Numerical Methods in Engineering and Applied Science

Lecture 3.

Let $f(x)$ be a sufficiently smooth function of $x \in \mathcal{R}$. To derive a first-order one-sided finite-difference approximation to its fist derivative at a point $x = x_0$, let us evaluate f at $x_1 = x_0 + h$, where h is small. Consider the Taylor series

$$f(x_1) = f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(x_0) + \frac{h^3}{6} f'''(x_0) + \frac{h^4}{24} f''''(\xi). \tag{1}$$

After rearranging the terms we obtain

$$hf'(x_0) = f(x_1) - f(x_0) - \frac{h^2}{2} f''(x_0) - \frac{h^3}{6} f'''(x_0) - \frac{h^4}{24} f''''(\xi). \tag{2}$$

Then we divide by h:

$$f'(x_0) = \frac{f(x_1) - f(x_0)}{h} - \frac{h}{2} f''(x_0) - \frac{h^2}{6} f'''(x_0) - \frac{h^3}{24} f''''(\xi). \tag{3}$$

Let us introduce the notation $R(x)$ for the truncation error,

$$R(x_0) = \frac{h}{2} f''(x_0) + \frac{h^2}{6} f'''(x_0) + \frac{h^3}{24} f''''(\xi). \tag{4}$$

Then we obtain

$$f'(x_0) = \frac{f(x_1) - f(x_0)}{h} - R(x_0) \tag{5}$$

and

$$\frac{f(x_1) - f(x_0)}{h} = f'(x_0) + R(x_0). \tag{6}$$

Let's consider again the truncation error,

$$R(x_0) = \frac{h}{2} f''(x_0) + \frac{h^2}{6} f'''(x_0) + \frac{h^3}{24} f''''(\xi). \tag{7}$$

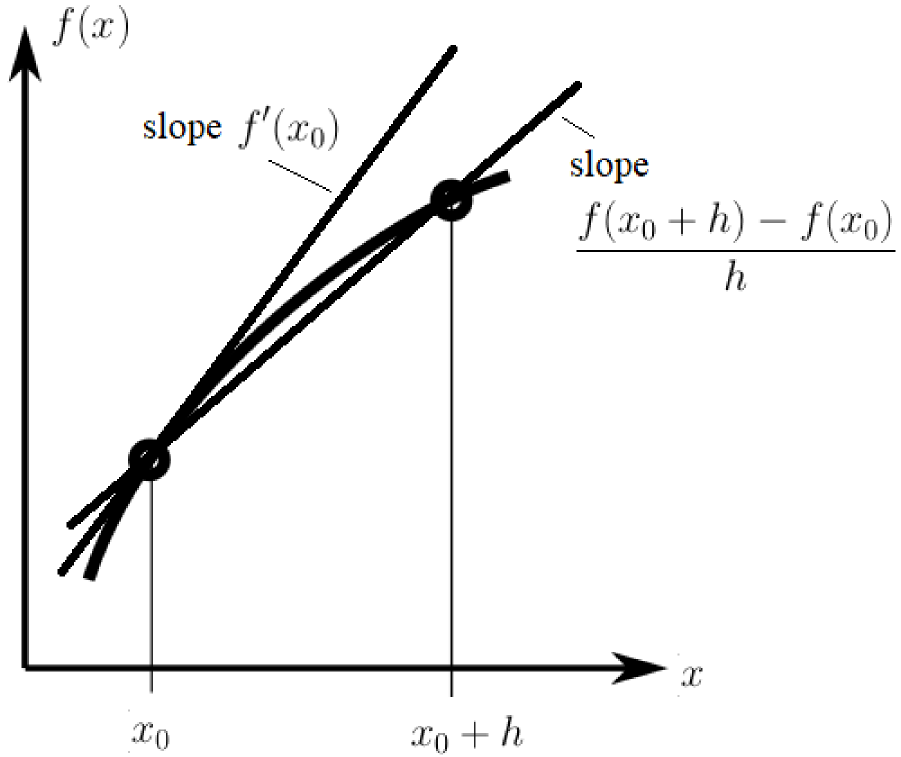
When h is sufficiently small, the second and third terms are negligibly small, compared to the first term in the right-hand side. In other words,

$$R(x_0) \sim \frac{h}{2} f''(x_0) \tag{8}$$

as $h \to 0$. We can rewrite this as

$$\left| \frac{f(x_0 + h) - f(x_0)}{h} - f'(x_0) \right| \sim \frac{h}{2} |f''(x_0)| \tag{9}$$

