CE 601: Numerical Methods

Lecture 19

Numerical Differentiation

Course Coordinator:
Dr. Suresh A. Kartha,
Associate Professor,
Department of Civil Engineering,
IIT Guwahati.

Numerical Differentiation

→ We already discussed that if polynomials are used as approximating functions for the actual functions, then these polynomials can be mostly used to find the derivatives of the actual function.

i.e. if $f(x) \approx P_n(x)$

then $f'(x) \approx P_n'(x)$

→ While using Newton's forward difference polynomial, we have seen that error

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

where $x_0 \le \zeta \le x_n$.

This means $P_n(x)$ has an error of $O(\Delta x^{n+1})$

$\rightarrow$ We have also seen that

$$f'(x) \approx P_n'(x) = \frac{1}{\Delta x}\left[\Delta f_0 + \frac{2s-1}{2}\Delta^2 f_0 + \frac{3s^2-6s+2}{6}\Delta^3 f_0 + \cdots\right] \text{ and}$$

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

$\rightarrow$ To obtain now various difference difference formulas

Now keep the base point as x_0.

$\therefore$ Newton's forward difference polynomial:

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

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

Here at $x = x_0$ i.e. $s = 0$,

i.e. $P_n(x_0) = f_0$

$$P_n'(x_0) = \frac{1}{\Delta x}\left[\Delta f_0 - \frac{1}{2}\Delta^2 f_0 + \frac{1}{3}\Delta^3 f_0 + \cdots\right]$$

$$P_n''(x_0) = \frac{1}{\Delta x^2}\left[\Delta^2 f_0 - \Delta^3 f_0 + \frac{11}{12}\Delta^4 f_0 + \cdots\right]$$

→ These equations for $P_n'(x_0)$ and $P_n''(x_0)$ are one-sided forward difference forms to approximate derivatives.

→ For $E(x)$ for the polynomial $P_n(x)$ approximating $f(x)$, $P_n'(x)$ will be having error

$$\frac{d}{dx}\left(E(x)\right) = \frac{d}{dx}\left[\frac{s(s-1)(s-2)\cdots(s-n)}{(n+1)!}(\Delta x)^{n+1} f^{(n+1)}(\zeta)\right]\frac{ds}{dx}$$

$$= \frac{(\Delta x)^n f^{(n+1)}(\zeta)}{(n+1)!}\frac{d}{dx}\left[\begin{array}{l}(s-1)(s-2)\cdots(s-n) + s(s-2)\cdots(s-n)\\ + \cdots + s(s-1)(s-2)\cdots(s-(n-1))\end{array}\right]$$

At $x = x_0$, i.e. $s = 0$, we have:

$$\frac{d}{dx}\ \mathrm{E}(x_0) = \frac{(-1)^n}{(n+1)!}(\Delta x)^n n!\, f^{(n+1)}(\zeta) = \frac{(-1)^n}{n+1}(\Delta x)^n f^{(n+1)}(\zeta)$$

That is we are having error of the order (Δx^n). Now as $\Delta x \to 0$,

$P_n(x_0) \to O(\Delta x^{n+1})$

$P_n'(x_0) \to O(\Delta x^n)$; (e.g. $P_1'(x_0) \to O(\Delta x^1)$; $P_2'(x_0) \to O(\Delta x^2)$)

Similarly, $P_n''(x_0) \to O(\Delta x^{n-1})$; (e.g. $P_2''(x_0) \to O(\Delta x)$; $P_3''(x_0) \to O(\Delta x^2)$...)

$\to$ These are one-sided forward difference formulas, we need to expand them to get difference formulas.

If the base point is x_0 and if we evaluate the derivatives at $x = x_1$.

Then s=1,

$$P_n'(x_1) = \frac{1}{\Delta x}\left[\Delta f_0 + \frac{1}{2}\Delta^2 f_0 - \frac{1}{6}\Delta^3 f_0 + \cdots\right]$$

$$P_n''(x_1) = \frac{1}{\Delta x^2}\left[\Delta^2 f_0 - \frac{1}{12}\Delta^4 f_0 + \cdots\right]$$

These are centered difference forms for first and second derivatives using Newton's polynomials.

You can see, $P_1'(x_1) \rightarrow O(\Delta x)$

$$P_2'(x_1) \rightarrow O(\Delta x^2)$$

Now see that $P_2''(x_1) \rightarrow O(\Delta x^2)$.

