Numerical Differentiation

→ The method of obtaining the derivative of a function using a numerical technique is known as Numerical differentiation.

→ There are essentially two situation where numerical differentiation is required, they are:

(i) The function values are known but the function is unknown — such ~~that~~ functions are called tabulated function.

(ii) The functions to be differentiated is complicated and therefore, it is difficult to differentiate (various) numerically, differentiation method can be applied to both tabulated & continuous function.

∘ Forward Difference Quotient:

consider a small increment $\Delta x = h$ in x. According to Taylor's theorem, we have.

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\theta)$$

for $x \le \theta \le x+h$. By rearranging the terms, we got

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h^2}{2} f''(\theta)$$

Thus, if h is choosen to be sufficiently small, $f'(x)$ can be approximated by

$$\boxed{f'(x) = \frac{f(x+h) - f(x)}{h}} \quad \rightarrow (1)$$

with a trancation error of

$$\boxed{E_t(h) = -\frac{h}{2} f''(\theta)} \quad \rightarrow (2)$$

Equation (1) is called the first order forward difference quotient. This is also known as two-point formula. The truncation error ~~descends~~ is in the order of h and can be decreased by decreasing h.

Similarly, we can show that the first-order backward difference quotient is

$$\boxed{f'(x) = \frac{f(x) - f(x-h)}{h}} \quad \to (3)$$

Q. Estimate appx. derivative of $f(x) = x^2$ at $x=1$, for $h = 0.2, 0.1, 0.05$, and 0.01 using the first-order forward difference formula.

Ans:
$$f'(x) = \frac{f(x+h) - f(x)}{h}$$

$$\therefore \quad f'(1) = \frac{f(1+h) - f(1)}{h}$$

$\therefore$ for $h = 0.2$:
$$f'(1) = \frac{f(1.2) - f(1)}{0.2} = 2.2$$

$\therefore$ for $h = 0.1$
$$f'(1) = \frac{f(1.1) - f(1)}{0.1} = 2.1$$

$\therefore$ for $h = 0.05$
$$f'(1) = \frac{f(1.05) - f(1)}{0.05} = 2.05$$

$\therefore$ for $h = 0.01$
$$f'(1) = \frac{f(1.01) - f(1)}{0.01} = 2.01$$

now, by calculas
$$\left.\frac{dx^2}{dx}\right|_{x=1} = \left.2x\right|_{x=1} = 2$$

Note: The derivative approximation approaches the exact values as h decreases. The truncation error increases proportionally with increase of h.

• **Q.** Compute the appx. derivatives of $f(x) = \sin x$ at $x = 0.45$ radians at increasing values of h from 0.01 to 0.04 with a step size of 0.05.

Ans: $f(x) = \sin x$

Using two point formula,

$$f'(x) = \frac{f(x+h) - f(x)}{h}$$

given, $x = 0.45$ radians

$\therefore \; f(x) = \sin(0.45) = 0.4350$ (rounded to 4 digits)

h	$f(x+h)$	$f'(x)$	Error
0.010	0.4439	0.8900	0.0104
0.015	0.4484	0.8933	0.0071
0.020	0.4529	0.8950	0.0054
0.025	0.4573	0.8935	0.0069
0.030	0.4618	0.8933	0.0071
0.035	0.4662	0.8914	0.0090
0.040	0.4706	0.8900	0.0104

◦ **Central Difference Quotient:**

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(\theta_1) \rightarrow (1)$$

Similarly,

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(\theta_1) \rightarrow (2)$$

Subtracting (2) from (1),

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3!}[f'''(\theta_1) + f'''(\theta_2)] \rightarrow (3)$$

Thus, we have

$$\boxed{f'(x) = \frac{f(x+h) - f(x-h)}{2h}} \rightarrow (4)$$

with the truncation error of,

$$E_6(h) = -\frac{h^2}{12}\left[f'''(\theta_1) + f'''(\theta_2)\right] = -\frac{h^2}{6} f'''(\theta)$$

which is of order h^2. (4) is called the <u>second-order central difference quotient</u>.

Note, this is the avg. of forward difference quotient & backward ~~differen~~ difference quotient. This is also known as three point formula.

Note! The approximation in three point formula.

Q. Estimate approximation derivative of $f(x) = x^2$ at $x = 1$, $h = 0.2, 0.1, 0.05$ using central difference quotient.

Ans: At $x = 1$,

$$f'(1) = \frac{f(1+h) - f(1-h)}{2h}$$

$\therefore$ for $h = 0.2$,

$$f'(1) = \frac{f(1.2) - f(0.8)}{2 \times 0.2} = 2$$

$\therefore$ for $h = 0.1$

$$f'(1) = \frac{f(1.1) - f(0.9)}{2 \times 0.2} = 2$$

$\therefore$ for $h = 0.05$

$$f'(1) = \frac{f(1.05) - f(0.95)}{2 \times 0.05} = 2$$

Analytical value,

$$\left.\frac{dx^2}{dx}\right|_{x=1} = 2$$

$\therefore$ Error at each case (each h) is 0.

