Numerical Differentiation

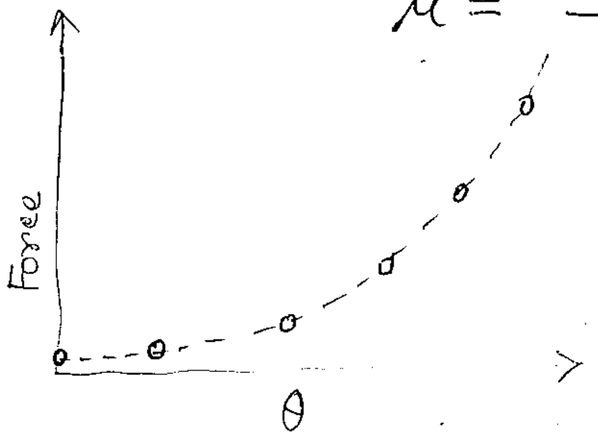
This normally arises

1. To approximate the derivative of a fn^c
2. To derive formulas to approximate the derivatives of a function in terms of linear combination of function values

Approximating derivative:

For example. coefficient of friction μ

$$\mu = \frac{dF/d\theta}{F(\theta)}, \quad \text{where } \frac{dF}{d\theta} \text{ is the rate of change of force.}$$



* We can approximate the fn^c by a polynomial.
* Then, we can take the derivative.

Deriving the formulas for derivative

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0+h) - f(x_0)}{h}$$

As we see, we can generate an approximation to $f'(x_0)$. We can use different approaches to approximate.

1. Lagrange polynomial
2. Taylor series expansion

So, First derivative of an arbitrary function "f" at x_0 is approximated using Lagrange polynomial as follows :

Let's assume that data from another point $x = x_1$. Now we can interpolate through $x = x_0$ and $x = x_1$

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

✓ Lagrange polynomial is chosen as it clearly isolates the dependence of the polynomial on the function values being interpolated.

Now, we differentiate $f(x)$ w.r.t x. Thus, we obtain,

$$f'(x) = \frac{d}{dx}\left[\frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1) + f[x_0, x_1, x_2] (x - x_0)(x - x_1) \right]$$

$$= \frac{1}{x_0 - x_1} f'(x_0) + \frac{1}{x_1 - x_0} f'(x_1) + (x - x_0)(x - x_1) \frac{d}{dx} f[x_0, x_1, x_2]$$

$$+ f[x_0, x_1, x_2] \frac{d}{dx} (x^2 - x x_0 - x x_1 + x_1 x_0)$$

$$= \frac{1}{x_0 - x_1} f'(x_0) + \frac{1}{x_1 - x_0} f'(x_1) + (x - x_0)(x - x_1) \frac{d}{dx} f[x_0, x_1, x_2]$$

$$+ f[x_0, x_1, x_2] (2x - x_0 - x_1) \quad \cdots ①$$

We evaluate $f'(x)$ at $x = x_0$. This simplifies ① to,

$$f'(x_0) = \frac{1}{x_0 - x_1} f'(x_0) + \frac{1}{x_1 - x_0} f'(x_1) + 0 + f[x_0, x_1, x_2] (x_0 - x_1)$$

$$= \frac{1}{x_0 - x_1} f'(x_0) + \frac{1}{x_1 - x_0} f'(x_1) + f[x_0, x_1, x_2] (x_0 - x_1)$$

If "f" has two continuous derivatives —

$$f[x_0, x_1, x_2] = \frac{f''(\xi)}{2}$$

There exists ξ between x_0 and x_1

So, we obtain,

$$f'(x_0) = \frac{f(x_1) - f(x_0)}{(x_1 - x_0)} + \frac{x_0 - x_1}{2} f''(\xi) \quad \cdots \cdots (2)$$

Generally, uniformly, or equally, spaced points are used for developing numerical differentiation formula.

That's $x_1 = x_0 + h$ can be used, where h is the spacing between two successive points.

From (2)

$$f'(x_0) = \frac{f(x_1) - f(x_0)}{(x_1 - x_0)} + \frac{x_0 - x_1}{2} f''(\xi)$$

$$= \frac{f(x_0 + h) - f(x_0)}{(x_0 + h - x_0)} + \frac{x_0 - x_0 - h}{2} f''(\xi)$$

$$= \frac{f(x_0 + h) - f(x_0)}{h} + \frac{-h}{2} f''(\xi)$$

$$= \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(\xi) \quad \cdots \cdots (3)$$

where $x_0 < \xi < x_0 + h$.

Here, approximation in (3) uses data to the right of the x_0, thus it is referred as the FORWARD DIFFERENCE

~~BACKWARD~~ Alternative Formula : Taylor series

Difference approximation is also possible using Taylor series expansion :

$$f(x_0+h) = f(x_0) + h f'(x_0) + \frac{h^2}{2} f''(\xi)$$

$$\Rightarrow \quad h f'(x_0) = -f(x_0) - \frac{h^2}{2} f''(\xi) + f(x_0+h)$$

$$\Rightarrow \quad f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h} - \frac{h}{2} f''(\xi)$$

Similar to derivation done ~~in~~ using divided difference method.

