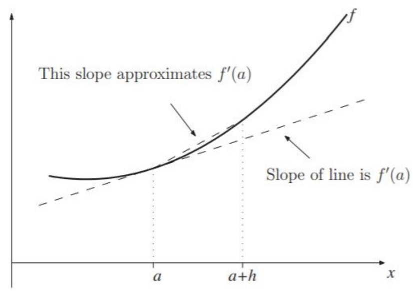
Numerical differentiation: In this section we are dealing with the different ways of numerically approximating the derivatives of the function.

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



Consider the shorter broken line as shown in the above, where h is small enough.

$$f'(a) \approx \text{ slope of short broken line}$$

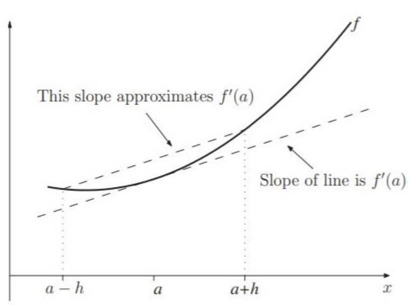
$$= \frac{\textit{difference in the } y-\textit{values}}{\textit{difference in the } x-\textit{value}} = \frac{f(a+h)-f(a)}{h}$$

This is called a one-sided difference or forward difference approximation to the derivative of $f(x)$. 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

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

This is another one-sided difference, called a backward difference, approximation to $f'(a)$.

A third method for approximating the first derivative of f can be seen in this way.



$f'(a) \approx$ slope of short broken line $= \dfrac{\textit{difference in the } y-\textit{values}}{\textit{difference in the } x-\textit{value}} = \dfrac{f(a+h)-f(a-h)}{2h}$

This is called a central difference approximation to $f'(a)$.

Note: In practice, the central difference formula is the most accurate.

Example 1: Use a forward difference, and the values of h given below, to approximate the derivative of $\cos(x)$ at $x = \dfrac{\pi}{3}$.

i) $h = 0.1$ ii) $h = 0.01$ iii) $h = 0.001$ iv) $h = 0.0001$

Solution:

i) $f'(a) = \dfrac{\cos(a+h)-\cos(a)}{h} = \dfrac{0.41104381-0.5}{0.1} = -0.88956192$

ii) $f'(a) = \dfrac{\cos(a+h)-\cos(a)}{h} = \dfrac{0.49131489-0.5}{0.01} = -0.86851095$

iii) $f'(a) = \dfrac{\cos(a+h)-\cos(a)}{h} = \dfrac{0.49913372-0.5}{0.001} = -0.86627526$

iv) $f'(a) = \dfrac{\cos(a+h)-\cos(a)}{h} = \dfrac{0.49991339-0.5}{0.0001} = -0.86605040$

The advantage of doing a simple example first is that we can compare these approximations with the exact values.

$$f'(a) = -\sin(\pi/3) = \frac{-\sqrt{3}}{2} = -0.86602540$$

Note that the accuracy levels of the four approximations are:

i) 1 d.p ii) 2 d.p iii) 3 d.p iv) 4 d.p

The errors reduce by about a factor of 10 each time.

Example 2: Use a central difference, and the values of h given below, to approximate the derivative of $\cos(x)$ at $x = \dfrac{\pi}{3}$.

i) $h = 0.1$ ii) $h = 0.01$ iii) $h = 0.001$ iv) $h = 0.0001$

Solution:

i) $f'(a)=\dfrac{\cos(a+h)-\cos(a-h)}{2h}=\dfrac{0.41104381-0.58396036}{0.2}=-0.86458275$

ii) $f'(a)=\dfrac{\cos(a+h)-\cos(a-h)}{2h}=\dfrac{0.49131489-0.50863511}{0.02}=-0.86601097$

iii) $f'(a)=\dfrac{\cos(a+h)-\cos(a-h)}{2h}=\dfrac{0.49913372-0.50086578}{0.002}=-0.86602526$

iv) $f'(a)=\dfrac{\cos(a+h)-\cos(a-h)}{2h}=\dfrac{0.49991339-0.50008660}{0.0002}=-0.86602540$

This time successive approximations generally have two extra accurate decimal places.

Example 3: The distance y of a runner from a fixed point is measured (in meters) at intervals of half a second. The data obtained are:

t:	*0.0*	*0.5*	*1.0*	*1.5*	*2.0*
y:	*0.00*	*3.65*	*6.80*	*9.90*	*12.15*

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

Solution:

$$y'(0.5)\approx\frac{y(1.0)-y(0.0)}{2(0.5)}=6.80\,m\,s^{-1}$$

$$y'(1.25)\approx\frac{y(1.5)-y(1.0)}{2(0.25)}=6.20\,m\,s^{-1}$$

Note: We can find velocity by interpolation method also.

t	y	$[t_i\,t_{i+1}]$	$[t_i\,t_{i+1}\,t_{i+2}]$	$[t_i\,t_{i+1}\,t_{i+2}\,t_{i+3}]$	$[t_i\,t_{i+1}\,t_{i+2}\,t_{i+3}\,t_{i+4}]$
$t_0=0$	0.0				
		7.3			
$t_1=0.5$	3.65		-1		
		6.3		0.6	
$t_2=1.0$	6.8		-0.1		-0.0833
		6.2		-1.066	
$t_3=1.5$	9.9		-1.7		
		4.5			
$t_4=2.0$	12.15				

