Overview

- Differentiation at multiple grid points
- Differentiation matrix as the discrete version of the differentiation operator

- Consider $f\colon \mathbb{R} \to \mathbb{R}$, sampled at $\{x_0, x_1, \dots, x_n\}$, $f_j \equiv f(x_j)$, $\boldsymbol{f} = [\ f_0 \ \ \dots \ \ f_n\ ]^T$
- Evaluate f' at points $\{x'_0, x'_1, \dots, x'_m\}$, $f'_j \cong f'(x'_j)$, $\boldsymbol{f}' = [\ f'_0 \ \ \dots \ \ f'_m\ ]^T$
- Finite difference formulas: derivative approximations as linear combinations

$$\boldsymbol{f}' = \boldsymbol{D}\boldsymbol{f}, \boldsymbol{D} = [d_{ij}], d_{ij} = \frac{l'_j(x'_i)}{l_j(x_j)}, l_j(t) = \prod_{k=0}^{n}{}' (t - x_k)$$

$$p(t) = \sum_{j=0}^{n} f_j \ell_j(t) \Rightarrow p'(t) = \sum_{j=0}^{n} f_j \ell'_j(t)$$

$$f'(x'_i) \cong \sum_{j=0}^{n} f_j \ell'_j(x'_i) = \sum_{j=0}^{n} f_j \frac{l'_j(x'_i)}{l_j(x_j)}$$

- $f : \mathbb{R} \to \mathbb{R}$, sampled at $\{x_0, x_1, \ldots, x_n\}$, $f_j \equiv f(x_j)$, $\boldsymbol{f} = [\; f_0 \;\; \ldots \;\; f_n \;]^T$
- Evaluate f' at points $\{x_1, \ldots, x_{n-1}\}$, $f_j' \cong f'(x_j)$, $\boldsymbol{f}' = [\; f_1' \;\; \ldots \;\; f_{n-1}' \;]^T$
- Centered finite difference $f_j' \cong (f_{j+1} - f_{j-1}) / (2h)$

$$\boldsymbol{f}' = \boldsymbol{D}_{2h} \boldsymbol{f} \Rightarrow \begin{bmatrix} f_1' \\ f_2' \\ \vdots \\ f_{n-1}' \end{bmatrix} = \frac{1}{2h} \begin{bmatrix} -1 & 0 & 1 & & & \\ & -1 & 0 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} f_0 \\ f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix},$$

- Sampling at half interval: $\{x_0, x_{1/2}, \ldots, x_n\}$, $f_j \equiv f(x_j)$, $\boldsymbol{f} = [\; f_0 \;\; \ldots \;\; f_n \;]^T$

$$\boldsymbol{f}' = \boldsymbol{D}_{h} \boldsymbol{f} \Rightarrow \begin{bmatrix} f_1' \\ f_2' \\ \vdots \\ f_{n-1}' \end{bmatrix} = \frac{1}{h} \begin{bmatrix} -1 & 0 & 1 & & & \\ & -1 & 0 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} f_{1/2} \\ f_1 \\ f_{3/2} \\ \vdots \\ f_{n-1/2} \end{bmatrix},$$

Differentiation matrix = discrete differentiation operator

- Calculus: differentiation operator $D = \mathrm{d}/\mathrm{d}t$, higher order derivatives:

$$f^{(k)}(t) = \frac{\mathrm{d}^k}{\mathrm{d}t^k} f(t) = D^k f = D(D(\ldots D(f)))$$

- Similar properties hold for differentation matrices, e.g., $\boldsymbol{f}'' = \boldsymbol{D}_h \boldsymbol{D}_h \boldsymbol{f}$

$$\boldsymbol{D}_h \boldsymbol{D}_h = \frac{1}{h^2} \begin{bmatrix} -1 & 0 & 1 & & & \\ & -1 & 0 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} -1 & 0 & 1 & & & \\ & -1 & 0 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 0 & 1 \end{bmatrix} \Rightarrow$$

$$\boldsymbol{D}_h^2 = \frac{1}{h^2} \begin{bmatrix} 1 & 0 & -2 & 0 & 1 & & \\ & 1 & 0 & -2 & 0 & 1 & \\ & & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix} \Rightarrow$$

$$f_n'' \cong \frac{f_{n-1} - 2 f_n + f_{n+1}}{h^2}$$

- Applying $\boldsymbol{D}_h^2$ to $\boldsymbol{f}$ leads to

$$f_n'' \cong \frac{f_{n-1} - 2f_n + f_{n+1}}{h^2}$$

- Taylor series analysis

$$f_{n+1} = f(x_{n+1}) = f_n + f_n' \cdot h + \frac{1}{2} f_n'' \cdot h^2 + \frac{1}{6} f_n''' h^3 + \cdots$$
$$f_{n-1} = f(x_{n-1}) = f_n - f_n' \cdot h + \frac{1}{2} f_n'' \cdot h^2 - \frac{1}{6} f_n''' h^3 + \cdots$$

$$\frac{1}{h^2}(f_{n-1} - 2f_n + f_{n+1}) = f_n'' + \frac{1}{12} f_n^{(\mathrm{iv})} h^2 = f_n'' + \mathcal{O}(h^2)$$