- <u>Elaboration of the difference formula</u>
- From the one-sided forward difference formula:

$$P_n'(x_0) = \frac{1}{\Delta x}\left[\Delta f_0 - \frac{1}{2}\Delta^2 f_0 + \frac{1}{3}\Delta^3 f_0 - \cdots\right]$$

$$\text{For } n = 1,\ P_1'(x_0) = \frac{\Delta f_0}{\Delta x} \quad \rightarrow O(\Delta x)$$

x	f	Δf	$\Delta^2 f$	$\Delta^3 f$
x_0	f_0			
		$f_1 - f_0$		
x_1	f_1		$f_2 - 2f_1 + f_0$	
		$f_2 - f_1$		$f_3 - 3f_2 + 3f_1 - f_0$
x_2	f_2		$f_3 - 2f_2 + f_1$	:
		$f_3 - f_2$	:	$f_n - 3 f_{n-1} + 3 f_{n-2} - f_{n-3}$
:	:	:	$f_n - 2 f_{n-1} - f_{n-2}$	
		$f_n - f_{n-1}$		
x_n	f_n			

i.e. $$\boxed{P_1'(x_0) = \frac{f_1 - f_0}{\Delta x} \rightarrow O(\Delta x)}$$

Similarly,

$$P_2'(x_0) = \frac{1}{\Delta x}\left[\Delta f_0 - \frac{1}{2}\Delta^2 f_0\right] + O(\Delta x^2)$$

$$= \frac{2\Delta f_0 - \Delta^2 f_0}{2\Delta x} + O(\Delta x^2)$$

$$= \frac{2\ \ f_1 - f_0\ \ -\ \ f_0 - 2 f_0 + f_0}{2\Delta x} + O(\Delta x^2)$$

$$\boxed{\left.\frac{df}{dx}\right|_{x=x_0} \cong P_2'(x_0) = \frac{f_2 + 4 f_1 - 3 f_0}{2\Delta x} \rightarrow O(\Delta x^2)}$$

This is second degree approximation for the first derivative with order of approximation $O(\Delta x^2)$.

In a similar note:

$\Rightarrow$ The second derivative

$$P_n''(x_0) = \frac{1}{\Delta x^2}\left[\Delta^2 f_0 - \Delta^3 f_0 + \cdots\right]$$

For $P_2''(x_0) = \frac{1}{\Delta x^2}\left[\Delta^2 f_0\right] + O(\Delta x)$

i.e. $\boxed{P_2''(x_0) = \frac{f_2 - 2f_1 + f_0}{\Delta x^2} \rightarrow O(\Delta x)}$

$$P_3''(x_0) = \frac{1}{\Delta x^2}\left[\Delta^2 f - \Delta^3 f\right] \rightarrow O(\Delta x^2)$$

$$= \frac{(f_2 - 2f_1 + f_0) - (f_3 - 3f_2 + 3f_1 - f_0)}{\Delta x^2} \rightarrow O(\Delta x^2)$$

i.e. $\boxed{P_3''(x_0) = \frac{-f_3 + 4f_2 - 5f_1 + 2f_0}{\Delta x^2} \rightarrow O(\Delta x^2)}$

$\Rightarrow$ The centered difference formulas for these derivatives

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

$\rightarrow$ To get the first degree, first order approx.

$$P_1'(x_1) = \frac{1}{\Delta x}\ \Delta f_0 \ \rightarrow O(\Delta x)$$

The method will not work.

$\rightarrow$ To get the second degree, second order approx.

$$\therefore P_2'(x_1) = \frac{1}{\Delta x}\left[\Delta f_0 + \frac{1}{2}\Delta^2 f_0\right] \rightarrow O(\Delta x^2)$$

$$= \frac{1}{2\Delta x}\left[2\Delta f_0 + \Delta^2 f_0\right] \rightarrow O(\Delta x^2) = \frac{2(f_1 - f_0) + (f_2 - 2f_1 + f_0)}{2\Delta x} \rightarrow O(\Delta x^2)$$

or, $$\boxed{\left.\frac{df}{dx}\right|_{x=x_1} \cong P_2'(x_1) = \frac{f_2 - f_0}{2\Delta x} \rightarrow O(\Delta x^2)}$$

Similarly the second derivative: $P_n''(x_1) = \frac{1}{\Delta x^2}\left[\Delta^2 f_0 - \frac{1}{12}\Delta^4 f_0 + \cdots\right]$

i.e. $P_2''(x_1) = \frac{1}{\Delta x^2}\left[\Delta^2 f_0\right] \to O(\Delta x^2)$

$$\boxed{P_2''(x_1) = \frac{f_2 - 2f_1 + f_0}{\Delta x^2} \to O(\Delta x^2)}$$