The Newton's divided difference formula is

$$\begin{aligned}y(t)&=y_0+(t-t_0)[t_0\,t_1]+(t-t_0)(t-t_1)[t_0\,t_1\,t_2]\\&\quad+(t-t_0)(t-t_1)(t-t_2)[t_0\,t_1\,t_2\,t_3]+(t-t_0)(t-t_1)(t-t_2)(t-t_3)[t_0\,t_1\,t_2\,t_3\,t_4]\end{aligned}$$

$$y(t) = 0 + t(7.3) + t(t-0.5)(-1) + t(t-0.5)(t-1)(0.6) + t(t-0.5)(t-1)(t-1.5)(-0.833)$$

$$y(t) = (7.3)t - (t^2 - 0.5t) + (t^3 - 1.5t^2 + 0.5t)(0.6) - (t^4 - 3t^3 + 2.75t^2 - 0.75t)(0.833)$$

$$y'(t) = (7.3) - (2t - 0.5) + (3t^2 - 2(1.5)t + 0.5)(0.6) - (4t^3 - 9t^2 + 2(2.75)t - 0.75)(0.833)$$

$$y'(0.5) = (7.3) - (2(0.5) - 0.5) + (3(0.5)^2 - 2(1.5)(0.5) + 0.5)(0.6)$$
$$- (4(0.5)^3 - 9(0.5)^2 + 2(2.75)(0.5) - 0.75)(0.833)$$

$$y'(0.5) = 7.3 - 0.5 - 0.15 + 0.20825 = 6.85\, m\, s^{-1}$$

Derivatives using Newton's forward difference table: Consider Newton's forward difference formula

$$y(x) = y_0 + k\Delta y_0 + \frac{k(k-1)}{2!}\Delta^2 y_0 + \frac{k(k-1)(k-2)}{3!}\Delta^3 y_0 + ... + \Delta^k y_0 \qquad (1)$$

$$x = x_0 + kh \text{ or } k = \frac{x - x_0}{h} \text{ (say)}$$

$$\frac{dy}{dx} = \frac{dy}{dk}\frac{dk}{dx} = \frac{1}{h}\frac{dy}{dk}$$

$$\frac{dy}{dx} = \frac{1}{h}\frac{dy}{dk} = \frac{1}{h}\left(\Delta y_0 + \frac{(2k-1)}{2}\Delta^2 y_0 + \frac{3k^2 - 6k + 2}{6}\Delta^3 y_0 + - - -\right)$$

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

Similarly, the second derivative can be written as

$$\frac{d^2 y}{dx^2} = \frac{1}{h^2}\left(\Delta^2 y_0 + (k-1)\Delta^3 y_0 + \frac{(6k^2 - 18k + 11)}{12}\Delta^4 y_0 + - - -\right)$$

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

Derivatives using Newton's forward difference table: Consider Newton's backward difference formula

$$y(x) = y_n + k\nabla y_n + \frac{k(k+1)}{2!}\nabla^2 y_n + \frac{k(k+1)(k+3)}{3!}\nabla^3 y_n + ...$$

where, $x = x_n + kh$ or $k = \frac{x - x_n}{h}$ (say)

$$\frac{dy}{dx} = \frac{dy}{dk}\frac{dk}{dx} = \frac{1}{h}\frac{dy}{dk}$$

$$\frac{dy}{dx} = \frac{1}{h}\frac{dy}{dk} = \frac{1}{h}\left(\nabla y_n + \frac{(2k+1)}{2}\nabla^2 y_n + \frac{(3k^2+6k+2)}{6}\nabla^3 y_n + ---\right)$$

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

Similarly, the second derivative can be written as

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

Derivatives using central difference table: Consider the Stirling's interpolation formula

$$y_p = y_0 + k\left(\frac{\Delta y_0 + \Delta y_{-1}}{2}\right) + \frac{k^2}{2!}\Delta^2 y_{-1} + \frac{k(k^2-1)}{3!}\left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right) + \frac{k^2(k^2-1)}{4!}\Delta^4 y_{-2} + ...$$

where $k = \frac{x - x_0}{h}$. Then, $\frac{dy}{dx} = \frac{dy}{dk}\frac{dk}{dx} = \frac{1}{h}\frac{dy}{dk}$

$$\frac{dy}{dx} = \frac{1}{h}\frac{dy}{dk} = \frac{1}{h}\left(\begin{array}{l}\left(\frac{\Delta y_0 + \Delta y_{-1}}{2}\right) + k\Delta^2 y_{-1} + \frac{(3k^2-1)}{12}\left(\Delta^3 y_{-1} + \Delta^3 y_{-2}\right) + \\ \frac{(2k^3-k)}{12}\Delta^4 y_{-2} + \frac{(5k^4-15k^2+4)}{240}\left(\Delta^5 y_{-2} + \Delta^5 y_{-3}\right) ---\end{array}\right)$$

$$\left(\frac{dy}{dx}\right)_{x=0} = \frac{1}{h}\left(\left(\frac{\Delta y_0 + \Delta y_{-1}}{2}\right) - \frac{1}{12}\left(\Delta^3 y_{-1} + \Delta^3 y_{-2}\right) + \frac{1}{60}\left(\Delta^5 y_{-2} + \Delta^5 y_{-3}\right) + --\right)$$

Similarly,

$$\frac{d^2 y}{dx^2} = \frac{1}{h^2}\left(\Delta^2 y_{-1} - \frac{1}{12}\Delta^4 y_{-2} + ---\right)$$

Example 1: A jet fighter's position on an aircraft carrier's runway was timed during landing:

$t\ (sec)$	1.0	1.1	1.2	1.3	1.4	1.5	1.6
$y\ (m)$	7.989	8.403	8.781	9.129	9.451	9.750	10.031

where y is the distance from the end of the carrier. Estimate the velocity and acceleration at $t = 1.1$, $t = 1.6$ and $t = 1.3$ using numerical differentiation.

