Chapter 8

Numerical Differentiation

Core Topics

(i) Finite Difference Approximation of the Derivative (8.2).

(ii) Finite Difference using the Taylor Series Expansion (8.3)

(iii) Summary of Finite Difference Formulas for Numerical Differentiation (8.4).

(iv) Differentiation Formulas using Lagrange Polynomials (8.5)

(v) Differentiation using Curve Fitting (8.6)

(vi) Use of MATLAB built-in Functions for Numerical Differentiation (8.7).

(vii) Richardson's Extrapolation (8.8)

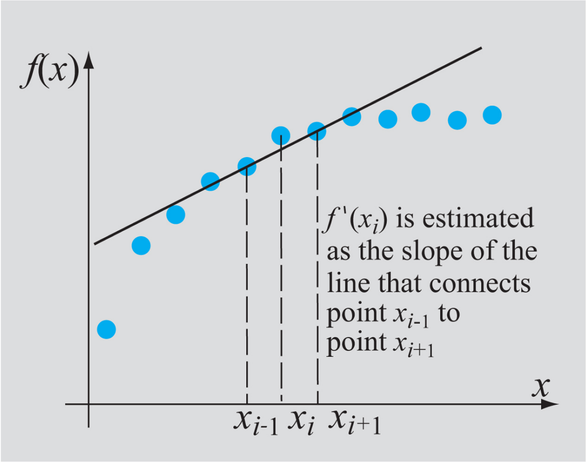
(viii) Error in Numerical Differentiation (8.9)

(ix) Numerical Partial Differentiation (8.10)

Background:

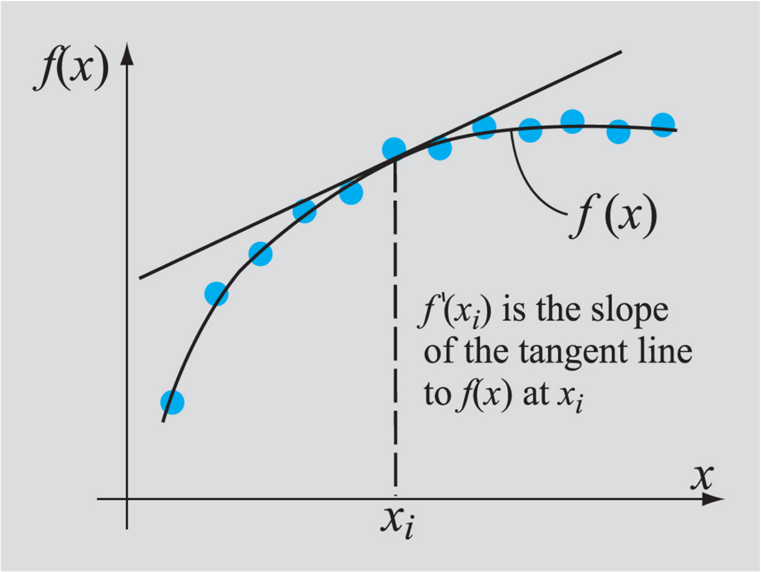
Numerical differentiation is needed where the function in question cannot be differentiated analytically, cannot be differentiated easily and/or there are very many differentiations to be performed.

The simplest approach is to use the finite difference approximation for the derivative. This approach calculates the derivative $f'(x_i)$ by obtaining the slope of the line containing $f'(x_{i-1})$ and $f'(x_{i+1})$ which are experimental data points or values of a discretised continuous function.



Background:

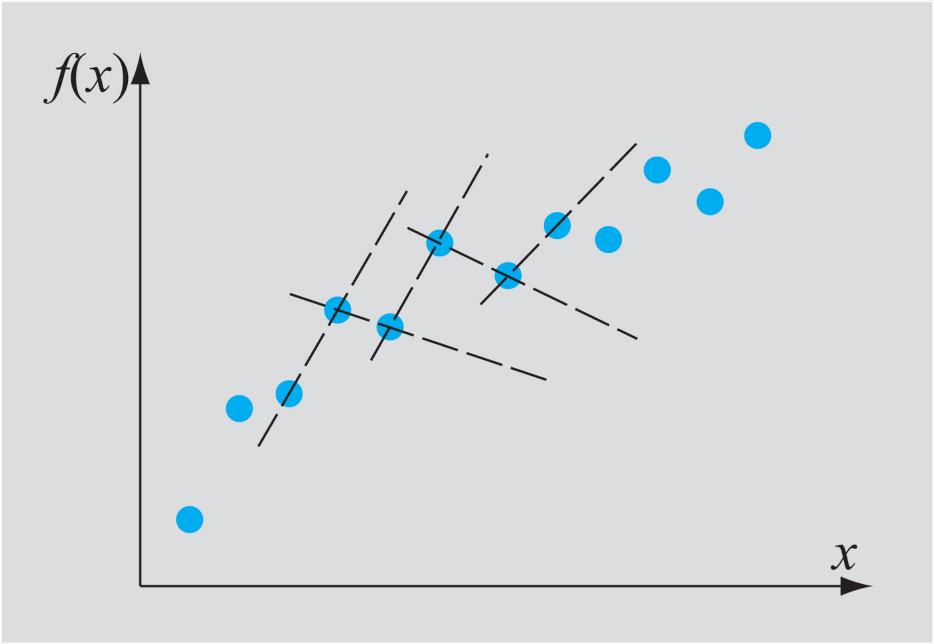
Another approach is to obtain an analytic expression for $f(x)$ by curve fitting and differentiating the resulting analytic expression.



(b)

Background:

Oftentimes there is a lot of scatter in experimental data which means that there can be large inaccuracies in differentiation using the finite difference method. This can be remedied by using higher order finite difference approximations which we will see later.

