is the error in the interpolation polynomial $P(x)$, then the error of the derivative $P'(x)$ is given by the relation

$$r(x) = R'(x) = f'(x) - P'(x).$$

Thus the error of the derivative of an interpolation polynomial is equal to the derivative of the error in that interpolation polynomial. This is also true for the higher-order derivatives.

10.2 NUMERICAL DIFFERENTIATION FORMULAE BASED ON EQUALLY SPACED DATA

10.2.1 NUMERICAL DIFFERENTIATION BASED ON NEWTON'S FORWARD DIFFERENCES

Consider a function $y(x)$ specified at equally spaced $(n+1)$ points x_i $(i=0,1,2,\ldots,n)$ in some interval $[a,b]$ by the relation

$$y_i = f(x_i).$$

We assume that the appropriate derivatives of $f(x)$ exist. Replacing the function $y(x)$ by Newton's interpolation polynomial (see section 5.2) we have

$$y_p \approx y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \frac{p(p-1)(p-2)(p-3)}{4!}\Delta^4 y_0 + \ldots,$$

or

$$y_p \approx y_0 + p\Delta y_0 + \frac{p^2-p}{2!}\Delta^2 y_0 + \frac{p^3-3p^2+2p}{3!}\Delta^3 y_0 + \frac{p^4-6p^3+11p^2-6p}{4!}\Delta^4 y_0 + \ldots, \quad (10.1)$$

where

$$p = \frac{x-x_0}{h} \text{ and } h = x_{i+1} - x_i \quad (i = 0,1,2,\ldots).$$

Now $\dfrac{dy}{dx} = \dfrac{dy}{dp} \times \dfrac{dp}{dx} = \dfrac{dy}{dp}\left(\dfrac{1}{h}\right) = \dfrac{1}{h}\dfrac{dy}{dp}$.

From (10.1) we get

$$\frac{dy_p}{dx} = y'_p \approx \frac{1}{h}\frac{d}{dp}\left[y_0 + p\Delta y_0 + \frac{p^2-p}{2!}\Delta^2 y_0 + \frac{p^3-3p^2+2p}{3!}\Delta^3 y_0 + \ldots\right]$$

$$y'_p \approx \frac{1}{h}\left[\Delta y_0 + \frac{2p-1}{2!}\Delta^2 y_0 + \frac{3p^2-6p+2}{3!}\Delta^3 y_0 + \dots\right] \qquad (10.2)$$

Since

$$\frac{d^2y}{dx^2} = \frac{d}{dx}\left[\frac{1}{h}\frac{dy}{dp}\right] = \frac{dp}{dx}\frac{d}{dp}\left[\frac{1}{h}\frac{dy}{dp}\right] = \frac{1}{h^2}\frac{d^2y}{dp^2},$$

in general

$$\frac{d^n y}{dx^n} = \frac{1}{h^n}\frac{d^n y}{dp^n}.$$

Thus

$$y''_p \approx \frac{1}{h^2}\left[\Delta^2 y_0 + (p-1)\Delta^3 y_0 + \frac{6p^2-18p+11}{12}\Delta^4 y_0 + \dots\right] \qquad (10.3)$$

$$y'''_p \approx \frac{1}{h^3}\left[\Delta^3 y_0 + \frac{2p-3}{2}\Delta^4 y_0 + \dots\right] \qquad (10.4)$$

$$y^{iv}_p \approx \frac{1}{h^4}[\Delta^4 y_0 + \dots] \qquad (10.5)$$

The formulae (10.2)-(10.5) are used to find derivatives at an interpolated point i.e. at a point other than a tabulated value of x. When seeking the derivatives y'_p, y''_p, ... at fixed point x, one should choose for x_0 the closest tabular value of the argument.