Solution:

$$\begin{array}{cccccccc}
t & y & \Delta y & \Delta^2 y & \Delta^3 y & \Delta^4 y & \Delta^5 y & \Delta^6 y \\
1.0 & 7.989 & & & & & & \\
 & & 0.414 & & & & & \\
1.1 & 8.403 & & -0.036 & & & & \\
 & & 0.378 & & 0.006 & & & \\
1.2 & 8.781 & & -0.030 & & -0.002 & & \\
 & & 0.348 & & 0.004 & & 0.001 & \\
1.3 & 9.129 & & -0.026 & & -0.001 & & 0.002 \\
 & & 0.322 & & 0.003 & & 0.003 & \\
1.4 & 9.451 & & -0.023 & & 0.002 & & \\
 & & 0.299 & & 0.005 & & & \\
1.5 & 9.750 & & -0.018 & & & & \\
 & & 0.281 & & & & & \\
1.6 & 10.031 & & & & & &
\end{array}$$

Here we use Newton's forward difference formula to find the velocity and acceleration at $t = 1.1$ (the point is nearer to the first tabular value).

$$\left(\frac{dy}{dt}\right)_{t=t_0} = \frac{1}{h}\left(\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \frac{1}{5}\Delta^5 y_0\right)$$

$$\left(\frac{dy}{dt}\right)_{t=1.1} = \frac{1}{0.1}\left(0.378 - \frac{1}{2}(-0.03) + \frac{1}{3}(0.004) - \frac{1}{4}(-0.001) + \frac{1}{5}(0.003)\right) = 3.9518$$

$$\left(\frac{d^2y}{dt^2}\right)_{t=t_0} = \frac{1}{h^2}\left(\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 - \frac{5}{6}\Delta^5 y_0\right)$$

$$\left(\frac{d^2y}{dt^2}\right)_{t=1.1} = \frac{1}{(0.1)^2}\left((-0.03) - 0.004 + \frac{11}{12}(-0.001) - \frac{5}{6}(0.003)\right) = -3.7417$$

To find velocity and acceleration at $t = 1.6$ (the point is the end point), we use Newton's backward difference formula.

$$\left(\frac{dy}{dt}\right)_{t=t_n} = \frac{1}{h}\left(\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \frac{1}{4}\nabla^4 y_n + \frac{1}{5}\nabla^5 y_n + \frac{1}{6}\nabla^6 y_n\right)$$

$$\left(\frac{dy}{dt}\right)_{t=1.6}=\frac{1}{0.1}\left(0.281+\frac{1}{2}(-0.018)+\frac{1}{3}(0.005)+\frac{1}{4}(0.002)+\frac{1}{5}(0.003)+\frac{1}{6}(0.002)\right)=2.751$$

$$\left(\frac{d^2y}{dt^2}\right)_{t=t_n}=\frac{1}{h^2}\left(\nabla^2 y_n+\nabla^3 y_n+\frac{11}{12}\nabla^4 y_n+\frac{5}{6}\nabla^5 y_n\right)$$

$$\left(\frac{d^2y}{dt^2}\right)_{t=1.6}=\frac{1}{(0.1)^2}\left(-0.018+0.005+\frac{11}{12}(0.002)+\frac{5}{6}(0.003)\right)=-0.8666$$

Finally, to find the velocity and acceleration at time $t=1.3$ we use central difference formula:

$$\left(\frac{dy}{dt}\right)_{t=0}=\frac{1}{h}\left(\left(\frac{\Delta y_0+\Delta y_{-1}}{2}\right)-\frac{1}{12}\left(\Delta^3 y_{-1}+\Delta^3 y_{-2}\right)+\frac{1}{60}\left(\Delta^5 y_{-2}+\Delta^5 y_{-3}\right)+--\right)$$

$$\left(\frac{dy}{dt}\right)_{t=0}=\frac{1}{0.1}\left(\frac{1}{2}(0.322+0.348)-\frac{1}{12}(0.003+0.004)+\frac{1}{60}(0.003+0.001)+--\right)=13.39$$

$$\left(\frac{d^2y}{dt^2}\right)_{t=1.3}=\frac{1}{h^2}\left(\Delta^2 y_{-1}-\frac{1}{12}\Delta^4 y_{-2}+---\right)=\frac{1}{(0.1)^2}\left(-0.026-\frac{1}{12}(-0.001)\right)=-2.591667$$

Maxima and Minima of a tabulated function: To find the maxima and minima of a function $y=f(x)$, we follow the following procedure.

i) Find $\frac{dy}{dx}$ and equate to zero. And solving for x.

ii) If $\frac{d^2y}{dx^2}$ at x is (-)ve, then y has maximum and if $\frac{d^2y}{dx^2}$ at x is (+)ve then y has minimum at the point x.

