CentraleSupelec **Numerical Methods, S8**

Finite Differences & ODE

1 Finite Differences

The first objective of this workshop is to implement and evaluate finite differences methods. To do so, the following analytical solution is investigated:

$$f(x) = \frac{\sin(x)}{x^3} \tag{1}$$

This function has the following first and second order derivatives:

$$\frac{\mathrm{d}f(x)}{\mathrm{d}x} = \frac{x\cos(x) - 3\sin(x)}{x^4}, \qquad \frac{\mathrm{d}^2 f(x)}{\mathrm{d}x^2} = \frac{-x^2\sin(x) - 6x\cos(x) + 12\sin(x)}{x^5} \tag{2}$$

The derivation of finite difference formulae is based on the Taylor-Expansion of a function around at a specific position:

$$f(x+h) = f(x) + \sum_{k=1}^{\infty} \frac{h^k}{k!} \left.\frac{\mathrm{d}^k f}{\mathrm{d}x^k}\right|_x \tag{3}$$

where h is the uniform spacing between each grid points.

1.1 First order derivatives

We first evaluate finite difference formula for the first order derivative $\frac{\mathrm{d}f}{\mathrm{d}x}$. Considering the following first and second order methods:

$$1^{st} \text{ order:} \quad \frac{\mathrm{d}f}{\mathrm{d}x} = \frac{f(x+h) - f(x)}{h} + \mathcal{O}(h) \tag{4}$$

$$2^{nd} \text{ order:} \quad \frac{\mathrm{d}f}{\mathrm{d}x} = \frac{f(x+h) - f(x-h)}{2h} + \mathcal{O}(h^2) \tag{5}$$

The objective is to write a python code in order to evaluate their accuracy:

1. In a module file, define two separated functions that evaluate the finite difference approximation of $\frac{\mathrm{d}f}{\mathrm{d}x}$ at first order and at second order. The input arguments of each function are the point where to evaluate the derivative x_0, the spacing h and the function to evaluate $func$.
2. In a main script file, import all functions of the previously defined module.
3. Define the functions f(x) and $\frac{\mathrm{d}f}{\mathrm{d}x}$.
4. Define the point $x_0 = 4$ where all derivatives are evaluated.
5. For different spacings h, evaluate the error made by the two finite difference methods.
6. Plot errors of each method with the adequate labels and titles, and conclude on the order of accuracy.
7. Find the constraints that a finite-difference approximation needs to fulfil to achieve a fourth order accuracy using a stencil of 4Δ. Then, write a fourth order approximation of $\frac{\mathrm{d}f}{\mathrm{d}x}$.
8. Implement and evaluate this fourth order method. Plot the error.

1.2 Second order derivatives

For a second order derivative $\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}$, we consider the two following second order methods with stencils $2h$ and $4h$:

$$2^{nd} \text{ order (2h):} \quad \frac{\mathrm{d}^2 f}{\mathrm{d}x^2} = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \mathcal{O}(h^2) \tag{6}$$

$$2^{nd} \text{ order (4h):} \quad \frac{\mathrm{d}^2 f}{\mathrm{d}x^2} = \frac{f(x+2h) - 2f(x) + f(x-2h)}{4h^2} + \mathcal{O}(h^2) \tag{7}$$

9. In your finite difference module file, add these two formula.
10. In your main script, define the function $\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}$.
11. For different spacing h, evaluate the error made by the two finite difference methods.
12. Plot errors of each method will the adequate labels and titles, and conclude on the order of accuracy.
13. Find the constraints that a finite-difference approximation needs to fulfil a fourth order accuracy using a stencil of 4Δ. Then, write a fourth order approximation of $\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}$.
14. Implement and evaluate this fourth order method. Plot the error.

2 Ordinary Differential Equations

Let us consider the following initial value problem:

$$\frac{\mathrm{d}Y(t)}{\mathrm{d}t} = F(t, Y(t)) \tag{8}$$

$$Y(t=0) = Y_0 \tag{9}$$

Considering a time-marching method, we use a discretized time vector $t_n = n\Delta t$. By integrating in time over the time interval $[t_n, t_{n+1}]$, we obtain the following update formula:

$$Y(t_{n+1}) = Y_n + \int_{t_n}^{t_{n+1}} F(\tau, Y(\tau))\mathrm{d}\tau \tag{10}$$

The time evolution of the right hand side is required to close the equation. The simpler strategy consists in considering that $F(\tau, Y(\tau)) = F(t_n, Y(t_n))$, which leads to the following scheme know as the Forward Euler's method:

$$Y(t_{n+1}) = Y_n + \Delta t F(t_n, Y(t_n)) \tag{11}$$

As a first introduction, we will investigate the following scalar ODE:

$$\frac{\mathrm{d}y(t)}{\mathrm{d}t} = -y \tag{12}$$

1. Find the analytical solution of $y(t)$ with the initial condition $y(t=0) = y_0$
2. Implement the Forward Euler's method. The initial condition is $y_0 = 1$. Choose an initial time step $\Delta t = 0.1s$ and a final time $T_{max} = 4s$.
3. Compare the results of the Euler's method to the analytical solution.
4. For different time steps, evaluate the error of this method compared to the analytical solution, and plot it. What is the order of accuracy?
5. What happen when the time step is larger than $1s$? Find K such that the forward Euler's method is written in the form $y^n = K^n y_0$. What is the constraint on K for the solution to be bounded?What is the consecutive constraint on Δt?