5 Numerical Differentiation

Given the function $f(x)$, compute $d^n f/dx^n$ at given x

5.1 Introduction

Numerical differentiation deals with the following problem: We are given the function $y = f(x)$ and wish to obtain one of its derivatives at the point $x = x_k$. The term "given" means that we either have an algorithm for computing the function or possess a set of discrete data points (x_i, y_i), $i = 0, 1, \ldots, n$. In either case, we have access to a finite number of (x, y) data pairs from which to compute the derivative. If you suspect by now that numerical differentiation is related to interpolation, you are right – one means of finding the derivative is to approximate the function locally by a polynomial and then differentiate it. An equally effective tool is the Taylor series expansion of $f(x)$ about the point x_k, which has the advantage of providing us with information about the error involved in the approximation.

Numerical differentiation is not a particularly accurate process. It suffers from a conflict between roundoff errors (due to limited machine precision) and errors inherent in interpolation. For this reason, a derivative of a function can never be computed with the same precision as the function itself.

5.2 Finite Difference Approximations

The derivation of the finite difference approximations for the derivatives of $f(x)$ is based on forward and backward Taylor series expansions of $f(x)$ about x, such as

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) + \cdots \tag{a}$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) - \cdots \tag{b}$$

$$f(x+2h) = f(x) + 2hf'(x) + \frac{(2h)^2}{2!}f''(x) + \frac{(2h)^3}{3!}f'''(x) + \frac{(2h)^4}{4!}f^{(4)}(x) + \cdots \quad \text{(c)}$$

$$f(x-2h) = f(x) - 2hf'(x) + \frac{(2h)^2}{2!}f''(x) - \frac{(2h)^3}{3!}f'''(x) + \frac{(2h)^4}{4!}f^{(4)}(x) - \cdots \quad \text{(d)}$$

We also record the sums and differences of the series:

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

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3}f'''(x) + \ldots \quad \text{(f)}$$

$$f(x+2h) + f(x-2h) = 2f(x) + 4h^2 f''(x) + \frac{4h^4}{3}f^{(4)}(x) + \cdots \quad \text{(g)}$$

$$f(x+2h) - f(x-2h) = 4hf'(x) + \frac{8h^3}{3}f'''(x) + \cdots \quad \text{(h)}$$

Note that the sums contain only even derivatives, whereas the differences retain just the odd derivatives. Equations (a)–(h) can be viewed as simultaneous equations that can be solved for various derivatives of $f(x)$. The number of equations involved and the number of terms kept in each equation depend on the order of the derivative and the desired degree of accuracy.

First Central Difference Approximations

The solution of Eq. (f) for $f'(x)$ is

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

or

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + \mathcal{O}(h^2) \quad (5.1)$$

which is called the *first central difference approximation* for $f'(x)$. The term $\mathcal{O}(h^2)$ reminds us that the truncation error behaves as h^2.

Similarly, Eq. (e) yields the first central difference approximation for $f''(x)$:

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

or

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \mathcal{O}(h^2) \quad (5.2)$$

Central difference approximations for other derivatives can be obtained from Eqs. (a)–(h) in the same manner. For example, eliminating $f'(x)$ from Eqs. (f) and (h) and solving for $f'''(x)$ yields

$$f'''(x) = \frac{f(x+2h) - 2f(x+h) + 2f(x-h) - f(x-2h)}{2h^3} + \mathcal{O}(h^2) \quad (5.3)$$

	$f(x-2h)$	$f(x-h)$	$f(x)$	$f(x+h)$	$f(x+2h)$
$2hf'(x)$		-1	0	1	
$h^2 f''(x)$		1	-2	1	
$2h^3 f'''(x)$	-1	2	0	-2	1
$h^4 f^{(4)}(x)$	1	-4	6	-4	1

Table 5.1 Coefficients of central finite difference approximations of $\mathcal{O}(h^2)$

The approximation

$$f^{(4)}(x) = \frac{f(x+2h) - 4f(x+h) + 6f(x) - 4f(x-h) + f(x-2h)}{h^4} + \mathcal{O}(h^2) \tag{5.4}$$

is available from Eqs. (e) and (g) after eliminating $f''(x)$. Table 5.1 summarizes the results.

First Noncentral Finite Difference Approximations

Central finite difference approximations are not always usable. For example, consider the situation where the function is given at the n discrete points $x_0, x_1, \ldots, x_n$. Because central differences use values of the function on each side of x, we would be unable to compute the derivatives at x_0 and x_n. Clearly, there is a need for finite difference expressions that require evaluations of the function on only one side of x. These expressions are called *forward* and *backward* finite difference approximations.

