

Lectures on Modeling and Simulation 1

Exercises 1

Pendulum equation, Euler's method, MATLAB plotting, MATLAB-ODE-Integrators

1.1 For the solution of the pendulum equation a constant length l of the pendulum is presumed:

$$\begin{aligned}\dot{\varphi} &= \omega \\ \dot{\omega} &= -\frac{g}{l} \cdot \sin(\varphi)\end{aligned}$$

- a) Implement the true solution of the linearized pendulum equation ($\sin(\varphi) \approx \varphi$) with a visualization of the results in the time course.
 - b) Make the calculation and visualization available as MATLAB functions for later reuse. Arguments of the functions are initial values and parameters.
 - c) What does happen if the damping becomes stronger?
- 1.2 An oscillation is regarded to be damped.
- a) Implement Euler's method in MATLAB analogous to the pattern in the lecture.
 - b) Plot the results ($\varphi(t)$, $\omega(t)$) in the course of time.
 - c) Speed up the MATLAB program by preallocating memory cells for the result vectors.
- 1.3 The pendulum equation is considered again.
- a) Visualize the numerical solution (1.2) by comparison with the true solution (1.1).
 - b) Now, vary the increment Δt . For which value of Δt is the numerical solution sufficiently accurate? What happens if the increment Δt becomes too large or much too large?
 - c) Replace φ by $\sin(\varphi)$ again. From which initial excursion of the pendulum on does the linearized solution (1.1) **not** describe the true shape of the numerical solution sufficiently accurate?
- 1.4 The nonlinear pendulum equations are considered again.
- a) Implement a MATLAB function for the righthand side of the differential equation system. It should be called like
$$\text{dphidt} = \text{pendulum}(\text{t}, \text{phi}).$$
 - b) Solve now the equations with one of the given MATLAB integrationprocedures `ode23`, `ode45`, ... and plot the results as well as the stepsize automatically chosen by the solver in the time course.
 - c) Become familiar with the function `odeset`. Check out the options to trigger the methods particularly with regard to the parameters `RelTol`, `AbsTol`, `InitialStep`, `MaxStep`.
 - d) How many steps are necessary and how much computing time is required respectively to solve the pendulum equations sufficiently accurate?

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Exercises 2

SIMULINK

2.1 A simulation for the fairground swing has to be implemented with SIMULINK. The system is modeled with the angle φ and the angular momentum L as state variables as:

$$\begin{aligned}\dot{L} &= -m \cdot g \cdot l \cdot \sin \varphi - \frac{d}{m \cdot l^2} \cdot L \\ \dot{\varphi} &= \frac{1}{m \cdot l^2} \cdot L\end{aligned}$$

- Write these equations as a SIMULINK block diagram using integrators, gains, trigonometric functions and summation blocks.
 - Arrange the blocks “nicely” and implement the diagram with SIMULINK. The parameters are $m = 100$, $g = 9.81$, $l = 2.5$, $d = 100$.
 - Specify the initial values $\varphi = 1$, $L = 0$. Where must this information be filled in?
 - Simulate the system and visualize φ and $\omega = \frac{1}{ml^2}L$ with a time plot and a state space plot by using oscilloscopes. Adjust the simulation time suitably.
- 2.2 The fairground swing model will now be combined to a new SIMULINK block with input l , output φ , ω and a parameter mask for m and d .
- Introduce an input port for l and change the block diagram appropriately, i.e. change the constant l into a signal $l(t)$. Multiplication and squaring block must be used for that.
 - Remove the oscilloscopes and convert the diagram into a SIMULINK block. Test the new block with a constant input and external oscilloscopes.
 - Introduce the parameters m , d instead of their fixed values and specify a mask for the input of these parameters. Test the mask by varying these parameters.
 - Duplicate the swing block and simultaneously simulate two different swings.
- 2.3 Different ODE solvers shall be compared for the fairground swing example.
- Start with the fixed step size Runge-Kutta schemes. Introduce an output of the state to the MATLAB workspace in order to compare different results. Now select the Runge-Kutta scheme of order 5 and vary the step size Δt until the result becomes stable up to 4 digits.
 - Find the step size Δt that produces 4 digits of precision for all Runge-Kutta schemes of order 1-5. Compare the results with respect to computational complexity.
 - Now switch to the variable step size Runge-Kutta 4/5 method. Adjust the absolute precision parameter of the method so that 4 digits of precision are obtained. Does the absolute precision parameter really agree with the finally obtained precision?
 - Output the times and state of the most recent simulation to the workspace. Use the MATLAB function `diff()` to inspect the time steps taken by the method. Are these time steps correlated to the systems dynamics?

