Numerical Differentiation

Why do we need this?

→ If we cannot completely differentiate the natural function

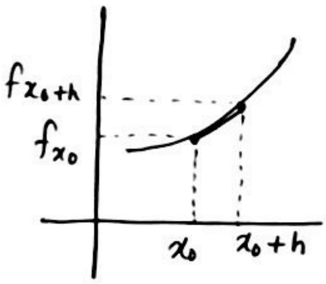
→ function complexity eg. experimental data

→ no explicit function available

→ computational efficiency

Therefore, we do approximation of the derivatives. There are 3 ways :
- forward difference
- backward difference
- central difference.

Forward difference



we use forward difference if we know the current node and future node

h = step size

Formula : $f'(x) = \dfrac{f(x_0+h) - f(x_0)}{h}$

Ex: $f(x) = x^2 + 10x$ Actual $= f'(x) = 2x + 10 = 2(2)+10 = 14$

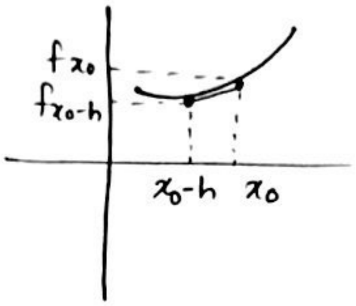
Find $f'(x)$ using forward diff. at $x = 2$, $h = 0.1$

$$f'(2) = \frac{f(2+0.1) - f(2)}{0.1} = \frac{f(2.1) - f(2)}{0.1}$$

$$= \frac{25.41 - 24}{0.1}$$

$$= 14.1$$

Backward difference



We use backward difference when we have the value of current node and previous node

Formula : $f'(x) = \dfrac{f(x_0) - f(x_0-h)}{h}$

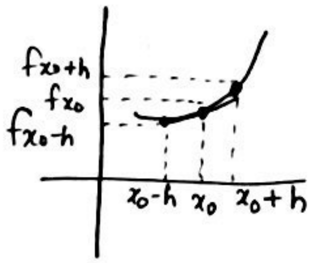
Ex: $f(x) = x^3 - 4x + 1$

Find the value of $f'(x)$ using backward diff. at $x=2$, $h=0.1$

$$f'(x) = \frac{f(2) - f(2-0.1)}{0.1}$$
$$= 7.41$$

Actual $= 3x^2 - 4$
$= 3(2)^2 - 4$
$= 8$

Central Difference



We use central difference when we have the value of current node, previous node and future node.

Formula : $f'(x) = \dfrac{f(x_0+h) - f(x_0-h)}{2h}$

Ex: $f(x) = x^3 - 4x + 1$

Find the value of $f'(x)$ using central diff. at $x=2$, $h=0.1$

$$f'(2) = \frac{f(2+0.1) - f(2-0.1)}{2h}$$

$$= 8.01$$

Now, let's take the same example and calculate $f'(x)$ using forward diff. at $x=2$, $h=0.1$

$f(x) = x^3 - 4x + 1$ Actual value $= 8$ [calc. previously]

$$f'(2) = \frac{f(2.1) - f(2)}{0.1}$$

$$= 8.61$$

comparing all three values, we can see that central difference gives minimum error than backward and forward differences.

Actual $= 8$

C.D $= 8.01 \Leftarrow$ best approximation
B.D $= 7.41$
F.D $= 8.61$

From our observation, we can see that the derivative calculated using the numerical difference methods are just an approximation. There are some errors to this value. After incorporating these truncation error; we get:

forward difference, $f'(x) = \underbrace{\frac{f(x+h) - f(x)}{h}}_{\text{approximate value}} - \underbrace{\frac{f''(\xi)}{2}(h)}_{\text{truncation error/ upper bound error}}$

backward difference, $f'(x) = \frac{f(x) - f(x-h)}{h} - \frac{f''(\xi)(h)}{2}$

central difference, $f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{f'''(\xi)(h)^2}{3!}$

From here, we get:

Error $\propto h \rightarrow$ forward and backward difference

Error $\propto h^2 \rightarrow$ central difference

$\boxed{\downarrow h \quad \downarrow \text{error}}$

Truncation error = | actual value − calculated value using FD/BD/CD |

$$\text{relative error} = \frac{|\text{actual} - \text{calc.}|}{|\text{actual}|}$$

* if the question says to calculate upper bound of truncation error, then we use the formula.

Ex: $f(x) = x\sin(x) + x^2\cos(x)$, $h = 0.2$

Calculate error bound, using $\xi \rightarrow [1.0, 1.4]$ by central difference.

$$\left| f^3(\xi)\frac{h^2}{3!} \right|$$

$$f'(x) = \sin x + x\cos x + 2x\cos x - x^2\sin x$$
$$= \sin x + 3x\cos x - x^2\sin x$$

$$f''(x) = 4\cos x - \cancel{5x\cos}\ 5x\sin x - x^2\cos x$$

$$f'''(x) = -9\sin x - 7x\cos x + x^2\sin(x)$$

$$\left|\frac{(0.2)^2}{3!}\right| \left| -9\sin(\xi) - 7(\xi)\cos(\xi) + (\xi)^2\sin(\xi) \right|$$

$$\left|\frac{(0.2)^2}{6}\right| \left| 9\sin(1.4) + 7(1.4)\cos(1.0) + (1.4)^2\sin(1.4) \right|$$

We always do modulus on individual continuous function including the coefficient for all upper bound of error.
Hence -9 sin(xi) becomes |-9sin(xi)|, -7xicos(xi) becomes |-7 xi cos(xi)|.

