

### Lösningar till tenta i matematisk modellering, MMG510, MVE160

Problems from the topics for which a student has got bonus points should not be solved at the examination.

#### 1. Lyapunov functions and stability of stationary points.

a) Formulate a criteria for asymptotically stable stationary point using a Lyapunov function that is not a strong Lyapunov function. **(2p)**

b) Consider the system of ODE: 
$$\begin{aligned}x' &= y \\ y' &= -y + y^3 - x^5\end{aligned}$$

Find a Lyapunov function  $V(x, y)$  for the given equation and show that the stationary point in the origin is asymptotically stable. **(2p)**

**Hint.** Use  $V(x, y)$  in the form  $V(x, y) = ax^6 + by^2$  and choose the parameters  $a, b$  so that  $V(x, y)$  would be a Lyapunov function

**Solution** A stationary point  $x_*$  is asymptotically stable if there is a neighborhood  $N$  of this point such that for any initial point  $x(o) \in N$  the corresponding trajectory  $x(t) \rightarrow x_*$  for  $t \rightarrow +\infty$ .

If there is a Lyapunov function such that  $V' \leq 0$  and is  $V' = 0$  on a set that does not include parts of trajectories except the stationary point in the origin then the stationary point in the origin is asymptotically stable. The Lyapunov function is not a strong Lyapunov function in this case but an additional analysis implies the asymptotic stability because trajectories leave the set where  $V' = 0$  and cannot stay there.

$$V'(x, y) = \frac{\partial V}{\partial x}y + \frac{\partial V}{\partial y}(-y + y^3 - x^5) = 6ax^5y - 2by^2 + 2by^4 - 2bx^5y$$

Taking  $6a = 2b$  and  $a = 1$  makes  $V'(x, y) = 6y^2(y^2 - 1) < 0$  for  $|y| < 1$  and  $y \neq 0$ .

For  $y = 0$   $y' = -x^5$  and therefore  $y' = 0$  only for  $x = 0$ . It implies that the origin is asymptotically stable.

#### 2. Limit cycles

Formulate the Poincare - Bendixsons sats and use it to show that the following system of ODE has a limit cycle in a "ring shaped" domain around the origin.

$$\begin{aligned}x' &= x^3 + y - x^3(x^2 + 4y^2); \\ y' &= -x + y^3 - y^3(x^2 + 4y^2)\end{aligned} \tag{4p}$$

**Hint.** Combine equations to get an expression for the derivative  $(x^2 + y^2)'$  and use its properties.

**Solution** Multiplying the equations by  $x$  and  $y$  and adding we get an expression for  $(r^2)'$  where  $r^2 = x^2 + y^2$

$$(r^2)' = 2(x^4 + y^4)(1 - x^2 - 4y^2)$$

We observe that for points inside the ellipse  $x^2 + 4y^2 = 1$  the distance  $r$  to the origin increases. For points outside the ellipse  $x^2 + 4y^2 = 1$  the distance  $r$  to the origin decreases. It means that for example the elliptic ring  $0.5 < x^2 + 4y^2 < 2$  is an invariant set for the system. On the other hand the only stationary point for this system is the origin, because outside the origin the only set where  $r' = 0$  is the ellipse  $x^2 + 4y^2 = 1$  but there are no stationary points on it because on this ellipse  $x' = y$  and  $y' = -x$ .

### 3. Asymptotic methods for ODE

a) Describe the idea of the direct asymptotic expansion of solutions to an ODE with a small parameter  $\epsilon \ll 1$ .

Consider the equation  $u'' + u = \epsilon (u')^2 u$ .

Write down equations for the terms of order zero and order one with respect to  $\epsilon \ll 1$  in a direct expansion for the solution  $u(t, \epsilon)$ . Explain what kind of terms in the expansion are called secular terms and why they appear. **(2p)**

b) Describe the idea of the Linstedt-Poincaré method or the averaging method. Write down equations for the terms of the zero and the first order for the given ODE. Clarify how the secular terms in the expansion can be eliminated. **(2p)**

( Find useful trigonometric formulas at the backside of this paper.)

**You do not need to solve equations completely here!**

#### Solution

a) The idea with direct expansion is to represent the solution as a part of power series in  $\epsilon$  for example up to the terms of order one:  $u = u_0 + \epsilon u_1 + O(\epsilon^2)$ . By putting this expression into the equation and after excluding terms of order higher than one we get:

$$u_0'' + u_0 + \epsilon(u_1'' + u_1) = \epsilon u_0 (u_0')^2 + O(\epsilon^2)$$

The equation must be satisfied for all  $\epsilon$ . It implies terms in front of different powers of  $\epsilon$  shall be zero,

$$\begin{aligned} \epsilon^0 : \quad & u_0'' + u_0 = 0, \\ \epsilon^1 : \quad & (u_1'' + u_1) = u_0 (u_0')^2. \end{aligned}$$

The first equation for  $u_0$  is solved explicitly and implies an equation for  $u_1$ :

$$u_0 = A \cos(t + \beta)$$

with arbitrary constants  $A$  and  $\beta$  is the general solution to the first equation.

