Dr. rer.nat. Julian Koellermeier, Safiere Kuijpers, M.Sc.

Differential Equations In Science And Engineering | 23/24 IIa
Sample Solution Examination | 02.04.2024

Exercise 1.
We consider the following system (1) of chemical reactions for the four species A, B, C, D:

$$\begin{aligned} A + B &\xrightarrow{k_1} 2B \\ B + 2C &\xrightarrow{k_2} 3C \\ C + D &\xrightarrow{k_3} D \end{aligned} \tag{1}$$

a) Draw the reaction network.

b) Derive the stoichiometric net coefficients, the reaction rates, the production rates, and the corresponding system of ODEs that describes the dynamics of the species' concentrations denoted by n_A, n_B, n_C, n_D.

c) Show that the system has <u>no</u> conserved quantity that includes any of the species A, B, C.

d) We now want to change the last reactions of the system (1) such that the whole changed system has the conserved quantity $n_A + n_B + n_C + n_D$.

   Write down <u>two</u> examples for a changed last reaction.

   Show that in the changed systems $n_A + n_B + n_C + n_D$ is conserved.

0.5+2+1+1.5 points

Solution.

a) The reaction network is given by

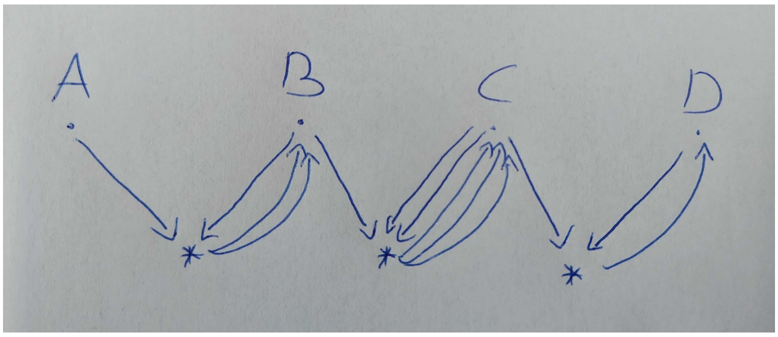

Abbildung 1: Reaction network.

Full points are only given if it is clear where the reaction happens (indicated by the stars in Figure 1). Otherwise the reaction network would not be generalizable for autocatalytic reactions that have product species.

b) We have 4 substances A, B, C, D, so $N = 4$ and 3 reactions, so $M = 3$.

   The stoichiometric coefficients are given by the following table:

$\gamma_{i,m}$	1	2	3
A	-1	0	0
B	1	-1	0
C	0	1	-1
D	0	0	0

The reaction rates are given by

$$\begin{aligned}
\lambda_1 &= k_1(T) \cdot n_A \cdot n_B \\
\lambda_2 &= k_2(T) \cdot n_B \cdot (n_C)^2 \\
\lambda_3 &= k_3(T) \cdot n_C \cdot n_D
\end{aligned}$$

The production rates R_i of the substances are then given by $R_i = \sum_{m=1}^{3} \gamma_{i,m}\lambda_m$:

$$\begin{aligned}
R_A &= -\lambda_1 \\
R_B &= +\lambda_1 - \lambda_2 \\
R_C &= +\lambda_2 - \lambda_3 \\
R_D &= 0
\end{aligned}$$

This leads to the following ODE system

$$\begin{aligned}
\frac{dn_A}{dt} &= -k_1(T) n_A n_B \\
\frac{dn_B}{dt} &= +k_1(T) n_A n_B - k_2(T) \cdot n_B \cdot (n_C)^2 \\
\frac{dn_C}{dt} &= +k_2(T) \cdot n_B \cdot (n_C)^2 - k_3(T) \cdot n_C \cdot n_D \\
\frac{dn_D}{dt} &= 0.
\end{aligned}$$

c) For conservation, we try to solve $\sum_{i=1}^{N} \alpha_i \gamma_{i,m} = 0$ for $m = 1, 2, 3$. This leads to

$$\begin{aligned}
-\alpha_A + \alpha_B &= 0 \\
-\alpha_B + \alpha_C &= 0 \\
-\alpha_C &= 0.
\end{aligned}$$

The only solution is $\alpha_A = \alpha_B = \alpha_C = 0$. This means that only n_D is conserved.

d) When changing the last equation of (1) to

$$C + (K) \cdot D \xrightarrow{k_3} (K+1) \cdot D, \tag{2}$$

for any integer $K \in \mathbb{N}$, then the last equation for the computation of the conserved quantities reads

$$-\alpha_C + \alpha_D = 0.$$

Which leads to the solution $\alpha_A = \alpha_B = \alpha_C = \alpha_D$, so that for example $n_A + n_B + n_C + n_D$ is constant.

