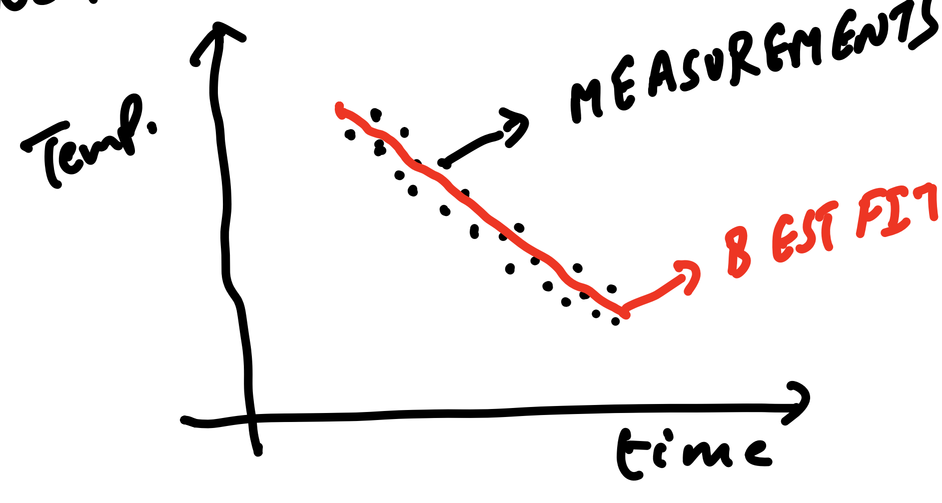
DS 288: NUMERICAL METHODS

SEP-9-2021

CURVE FITTING (§8.1)

- SO FAR ALL INTERPOLANTS PASS EXACTLY THROUGH DATA POINTS OF $f(x_j)$
- THERE ARE MANY SITUATIONS WHERE DATA HAS ERROR. FITTING A FUNCTION THAT MATCHES THESE DATA POINTS IS NOT RIGHT. & MAY NOT BE POSSIBLE TO MATCH.



BEST FIT : FITTING A STRAIGHT LINE

- DEFINE "BEST" IN MANY WAYS

* COMMON ONE

- MINIMIZE THE SUM OF SQUARED ERRORS : LEAST SQUARES CURVE FIT

$$\text{ERROR } E = \sum_{j=0}^{N} \left[f(x_j) - \tilde{P}(x_j) \right]^2$$

$\tilde{P}(x) \rightarrow$ APPROXIMATING FUNCTION (NEED NOT BE A POLYNOMIAL)

↳ PROVIDES BEST FIT TO THE "DATA" $f(x_j)$ BY MINIMIZING 'E'

WE NEVER DEMAND $E = 0$

DEMAND IS E TO BE POSSIBLE MINIMUM.

Ex: (i) STRAIGHT LINE THROUGH DAT

"LINEAR LEAST SQUARES FIT"

$$\tilde{P}(x) = P_1(x) = a_0 + a_1 x \quad [y = mx + b]$$

$$\text{ERROR } E = \sum_{j=0}^{N} \left[f(x_j) - (a_0 + a_1 x_j) \right]^2$$

UNKNOWNS: a_0 & a_1

MINIMIZE 'E' W.R. TO a_0 & a_1

$$\frac{\partial E}{\partial a_0} = \frac{\partial E}{\partial a_1} = 0 \quad (\text{REQUIREMENT})$$

$$\frac{\partial E}{\partial a_0} = 0 = 2 \sum_{j=0}^{N} \left[f(x_j) - (a_0 + a_1 x_j) \right] (-1)$$

$$\frac{\partial E}{\partial a_1} = 0 = 2 \sum_{j=0}^{N} \left[f(x_j) - (a_0 + a_1 x_j) \right] (-x_j)$$

