Imperial College London

19 October 2007

**Department of Bioengineering**
**MEng/BEng in Biomedical Engineering**

**BE3-H36/BE4-H36 – Modelling in Biology (MiB)**

## ***Assignment 1: Building up some tools of the trade***

To be returned by **Monday, 5 November 2007**

Your coursework should contain: handwritten calculations if appropriate, annotated Matlab graphs and figures, short pieces of code, and succinct answers to the questions. You are encouraged to discuss with other students and to use the *Matlab Help*, but your answers should be *yours*, i.e., written by you, in your own words, showing your own understanding. You must produce your own code and submit it when appropriate.

### Question 1: Simple numerics on the single exponential

Consider the simplest of ODEs, which we saw in class: $\dot{x} = -kx$, and for concreteness make $k = 2/3$.

1. (a) Taking as initial condition $x_0 = 10$, use Matlab to integrate this equation numerically for $0 \leq t \leq 5$ and plot $x$ as a function of time.

   (b) Obtain the analytical solution to this equation and plot it on the same figure.

   (c) Use Matlab to obtain the mean squared error of the numerical solution with respect to the true analytical solution.

   [*Read the Matlab Help, which will tell you that the fourth order Runge-Kutta method* `ode45` *should be your initial method of choice for general problems.*]

2. (a) By default, `ode45` does not give the solution at fixed points in time. Confirm this in the numerical solution obtained in 1. Can you deduce why/when `ode45` takes smaller or larger steps?

   (b) Read the Matlab Help to find out how to force `ode45` to give values of $x$ at `t=[0:0.01:5]`. Calculate the mean squared error of this numerical solution compared with the analytical solution.

   (c) Use now the `diff` function in Matlab to calculate the discrete difference between equally spaced values of $x$: $x(t+0.01)-x(t)$, for `t=[0.01:0.01:5]`. Plot now $[x(t+0.01)-x(t)]/x(t)$ as a function of time. Carry out some simple calculations to explain the limit of this plot at small $t$. What is the reason for the oscillations at large $t$?

### Question 2: Your first algorithmic implementation—Euler method

[*Although Runge-Kutta is most useful in practice, you will now implement the simplest integration algorithm: Euler's method. Euler-type algorithms must be used when integrating numerically stochastic differential equations, as in part 2 of this question.*]

1. **Deterministic Euler algorithm** – Write a short Matlab code to implement Euler's method and solve numerically the same equation as in Question 1:

$$x(t+h) = x(t) + h\,[-k\,x(t)] \qquad \text{with} \qquad k = 2/3,\ h = 0.01,\ x(0) = 10,\ t \in [0, 85]$$

   (a) Calculate the mean squared error of this solution with respect to the analytical solution.

   (b) Repeat the numerical calculation with $h = 0.001$ and calculate the mean squared error. Explain the differences for both values of $h$. Compare the error to the Runge-Kutta method.

   (c) Save your code in a file `euler.m` and submit it with your assignment.

2. **Stochastic Euler algorithm** – We will now implement an Euler algorithm for the integration of the *Stochastic Differential Equation* associated with the ODE of Question 1:

$$dx = -kxdt + \sigma dW$$

   where $\sigma$ is the amplitude of the random noise process $dW$. The algorithm follows similar lines to the above Euler method so you should build on your programme `euler.m`.

   Take $k = 2/3,\ h = 0.01,\ x(0) = 10,\ t \in [0, 5]$ and $\sigma = 0.2$ and implement:

$$x(t+h) = x(t) + h\,[-k\,x(t)] + \sigma\sqrt{h} * \texttt{randn},$$

   where `randn` is a Matlab function that generates a random number drawn from a *Gaussian distribution* of mean zero and unit variance (see the Matlab Help).

   (a) Save your code in a file `eulerSDE.m` and submit it with your coursework.

   (b) i. Run `eulerSDE.m` 15 times and superimpose the plots of $x(t)$ as a function of time.

   ii. Using these fifteen trajectories, calculate the average trajectory as a function of time. Explain how these trajectories are related to the results in Question 1.

   (c) i. Run `eulerSDE.m` with $x(0) = 0$, $\sigma = 0.1$ and $h = 0.01$ for a long time, $t \gg 5$. (Note the initial condition is zero now.) Plot the histogram of the values of $x(t)$, using the Matlab command `hist`.

   ii. Repeat this calculation but now with $\sigma = 5$ and plot the corresponding histogram.

   iii. Using the Matlab commands `mean` and `std` calculate the means and standard deviations of the two distributions obtained above. Explain the difference in the width (i.e., the `std`) of the histograms for the two values of $\sigma$.

## Question 3: *Probably* your first Monte Carlo programmes

[*An important skill in 'Modelling' is being able to understand other people's code, translating it back to a physical, biological or mathematical picture. This is the goal of this exercise.*]

1. Run the following lines of code in Matlab:

```
clear;
i=0;
for N=[100 1000 5e3 1e4 5e4 1e5 5e5];
   i=i+1;
   pp=rand(N,2);
   P=4*mean((pp(:,1).^2+pp(:,2).^2)<=1);
   A(i,:)=[N P];
end
```

(a) Explain briefly the meaning of the code. What is the difference between `rand` and `randn`?

