# Interpolation 

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## A- NEWTON'S DIVIDED-DIFFERENCE <br> INTERPOLATING POLYNOMIAL

As stated above, there are a variety of alternative forms for expressing an interpolating polynomial. Newton's divided-difference interpolating polynomial is among the most popular and useful forms. Before presenting the general equation, we will introduce the first- and secondorder versions because of their simple visual interpretation.

## 1- Linear Interpolation

The simplest form of interpolation is to connect two data points with a straight line. This technique, called linear interpolation.

Given $\left(x_{0}, y_{0}\right)$ and $\left(x_{1}, y_{1}\right)$

$$
\begin{gathered}
\frac{y_{1}-y_{0}}{x_{1}-x_{0}}=\frac{f_{1}(x)-y_{0}}{x-x_{0}} \\
f_{1}(x)=y_{0}+\frac{y_{1}-y_{0}}{x_{1}-x_{0}}\left(x-x_{0}\right)
\end{gathered}
$$

$f_{1}(x)$ : first order interpolation
A smaller interval, i.e., $\left|x_{1}-x_{0}\right|$ closer to zero, leads to better approximation.

Example: Given $\ln 1=0, \ln 6=1.791759$, use linear interpolation to find $\ln 2$.
Solution:
$f_{1}(2)=\ln 2=\ln 1+\frac{\ln 6-\ln 1}{6-1} \times(2-1)=0.3583519$
True solution: $\ln 2=0.6931472$.
$\epsilon_{t}=\left|\frac{f_{1}(2)-\ln 2}{\ln 2}\right| \times 100 \%=\left|\frac{0.3583519-0.6931472}{0.6931472}\right| \times 100 \%=48.3 \%$


Figure 2: A smaller interval provides a better estimate

## 2- Quadratic Interpolation

An error maybe resulted from our approximating a curve with a straight line. Consequently, a strategy for improving the estimate is to introduce some curvature into the line connecting the points. If three data points
are available, this can be accomplished with a second-order polynomial (also called a quadratic polynomial or a parabola.

Given 3 data points, $\left(x_{0}, y_{0}\right),\left(x_{1}, y_{1}\right)$, and $\left(x_{2}, y_{2}\right)$, we can have a second order polynomial

$$
\begin{align*}
& f_{2}(x)=b_{0}+b_{1}\left(x-x_{0}\right)+b_{2}\left(x-x_{0}\right)\left(x-x_{1}\right) \\
& f_{2}\left(x_{0}\right)=b_{0}=y_{0} \\
& f_{2}\left(x_{1}\right)=b_{0}+b_{1}\left(x_{1}-x_{0}\right)=y_{1}, \rightarrow b_{1}=\frac{y_{1}-y_{0}}{x_{1}-x_{0}} \\
& f_{2}\left(x_{2}\right)=b_{0}+b_{1}\left(x_{2}-x_{0}\right)+b_{2}\left(x_{2}-x_{0}\right)\left(x_{2}-x_{1}\right)=y_{2}, \rightarrow b_{2}=\frac{\frac{y_{2}-y_{1}}{x_{2}-x_{1}}-\frac{y_{1}-y_{0}}{x_{2}-x_{0}}}{x_{2}-x_{0}} \tag{*}
\end{align*}
$$

Proof (*):

$$
\begin{aligned}
b_{2} & =\frac{y_{2}-b_{0}-b_{1}\left(x_{2}-x_{0}\right)}{\left(x_{2}-x_{0}\right)\left(x_{2}-x_{1}\right)}=\frac{y_{2}-y_{0}-\frac{\left(y_{1}-y_{0}\right)\left(x_{2}-x_{0}\right)}{x_{1}-x_{0}}}{\left(x_{2}-x_{0}\right)\left(x_{2}-x_{1}\right)} \\
& =\frac{\left(y_{2}-y_{0}\right)\left(x_{1}-x_{0}\right)-\left(y_{1}-y_{0}\right)\left(x_{2}-x_{0}\right)}{\left(x_{2}-x_{0}\right)\left(x_{2}-x_{1}\right)\left(x_{1}-x_{0}\right)} \\
& =\frac{y_{2}\left(x_{1}-x_{0}\right)-y_{0} x_{1}+y_{0} x_{0}-\left(y_{1}-y_{0}\right) x_{2}+y_{1} x_{0}-y_{0} x_{0}}{\left(x_{2}-x_{0}\right)\left(x_{2}-x_{1}\right)\left(x_{1}-x_{0}\right)} \\
& =\frac{y_{2}\left(x_{1}-x_{0}\right)-y_{1} x_{1}+y_{1} x_{0}-\left(y_{1}-y_{0}\right) x_{2}+y_{1} x_{1}-y_{0} x_{1}}{\left(x_{2}-x_{0}\right)\left(x_{2}-x_{1}\right)\left(x_{1}-x_{0}\right)} \\
& =\frac{\left(y_{2}-y_{1}\right)\left(x_{1}-x_{0}\right)-\left(y_{1}-y_{0}\right)\left(x_{2}-x_{1}\right)}{\left(x_{2}-x_{0}\right)\left(x_{2}-x_{1}\right)\left(x_{1}-x_{0}\right)}
\end{aligned}
$$

Comments: In the expression of $f_{2}(x)$,

- $b_{0}+b_{1}\left(x-x_{0}\right)$ is linear interpolating from $\left(x_{0}, y_{0}\right)$ and $\left(x_{1}, y_{1}\right)$, and - $+b_{2}\left(x-x_{0}\right)\left(x-x_{1}\right)$ introduces second order curvature.

Example: Given $\ln 1=0, \ln 4=1.386294$, and $\ln 6=1.791759$, find $\ln 2$.
Solution:

$$
\begin{aligned}
& \left(x_{0}, y_{0}\right)=(1,0),\left(x_{1}, y_{1}\right)=(4,1.386294),\left(x_{2}, y_{2}\right)=(6,1.791759) \\
& b_{0}=y_{0}=0 \\
& b_{1}=\frac{y_{1}-y_{0}}{x_{1}-x_{0}}=\frac{1.386294-0}{4-1}=0.4620981 \\
& b_{2}=\frac{\frac{y_{2}-y_{1}}{x_{2}-x_{1}}-\frac{y_{1}-y_{0}}{x_{1}-x_{0}}}{x_{2}-x_{0}}=\frac{1.791759-1.386294}{6-4}-0.4620981 \\
& 6-1 \\
& f_{2}(x)=0.4620981(x-1)-0.0518731(x-1)(x-4) \\
& f_{2}(2)=0.565844 \\
& \epsilon_{t}=\left|\frac{f_{2}(2)-\ln 2}{\ln 2}\right| \times 100 \%=18.4 \%
\end{aligned}
$$



Figure 3: Quadratic interpolation provides a better estimate than linear interpolation


Figure 4: Linearization of nonlinear relationships

# Interpolation Part II 

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## A- NEWTON'S DIVIDED-DIFFERENCE INTERPOLATING POLYNOMIAL

B-LAGRANGE INTERPOLATING POLYNOMIALS

The Lagrange interpolating polynomial is a reformulation of the Newton's interpolating polynomial that avoids the computation of divided differences. The basic format is

$$
f_{n}(x)=\sum_{i=0}^{n} L_{i}(x) f\left(x_{i}\right)
$$

where $L_{i}(x)=\prod_{j=0, j \neq i}^{n} \frac{x-x_{j}}{x_{i}-x_{j}}$
Linear Interpolation $(n=1)$
$f_{1}(x)=\sum_{i=0}^{1} L_{i}(x) f\left(x_{i}\right)=L_{0}(x) y_{0}+L_{1}(x) y_{1}=\frac{x-x_{1}}{x_{0}-x_{1}} y_{0}+\frac{x-x_{0}}{x_{1}-x_{0}} y_{1}$
$\left(f_{1}(x)=y_{0}+\frac{y_{1}-y_{0}}{x_{1}-x_{0}}\left(x-x_{0}\right)\right)$
Second Order Interpolation $(n=2)$
$f_{2}(x)=\sum_{i=0}^{2} L_{i}(x) f\left(x_{i}\right)=L_{0}(x) y_{0}+L_{1}(x) y_{1}+L_{2}(x) y_{2}=\frac{\left(x-x_{1}\right)\left(x-x_{2}\right)}{\left(x_{0}-x_{1}\right)\left(x_{0}-x_{2}\right)} y_{0}+$ $\frac{\left(x-x_{0}\right)\left(x-x_{2}\right)}{\left(x_{1}-x_{0}\right)\left(x_{1}-x_{2}\right)} y_{1}+\frac{\left(x-x_{0}\right)\left(x-x_{1}\right)}{\left(x_{2}-x_{0}\right)\left(x_{2}-x_{1}\right)} y_{2}$

Solution:

$$
\begin{aligned}
& \left(x_{0}, y_{0}\right)=(1,0),\left(x_{1}, y_{1}\right)=(4,1.386294),\left(x_{2}, y_{2}\right)=(6,1.791759) \\
& f_{1}(x)=y_{0}+\frac{y_{1}-y_{0}}{x_{1}-x_{0}}\left(x-x_{0}\right)=\frac{x-4}{1-4} \times 0+\frac{x-1}{4-1} \times 1.386294=0.4620981 \\
& f_{2}(x)=\frac{\left(x-x_{1}\right)\left(x-x_{2}\right)}{\left(x_{0}-x_{1}\right)\left(x_{0}-x_{2}\right)} y_{0}+\frac{\left(x-x_{0}\right)\left(x-x_{2}\right)}{\left(x_{1}-x_{0}\right)\left(x_{1}-x_{2}\right)} y_{1}+\frac{\left(x-x_{0}\right)\left(x-x_{1}\right)}{\left(x_{2}-x_{0}\right)\left(x_{2}-x_{1}\right)} y_{2}=\frac{(x-4)(x-6)}{(1-4)(1-6)} \times 0+ \\
& \frac{(x-1)(x-6)}{(4-1)(4-6)} \times 1.386294+\frac{(x-1)(x-4)}{(6-1)(6-4)} \times 1.791760=0.565844
\end{aligned}
$$

Example: Find $f(2.6)$ by interpolating the following table of values.

| $i$ | $x_{i}$ | $y_{i}$ |
| :---: | :---: | :---: |
| 1 | 1 | 2.7183 |
| 2 | 2 | 7.3891 |
| 3 | 3 | 20.0855 |

(1) Use Lagrange interpolation

$$
\begin{aligned}
& f_{2}(x)=\sum_{i=1}^{3} L_{i}(x) f\left(x_{i}\right), L_{i}(x)=\prod_{j=1, j \neq i}^{3} \frac{x-x_{j}}{x_{i}-x_{j}} \\
& L_{1}(x)=\frac{\left(x-x_{2}\right)\left(x-x_{3}\right)}{\left(x_{1}-x_{2}\right)\left(x_{1}-x_{3}\right)}=\frac{(2.6-2)(2.6-3)}{(1-2)(1-3)}=-0.12 \\
& L_{2}(x)=\frac{\left(x-x_{1}\right)\left(x-x_{3}\right)}{\left(x_{2}-x_{1}\right)\left(x_{2}-x_{3}\right)}=\frac{(2.6-1)(2.6-3)}{(2-1)(2-3)}=0.64 \\
& L_{3}(x)=\frac{\left(x-x_{1}\right)\left(x-x_{2}\right)}{\left(x_{3}-x_{1}\right)\left(x_{3}-x_{2}\right)}=\frac{(2.6-1)(2.6-2)}{(3-1)(3-2)}=0.48
\end{aligned}
$$

$f_{2}(2.6)=-0.12 \times 2.7183+0.64 \times 7.3891+0.48 \times 20.08853=14.0439$
(2) use Newton's interpolation
$f_{2}(x)=b_{0}+b_{1}\left(x-x_{1}\right)+b_{2}\left(x-x_{1}\right)\left(x-x_{2}\right)$
$b_{0}=y_{1}=2.7183$
$b_{1}=\frac{y_{2}-y_{1}}{x_{2}-x_{1}}=\frac{7.3891-2.7183}{2-1}=4.6708$
$b_{2}=\frac{\frac{y_{2}-y_{1}}{x_{2}-x_{1}}-\frac{y_{1}-y_{0}}{x_{1}-x_{0}}}{x_{2}-x_{0}}=\frac{\frac{20.0855-7.3891}{3-2}-4.6708}{3-1}=4.0128$
$f_{2}(2.6)=2.7183+4.6708 \times(2.6-1)+4.0128 \times(2.6-1)(2.6-2)=14.0439$
(3) Use the straightforward method
$f_{2}(x)=a_{0}+a_{1} x+a_{2} x^{2}$

$$
\begin{aligned}
& a_{0}+a_{1}+a_{2} \times 1^{2}=2.7183 \\
& a_{0}+a_{1}+a_{2} \times 2^{2}=7.3891 \\
& a_{0}+a_{1}+a_{2} \times 3^{2}=20.0855
\end{aligned}
$$

or

$$
\left[\begin{array}{lll}
1 & 1 & 1 \\
1 & 2 & 4 \\
1 & 3 & 9
\end{array}\right]\left[\begin{array}{l}
a_{0} \\
a_{1} \\
a_{2}
\end{array}\right]=\left[\begin{array}{l}
2.7183 \\
7.3891 \\
20.0855
\end{array}\right]
$$

$\left[\begin{array}{lll}a_{0} & a_{1} & a_{2}\end{array}\right]^{\prime}=[6.0732 ;-7.36784 .0129]^{\prime}$
$f(2.6)=6.0732-7.3678 \times 2.6+4.01219 \times 2.6^{2}=14.044$.

## Example:

| $x_{i}$ | 1 | 2 | 3 | 4 |
| :---: | :---: | :---: | :---: | :---: |
| $y_{i}$ | 3.6 | 5.2 | 6.8 | 8.8 |

Model: $y=a x^{b} e^{c x}$
$\ln y=\ln a+b \ln x+c x$. Let $Y=\ln y, a_{0}=\ln a, a_{1}=b, x_{1}=\ln x, a_{2}=c$, and $x_{2}=x$, then we have $Y=a_{0}+a_{1} x_{1}+a_{2} x_{2}$.

| $x_{1, i}$ | 0 | 0.6931 | 1.0986 | 1.3863 |
| :---: | :---: | :---: | :---: | :---: |
| $x_{2, i}$ | 1 | 2 | 3 | 4 |
| $Y_{i}$ | 1.2809 | 1.6487 | 1.9169 | 2.1748 |

$\sum x_{1, i}=3.1781, \sum x_{2, i}=10, \sum x_{1, i}^{2}=3.6092, \sum x_{2, i}^{2}=30, \sum x_{1, i} x_{2, i}=$ 10.2273, $\sum Y_{i}=7.0213, \sum x_{1, i} Y_{i}=6.2636, \sum x_{2, i} Y_{i}=19.0280 . n=4$.

$$
\left[\begin{array}{lll}
1 & \sum x_{1, i} & \sum x_{2, i} \\
\sum x_{1, i} & \sum x_{1, i}^{2} & \sum x_{2, i} x_{1, i} \\
\sum x_{2, i} & \sum x_{1, i} x_{2, i} & \sum x_{2, i}^{2}
\end{array}\right]\left[\begin{array}{l}
a_{0} \\
a_{1} \\
a_{2}
\end{array}\right]=\left[\begin{array}{l}
\sum Y_{i} \\
\sum x_{1, i} Y_{i} \\
\sum x_{2, i} Y_{i}
\end{array}\right]
$$

$\left[\begin{array}{lll}4 & 3.1781 & 10 \\ 3.1781 & 3.6092 & 10.2273 \\ 10 & 10.2273 & 30\end{array}\right]\left[\begin{array}{l}a_{0} \\ a_{1} \\ a_{2}\end{array}\right]=\left[\begin{array}{l}7.0213 \\ 6.2636 \\ 19.0280\end{array}\right]$
$\left[\begin{array}{lll}a_{0} & a_{1} & a_{2}\end{array}\right]^{\prime}=\left[\begin{array}{lll}7.0213 & 6.2636 & 19.0280\end{array}\right]^{\prime}$
$a=e^{a_{0}}=1.2332, b=a_{1}=-1.4259, c=a_{2}=1.0505$, and
$y=a x^{b} e^{c x}=1.2332 \cdot x^{-1.4259} \cdot e^{1.0505 x}$.


Figure 4: Linearization of nonlinear relationships

## Numrical Differentiation

We have already introduced the notion of numerical differentiation. Recall that we employed Taylor series expansions to derive finite-divided-difference approximations of derivatives. In Chap. 4, we developed forward, backward, and centered difference approximations of first and higher derivatives. Recall that, at best, these estimates had errors that were $\mathrm{O}\left(\mathrm{h}^{2}\right)$ —that is, their errors were proportional to the square of the step size. This level of accuracy is due to the number of terms of the Taylor series that were retained during the derivation of these formulas. We will now illustrate how to develop more accurate formulas by retaining more terms.