2 EQNS & 2 UNKNOWNS.

THESE EQUATIONS ARE KNOWN AS NORMAL EQUATIONS

$$\sum_{j=0}^{N}{}' = N+1 \qquad \sum_{j=1}^{m}{}' \Rightarrow m$$

$$Y_j = f(x_j)$$

$$a_0 m + a_1 \sum_{j=1}^{m}{}' x_j = \sum_{j=1}^{m}{}' Y_j .$$

$$a_0 \sum_{j=1}^{m}{}' x_j + a_1 \sum_{j=1}^{m}{}' x_j^2 = \sum_{j=1}^{m}{}' x_j Y_j .$$

a_0 & a_1 → WRITE IT OUT.

$$a_0 = \frac{\sum' x_j^2 \sum' Y_j - \sum x_j Y_j \sum x_j}{m \sum' x_j^2 - \left(\sum x_j\right)^2} \qquad \left[\sum{}' \to \sum_{j=1}^{m}\right]$$

$$a_1 = \frac{m \sum' x_j Y_j - \sum' x_j \sum Y_j}{m \sum' x_j^2 - \left(\sum x_j\right)^2}$$

IN GENERAL

$$\tilde{p}(x) = P_N(x) = a_n x^n + a_{n-1} x^{n-1} + \dots + a_1 x + a_0$$

$N+1$ TERMS $\{a_i\}$

$$E = \sum_{i=1}^{m} \Big[f(x_i) - \underbrace{P_N(x_i)}_{= \sum_{k=0}^{N} a_k x_i^k} \Big]^2$$

REQUIRE $\dfrac{\partial E}{\partial a_j} = 0 \quad j = 0, 1, 2 \dots N$

$m \to$ NO. OF DATA POINTS

$N \to$ ORDER OF POLYNOMIAL

$$\frac{\partial E}{\partial a_j} = -2 \sum_{i=1}^{m} y_i x_i^j + 2 \sum_{k=0}^{N} a_k \sum_{i=1}^{m} x_i^{j+k}$$

$N+1 \to$ NORMAL EQUATIONS

$\hookrightarrow$ NO. OF UNKNOWNS

$$\underline{A} = \underline{\underline{X}}^{-1} \underline{b} \quad \text{X} \to \text{DATA POINTS}$$

$\hookrightarrow [a_0, \dots a_N]^T$

WHAT IF $\tilde{p}(x)$ IS NOT POLYNOMIAL?

Ex :- $\tilde{p}(x) = b e^{ax}$

$$E = \sum_{i=1}^{m} \left[f(x_i) - b e^{a x_i} \right]^2$$

$y_i = f(x_i)$

NORMAL EQUATIONS.

$$\frac{\partial E}{\partial b} = 0 = 2 \sum_{i=1}^{m} \left[y_i - b e^{a x_i} \right] \left(-e^{a x_i} \right)$$

$$\frac{\partial E}{\partial a} = 0 = 2 \sum_{i=1}^{m} \left[y_i - b e^{a x_i} \right] \left(-b x_i e^{a x_i} \right)$$

$$\Rightarrow \; b \sum_{i=1}^{m} e^{2 a x_i} = \sum y_i e^{a x_i}$$

$$b \sum_{i=1}^{m} x_i e^{2 a x_i} = \sum_{i=1}^{m} x_i y_i e^{a x_i}$$

NO EXACT SOLUTION (CAN NOT WRITE A LINEAR SYSTEM OF EQUATIONS IN TERMS OF a & b)

CONSIDER CHANGE OF VARIABLE

CONSIDER

$$\ln y = \ln(be^{ax}) = \ln b + ax$$

NOW APPLY LEAST SQUARES. TO FIND $\ln b$ & a WHICH MINIMIZES 'E'. IN TERMS OF $\{x_i\}$ & $\{\ln y_i\}$

[[PRACTISE IN HW#4]]

<u>LEAST SQUARES IN CONTINUUM</u>

(§8.2) - ORTHOGNAL POLYNOMIAL

FIND THE POLYNOMIAL P_N WHICH MINIMIZES THE ERROR E OVER INTERVAL $[a,b]$

$$E = \int_a^b [f(x) - P_N(x)]^2 \, dx$$

WHERE $P_N(x) = \sum_{K=0}^{N} a_K x^K$

→ N^{TH} ORDER POLYNOMIAL

N+1 COEFFICIENTS → UNKNOWNS

N+1 EQUATIONS (NORMAL)

