Finite Difference Method:
Approximate the derivatives

Taylor Expansion

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

$$f(x_0 + \Delta x) = f(x_0) + \int_{x_0}^{x_0 + \Delta x} f'(x) dx$$

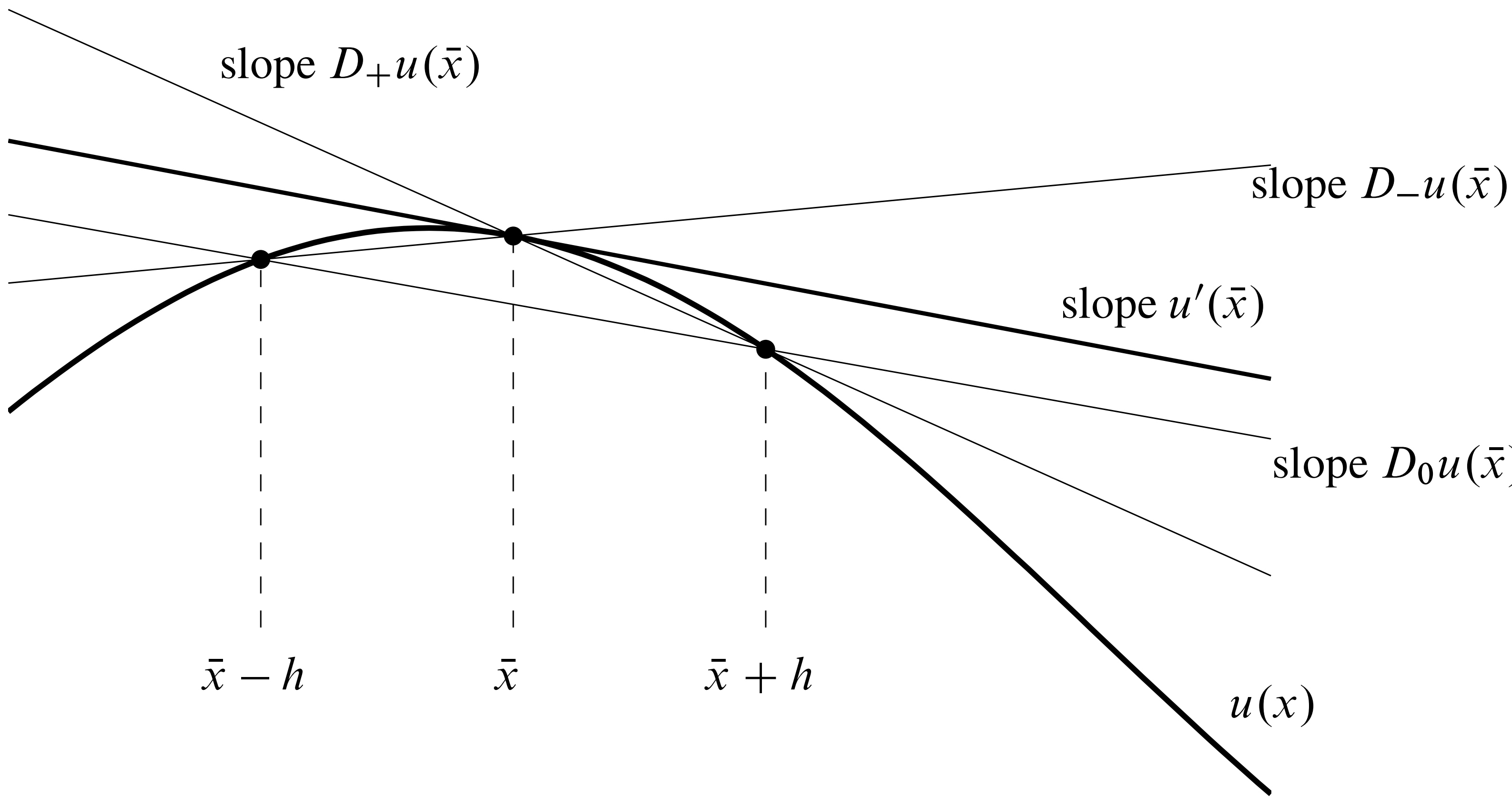
$$\to f(x_0 + \Delta x) = f(x_0) + \int_{x_0}^{x_0 + \Delta x_0} \left(f'(x_0) + \int_{x_0}^{x_0 + \Delta x_0} f''(x_2) dx_2 \right) dx$$

