CE 601: Numerical Methods

Lecture 18

Multi-Variate Regression; Numerical Differentiation

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- We have already discussed on using method of least squares to fit polynomials (approximately-fit polynomials) for the given data set
- This process of fitting is called <u>regression</u>.
- We can also do regression for multi-variate cases.

Say if $f = f(x, y)$

We want to approximate the actual function 'f' with a multi-variate polynomial 'Z'.

i.e. $f \approx Z = f(x, y)$

Then $Z = A + Bx + Cy$ (Linear regression)

$$\therefore e_i = f_i - Z_i$$

Minimize sum of square of errors

i.e. $\sum e_i^2 = \sum_{i=0}^{n} (f_i - y_i)^2 = S$

Criteria for minimisation: $\frac{\partial S}{\partial A} = 0, \frac{\partial S}{\partial B} = 0, \frac{\partial S}{\partial C} = 0.$

You will get the normal equations:

$$\begin{bmatrix} (n+1) & \sum x_i & \sum y_i \\ \sum x_i & \sum x_i^2 & \sum x_i y_i \\ \sum y_i & \sum x_i y_i & \sum y_i^2 \end{bmatrix} \begin{Bmatrix} A \\ B \\ C \end{Bmatrix} = \begin{Bmatrix} \sum f_i \\ \sum x_i f_i \\ \sum y_i f_i \end{Bmatrix}$$

$\rightarrow$ If you have higher degree multi-variate polynomial approximations, say, $Z = a_0 + a_1 x + b_1 y + a_2 x^2 + b_2 y^2 + c_2 xy$

There are 6 parameters: $a_0, a_1, b_1, a_2, b_2, c_2$

$\rightarrow$ You require that many number of normal equations to find these parameters or coefficients.

Extension of Method of Least Squares to fit non-linear curves that are not polynomials

- We have seen till now, this regressive technique to get polynomials for a given data set

  → The polynomials may be linear or non-linear.

Q. What happens if polynomial fitting is not suitable for certain types of data

Soln. You may have to go for some other non-linear curve fitting.

Power equation $y = Ax^B$

Exponential equation $y= Ae^{Bx}$

To fit such non-linear equation, we can apply the method of least squares.

1) Power fit

For the data set (x_i, f_i), if $f \approx y(x)$ is more appropriate where $y = ax^b$ (The power equation)

We will linearise this expression:

$ln(y) = ln(a) + b\ ln(x)$

$\boxed{Y = A + B X}$, where $Y = ln(y)$, $A = ln(a)$, $B = b$, $X = ln(x)$.

Once, this form is made, the earlier description is used to find A and B and then $a = e^A$.

2) Exponential fit

If $f \approx y(x)$, where $y = a\ e^{bx}$,

then again, $ln(y) = ln(a) + bx$. Now linearise it and follow the same procedure as before.

3) Non-linear equation: Say if we want to fit,

$y = \dfrac{A}{1+Bx}$ or $y = \dfrac{A}{B+e^{Cx}}$ etc., then the above linearisation procedure will not work.

Define $e_i^2 = (f_i - y_i)^2$ and $S = \sum_{i=0}^{n}(f_i - y_i)^2 = \sum_{i=0}^{n}\left(f_i - \dfrac{A}{1+Bx_i}\right)^2$

or for the other function $S = \sum_{i=0}^{n}\left(f_i - \dfrac{A}{B+e^{Cx_i}}\right)^2$

For minimum S, we want

$\dfrac{\partial S}{\partial A} = 0$ and $\dfrac{\partial S}{\partial B} = 0$ and/or $\dfrac{\partial S}{\partial C} = 0$

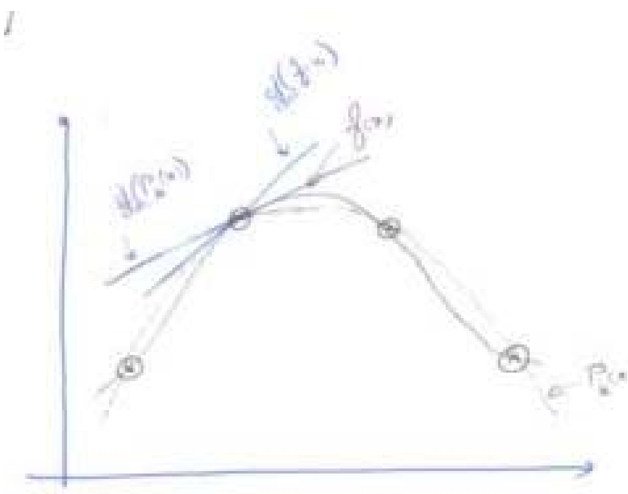
i.e. $\dfrac{\partial S}{\partial A} = 0 = \sum_{i=0}^{n} 2\left(f_i - \dfrac{A}{1+Bx_i}\right)\left(\dfrac{-1}{1+Bx_i}\right)$

$$\frac{\partial S}{\partial B} = 0 = \sum_{i=0}^{n} 2\left(f_i - \frac{A}{1+Bx_i}\right)\left(\frac{-x_i A}{(1+Bx_i)^2}\right)$$

This is a system of non-linear equations in A and B. We can use Newton's iteration method to solve such non-linear systems and find the coefficients A and B.

Numerical Differentiation

We need the exactly fit or approximately fit polynomials to interpolate function values for a given data set (x_i, f_i), $i = 1, 2, 3, \ldots, n$.