## 1- HIGH-ACCURACY DIFFERENTIATION FORMULA

As noted above, high-accuracy divided-difference formulas can be generated by including additional terms from the Taylor series expansion. For example, the forward Taylor series expansion can be written as [Eq. (4.21)]

$$
\begin{equation*}
f\left(x_{i+1}\right)=f\left(x_{i}\right)+f^{\prime}\left(x_{i}\right) h+\frac{f^{\prime \prime}\left(x_{i}\right)}{2} h^{2}+\cdots \tag{23.1}
\end{equation*}
$$

which can be solved for

$$
\begin{equation*}
f^{\prime}\left(x_{i}\right)=\frac{f\left(x_{i+1}\right)-f\left(x_{i}\right)}{h}-\frac{f^{\prime \prime}\left(x_{i}\right)}{2} h+O\left(h^{2}\right) \tag{23.2}
\end{equation*}
$$

In Chap. 4, we truncated this result by excluding the second- and higher-derivative terms and were thus left with a final result of

$$
\begin{equation*}
f^{\prime}\left(x_{i}\right)=\frac{f\left(x_{i+1}\right)-f\left(x_{i}\right)}{h}+O(h) \tag{23.3}
\end{equation*}
$$

In contrast to this approach, we now retain the second-derivative term by substituting the following approximation of the second derivative [recall Eq. (4.24)]

$$
\begin{equation*}
f^{\prime \prime}\left(x_{i}\right)=\frac{f\left(x_{i+2}\right)-2 f\left(x_{i+1}\right)+f\left(x_{i}\right)}{h^{2}}+O(h) \tag{23.4}
\end{equation*}
$$

into Eq. (23.2) to yield

$$
f^{\prime}\left(x_{i}\right)=\frac{f\left(x_{i+1}\right)-f\left(x_{i}\right)}{h}-\frac{f\left(x_{i+2}\right)-2 f\left(x_{i+1}\right)+f\left(x_{i}\right)}{2 h^{2}} h+O\left(h^{2}\right)
$$

or, by collecting terms,

$$
\begin{equation*}
f^{\prime}\left(x_{i}\right)=\frac{-f\left(x_{i+2}\right)+4 f\left(x_{i+1}\right)-3 f\left(x_{i}\right)}{2 h}+O\left(h^{2}\right) \tag{23.5}
\end{equation*}
$$

Notice that inclusion of the second-derivative term has improved the accuracy to $O\left(h^{2}\right)$. Similar improved versions can be developed for the backward and centered formulas as well as for the approximations of the higher derivatives. The formulas are summarized in Figs. 23.1 through 23.3 along with all the results from Chap. 4. The following example illustrates the utility of these formulas for estimating derivatives.

## FIGURE 23.1

Forward finite-divided-difference formulas: two versions are presented for each derivative. The latter version incorporates more terms of the Taylor series expansion and is, consequently, more accurate.

First Derivative Error

$$
\begin{align*}
& f^{\prime}\left(x_{i}\right)=\frac{f\left(x_{i+1}\right)-f\left(x_{i}\right)}{h}  \tag{h}\\
& f^{\prime}\left(x_{i}\right)=\frac{-f\left(x_{i+2}\right)+4 f\left(x_{i+1}\right)-3 f\left(x_{i}\right)}{2 h} \tag{2}
\end{align*}
$$

Second Derivative

$$
\begin{align*}
& f^{\prime \prime}\left(x_{i}\right)=\frac{f\left(x_{i+2}\right)-2 f\left(x_{i+1}\right)+f\left(x_{i}\right)}{h^{2}}  \tag{h}\\
& f^{\prime \prime}\left(x_{i}\right)=\frac{-f\left(x_{i+3}\right)+4 f\left(x_{i+2}\right)-5 f\left(x_{i+1}\right)+2 f\left(x_{i}\right)}{h^{2}} \tag{2}
\end{align*}
$$

Third Derivative

$$
\begin{align*}
& f^{\prime \prime \prime}\left(x_{i}\right)=\frac{f\left(x_{i+3}\right)-3 f\left(x_{i+2}\right)+3 f\left(x_{i+1}\right)-f\left(x_{i}\right)}{h^{3}}  \tag{h}\\
& f^{\prime \prime \prime}\left(x_{i}\right)=\frac{-3 f\left(x_{i+4}\right)+14 f\left(x_{i+3}\right)-24 f\left(x_{i+2}\right)+18 f\left(x_{i+1}\right)-5 f\left(x_{i}\right)}{2 h^{3}}
\end{align*}
$$

Fourth Derivative

$$
\begin{align*}
& f^{\prime \prime \prime}\left(x_{i}\right)=\frac{f\left(x_{i+4}\right)-4 f\left(x_{i+3}\right)+6 f\left(x_{i+2}\right)-4 f\left(x_{i+1}\right)+f\left(x_{i}\right)}{h^{4}}  \tag{h}\\
& f^{\prime \prime \prime}\left(x_{i}\right)=\frac{-2 f\left(x_{i+5}\right)+11 f\left(x_{i+4}\right)-24 f\left(x_{i+3}\right)+26 f\left(x_{i+2}\right)-14 f\left(x_{i+1}\right)+3 f\left(x_{i}\right)}{h^{4}} \tag{2}
\end{align*}
$$

First Derivative Error

$$
\begin{equation*}
f^{\prime}\left(x_{i}\right)=\frac{f\left(x_{i}\right)-f\left(x_{i-1}\right)}{h} \tag{h}
\end{equation*}
$$

$$
\begin{equation*}
f^{\prime}\left(x_{i}\right)=\frac{3 f\left(x_{i}\right)-4 f\left(x_{i-1}\right)+f\left(x_{i-2}\right)}{2 h} \tag{2}
\end{equation*}
$$

Second Derivative

$$
f^{\prime \prime}\left(x_{i}\right)=\frac{f\left(x_{i}\right)-2 f\left(x_{i-1}\right)+f\left(x_{i-2}\right)}{h^{2}} \quad O(h)
$$

$$
f^{\prime \prime}\left(x_{i}\right)=\frac{2 f\left(x_{i}\right)-5 f\left(x_{i-1}\right)+4 f\left(x_{i-2}\right)-f\left(x_{i-3}\right)}{h^{2}}
$$

Third Derivative

$$
f^{\prime \prime \prime}\left(x_{i}\right)=\frac{f\left(x_{i}\right)-3 f\left(x_{i-1}\right)+3 f\left(x_{i-2}\right)-f\left(x_{i-3}\right)}{h^{3}} \quad O(h)
$$

$$
f^{\prime \prime \prime}\left(x_{i}\right)=\frac{5 f\left(x_{i}\right)-18 f\left(x_{i-1}\right)+24 f\left(x_{i-2}\right)-14 f\left(x_{i-3}\right)+3 f\left(x_{i-4}\right)}{2 h^{3}} \quad O\left(h^{2}\right)
$$

Fourth Derivative

$$
f^{\prime \prime \prime \prime}\left(x_{i}\right)=\frac{f\left(x_{i}\right)-4 f\left(x_{i-1}\right)+6 f\left(x_{i-2}\right)-4 f\left(x_{i-3}\right)+f\left(x_{i-4}\right)}{h^{4}}
$$

$$
O(h)
$$

$$
f^{\prime \prime \prime \prime}\left(x_{i}\right)=\frac{3 f\left(x_{i}\right)-14 f\left(x_{i-1}\right)+26 f\left(x_{i-2}\right)-24 f\left(x_{i-3}\right)+11 f\left(x_{i-4}\right)-2 f\left(x_{i-5}\right)}{h^{4}}
$$

FIGURE 23.3
Centered finite-divideddifference formulas: two
versions are presented for each derivative. The latter version incorporates more terms of the Taylor series expansion and is, consequently, more accurate.

First Derivative Error

$$
f^{\prime}\left(x_{i}\right)=\frac{f\left(x_{i+1}\right)-f\left(x_{i-1}\right)}{2 h} \quad O\left(h^{2}\right)
$$

$$
f^{\prime}\left(x_{i}\right)=\frac{-f\left(x_{i+2}\right)+8 f\left(x_{i+1}\right)-8 f\left(x_{i-1}\right)+f\left(x_{i-2}\right)}{12 h}
$$

$$
O\left(h^{4}\right)
$$

Second Derivative

$$
\begin{align*}
& f^{\prime \prime}\left(x_{i}\right)=\frac{f\left(x_{i+1}\right)-2 f\left(x_{i}\right)+f\left(x_{i-1}\right)}{h^{2}}  \tag{2}\\
& f^{\prime \prime}\left(x_{i}\right)=\frac{-f\left(x_{i+2}\right)+16 f\left(x_{i+1}\right)-30 f\left(x_{i}\right)+16 f\left(x_{i-1}\right)-f\left(x_{i-2}\right)}{12 h^{2}} \tag{4}
\end{align*}
$$

Third Derivative

$$
\begin{aligned}
& f^{\prime \prime \prime}\left(x_{i}\right)=\frac{f\left(x_{i+2}\right)-2 f\left(x_{i+1}\right)+2 f\left(x_{i-1}\right)-f\left(x_{i-2}\right)}{2 h^{3}} \\
& f^{\prime \prime \prime}\left(x_{i}\right)=\frac{-f\left(x_{i+3}\right)+8 f\left(x_{i+2}\right)-13 f\left(x_{i+1}\right)+13 f\left(x_{i-1}\right)-8 f\left(x_{i-2}\right)+f\left(x_{i-3}\right)}{8 h^{3}}
\end{aligned}
$$

Fourth Derivative

$$
\begin{equation*}
f^{\prime \prime \prime \prime}\left(x_{i}\right)=\frac{f\left(x_{i+2}\right)-4 f\left(x_{i+1}\right)+6 f\left(x_{i}\right)-4 f\left(x_{i-1}\right)+f\left(x_{i-2}\right)}{h^{4}} \tag{2}
\end{equation*}
$$

$f^{\prime \prime \prime \prime}\left(x_{i}\right)=\frac{-f\left(x_{i+3}\right)+12 f\left(x_{i+2}\right)-39 f\left(x_{i+1}\right)+56 f\left(x_{i}\right)-39 f\left(x_{i-1}\right)+12 f\left(x_{i-2}\right)-f\left(x_{i-3}\right)}{6 h^{4}}$

EXAMPLE 23.1 High-Accuracy Differentiation Formulas
Problem Statement. Recall that in Example 4.4 we estimated the derivative of

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

at $x=0.5$ using finite divided differences and a step size of $h=0.25$,

|  | Forward <br> $\boldsymbol{O}(\boldsymbol{h})$ | Backward <br> $\boldsymbol{O}(\boldsymbol{h})$ | Centered <br> $\boldsymbol{O}\left(\boldsymbol{h}^{\mathbf{2}}\right)$ |
| :--- | :---: | :---: | :---: |
| Estimate | -1.155 | -0.714 | -0.934 |
| $\boldsymbol{\varepsilon}_{t}(\%)$ | -26.5 | 21.7 | -2.4 |

where the errors were computed on the basis of the true value of -0.9125 . Repeat this computation, but employ the high-accuracy formulas from Figs. 23.1 through 23.3.
Solution. The data needed for this example are

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

The forward difference of accuracy $O\left(h^{2}\right)$ is computed as (Fig. 23.1)

$$
f^{\prime}(0.5)=\frac{-0.2+4(0.6363281)-3(0.925)}{2(0.25)}=-0.859375 \quad \varepsilon_{t}=5.82 \%
$$

The backward difference of accuracy $O\left(h^{2}\right)$ is computed as (Fig. 23.2)

$$
f^{\prime}(0.5)=\frac{3(0.925)-4(1.1035156)+1.2}{2(0.25)}=-0.878125 \quad \varepsilon_{t}=3.77 \%
$$

The centered difference of accuracy $O\left(h^{4}\right)$ is computed as (Fig. 23.3)

$$
f^{\prime}(0.5)=\frac{-0.2+8(0.6363281)-8(1.1035156)+1.2}{12(0.25)}=-0.9125 \quad \varepsilon_{t}=0 \%
$$

The centered difference of accuracy $O\left(h^{4}\right)$ is computed as (Fig. 23.3)

$$
f^{\prime}(0.5)=\frac{-0.2+8(0.6363281)-8(1.1035156)+1.2}{12(0.25)}=-0.9125 \quad \varepsilon_{t}=0 \%
$$

As expected, the errors for the forward and backward differences are considerably more accurate than the results from Example 4.4. However, surprisingly, the centered difference yields a perfect result. This is because the formulas based on the Taylor series are equivalent to passing polynomials through the data points.

## 2- RICHARDSON EXTRAPOLATION

To this point, we have seen that there are two ways to improve derivative estimates when employing finite divided differences: (1) decrease the step size or (2) use a higher-order formula that employs more points. A third approach, based on Richardson extrapolation, uses two derivative estimates to compute a third, more accurate approximation.

Recall from Sec. 22.2.1 that Richardson extrapolation provided a means to obtain an improved integral estimate $I$ by the formula [Eq. (22.4)]

$$
\begin{equation*}
I \cong I\left(h_{2}\right)+\frac{1}{\left(h_{1} / h_{2}\right)^{2}-1}\left[I\left(h_{2}\right)-I\left(h_{1}\right)\right] \tag{23.6}
\end{equation*}
$$

where $I\left(h_{1}\right)$ and $I\left(h_{2}\right)$ are integral estimates using two step sizes $h_{1}$ and $h_{2}$. Because of its convenience when expressed as a computer algorithm, this formula is usually written for the case where $h_{2}=h_{1} / 2$, as in

$$
\begin{equation*}
I \cong \frac{4}{3} I\left(h_{2}\right)-\frac{1}{3} I\left(h_{1}\right) \tag{23.7}
\end{equation*}
$$

In a similar fashion, Eq. (23.7) can be written for derivatives as

$$
\begin{equation*}
D \cong \frac{4}{3} D\left(h_{2}\right)-\frac{1}{3} D\left(h_{1}\right) \tag{23.8}
\end{equation*}
$$

For centered difference approximations with $O\left(h^{2}\right)$, the application of this formula will yield a new derivative estimate of $O\left(h^{4}\right)$.

## EXAMPLE 23.2 Richardson Extrapolation

Problem Statement. Using the same function as in Example 23.1, estimate the first derivative at $x=0.5$ employing step sizes of $h_{1}=0.5$ and $h_{2}=0.25$. Then use Eq. (23.8) 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

$$
D(0.5)=\frac{0.2-1.2}{1}=-1.0 \quad \varepsilon_{t}=-9.6 \%
$$

and

$$
D(0.25)=\frac{0.6363281-1.1035156}{0.5}=-0.934375 \quad \varepsilon_{t}=-2.4 \%
$$

The improved estimate can be determined by applying Eq. (23.8) to give

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

which for the present case is a perfect result.

The previous example yielded a perfect result because the function being analyzed was a fourth-order polynomial. The perfect outcome was due to the fact that Richardson extrapolation is actually equivalent to fi tting a higher-order polynomial through these data and then evaluating the derivatives by centered divided differences. Thus, the present case matched the derivative of the fourth-order
polynomial precisely. For most other functions, of course, this would not occur and our derivative estimate would be improved.
but not perfect. Consequently, as was the case for the application of
Richardson extrapolation, the approach can be applied iteratively using a Romberg algorithm until the result falls below an acceptable error criterion

## Numrical Integration: applications

## using Newton-Cotes Integration <br> Formulas

## Dr Jalil Kwad <br> University of Anbar Department of civil Engineering

The Newton-Cotes formulas are the most common numerical integration schemes. They are based on the strategy of replacing a complicated function or tabulated data with an approximating function that is easy to integrate.
Closed and open forms of the Newton-Cotes formulas are available. The closed forms are those where the data points at the beginning and end of the limits of integration are known. The open forms have integration limits that extend beyond the range of the data.


The difference between (a) closed and (b) open integration formulas.

## Closed forum:

## 1- Trapezium Rule

Finding a definite integral can be thought of as determining the area under the curve. Some integrals are difficult to evaluate exactly and so numerical methods are needed.


