Numerical Methods

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Aims

In this lecture, we will . . .

- find the approximate solutions of derivative (first- and second-order) and antiderivative (definite integral only).

Numerical Differentiation and Integration

In this chapter we deal with techniques for approximating numerically the two fundamental operations of the calculus, differentiation and integration. Both of these problems may be approached in the same way. Although both numerical differentiation and numerical integration formulas will be discussed, it should be noted that numerical differentiation is inherently much less accurate than numerical integration, and its application is generally avoided whenever possible. Nevertheless, it has been used successfully in certain applications.

Important Points

I. Here we shall find the approximate solutions of derivative (first- and second-order) and antiderivative (definite integral only).
II. Given data points should be equally spaced only (length of each subinterval should be same). Smaller the length of the interval better the approximation.
III. Numerical methods for differentiation and integration can be derived using Lagrange interpolating polynomial at equally-spaced data points.
IV. Error term for each numerical method will be discuss which helps to look for the maximum error in the approximation.
V. Two-point formula (for first derivative) and three-point formulas (for first and second derivatives) for numerical differentiation and Trapezoidal and Simpson's rules for numerical integration will be discuss here.

Numerical Differentiation

Firstly, we discuss the numerical process for approximating the derivative of the function $f(x)$ at the given point. A function $f(x)$, known either explicitly or as a set of data points, is replaced by a simpler function. A polynomial $p(x)$ is the obvious choice of *approximating function*, since the operation of differentiation is then easily performed. The polynomial $p(x)$ is differentiated to obtain $p'(x)$, which is taken as an approximation to $f'(x)$ for any numerical value of x. Geometrically, this is equivalent to replacing the slope of $f(x)$, at x, by that of $p(x)$. Here, numerical differentiation are derived by differentiating interpolating polynomials. We now turn our attention to the numerical process for approximating the derivative of a function $f(x)$ at x, that is

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}, \quad \text{provided the limit exits.} \tag{1}$$

In principle, it is always possible to determine an analytic form (1) of a derivative for a given function. In some cases, however, the analytic form is very complicated, and a numerical approximation of the derivative may be sufficient for our purpose. The formula (1) provides an obvious way to get an approximation to $f'(x)$; simply compute

$$D_h f(x) = \frac{f(x+h) - f(x)}{h}, \tag{2}$$

for small values of stepsize h, called numerical differentiation formula for (1).

Here, we shall derive some formulas for estimating derivatives but we should avoid as far as possible, numerically calculating derivatives higher than the first, as the error in their evaluation increases with their orders. In spite of some inherent shortcomings, numerical differentiation is important to derive formulas for solving integrals and the numerical solution of both ordinary and partial differential equations.

There are three different approaches for deriving the numerical differentiation formulas. The first approach is based on the Taylor expansion of a function about a point, the second is to use difference operators, and the third approach to numerical differentiation is to fit a curve with a simple form to a function, and then to differentiate the curve-fit function. For example, the polynomial interpolation or spline methods of the Chapter 4 can be used to fit a curve to *tabulated data* for a function and the resulting polynomial or spline can then be differentiated. When a function is represented by a table of values, the most obvious approach is to differentiate the Lagrange interpolation formula

$$f(x) = p_n(x) + \frac{f^{(n+1)}(\eta(x))}{(n+1)!}\prod_{i=0}^{n}(x - x_i), \tag{3}$$

where the first term $p_n(x)$ of the right hand side is the Lagrange interpolating polynomial of degree n and the second term is its error term.

It is interesting to note that the process of numerical differentiation may be less satisfactory than interpolation the closeness of the ordinates of $f(x)$ and $p_n(x)$ on the interval of interest does not guarantee the closeness of their respective derivatives. Note that the derivation and analysis of formulas for numerical differentiation is considerably simplifies when the data is equally spaced. It will be assumed, therefore, that the points x_i are given by $x_i = x_0 + ih, (i = 0, 1, \ldots, n)$ for some fixed tabular interval h.

Numerical Differentiation Formulas

Here, we will find the approximation of first and second derivative of a function at a given arbitrary point x. For the approximation of the first derivative of a function we will use two-point formula, three-point formula, and Richardson's extrapolation formula. While for second derivative approximation we will discuss three-point formula only.

First Derivative Numerical Formulas

To obtain general formula for approximation of the first derivative of a function $f(x)$, we consider that $\{x_0, x_1, \ldots, x_n\}$ are $(n+1)$ distinct equally spaced points in some interval I and function $f(x)$ is continuous and its $(n+1)th$ derivatives exist in the given interval, that is, $f \in C^{n+1}(I)$. Then by differentiating (3) with respect to x and at $x = x_k$, we have

$$f'(x_k) = \sum_{i=0}^{n} f(x_i) L_i'(x_k) + \frac{f^{(n+1)}(\eta(x_k))}{(n+1)!} \prod_{\substack{i=0 \\ i \neq k}}^{n} (x_k - x_i). \tag{4}$$

The formula (4) is called the *(n+1)-point formula* to approximate $f'(x_k)$ with its error term. From this formula we can obtain many numerical differentiation formulas but here we shall discuss only two formulas to approximate (1) at given point $x = x_k$. First one is called the *two-point formula* and its error term which we can get from (4) by taking $n = 1$ and $k = 0$. The second numerical differentiation formula is called the *three-point formula* and its error term which can be obtained from (4) when $n = 2$ and $k = 0, 1, 2$.