Noncentral finite differences can also be obtained from Eqs. (a)–(h). Solving Eq. (a) for $f'(x)$, we get

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2}f''(x) - \frac{h^2}{6}f'''(x) - \frac{h^3}{4!}f^{(4)}(x) - \cdots$$

Keeping only the first term on the right-hand side leads to the *first forward difference approximation*

$$f'(x) = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h) \tag{5.5}$$

Similarly, Eq. (b) yields the *first backward difference approximation*

$$f'(x) = \frac{f(x) - f(x-h)}{h} + \mathcal{O}(h) \tag{5.6}$$

Note that the truncation error is now $\mathcal{O}(h)$, which is not as good as $\mathcal{O}(h^2)$ in central difference approximations.

We can derive the approximations for higher derivatives in the same manner. For example, Eqs. (a) and (c) yield

$$f''(x) = \frac{f(x+2h) - 2f(x+h) + f(x)}{h^2} + \mathcal{O}(h) \tag{5.7}$$

The third and fourth derivatives can be derived in a similar fashion. The results are shown in Tables 5.2a and 5.2b.

	$f(x)$	$f(x+h)$	$f(x+2h)$	$f(x+3h)$	$f(x+4h)$
$hf'(x)$	-1	1			
$h^2 f''(x)$	1	-2	1		
$h^3 f'''(x)$	-1	3	-3	1	
$h^4 f^{(4)}(x)$	1	-4	6	-4	1

Table 5.2a Coefficients of forward finite difference approximations of $\mathcal{O}(h)$

	$f(x-4h)$	$f(x-3h)$	$f(x-2h)$	$f(x-h)$	$f(x)$
$hf'(x)$				-1	1
$h^2 f''(x)$			1	-2	1
$h^3 f'''(x)$		-1	3	-3	1
$h^4 f^{(4)}(x)$	1	-4	6	-4	1

Table 5.2b Coefficients of backward finite difference approximations of $\mathcal{O}(h)$

Second Noncentral Finite Difference Approximations

Finite difference approximations of $\mathcal{O}(h)$ are not popular, for reasons to be explained shortly. The common practice is to use expressions of $\mathcal{O}(h^2)$. To obtain noncentral difference formulas of this order, we have to retain more terms in the Taylor series. As an illustration, we derive the expression for $f'(x)$. We start with Eqs. (a) and (c), which are

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{6} f'''(x) + \frac{h^4}{24} f^{(4)}(x) + \cdots$$

$$f(x+2h) = f(x) + 2hf'(x) + 2h^2 f''(x) + \frac{4h^3}{3} f'''(x) + \frac{2h^4}{3} f^{(4)}(x) + \cdots$$

We eliminate $f''(x)$ by multiplying the first equation by 4 and subtracting it from the second equation. The result is

$$f(x+2h) - 4f(x+h) = -3f(x) - 2hf'(x) + \frac{h^4}{2} f^{(4)}(x) + \cdots$$

Therefore,

$$f'(x) = \frac{-f(x+2h) + 4f(x+h) - 3f(x)}{2h} + \frac{h^2}{4} f^{(4)}(x) + \cdots$$

or

$$f'(x) = \frac{-f(x+2h) + 4f(x+h) - 3f(x)}{2h} + \mathcal{O}(h^2) \tag{5.8}$$

Equation (5.8) is called the *second forward finite difference approximation*.

The derivation of finite difference approximations for higher derivatives involve additional Taylor series. Thus the forward difference approximation for $f''(x)$ utilizes

	$f(x)$	$f(x+h)$	$f(x+2h)$	$f(x+3h)$	$f(x+4h)$	$f(x+5h)$
$2hf'(x)$	-3	4	-1			
$h^2 f''(x)$	2	-5	4	-1		
$2h^3 f'''(x)$	-5	18	-24	14	-3	
$h^4 f^{(4)}(x)$	3	-14	26	-24	11	-2

Table 5.3a Coefficients of forward finite difference approximations of $\mathcal{O}(h^2)$

	$f(x-5h)$	$f(x-4h)$	$f(x-3h)$	$f(x-2h)$	$f(x-h)$	$f(x)$
$2hf'(x)$				1	-4	3
$h^2 f''(x)$			-1	4	-5	2
$2h^3 f'''(x)$		3	-14	24	-18	5
$h^4 f^{(4)}(x)$	-2	11	-24	26	-14	3

Table 5.3b Coefficients of backward finite difference approximations of $\mathcal{O}(h^2)$

series for $f(x+h)$, $f(x+2h)$, and $f(x+3h)$; the approximation for $f'''(x)$ involves Taylor expansions for $f(x+h)$, $f(x+2h)$, $f(x+3h)$, $f(x+4h)$, and so on. As you can see, the computations for high-order derivatives can become rather tedious. The results for both the forward and backward finite differences are summarized in Tables 5.3a and 5.3b.

