MATEMATIK	Datum: 2010-05-25	Tid: 8:30
GU, Chalmers	Hjälpmedel: Beta	
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Tenta i matematisk modellering, MMG510, MVE160

1. **Linear systems.**

Consider the following ODE:

$\dfrac{d\overrightarrow{r}(t)}{dt} = A\overrightarrow{r}(t),\ \overrightarrow{r}(t) = \begin{bmatrix} r_1(t) \\ r_2(t) \end{bmatrix}$ with $A = \begin{bmatrix} 1 & -4 \\ -2 & 1 \end{bmatrix}$,

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

Find which type has the stationary point at the origin and give a possibly exact sketch of the phase portrait. **(2p)**

Solution

Eigenvectors and eigen values of the matrix $\begin{bmatrix} 1 & -4 \\ -2 & 1 \end{bmatrix}$ are: $\left\{ \begin{bmatrix} \sqrt{2} \\ 1 \end{bmatrix} \right\} \leftrightarrow \lambda_1 = 1 - 2\sqrt{2} < 0$, $\left\{ \begin{bmatrix} -\sqrt{2} \\ 1 \end{bmatrix} \right\} \leftrightarrow \lambda_1 = 2\sqrt{2} + 1 > 0$

The change of variables $\overrightarrow{r} = \begin{bmatrix} \sqrt{2} & -\sqrt{2} \\ 1 & 1 \end{bmatrix} \overrightarrow{y}$ reduces the system to two independent equations:$y_1' = \left(1 - 2\sqrt{2}\right) y_1$ and $y_2' = \left(1 + 2\sqrt{2}\right) y_2$.

The solution can be expressed in the form: $\overrightarrow{r}(t) = M^{-1}\exp(tD)M\ \overrightarrow{r}(0)$, where

$M = \begin{bmatrix} \sqrt{2} & -\sqrt{2} \\ 1 & 1 \end{bmatrix}$, $M^{-1} = \begin{bmatrix} \frac{1}{4}\sqrt{2} & \frac{1}{2} \\ -\frac{1}{4}\sqrt{2} & \frac{1}{2} \end{bmatrix}$, $D = \begin{bmatrix} 1 - 2\sqrt{2} & 0 \\ 0 & 1 + 2\sqrt{2} \end{bmatrix}$,

$\exp(tD) = \begin{bmatrix} \exp\left(t(1 - 2\sqrt{2})\right) & 0 \\ 0 & \exp\left(t\left(1 + 2\sqrt{2}\right)\right) \end{bmatrix}$

It is in fact the evolution operator :

$$\varphi_t(\overrightarrow{r}(0)) = M^{-1}\exp(tD)M = \begin{bmatrix} \frac{1}{4}\sqrt{2} & \frac{1}{2} \\ -\frac{1}{4}\sqrt{2} & \frac{1}{2} \end{bmatrix} \begin{bmatrix} \exp\left(t(1 - 2\sqrt{2})\right) & 0 \\ 0 & \exp\left(t\left(1 + 2\sqrt{2}\right)\right) \end{bmatrix} \begin{bmatrix} \sqrt{2} & -\sqrt{2} \\ 1 & 1 \end{bmatrix} \overrightarrow{r}(0)$$

$$\begin{bmatrix} \frac{1}{2}e^{t\left(-2\sqrt{2}+1\right)} + \frac{1}{2}e^{t\left(2\sqrt{2}+1\right)} & -\frac{1}{2}e^{t\left(-2\sqrt{2}+1\right)} + \frac{1}{2}e^{t\left(2\sqrt{2}+1\right)} \\ -\frac{1}{2}e^{t\left(-2\sqrt{2}+1\right)} + \frac{1}{2}e^{t\left(2\sqrt{2}+1\right)} & \frac{1}{2}e^{t\left(-2\sqrt{2}+1\right)} + \frac{1}{2}e^{t\left(2\sqrt{2}+1\right)} \end{bmatrix}$$

$$\varphi_t(\overrightarrow{r}(0)) = e^{t\left(-2\sqrt{2}+1\right)} \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix} \overrightarrow{r}(0) + e^{t\left(2\sqrt{2}+1\right)} \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} \overrightarrow{r}(0)$$

An alternative solution uses the method by Sylvester.