Two-point Formula

Consider two distinct points x_0 and x_1, then, to find the approximation of (1), the first derivative of a function at given point, take $x_0 \in (a, b)$, 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 $x_1 \in [a, b]$. Consider the linear Lagrange *interpolating polynomial* $p_1(x)$ which interpolate $f(x)$ at the given points is

$$f(x) = p_1(x) = \left(\frac{x - x_1}{x_0 - x_1}\right) f(x_0) + \left(\frac{x - x_0}{x_1 - x_0}\right) f(x_1). \tag{5}$$

By taking derivative of (5) with respect to x and at $x = x_0$, we obtain

$$f'(x)|_{x=x_0} \approx p_1'(x)|_{x=x_0} = -\frac{f(x_0)}{x_0 - x_1} + \frac{f(x_1)}{x_1 - x_0}.$$

Simplifying the above expression, we have

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

which can be written as

$$f'(x_0) \approx \frac{f(x_0 + h) - f(x_0)}{h} = D_h f(x_0). \tag{6}$$

It is called the *two-point formula* for smaller values of h. For $h > 0$, sometime the formula (6) is also called the *two-point forward-difference formula* because it involves only differences of a function values forward from $f(x_0)$.

The two-point *forward-difference formula* has a simple *geometric interpretation* as the slope of the forward *secant line*, as shown in Figure 1.

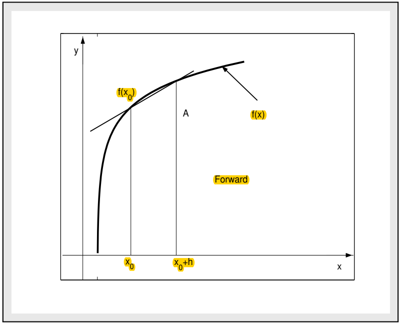

Figure: Forward-difference approximations.

Note that if $h < 0$, then the formula (6) is also called the *two-point backward-difference formula*, which can be written as

$$f'(x_0) \approx \frac{f(x_0) - f(x_0 - h)}{h}. \tag{7}$$

In this case, a value of x behind the point of interest is used. The formula (7) is useful in cases where the independent variable represents time. If x_0 denotes the present time, the *backward-difference formula* uses only present and past samples, it does not rely on future data samples that may not yet be available in a real time application.

The geometric interpretation of the two-point backward-difference formula, as the slope of the backward secant line, is shown in Figure 2.

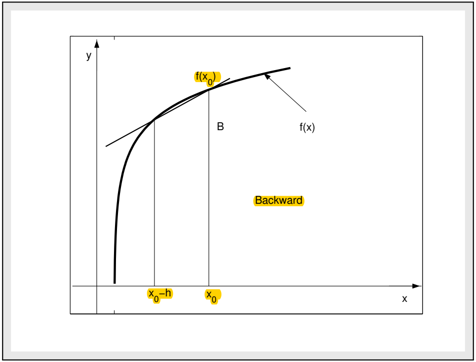

Figure: Backward-difference approximations.

Example 0.1

Let $f(x) = e^x$ and $h = 0.1, h = 0.01$. Use two-point forward difference formula to approximate $f'(2)$. For which value of h we have better approximation and why ?

Solution. Using the formula (6), with $x_0 = 2$, we have

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

Then for $h = 0.1$, we get

$$f'(2) \approx \frac{f(2.1) - f(2)}{0.1} \approx \frac{e^{2.1} - e^2}{0.1} = 7.7712.$$

Similarly, by using $h = 0.01$, we obtain

$$f'(2) \approx \frac{(e^{2.01} - e^2)}{0.01} = 7.4262.$$

Since the exact solution of $f'(2) = e^2$ is, 7.3891, so the corresponding actual errors with $h = 0.1$ and $h = 0.01$ are, -0.3821 and -0.0371 respectively. This shows that the approximation obtained with $h = 0.01$ is better than the approximation with $h = 0.1$. •

Error Term of Two-point Formula

The formula (6) is not very useful, therefore, let us attempt to find the error involves in our first numerical differentiation formula (6). Consider the *error term* for the linear Lagrange polynomial which can be written as

$$f(x) - p_1(x) = \frac{f''(\eta(x))}{2!} \prod_{i=0}^{1} (x - x_i),$$

for some unknown point $\eta(x) \in (x_0, x_1)$. By taking derivative of above equation with respect to x and at $x = x_0$, we have

$$\begin{aligned} f'(x_0) \quad - \quad p_1'(x_0) &= \left(\frac{d}{dx} f''(\eta(x)) \Big|_{x=x_0} \right) \frac{(x - x_0)(x - x_1)}{2} \\ &+ \quad \frac{f''(\eta(x_0))}{2} \left(\frac{d}{dx} (x^2 - x(x_0 + h) - x x_0 + x_0(x_0 + h)) \Big|_{x=x_0} \right). \end{aligned}$$

Since $\dfrac{d}{dx} f''(\eta(x)) = 0$ only if $x = x_0$, so error in the forward-difference formula (6) is

$$E_F(f, h) = f'(x_0) - D_h f(x_0) = -\frac{h}{2} f''(\eta(x)), \quad \text{where} \quad \eta(x) \in (x_0, x_1), \tag{8}$$

which is called the *error formula* of the two-point formula (6). Hence the formula (6) can be written as

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(\eta(x)), \quad \text{where} \quad \eta \in (x_0, x_1). \tag{9}$$

The formula (9) is more useful than the formula (6) because now on a large class of function, an error term is available along with the basic numerical formula.

