

Numerical Differentiation

What is derivative in action?

- Given is the position $x(t)$ in meters of an object at time t , the first derivative with respect to t , $x'(t)$, is the velocity in meters/second (note: The integral of velocity is position to within a constant)
- Given is the velocity $v(t)$ in meters/second of an object at time t , the first derivative with respect to t , $v'(t)$, is the acceleration in meters/second squared

Need and Scope

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



Why do we need to approximate derivatives at all?



There are essential two situations where numerical differentiation is required. They are:

1. The function values are known but the function is unknown. We may still be interested in studying changes in the data, which are related, of course, to derivatives.
2. The function to be differentiated is complicated and, therefore, it is difficult to differentiate. It might be significantly simpler to approximate the derivative instead of computing its exact value.

What is derivative?

- According to the dictionary differentiation means “mark off by differences”.
- The derivative which is fundamental concept of differentiation is rate of change of dependent variable with respect independent variable.
- $\frac{dy}{dx} = \lim_{\Delta x \rightarrow 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$
- Where, $f(x)$ or y is independent variable and x is dependent variable.
- $\frac{dy}{dx}$ or $f'(x)$ is first derivative of $f(x)$ or y with respect to x evaluated at x_i
- derivative of $f(x)$ at x is the slope of the line tangent to $f(x)$ at x
- Numerical differentiation methods that could be applied to both tabulated and continuous function.

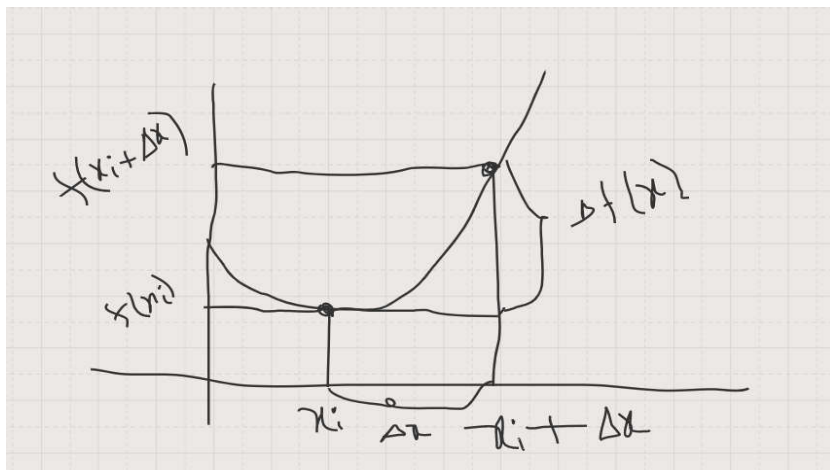


Figure 1: Graphical Representation of Differentiation

Differentiating Continuous Functions

- Numerical algorithms for computing the derivative of a function require the estimate of the slope of the function for some particular range of x values.
- Here, the numerical process of approximating the derivative $f'(x)$ of a function $f(x)$ is carried out when the function is continuous and itself available.

Forward and Backward Difference Quotient

$$\text{Forward Difference formula: } f'(x) = \frac{f(x+h) - f(x)}{h}$$

$$\text{Backward Difference formula: } f'(x) = \frac{f(x) - f(x-h)}{h}$$

Derivation of Forward Difference Formula:

Let $y = f(x)$, be a solution of the equation. Consider a small increment in $\Delta x = h$ in x . According to Taylor’s theorem, we have:

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

for $x \leq \theta \leq x+h$. By rearranging the terms, we get

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

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

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

- Since this approximation of the derivative at x is based on the values of the function at x and $x + h$, the approximation (1) is called a forward different quotient or two point formula.
- The $E_t(h) = -\frac{h}{2} f''(x)$ is the error term. Since the approximation (2) can be thought of as being obtained by truncating this term from the exact formula (1), this error is called the truncation error. The small parameter h denotes the distance between the two points x and $x+h$. As this distance tends to zero, i.e., $h \rightarrow 0$, the two points approach each other and we expect the approximation (2) to improve.
- The “speed” in which the error goes to zero as $h \rightarrow 0$ is called the rate of convergence. The truncation error is in the order of ‘ h ’ and can be decreased by decreasing ‘ h ’. When the truncation error is of the order of $O(h)$, we say that the method is a first order method. We refer to a methods as a p^{th} order method if the truncation error is of the order of $O(h^p)$.

