Lecture 27: Difference formulas using Newton's polynomials

(03-Oct-2012)

NUMERICAL DIFFERENTIATION - - -

LECTURE 27
03-OCT-2012

In the last class we discussed that in numerical methods, the differentiation of any functions are done by using approximate forms like - <u>numerical differentiation</u>.

→ If the discrete data sets are approximated by polynomial expressions, then the derivatives (or differentiations) can also be obtained by differentiating the polynomial.

→ For equally spaced data set you have seen the one-sided forward difference formulas for first and second derivatives (using Newton's forward difference polynomial) as:

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

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

The error expression was given as:

$$\frac{d}{dx}\left(\text{Error}\,(x_0)\right) = \frac{(-1)^n}{(n+1)}(\Delta x)^n f^{(n+1)}(\xi)$$

$$x_0 \le \xi \le x_n$$

Therefore error for first derivative was of $O(\Delta x^n)$

That is, the order of first derivative got reduced by one degree compared to the ~~actual~~ polynomial $P_n(x)$.

Therefore, from the one sided forward difference formulas

$P_1'(x_0) \rightarrow O(\Delta x)$

$P_2'(x_0) \rightarrow O(\Delta x^2)$

$P_3'(x_0) \rightarrow O(\Delta x^3)$

$\vdots$

$P_n'(x_0) \rightarrow O(\Delta x^n)$

→ Now $\quad P_n''(x_0) \rightarrow O(\Delta x^{n-1})$

i.e. $P_1''(x_0) \rightarrow$ Not possible

$P_2''(x_0) \rightarrow O(\Delta x)$

$P_3''(x_0) \rightarrow O(\Delta x^2)$ etc.

⇒ If $s = 1.0$ in Newton's forward difference polynomial then $x = x_1$

$$P_n(x_1) = f_0 + \Delta f_0$$

$$P_n'(x_1) = \frac{1}{\Delta x}\left[\Delta f_0 + \frac{2-1}{2}\Delta^2 f_0 + \frac{3-6+2}{6}\Delta^3 f_0 + \frac{4-18+22-6}{24}\Delta^4 f_0 + \cdots\right]$$

$$\left(\because\ P_n'(x) = \frac{1}{\Delta x}\left[\Delta f_0 + \frac{2s-1}{2}\Delta^2 f_0 + \frac{3s^2-6s+2}{6}\Delta^3 f_0 + \frac{1}{24}(4s^3-18s^2+22s-6)\Delta^4 f_0 + \cdots\right]\right)$$

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

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

$P_n'(x_1)$ and $P_n''(x_1)$ are expressions for centered difference formulas for first and second derivatives. This is because the differences are calculated centered at $x = x_1$.

Now $P_1'(x_1) \Rightarrow O(\Delta x)$ same as one-sided forward difference

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

However, $P_2''(x_1) \rightarrow$ of what order

As this is a second degree polynomial

$P_2(x_1) \rightarrow O(\Delta x^3)$

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

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

$\therefore \quad P_2'' x_1 = \frac{1}{(\Delta x)^2}\left[\Delta^2 f_0\right] \rightarrow \frac{O(\Delta x^4)}{(\Delta x^2)} \rightarrow O(\Delta x^2)$

From Example (from Hoffman, 2001 Page 259)

For the given data set, evaluate $P_n'(3.5)$ and $P_n''(3.5)$ using forward and centered difference formulas.

x	$f(x)$	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		8×10^{-6}
		−0.007508		−0.000032	
3.7	0.270270		0.000396		
		−0.007112			
3.8	0.263158				

$$P_n'(x) = \frac{1}{\Delta x}\left[\Delta y_0 + \frac{2s-1}{2}\Delta^2 y_0 + \frac{3s^2-6s+2}{6}\Delta^3 y_0 + \cdots\right]$$

$$P_n''(x) = \frac{1}{(\Delta x)^2}\left[\Delta^2 y_0 + (s-1)\Delta^3 y_0 + \cdots\right]$$

To evaluate $P_n'(3.5)$ using one-sided forward difference formula.