Note that the formula (9) may also be derived from the Taylor's theorem. Expansion of function $f(x_1)$ about x_0 as far as term involving h^2 gives

$$f(x_1) = f(x_0) + hf'(x_0) + \frac{h^2}{2!} f''(\eta(x)). \tag{10}$$

From this the result follows by subtracting $f(x_0)$ both sides and dividing both sides by h and put $x_1 = x_0 + h$.

Example 0.2

Let $f(x) = x^3$ be defined in the interval $[0.2, 0.3]$. Use the error formula (8) of two-point formula for the approximation of $f'(0.2)$ to compute a value of η.

Solution. Since the exact value of the first derivative of the function at $x_0 = 0.2$ is

$$f'(x) = 3x^2 \quad \text{and} \quad f'(0.2) = 3(0.2)^2 = 0.12,$$

and the approximate value of $f'(0.2)$ using two point formula is

$$f'(0.2) \approx \frac{f(0.3) - f(0.2)}{0.1} = \frac{(0.3)^3 - (0.2)^3}{0.1} = 0.19,$$

so error E can be calculated as

$$E = 0.12 - 0.19 = -0.07.$$

Using the formula (6) and $f''(\eta) = 6\eta$, we have

$$-0.07 = -\frac{0.1}{2} 6\eta,$$

and solving for η, we get $\eta = 0.233$. •

Example 0.3

Let $f(x) = x^2 \cos x$ and $h = 0.1$. Then
(a) Compute the approximate value of $f'(1)$ using forward difference two-point formula (6).
(b) Compute the *error bound* for your approximation using the formula (8).
(c) Compute the absolute error.
(d) What best maximum value of stepsize h required to obtain the approximate value of $f'(1)$ correct to 10^{-2}.

Solution. *(a)* Given $x_0 = 1$, $h = 0.1$, then by using the formula (6), we have

$$f'(1) \approx \frac{f(1+0.1) - f(1)}{0.1} = \frac{f(1.1) - f(1)}{0.1} = D_h f(1).$$

Thus

$$f'(1) \approx \frac{(1.1)^2 \cos(1.1) - (1)^2 \cos(1)}{0.1} \approx \frac{0.5489 - 0.5403}{0.1} = 0.0860,$$

which is the required approximation of $f'(x)$ at $x = 1$.
(b) To find the error bound, we use the formula (8), which gives

$$E_F(f,h) = -\frac{0.1}{2} f''(\eta(x)), \quad \text{where} \quad \eta(x) \in (1, 1.1),$$

or

$$|E_F(f,h)| = \left| -\frac{0.1}{2} \right| |f''(\eta(x))|, \quad \text{for} \quad \eta \in (1, 1.1).$$

The second derivative $f''(x)$ of the function can be found as

$$f(x) = x^2 \cos x, \quad \text{gives} \quad f''(x) = (2 - x^2)\cos x - 4x \sin x.$$

The value of the second derivative $f''(\eta(x))$ cannot be computed exactly because $\eta(x)$ is not known. But one can bound the error by computing the largest possible value for $|f''(\eta(x))|$. So bound $|f''|$ on $[1, 1.1]$ can be obtain

$$M = \max_{1 \leq x \leq 1.1} |(2 - x^2)\cos x - 4x \sin x| = 3.5630,$$

at $x = 1.1$. Since $|f''(\eta(x))| \leq M$, therefore, for $h = 0.1$, we have

$$|E_F(f, h)| \leq \frac{0.1}{2} M = 0.05(3.5630) = 0.1782,$$

which is the possible maximum error in our approximation.

(c) Since the exact value of the derivative $f'(1)$ is 0.2392, therefore the absolute error $|E|$ can be computed as follows:

$$|E| = |f'(1) - D_h f(1)| = |0.2391 - 0.0860| = 0.1531.$$

(d) Since the given accuracy required is 10^{-2}, so

$$|E_F(f,h)| = |-\frac{h}{2} f''(\eta(x))| \leq 10^{-2},$$

for $\eta(x) \in (1, 1.1)$. This gives

$$\frac{h}{2} M \leq 10^{-2}, \quad \text{or} \quad h \leq \frac{(2 \times 10^{-2})}{M}.$$

Using $M = 3.5630$, we obtain

$$h \leq \frac{2}{356.3000} = 0.0056,$$

which is the best maximum value of h to get the required accuracy. •

The truncation error in the approximation of (9) is roughly proportional to stepsize h used in its computation. The situation is made worse by the fact that the round-off error in computing the approximate derivative (6) is roughly proportion to $\frac{1}{h}$. The overall error therefore is of the form

$$E = ch + \frac{\delta}{h},$$

where c and δ are constants. This places serve restriction on the accuracy that can be achieved with this formula.