Consider the Newton's forward interpolation formula,

$$y(x)=y_0+k\Delta y_0+\frac{k(k-1)}{2!}\Delta^2 y_0+\frac{k(k-1)(k-2)}{3!}\Delta^3 y_0+....+\Delta^k y_0$$

$$x=x_0+kh \text{ or } k=\frac{x-x_0}{h} \text{ (say)}$$

Then, $\frac{dy}{dx} = \frac{dy}{dk}\frac{dk}{dx} = \frac{1}{h}\frac{dy}{dk}$

$$\frac{dy}{dx} = \frac{1}{h}\frac{dy}{dk} = \frac{1}{h}\left(\Delta y_0 + \frac{(2k-1)}{2}\Delta^2 y_0 + \frac{3k^2-6k+2}{6}\Delta^3 y_0 + --- \right)$$

We know that for extreme values, $\frac{dy}{dx} = 0$

$$\Delta y_0 + \frac{(2k-1)}{2}\Delta^2 y_0 + \frac{3k^2-6k+2}{6}\Delta^3 y_0 + --- = 0$$

Since, the higher differences are very small, we can neglect the higher differences from the above equation.

$$\Delta y_0 + \frac{(2k-1)}{2}\Delta^2 y_0 + \frac{3k^2-6k+2}{6}\Delta^3 y_0 = 0$$

The values of Δy_0, $\Delta^2 y_0$ and $\Delta^3 y_0$ taken from the difference table and substitute in the above equation. And then solve the quadratic equation for k. Using $x = x_0 + kh$, we get the critical values at which y is maximum or minimum.

Example 1: From the following table, find the extreme values of y.

x:	*3*	*4*	*5*	*6*	*7*	*8*
y:	*0.205*	*0.240*	*0.259*	*0.262*	*0.250*	*0.224*

Solution: The forward difference table for the given data:

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$
3	0.205			
		0.035		
4	0.240		−0.016	
		0.019		0.000
5	0.259		−0.016	
		0.003		0.001
6	0.262		−0.015	
		−0.012		0.001
7	0.250		−0.014	
		−0.026		
8	0.224			

Newton's forward difference formula for the first derivative gives,

$$\Delta y_0 + \frac{(2k-1)}{2}\Delta^2 y_0 + \frac{3k^2-6k+2}{6}\Delta^3 y_0 = 0$$

If we choose, $x_0 = 3$, then $y_0 = 0.205$, $\Delta y_0 = 0.035$, $\Delta^2 y_0 = -0.016$ and $\Delta^3 y_0 = 0.000$

$$\left(0.035\right)+\frac{\left(2k-1\right)}{2}\left(-0.016\right)+\frac{\left(3k^2-6k+2\right)}{6}\left(0.000\right)=0$$

$0.035-\left(2k-1\right)\left(0.008\right)=0$ which implies that $k=2.6875$

Therefore, the critical point $x=x_0+kh=3+\left(2.6875\right)1=5.6875$

From the Newton's forward difference table, we write the second derivative,

$$\frac{d^2y}{dx^2}=\frac{1}{h^2}\left(\Delta^2y_0+\left(k-1\right)\Delta^3y_0+\frac{\left(6k^2-18k+11\right)}{12}\Delta^4y_0+---\right)$$

$$\frac{d^2y}{dx^2}=\left(\left(0.035\right)+\left(2.6875-1\right)\left(0.000\right)+\frac{\left(6\left(2.6875\right)^2-18\left(2.6875\right)+11\right)}{12}\left(0.001\right)\right)<0$$

Therefore, the function will have maximum at the point $x=5.6875$ and the maximum value is

$$y\left(x\right)=y_0+k\Delta y_0+\frac{k\left(k-1\right)}{2!}\Delta^2y_0+\frac{k\left(k-1\right)\left(k-2\right)}{3!}\Delta^3y_0+--$$

$$y\left(5.6875\right)=0.205+\left(2.6875\right)\left(0.035\right)+\frac{\left(2.6875\right)\left(2.6875-1\right)}{2!}\left(-0.016\right)=0.2628$$

Comment: If you choose $x_0=5$, then we have $y_0=0.259$, $\Delta y_0=0.003$, $\Delta^2y_0=-0.015$ and $\Delta^3y_0=0.001$. So that

$$\left(0.035\right)+\frac{\left(2k-1\right)}{2}\left(-0.015\right)+\frac{\left(3k^2-6k+2\right)}{6}\left(0.001\right)=0$$

$$0.003k^2-0.096k+0.065=0$$

The roots are: $k=31.3080,\ 0.6920$. Therefore, the critical points are:

$x=x_0+kh=5+\left(0.6920\right)1=5.692$

$x=x_0+kh=5+\left(31.3080\right)1=36.3080$, which is out range.

Example 2: Find the extreme values of the function y from the following table:

x:	-2	-1	0	1	2	3	4
y:	2	-0.25	0	-0.25	2	15.75	56

Solution:

$$
\begin{array}{ccccccc}
x & y & \Delta y & \Delta^2 y & \Delta^3 y & \Delta^4 y & \Delta^5 y \\
-2 & 2 & & & & & \\
 & & -2.25 & & & & \\
-1 & -0.25 & & 2.5 & & & \\
 & & 0.25 & & -3 & & \\
0 & 0 & & -0.5 & & 6 & \\
 & & -0.25 & & 3 & & 0 \\
1 & -0.25 & & 2.5 & & 6 & \\
 & & 2.25 & & 9 & & 0 \\
2 & 2 & & 11.5 & & 6 & \\
 & & 13.75 & & 15 & & \\
3 & 15.75 & & 26.5 & & & \\
 & & 40.25 & & & & \\
4 & 56 & & & & &
\end{array}
$$

