Lecture 28: Difference formulas

(04-Oct-2012)

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DIFFERENCE FORMULAS

In the last class we have seen how Newton's polynomials are used to develop difference formulas ~~using~~ for various derivatives.

In the last day's uploaded notes - a short description on one-sided backward difference formulas were also given. These formula for $P_n'(x_0)$ and $P_n''(x_0)$ were developed from Newton's backward difference polynomial.

* Now recall the one-sided forward difference formula

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

As suggested, on truncating after the first term, we have

$$P_1'(x_0) = \frac{\Delta f_0}{\Delta x} + O(\Delta x)$$

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

x	f	Δf	$\Delta^2 f$
x_0	f_0		
		$(f_1 - f_0)$	
x_1	f_1		$f_2 - 2f_1 + f_0$
		$(f_2 - f_1)$	
x_2	f_2		$f_3 - 2f_2 + f_1$
		$(f_3 - f_2)$	
x_3	f_3		

Ill^y. On truncating after second term:

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

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

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

$$\text{i.e. } P_2'(x_0) = \frac{-f_2 + 4f_1 - 3f_0}{2\Delta x} + O(\Delta x^2)$$

The second derivative using one-sided forward difference :

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

Now $\quad P_2''(x_0) = \frac{1}{(\Delta x)^2} \Delta^2 f_0 + O(\Delta x)$

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

(Please note that there was typing mistake in last class's notes)

IIIly $\quad P_3''(x_0) = \frac{1}{(\Delta x)^2}\left[\Delta^2 f_0 - \Delta^3 f_0 \right] + O(\Delta x^2)$

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

$$= \frac{-f_3 + 4f_2 - 5f_1 + 2f_0}{(\Delta x)^2} + O(\Delta x^2)$$

⇒ You can also use centered-difference to derive difference formulas.

Please recall

$$P_n'(x_1) = \frac{1}{\Delta x}\left[\Delta f_0 + \frac{1}{2}\Delta^2 f_0 - \frac{1}{6}\Delta^3 f_0 + \frac{1}{12}\Delta^4 f_0 + \cdots \right]$$

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

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

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

i.e. $\quad P_2'(x_1) = \dfrac{f_2 - f_0}{2\Delta x} + O(\Delta x^2)$

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

i.e. $\quad P_2''(x_1) = \frac{1}{(\Delta x)^2}\Delta^2 f_0 \quad + \quad O(\Delta x^2)$

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

Example:

Calculate second-order forward and centered difference approximations for $f'(3.6)$ and $f''(3.6)$ for the yesterday's example.

Soln.

Given

x	f
3.4	0.294118
3.5	0.285714
3.6	0.277778
3.7	0.270270
3.8	0.263158

⇒ To evaluate $f'(3.6)$ using second-order forward difference

$f'(3.6) \approx P_2'(x_0)$

where $x_0 = 3.6$, $f_0 = 0.277778$

$$\therefore P_2'(x_0) = \frac{-f_2 + 4f_1 - 3f_0}{2\Delta x} = \frac{-0.263158 + 4\times 0.270270 - 3\times 0.277778}{2\times 0.1}$$

$$= -0.07706$$

⇒ To evaluate $f'(3.6)$ using second-order centered difference

$f'(3.6) \approx P_2'(x_1)$; where $x_0 = 3.5$, $x_1 = 3.6$

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

$$= \frac{0.270270 - 0.285714}{2\times 0.1} = -0.07722 \quad O(\Delta x^2)$$

Similarly for second derivative

$\Rightarrow$ Using second-order forward difference if $x_0 = 3.5$

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

$$= \frac{0.270270 - 2 \times 0.277778 + 0.285714}{(0.1)^2}$$

$$= \underline{\underline{0.0428}}$$

~~$\Rightarrow$ Using second-order centered difference~~

But if you have consider $f''(3.6) \approx P_2''(3.6)$, then using forward difference you may get:

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

$$= \frac{0.263158 - 2 \times 0.270270 + 0.277778}{(0.1)^2} + O(\Delta x)$$

$$= \underline{\underline{0.0396}}$$

$\Rightarrow$ Using centered difference

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

$$= \underline{\underline{0.0428}}$$

There is definitely difference in the results in the above two schemes:

To Obtain Difference Formulas using Taylor's Series

→ The difference formulas for first and second derivatives developed using Newton's polynomials was discussed in the previous section.