This is a first-order one-sided FD scheme: $D_+ f(x) = (f(x+h) - f(x))/h$



A central scheme can be derived similarly.

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(x_0) + \frac{h^3}{6}f'''(x_0) + \frac{h^4}{24}f''''(\xi_1), \tag{10}$$

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2}f''(x_0) - \frac{h^3}{6}f'''(x_0) + \frac{h^4}{24}f''''(\xi_2). \tag{11}$$

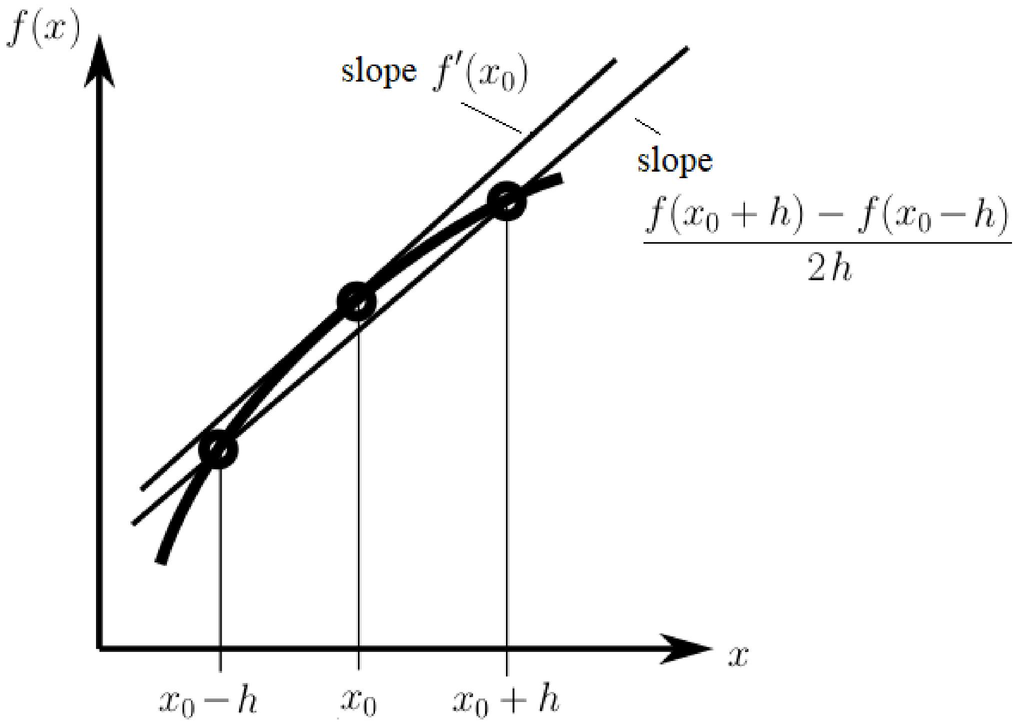
Therefore,

$$f(x_0 + h) - f(x_0 - h) = 2hf'(x_0) + \frac{h^3}{3}f'''(x_0) + O(h^5) \tag{12}$$

and

$$\frac{f(x_0 + h) - f(x_0 - h)}{2h} - f'(x_0) = \frac{h^2}{6}f'''(x_0) + O(h^4). \tag{13}$$

This is a second-order central FD scheme: $D_0 f(x) = (f(x+h) - f(x-h))/2h$



We found that

$$|D_+ f(x) - f'(x)| \sim \frac{h}{2}|f''(x)| \tag{14}$$

$$|D_0 f(x) - f'(x)| \sim \frac{h^2}{6}|f'''(x)|, \tag{15}$$

In general, for any finite-difference approximation,

$$|Df(x) - f'(x)| \sim Ch^p, \tag{16}$$

where C and p do not depend on h.

