4.9 Numerical Differentiation

At the beginning of this chapter we stated that derivative approximations are not as frequently needed as integral approximations. This is true for the approximation of single derivatives, but derivative approximation formulas are used extensively for approximating the solutions to ordinary and partial differential equations, a subject we consider in Chapters 11 and 12.

The derivative of the function f at x_0 is defined as

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

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 the 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, $P_{0,1}$, 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 number $\xi(x)$ in $[a, b]$. Differentiating this equation gives

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

so

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

with error

$$\frac{2(x - x_0) - h}{2} f''(\xi(x)) + \frac{(x - x_0)(x - x_0 - h)}{2} D_x(f''(\xi(x))).$$

Difference equations were used and popularized by Isaac Newton in the last quarter of the 17th century, but many of these techniques had previously been developed by Thomas Harriot (1561–1621) and Henry Briggs (1561–1630). Harriot made significant advances in navigation techniques, and Briggs was the person most responsible for the acceptance of logarithms as an aid to computation.

There are two terms for the error in this approximation. The first term involves $f''(\xi(x))$, which can be bounded if we have a bound for the second derivative of f. The second part of the truncation error involves $D_x f''(\xi(x)) = f'''(\xi(x)) \cdot \xi'(x)$, which generally cannot be estimated because it contains the unknown term $\xi'(x)$. However, when x is x_0, the coefficient of $D_x f''(\xi(x))$ is zero. In this case, the formula simplifies to the following:

Two-Point Formula

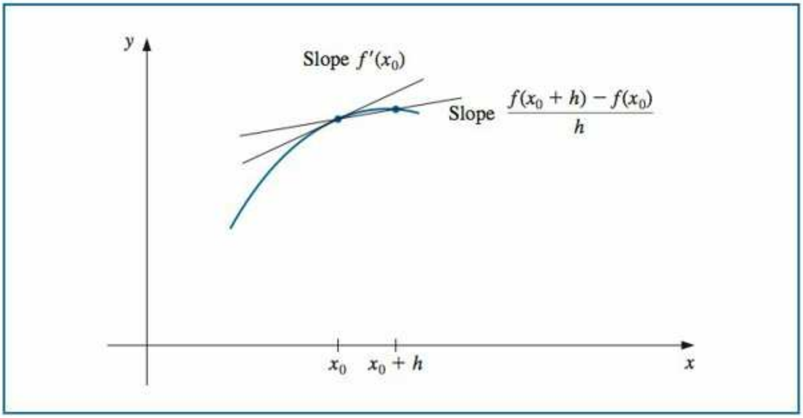
If f'' exists on the interval containing x_0 and $x_0 + h$, then

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

for some number ξ between x_0 and $x_0 + h$.

Suppose that M is a bound on $|f''(x)|$ for $x \in [a, b]$. Then 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 $M|h|/2$. This is a two-point formula known as the **forward-difference formula** if $h > 0$ (see Figure 4.20) and the **backward-difference formula** if $h < 0$.

Figure 4.20



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 4.9.

Table 4.9

h	$f(1.8+h)$	$\dfrac{f(1.8+h)-f(1.8)}{h}$	$\dfrac{\lvert h\rvert}{2(1.8)^2}$
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 $f \in C^{n+1}(I)$. Then

$$f(x) = \sum_{j=0}^{n} f(x_j)L_j(x) + \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} f^{(n+1)}(\xi(x))$$

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

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

Again we have a problem with the second part of the truncation error unless x is one of the numbers x_k. In this case, the multiplier of $D_x[f^{(n+1)}(\xi(x))]$ is zero, and the formula becomes

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

Three-Point Formulas

Applying this technique using the second Lagrange polynomial at x_0, $x_1 = x_0 + h$, and $x_2 = x_0 + 2h$ produces the following formula.

Three-Point Endpoint Formula

If f''' exists on the interval containing x_0 and $x_0 + 2h$, then

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

for some number ξ between x_0 and $x_0 + 2h$.

This formula is useful when approximating the derivative at the endpoint of an interval. This situation occurs, for example, when approximations are needed for the derivatives used for the clamped cubic splines. Left endpoint approximations are found using $h > 0$, and right endpoint approximations using $h < 0$.

When approximating the derivative of a function at an interior point of an interval, it is better to use the formula that is produced from the second Lagrange polynomial at $x_0 - h$, x_0, and $x_0 + h$.