→ The same formulas can be derived using Taylor's series approach as well.

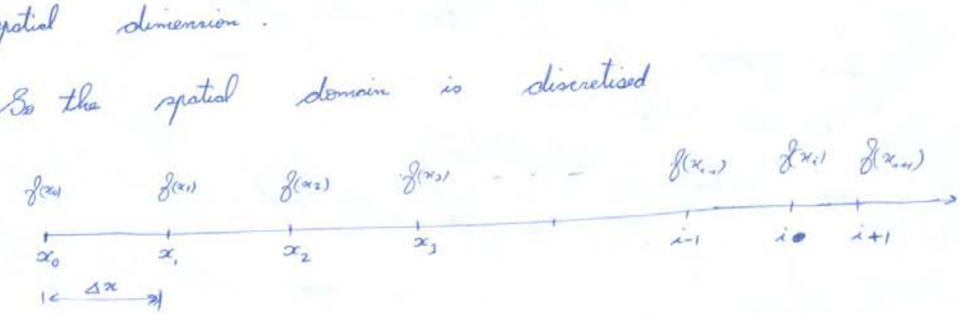
If 'f' is function of only 'x' and if at $x = x_0$, $f(x_0) = f_0$ is known to you, then we can define for equally spaced data at the function $f(x)$

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

This is an infinite series.

→ In this case we usually consider x representing spatial dimension.

So the spatial domain is discretised



→ If your function f is varying only with respect to time 't' and say at $t = t_0$, $f(t_0)$ is the function value

Then we can say:

$$f(t) = f(t_0) + \left.\frac{df}{dt}\right|_{t_0} \Delta t + \frac{1}{2}\left.\frac{d^2f}{dt^2}\right|_{t_0} (\Delta t)^2 + \cdots\cdots$$

Now if the function 'f' varies both w.r.t x ~~and~~ (space) and t (time), then say at $f(x_0, t_0)$ the function value is known:

$$f(x,t) = f(x_0,t_0) + \left(\left.\frac{\partial f}{\partial x}\right|_{(x_0,t_0)} \Delta x + \left.\frac{\partial f}{\partial t}\right|_{(x_0,t_0)} \Delta t \right)$$

$$+ \frac{1}{2!}\left(\left.\frac{\partial^2 f}{\partial x^2}\right|_{(x_0,t_0)} \Delta x^2 + \left.\frac{\partial^2 f}{\partial t^2}\right|_{(x_0,t_0)} \Delta t^2 + 2\left.\frac{\partial^2 f}{\partial x \partial t}\right|_{(x_0,t_0)} \Delta x \Delta t \right)$$

$$+ \cdots\cdots$$

Please note:

$\Rightarrow$ The continuous spatial domain is discretized as discrete points $x_0, x_1, x_2, \cdots x_n$

$\Rightarrow$ The continuous time domain is discretized into $t_0, t_1, t_2, \ldots$ discrete times.

In Taylor's series, we have to note that, the function 'f' has to be differentiated w.r.t 'x' and 't' and they are partial differentiations.

However if $f(x,t) = f(x)$. That is not varying w.r.t ~~for~~ 't'. Then we can ~~say~~ differentiate fully w.r.t 'x' i.e $\frac{df}{dx}$ or $\frac{d^2f}{dx^2}$, etc.

