

Finite Differencing (D2.1; assumed review)

$$f(x_0 + \Delta x) = f(x_0) + \Delta x f'_x(x_0) + \frac{(\Delta x)^2}{2} f''_{xx}(x_0) \dots$$

$$f'_x(x_0) = \underbrace{\frac{f(x_0 + \Delta x) - f(x_0)}{\Delta x}}_{\text{forward difference}} + \underbrace{\mathcal{O}\left(\frac{\Delta x}{2}\right) f''_{xx}(x_0)}_{\text{local truncation error (LTE)}} \dots = O(\Delta x)$$

If truncation error is $O(\Delta x^m)$, method is m 'th order accurate.

Difference operators make for compact notation.

$$\delta_{nx} f(x) = \frac{1}{n\Delta x} \left\{ f\left(x + \frac{n\Delta x}{2}\right) - f\left(x - \frac{n\Delta x}{2}\right) \right\} \quad \text{centered difference of span } n\Delta x$$

$$\delta_{nx}^F f(x) = \frac{1}{n\Delta x} \left\{ f(x + n\Delta x) - f(x) \right\}$$

$$\delta_{nx}^B f(x) = \frac{1}{n\Delta x} \left\{ f(x) - f(x - n\Delta x) \right\}$$

$$\delta_{2x} f = f'_x(x) + \frac{(\Delta x)^2}{6} f'''_{xxx}(x) + O(\Delta x^4) \quad \text{2nd order approx to } f'_x$$

$$\begin{aligned} \delta_x^2 f &= \frac{\delta_x \left\{ f\left(x + \frac{\Delta x}{2}\right) - f\left(x - \frac{\Delta x}{2}\right) \right\}}{\Delta x} = \frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{(\Delta x)^2} \\ &= f''_{xx} + \frac{(\Delta x)^2}{12} f''''_{xxxx} + O(\Delta x^4) \dots \end{aligned}$$

They also allow higher-order accurate formulas to be derived, e.g.

$$\begin{aligned} f'_x(x) &= \delta_{2x} f - \frac{(\Delta x)^2}{6} f'''_{xxx}(x) + O(\Delta x^4) \\ &= \delta_{2x} f - \frac{(\Delta x)^2}{6} \left(\delta_x^2 f_x + O(\Delta x^4) \right) + O(\Delta x^4) \\ &= \left\{ 1 - \frac{(\Delta x)^2}{6} \delta_x^2 \right\} \delta_{2x} f + O(\Delta x^4) \end{aligned}$$

Boundary conditions

Heat Eqn: $\frac{\partial \psi}{\partial t} = k \frac{\partial^2 \psi}{\partial x^2} \quad 0 \leq x \leq L$

$$\psi(x, 0) = f(x)$$

$$\partial \psi(0, t) = g(t)$$

$$\frac{\partial \psi}{\partial x}(L, t) = 0.$$

Discretize in x only for now: at $x_k = k\Delta x$, $k=0, \dots, N$, $\Delta x = \frac{L}{N}$:

$$\frac{\partial \psi_k}{\partial t} = k \delta_x^2 \psi_k + O(\Delta x^2), k=1, \dots, N-1$$

$$\psi_0(t) = g(t)$$

$$\left. \begin{array}{c} 0 \\ \dots \\ \dots \\ \dots \\ N+1 \\ x \end{array} \right\}$$

For $\psi_N(t)$, two alternatives:

(1) Use a one-sided formula, e.g.

$$\begin{aligned} \left(\frac{\partial^2 \psi}{\partial x^2} \right)_N &= \delta_x^B \left(\frac{\partial \psi}{\partial x} \right)_N + O(\Delta x) \\ &= \frac{\left(\frac{\partial \psi}{\partial x} \right)_N^0 - \left(\frac{\partial \psi}{\partial x} \right)_{N-1}}{\Delta x} + O(\Delta x) \end{aligned}$$

$$\approx - \frac{\psi_{N-1}}{\Delta x} + O(\Delta x) \quad \dots \text{only 1st order accurate.}$$

(1b) Use a 2nd order accurate one-sided formula

$$\left(\frac{\partial^2 \psi}{\partial x^2} \right)_N = \left[\frac{\partial}{\partial x} \left(\frac{\partial \psi}{\partial x} \right) \right]_N$$

$$\delta_x^B f = \frac{f(x) - f(x-\Delta x)}{\Delta x} = f'(x) - \frac{\Delta x}{2} f''(x) + O(\Delta x)^2$$

$$\delta_{2x}^B f = \frac{f(x) - f(x-2\Delta x)}{2\Delta x} = f'(x) - \Delta x f''(x) + O(\Delta x)^2$$

$$\Rightarrow f'(x) = 2\delta_x^B f - \delta_{2x}^B f + O(\Delta x)^2$$

$$\Rightarrow \left(\frac{\partial^2 \psi}{\partial x^2} \right)_N = 2 \frac{\left(\frac{\partial \psi}{\partial x} \right)_{N-1} - \left(\frac{\partial \psi}{\partial x} \right)_N^0}{\Delta x} - \frac{\left(\frac{\partial \psi}{\partial x} \right)_{N-2} - \left(\frac{\partial \psi}{\partial x} \right)_N^0}{2\Delta x} + O(\Delta x)^2$$

Now find third order accurate formulas for $\left(\frac{\partial \psi}{\partial x} \right)_{N-1}$ and $\left(\frac{\partial \psi}{\partial x} \right)_{N-2}$... complicated.

(2) Use an image point x_{N+1}

$$\text{B.C.} \Rightarrow \delta_{2x} \psi_N = 0 \text{ to } O(\Delta x^2) \Rightarrow \psi_{N+1} = \psi_{N-1} + O(\Delta x^2)$$

and now all points are defined.

$$\left(\frac{\partial^2 \psi}{\partial x^2} \right)_N = \frac{\psi_{N+1} - 2\psi_N + \psi_{N-1}}{(\Delta x)^2} = \frac{2(\psi_N - \psi_{N-1})}{(\Delta x)^2} = - \frac{\delta_x^F \psi_{N-1}}{\Delta x} + O(\Delta x^2).$$

Periodic BC's: $\psi_0 = \psi_N, \psi_{N+1} = \psi_1$