$$= f(x_0) + f'(x_0)\Delta x + \left(\int_{x_0}^{x_0 + \Delta x_0} f''(x) dx \right)^2$$

$$= f(x_0) + f'(x_0)\Delta x + f''(x_0)\frac{\Delta x^2}{2} + \left(\int_{x_0}^{x_0 + \Delta x_0} f'''(x) dx \right)^3$$

$$\Rightarrow f(x_0 + \Delta x) = f(x_0) + f'(x_0)\Delta x + f''(x_0)\frac{\Delta x^2}{2} + f'''(x_0)\frac{\Delta x^3}{3!} + \ldots$$

Using two neighboring points to approximate first derivatives



One-sided Differences

$$D_-u(\bar{x}) = \frac{u(\bar{x}) - u(\bar{x}-h)}{h}$$

$$D_+u(\bar{x}) = \frac{u(\bar{x}+h) - u(\bar{x})}{h}$$

Take the average of the two: Centered-difference

$$D_0u(\bar{x}) = \frac{u(\bar{x}+h) - u(\bar{x}-h)}{2h}$$

Example: $u(x) = sin(x)$

Evaluate $u'(x)$ at $x=1$ using D_- , D_+, D_0.

Let's code this.

Second order derivatives

$$D_0(D_0(u(\bar{x})) = \frac{D_0(\bar{x}+h/2) - D_0(\bar{x}-h/2)}{h} = \frac{\frac{u(\bar{x}+h)-u(\bar{x})}{h} - \frac{u(\bar{x})-u(\bar{x}-h)}{h}}{h}$$

$$= \frac{u(\bar{x}+h) - 2u(\bar{x}) + u(\bar{x}-h)}{h^2}$$

$$D_+(D_-(u(\bar{x})) = \frac{D_-(\bar{x}+h) - D_-(\bar{x})}{h} = \frac{\left(\frac{u(\bar{x}+h)-u(\bar{x})}{h}\right) - \left(\frac{u(\bar{x})-u(\bar{x}-h)}{h}\right)}{h}$$

Let's see the error again for u(x)=sin(x)

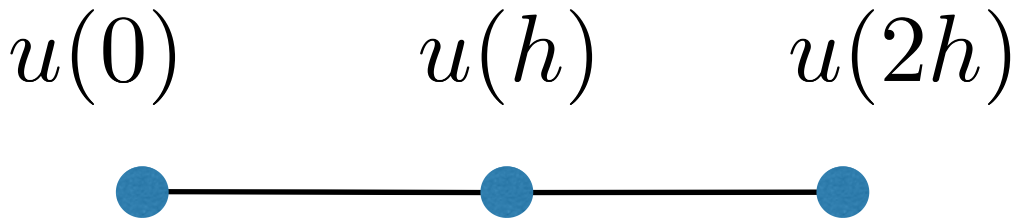
We can derive this expression from Taylor expansion

$$u(\bar{x}-h) = u(\bar{x}) - u'(\bar{x})h + u''(\bar{x})\frac{h^2}{2}$$

$$u(\bar{x}+h) = u(\bar{x}) + u'(\bar{x})h + u''(\bar{x})\frac{h^2}{2}$$

$$\begin{bmatrix} -h & h^2/2 \\ h & h^2/2 \end{bmatrix} \begin{bmatrix} u'(\bar{x}) \\ u''(\bar{x}) \end{bmatrix} = \begin{bmatrix} u(\bar{x}-h) - u(\bar{x}) \\ u(\bar{x}+h) - u(\bar{x}) \end{bmatrix}$$

Finite Difference formulations for boundary points



$$u(h) = u(0) + hu'(0) + (h^2/2)u''(0)$$

$$u(2h) = u(0) + 2hu'(0) + (2h^2)u''(0)$$

$$u'(0) = \frac{4u(h) - 3u(0) - u(2h)}{2h}$$

$$u''(0) = \frac{u(2h) - 2u(h) + u(0)}{h^2}$$

Lagrange Interpolation Function

Given the data values u_i at the locations **x_j, $j = -l+i, \ldots, i, \ldots, i+r$**, the Lagrange interpolation polynomial based on the values **$u_j = u(x_j)$**, becomes

$$p_j(x) = \sum_{i=0}^{j} L_{i,j}(x) u_i, \qquad j = -l + i, ..., i, .., i + r$$

$$L_{i,j} = \frac{(x - x_{i-l})...(x - x_{i-1})(x - x_{i+1})...(x - x_{i+r})}{(x_i - x_{i-l})...(x_i - x_{i-1})(x_i - x_{i+1})...(x_i - x_{i+r})}$$