Then from our given/calculated range, we check which gives the highest value. In this case sin(1.4) > sin(1.0) and cos(1.0) > cos(1.4)

Proof of the formula : $f'(x) = \frac{f(x+h)-f(x)}{h} - \frac{f''(\xi)h}{2}$

$$\left.\begin{array}{l} x_0 \to x = x_0 \\ x_1 \to x+h = x_0+h \end{array}\right\} 2 \text{ nodes, degree} = 1$$

Using lagrange:

$$f(x) = P_1(x) + \text{error}$$

$$P_1(x) = f(x_0)\, l_0(x) + f(x_1)\, l_1(x)$$

uv differentiation

~~$f(x_0) \to$~~

$$f(x) = \frac{x-x_1}{x_0-x_1} f(x_0) + \frac{x-x_0}{x_1-x_0} f(x_1) + \overbrace{\frac{f''(\xi)}{2}}^{u}\,\overbrace{(x-x_0)(x-x_1)}^{v}$$

$$f'(x) = \frac{1}{x_0-x_1} f(x_0) + -\frac{1}{x_1-x_0} f(x_1) + \frac{f'''(\xi)}{2}\frac{d\xi}{dx}(x-x_0)(x-x_1)$$

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

Plugging $x = x_0$, $x_1 = x_0+h$

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

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

The other formulas are derived in the same way.

Let us see some examples where as we decrease h, error decreases

Example: $f(x) = \ln(x)$

$$f'(x) = \frac{1}{x} = \frac{1}{2} = 0.5$$

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

Using forward difference, at $x_0 = 2$.

h	$f'(2)$	Truncation Error
1	0.405465	0.5 − 0.405465 = 0.0945349
0.1	0.487902	0.5 − 0.487902 = 0.0120984
0.01	0.498754	0.5 − 0.498754 = 0.00124585
0.001	0.499875	0.5 − 0.499875 = 0.00012

Truncation error = |actual − calc. from FD|

We can see that step size is decreasing by 10, the error is also decreasing by 10.

[error $\propto h$]

For Central Difference,

if step size decreases by 10,
error reduces by $10^2 = 100$ [error $\propto h^2$]

More examples

x	4.0	4.1	4.2	4.3	4.4
$f(x)$	16	18	20	21	22

a) Using backward difference, calculate $f'(4.2)$

Now, h (step size is not given)

h is the difference between the nodes

$\rightarrow (4.1 - 4.0) = 0.1 = h$

So many values of x given. Which ones to take?

$x \rightarrow 4.2$ (question)

So, this is x_0. We need $x_0 - h \rightarrow$ the previous node, so we are going to take $x = 4.2, 4.1$

$$f'(4.2) = \frac{f(4.2) - f(4.1)}{0.1}$$

$$= \frac{20 - 18}{0.1}$$

$$= 20$$

b) Calc. forward difference : $f'(4.3)$

$x \rightarrow 4.3,\ 4.4$

$\hookrightarrow x_0 + h$

$$f'(4.3) = \frac{f(4.4) - f(4.3)}{0.1}$$

$$= \frac{22 - 21}{0.1}$$

$$= 10$$

Till now, we have seen that if step size decreases, truncation error also decreases. What about rounding error?

Especially for central difference,

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

→ smaller h, better result

→ if h is very small, $f(x+h)$ and $f(x-h)$ will have similar values

→ subtracting 2 similar values/close values, gives "loss of significance" → Chapter 1

→ Therefore rounding error increases.

From chapter 1 :

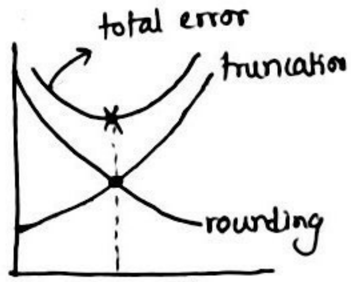
$$\delta = \frac{|fl(x) - x|}{|x|}$$

$$fl(x) = (1+\delta)x$$

⋮

$$fl[fl(x_1+h)] = (1+\delta_1) f(x_1+h)$$

$$fl[f(x_1-h)] = (1+\delta_2) f(x_1-h)$$



optimal value of h.

which value of h to choose?

$$\left| \text{actual value of differentiation} - \text{value of differentiation by numerical approach} \right|$$

$$= \text{Error}$$

$$\text{Error} \leq \underbrace{\frac{|f'''(\xi)|\, h^2}{6}}_{\text{truncation error}} + \underbrace{\varepsilon_M \cdot \frac{|f(x_1+h) + f(x_1-h)|}{2h}}_{\text{rounding error.}}$$