Errors in Finite Difference Approximations

Observe that in all finite difference expressions, the sum of the coefficients is zero. The effect on the *roundoff error* can be profound. If h is very small, the values of $f(x)$, $f(x \pm h)$, $f(x \pm 2h)$, and so forth will be approximately equal. When they are multiplied by the coefficients and added, several significant figures can be lost. On the other hand, we cannot make h too large, because then the *truncation error* would become excessive. This unfortunate situation has no remedy, but we can obtain some relief by taking the following precautions:

- Use double-precision arithmetic.
- Employ finite difference formulas that are accurate to at least $\mathcal{O}(h^2)$.

To illustrate the errors, let us compute the second derivative of $f(x) = e^{-x}$ at $x = 1$ from the central difference formula, Eq. (5.2). We carry out the calculations with six- and eight-digit precision, using different values of h. The results, shown in Table 5.4, should be compared with $f''(1) = e^{-1} = 0.367\,879\,44$.

In the six-digit computations, the optimal value of h is 0.08, yielding a result accurate to three significant figures. Hence, three significant figures are lost because of a combination of truncation and roundoff errors. Above optimal h, the dominant error is due to truncation; below it, the roundoff error becomes pronounced. The best result obtained with the eight-digit computation is accurate to four significant figures.

h	6-digit precision	8-digit precision
0.64	0.380 610	0.380 609 11
0.32	0.371 035	0.371 029 39
0.16	0.368 711	0.368 664 84
0.08	0.368 281	0.368 076 56
0.04	0.368 75	0.367 831 25
0.02	0.37	0.3679
0.01	0.38	0.3679
0.005	0.40	0.3676
0.0025	0.48	0.3680
0.00125	1.28	0.3712

Table 5.4 $(e^{-x})''$ at $x = 1$ from central finite difference approximation

Because the extra precision decreases the roundoff error, the optimal h is smaller (about 0.02) than in the six-figure calculations.

5.3 Richardson Extrapolation

Richardson extrapolation is a simple method for boosting the accuracy of certain numerical procedures, including finite difference approximations (we also use it later in other applications).

Suppose that we have an approximate means of computing some quantity G. Moreover, assume that the result depends on a parameter h. Denoting the approximation by $g(h)$, we have $G = g(h) + E(h)$, where $E(h)$ represents the error. Richardson extrapolation can remove the error, provided that it has the form $E(h) = ch^p$, c and p being constants. We start by computing $g(h)$ with some value of h, say, $h = h_1$. In that case we have

$$G = g(h_1) + ch_1^p \tag{i}$$

Then we repeat the calculation with $h = h_2$, so that

$$G = g(h_2) + ch_2^p \tag{j}$$

Eliminating c and solving for G, Eqs. (i) and (j) yield

$$G = \frac{(h_1/h_2)^p g(h_2) - g(h_1)}{(h_1/h_2)^p - 1} \tag{5.8}$$

which is the *Richardson extrapolation formula*. It is common practice to use $h_2 = h_1/2$, in which case Eq. (5.8) becomes

$$G = \frac{2^p g(h_1/2) - g(h_1)}{2^p - 1} \tag{5.9}$$

Let us illustrate Richardson extrapolation by applying it to the finite difference approximation of $(e^{-x})''$ at $x = 1$. We work with six-digit precision and utilize the results in Table 5.4. Because the extrapolation works only on the truncation error, we must confine h to values that produce negligible roundoff. In Table 5.4 we have

$$g(0.64) = 0.380\,610 \qquad g(0.32) = 0.371\,035$$

The truncation error in central difference approximation is $E(h) = \mathcal{O}(h^2) = c_1 h^2 + c_2 h^4 + c_3 h^6 + \ldots$. Therefore, we can eliminate the first (dominant) error term if we substitute $p = 2$ and $h_1 = 0.64$ in Eq. (5.9). The result is

$$G = \frac{2^2 g(0.32) - g(0.64)}{2^2 - 1} = \frac{4(0.371\,035) - 0.380\,610}{3} = 0.\,367\,84\,3$$

which is an approximation of $(e^{-x})''$ with the error $\mathcal{O}(h^4)$. Note that it is as accurate as the best result obtained with eight-digit computations in Table 5.4.