LINEAR SYSTEM OF EQUATIONS:

$(N+1) \times (N+1)$

→ OPERATIONS $O((N+1)^3)$

EXPRESS $P_N(x)$ IN TERMS OF

ORTHOGNAL BASIS FUNCTION

$$P(x) = \sum_{K=0}^{N} a_K \phi_K(x)$$

$\phi_K(x)$ — BASIS FUNCTIONS WHICH
ARE ORTHOGONAL ON [a, b]
W.R.T. WEIGHTING FUNCTION
$w(x)$

→ MAY NOT BE POLYNOMIAL

i.e. $\int_a^b w(x)\, \phi_j(x)\, \phi_i(x)\, dx = \begin{cases} 0 & i \neq j \\ \alpha_j & i = j \end{cases}$

[ORTHONORMAL $= \delta_{ij}$]

Ex: FOURIER SERIES.

$w(x) = 1 \qquad [a, b] = [-\pi, \pi]$

$\phi_j(x) = \begin{cases} \sin jx \\ \text{or } \cos jx \end{cases} \Rightarrow \alpha_j = \pi$

WEIGHTED ERROR

$$E = \int_a^b w(x) \left[f(x) - \sum_{k=0}^{N-1} a_k \phi_k(x) \right]^2 dx$$

MINIMIZE E

$$\frac{\partial E}{\partial a_i} = 0 = \int_a^b w(x) \left[f(x) - \sum_{k=0}^{N-1} a_k \phi_k(x) \right] \phi_i(x)\, dx$$

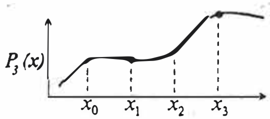
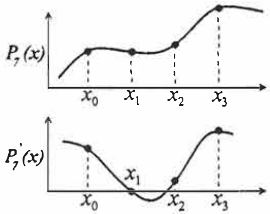
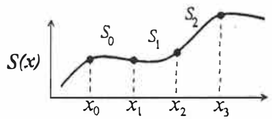
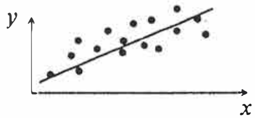
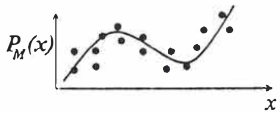
$$\sum_{k=0}^{N} a_k \underbrace{\int_a^b w(x)\,\phi_k(x)\,\phi_i(x)\,dx}_{=\begin{cases}0 & i\neq k\\ \alpha_k & i=k\end{cases}} = \int_a^b f(x)\,\phi_i(x)\,w(x)\,dx$$

$$\boxed{a_i = \frac{1}{\alpha_i}\int_a^b f(x)\,\phi_i(x)\,w(x)\,dx}$$

COEFFICIENTS FOR ORTHOGNAL BASIS FUNCTION.

((HAND OUT ON SUMMARY OF INTERPOLATION METHODS))

Summary of Interpolation Methods

Method	Data Error Tolerated	Points Matched Exactly	Local/Global Characteristics	Graphical Interpretation	Error Term
Lagrange	small	$N+1$	global		$\frac{f^{(N+1)}(\xi)}{(N+1)!}\prod_{i=0}^{N}(x-x_i)$
Hermite	small	$2N+2$ $(N+1$ deriv.$)$	global		$\frac{f^{(2N+2)}(\xi)}{(2N+2)!}\prod_{i=0}^{N}(x-x_i)^2$
Cubic Spline	small	$N+1$ (contin. P',P'')	local		$\max\lvert f(x)-S(x)\rvert \le$ $\max\frac{\lvert f^{(4)}(x)\rvert}{384}\cdot\max\,(x_{j+1}-x_j)$ $x\in[x_0,x_n]\,;\;\; j\in[0,n]$
Least Squares (straight line)	large	none	global		$\sum_{j=0}^{N}[f(x_j)-(a+bx_j)]^2$ $\neq 0$
Least Squares (polynomial)	large	none	global		$\sum_{j=0}^{N}\left[f(x_j)-\sum_{i=0}^{M}a_i x_j^i\right]^2$ $\neq 0$