Consider the function $f(x)$:

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

$$\cdots + \frac{1}{n!} \left.\frac{d^nf}{dx^n}\right|_{x_0} (\Delta x)^n + \cdots$$

This series if you truncate at $\left.\frac{d^nf}{dx^n}\right|_{x_0}$ term

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

$$\cdots + \frac{1}{n!} \left.\frac{d^nf}{dx^n}\right|_{x_0} (\Delta x)^n + \underbrace{R^{(n+1)}}_{\text{Remainder}}$$

Remainder $\quad R^{(n+1)} = \frac{1}{(n+1)!} \left.\frac{d^{(n+1)}f}{dx^{n+1}}\right|_{(x=\xi)} \Delta x^{n+1}$

where $\quad x_0 \le \xi \le x_0 + \Delta x$

i.e. If we truncate Taylor's series, the order of approximation can be given as $O(\Delta x^{n+1})$.

$\Rightarrow$ As suggested earlier if the spatial domain is discretised at equal space

Using $x = x_i$ as base point, we can develop Taylor's series:

i.e. $f(x_i + \Delta x) = f(x_i) + \left.\frac{df}{dx}\right|_{x_i} \Delta x + \frac{1}{2!} \left.\frac{d^2f}{dx^2}\right|_{x_i} (\Delta x)^2 + \frac{1}{6} \left.\frac{d^3f}{dx^3}\right|_{x_i} (\Delta x)^3$

i.e. $f(x_{i+1}) \qquad + \cdots\cdots \qquad \rightarrow$ (A)

And

$$f(x_i - \Delta x) = f(x_{i-1}) = f(x_i) - \left.\frac{df}{dx}\right|_{x_i} \Delta x + \frac{1}{2} \left.\frac{d^2 f}{dx^2}\right|_{x_i} (\Delta x)^2$$

$$- \frac{1}{6} \left.\frac{d^3 f}{dx^3}\right|_{x_i} (\Delta x)^3 + \cdots \rightarrow B$$

$\Rightarrow$ Eqn A − B gives:

$$f_{i+1} - f_{i-1} = 2 \left.\frac{df}{dx}\right|_{x_i} \Delta x + \frac{1}{3} \left.\frac{d^3 f}{dx^3}\right|_{x_i} (\Delta x)^3 + \cdots$$

If we are truncating Taylor's series at $\frac{d^3 f}{dx^3}$ term:

$$\left.\frac{df}{dx}\right|_{x_i} = f'(x_i) = \frac{f_{i+1} - f_{i-1}}{2\Delta x} - \frac{1}{6} f^{(3)}(\xi) \Delta x^2$$

where $x_{i-1} \leq \xi \leq x_{i+1}$

i.e. $$\boxed{f'(x_i) = \frac{f_{i+1} - f_{i-1}}{2\Delta x} - \frac{1}{6} f^{(3)}(\xi) \Delta x^2}$$

$\rightarrow O(\Delta x^2)$

This $O(\Delta x^2)$ finite-difference approximation for $f'(x_i)$.

$\Rightarrow$ If A + B is taken:

$$f_{i+1} + f_{i-1} = 2 f_i + f''(x_i) \Delta x^2 + \frac{1}{12} f^{(4)}(x_i) \Delta x^4 + \cdots$$

Truncating at fourth order:

$$\boxed{f''(x_i) \Delta x^2 = \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} - \frac{1}{12} f^{(4)}(\xi) \Delta x^2}$$

This is again finite-difference approximation for second derivative

If function f is w.r.t time 't' only, then the same logic of obtaining difference equations ~~are~~ are applicable for this case.

In the case of time differentiation

$$\left.\frac{df}{dt}\right|_{t=t_n} = \frac{f(t_{n+1}) - f(t_{n-1})}{2\Delta t} + O(\Delta t^2)$$

$$\left.\frac{d^2 f}{dt^2}\right|_{t=t_n} = \frac{f(t_{n+1}) - 2f(t_n) - f(t_{n-1})}{(\Delta t)^2} + O(\Delta t^2)$$

You can go through the various difference formulas provided in the text book.