By taking the logarithm, we obtain

$$\log|Df(x) - f'(x)| \sim \log C + p \log h, \tag{17}$$

therefore, the plot of $\log|Df(x) - f'(x)|$ versus $\log h$ looks like a straight line.

One can use a similar approach to derive a central scheme for the second derivative.
We will obtain

$$D^{(2)}f(x) = \frac{\alpha f(x-h) + \beta f(x) + \gamma f(x+h)}{h^2} \tag{18}$$

and

$$\left| D^{(2)}f(x) - f''(x) \right| \sim Ch^p. \tag{19}$$

Question: $\alpha =?$ $\beta =?$ $\gamma =?$ $C =?$ Maximum possible $p =?$

One can derive finite-difference schemes by the process of local interpolation and differentiation.

For example, $D_0 f(x)$ can be derived as follows:

- *Let* $p(x)$ *be the unique polynomial of degree* ≤ 2 *with* $p(x_0 - h) = f(x_0 - h)$, $p(x_0) = f(x_0)$ *and* $p(x_0 + h) = f(x_0 + h)$.
- Set $D_0 f(x) = p'(x_0)$.

The interpolant is given by

$$p(x) = f(x_0 - h)a_{-1}(x) + f(x_0)a_0(x) + f(x_0 + h)a_1(x), \tag{20}$$

where

$$a_{-1}(x) = \frac{(x - x_0)(x - (x_0 + h))}{2h^2}, a_0(x) = -\frac{(x - (x_0 - h))(x - (x_0 + h))}{h^2},$$
$$a_1(x) = \frac{(x - (x_0 - h))(x - x_0)}{2h^2}. \tag{21}$$

$p(x)$ is a *Lagrange polynomial.* Higher degree Lagrange polynomials can be used to construct finite-difference schemes of higher order. For example, a fourth-order central scheme: For example, a fourth-order scheme can be derived as follows:

- *Let $p(x)$ be the unique polynomial of degree ≤ 4 with $p(x_0 \pm 2h) = f(x_0 \pm 2h)$, $p(x_0 \pm h) = f(x_0 \pm h)$ and $p(x_0) = f(x_0)$.*
- Set $D_{0IV}f(x) = p'(x_0)$.

The interpolant is given by

$$p(x) = \sum_{j=-2}^{2} f(x_0 + jh)a_j(x), \tag{22}$$

where

$$a_j(x) = \prod_{\substack{-2\leq m\leq 2 \\ m\neq j}} \frac{x - (x_0 + mh)}{(j - m)h}. \tag{23}$$

We obtain

$$D_{0IV} f(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h}. \tag{24}$$

Wikipedia page on Lagrange polynomials:
`https://en.wikipedia.org/wiki/Lagrange_polynomial`

Wikipedia page on finite difference coefficients:
`https://en.wikipedia.org/wiki/Finite_difference_coefficient`
For the original source, see B. Fornberg, "Generation of Finite Difference Formulas on Arbitrarily Spaced Grids", *Mathematics of Computation*, **51** (184): 699–706 (1988).