Example 0.4

Consider $f(x) = x^2 \cos x$ and $x_0 = 1$. To show the effect of *rounding error*, the values $\tilde{f}_i$ are obtained by rounding $f(x_i)$ to seven *significant digits*, compute the *total error* for $h = 0.1$ and also, find the optimum h.

Solution. Given $|\epsilon_i| \leq \frac{1}{2} \times 10^{-7} = \delta$ and $h = 0.1$. Now to calculate the total error, we use

$$E(h) = \frac{h}{2} M + \frac{10^{-t}}{h},$$

where

$$M = \max_{1 \leq x \leq 1.1} |(2 - x^2)\cos x - 4x \sin x| = 3.5630.$$

Then

$$E(h) = \frac{0.1}{2}(3.5630) + \frac{10^{-7}}{0.1} = 0.17815 + 0.000001 = 0.178151.$$

Now to find the optimum h, we use

$$h = h_{opt} = \sqrt{\frac{2}{M} \times 10^{-t}} = \sqrt{\frac{2}{3.5630} \times 10^{-7}} = 0.00024,$$

which is the smallest value of h, below which the total error will begin to increase. Note that for

$$\begin{array}{ll} h = 0.00024, & E(h) = 0.000844, \\ h = 0.00015, & E(h) = 0.000934, \\ h = 0.00001, & E(h) = 0.010018. \end{array}$$

Three-point Central Difference Formula

Consider the quadratic Lagrange interpolating polynomial $p_2(x)$ to the three distinct equally spaced points x_0, x_1, and x_2, with $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$, for smaller value h, we have

$$\begin{aligned} f(x) = p_2(x) &= \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) \\ &+ \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2). \end{aligned}$$

Now taking the derivative of the above expression with respect to x and then take $x = x_k$, for $k = 0, 1, 2$, we have

$$\begin{aligned} f'(x_k) &\approx \frac{(2x_k-x_1-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(2x_k-x_0-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) \\ &+ \frac{(2x_k-x_0-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2). \end{aligned} \tag{11}$$

Three different numerical differentiation formulas can be obtained from (11) by putting $x_k = x_0$, or $x_k = x_1$ or $x_k = x_2$, which are use to find the approximation of the first derivative of a function defined by the formula (1) at the given point. Firstly, we take $x_k = x_1$, then the formula (11) becomes

$$\begin{aligned} f'(x_1) &\approx \frac{(2x_1 - x_1 - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(2x_1 - x_0 - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) \\ &+ \frac{(2x_1 - x_0 - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2). \end{aligned}$$

After, simplifying, and replacing $x_0 = x_1 - h, x_2 = x_1 + h$, we obtain

$$f'(x_1) \approx \frac{f(x_1 + h) - f(x_1 - h)}{2h} = D_h f(x_1). \tag{12}$$

It is called the *three-point central-difference formula* for finding the approximation of the first derivative of a function at the given point x_1.
Note that the formulation of the formula (12) uses data points that are centered about the point of interest x_1 even though it does not appear in the right side of (12).

Error Formula of Central Difference Formula

The formula (12) is not very useful, therefore, let us attempt to find the error involve in the formula (12) for numerical differentiation. Consider the error term for the quadratic Lagrange polynomial which can be written as

$$f(x) - p_2(x) = \frac{f'''(\eta(x))}{3!} \prod_{i=0}^{2} (x - x_i),$$

for some unknown point $\eta(x) \in (x_0, x_2)$. By taking derivative of the above equation with respect to x and then taking $x = x_1$, we have

$$f'(x_1) - p_2'(x_1) = \left(\frac{d}{dx} f'''(\eta(x)) \Big|_{x=x_1} \right) \frac{(x - x_0)(x - x_1)(x - x_2)}{6}$$

$$+ \quad \frac{f'''(\eta(x_1))}{6} \Big((x - x_1)(x - x_2) + (x - x_0)(x - x_2) + (x - x_0)(x - x_1) \Big|_{x=x_1} \Big).$$

Since $\dfrac{d}{dx} f'''(\eta(x)) = 0$ only if $x = x_1$, therefore the error formula of the central-difference formula (12) can be written as

$$E_C(f, h) = f'(x_1) - D_h f(x_1) = -\frac{h^2}{6} f'''(\eta(x_1)), \tag{13}$$

where $\eta(x_1) \in (x_1 - h, x_1 + h)$.

Hence the formula (12) can be written as

$$f'(x_1) = \frac{f(x_1 + h) - f(x_1 - h)}{2h} - \frac{h^2}{6} f'''(\eta(x_1)), \tag{14}$$

where $\eta(x_1) \in (x_1 - h, x_1 + h)$. The formula (14) is more useful than the formula (12) because now on a large class of function, an error term is available along with the basic *numerical formula*.

Example 0.5

Let $f(x) = x^2 + \cos x$ and $h = 0.1$. Then
(a) Compute the approximate value of $f'(1)$ by using three-point central difference formula (12).
(b) Compute the error bound for your approximation using (13).
(c) Compute the absolute error.
(d) What is the best maximum value of stepsize h required to obtain the approximate value of $f'(1)$ correct to 10^{-2}.