Say, $f(x) = P_k(x)$ (k^{th} degree polynomial)

$$\therefore\ f'(x) = P_k'(x);\ \text{i.e. } \frac{d}{dx}\big(f(x)\big) = \frac{d}{dx}\big(P_k(x$$

However, if we plot the data sometimes the derivatives at the data point may not be the same as in obvious from the difference in slope of $f(x)$ and $P_k(x)$.

$\therefore\ f'(x) = P_k'(x)$ (may not be true everytime).

Recall in the exactly fit polynomial. We used direct method.

$$f(x) \approx P_k(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_k x^k$$

$$\therefore\ f'(x) \approx P_k'(x) = a_1 + 2a_2 x + \cdots + k a_k x^{k-1}$$

- We can also use divided difference polynomials:

x	y	$y_i^{(1)}$	$y_i^{(2)}$	$y_i^{(3)}$
x_0	y_0			
		$y_0^{(1)}$		
x_1	y_1		$y_0^{(2)}$	
				$y_0^{(3)}$
x_2	y_2	$y_1^{(1)}$	$\vdots$	
$\vdots$	$\vdots$	$\vdots$	$y_{n-2}^{(2)}$	
		$y_{n-1}^{(1)}$		
x_n	y_n			

The divided differences $f_i^{(1)} = f[x_i, x_{i+1}] = \dfrac{f_{i+1} - f_i}{x_{i+1} - x_i}$

You can apply this polynomial this polynomial for uniformly spaced data.

$$f(x) \approx P_n(x) = f_i^{(0)} + (x - x_0) f_i^{(1)} + (x - x_0)(x - x_1) f_i^{(2)}$$

$$+ \ldots + (x - x_0)(x - x_1) \cdots (x - x_{n-1}) f_i^{(n)}$$

$$\therefore f'(x) \approx P_n'(x) = f_i^{(1)} + (2x - (x_0 - x_1)) f_i^{(2)} + \ldots$$

Similarly, you can find $f''(x) \approx P_n''(x)$, etc.

For equally spaced data, we may use Newton's forward

or backward difference polynomial to approximate a function.

x	f	Δf	$\Delta^2 f$	$\Delta^3 f$
x_0	f_0			
		Δf_0		
x_1	f_1		$\Delta^2 f_0$	
				$\Delta^3 f_1$
		Δf_1		
x_2	f_2		$\Delta^2 f_1$	
		Δf_2		
x_3	f_3			

$\Delta f_i = f_{i+1} - f_i;\ \Delta^2 f_i = \Delta f_{i+1} - \Delta f$

Recall Newton's forward difference polynomial

$$P_n(x) = f_0 + s\Delta f_0 + \frac{s(s-1)}{2}\Delta^2 f_0 + \frac{s(s-1)(s-2)}{6}\Delta^3 f_0$$

$$+\cdots+\frac{s(s-1)(s-2)\cdots(s-(n-1))}{n!}\Delta^n f_0, \text{ where } s = \frac{x-x_0}{\Delta x}.$$

The error in this n^{th} degree polynomial can be given as:

$$E(x) = \frac{s(s-1)(s-2)\cdots(s-n)}{(n+1)!}\Delta x^{n+1} f_0 + \frac{s(s-1)(s-2)\cdots(s-n-1)}{(n+2)!}\Delta x^{n+2} f_0 + \cdots$$

We can write when $\Delta x \to 0$,

$$\lim_{\Delta x \to 0}\frac{\Delta^2 y}{\Delta x^2} = \frac{d^2 y}{dx^2}; \quad (\text{i.e. } y^{(2)}); \quad \therefore \Delta^2 y \approx \Delta x^2 y^{(2)}$$

In a similar sense:

$$E(x) = \frac{s(s-1)(s-2)\cdots(s-n)}{(n+1)!}(\Delta x)^{n+1} f^{(n+1)}(\zeta)$$

where $\Delta^{(n+1)} f \to (\Delta x)^{n+1} f^{(n+1)}(\zeta);\ x_0 \le \zeta \le x_n.$

$\therefore$ Actual function, $f(x) = P_n(x) + E(x)$

However we suggest $f(x) \approx P_n(x)$

$$\therefore\ f'(x) \approx \frac{d}{dx}\left(P_n(x)\right)$$

From $s = \dfrac{x - x_0}{\Delta x}$, $\therefore \dfrac{ds}{dx} = \dfrac{1}{\Delta x}$ (Constant)

$$\therefore \frac{d}{dx}\left(P_n(x)\right) = \frac{d}{ds}\left(P_n(s)\right)\frac{ds}{dx} = \frac{1}{\Delta x}\frac{d}{ds}\left(P_n(s)\right)$$

i.e. $P_n'(x) = \dfrac{1}{\Delta x}\left[\Delta f_0 + \dfrac{2s-1}{2}\Delta^2 f_0 + \dfrac{3s^2 - 6s + 2}{6}\Delta^3 f_0 + \cdots\right]$

Similarly, $\dfrac{d}{dx}\left(E(x)\right) = \dfrac{1}{\Delta x}\dfrac{d}{ds}\left(E(s)\right)$.

Also $f''(x) \approx P_n''(x) = \dfrac{d}{dx}\left(P_n'(x)\right) = \dfrac{d}{ds}\left(P_n'(s)\right)\dfrac{ds}{dx}$

$$= \frac{1}{(\Delta x)^2}\left[\Delta^2 f_0 + (s-1)\Delta^3 f_0 + \frac{6s^2 - 18s + 11}{12}\Delta^4 f_0 + \cdots\right]$$