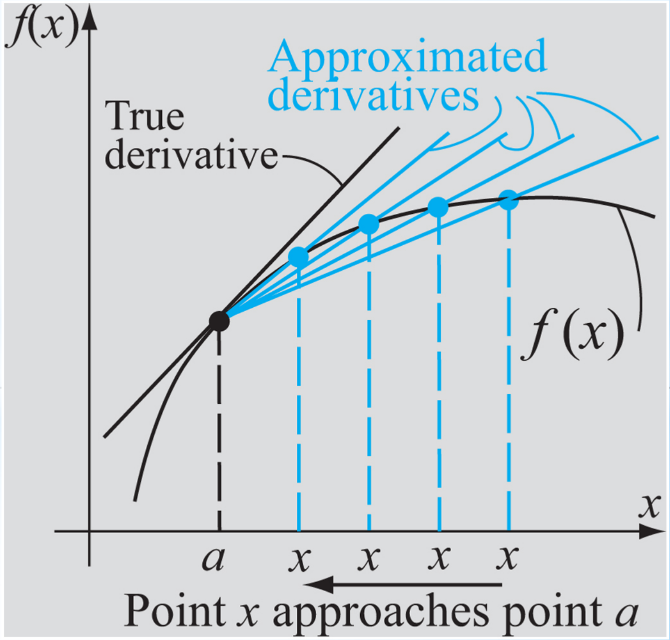


Finite Difference Approximation of the Derivative:

The derivative $f'(x)$ of a function $f(x)$ at the point $x = a$ is defined by:

$$\left.\frac{df(x)}{dx}\right|_{x=a} = f'(a) = \lim_{x \to a} \frac{f(x) - f(a)}{x - a} \tag{8.4}$$

This is the slope of the tangent to the function $f(x)$ at the point $x = a$. The derivative is obtained by choosing a point x close to a and calculating the slope of the line containing the two points. Clearly the closer x is to a the more accurate the result.



Finite Difference Approximation of the Derivative:

In finite difference approximations of the derivative, values of the function at different points in the neighbourhood of $x = a$ are used for estimating the slope. Three such fundamental variants exist:

1. The forward difference formula:

$$\left.\frac{df}{dx}\right|_{x=x_i} = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} \tag{8.5}$$

2. The backward difference formula:

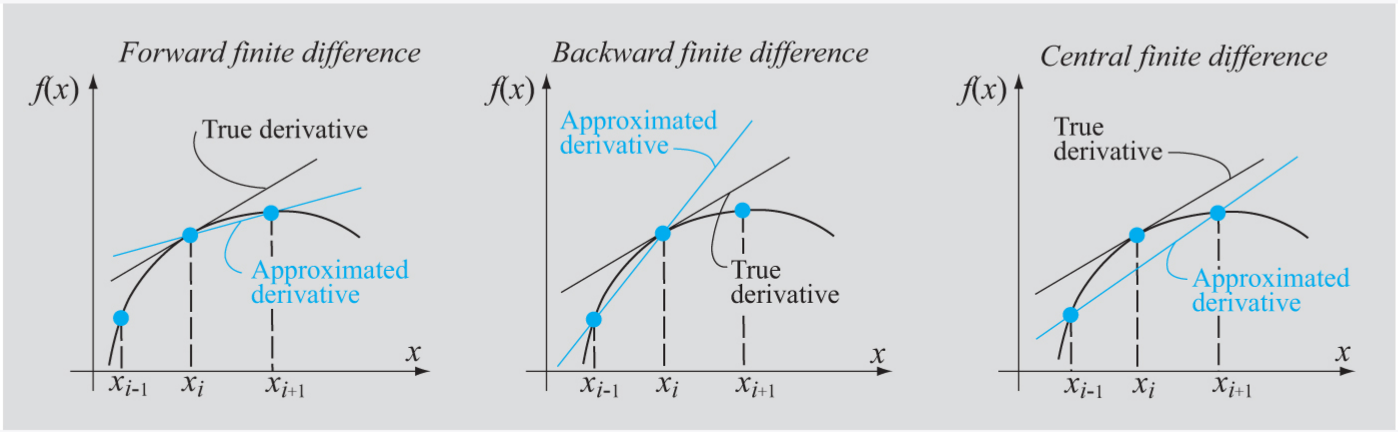
$$\left.\frac{df}{dx}\right|_{x=x_i} = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} \tag{8.6}$$

3. The central difference formula:

$$\left.\frac{df}{dx}\right|_{x=x_i} = \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}} \tag{8.7}$$

Finite Difference Approximation of the Derivative:

If the function is slowly varying then the central difference formula is usually the most accurate. That being said all are accurate if the spacings between the points are made very small.



Example:

Example 8-1: Comparing numerical and analytical differentiation.

Consider the function $f(x) = x^3$. Calculate its first derivative at point $x = 3$ numerically with the forward, backward, and central finite difference formulas and using:
(a) Points $x = 2$, $x = 3$, and $x = 4$.
(b) Points $x = 2.75$, $x = 3$, and $x = 3.25$.
Compare the results with the exact (analytical) derivative.

SOLUTION

***Analytical differentiation*:** The derivative of the function is $f'(x) = 3x^2$, and the value of the derivative at $x = 3$ is $f'(3) = 3 \cdot 3^2 = 27$.