Example: j=(i-1,i, i+1)

$$p(x) = \frac{(x - x_i)(x - x_{i+1})}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} u_{i-1} + \frac{(x - x_{i-1})(x - x_{i+1})}{(x_i - x_{i-1})(x_i - x_{i+1})} u_i + \frac{(x - x_{i-1})(x - x_i)}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} u_{i+1}$$

Nonuniform points

When gradients of the computed variable are nonuniform in space.
Example: Advection-diffusion equation with *Pe>>1*.

$$p(x) = \frac{(x-x_i)(x-x_{i+1})}{(x_{i-1}-x_i)(x_{i-1}-x_{i+1})}u_{i-1} + \frac{(x-x_{i-1})(x-x_{i+1})}{(x_i-x_{i-1})(x_i-x_{i+1})}u_i + \frac{(x-x_{i-1})(x-x_i)}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)}u_{i+1}$$

$$u'(x_i) = -\frac{h_2}{h_1(h_1+h_2)}u(x_{i-1}) + \left(\frac{1}{h_1} - \frac{1}{h_2}\right)u(x) + \frac{h_1}{h_1(h_1+h_2)}u(x_{i+1})$$

$$u''(x_i) = \frac{2}{h_1+h_2}\left[\frac{1}{h_1}u(x_{i-1}) - \frac{(h_1+h_2)}{h_1 h_2}u(x_i) + \frac{1}{h_2}u(x_{i+1})\right]$$

Determining the error using Taylor expansion

- Equally spaced

$$u(\bar{x}+h) = u(\bar{x}) + u'(\bar{x})h + u''(\bar{x})\frac{h^2}{2} + u'''(\bar{x})\frac{h^3}{3!} + u''''(\bar{x})\frac{h^4}{4!}$$

$$u(\bar{x}-h) = u(\bar{x}) - u'(\bar{x})h + u''(\bar{x})\frac{h^2}{2} - u'''(\bar{x})\frac{h^3}{3!} + u''''(\bar{x})\frac{h^4}{4!}$$

$$D_{-}u(\bar{x}) = \frac{u(\bar{x}) - u(\bar{x}-h)}{h} = u'(\bar{x}) + u''(\bar{x})\frac{h}{2} + \mathcal{O}(h^2)$$

$$D_{+}u(\bar{x}) = \frac{u(\bar{x}+h) - u(\bar{x})}{h} = u'(\bar{x}) + u''(\bar{x})\frac{h}{2} + \mathcal{O}(h^2)$$

$$D_{0}u(\bar{x}) = \frac{u(\bar{x}+h) - u(\bar{x}-h)}{2h} = u'(\bar{x}) + u'''(\bar{x})\frac{h^2}{3!} + \mathcal{O}(h^3)$$

$$D_{0}^{2}u(\bar{x}) - \frac{u(\bar{x}-h) - 2u(\bar{x}) + u(\bar{x}+h)}{h^2} = u''''\frac{h^2}{4!} + \mathcal{O}(h^3)$$

Oder of accuracy: Boundary Points

$$u(h) = u(0) + hu'(0) + (h^2/2)u''(0) + (h^3/3!)u'''(0) + (h^4/4!)u''''(0) + \ldots$$
$$u(2h) = u(0) + 2hu'(0) + (2h^2)u''(0) + (8h^3/3!)u'''(0) + (16h^4/4!)u''''(0) + \ldots$$

$$u'(0) = \frac{4u(h) - 3u(0) - u(2h)}{2h} \qquad u''(0) = \frac{u(2h) - 2u(h) + u(0)}{h^2}$$

$$u'(0) - \frac{4u(h) - 3u(0) - u(2h)}{2h} = \boxed{-(h^2/3)u'''(0)} + \mathcal{O}(h^3)$$

$$u''(0) - \frac{u(2h) - 2u(h) + u(0)}{h^2} = \boxed{hu'''(0)} + \mathcal{O}(h^2)$$

The second derivative approximation reduces to first-order accurate for boundary points.