Solution. *(a)* Given $x_1 = 1, h = 0.1$, then using the formula (12), we have

$$f'(1) \approx \frac{f(1+0.1) - f(1-0.1)}{2(0.1)} = \frac{f(1.1) - f(0.9)}{0.2} = D_h f(1).$$

Then

$$f'(1) \approx \frac{[(1.1)^2 + \cos(1.1)] - [(0.9)^2 + \cos(0.9)]}{0.2} \approx \frac{1.6636 - 1.4316}{0.2} = 1.1600.$$

(b) By using the error formula (13), we have

$$E_C(f,h) = -\frac{(0.1)^2}{6} f'''(\eta(x_1)), \quad \text{for} \quad \eta(x_1) \in (0.9, 1.1),$$

or

$$|E_C(f,h)| = \left| -\frac{(0.1)^2}{6} \right| |f'''(\eta(x_1))|, \quad \text{for} \quad \eta(x_1) \in (0.9, 1.1).$$

Since

$$f'''(\eta(x_1)) = \sin \eta(x_1).$$

This formula cannot be computed exactly because $\eta(x_1)$ is not known. But one can bound the error by computing the largest possible value for $|f'''(\eta(x_1))|$. So bound $|f'''|$ on $[0.9, 1.1]$ is

$$M = \max_{0.9 \leq x \leq 1.1} |\sin x| = 0.8912,$$

at $x = 1.1$. Thus, for $|f'''(\eta(x_1))| \leq M$ and $h = 0.1$, gives

$$|E_C(f,h)| \leq \frac{0.01}{6} M = \frac{0.01}{6}(0.8912) = 0.0015,$$

which is the possible *maximum error* in our approximation.

(c) Since the exact value of the derivative $f'(1)$ is, 0.2391, therefore, the absolute error $|E|$ can be computed as follows

$$|E| = |f'(1) - D_h f(1)| = |(2 - \sin 1) - 1.1600| = |1.1585 - 1.1600| = 0.0015.$$

(d) Since the given accuracy required is 10^{-2}, so

$$|E_C(f,h)| = \left| -\frac{h^2}{6} f'''(\eta(x_1)) \right| \leq 10^{-2},$$

for $\eta(x_1) \in (0.9, 1.1)$. Then

$$\frac{h^2}{6} M \leq 10^{-2}.$$

Solving for h and taking $M = 0.8912$, we obtain

$$h^2 \leq \frac{6}{0.8912} = 0.0673, \quad \text{and} \quad h \leq 0.2594.$$

So the best value of h is 0.25.

Three-point Forward and Backward Difference Formulas

Similarly, the two other three-point formulas can be obtained by taking $x_k = x_0$ and $x_k = x_2$ in the formula (11). Firstly, by taking $x_k = x_0$ in the formula (11) and then after simplifying, we have

$$f'(x_0) \approx \frac{-3f(x_0) + 4f(x_0+h) - f(x_0+2h)}{2h} = D_h f(x_0), \tag{15}$$

which is called the *three-point forward-difference formula* which is use to approximate the formula (1) at given point $x = x_0$. The error term of this approximation formula can be obtain in the similar way as we obtained for the central-difference formula and it is

$$E_F(f,h) = \frac{h^2}{3} f'''(\eta(x_0)), \tag{16}$$

where $\eta(x_0) \in (x_0, x_0+2h)$. Similarly, taking $x_k = x_2$ in the formula (11), and after simplifying, we obtain

$$f'(x_2) \approx \frac{f(x_2-2h) - 4f(x_2-h) + 3f(x_2)}{2h} = D_h f(x_2), \tag{17}$$

which is called the *three-point backward-difference formula* which is use to approximate the formula (1) at given point $x = x_2$. It has the error term of the form

$$E_B(f,h) = \frac{h^2}{3} f'''(\eta(x_2)), \tag{18}$$

where $\eta(x_2) \in (x_2 - 2h, x_2)$.

Note that the *backward-difference formula* (17) can be obtained from the *forward-difference formula* by replacing h with $-h$. Also, note that the error in (12) is approximately half the error in (15) and (17). This is reasonable since in using the central-difference formula (12) data is being examined on both sides of point x_1, and for others in (15) and (17) only on one side. Note that in using the central-difference formula, a function $f(x)$ needs to be evaluated at only two points, whereas in using the other two formulas, we need the values of a function at three points. The approximations in using the formulas (15) and (17) are useful near the ends of the required interval, since the information about a function outside the interval may not be available. Thus the central-difference formula (12) is superior to both the forward-difference formula (15) and the backward-difference formula (17). The central-difference represents the average of the forward-difference and the backward-difference.

Example 0.6

Consider the following table for set of data points

x	1	1.6	2	2.3	2.8	3	3.9	4	4.8	5
$f(x)$	0.00	0.47	0.69	0.83	1.03	1.10	1.36	1.39	1.57	1.61

(a) Use three-point formula for smaller value of h to find approximation of $f'(3)$.
(b) The function tabulated is $\ln x$, find error bound and absolute error for the approximation
of $f'(3)$.
(c) What is the best maximum value of stepsize h required to obtain the approximate value of $f'(3)$ within the accuracy 10^{-4}.