Put $x_0 = 3.5$, ~~and $s = 0.0$~~ $\therefore y_0 = 0.285714$, and $s = 0.0$

Then $P_n'(3.5) = \frac{1}{0.1}\left[(-0.007936) + \left(-\frac{1}{2}\right)\times(0.000428) + \frac{1}{3}\times(-0.000032)\right]$

$= -0.081607$

If you had taken
$P_1'(3.5) = -0.07936 \rightarrow O(\Delta x)$
$P_2'(3.5) = -0.081500 \rightarrow O(\Delta x^2)$
$P_3'(3.5) = -0.081607 \rightarrow O(\Delta x^3)$

Similarly $P_n''(3.5) = \frac{1}{(0.1)^2}\left[(0.000428) - (-0.000032)\right]$

Here $P_2''(3.5) = 0.04280 \rightarrow O(\Delta x)$
$P_3''(3.5) = 0.0460 \rightarrow O(\Delta x^2)$

To evaluate $P_n'(3.5)$ & $P_n''(3.5)$ using centered difference formula

Now put $x_0 = 3.4$, $\therefore y_0 = 0.294118$, and $s = 1.0$

i.e. $x_1 = 3.5$.

$\therefore P_n'(3.5) = \frac{1}{\Delta x}\left[\Delta y_0 + \frac{1}{2}\Delta^2 y_0 - \frac{1}{6}\Delta^3 y_0 + \frac{1}{12}\Delta^4 y_0 + \cdots\right]$

i.e. $P_n'(3.5) = \frac{1}{(0.1)}\left[(-0.008404) + \frac{1}{2}(0.000468) - \frac{1}{6}\times(-0.00004) + \frac{1}{12}\times 8\times10^{-6}\right]$

$\therefore P_1'(3.5) = -0.08404 \rightarrow O(\Delta x)$

$P_2'(3.5) = -0.0817 \rightarrow O(\Delta x^2)$

$P_3'(3.5) = -0.081633$

$P_4'(3.5) = -0.081626$

Similarly

$$P_n''(3.5) = \frac{1}{(0.1)^2}\left[\Delta^2 f_0 - \frac{1}{12}\Delta^4 f_0 \cdots\right]$$

Again $P_2''(3.5) = \frac{1}{(0.1)^2}\left[(0.000468)\right]$

$= 0.0468$

$P_3''(3.5) \Rightarrow$ Not possible to evaluate

$$P_4''(3.5) = \frac{1}{(0.1)^2}\left[0.000468 - \frac{1}{12} \times 8 \times 10^{-6}\right]$$

$= 0.0467333$

You can see that centered difference formula behaves better for numerically differentiating the functions.

Newton's Backward Difference Polynomial

The Newton's backward difference polynomial was given as:

$$P_n(x) = f_0 + s\,\nabla f_0 + \frac{s(s+1)}{2!}\nabla^2 f_0 + \frac{s(s+1)(s+2)}{3!}\nabla^3 f_0 + \cdots$$

where $s = \dfrac{x - x_0}{\Delta x}$

Now if we are approximating the actual function $f(x)$ by Newton's backward difference polynomial $P_n(x)$, then

$$f'(x) \approx P_n'(x) = \frac{1}{\Delta x}\frac{d}{ds}(P_n(s))$$

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

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

Again at $\underline{x = x_0}$, we have $s = 0.0$

$$\boxed{\begin{aligned} P_n'(x_0) &= \frac{1}{\Delta x}\left[\nabla f_0 + \frac{1}{2}\nabla^2 f_0 + \frac{1}{3}\nabla^3 f_0 + \cdots\right] \\ P_n''(x_0) &= \frac{1}{(\Delta x)^2}\left[\nabla^2 f_0 + \nabla^3 f_0 + \cdots\cdots\right] \end{aligned}}$$

These are one-sided backward-difference formulas.

IIly when $s = -1.0$, we have $x = x_{-1}$

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

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

$\Rightarrow$ Let us elaborate these difference formulas

<u>Difference Formulas</u>

The one-sided forward difference formula

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

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

When we truncate after the first term

i.e. $$P_n'(x_0) = \frac{\Delta f_0}{\Delta x} + O(\Delta x)$$

$$\therefore \quad P_1'(x_0) = \frac{f_1 - f_0}{x_1 - x_0} + O(\Delta x)$$

→ If we truncate after the second order term:

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

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

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

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

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

⇒ The one-sided forward difference for second derivative

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

If we truncate after first term:

$$P_n''(x_0) = \frac{1}{(\Delta x)^2} \cdot \Delta^2 f_0 + O(\Delta x)$$

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

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

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

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