NUMERICAL DIFFERENTIATION AT TABULATED POINTS:

It is often required to find the derivatives at tabulated value of x. The numerical differentiation formulae are simplified in this case. Each tabular value may be taken as the initial value, we set $x = x_0$, then $p = 0$. Thus

$$(y')_{x_0} \approx \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \dots\right] \qquad (10.2')$$

$$(y'')_{x_0} \approx \frac{1}{h^2}\left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 - \frac{5}{6}\Delta^5 y_0 + \dots\right] \qquad (10.3')$$

$$(y''')_{x_0} \approx \frac{1}{h^3}\left[\Delta^3 y_0 - \frac{3}{2}\Delta^4 y_0 + \dots\right] \qquad (10.4')$$

EXAMPLE 10.1: Find the first and second derivatives of the function tabulated below at the points x = 2.31 and 3.0.

x	0	1	2	3	4	5	6
y	2	3	10	29	66	127	218

SOLUTION: Construct a difference table as given below.

Table 10.1 Difference Table for Derivative Approximation

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$
0	2				
		1			
1	3		6		
		7		6	
2	10		12		0
		19		6	
3	29		18		0
		37		6	
4	66		24		0
		61		6	
5	127		30		
		91			
6	218				

When x = 2.31.

Take $x_0 = 2$, then $p = 0.31$.

Here $h = 1$, $y_0 = 10$, $\Delta y_0 = 19$, $\Delta^2 y_0 = 18$, $\Delta^3 y_0 = 6$, $\Delta^4 y_0 = 0$.

Using formulae (10.2) and (10.3) we obtain

$$y'_p \approx \frac{1}{h}\left[19 + \frac{2(0.31) - 1}{2}18 + \frac{3(0.31)^2 - 6(0.31) + 2}{6}6\right]$$

$$= [19 - 3.42 + 0.4283]$$

$$= 16.0083 \approx 16.008$$

and $\quad y''_p \approx (1/1^2)[18 + (0.31 - 1)6] = 13.86.$

When x = 3.

In this case we choose $x_0 = 3$, then

$$\Delta y_0 = 37, \quad \Delta^2 y_0 = 24, \quad \Delta^3 y_0 = 6.$$

Using formulae (10.2′) and (10.3′) we get

$$y'_{x_0} \approx \frac{1}{1}\left[37 - \frac{1}{2}(24) + \frac{1}{3}(6)\right]$$

$$= 37 - 12 + 2 = 27$$

and

$$y''_{x_0} \approx \frac{1}{1^2}\left[24 - 6\right] = 18.$$

To estimate the accuracy of these values, we note that as the table represents the polynomial $y = x^3 + 2$,

$$y' = 3x^2, \quad y'' = 6x.$$

Hence

$$y'(2.31) = 3(2.31)^2 = 16.0083 \approx 16.008$$

$$y'(3) = 3(3)^2 = 27$$
$$y''(2.31) = 6(2.31) = 13.86$$
$$y''(3) = 6(3) = 18.$$

Thus the results are correct to the given digits.

10.2.2 NUMERICAL DIFFERENTIATION BASED ON NEWTON'S BACKWARD DIFFERENCES

We know that Newton's backward difference formula (5.2) is

$$y_p \approx y_0 + p\nabla y_0 + \frac{p(p+1)}{2!}\nabla^2 y_0 + \frac{p(p+1)(p+2)}{3!}\nabla^3 y_0 + \frac{p(p+1)(p+2)(p+3)}{4!}\nabla^4 y_0 + \ldots$$

$$= y_0 + p\nabla y_0 + \frac{p^2+P}{2!}\nabla^2 y_0 + \frac{p^3+3p^2+2p}{3!}\nabla^3 y_0 + \frac{p^4+6p^3+11p^2+6p}{4!}\nabla^4 y_0 + \ldots$$

