CHN-323
Computer Applications in Chemical Engineering

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Interpretation

- What will be f(3.5)?

x	$f(x)$
2	8
3	27
4	64
5	125
6	216

Difference operators

- Let us say we have a data set

$$\{(f_j, x_j) \mid \quad j = 1, 2, \ldots., m\}$$

- Data is equally spaced

$$x_{i+1} = x_i + h$$
$$where\ i = 1, 2, \ldots., m-1$$

- h: step size, discretization interval

- $\Delta f_i = f_{i+1} - f_i$ Forward difference operator
- $\nabla f_i = f_i - f_{i-1}$ Backward difference operator
- $E f_i = f_{i+1}$ Shift operator

Difference operators: higher order

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

$$= (f_{i+2} - f_{i+1}) - (f_{i+1} - f_i)$$

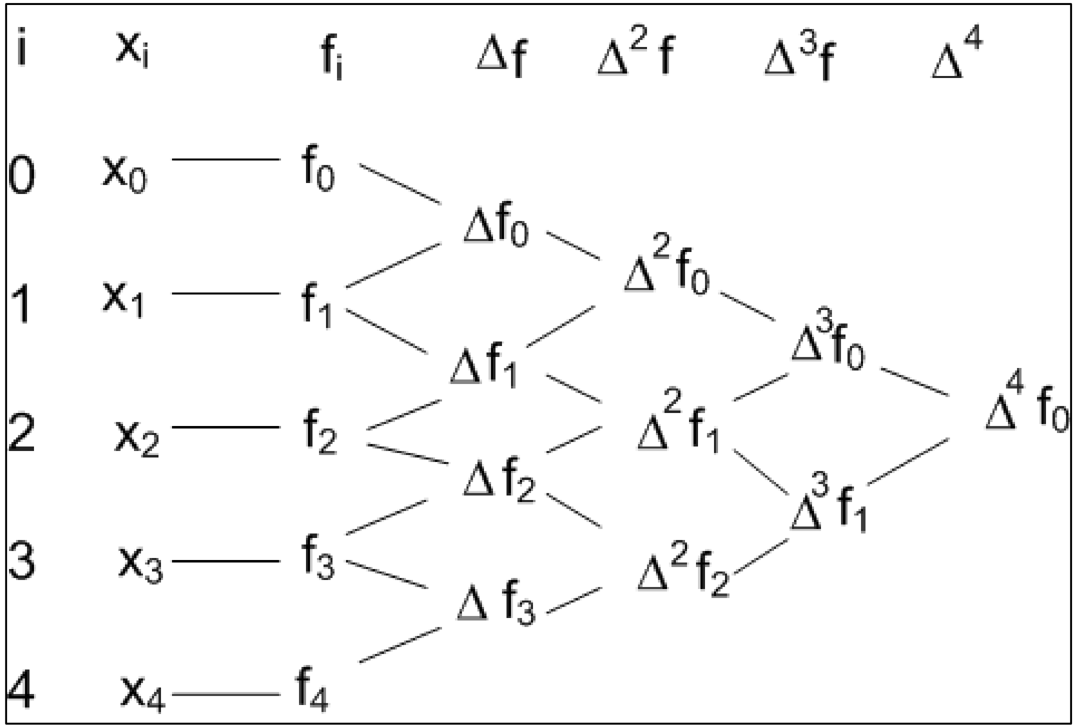
$$= f_{i+2} - 2f_{i+1} + f_i$$

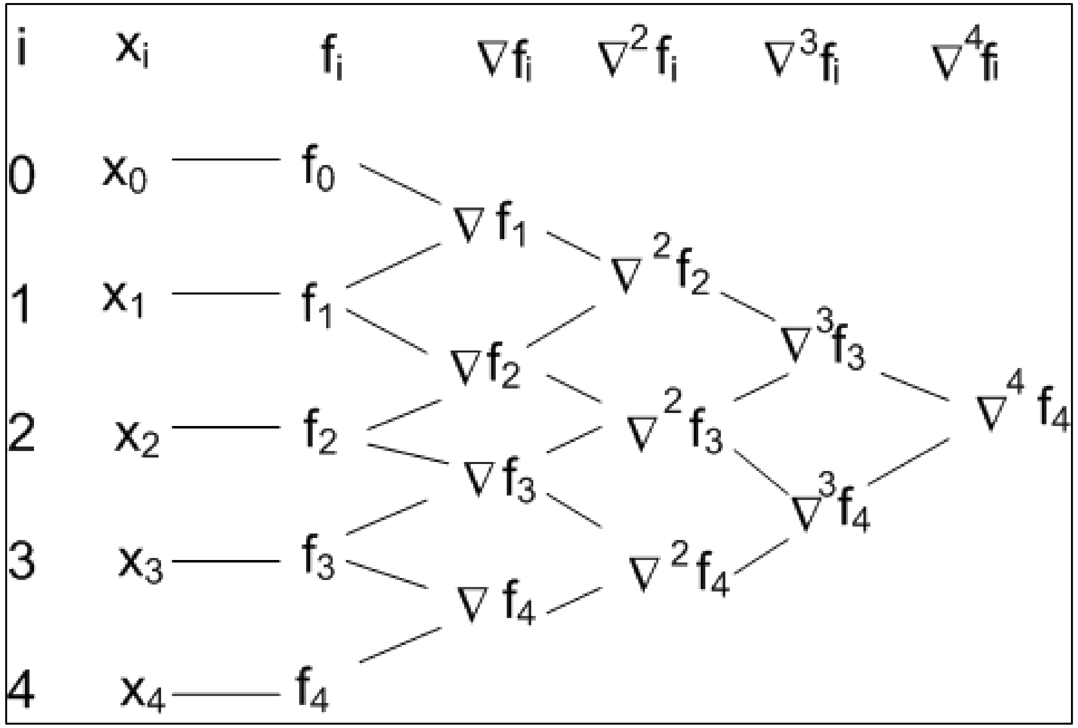
- $\Delta^3 f_i = \Delta^2(\Delta f_i) = \Delta^2(f_{i+1} - f_i) = \Delta^2(f_{i+1}) - \Delta^2(f_i)$