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Exercises 3

Distribution functions

3.1 Consider the three following probability functions.

$$d_x(\xi) = c \cdot \begin{cases} \xi, & 0 \leq \xi \leq 1 \\ 0, & \text{otherwise} \end{cases}$$

$$d_x(\xi) = c \cdot \begin{cases} 1, & a \leq \xi \leq b \\ 0, & \text{otherwise} \end{cases}$$

$$d_x(\xi) = c \cdot \begin{cases} 1, & \xi = 1, 2, 3, 4, 5, 6 \\ 0, & \text{otherwise} \end{cases}$$

$$d_x(\xi) = c \cdot \begin{cases} 1, & \xi = -1 \\ 2, & \xi = 0 \\ 3, & \xi = 1 \\ 0, & \text{otherwise} \end{cases}$$

Which of these distributions is continuous and which one is discrete? For each of the three distributions :

- Determine the constant value c .
- Calculate the moments M_1 and M_2 .
- Calculate the variance and the standard deviation.
- Determine the cumulative distribution function $D_x(\xi)$.
- Evaluate the 1st quartiles, the medians and the 3rd quartiles.

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Exercises 4

Stochastic Simulation, Random Number Generation, Sample evaluation, Testing

4.1 Standard statistical estimation procedures:

- Generate a sample of 1000 n_{μ,σ^2} normally distributed random numbers with $\mu = 2.0$, $\sigma = 0.6$. Use MATLAB's `randn()` generator and an appropriate scaling and translation. What are the scaling and translation constants?
- Compute the sample mean value and standard deviation. Repeat this for different samples.
- Draw a histogram with a different number of boxes from $m = 1$ to $m = 1000$. What is an optimal value of m ? Why?
- Plot the empirical cumulative distribution function, i.e. plot the numbers $\frac{1}{1000}, \frac{2}{1000}, \dots, 1$ over the sorted sample values.
- Compute the median, first and third quartile of the sample by computing the 250th, 500th and 750th of the sorted values.

4.2 Take the sample from exercise 1 to test the data for a uniform distribution

- Assume that the data is uniformly $U_{[a,b]}$ distributed. Find a good estimate of a and b from the data.
- Scale and translate the data to the interval $[0, 1]$. What are the scaling and transformation constants? You are losing 2 degrees of freedom (for a and b) by this procedure.
- Draw a histogram of the $[0, 1]$ scaled data with $m = 10$ boxes. Compute the histogram values H_1, \dots, H_{10} and the sum of squares $SSQ = \frac{1}{100} \sum_{i=1}^{10} (H_i - 100)^2$.
- Carry out the χ^2 -test with 7 degrees of freedom (2 degrees are lost for a, b and one is lost because $H_{10} = 1000 - \sum_{i=1}^9 H_i$ is redundant). Take a confidence level of $\alpha = 90\%$ and $\alpha = 99\%$. At which level would the test be exactly passed, i.e. what is the p -value?

