Ordinary Differential Equations
Part 1

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SCUOLA DI INGEGNERIA INDUSTRIALE
E DELL'INFORMAZIONE

Calcoli di Processo dell' Ingegneria Chimica

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Ordinary Differential Equations

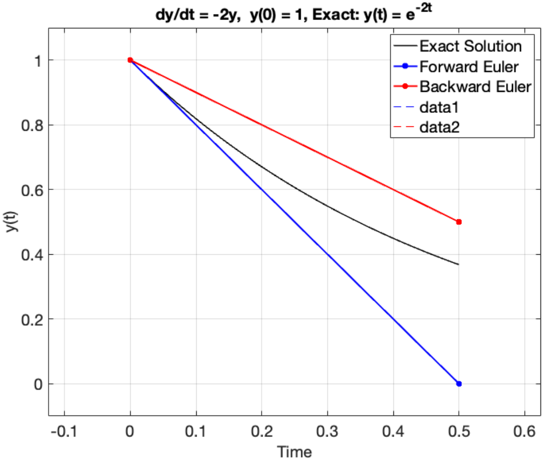
We will discuss different methods to approximate numerically the solution of the following Ordinary Differential Equation:

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

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**):

$$y_{n+1} = y_n + hy'_{n+1}$$

Exercises

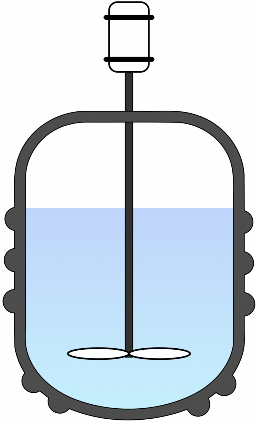
Exercises

- 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 occuring inside an isothermal batch reactor, in which takes place the following first order irreversible reaction:

$$A \rightarrow B \quad k = 0.01 \;\left[s^{-1}\right]$$

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:

$$\begin{cases} R_A = -k \cdot C_A \\ R_B = k \cdot C_B \end{cases} \qquad \begin{cases} \dfrac{dC_A}{dt} = -k \cdot C_A \\ \dfrac{dC_B}{dt} = k \cdot C_A \end{cases}$$

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!