Solution. *(a)* For the given table of data points, we can use all three-points formulas as for the central difference we can take

$$x_0 = x_1 - h = 2, \quad x_1 = 3, \quad x_2 = x_1 + h = 4, \quad \text{gives} \quad h = 1,$$

for the forward difference formula we can take

$$x_0 = 3, \quad x_1 = x_0 + h = 3.9, \quad x_2 = x_0 + 2h = 4.8, \quad \text{gives} \quad h = 0.9,$$

and for the backward difference formula we can take

$$x_0 = x_2 - 2h = 1.6, \quad x_1 = x_2 - h = 2.3, \quad x_2 = 3, \quad \text{gives} \quad h = 0.7.$$

Since we know that smaller the vale of h better the approximation of the derivative of the function, therefore, for the given problem, backward difference is the best formula to find approximation of $f'(3)$ as

$$f'(3) \approx \frac{f(1.6) - 4f(2.3) + 3f(3)}{2(0.7)} \approx \frac{[0.47 - 4(0.83) + 3(1.10)]}{1.4} = 0.3214.$$

(b) Using error term of backward difference formula, we have

$$E_B(f,h) = \frac{h^2}{3} f'''(\eta), \quad \text{or} \quad |E_B(f,h)| \leq \frac{h^2}{3} |f'''(\eta)|.$$

Taking $|f'''(\eta(x_2))| \leq M = \max_{1.6 \leq x \leq 3} |f'''(x)| = \max_{1.6 \leq x \leq 3} |2/x^3| = 0.4883$. Thus using $h = 0.7$, we obtain

$$|E_B(f,h)| \leq \frac{(0.7)^2}{3}(0.4883) = 0.0798,$$

the required error bounds for the approximations. To compute the absolute error we do as

$$|E| = |f'(3) - 0.3214| = |0.3333 - 0.3214| = 0.0119.$$

(c) Since the given accuracy required is 10^{-4}, so

$$|E_B(f,h)| = \left|\frac{h^2}{3} f'''(\eta)\right| \leq 10^{-4},$$

for $\eta \in (1.6, 3)$. Then

$$\frac{h^2}{3} M \leq 10^{-4}.$$

Solving for h by taking $M = 0.4883$, we obtain

$$h^2 \leq \frac{3 \times 10^{-4}}{0.4883} = 0.0248,$$

and so $h = 0.025$ the best maximum value of h. $\bullet$

Example 0.7

Use the three-point formulas (12), (15) and (17) to approximate the first derivative of the function $f(x) = e^x$ at $x = 2$, take $h = 0.1$. Also, compute the error bound for each approximation.

Solution. Given $f(x) = e^x$ and $h = 0.1$, then
Central-difference formula:

$$f'(2) \approx \frac{(f(2.1) - f(1.9))}{2h} = \frac{(e^{2.1} - e^{1.9})}{0.2} = 7.4014.$$

Forward-difference formula:

$$f'(2) \approx \frac{-3f(2) + 4f(2.1) - f(2.2)}{2h} \approx \frac{-3e^2 + 4e^{2.1} - e^{2.2}}{0.2} = 7.3625.$$

Backward difference formula:

$$f'(2) \approx \frac{f(1.8) - 4f(1.9) + 3f(2)}{2h} \approx \frac{e^{1.8} - 4e^{1.9} + 3e^2}{0.2} = 7.3662.$$

Since the exact solution of the first derivative of the given function at $x = 2$ is 7.3891, so the corresponding actual errors are, $-0.0123, 0.0266$ and 0.0229 respectively. This shows that the approximate solution got by using the central-difference formula is closer to exact solution as compared with the other two difference formulas.

The error bounds for the approximations got by (12), (15), and (17) are as follows:
Central-difference formula:

$$E_C(f,h) = -\frac{h^2}{6} f'''(\eta(x_1)), \quad \text{or} \quad |E_C(f,h)| \leq \frac{h^2}{6} |f'''(\eta(x_1))|.$$

Taking $|f'''(\eta(x_1))| \leq M = \max_{1.9 \leq x \leq 2.1} |e^x| = e^{2.1}$ and $h = 0.1$, we obtain

$$|E_C(f,h)| \leq \frac{(0.1)^2}{6} e^{2.1} = 0.0136.$$

Forward-difference formula:

$$E_F(f,h) = \frac{h^2}{3} f'''(\eta(x_0)), \quad \text{or} \quad |E_F(f,h)| \leq \frac{h^2}{3} |f'''(\eta(x_0))|.$$

Taking $|f'''(\eta(x_0))| \leq M = \max\limits_{2 \leq x \leq 2.2} |e^x| = e^{2.2}$ and $h = 0.1$, we obtain

$$|E_F(f,h)| \leq \frac{(0.1)^2}{3} e^{2.2} = 0.0301.$$

Backward difference formula:

$$E_B(f,h) = \frac{h^2}{3} f'''(\eta(x_2)), \quad \text{or} \quad |E_B(f,h)| \leq \frac{h^2}{3} |f'''(\eta(x_2))|.$$

Taking $|f'''(\eta(x_2))| \leq M = \max_{1.8 \leq x \leq 2} |e^x| = e^2$ and $h = 0.1$, we obtain

$$|E_B(f,h)| \leq \frac{(0.1)^2}{3} e^2 = 0.0246.$$

Thus we got the required error bounds for the approximations.