Three-Point Midpoint Formula

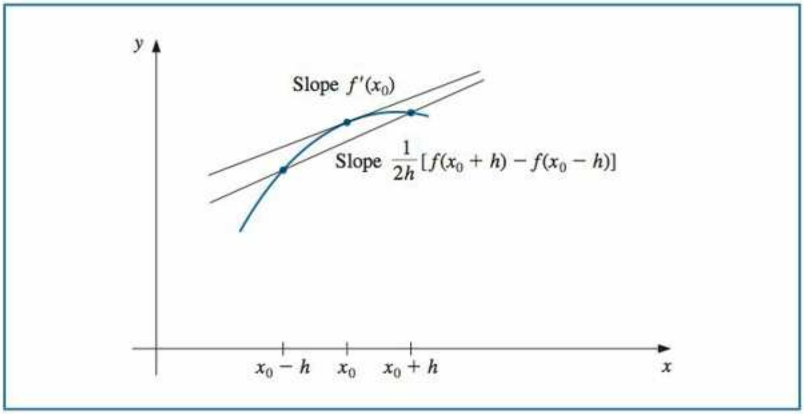
If f''' exists on the interval containing $x_0 - h$ and $x_0 + h$, then

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

for some number ξ between $x_0 - h$ and $x_0 + h$.

The error in the Midpoint formula is approximately half the error in the Endpoint formula and f needs to be evaluated at only two points whereas in the Endpoint formula three evaluations are required. Figure 4.21 gives an illustration of the approximation produced from the Midpoint formula.

Figure 4.21



These methods are called *three-point formulas* (even though the third point, $f(x_0)$, does not appear in the Midpoint formula). Similarly, there are *five-point formulas* that involve evaluating the function at two additional points, whose error term is $O(h^4)$. These formulas are generated by differentiating fourth Lagrange polynomials that pass through the evaluation points. The most useful is the Midpoint formula.

Five-Point Formulas

Five-Point Midpoint Formula

If $f^{(5)}$ exists on the interval containing $x_0 - 2h$ and $x_0 + 2h$, then

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

for some number ξ between $x_0 - 2h$ and $x_0 + 2h$.

There is another five-point formula that is useful, particularly with regard to the clamped cubic spline interpolation.

Five-Point Endpoint Formula

If $f^{(5)}$ exists on the interval containing x_0 and $x_0 + 4h$, then

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

for some number ξ between x_0 and $x_0 + 4h$.

Left-endpoint approximations are found using $h > 0$, and right-endpoint approximations are found using $h < 0$.

Example 2 Values for $f(x) = xe^x$ are given in Table 4.10. Use all the applicable three-point and five-point formulas to approximate $f'(2.0)$.

Table 4.10

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

Solution The data in the table permit us to find four different three-point approximations:

Three-Point Endpoint Formula with $h = 0.1$:

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

Three-Point Endpoint Formula with $h = -0.1$:

$$\frac{1}{-0.2}[-3f(2.0) + 4f(1.9) - f(1.8)] = -5[-3(14.778112) + 4(12.703199) - 10.889365)] = 22.054525,$$

Three-Point Midpoint Formula with $h = 0.1$:

$$\frac{1}{0.2}[f(2.1) - f(1.9)] = 5(17.148957 - 12.703199) = 22.228790,$$

Three-Point Midpoint Formula with $h = 0.2$:

$$\frac{1}{0.4}[f(2.2) - f(1.8)] = \frac{5}{2}(19.855030 - 10.889365) = 22.414163.$$

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

Five-Point Midpoint Formula with $h = 0.1$:

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

If we had no other information, we would accept the five-point midpoint approximation using $h = 0.1$ as the most accurate. The true value for this problem is $f'(2.0) = (2+1)e^2 = 22.167168$. ■

Round-Off Error Instability

It is particularly important to pay attention to round-off error when approximating derivatives. When approximating integrals in Section 4.3, we found that reducing the step size in the Composite Simpson's rule reduced the truncation error, and, even though the amount of calculation increased, the total round-off error remained bounded. This is not the case when approximating derivatives.

When applying a numerical differentiation technique, the truncation error will also decrease if the step size is reduced, but only at the expense of increased round-off error. To see why this occurs, let us examine more closely the Three-Point Midpoint formula:

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

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 computed values $\tilde{f}(x_0+h)$ and $\tilde{f}(x_0-h)$ are related to the true values $f(x_0+h)$ and $f(x_0-h)$ by

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

In this case, the total error in the approximation,

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

is due in part to round-off and in part to truncating. If we assume that the round-off errors, $e(x_0 \pm h)$, for the function evaluations 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 portion of the error, $h^2M/6$, we must reduce h. But as h is reduced, the round-off portion of the error, ε/h, grows. In practice, then, it is seldom advantageous to let h be too small, since the round-off error will dominate the calculations.

Illustration Consider using the values in Table 4.11 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 4.12.

Table 4.11

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 4.12

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 13) 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 4.12.

