

F DFI L'INFORMAZIONE

SCUOLA DI INGEGNERIA INDUSTRIALE

Ordinary Differential Equations Part 1

Calcoli di Processo dell' Ingegneria Chimica

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Ordinary Differential Equations

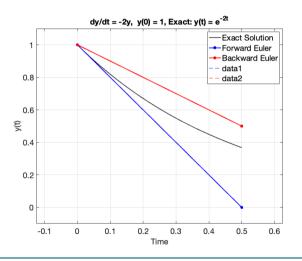
We will discuss different methods to approximate numerically the solution of the following Ordinary Differential Equation:

$$\frac{dy}{dt} = f(t, y, \Theta)$$

Generally speaking we are going to solve what it is usually called an **IVP** (Initial Value Problems), a differential equation associated with a set of initial conditions.

$$\begin{cases} \frac{dC_A}{dt} = -C_A \\ C_A(t = t^*) = C_A^* \end{cases}$$

Methods

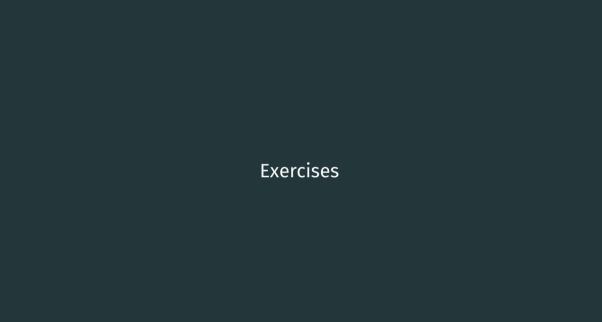


Forward Euler (explicit):

$$y_{n+1} = y_n + hy_n'$$

Backward Euler (implicit):

$$y_{n+1} = y_n + \frac{h}{h} y'_{n+1}$$



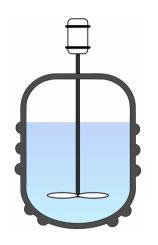
Exercises

▶ Implement in MATLAB a function to perform the integration exploiting Euler forward and Backward method and test it on the ODE reported below then study the behaviour of the algorithms with respect to a multiplication factor k. (Analytical solution: $x = x_0 exp(-t)$)

$$\frac{dx}{dt} = -k * x$$

➤ Solve the system of ODE reported below exploiting the builtin MATLAB function ode45.

$$\begin{cases} \frac{dC_A}{dt} = -C_A \\ \frac{dC_B}{dt} = C_A - C_B \\ \frac{dC_C}{dt} = C_B \end{cases}$$



Design of isothermal batch reactor.

Compute the conversion (hereinafter denoted as X_A) of the reactant A occurring inside an isothermal batch reactor, in which takes place the following first order irreversible reaction:

$$A \to B \ k = 0.01 \ [s^{-1}]$$

Let's define the reaction rate (r) as:

$$r = k \cdot C_A$$

Now write the rate of production/consumption of the two species taking part into the reaction:

$$\begin{cases} R_A = -k \cdot C_A \\ R_B = k \cdot C_B \end{cases}$$

$$\begin{cases} \frac{dC_A}{dt} = -k \cdot C_A \\ \frac{dC_B}{dt} = k \cdot C_A \end{cases}$$

Now let's focus on the first equation of the system:

$$\frac{dC_A}{dt} = -k \cdot C_A \quad \text{given} \quad X_A = \frac{C_A^0 - C_A}{C_A^0}$$

So the equation will become:

$$-C_A^0 \cdot \frac{dX}{dt} = -k \cdot C_A^0 \cdot (1 - X)$$

$$\frac{dX}{dt} = k \cdot (1 - X) \quad \text{with} \quad X(t = 0) = 0$$

So the solution of the ordinary differential equation will be $X(t) = 1 - exp(-k \cdot t)$

► Solve the system of equations of Lotka-Volterra (x prey and y predator) and The Lorenz attractor to emulate a chaotic system:

Lotka-Volterra

$$\begin{cases} \frac{dx}{dt} = (\alpha - \beta y)x \\ \frac{dy}{dt} = (\gamma x - \delta)y \end{cases}$$

$$\alpha=$$
 0.3, $\beta=$ 0.15, $\gamma=$ 0.1, $\delta=$ 0.1.

Lorentz

$$\begin{cases} \frac{dx}{dt} = \sigma(y - x) \\ \frac{dy}{dt} = x(\rho - z) - y \\ \frac{dz}{dt} = xy - \beta z \end{cases}$$

$$\beta = 8/3$$
, $\sigma = 10$, $\rho = 10$.

Thank you for the attention!