Similarly, the approximation of the derivative at x that is based on the values of the function at $x - h$ and x , i.e.

$$f'(x) = \frac{f(x) - f(x - h)}{h} \dots\dots\dots(3) \text{ is called a backward differencing.}$$

Example: Estimate approximate 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.

Solution:

Analytical Method: $f'(x) = 2x$, i.e. $f'(x=1) = 2 * 1 = 2$ (true value)

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

Therefore,

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

Derivative approximations are tabulated below:

<i>H</i>	<i>f' (1)</i>	Error
0.2	2.2	0.2
0.1	2.1	0.1
0.05	2.05	0.05
0.01	2.01	0.01

Conclusively, it is found that the derivative approximation approaches the exact value as ‘*h*’ decreases. The truncation error decreases proportionally with decrease in ‘*h*’. There is no round off error.

Central Difference Quotient

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

Derivation of Central Difference Formula:

Equation (2) was obtained using the linear approximation to $f(x)$. This would give large truncation error if the functions were of higher order. In such cases, we can reduce truncation errors for a given ‘*h*’ by using a quadratic approximation rather than a linear one. This can be achieved by the following form of Taylor’s Expansion.

According to Taylor’s theorem, we have

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

Similarly,

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

by subtracting, we obtain

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

Thus, we have

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

with a truncation error of

$$E_t(h) = -2 * \frac{h^2}{12} f'''(x) = -\frac{h^2}{6} f'''(x), \text{ which is order of 'h}^2\text{'}$$

This is called the second order *central difference quotient or three point formula*.

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

Solution:

We have: $f(x) = x^2$, i.e. $f'(x=1) = 2x = 2$ (true value)

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

Therefore,

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

Derivative approximations are tabulated below: (*forward difference quotient*)

<i>h</i>	<i>f' (1)</i>	Error
0.2	2.2	0.2
0.1	2.1	0.1
0.05	2.05	0.05
0.01	2.01	0.01

Derivative approximations are tabulated below: (*central difference quotient*)

<i>H</i>	<i>f' (1)</i>	Error
0.2	2.0	0
0.1	2.0	0
0.05	2.0	0
0.01	2.0	0

Higher-order Derivatives

We can also obtain approximations of higher order derivatives using Taylor's Series Expansion.

As we know that:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + R_1 \dots \dots \dots (4)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(x) + R_2 \dots \dots \dots (5)$$

Where error terms,

$$R_1 = \frac{h^4}{4!} f^{iv}(\theta_1) \text{ and}$$

$$R_2 = \frac{h^4}{4!} f^{iv}(\theta_2)$$

So, the addition of two expansions gives:

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

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

Therefore, the approximation of 2nd derivative is:

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

With truncation error:

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

i.e.

$$E_t(h) = -\frac{1}{h^2} \frac{2h^4}{4!} \{f^4(\theta_1) + f^4(\theta_2)\} = -\frac{h^2}{12} f^4(\theta)$$

So, the error is of order h^2

Example:

Find the approximation to second derivative of $\cos(x)$ at $x = 0.75$ radian with $h = 0.01$. Compare with the true value.

Solution:

We have given: $y = f(x) = \cos(x)$

Then: $y' = f'(x) = -\sin(x)$ and $y'' = f''(x) = -\cos(x)$

Therefore Exact Value: $f''(x=0.75) = -\cos(0.75) = -0.7316888$

Using the formula at $h = 0.01$

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = \frac{f(0.76) - 2f(0.75) + f(0.74)}{0.0001}$$

$$f''(x) = \frac{0.7248360 - 2(0.7316888) + 0.7384685}{0.0001}$$

$$f''(x) = \frac{1.4633046 - 1.4633778}{0.0001} = -0.7300000$$

Error: $\text{abs}(0.7316888 - 0.7300000) = 0.0016888$

Differentiating Tabulated Functions

If we are given a set of data points (x_i, f_i) , for $i = 0, 1, 2 \dots n$, which corresponds to the values of an unknown function $f(x)$ and we wish to estimate the derivative at these points. Assume that the points are equally spaced with a step size of 'h'. When function values are available in tabulated form, we may approximate this function by an interpolation polynomial $P(x)$ and then differentiate $P(x)$. If we consider the quadratic approximation, we need to use three points as referenced by Newton Polynomial Form:

i.e. $P_2(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) \dots \dots \dots (1)$