We will use the variable  $\phi = t + \beta$  to make formulas shorter.

$$u_1'' + u_1 = A^3 (\sin(\phi))^2 \cos(\phi)$$

$$\sin^2(\phi) = (1 - \cos(2\phi))/2$$

$$(\sin(\phi))^2 \cos(\phi) = 1/2[(1 - \cos(2\phi)) \cos(\phi)] = 1/2[\cos(\phi) - 1/2(\cos(\phi) + \cos(3\phi))] = 1/4(\cos(\phi) - \cos(3\phi))$$

Therefore

$$u_1'' + u_1 = \frac{A^3}{4} (\cos(\phi) - \cos(3\phi))$$

The general solution to the last equation for  $u_1$  is a sum of the general solution to the homogeneous equation and two particular solutions with the right hand sides  $\frac{A^3}{4} \cos(\phi)$  and  $-\frac{A^3}{4} \cos(3\phi)$ : The frequency of the first right hand side is the same as one in the equation. This situation is called resonance and it makes that the particular solution shall be taken as  $C_1 \phi \cos(\phi)$  with some constant  $C_1$ . Such terms, increasing in absolute value with  $\phi \rightarrow \infty$  are called secular terms and do not satisfy our hypothesis on the structure of solution where  $\epsilon u_1$  shall be of order  $\epsilon$ . The frequency of the second right hand side is not present in the equation, therefore corresponding particular solution can be taken in the same form as the right hand side:  $C_2 \cos(3\phi)$  with some constant  $C_2$ . Therefore the term of the first order in the direct expansion is

$$u_1(t) = C_0 \cos(t + \beta) + C_1 t \cos(t + \beta) + C_2 \sin(3(t + \beta))$$

Constants here can be defined by putting this expression into the equation and by using possible initial conditions.

b) The idea of the Linstedt-Poincare method is to introduce a more complicated dependence of solution on the parameter  $\epsilon$ . Namely we introduce a new timescale  $\tau = \omega(\epsilon)t$  depending in  $\epsilon$  and make the corresponding change of variables in the equation.

$$\omega^2 u'' + u = \epsilon u (u')^2$$

Then we expand both the solution  $u$  and the frequency  $\omega$  in powers of  $\epsilon$  up to the first order:

$$u = u_0 + \epsilon u_1 + \dots$$

$$\omega = 1 + \epsilon \omega_1 + \dots$$

Using these expressions we come to equations for  $u_0$  and  $u_1$ :

$$\epsilon^0 : \quad u_0'' + u_0 = 0,$$

$$\epsilon^1 : \quad (u_1'' + u_1) = u_0 (u_0')^2 + 2\omega_1 u_0''.$$

where a new term appears in the second equation comparing with the case of direct expansion.

General solution to the equation for  $u_0$  is

$$u_0 = A \cos(\tau + \beta)$$

The equation for  $u_1$  transforms to:

$$u_1'' + u_1 = A^3 \cos(\tau + \beta) (\sin(\tau + \beta))^2 - 2A\omega_1 \cos(\tau + \beta).$$

Using the same trigonometric formulas as in the case of direct expansion we come to the equation

$$u_1'' + u_1 = \frac{A^3}{4} (\cos(\tau + \beta) - \cos(3(\tau + \beta))) - 2A\omega_1 \cos(\tau + \beta).$$

Choosing the free constant  $\omega_1$  as  $\omega_1 = A^2/8$  we get an equation that has no resonant terms in the right hand side and therefore no secular terms in the solution.

b) The idea of the averaging method is to represent the solution to the nonlinear equation

$$u'' + u = \epsilon (u')^2 u.$$

in the form  $u = A(t) \cos(t + \beta(t))$  similar to solution of the linear equation with  $\epsilon = 0$ , but with the amplitude  $A$  and the phase  $\beta$  depending on time  $t$ . We require also that  $u' = -A(t) \sin(t + \beta(t))$  as the solution to the linear equation. We can do it because we have now two unknown functions  $A(t)$  and  $\beta(t)$  instead of one in the original formulation. We use the expressions

$$\begin{aligned} u &= A(t) \cos(t + \beta(t)) \\ u' &= -A(t) \sin(t + \beta(t)) \end{aligned}$$

and the equation

$$u'' + u = \epsilon (u')^2 u.$$

to get differential equations for new unknown functions  $A(t)$  and  $\beta(t)$ . After differentiating  $A(t) \cos(t + \beta(t))$  with respect to time two times we get that

$$u' = -A \sin(t + \beta) + A' \cos(t + \beta) - A\beta' \sin(t + \beta)$$

and

$$u'' = -A \cos(t + \beta) - A' \sin(t + \beta) - A\beta' \cos(t + \beta)$$

that together with the postulated expression for  $u'$  above and with the equation implies:

$$A' \cos(t + \beta) - A\beta' \sin(t + \beta) = 0$$

$$A' \sin(t + \beta) + A\beta' \cos(t + \beta) = -\epsilon A^3 \cos(t + \beta)(\sin(t + \beta))^2$$