Second Derivative Numerical Formula

It is also possible to estimate second and higher order derivatives numerically. Formulas for *higher derivatives* can be found by differentiating the interpolating polynomial repeatedly or using the Taylor's theorem. Since the *two-point* and *three-point* formulas for the approximation of the first derivative of a function were derived by differentiating the Lagrange interpolation polynomials for $f(x)$ but the derivation of the higher-order can be tedious. Therefore, we shall use here the Taylor's theorem for finding the *three-point* central-difference formulas for finding approximation of the second derivative $f''(x)$ of a function $f(x)$ at the given point $x = x_1$. The process used to obtain numerical formulas for first and second derivatives of a function can be readily extended to third- and higher-order derivatives of a function.

Three-point Central Difference Formula

To find the three-point central-difference formula for the approximation of the second derivative of a function at given point, we use the third-order Taylor's theorem by expanding a function $f(x)$ about a point x_1 and evaluate at $x_1 + h$ and $x_1 - h$. Then

$$f(x_1 + h) = f(x_1) + hf'(x_1) + \frac{1}{2}h^2 f''(x_1) + \frac{1}{6}h^3 f'''(x_1) + \frac{1}{24}h^4 f^{(4)}(\eta_1(x)),$$

and

$$f(x_1 - h) = f(x_1) - hf'(x_1) + \frac{1}{2}h^2 f''(x_1) - \frac{1}{6}h^3 f'''(x_1) + \frac{1}{24}h^4 f^{(4)}(\eta_2(x)),$$

where $(x_1 - h) < \eta_2(x) < x_1 < \eta_1(x) < (x_1 + h)$.
By adding these equations and simplifies, we have

$$f(x_1 + h) + f(x_1 - h) = 2f(x_1) + h^2 f''(x_1) + \frac{(f^{(4)}(\eta_1(x)) + f^{(4)}(\eta_2(x)))}{24} h^4.$$

Solving this equation for $f''(x_1)$, we obtain

$$f''(x_1) = \frac{f(x_1 - h) - 2f(x_1) + f(x_1 + h)}{h^2} - \frac{h^4}{24}\left[f^{(4)}(\eta_1(x)) + f^{(4)}(\eta_2(x))\right].$$

If $f^{(4)}$ is continuous on $[x_1 - h, x_1 + h]$, then by using the Intermediate Value Theorem, the above equation can be written as

$$f''(x_1) = \frac{f(x_1 - h) - 2f(x_1) + f(x_1 + h)}{h^2} - \frac{h^4}{12} f^{(4)}(\eta(x_1)).$$

Then the following formula

$$f''(x_1) \approx \frac{f(x_1 - h) - 2f(x_1) + f(x_1 + h)}{h^2} = D_h^2 f(x_1), \tag{19}$$

is called the *three-point central-difference formula* for the approximation of the second derivative of a function $f(x)$ at the given point $x = x_1$.

Note that the *error term* of the three-point central-difference formula (19) for the approximation of the second derivative of a function $f(x)$ at the given point $x = x_1$ is of the form

$$E_C(f,h) = -\frac{h^2}{12} f^{(4)}(\eta(x_1)), \tag{20}$$

for some unknown point $\eta(x_1) \in (x_1 - h, x_1 + h)$.

Example 0.8

Let $f(x) = x \ln x + x$ and $x = 0.9, 1.3, 2.1, 2.5, 3.2$. Then find the approximate value of $f''(x) = \frac{1}{x}$ at $x = 1.9$. Also, compute the absolute error.

Solution. Given $f(x) = x \ln x + x$, then one can easily find second derivative of the function as

$$f'(x) = \ln x + 2 \quad \text{and} \quad f''(x) = \frac{1}{x}.$$

To find the approximation of $f''(x) = \frac{1}{x}$ at the given point $x_1 = 1.9$, we use the three-point formula (19)

$$f''(x_1) \approx \frac{f(x_1 + h) - 2f(x_1) + f(x_1 - h)}{h^2} = D_h^2 f(x_1).$$

Taking the three points $1.3, 1.9$ and 2.5 (equally spaced), giving $h = 0.6$, we have

$$\begin{aligned} f''(1.9) &\approx \frac{f(2.5) - 2f(1.9) + f(1.3)}{0.36} \\ &\approx \frac{((2.5 \ln 2.5 + 2.5) - 2(1.9 \ln 1.9 + 1.9) + (1.3 \ln 1.3 + 1.3))}{0.36} \\ &\approx \frac{4.7907 - 6.2391 + 1.6411}{0.36} = 0.5353 = D_h^2 f(1.9). \end{aligned}$$

Since the exact value of $f''(1.9)$ is $\frac{1}{1.9} = 0.5263$, therefore, the absolute error $|E|$ can be computed as follows:

$$|E| = |f''(1.9) - D_h^2 f(1.9)| = |0.5263 - 0.5353| = 0.009.$$

Example 0.9

Let $f(x) = x^2 + \cos x$. Then
(a) Compute the approximate value of $f''(x)$ at $x = 1$, taking $h = 0.1$ using (19).
(b) Compute the error bound for your approximation using (20).
(c) Compute the absolute error.
(d) What is the best maximum value of stepsize h required to obtain the approximate value of $f''(1)$ within the accuracy 10^{-2}.