Courtesy: Prof. Simon Shepard

CH #4 NUMERICAL DIFFERENTIATION

- LOOKING FOR WAYS TO APPROXIMATE FUNCTION DERIVATIVES WITH COMBINATIONS OF FUNCTION EVALUATIONS AT DISCRETE POINTS

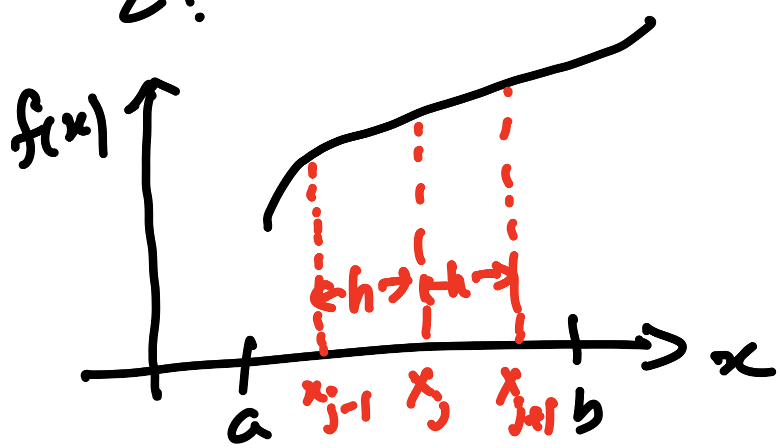
[RECALL:
SECANT METHOD $f'(p_n) = \dfrac{f(p_n) - f(p_{n-1})}{p_n - p_{n-1}}$]

TEXT: CONSTRUCT A POLYNOMIAL APPROXIMATION TO $f(x)$ THROUGH EVENLY SPACED SAMPLES OF $f(x_i)$, THEN DIFFERENTIATE THE POLYNOMIAL

IN CLASS: USE A TAYLOR SERIES EXPANSION.

- EXPAND $f(x)$ about x_j, THE POINT WHERE DERIVATIVE IS NEEDED/TO BE COMPUTED

$$f(x) = f(x_j) + f'(x_j)(x - x_j) + \frac{f''(x_j)}{2!}(x - x_j)^2 + \cdots \quad \text{\textcircled{*}}$$



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

(EQUAL-SPACED SAMPLES)

NOTATION: $f_j \equiv f(x_j)$

LET $x = x_{j+1}$ IN $\circledast$

$$f_{j+1} = f_j + h f_j' + \frac{h^2}{2} f_j'' + \cdots$$

IF h IS SMALL, THEN HIGHER ORDER TERMS (f_j'', f_j''' ...) WILL DIMINISH FASTER

$$f_{j+1} = f_j + h f_j' + C_1 h^2 \quad C_1 = \frac{f_j''}{2}$$

$$f_j' = \frac{f_{j+1} - f_j}{h} + \underbrace{O(h)}_{\text{ERROR TERM}}$$

$\swarrow$

APPROXIMATION TO FIRST DERIVATIVE TO ORDER OF 'h' ACCURACY $= \frac{f_j'' h}{2}$

EXACT: $$f_j' = \frac{f_{j+1} - f_j}{h} - \frac{f''(\xi)\,h}{2}$$

$$\xi \in [x_j, x_{j+1}]$$

DEFINE $\Delta f_j \equiv f_{j+1} - f_j \equiv$ FIRST FORWARD DIFFERENCE

$$\boxed{f_j' = \frac{\Delta f_j}{h}}$$

FIRST FORWARD DIFFERENCE APPROX. TO $O(h)$.

