Technische Universität München
Lehrstuhl für Informatik V
Dr. T. Neckel
M.Sc. D. Jarema

WS 2015/16
Scientific Computing
09.11.2015/11.11.2015

Worksheet 3
Sample Solutions

Continuous Models: Ordinary Differential Equations

Ordinary differential equations or ODEs are often used to describe *continuous problems* such as time-dependent phenomena. They contain a function $u(t)$ of one independent variable t and its derivatives du/dt, $f(t, u, du/dt, d^2u/dt^2, ..., d^nu/dt^n) = 0$. For ODE problems of the form

$$\frac{du(t)}{dt} = f(t) \cdot g(u),$$

the solution of the underlying problem can be determined via separation of variables:

1. For $g(u) \neq 0$, divide by $g(u)$:
$$\frac{1}{g(u)} \frac{du}{dt} = f(t)$$
2. Solve the integral equation:
$$\int \frac{1}{g(u)} du = \int f(t) dt$$
3. Solve the arising equation for u, i.e. write the equation as $u(t) = ...$.

(H) Exercise 1: Radioactive Decay

In radioactive decay, radioactive material is turned into more stable chemical elements. Let $N(t = 0)$ denote the original number of atoms. Then, $\lambda N(t)$ atoms ($0 < \lambda < 1$) are expected to mutate over an infinitesimal time interval. This yields the following ordinary differential equation:

$$\frac{dN(t)}{dt} = -\lambda N(t) \tag{1}$$

(a) Solve the ODE (1) via separation of variables. How many solutions do we obtain? Under which assumption do we obtain a unique solution?

(b) The *half-life* t_H is the time after which 50% of the original material has mutated. Compute the half-life depending on an arbitrary choice of λ. How does the initial amount of atoms influence the half-life?

(c) General chemical reactions for a substance $N(t)$ can be modeled analogously to the radioactive decay. However, the substance may not only vanish, but it can also be created, e.g. due to other chemical reactions which happen simultaneously and don't necessarily depend on $N(t)$. How does the respective model for the substance $N(t)$ look like? Can you still solve the problem via separation of variables?

Solution:

(a) One trivial solution to the problem is $N(t) = 0$. For all functions $N(t) \neq 0$, we can apply the separation of variables as follows:

$$\begin{aligned} \frac{dN(t)}{dt} &= -\lambda N(t) \\ \frac{1}{N(t)}\frac{dN(t)}{dt} &= -\lambda \\ \int_N \frac{1}{N} dN &= \int_t -\lambda dt \\ \ln(N(t)) &= -\lambda t + C \\ N(t) &= e^{-\lambda t + C} \end{aligned}$$

where $C \in \mathbb{R}$ is an additional constant arising from the integration. Since C is an arbitrary real number, we obtain an infinite number of solutions. Using the assumption that we have $N(t = 0) = N_0 > 0$ atoms at the very beginning, fixes our constant:

$$N(t = 0) = e^{-\lambda 0 + C} = e^C \stackrel{!}{=} N_0 \Leftrightarrow C = \ln(N_0)$$

We hence obtain a unique solution if we know the *initial condition* of our problem.

(b) From the definition of the half-life, we search for the time t where $N(t) = 0.5N(t = 0) = 0.5N_0$. We hence obtain:

$$N_0 e^{-\lambda t} \stackrel{!}{=} 0.5N_0 \Leftrightarrow e^{-\lambda t} = 0.5 \Leftrightarrow t = -\frac{\ln(0.5)}{\lambda}$$

The half-life is independent of N_0.

(c) In the generalized case, we have an additional source term $q(t)$: $dN(t)/dt = -\lambda N(t) + q(t)$. The coefficient λ denotes the respective reaction constant. If $q(t)$ is bigger than zero, then new material of N is created. If it is smaller than zero, the substance is further reduced. For a general term $q(t)$, a splitting of the right hand side of the differential equation $f(t) \cdot g(N)$ is not possible anymore. The ansatz of separation of variables can therefore not work anymore. Other solution strategies are hence required (see for example theory on variation of constants for inhomogeneous ordinary differential equations).

(H) Exercise 2: Eigenvalues of Differential Operators

Given an operator L, a real number λ is called *eigenvalue* of L, if

$$L(u) = \lambda u \tag{2}$$

for a non-zero function u. The function u is called *eigenfunction*.
Consider the case $L(u) := -\frac{d^2u}{dx^2}$.

