May 3, 2022 (Due: 08:00 May 10, 2022)

1. The classical Runge–Kutta method (RK4) for solving the IVP

$$\begin{cases} u'(t) = f\big(t, u(t)\big), & (t > 0) \\ u(0) = u_0 \end{cases}$$

reads

$$u_{n+1} = u_n + \frac{h}{6}(k_1 + 2k_2 + 2k_3 + k_4),$$

where

$$\begin{aligned} k_1 &= f(t_n, u_n), \\ k_2 &= f\Big(t_n + \frac{1}{2}h, u_n + \frac{1}{2}hk_1\Big), \\ k_3 &= f\Big(t_n + \frac{1}{2}h, u_n + \frac{1}{2}hk_2\Big), \\ k_4 &= f(t_n + h, u_n + hk_3). \end{aligned}$$

Determine (numerically) the order of global truncation error (GTE) for RK4.
2. Let us consider the following family of methods

$$u_{k+1} = u_k + h\big(\theta f(t_{k+1}, u_{k+1}) + (1-\theta) f(t_k, u_k)\big)$$

to approximate the solution of the IVP

$$\begin{cases} u'(t) = f\big(t, u(t)\big), & (t > 0), \\ u(0) = u_0, \end{cases}$$

where $\theta \in [0, 1]$ is a parameter to be chosen. When this family of methods is applied to solve the model problem

$$\begin{cases} u'(t) = -\lambda u(t), & t > 0, \\ u(0) = u_0, \end{cases}$$

where λ is a given positive real number, the step size h needs to be chosen inside a certain region (the so-called *stable region*) to preserve the decay property of the solution. Determine (in terms of θ), the values of h for which the computed solution converges to 0 as $k \to \infty$. Note that by default h is a positive real number in practice.
3. Bacteria growing in a batch reactor utilize a soluble food source (substrate) as depicted in Figure 1. The uptake of the substrate is represented by a logistic

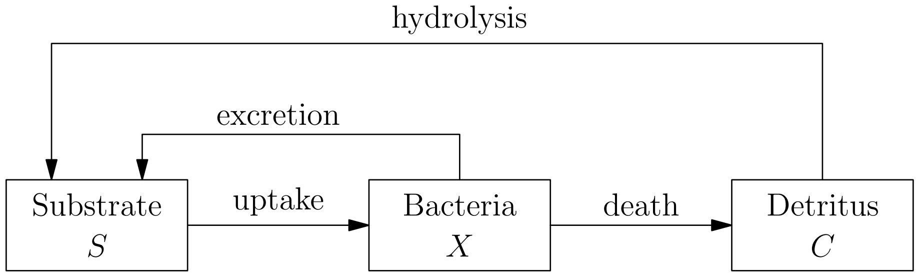

Figure 1: A batch reactor for bacteria growth.

model with Michaelis–Menten limitation. Death of the bacteria produces detritus which is subsequently converted to the substrate by hydrolysis. In addition, the bacteria also excrete some substrate directly. Death, hydrolysis and excretion are all simulated as first-order reactions.

Mass balances can be written as

$$\begin{cases} X' = \mu_{\max}\Big(1 - \dfrac{X}{K}\Big)\Big(\dfrac{S}{K_S + S}\Big)X - k_d X - k_e X \\ C' = k_d X - k_h C \\ S' = k_e X + k_h C - \mu_{\max}\Big(1 - \dfrac{X}{K}\Big)\Big(\dfrac{S}{K_S + S}\Big)X \end{cases}$$

where X, C, and S are the concentrations [mg·L^{-1}] of bacteria, detritus, and substrate, respectively;
$\mu_{\max}$ is the maximum growth rate [d^{-1}];
K is the logistic carrying capacity [mg·L^{-1}];
K_S is the Michaelis–Menten half-saturation constant [mg·L^{-1}];
k_d, k_e, and k_h, respectively, are the death rate [d^{-1}], the excretion rate [d^{-1}], and the hydrolysis rate [d^{-1}].

Simulate the concentrations from $t = 0$ to $100\,\mathrm{d}$, given the initial conditions $X(0) = 1\,\mathrm{mg{\cdot}L^{-1}}$, $S(0) = 100\,\mathrm{mg{\cdot}L^{-1}}$, and $C(0) = 0\,\mathrm{mg{\cdot}L^{-1}}$. Employ the following parameters in your calculation:

$$\mu_{\max} = 10\,\mathrm{d}^{-1}, \quad K = 10\,\mathrm{mg{\cdot}L^{-1}}, \quad K_S = 10\,\mathrm{mg{\cdot}L^{-1}}, \quad k_d = k_e = k_h = 0.1\,\mathrm{d}^{-1}.$$

Find stationary concentrations and visualize your solution.

4. A spring–mass system as shown in Figure 2 can be modeled by the following second order ODE, under certain simplifying assumptions (e.g., small displacement, spring has no mass, no friction, etc.):

$$mx''(t) = -kx(t), \qquad x(0) = x_0, \qquad x'(0) = v_0,$$

where m is the weight of the mass and k is the spring constant.

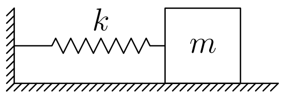

Figure 2: A simple spring–mass system.

(a) Find the exact solution $x(t)$.
(b) Transform the second order ODE to a first order one by introducing $u(t) = [x(t), x'(t)]^\top$.
(c) Solve the IVP in part (b) by Euler method, backward Euler method, trapezoidal method, and classical Runge–Kutta method, for a long time period. You may assume $m = k = 1$, and use a step size $h = 0.1$. Visualize your solutions using phase diagrams (i.e., plot the solutions in the u-plane). What can you say about long-term behavior of these methods?