Backward difference

In Backward difference, approximation uses $x_1 = x_0 - h$ (that's a point at the left of x_0)

with $x_1 = x_0 - h$, we obtain,

$$f'(x_0) = \frac{f(x_0) - f(x_0 - h)}{h} + \frac{h}{2} f''(\xi)$$

where $x_0 - h < \xi < x_0$.

Similarly, if Taylor's expansion is used for approximating $f(x_0-h)$, we obtain,

$$f(x_0-h) = f(x_0) - h f'(x_0) + \frac{h^2}{2} f''(\xi)$$

$$\Rightarrow \quad h f'(x_0) = f(x_0) + \frac{h^2}{2} f''(\xi) - f(x_0-h)$$

$$\Rightarrow \quad f'(x_0) = \frac{f(x_0) - f(x_0-h)}{h} + \frac{h}{2} f''(\xi)$$

Error Term

Formulation of the first-order derivative has errors associated with it.

Here, the approximation formulas from forward and backward difference introduce errors, which is proportional to the first power of the spacing between adjacent points. :

$$\text{error} \propto h$$

Since, error is proportional to first-order of "h", formulas we derive is known as

"first-order approximation of derivative"

W If a first-order formula is used, and the step size is cut by a factor 2, the error should drop by the same factor.

↳ Can be a way to verify one's implementation.

So,

Error $E = -\frac{1}{2} h f''(\xi)$ forward

$E = \frac{1}{2} h f''(\xi)$ backward

if, for every $t \in [a\ b]$, $f''(t) < M_2$, where M_2 is a positive constant

$$|E| = |\pm \tfrac{1}{2} h f''(\xi)|$$

$$\leqslant \tfrac{1}{2} h M_2$$

Thus, $|E| = O(h)$

Given $f(x) = e^x$. Approximate derivative at $x=0$ Using fwd difference method

h	$f'(x=0)$	Error	Ratio
0·2000	1·1070	0·1070	0
0·1000	1·0517	0·0517	2·0695
0·0500	1·0254	0·0254	2·0340
0·0250	1·0126	0·0126	2·0168
0·0125	1·0063	0·0063	2·0084

As h is reduced by "2" erro is reduced by a factor of two.

Central difference formula:

Function value $f(x)$ can be approximated/evaluated at values ~~lie~~ that lie to the left and right of x.

Assume that $f \in C^3[a,b]$ and that $x-h$, x, and $x+h$ points, all are within $[a,b]$. Then, first derivative at x can be evaluated as:

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

we can obtain (1) using Taylor's expansion as below

Central Difference Method

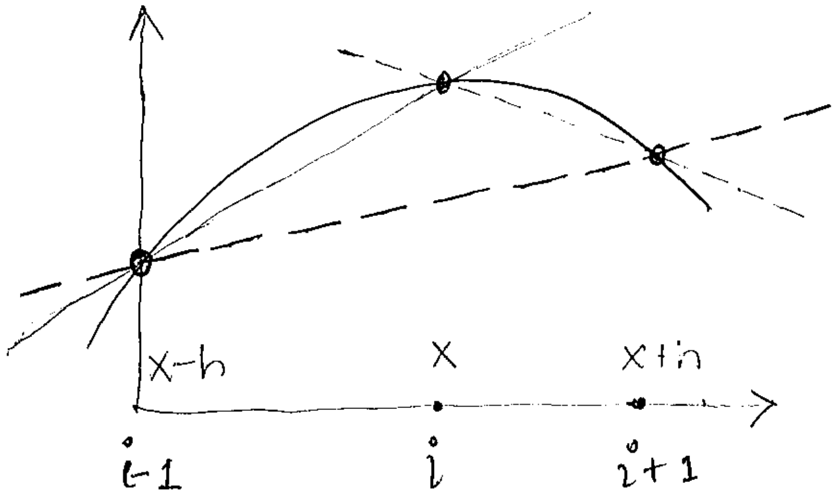
While the truncation error during discretization process reduces in $O(h)$, we can design a more accurate scheme of discretization; with error reduction in $O(h^2)$.

↓

Central Difference Method

↳ Widely used method to approximate the derivatives

Graphically,



Formula: Assume that $f \in C^3[a,b]$ and that $x+h$, $x-h$, and $x \in [a,b]$. Then.

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

Furthermore, there exists a number $c = c(x) \in [a,b]$

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

$$= -\frac{h^2 f'''(c)}{3!} = O(h^2)$$

Proof:

Using Taylor series expansion (2nd degree expansion), we can write

second degree Taylor expansion

could be c_1

(1) $$f(x+h) = f(x) + f'(x).h + \frac{f''(x).h^2}{2!} + \frac{f'''(x)h^3}{3!} + O(h^4)$$

c_2

(2) $$f(x-h) = f(x) - f'(x).h + \frac{f''(x).h^2}{2!} \quad \frac{f'''(x).h^3}{3!} + O(h^4)$$

By Subtracting (1) and (2)

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

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

Neglect

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

Assuming $f'''(x)$ is continuous and intermediate value theorem $\frac{f'''(c_1) + f'''(c_2)}{2}$

$= \frac{f'''(c)}{2}$

If we assume that $\frac{h^2 f'''(c)}{3!}$ does not change rapidly. Then, the truncation error reduces to zero as h^n. That's why error reduction is expressed as $O(h^2)$.