Note 1: In each case, the derivative is exactly for all values of h [for the last problem]. This is because the quadratic approximation for a quadratic function has been used.

Note 2: The 5 point central difference formula is given by ~~by~~ by,

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} \rightarrow (i)$$

~~Note 3: (i) is a fourth order approximation and the fr~~

Note 3: (i) is a fourth order approximation and the truncation ~~fraction~~ error is of order h^4. In this case truncation error approaches to 0 much faster compare to the point formula.

Q. Estimate the approximation derivative of $f(x) = 4x^3$ at $x=1$ and $h=0.1$ with 5 point central difference quotient.

Ans: $\therefore f'(1) = \frac{-f(1+2h) + 8f(1+h) - 8f(1-h) + f(1-2h)}{12h}$

for $h = 0.1$

$$\therefore f'(1) = \frac{-f(1.2) + 8f(1.1) - 8f(0.9) + f(0.8)}{12 \times 0.1}$$

$$= 12$$

- **Higher Order Derivative:**

We can also obtain approximations to higher order derivatives using Taylor's expansion. To illustrate this, we derive here the formula for $f''(x)$. We know,

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + R_1$$

and

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(x) + R_2$$

Adding these two expansions gives

$$f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + R_1 + R_2$$

Therefore,

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{(R_1 + R_2)}{h^2}$$

Thus, the approximation to second derivative is

$$\boxed{f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}}$$

The truncation error is,

$$E_t(h) = -\frac{R_1 + R_2}{h^2}$$

$$\cancel{= \frac{+}{h^2} h^4} = \frac{-1}{h^2} \frac{h^4}{4!} \left(f^{(4)}(\theta_1) + f^{(4)}(\theta_2) \right)$$

$$= -\frac{h^2}{12} f^{(4)}(\theta)$$

∴ The error is of order h^2

∴ Similarly, we can obtain other higher-order derivatives with the error of order h^3 and h^4.

Q. Use 3pt. formula to estimate 2nd order derivative of $x^2 + 2x + 1$ at $x = 0.5$ with $h = 0.01$

Ans: $f'(0.5) = \dfrac{f(0.5+h) - 2f(0.5) + f(0.5-h)}{h^2}$

At $h = 0.01$

$$f''(0.5) = \frac{f(0.51) - 2f(0.5) + f(0.49)}{h^2}$$

$$= 2$$

Q. $f(x) = \cos x$, find $f''(x)$ at $x = 0.75$ radian from $h = 0.01$ to 0.05 with step size 0.005.

Ans:- $f(x) = \cos x$

~~using loop~~

$$f''(x) = \cancel{\cos x}\ \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

Given, $x = 0.75$, $\therefore f(x) = \cos(0.75) = 0.7317$

$$\therefore f''(x) = \frac{f(0.75+h) - 2f(0.75) + f(0.75-h)}{h^2}$$

h	$f(x+h)$	$f(x-h)$	$f''(x)$
0.010	0.7248	0.7384	-2
0.015	0.7214	0.7418	~~208~~ -0.8889
0.020	0.7179	0.7452	-0.75
0.025	0.7144	0.7485	-0.8
0.030	0.7109	0.7518	-0.7778
0.035	0.7074	0.7550	-0.8163
0.040	0.7038	0.7584	-0.75
0.045	0.7003	0.7616	-0.7407
0.050	0.6967	0.7648	-0.76

Q. Apply 3 point formula of central quotient ~~difference~~ difference for finding $f'(x)$ at $x = 0.1$ with $h = 0.01$ of the following and find error:

(i) $\cosh x$

(ii) $e^x \sin x$

(iii) $\ln(1+x)$

(iv) $x^2 + 2x + 1$

(v) $1/(1+x^2)$

Ans: $f'(x) = \frac{f(x+h) - f(x-h)}{2h}$

given, $x = 1$ & $h = 0.1$

$\therefore f'(x) = \frac{f(1+0.1) - f(1-0.1)}{2 \times 0.1} = \frac{f(1.1) - f(0.9)}{0.2}$