The simplest of these methods is the trapezium rule which approximates the area under the curve by $n$ trapezia each of width $h$ as shown.
The formula for the area of the first of these trapezia is

$$
A=\frac{h}{2}\left(y_{0}+y_{1}\right)
$$

when we sum all these areas, we will get

$$
\int_{a}^{b} y \mathrm{~d} x \approx \frac{h}{2}\left[y_{0}+2\left(y_{1}+y_{2}+\ldots+y_{n-1}\right)+y_{n}\right]
$$

where $h=\frac{b-a}{n}$

## Example

1(i) Consider $I=\int_{1}^{2} x^{2} \mathrm{~d} x=\left[\frac{x^{3}}{3}\right]_{1}^{2}=\frac{2^{3}}{3}-\frac{1}{3}=\frac{7}{3} \quad \underline{\underline{=2.3}}$
(ii) We have, using trapezium rule with 1 interval $\quad I \approx \quad \frac{h}{2}\left(y_{0}+y_{1}\right) \quad h=\frac{2-1}{1}=1$

|  | $x$ | $y=x^{2}$ |
| :--- | :--- | :--- |
| $y_{0}$ | 1 | $1^{2}$ |
| $y_{1}$ | 2 | $2^{2}$ |

$$
\begin{aligned}
I \quad & \approx \frac{1}{2}\left(1^{2}+2^{2}\right) \quad=\frac{1}{2} \times 5 \\
& =2.5
\end{aligned}
$$

(iii) Using 2 intervals: $I \approx \quad \frac{h}{2}\left(y_{0}+2 y_{1}+y_{2}\right) \quad h=\frac{2-1}{2}=\frac{1}{2}$

|  | $x$ | $y=x^{2}$ |
| ---: | :--- | :--- |
| $y_{0}$ | 1 | $1^{2}$ |
| $y_{1}$ | $\frac{3}{2}$ | $\left(\frac{3}{2}\right)^{2}$ |
| $y_{2}$ | 2 | $2^{2}$ |
|  | $I$ | $\approx \frac{1}{4}\left(1^{2}+2\left(\frac{3}{2}\right)^{2}+2^{2}\right)$ |
|  | $=\frac{1}{4}\left(1+\frac{9}{2}+4\right)$ |  |
|  | $=\frac{19}{8}$ |  |
|  | $=$$=2.375$ |  |

(iv) Using 4 intervals: $I \approx \quad \frac{h}{2}\left(y_{0}+2\left(y_{1}+y_{2}+y_{3}\right)+y_{4}\right) \quad h=\frac{2-1}{4}=\frac{1}{4}$

|  | $x$ | $y=x^{2}$ | $=1$ |
| :--- | :--- | :--- | :--- |
| $y_{0}$ | 1 | $1^{2}$ | $=1.5625$ |
| $y_{1}$ | $\frac{5}{4}$ | $\left(\frac{5}{4}\right)^{2}$ |  |
| $y_{2}$ | $\frac{6}{4}$ | $\left(\frac{6}{4}\right)^{2}$ | $=2.25$ |
| $y_{3}$ | $\frac{7}{4}$ | $\left(\frac{7}{4}\right)^{2}$ | $=3.0625$ |
| $y_{4}$ | 2 | $2^{2}$ | $=4$ |

$I \quad \approx \frac{1}{8}(1+2(1.5625+2.25+3.0625)+4)$
$=\frac{1}{8}(18.75)$
$=2.34375$
2) Find the value of the integral $\int_{0}^{\frac{2 \pi}{3}} \sqrt{\sin (x)} \mathrm{d} x$ using the trapezium rule with (i) 4 intervals (ii) 8 intervals giving your answers to 3 dp Note we must work to at least 4 dp if the answer is required to 3dp.
i) with 4 intervals
first we need to work out $h$

$$
h=\frac{\frac{2 \pi}{3}-0}{4} \quad=\frac{\pi}{6}
$$

Now we need a table of values of $\sqrt{\sin (x)}$ for $x=0$ to $\frac{2 \pi}{3}$ in steps of $\frac{\pi}{6}$. These will be the values of $y_{0}, y_{1}, y_{2}, y_{3}$, and $y_{4}$.

| $x$ values |  | $\sqrt{\sin (x)}$ |  |
| :--- | :--- | :--- | :--- |
| 0 | $y_{0}$ | $\sqrt{\sin (0)}$ | 0.0000 |
| $\frac{\pi}{6}$ | $y_{1}$ | $\sqrt{\sin \left(\frac{\pi}{6}\right)}$ | 0.7071 |
| $\frac{2 \pi}{6}$ | $y_{2}$ | $\sqrt{\sin \left(\frac{2 \pi}{6}\right)}$ | 0.9306 |
| $\frac{3 \pi}{6}$ | $y_{3}$ | $\sqrt{\sin \left(\frac{3 \pi}{6}\right)}$ | 1 |
| $\frac{4 \pi}{6}=\frac{2 \pi}{3}$ | $y_{4}$ | $\sqrt{\sin \left(\frac{4 \pi}{6}\right)}$ | 0.9306 |

Then using formula for trapezium rule

$$
\begin{aligned}
\int_{0}^{\frac{2 \pi}{3}} \sqrt{\sin (x)} \mathrm{d} x & \approx \frac{h}{2}\left(y_{0}+2\left(y_{1}+y_{2}+y_{3}\right)+y_{4}\right) \\
\text { gives } \quad & =\frac{\frac{\pi}{6}}{2}(0+2(0.7071+0.9306+1)+0.9306) \quad=\frac{\frac{\pi}{6}}{2} \times 6.2060 \\
& =1.625 \text { to 3dp }
\end{aligned}
$$

ii) with 8 intervals
first we need to work out $h$

$$
h=\frac{\frac{2 \pi}{3}-0}{8} \quad=\frac{\pi}{12}
$$

Now we need a table of values of $\sqrt{\sin (x)}$ for $x=0$ to $\frac{2 \pi}{3}$ in steps of $\frac{\pi}{12}$. These will be the values of $y_{0}, y_{1}, y_{2}, y_{3}, \ldots . . y_{8}$.

| $x$ values |  | $\sqrt{\sin (x)}$ |  |
| :--- | :--- | :--- | :--- |
| 0 | $y_{0}$ | $\sqrt{\sin (0)}$ | 0.0000 |
| $\frac{\pi}{12}$ | $y_{1}$ | $\sqrt{\sin \left(\frac{\pi}{12}\right)}$ | 0.5087 |
| $\frac{2 \pi}{12}$ | $y_{2}$ | $\sqrt{\sin \left(\frac{\pi}{6}\right)}$ | 0.7071 |
| $\frac{3 \pi}{12}$ | $y_{3}$ | $\sqrt{\sin \left(\frac{\pi}{4}\right)}$ | 0.8409 |
| $\frac{4 \pi}{12}$ | $y_{5}$ | $\sqrt{\sin \left(\frac{\pi}{3}\right)}$ | 0.9306 |
| $\frac{5 \pi}{12}$ | $y_{6}$ | $\sqrt{\sin \left(\frac{5 \pi}{12}\right)}$ | 0.9828 |
| $\frac{6 \pi}{12}$ | $y_{7}$ | $\sqrt{\sin \left(\frac{\pi}{2}\right)}$ | 1 |
| $\frac{7 \pi}{12}$ | $y_{8}$ | $\sqrt{\sin \left(\frac{7 \pi}{12}\right)}$ | 0.9828 |
| $\frac{8 \pi}{12}=\frac{2 \pi}{3}$ |  | 0.9306 |  |

Then using formula for trapezium rule

$$
\begin{aligned}
& \frac{2 \pi}{\frac{2 \pi}{3}} \sqrt{\sin (x)} \mathrm{d} x \approx \frac{h}{2}\left(y_{0}+2\left(y_{1}+y_{2}+y_{3}+y_{4}+y_{5}+y_{6}+y_{7}\right)+y_{8}\right) \\
& \text { gives } \quad= \\
& \quad=\frac{\frac{\pi}{12}}{2} \times 12.8364 \quad=1.680 \text { to 3dp }
\end{aligned}
$$

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Closed and open forms of the Newton-Cotes formulas are available. The closed forms are those where the data points at the beginning and end of the limits of integration are known. The open forms have integration limits that extend beyond the range of the data.


The difference between (a) closed and (b) open integration formulas.

## Closed forum:

## 1- Trapezium Rule

## 2- SIMPSON'S RULES

Aside from applying the trapezoidal rule with finer segmentation, another way to obtain a more accurate estimate of an integral is to use higher-order polynomials to connect the points. For example, if there is an extra point midway between $f(a)$ and $f(b)$, the three points can be connected with a parabola (Fig.a). If there are two points equally spaced between $f(a)$ and $f(b)$, the four points can be connected with a third-order polynomial (Fig.b). The formulas that result from taking the integrals under these polynomials are called Simpson's rules.

(a)Graphical depiction of Simpson's $1 / 3$ rule: It consists of taking the area under a parabola connecting three points. (b) Graphical depiction of Simpson's $3 / 8$ rule: It consists of taking the area under a cubic equation connecting four points.

## a- Simpson's 1/3 Rule

Simpson's $1 / 3$ rule results when a second-order interpolating polynomial is substituted into Eq. (21.1):

$$
I=\int_{a}^{b} f(x) d x \cong \int_{a}^{b} f_{2}(x) d x
$$

If $a$ and $b$ are designated as $x_{0}$ and $x_{2}$ and $f_{2}(x)$ is represented by a second-order Lagrange polynomial [Eq. (18.23)], the integral becomes

$$
\begin{aligned}
I= & \int_{x_{0}}^{x_{2}}\left[\frac{\left(x-x_{1}\right)\left(x-x_{2}\right)}{\left(x_{0}-x_{1}\right)\left(x_{0}-x_{2}\right)} f\left(x_{0}\right)+\frac{\left(x-x_{0}\right)\left(x-x_{2}\right)}{\left(x_{1}-x_{0}\right)\left(x_{1}-x_{2}\right)} f\left(x_{1}\right)\right. \\
& \left.+\frac{\left(x-x_{0}\right)\left(x-x_{1}\right)}{\left(x_{2}-x_{0}\right)\left(x_{2}-x_{1}\right)} f\left(x_{2}\right)\right] d x
\end{aligned}
$$

After integration and algebraic manipulation, the following formula results:

$$
\begin{equation*}
I \cong \frac{h}{3}\left[f\left(x_{0}\right)+4 f\left(x_{1}\right)+f\left(x_{2}\right)\right] \tag{21.14}
\end{equation*}
$$

where, for this case, $h=(b-a) / 2$. This equation is known as Simpson's $1 / 3$ rule. It is the second Newton-Cotes closed integration formula. The label " $1 / 3$ " stems from the fact that $h$ is divided by 3 in Eq. (21.14). An alternative derivation is shown in Box 21.3 where the Newton-Gregory polynomial is integrated to obtain the same formula.

As was done for the trapezoidal rule, Simpson's 1y3 rule can be derived by integrating the forward Newton-Gregory interpolating polynomial:

the function is fitted by parabolas which give a more accurate result.


There must be an even number, $n$, of intervals each of width $h$.

$$
\int_{a}^{b} y \mathrm{~d} x \approx \frac{h}{3}\left[y_{0}+4\left(y_{1}+y_{3}+\ldots+y_{n-1}\right)+2\left(y_{2}+y_{4}+\ldots+y_{n-2}\right)+y_{n}\right]
$$

where

$$
h=\frac{b-a}{n}
$$

## Ex:

## Single Application of Simpson's 1/3 Rule

Problem Statement. Use Eq. (21.15) to integrate

$$
f(x)=0.2+25 x-200 x^{2}+675 x^{3}-900 x^{4}+400 x^{5}
$$

from $a=0$ to $b=0.8$. Recall that the exact integral is 1.640533 . Solution.

$$
f(0)=0.2 \quad f(0.4)=2.456 \quad f(0.8)=0.232
$$

Therefore, Eq. (21.15) can be used to compute

$$
I \cong 0.8 \frac{0.2+4(2.456)+0.232}{6}=1.367467
$$

## Roots: Open Methods

Years ago, you learned to use the quadratic formula

$$
\begin{equation*}
x=\frac{-b \pm \sqrt{b^{2}-4 a c}}{2 a} \tag{PT2.1}
\end{equation*}
$$

to solve

$$
\begin{equation*}
f(x)=a x^{2}+b x+c=0 \tag{PT2.2}
\end{equation*}
$$

The values calculated with Eq. (PT2.1) are called the "roots" of Eq. (PT2.2). They represent the values of $x$ that make Eq. (PT2.2) equal to zero. Thus, we can defi ne the root of an equation as the value of $x$ that makes $f(x) 50$. For this reason, roots are sometimes called the zeros of the equation. Although the quadratic formula is handy for solving Eq. (PT2.2), there are many other functions for which the root cannot be determined so easily. For these cases, the numerical methods described

## Solving equations numerically



Some equations can't be solved algebraically

and we have to use numerical methods.


## 1. Interval bisector method

Example: Solve $3+4 x-x^{4}=0$.

## Solution

If we plot $f(x)=3+4 x-x^{4}$ we see that the curve crosses the $x$-axis between $x=1$ and $x=2$.


Therefore there is a root (solution) to the equation $3+4 x-x^{4}=0$ between $x=1$ and $x=2$. If we want a better approximation we can narrow down the interval.

Let

$$
f(x)=3+4 x-x^{4}
$$

then

$$
f(1)=3+4-1=6>0
$$

and

$$
f(2)=3+8-16=-5<0
$$

therefore there is a root in the interval $x=1$ to $x=2$

we can work out $f(1.5)$

$$
\begin{aligned}
& f(1.5)=3+4 \times 1.5-1.5^{4}=3.9>0
\end{aligned} \quad \therefore \text { the root lies between } 1.5 \text { and } 20 \text { and } 2
$$

if we carry on like this, we can get an accurate enough solution

$$
\begin{aligned}
f(1.8)= & -0.2976<0 \quad \therefore \text { the root lies between } 1.75 \text { and } 1.8 \\
& 1.75<x<1.8 \\
& \therefore \text { the root is } \mathbf{1 . 8} \text { to } \mathbf{1} \text { d.p }
\end{aligned}
$$

Example 2. Show that the equation $\ln (1+x)-e^{-x}-1=0$ has a root between $x=1.5$ and $x=2.5$.

Find this root to 1 d.p.
Solution
Let

$$
\begin{aligned}
& f(x)=\ln (1+x)-e^{-x}-1 \\
& f(1.5)=-0.306<0
\end{aligned}
$$

$f(2.5)=0.171>0 \quad \therefore$ the root lies between 1.5 and
2.5
$f(2.0)=-0.0367<0 \quad \therefore$ the root lies between 2.0 and
2.5

$$
f(2.25)=0.0732>0 \quad \therefore \text { the root lies between } 2.0 \text { and }
$$

2.25

$$
f(2.1)=0.009>0 \quad \therefore \text { the root lies between } 2.0 \text { and }
$$

2.1 $f(2.05)=\quad \therefore 0 \quad \therefore$ the root lies between 2.05 and
2.1
$2.05<x<2.1$
$\therefore$ the root is 2.1 to 1 d.p

## Exercise

1. Show that $x^{3}=14$ has a root between 2 and 3 . Find this root to 1 dp .
2. Show that $2^{x}=8 x$ has 2 roots, the first lying between 0 and 1 and the second between 5 and 6 . Find both of the roots to 1 dp .
Answers
3. Let

$$
f(x)=x^{3}-14
$$

$$
f(2)=2^{3}-14<0
$$

$$
f(3)=3^{3}-14>0 \quad \text { therefore root lies between } 2 \text { and } 3
$$

$$
f(2.5)=2.5^{3}-14>0 \quad \text { therefore root lies between } 2 \text { and } 2.5
$$

$$
f(2.25)<0 \quad \text { therefore root lies between } 2.25 \text { and } 2.5
$$

$$
f(2.3)<0 \quad \text { therefore root lies between } 2.3 \text { and } 2.5
$$

$f(2.4)<0 \quad$ therefore root lies between 2.4 and 2.5
$f(2.45)>0 \quad$ therefore root lies between 2.4 and 2.45
$2.4<x<2.45$

## $\therefore$ the root is 2.4 to $1 \mathbf{d p}$

2. Show that $2^{x}=8 x$ has 2 roots, the first lying between 0 and 1 and the second between 5 and 6 . Find both of the roots to 1 dp .

Let $f(x)=2^{x}-8 x$ $f(0)=1-0>0$
$f(1)=2-8<0 \quad \therefore$ the root lies between 0 and 1
$f(0.5)<0 \quad \therefore$ the root lies between 0 and 0.5
$f(0.25)<0 \quad \therefore$ the root lies between 0 and 0.25
$f(0.1)>0 \quad \therefore$ the root lies between 0.1 and 0.25
$f(0.2)<0 \quad \therefore$ the root lies between 0.1 and 0.2
$f(0.15)<0 \quad \therefore$ the root lies between 0 and 0.15
$\therefore$ the root is 0.1 to 1 dp

To find the other root,

$$
\begin{aligned}
& f(5)=2^{5}-8 \times 5=-8<0 \\
& f(6)=2^{6}-8 \times 6=16>0
\end{aligned}
$$

| $f(5.5)=1.25>0$ | $\therefore$ the root lies between 5 and 5.5 |
| :--- | :--- |
| $f(5.25)<0$ | $\therefore$ the root lies between 5.25 and 5.5 |
| $f(5.4)<0$ | $\therefore$ the root lies between 5.4 and 5.5 |
| $f(5.45)>0$ | $\therefore$ the root lies between 5.4 and 5.45 |

$5.4<x<5.45$
$\therefore$ the root is 5.4 to 1 dp
2. Fixed point iteration $\quad x=g(x)$

This is also repetitive procedure which leads us closer and closer to the precise answer

Example 1
Consider the equation $\quad x^{2}-5 x+2=0$

$f(0)=0^{2}-5(0)+2=2>0$
$f(1)=1^{2}-5(1)+2=-2<0$
$\therefore f(x)$ must be 0 between 0 and 1 and so one solution lies between 0 and 1
Similarly
$f(4)=4^{2}-5(4)+2=-2<0$
$f(5)=5^{2}-5(5)+2=2>0$
$\therefore f(x)$ must be 0 between 4 and 5 and so the other solution lies between 4 and 5
Rearranging the equation

$$
\begin{aligned}
& x^{2}-5 x+2=0 \\
& x^{2}=5 x-2 \\
& x= \pm \sqrt{5 x-2}
\end{aligned}
$$

make an iterative formula $\quad x_{n+1}=\sqrt{5 x_{n}-2}$
(we need + ve square root for $5 x_{n}-2>0$ for all $n$ )
we can now use this to get a sequence of solutions which get closer and closer to the root.
We will start with

$$
\begin{array}{ll}
x_{0}=4 & =4.242640687 \\
x_{1}=\sqrt{ }\{5(4)-2\} & =4.38328683 \\
x_{2}=\sqrt{ }\{5(4.242640687)-2\} & =4.4627832029 \\
x_{3}=\sqrt{ }\{5(4.38328 \ldots \ldots-2\} & =4.507096199 \\
x_{4}= & =4.531609096 \\
x_{5}= & =4.545112262 \\
x_{6}= & =4.552533505 \\
x_{7}= & =4.556607019 \\
x_{8}= & =4.55884142
\end{array}
$$

To find the other root, we need to re-arrange the equation $x^{2}-5 x+2=0$ in a different way: Let's try


Let $x_{0}=4$ then

$$
\begin{aligned}
& x_{1}=3.6 \\
& x_{2}=2.992 \\
& x_{3}=2.1904128 \\
& x_{4}=1.359581647 \\
& x_{5}=0.76969245 \\
& x_{6}=0.518485293 \\
& x_{7}=0.4537654 \\
& x_{8}=0.441180607 \\
& x_{9}=0.438928065 \\
& x_{10}=0.438531569
\end{aligned}
$$

$\therefore x=0.44$ (to 2 dp ) ie the smaller root

So how we arrange the equation and the starting value we choose can lead us to different roots

We find $\quad x^{2}=5 x-2 \quad x^{2}=5 x-2$ gives $\boldsymbol{x}=4.56$ to $\mathbf{2 ~ d p}$

Or $\quad x^{2}=5 x-2 \quad \therefore x=5-\frac{2}{x} \quad$ gives $x=4.56$ to 2 dp

$$
5 x=x^{2}+2 \quad \therefore x=\frac{x^{2}+2}{5} \quad \text { gives } x=\mathbf{0 . 4 4} \text { (to } 2 \mathrm{dp} \text { ) ie the smaller root }
$$

Or
$x(x-5)=-2 \quad \therefore x=\frac{-2}{x-5} \quad$ gives $\quad x=0.44$ (to 2 dp ) ie the smaller root

Some of the iteration formulae lead to the first root and some to the second root
Generally, when an equation has two or more roots, a single arrangement will not find them all.