Then: $P'_2(x) = a_1 + a_2\{(x - x_0) + (x - x_1)\} \dots \dots \dots (2)$

Let first consider the linear equation

$$P_1(x) = a_0 + a_1(x - x_0) + R_1$$

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

$$P'_1(x) = a_1 + \frac{dR_1}{dx}$$

Then the approximate derivate of the function $f(x)$ is given by

$$P'_1(x) = f'(x) = a_1$$

We know that according to Newton divide difference table:

$$\begin{aligned} a_1 &= f[x_0, x_1] \\ &= \frac{f(x_1) - f(x_0)}{x_1 - x_0} \end{aligned}$$

On substituting

$$\begin{aligned} h &= x_1 - x_0 \\ x_1 &= x + h \\ x_0 &= x \end{aligned}$$

we get

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

This is the familiar **two-point** forward difference formula.

Now, let us consider the quadratic approximation. 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

$$f'(x) = a_1 + a_2 [(x - x_0) + (x - x_1)] \dots \dots \dots (3)$$

Let $x_0 = x$,
 $x_1 = x + h$,
 $x_2 = x + 2h$,

Then

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

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

$$\begin{aligned} &= \frac{\frac{f(x_2) - f(x_1)}{x_2 - x_1} - \frac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0} \\ &= \frac{\frac{f(x_2) - f(x_1)}{h} - \frac{f(x_1) - f(x_0)}{h}}{2h} \\ &= \frac{f(x_2) - 2f(x_1) + f(x_0)}{2h^2} \\ &= \frac{f(x+2h) - 2f(x+h) + f(x)}{2h^2} \end{aligned}$$

Substituting for a_1 and a_2 , at (3) we get:

$$f'(x) = \frac{f(x+h) - f(x)}{h} + \frac{f(x+2h) - 2f(x+h) + f(x)}{2h^2} [(x - x_0) + (x - x_1)]$$

Replace $x = x_0$

$$\begin{aligned} f'(x) &= \frac{f(x+h) - f(x)}{h} + \frac{f(x+2h) - 2f(x+h) + f(x)}{2h^2} [(0) + (-h)] \\ &= \frac{2f(x+h) - 2f(x) - f(x+2h) + 2f(x+h) - f(x)}{2h} \end{aligned}$$

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

This is a **three-point** forward difference formula.

Similarly, three-point backward difference formula is given by [replacing $h = -h$]

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

Similarly, we can obtain three-point central difference formula.

Let

$$x_0 = x,$$

$$x_1 = x - h,$$

$$x_2 = x + h.$$

Thus,

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

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

Substituting these values, we get

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

Example: The table below gives the values of distance travelled by a car at various time intervals during the initial running

Time, t(s)	5	6	7	8	9
Distance travelled, s(t), (km)	10.0	14.5	19.5	25.5	32.0

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

Solution:

At $t = 5$, we use the three-point forward difference formula.

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

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

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

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

$$v(5) = \frac{s(8) - s(6)}{2(1)} = \frac{25.5 - 14.5}{2} = 5.5 \text{ km/s}$$

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

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

$$v(9) = \frac{3s(9) - 4s(8) + s(7)}{2(1)} = \frac{3(32) - 4(25.5) + 19.5}{2} = 6.75 \text{ km/s}$$

Higher Order Derivative using Newton Divide Difference Formula

Forward

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

Backward

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

Central

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

Example: The table below gives the values of distance travelled by a car at various time intervals during the initial running

Time, t(s)	5	6	7	8	9
Distance travelled, s(t), (km)	10.0	14.5	19.5	25.5	32.0

Estimate acceleration at time $t = 7$ s.