4.3 Take the sample from exercise 1 to test the data for a normal distribution.

- Assume that the data is normally n_{μ,σ^2} distributed. Find a good estimate of μ and σ from the data.
- Assuming a n_{μ,σ^2} distribution transform the data to a $U_{[0,1]}$ distribution by using the n_{μ,σ^2} cumulative probability density function. You are losing 2 degrees of freedom (for μ and σ) by this procedure.
- Draw a histogram of the $[0, 1]$ transformed data with $m = 10$ boxes. Compute the histogram values H_1, \dots, H_{10} and the sum of squares $SSQ = \frac{1}{100} \sum_{i=1}^{10} (H_i - 100)^2$.
- Carry out the χ^2 -test with 7 degrees of freedom (2 degrees are lost for μ, σ^2 and one is lost because $H_{10} = 1000 - \sum_{i=1}^9 H_i$ is redundant). Take a confidence level of $\alpha = 90\%$ and $\alpha = 99\%$. At which level would the test be exactly passed, i.e. what is the p -value?

- e) Compare the results with those of exercise 2. Which random number generator would you prefer to simulate data like that in the sample? Assume that you have tested a third distribution (e.g a beta distribution) and both normal distributions and the beta distribution pass the χ^2 -test on a 90% confidence level. Which one would you take? Why?

4.4 A sun collector supplies the electricity of a parking meter. If the energy supply is too low additional energy has to be fed in from the electricity net.

- a) The sunshine intensity X is assumed to be n_{μ, σ^2} normally distributed with $\mu = 2.0$, $\sigma = 0.6$. Generate a sample x_1, \dots, x_{1000} with this distribution.
- b) The power output of the collector is given by a saturating characteristics

$$y = y_{\max} \cdot \frac{x}{x + y_{\text{half}}}$$

with $y_{\max} = 2.0$, $y_{\text{half}} = 1.0$. Compute a sample of y from the sample of x .

- c) Draw a suitable histogram of the y sample. What is the reason for the unsymmetry of the histogram?
- d) If $y < y_{\min} = 1.5$ additional energy supply has to be purchased. The resulting cost function is:

$$z = \max(0, y_{\min} - y)$$

Compute z from y and draw another histogram. Which kind of distribution has z (continuous or discrete)?

4.5 Compare the experiment from exercise 3 with a second experiment using another type of collector: $y_{\max} = 1.8$, $y_{\text{half}} = 0.7$ and another data set x .

- a) Compute the mean electricity purchase with a 90% confidence interval. Compare the result with that of exercise 4. Which collector performs better?
- b) Carry out a t -test on a 90% confidence level to decide whether there is a significant difference between collector 1 and 2.
- c) Draw a figure where the electricity cost of collector 1 is plotted against that of collector 2. Use a dot for each value pair. How should this figure look like if one collector is far better than the other?
- d) Repeat the experiment by taking the *same* x dataset for both collectors. Then repeat steps a), b), c). What is the difference? Are you now able to decide which of the two collectors is the better one? Can you now tell what the best collector is?

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Exercises 1

Order analysis

1.1 Determine the order of the following numerical approximations with regard to Δx :

a) $f'(x) \approx \frac{f(x+\Delta x) - f(x)}{\Delta x}$ (differential quotient)

b) $f'(x) \approx \frac{f(x+\Delta x) - f(x-\Delta x)}{2\Delta x}$ (symmetrical differential quotient)

c) $f''(x) \approx \frac{f(x+\Delta x) - 2f(x) + f(x-\Delta x)}{\Delta x^2}$ (difference quotient for the 2nd derivative)

d) $\int_x^{x+\Delta x} f(\xi) d\xi \approx f(x) \cdot \Delta x$ (rectangular rule for numerical integration)

e) $\int_x^{x+\Delta x} f(\xi) d\xi \approx \frac{1}{2} (f(x+\Delta x) + f(x)) \cdot \Delta x$ (trapezoid rule for numerical integration)

Hint: Develop only the numerators of the fractions in 1, 2, 3.