(i) $f'(x) = 1.1772$

by calculus:

$$\frac{d}{dx} \cosh x \Big|_{x=1} = 0.1752$$

$\therefore$ error $= |0.1752 - 0.1772| = 0.998$

(ii) $f'(x) = 3.7533$

by calculus:

$$\frac{d}{dx} e^x \sin x \Big|_{x=1} = 3.7560$$

$\therefore$ error $= |3.7560 - 3.7533| = 0.0027$

(iii) $f'(x) = 0.5004$

by calculus:

$$\frac{d}{dx} \ln(1+x) \Big|_{x=1} = 0.5$$

$\therefore$ error $= |0.5 - 0.5004| = 0.0004$

(iv) $f'(x) = 4$

by calculus,

$$\frac{d}{dx} (x^2 + 2x + 1) \Big|_{x=1} = 4$$

$\therefore$ error $= |4 - 4| = 0$

(v) $f'(x) = \cancel{-0.4999} = \cancel{0.5}\ -0.49998$

by calculus,

$$\frac{d}{dx}\left(\frac{1}{1+x^2}\right)\Bigg|_{x=1} = -0.5$$

$\therefore$ error: $\left|-0.5 + 0.49998\right| = 0.00002$

- **Differentiating Tabulated Functions:**

Suppose that we are given a set of data points (x_i, f_i) $i = 0, 1, \dots, n$ which correspond to the values of an unknown function $f(x)$ and we wish ~~to~~ to estimate the ~~es~~ derivatives at these points. Assume that the points equally spaced with a step size of h.

When function values are ~~va~~ available in tabulated form, we may approximate this function by an interpolation polynomial $p(x)$ and the differentiate $p(x)$.

We will use here Newton's Interpolation polynomial.

Let, us consider the linear equation,

$$p_1(x) = a_0 + a_1(x - x_0) + R_1$$

where R_1 is the remainder term used for estimation. Upon differentiation of this formula, we obtain,

$$p_1'(x) = a_1 + \frac{dR_1}{dx}$$

Then the approximate derivative of ~~notebook~~ the function $f(x)$ is given by,

$$f'(x) = p_1'(x) = a_1$$

We know that,

$$a_1 = f[x_0, x_1]$$

$$= \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

On substituting,

$$h = x_1 - x_0$$

$$x_1 = x + h$$

$$x_0 = x$$

we get

$$\boxed{f'(x) = \frac{f(x+h) - f(x)}{h}} \longrightarrow (1)$$

This is the two-point forward difference formula.

Let us consider the quadratic approx. Here, we need to use three points. Thus,

$$p_2(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + R_2$$

Then, $p_2'(x) = a_1 + a_2[(x - x_0) + (x - x_1)] + \frac{dR_2}{dx}$

Thus we obtain

$$f'(x) = a_1 + a_2[(x - x_0) + (x - x_1)] \longrightarrow (2)$$

let, $x_0 = x$, $x_1 = x + h$, $x_2 = x + 2h$, then

$$a_1 = \frac{f(x+h) - f(x)}{h}$$

$$a_2 = f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}$$

$$= \frac{\frac{f(x_2) - f(x_1)}{x_2 - x_1} - \frac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0}$$

$$= \frac{f(x+2h) - 2f(x+h) + f(x)}{2h^2}$$

Substituting for a_1 & a_2 in (2) ~~and~~, we get,

$$\boxed{f'(x) = \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h}} \rightarrow (3)$$

This is a three-point forward difference formula.

We can obtain a three-point backward difference formula by replacing h by $-h$ in (3). The 3 point backward difference formula is given by

$$\boxed{f'(x) = \frac{3f(x) - 4f(x-h) - f(x-2h)}{2h}} \rightarrow (4)$$

Similarly, we can obtain the three-point difference formula by letting $x_0 = x, x_1 = x+h, x_1 = x+h$ in (2). Thus,

$$a_1 = \frac{f(x) - f(x-h)}{h}$$

$$a_2 = \frac{f(x+h) - 2f(x) + f(x-h)}{2h^2}$$

Substituting a_1 & a_2 in (2) we get,

$$\boxed{f'(x) = \frac{\cancel{f(x)} \cdot f(x+h) - f(x-h)}{2h}} \rightarrow (5)$$

This is the three point central difference formula.

Q. The table below gives the values of distance travelled by a car at various time intervals during the initial ~~...~~ running.

Time 't' t(s)	5	6	7	8	9
Distance s(t)	10.0	14.5	19.5	25.5	320

Estimate velocity at time $t=5$, $t=7$ and $t=9$

Ans: We know, velocity is the derivative of ~~de~~ displacement

At, $t=5$, we can use forward difference formula;

$$v(t) = \frac{-3s(t) + 4s(t+h) - s(t+2h)}{2h}$$

then,

$$v(5) = \frac{-3(10) + 4(14.5) - 19.5}{2(1)} = 4.25 \text{ km/s}$$

At $t=7$, we use three point central difference formula.

