## NUMERICAL DIFFERENTIATION \& INTEGRATION

## Numerical Differentiation

## 1- Using Taylor Series

## -First derivatives

Our aim is to approximate the slope of a curve $f$ at a particular point $x=a$ in terms of $f$ (a) and the value of $f$ at a nearby point where $x=a+h$.

$f^{\prime}(a) \approx$ slope of short broken line $=\frac{\text { difference in the } y \text {-values }}{\text { difference in the } x \text {-values }}=\frac{f(a+h)-f(a)}{h}$.

This is called a forward difference approximation to the derivative of $f$.

A second version of this arises on considering a point to the left of a, rather than to the right as we did above. In this case we obtain the approximation

$$
f^{\prime}(a) \approx \frac{f(a)-f(a-h)}{h}
$$

This is another difference, called a backward difference, approximation to $f^{\prime}(a)$.
A third method for approximating the first derivative of $f$ can be seen in the next diagram

$f^{\prime}(a) \approx$ slope of short broken line $=\frac{\text { difference in the } y \text {-values }}{\text { difference in the } x \text {-values }}=\frac{f(x+h)-f(x-h)}{2 h}$

This is called a central difference approximation to $f^{\prime \prime}(\mathbf{a})$.
In practice, the central difference formula is the most accurate.

## RELATIVE ERROR

$$
\left|\epsilon_{t}\right|=\left|\frac{\text { exact solution }- \text { numerical solution }}{\text { exact solution }}\right| \times 100 \%
$$

## Example

Use a forward difference, and the values of $h$ shown, to approximate the derivative of $\cos (x)$ at $x=\pi / 3$.
(a) $\mathrm{h}=0.1$, (b) $\mathrm{h}=0.0001$

$$
\begin{aligned}
& f^{\prime}(a) \approx \frac{\cos (a+h)-\cos (a)}{h}=\frac{0.41104381-0.5}{0.1}=-0.88956192 \\
& f^{\prime}(a) \approx \frac{\cos (a+h)-\cos (a)}{h}=\frac{0.49991339-0.5}{0.0001}=-0.86605040
\end{aligned}
$$

## H.W.

Let $\mathrm{f}(\mathrm{x})=\ln (\mathrm{x})$ and $\mathrm{a}=3$. Using both a forward and a central difference, and working to 8 decimal places, approximate $\mathrm{f}^{\prime}$ (a) using $\mathrm{h}=0.1$ and $\mathrm{h}=0.01$.

## Example

The distance $x$ of a runner from a fixed point is measured (in meters) at intervals of half a second. The data obtained is

| $t$ | 0.0 | 0.5 | 1.0 | 1.5 | 2.0 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $x$ | 0.00 | 3.65 | 6.80 | 9.90 | 12.15 |

Use central differences to approximate the runner's velocity at times $t=0.5 \mathrm{~s}$, and $\mathrm{t}=1.25 \mathrm{~s}$.

## Solution

Our aim here is to approximate $x^{\prime}(t)$. The choice of $h$ is dictated by the available data. Using data with $t=0.5 \mathrm{~s}$ at its centre we obtain

$$
x^{\prime}(0.5) \approx \frac{x(1.0)-x(0.0)}{2 \times 0.5}=6.80 \mathrm{~m} / \mathrm{s}
$$

Data centred at $t=1.25 \mathrm{~s}$ gives us the approximation

$$
x^{\prime}(1.25) \approx \frac{x(1.5)-x(1.0)}{2 \times 0.25}=6.20 \mathrm{~m} / \mathrm{s}
$$

Note the value of $h$ used.
H.W.

The velocity v (in $\mathrm{m} / \mathrm{s}$ ) of a rocket measured at half second intervals is

| $t$ | 0.0 | 0.5 | 1.0 | 1.5 | 2.0 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $v$ | 0.000 | 11.860 | 26.335 | 41.075 | 59.051 |

Use central differences to approximate the acceleration of the rocket at times $t=1.0 \mathrm{~s}$ and $\mathrm{t}=$ 1.75 s .