$$= (f_{i+3} - 2f_{i+2} + f_{i+1}) - (f_{i+2} - 2f_{i+1} + f_i)$$

$$= f_{i+3} - 3f_{i+2} + 3f_{i+1} - f_i$$

Difference tables





Shift operator

- $Ef_i = f_{i+1}$ what are f_i and f_{i+1}?
- $E^2 f_i = f_{i+2}$

$$Ef(x_i) = f(x_i + h)$$

- We know that $\Delta f_i = f_{i+1} - f_i$
- This can be rewritten as $\Delta f_i = Ef_i - f_i = (E-1)f_i$

$$\Delta = (E-1)$$

Or $E = (1+\Delta)$

- Generalizing this, $E^\alpha = (1+\Delta)^\alpha$

- Exercise: Prove that $E^2 = (1+\Delta)^2$

Polynomial approximation of dataset

- Our data set

$$\{(f_j, x_j)| \quad j = 1, 2, \ldots., m\}$$

This can be approximated as

$$f(x) = P_n(x) + R(x)$$

Where $P_n(x)$ is the polynomial approximation of f(x) and R(x) is the residual error.

- What will be f(3.5)?

x	*f(x)*
2	8
3	27
4	64
5	125
6	216

- In other words, we need to find $f(3+0.5)$ or $f(2+1.5)$ or $f(4-0.5)$.