(a) Show that all values $\lambda_k := (k\pi)^2$, $k \in \mathbb{N}$, are eigenvalues of L with corresponding eigenfunctions $u_k(x) := \sin(k\pi x)$, i.e. show that they solve the eigenvalue problem

$$L(u_k) = \lambda_k u_k, \quad u_k(0) = u_k(1) = 0 \tag{3}$$

on the unit interval.

(b) How does the problem from (a) translate to higher-dimensional problems, i.e. which functions u and scalars λ can you identify from the one-dimensional case which fulfill

$$-\sum_{d=1}^{D} \frac{\partial^2 u}{\partial x_d^2} = \lambda u, \quad u\|_{\partial\Omega} = 0 \tag{4}$$

where $\Omega = [0;1]^D$ is the unit hypercube and $\partial\Omega$ its boundary?

Solution:

(a) Computing the second derivative of u_k yields:

$$\frac{d^2u_k}{dx^2} = k\pi\frac{d(\cos(k\pi x))}{dx} = -(k\pi)^2\sin(k\pi x) = -(k\pi)^2 u_k$$

Each function u_k further automatically fulfills the boundary conditions $u(0) = u(1) = 0$.

(b) For a D-dimensional problem, consider the function

$$u_k(x) := \Pi_{d=1}^{D} \sin(k_d \pi x_d),$$

where $k_d \in \mathbb{N}$ and $k = (k_1, k_2, \cdots, k_n) \in \mathbb{N}^n$ is multi-index. Each second partial derivative yields again

$$-\frac{\partial^2 u_k}{\partial x_d^2} = (k_d\pi)^2 u_k.$$

With the sum over all respective derivatives, we see that u_k is an eigenfunction of the system. The respective eigenvalue is $\lambda_k = \sum\limits_{d=1}^{D}(k_d\pi)^2$.

(I) Exercise 3: Population Models with One Species

Direction Fields

Name the corresponding models and provide the dynamics equations (basic equation without values of coefficients) for the direction fields provided in Figure 1.

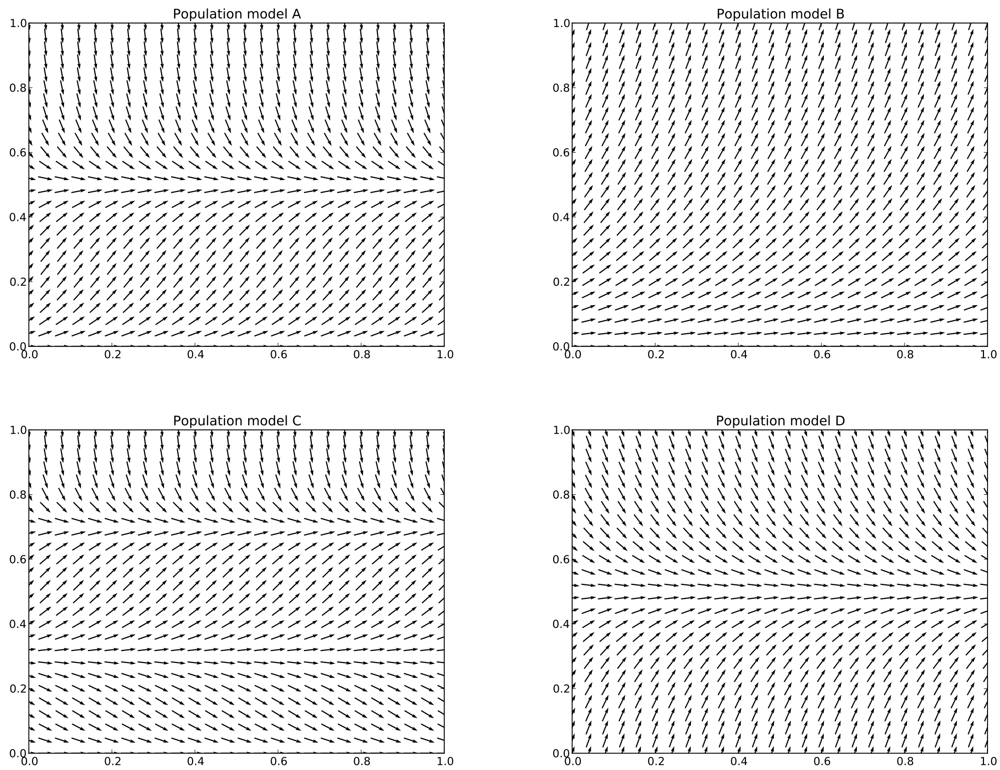

Figure 1: Direction fields for different population models with one species.