EXAMPLE 5.1

Given the evenly spaced data points

x	0	0.1	0.2	0.3	0.4
$f(x)$	0.0000	0.0819	0.1341	0.1646	0.1797

compute $f'(x)$ and $f''(x)$ at $x = 0$ and 0.2 using finite difference approximations of $\mathcal{O}(h^2)$.

Solution We use finite difference approximations of $\mathcal{O}(h^2)$. From the forward difference tables Table 5.3a, we get

$$f'(0) = \frac{-3f(0) + 4f(0.1) - f(0.2)}{2(0.1)} = \frac{-3(0) + 4(0.0819) - 0.1341}{0.2} = 0.967$$

$$\begin{aligned} f''(0) &= \frac{2f(0) - 5f(0.1) + 4f(0.2) - f(0.3)}{(0.1)^2} \\ &= \frac{2(0) - 5(0.0819) + 4(0.1341) - 0.1646}{(0.1)^2} = -3.77 \end{aligned}$$

The central difference approximations in Table 5.1 yield

$$f'(0.2) = \frac{-f(0.1) + f(0.3)}{2(0.1)} = \frac{-0.0819 + 0.1646}{0.2} = 0.4135$$

$$f''(0.2) = \frac{f(0.1) - 2f(0.2) + f(0.3)}{(0.1)^2} = \frac{0.0819 - 2(0.1341) + 0.1646}{(0.1)^2} = -2.17$$

EXAMPLE 5.2

Use the data in Example 5.1 to compute $f'(0)$ as accurately as you can.

Solution One solution is to apply Richardson extrapolation to finite difference approximations. We start with two forward difference approximations of $\mathcal{O}(h^2)$ for $f'(0)$:

one using $h = 0.2$ and the other one $h = 0.1$. Referring to the formulas of $O(h^2)$ in Table 5.3a, we get

$$g(0.2) = \frac{-3f(0) + 4f(0.2) - f(0.4)}{2(0.2)} = \frac{3(0) + 4(0.1341) - 0.1797}{0.4} = 0.8918$$

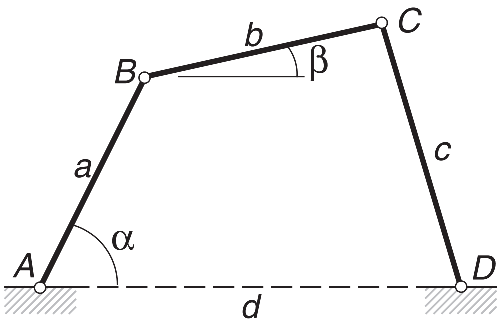
$$g(0.1) = \frac{-3f(0) + 4f(0.1) - f(0.2)}{2(0.1)} = \frac{-3(0) + 4(0.0819) - 0.1341}{0.2} = 0.9675$$

Recall that the error in both approximations is of the form $E(h) = c_1 h^2 + c_2 h^4 + c_3 h^6 + \ldots$. We can now use Richardson extrapolation, Eq. (5.9), to eliminate the dominant error term. With $p = 2$ we obtain

$$f'(0) \approx G = \frac{2^2 g(0.1) - g(0.2)}{2^2 - 1} = \frac{4(0.9675) - 0.8918}{3} = 0.9927$$

which is a finite difference approximation of $O(h^4)$.

EXAMPLE 5.3



The linkage shown has the dimensions $a = 100$ mm, $b = 120$ mm, $c = 150$ mm, and $d = 180$ mm. It can be shown by geometry that the relationship between the angles α and β is

$$(d - a\cos\alpha - b\cos\beta)^2 + (a\sin\alpha + b\sin\beta)^2 - c^2 = 0$$

For a given value of α, we can solve this transcendental equation for β by one of the root-finding methods in Chapter 2. This was done with $\alpha = 0^\circ, 5^\circ, 10^\circ, \ldots, 30^\circ$, the results being

α (deg)	0	5	10	15	20	25	30
β (rad)	1.6595	1.5434	1.4186	1.2925	1.1712	1.0585	0.9561

If link AB rotates with the constant angular velocity of 25 rad/s, use finite difference approximations of $O(h^2)$ to tabulate the angular velocity $d\beta/dt$ of link BC against α.