Or $f(x_i+\alpha h)$

- $f(x_i+\alpha h)=E^{\alpha}f(x_i)=(1+\Delta)^{\alpha}f(x_i)$

- Using binomial theorem, we can write

$$f(x_i + \alpha h) = \left[1 + \alpha\Delta + \frac{\alpha(\alpha-1)}{2!}\Delta^2 + \frac{\alpha(\alpha-1)(\alpha-2)}{3!}\Delta^3 + \cdots\right] f(x_i)$$

- Can choose α to be 0, 1, …, m-1 and indeed other non-integer real values to reach any x value in $[x_1, x_m]$

Numerical differentiation

- We need to estimate $\frac{df}{dx}$

- We have already written

$$f(x) = f(x_i + \alpha h) = \left[1 + \alpha\Delta + \frac{\alpha(\alpha-1)}{2!}\Delta^2 + \frac{\alpha(\alpha-1)(\alpha-2)}{3!}\Delta^3 + \cdots\right] f(x_i)$$

- $\frac{df}{dx} = \frac{df}{d\alpha} * \frac{d\alpha}{dx} = \frac{df}{d\alpha} * \frac{1}{h}$ Since $x = x_i + \alpha h \rightarrow \frac{d\alpha}{dx} = \frac{1}{h}$

- Thus we can write

$$f'(x) \approx \frac{1}{h}\left[\Delta + \frac{\alpha+(\alpha-1)}{2}\Delta^2 + \frac{\{\alpha(\alpha-1)+(\alpha-1)(\alpha-2)+\alpha(\alpha-2)\}}{6}\Delta^3 + \cdots\right] f(x_i)$$

- For x_1, $\alpha = 0$

$$f'(x_1) \approx \frac{1}{h}\left[\Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 + \cdots \pm \frac{1}{m-1}\Delta^{m-1}\right] f(x_1) + O(h^{m-1})$$

- Consider only the first term

$$f'(x_1) \approx \frac{1}{h}\Delta f(x_1) + O(h)$$
$$\approx \frac{1}{h}\{f_2 - f_1\} + O(h)$$

Two-points (2P)
First order accurate (FOA)
Forward difference (FDA)

Generalized form: $f'(x_i) \approx \frac{1}{h}\{f_{i+1} - f_i\} + O(h)$

- Consider the first two terms

$$f'(x_1) \approx \frac{1}{h}\left[\Delta f(x_1) - \frac{1}{2}\Delta^2 f(x_1)\right] + O(h^2)$$
$$\approx \frac{1}{h}\left[(f_2 - f_1) - \frac{1}{2}(f_1 - 2f_2 + f_3)\right] + O(h^2)$$
$$\approx \frac{1}{2h}[-3f_1 + 4f_2 - f_3] + O(h^2)$$

3P, SOA, FDA

Generalized form: $f'(x_i) \approx \frac{1}{2h}[-3f_i + 4f_{i+1} - f_{i+2}] + O(h^2)$

- For x_2, $\alpha = 1$

$$f'(x_2) \approx \frac{1}{h}\left[\Delta + \frac{1}{2}\Delta^2 - \frac{1}{6}\Delta^3 + \cdots\right] f(x_1) + O(h^{m-1})$$

- Consider the first two terms

$$f'(x_2) \approx \frac{1}{h}\left[\Delta f(x_1) + \frac{1}{2}\Delta^2 f(x_1)\right] + O(h^2)$$

$$\approx \frac{1}{h}\left[(f_2 - f_1) + \frac{1}{2}(f_1 - 2f_2 + f_3)\right] + O(h^2)$$

$$\approx \frac{1}{2h}[f_3 - f_1] + O(h^2)$$

2P, SOA, CDA

- Generalizing this, we can write another formula for $f'(x_i)$

$$f'(x_i) \approx \frac{1}{2h}\{f_{i+1} - f_{i-1}\} + O(h^2)$$

First Derivative		
Method	**Formula**	**Truncation Error**
Two-point forward difference	$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
Three-point forward difference	$f'(x_i) = \dfrac{-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2})}{2h}$	$O(h^2)$
Two-point central difference	$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_{i-1})}{2h}$	$O(h^2)$
Two-point backward difference	$f'(x_i) = \dfrac{f(x_i) - f(x_{i-1})}{h}$	$O(h)$
Three-point backward difference	$f'(x_i) = \dfrac{f(x_{i-2}) - 4f(x_{i-1}) + 3f(x_i)}{2h}$	$O(h^2)$