Numerical differentiation

(a) The points used for numerical differentiation are:

x:	2	3	4
$f(x)$:	8	27	64

Using Eqs. (8.5) through (8.7), the derivatives using the forward, backward, and central finite difference formulas are:

Forward finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(4)-f(3)}{4-3} = \frac{64-27}{1} = 37 \qquad error = \left|\frac{37-27}{27}\cdot 100\right| = 37.04\,\%$$

Backward finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(3)-f(2)}{3-2} = \frac{27-8}{1} = 19 \qquad error = \left|\frac{19-27}{27}\cdot 100\right| = 29.63\,\%$$

Central finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(4)-f(2)}{4-2} = \frac{64-8}{2} = 28 \qquad error = \left|\frac{28-27}{27}\cdot 100\right| = 3.704\,\%$$

(b) The points used for numerical differentiation are:

x:	2.75	3	3.25
$f(x)$:	2.75^3	3^3	3.25^3

Using Eqs. (8.5) through (8.7), the derivatives using the forward, backward, and central finite difference formulas are:

Forward finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(3.25)-f(3)}{3.25-3} = \frac{3.25^3-27}{0.25} = 29.3125 \qquad error = \left|\frac{29.3125-27}{27}\cdot 100\right| = 8.565\ \%$$

Backward finite difference:

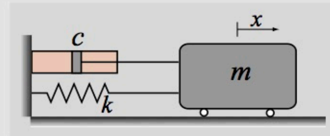
$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(3)-f(2.75)}{3-2.75} = \frac{27-2.75^3}{0.25} = 24.8125 \qquad error = \left|\frac{24.8125-27}{27}\cdot 100\right| = 8.102\ \%$$

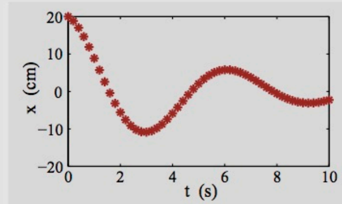
Central finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(3.25)-f(2.75)}{3.25-2.75} = \frac{3.25^3-2.75^3}{0.5} = 27.0625 \qquad error = \left|\frac{27.0625-27}{27}\cdot 100\right| = 0.2315\ \%$$

The results show that the central finite difference formula gives a more accurate approximation. This will be discussed further in the next section. In addition, smaller separation between the points gives a significantly more accurate approximation.

Example 8-2: Damped vibrations.





In a vibration experiment, a block of mass m is attached to a spring of stiffness k, and a dashpot with damping coefficient c, as shown in the figure. To start the experiment the block is moved from the equilibrium position and then released from rest. The position of the block as a function of time is recorded at a frequency of 5 Hz (5 times a second). The recorded data for the first 10 s is shown in the figure. The data points for $4 \le t \le 8$ s are given in the table below.

(a) The velocity of the block is the derivative of the position w.r.t. time. Use the central finite difference formula to calculate the velocity at time $t = 5$ and $t = 6$ s.

(b) Write a user-defined MATLAB function that calculates the derivative of a function that is given by a set of discrete points. Name the function `dx=derivative(x,y)` where `x` and `y` are vectors with the coordinates of the points, and `dx` is a vector with the value of the derivative $\frac{dy}{dx}$ at each point. The function should calculate the derivative at the ***first*** and ***last*** points using the ***forward*** and ***backward finite difference formulas***, respectively, and using the central finite difference formula for all of the other points.

Use the given data points to calculate the velocity of the block for $4 \le t \le 8$ s. Calculate the acceleration of the block by differentiating the velocity. Make a plot of the displacement, velocity, and acceleration, versus time for $4 \le t \le 8$ s.

t (s)	4.0	4.2	4.4	4.6	4.8	5.0	5.2	5.4	5.6	5.8	6.0	6.2	6.4	6.6
x (cm)	−5.87	−4.23	−2.55	−0.89	0.67	2.09	3.31	4.31	5.06	5.55	5.78	5.77	5.52	5.08

t (s)	6.8	7.0	7.2	7.4	7.6	7.8	8.0
x (cm)	4.46	3.72	2.88	2.00	1.10	0.23	−0.59

SOLUTION

(a) The velocity is calculated by using Eq. (8.7):

for $t = 5$ s: $$\left.\frac{dx}{dt}\right|_{x=5} = \frac{f(5.2)-f(4.8)}{5.2-4.8} = \frac{3.31-0.67}{0.4} = 6.6 \quad \text{cm/s}$$

for $t = 6$ s: $$\left.\frac{dx}{dt}\right|_{x=5} = \frac{f(6.2)-f(5.8)}{6.2-5.8} = \frac{5.77-5.55}{0.4} = 0.55 \quad \text{cm/s}$$

(b) The user-defined function `dx=derivative(x,y)` that is listed next calculates the derivative of a function that is given by a set of discrete points.

Program 8-1: Function file. Derivative of a function given by points.

```
function dx = derivative(x,y)
% derivative calculates the derivative of a function that is given by a set
% of points. The derivatives at the first and last points are calculated by
% using the forward and backward finite difference formula, respectively.
% The derivative at all the other points is calculated by the central
```

Example:

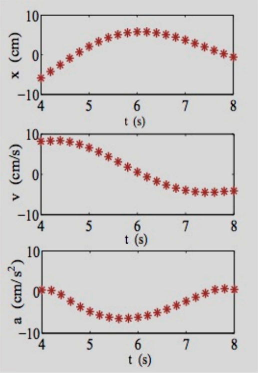
```
% finite difference formula.
% Input variables:
% x  A vector with the coordinates x of the data points.
% y  A vector with the coordinates y of the data points.
% Output variable:
% dx  A vector with the value of the derivative at each point.

n = length(x);
dx(1) = (y(2) - y(1))/(x(2) - x(1));
for i = 2:n - 1
   dx(i) = (y(i + 1) - y(i - 1))/(x(i + 1) - x(i - 1));
end
dx(n) = (y(n) - y(n - 1))/(x(n) - x(n - 1));
```

The user-defined function `derivative` is used in the following script file. The program determines the velocity (the derivative of the given data points) and the acceleration (the derivative of the velocity) and then displays three plots.

```
t = 4:0.2:8;
x = [-5.87 -4.23 -2.55 -0.89 0.67 2.09 3.31 4.31 5.06 5.55 5.78 5.77 5.52 5.08 4.46
3.72 2.88 2.00 1.10 0.23 -0.59];
vel = derivative(t,x)
acc = derivative(t,vel);
subplot (3,1,1)
plot(t,x)
subplot (3,1,2)
plot(t,vel)
subplot (3,1,3)
plot(t,acc)
```

When the script file is executed, the following plots are displayed (the plots were formatted in the Figure Window):



Finite Difference Formulas using the Taylor Series Expansion:

The forward, backward and central difference formulae, as well as other finite difference formulas, can be obtained using the Taylor Series expansion of $f(x)$. The advantage of using the Taylor Series expansion is that an estimate of the error in the approximation can be obtained.