Solution The angular speed of BC is

$$\frac{d\beta}{dt} = \frac{d\beta}{d\alpha}\frac{d\alpha}{dt} = 25\frac{d\beta}{d\alpha}\ \text{rad/s}$$

where $d\beta/d\alpha$ can be computed from finite difference approximations using the data in the table. Forward and backward differences of $\mathcal{O}(h^2)$ are used at the endpoints, central differences elsewhere. Note that the increment of α is

$$h = (5\,\text{deg})\left(\frac{\pi}{180}\text{rad / deg}\right) = 0.087\,266\,\text{rad}$$

The computations yield

$$\dot{\beta}(0^\circ) = 25\frac{-3\beta(0^\circ) + 4\beta(5^\circ) - \beta(10^\circ)}{2h} = 25\frac{-3(1.6595) + 4(1.5434) - 1.4186}{2\,(0.087\,266)}$$
$$= -32.01\,\text{rad/s}$$
$$\dot{\beta}(5^\circ) = 25\frac{\beta(10^\circ) - \beta(0^\circ)}{2h} = 25\frac{1.4186 - 1.6595}{2(0.087\,266)} = -34.51\,\text{rad/s}$$

and so forth.

The complete set of results is

α (deg)	0	5	10	15	20	25	30
$\dot{\beta}$ (rad/s)	−32.01	−34.51	−35.94	−35.44	−33.52	−30.81	−27.86

5.4 Derivatives by Interpolation

If $f(x)$ is given as a set of discrete data points, interpolation can be a very effective means of computing its derivatives. The idea is to approximate the derivative of $f(x)$ by the derivative of the interpolant. This method is particularly useful if the data points are located at uneven intervals of x, when the finite difference approximations listed in the last section are not applicable.[1]

Polynomial Interpolant

The idea here is simple: fit the polynomial of degree n

$$P_{n-1}(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

through $n+1$ data points and then evaluate its derivatives at the given x. As pointed out in Section 3.2, it is generally advisable to limit the degree of the polynomial to less than 6 in order to avoid spurious oscillations of the interpolant. Because these oscillations are magnified with each differentiation, their effect can devastating. In view of this limitation, the interpolation is usually a local one, involving no more than a few nearest-neighbor data points.

For evenly spaced data points, polynomial interpolation and finite difference approximations produce identical results. In fact, the finite difference formulas are equivalent to polynomial interpolation.

[1] It is possible to derive finite difference approximations for unevenly spaced data, but they would not be as accurate as the formulas derived in Section 5.2.

Several methods of polynomial interpolation were introduced in Section 3.2. Unfortunately, none of them are suited for the computation of derivatives of the interpolant. The method that we need is one that determines the coefficients $a_0, a_1, \ldots, a_n$ of the polynomial. There is only one such method discussed in Chapter 3: the *least-squares fit*. Although this method is designed mainly for smoothing of data, it will carry out interpolation if we use $m = n$ in Eq. (3.22) – recall that m is the degree of the interpolating polynomial and $n+1$ represents the number of data points to be fitted. If the data contains noise, then the least-squares fit should be used in the smoothing mode, that is, with $m < n$. After the coefficients of the polynomial have been found, the polynomial and its first two derivatives can be evaluated efficiently by the function `evalPoly` listed in Section 4.7.

Cubic Spline Interpolant

Because of to its stiffness, the cubic spline is a good global interpolant; moreover, it is easy to differentiate. The first step is to determine the second derivatives k_i of the spline at the knots by solving Eqs. (3.11). This can be done with the function `curvatures` in the module `cubicSpline` listed in Section 3.3. The first and second derivatives are then computed from

$$\begin{aligned} f'_{i,i+1}(x) = &\frac{k_i}{6}\left[\frac{3(x-x_{i+1})^2}{x_i - x_{i+1}} - (x_i - x_{i+1})\right] \\ &- \frac{k_{i+1}}{6}\left[\frac{3(x-x_i)^2}{x_i - x_{i+1}} - (x_i - x_{i+1})\right] + \frac{y_i - y_{i+1}}{x_i - x_{i+1}} \end{aligned} \tag{5.10}$$

$$f''_{i,i+1}(x) = k_i \frac{x - x_{i+1}}{x_i - x_{i+1}} - k_{i+1}\frac{x - x_i}{x_i - x_{i+1}} \tag{5.11}$$

which are obtained by differentiation of Eq. (3.10).

EXAMPLE 5.4
Given the data

x	1.5	1.9	2.1	2.4	2.6	3.1
$f(x)$	1.0628	1.3961	1.5432	1.7349	1.8423	2.0397

compute $f'(2)$ and $f''(2)$ using (1) polynomial interpolation over three nearest-neighbor points and (2) the natural cubic spline interpolant spanning all the data points.