Each iteration formula may give only one root, so that for an equation with 3 roots, you may need 3 iteration formulae, and so on.


## Starting points for iteration

It saves time if you can use a starting point which is close to the root.
To do this, find an interval in which a root lies. That is find two values $a$ and $b$ such that if $f(a)>0$ then $f(b)<0$
The method converges for $\left|\mathrm{g}^{\prime}(x)\right|<1$



## Example 2

Show that the equation $\ln x-x+2=0$ has a root between 3 and 4 .
By using the iteration formula $x_{n+1}=2+\ln x_{n}$ and starting with $x_{0}=3$, find to 3 s.f. a root of the equation $\ln x-x+2=0$

## Solution

Let $f(x)=\ln x-x+2$ then
Then $f(3)=\ln 3-3+2=0.0986>0$
$f(4)=\ln 4-4+2=-0.6137<0$
$\therefore$ a root to the equation lies between 3 and 4

$$
\begin{aligned}
x_{n+1}= & 2+\ln x_{n} \\
x_{0} & =3 \\
x_{1} & =3.098612289 \\
x_{2} & =3.130954361 \\
x_{3} & =3.141337866 \\
x_{4} & =3.144648781 \\
x_{5} & =3.145702209 \\
x_{6} & =3.146037143 \\
x_{7} & =3.146433611 \\
x_{8} & =3.146177452 \\
x_{9} & =3.146188209
\end{aligned}
$$

## $\therefore \boldsymbol{x}=3.15$ to 3 s.f.

http://www.youtube.com/watch?v=OLqdJMjzib8

## Exercise

1. Show that the equation $x^{3}-x-2=0$ has a root between 1 and 2 , and can be arranged in the form $x=\sqrt[3]{x+2}$.

Use the iterative formula

$$
x_{n+1}=\sqrt[3]{x_{n}+2} \quad \text { to find the value of the root to } 3 \text { d.p. }
$$

2. Show that the equation $e^{-x}-x+2=0$ has a root between 2 and 3 .

Use the iterative formula

$$
x_{n+1}=e^{-x_{n}}+2 \quad \text { to find the value of the root to } 3 \text { d.p. }
$$

3. Show that the equation $e^{x}+x-6=0$ has a root between 1 and 2 .

Show that the equation can be arranged in the form $x=\ln (6-x)$.
Use the iterative formula

$$
x_{n+1}=\ln \left(6-x_{n}\right) \quad \text { to find the value of the root to } 3 \text { d.p. }
$$

Ans.

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## Ordinary Differential Equations

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## Runge-Kutta Methods

Although it is possible to derive solution formulas for some ordinary differential equations many differential equations arising in applications are so complicated that it is impractical to have solution formulas. Even when a solution formula is available, it may involve integrals that can be calculated only by using a numerical quadrature formula. In either situation, numerical methods provide a powerful alternative tool for solving the differential equation.

This chapter is devoted to solving ordinary differential equations of the form

$$
\frac{d y}{d x}=f(x, y)
$$

In Chap. 1, we used a numerical method to solve such an equation for the velocity of the falling parachutist. Recall that the method was of the general form

$$
\text { New value }=\text { old value }+ \text { slope } \times \text { step size }
$$

or, in mathematical terms,

$$
\begin{equation*}
y_{i+1}=y_{i}+\phi h \tag{25.1}
\end{equation*}
$$

According to this equation, the slope estimate of $\phi$ is used to extrapolate from an old value $y_{i}$ to a new value $y_{i+1}$ over a distance $h$ (Fig. 25.1). This formula can be applied step by step to compute out into the future and, hence, trace out the trajectory of the solution.


Graphical depiction of a one step method.
All one-step methods can be expressed in this general form, with the only difference being the manner in which the slope is estimated. As in the falling parachutist problem, the simplest approach is to use the differential equation to estimate the slope in the form of the fi rst derivative at xi. In other words, the slope at the beginning of the interval is taken as an approximation of the average slope over the whole interval. This approach, called Euler's method, is discussed in the fi rst part of this chapter. This is followed by other one-step methods that employ alternative slope estimates that result in more accurate predictions. All these techniques are generally called Runge-Kutta methods.


## Euler's method

## EULER'S METHOD

The first derivative provides a direct estimate of the slope at $x_{i}$ (Fig. 25.2):

$$
\phi=f\left(x_{i}, y_{i}\right)
$$

where $f\left(x_{i}, y_{i}\right)$ is the differential equation evaluated at $x_{i}$ and $y_{i}$. This estimate can be substituted into Eq. (25.1):

$$
\begin{equation*}
y_{i+1}=y_{i}+f\left(x_{i}, y_{i}\right) h \tag{25.2}
\end{equation*}
$$

This formula is referred to as Euler's (or the Euler-Cauchy or the point-slope) method. A new value of $y$ is predicted using the slope (equal to the first derivative at the original value of $x$ ) to extrapolate linearly over the step size $h$ (Fig. 25.2).

## Euler's Method

Problem Statement. Use Euler's method to numerically integrate Eq. (PT7.13):

$$
\frac{d y}{d x}=-2 x^{3}+12 x^{2}-20 x+8.5
$$

from $x=0$ to $x=4$ with a step size of 0.5 . The initial condition at $x=0$ is $y=1$. Recall that the exact solution is given by Eq. (PT7.16):

$$
y=-0.5 x^{4}+4 x^{3}-10 x^{2}+8.5 x+1
$$

Solution. Equation (25.2) can be used to implement Euler's method:

$$
y(0.5)=y(0)+f(0,1) 0.5
$$

where $y(0)=1$ and the slope estimate at $x=0$ is

$$
f(0,1)=-2(0)^{3}+12(0)^{2}-20(0)+8.5=8.5
$$

Therefore,

$$
y(0.5)=1.0+8.5(0.5)=5.25
$$

The true solution at $x=0.5$ is

$$
y=-0.5(0.5)^{4}+4(0.5)^{3}-10(0.5)^{2}+8.5(0.5)+1=3.21875
$$

Thus, the error is

$$
E_{t}=\text { true }- \text { approximate }=3.21875-5.25=-2.03125
$$

or, expressed as percent relative error, $\varepsilon_{t}=-63.1 \%$. For the second step,

$$
\begin{aligned}
y(1) & =y(0.5)+f(0.5,5.25) 0.5 \\
& =5.25+\left[-2(0.5)^{3}+12(0.5)^{2}-20(0.5)+8.5\right] 0.5 \\
& =5.875
\end{aligned}
$$

The true solution at $x=1.0$ is 3.0 , and therefore, the percent relative error is $-95.8 \%$. The computation is repeated, and the results are compiled in Table 25.1 and Fig. 25.3.

TABLE 25.1 Comparison of true and approximate values of the integral of $y^{\prime}=-2 x^{3}+12 x^{2}-20 x+8.5$, with the initial condition that $y=1$ at $x=0$. The approximate values were computed using Euler's method with a step size of 0.5 . The local error refers to the error incurred over a single step. It is calculated with a Taylor series expansion as in Example 25.2. The global error is the total discrepancy due to past as well as present steps.

|  |  |  | Percent Relative Error |  |
| :---: | :---: | :---: | :---: | ---: |
| $\boldsymbol{x}$ | $\boldsymbol{y}$ true | $\boldsymbol{y}$ Euler | Global | Local |
| 0.0 | 1.00000 | 1.00000 |  |  |
| 0.5 | 3.21875 | 5.25000 | -63.1 | -63.1 |
| 1.0 | 3.00000 | 5.87500 | -95.8 | -28.1 |
| 1.5 | 2.21875 | 5.12500 | -131.0 | -1.4 |
| 2.0 | 2.00000 | 4.50000 | -125.0 | 20.3 |
| 2.5 | 2.71875 | 4.75000 | -74.7 | 17.2 |
| 3.0 | 4.00000 | 5.87500 | -46.9 | 3.9 |
| 3.5 | 4.71875 | 7.12500 | -51.0 | -11.3 |
| 4.0 | 3.00000 | 7.00000 | -133.3 | -53.1 |



## FIGURE 25.3

Comparison of the true solution with a numerical solution using Euler's method for the integral of $y^{\prime}=-2 x^{3}+12 x^{2}-20 x+8.5$ from $x=0$ to $x=4$ with a step size of 0.5 . The initial condition at $x=0$ is $y=1$.

## PARTIAL DIFFERENTIAL <br> EQUATION:

Finite Difference: Elliptic Equations

Elliptic equations in engineering are typically used to characterize steady-state, boundary value problems. Before demonstrating how they can be solved, we will illustrate how a simple case-the Laplace equation-is derived from a physical problem context.

Laplace's equation

From the equation above, $k\left(\frac{\partial^{2} T}{\partial x^{2}}+\frac{\partial^{2} T}{\partial y^{2}}\right)=\frac{\partial T}{\partial t}$ it is clear that if the heat flow is steady, i.e. time independent, then $\frac{\partial T}{\partial t}=0$ so the temperature satisfies the equation

$$
\frac{\partial^{2} T}{\partial x^{2}}+\frac{\partial^{2} T}{\partial y^{2}}=0
$$

This gives us the two-dimensional Laplace equation

$$
\frac{\partial^{2} V}{\partial x^{2}}+\frac{\partial^{2} V}{\partial y^{2}}=0 \quad \text { used to model equilibrium situations. }
$$

Laplace's equation arises in
$>$ Electrostatics ( $V$ being the electrostatic potential in a free charge region)
$>$ Gravitation ( $V$ being the gravitational potential in free space)
$>$ Steady state flow of inviscid fluids
$>$ Steady state heat conduction
We can also have a three-dimensional version of Laplace's equation, and a polar coordinate form when
 we consider circular sheets.
There are other important partial differential equations in science and engineering, such as Poisson's equation, Helmholtz's equation, Schrödinger's equation and Tranverse vibrations equation.

We will look at some solutions to the Wave, Heat Conduction and Laplace's equations.
Examples
Show that $f=x^{2}-y^{2}$ satisfies Laplace's equation

$$
\begin{array}{ll}
\frac{\partial f}{\partial x}=2 x & \frac{\partial f}{\partial y}=-2 y \\
\frac{\partial^{2} f}{\partial x^{2}}=2 & \frac{\partial^{2} f}{\partial y^{2}}=-2
\end{array}
$$

Laplace's equation is $\frac{\partial^{2} f}{\partial x^{2}}+\frac{\partial^{2} f}{\partial y^{2}}=0$
here

$$
\frac{\partial^{2} f}{\partial x^{2}}+\frac{\partial^{2} f}{\partial y^{2}}=2-2 \quad=0
$$

hence, $\quad f=x^{2}-y^{2}$ satisfies Laplace's equation
ii) Show that $f=3 x^{2} y-y^{3}$ satisfies Laplace's equation

$$
\begin{array}{lr}
\frac{\partial f}{\partial x}=6 x y & \frac{\partial f}{\partial y}=3 x^{2}-3 y^{2} \\
\frac{\partial^{2} f}{\partial x^{2}}=6 y & \frac{\partial^{2} f}{\partial y^{2}}=-6 y \\
\frac{\partial^{2} f}{\partial x^{2}}+\frac{\partial^{2} f}{\partial y^{2}} & =6 y-6 y=0
\end{array}
$$

hence
hence, $f=3 x^{2} y-y^{3}$ satisfies Laplace's equation
iii) Show that $f=\ln \left(x^{2}+y^{2}\right)$ satisfies Laplace's equation

$$
\begin{array}{ll}
\frac{\partial f}{\partial x}=\frac{2 x}{x^{2}+y^{2}} & \frac{\partial f}{\partial y}=\frac{2 y}{x^{2}+y^{2}} \\
\frac{\partial^{2} f}{\partial x^{2}}=\frac{\left(x^{2}+y^{2}\right) 2-2 x \times 2 x}{\left(x^{2}+y^{2}\right)^{2}} & =\frac{2 y^{2}-2 x^{2}}{\left(x^{2}+y^{2}\right)^{2}}
\end{array}
$$

$$
\begin{aligned}
& \frac{\partial^{2} f}{\partial x^{2}}=\frac{\left(x^{2}+y^{2}\right) 2-2 x \times 2 x}{\left(x^{2}+y^{2}\right)^{2}}=\frac{2 y^{2}-2 x^{2}}{\left(x^{2}+y^{2}\right)^{2}} \\
& \frac{\partial^{2} f}{\partial y^{2}}=\frac{\left(x^{2}+y^{2}\right) 2-2 y \times 2 y}{\left(x^{2}+y^{2}\right)^{2}}=\frac{2 x^{2}-2 y^{2}}{\left(x^{2}+y^{2}\right)^{2}}
\end{aligned}
$$

hence $\quad \frac{\partial^{2} f}{\partial x^{2}}+\frac{\partial^{2} f}{\partial y^{2}}=0$

## hence, $\quad f$ satisfies Laplace's equation

above functions are said to be solutions of Laplace's equation.
iv) Show that $f=\sin 2 x \cos 3 t$ satisfies the wave equation $\frac{\partial^{2} f}{\partial x^{2}}=\frac{1}{c^{2}} \frac{\partial^{2} f}{\partial t^{2}}$ if $\quad c= \pm \frac{3}{2}$

$$
\begin{aligned}
& \qquad \frac{\partial f}{\partial x}=2 \cos 2 x \cos 3 t \\
& \frac{\partial^{2} f}{\partial x^{2}}=-4 \sin 2 x \cos 3 t \quad \frac{\partial f}{\partial t}=-3 \sin 2 x \sin 3 t \\
& \text { therefore, if } \quad \frac{\partial^{2} f}{\partial t^{2}}=-9 \sin 2 x \cos 3 t \\
& \frac{\partial^{2} f}{\partial x^{2}}=\frac{1}{c^{2}} \frac{\partial^{2} f}{\partial t^{2}} \\
& -4 \sin 2 x \cos 3 t=\frac{1}{c^{2}}(-9 \sin 2 x \cos 3 t) \\
& 4
\end{aligned}
$$

v) The temperature gradient $T$ at a point in a solid is $T=e^{-4 t} \sin 2 x$. Show that T satisfies the heat conduction equation with $k=1$.

$$
\begin{array}{r}
\frac{\partial T}{\partial t}=-4 e^{-4 t} \sin 2 x \quad \frac{\partial T}{\partial x}=2 e^{-4 t} \cos 2 x \\
\frac{\partial^{2} T}{\partial x^{2}}=-4 e^{-4 t} \sin 2 x
\end{array}
$$

therefore, if

$$
\begin{aligned}
& \frac{\partial^{2} T}{\partial x^{2}}=k \frac{\partial T}{\partial t} \\
& -4 e^{-4 t} \sin 2 x=k\left(-4 e^{-4 t} \sin 2 x\right)
\end{aligned}
$$

which is true when $k=1$

This represents a bar at end $x=0$, the temperature varies along the bar, decaying exponentially with $t$.
vi) Consider $y^{2} \frac{\partial^{L} f}{\partial x^{2}}+\frac{1}{y} \frac{\partial f}{\partial y}-\frac{\partial^{L} f}{\partial y^{2}}=0$.