(b) To what number does `P` converge as you make `N` large? Explain this limiting behaviour of `P` using a sketch.

(c) Explain the following statement: *The above Matlab operation is equivalent to throwing darts blindfolded at a blank square, and counting how many times your dart falls in a certain region.* Which region is that?

2. The Matlab programme above is a simple example of Monte Carlo (as in the Casino in Monaco) techniques, a direct application of probability theory to solve deterministic problems. Based on your understanding of the problem above, run and interpret the following short codes:

*Program 1:*

```
clear; Q=0; Nfinal=1e6;
for N=1:Nfinal;
    pp=rand(1,2);
    Q=Q+(1./(1+pp(1,1).^2)>=pp(1,2));
end
P1=Q/Nfinal
```

*Program 2:*

```
clear; Q=0; Nfinal=1e6;
for N=1:Nfinal;
    pp=rand(1,2);
    Q=Q+(pp(1,1)./(1+pp(1,1).^2)>=pp(1,2));
end
P2=Q/Nfinal
```

What is the limiting value of `P1` and `P2` as `Nfinal` $\to \infty$? Explain briefly how you got your answer.

### Question 4: Normal modes and systems of coupled harmonic (linear) oscillators

1. Consider the following system of coupled differential equations corresponding to a system of linear *overdamped* oscillators:

$$
\begin{aligned}
\dot{x}_1 &= -k(x_1 - x_2) - k(x_1 - x_4) \\
\dot{x}_2 &= -k(x_2 - x_3) - k(x_2 - x_1) \\
\dot{x}_3 &= -k(x_3 - x_4) - k(x_3 - x_2) \\
\dot{x}_4 &= -k(x_4 - x_3) - k(x_4 - x_1), \qquad k = 1
\end{aligned}
$$

(a) Draw a sketch of the physical system that originated these equations.

(b) Use Matlab to integrate them for $t \in [0, 4]$ with an initial condition

$$\mathbf{x}^{(0)} = (x_1(0), x_2(0), x_3(0), x_4(0)) = (4, 7, -3, -0.4).$$

Plot the result of the integration for the four coordinates as a function of time.

[*Use the Matlab Help to learn how to integrate systems of ODES with* `ode45`. *Create a function that contains your right hand side which should take a vector as an input and return a vector as an output.*]

(c) Follow what we did in class and write the equation in matrix-vector form

$$\dot{\mathbf{x}} = A\mathbf{x},$$

where $A_{4\times4}$ is a matrix and $\mathbf{x}_{4\times1}$ is a vector. Use the Matlab command `eig` to calculate the eigenvalues and eigenvectors of $A$.

(d) What is the meaning of the eigenvector with the maximum eigenvalue? Interpret the other eigenvectors of the problem as vibrational modes.

[*For inspiration, you can think of the vibrational spectrum of the molecule cyclobutadiene, even though this is not a chemically stable molecule.*]

(e) Using your numerical results obtained in 1b, plot the time evolution of a variable that is the sum of all four coordinates, i.e., $X(t) = \sum_{i=1}^{4} x_i(t)$. Explain what happens in light of the results of 1c.

2. Consider now the following system of ODEs:

$$\begin{aligned}
\dot{x}_1 &= -k(x_1 - x_2) - kx_1 \\
\dot{x}_2 &= -k(x_2 - x_3) - k(x_2 - x_1) \\
\dot{x}_3 &= -k(x_3 - x_4) - k(x_3 - x_2) \\
\dot{x}_4 &= -k(x_4 - x_3) - kx_4, \qquad k = 1
\end{aligned}$$

(a) As you did in 1c, write down the matrix $A_{4\times4}$ associated with this linear system and find its eigenvalues and eigenvectors with Matlab.

(b) Compare the maximum eigenvalue of this system and that of 1. What would be the result of the simulation if you were to repeat the calculation in 1e. To aid your explanation, add a sketch of the physical system of springs behind the equations and compare it with that in 1.

## Question 5: A very familiar second order system

Consider the second order linear ordinary differential equation

$$\frac{d^2y}{dt^2} + \eta\frac{dy}{dt} + y = 0$$

1. Write the equation as a system of two first order ODEs and integrate it numerically with Matlab's `ode45`, with initial conditions $\{y(0) = 2,\ \dot{y}(0) = 10\}$ and $t \in [0, 60]$. Perform the calculation for three different dampings: $\eta = \{0, 0.02, 5\}$. Plot the three trajectories $y(t)$ as a function of time on the same figure.

2. Represent the same trajectories in phase space by plotting $\dot{y}$ as a function of $y$ for the three different values of $\eta$.

3. Explain the difference between the cases with $\eta = 0.02$ and $\eta = 5$ in the phase plane. How does that relate to your previous knowledge of oscillations? At what value of $\eta$ does one expect to switch from one behaviour to the other?