Exercise 2.

The system of chemical reactions from exercise (1), can be simplified assuming constant populations n_A and n_D, and the scalings $x = \frac{n_B}{n_{B_0}}$, $z = \frac{n_C}{n_{C_0}}$. The simplified system reads

$$\begin{aligned} \frac{dx}{dt} &= \alpha x - \beta x z^2, \\ \frac{dz}{dt} &= \beta x z^2 - \gamma z. \end{aligned}$$

where $\alpha, \beta, \gamma \in \mathbb{R}_+$ are some positive constants.

a) Compute the two steady states of this ODE system, including the non-trivial steady state $(x_s, z_s) = \left(\frac{\gamma}{\sqrt{\alpha\beta}}, \sqrt{\frac{\alpha}{\beta}}\right)$.

b) Find all possible parameters α, β, γ such that the Jacobian of the non-trivial steady state has two real eigenvalues with the same sign.

   Characterise the stability behavior of both steady states for that case.

c) We now interpret the ODE system as a model for the population dynamics of a prey species x and a predator species z.

   i) What is then the physical meaning of the parameters α, β, γ?

   ii) What is different with respect to the standard Lotka-Volterra model discussed in the lectures?

   iii) What process is modeled by that difference?

1+2.5+1.5 points

Solution.

a) The condition for steady state is that temporal derivatives vanish.

   We get from $\frac{dx}{dt} = 0$ and $\frac{dz}{dt} = 0$ via direct computation that the following three steady states exist:

   (1) $x = 0$ and $z = 0$,

   (2) $x = \frac{\gamma}{\sqrt{\alpha\beta}}$ and $z = \sqrt{\frac{\alpha}{\beta}}$.

   Note that for the non-trivial steady state, only the positive solution makes sense.

b) We compute the Jacobian

$$\begin{pmatrix} \alpha - \beta z^2 & -2\beta x z \\ \beta z^2 & 2\beta x z - \gamma \end{pmatrix}.$$

   For stability of the non-trivial steady state, we compute the Jacobian at that steady states and compute the eigenvalues, which characterize the stability.

   The Jacobian at the non-trivial steady state reads:

$$A = \begin{pmatrix} 0 & -2\gamma \\ \alpha & \gamma \end{pmatrix}$$

   We observe $tr(A) = P = \gamma$ and $det(A) = Q = 2\gamma\alpha$.

   The eigenvalues are then given by

$$\begin{aligned} \lambda_{1,2} &= \frac{1}{2}\left(P \pm \sqrt{P^2 - 4Q}\right) \\ &= \frac{1}{2}\left(\gamma \pm \sqrt{\gamma^2 - 8\gamma\alpha}\right). \end{aligned}$$

so that real eigenvalues are obtained for $\gamma^2 - 8\gamma\alpha \geq 0$.

This means that $\frac{\gamma}{8} \geq \alpha$.

Two eigenvalues with positive real part are obtained when $\gamma - \sqrt{\gamma^2 - 8\gamma\alpha} > 0$.

This means that $\gamma^2 > \gamma^2 - 8\gamma\alpha$ and thus $0 > -8\gamma\alpha$, which is already true for $\gamma > 0$, $\alpha > 0$.

Note, that two eigenvalues with negative real part are not possible.

So the only additional condition for two real eigenvalues with the same (positive) sign is $\frac{\gamma}{8} \geq \alpha$.

For the non-trivial steady-state, the stability behavior is characterised by an unstable focus.

For the trivial steady-state, the Jacobian is given by

$$A = \begin{pmatrix} \alpha & 0 \\ 0 & -\gamma \end{pmatrix}$$

We directly find the eigenvalues $\lambda_1 = \alpha$ and $\lambda_2 = -\gamma$. Both eigenvalues are real and they have different signs.

For the trivial steady-state, the stability behavior is therefore characterised by an unstable saddle point.

c) i)
  * α is the specific natural reproduction rate of prey
  * β is the hunting rate
  * γ is the death rate of predators

  ii) The z^2 is different w.r.t. the standard Lotka-Volterra model.

  iii) It means that the probability of prey being hunted is proportional to the probability of two predators coming together. This means that predators are hunting collectively. More specifically, they hunt in couples.

Exercise 3.

We consider the scalar wave equation

$$\frac{\partial^2}{\partial t^2}u - c\frac{\partial^2}{\partial x^2}u = 0, \quad c \in \mathbb{R}, \tag{3}$$

with constant wave velocity c.
We want to perform a linear stability analysis of equation (3) using the wave ansatz

$$u(t,x) = u_0 \cdot e^{i(kx-\omega t)}, \tag{4}$$

for wave number $k \in \mathbb{R}$, wave frequencies $\omega \in \mathbb{C}$ and amplitude $u_0 \in \mathbb{R}$.

a) What wave frequencies ω in (4) lead to a non-increasing, i.e. stable, wave in time?

b) Insert the wave ansatz (4) into the wave equation (3) to derive a stability condition for the wave equation. Show that the stability condition is equivalent to $c \geq 0$.

c) What is the physical interpretation of this stability condition and does it make sense?

