MATEMATIK | Datum: 2010-06-01 | Tid: 8:30
GU, Chalmers | Hjälpmedel: Beta
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Lösningar till tenta i matematisk modellering, MMG510, MVE160

1. **Linear systems.**

Consider the following ODE:

$$\frac{d\overrightarrow{r}(t)}{dt} = A\overrightarrow{r}(t),\ \overrightarrow{r}(t) = \begin{bmatrix} r_1(t) \\ r_2(t) \end{bmatrix} \text{ with } A = \begin{bmatrix} -1 & -4 \\ 1 & -1 \end{bmatrix},$$

Find the evolution operator for this system. **(2p)**

Find which type has the stationary point at the origin and give a sketch of the phase portrait with marked directions of trajectories. **(2p)**

Solution

The evolution operator is $\varphi_t(\overrightarrow{r}(0)) = \exp(t\,A)\overrightarrow{r}(0)$ where $\exp(t\,A) = \sum_{k=0}^{+\infty} \frac{A^k t^k}{k!}$. Solution reduces to a reasonable calculation of $\exp(t\,A)$. We start from computation of eigenvalues to the matrix A.

$\begin{bmatrix} -1 & -4 \\ 1 & -1 \end{bmatrix}$, eigenvalues: $\lambda_1 = -1-2i$, $\lambda_2 = -1+2i$.

In the case with complex eigenvalues it is easier to use the method by Sylvester to compute $\exp(t\,A)$.

Define matrices Q_1 and Q_2:

$$Q_1 = \frac{A-\lambda_2 I}{\lambda_1-\lambda_2} = \frac{1}{(-1-2i)-(-1+2i)}\left(\begin{bmatrix} -1 & -4 \\ 1 & -1 \end{bmatrix} - \begin{bmatrix} -1+2i & 0 \\ 0 & -1+2i \end{bmatrix}\right) = \frac{1}{4}i\begin{bmatrix} -2i & -4 \\ 1 & -2i \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & -i \\ \frac{1}{4}i & \frac{1}{2} \end{bmatrix},$$

$$Q_2 = \frac{A-\lambda_1 I}{\lambda_2-\lambda_1} = \frac{1}{(-1+2i)-(-1-2i)}\left(\begin{bmatrix} -1 & -4 \\ 1 & -1 \end{bmatrix} - \begin{bmatrix} -1-2i & 0 \\ 0 & -1-2i \end{bmatrix}\right) = -\frac{1}{4}i\begin{bmatrix} 2i & -4 \\ 1 & 2i \end{bmatrix} = \begin{bmatrix} \frac{1}{2} & i \\ -\frac{1}{4}i & \frac{1}{2} \end{bmatrix}$$

with properties: $Q_1Q_2 = 0$; $Q_1^2 = Q_1$; $Q_2^2 = Q_2$;

$A = \lambda_1 Q_1 + \lambda_2 Q_2$;

The evolution operator is $\varphi_t(\overrightarrow{r}(0)) = \exp(t\,A)\overrightarrow{r}(0)$ where

$$\exp(t\,A) = \sum_k \frac{A^k t^k}{k!} = \sum_k \frac{(\lambda_1 Q_1 + \lambda_2 Q_2)^k t^k}{k!} = \sum_k \frac{(\lambda_1)^k t^k}{k!} Q_1 + \sum_k \frac{(\lambda_2)^k t^k}{k!} Q_2 = e^{t\lambda_1} Q_1 + e^{t\lambda_2} Q_2 = e^{t(-1-2i)} Q_1 + e^{t(-1+2i)} Q_2 =$$

$$e^{t(-1-2i)}\begin{bmatrix} \frac{1}{2} & -i \\ \frac{1}{4}i & \frac{1}{2} \end{bmatrix} + e^{t(-1+2i)}\begin{bmatrix} \frac{1}{2} & i \\ -\frac{1}{4}i & \frac{1}{2} \end{bmatrix} = \begin{bmatrix} \frac{1}{2}e^{-(1+2i)t} + \frac{1}{2}e^{-(1-2i)t} & -ie^{-(1+2i)t} + ie^{-(1-2i)t} \\ \frac{1}{4}ie^{-(1+2i)t} - \frac{1}{4}ie^{-(1-2i)t} & \frac{1}{2}e^{-(1+2i)t} + \frac{1}{2}e^{-(1-2i)t} \end{bmatrix} =$$

$$e^{-t}\begin{bmatrix} \frac{1}{2}e^{-(2i)t} + \frac{1}{2}e^{-(-2i)t} & -ie^{-(2i)t} + ie^{-(-2i)t} \\ \frac{1}{4}ie^{-(2i)t} - \frac{1}{4}ie^{-(-2i)t} & \frac{1}{2}e^{-(2i)t} + \frac{1}{2}e^{-(-2i)t} \end{bmatrix} = e^{-t}\begin{bmatrix} \cos 2t & -2\sin 2t \\ \frac{1}{2}\sin 2t & \cos 2t \end{bmatrix}$$

The fixed point in the origin is the stable focus because the real part of the eigenvalues is negative. Spirals go counterclockwise around the origin that is easy to see from the formula for the evolution operator by inspecting solutions for simple initial vectors $\overrightarrow{r}(0) = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ or $\overrightarrow{r}(0) = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$.