Show that $f=4 x^{3}+3 x y^{4}$ satisfies this equation.

$$
\begin{array}{ll}
\frac{\partial f}{\partial x}=12 x^{2}+3 y^{4} & \frac{\partial f}{\partial y}=12 x y^{3} \\
\frac{\partial^{2} f}{\partial x^{2}}=24 x & \frac{\partial^{2} f}{\partial y^{2}}=36 x y^{2} \\
y^{2} \frac{\partial^{2} f}{\partial x^{2}}+\frac{1}{y} \frac{\partial f}{\partial y}-\frac{\partial^{2} f}{\partial y^{2}} & =y^{2}(24 x)+\frac{1}{y}\left(12 x y^{3}\right)-36 x y^{2} \\
& =24 x y^{2}+12 x y^{2}-36 x y^{2}=0 \text { as required }
\end{array}
$$

therefore the given function $f$ satisfies this equation
vii) If $f=x^{4}+a x^{2} y^{2}+b y^{4}$ where $a$ and $b$ are constants, show that $x \frac{\partial f}{\partial x}+y \frac{\partial f}{\partial y}=4 f$

$$
\frac{\partial f}{\partial x}=4 x^{3}+2 a x y^{2} \quad \frac{\partial f}{\partial y}=2 a x^{2} y+4 b y^{3}
$$

therefore

$$
\begin{aligned}
x \frac{\partial f}{\partial x}+y \frac{\partial f}{\partial y}=4 x^{4} & +2 a x^{2} y^{2}+2 a x^{2} y^{2}+4 b y^{4} \\
& =4\left(x^{4}+a x^{2} y^{2}+b y^{4}\right) \\
& =4 f \quad \text { as required }
\end{aligned}
$$

viii) For $f=x^{4}+a x^{2} y^{2}+b y^{4}$, find the constants $a$ and $b$ so that $f$ satisfies Laplace's equation.

$$
\frac{\partial f}{\partial x}=4 x^{3}+2 a x y^{2} \quad \frac{\partial f}{\partial y}=2 a x^{2} y+4 b y^{3}
$$

so

$$
\frac{\partial^{2} f}{\partial x^{2}}=12 x^{2}+2 a y^{2} \quad \frac{\partial^{2} f}{\partial y^{2}}=2 a x^{2}+12 b y^{2}
$$

using Laplace's equation $\frac{\partial^{2} f}{\partial x^{2}}+\frac{\partial^{2} f}{\partial y^{2}}=12 x^{2}+2 a y^{2}+2 a x^{2}+12 b y^{2}$

$$
=x^{2}(12+2 a)+y^{2}(2 a+12 b)
$$

this will be equal to zero when

$$
12+2 a=0 \quad a=-6
$$

and $\quad 2 a+12 b=0 \quad b=1$
so $\quad \underline{\underline{f=x^{4}}-6 x^{2} y^{2}+y^{4}} \underline{\underline{\text { satisfies Laplace's equation }}}$
ix) If $u=(1+x) \sinh (5 x-2 y)$ verify that $4 \frac{\partial^{2} u}{\partial x^{2}}+20 \frac{\partial^{2} u}{\partial x \partial y}+25 \frac{\partial^{2} u}{\partial y^{2}}=0$

$$
\begin{aligned}
& \frac{\partial u}{\partial x}=\sinh (5 x-2 y)+5(1+x) \cosh (5 x-2 y) \\
& \frac{\partial^{2} u}{\partial x^{2}}=5 \cosh (5 x-2 y)+5 \cosh (5 x-2 y)+25(1+x) \sinh (5 x-2 y) \\
& =10 \cosh (5 x-2 y)+25(1+x) \sinh (5 x-2 y)
\end{aligned}
$$

$$
\begin{aligned}
& \frac{\partial u}{\partial y}=-2(1+x) \cosh (5 x-2 y) \\
& \frac{\partial^{2} u}{\partial x \partial y}=-2 \cosh (5 x-2 y)-10(1+x) \sinh (5 x-2 y) \\
& \frac{\partial^{2} u}{\partial y^{2}}=4(1+x) \sinh (5 x-2 y) \\
& 4 \frac{\partial^{2} u}{\partial x^{2}}+20 \frac{\partial^{2} u}{\partial x \partial y}+25 \frac{\partial^{2} u}{\partial y^{2}}
\end{aligned}
$$

therefore

$$
\begin{array}{cc}
=40 \cosh (5 x-2 y) & +100(1+x) \sinh (5 x-2 y) \\
-40 \cosh (5 x-2 y) & -200(1+x) \sinh (5 x-2 y) \\
& +100(1+x) \sinh (5 x-2 y) \\
=0 & \text { as required }
\end{array}
$$

## Lecture: Round-off Error:

## Definition and Examples

Summary: There are two sources of error - one comes from approximating numbers and another from approximating mathematical procedures. In this lecture, the error, round-off error, that is a result of approximating numbers is defined and shown through an example.

Learning Objectives: After this lecture, you will be able to identify and calculate one of the two sources of errors in numerical methods - round-off errors.

## SOURCE OF ERROR: Round-off Error

In this segment we're going to talk about round-off errors. There are several possibilities of error whenever you're going to use numerical methods, but we want to concentrate here on just two errors, one is the round-off error and the other is the truncation error.
So those are the sources of error which we are going to talk about, because those are the ones which are coming from something on which you may or may not have as much control as other errors, like for example if you have made a mistake in programming, or if your logic is wrong, those are not the kind of errors which we are talking about when we talk about numerical methods.
So you're going to have two sources of error, which you are going to have. One is round-off error and the other one is called truncation error. And let's go ahead and concentrate on what round-off error is.


Now round-off error is defined as follows, it is basically the error which comes from error created due to approximate representation of numbers. So the round-off error is simply the error created by the approximate representation of numbers, because in a computer you'll be able to only represent a number only so approximately. For example, if you have a number like 1 divided by 3 , and you had a
six significant digit computer let's suppose in the decimal notation, then this can be only approximated as 0.333333 a simple rational number like 1 divided by 3 cannot be written exactly in the decimal format. So the amount of round-off error which you are getting here is the difference between the value of 1 divided by 3 and the value of 0.333333 . So in this case, this error is 0.0000003333 and so on and so forth.
You're going to get similar round-off errors from other numbers also, like, you may have pi, that also cannot be represented exactly, even in a decimal format, and then square root of 2 , things like that.
So you're finding out there are many, many numbers, individual numbers, like 1 divided by 3 , or pi, or square root of 2 , which cannot be represented exactly in a computer.
So that's why this creates the round-off error, the round-off error is the difference between what you want to, what you want to be able to approximate, of what you want to be able to denote, and what you are able to get as its approximation. So that's the, that's what we call as round-off error. So that's the end of this particular segment here.

## Truncation Error: Definition

Summary: There are two sources of error - one comes from approximating numbers and another from approximating mathematical procedures. In this lecture, the error, called truncation error, that is a result of approximating mathematical procedures is defined.

Learning Objectives: After this lecture, you will be able to identify and calculate one of the two sources of errors in numerical methods - truncation errors.

In this segment we're going to talk about truncation error. I want to say that we have sources of error in numerical methods. And we're not talking about the errors which are created by writing the wrong program, so far as logic or syntax is concerned, but the errors which are inherent when you are using numerical methods, and one is called the round-off error, and the other one is called the truncation error. So in this segment we're going to talk about, what does it mean when we say that, hey, we are having a truncation error? So let's go ahead and write down the definite of truncation error.
Truncation error is defined as the error created by truncating a mathematical procedure

Now, some people don't like the word truncating in the definition of truncation error itself, because they say that it doesn't mean much. So I'm going to cross it off there, and I'm going to say, hey, approximating a mathematical procedure. So if you're going to approximate a mathematical procedure, it is going to create some error, and that error is associated with truncation error. Please don't think that truncation error is something which is associated with rounding off numbers. It is, truncation error is related to the error which is created by approximating, not numbers, but a mathematical procedure. Examples of truncation error as follows, so let's look at some examples. In this segment I'm just going to enumerate the examples, and then we will have three more segments, which will show each individual example with some numbers.


One of the examples is, let's suppose you are using Maclaurin series. The Maclaurin series for e to the power $x$ is 1 plus $x$ plus $x$ squared by factorial 2 plus $x$ cubed by factorial 3 , and plus so on and so forth.

So you have infinite number of terms in this particular series for e to the power $x$. So if you want to calculate e to the power $x$ at some value of $x$, let's suppose. And let's suppose if somebody says, hey, calculate e to the power 0.5 , so I would say 1 plus 0.5 plus 0.5 squared divided by 2 factorial plus 0.5 cubed, factorial 3, and so on and so forth. Now you can realize that since there are infinite terms in this Maclaurin series to calculate e to the power 0.5 , I don't have the privilege or the luxury to use all the terms, all the infinite number of terms which I have in that particular series. If somebody were to say, hey, I'm going to use only the first three terms of the series to calculate my value of e to the power 0.5.


So what's happening is that you are not accounting for these other infinite terms after the fourth term, you're not accounting for those terms at all in your calculation e to the power 0.5 , and whatever is leftover is your truncation error. Because what you did was, the original mathematical procedure required you to use infinite number of terms, but you are using only three terms, so whatever is leftover is truncation error, because you have basically truncated a procedure, a mathematical procedure requiring you to use infinite number of terms, and you're using only a few terms out of that . . . out of that series there. Now what happens is that, in the past, I used to give only this as an example of truncation error, and many students would think that truncation error is something which is only related to series. But there are other examples where you will see how a mathematical procedure gets truncated. So let's look at that.

For both types, the relationship between the exact, or true, result and the approximation can be formulated as

$$
\begin{equation*}
\text { True value }=\text { approximation }+ \text { error } \tag{3.1}
\end{equation*}
$$

By rearranging Eq. (3.1), we find that the numerical error is equal to the discrepancy between the truth and the approximation, as in

$$
\begin{equation*}
E_{t}=\text { true value }- \text { approximation } \tag{3.2}
\end{equation*}
$$

$$
\text { True fractional relative error }=\frac{\text { true error }}{\text { true value }}
$$

where, as specified by Eq. (3.2), error $=$ true value - approximation. The relative error can also be multiplied by 100 percent to express it as

$$
\begin{equation*}
\varepsilon_{t}=\frac{\text { true error }}{\text { true value }} 100 \% \tag{3.3}
\end{equation*}
$$

where $\varepsilon_{t}$ designates the true percent relative error.

## Calculation of Errors

Problem Statement. Suppose that you have the task of measuring the lengths of a bridge and a rivet and come up with 9999 and 9 cm , respectively. If the true values are 10,000 and 10 cm , respectively, compute (a) the true error and (b) the true percent relative error for each case.
Solution.
(a) The error for measuring the bridge is [Eq. (3.2)]
$E_{t}=10,000-9999=1 \mathrm{~cm}$

## and for the rivet it is

$$
E_{t}=10-9=1 \mathrm{~cm}
$$

## (b) The percent relative error for the bridge is [Eq. (3.3)]

$$
\varepsilon_{t}=\frac{1}{10,000} 100 \%=0.01 \%
$$

and for the rivet it is

$$
\varepsilon_{t}=\frac{1}{10} 100 \%=10 \%
$$

Notice that for Eqs. (3.2) and (3.3), E and e are subscripted with a to signify that the error is normalized to the true value. In Example 3.1, we were provided with this value. However, in actual situations such information is rarely available. For numerical methods, the true value will be known only when we deal with functions that can be solved analytically. Such will typically be the case when we investigate the theoretical behavior of a particular technique for simple systems. However, in real-world applications, we will obviously not know the true answer a priori. For these situations, an alternative is to normalize the error using the best available estimate of the true value, that is, to the approximation itself, as in

$$
\begin{equation*}
\varepsilon_{a}=\frac{\text { approximate error }}{\text { approximation }} 100 \% \tag{3.4}
\end{equation*}
$$

where the subscript a signifi es that the error is normalized to an approximate value. Note also that for real-world applications, Eq. (3.2) cannot be used to calculate the error term for Eq. (3.4). One of the challenges of numerical methods is to determine error estimates in the absence of knowledge regarding the true value. For example, certain numerical methods use an iterative approach to compute answers. In such an approach, a present approximation is made on the basis of a previous approximation. This process is performed repeatedly, or iteratively, to successively compute (we hope) better and better approximations. For such cases, the error is often estimated as the difference between previous and current approximations. Thus, percent relative error is determined according to

$$
\begin{equation*}
\varepsilon_{a}=\frac{\text { current approximation }- \text { previous approximation }}{\text { current approximation }} 100 \% \tag{3.5}
\end{equation*}
$$

## Error Estimates for Iterative Methods

Problem Statement. In mathematics, functions can often be represented by infinite series. For example, the exponential function can be computed using

$$
\begin{equation*}
e^{x}=1+x+\frac{x^{2}}{2}+\frac{x^{3}}{3!}+\cdots+\frac{x^{n}}{n!} \tag{E3.2.1}
\end{equation*}
$$

Thus, as more terms are added in sequence, the approximation becomes a better and better estimate of the true value of $e^{x}$. Equation (E3.2.1) is called a Maclaurin series expansion.

Starting with the simplest version, $e^{x}=1$, add terms one at a time to estimate $e^{0.5}$. After each new term is added, compute the true and approximate percent relative errors with Eqs. (3.3) and (3.5), respectively. Note that the true value is $e^{0.5}=1.648721 \ldots$. Add terms until the absolute value of the approximate error estimate $\varepsilon_{a}$ falls below a prespecified error criterion $\varepsilon_{s}$ conforming to three significant figures.
Solution. First, Eq. (3.7) can be employed to determine the error criterion that ensures a result is correct to at least three significant figures:

$$
\varepsilon_{s}=\left(0.5 \times 10^{2-3}\right) \%=0.05 \%
$$

Thus, we will add terms to the series until $\varepsilon_{a}$ falls below this level.
The first estimate is simply equal to Eq. (E3.2.1) with a single term. Thus, the first estimate is equal to 1 . The second estimate is then generated by adding the second term, as in

$$
e^{x}=1+x
$$

or for $x=0.5$,

$$
e^{0.5}=1+0.5=1.5
$$

This represents a true percent relative error of [Eq. (3.3)]

$$
\varepsilon_{t}=\frac{1.648721-1.5}{1.648721} 100 \%=9.02 \%
$$

Equation (3.5) can be used to determine an approximate estimate of the error, as in

$$
\varepsilon_{a}=\frac{1.5-1}{1.5} 100 \%=33.3 \%
$$

Because $\varepsilon_{a}$ is not less than the required value of $\varepsilon_{s}$, we would continue the computation by adding another term, $x^{2} / 2$ !, and repeating the error calculations. The process is continued until $\varepsilon_{a}<\varepsilon_{s}$. The entire computation can be summarized as

| Terms | Result | $\boldsymbol{\varepsilon}_{\boldsymbol{q}}(\%)$ | $\boldsymbol{\varepsilon}_{\boldsymbol{a}}(\%)$ |
| :---: | :--- | :---: | :---: |
| 1 | 1 | 39.3 |  |
| 2 | 1.5 | 9.02 | 33.3 |
| 3 | 1.625 | 1.44 | 7.69 |
| 4 | 1.645833333 | 0.175 | 1.27 |
| 5 | 1.648437500 | 0.0172 | 0.158 |
| 6 | 1.648697917 | 0.00142 | 0.0158 |

## Matrices Part I

1. Introduction and definitions
2. Special matrices
3. Addition and subtraction of matrices
4. Multiplication of a matrix by a number
5. Multiplication of two matrices together

## 1. Introduction and definitions

A matrix is a set of numbers arranged in rows $\longleftrightarrow$ and columns to form a rectangle, and enclosed in brackets ( ).

Note: 1 matrix, 2 matrices
For example $\left(\begin{array}{lll}5 & 7 & 2 \\ 6 & 3 & 8\end{array}\right) \longleftrightarrow$ rows
$\downarrow$ columns
This matrix has 2 rows and 3 columns, this is a $2 \times 3$ matrix (we say 2 by 3 matrix)
the $5,7,2,6,3,8$ are elements of the matrix.
$\left(\begin{array}{lll}2 & 5 & 9\end{array}\right)$ is a row matrix of order $1 \times 3$
$\left(\begin{array}{l}2 \\ 4 \\ 7\end{array}\right) \quad$ is a column vector of order $3 \times 1$

We can refer to each element of the matrix by its position within the matrix. That is, by its row number and column number

$$
\left(\begin{array}{lll}
a_{11} & a_{12} & a_{13} \\
a_{21} & a_{22} & a_{23} \\
a_{31} & a_{32} & a_{33}
\end{array}\right) \quad \begin{gathered}
\\
\end{gathered}
$$

We usually identify matrices by a capital letter, so for example

$$
A=\left(\begin{array}{ll}
2 & 5 \\
-1 & 0.6 \\
4 & 3
\end{array}\right) \quad \text { The order (or size) of this matrix is } 3 \times 2
$$

## 2. Special matrices

a) A matrix that has the same number of rows as columns is a square matrix

For example

$$
B=\left(\begin{array}{lrr}
4 & -1.5 & 2.6 \\
7.3 & -9.1 & 4.2 \\
0.3 & 2.5 & -9.2
\end{array}\right)
$$

b) A matrix that only has values on the "leading diagonal" is a diagonal matrix, (all other elements are equal to 0 )

For example

$$
C=\left(\begin{array}{rrr}
4 & 0 & 0 \\
0 & -9.1 & 0 \\
0 & 0 & -9.2
\end{array}\right)
$$

c) A matrix that only has the value 1 on the "leading diagonal" is the identity matrix, (all other elements are 0 )

For example

$$
I=\left(\begin{array}{lll}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{array}\right)
$$

We call this matrix $I$
d) A matrix is lower triangular if $a_{i j}=0$ for $i<j$

$$
D=\left(\begin{array}{lll}
1 & 0 & 0 \\
2 & 3 & 0 \\
-1 & 4 & -2
\end{array}\right)
$$

and is upper triangular if $a_{i j}=0$ for $i>j$

$$
E=\left(\begin{array}{rrr}
1 & 5 & -7 \\
0 & 3 & 2 \\
0 & 0 & -2
\end{array}\right)
$$

e) The zero or null matrix has all elements equal to zero.

$$
N=\left(\begin{array}{lll}
0 & 0 & 0 \\
0 & 0 & 0
\end{array}\right)
$$

f) The transpose of an $m \times n$ matrix A is the $n \times m$ matrix $\mathrm{A}^{\mathrm{T}}$ with the $(i, j)^{t h}$ element of $\left(a^{T}\right)_{i j}=a_{j i}$ (i.e. the rows and columns are interchanged).
So if $A=\left(\begin{array}{lllll}1 & -2 & 1 & 0 & 3 \\ 2 & 3 & 1 & 2 & -1 \\ -1 & 4 & -2 & 1 & -2 \\ -3 & 1 & 1 & -1 & 3 \\ 0 & -1 & 1 & -2 & 4\end{array}\right)$ then $A^{T}=\left(\begin{array}{lllll}1 & 2 & -1 & -3 & 0 \\ -2 & 3 & 4 & 1 & -1 \\ 1 & 1 & -2 & 1 & 1 \\ 0 & 2 & 1 & -1 & -2 \\ 3 & -1 & -2 & 3 & 4\end{array}\right)$
The transpose of a row matrix is a column matrix and vice-versa.
The transpose of the transpose of a matrix is the original matrix i.e. $\left(A^{T}\right)^{T}=A$
g) If the square matrix $A$ is equal to its transpose i.e. $A=A^{T}$ then A is symmetric.

$$
A=\left(\begin{array}{lllll}
1 & -2 & 1 & 0 & 3 \\
-2 & 3 & 4 & 1 & -1 \\
1 & 4 & -2 & 1 & -4 \\
0 & 1 & 1 & -1 & -2 \\
3 & -1 & -4 & -2 & 4
\end{array}\right)=A^{T}
$$

h) Two matrices are said to be equal if each of the corresponding elements of the two matrices are equal

$$
\left(\begin{array}{lll}
a_{11} & a_{12} & a_{13} \\
a_{21} & a_{22} & a_{23}
\end{array}\right)=\left(\begin{array}{lll}
5 & 7 & 8 \\
2 & 3 & 6
\end{array}\right) \text { implies } a_{11}=5 \text { etc. }
$$

## 3. Addition and subtraction of matrices

Two (or more) matrices can only be added or subtracted if they are the same size (that is, they have the same number of rows and the same number of columns). We add or subtract the corresponding elements.

