Scientific Computing

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 $u(t) = ...$.

Exercise 6: 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 equation from above via separation of variables. How many solutions do we obtain? Under which assumption do we obtain a unique solution?

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

(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. How does the respective model for the substance $N(t)$ look like? Can you still solve the problem via separation of variables?

(d) Write a maple worksheet that exactly solves Eq. (1) and the extended model for chemical reactions for $\lambda = 0.1$ and $N(t = 0) = 10^3$ atoms.

Note: For an introduction to maple, see amongst others:
http://wofford-ecs.org/IntroComputationalScience/_dataFilePages/maple.htm.

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:

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

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

$$\int_N \frac{1}{N} dN = \int_t -\lambda dt$$

$$\log(N(t)) = -\lambda t + C$$

$$N(t) = e^{-\lambda t + C}$$

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:

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

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

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

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

The half-live is independent from N_0.

(c) In the generalised 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).

(d) See ws3.mw.

Exercise 7: Eigenvalues of Differential Operators

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

$$L(u) = \lambda u \qquad (2)$$

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

(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

$$L(u_k) = \lambda_k u_k, \quad u_k(0) = u_k(1) = 0 \qquad (3)$$

on the unit interval.

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

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

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

Solution:

(a) Computing the second derivative of u_k yields:

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

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

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

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

with $k_d \in \mathbb{N}$. 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 evolves at $\lambda_k = \sum_{d=1}^{D} (k_d \pi)^2$.

Exercise 8 (Homework, discrete population dynamics): Game of Life

Considering the "Game of Life" (as introduced in the lecture), which initial configurations yield stable cell configurations or respective periodic cycles? Investigate the behaviour for different start configurations with no more than four cells.
Remark: This exercise is marked as homework. It will not be discussed in the exercise course.