1+3+1 points

Solution.

a) Stability in time means that the wave solution does not increase with t.

Using $\omega = Re(\omega) + iIm(\omega))$, we get that

$$i(-\omega t) = -i(Re(\omega) + iIm(\omega))t = -iRe(\omega)t + Im(\omega)t.$$

The term $-iRe(\omega)t$ is an oscillation in time and not increasing with t. The term $Im(\omega)t$ is potentially increasing and has to be smaller or equal than 0 for stability. (it is ok if the students say equal zero and smaller than zero).

This means that $\omega \in \mathbb{C}$ has to have negative imaginary part: $Im(\omega) < 0$.

b) We use that the derivatives of the wave ansatz (4) are

$$\begin{aligned}
\frac{\partial}{\partial t}u &= -\omega i u, \\
\frac{\partial^2}{\partial t^2}u &= -\omega^2 u, \\
\frac{\partial}{\partial x}u &= kiu, \\
\frac{\partial^2}{\partial x^2}u &= -k^2 u.
\end{aligned}$$

Inserting this into the wave equation (3) yields

$$\begin{aligned}
\frac{\partial^2}{\partial t^2}u - c\frac{\partial^2}{\partial x^2}u &= 0 \\
\Rightarrow (-\omega i)^2 u + ck^2 u &= 0 \\
\Rightarrow (ck^2 - \omega^2)u &= 0.
\end{aligned}$$

Non-trivial solutions are given by

$$ck^2 - \omega^2 = 0,$$

which leads to

$$\omega = \pm\sqrt{ck^2}. \tag{5}$$

Using the solution of part a), stable solutions are given by $Im(\omega) < 0$. From (5) we see that there will always be a positive and negative solution so the imaginary part needs to be zero overall. This requires

$$c \geq 0.$$

c) We have $c \geq 0$. This means that the wave velocity needs to be positive. Waves need to move forward in time, not backward. For positive wave velocity $c \geq 0$, there will be two waves with real wave speeds $\omega = \pm\sqrt{ck^2}$, moving to the left and right, respectively. This is physical for traveling waves.

Exercise 4.

The shallow water equations for water height $h(t,x)$ and vertical velocity $u(t,x)$ are

$$\partial_t \begin{pmatrix} h \\ hu \end{pmatrix} + \partial_x \begin{pmatrix} hu \\ hu^2 + \cos(\alpha) g \frac{h^2}{2} \end{pmatrix} = -\frac{1}{\lambda} \begin{pmatrix} 0 \\ u \end{pmatrix}, \tag{6}$$

where $h(t,x)$ and $u(t,x)$ are the unknowns and g, λ, α are parameters.

a) What physical interpretations do the equations (6) have and what are the main assumptions for their derivation?

b) Show that the system (6) can be written in the following (so-called primitive variable) form:

$$\partial_t \begin{pmatrix} h \\ u \end{pmatrix} + \begin{pmatrix} u & h \\ \cos(\alpha) g & u \end{pmatrix} \cdot \partial_x \begin{pmatrix} h \\ u \end{pmatrix} = -\frac{1}{\lambda h} \begin{pmatrix} 0 \\ u \end{pmatrix}, \tag{7}$$

c) Assume the spatially homogeneous case in which all spatial derivatives vanish, i.e. $\partial_x h = 0$, $\partial_x u = 0$. For this case, derive the solution of the shallow water equations (6).

d) What problem can appear for numerical schemes trying to solve the homogeneous shallow water equations?

1.5+1.5+1.5+0.5 points

Solution.

a) The first equation is derived from the vertical average of the conservation of mass (also-called continuity equation). The second equation is derived from the vertical average of the conservation of momentum in x-direction.

   The main assumptions for the derivation are:

   - incompressibility or $\rho = const.$
   - shallowness or $\frac{H}{L} = \epsilon \ll 1$.
   - plane with inclination angle α.
   - friction is modeled using a slip law at the bottom with slip length $\lambda > 0$ (that leads to a relaxation of u towards zero with relaxation time $\frac{1}{\lambda}$).
   - gravity is modeled using a gravity constant gravitational acceleration g.

b) The first equation of (7) is derived from the first equation of (6).

   The second equation of (7) is derived from the second equation of (6) using the first equation obtained before.

c) The height is constant and the velocity is decaying exponentially.

d) A small value for $h\lambda$ leads to stiffness, which means that the system requires a small time step for a standard explicit scheme.