The Two Point Forward Difference Formula:

Assuming that points are evenly spaced we can write:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(x_i)}{4!}h^4 + \dots \qquad (8.8)$$

This can be written:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(\xi)}{2!}h^2 \qquad (8.9)$$

where $h = x_{i+1} - x_i$ and $\xi \in]x_i, x_{i+1}[$

Finite Difference Formulas using the Taylor Series Expansion:

Solving for $f'(x_i)$ yields:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(\xi)}{2!}h \qquad (8.10)$$

An approximate value of the derivative $f'(x_i)$ can be calculated if the second term on the r.h.s. of Equation (8.10) is ignored. Ignoring this term introduces a truncation error which is said to be in the 'order of h', written $O(h)$, since it is proportional to h.

$$truncation\ \ error = -\frac{f''(\xi)}{2!}h = O(h) \qquad (8.11)$$

Using this notation we can write the forward difference formula as:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h) \qquad (8.12)$$

Finite Difference Formulas using the Taylor Series Expansion:

The Two-Point Backward Difference Formula:

Using Taylor's Theorem we can write:

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(x_i)}{4!}h^4 + \dots \qquad (8.13)$$

As before this reduces to:

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + \frac{f''(\xi)}{2!}h \qquad (8.15)$$

where $h = x_i - x_{i-1}$ and $\xi \in]x_{i-1}, x_i[$

This in turn gives:

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + O(h) \qquad (8.16)$$

Finite Difference Formulas using the Taylor Series Expansion:

The Two-Point Central Difference Formula for the First Derivative:

We write:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(\xi_1)}{3!}h^3 \qquad (8.17)$$

where $\xi_1 \in \,]x_i, x_{i+1}[$ and $h = x_{i+1} - x_i$

Now write:

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(\xi_2)}{3!}h^3 \qquad (8.18)$$

where $\xi_1 \in \,]x_{i-1}, x_i[$ and $h = x_i - x_{i-1}$

Finite Difference Formulas using the Taylor Series Expansion:

The spacings between points are equal ($h = x_{i+1} - x_i = x_i - x_{i-1}$) then subtracting Equation (8.18) from (8.17) gives:

$$f(x_{i+1}) - f(x_{i-1}) = 2f'(x_i)h + \frac{f'''(\xi_1)}{3!}h^3 + \frac{f'''(\xi_2)}{3!}h^3 \qquad (8.19)$$

Solving for $f'(x_i)$ gives:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2) \qquad (8.20)$$

This gives us the noteworthy result that the central difference formula is more accurate than the forward and backward difference formulae because the order of the truncation error is $O(h^2)$ as opposed to $O(h)$.

Finite Difference Formulas using the Taylor Series Expansion:

At the endpoints it is not possible to use the central difference formula for the derivative. One can use the forward and backward difference formulae but the truncation error is $O(h)$ as opposed to $O(h^2)$ (for the central difference formula). It would therefore be useful if we could obtain a difference formula for the endpoints that has the smaller truncation error of $O(h^2)$.

To this end we derive the three point forward and backward difference formulae for use at the endpoints. These formulae have a truncation error of $O(h^2)$.

Finite Difference Formulas using the Taylor Series Expansion:

Letting the endpoint be x_i then:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(\xi_1)}{3!}h^3 \qquad (8.21)$$

$$f(x_{i+2}) = f(x_i) + f'(x_i)2h + \frac{f''(x_i)}{2!}(2h)^2 + \frac{f'''(\xi_2)}{3!}(2h)^3 \qquad (8.22)$$

where $\xi_1 \in \,]x_i, x_{i+1}[$ and $\xi_2 \in \,]x_i, x_{i+2}[$

Multiplying Equation (8.21) by 4 and subtracting from (8.22) gives:

$$4f(x_{i+1}) - f(x_{i+2}) = 3f(x_i) + 2f'(x_i)h + \frac{4f'''(\xi_1)}{3!}h^3 - \frac{f'''(\xi_2)}{3!}(2h)^3 \quad (8.23)$$

Finite Difference Formulas using the Taylor Series Expansion:

Solving for $f'(x_i)$ gives:

$$f'(x_i) = \frac{-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2})}{2h} + O(h^2) \qquad (8.24)$$

This is our desired three –point forward difference formula for use at one of the endpoints of the function with a truncation error of $O(h^2)$.

In like fashion a three-point backward difference formula can be derived for use at the other endpoint:

$$f'(x_i) = \frac{f(x_{i-2}) - 4f(x_{i-1}) + 3f(x_i)}{2h} + O(h^2) \qquad (8.25)$$

Example:

Example 8-3: Comparing numerical and analytical differentiation.

Consider the function $f(x) = x^3$. Calculate the first derivative at point $x = 3$ numerically with the three-point forward difference formula, using:

(*a*) Points $x = 3$, $x = 4$, and $x = 5$.

(*b*) Points $x = 3$, $x = 3.25$, and $x = 3.5$.

Compare the results with the exact value of the derivative, obtained analytically.

SOLUTION

Analytical differentiation: The derivative of the function is $f'(x) = 3x^2$, and the value of the derivative at $x = 3$ is $f'(3) = 3 \cdot 3^2 = 27$.