Newton's forward difference formula for the first derivative gives,

$$\Delta y_0 + \frac{(2k-1)}{2}\Delta^2 y_0 + \frac{3k^2-6k+2}{6}\Delta^3 y_0 = 0$$

Taking $x_0 = 0$, then we have $y_0 = 0$, $\Delta y_0 = -0.25$, $\Delta^2 y_0 = 2.5$ and $\Delta^3 y_0 = 9$. So that

$$(-0.25) + \frac{(2k-1)}{2}(2.5) + \frac{(3k^2-6k+2)}{6}(9) = 0$$

$4.5k^2 - 7.5k + 1.55 = 0$ implies that $k = 1.4249,\ 0.2417$

Therefore, the critical points are:

$$x = x_0 + kh = 0 + (1.4249)1 = 1.4249$$

$$x = x_0 + kh = 0 + (0.2417)1 = 0.2417$$

Now we have to find the second derivative at these points to decide extremum of the given data:

From the Newton's forward difference table, the second derivative,

$$\frac{d^2y}{dx^2} = \frac{1}{h^2}\left(\Delta^2 y_0 + (k-1)\Delta^3 y_0 + \frac{(6k^2-18k+11)}{12}\Delta^4 y_0 + ---\right)$$

$$\left(\frac{d^2y}{dx^2}\right)_{k=1.4249} = 2.5 + (1.4249-1)(9) + \frac{\left(6(1.4249)^2 - 18(1.4249) + 11\right)}{12}(6) > 0$$

$$\left(\frac{d^2y}{dx^2}\right)_{k=0.2417} = 2.5+(0.2417-1)(9)+\frac{\left(6(0.2417)^2-18(0.2417)+11\right)}{12}(6)<0$$

Therefore, the function will have maximum at $x=0.2417$ and minimum at $x=1.4249$.

Numerical integration: We will now discuss some methods that can be used to approximate integrals. Attention will be paid to how we ensure that such approximations can be guaranteed to be of a certain level of accuracy.

Our aim is to describe some numerical methods for approximating integrals of the form

$$\int_a^b f(x)\,dx$$

The first step in numerical integration methods is to replace the function to be integrand $f(x)$ by a simple polynomial $q_{n-1}(x)$ of degree $n-1$ which coincides with $f(x)$ at n points x_i, where $i = 0,1,2,...,n-1$. Thus,

$$\int_a^b f(x)\,dx \simeq \int_a^b q_{n-1}(x)\,dx \qquad (1)$$

where $q_{n-1}(x) = a_0 + a_1x + a_2x^2 + ... + a_{n-1}x^{n-1}$. The a_i's are constant coefficients.

The approximating polynomial $q_{n-1}(x)$ is always integrated exactly, so the accuracies of different methods depend on how closely $q_{n-1}(x)$ fits the actual function $f(x)$ under consideration.

Note: For a cubic function, fourth differences are zero. In general for n^{th} degree polynomial, the n^{th} differences are constants (i.e., $\Delta^3 y$ are constants for a fourth degree polynomial) and hence $(n+1)^{th}$ differences are zero.

The formula we get from Eqn. (1) will not be exact because the polynomial is not identical with $f(x)$. We get an expression for the error by integrating the error term. Let the interval $[a,b]$ be divided into n equal sub intervals such that $a = x_0 < x_1 < x_2 < ... < x_n = b$. Clearly, $x_2 = x_0 + 2h$ and in general $x_n = x_0 + nh$

$$I = \int_{x_0}^{x_n} y\,dx = \int_a^b y\,dx$$

Approximating y by Newton's forward difference, we obtain

$$I = \int_{x_0}^{x_n} \left(y_0 + k\Delta y_0 + \frac{k(k-1)}{2!}\Delta^2 y_0 + \frac{k(k-1)(k-2)}{3!}\Delta^3 y_0 + ... \right) dx$$

where, $k = \frac{x - x_0}{h}$ i.e., $x = x_0 + hk$ so that $dx = h\ dk$

The above integral becomes,

$$I = h\int_0^n \left(y_0 + k\Delta y_0 + \frac{k(k-1)}{2!}\Delta^2 y_0 + \frac{k(k-1)(k-2)}{3!}\Delta^3 y_0 + \dots \right) dk$$

$$I = nh\left(y_0 + \frac{n}{2}\Delta y_0 + \frac{n(2n-3)}{12}\Delta^2 y_0 + \frac{n(n-2)^2}{24}\Delta^3 y_0 + \dots \right)$$

From this general formula, we can obtain different formulae by putting $n = 1, 2, 3, ..$ etc. we divide here a few of these formulae but it should be mentioned that the repeated trapezoidal and Simpson's $\frac{1}{3}$ rules give sufficient accuracy for use in practical problems.

Trapezoidal rule (or two-point rule):

Put $n = 1$ in the general formula (1), then two data points gives only Δy and $\Delta^2 y = \dots = 0$ or two data points means a first order polynomial $a_0 + a_1 x$, as result $\Delta^2 y = 0$.

$$I = \int_{x_0}^{x_1} y\, dx = h\left(y_0 + \frac{1}{2}\Delta y_0 \right) = h\left(y_0 + \frac{y_1 - y_0}{2} \right) = \frac{h}{2}(y_0 + y_1)$$

If we have n integrals,

$$I = \frac{h}{2}\left[(y_0 + y_1) + (y_1 + y_2) + (y_2 + y_3) + \dots (y_{n-1} + y_n) \right]$$

$$I = \frac{h}{2}\left[y_0 + 2(y_1 + y_2 + y_3 + \dots + y_{n-1}) + y_n \right]$$

This is known as Trapezoidal rule. It can be shown that Trapezoidal rule has a dominant error term of the form $\frac{-1}{12}h^3 f''(x_0)$ where x_0 is the lower limit of integration.

