Overview

- Approximate derivative by derivative of approximation
- Finite difference formulas from Taylor series

- $f\colon \mathbb{R} \to \mathbb{R}$ differentiable up to order k, $f \in C^{(k)}(\mathbb{R})$
- The derivative of f is the function $f' \in C^{(k-1)}(\mathbb{R})$

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

- The differentiation operator $D = \frac{\mathrm{d}}{\mathrm{d}x}$ is linear

$$D(\alpha f + \beta g) = \alpha D(f) + \beta D(g)$$

- Geometric interpretation of derivatives:
  - first derivative: slope of tangent
  - second derivative: related to curvature

$$\kappa = \frac{|f''(x)|}{\sqrt{1 + (f'(x))^2}}$$

- Consider $f\colon \mathbb{R}\to\mathbb{R}$, $f\in C^{(k)}(\mathbb{R})$, $f(x)$ difficult to compute
- Approximation $g\colon \mathbb{R}\to\mathbb{R}$, $f\in C^{(k)}(\mathbb{R})$, $g(x)$ simpler to compute

$$g \cong f$$

  Examples: interpolation, least squares
- Basic idea: approximation of derivative = derivative of approximation

$$f'(x) \cong g'(x)$$

- Example: consider data $\mathcal{D}=\{(x_0, f_0),(x_1, f_1)\}$. Interpolant is

$$g(t)=p_1(t)=\sum_{i=0}^{1} f_i\,\ell_i(t), \ell_0(t)=\frac{t-x_1}{x_0-x_1}, \ell_1(t)=\frac{t-x_0}{x_1-x_0}$$

$$f'(t)\cong p_1'(t)=\sum_{i=0}^{1} f_i\,\ell_i'(t)=\frac{f_0}{x_0-x_1}+\frac{f_1}{x_1-x_0}=\frac{f_1-f_0}{x_1-x_0}$$

- For data $\mathcal{D}=\{(x_0, f_0), \ldots, (x_n, f_n)\}$ differentiation of the Lagrange form

$$p_n(t)=\sum_{i=0}^{n} f_i\,\ell_i(t)$$

leads to $n+1$ derivatives of n^{th} degree polynomials

$$p_n'(t)=\sum_{i=0}^{n} f_i\,\ell_i'(t)$$

- The Newton form

$$p(t)=[f_0]+[f_1, f_0](t-x_0)+\cdots+[f_n, \ldots, f_0](t-x_0)\cdot\ldots\cdot(t-x_{n-1})$$

requires less effort, $n+1$ derivative of polynomials of degree $0, 1, \ldots, n$

- Often $x_k = x_0 + kh, h = (x_n - x_0)/n$, i.e., f sampled at equidistant points
- Sample point positions with respect to evaluation point:
  - Left sample points $\mathcal{L} = \{(x_{n-k}, f_{n-k}), (x_{n-k+1}, f_{n-k+1}), \ldots, (x_n, f_n)\}$
  - Centered sample points $\mathcal{C} = \{(x_{n-k}, f_{n-k}), \ldots, (x_n, f_n), \ldots, (x_{n+k}, f_{n+k})\}$
  - Right sample points $\mathcal{R} = \{(x_n, f_n), (x_{n+1}, f_{n+1}) \ldots, (x_{n+k}, f_{n+k})\}$

$$
\begin{array}{lll}
 & f_n' & f_n'' \\
\text{Centered} & \dfrac{f_{n+1} - f_{n-1}}{2h} & \dfrac{f_{n+1} - 2f_n + f_{n-1}}{h^2} \\
\text{Forward} & \dfrac{f_{n+1} - f_n}{h} & \dfrac{2f_n - 5f_{n+1} + 4f_{n+2} - f_{n+3}}{h^2} \\
\text{Backward} & \dfrac{f_n - f_{n-1}}{h} & \dfrac{2f_n - 5f_{n-1} + 4f_{n-2} - f_{n-3}}{h^2} \\
\text{Forward} & \dfrac{-3f_n + 4f_{n+1} - f_{n+2}}{2h} & \\
\text{Backward} & \dfrac{3f_n - 4f_{n-1} + f_{n-2}}{2h} &
\end{array}
$$

- Consider $f\colon\mathbb{R}\to\mathbb{R}$, $f\in\mathbb{C}^{(N)}(\mathbb{R})$, hard to compute, known at sample points $x_j = x_n + jh$, $j\in\{0,\pm 1,\pm 2,\dots\}$, $f_j \equiv f(x_j)$
- An alternative approach to obtaining approximations of $f_n^{(k)} \equiv f^{(k)}(x_n)$ from the sample points is through linear combinations of Taylor series

$$f(x_{n+j}) = f_n + \frac{1}{1!}f_n'\cdot(jh) + \frac{1}{2!}f_n''\cdot(jh)^2 + \frac{1}{3!}f_n'''\cdot(jh)^3 + \cdots$$

- Example:

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

Eliminate f_n'' from above and obtain

$$f_n' = \frac{f_{n+1} - f_{n-1}}{2h} + \frac{1}{3}f_n'''h^2 + \cdots = \frac{f_{n+1} - f_{n-1}}{2h} + \mathcal{O}(h^2)$$

- Taylor series expansions are used to obtain the *order of accuracy* of a formula (do not confuse with order of convergence of a sequence)
- From previous example

$$f_n' = \frac{f_{n+1} - f_{n-1}}{2h} + \frac{1}{3} f_n''' h^2 + \cdots = \frac{f_{n+1} - f_{n-1}}{2h} + \mathcal{O}(h^2)$$

hence the approximation $f_n' \cong (f_{n+1} - f_{n-1})/(2h)$ is of second order (of accuracy)

- Example: determine order of accuracy of $f_n' \cong (-3f_n + 4f_{n+1} - f_{n+2})/(2h)$

$$\begin{aligned} -3f_n &= -3f_n \\ 4f_{n+1} &= 4f_n + 4f_n' \cdot h + 2f_n'' \cdot h^2 + \frac{2}{3} f_n''' h^3 + \cdots \\ -f_{n+2} &= -f_n - f_n' \cdot (2h) - \frac{1}{2} f_n'' \cdot (2h)^2 - \frac{1}{6} f_n'''(2h)^3 - \cdots \end{aligned} \quad \Rightarrow$$

$$(-3f_n + 4f_{n+1} - f_{n+2})/(2h) = f_n' - \frac{2}{3} f_n''' h^2 = f_n' + \mathcal{O}(h^2), \text{second order.}$$

- Position of evaluation of derivative point w.r.t. sample points
  - left: evaluate $f_n^{(k)}$ using sample points $f_{n+j}, j \leqslant 0$

$$f_n' = \frac{f_n - f_{n-1}}{h} + \mathcal{O}(h)$$

  - right: evaluate $f_n^{(k)}$ using sample points $f_{n+j}, j \geqslant 0$

$$f_n' = \frac{f_{n+1} - f_n}{h} + \mathcal{O}(h)$$

  - centered: evaluate $f_n^{(k)}$ using sample points $f_{n+j}, -m \leqslant j \leqslant m$

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

(note higher order accurach of centered formulas)