Numerical differentiation

(*a*) The points used for numerical differentiation are:

x:	3	4	5
$f(x)$:	27	64	125

Using Eq. (8.24), the derivative using the three-point forward difference formula is:

$$f'(3) = \frac{-3f(3)+4f(4)-f(5)}{2\cdot 1} = \frac{-3\cdot 27+4\cdot 64-125}{2} = 25 \qquad error = \left|\frac{25-27}{27}\right|\cdot 100 = 7.41\ \%$$

(*b*) The points used for numerical differentiation are:

x:	3	3.25	3.5
$f(x)$:	27	3.25^3	3.5^3

Using Eq. (8.24), the derivative using the three points forward finite difference formula is:

$$f'(3) = \frac{-3f(3)+4f(3.25)-f(3.5)}{2\cdot 0.25} = \frac{-3\cdot 27+4\cdot 3.25^3-3.5^3}{0.5} = 26.875$$

$$error = \left|\frac{26.875-27}{27}\right|\cdot 100 = 0.46\ \%$$

The results show that the three-point forward difference formula gives a much more accurate value for the first derivative than the two-point forward finite difference formula in Example 8-1. For $h = 1$ the error reduces from 37.04% to 7.4%, and for $h = 0.25$ the error reduces from 8.57% to 0.46%.

Finite Difference Formulas using the Taylor Series Expansion:

The Three point Central Difference Formula for the Second Derivative:

We write:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(\xi_1)}{4!}h^4 \qquad (8.26)$$

and

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(\xi_2)}{4!}h^4 \qquad (8.27)$$

where $\xi_1 \in]x_i, x_{i+1}[$ and $\xi_2 \in]x_i, x_{i-1}[$

Finite Difference Formulas using the Taylor Series Expansion:

Adding Equations (8.26) and (8.27) gives:

$$f(x_{i+1}) + f(x_{i-1}) = 2f(x_i) + 2\frac{f''(x_1)}{2!}h^2 + \frac{f^{(4)}(\xi_1)}{4!}h^4 + \frac{f^{(4)}(\xi_2)}{4!}h^4 \quad (8.28)$$

Solving for $f''(x_i)$ gives:

$$f''(x_i) = \frac{f(x_{i-1}) - 2f(x_i) + f(x_{i+1})}{h^2} + O(h^2) \quad (8.29)$$

This is a three-point central difference formula that provides an estimate of the second derivative at the point x_i in terms of the value of the function at that point, the previous point x_{i-1} and the next point x_{i+1} with a truncation error of $O(h^2)$.

The same procedure can be used to obtain higher order formulae involving more points.

Finite Difference Formulas using the Taylor Series Expansion:

Three-Point Forward and Backward Difference Formulae for the Second Derivative:

The Three-Point Forward Difference Formula for the second derivative can be obtained by multiplying Equation (8.21) by 2 and subtracting it from (8.22) – eliminating $f'(x_i)$.

$$f''(x_i) = \frac{f(x_i) - 2f(x_{i+1}) + f(x_{i+2})}{h^2} + O(h) \qquad (8.31)$$

Likewise a Three-Point Backward Difference Formula for the second derivative is obtained:

$$f''(x_i) = \frac{f(x_{i-2}) - 2f(x_{i-1}) + f(x_i)}{h^2} + O(h) \qquad (8.32)$$

Example:

Example 8-4: Comparing numerical and analytical differentiation.

Consider the function $f(x) = \frac{2^x}{x}$. Calculate the second derivative at $x = 2$ numerically with the three-point central difference formula using:

(a) Points $x = 1.8$, $x = 2$, and $x = 2.2$.

(b) Points $x = 1.9$, $x = 2$, and $x = 2.1$.

Compare the results with the exact (analytical) derivative.

SOLUTION

Analytical differentiation: The second derivative of the function $f(x) = \frac{2^x}{x}$ is:

$$f''(x) = \frac{2^x[\ln(2)]^2}{x} - \frac{2 \cdot 2^x \ln(2)}{x^2} + \frac{2 \cdot 2^x}{x^3}$$

and the value of the derivative at $x = 2$ is $f''(2) = 0.574617$.

Numerical differentiation

(a) The numerical differentiation is done by substituting the values of the points $x = 1.8$, $x = 2$, and $x = 2.2$ in Eq. (8.29). The operations are done with MATLAB, in the Command Window:

```
>> xa = [1.8 2 2.2];
>> ya = 2.^xa./xa;
>> df = (ya(1) - 2*ya(2) + ya(3))/0.2^2
df =
   0.57748177389232
```

(b) The numerical differentiation is done by substituting the values of the points $x = 1.9$, $x = 2$, and $x = 2.1$ in Eq. (8.29). The operations are done with MATLAB, in the Command Window:

```
>> xb = [1.9 2 2.1];
>> yb = 2.^xb./xb;
>> dfb = (yb(1) - 2*yb(2) + yb(3))/0.1^2
dfb =
   0.57532441566441
```

Error in part (a): $error = \frac{0.577482 - 0.574617}{0.574617} \cdot 100 = 0.4986\ \%$

Error in part (b): $error = \frac{0.575324 - 0.574617}{0.574617} \cdot 100 = 0.1230\ \%$

The results show that the three-point central difference formula gives a quite accurate approximation for the value of the second derivative.

Differentiation Formulae Using Lagrange Polynomials:

Differentiation formulae can also be derived using Lagrange Polynomials. For the first derivative the two-point central, three-point forward and three-point backward difference formulae are obtained by considering three points (x_i, y_i), (x_{i+1}, y_{i+1}) and (x_{i+2}, y_{i+2}).
The polynomial, in Lagrange form, that passes through these points is given by:

$$f(x) = \frac{(x-x_{i+1})(x-x_{i+2})}{(x_i-x_{i+1})(x_i-x_{i+2})} y_i + \frac{(x-x_i)(x-x_{i+2})}{(x_{i+1}-x_i)(x_{i+1}-x_{i+2})} y_{i+1} + \frac{(x-x_i)(x-x_{i+1})}{(x_{i+2}-x_i)(x_{i+2}-x_{i+1})} y_{i+2} \tag{8.33}$$

Differentiation Formulae Using Lagrange Polynomials:

Differentiating Equation (8.33) gives:

$$f'(x) = \frac{2x - x_{i+1} - x_{i+2}}{(x_i - x_{i+1})(x_i - x_{i+2})} y_i + \frac{2x - x_i - x_{i+2}}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})} y_{i+1} + \frac{2x - x_i - x_{i+1}}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} y_{i+2} \qquad (8.34)$$

The first derivative at any one of the three points, (x_i, y_i), (x_{i+1}, y_{i+1}) and (x_{i+2}, y_{i+2}), is obtained by substituting the corresponding value of x in Equation (8.34).