Note:

i) Global error $\approx$ n (local error)

ii) From (1), local error $\approx h\left(\frac{-1}{12}\right)\Delta^2 y_0 = \left| \frac{h}{12} h^2 (y'')_{x_0} \right| = \frac{h^3}{12} f''(x_0)$

Truncation error in Trapezoidal Rule: Consider the Taylor series expansion of $y = f(x)$ around the point $x = x_0$.

$$y = f(x) = y_0 + \frac{(x - x_0)}{1!} y_0' + \frac{(x - x_0)^2}{2!} y_0'' + \ldots \qquad (1)$$

Now integrate (1) with respect to x between x_0 to x_1, we get

$$\int_{x_0}^{x_1} f(x)\,dx = \int_{x_0}^{x_1} \left(y_0 + \frac{(x - x_0)}{1!} y_0' + \frac{(x - x_0)^2}{2!} y_0'' + \ldots \right) dx$$

$$\int_{x_0}^{x_1} f(x)\,dx = \left(y_0\, x + \frac{(x - x_0)^2}{2!} y_0' + \frac{(x - x_0)^3}{3!} y_0'' + \ldots \right)_{x_0}^{x_1}$$

$$\int_{x_0}^{x_1} f(x)\,dx = \left(y_0\, x_1 + \frac{(x_1 - x_0)^2}{2!} y_0' + \frac{(x_1 - x_0)^3}{3!} y_0'' + \ldots \right) - y_0\, x_0$$

$$\int_{x_0}^{x_1} f(x)\,dx = \left(y_0 (x_1 - x_0) + \frac{(x_1 - x_0)^2}{2!} y_0' + \frac{(x_1 - x_0)^3}{3!} y_0'' + \ldots \right)$$

$$\int_{x_0}^{x_1} f(x)\,dx = y_0\, h + \frac{h^2}{2!} y_0' + \frac{h^3}{3!} y_0'' + \ldots, \text{ where } h = x_1 - x_0 \qquad (2)$$

The area of the first trapezoid in the interval (x_0, x_1) is

$$A_0 = \frac{1}{2} h (y_0 + y_1) \qquad (3)$$

Putting $x = x_1$ in (1), we get

$$y_1 = y_0 + \frac{(x_1 - x_0)}{1!} y_0' + \frac{(x_1 - x_0)^2}{2!} y_0'' + \ldots$$

$$y_1 = y_0 + \frac{h}{1!} y_0' + \frac{h^2}{2!} y_0'' + \ldots$$

Substituting y_1 value in (3), we get

$$A_0 = \frac{1}{2} h \left(2 y_0 + \frac{h}{1!} y_0' + \frac{h^2}{2!} y_0'' + \ldots \right)$$

$$A_0 = hy_0 + \frac{h^2}{2!} y_0' + \frac{h^3}{2.2!} y_0'' + \dots \tag{4}$$

From (2) and (4),

$$\int_{x_0}^{x_1} f(x)\,dx - A_0 = h^3 \left(\frac{1}{3!} - \frac{1}{2.2!} \right) y_0'' + \dots$$

The error in the interval (x_0, x_1) is $\frac{-h^3}{12} y_0''$.

In general, E_n denote the error in the trapezoidal rule with n subintervals, then

$$E_n \le \frac{h^3}{12} \left(\underset{1st\ Interval}{Max} |y''| + \underset{2nd\ Interval}{Max} |y''| + \underset{3rd\ Interval}{Max} |y''| + \dots + \underset{nth\ Interval}{Max} |y''| \right)$$

The process of working out the maximum value of $|y''|$ separately in each subinterval is very time-consuming. We can obtain a more user-friendly, if else accurate, error bound by replacing each term in the last bracket above with the biggest one. Hence, we obtain

$$E_n \le \frac{n\,h^3}{12} \underset{a \le x \le b}{Max} |y''| = \frac{(b-a)h^2}{12} \underset{a \le x \le b}{Max} |y''|$$

Example 1: Use trapezium rule to approximate the integral $\int_0^2 \cosh(x)\, dx$ by dividing the interval into 4 subintervals.

Solution: Here, $h = \frac{2-0}{4} = 0.5$

x_n	0	0.5	1	1.5	2
$f_n = \cosh(x_n)$	1.0000	1.127626	1.543081	2.352410	3.762196

$$\int_0^2 \cosh(x)\, dx \approx \frac{1}{2} h \left(f_0 + f_4 + 2(f_1 + f_2 + f_3) \right)$$

$$\int_0^2 \cosh(x)\, dx \approx \frac{1}{2} (0.5) \left(1 + 3.762196 + 2(1.127626 + 1.543081 + 2.35241) \right)$$

$$\int_0^2 \cosh(x)\, dx \approx 3.452107$$

Comment: The exact value is 3.6269

Example 2: The function $f(x)$ is known to have a second derivative with the property that $|f''(x)| < 12$ for x between 0 and 4. Using the error bound, determine how many subintervals are required so that the trapezium rule used to approximate $\int_0^4 f(x)\,dx$ can be guaranteed to be in error by less than $\frac{10^{-3}}{2}$.

