Numerical Differentiation

Wednesday, 18 December 2024 6:13 pm

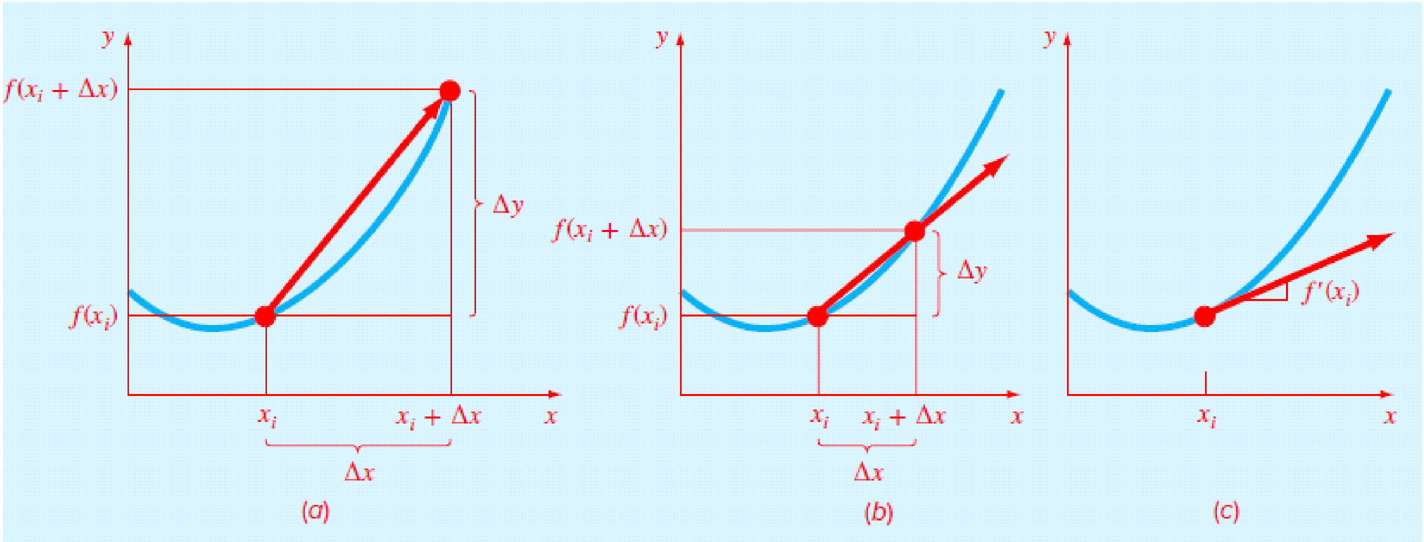
Numerical Differentiation

21.1.1 What Is Differentiation?

Calculus is the mathematics of change. Because engineers and scientists must continuously deal with systems and processes that change, calculus is an essential tool of our profession. Standing at the heart of calculus is the mathematical concept of differentiation.

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$



For example, the forward Taylor series expansion can be written as [recall Eq. (4.13)]

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \cdots \tag{21.12}$$

which can be solved for

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(x_i)}{2!}h + O(h^2) \tag{21.13}$$

In Chap. 4, we truncated this result by excluding the second- and higher-derivative terms and were thus left with a forward-difference formula:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h) \tag{21.14}$$

In contrast to this approach, we now retain the second-derivative term by substituting the following forward-difference approximation of the second derivative [recall Eq. (4.27)]:

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h) \tag{21.15}$$

into Eq. (21.13) to yield

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{2h^2}h + O(h^2) \tag{21.16}$$

or, by collecting terms:

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2) \tag{21.17}$$

Problem Statement. Recall that in Example 4.4 we estimated the derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at $x = 0.5$ using finite-differences and a step size of $h = 0.25$. The results are summarized in the following table. Note that the errors are based on the true value of $f'(0.5) = -0.9125$.