Differentiation Formulae Using Lagrange Polynomials:

$$f'(x_i)=\frac{2x_i-x_{i+1}-x_{i+2}}{(x_i-x_{i+1})(x_i-x_{i+2})}y_i+\frac{x_i-x_{i+2}}{(x_{i+1}-x_i)(x_{i+1}-x_{i+2})}y_{i+1}+\frac{x_i-x_{i+1}}{(x_{i+2}-x_i)(x_{i+2}-x_{i+1})}y_{i+2} \quad (8.35)$$

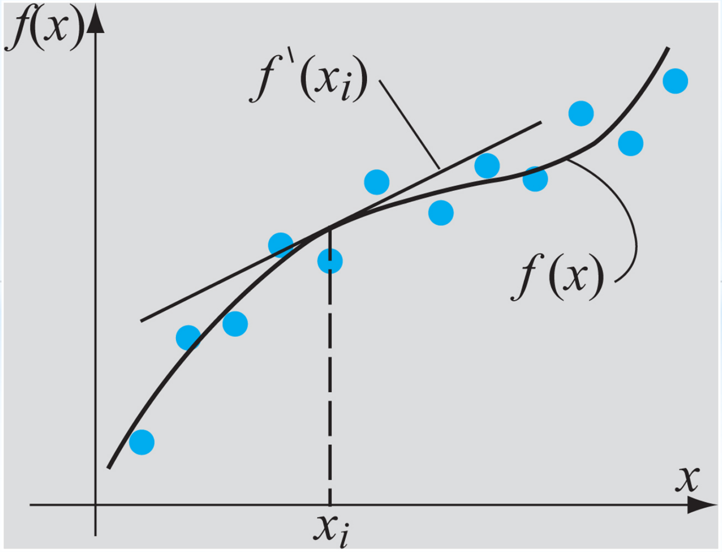
$$f'(x_{i+1})=\frac{x_{i+1}-x_{i+2}}{(x_i-x_{i+1})(x_i-x_{i+2})}y_i+\frac{2x_{i+1}-x_i-x_{i+2}}{(x_{i+1}-x_i)(x_{i+1}-x_{i+2})}y_{i+1}+\frac{x_{i+1}-x_i}{(x_{i+2}-x_i)(x_{i+2}-x_{i+1})}y_{i+2} \quad (8.36)$$

$$f'(x_{i+2})=\frac{x_{i+2}-x_{i+1}}{(x_i-x_{i+1})(x_i-x_{i+2})}y_i+\frac{x_{i+2}-x_i}{(x_{i+1}-x_i)(x_{i+1}-x_{i+2})}y_{i+1}+\frac{2x_{i+2}-x_i-x_{i+1}}{(x_{i+2}-x_i)(x_{i+2}-x_{i+1})}y_{i+2} \quad (8.37)$$

These are the three-point forward difference, two-point central difference and three point backward difference formulae respectively. The advantage of these formulae is that points do not have to be evenly spaced. However there is no estimate for the magnitude of the error.

Differentiation using Curve Fitting:

Differentiation may also be performed by finding an analytic function that approximates the data. The value of the derivative at a point can then be found by differentiating analytically. This procedure is preferred if there is a lot of scatter in the data. Curve fitting smooths out the scatter and so enhances the accuracy of the estimate of the derivative. Again however, unlike using finite difference formulae using the Taylor Series expansion there is no error estimate.



Example:

Example 8-5: Using Richardson's extrapolation in differentiation.

Use Richardson's extrapolation with the results in Example 8-4 to calculate a more accurate approximation for the derivative of the function $f(x) = \frac{2^x}{x}$ at the point $x = 2$.

Compare the results with the exact (analytical) derivative.

SOLUTION

In Example 8-4 two approximations of the derivative of the function at $x = 2$ were calculated using the central difference formula in which the error is $O(h^2)$. In one approximation $h = 0.2$, and in the other $h = 0.1$. The results from Example 8-4 are:

for $h = 0.2$, $f''(2) = 0.577482$. The error in this approximation is 0.5016 %.

for $h = 0.1$, $f''(2) = 0.575324$. The error in this approximation is 0.126 %.

Richardson's extrapolation can be used by substituting these results in Eq. (8.45) (or Eq. (8.53)):

$$D = \frac{1}{3}\left(4D\left(\frac{h}{2}\right) - D(h)\right) + O(h^4) = \frac{1}{3}(4 \cdot 0.575324 - 0.577481) = 0.574605$$

The error now is $error = \frac{0.574605 - 0.5746}{0.5746} \cdot 100 = 0.00087$ %

This result shows that a much more accurate approximation is obtained by using Richardson's extrapolation.

Error in Numerical Differentiation:

We have seen with finite difference formulae derived using the Taylor Series expansion that truncation errors of various orders of the spacing, h, were obtained. Since for a discrete set of data points h is fixed (the interval between data points) so it is not possible to reduce the error by reducing h. We can however use a difference formula with a higher order truncation error to get greater accuracy.

On the other hand if the function to be differentiated is continuous then we can reduce h and so get greater accuracy – or so it would seem! However there is also a round-off error resulting from the finite precision of the computer being used. This means that even though h can be made vanishingly small the round-off error remains or can even grow as h is made smaller and smaller. The following example illustrates this point.