## Second derivatives

A central difference approximation to the second derivative $f "(a)$ is:

$$
f^{\prime \prime}(a) \approx \frac{f(a+h)-2 f(a)+f(a-h)}{h^{2}}
$$

## Example

The distance x of a runner from a fixed point is measured (in meters) at intervals of half a second. The data obtained is

| $t$ | 0.0 | 0.5 | 1.0 | 1.5 | 2.0 |
| :---: | :---: | :---: | :---: | :---: | :---: |
| $x$ | 0.00 | 3.65 | 6.80 | 9.90 | 12.15 |

Use a central difference to approximate the runner's acceleration at time $\mathrm{t}=1.5 \mathrm{~s}$.

Using data with $t=1.5 \mathrm{~s}$ at its centre we obtain

$$
x^{\prime \prime}(1.5) \approx \frac{x(2.0)-2 x(1.5)+x(1.0)}{0.5^{2}}=-3.40 \mathrm{~m} / \mathrm{s}^{2}
$$

from which we see that the runner is slowing down.

## H.W.

The distance $x$, measured in meters, of a downhill skier from a fixed point is measured at intervals of 0.25 s . The data gathered is

| $t$ | 0 | 0.25 | 0.5 | 0.75 | 1 | 1.25 | 1.5 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $x$ | 0 | 4.3 | 10.2 | 17.2 | 26.2 | 33.1 | 39.1 |

Use a central difference to approximate the skier's velocity and acceleration at the times $\mathrm{t}=0.25 \mathrm{~s}, 0.75 \mathrm{~s}$ and 1.25 s . Give your answers to 1 decimal place.

## 2- Using Newton's Forward Difference Formula

$$
\begin{aligned}
f(x) \approx P_{n}(x)= & f\left(x_{0}\right)+s \Delta f\left(x_{0}\right)+\frac{s(s-1)}{2!} \Delta^{2} f\left(x_{0}\right)+\frac{s(s-1)(s-2)}{3!} \Delta^{3} f\left(x_{0}\right) \\
& \ldots \frac{s(s-1)(s-2) \cdots(s-n+1)}{n!} \Delta^{n} f\left(x_{0}\right)
\end{aligned}
$$

where

$$
x=x_{0}+s h
$$

We use $p_{n}(x)$ to calculate the derivatives of $f$.

That is $f^{\prime}(x) \simeq p_{n}^{\prime}(x)$ for all $x \in\left[x_{0}, x_{n}\right]$.

For a given $x$,

$$
\begin{gathered}
f^{\prime}(x) \simeq p_{n}^{\prime}(x) \\
=\frac{d p_{n} d s}{d s} \frac{d s}{d x} \\
=\frac{1}{h} \frac{d p_{n}}{d s}
\end{gathered}
$$

Similarly,

$$
\begin{aligned}
& f^{\prime \prime}(x) \simeq \frac{d^{2} p_{n}}{d x^{2}} \\
& \quad \frac{d}{d x}\left(\frac{d p_{n}}{d x}\right) \\
& =\frac{d}{d x}\left(\frac{d p_{n}}{d s} \frac{d s}{d x}\right) \\
& =\frac{1}{h} \frac{d}{d x}\left(\frac{d p_{n}}{d s}\right)
\end{aligned}
$$

$$
\begin{gathered}
=\frac{1}{h}\left(\frac{d^{2} p_{n}}{d s^{2}} \frac{1}{h}\right) \\
=\frac{1}{h^{2}} \frac{d^{2} p_{n}}{d s^{2}}
\end{gathered}
$$

## Thus in general,

$$
f^{(k)}(x)=\frac{1}{h^{k}} \frac{d^{k} p_{n}}{d s^{k}}
$$

## EXAMPLE

Using Taylor series expansion (forward formula) and Newton forward divided difference, compute first and second derivative at $\mathbf{x}=\mathbf{2}$ for the following tabulated function

| $x$ | 1 | 2 | 3 | 4 |
| :---: | :---: | :---: | :---: | :---: |
| $f(x)$ | 2 | 5 | 7 | 10 |