1.2 The vectorial linear differential equation system

$$\dot{\mathbf{x}} = \mathbf{A} \cdot \mathbf{x}, \quad \mathbf{x}(0) = \mathbf{x}_0$$

and the scalar nonlinear differential equation system

$$\dot{x} = x^2, \quad x(0) = 1$$

are considered.

a) Develop a solution in terms of Taylor-series for each case:

$$x(\Delta t) = x(0) + \dot{x}(0) \cdot \Delta t + \frac{1}{2} \ddot{x}(0) \cdot \Delta t^2 + \dots + \frac{1}{n!} x^{(n)}(0) \cdot \Delta t^n + o(\Delta t^n)$$

b) Compare the results with the true solutions

$$\mathbf{x}(t) = \mathbf{x}_0 \cdot \exp(\mathbf{A} \cdot t)$$

respectively

$$x(t) = \frac{1}{1-t}$$

c) Compute one Runge-Kutta step with the methods from the 1st to 4th order for both examples. Compare the results with 1). How large is the error of the approximation for each case?

d) Exert the Adam-Bashfort method for both examples. Start with first order step and increase the order with every following step.

e) To determine the order of the approximation of the Adam-Bashfort method the order of the first multistep has to be calculated with regard to the *exact* solution:

$$\begin{aligned} x(0) &= \mathbf{x}_0 \\ x(\Delta t) &= \mathbf{x}_0 \cdot \exp(\mathbf{A} \cdot \Delta t) \\ &\vdots \\ x((n-1) \cdot \Delta t) &= \mathbf{x}_0 \cdot \exp((n-1) \cdot \mathbf{A} \cdot \Delta t) \end{aligned}$$

f) Substitute the Taylor Series of $\exp(k \cdot \mathbf{A} \cdot \Delta t)$ into the Adams-Bashfort formulas.

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Exercises 2

Integration Error, Step Size Control, Stationary Systems

2.1 One of the the most famous ecological model is the Lotka-Volterra model of a predator-prey interrelationship:

$$\begin{aligned}\dot{x} &= ax - cxy, & x(0) &= x_0 \\ \dot{y} &= -by + dxy, & y(0) &= y_0\end{aligned}$$

Here x is the number of prey individuals (e.g. insects) and y the number of predators (e.g. birds).

- Discuss the meaning of the model equations. What are the model assumptions? What are reasonable values of a, b, c, d ?
- Show that the invariant

$$a \cdot \ln y + b \cdot \ln x - cy - dx = \text{const}$$

always holds.

Hint: Derive the equation with respect to t . What ist the value of the constant?

- A SIMULINK implementation of the Lotka-Volterra model is supplied. For simplicity $a = b = c = d = 1$. Try different fixed step size solvers and discuss the error in the invariant by plotting the error over time. Compare with a niveau plot of the invariant.
 - Compute the total error of the invariant after the simulation time $T = 40$ for different Runge-Kutta methods and different step sizes. Determine the error order of each method from a log-log-plot.
 - Now switch to step size controlled Runge-Kutta methods. Explore the behavior of these methods for different absolute and relative error tolerances. Is the step size control related to the dynamics of the system?
 - Do the fixed tolerances really specify the total error after time T ?
- 2.2 Both the Lotka-Volterra system from Exercise 1 and the pendulum equations

$$\begin{aligned}\dot{\varphi} &= \omega \\ \dot{\omega} &= -\frac{d\omega}{ml^2} - \frac{g}{l} \sin \varphi\end{aligned}$$

are supplied as a SIMULINK implementation. For simplicity take $d = m = l = g = 1$.

- Explicitly determine all stationary states for both systems. Which of them are stable?
- Use the SIMULINK function `trim()` to determine the stationary states numerically. Change the initial values.
- Try to compute the stable stationary states with an ODE solver and a large step size.

