CE 601: Numerical Methods

Lecture 20

Numerical Differentiation-2 (contd.)

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We discussed in the last class on development of one-sided forward difference form (in general):

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

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

and the centered-difference form:

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

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

We also discussed the development of difference formulas for derivatives.

$\rightarrow$ The one-sided forward difference formulas for first, second derivatives, etc

$$\left.\frac{df}{dx}\right|_{x=x_0} \approx P_1'(x_0) = \frac{f_1 - f_0}{\Delta x} \rightarrow O(\Delta x)$$

$$\left.\frac{d^2 f}{dx^2}\right|_{x=x_0} \approx P_2''(x_0) = \frac{f_2 - 2f_1 + f_0}{\Delta x^2} \rightarrow O(\Delta x), \text{ etc.}$$

$\rightarrow$ The centered-difference formulas for first, second derivatives etc.

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

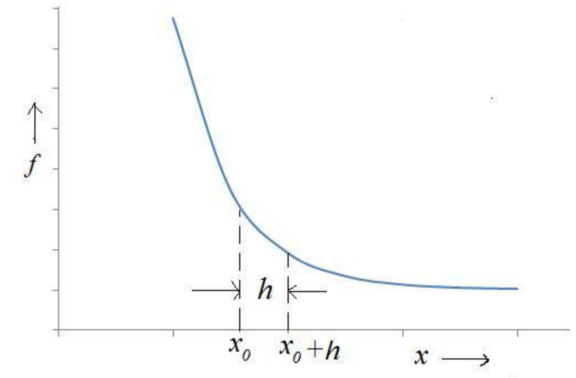
$$\left.\frac{d^2 f}{dx^2}\right|_{x=x_1} \approx P_2''(x_1) = \frac{f_2 - 2f_1 + f_0}{\Delta x^2} \rightarrow O(\Delta x^2)$$

Q1. Why do you require numerical differentiation?

- If there exist only discrete data, then to understand the changing behavior in data, we need to find the derivatives of the actual function. In such situation, we can approximate the derivative by numerical differentiation.
- Sometimes, even if the actual function is available, it may be difficult to perform the differentiation or evaluate derivatives. In those cases also numerical differentiation is useful.

Q2. How do we know that higher order approximations are better (i.e. *$O(\Delta x^2)$* is better than *$O(\Delta x)$,* etc.)?

- For this we need to go back into the definition from fundamental calculus.
- For derivative of a function *f* w.r.t. *x,* we know,



$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

Or, $f'(x = x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}$

where h is a very small interval considered.

- So while using numerical differentiation, we are now approximating for the given discrete data.

$f'(x_0) \approx P_1'(x_0)$

Then $f'(x_0) = \frac{f_1 - f_0}{\Delta x} - \frac{1}{2} \frac{(\Delta x)^2}{\Delta x} f''(\zeta);$

where $x_0 \leq \zeta \leq x_1$

$\therefore$ If actual second derivative $f''(\zeta)$ exists, we can now say that, the approximation error is $\frac{1}{2}.\Delta x. f''(\zeta)$

$\therefore \; f'(x_0) = \frac{f_1 - f_0}{\Delta x} \qquad \text{if } \Delta x \to 0$

i.e. In actual: $f'(x_0) = \frac{f_1 - f_0}{\Delta x} - \frac{1}{2} \Delta x f''(\zeta)$

If we want to approximate $f'(x_0) \approx P_1'(x_0)$,

some truncation error will exist $\frac{1}{2}\ \Delta x\ \ f''(\zeta)$

This approximation error due to truncation will vanish as $\Delta x \to 0$.

Here the speed in which the error goes to zero as $\Delta x \to 0$

is the rate of convergence.

If the truncation error is of order $O(\Delta x) \to$ First order approximation.

For second derivative: $P_2''(x_1) = \dfrac{f_2 - 2f_1 + f_0}{\Delta x^2} \to O(\Delta x^2)$

This is a second order method. Here the speed of truncation error approaching zero is more.

($\because$ Ultimately, we want the derivative at $x = x_1$).

Difference Formulas Using Taylor's series

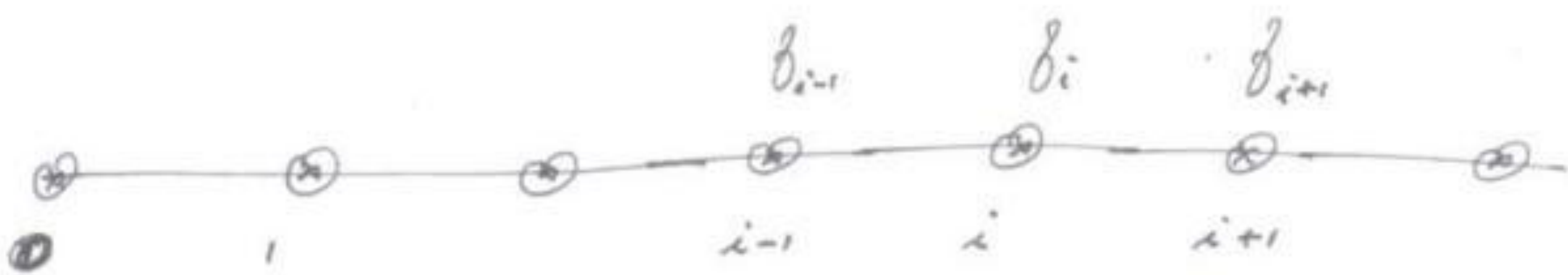
- Using Taylor's series one can obtain a function if the function value at any independent variable $x = x_0$ is known, if the data is uniformly spaced.

