Lecture 18. 3.25.2019

§ 4.1 Numerical differentiation

Given $f(x)$

Goal: approximate $f'(x)$ using $f(x)$

One idea: $f(x) \leftarrow P(x)$ ↓ interpolation

$$\downarrow$$

$$f'(x) \approx P'(x)$$

with (x_j, y_j) $j = 1, 2, \dots, n+1$

$y_j = f(x_j)$

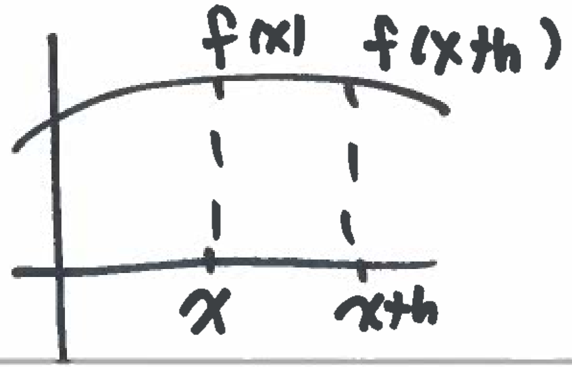
$x_{j+1} - x_j = h$

(equally spacing)

$n = 1$

$$f'(x) \sim \frac{f(x+h) - f(x)}{h}$$ forward difference

$$f'(x) \sim \frac{f(x) - f(x-h)}{h}$$ backward differen (e



error : $O(h)$ $\leftarrow$ Mh

first order in h

$O(h) \leq Mh$

M independent of h

'1st order accurate'

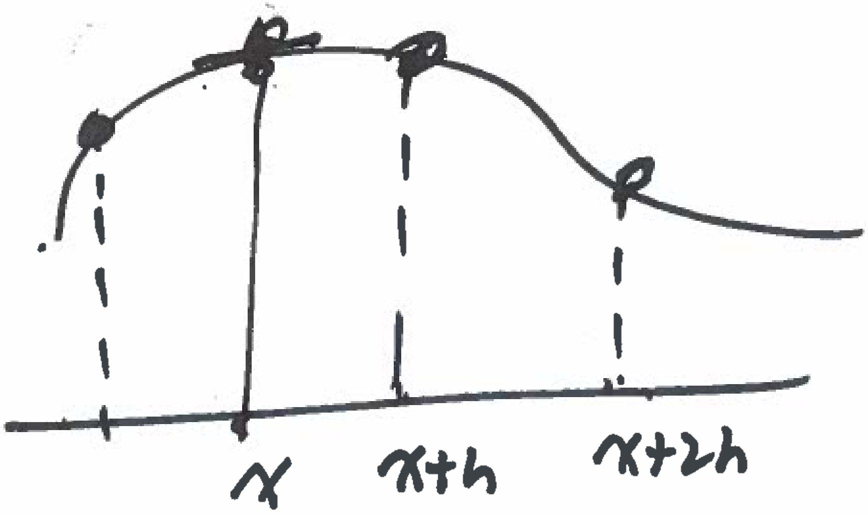
$n = 2$

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

one-sided

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

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



Error = $O(h^2)$

2nd order approximation.

One can find the coefficients in the approximation based on Taylor series expansion, and learn about the order of accuracy.

Example: Given $f(x)$ $(h>0)$

1) Approximate $f'(x)$ using $f(x)$, $f(x+h)$, $f(x+2h)$ linear combination

- up to 2nd order accurate (error $= O(h^2)$)

- what about approximations of 3rd order? what about 1st order?

2) Approximate $f''(x)$ using $f(x)$, $f(x+h)$, $f(x+2h)$,

up to 1st order, possibly 2nd order accuracy

Using Taylor series expansion.

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

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

$$\gamma \cdot \left\{ f(x) = f(x) \right.$$

Based on those

$$\alpha f(x+2h) + \beta f(x+h) + \gamma f(x)$$

$$= (\alpha+\beta+\gamma) f(x) + (2\alpha+\beta) h f'(x) + \frac{4\alpha+\beta}{2} h^2 f''(x) + \frac{8\alpha+\beta}{6} h^3 f'''(x) + O(h^4)$$

To approximate $f'(x)$.

we first require

$$\alpha + \beta + \gamma = 0 \quad \text{---- consistency}$$

also require $2\alpha + \beta \neq 0$

RHS

$$\Rightarrow \frac{\alpha f(x+2h) + \beta f(x+h) + \gamma f(x)}{(2\alpha+\beta)h} = f'(x)$$

LHS

$$+ \frac{4\alpha+\beta}{2(2\alpha+\beta)} h f''(x)$$

$$+ \frac{8\alpha+\beta}{6(2\alpha+\beta)} h^2 f'''(x)$$

$$+ O(h^3)$$

To get 2nd order approximation for $f'(x)$

we require $4\alpha + \beta = 0$

So far we have

$$\left\{\begin{array}{l} \alpha+\beta+\gamma=0 \\ 4\alpha+\beta=0 \end{array}\right\} \Rightarrow \beta=-4\alpha$$

$$\gamma=-\alpha-\beta=-\alpha+4\alpha=3\alpha$$

now we have $\left\{\begin{array}{l} \alpha \\ \beta=-4\alpha \\ \gamma=3\alpha \end{array}\right.$

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

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

$$RHS=\boxed{f'(x)}+\frac{8\alpha+\beta}{6(2\alpha+\beta)}h^2f'''(x)+O(h^3)$$

$$=f'(x)\underbrace{-\frac{1}{3}h^2f'''(x)+O(h^3)}$$

error $= O(h^2)$

Remark: 1) it is impossible to get a 3rd order approximation for $f'(x)$, simply based on $f(x)$, $f(x+h)$, $f(x+2h)$

2) what about first order?

$$\alpha + \beta + \sigma = 0$$

$$4\alpha + \beta \neq 0$$

$$2\alpha + \beta \neq 0$$

one example: we require

$$3\alpha + \beta = 0$$

lead to a first order approximation.