Population Dynamics

Consider the following one-species population model

$$\frac{dp}{dt} = f(p) = -r\left(1 - \frac{p}{k}\right)\left(1 - \frac{p}{l}\right), \tag{5}$$

with $p(0) = p_0 \geq 0$ and $r > 0$, $0 < l < k$.

(a) Compute the critical points. Are they stable or not?

(b) Determine the limit $\lim_{t\to\infty} p(t)$ for

I) $0 \leq p_0 < l$,

II) $p_0 = l$,

III) $l < p_0 < k$,

IV) $p_0 = k$,

V) $p_0 > k$,

and sketch the trajectories of the solution $p(t)$ for each of the five cases.

(c) Name one reason why the model is not a realistic population model.

Solution:

Direction Fields

(A) Verhulst model – logistic growth.

$$\frac{dp}{dt} = \alpha \left(1 - \frac{p(t)}{\beta}\right) p(t).$$

(B) Malthus model – exponential growth.

$$\frac{dp}{dt} = r \cdot p(t), \quad r > 0.$$

(C) Verhulst model – logistic growth with thresholds.

$$\frac{dp}{dt} = \alpha \left(1 - \frac{p(t)}{\beta}\right)\left(1 - \frac{p(t)}{\delta}\right) p(t), \quad \alpha < 0.$$

(D) Verhulst model – saturation.

$$\frac{dp}{dt} = \alpha - \beta \cdot p(t).$$

Population Dynamics

(a) Critical points:

$$\frac{dp}{dt} = -r\left(1 - \frac{p}{k}\right)\left(1 - \frac{p}{l}\right) = 0 \quad \leftrightarrow \quad p = k \quad \text{or} \quad p = l$$

Stability of the critical points:

$$\frac{df}{dp}(p) = -r\left(1 - \frac{p}{k}\right)\left(-\frac{1}{l}\right) - r\left(-\frac{1}{k}\right)\left(1 - \frac{p}{l}\right) = r\frac{l + k - 2p}{kl}.$$

When $r > 0$, $0 < l < k$ we obtain:

$$\frac{df}{dp}(l) = r\frac{l + k - 2l}{kl} > 0 \quad \rightarrow \text{unstable critical point at } p = l.$$

$$\frac{df}{dp}(k) = r\frac{l + k - 2k}{kl} < 0 \quad \rightarrow \text{stable critical point at } p = k.$$

(b) Limit for $t \to \infty$:

I) smallest critical point at $p = l$, unstable

$$\lim_{t\to\infty} p(t) = -\infty \quad \text{for} \quad 0 \le p_0 < l,$$

II) critical point at $p = l$,

$$\lim_{t\to\infty} p(t) = l \quad \text{for} \quad p_0 = l,$$

III) unstable critical point at $p = l$, stable critical point at $p = k$, no critical points in between

$$\lim_{t\to\infty} p(t) = k \quad \text{for} \quad l < p_0 < k,$$

IV) critical point at $p = k$

$$\lim_{t\to\infty} p(t) = k \quad \text{for} \quad p_0 = k,$$

V) biggest critical point at $p = k$, stable

$$\lim_{t\to\infty} p(t) = k \quad \text{for} \quad p_0 > k.$$

The trajectories are demonstrate in Figure 2.

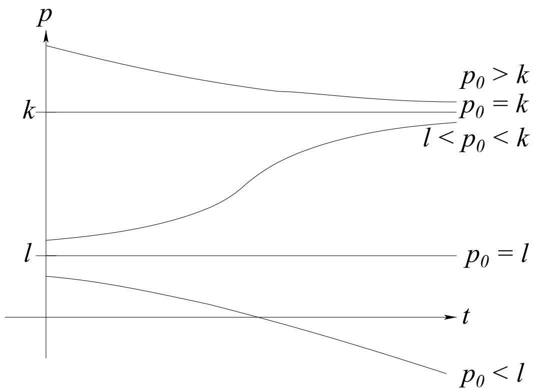

Figure 2: Sketches of some of the trajectories for the population dynamics.

(c) $\lim_{t\to\infty} p = -\infty$ for $p_0 < l$, but only positive population numbers $p > 0$ have physical meaning.