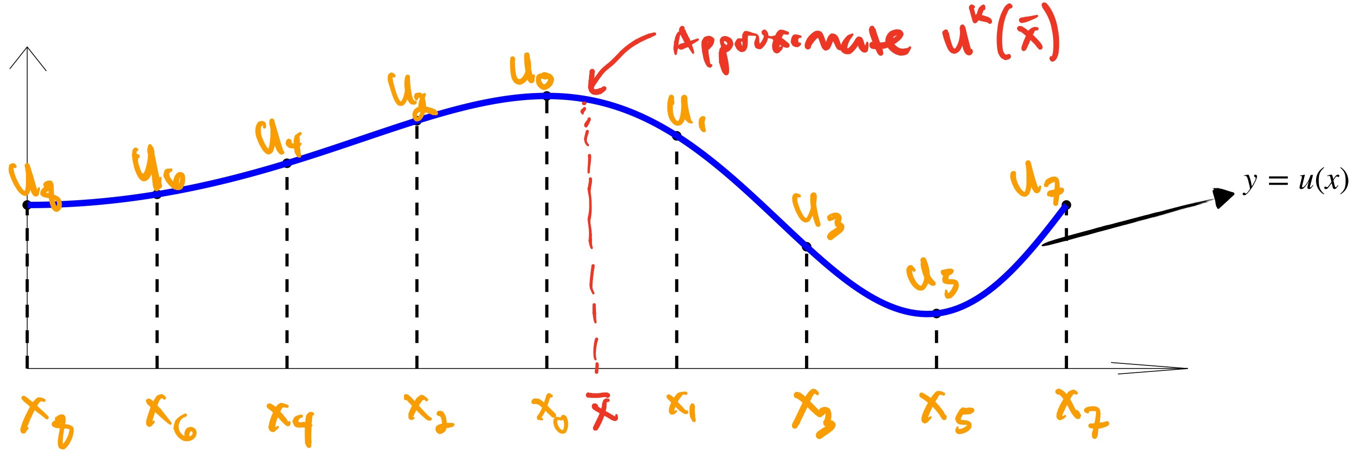
Finite Differences

Method 2 & 3: Polynomial interpolation and method of undetermined coefficients



Goal is to approximate kth derivative of u at $\bar{x}$ with a formula of the form:

$x_0 = 0$

$x_1 = h$ $\quad n=2$

$x_2 = -h$

$$\left.\frac{d^k u}{dx^k}\right|_{x=\bar{x}} \approx \sum_{j=0}^{n} c_j^k u_j$$

weight

$$u'(x_0) = \frac{1}{2h}u(x_1) - \frac{1}{2h}u(x_2) = c_1^1 u_1 - c_2^1 u_2$$

$\bar{x} = x_0$

Question: How do we determine the coefficients c_j^k?

Given $u_0, u_1, \ldots, u_n$, k, $x_0, x_1, \ldots, x_n$

Method 2: Polynomial interpolation

Recall Lagrange's interpolation formula:

$$p_n(x) = \sum_{j=0}^{n} L_j(x)u_j \qquad \text{where} \qquad L_j(x) = \underbrace{\frac{(x-x_0)(x-x_1)\cdots(x-x_{j-1})(x-x_{j+1})\cdots(x-x_n)}{(x_j-x_0)(x_j-x_1)\cdots(x_j-x_{j-1})(x_j-x_{j+1})\cdots(x_j-x_n)}}_{n^{th}\text{ degree polynomial}}$$

n^{th} degree polynomial

$$L_j(x_i) = \begin{cases} 1 & \text{if } i=j \\ 0 & \text{if } i \neq j \end{cases}$$

Guarantees that: $p_n(x_i) = u_i$, $i = 0, 1, \dots, n$

Cardinal property

Ex. $x_0 = 1$, $x_1 = 3$, $x_2 = 3.5$.

$$P_2(x) = \frac{(x-3)(x-3.5)}{(1-3)(1-3.5)}u_0 + \frac{(x-1)(x-3.5)}{(3-1)(3-3.5)}u_1 + \frac{(x-1)(x-3)}{(3.5-1)(3.5-3)}u_2$$

$$P_2(3) = 0 + u_1 + 0$$

Approximate:

$$\frac{d^k}{dx^k}u\Big|_{x=\bar{x}} \approx \frac{d^k}{dx^k}P_n\Big|_{x=\bar{x}} = \frac{d^k}{dx^k}\left(\sum_{j=0}^{n} L_j(x)\,u_j\right)\Big|_{x=\bar{x}}$$

$$= \sum_{j=0}^{n} \underbrace{\left[\frac{d^k}{dx^k}L_j(x)\Big|_{x=\bar{x}}\right]}_{c_j^k} u_j$$

$$= \sum_{j=0}^{n} c_j^k\,u_j$$

Error error analysis follows the error in the polynomial interpolation.

Method 3: Method of undetermined coefficients

$$\frac{d^k}{dx^k}u\Big|_{x=\bar{x}} \approx \sum_{j=0}^{n} c_j^k u_j$$

- Choose $\{c_j^k\}_{j=0}^n$ so that the formula is exact for as high degree polynomials as possible.