Example:

Example 8-6: Comparing numerical and analytical differentiation.

Consider the function $f(x) = e^x$. Write an expression for the first derivative of the function at $x = 0$ using the two-point central difference formula in Eq. (8.20). Investigate the effect that the spacing, h, between the points has on the truncation and round-off errors.

SOLUTION

The two-point central difference formula in Eq. (8.20) is:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - 2\frac{f'''(\xi)}{3!}h^2$$

where ξ is a value of x between x_{i-1} and x_{i+1}

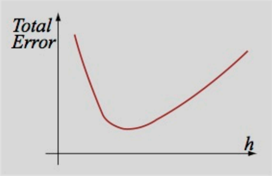
The points used for calculating the derivative of $f(x) = e^x$ at $x = 0$ are $x_{i-1} = -h$ and $x_{i+1} = h$. Substituting these points in the formula gives:

$$f'(0) = \frac{e^h - e^{-h}}{2h} - 2\frac{f'''(\xi)}{3!}h^2 \tag{8.55}$$

When the computer calculates the values of e^h and e^{-h}, a round-off error is introduced, since the computer has finite precision. Consequently, the terms e^h and e^{-h} in Eq. (8.55) are replaced by $e^h + R_1$ and $e^{-h} + R_2$ where now e^h and e^{-h} are the exact values, and R_1 and R_2 are the round-off errors:

$$f'(0) = \frac{e^h + R_1 - e^{-h} - R_2}{2h} - 2\frac{f'''(\xi)}{3!}h^2 = \frac{e^h - e^{-h}}{2h} + \frac{R_1 - R_2}{2h} - 2\frac{f'''(\xi)}{3!}h^2 \tag{8.56}$$

In Eq. (8.56) the last term on the right-hand side is the truncation error. In this term, the value of $f'''(\xi)$ is not known, but it is bounded. This means that as h decreases the truncation error decreases. The round-off error is $(R_1 - R_2)/(2h)$. As h decreases the round-off error increases. The total error is the sum of the truncation error and round-off error. Its behavior is shown schematically in the figure on the right. As h decreases, the total error initially decreases, but after a certain value (which depends on the precision of the computer used) the total error increases as h decreases further.



Numerical Partial Differentiation:

The finite difference formulae obtained earlier can also be used to obtain partial derivatives. For a function $f(x, y)$ the partial derivatives with respect to x and y at that point (a, b) are:

$$\left.\frac{\partial f(x,y)}{\partial x}\right|_{\substack{x=a\\y=b}} = \lim_{x \to a} \frac{f(x,b) - f(a,b)}{x-a} \qquad (8.57)$$

$$\left.\frac{\partial f(x,y)}{\partial y}\right|_{\substack{x=a\\y=b}} = \lim_{y \to b} \frac{f(a,y) - f(a,b)}{y-b} \qquad (8.58)$$

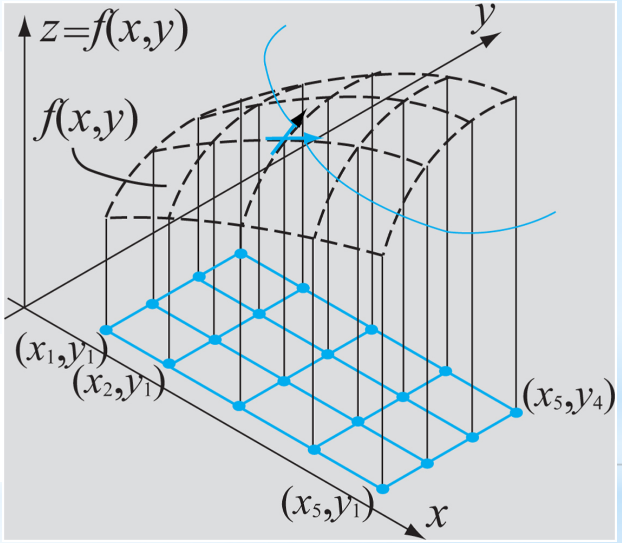
This means that the finite difference formulae for functions of a single variable can be extended to calculating the partial derivatives with respect to a particular variable of functions of two or more independent variables simply by holding the other variables constant.

Numerical Partial Differentiation:

For example an approximation for the partial derivative at the point (x_i, y_i) with the two-point forward difference formula is:

$$\left.\frac{\partial f}{\partial x}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{f(x_{i+1}, y_i) - f(x_i, y_i)}{h_x}$$

$$\left.\frac{\partial f}{\partial y}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{f(x_i, y_{i+1}) - f(x_i, y_i)}{h_y}$$



Numerical Partial Differentiation:

In the same way the two-point backward and central difference formulae are:

$$\left.\frac{\partial f}{\partial x}\right|_{\substack{x=x_i\\ y=y_i}} = \frac{f(x_i, y_i) - f(x_{i-1}, y_i)}{h_x} \qquad \left.\frac{\partial f}{\partial y}\right|_{\substack{x=x_i\\ y=y_i}} = \frac{f(x_i, y_i) - f(x_i, y_{i-1})}{h_y} \qquad (8.61)$$

$$\left.\frac{\partial f}{\partial x}\right|_{\substack{x=x_i\\ y=y_i}} = \frac{f(x_{i+1}, y_i) - f(x_{i-1}, y_i)}{2h_x} \qquad \left.\frac{\partial f}{\partial y}\right|_{\substack{x=x_i\\ y=y_i}} = \frac{f(x_i, y_{i+1}) - f(x_i, y_{i-1})}{2h_y} \qquad (8.62)$$

The second partial derivatives with the three-point central difference formulae are:

$$\left.\frac{\partial^2 f}{\partial x^2}\right|_{\substack{x=x_i\\ y=y_i}} = \frac{f(x_{i-1}, y_i) - 2f(x_i, y_i) + f(x_{i+1}, y_i)}{h_x^2} \qquad (8.63)$$

$$\left.\frac{\partial^2 f}{\partial y^2}\right|_{\substack{x=x_i\\ y=y_i}} = \frac{f(x_i, y_{i-1}) - 2f(x_i, y_i) + f(x_i, y_{i+1})}{h_y^2} \qquad (8.64)$$

Numerical Partial Differentiation :

The second order partial derivative can also be mixed:

$$\frac{\delta^2 f}{\delta x \delta y} = \frac{\delta}{\delta y}\left(\frac{\delta f}{\delta x}\right) == \frac{\delta}{\delta x}\left(\frac{\delta f}{\delta y}\right)$$

A finite difference formula for the mixed derivative can be obtained by using the first-order finite difference formulae for partial derivatives.