	Backward $O(h)$	Centered $O(h^2)$	Forward $O(h)$
Estimate	−0.714	−0.934	−1.155
ε_t	21.7%	−2.4%	−26.5%

First Derivative	Error
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$	$O(h^2)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$	$O(h)$
$f''(x_i) = \dfrac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}$	$O(h^2)$

First Derivative	Error
$f'(x_i) = \dfrac{f(x_i) - f(x_{i-1})}{h}$	$O(h)$
$f'(x_i) = \dfrac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h}$	$O(h^2)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}$	$O(h)$
$f''(x_i) = \dfrac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2}$	$O(h^2)$

First Derivative	Error
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_{i-1})}{2h}$	$O(h^2)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}$	$O(h^4)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}$	$O(h^2)$
$f''(x_i) = \dfrac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2}$	$O(h^4)$

Solution. The data needed for this example are

$$
\begin{array}{ll}
x_{i-2} = 0 & f(x_{i-2}) = 1.2 \\
x_{i-1} = 0.25 & f(x_{i-1}) = 1.1035156 \\
x_i = 0.5 & f(x_i) = 0.925 \\
x_{i+1} = 0.75 & f(x_{i+1}) = 0.6363281 \\
x_{i+2} = 1 & f(x_{i+2}) = 0.2
\end{array}
$$

The forward difference of accuracy $O(h^2)$ is computed as (Fig. 21.3)

$$f'(0.5) = \frac{-0.2 + 4(0.6363281) - 3(0.925)}{2(0.25)} = -0.859375 \qquad \varepsilon_t = 5.82\%$$

The backward difference of accuracy $O(h^2)$ is computed as (Fig. 21.4)

$$f'(0.5) = \frac{3(0.925) - 4(1.1035156) + 1.2}{2(0.25)} = -0.878125 \qquad \varepsilon_t = 3.77\%$$

The centered difference of accuracy $O(h^4)$ is computed as (Fig. 21.5)

$$f'(0.5) = \frac{-0.2 + 8(0.6363281) - 8(1.1035156) + 1.2}{12(0.25)} = -0.9125 \qquad \varepsilon_t = 0\%$$

RICHARDSON EXTRAPOLATION

$$D = \frac{4}{3}D(h_2) - \frac{1}{3}D(h_1)$$

Richardson Extrapolation

Problem Statement. Using the same function as in Example 21.1, estimate the first derivative at $x = 0.5$ employing step sizes of $h_1 = 0.5$ and $h_2 = 0.25$. Then use Eq. (21.20) to compute an improved estimate with Richardson extrapolation. Recall that the true value is -0.9125.

Solution. The first-derivative estimates can be computed with centered differences as

$$D(0.5) = \frac{0.2 - 1.2}{1} = -1.0 \qquad \varepsilon_t = -9.6\%$$

and

$$D(0.25) = \frac{0.6363281 - 1.103516}{0.5} = -0.934375 \qquad \varepsilon_t = -2.4\%$$

The improved estimate can be determined by applying Eq. (21.20) to give

$$D = \frac{4}{3}(-0.934375) - \frac{1}{3}(-1) = -0.9125$$

which for the present case is exact.

DERIVATIVES OF UNEQUALLY SPACED DATA

For example, you can fit a second-order Lagrange polynomial to three adjacent points (x_0, y_0), (x_1, y_1), and (x_2, y_2). Differentiating the polynomial yields:

$$f'(x) = f(x_0)\frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} + f(x_1)\frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} + f(x_2)\frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} \tag{21.21}$$

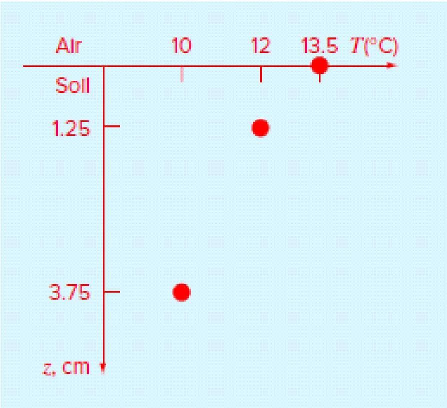
Differentiating Unequally Spaced Data

Problem Statement. As in Fig. 21.6, a temperature gradient can be measured down into the soil. The heat flux at the soil-air interface can be computed with Fourier's law (Table 21.1):

$$q(z = 0) = -k\left.\frac{dT}{dz}\right|_{z=0}$$

where $q(z)$ = heat flux (W/m^2), k = coefficient of thermal conductivity for soil [= 0.5 W/(m · K)], T = temperature (K), and z = distance measured down from the surface into the soil (m). Note that a positive value for flux means that heat is transferred from the air to the soil. Use numerical differentiation to evaluate the gradient at the soil-air interface and employ this estimate to determine the heat flux into the ground.

