Responsible TA:
Jiwoo Oh
jiwoo.oh@chem.ethz.ch

Statistical and Numerical Methods
Exercise 7, HS 2024

12/11/2024

# 1 ODE Stability Region (Core)

The second order Heun method reads

$$
\begin{aligned}
k_1 &= f(t_n, y_n) \\
k_2 &= f(t_n + h, y_n + hk_1) \\
y_{n+1} &= y_n + \frac{h}{2}(k_1 + k_2)
\end{aligned}
\tag{1}
$$

1. Find the stability interval for the second order Heun method (by hand).
   - Use the Dahlquist test equation
     $$f(t, y) = \lambda y(t)$$
   - Find an expression of the form `abs(...) < 1` that guarantees stability if it is fulfilled
2. Try to use the definition of the absolute value of a complex number to find an expression that does not contain the absolute value operator so that you can use the function `draw_stabfunc` (given online) to plot the stability region.
   - The easiest approach is to substitute a complex number w for $h\lambda$, defined as $w = a + ib$, and then applying the definition of absolute value:
     $$
     \begin{aligned}
     w &= h\lambda = a + ib \\
     a &= \text{Re}(w) = \text{Re}(h\lambda) \\
     b &= \text{Im}(w) = \text{Im}(h\lambda) \\
     |w| &= \sqrt{a^2 + b^2}
     \end{aligned}
     $$
   - Note that for this, you will have to multiply out the square of w (remember that $i^2 = -1$). Before you resolve the absolute value bring the complex number into the form $c + id$

# 2 Stiff ODEs (Core)

Consider a batch reactor with second order reactions

$$
\begin{aligned}
\frac{dA}{dt} &= -2k_1 A^2 \\
\frac{dB}{dt} &= k_1 A^2 - 2k_2 B^2
\end{aligned}
\tag{2}
$$

1. Solve the batch reactor and plot the solutions
   - Use $k_1 = 1000$; $k_2 = 0.1$; $y_0$= [1, 0.1] and tSpan = [0, 1]
   - Do you expect the system to be stiff? Use the linearization method to check the stiffness ratio at y = $y_0$ (by hand) by calculating the eigenvalues of the Jacobain of the system.
   - Remember that the eigenvalues of a matrix can be calculated by solving $\det(\mathbf{J} - \lambda\mathbf{I}) = 0$ for $\lambda$
   - The determinant of a 2x2 matrix is
     $$\det\begin{pmatrix} j_{11} & j_{12} \\ j_{21} & j_{22} \end{pmatrix} = j_{11}j_{22} - j_{21}j_{12}$$
   - Use ode45 to solve the system and plot the solutions. Is it stiff? Looking at the Jacobian, can you say why? Note how y changes and how it changes the Jacobian and its eigenvalues.

# 3 Stiff ODE 2

We consider the Van der Pol ODE

$$\ddot{y}(t) = \mu(1 - y^2(t))\dot{y}(t) - y(t) \tag{3}$$

with $\mu$ = 1000 and t $\in$ [0, 3000] with the following initial values

$$y(0) = 2, \;\; \dot{y}(0) = 0 \tag{4}$$

1. Run `StiffVanDerPol.m` which solves the IVP numerically using Matlab's `ode45` and `ode23s`. **Note**: The computation with ode45 can take a few minutes.

2. Based on the resulting plots, can you explain the large difference in run time?