MATEMATIK	Datum: 2011-05-26	Tid: 8:30
GU, Chalmers	Hjälpmedel: Inga	
A.Heintz	Telefonvakt:	Tel.: 0762-721860.

Lösningar till tenta i matematisk modellering, MMG510, MVE160

1. **Linear systems**

   Consider the following ODE:

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

   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)**

   Eigenvectors and eigenvalues to A: $\left\{\begin{bmatrix} 1 \\ 1 \end{bmatrix}\right\} \leftrightarrow \lambda_1 = -1$; $\left\{\begin{bmatrix} -1 \\ 1 \end{bmatrix}\right\} \leftrightarrow \lambda_2 = 3$.

   One can use the change of variables $x = My$ with matrix M having eigenvectors as columns: $M = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}$ and inverse matrix $M^{-1} = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}^{-1} = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix}$ to compute the evolution operator:

   $\exp(t\,A) = M\exp(D)M^{-1} = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} \exp(-t) & 0 \\ 0 & \exp(3t) \end{bmatrix}\begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix} =$

   $\begin{bmatrix} \frac{1}{2}e^{-t} + \frac{1}{2}e^{3t} & \frac{1}{2}e^{-t} - \frac{1}{2}e^{3t} \\ \frac{1}{2}e^{-t} - \frac{1}{2}e^{3t} & \frac{1}{2}e^{-t} + \frac{1}{2}e^{3t} \end{bmatrix} = e^{-t}\begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} + e^{3t}\begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix}$.

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

   $Q_1 = \frac{A-\lambda_2 I}{\lambda_1-\lambda_2} = \frac{1}{-1-3}\left(\begin{bmatrix} 1 & -2 \\ -2 & 1 \end{bmatrix} - \begin{bmatrix} 3 & 0 \\ 0 & 3 \end{bmatrix}\right) = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix}$,

   $Q_2 = \frac{A-\lambda_1 I}{\lambda_2-\lambda_1} = \frac{1}{3+1}\left(\begin{bmatrix} 1 & -2 \\ -2 & 1 \end{bmatrix} - \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}\right) = \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix}$

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

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

   $\exp(t\,A) = \sum_k \frac{A^k t^k}{k!} = \sum_k \frac{(\lambda_1 Q_1 + \lambda_2 Q_2)^k\, t^k}{k!} = \sum_k \frac{(\lambda_1)^k\, t^k}{k!} Q_1 + \sum_k \frac{(\lambda_2)^k\, t^k}{k!} Q_2 = e^{-t}Q_1 + e^{3t}Q_2$.

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

   eigenvectors - $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ and $\begin{bmatrix} -1 \\ 1 \end{bmatrix}$ that have angle $\pi/4$ with x- axis. Trajectories tend to the line parallel to $\begin{bmatrix} -1 \\ 1 \end{bmatrix}$ when time goes to $+\infty$.

2. **Lyapunovs functions and stability of stationary points.** Formulate the criterion for asymptotic stability of a stationary point of an ODE using only a weak Lyapunov function**.**

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

   Show that $V(x, y) = x^2 + y^2$ is a weak Lyapunov function and decide if the stationary point at the origin is asymptotically stable. **(4p)**

$\frac{d}{dt}(V) = \nabla V \cdot \begin{bmatrix} -x+y^2 \\ -xy-x^2 \end{bmatrix} = \begin{bmatrix} 2x \\ 2y \end{bmatrix} \cdot \begin{bmatrix} -x+y^2 \\ -xy-x^2 \end{bmatrix} = 2x\left(-x+y^2\right) + 2y\left(-xy-x^2\right) =$
$-2x^2 - 2x^2y = -2x^2(1+y)$;

For $|y| < 1$ $\frac{d}{dt}(V) \leq 0$. It implies that the origin is a stable stationary point. On the line $x = 0$ $\frac{d}{dt}(V) = 0$ so V is only a weak Lyapunovs funktion. But we observe that on the line $x = 0$ the velocity is not zero $-x + y^2 \neq 0$ exept the stationary point itself. It implies that the origin is an asymptoticaly stable stationary point.