FIGURE 21.6
Temperature versus depth into the soil.



Solution. Equation (21.21) can be used to calculate the derivative at the air-soil interface as

$$f'(0) = 13.5\,\frac{2(0) - 0.0125 - 0.0375}{(0 - 0.0125)(0 - 0.0375)} + 12\,\frac{2(0) - 0 - 0.0375}{(0.0125 - 0)(0.0125 - 0.0375)}$$
$$+ 10\,\frac{2(0) - 0 - 0.0125}{(0.0375 - 0)(0.0375 - 0.0125)}$$
$$= -1440 + 1440 - 133.333 = -133.333 \text{ K/m}$$

which can be used to compute

$$q(z = 0) = -0.5\,\frac{\text{W}}{\text{m K}}\left(-133.333\,\frac{\text{K}}{\text{m}}\right) = 66.667\,\frac{\text{W}}{\text{m}^2}$$

21.1 Compute forward and backward difference approximations of $O(h)$ and $O(h^2)$, and central difference approximations of $O(h^2)$ and $O(h^4)$ for the first derivative of $y = \sin x$ at $x = \pi/4$ using a value of $h = \pi/12$. Estimate the true percent relative error ε_t for each approximation.

21.2 Use centered difference approximations to estimate the first and second derivatives of $y = e^x$ at $x = 2$ for $h = 0.1$. Employ both $O(h^2)$ and $O(h^4)$ formulas for your estimates.

21.4 Use Richardson extrapolation to estimate the first derivative of $y = \cos x$ at $x = \pi/4$ using step sizes of $h_1 = \pi/3$ and $h_2 = \pi/6$. Employ centered differences of $O(h^2)$ for the initial estimates.

21.5 Repeat Prob. 21.4, but for the first derivative of ln x at $x = 5$ using $h_1 = 2$ and $h_2 = 1$.

21.6 Employ Eq. (21.21) to determine the first derivative of $y = 2x^4 - 6x^3 - 12x - 8$ at $x = 0$ based on values at $x_0 = -0.5$, $x_1 = 1$, and $x_2 = 2$. Compare this result with the true value and with an estimate obtained using a centered difference approximation based on $h = 1$.

DERIVATIVES USING NEWTON'S FORWARD INTERPOLATION FORMULA

$$Dy_0 = \left(\frac{dy}{dx}\right)_{x=x_0} = \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \ldots\right]$$

$$D^2 y_0 = \left(\frac{d^2 y}{dx^2}\right)_{x=x_0} = \frac{1}{h^2}\left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 + \ldots\right]$$

DERIVATIVES USING NEWTON'S BACKWARD INTERPOLATION FORMULA

$$\left(\frac{dy}{dx}\right)_{x=x_n} = \frac{1}{h}\left[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \frac{1}{3}\nabla^3 y_n + \frac{1}{4}\nabla^4 y_n + \dots\right],$$

$$\left(\frac{d^2y}{dx^2}\right)_{x=x_n} = \frac{1}{h^2}\left[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \dots\right].$$

DERIVATIVES USING STIRLING'S FORMULA

$$\left(\frac{dy}{dx}\right)_{x=x_0} = \frac{1}{h}\left[\frac{\Delta y_0 + \Delta y_{-1}}{2} - \frac{1}{6}\frac{\left(\Delta^3 y_{-1} + \Delta^3 y_{-2}\right)}{2} + \frac{1}{30}\frac{\left(\Delta^5 y_{-2} + \Delta^5 y_{-3}\right)}{2} + \dots\right]$$