If instead we want to approximate $f''(x)$ using $f(x)$, $f(x+h)$, $f(x+2h)$

we require

$$\left.\begin{aligned} \alpha+\beta+\gamma &= 0 \\ 2\alpha+\beta &= 0 \\ 4\alpha+\beta &\neq 0 \end{aligned}\right) \Rightarrow \begin{aligned} \beta &= -2\alpha \\ \gamma &= -\alpha-\beta \\ &= \alpha \end{aligned}$$

$$\Rightarrow \frac{\alpha f(x+2h)+\beta f(x+h)+\gamma f(x)}{\left(\frac{4\alpha+\beta}{2}\right)h^2} = f''(x)$$

$$+ \frac{8\alpha+\beta}{6} \Big/ \left(\frac{4\alpha+\beta}{2}\right) * h f'''(x) + O(h^2)$$

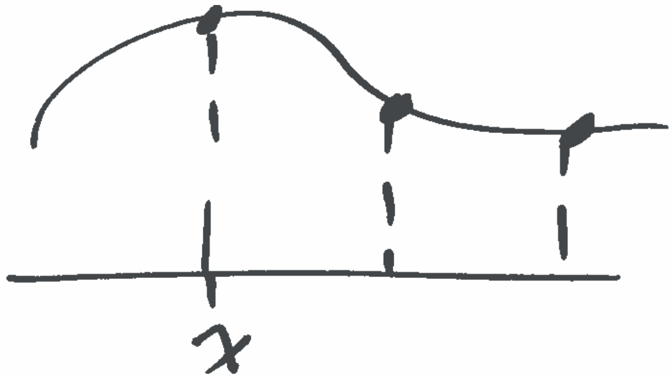
$$\Rightarrow \frac{f(x+2h)-2f(x+h)+f(x)}{h^2}$$

$$= f''(x) + hf'''(x) + O(h^2)$$

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

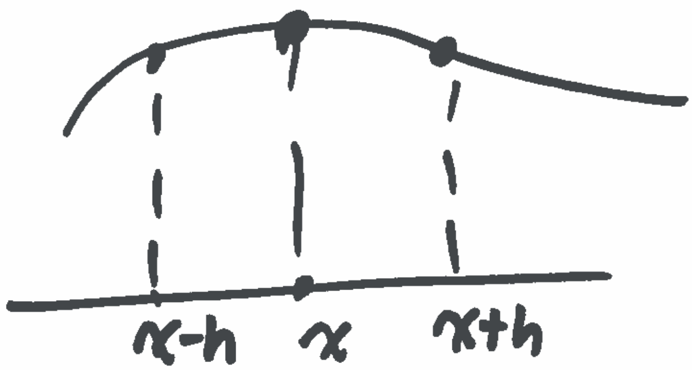
"first order"

2nd order: impossible.



one-sided

not possible to lead to 2nd order approximate for $f''(x)$



central

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

2nd order approximation

("central")

Richardson Extrapolation

to enhance the accuracy.

Recall

$$\underbrace{f'(x)}_{Q} = \underbrace{\frac{f(x+h)-f(x)}{h}}_{F(h)} \underbrace{- \frac{h}{2} f''(x) + O(h^2)}_{\text{error } O(h)}$$

General setting: to approximate a quantity Q, with $F_n(h)$, where $F_n(h)$ is nth order accurate

$$(*1) \quad Q = F_n(h) + K h^n + O(h^{n+1})$$

Now halve the step size

$$(*2) \quad Q = F_n\left(\frac{h}{2}\right) + K\left(\frac{h}{2}\right)^n + O\left(\left(\frac{h}{2}\right)^{n+1}\right)$$

$$(*2) \cdot 2^n \Leftrightarrow \quad 2^n Q = 2^n F_n\left(\frac{h}{2}\right) + K h^n + \frac{2^n}{2^{n+1}} O(h^{n+1})$$

$$\Rightarrow (2^n-1)Q = 2^n F_n(\tfrac{h}{2}) - F_n(h) + O(h^{n+1})$$

$$\Leftrightarrow Q = \boxed{\frac{2^n F_n(\frac{h}{2}) - F_n(h)}{2^n-1}} + O(h^{n+1})$$

$\downarrow$

This gives a new approximation of $(n+1)$-th order accurate. for Q.

Example. $Q = f'(x)$

$$F_1(h) = \frac{f(x+h) - f(x)}{h}. \quad (n=1).$$

$$\frac{2^n F_n(\frac{h}{2}) - F_n(h)}{2^n-1}$$

$$= 2\left(\frac{f(x+\frac{h}{2}) - f(x)}{h/2}\right) - \frac{f(x+h) - f(x)}{h}$$

$$= \left(4f(x+\tfrac{h}{2}) - 3f(x) - f(x+h)\right)/h.$$

This gives a 2nd order
approximation for $f'(x)$

let $\hat{h} = \frac{h}{2}$

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

Related to
some approximation
we've derived