- There are $n+1$ parameters $\{c_j^k\}_{j=0}^n$, so we can hope to make the formula exact for polynomials:

$$\{1, x, x^2, \ldots, x^n\}$$

- Better to work with polynomials:

$$\Big\{ \underset{i=0}{1},\ \underset{i=1}{x-\bar{x}},\ \underset{i=2}{\frac{(x-\bar{x})^2}{2!}},\ \frac{(x-\bar{x})^3}{3!},\ \ldots,\ \underset{i=n}{\frac{(x-\bar{x})^n}{n!}} \Big\}$$

Set of equations: For $i = 0, 1, \cdots, n$

$$\frac{1}{i!} \sum_{j=0}^{n} c_j^k (x_j - \bar{x})^i = \frac{1}{i!} \frac{d^k}{dx^k} (x - \bar{x})^i \Big|_{x=\bar{x}}$$

$$= \begin{cases} 1 & \text{if } i = k \\ 0 & \text{otherwise} \end{cases}$$

Leads to a Vandermonde type linear system:

System:

$$\begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ (x_0-\bar{x}) & (x_1-\bar{x}) & (x_2-\bar{x}) & \cdots & (x_n-\bar{x}) \\ \frac{(x_0-\bar{x})^2}{2!} & \frac{(x_1-\bar{x})^2}{2!} & \frac{(x_2-\bar{x})^2}{2!} & \cdots & \frac{(x_n-\bar{x})^2}{2!} \\ \vdots & & & & \\ \frac{(x_0-\bar{x})^n}{n!} & \frac{(x_1-\bar{x})^n}{n!} & \frac{(x_2-\bar{x})^n}{n!} & \cdots & \frac{(x_n-\bar{x})^n}{n!} \end{bmatrix} \begin{bmatrix} c_0^k \\ c_2^k \\ c_3^k \\ \vdots \\ c_n^k \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{bmatrix}$$

k^{th} row where you count from zero

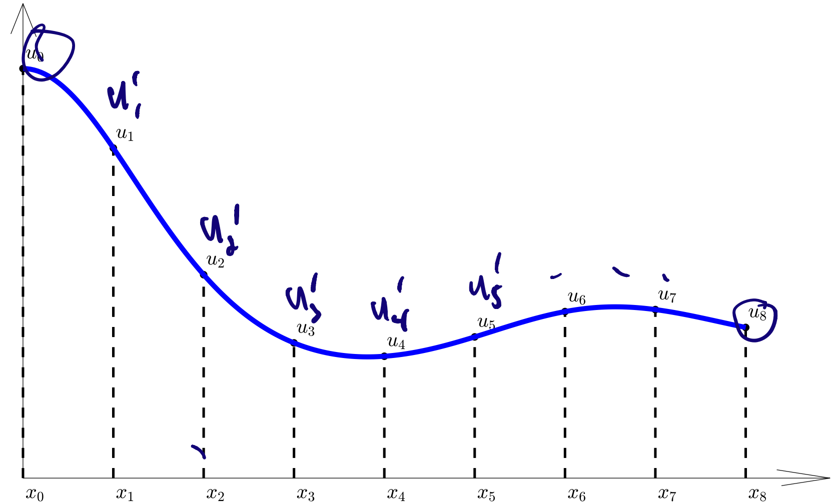
- This gives the same result as Method 2 for the coefficients, using exact arithmetic.
- Method 3 is numerically unstable for large n.

Fornberg's algorithm

- Clever algorithm for doing the computations in method 2.
- Webpage, links to codes for this algorithm: weights

Differentiation matrices

- Discrete form of a differential operator
- Operates on a vector of function samples
- Produces a vector containing approximations of some derivative.



Example: first derivative

$$\frac{1}{2h}\begin{bmatrix} -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} u_0 \\ u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \\ u_8 \end{bmatrix} = \begin{bmatrix} u_1' \\ u_2' \\ u_3' \\ u_4' \\ u_5' \\ u_6' \\ u_7' \end{bmatrix} + \begin{bmatrix} \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \end{bmatrix}$$

$$-\frac{1}{2h}u_0 + \frac{1}{2h}u_1 = u_1' + O(h^2)$$

$$\Rightarrow \frac{1}{2h}u_1 = u_1' + \frac{1}{2h}u_0 + O(h^2)$$

Or we can produce a square differentiation matrix by accounting for the boundaries:

$$\frac{1}{2h}\begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \end{bmatrix} = \begin{bmatrix} u_1' \\ u_2' \\ u_3' \\ u_4' \\ u_5' \\ u_6' \\ u_7' \end{bmatrix} + \frac{1}{2h}\begin{bmatrix} u_0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -u_8 \end{bmatrix} + \begin{bmatrix} \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \end{bmatrix}$$

Example: second derivative

$$\frac{1}{h^2}\begin{bmatrix} -2 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -2 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -2 \end{bmatrix}\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \\ u_6 \\ u_7 \end{bmatrix} = \begin{bmatrix} u_1'' \\ u_2'' \\ u_3'' \\ u_4'' \\ u_5'' \\ u_6'' \\ u_7'' \end{bmatrix} - \frac{1}{h^2}\begin{bmatrix} u_0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ u_8 \end{bmatrix} + \begin{bmatrix} \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \\ \mathcal{O}(h^2) \end{bmatrix}$$