Numerical Differentiation

Laura Grigori

EPFL and PSI
slides based on lecture notes/slides from L. Dede/S. Deparis

October 15, 2024

Plan

Goals

Given $f \in C^1((a,b))$, approximate $f'(x)$ for some $x \in (a,b) \subseteq \mathbb{R}$
Examples:

- For known function $f(x)$, it might be too expensive to explicitly evaluate $f'(x)$ for some $x \in (a,b)$
- Numerical derivation is necessary if only the set of data couples $\{(x_i, y_i)\}_{i=0}^n$ is provided and not $f(x)$ from which these are eventually obtained
  - It might still be required to have the first derivative of the unknown function $f(x)$ at one or all the nodes $\{x_i\}_{i=0}^n$

Plan

Finite Differences Schemes

- Forward and backward finite differences
- Centered finite differences

Forward and backward finite differences

Definition (4.1)

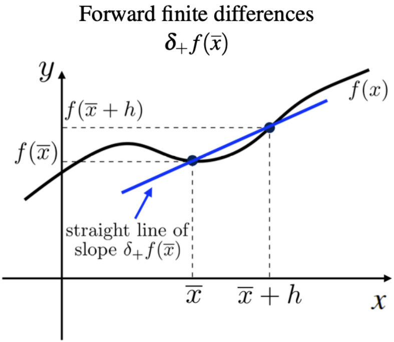
Given a function $f(x)$ and the step size $h > 0$, the approximation of $f'(\bar{x})$ at some $\bar{x} \in (a, b) \subseteq \mathbb{R}$ by the forward finite differences scheme is defined as:

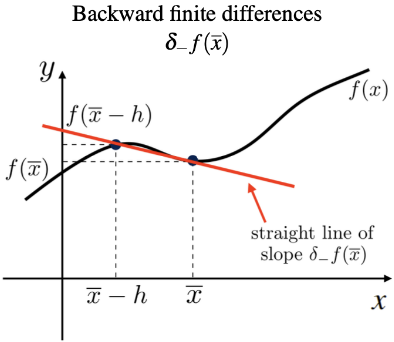
$$\boxed{\delta_+ f(\bar{x}) := \frac{f(\bar{x}+h) - f(\bar{x})}{h},} \tag{1}$$

while by the backward finite differences scheme as:

$$\boxed{\delta_- f(\bar{x}) := \frac{f(\bar{x}) - f(\bar{x}-h)}{h}.} \tag{2}$$

Forward and backward finite differences





$$\delta_+ f(\bar{x}) := \frac{f(\bar{x}+h) - f(\bar{x})}{h}$$

$$\delta_- f(\bar{x}) := \frac{f(\bar{x}) - f(\bar{x}-h)}{h}$$

Error of forward/backward finite differences

Proposition (4.1)

If $f \in C^2((a,b))$ and $\bar{x} \in (a,b)$, the error $E_+ f(\bar{x})$ for forward finite differences scheme is:

$$\boxed{E_+ f(\bar{x}) := f'(\bar{x}) - \delta_+ f(\bar{x}) = -\frac{1}{2} h f''(\xi_+) \quad \text{for some}\, \xi_+ \in [\bar{x}, \bar{x}+h],} \tag{3}$$

while the error $E_- f(\bar{x})$ for backward finite differences is:

$$\boxed{E_- f(\bar{x}) := f'(\bar{x}) - \delta_- f(\bar{x}) = \frac{1}{2} h f''(\xi_-) \quad \text{for some}\, \xi_- \in [\bar{x}-h, \bar{x}].} \tag{4}$$

Error of forward/backward finite differences

Proof of Prop. 4.1 (Forward finite differences scheme)
Consider the Taylor expansion of $f(\bar{x}+h)$ around $\bar{x}$, obtaining

$$f(\bar{x}+h) = f(\bar{x}) + f'(\bar{x})h + \frac{1}{2}f''(\xi_+)h^2 \quad \text{for some}\,\xi_+ \in [\bar{x}, \bar{x}+h].$$

Since the error is:

$$E_+ f(\bar{x}) := f'(\bar{x}) - \delta_+ f(\bar{x}),$$

the result follows.

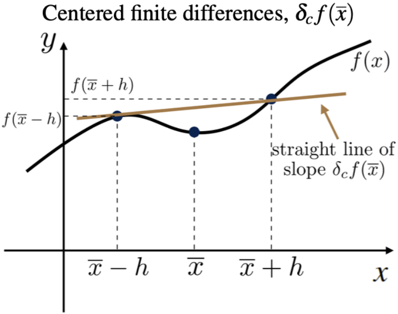
Remarks for forward/backward finite differences

- The forward and backward finite differences schemes are methods of order 1;
  the errors $E_+f(\bar{x})$ and $E_-f(\bar{x})$ converge to zero with order 1 in the step size h
- If $f \in \mathbb{P}_1$, we have $\delta_+f(\bar{x}) = \delta_-f(\bar{x}) = f'(\bar{x})$ for all $\bar{x} \in \mathbb{R}$.