CAN ALSO DO A "BACKWARD DIFFERENCE"

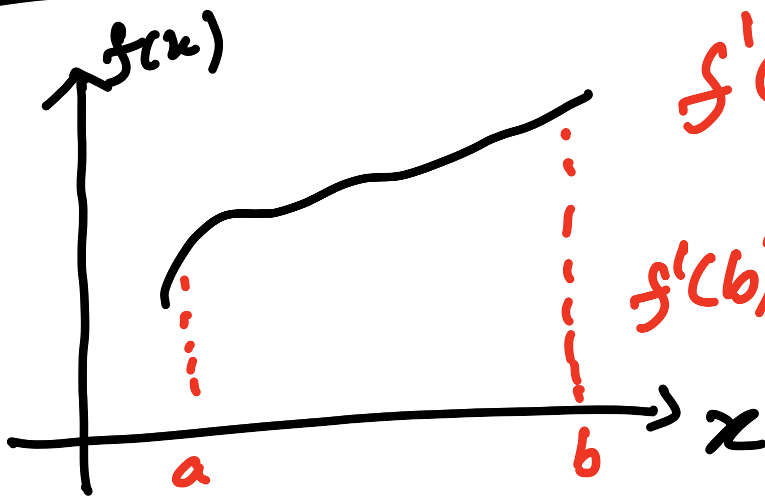
EVALUATE $x = x_{j-1}$ IN $*$

$$\Rightarrow f_j' = \frac{f_j - f_{j-1}}{h} + O(h) \qquad h = x_j - x_{j-1}$$

DEFINE $\nabla f_j = f_j - f_{j-1}$ FIRST BACKWARD DIFFERENCE

$$\boxed{f_j' = \frac{\nabla f_j}{h}}$$

FIRST BACKWARD DIFFERENCE APPROX. TO $O(h)$



$f'(a) \rightarrow$ FORWARD ONLY

$f'(b) \rightarrow$ BACKWARD ONLY

SECOND DERIVATIVE f_j''

$$f_{j+1} = f_j + h f_j' + \frac{h^2}{2} f_j'' + \frac{h^3}{3!} f_j''' + \dots \quad \llcorner (+)$$

$x = x_{j+2}$ IN $(*)$

$$f_{j+2} = f_j + 2h f_j' + \frac{(2h)^2}{2!} f_j'' + \frac{(2h)^3}{3!} f_j''' + \dots \quad \llcorner (\times)$$

$$[x_{j+2} - x_j = 2h]$$

DO $(\times) - 2(+)$

$$f_{j+2} - 2f_{j+1} = -f_j + f_j'' h^2 + f_j''' h^3 + \cdots$$

SOLVE FOR f_j''

$$f_j'' = \frac{f_{j+2} - 2f_{j+1} + f_j}{h^2} + O(h)$$

$$\equiv f'''(\xi)\, h$$

$$\xi \in [x_j, x_{j+2}]$$

$$\Delta^2 f_j = \Delta(\Delta f_j) = \Delta(f_{j+1} - f_j)$$

$$= \Delta(f_{j+1}) - \Delta(f_j)$$

$$= f_{j+2} - f_{j+1} - (f_{j+1} - f_j)$$

$$= f_{j+2} - 2f_{j+1} + f_j$$

$$\boxed{f_j'' = \frac{\Delta^2 f_j}{h^2}}$$

SECOND FORWARD DIFFERENCE APPROX. TO f_j'' TO $O(h)$

SIMILARLLY

$$\boxed{f_j'' = \frac{\nabla^2 f_j}{h^2}}$$

SECOND BACKWARD APPROX OF f_j'' TO $O(h)$

$f_j'' \rightarrow$ 2 TAYLOR EXPANSIONS

[1 IS AROUND x_{j+1} &

2 IS AROUND x_{j+2}]

f_j''' NEED 3 TAYLOR EXPANSIONS

$$\boxed{f_j''' = \frac{\Delta^3 f_j}{h^3}}$$

THIRD FORWARD DIFFERENCE APPROX. TO f_j''' TO $O(h)$

$$f_j''' = \frac{f_{j+3} - 3f_{j+2} + 3f_{j+1} - f_j}{h^3} + O(h)$$

FUNCTION EVALUATIONS $\rightarrow$ 4

IN GENERAL, ONE CAN CONSTRUCT APPROXIMATION TO N^{TH} ORDER DERIVATIVE OF f AT x_j $(\equiv f_j^{N})$ TO ACCURACY $O(h)$ USING WEIGHTED SUM OF 'N' TAYLOR EXPANSIONS REQUIRING 'N+1' FUNCTION EVALUATIONS TO $O(h)$ [TRUE FOR BOTH FORWARD & BACKWARD]