2. **Ljapunovs functions and stability of stationary points.**

   Consider the system of equations: $\begin{cases} x' = -x + 2xy^2 \\ y' = -(1-x^2)y^3 \end{cases}$

   Show that the origin is an stable fixed point. **(4p)**

   Solution

   $V(x,y) = x^2 + y^2$

   $V' = 2x\left(-x + 2xy^2\right) + 2y\left(-(1-x^2)y^3\right) = -2x^2 + 4x^2y^2 - 2y^4\left(1-x^2\right) =$
   $-2x^2\left(1-2y^2\right) - 2y^4\left(1-x^2\right)$

   We see that $V' < 0$ for $|x| < 1$ and $|y| < \sqrt{1/2}$

3. **Periodic solutions to ODE.**

   Use Poincare - Bendixsons theory to show that the system of equations

   $$\begin{cases} x' = x - 2y - x\left(x^2 + y^2\right) \\ y' = 2x + y - y\left(x^2 + y^2\right) \end{cases}$$

   has at least one periodic solution. **(4p)**

   Solution

   $r^2 = \left(x^2 + y^2\right)$

   $0.5\left(r^2\right)' = \left(x^2 + y^2\right)\left(1 - \left(x^2 + y^2\right)\right) = r^2\left(1 - r^2\right)$

   $r' = r\left(1 - r^2\right) > 0, \quad r < 1$

   $r' = r\left(1 - r^2\right) < 0, \quad r > 1$

   the only fixpoint is the origin.$r' = 0$ if $r = 0$ or $r = 1$. In the second case $x' = -2y$, $y' = 2x$ therefore the only fixpoint is in the origin $x = y = 0$. Therefore the ring $0.5 < r < 2$ is an invariant set without fixpoints and must include at least one periodic trajectory.

4. **Hopf bifurcation.**

   Explain the notion Hopf bifurcation.

   Show that the system $\begin{cases} x' = \mu x + y \\ y' = -x - y^3 \end{cases}$

   has a Hopf bifurcation at $\mu = 0$. **(4p)**

   Solution

   The matrix $\begin{bmatrix} \mu & 1 \\ -1 & 0 \end{bmatrix}$ of the linearised system has eigenvalues: $\lambda_1 = \frac{1}{2}\mu - \frac{1}{2}\sqrt{\mu^2 - 4}, \lambda_2 = \frac{1}{2}\mu + \frac{1}{2}\sqrt{\mu^2 - 4}$.

   For $|\mu| < 2$ $\operatorname{Re}\lambda_{1,2}(\mu) = \frac{1}{2}\mu$. $\left.\frac{d}{d\mu}\lambda_{1,2}(\mu)\right|_{\mu=0} = 1/2 > 0$.

   The asymptotic stability of the fixed point in the origin for $\mu = 0$ is necessary to investigate.

   $$\begin{cases} x' = y \\ y' = -x - y^3 \end{cases}$$

   We try the function $V(x,y) = x^2 + y^2$ to check the stability.

$V' = 2xy - 2yx - 2y^4 = -2y^4 \le 0$. It implies the neutral stability of the fixed point. $V' = 0$ on the line $y = 0$.

This line does not include whole trajectories exept the origin because the velocities of the system cross the line $y = 0$ in all points exept the origin: $y' = x \neq 0$ for all points exept the origin.

5. **Chemical reactions by Gillespies method**

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

a) Write down differential equations for the number of particles for these reactions. **(2p)**

b) Give formulas for the algorithm that shell model these reactions stochastically by Gillespies method. **(2p)**

Solution

Equations for the numbers of particles are:

$X' = -c_1 X \frac{1}{2} Z^2 + c_2 W$

$Z' = -c_1 X Z^2 + c_2 2W$

$W' = c_1 X \frac{1}{2} Z^2 - c_2 W - c_3 W Z + c_4 P Z$

$P' = -c_4 P Z + c_3 W Z$

b) **Gillespies method.**

$P(\tau, \mu) d\tau$ is the probability that the reaction of type μ will take place during the time interval $d\tau$ after the time τ when no reactions were observed.

$P(\tau, \mu) = P_0(\tau) h_\mu c_\mu d\tau$.

Here $P_0(\tau)$ is the probability that no reactions will be observed during time τ.

$h_\mu c_\mu d\tau$ is the probability that only the reaction μ will be observed during the time $d\tau$.

h_μ is the number of combinations of particles necessary for the reaction μ. For reaction 1 in the example $h_1 = X \frac{1}{2} Z^2$, for reaction 2 $h_2 = W$, for reaction 3 $h_3 = WZ$, for reaction 4 $h_4 = PZ$.

For $P_0(\tau) = exp(-a\tau)$ with $a = \sum_{\mu=1}^{4} h_\mu c_\mu$.

Algorith to model reactions:

0) initialize variables X, Z, W, P for time $t = 0$.

1) Compute h_i, a for actual values of variables.

2) Generate two random numbers r and p uniformly distributed over the interval $(0, 1)$.

Random time τ before the next reaction is $\tau = 1/a \ln(1/r)$.

Choose the next reaction μ so that $\sum_{i=1}^{\mu-1} h_i c_i \le p\,a \le \sum_{i=1}^{\mu} h_i c_i$.

3) Add τ to the time variable t.Change the numbers of particles after the chosen reaction:

$\mu = 1 \quad \rightarrow X = X - 1,\ Z = Z - 2,\ W = W + 1.$

$\mu = 2 \quad \rightarrow X = X + 1,\ Z = Z + 2,\ W = W - 1.$

$\mu = 3 \quad \rightarrow P = P + 1,\ W = W - 1.$

$\mu = 4 \quad \rightarrow P = P - 1,\ W = W + 1.$

3) If time is larger then the maximal time we are interested in - finish computation, otherwise go to the step 1.

Max. 20 points;

For GU: **VG:** 15 points; **G:** 10 points. For Chalmers: **5:** 17 points; **4:** 14 points; **3**: 10 points;
Total points for the course will be an average of points for the project (60%) and for this exam (40%).