

Tenta i matematisk modellering, MMG510, MVE160

1. Linear systems.

Consider the following ODE:

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

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

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

Eigenvectors and eigenvalues of the matrix $\begin{bmatrix} 1 & -2 \\ -1 & -1 \end{bmatrix}$, are: $\left\{ \begin{bmatrix} -\sqrt{3}-1 \\ 1 \end{bmatrix} \right\} \leftrightarrow \lambda_1 = \sqrt{3}$, $\left\{ \begin{bmatrix} \sqrt{3}-1 \\ 1 \end{bmatrix} \right\} \leftrightarrow \lambda_2 = -\sqrt{3}$

The change of variables $\vec{r} = \begin{bmatrix} -\sqrt{3}-1 & \sqrt{3}-1 \\ 1 & 1 \end{bmatrix} \vec{y}$ reduces the system to two independent equations: $y_1' = \sqrt{3}y_1$ and $y_2' = -\sqrt{3}y_2$.

Sylvester's method uses matrices $Q_1 = \frac{A-\lambda_2 I}{\lambda_1-\lambda_2}$ and $Q_2 = \frac{A-\lambda_1 I}{\lambda_2-\lambda_1}$ such that $A = Q_1 + Q_2$ and the evolution operator $\exp(At) = \exp(\lambda_1 t)Q_1 + \exp(\lambda_2 t)Q_2$

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

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

The stationary point is a saddle point. Trajectories are hyperbolas that tend to lines through the origin parallel to eigenvectors.

2. Ljapunovs functions and stability of fixed points.

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

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

We try if function $V(x, y) = x^2 + y^2$ is a Lyapunov's function in some neighbourhood of origin.

$$V' = 2x(-x + 2xy \sin(y)) + 2y(-\cos(x)y) = -2x^2 - 2y^2 + 4x^2y \sin(y) + 2y^2(1 - \cos(y)) = -2(x^2 + y^2) + 2(x^4 + y^4) + x^2O(y^3) + 2y^2O(y^2)$$

where $O(z)/z < const$ when $z \rightarrow 0$. It shows that in a small neighbourhood of the origin all terms in V' are dominated by $-2(x^2 + y^2)$ and that V is a strong Lyapunov's function and the origin is an asymptotically stable point for the system.

3. Periodic solutions to ODE

Show that the system of equations

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

has at least one periodic solution. (4p)

We consider the equation for the function $\varphi(x, y) = 2x^2 + y^2$ by multiplying the first equation by $2x$ and the second equation by y .

$$\begin{cases} 2xx' = 2xx - 4xy - 2x^2(2x^2 + y^2) \\ yy' = 4xy + y^2 - y^2(2x^2 + y^2) \end{cases} \implies 0.5\varphi' = 0.5(2x^2 + y^2)' = (2x^2 + y^2) - (2x^2 + y^2)^2 = \varphi(x, y)(1 - \varphi(x, y))$$

We observe that for (x, y) on the ellipse ring $2x^2 + y^2 = 0.5$ we get $\varphi' > 0$ and on the ellipse $2x^2 + y^2 = 2$ we get $\varphi' < 0$. It implies that the elliptic ring $0.5 < 2x^2 + y^2 < 2$ is the invariant set for the system. On the other hand on the ellipse $2x^2 + y^2 = 1$ where $\varphi' = 0$ velocities are not zero and system has no stationary points in the ring $0.5 < 2x^2 + y^2 < 2$. Poincaré-Bendixson theorem implies that it must be a periodic solution inside this ring.

4. Hopf bifurcation.

Explain the notion Hopf bifurcation.

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

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

The linearization of the equation around the origin is
$$\begin{cases} x' = y \\ y' = -x + \mu y \end{cases}$$

The matrix $\begin{pmatrix} 0 & 1 \\ -1 & \mu \end{pmatrix}$, has eigenvalues: $\lambda_1 = \frac{1}{2}\mu - \frac{1}{2}i\sqrt{4 - \mu^2}$; $\lambda_2 = \frac{1}{2}\mu + \frac{1}{2}i\sqrt{4 - \mu^2}$.

The system stable focus for $\mu < 0$ and unstable focus for $\mu > 0$. $\frac{d\text{Re}\lambda_i(\mu)}{d\mu} > 0$.

We check stability of the stationary point in the origin for $\mu = 0$, by computing $(x^2 + y^2)'$: $0.5(x^2 + y^2)' = -y^4 \leq 0$. It implies that $(x^2 + y^2)$ is a weak Lyapunov function.

On the other hand system has no trajectories imbedded in the line $y = 0$, because $y' = -x$ on this line and trajectories cross it everywhere except the origin. It implies that the origin is even asymptotically stable stationary point. It implies that the system has a Hopf bifurcation for $\mu = 0$. For $\mu < 0$ system has stable focus in the origin. When μ changes from negative to positive value it appears a limit cycle around the origin and the stationary point becomes unstable.

5. Chemical reactions by Gillespie's method

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

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

$$X' = -c_1PX + c_2W$$

$$P' = -c_1PX + c_3\frac{1}{2}Z(Z - 1) - c_4P$$

$$W' = c_1PX - c_2W$$

$$Z' = -c_3Z(Z - 1) + c_42P$$

b) Give formulas for the algorithm that models these reactions stochastically by Gillespie's method. (2p)

$P(\tau, \mu)d\tau$ 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.

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

$h_\mu c_\mu d\tau$ 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: $h_1 = XP$, for reaction 2: $h_2 = W$, for reaction 3: $h_3 = \frac{1}{2}Z(Z - 1)$, for reaction 4: $h_4 = P$.

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

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

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

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

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

$$\mu = 3 \rightarrow Z = Z - 2, P = P + 1.$$

$$\mu = 4 \rightarrow Z = Z + 2, P = P - 1.$$

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 together with bonus points for home assignments(40%).