Let us now consider the following boundary-value problem:

$$\begin{aligned} -u''(x) &= f(x), \qquad \forall x \in]0,1[, \\ u(0) &= u(1) = 0 \end{aligned} \tag{25}$$

We divide the domain using a set of discrete points

$$x_0 = 0 < x_1 < x_2 < ... < x_N < x_{N+1} = 1 \tag{26}$$

with a constant step $h = x_{i+1} - x_i$, $\forall i \in [0, N]$.
We then write the differential at the discrete points,

$$-u''(x_i) = f(x_i), \qquad \forall i \in 1, ..., N. \tag{27}$$

Consider the Taylor series

$$u(x_{i+1}) = u(x_i) + hu'(x_i) + \frac{h^2}{2}u''(x_i) + \frac{h^3}{6}u'''(x_i) + \frac{h^4}{24}u''''(\xi_i), \tag{28}$$

and

$$u(x_{i-1}) = u(x_i) - hu'(x_i) + \frac{h^2}{2}u''(x_i) - \frac{h^3}{6}u'''(x_i) + \frac{h^4}{24}u''''(\eta_i), \qquad (29)$$

where $\xi_i \in [x_i, x_{i+1}]$ and $\eta_i \in [x_{i-1}, x_i]$. After summing up the two series, we obtain

$$u(x_{i+1}) + u(x_{i-1}) = 2u(x_i) + h^2u''(x_i) + O(h^4), \qquad (30)$$

which suggests that it may be reasonable to approximate $u''(x_i)$ with the finite difference

$$\frac{u(x_{i-1}) - 2u(x_i) + u(x_{i+1})}{h^2}. \qquad (31)$$

This constitutes a second-order accurate approximation to the second derivative operator, as it can be shown that

$$R_i = u''(x_i) - \frac{u(x_{i-1}) - 2u(x_i) + u(x_{i+1})}{h^2} = O(h^2). \qquad (32)$$

R_i is the **consistency** error.

Let us now consider the following finite difference equation

$$-\frac{u_{i-1} - 2u_i + u_{i+1}}{h^2} = f_i, \qquad i = 1, ..., N, \tag{33}$$

where $f_i = f(x_i)$ and u_i are unknowns. It can be shown that finite-difference solution u_i **converges** *with the second order* to the exact solution $u(x_i)$ of the boundary-value problem:

$$|u_i - u(x_i)| \leq \frac{1}{12}||u''''||_\infty h^2. \tag{34}$$

The finite-difference problem can be written in an alternative form

$$u_{i-1}\left(-\frac{1}{h^2}\right) + u_i\left(\frac{2}{h^2}\right) + u_{i+1}\left(-\frac{1}{h^2}\right) = f_i, \qquad i = 1, ..., N, \tag{35}$$

$$u_0 = 0, \tag{36}$$

$$u_{N+1} = 0. \tag{37}$$

It is written the matrix form as

$$D^{(2)}\boldsymbol{U} = \boldsymbol{b} \tag{38}$$

where

$$D^{(2)} = \frac{1}{h^2}\begin{pmatrix} 2 & -1 & & & & & \\ -1 & 2 & -1 & & & & \\ & -1 & 2 & -1 & & & \\ & & & & \cdots & & \\ & & & & -1 & 2 & -1 \\ & & & & & -1 & 2 \end{pmatrix} \tag{39}$$

$$\boldsymbol{U} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-1} \\ u_N \end{pmatrix}, \quad \boldsymbol{b} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_{N-1} \\ f_N \end{pmatrix} \tag{40}$$

This tri-diagonal linear system can be solved by Gaussian elimination.

Note that the same matrix $D^{(2)}$ can be used to compute the derivative of u by matrix-vector multiplication when the values of $\boldsymbol{U}$ are given. It is called a *differentiation matrix* The differentiation matrix (41) in this case assumes that $u_0 = 0$ and $u_{N+1} = 0$. If this is not the case, the first and the last lines in $D^{(2)}$ should be modified such as to use one-sided schemes or different boundary conditions.

For example, let us introduce periodic boundary conditions, such that $x_0 = x_N$ and $x_{N+1} = x_1$. In that case we obtain

$$D^{(2)} = \frac{1}{h^2} \begin{pmatrix} 2 & -1 & & & & & & -1 \\ -1 & 2 & -1 & & & & & \\ & -1 & 2 & -1 & & & & \\ & & & & \cdots & & & \\ & & & & & -1 & 2 & -1 \\ -1 & & & & & & -1 & 2 \end{pmatrix} \tag{41}$$