Solution of Part (1) The interpolant is $P_2(x) = a_0 + a_1 x + a_2 x^2$ passing through the points at $x = 1.9, 2.1$, and 2.4. The normal equations, Eqs. (3.22), of the least-squares fit are

$$\begin{bmatrix} n & \sum x_i & \sum x_i^2 \\ \sum x_i & \sum x_i^2 & \sum x_i^3 \\ \sum x_i^2 & \sum x_i^3 & \sum x_i^4 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum y_i \\ \sum y_i x_i \\ \sum y_i x_i^2 \end{bmatrix}$$

After substituting the data, we get

$$\begin{bmatrix} 3 & 6.4 & 13.78 \\ 6.4 & 13.78 & 29.944 \\ 13.78 & 29.944 & 65.6578 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 4.6742 \\ 10.0571 \\ 21.8385 \end{bmatrix}$$

which yields $\mathbf{a} = \begin{bmatrix} -0.7714 & 1.5075 & -0.1930 \end{bmatrix}^T$.

The derivatives of the interpolant are $P_2'(x) = a_1 + 2a_2 x$ and $P_2''(x) = 2a_2$. Therefore,

$$f'(2) \approx P_2'(2) = 1.5075 + 2(-0.1930)(2) = 0.7355$$

$$f''(2) \approx P_2''(2) = 2(-0.1930) = -0.3860$$

Solution of Part (2) We must first determine the second derivatives k_i of the spline at its knots, after which the derivatives of $f(x)$ can be computed from Eqs. (5.10) and (5.11). The first part can be carried out by the following small program:

```
#!/usr/bin/python
## example5_4
from cubicSpline import curvatures
from LUdecomp3 import *
from numpy import array

xData = array([1.5, 1.9, 2.1, 2.4, 2.6, 3.1])
yData = array([1.0628, 1.3961, 1.5432, 1.7349, 1.8423, 2.0397])
print curvatures(xData,yData)
raw_input("Press return to exit")
```

The output of the program, consisting of k_0 to k_5, is

```
[ 0.   -0.4258431 -0.37744139 -0.38796663 -0.55400477   0.   ]
Press return to exit
```

Because $x = 2$ lies between knots 1 and 2, we must use Eqs. (5.10) and (5.11) with $i = 1$. This yields

$$\begin{aligned} f'(2) \approx f'_{1,2}(2) &= \frac{k_1}{6}\left[\frac{3(x-x_2)^2}{x_1-x_2} - (x_1-x_2)\right] \\ &\quad - \frac{k_2}{6}\left[\frac{3(x-x_1)^2}{x_1-x_2} - (x_1-x_2)\right] + \frac{y_1-y_2}{x_1-x_2} \\ &= \frac{(-0.4258)}{6}\left[\frac{3(2-2.1)^2}{(-0.2)} - (-0.2)\right] \\ &\quad - \frac{(-0.3774)}{6}\left[\frac{3(2-1.9)^2}{(-0.2)} - (-0.2)\right] + \frac{1.3961-1.5432}{(-0.2)} \\ &= 0.7351 \end{aligned}$$

$$f''(2) \approx f''_{1,2}(2) = k_1 \frac{x - x_2}{x_1 - x_2} - k_2 \frac{x - x_1}{x_1 - x_2}$$
$$= (-0.4258) \frac{2 - 2.1}{(-0.2)} - (-0.3774) \frac{2 - 1.9}{(-0.2)} = -0.4016$$

Note that the solutions for $f'(2)$ in parts (1) and (2) differ only in the fourth significant figure, but the values of $f''(2)$ are much further apart. This is not unexpected, considering the general rule: The higher the order of the derivative, the lower the precision with which it can be computed. It is impossible to tell which of the two results is better without knowing the expression for $f(x)$. In this particular problem, the data points fall on the curve $f(x) = x^2 e^{-x/2}$, so that the "true" values of the derivatives are $f'(2) = 0.7358$ and $f''(2) = -0.3679$.