Examples
a) $\left(\begin{array}{lll}4 & 2 & 3 \\ 5 & 7 & 6\end{array}\right)+\left(\begin{array}{rrr}1 & 8 & 9 \\ 3 & 0.5 & -4\end{array}\right)$

$$
\begin{aligned}
& =\left(\begin{array}{lll}
4+1 & & 2+8 \\
5+3 & & 7+0.5
\end{array}\right. \\
& =\left(\begin{array}{lll}
5 & 10 & 12 \\
8 & 7.5 & 2
\end{array}\right)
\end{aligned}
$$

b) $\left(\begin{array}{ll}6 & 5 \\ 9 & -4 \\ 2.5 & -3.2\end{array}\right)-\left(\begin{array}{cc}3 & 7 \\ 1 & 2.3 \\ -4.2 & -2.1\end{array}\right)=\left(\begin{array}{lc}6-3 & 5-7 \\ 9-1 & -4-2.3 \\ 2.5+4.2 & -3.2+2.1\end{array}\right)$

$$
=\left(\begin{array}{ll}
3 & -2 \\
8 & -6.3 \\
6.7 & -1.1
\end{array}\right)
$$

c) If $A=\left(\begin{array}{cc}6 & 1 \\ 3 & 2 \\ 0 & -0.5\end{array}\right), B=\left(\begin{array}{ll}2 & -1 \\ 9 & -3 \\ 4 & 0\end{array}\right) \quad$ and $C=\left(\begin{array}{ll}2 & 1 \\ 5 & 9\end{array}\right)$
find (i) $A+B$
(ii) $B+C$
(iii) $B-A$
(i) $A+B=\left(\begin{array}{cc}6 & 1 \\ 3 & 2 \\ 0 & -0.5\end{array}\right)+\left(\begin{array}{ll}2 & -1 \\ 9 & -3 \\ 4 & 0\end{array}\right) \quad=\xlongequal{\left(\begin{array}{ll}8 & 0 \\ 12 & -1 \\ 4 & -0.5\end{array}\right)}$
(ii) $\quad B+C$ not possible
(iii) $\quad B-A=\left(\begin{array}{ll}2 & -1 \\ 9 & -3 \\ 4 & 0\end{array}\right)-\left(\begin{array}{cc}6 & 1 \\ 3 & 2 \\ 0 & -0.5\end{array}\right)=\left(\begin{array}{rr}-4 & -2 \\ 6 & -5 \\ 4 & 0.5\end{array}\right)$

## 4. Multiplication of a matrix by a number

We can multiply a matrix by a single number (a scalar). Each individual element of the matrix is multiplied by the number,

$$
\text { so if } \begin{aligned}
A & =\left(\begin{array}{ll}
6 & 1 \\
3 & 2 \\
0 & -0.5
\end{array}\right) \text { and } B=\left(\begin{array}{ll}
2 & -1 \\
9 & -3 \\
4 & 0
\end{array}\right) \\
4 A & =\left(\begin{array}{ll}
4 \times 6 & 4 \times 1 \\
4 \times 3 & 4 \times 2 \\
4 \times 0 & 4 \times-0.5
\end{array}\right)
\end{aligned}
$$

$$
\text { and } \quad \frac{1}{2} B=\left(\begin{array}{ll}
\frac{1}{2} \times 2 & \frac{1}{2} \times-1 \\
\frac{1}{2} \times 9 & \frac{1}{2} \times-3 \\
\frac{1}{2} \times 4 & \frac{1}{2} \times 0
\end{array}\right)=\left(\begin{array}{cc}
1 & -0.5 \\
4.5 & -1.5 \\
2 & 0
\end{array}\right)
$$

$$
\text { then } \quad 4 A+\frac{1}{2} B=\left(\begin{array}{lr}
24 & 4 \\
12 & 8 \\
0 & -2
\end{array}\right)+\left(\begin{array}{lr}
1 & -0.5 \\
4.5 & -1.5 \\
2 & 0
\end{array}\right)
$$

$$
=\underline{\left(\begin{array}{cc}
25 & 3.5 \\
16.5 & 6.5 \\
2 & -2
\end{array}\right)}
$$

We now have the properties

Commutative law:
Associative law:
Distributive law:

$$
A+B=B+A
$$

$$
(A+B)+C=A+(B+C)
$$

$$
\lambda(A+B)=\lambda A+\lambda B
$$

These show we can treat matrices as if they are 'number' as far as addition and multiplication by a scalar are concerned.
They are not numbers however, and the differences start to appear when we try to multiply two matrices together.

## 5. Multiplication of two matrices together

This can only be done if the number of columns in the first matrix is the same as the number of rows in the second matrix.
That is; $C=A \times B$ is only possible if the number of columns in $A$ is the same as the number of rows in matrix $B$. Then,
the number of rows in $C=$ number of rows in $A$
number of columns in $C=$ number of columns in $B$
so if $A$ is a $p \times q$ matrix and $B$ is a $q \times s$ matrix, $C$ is a $p \times s$ matrix.
i.e. $(p \times q) \times(q \times s) \rightarrow(p \times s)$ matrix

## Examples

a) Find $A B$ if $A=\left(\begin{array}{ll}1 & 4 \\ 6 & 3\end{array}\right)$ and $B=\binom{2}{5}$

$$
\begin{align*}
A B & =\left(\begin{array}{ll}
1 & 4 \\
6 & 3
\end{array}\right)\binom{2}{5} \\
& =\binom{1 \times 2+4 \times 5}{6 \times 2+3 \times 5} \tag{22}
\end{align*}
$$

Each element in a row in the first matrix is multiplied by the corresponding element in the column of the second matrix and the results summed to give a single value.
The position of this value in the resulting matrix corresponds to the row number from the first matrix and the column number from the second.
b) Find $C D$ where $C=\left(\begin{array}{lll}1 & 4 & 9 \\ 2 & 0 & 1\end{array}\right)$ and $D=\left(\begin{array}{rr}1 & 9 \\ 8 & 7 \\ -7 & 3\end{array}\right)$

$$
\begin{aligned}
C D= & =\left(\begin{array}{lll}
1 & 4 & 9 \\
2 & 0 & 1
\end{array}\right)\left(\begin{array}{rr}
1 & 9 \\
8 & 7 \\
-7 & 3
\end{array}\right) \\
& =\left(\begin{array}{ll}
1 \times 1+4 \times 8+9 \times-7 & 1 \times 9+4 \times 7+9 \times 3 \\
2 \times 1+0 \times 8+1 \times-7 & 2 \times 9+0 \times 7+1 \times 3
\end{array}\right) \\
& =\left(\begin{array}{ll}
-30 & 64 \\
-5 & 21
\end{array}\right)
\end{aligned}
$$

c) Find $S T$ where $S=\left(\begin{array}{rrr}2 & -1 & 1 \\ 0 & 1 & 3 \\ 4 & 2 & -1\end{array}\right)$ and $T=\left(\begin{array}{rr}2 & 1 \\ -1 & 3 \\ 1 & -1\end{array}\right)$

$$
\begin{aligned}
S T & =\left(\begin{array}{ccc}
2 & -1 & 1 \\
0 & 1 & 3 \\
4 & 2 & -1
\end{array}\right)\left(\begin{array}{rr}
2 & 1 \\
-1 & 3 \\
1 & -1
\end{array}\right) \\
& =\left(\begin{array}{cc}
2 \times 2+-1 \times-1+1 \times 1 & 2 \times 1+-1 \times 3+1 \times-1 \\
0 \times 2+ & 1 \times-1+3 \times 1 \\
4 \times 2+2 \times-1+-1 \times 1 & 0 \times 1+1 \times 3+3 \times-1 \\
4 \times 1+2 \times 3+-1 \times-1
\end{array}\right) \\
& =\left(\begin{array}{rr}
6 & -2 \\
2 & 0 \\
5 & 11
\end{array}\right)
\end{aligned}
$$

Note: TS is not possible
If we are given two matrices $A$ and $B$, and we can find both $A B$ and $B A$, in general $A B \neq B A$. In the case where $A B=B A$. , $A$ and $B$ are said to commute.
d) If $A=\left(\begin{array}{ll}2 & -1\end{array}\right), \quad B=\left(\begin{array}{lll}1 & 5 & -1 \\ 2 & 3 & -4\end{array}\right)$ and $C=\left(\begin{array}{l}1 \\ 3 \\ 2\end{array}\right)$

$$
\begin{aligned}
A(B C) & =\left(\begin{array}{ll}
2 & -1
\end{array}\right)\left(\begin{array}{lll}
1 & 5 & -1 \\
2 & 3 & -4
\end{array}\right)\left(\begin{array}{l}
1 \\
3 \\
2
\end{array}\right) \\
& =\left(\begin{array}{ll}
2 & -1
\end{array}\right)\binom{14}{3}
\end{aligned}
$$

and

$$
\begin{aligned}
& (A B) C=\left(\begin{array}{ll}
2 & -1
\end{array}\right)\left(\begin{array}{lll}
1 & 5 & -1 \\
2 & 3 & -4
\end{array}\right)\left(\begin{array}{l}
1 \\
3 \\
2
\end{array}\right) \\
& =\left(\begin{array}{lll}
0 & 7 & 2
\end{array}\right)\left(\begin{array}{l}
1 \\
3 \\
2
\end{array}\right)
\end{aligned}
$$

We now have the properties
Commutative law:
Matrices do not usually commute, i.e. $A B \neq B A$
Associative law:

$$
A(B C)=(A B) C
$$

Distributive law (over scalar multiplication): $\quad \lambda(A B)=(\lambda A) B=A(\lambda B)$
Distributive law (over addition):

$$
A(B+C)=A B+A C
$$

Multiplication by a unit matrix:

$$
I A=A=A I
$$

Transpose of a product:
$(A B)^{T}=B^{T} A^{T}$

Transpose of a sum:
$(A+B)^{T}=A^{T}+B^{T}$

## Matrices Part II

6. Transformation of matrices
7. The inverse of a $2 \times 2$ matrix
8. The determinant of a $2 \times 2$ matrix
9. Applications of matrices to solving two simultaneous equations
10. The determinant of a $3 \times 3$ matrix, cofactors, minors and adjoint
11. Properties of determinants
12. Inverse of a $3 \times 3$ Matrix

## 6. Transformations of a matrix




If for every point $Q(u, v)$ in the $u-v$ plane there is a corresponding point $P(x, y)$ in the $x-y$ plane, then there is a relationship between the two sets of co-ordinates.
In the simple case of scaling the co-ordinate where $u=a x$ and $v=b y$ we have a linear transformation which we can write in matrix from as

$$
\binom{u}{v}=\left(\begin{array}{ll}
a & 0 \\
0 & b
\end{array}\right)\binom{x}{y}
$$

The matrix $\left(\begin{array}{ll}a & 0 \\ 0 & b\end{array}\right)$ then provides the transformation between the vector $\binom{x}{y}$ (representing the point $(x, y))$ in one set of co-ordinates and the vector $\binom{u}{v}$ (representing the point $\left.(u, v)\right)$ in the other set of co-ordinates.

## Examples

1. Consider the square with vertices at $(0,0),(1,0),(1,1)$ and $(0,1)$, and the matrix $\mathrm{A}=\left(\begin{array}{ll}a_{11} & a_{12} \\ a_{21} & a_{22}\end{array}\right)$. Then using matrix multiplication the vertices are transformed to;

$$
\left.\begin{array}{ll} 
& \left(\begin{array}{ll}
a_{11} & a_{12} \\
a_{21} & a_{22}
\end{array}\right)\binom{0}{0}=\binom{0}{0} \\
& \left(\begin{array}{ll}
a_{11} & a_{12} \\
a_{21} & a_{22}
\end{array}\right)\binom{1}{0}=\binom{a_{11}}{a_{21}} \\
& \left(\begin{array}{ll}
a_{11} & a_{12} \\
a_{21} & a_{22}
\end{array}\right)\binom{1}{1}=\binom{a_{11}+a_{12}}{a_{21}+a_{22}} \\
\text { and } \quad & \left(\begin{array}{ll}
a_{11} & a_{12} \\
a_{21} & a_{22}
\end{array}\right)
\end{array}\right)\binom{0}{1}=\binom{a_{12}}{a_{22}} . ~ \$
$$

The 'new square' is defined by the points

$$
(0,0),\left(a_{11}, a_{21}\right),\left(a_{11}+a_{12}, a_{21}+a_{22}\right) \text { and }\left(a_{12}, a_{22}\right)
$$

2. A square has vertices at $(0,0),(1,0),(1,1)$ and $(0,1)$, and is transformed by the following matrices. Determine the positions of the new vertices in each case.
i) $\quad \mathrm{A}=\left(\begin{array}{ll}3 & 0 \\ 0 & \frac{1}{2}\end{array}\right)$

By matrix multiplication $\quad\left(\begin{array}{ll}3 & 0 \\ 0 & \frac{1}{2}\end{array}\right)\binom{0}{0}=\binom{0}{0}$

$$
\begin{aligned}
\left(\begin{array}{ll}
3 & 0 \\
0 & \frac{1}{2}
\end{array}\right)\binom{1}{0}=\binom{3}{0} \\
\left(\begin{array}{ll}
3 & 0 \\
0 & \frac{1}{2}
\end{array}\right)\binom{1}{1}=\binom{3}{\frac{1}{2}} \\
\text { and } \quad\left(\begin{array}{ll}
3 & 0 \\
0 & \frac{1}{2}
\end{array}\right)\binom{0}{1}=\binom{0}{\frac{1}{2}} .
\end{aligned}
$$



The vertices are at

$$
(0,0),(3,0),\left(3, \frac{1}{2}\right) \text { and }\left(0, \frac{1}{2}\right)
$$

ii) $\quad \mathrm{A}=\frac{1}{\sqrt{2}}\left(\begin{array}{cc}1 & -1 \\ 1 & 1\end{array}\right)$

By matrix multiplication $\quad \frac{1}{\sqrt{2}}\left(\begin{array}{cc}1 & -1 \\ 1 & 1\end{array}\right)\binom{0}{0}=\binom{0}{0}$

$$
\frac{1}{\sqrt{2}}\left(\begin{array}{cc}
1 & -1 \\
1 & 1
\end{array}\right)\binom{1}{0}=\binom{\frac{1}{\sqrt{2}}}{\frac{1}{\sqrt{2}}}
$$

$$
\frac{1}{\sqrt{2}}\left(\begin{array}{cc}
1 & -1 \\
1 & 1
\end{array}\right)\binom{1}{1}=\binom{0}{\sqrt{2}}
$$

and


The vertices are at

$$
\underline{(0,0),\left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right),(0, \sqrt{2}) \xlongequal{\text { and }}\left(-\frac{1}{\sqrt{2}}, \sqrt{2}\right)}
$$

## 7. The inverse of a matrix

Let $A$ be a square $n \times n$ matrix. Then $B$ is the inverse of $A$ if it satisfies the equations

$$
A B=I=B A,
$$ where $I$ is the Identity matrix.

If so, then $B$ is denoted as $A^{-1}$.
$A^{-1}$ is called the inverse of $A$ and we have the equation $A A^{-1}=I=A^{-1} A$
We use the inverse of a matrix for division. Note: the inverse of a matrix does not always exist!

## Example

Verify that if $A=\left(\begin{array}{cr}2 & -1 \\ -1 & 1\end{array}\right)$ then its inverse is $A^{-1}=\left(\begin{array}{ll}1 & 1 \\ 1 & 2\end{array}\right)$.
Using $A A^{-1}=I$

$$
\left(\begin{array}{lr}
2 & -1 \\
-1 & 1
\end{array}\right)\left(\begin{array}{ll}
1 & 1 \\
1 & 2
\end{array}\right)=\left(\begin{array}{ll}
1 & 0 \\
0 & 1
\end{array}\right) \text { as required }
$$

and

$$
A^{-1} A=I
$$

$$
\left(\begin{array}{ll}
1 & 1 \\
1 & 2
\end{array}\right)\left(\begin{array}{lr}
2 & -1 \\
-1 & 1
\end{array}\right)=\left(\begin{array}{ll}
1 & 0 \\
0 & 1
\end{array}\right) \text { as required. }
$$

We use the inverse of a matrix to solve a set of linear equations $A x=b$.
Then, if $A^{-1}$ exists, the solution is given by $x=A^{-1} b$

To find the inverse of a $2 \times 2$ matrix

If $A=\left(\begin{array}{ll}a & b \\ c & d\end{array}\right)$, then $A^{-1}=\frac{1}{a d-b c}\left(\begin{array}{lr}d & -b \\ -c & a\end{array}\right)$

```
Step 1: work out ad - bc
Step 2: swap elements on leading diagonal
Step 3: change signs of other elements
Step 4: multiply by }\frac{1}{ad-bc
```


## Example

Find the inverse of $A=\left(\begin{array}{rr}6 & 5 \\ -2 & 3\end{array}\right)$ and show that $A A^{-1}=A^{-1} A=I$.