Therefore

$$y'_p \approx \frac{1}{h}\left[\nabla y_0 + \frac{1}{2}(2p+1)\nabla^2 y_0 + \frac{3p^2+6p+2}{6}\nabla^3 y_0 + \frac{2p^3+9p^2+11p+3}{12}\nabla^4 y_0 + \ldots\right] \quad (10.9)$$

$$y''_p \approx \frac{1}{h^2}\left[\nabla^2 y_0 + (p+1)\nabla^3 y_0 + \frac{6p^2+18p+11}{12}\nabla^4 y_0 + \ldots\right] \quad (10.10)$$

$$y_p''' = \frac{1}{h^3}\left[\nabla^3 y_0 + \frac{1}{2}(2p+3)\nabla^4 y_0 + \ldots\right] \tag{10.11}$$

$$y_p^{iv} = \frac{1}{h^4}\left[\nabla^4 y_0 + \ldots\right] \tag{10.12}$$

and so on.

If $p = 0$, we obtain

$$y'_{x_0} \approx \frac{1}{h}\left[\nabla y_0 + \frac{1}{2}\nabla^2 y_0 + \frac{1}{3}\nabla^3 y_0 + \frac{1}{4}\nabla^4 y_0 + \ldots\right] \tag{10.9'}$$

$$y''_{x_0} \approx \frac{1}{h^2}\left[\nabla^2 y_0 + \nabla^3 y_0 + \frac{11}{12}\nabla^4 y_0 + \ldots\right] \tag{10.10'}$$

$$y'''_{x_0} \approx \frac{1}{h^3}\left[\nabla^3 y_0 + \frac{3}{2}\nabla^4 y_0 + \ldots\right] \tag{10.11'}$$

To express the derivatives in terms of functional values we retain one, two and three terms of (10.9′) and obtain, respectively, two-point, three-point, and four-point backward formulae.

$$y'_{x_0} \approx \frac{1}{h}[y_0 - y_{-1}] \tag{10.13}$$

$$y'_{x_0} \approx \frac{1}{2h}[3y_0 - 4y_{-1} + y_{-2}] \tag{10.14}$$

$$y'_{x_0} \approx \frac{1}{6h}[11y_0 - 18y_{-1} + 9y_{-2} - 2y_{-3}]. \tag{10.15}$$

EXAMPLE 10.2: Find the first and second derivatives of the function tabulated in Example 10.1 at the points $x = 5$ and 5.7.

SOLUTION: To estimate the desired derivatives, we use the numerical differentiation formula based on Newton's backward differences.

When $x = 5$, we take $x_0 = 5$. Then

$$\nabla y_0 = 61,\ \nabla^2 y_0 = 24,\ \nabla^3 y_0 = 6,\ \nabla^4 y_0 = 0.$$

Thus the differentiation formulae (10.9′) and (10.10′) yeild respectively

$$y'_{x_0} \approx \frac{1}{1}\left[61 + \frac{1}{2}(24) + \frac{1}{3}(6)\right] = 61 + 12 + 2 = 75$$

and

$$y''_{x_0} \approx \frac{1}{1}[24 + 6] = 30.$$

When $x = 5.7$.
Take $x_0 = 6$, then $p = 5.7 - 6 = -0.3$, and

$$\nabla y_0 = 91,\ \nabla^2 y_0 = 30,\ \nabla^3 y_0 = 6,\ \nabla^4 y_0 = 0.$$

Using (10.9) and (10.10) respectively, we obtain

$$y'_p \approx \frac{1}{1}\left[91 + \frac{1}{2}(-0.6 + 1)30 + \frac{3(0.09) - 1.8 + 2}{6}6\right]$$

$$= [91 + 6 + 0.47] = 97.47$$

and

$$y''_p \approx \frac{1}{1^2}[30 + (-0.3 + 1)6] = 30 + 4.2 = 34.2.$$

Let us estimate the accuracy of these results. We know that

$$y = x^3 + 2.$$

Thus

$$y'_x = 3x^2,\ y''_x = 6x.$$

Therefore

$$y'(5) = 3(25) = 75$$
$$y'(5.7) = 3(32.49) = 97.47$$
$$y''(5) = 6(5) = 30$$
$$y''(5.7) = 6(5.7) = 34.2.$$

Hence the results are accurate to the given digits.