EXAMPLE 5.5

Determine $f'(0)$ and $f'(1)$ from the following noisy data:

x	0	0.2	0.4	0.6
$f(x)$	1.9934	2.1465	2.2129	2.1790
x	0.8	1.0	1.2	1.4
$f(x)$	2.0683	1.9448	1.7655	1.5891

Solution We used the program listed in Example 3.10 to find the best polynomial fit (in the least-squares sense) to the data. The program was run three times with the following results:

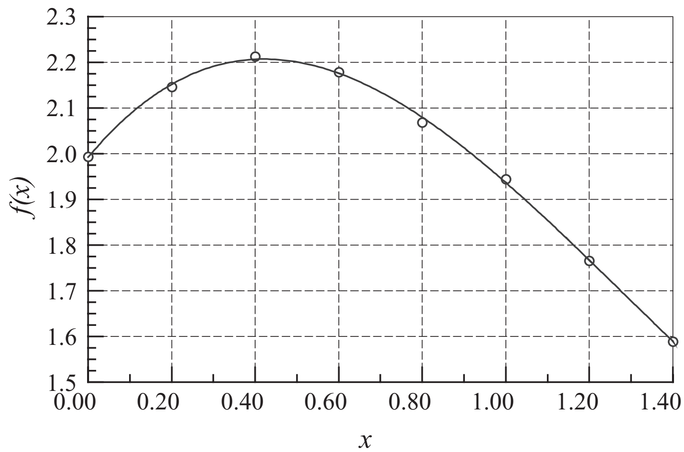
```
Degree of polynomial ==> 2
Coefficients are:
[ 2.0261875   0.64703869 -0.70239583]
Std. deviation = 0.0360968935809

Degree of polynomial ==> 3
Coefficients are:
[ 1.99215     1.09276786 -1.55333333  0.40520833]
Std. deviation = 0.0082604082973

Degree of polynomial ==> 4
Coefficients are:
[ 1.99185568  1.10282373 -1.59056108  0.44812973 -0.01532907]
Std. deviation = 0.00951925073521

Degree of polynomial ==>
Finished. Press return to exit
```

Based on standard deviation, the cubic seems to be the best candidate for the interpolant. Before accepting the result, we compare the plots of the data points and the interpolant – see the figure. The fit does appear to be satisfactory.



Approximating $f(x)$ by the interpolant, we have

$$f(x) \approx a_0 + a_1 x + a_2 x^2 + a_3 x^3$$

so that

$$f'(x) \approx a_1 + 2a_2 x + 3a_3 x^2$$

Therefore,

$$f'(0) \approx a_1 = 1.093$$

$$f'(1) = a_1 + 2a_2 + 3a_3 = 1.093 + 2(-1.553) + 3(0.405) = -0.798$$

In general, derivatives obtained from noisy data are at best rough approximations. In this problem, the data represents $f(x) = (x+2)/\cosh x$ with added random noise. Thus, $f'(x) = \left[1 - (x+2)\tanh x\right]/\cosh x$, so that the "correct" derivatives are $f'(0) = 1.000$ and $f'(1) = -0.833$.

PROBLEM SET 5.1

1. Given the values of $f(x)$ at the points x, $x - h_1$, and $x + h_2$, where $h_1 \neq h_2$, determine the finite difference approximation for $f''(x)$. What is the order of the truncation error?
2. Given the first backward finite difference approximations for $f'(x)$ and $f''(x)$, derive the first backward finite difference approximation for $f'''(x)$ using the operation $f'''(x) = \left[f''(x)\right]'$.
3. Derive the central difference approximation for $f''(x)$ accurate to $\mathcal{O}(h^4)$ by applying Richardson extrapolation to the central difference approximation of $\mathcal{O}(h^2)$.
4. Derive the second forward finite difference approximation for $f'''(x)$ from the Taylor series.
5. Derive the first central difference approximation for $f^{(4)}(x)$ from the Taylor series.

6. Use finite difference approximations of $O(h^2)$ to compute $f'(2.36)$ and $f''(2.36)$ from the data

x	2.36	2.37	2.38	2.39
$f(x)$	0.85866	0.86289	0.86710	0.87129

7. Estimate $f'(1)$ and $f''(1)$ from the following data:

x	0.97	1.00	1.05
$f(x)$	0.85040	0.84147	0.82612

8. Given the data

x	0.84	0.92	1.00	1.08	1.16
$f(x)$	0.431711	0.398519	0.367879	0.339596	0.313486

calculate $f''(1)$ as accurately as you can.

9. Use the data in the table to compute $f'(0.2)$ as accurately as possible.

x	0	0.1	0.2	0.3	0.4
$f(x)$	0.000 000	0.078 348	0.138 910	0.192 916	0.244 981

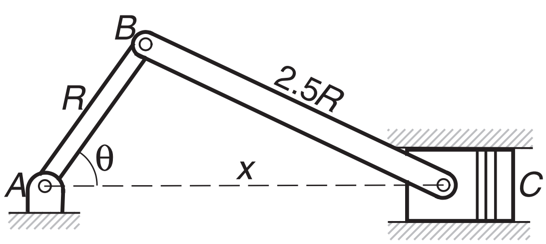
10. Using five significant figures in the computations, determine $d(\sin x)/dx$ at $x = 0.8$ from (a) the first forward difference approximation and (b) the first central difference approximation. In each case, use h that gives the most accurate result (this requires experimentation).