These equations can be made simpler by multiplying the first by  $\cos(t + \beta)$  and the second by  $\sin(t + \beta)$  and adding:

$$A' = \epsilon A^3 \sin(t + \beta)^3 \cos(t + \beta)$$

$$\beta' = \epsilon A^2 \sin(t + \beta)^2 \cos(t + \beta)^2$$

Therefore  $A$  and  $\beta$  change slowly with time. It makes that derivatives of  $A$  and  $\beta$  are approximately equal to the mean values of the right hand sides of the last equations over the interval  $[0, 2\pi]$ . To compute these averages we transform the expressions in the right hand side to linear combinations of trigonometric functions.

$$\sin(\phi)^3 \cos(\phi) = (1 - \cos(2\phi))/2 \sin(\phi) \cos(\phi) = (1 - \cos(2\phi)) \sin(2\phi)/4 = \sin(2\phi)/4 - \sin(4\phi)/8.$$

It shows that the first right hand side has the average zero over the interval  $[0, 2\pi]$  and approximately

$$A' = 0$$

$\sin(\phi)^2 \cos(\phi)^2 = 1/4 \sin(2\phi)^2 = 1/8(1 - \cos(4\phi))$  It implies that the approximate relation

$$\beta' = \epsilon A^2 1/8$$

Therefore  $A = A_0 = \text{const}$  and  $\beta(t) = \epsilon A_0^2 1/8 t + \beta_0$  and the solution to the original problem has the approximate form

$$u(t) = A_0 \cos((1 + \epsilon A_0^2 1/8)t + \beta_0)$$

that coincides with the result by the Linstedt-Poincare method.

#### 4. Chemical reactions and the Gillespie method

Consider the following reactions:  $X+X \xrightleftharpoons[c_2]{c_1} W$ ,  $W+X \xrightleftharpoons[c_4]{c_3} P$  where  $c_i dt$  is the probability that during time  $dt$  the reaction with index  $i$  will take place.  $i = 1, 2, 3, 4$ .

- Write differential equations for the number of particles for these reactions. **(2p)**
- Give formulas for the Gillespie algorithm that would model stochastically these reactions by the Gillespie method. **(2p)**

#### Solution

a) Observe that the reaction  $c_1$  takes out of the game **two**  $X$  particles and reaction 2 adds two  $X$  particles. It makes that we multiply by 2 the terms with  $c_1 X(X - 1)/2$  and with  $c_2 W$  in the balance equation for  $X$ .

$$X' = -2c_1 X(X - 1)/2 + 2c_2 W - c_3 W X + c_4 P$$

$$W' = c_1 X(X - 1)/2 - c_2 W - c_3 W X + c_4 P$$

$$P' = c_3 W X - c_4 P$$

b) The Gillespie algorithm for this particular system is the following:

0) Put initial values of the numbers of particles of each type  $X, W, Q, P$ . and set time variable  $t = 0$ .

1) compute weights in the method  $h_1 = X(X - 1)/2$ ,  $h_2 = W$ ,  $h_3 = W X$ ,  $h_4 = P$ .

$$a = h_1 c_1 + h_2 c_2 + h_3 c_3 + h_4 c_4$$

2) Generate two random numbers  $r$  and  $p$  uniformly distributed on a unit interval. Calculate the random “waiting time”  $\tau$  before the next reaction after the formula  $\tau = 1/a \ln(1/r)$ . Calculate the random number  $k$  of the reaction that will take place during short time after we choose the number  $k$  such that

$$\sum_{i=1}^k h_i c_i \leq pa \leq \sum_{i=1}^{k+1} h_i c_i$$

3) Perform changes due to the chosen reaction

$$k = 1: X \rightarrow X - 2, W \rightarrow W + 1;$$

$$k = 2: X \rightarrow X + 2, W \rightarrow W - 1;$$

$$k = 3: X \rightarrow X - 1, W \rightarrow W - 1, P \rightarrow P + 1;$$

$$k = 4: X \rightarrow X + 1, W \rightarrow W + 1, P \rightarrow P - 1;$$

Max. 16 points;

For GU: **VG**: 13 points; **G**: 8 points;

For Chalmers: **5**: 14 points; **4**: 11 points; **3**: 8 points;