Solution: Here we require that,

$$(12)\frac{(b-a)h^2}{12} < 0.0005$$

$$4h^2 < 0.0005$$

This implies that $h^2 < 0.000125$ and therefore, $h < 0.0111803$

Now, $n = \frac{b-a}{h} = \frac{4}{h} > 357.7708$

We conclude that the smallest number of subintervals which guarantees an error smaller than 0.0005 is $n = 358$.

Three point rule (Simpson's $\frac{1}{3}$ rule):

This rule fits a parabola over each set of three points. For a quadratic function $a_0 + a_1 x + a_2 x^2$ (i.e., $\Delta^3 y = 0$), the rule is

$$\int_{x_0}^{x_2} y\,dx = 2h\left(y_0 + \Delta y_0 + \frac{1}{6}\Delta^2 y_0\right) = 2h\left(y_0 + (y_1 - y_0) + \frac{1}{6}(y_2 - 2y_1 + y_0)\right)$$

$$\int_{x_0}^{x_2} y\,dx = \frac{h}{3}(y_0 + 4y_1 + y_2)$$

Since each subdomain requires two intervals, this rule requires the division of the whole range into an even number of sub intervals of width h. For the whole domain

$$\int_{x_0}^{x_n} y\,dx = \frac{h}{3}\left[(y_0 + 4y_1 + y_2) + (y_2 + 4y_3 + y_4) + (y_4 + 4y_5 + y_6) + (y_{n-2} + 4y_{n-1} + y_n)\right]$$

$$\int_{x_0}^{x_n} y\,dx = \frac{h}{3}\left[y_0 + 4\left(y_1 + y_3 + y_5 + \ldots + y_{n-1}\right) + 2\left(y_2 + y_4 + y_6 + \ldots + y_{n-2}\right) + y_n\right]$$

Because of the $\frac{h}{3}$ factor, it is called Simpson's $\frac{1}{3}$ rule.

Truncation error in Simpson's one third rule: It can be shown that Simpson's $\frac{1}{3}$ rule has a dominant error of the form $\frac{-1}{180}h^5 f^{iv}(x)$. In general, In general, E_n denote the error in the trapezoidal rule with n subintervals, then

$$E_n \le \frac{n h^5}{180} \underset{a \le x \le b}{Max} |y''| = \frac{(b-a)h^4}{180} \underset{a \le x \le b}{Max} |y''|$$

Example 1: Use Simpson's one third rule to approximate the integral $\int_0^2 \cosh(x)\,dx$ by dividing the interval into 4 subintervals.

Solution: Here, $h = \frac{2-0}{4} = 0.5$

x_n	0	0.5	1	1.5	2
$f_n = \cosh(x_n)$	1.0000	1.127626	1.543081	2.352410	3.762196

$$\int_0^2 \cosh(x)\,dx \approx \frac{1}{3}h\left(f_0 + 4\left(f_1 + f_3\right) + 2\left(f_2\right) + f_4\right)$$

$$\int_0^2 \cosh(x)\,dx \approx \frac{1}{3}(0.5)\left(1 + 4(1.127626 + 2.35241) + 2(1.543081) + 3.762196\right) = 3.628083$$

Comment: Note that approximation value is very closer to the exact value of 3.626860 than we obtained when using the trapezoidal rule with the same number of subintervals.

Example 2: The function $f(x)$ is known to have a fourth derivative with the property that $\left|f^{iv}(x)\right| < 5$ for x between 1 and 5. Determine how many subintervals are required so that the Simpson's one third rule used to approximate $\int_1^5 f(x)\,dx$ can be guaranteed to be in error by less than 0.005.

Solution: Here we require that,

$$\left|f^{iv}(x)\right|\frac{(b-a)h^4}{180} < 0.005$$

$$(5)\frac{4h^4}{180} < 0.005$$

$h^4 < 0.045$ and therefore, $h < 0.460578$

Now, $n = \dfrac{b-a}{h} = \dfrac{4}{h} > 8.684741$

For the Simpson's one third rule, the number of intervals must be an even number and we conclude that the smallest number of subintervals which guarantees an error smaller than 0.005 is $n = 10$.

Simpson's $\frac{3}{8}$ rule:

Put $n = 3$ in the general form of (1) (i.e., we need four points $a_0 + a_1x + a_2x^2 + a_3x^3$ so that $\Delta^4 y = 0$),

$$\int_{x_0}^{x_3} y\,dx = 3h\left(y_0 + \frac{3}{2}\Delta y_0 + \frac{3}{4}\Delta^2 y_0 + \frac{1}{8}\Delta^3 y_0\right)$$

$$\int_{x_0}^{x_3} y\,dx = 3h\left(y_0 + \frac{3}{2}(y_1 - y_0) + \frac{3}{4}(y_2 - 2y_1 + y_0) + \frac{1}{8}(y_3 - 3y_2 + 3y_1 - y_0)\right)$$

$$\int_{x_0}^{x_3} y\,dx = \frac{3h}{8}(y_0 + 3y_1 + 3y_2 + y_3)$$

Similarly,

$$\int_{x_3}^{x_6} y\,dx = \frac{3h}{8}\left(y_3 + 3y_4 + 3y_5 + y_6\right) \text{ and so on.}$$

Summing up all these, we get

$$\int_{x_0}^{x_n} y\,dx = \frac{3h}{8}\left[\left(y_0 + 3y_1 + 3y_2 + y_3\right) + \left(y_3 + 3y_4 + 3y_5 + y_6\right) + .. + \left(y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n\right)\right]$$

$$\int_{x_0}^{x_n} y\,dx = \frac{3h}{8}\left[y_0 + 3y_1 + 3y_2 + 2y_3 + 3y_4 + 3y_5 + 2y_6 + .. + 2y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n\right]$$

Because of the common factor $\frac{3h}{8}$, it is called $\frac{3}{8}$ rule. It is not that accurate as $\frac{1}{3}$ rule. The error term is $O\left(\frac{-3}{80}h^5 f^{iv}\left(\bar{x}\right)\right)$.