Solution:

Acceleration is given by the second derivative of $s(t)$. Therefore,

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

$$a(7) = \frac{25.5 - 2(19.5) + 14.5}{1} = 1.0 \text{ km/s}^2$$

Summary: Formulas Differentiating Tabulated Functions

Three-point forward difference formula	$f'(x) = \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h}$
Three-point backward difference formula	$f'(x) = \frac{3f(x) - 4f(x-h) + f(x-2h)}{2h}$
Three-point central difference formula	$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$
Five-point forward difference formula	$f''(x) = \frac{2f(x) - 5f(x+h) + 4f(x+2h) - f(x+3h)}{h^2}$
Five-point backward difference formula	$f''(x) = \frac{2f(x) - 5f(x-h) + 4f(x-2h) - f(x-3h)}{h^2}$
Five-point central difference formula	$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$

Derivatives using Newton’s forward interpolation formula for non-tabulated value

- When the values of the arguments are equally spaced and we are to find the derivative for some given x lying near the beginning of the table, we can represent the function by *Newton’s forward interpolation formula*.
- When the value of $\frac{dy}{dx}$ is required at the point near the end of the table we use *Newton’s backward interpolation formula* and we may use suitable *central difference interpolation formula* when the derivation is to be found at some point lying near the middle of the tabulated values.
- If the values of arguments x are not equally spaced, we should use *Newton’s divided difference formula* to approximate the function $y = f(x)$.

Consider Newton’s forward interpolation formula

$$y = y_0 + u \Delta y_0 + \frac{u(u-1)}{2!} \Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!} \Delta^3 y_0 + \dots \text{----- (6)}$$

where $u = \frac{x - x_0}{h}$ ----- (7)

Differentiating (6) with respect to u we get,

$$\frac{dy}{du} = \Delta y_0 + \frac{2u - 1}{2!} \Delta^2 y_0 + \frac{3u^2 - 6u + 2}{3!} \Delta^3 y_0 \dots \dots \dots (8)$$

Differentiating (7) with respect to x we get,

$$\frac{du}{dx} = \frac{1}{h} \text{ ----- (9)}$$

Now from equations (8) and (9)

$$\begin{aligned} \frac{dy}{dx} &= \frac{dy}{du} \cdot \frac{du}{dx} \\ \Rightarrow \frac{dy}{dx} &= \frac{1}{h} [\Delta y_0 + \frac{2u-1}{2!} \Delta^2 y_0 + \frac{3u^2-6u+2}{3!} \Delta^3 y_0 \dots \dots] \text{ ----- (10)} \end{aligned}$$

Expression (10) gives the value of $\frac{dy}{dx}$ at any x which is not tabulated.

For tabulated values of x, particularly when $x = x_0$ and $u = 0$, we have

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

Differentiating (10) with respect to x we get

$$\frac{d^2y}{dx^2} = \frac{1}{h^2} [\Delta^2 y_0 + (u - 1) \Delta^3 y_0 + \frac{6u^2 - 18u + 11}{12} \Delta^4 y_0 \dots \dots]$$

Putting $u = 0$ we have

$$\frac{d^2y}{dx^2} \Big|_{x=x_0} = \frac{1}{h^2} [\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12} \Delta^4 y_0 - \dots \dots]$$

Formula for computing higher order derivation may be obtained by successive differentiation.

Example: From the table of values given below find $\frac{dy}{dx}$ and $\frac{d^2y}{dx^2}$ for $x = 1$.

x	y	Δ	Δ^2	Δ^3	Δ^4	Δ^5
1	1	7				
2	8	19	12	6		
3	27	37	18	6	0	
4	64	61	24	6	0	0
5	125	91	30			
6	216					

We have, $x_0=1, h = 1, x = 1.$
 $\therefore u = 0$

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

$$\begin{aligned} \therefore \left(\frac{dy}{dx}\right)_{x=1} &= \frac{1}{1} \left[7 - \frac{1}{2} (12) + \frac{1}{3} (6) - 0 \right] \\ &= 7 - 6 + 2 \\ &= 3 \end{aligned}$$

$$\begin{aligned} \left(\frac{d^2y}{dx^2}\right)_{x=1} &= \frac{1}{h^2} \left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12} \Delta^4 y_0 - \dots \right] \\ &= \frac{1}{1} (12 - 6 + 0) \\ &= 6 \end{aligned}$$

Home Task: Find $\frac{dy}{dx}$ and $\frac{d^2y}{dx^2}$ for $x = 2$ and $x = 1.5$ for the above table.