Step 1: $a d-b c \quad=18+10 \quad=28$
Step2: swap $\quad\left(\begin{array}{rr}3 & 5 \\ -2 & 6\end{array}\right)$
Step 3: $\quad$ signs $\quad\left(\begin{array}{rr}3 & -5 \\ 2 & 6\end{array}\right)$
Step 4: multiply $\quad A^{-1}=\frac{1}{28}\left(\begin{array}{lr}3 & -5 \\ 2 & 6\end{array}\right)$

Check:

$$
\begin{aligned}
& A A^{-1}=\frac{1}{28}\left(\begin{array}{rr}
6 & 5 \\
-2 & 3
\end{array}\right)\left(\begin{array}{rr}
3 & -5 \\
2 & 6
\end{array}\right) \\
& =\frac{1}{28}\left(\begin{array}{rr}
6 \times 3+5 \times 2 & 6 \times-5+5 \times 6 \\
-2 \times 3+3 \times 2 & -2 \times-5+3 \times 6
\end{array}\right) \\
& =\frac{1}{28}\left(\begin{array}{ll}
28 & 0 \\
0 & 28
\end{array}\right) \\
& =\left(\begin{array}{ll}
1 & 0 \\
0 & 1
\end{array}\right) \quad \text { the identity matrix } \\
& A^{-1} A=\frac{1}{28}\left(\begin{array}{rr}
3 & -5 \\
2 & 6
\end{array}\right)\left(\begin{array}{rr}
6 & 5 \\
-2 & 3
\end{array}\right) \\
& =\frac{1}{28}\left(\begin{array}{ll}
3 \times 6+(-5 \times-2) & 3 \times 5+(-5 \times 3) \\
2 \times 6+6 \times-2 & 2 \times 5+6 \times 3
\end{array}\right) \\
& =\frac{1}{28}\left(\begin{array}{ll}
28 & 0 \\
0 & 28
\end{array}\right) \\
& =\left(\begin{array}{ll}
1 & 0 \\
0 & 1
\end{array}\right) \quad \text { the identity matrix }
\end{aligned}
$$

## 8. The determinant of a $2 \times 2$ matrix

The quantity $a d-b c$ is called the determinant of the matrix $A$, the notation is $|A|$.

If $A=\left(\begin{array}{ll}a & b \\ c & d\end{array}\right)$ then $|A|=\left|\begin{array}{ll}a & b \\ c & d\end{array}\right| \quad=a d-b c$
Sometimes, the determinant $|A|$ of the matrix $A$ is equal to zero.
Then $A$ is called a singular matrix and it does not have an inverse.

## 9. Applications of matrices to solving two simultaneous equations

a) Applying Kirchoff's law to a circuit gives the following equations

$$
\begin{aligned}
30 i_{1}-10 i_{2} & =12 \\
-10 i_{1}+35 i_{2} & =5 \text { where } i_{1} \text { and } i_{2} \text { represent current. }
\end{aligned}
$$

Solve the equations for $i_{1}$ and $i_{2}$.
First write equations as matrices

$$
\left(\begin{array}{lr}
30 & -10 \\
-10 & 35
\end{array}\right)\binom{i_{1}}{i_{2}}=\binom{12}{5}
$$

or

$$
A X=B
$$

where

$$
A=\left(\begin{array}{rr}
30 & -10 \\
-10 & 35
\end{array}\right), \quad X=\binom{i_{1}}{i_{2}} \quad \text { and } B=\binom{12}{5}
$$

We want to find

$$
X=\binom{i_{1}}{i_{2}} \quad \text { to solve our equations. }
$$

Now if
Then
but
so
$A X=B$ and we can find the inverse matrix $A^{-1}$
$A^{-1} A X=A^{-1} B$
$A^{-1} A=I$
$X=A^{-1} B$

That is, to solve for $X$ we
find the inverse matrix $A^{-1}$ and multiply it by matrix $B$.
In this example, $\quad A=\left(\begin{array}{rr}30 & -10 \\ -10 & 35\end{array}\right)$,
So

$$
|A|=30 \times 35-(-10) \times(-10)=950
$$

So

$$
A^{-1}=\frac{1}{950}\left(\begin{array}{cc}
35 & 10 \\
10 & 30
\end{array}\right) \quad=\frac{1}{190}\left(\begin{array}{ll}
7 & 2 \\
2 & 6
\end{array}\right)
$$

then

$$
\begin{aligned}
X=A^{-1} B & =\frac{1}{190}\left(\begin{array}{ll}
7 & 2 \\
2 & 6
\end{array}\right)\binom{12}{5} \\
& =\frac{1}{190}\binom{84+10}{24+30} \\
& =\binom{0.495}{0.284}
\end{aligned}
$$

The solution to the simultaneous equations is $i_{1}=0.495, \quad i_{2}=0.284$
b) Solve the simultaneous equations

$$
\begin{aligned}
& 5.2 x-0.3 y=12.66 \\
& 2.1 \boldsymbol{x}+1.6 \boldsymbol{y}=4.08
\end{aligned}
$$

First write equations as matrices

$$
\begin{array}{ll} 
& \left(\begin{array}{rr}
5.2 & -0.3 \\
2.1 & 1.6
\end{array}\right)\binom{x}{y}=\binom{12.66}{4.08} \\
\text { or } & A X=B \\
\text { Here, } & A=\left(\begin{array}{rr}
5.2 & -0.3 \\
2.1 & 1.6
\end{array}\right), \\
\text { so } & |A|=5.2 \times 1.6-2.1 \times(-0.3)=8.95 \\
\text { So } & A^{-1}=\frac{1}{8.95}\left(\begin{array}{rr}
1.6 & 0.3 \\
-2.1 & 5.2
\end{array}\right)
\end{array}
$$

then

$$
\begin{aligned}
X=A^{-1} B & =\frac{1}{8.95}\left(\begin{array}{rr}
1.6 & 0.3 \\
-2.1 & 5.2
\end{array}\right)\binom{12.66}{4.08} \\
& =\frac{1}{8.95}\binom{20.256+1.224}{-26.586+21.216} \\
& =\frac{1}{8.95}\binom{21.48}{-5.37} \\
& =\binom{2.4}{-0.6}
\end{aligned}
$$

The solution to the simultaneous equations is $x=2.4$, $y=-0.6$
10. The Determinant of a $3 \times 3$ matrix, minors, cofactors and adjoint

For a $3 \times 3$ matrix where $A=\left(\begin{array}{lll}a_{1} & b_{1} & c_{1} \\ a_{2} & b_{2} & c_{2} \\ a_{3} & b_{3} & c_{3}\end{array}\right)$
The determinant is defined as
or $\quad|A|=a_{1}\left|\begin{array}{ll}b_{2} & c_{2} \\ b_{3} & c_{3}\end{array}\right|-b_{1}\left|\begin{array}{ll}a_{2} & c_{2} \\ a_{3} & c_{3}\end{array}\right|+c_{1}\left|\begin{array}{ll}a_{2} & b_{2} \\ a_{3} & b_{3}\end{array}\right|$
Example

$$
\text { if } \begin{aligned}
A=\left(\begin{array}{ccc}
6 & 3 & -2 \\
2 & 1 & 5 \\
7 & 4 & -4
\end{array}\right) \quad \text { then }|A| & =6\left|\begin{array}{cc}
1 & 5 \\
4 & -4
\end{array}\right|-3\left|\begin{array}{cc}
2 & 5 \\
7 & -4
\end{array}\right|+(-2)\left|\begin{array}{ll}
2 & 1 \\
7 & 4
\end{array}\right| \\
& \xlongequal{=-17}
\end{aligned}
$$

## The Minor of a $3 \times 3$ matrix

The $\left|\begin{array}{ll}b_{2} & c_{2} \\ b_{3} & c_{3}\end{array}\right|$ is the minor for $a_{1}$
and the minor for $a_{2}$ is $\left|\begin{array}{ll}b_{1} & c_{1} \\ b_{3} & c_{3}\end{array}\right|$
that is, the row and column containing the element are ignored and the $2 \times 2$ determinant of the remaining rows and columns is calculated.

## Cofactors of a $3 \times 3$ matrix

Associated with each minor is a sign $\left(\begin{array}{lll}+ & - & + \\ - & + & - \\ + & - & +\end{array}\right)$
A minor together with its associated sign is called the cofactor

The cofactor of $a_{2}$ is denoted by $A_{2}$

$$
\text { where } A_{2}=-\left|\begin{array}{ll}
b_{1} & c_{1} \\
b_{3} & c_{3}
\end{array}\right|
$$

Thus we can define the determinant of $A$ as $a_{1} A_{1}+b_{1} B_{1}+c_{1} C_{1}$

## Adjoint of a square matrix

To form the Adjoint of a matrix, it is the transpose of the matrix of cofactors.
Step1: Form a new matrix $C$ of the cofactors
e.g. $A=\left(\begin{array}{ccc}4 & 2 & -1 \\ 7 & 8 & -2 \\ 4 & -1 & 5\end{array}\right)$ then
$C=\left(\begin{array}{rlr}\left|\begin{array}{rr}8 & -2 \\ -1 & 5\end{array}\right| & -\left|\begin{array}{rr}7 & -2 \\ 4 & 5\end{array}\right| & \left|\begin{array}{rr}7 & 8 \\ 4 & -1\end{array}\right| \\ -\left|\begin{array}{rr}2 & -1 \\ -1 & 5\end{array}\right| & -\left|\begin{array}{rr}4 & -1 \\ 4 & 5\end{array}\right| & -\left|\begin{array}{rr}4 & 2 \\ 4 & -1\end{array}\right| \\ \left|\begin{array}{rr}2 & -1 \\ 8 & -2\end{array}\right| & -\left|\begin{array}{rr}4 & -1 \\ 7 & -2\end{array}\right| & \left|\begin{array}{rrr}4 & 2 \\ 7 & 8\end{array}\right|\end{array}\right)=\left(\begin{array}{rrr}38 & -43 & -39 \\ -9 & 24 & 12 \\ 4 & 1 & 18\end{array}\right)$

Step 2: form the transpose of C
$C^{T}=\left(\begin{array}{ccc}38 & -9 & 4 \\ -43 & 24 & 1 \\ -39 & 12 & 18\end{array}\right)$ this is called the Adjoint denoted by adjA
Remember $\quad \operatorname{adj} A=C^{T}$

## 11. Properties of determinants include:

For the $n \times n$ matrices $A$ and $B$
$>\quad$ if $A$ is diagonal or triangular, then $|A|=a_{11} a_{22} a_{33} a_{44} \ldots a_{n n}$.
That is, the determinant is the product of the elements on the diagonal.
$>\quad|A B|=|A| \times|B|$
$>\quad|A|=\left|A^{T}\right|$
$>\quad|\lambda A|=\lambda^{n}|A|$
There are several properties which help to simplify finding the determinant of a matrix
$>\quad$ If two rows or columns are equal, or proportional, then the determinant $=0$.
$>$ Multiplying a row, or a column, by a scalar multiplies the determinant by that scalar.
$>$ Interchanging two rows, or columns, changes the sign of the determinant.
$>$ Adding multiples of a row to another row does not change the value of the determinant.
$>$ Adding multiples of a column to another column does not change the value of the determinant.

## Examples

1) Find the value of the determinant of $A=\left(\begin{array}{cccc}1 & 2 & -2 & 4 \\ 0 & -1 & 3 & 6 \\ 0 & 2 & 1 & 4 \\ 0 & 0 & 0 & 3\end{array}\right)$

$$
\begin{aligned}
|A|=\left|\begin{array}{cccc}
1 & 2 & -2 & 4 \\
0 & -1 & 3 & 6 \\
0 & 2 & 1 & 4 \\
0 & 0 & 0 & 3
\end{array}\right| & =1 \times\left|\begin{array}{ccc}
-1 & 3 & 6 \\
2 & 1 & 4 \\
0 & 0 & 3
\end{array}\right| \\
& =-1 \times\left|\begin{array}{ll}
1 & 4 \\
0 & 3
\end{array}\right|-3 \times\left|\begin{array}{cc}
2 & 4 \\
0 & 3
\end{array}\right|+6 \times\left|\begin{array}{cc}
2 & 1 \\
0 & 0
\end{array}\right| \\
& =-1 \times 3-3 \times 6+6 \times 0 \quad=-21
\end{aligned}
$$

2) Find the value of the determinant of $B=\left(\begin{array}{cccc}1 & 2 & 5 & 4 \\ 1 & -1 & 5 & 6 \\ 1 & 2 & 5 & 4 \\ 1 & 0 & 5 & 3\end{array}\right)$

Here, $|B|=0 \quad$ because row 3 is equal to row 1
(or also because column 3 is a multiple of column 1)

## 12. Inverse of a $3 \times 3$ Matrix

For a $3 \times 3$ matrix $A$ its inverse $A^{-1}=\frac{1}{|A|} \times C^{T}$

To find the inverse of a matrix $A^{-1}$
Step 1: Calculate the determinant $|A|$
Step 2: Form a new matrix $C$ of the cofactors
Step 3: Form the transpose of $C$, the adjoint of $A$
Step 4: Use $A^{-1}=\frac{1}{|A|} \times C^{T}$

Example if $A=\left(\begin{array}{ccc}6 & 3 & -2 \\ 2 & 1 & 5 \\ 7 & 4 & -4\end{array}\right)$ then

$$
\begin{aligned}
&|A|=6(-4-20)-3(-8-35)-2(8-7) \\
&=-17 \\
& C=\left(\begin{array}{ccc}
-24 & 43 & 1 \\
4 & -10 & -3 \\
17 & -34 & 0
\end{array}\right) \\
& C^{T}=\left(\begin{array}{ccc}
-24 & 4 & 17 \\
43 & -10 & -34 \\
1 & -3 & 0
\end{array}\right)
\end{aligned}
$$

$$
A^{-1}=-\frac{1}{17} \times\left(\begin{array}{ccc}
-24 & 4 & 17 \\
43 & -10 & -34 \\
1 & -3 & 0
\end{array}\right)
$$

$$
A^{-1} A=-\frac{1}{17} \times\left(\begin{array}{ccc}
-24 & 4 & 17 \\
43 & -10 & -34 \\
1 & -3 & 0
\end{array}\right)\left(\begin{array}{ccc}
6 & 3 & -2 \\
2 & 1 & 5 \\
7 & 4 & -4
\end{array}\right)
$$

$$
A^{-1} A=-\frac{1}{17} \times\left(\begin{array}{ccc}
-17 & 0 & 0 \\
0 & -17 & 0 \\
0 & 0 & -17
\end{array}\right)=\left(\begin{array}{lll}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{array}\right)
$$

## Curve Fitting Part I

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## Introduction to Curve Fitting

Introduction Historians attribute the phrase regression analysis to Sir Francis Galton (1822-1911), a British anthropologist and meteorologist, who used the term regression in an address that was published in Nature in 1885. Galton used the term while talking of his discovery that offspring of seeds "did not tend to resemble their parent seeds in size, but to be always more mediocre [i.e., more average] than they.... The experiments showed further that the mean filial regression towards mediocrity was directly proportional to the parental deviation from it." The content of Galton's paper would probably be called correlation analysis today, a term which he also coined. However, the term regression soon was applied to situations other than Galton's and it has been used ever since. Regression Analysis refers to the study of the relationship between a response (dependent) variable, Y , and one or more independent variables, the X's. When this relationship is reasonably approximated by a straight line, it is said to be linear, and we talk of linear regression. When the relationship follows a curve, we call it curvilinear regression. Usually, you assume that the independent variables are measured exactly (without random error) while the dependent variable is measured with random error. Frequently, this assumption is not completely true, but when it cannot be justified, a much more complicated fitting procedure is required. However, if the size of the measurement error in an independent variable is small relative to the range of values of that variable, least squares regression analysis may be used with legitimacy.

## Two types of curve fitting

- Least square regression

Given data for discrete values, derive a single curve that represents the general trend of the data.

- When the given data exhibit a significant degree of error or noise.

Given data for discrete values, fit a curve or a series of curves that pass directly through each of the points.

- When data are very precise.



## PART I: Least square regression

There are several models of this method:
Straight line, Polynomial model, Power model, Exponential model, Logarithmic model $\qquad$ etc.

1- $\quad$ Simple Linear Regression (straight line)
Fitting a straight line to a set of paired observations $\left(x_{1}, y_{1}\right),\left(x_{2}, y_{2}\right), \ldots,\left(x_{n}, y_{n}\right)$. Mathematical expression for the straight line (model)

$$
y=a_{0}+a_{1} x
$$

where $a_{0}$ is the intercept, and $a_{1}$ is the slope.
Define

$$
e_{i}=y_{i, \text { measured }}-y_{i, \text { model }}=y_{i}-\left(a_{0}+a_{1} x_{i}\right)
$$

Criterion for a best fit:

$$
\min S_{r}=\min _{a_{0}, a_{1}} \sum_{i=1}^{n} e_{i}^{2}=\min _{a_{0}, a_{1}} \sum_{i=1}^{n}\left(y_{i}-a_{0}-a_{1} x_{i}\right)^{2}
$$

Find $a_{0}$ and $a_{1}$ :

$$
\begin{align*}
& \frac{\partial S_{r}}{\partial a_{0}}=-2 \sum_{i=1}^{n}\left(y_{i}-a_{0}-a_{1} x_{i}\right)=0  \tag{1}\\
& \frac{\partial S_{r}}{\partial a_{1}}=-2 \sum_{i=1}^{n}\left[\left(y_{i}-a_{0}-a_{1} x_{i}\right) x_{i}\right]=0 \tag{2}
\end{align*}
$$

From (1), $\sum_{i=1}^{n} y_{i}-\sum_{i=1}^{n} a_{0}-\sum_{i=1}^{n} a_{1} x_{i}=0$, or

$$
\begin{equation*}
n a_{0}+\sum_{i=1}^{n} x_{i} a_{1}=\sum_{i=1}^{n} y_{i} \tag{3}
\end{equation*}
$$

From (2), $\sum_{i=1}^{n} x_{i} y_{i}-\sum_{i=1}^{n} a_{0} x_{i}-\sum_{i=1}^{n} a_{1} x_{i}^{2}=0$, or

$$
\begin{equation*}
\sum_{i=1}^{n} x_{i} a_{0}+\sum_{i=1}^{n} x_{i}^{2} a_{1}=\sum_{i=1}^{n} x_{i} y_{i} \tag{4}
\end{equation*}
$$

(3) and (4) are called normal equations.