There fore,

$$v(7) = \frac{s(8) - s(6)}{2h} = \frac{25.5 - 14.5}{2} = 5.5 \text{ km/s}$$

At $t=9$, we use the backward difference formula.

$$v(9) = \frac{3s(9) - 4s(8) + s(7)}{2h}$$

$$= \frac{3(32) - 4(25.5) + 19.5}{2} = 6.75 \text{ km/s}$$

- **Higher order derivative in Tabulated form:**

Second and higher order derivative can be obtained from the Newton's divided difference formula.

The second order differentiation:

(i) Forward: $$f''(x) = \frac{2f(x) - 5f(x+h) + 4(x+2h) - 4(x+3h)}{h^2}$$

(ii) Backward: $$f''(x) = \frac{2f(x) - 5f(x-h) + 4f(x-2h) - 4(x-3h)}{h^2}$$

(iii) Central: $$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

Q. Use the table of the data given:

time	5	6	7	8	9
Distance	10.0	14.5	19.5	25.5	32.0

to estimate accelaration at $t=7$.

$$a'(t) = \frac{f(t+h) - 2f(t) + f(t-h)}{h^2}$$

$$= \frac{f(8) - 2f(7) + f(6)}{1^2}$$

$$= \frac{25.5 - 2\times 19.5 + 14.5}{1^2}$$

$$= 1 \text{ km/s}^2$$

○ Richardson Extrapolation:

Let, us assume

$$x_k = x^* + Mh^n \quad \longrightarrow (1)$$

x_k is the k^{th} estimate of sol^n x^* and Mh^n is the error term.

Let us replace, h by rh & obtain another estimate for x^*

$$x_{k+1} = x^* + Mr^n h^n \quad \longrightarrow (2)$$

Multiplying (1) by r^n & solving for x^*,

$$\boxed{x^* = x_R = \frac{x_{k+1} - r^n x_k}{1 - r^n}} \quad \longrightarrow (3)$$

This is known as Richardson extrapolation estimate.

Using this we can obtain a higher-order formula from a lower-order formula, thus improving the accuracy of the estimates. This process is called extrapolation

Now let,

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(\theta)$$

$$= D(h) - \frac{h^2}{6} f'''(\theta) \quad \longrightarrow (4)$$

where $D(h)$ is the estimate obtained using h as step size.
Note that, $f'(x)$ is the exact solⁿ which is usually appx. by $D(h)$. If we remove the error term then we can obtain a better approximation.

Now, let us obtain better approximation for $f'(x)$ by replacing h by rh. Thus,

$$f'(x) = \frac{f(x+rh) - f(x-rh)}{2hr} - \frac{h^2 r^2}{6} f''(\theta)$$

$$= D(rh) - \frac{h^2 r^2}{6} f''(\theta) \rightarrow (5)$$

We can eliminate the error term by multiplying (4) by r^2 & subtracting it with (5),

$$f'(x) = \frac{D(rh) - r^2 D(h)}{1-r^2} \rightarrow (6)$$

This would give a better estimate of $f'(x)$ as we have eliminated the error term h^2; (6) becomes

$$f'(x) = \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h} \rightarrow (7)$$

Note that this is a five-point central difference formula which contains error only in the order in h^4. We can repeat this process further to eliminate the error term containing h^4 and so on.

One of the most common choices of r is 0.5. Letting $r = 1/2$, (6) becomes

$$f'(x) = \frac{f(x-h) - 8(x-h/2) + 8f(x+h/2) - f(x+h)}{6h} \rightarrow (8)$$

Note that the use of this formula depends on the availability of function at $x \pm h/2$.

Q. Estimate first derivative at $x = 0.5$ from the given data using Richardson Extrapolation.

x	-0.5	-0.25	0	0.25	0.5	0.75	1.0
$f(x) = e^x$	0.6065	0.7788	1.0000	1.2840	1.6487	2.1170	2.7183

x	1.25	1.5
$f(x)$	3.4903	4.4817

Ans: Let, us estimate $f'(x)$ at $x = 0.5$ & assume $h = 0.5$ & $r = 1/2$.

Then using three-point central formula, we have,

$$D(h) = D(0.5) = \frac{f(1.0) - f(0)}{2 \times 0.5} = 1.7183$$

$$D(rh) = D(0.25) = \frac{f(0.75) - f(0.25)}{0.5} = 1.666$$

$$f'(x) = \frac{D(rh) - r^2 D(h)}{1 - r^2}$$

$$\therefore f'(0.5) = \frac{1.666 - (0.25 \times 1.7183)}{0.75}$$

$$= 1.6486$$