11. ■ Use polynomial interpolation to compute f' and f'' at $x = 0$, using the data

x	−2.2	−0.3	0.8	1.9
$f(x)$	15.180	10.962	1.920	−2.040

Given that $f(x) = x^3 - 0.3x^2 - 8.56x + 8.448$, gauge the accuracy of the result.

12. ■

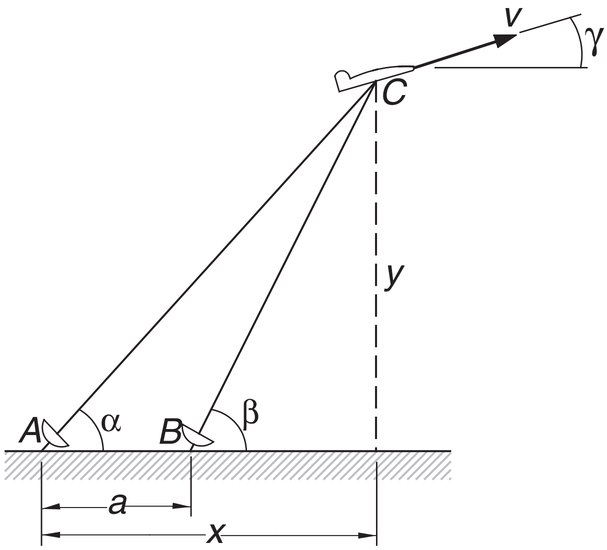


The crank AB of length $R = 90$ mm is rotating at constant angular speed of $d\theta/dt = 5000$ rev/min. The position of the piston C can be shown to vary with the angle θ as

$$x = R\left(\cos\theta + \sqrt{2.5^2 - \sin^2\theta}\right)$$

Write a program that computes the acceleration of the piston at $\theta = 0°, 5°, 10°, \ldots, 180°$ by numerical differentiation.

13. ■



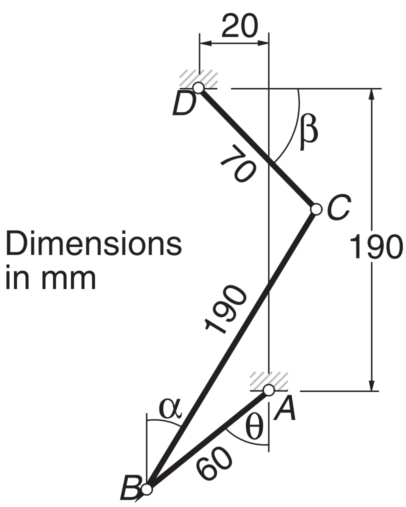
The radar stations A and B, separated by the distance $a = 500$ m, track the plane C by recording the angles α and β at 1-second intervals. If three successive readings are

t (s)	9	10	11
α	54.80°	54.06°	53.34°
β	65.59°	64.59°	63.62°

calculate the speed v of the plane and the climb angle γ at $t = 10$ s. The coordinates of the plane can be shown to be

$$x = a\frac{\tan\beta}{\tan\beta - \tan\alpha} \qquad y = a\frac{\tan\alpha\tan\beta}{\tan\beta - \tan\alpha}$$

14. ■



Geometric analysis of the linkage shown resulted in the following table relating the angles θ and β:

θ (deg)	0	30	60	90	120	150
β (deg)	59.96	56.42	44.10	25.72	−0.27	−34.29

Assuming that member AB of the linkage rotates with the constant angular velocity $d\theta/dt = 1$ rad/s, compute $d\beta/dt$ in rad/s at the tabulated values of θ. Use cubic spline interpolation.

15. ■ The relationship between stress σ and strain ε of some biological materials in uniaxial tension is

$$\frac{d\sigma}{d\varepsilon} = a + b\sigma$$

where a and b are constants. The following table gives the results of a tension test on such a material:

Strain ε	Stress σ (MPa)
0	0
0.05	0.252
0.10	0.531
0.15	0.840
0.20	1.184
0.25	1.558
0.30	1.975
0.35	2.444
0.40	2.943
0.45	3.500
0.50	4.115

Write a program that plots the tangent modulus $d\sigma/d\varepsilon$ versus σ and computes the parameters a and b by linear regression.