10.2.3 NUMERICAL DIFFERENTIATION BASED ON STIRLING'S FORMULA

The numerical differentiation formulae discussed in Sec. (10.2.1) & (10.2.2) for a function $y(x)$ at a point $x = x_0$ have the disadvantage that they only take one-sided values of the function. The formulae of sec. (10.2.1) employ values of the function for $x > x_0$ while the formulae of sec. (10.2.2) employ values of the function for $x < x_0$. However, a relatively higher accuracy is ensured by the symmetric formulae of differentiation which employ the values of the given function $y(x)$ both for $x > x_0$ and $x < x_0$. These formulae are generally called central difference formulae. Any one of the central difference interpolation formulae can be used to give a formula for derivatives. We will derive only the formulae based on Stirling's and Bessel's interpolation formulae.

Let $\ldots, x_{-2}, x_{-1}, x_0, x_1, x_2, \ldots$ be a set of equally spaced points with $x_{i+1} = x_i+h$. Suppose that $y_i = f(x_i)$ give the corresponding values of the given function $y=f(x)$. Replacing the given function y by the Stirling's interpolation polynomial (Sec.5.5) and setting $p = (x - x_0)/h$, we obtian

$$y_p \approx y_0 + p\mu\delta y_0 + \frac{p^2}{2!}\delta^2 y_0 + \frac{p(p^2-1)}{3!}\mu\delta^3 y_0 + \frac{p^2(p^2-1)}{4!}\delta^4 y_0 + \ldots$$

or

$$y_p \approx y_0 + p\,\frac{\Delta y_{-1}+\Delta y_0}{2} + \frac{p^2}{2!}\Delta^2 y_{-1} + \frac{p(p^2-1)}{3!}\,\frac{\Delta^3 y_{-2}+\Delta^3 y_{-1}}{2} +$$

$$\frac{p^2(p^2-1)}{4!}\Delta^4 y_{-2} + \frac{p(p^2-1)(p^2-2^2)}{5!}\,\frac{\Delta^5 y_{-3}+\Delta^5 y_{-2}}{2} + \ldots$$

Since $\dfrac{dy}{dx} = \dfrac{dy}{dp}\dfrac{dp}{dx} = \dfrac{1}{h}\dfrac{dy}{dp}$, thus from the above relation we get

$$y'_p \approx \frac{1}{h}\Bigg[\frac{\Delta y_{-1}+\Delta y_0}{2} + p\Delta^2 y_{-1} + \frac{3p^2-1}{3!}\,\frac{\Delta^3 y_{-2}+\Delta^3 y_{-1}}{2} + \frac{4p^3-2p}{4!}\Delta^4 y_{-2}$$

$$+ \frac{5p^4-15p^2+4}{5!}\,\frac{\Delta^5 y_{-3}+\Delta^5 y_{-2}}{2} + \ldots\Bigg] \qquad (10.16)$$

$$y''_p \approx \frac{1}{h^2}\Bigg[\Delta^2 y_{-1} + p\,\frac{\Delta^3 y_{-2}+\Delta^3 y_{-1}}{2} + \frac{6p^2-1}{12}\Delta^4 y_{-2} + \frac{2p^3-3p}{12}\,\frac{\Delta^5 y_{-3}+\Delta^5 y_{-2}}{2}$$

$$+\ldots\Bigg] \qquad (10.17)$$

$$y'''_p \approx \frac{1}{h^3}\Bigg[\frac{\Delta^3 y_{-2}+\Delta^3 y_{-1}}{2} + p\Delta^4 y_{-2} + \frac{2p^2-1}{4}\,\frac{\Delta^5 y_{-3}+\Delta^5 y_{-2}}{2} + \ldots\Bigg] \qquad (10.18)$$

$$y_p^{IV} \approx \frac{1}{h^4}\left[\Delta^4 y_{-2} + p\frac{\Delta^5 y_{-3} + \Delta^5 y_{-2}}{2} + \dots\right] \quad (10.19)$$

$$y_p^{V} \approx \frac{1}{h^5}\left[\frac{\Delta^5 y_{-3} + \Delta^5 y_{-2}}{2} + \dots\right]. \quad (10.20)$$