3. **Periodical solutions to ODE.**

Formulate the Poincare - Bendixson theorem. Use Poincare - Bendixsons theorem to show that the system of equations.

$$\begin{cases} x' = -y + x(1 - x^2 - y^4) \\ y' = x + y(1 - x^2 - y^4) \end{cases}$$

has at least one periodical solution.

Hint. Use polar coordinates and write down an equation for r. **(4p)**

If an ODE in plane has a compact positively invariant set U without stationary points, there must be at least one periodical solution in U.

Multipluing the first equation by x and the second by y and adding them we get an equation for $r = \sqrt{x^2 + y^2}$.

$xx' + yy' = 0.5\left(r^2\right)' = x\left[-y + x(1 - x^2 - y^4)\right] + y\left[x + y(1 - x^2 - y^4)\right] = \left(x^2 + y^2\right)(1 - x^2 - y^4)$

We observe that $\left(r^2\right)' > 0$ for $r \leq \sqrt{0.5}$ and $\left(r^2\right)' < 0$ for $r \leq \sqrt{2}$. It implies that the ring $\sqrt{0.5} \leq r \leq \sqrt{2}$ is a positively invariant set for the system. It is easy to see that the origin is the only stationary point, because for a stationary (x, y)point outside the origin $(1 - x^2 - y^4)$. Therefore there must be at least one periodic solution in the ring $\sqrt{0.5} \leq r \leq \sqrt{2}$.

4. **Hopf bifurcation.**

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

has a Hopf bifurcation for $\mu = 0$ and explain what does it mean. **(4p)**

The linearised system has matrix $\begin{bmatrix} 0 & 1 \\ -1 & \mu \end{bmatrix}$, with complex eigenvalues $\lambda_{1,2} = \frac{1}{2}\mu \pm \frac{1}{2}\sqrt{\mu^2 - 4}$.

For $-2 < \mu < 0$ the system has a stable stationary point in the origin. For $0 < \mu < 2$ the system has an unstable stationary point in the origin. When $\mu = 0$ one cannot use linearization to make conclusions on stability. We try to use $V(x, y) = x^2 + y^2$ as Lyapunovs function for the system

$\begin{cases} x' = y - x^3 \\ y' = -x - x^2 y \end{cases}$. $\frac{d}{dt}(V) = \nabla V \cdot \begin{bmatrix} y - x^3 \\ -x - x^2 y \end{bmatrix} = -x^4 - x^2y^2 = -x^2\left(x^2 + y^2\right) \leq 0$

for $x = 0$ we observe that $x' = y \neq 0$ outside the origin. It implies that the trajectory goes out for the line $x = 0$

everywhere exept the origin and the origin is an asymptotically stable stationary point.

5. **Chemical reactions by Gillespies method**

Consider the following reactions: $X + Z \underset{c_2}{\overset{c_1}{\rightleftarrows}} W, \qquad W + W \underset{c_4}{\overset{c_3}{\rightleftarrows}} P$ 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)**

Equations for the numbers of particles are:

$X' = -c_1XZ + c_2W$

$Z' = -c_1XZ + c_2W$

$W' = c_1XZ - c_2W - c_3W^2 + 2c_4P$

$P' = -c_4P + c_3\frac{1}{2}W^2$

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 reaktion 1 in the example det $h_1 = X \cdot Z$, för reaktion 2 är det $h_2 = W$, för reaktion 3 är det $h_3 = 0.5W(W-1)$.

$P_0(\tau) = exp(-a\tau)$ with $a = \sum_{\mu=1}^{3} h_\mu c_\mu$.

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:

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

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

$\mu = 3 \quad \to P = P + 1,\ W = W - 2.$

$\mu = 4 \quad \to P = P - 1,\ W = W + 2$

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%).