MATEMATIK
GU, Chalmers
A.Heintz

Datum: 2013-01-15
Hjälpmedel: Beta
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Tid: 8:30

Tel.: 0762-721860.

Tenta i matematisk modellering, MMG510, MVE160

1. **Liapunovs theory**

   Formulate and give a proof for Liapunovs theorem on instability of a fixed point together with definitions of the notions used in the formulation. (4p)

2. **Linear systems**

   Consider the following ODE:
   $\frac{d\vec{r}(t)}{dt} = A\vec{r}(t)$, $\vec{r}(t) = \begin{bmatrix} r_1(t) \\ r_2(t) \end{bmatrix}$ with a constant matrix A defined as $A = 2I + C = -2\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$.

   Define the evolution operator for this system. (4p)

3. **Liapunovs theory**

   Consider the following system of ODE and investigate stability of the fixed point in the origin. (4p)

   $$\begin{cases} x' = x^3 + 2xy^2 \\ y' = x^2 y \end{cases}$$

4. **Periodic solutions to ODE.**

   Show that the following system of ODE has a periodic solution.

   $$\begin{cases} x' = y \\ y' = -x + y(1 - 3x^2 - 2y^2) \end{cases}$$

   Hint: transform the system to polar coordinates and consider the equation for polar radius. (4p)

5. **Chemical reactions by Gillespies method**

   Consider the following reactions: $X + Z \underset{c_2}{\overset{c_1}{\rightleftarrows}} W$, $\quad W \underset{c_4}{\overset{c_3}{\rightleftarrows}} P$ where $c_i\,dt$ with $c_i > 0$ is the probability that during time dt the reaction with index i will take place $i = 1, 2, 3$.

   a) Using mass action law write down differential equations for the number of particles for these reactions. (2p)

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

   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 the average of points for the project (60%) and for this exam together with bonus points for home assingments (40%).

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Datum: 2013-01-15 Tid: 8:30
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Telefonvakt: Peter Helgesson Tel.: 0762-721860.

Lösningar till tenta i matematisk modellering, MMG510, MVE160

1. **Liapunovs theory.**

   Formulate and give a proof for Liapunovs theorem on instability of a fixed point together with definitions of the notions used in the formulation. See the book by Arrowsmith Place.
   (4p)

2. **Linear systems**

   Consider the following ODE:
   $\frac{d\vec{r}(t)}{dt} = A\vec{r}(t)$, $\vec{r}(t) = \begin{bmatrix} r_1(t) \\ r_2(t) \end{bmatrix}$ with a constant matrix A defined as $A = -2I + C =$ $-2\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}$.

   Define the evolution operator for this system. **(4p)**

   Evolution operator is operator maps the initial data $\vec{r}_0$ into the solution: $\vec{r}(t) = \exp(At)\vec{r}_0$.

   The matrix $\exp(At)$ can be computed using series $\exp(At) = I + At + \frac{A^2t^2}{2!} + \frac{A^3t^3}{3!} + \frac{A^4t^4}{4!} + \ldots$

   Considering $A = \lambda I + C$ with arbitrary λ we observe that $C^2 = 0$. It implies that

   $A^2 = 2\lambda C + \lambda^2 I$; $A^3 = \left(\lambda^2 I + 2\lambda C\right)(\lambda I + C) = 3C\lambda^2 + I\lambda^3$;

   $A^4 = \left(3C\lambda^2 + I\lambda^3\right)(\lambda I + C) = 4C\lambda^3 + I\lambda^4$, etc. $A^n = nC\lambda^{n-1} + I\lambda^n$

   Substituting these expressions into the series for $\exp(At)$ we obtain

   $\exp(At) = \left(I + I(\lambda t) + \frac{I(\lambda t)^2}{2!} + \frac{I(\lambda t)^3}{3!} + \frac{I(\lambda t)^4}{4!} + \ldots\right) +$

   $\left(I + I(\lambda t) + \frac{I(\lambda t)^2}{2!} + \frac{I(\lambda t)^3}{3!} + \frac{I(\lambda t)^4}{4!} + \ldots\right) Ct = \exp(\lambda t)(I + tC)$

   At the end we can substitute $\lambda = -2$.

3. **Liapunovs functions and stability**

   Consider the following system of ODE and investigate stability of the fixed point in the origin.
   (4p)

   $$\begin{cases} x' = x^3 + 2xy^2 \\ y' = x^2 y \end{cases}$$

   Consider test function $V(x,y) = x^2 + y^2$. $V(x,y) \geq 0$. $V(0,0) = 0$.

   $V' = 2x(x^3 + 2xy^2) + 2yx^2y = 2x^4 + 6x^2y^2 = 2x^2\left(x^2 + 3y^2\right) > 0$.

   It implies that the origin is an unstable equilibrium point.

4. **Periodic solutions to ODE.**

   Show that the following system of ODE has a periodic solution.

   $$\begin{cases} x' = y \\ y' = -x + y(1 - 3x^2 - 2y^2) \end{cases}$$

   Hint: transform the system to polar coordinates and consider the equation for polar radius.

   (4p)

$r' = r\sin^2(\theta)(1 - 3r^2\cos^2(\theta) - 2r\sin^2(\theta))$

We observe that for small enough r $\quad r' \geq 0$,

for example for $r = 0.5$: $r' = 0.25\sin^2(\theta)(1 - 0.5\cos^2(\theta)) \geq 0$

One observes also from the equation for r' that

$r' \leq r\sin^2(\theta)(1 - 2r^2)$ that makes $r' \leq 0$ for $r \leq 1/\sqrt{2}$. Equality is attained only for $\theta = 0, \theta = \pi$.

It makes the ring $0.5 < r < 1/\sqrt{2}$ a positively invariant set for the system.

The only fixpoint of the sistem is the origin, therefore by the Poincare-Bendixson theorem it must have a periodic solution in this ring.

5. **Chemical reactions by Gillespies method**

Consider the following reactions: $X + Z \underset{c_2}{\overset{c_1}{\rightleftarrows}} W, \qquad W \underset{c_4}{\overset{c_3}{\rightleftarrows}} P$ where $c_i\,dt$ with $c_i > 0$ is the probability that during time dt the reaction with index i will take place $i = 1, 2, 3$.

a) Using mass action law write down differential equations for the number of particles for these reactions. **(2p)**

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

a)

$X' = -c_1XZ + c_2W$

$Z' = -c_1XZ + c_2W$

$W' = c_1XZ - (c_2 + c_3)W$

$P' = c_3W$

b) **Gillespies metod.**

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

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

Here $P_0(\tau)$ is the probability that no rections are observed during the time τ.

$h_\mu c_\mu d\tau$ is the probability that just the reaction μ happen during time $d\tau$.

h_μ is the number of combinations of particles for actual nubers X, Z, W, P that can make input to the reaction μ. For reaction 1 in the example $h_1 = X \cdot Z$, for reaction 2 it is $h_2 = W$, for reaction 3 it is $h_3 = W$,for reaction 4 it is $h_4 = P$.

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

The algorithm for stochastic modelling consists of the following steps.

0) inicializing variables X, Z, W, P and time $t = 0$.

1) compute h_i, a.

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

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

Choose next reaction μ so that $\sum_{i=1}^{\mu-1} h_ic_i \leq p\,a \leq \sum_{i=1}^{\mu} h_ic_i$.

3) Add time τ to the time variable t. Change variables X, Z, W, P representing numbers of particles according to the chosen reaction:

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

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

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

3) If time t is larger than the maximal time finish computations otherwise go to the step 1.

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