## SOLUTION

| $x$ | $f(x)$ | $\Delta$ | $\Delta^{2}$ | $\Delta^{3}$ |
| :---: | :---: | :---: | :---: | :---: |
| 1 | 2 |  |  |  |
| 2 | 5 |  | -1 |  |
| 3 | 7 |  | 1 |  |
| 4 | 10 |  |  |  |

Here $\mathrm{h}=1$
Using Taylor Series

$$
\begin{gathered}
f^{\prime}(2)=\frac{f(2+h)-f(2)}{h}=\frac{f(3)-f(2)}{1}=2 \\
f^{\prime \prime}(2)=\frac{f(2+h)-2 f(2)+f(2-h)}{h^{2}}=\frac{f(3)-2 f(2)+f(1)}{1}=-1
\end{gathered}
$$

Using Newton Forward Divided Difference Formula

$$
\mathrm{S}=\left(\mathrm{x}-\mathrm{x}_{\mathrm{o}}\right) / \mathrm{h}
$$

$$
\begin{aligned}
& f(x) \approx P_{n}(x)=f\left(x_{0}\right)+s \Delta f\left(x_{0}\right)+\frac{s(s-1)}{2!} \Delta^{2} f\left(x_{0}\right)+\frac{s(s-1)(s-2)}{3!} \Delta^{3} f\left(x_{0}\right) \\
& f^{\prime}(x) \approx \frac{1}{h} \frac{d p_{n}}{d s}=\frac{1}{h}\left[\Delta f\left(x_{0}\right)+\frac{2 s-1}{2!} \Delta^{2} f\left(x_{0}\right)+\frac{3 s^{2}-6 s+2}{3!} \Delta^{3} f\left(x_{0}\right)\right]
\end{aligned}
$$

Here $x=2, x_{0}=1, s=1$ and $h=1$

$$
\begin{gathered}
f^{\prime}(2)=3-\frac{1}{2}-\frac{1}{3}=13 / 6 \\
f^{\prime \prime}(x) \approx \frac{1}{h^{2}} \frac{d^{2} p_{n}}{d s^{2}}=\frac{1}{h^{2}}\left[\Delta^{2} f\left(x_{0}\right)+(s-1) \Delta^{3} f\left(x_{0}\right)\right] \\
f^{\prime \prime}(2)=-1
\end{gathered}
$$

H.W.

Calculate $f^{(4)}(0.15)$

| $x$ | 0.1 | 0.2 | 0.3 | 0.4 | 0.5 | 0.6 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $f(X)$ | 0.425 | 0.475 | 0.400 | 0.450 | 0.525 | 0.575 |

Newton's forward difference formula:

$$
\begin{aligned}
& p_{5}(x)=f\left(x_{0}\right)+s \triangle^{1} f\left(x_{0}\right)+\frac{s^{2}-s}{2} \triangle^{2} f\left(x_{0}\right)+\frac{s^{3}-3 s^{2}+2 s}{6} \Delta^{3} f\left(x_{0}\right)+ \\
& +\frac{s^{4}-6 s^{3}+11 s^{2}-6 s}{24} \Delta^{4} f\left(x_{0}\right)+\frac{s^{5}-10 s^{4}+35 s^{3}-50 s^{2}+24 s}{120} \Delta^{5} f\left(x_{0}\right)
\end{aligned}
$$

Differentiating this 4-times we get,

$$
\begin{aligned}
& \frac{d^{4} f}{d x^{4}} \simeq \frac{d p_{5}^{4}}{d x^{4}}=\frac{1}{h^{4}}\left[\triangle^{4} f\left(x_{0}\right)+\frac{1}{5}(5 s-10) \triangle^{5} f\left(x_{0}\right)\right. \\
& =\frac{1}{(0.1)^{4}}[-035+(0.5-2)(0.4)]=-95.00 \times 10^{2}
\end{aligned}
$$