- Second order derivatives
- We have already written

$$f(x) = f(x_i + \alpha h) = \left[1 + \alpha\Delta + \frac{\alpha(\alpha-1)}{2!}\Delta^2 + \frac{\alpha(\alpha-1)(\alpha-2)}{3!}\Delta^3 + \cdots\right] f(x_i)$$

- $\frac{d^2 f}{dx^2} = \frac{d}{dx}\left[\frac{df}{d\alpha} * \frac{d\alpha}{dx}\right] = \frac{d}{d\alpha}\left[\frac{df}{d\alpha} * \frac{d\alpha}{dx}\right]\frac{d\alpha}{dx} = \frac{1}{h^2}\frac{d^2 f}{d\alpha^2}$

- Thus we can write

$$f''(x) \approx \frac{1}{h^2}\left[\Delta^2 + \frac{\{\alpha+(\alpha-1)+(\alpha-1)+(\alpha-2)+\alpha+(\alpha-2)\}}{6}\Delta^3 + \cdots\right] f(x_i)$$

- For x_1, $\alpha = 0$

$$f''(x_1) \approx \frac{1}{h^2}\left[\Delta^2 - \Delta^3 + \frac{11}{12}\Delta^4 + \cdots\right] f(x_1)$$

- Consider only the first term

$$f''(x_1) \approx \frac{1}{h^2}[\Delta^2 f(x_1)] + O(h)$$
$$\approx \frac{1}{h^2}\{f_1 - 2f_2 + f_3\} + O(h)$$

3P, FOA, FDA

Generalized form: $f''(x_i) \approx \frac{1}{h^2}\{f_i - 2f_{i+1} + f_{i+2}\} + O(h)$

- Consider the first two terms

$$f''(x_1) \approx \frac{1}{h^2}[\Delta^2 f(x_1) - \Delta^3 f(x_1)] + O(h^2)$$
$$\approx \frac{1}{h^2}\{2f_1 - 5f_2 + 4f_3 - f_4\} + O(h^2)$$

4P, SOA, FDA

Generalized form: $f''(x_i) \approx \frac{1}{h^2}\{2f_i - 5f_{i+1} + 4f_{i+2} - f_{i+3}\} + O(h^2)$

- For x_2, $\alpha = 1$

$$f''(x_2) \approx \frac{1}{h^2}[\Delta^2 + 0\Delta^3 + \cdots]f(x_1)$$

- Consider the first two terms

$$f''(x_2) \approx \frac{1}{h^2}[\Delta^2 f(x_1)] + O(h^2)$$

$$\approx \frac{1}{h^2}\{f_1 - 2f_2 + f_3\} + O(h^2)$$

3P, SOA, CDA

- Generalizing this, we can write another formula for $f''(x_i)$

$$f''(x_i) \approx \frac{1}{h^2}\{f_{i-1} - 2f_i + f_{i+1}\} + O(h^2)$$

Second Derivative		
Method	**Formula**	**Truncation Error**
Three-point forward difference	$f''(x_i) = \dfrac{f(x_i) - 2f(x_{i+1}) + f(x_{i+2})}{h^2}$	$O(h)$
Four-point forward difference	$f''(x_i) = \dfrac{2f(x_i) - 5f(x_{i+1}) + 4f(x_{i+2}) - f(x_{i+3})}{h^2}$	$O(h^2)$
Three-point central difference	$f''(x_i) = \dfrac{f(x_{i-1}) - 2f(x_i) + f(x_{i+1})}{h^2}$	$O(h^2)$
Three-point backward difference	$f''(x_i) = \dfrac{f(x_{i-2}) - 2f(x_{i-1}) + f(x_i)}{h^2}$	$O(h)$
Four-point backward difference	$f''(x_i) = \dfrac{-f(x_{i-3}) + 4f(x_{i-2}) - 5f(x_{i-1}) + 2f(x_i)}{h^2}$	$O(h^2)$

Example

- What is f′(3.5)?
  - Using 2P, FOA, FDA
  - Using 2P, FOA, BDA
  - Using 2P, SOA, CDA

x	f(x)
3.4	0.294118
3.5	0.285714
3.6	0.277778

- What is f″(3.5)?
  - Using 3P, SOA, CDA