In practice, we cannot compute an optimal h to use in approximating the derivative, because 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 Midpoint formula, but similar difficulties occur with all the differentiation formulas. The reason for the problems can be traced to the need to divide by a power of h. As we found in Section 1.4 (see, in particular, Example 1), division by small numbers tends to exaggerate round-off error, and this operation should be avoided if possible. In the case of numerical differentiation, it is impossible to avoid the problem entirely, although the higher-order methods reduce the difficulty.

Keep in mind that, as an approximation method, numerical differentiation is unstable, because the small values of h needed to reduce truncation error cause the round-off error to grow. This is the first class of unstable methods that we have encountered, and these techniques would be avoided if it were possible. However it is not, because these formulas are needed in Chapters 11 and 12 for approximating the solutions of ordinary and partial-differential equations.

Keep in mind that difference method approximations can be unstable.

Methods for approximating higher derivatives of functions using Taylor polynomials can be derived as was done when approximating the first derivative or by using an averaging technique that is similar to that used for extrapolation. These techniques, of course, suffer from the same stability weaknesses as the approximation methods for first derivatives, but they are needed for approximating the solution to boundary value problems in differential equations. The only one we will need is a Three-Point Midpoint formula, which has the following form.

Three-Point Midpoint Formula for Approximating f''

If $f^{(4)}$ exists on the interval containing $x_0 - h$ and $x_0 + h$, then

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

for some number ξ between $x_0 - h$ and $x_0 + h$.

EXERCISE SET 4.9

1. Use the forward-difference formulas and backward-difference formulas to determine each missing entry in the following tables.

a.

x	$f(x)$	$f'(x)$
0.5	0.4794	
0.6	0.5646	
0.7	0.6442	

b.

x	$f(x)$	$f'(x)$
0.0	0.00000	
0.2	0.74140	
0.4	1.3718	

2. The data in Exercise 1 were taken from the following functions. Compute the actual errors in Exercise 1, and find error bounds using the error formulas.

a. $f(x) = \sin x$ b. $f(x) = e^x - 2x^2 + 3x - 1$

3. 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	

b.

x	$f(x)$	$f'(x)$
8.1	16.94410	
8.3	17.56492	
8.5	18.19056	
8.7	18.82091	

c.

x	$f(x)$	$f'(x)$
2.9	−4.827866	
3.0	−4.240058	
3.1	−3.496909	
3.2	−2.596792	

d.

x	$f(x)$	$f'(x)$
2.0	3.6887983	
2.1	3.6905701	
2.2	3.6688192	
2.3	3.6245909	

4. The data in Exercise 3 were taken from the following functions. Compute the actual errors in Exercise 3, and find error bounds using the error formulas.

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

c. $f(x) = x \cos x - x^2 \sin x$ d. $f(x) = 2(\ln x)^2 + 3 \sin x$

5. Use the formulas given in this section to determine, as accurately as possible, approximations for each missing entry in the following tables.

a.

x	$f(x)$	$f'(x)$
2.1	−1.709847	
2.2	−1.373823	
2.3	−1.119214	
2.4	−0.9160143	
2.5	−0.7470223	
2.6	−0.6015966	

b.

x	$f(x)$	$f'(x)$
−3.0	9.367879	
−2.8	8.233241	
−2.6	7.180350	
−2.4	6.209329	
−2.2	5.320305	
−2.0	4.513417	

6. 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. $f(x) = \tan x$ b. $f(x) = e^{x/3} + x^2$

7. Let $f(x) = \cos \pi x$. Use the Three-Point Midpoint formula for f'' and the values of $f(x)$ at $x = 0.25$, 0.5, and 0.75 to approximate $f''(0.5)$. Compare this result to the exact value and to the approximation found in Exercise 7 of Section 3.5. Explain why this method is particularly accurate for this problem.

8. Let $f(x) = 3xe^x - \cos x$. Use the following data and the Three-Point Midpoint formula for f'' to approximate $f''(1.3)$ with $h = 0.1$ and with $h = 0.01$.

x	1.20	1.29	1.30	1.31	1.40
$f(x)$	11.59006	13.78176	14.04276	14.30741	16.86187

Compare your results to $f''(1.3)$.

9. Use the following data and the knowledge that the first five derivatives of f were bounded on $[1, 5]$ by 2, 3, 6, 12, and 23, respectively, to approximate $f'(3)$ as accurately as possible. Find a bound for the error.

x	1	2	3	4	5
$f(x)$	2.4142	2.6734	2.8974	3.0976	3.2804

10. Repeat Exercise 9, assuming instead that the third derivative of f is bounded on $[1, 5]$ by 4.

11. Analyze the round-off errors for the formula

$$f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} - \frac{h}{2}f''(\xi_0).$$

Find an optimal $h > 0$ in terms of a bound M for f'' on $(x_0, x_0 + h)$.