Solution. *(a)* Given $x_1 = 1, h = 0.1$, then the formula (19) becomes

$$f''(1) \approx \frac{f(1+0.1) - 2f(1) + f(1-0.1)}{(0.1)^2} = D_h^2 f(1),$$

or

$$\begin{aligned} f''(1) &\approx \frac{f(1.1) - 2f(1) + f(0.9)}{0.01} \\ &\approx \frac{[(1.1)^2 + \cos(1.1)] - 2[1^2 + \cos(1)] + [(0.9)^2 + \cos(0.9)]}{0.01} \\ &\approx \frac{1.6636 - 3.0806 + 1.4316}{0.01} \approx 1.4600 = D_h^2 f(1). \end{aligned}$$

(b) To compute the error bound for our approximation in part (a), we use the formula (20) and have

$$E_C(f,h) = -\frac{h^2}{12} f^{(4)}(\eta(x_1)), \quad \text{for} \quad \eta(x_1) \in (0.9, 1.1),$$

or

$$|E_C(f,h)| = \left| -\frac{h^2}{12} \right| |f^{(4)}(\eta(x_1))|, \quad \text{for} \quad \eta(x_1) \in (0.9, 1.1).$$

The fourth derivative of the given function at $\eta(x_1)$ is

$$f^{(4)}(\eta(x_1)) = \cos \eta(x_1),$$

and it cannot be computed exactly because $\eta(x_1)$ is not known. But one can bound the error by computing the largest possible value for $|f^{(4)}(\eta(x_1))|$. So bound $|f^{(4)}|$ on the interval $(0.9, 1.1)$ is

$$M = \max_{0.9 \le x \le 1.1} |\cos \eta(x_1)| = 0.4536,$$

at $x = 1.1$, Thus, for $|f^{(4)}(\eta(x))| \le M$, we have

$$|E_C(f,h)| \le \frac{h^2}{12} M.$$

Taking $M = 0.4536$ and $h = 0.1$, we obtain

$$|E_C(f,h)| \le \frac{0.01}{12}(0.4536) = 0.0004,$$

which is the possible maximum error in our approximation.

(c) Since the exact value of $f''(1)$ is

$$f''(1) = (2 - 1^2)\cos 1 - 4(1)\sin 1 = -2.8256,$$

therefore, the absolute error $|E|$ can be computed as follows:

$$|E| = |f''(1) - D_h^2 f(1)| = |1.4597 - 1.4600| = 0.0003.$$

(d) Since the given accuracy required is 10^{-2}, so

$$|E_C(f,h)| = \left| -\frac{h^2}{12} f^{(4)}(\eta(x_1)) \right| \leq 10^{-2},$$

for $\eta(x_1) \in (0.9, 1.1)$. Then for $|f^{(4)}(\eta(x_1))| \leq M$, we have

$$\frac{h^2}{12} M \leq 10^{-2}.$$

Solving for h^2, we obtain

$$h^2 \leq \frac{(12 \times 10^{-2})}{M} = \frac{(12 \times 10^{-2})}{0.4536} = 0.2646,$$

and it gives the value of h as

$$h \leq 0.5144.$$

Thus the best maximum value of h is 0.5. •

Formulas for Computing Derivatives

For convenience, we collect following some useful central-difference, forward-difference and backward-difference formulas for computing different orders derivatives.

Central Difference Formulas

The central-difference formula (12) for first derivative $f'(x_1)$ of a function required that a function can be computed at points that lies on both sides of x_1. The Taylor series can be used to obtain central-difference formulas for higher derivatives. The most usable are those of order $O(h^2)$ and $O(h^4)$ and are given as follows:

$$
\begin{aligned}
f'(x_0) &= \frac{f_1 - f_{-1}}{2h} + O(h^2) \\
f'(x_0) &= \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h} + O(h^4) \\
f''(x_0) &= \frac{f_1 - 2f_0 + f_{-1}}{h^2} + O(h^2) \\
f''(x_0) &= \frac{-f_2 + 16f_1 - 30f_0 + 16f_{-1} - f_{-2}}{12h^2} + O(h^4) \\
f'''(x_0) &= \frac{f_2 - 2f_1 + 2f_{-1} - f_{-2}}{2h^3} + O(h^2) \\
f'''(x_0) &= \frac{-f_3 + 8f_2 - 13f_1 + 13f_{-1} - 8f_{-2} + f_{-3}}{8h^3} + O(h^4) \\
f^{(4)}(x_0) &= \frac{f_2 - 4f_1 + 6f_0 - 4f_{-1} + f_{-2}}{h^4} + O(h^2) \\
f^{(4)}(x_0) &= \frac{-f_3 + 12f_2 - 39f_1 + 56f_0 - 39f_{-1} + 12f_{-2} - f_{-3}}{6h^4} + O(h^4)
\end{aligned}
$$

Summary

In this lecture, we ...

- found the approximate solutions of derivative (first- and second-order) and antiderivative (definite integral only).