Differentiating (20) w.r.t. x and putting $x = x_0$ we get

$$\left(\frac{d^2y}{dx^2}\right)_{x=x_0} = \frac{1}{h^2}\left[\Delta^2 y_{-1} - \frac{1}{12}\Delta^4 y_{-2} + \dots\right].$$

Example 8.1 *From the table of values below compute* $\frac{dy}{dx}$ *and* $\frac{d^2y}{dx^2}$ *for* $x = 1$

x	1	2	3	4	5	6
y	1	8	27	64	125	216

Solution The difference table is

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$
1	1				
		7			
2	8		12		
		19		6	
3	27		18		0
		37		6	
4	64		24		0
		61		6	
5	125		30		
		91			
6	216				

We have $x_0 = 1$, $h = 1$. $x = 1$ is at the beginning of the table.

$\therefore$ We use Newtons forward formula

$$\left(\frac{dy}{dx}\right)_{x=x_0} = \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \dots\right]$$

$$\Rightarrow \left(\frac{dy}{dx}\right)_{x=1} = \frac{1}{h}\left[7 - \frac{1}{2}12 + \frac{1}{3}6 - 0 + \dots\right]$$

$$= 7 - 6 + 2 = 3$$

and

$$\left(\frac{d^2y}{dx^2}\right)_{x=x_0} = \frac{1}{h^2}\left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 - \dots\right]$$

$$\Rightarrow \left(\frac{d^2y}{dx^2}\right)_{x=1} = \frac{1}{1^2}\left[12 - 6\right] = 6$$

$$\therefore \left(\frac{dy}{dx}\right)_{x=1} = 3, \left(\frac{d^2y}{dx^2}\right)_{x=1} = 6.$$

Example 8.2 *From the following table of values of x and y find* $\frac{dy}{dx}$ *and* $\frac{d^2y}{dx^2}$ *for* $x = 1.05$.

x	1.00	1.05	1.10	1.15	1.20	1.25	1.30
y	1.00000	1.02470	1.04881	1.07238	1.09544	1.11803	1.14017

Solution The difference table is as follows

x	y	Δ	Δ^2	Δ^3	Δ^4	Δ^5
1.00	1.00000					
		0.02470				
1.05	1.02470		–0.00059			
		0.002411		–0.00002		
1.10	1.04881		–0.00054		0.00003	
		0.02357		–0.00001		–0.00006
1.15	1.07238		–0.00051		–0.00003	
		0.02306		–0.00002		
1.20	1.09544		–0.00047			
		0.02259				
1.25	1.11803		–0.00045			
		0.02214				
1.30	1.14017					

Taking $x_0 = 1.05$, $h = 0.05$ we have

$$\Delta y_0 = 0.02411,$$
$$\Delta^2 y_0 = -0.00054,$$
$$\Delta^3 y_0 = 0.00003,$$
$$\Delta^4 y_0 = -0.00001,$$
$$\Delta^5 y_0 = -0.00003,$$

from Newton's formula

$$\left(\frac{dy}{dx}\right)_{x=x_0} = \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 - \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \ldots\right]$$

$$\therefore \left(\frac{dy}{dx}\right)_{x=1.05} = \frac{1}{0.05}\left[0.02411 - \frac{0.00054}{2} + \frac{1}{3}(0.00003)\right] + \frac{1}{0.05}\left[-\frac{1}{4}(0.00001) + \frac{1}{5}(0.00003)\right]$$

$$\therefore \left(\frac{dy}{dx}\right)_{x=1.05} = 0.48763$$

and $$\left(\frac{d^2y}{dx^2}\right)_{x=x_0} = \frac{1}{h^2}\left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 - \frac{5}{6}\Delta^5 y_0 + \ldots\right]$$

$$\Rightarrow \left(\frac{d^2y}{dx^2}\right)_{x=1.05} = \frac{1}{(1.05)^2}\left[-0.00054 - 0.0003 + \frac{11}{12}(0.00001) - \frac{5}{6}(-0.00003)\right]$$

$$\left(\frac{d^2y}{dx^2}\right)_{x=1.05} = -0.2144.$$