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Exercises 3

Stationary and Stiff Systems

3.1 The pendulum equations from Exercise 2.2 M&S2 are regarded again.

- Try to find stationary states by the fixed point method. Try to find matrices that facilitate or speed up convergence. What are the eigenvalues in stationary state?
- Use Newton's method to find stationary states. How does the method behave?
- Use the gradient method to determine the stationary states.

3.2 A famous time-dependent equation is the Kepler equation

$$\varphi - e \cdot \sin \varphi = \omega \cdot t.$$

It describes the angular position $\varphi(t)$ of a planet on an elliptical orbit around the sun. Here ω is the mean angular velocity of the planet and $0 \leq e \leq 1$ is the eccentricity of the orbit. Assume that $\omega = 1$ and $e = 0.5$

- Find values of t for which the equation is easy to solve. Start with this solution.
- Use a successive Newton iteration to solve the equation for some step sizes Δt .
- Formulate the continuation ODE and use an ODE solver to solve this equation.
- Use the predictor-corrector method (Euler + Newton) instead.

3.3 The differential equation

$$\begin{aligned}\dot{x} &= -\lambda \cdot (x^2 + y^2 - 1) \cdot x - y & \lambda > 0 \\ \dot{y} &= -\lambda \cdot (x^2 + y^2 - 1) \cdot y + x\end{aligned}$$

describes a limit cycle, i.e. any trajectory in the phase plane converges towards the circle

$$x^2 + y^2 = 1$$

A SIMULINK model of this ODE is supplied.

- Show that the variable $z = x^2 + y^2$ fulfills the differential equation

$$\dot{z} = -2\lambda [z - 1] \cdot z.$$

How does z behave for $z \approx 1$? What does this mean for the original equation? What happens for $z = 1$?

- For $\lambda \gg 1$ the system becomes stiff. What is the "slow" and the "fast" process in the phase plane.
- Plot the solution in the xy -plane for $\lambda = 10^k$, $k = -1, 0, 1, 2, 3, 4, 5$. Use ODE45 for the solution. Can you see the stiffness in the phase plane? How does computation time evolve?
- For $\lambda = 1000$ take a fixed step size with ODE5. From what Δt on does the solution become unstable?
- for $\lambda = 10000$ use different step-size-controlled solvers. Which one is the best?

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Exercises 4

Stiff and Differential Algebraic Systems

4.1 Implicit Euler Scheme

- a) Formulate the implicit Euler method for the differential equation

$$\dot{x} = -x^2, \quad x(0) = 1$$

- b) How does the result behave for $\Delta t \rightarrow 0$ and $\Delta t \rightarrow \infty$?
c) What do the two branches of the solution mean? Why is only one branch taken for a numerical solution?
Hint: The true solution of the equation is: $x(t) = \frac{1}{x_0 \cdot t + 1}$
d) Formulate the Newton step for solving the implicit equation numerically.
e) Use the Newton method on the MATLAB command line for one time step Δt .
f) How large can Δt be taken until the Newton step diverges?

4.2 Gauss-Radau Schemes

- a) Formulate the Gauss-Radau scheme of order 2, 3, 4 for the ODE

$$\dot{x} = -x^2, \quad x(0) = 1.$$

- b) Give the first Newton step for solving the resulting nonlinear equation system.

4.3 Consider the differential algebraic equation

$$\begin{aligned} \dot{x} &= x - y, & x(0) &= 2 \\ x \cdot y &= 1 \end{aligned}$$

- a) Determine a consistent initial condition for y .
b) Transform the equation into an ODE by computing the time derivative of the algebraic equation.
c) Transform the equation into an ODE by solving the second equation and substitution into the first equation.

4.4 DAE index

Determine the differentiation index of the following DAE-systems and transform each system into an ODE system.

$$\begin{aligned} \dot{x}_2 &= -x_1 + f_1(t) \\ \dot{x}_3 &= -x_2 + f_2(t) \\ &\vdots \\ \dot{x}_n &= -x_{n-1} + f_{n-1}(t) \\ x_n &= f_n(t) \end{aligned}$$