Error Analysis

Since, analytical methods give exact answers; the numerical techniques provide only approximations to derivatives. Numerical differentiation methods are very sensitive to round off errors, in addition to the truncation error introduced by the methods of themselves. So, it is necessary to discuss the errors and ways to minimize them.

If $E_r(h)$ is the round off error introduced in an approximation of derivative, and $E_t(h)$ is the truncation error then the total error is given by:

$$E(h) = E_r(h) + E_t(h) \dots \dots \dots (11)$$

Calculation of Round off error $E_r(h)$:

Now consider two point formulae for the purpose of analysis.

$$f'(x) = \frac{f(x+h) - f(x)}{h} = \frac{f_1 - f_0}{h}$$

If we assume round off error in f_1 and f_0 as e_1 and e_0 respectively, then:

$$f'(x) = \frac{(f_1 + e_1) - (f_0 + e_0)}{h} = \frac{(f_1 - f_0)}{h} + \frac{(e_1 - e_0)}{h}$$

If e_1 and e_0 are of magnitude of e and opposite sign, then bound of round off error:

$$|E_r(h)| \leq \frac{2e}{h}$$

Calculation of Truncation error $E_t(h)$:

We know, the truncation error for two point formula is:

$$|E_t(h)| \leq -\frac{h}{2} f''(\theta) \leq \frac{M_2 h}{2}$$

M_2 is the bound given by $M_2 = \max |f''(\theta)| \{ \because x \leq \theta \leq (x+h) \}$

Thus the boundary for total error in the derivative is:

$$|E(h)| \leq \frac{M_2 h}{2} + \frac{2e}{h} \dots \dots \dots (12)$$

We can obtain a rough estimation of h that gives us minimum error, by differentiating equation (12) with respect to h , we get:

$$|E'(h)| \leq \frac{M_2}{2} - \frac{2e}{h^2}$$

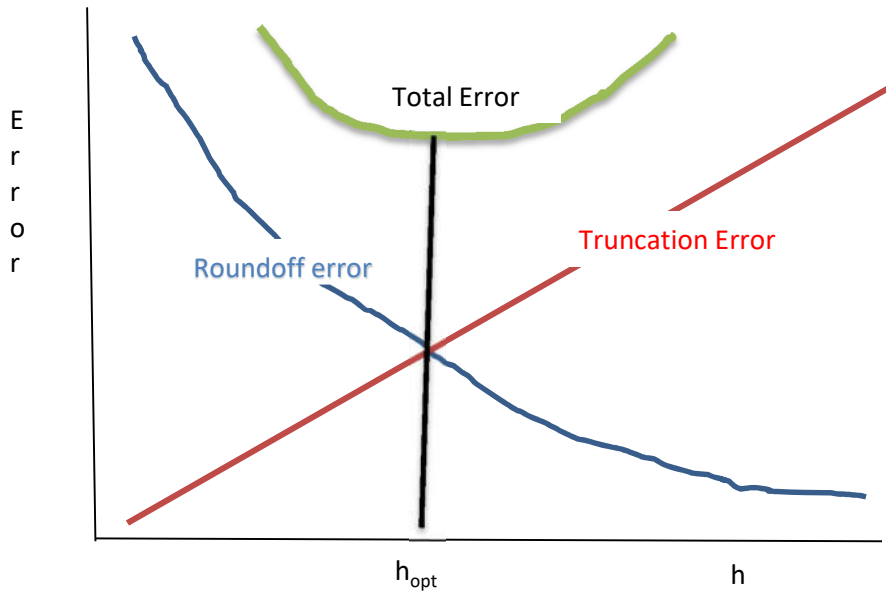
Now, we know that $E(h)$ is minimum when $E'(h) = 0$, solving for h we get h_{opt}

$$0 \leq \frac{M_2}{2} - \frac{2e}{h^2}$$

$$h_{opt} = 2 \sqrt{\frac{e}{M_2}}$$

Where h_{opt} is optimum step size, substituting this value in equation (12) we get:

$$E(h_{opt}) = 2\sqrt{eM_2}$$



Example:

Compute the approximate derivative of $f(x) = \sin(x)$ at $x = 0.45$ radian at increasing value of 'h' from 0.01 to 0.04 with a step size of 0.005. Analyze the total error. What is the optimum step size?

Solution:

We have given: $y = f(x) = \sin(x)$ and $f'(x) = \cos(x)$

Using forward difference formula:

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

Given $x = 0.45$ radian

So, $f(x=0.45\text{rad}) = \sin(0.45\text{rad}) = 0.4350$ (rounded to four digits)

And $f'(x=0.45\text{rad}) = \cos(0.45\text{rad}) = 0.9004$

Table below gives the approximate derivatives of $\sin x$ at $x=0.45$ using various value of h

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

The total error decreases from 0.0104 (at $h = 0.01$) till $h = 0.02$ and again increases when 'h' is increased. Since, we have used four significant digits; the bound for round off error 'e' is 0.5×10^{-4} .

For the two point formula, the bound M_2 is given by:

$$M_2 = \max |f''(\theta)| \quad \text{for: } 0.41 \leq \theta \leq 0.49$$

$$\text{i. e. } M_2 = |-\sin 0.49| = 0.4706$$

Therefore the optimum step size:

$$h_{opt} = 2 \sqrt{\frac{e}{M_2}} = 2 \sqrt{\frac{0.5 \times 10^{-4}}{0.4706}} = 0.0206$$

Richardson Extrapolation

Two ways to improve derivative estimates, when employing finite difference:

1. Decrease the step size
2. Use higher order formula that employs more points

Richardson Extrapolation:

- Uses two derivative estimation to compute the third to get more accurate approximation.
- Based on model for the error in numerical process.
- Used to improve the estimates of numerical solutions.

Assume,

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

$x_k \rightarrow k^{\text{th}}$ estimation of the solution x^*

$Mh^n \rightarrow$ is the error term

Replace $h = rh$

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

Multiplying equation (1) by r^n and solving for x^* we get,

$$x^* = x_r = \frac{x_{k+1} - r^n x_k}{1 - r^n} \dots \dots \dots (3)$$

Equation (3) is known as Richardson Extrapolation.

Derivation of Richardson Extrapolation using three point central difference formula:

Three point central difference formula:

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

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

Let $h = rh$

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

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

Multiplying equation (4) by r^2 and subtracting from (5)

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

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

Equation 6 is Richardson extrapolation formula using three point central difference formula and get better approximation of $f'(x)$ by eliminating error term h^2 . The most common choice of r is $r = 0.5$.

Example:

Show that, using the data given below, Richardson extrapolation technique can provide better estimates for $f'(x)$ at $x = 0.5$ and assume $h = 0.5 ; r = 0.5$.

X	-0.5	-0.25	0	0.25	0.5	0.75	1.0	1.25	1.5
f(x)	0.6065	0.7788	1.0000	1.2840	1.6487	2.1170	2.7183	3.4903	4.4871

Solution:

Using three point central difference formula:

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

$$D(rh) = D(0.25) = \frac{f(x + h) - f(x - h)}{2h} = \frac{f(0.75) - f(0.25)}{2 * 0.5 * 0.5} = 1.666$$

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

Therefore,

$$f'(0.5) = \frac{1.666 - (1.7183) * (0.5)^2}{0.75} = 1.6486$$

Correct Value of $f'(0.5) = e^x = e^{0.5} = 1.6487$

$$\text{Relative \% Error} = \frac{1.6487 - 1.6486}{1.6487} * 100\% = 0.01\%$$