Romberg integration: We can combine two estimates of the integral that have h values in $2:1$ ratio. We may then obtain a better estimate.

Better estimate = more accurate estimate + $\frac{1}{2^n - 1}$ (more accurate – less accurate)

where, $n =$ power of h that appears in global error.

For Trapezoidal rule, this method helps us to find a good estimate of the integral which is as good that of Simpson's $\frac{1}{3}$ rule.

Note:

i) For Trapezoidal rule, $n = 2$

ii) For Simpson's rule, $n = 3$

The following problem illustrates all those techniques.

Problem: Find the value of $\int_{\pi/4}^{\pi/2} \sin x\ dx$

Solution:

Exact value: $\int_{\pi/4}^{\pi/2} \sin x\ dx = \left(-\cos x\right)_{\pi/4}^{\pi/2} = 0.7071$

Trapezoidal rule: suppose we have three sub divisions, $h = \frac{1}{3}\left(\frac{\pi}{2} - \frac{\pi}{4}\right) = \frac{\pi}{12}$

$$\int_{x_0}^{x_n} y(x)\, dx = \frac{h}{2}\left[y_0 + 2\left(y_1 + y_2 + y_3 + ... + y_{n-1} \right) + y_n \right]$$

$$\int_{\pi/4}^{\pi/2} \sin x\ dx = \frac{1}{2}\frac{\pi}{12}\left(\sin\left(\frac{\pi}{4}\right) + 2\left(\sin\left(\frac{\pi}{3}\right) + \sin\left(\frac{5\pi}{12}\right) \right) + \sin\left(\frac{\pi}{2}\right) \right)$$

$$= \frac{\pi}{24}\left(0.7071 + 2\left(0.8660 + 0.9659\right) + 1 \right) = 0.7031$$

Simpson's rule: We should have even number of sub intervals. Consider four sub intervals so that $h = \frac{1}{4}\left(\frac{\pi}{2} - \frac{\pi}{4}\right) = \frac{\pi}{16}$

$$\int_{x_0}^{x_n} y\, dx = \frac{h}{3}\left[y_0 + 4\left(y_1 + y_3\right) + 2\left(y_2\right) + y_4 \right]$$

$$\int_{\pi/4}^{\pi/2} \sin x\ dx = \frac{1}{3}\frac{\pi}{16}\left(\sin\left(\frac{\pi}{4}\right) + 4\left(\sin\left(\frac{5\pi}{16}\right) + \sin\left(\frac{7\pi}{16}\right) \right) + 2\sin\left(\frac{6\pi}{16}\right) + \sin\left(\frac{\pi}{2}\right) \right)$$

$$= \frac{\pi}{48}\left[0.7071 + 4\left(0.8315 + 0.9808\right) + 2\left(0.9239\right) + 1 \right] = 0.7071$$

Combination of Trapezoidal and Simpson's rule: Suppose we have four points as in the first formulation, where $h = \frac{\pi}{12}$

$$\int_{x_0}^{x_n} y\, dx = \frac{h}{3}\left(y_0 + 4y_1 + y_2\right) + \frac{h}{2}\left(y_2 + y_3\right)$$

$$\int_{\pi/4}^{\pi/2} \sin x\ dx = \frac{1}{3}\frac{\pi}{12}\left(\sin\left(\frac{\pi}{4}\right) + 4\left(\sin\left(\frac{\pi}{3}\right) + \sin\left(\frac{5\pi}{12}\right) \right) \right) + \frac{1}{2}\frac{\pi}{12}\left(\sin\left(\frac{5\pi}{12}\right) + \sin\left(\frac{\pi}{2}\right) \right)$$

$$\int_{\pi/4}^{\pi/2} \sin x\ dx = 0.4483 + 0.2573 = 0.7056$$

Romberg integration for this problem:

Consider Trapezoidal rule for two intervals so that $h = \frac{\pi}{8}$

Step 1: Consider Trapezoidal rule for two intervals

$$\int_{\pi/4}^{\pi/2} \sin x\ dx = \frac{\pi}{16}\left(0.7071 + 2\left(0.9239\right) + 1 \right) = 0.6980 \quad \text{(less accurate)}$$

Step 2: Consider four intervals

$$\int_{\pi/4}^{\pi/2} \sin x \; dx = \frac{\pi}{32}\left(0.7071 + 2\left(0.8315 + 0.9239 + 0.9808\right) + 1\right) = 0.7048$$

Step 3: Romberg rule

$$\int_{\pi/4}^{\pi/2} \sin x \; dx = 0.7048 + \frac{1}{2^2 - 1}\left(0.7048 - 0.6980\right) = 0.7071$$