Example:

Example 8-7: Numerical partial differentiation.

The following two-dimensional data for the x component of velocity u as a function of the two coordinates x and y is measured from an experiment:

	$x = 1.0$	$x = 1.5$	$x = 2.0$	$x = 2.5$	$x = 3.0$
$y = 1.0$	163	205	250	298	349
$y = 2.0$	228	291	361	437	517
$y = 3.0$	265	350	448	557	676

(*a*) Using central difference approximations, calculate $\partial u/\partial x$, $\partial u/(\partial y)$, $\partial^2 u/\partial y^2$, and $\partial^2 u/\partial x \partial y$ at the point $(2,2)$.

(*b*) Using a three-point forward difference approximation, calculate $\partial u/\partial x$ at the point (2,2).

(*c*) Using a three-point forward difference approximation, calculate $\partial u/\partial y$ at the point $(2,1)$.

SOLUTION

(*a*) In this part $x_i = 2$, $y_i = 2$, $x_{i-1} = 1.5$, $x_{i+1} = 2.5$, $y_{i-1} = 1$, $y_{i+1} = 3$, $h_x = 0.5$, $h_y = 1$.

Using Eqs. (8.59) and (8.60), the partial derivatives $\partial f/\partial x$ and $\partial u/\partial y$ are:

$$\left.\frac{\partial u}{\partial x}\right|_{\substack{x=x_i\\y=y_i}} = \frac{u(x_{i+1}, y_i) - u(x_{i-1}, y_i)}{2h_x} = \frac{u(2.5,2) - u(1.5,2)}{2 \cdot 0.5} = \frac{437-291}{1} = 146$$

$$\left.\frac{\partial u}{\partial y}\right|_{\substack{x=x_i\\y=y_i}} = \frac{u(x_i, y_{i+1}) - u(x_i, y_{i-1})}{2h_y} = \frac{u(2,3) - u(2,1)}{2 \cdot 1} = \frac{448-250}{2} = 99$$

The second partial derivative $\partial^2 u/\partial y^2$ is calculated with Eq. (8.64):

$$\left.\frac{\partial^2 u}{\partial y^2}\right|_{\substack{x=x_i\\y=y_i}} = \frac{u(x_i, y_{i-1}) - 2u(x_i, y_i) + u(x_i, y_{i+1})}{h_y^2} = \frac{250 - (2 \cdot 361) + 448}{1^2} = -24$$

The second mixed derivative $\partial^2 u/\partial x \partial y$ is given by Eq. (8.65):

$$\left.\frac{\partial^2 u}{\partial x \partial y}\right|_{\substack{x=x_i\\y=y_i}} = \frac{[u(x_{i+1}, y_{i+1}) - u(x_{i-1}, y_{i+1})] - [u(x_{i+1}, y_{i-1}) - u(x_{i-1}, y_{i-1})]}{2h_x \cdot 2h_y}$$

$$= \frac{[u(2.5,3) - u(1.5,3)] - [u(2.5,1) - u(1.5,1)]}{2 \cdot 0.5 \cdot 2 \cdot 1} = \frac{[557-350]-[298-205]}{2 \cdot 0.5 \cdot 2 \cdot 1} = 57$$

(*b*) In this part $x_i = 2$, $x_{i+1} = 2.5$, $x_{i+2} = 3.0$, $y_i = 2$, and $h_x = 0.5$. The formula for the partial derivative $\partial u/\partial x$ with the three-points forward finite difference formula can be written from the formula for the first derivative in Section 8.4.

$$\left.\frac{\partial u}{\partial x}\right|_{\substack{x=x_i\\y=y_i}} = \frac{-3u(x_i, y_i) + 4u(x_{i+1}, y_i) - u(x_{i+2}, y_i)}{2h_x} =$$

$$= \frac{-3u(2,2) + 4u(2.5,2) - u(3.0,2)}{2 \cdot 0.5} = \frac{-3 \cdot 361 + 4 \cdot 437 - 517}{2 \cdot 0.5} = 148$$

(*c*) In this part $y_i = 1$, $y_{i+1} = 2$, $y_{i+2} = 3$, $x_i = 2$, and $h_y = 1.0$. The formula for the partial derivative $\partial u/\partial y$ with the three-points forward difference formula can be written from the formula for the first derivative in Section 8.4.

$$\left.\frac{\partial u}{\partial y}\right|_{\substack{x=x_i\\y=y_i}} = \frac{-3u(x_i, y_i) + 4u(x_i, y_{i+1}) - u(x_i, y_{i+2})}{2h_y} =$$

$$= \frac{-3u(2,1) + 4u(2,2) - u(2,3)}{2 \cdot 1} = \frac{-3 \cdot 250 + 4 \cdot 361 - 448}{2 \cdot 1} = 123$$

Recommended Problems:

Problems to be solved by hand (do at least 1):

8.3, 8.8, 8.9

Problems to be programmed in MATLAB:

8.19

Problems in Science and Engineering (do at least 1):

8.31, 8.37

You should pick out problems that you find interesting/challenging and do these too.