From (3),

$$
a_{0}=\frac{1}{n} \sum_{i=1}^{n} y_{i}-\frac{1}{n} \sum_{i=1}^{n} x_{i} a_{1}=\bar{y}-\bar{x} a_{1}
$$

where $\bar{x}=\frac{1}{n} \sum_{i=1}^{n} x_{i}, \bar{y}=\frac{1}{n} \sum_{i=1}^{n} y_{i}$.
From (4), $\sum_{i=1}^{n} x_{i}\left(\frac{1}{n} \sum_{i=1}^{n} y_{i}-\frac{1}{n} \sum_{i=1}^{n} x_{i} a_{1}\right)+\sum_{i=1}^{n} x_{i}^{2} a_{1}=\sum_{i=1}^{n} x_{i} y_{i}$,

$$
a_{1}=\frac{\sum_{i=1}^{n} x_{i} y_{i}-\frac{1}{n} \sum_{i=1}^{n} x_{i} \sum_{i=1}^{n} y_{i}}{\sum_{i=1}^{n} x_{i}^{2}-\frac{1}{n}\left(\sum_{i=1}^{n} x_{i}\right)^{2}}
$$

or

$$
a_{1}=\frac{n \sum_{i=1}^{n} x_{i} y_{i}-\sum_{i=1}^{n} x_{i} \sum_{i=1}^{n} y_{i}}{n \sum_{i=1}^{n} x_{i}^{2}-\left(\sum_{i=1}^{n} x_{i}\right)^{2}}
$$

## Example:

| $x$ | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $y$ | 0.5 | 2.5 | 2.0 | 4.0 | 3.5 | 6.0 | 5.5 |

$\sum x_{i}=1+2+\ldots+7=28$
$\sum y_{i}=0.5+2.5+\ldots+5.5=24$
$\sum x_{i}^{2}=1^{2}+2^{2}+\ldots+7^{2}=140$
$\sum x_{i} y_{i}=1 \times 0.5+2 \times 2.5+\ldots+7 \times 5.5=119.5$
$a_{1}=\frac{n \sum_{i=1}^{n} x_{i} y_{i}-\sum_{i=1}^{n} x_{i} \sum_{i=1}^{n} y_{i}}{n \sum_{i=1}^{n} x_{i}^{2}-\left(\sum_{i=1}^{n} x_{i}\right)^{2}}=\frac{7 \times 119.5-28 \times 24}{7 \times 140-28^{2}}=0.8393$
$a_{0}=\bar{y}-\bar{x} a_{1}=\frac{1}{n} \sum y_{i}-a_{1} \frac{1}{n} \sum x_{i}=\frac{1}{7} \times 24-0.8393 \times \frac{1}{7} \times 28=0.07143$.
Model: $y=0.07143+0.8393 x$.

## Solution of a system of simultaneous equations:

Method 1: Matrix Method

Method 2: Cramer's Rule

## Method 3: Gaussian Elimination

## Method 1: Matrix Method

If $\quad A X=B \quad$ then $X=A^{-1} B \quad\left(\right.$ since $\left.A A^{-1}=I\right)$
To solve a system of simultaneous equations
Step 1: Write system in matrix form $A X=B$
Step 2: Find determinant $|A|$
Step 3: Find the matrix of co-factors $C$
Step 4: Transpose $C$ to give $C^{\mathrm{T}}$ (or the adjoint of $A$ )
Step 5: Find the inverse $A^{-1}$, using $A^{-1}=\frac{1}{|A|} \times C^{T}$
Step 6: Multiply $\quad A^{-1} B$ to give solution

When solving three simultaneous equations, we are finding the intersection (if it exists) of three planes.

## Example

1. Solve the system of simultaneous equations

$$
\begin{array}{ll}
3 x-y+4 z & =13 \\
5 x+y-3 z & =5 \\
x-y+z & =3
\end{array}
$$



Step 1: First, writing in matrix form $A X=B$

$$
\text { Here, }\left(\begin{array}{rrr}
3 & -1 & 4 \\
5 & 1 & -3 \\
1 & -1 & 1
\end{array}\right)\left(\begin{array}{l}
x \\
y \\
z
\end{array}\right)=\left(\begin{array}{r}
13 \\
5 \\
3
\end{array}\right)
$$

Step 2: Finding the determinant $|A|$

$$
A=\left(\begin{array}{rrr}
3 & -1 & 4 \\
5 & 1 & -3 \\
1 & -1 & 1
\end{array}\right)
$$

so

$$
\begin{aligned}
& |A|=3\left|\begin{array}{lr}
1 & -3 \\
-1 & 1
\end{array}\right|-(-1)\left|\begin{array}{rr}
5 & -3 \\
1 & 1
\end{array}\right|+4\left|\begin{array}{rr}
5 & 1 \\
1 & -1
\end{array}\right| \\
& |A|=3(1-3)+1(5+3)+4(-5-1) \\
& |A|=-22
\end{aligned}
$$

Step 3: Finding the matrix of co-factors $C$

$$
C=\left(\begin{array}{lll}
-2 & -8 & -6 \\
-3 & -1 & 2 \\
-1 & 29 & 8
\end{array}\right)
$$

Step 4: Transpose $C$ to give $C^{\mathrm{T}}$

$$
C^{T}=\left(\begin{array}{ccc}
-2 & -3 & -1 \\
-8 & -1 & 29 \\
-6 & 2 & 8
\end{array}\right)
$$

Step 5: Find inverse $A^{-1}$, using $A^{-1}=\frac{1}{|A|} \times C^{T}$

$$
A^{-1}=\frac{-1}{22}\left(\begin{array}{ccc}
-2 & -3 & -1 \\
-8 & -1 & 29 \\
-6 & 2 & 8
\end{array}\right)=\frac{1}{22}\left(\begin{array}{ccc}
2 & 3 & 1 \\
8 & 1 & -29 \\
6 & -2 & -8
\end{array}\right)
$$

Step 6: Multiply $A^{-1} B$ to give solution

$$
\begin{aligned}
& \left(\begin{array}{l}
x \\
y \\
z
\end{array}\right)=\frac{1}{22}\left(\begin{array}{lll}
2 & 3 & 1 \\
8 & 1 & -29 \\
6 & -2 & -8
\end{array}\right)\left(\begin{array}{r}
13 \\
5 \\
3
\end{array}\right) \\
& \left(\begin{array}{l}
x \\
y \\
z
\end{array}\right)=\left(\begin{array}{l}
2 \\
1 \\
2
\end{array}\right)
\end{aligned}
$$

## Method 2: Cramer's rule

Consider a system of two linear simultaneous equations,

$$
\begin{aligned}
& a_{1} x+b_{1} y=k_{1} \\
& a_{2} x+b_{2} y=k_{2}
\end{aligned}
$$

Cramer's rule states that

$$
x=\frac{\left|\begin{array}{ll}
k_{1} & b_{1} \\
k_{2} & b_{2}
\end{array}\right|}{\left|\begin{array}{ll}
a_{1} & b_{1} \\
a_{2} & b_{2}
\end{array}\right|}, \quad y=\frac{\left|\begin{array}{ll}
a_{1} & k_{1} \\
a_{2} & k_{2}
\end{array}\right|}{\left|\begin{array}{ll}
a_{1} & b_{1} \\
a_{2} & b_{2}
\end{array}\right|},
$$

## Example

Solve the simultaneous equations

By Cramer's rule

Cramer's rule can be extended to systems of linear equations with more than two unknowns.

$$
\begin{aligned}
& a_{1} x+b_{1} y+c_{1} z=k_{1} \\
& a_{2} x+b_{2} y+c_{2} z=k_{2} \\
& a_{3} x+b_{3} y+c_{3} z=k_{3}
\end{aligned}
$$

$$
\text { Consider } \quad a_{2} x+b_{2} y+c_{2} z=k_{2}
$$

Then Cramer's rule states that

$$
x=\frac{\left|\begin{array}{lll}
k_{1} & b_{1} & c_{1} \\
k_{2} & b_{2} & c_{2} \\
k_{3} & b_{3} & c_{3}
\end{array}\right|}{\left|\begin{array}{lll}
a_{1} & b_{1} & c_{1} \\
a_{2} & b_{2} & c_{2} \\
a_{3} & b_{3} & c_{3}
\end{array}\right|}, \quad y=\frac{\left|\begin{array}{lll}
a_{1} & k_{1} & c_{1} \\
a_{2} & k_{2} & c_{2} \\
a_{3} & k_{3} & c_{3}
\end{array}\right|}{\left|\begin{array}{lll}
a_{1} & b_{1} & c_{1} \\
a_{2} & b_{2} & c_{2} \\
a_{3} & b_{3} & c_{3}
\end{array}\right|}, \left.\quad z=\frac{\left|\begin{array}{lll}
a_{1} & b_{1} & k_{1} \\
a_{2} & b_{2} & k_{2} \\
a_{3} & b_{3} & k_{3}
\end{array}\right|}{\left|\begin{array}{lll}
a_{1} & b_{1} & c_{1} \\
a_{2} & b_{2} & c_{2} \\
a_{3} & b_{3} & c_{3}
\end{array}\right|} \right\rvert\,
$$

$$
\begin{aligned}
& x+y=3 \\
& 2 x+3 y=7 \\
& x=\frac{\left|\begin{array}{ll}
3 & 1 \\
7 & 3
\end{array}\right|}{\left|\begin{array}{ll}
1 & 1 \\
2 & 3
\end{array}\right|}, \\
& y=\frac{\left|\begin{array}{ll}
1 & 3 \\
2 & 7
\end{array}\right|}{\left|\begin{array}{ll}
1 & 1 \\
2 & 3
\end{array}\right|} \\
& x=\frac{9-7}{3-2}, \quad y=\frac{7-6}{3-2} \\
& x=2, \quad y=1
\end{aligned}
$$

Example
Solve the simultaneous equations

$$
\begin{aligned}
& x+2 y+z=2 \\
& 2 x-y-2 z=5 \\
& 2 x+2 y+3 z=7
\end{aligned}
$$

First, evaluate


$$
\begin{aligned}
&\left|\begin{array}{lll}
a_{1} & b_{1} & c_{1} \\
a_{2} & b_{2} & c_{2} \\
a_{3} & b_{3} & c_{3}
\end{array}\right|=\left|\begin{array}{ll}
1 & 2 \\
2 & 1 \\
2 & -1 \\
2 & 2
\end{array}\right| \\
&=1\left|\begin{array}{cc}
-1 & -2 \\
2 & 3
\end{array}\right|-2\left|\begin{array}{ll}
2 & -2 \\
2 & 3
\end{array}\right|+1\left|\begin{array}{ll}
2 & -1 \\
2 & 2
\end{array}\right| \\
&=1(-3+4)-2(6+4)+1(4+2) \\
&=1-20+6 \\
&=-13
\end{aligned}
$$

Now, find $x=\frac{\left|\begin{array}{lll}k_{1} & b_{1} & c_{1} \\ k_{2} & b_{2} & c_{2} \\ k_{3} & b_{3} & c_{3}\end{array}\right|}{\left|\begin{array}{llll}a_{1} & b_{1} & c_{1} \\ a_{2} & b_{2} & c_{2} \\ a_{3} & b_{3} & c_{3}\end{array}\right|}=\frac{\left|\begin{array}{lll}2 & 2 & 1 \\ 5 & -1 & -2 \\ 7 & 2 & 3\end{array}\right|}{-13}$
We want $\quad 2\left|\begin{array}{ll}-1 & -2 \\ 2 & 3\end{array}\right|-2\left|\begin{array}{cc}5 & -2 \\ 7 & 3\end{array}\right|+1\left|\begin{array}{ll}5 & -1 \\ 7 & 2\end{array}\right|$

$$
=2(-3+4)-2(15+14)+1(10+7)
$$

$$
=-39
$$

So

$$
x=\frac{-39}{-13} \quad \text { giving } \underline{\underline{x=3}}
$$

Second, find $y=\frac{\left|\begin{array}{lll}a_{1} & k_{1} & c_{1} \\ a_{2} & k_{2} & c_{2} \\ a_{3} & k_{3} & c_{3}\end{array}\right|}{\left|\begin{array}{llll}a_{1} & b_{1} & c_{1} \\ a_{2} & b_{2} & c_{2} \\ a_{3} & b_{3} & c_{3}\end{array}\right|}=\frac{\left|\begin{array}{lll}1 & 2 & 1 \\ 2 & 5 & -2 \\ 2 & 7 & 3\end{array}\right|}{-13}$

We want

$$
\begin{aligned}
& 1\left|\begin{array}{ll}
5 & -2 \\
7 & 3
\end{array}\right|-2\left|\begin{array}{cc}
2 & -2 \\
2 & 3
\end{array}\right|+1\left|\begin{array}{ll}
2 & 5 \\
2 & 7
\end{array}\right| \\
& =1(15+14)-2(6+4)+1(14-10) \\
& =13
\end{aligned}
$$

So $\quad y=\frac{13}{-13} \quad$ giving $\underline{\underline{y=-1}}$
Finally, find $z=\frac{\left|\begin{array}{lll}a_{1} & b_{1} & k_{1} \\ a_{2} & b_{2} & k_{2} \\ a_{3} & b_{3} & k_{3}\end{array}\right|}{\left|\begin{array}{llll}a_{1} & b_{1} & c_{1} \\ a_{2} & b_{2} & c_{2} \\ a_{3} & b_{3} & c_{3}\end{array}\right|}=\frac{\left|\begin{array}{lll}1 & 2 & 2 \\ 2 & -1 & 5 \\ 2 & 2 & 7\end{array}\right|}{-13}$
We want $\quad 1\left|\begin{array}{ll}-1 & 5 \\ 2 & 7\end{array}\right|-2\left|\begin{array}{ll}2 & 5 \\ 2 & 7\end{array}\right|+2\left|\begin{array}{ll}2 & -1 \\ 2 & 2\end{array}\right|$

$$
\begin{aligned}
& =1(-7-10)-2(14-10)+2(4+2) \\
& =-13
\end{aligned}
$$

So $\quad z=\frac{-13}{-13} \quad$ giving $\underline{\underline{z=1}}$

The solution to the simultaneous equations is

$$
x=3, y=-1, z=1
$$

Step 1 - form the augmented matrix
Step 2 - make all the first column values equal to zero, with the exception of one
Step 3 - make just two rows with a non zero value in the second column
Step 4 - interchange rows
Step 5 - detach the right hand column
Step 6 - back substitute, starting with bottom row


Carl Friedrich Gauss 1777 - 1855

German
Example
Solve the system of simultaneous equations

$$
\begin{array}{ll}
x+y+2 z & =9 \\
4 x+4 y-3 z & =3 \\
5 x+y+2 z & =13
\end{array}
$$

Step 1 - form the augmented matrix


$$
\left(\begin{array}{ccccc}
1 & 1 & 2 & : & 9 \\
4 & 4 & -3 & : & 3 \\
5 & 1 & 2 & : & 13
\end{array}\right)
$$

We want to reduce this matrix to one of the form

$$
\left(\begin{array}{llll}
a_{1} & 0 & 0 & d_{1} \\
0 & b_{2} & 0 & d_{2} \\
0 & 0 & c_{3} & d_{3}
\end{array}\right)
$$

Step 2 - make all the first column values equal to zero, with the exception of one Here, subtract 5 times row 1 from row 3, giving

$$
\left(\begin{array}{ccccc}
1 & 1 & 2 & : & 9 \\
4 & 4 & -3 & : & 3 \\
0 & -4 & -8 & : & -32
\end{array}\right)
$$

and, subtract 4 times row 1 from row 2, giving

$$
\left(\begin{array}{ccccc}
1 & 1 & 2 & : & 9 \\
0 & 0 & -11 & : & -33 \\
0 & -4 & -8 & : & -32
\end{array}\right)
$$

Step 3 - interchange rows 2 and 3

$$
\left(\begin{array}{ccccc}
1 & 1 & 2 & : & 9 \\
0 & -4 & -8 & : & -32 \\
0 & 0 & -11 & : & -33
\end{array}\right)
$$

Step 4 - divide row 3 by -11

$$
\left(\begin{array}{ccccc}
1 & 1 & 2 & : & 9 \\
0 & -4 & -8 & : & -32 \\
0 & 0 & 1 & : & 3
\end{array}\right)
$$

Step 5 - add 8 times row 3 to row 2

$$
\left(\begin{array}{ccccc}
1 & 1 & 2 & : & 9 \\
0 & -4 & 0 & : & -8 \\
0 & 0 & 1 & : & 3
\end{array}\right)
$$

Step 6 - divide row 2 by -4

$$
\left(\begin{array}{lllll}
1 & 1 & 2 & : & 9 \\
0 & 1 & 0 & : & 2 \\
0 & 0 & 1 & : & 3
\end{array}\right)
$$

Step 7 - subtract row 2 from row 1

$$
\left(\begin{array}{lllll}
1 & 0 & 2 & : & 7 \\
0 & 1 & 0 & : & 2 \\
0 & 0 & 1 & : & 3
\end{array}\right)
$$

Step 8 - subtract 2 times row 3 from row 1

$$
\left(\begin{array}{lllll}
1 & 0 & 0 & : & 1 \\
0 & 1 & 0 & : & 2 \\
0 & 0 & 1 & : & 3
\end{array}\right)
$$

The solution to the simultaneous equations is

$$
x=1, y=2, z=3
$$

