Zuse Institute Berlin (ZIB)
Freie Universität Berlin
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9. Homework
Numerics for Bioinformaticians
WS 2016/17

Deadline: January 11, 10:00 (**before** the lecture)

The homework should be worked out in groups of two or three students. Each solution sheet must contain the names and student numbers ('Matrikulationnummer') of all group members and the exercise group (Wednesday/Friday). Solutions to exercise 1, 2 & 3.d must be handed in in paper form, either hand written or printed out if generated electronically. Please staple all sheets.
Programming tasks must be submitted to max.kleist2@fu-berlin.de or BioInfNumerik@hotmail.com by email. Before sending it, please 'zip' it.

Exercise 1 (maximum likelihood estimate II, 3 points)
Consider the structural model $\mathcal{M}$:

$$x_{i|k} = k \cdot t_i + x_0$$

with $x_0 = 1$, assuming an additive error

$$y_i = x_{i|k} + \eta_i$$

where $\eta_i \sim \mathcal{N}(0, \sigma^2)\ \forall\ i$.
You are given the data points $z = (t_i, y_i)$ with $t = 1, 2$ and $y = 2.5, 5.5$. What is the maximum likelihood estimate of k?
Hint1: Use the formula for the log-likelihood.
Hint2: Take all derivatives with respect to k

$$\begin{bmatrix} \frac{d(-\log p_1)}{dk} \\ \frac{d(-\log p_2)}{dk} \end{bmatrix} \tag{1}$$

and note that they should sum up to 0.
Hint3: Substitute Gaussian density, substitute the model, solve for θ.

Exercise 2 (Predator-Prey model: Algebraic (3 Points))
Let us consider the predator-prey model,

$$x_1 \xrightarrow{k_0} x_1 + x_1 \tag{2}$$

$$x_1 + x_2 \xrightarrow{k_1} x_2 \tag{3}$$

$$x_1 + x_2 \xrightarrow{k_2} x_2 + x_2 \tag{4}$$

$$x_2 \xrightarrow{\delta} \emptyset \tag{5}$$

where x_1, x_2 denotes the population of prey and predators (x_2 eats x_1). The corresponding ODEs is given by:

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} x_1 &= x_1(k_0 - x_2 \cdot k_1 - x_2 \cdot k_2), \\ \frac{\mathrm{d}}{\mathrm{d}t} x_2 &= x_2(x_1 \cdot k_2 - \delta). \end{aligned} \tag{6}$$

a) Derive the two fixed points for the Predator-Prey model.

b) Derive the corresponding eigenvalues of the two fixed points.

c) What are the dynamic characteristics of the two fixed points?

Exercise 3 (Predator-Prey model: Implmentation (4 Points))
Fix the parameters to be 0.3, 0.01, 0.01 and 0.3 for k_0, k_1, k_2 and δ_2. At $t = 0$ set the initial value to $(x_1 = 20, x_2 = 20)$ and let $t_{final} = 50$.

a) Plot the phase space diagram of the Predator-Prey model.

b) Using the Explicit Euler method, plot the approximation of (6) for step sizes $h = 0.5, 0.1, 0.01$.

c) Now plot the approximation of (6) using the 4^{th} order Runge–Kutta method for $h = 0.5$.

d) Comment of what you are observing in regards to dynamics and numerics. (Write on the hand in sheet)

Hint: The code for Quiver function to draw the phase space diagram looks a bit like this:

```
import matplotlib.pyplot as plt

X = np.arange(0,80,3)
Y = np.arange(0,40,3)
XX,YY = np.meshgrid(X,Y)

U = XX*(k_0 - YY*(k_1 + k_2))
V = YY*(XX*k_2 -delta)

plt.quiver(XX,YY,U,V)
```

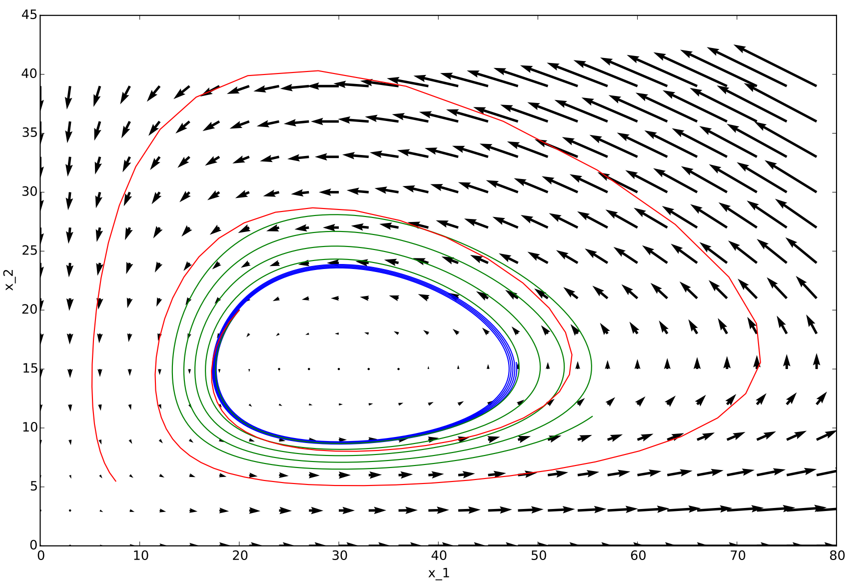

Figure 1: Mockup of the solution for Exercise 2. Please make sure you have all curves labeled and on a single plot, so one can compare them.