If we take $x=x_0$, then $p=0$ and formulae (10.16) - (10.20) take the form

$$y'_{x_0} \approx \frac{1}{h}\left[\frac{\Delta y_{-1} + \Delta y_0}{2} - \frac{1}{3!}\frac{\Delta^3 y_{-2} + \Delta^3 y_{-1}}{2} + \frac{4}{5!}\frac{\Delta^5 y_{-3} + \Delta^5 y_{-2}}{2} + \dots\right] \quad (10.16')$$

$$y''_{x_0} \approx \frac{1}{h^2}\left[\Delta^2 y_{-1} - \frac{1}{12}\Delta^4 y_{-2} + \dots\right] \quad (10.17')$$

$$y'''_{x_0} \approx \frac{1}{h^3}\left[\frac{\Delta^3 y_{-2} + \Delta^2 y_{-1}}{2} - \frac{1}{4}\frac{\Delta^5 y_{-3} + \Delta^5 y_{-2}}{2} + \dots\right] \quad (10.18')$$

$$y^{IV}_{x_0} \approx \frac{1}{h^4}\left[\Delta^4 y_{-2} + \dots\right] \quad (10.19')$$

$$y^{V}_{x_0} \approx \frac{1}{h^5}\left[\frac{\Delta^5 y_{-3} + \Delta^5 y_{-2}}{2} + \dots\right] \quad (10.20')$$

EXAMPLE 10.3: Find $y'(0.6)$ and $y''(0.6)$ for the function $y = y(x)$ given by the following table.

x	0.4	0.5	0.6	0.7	0.8
y	1.5836494	1.7974426	2.0442376	2.3275054	2.6510818

SOLUTION: First of all we construct the difference Table 10.2.

Take $x_0 = 0.6$, then $p = 0$, $h = 0.1$,

$\Delta y_0 = 0.2832678$, $\Delta y_{-1} = 0.2467950$, $\Delta^2 y_{-1} = 0.0364728$,
$\Delta^3 y_{-1} = 0.0038358$, $\Delta^3 y_{-2} = 0.0034710$, $\Delta^4 y_{-2} = 0.0003648$.

Table 10.2 Difference Table for Derivative Approximation

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$
0.4	1.5836494				
		0.2137932			
0.5	1.7974426		0.0330018		
		0.2467950		0.0034710	
0.6	2.0442376		0.0364728		0.0003648
		0.2832678		0.0038358	
0.7	2.3275054		0.0403086		
		0.3235764			
0.8	2.6510818				

Substituting these values in the formulae (10.16′) and (10.17′), respectively we get

$$y'_{x_0} \approx 10\left[\frac{0.2467950 + 0.2832678}{2} - \frac{1}{6}\,\frac{0.0034710 + 0.0038358}{2}\right]$$

$$= 10[0.2650314 - 0.0006089] = 2.6442 .$$

$$y''_{x_0} \approx 100\left[0.0364728 - \frac{1}{12}(0.0003648)\right]$$

$$= 100[0.0364728 - 0.0000304] = 3.6442.$$

As a check, we note that the tabulated function is

$$y = 2e^x - x - 1.$$

Thus $\quad y' = 2e^x - 1$

and $\quad y'' = 2e^x.$

Substituting $x = 0.6$; we obtain

$y' = $ [illegible]$.6442$, $y'' = 3.6442$.

By comparison of these values we note that the values found by numerical differentiation are correct to four decimal places in both cases.