One can also use a simpler approach by Sylvester. Define matrices Q_1 and Q_2:

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

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

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

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

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

The stationary point at the origin is a saddle point and trajectories are hyperbolas with asymptotic lines parallel to

eigenvectors - $\begin{bmatrix} \sqrt{2} \\ 1 \end{bmatrix}$ and $\begin{bmatrix} -\sqrt{2} \\ 1 \end{bmatrix}$. Trajectories tend to the line parallel to $\begin{bmatrix} -\sqrt{2} \\ 1 \end{bmatrix}$ when time goes to $+\infty$.

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

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

   Investigate stability of the fixed point in the origin. **(4p)**

   Solution. $V(x,y) = x^2 + y^2$ is positive definite. We check the sign of $V' = 2x\left(-x + 2xy^2\right) - 2y\left((1 - x^2)y^3\right) = -2x^2\left(1 - 2y^2\right) - 2(1 - x^2)y^4$

   Therefore $V' \leq 0$ for $(x,y) \neq (0,0)$, $|x| < 1$, and $|y| < \sqrt{1/2}$ and V is a strong Ljapunov function in the rectangle: $|x| < 1$, $|y| < \sqrt{1/2}$.

   It implies that the origin is an asymptotically stable fixed point.

3. **Periodic solutions to ODE.**

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

   $$\begin{cases} x' = \sin(y) + x(y^2 + 1) \\ y' = (x - 1)^2 + x^2 y \end{cases}$$

   does not have periodic solutions. **(4p)**

   Solution. For right hand side $\overrightarrow{f}$ we have $div(\overrightarrow{f}) = (y^2 + 1) + x^2 > 0$. It implies that the system cannot have a periodic solution.

4. **Hopf bifurcation.**

   Explain the notion Hopf bifurcation.

   Show that the system $\begin{cases} x' = \mu x + y - x^3 \cos(x) \\ y' = -x + \mu^2 y \end{cases}$

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

   Solution. The linearization around the origine gives the matrix:

   $\begin{bmatrix} \mu & 1 \\ -1 & \mu^2 \end{bmatrix}$, with eigenvalues: $\lambda_{1,2}(\mu) = \frac{1}{2}\mu + \frac{1}{2}\mu^2 \pm \frac{1}{2}\sqrt{\mu^2 - 2\mu^3 + \mu^4 - 4}$. It implies that $\lambda_{1,2}(0) = \pm i$, $\operatorname{Re}\lambda_{1,2}(0) = 0$ and $\frac{d}{d\mu}\left(\operatorname{Re}\lambda_{1,2}(\mu)\right)\Big|_{\mu=0} = \frac{1}{2} + \mu\Big|_{\mu=0} > 0$.

   Consider the system for $\mu = 0$:

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

   The function $V(x,y) = x^2 + y^2$ has the derivative along trajectories: $V'(x,y) = 2x\left(y - x^3\cos(x)\right) + 2y\,(-x) = -2x^4\cos(x) \leq 0$ for $|x| < \pi/2$ and $x \neq 0$

   Therefore V - is a weak Liapunov function. On the other hand for $x = 0$ we have $x' = y \neq 0$ for $y \neq 0$. It means that the line $x = 0$ (y - axis) does not include whole trajectories exept the origin. All trajectories coming to the y-axis outside the origin leave it immediately. It implies that the origin is an asymptotically stable fixpoint. Therefore Hopf bifurcation takes place at $\mu = 0$. When μ changes from negative values to positive values the stable focus becomes unstable focus surrounded by a limit cycle, that increases with μ.

5. **Chemical reactions by Gillespies method**

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

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:

$X' = -c_1XZ + c_2W$

$Z' = -c_1XZ + c_2W - c_3WZ + c_4P$

$W' = c_1XZ - c_2W - c_3WZ + c_4P$

$P' = -c_4P + c_3WZ$

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 $h_1 = X \cdot Z$, for reaction 2 $h_2 = W$, for reaction 3 $h_3 = WZ$, for reaction 4 $h_4 = P$.

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 $\sum_{i=1}^{\mu-1} h_i c_i \leq p\,a \leq \sum_{i}^{\mu} h_i c_i$.

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

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

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

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

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

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%).