Centered finite differences

Definition 4.2 Given $f(x)$ and step size $h > 0$, the approximation of $f'(\bar{x})$ at some $\bar{x} \in (a, b) \subseteq \mathbb{R}$ by the centered finite differences scheme is defined as:

$$\delta_c f(\bar{x}) := \frac{f(\bar{x}+h) - f(\bar{x}-h)}{2h}. \tag{5}$$



Error of centered finite differences

Proposition (4.2)

If $f \in C^3((a,b))$ and $\bar{x} \in (a,b)$, the error $E_c f(\bar{x})$ associated with the centered finite differences scheme is:

$$E_c f(\bar{x}) := f'(\bar{x}) - \delta_c f(\bar{x}) = -\frac{1}{12} h^2 \left[f'''(\xi_+) + f'''(\xi_-) \right]$$

for some $\xi_+ \in [\bar{x}, \bar{x} + h]$ and $\xi_- \in [\bar{x} - h, \bar{x}]$.

Error of centered finite differences

Proof of Prop. 4.2 Consider the Taylor expansion of $f(\bar{x}+h)$ around x,

$$f(\bar{x}+h) = f(\bar{x}) + f'(\bar{x})h + \frac{1}{2}f''(\bar{x})h^2 + \frac{1}{6}f'''(\xi_+)h^3 \quad \text{for some}\, \xi_+ \in [\bar{x}, \bar{x}+h];$$

similarly, the Taylor expansion of $f(\bar{x}-h)$ around x is

$$f(\bar{x}-h) = f(\bar{x}) - f'(\bar{x})h + \frac{1}{2}f''(\bar{x})h^2 - \frac{1}{6}f'''(\xi_-)h^3 \quad \text{for some}\, \xi_- \in [\bar{x}-h, \bar{x}].$$

Then, by applying the definition of the error $E_c f(\bar{x})$, the result follows.

Remarks

- The centered finite differences scheme is a method of order 2
  the error $E_c f(\bar{x})$ converges to zero with order 2 in the step size h
- If $f \in \mathbb{P}_2$, we have $\delta_c f(\bar{x}) = f'(\bar{x})$ for all $\bar{x} \in \mathbb{R}$

Approximating $f'(x)$ at multiple nodes

Goal: Approximate $f'(x)$ at multiple and equally spaced nodes in the interval $[a, b]$, that is $x_i = a + ih$ for all $i = 0, \dots, n$, with

$$h = \frac{b-a}{n}; \quad x_0 = a \,\text{and}\, x_n = b$$

- Consider the centered finite differences scheme at the nodes internal to the interval $[a, b]$, as:

$$\delta_c f(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} \quad \text{for all } i = 1, \dots, n-1$$

- Approximate $f'(x_0)$ and $f'(x_n)$ with the forward and backward finite differences schemes:

$$\delta_+ f(x_0) = \frac{f(x_1) - f(x_0)}{h} \quad \text{and} \quad \delta_- f(x_n) = \frac{f(x_n) - f(x_{n-1})}{h}.$$

$\rightarrow$ Method of order 2 for internal nodes $\{x_i\}_{i=1}^{n-1}$ and order 1 for x_0 and x_n

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$\rightarrow$ Method of order 2 for internal nodes $\{x_i\}_{i=1}^{n-1}$ and order 1 for x_0 and x_n

Approximating $f'(x)$ at multiple nodes

Restore the full convergence order 2 in h for all the nodes $\{x_i\}_{i=0}^{n}$ using the following finite differences schemes at x_0 and x_n:

$$\delta_{c,0} f(x_0) = \frac{-3f(x_0) + 4f(x_1) - f(x_2)}{2h}$$

and

$$\delta_{c,n} f(x_n) = \frac{f(x_{n-2}) - 4f(x_{n-1}) + 3f(x_n)}{2h}$$

because

- $\delta_{c,0} f(x_0) = (\Pi_{2,\{x_0,x_1,x_2\}} f)'(x_0)$ where $(\Pi_{2,\{x_0,x_1,x_2\}} f)'(x)$ is polynomial of degree 2 interpolating $f(x)$ at $\{x_i\}_{i=0}^{2}$
- $\delta_{c,n} f(x_n) = (\Pi_{2,\{x_{n-2},x_{n-1},x_n\}} f)'(x_n)$ where $(\Pi_{2,\{x_{n-2},x_{n-1},x_n\}} f)'(x)$ is polynomial of degree 2 interpolating $f(x)$ at $\{x_i\}_{i=n-2}^{n}$