12. All calculus students know that the derivative of a function f at x can be defined as

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

Choose your favorite function f, nonzero number x, and computer or calculator. Generate approximations $f_n'(x)$ to $f'(x)$ by

$$f_n'(x) = \frac{f(x+10^{-n}) - f(x)}{10^{-n}}$$

for $n = 1, 2, \ldots, 20$ and describe what happens.

13. Consider the function

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

where M is a bound for the third derivative of a function. Show that $e(h)$ has a minimum at $\sqrt[3]{3\varepsilon/M}$.

14. The forward-difference formula can be expressed as

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

Use extrapolation on this formula to derive an $O(h^3)$ formula for $f'(x_0)$.

15. In Exercise 7 of Section 3.4, data were given describing a car traveling on a straight road. That problem asked to predict the position and speed of the car when $t = 10$ s. Use the following times and positions to predict the speed at each time listed.

Time	0	3	5	8	10	13
Distance	0	225	383	623	742	993

16. In a circuit with impressed voltage $\mathcal{E}(t)$ and inductance L, Kirchhoff's first law gives the relationship

$$\mathcal{E}(t) = L\frac{di}{dt} + Ri,$$

where R is the resistance in the circuit and i is the current. Suppose we measure the current for several values of t and obtain:

t	1.00	1.01	1.02	1.03	1.0
i	3.10	3.12	3.14	3.18	3.24

where t is measured in seconds, i is in amperes, the inductance L is a constant 0.98 henries, and the resistance is 0.142 ohms. Approximate the voltage $\mathcal{E}(t)$ when $t = 1.00$, 1.01, 1.02, 1.03, and 1.04.

17. Derive a method for approximating $f''(x_0)$ whose error term is of order h^2 by expanding the function f in a third Taylor polynomial about x_0 and evaluating at $x_0 + h$ and $x_0 - h$.

4.10 Survey of Methods and Software

In this chapter we considered approximating integrals of functions of one, two, or three variables and approximating the derivatives of a function of a single real variable.

The Midpoint rule, Trapezoidal rule, and Simpson's rule were studied to introduce the techniques and error analysis of quadrature methods. Composite Simpson's rule is easy to use and produces accurate approximations unless the function oscillates in a subinterval of the interval of integration. Adaptive quadrature can be used if the function is suspected of oscillatory behavior. To minimize the number of nodes and also increase the accuracy, we studied Gaussian quadrature. Romberg integration was introduced to take advantage of the easily-applied Composite Trapezoidal rule and extrapolation.

Most software for integrating a function of a single real variable is based on the adaptive approach or extremely accurate Gaussian formulas. Cautious Romberg integration is an adaptive technique that includes a check to make sure that the integrand is smoothly behaved over subintervals of the integral of integration. This method has been successfully used in software libraries. Multiple integrals are generally approximated by extending good adaptive methods to higher dimensions. Gaussian-type quadrature is also recommended to decrease the number of function evaluations.

The main routines in both the IMSL and NAG Libraries are based on QUADPACK: *A Subroutine Package for Automatic Integration* by R. Piessens, E. de Doncker-Kapenga, C. W. Uberhuber, and D. K. Kahaner published by Springer-Verlag in 1983 [PDUK]. The routines are also available as public domain software, at http://www.netlib.org/quadpack. The main technique is an adaptive integration scheme based on the 21-point Gaussian-Kronrod rule using the 10-point Gaussian rule for error estimation. The Gaussian rule uses the 10 points $x_1, \ldots, x_{10}$ and weights $w_1, \ldots, w_{10}$ to give the quadrature formula $\sum_{i=1}^{10} w_i f(x_i)$ to approximate $\int_a^b f(x)dx$. The additional points $x_{11}, \ldots, x_{21}$ and the new weights $v_1, \ldots, v_{21}$ are then used in the Kronrod formula, $\sum_{i=1}^{21} v_i f(x_i)$. The results of the two formulas are compared to eliminate error. The advantage in using $x_1, \ldots, x_{10}$ in each formula is that f needs to be evaluated at only 21 points. If independent 10- and 21-point Gaussian rules were used, 31 function evaluations would be needed. This procedure also permits endpoint singularities in the integrand. Other subroutines allow user specified singularities and infinite intervals of integration. Methods are also available for multiple integrals.

Although numerical differentiation is unstable, derivative approximation formulas are needed for solving differential equations. The NAG Library includes a subroutine for the numerical differentiation of a function of one real variable, with differentiation to the fourteenth derivative being possible. An IMSL function uses an adaptive change in step size for finite differences to approximate a derivative of f at x to within a given tolerance. Both packages allow the differentiation and integration of interpolatory cubic splines.

For further reading on numerical integration, we recommend the books by Engels [E] and by Davis and Rabinowitz [DR]. For more information on Gaussian quadrature, see Stroud and Secrest [StS]. Books on multiple integrals include those by Stroud [Stro] and by Sloan and Joe [SJ].