i.e. at $x = x_0$, we have f_0, then

$$f(x) = f_0 + \left.\frac{df}{dx}\right|_{x_0} \Delta x + \frac{1}{2!}\left.\frac{d^2 f}{dx^2}\right|_{x_0} \Delta x^2 + \cdots + \frac{1}{n!}\left.\frac{d^n f}{dx^n}\right|_{x_0} \Delta x^n + \cdots$$

where $\Delta x = x - x_0$

One can also form Taylor's series function for multi-variate cases as well.



Taylor's series with base point at $x = x_i$ as:

$$f(x_i + \Delta x) = f_{i+1} = f_i + \Delta x f_i^{(1)} + \frac{(\Delta x)^2}{2!} f_i^{(2)} + \cdots + \frac{(\Delta x)^n}{n!} f_i^{(n)} + \cdots$$

Similarly, we can also write:

$$f(x_i - \Delta x) = f_{i-1} = f_i - \Delta x f_i^{(1)} + \frac{(\Delta x)^2}{2!} f_i^{(2)} - \cdots + \frac{(-\Delta x)^n}{n!} f_i^{(n)} + \cdots$$

Subtracting $f_{i+1} - f_{i-1},$ we get,

$$f_{i+1} - f_{i-1} = 2\Delta x f_i^{(1)} + \frac{1}{3}(\Delta x)^3 f_i^{(3)} + \frac{1}{60}(\Delta x)^5 f_i^{(1)} + \cdots$$

If we truncate the Taylor's series at $O(\Delta x^3),$ we get,

$$f_{i+1} - f_{i-1} = 2\Delta x f_i^{(1)} \rightarrow O(\Delta x^3)$$

or, $\boxed{f_i^{(1)} = \frac{f_{i+1} - f_{i-1}}{2\Delta x} \rightarrow O(\Delta x^2)}$

This is the centered-difference formula for first derivative at any $x = x_i$ by suggesting the order of approximations.

- <u>Example</u>
- Evaluate $P_n'(3.5)$ and $P_n''(3.5)$ using forward and centered difference formulas:

x	f	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$
3.4	***0.294118***				
		-0.008404			
3.5	***0.285714***		***0.000468***		
		-0.007936		***-0.00004***	
3.6	***0.277778***		***0.000428***		-7.2×10^{-5}
		-0.007508		***-0.000032***	
3.7	***0.270270***		***0.000396***		
		-0.007112			
3.8	***0.263158***				

Using forward difference:

$$P_1'(3.5) = \frac{f(3.6) - f(3.5)}{\Delta x} \rightarrow O(\Delta x)$$

$$= \frac{0.277778 - 0.285417}{0.1} = -0.07936$$

$$\text{and } P_2''(3.5) = \frac{f(3.7) - 2f(3.6) + f(3.5)}{\Delta x^2}$$

$$= \frac{0.27027 - 2 \times 0.277778 + 0.285714}{0.1^2} = 0.0428$$

$$\text{Again, } P_2'(3.5) = \frac{1}{\Delta x}\left[\Delta f_{3.5} - \frac{1}{2}\Delta^2 f_{3.5}\right] \rightarrow O(\Delta x^2)$$

$$= \frac{-f(3.7) + 4f(3.6) - 3f(3.5)}{2\Delta x}$$

$$= \frac{-0.27027 + 4 \times 0.277778 - 3 \times 0.285714}{2 \times 0.1} = -0.0815$$

Using centered difference

$$P_2\,'(3.5) == \frac{f(3.6) - f(3.4)}{2\Delta x}$$

$$= \frac{0.277778 - 0.294118}{2 \times 0.1} = -0.0817$$

$$P_2\,''(3.5) == \frac{f(3.6) - 2f(3.5) + f(3.4)}{(0.1)^2} = 0.0468$$

• You can also use Newton's backward difference polynomial, and develop difference difference formulas for derivatives.

$$P_n(x) = f_n + s\nabla f_n + \frac{s(s+1)}{2!}\nabla^2 f_n + \frac{s(s+1)(s+2)}{3!}\nabla^3 f_n + \cdots$$

$$+ \frac{s(s+1)(s+2)\cdots(s+n-1)}{n!}\nabla^n f_n$$

$$\therefore P_n\,'(x) = \frac{1}{\Delta x}\left[\nabla f_n + \frac{2s+1}{2}\nabla^2 f_n + \frac{3s^2+6s+2}{6}\nabla^3 f_n + \cdots\right]$$

$$P_n\,''(x) = \frac{1}{\Delta x^2}\left[\nabla^2 f_n + (s+1)\nabla^3 f_n + \cdots\right]$$

$$\text{e.g. } P_1\,'(x_n) = \frac{f_n - f_{n-1}}{\Delta x} \rightarrow O(\Delta x)$$

$$P_2\,''(x_n) = \frac{f_n - 2f_{n-1} + f_{n-2}}{\Delta x^2} \rightarrow O(\Delta x^2)$$