For computer simulation "h" can not be choosen too small.

$\downarrow$

We need approximation of $O(h^4)$

Central Difference For $f''(x)$

Consider Taylor's expansion

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

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

By adding (1) and (2)

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

Solving the Eq. 3 for $f''(x)$,

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

$$\Rightarrow \quad h^2 f''(x) = f(x+h) + f(x-h) - 2f(x) - \frac{h^4 f''''(x)}{12} \cdots$$

$$\Rightarrow \quad f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{h^2 f''''(x)}{12} \cdots \quad c$$

Precisely,

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

Comments: The above derivation truncates after the fourth derivative, and thus, there exists a value c that lies in $[x-h, x+h]$

So, approximating at $x = x_0$ $\quad f''(x_0) = \frac{f_1 - 2f_0 + f_{-1}}{h^2}$

Example :

Given, $f(x) = \cos x$

Find $f''(0.8) = ?$ (we approximate)

where $h = 0.1$, 0.01, and 0.001

Calculation at $x = 0.8$ for $h = 0.01$ is as follows:

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

$$= \frac{f(0.8+0.01) - 2f(0.8) + f(0.8-0.01)}{(0.01)^2}$$

$$= -0.69669\,0000$$

And error w.r.t true value $= f''(0.8) = -\cos(0.8)$

All the errors are as in below Table

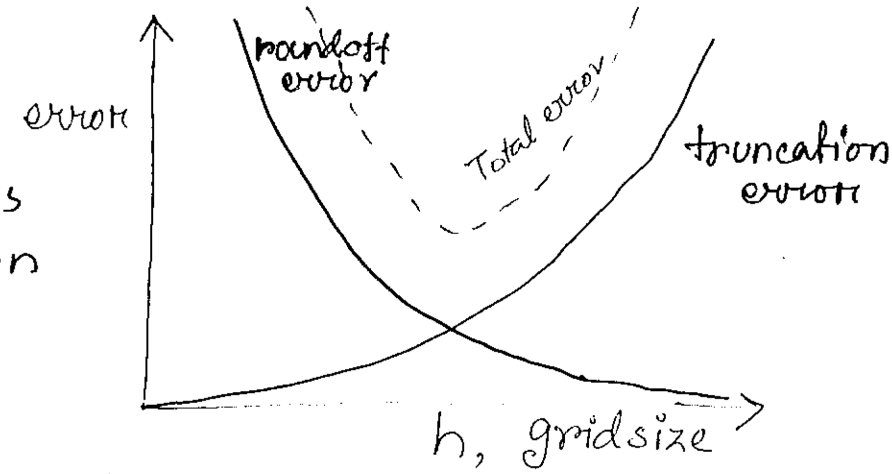
step size	Approximated of $f''(x)$	error
$h = 0.1$	-0.696126300	-0.000580409
$h = 0.01$	-0.69669000	-0.000016709
$h = 0.001$	-0.69600000	-0.000706709

Here, lowest error for $h = 0.01$!

We can do error analysis to find the answer of " why $h = 0.01$ performs better "

Error analysis

Let's taka a look at the error plot.



When gride size h is very small, truncation error reduces.

But

for smaller 'h', we need to perform more computations to get solutions for the same domain.

$\downarrow$ this leads to

increased roundoff error

Let's assume

$f_K = y_K + e_K$, here e_k is the error in the computation.

So,

$$f''(x_0) = \frac{y_1 - 2y_0 + y_{-1}}{h^2} + E(f,h)$$

$E(f,h)$ → Truncation error
→ Round off error

$$E(f,h) = \frac{e_1 - 2e_0 + e_{-1}}{h^2}$$

If we assume that, each error e_k is around ϵ, with signs that accumulate error, and $|f''''(x)| \leq M$ we get the error bound

$$|E(f,h)| \leq \frac{4\epsilon}{h^2} + \frac{Mh^2}{12}$$

If h is small, $\frac{4\epsilon}{h^2}$ due to round-off error is large.
When h is large, contribution $Mh^2/12$ is large.

Optimal size of h will minimize

$$g(h) = \frac{4\epsilon}{h^2} + \frac{Mh^2}{12}$$

☐ To find the minimum of a fn^c, we take derivative, and equate it to zero. so,

$g'(h) = 0$, provides h, for which $g(h)$ is minimum.

We obtain,

$$\frac{-8\epsilon}{h^3} + \frac{Mh}{6} = 0$$

$$\Rightarrow \quad h^4 = \frac{48\epsilon}{M} \quad \Big| \Rightarrow h = \left(\frac{48\epsilon}{M}\right)^{1/4}$$