# Mathematical Modelling in the Natural Sciences
# SS21, Exercises, Sheet 1

1. For the *Supersize Me!* problem suppose that the following data have been measured:

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n = 30;
t = linspace(0,30,n);
p = 1.0;
m = 231.48 + (84-231.48)exp(-t/361.11) + p*randn(1,n);
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   Formulate a method for estimating the parameter $\phi$ in the model

$$m'(t) = \epsilon/\kappa - m(t)\phi/\kappa, \quad m(0) = 84, \quad \epsilon = 5000, \quad \kappa = 7800$$

   and implement this method using Matlab. For different values of the noise level $p$, compare your result with the value of $\phi = 21.6$ used in the lecture notes. Hint: Consider using the $\ell_2-$ or the $\ell_1-$norm of the differences between simulated and measured data.

2. Develop a refinement of the *Supersize Me!* model which is intended to be more suitable for (a) very small or (b) very large values of $m$, and argue why your model is more suitable for these extreme cases. Hint: Consider the behavior of the steady state with respect to other parameters.

3. For the system of differential equations modelling the discovery of treasures by a random walk

$$\begin{aligned} p_0'(t) &= -\beta p_0(t) \\ p_n'(t) &= -\beta p_n(t) + \beta p_{n-1}(t), \quad n = 1, 2, \ldots, N-1 \qquad 0 \le t \le T \\ p_N'(t) &= \beta p_{N-1}(t) \end{aligned}$$

   determine the initial conditions which correspond to not having discovered any treasures at all at time $t = 0$. Choose values $\beta, T > 0$ and $N \in \mathbb{N}$ and solve the above system using Matlab plotting $\{p_n(t)\}_{n=0}^N$ together for $t \in [0, T]$. Given the values $\{p_n(t) : t \in [0, T]\}_{n=0}^N$ determine $E_N(t)$ the expected number of treasures discovered up to time $t$. Plot also $E_N(t)$ together with $E(t)$ presented in the lecture notes, and compare the two plots for ever larger $N$.

4. Let the data be given:

$$Y = \begin{bmatrix} 0 & 1 & 2 & 3 \\ 0 & 1 & 1 & 2 \end{bmatrix}.$$

   (a) Carry out PCA to determine $Y_\mathrm{c}$, $K = \frac{1}{4} Y_\mathrm{c} Y_\mathrm{c}^\top$, $V$ and $\Lambda = \mathrm{diag}\{\lambda_i\}$ with $KV = V\Lambda$ and $Y_\mathrm{s} = \Lambda^{-\frac{1}{2}} V^\top Y_\mathrm{c}$. Plot $Y$ and $Y_\mathrm{s}$.

   (b) Show that the sphered data satisfy $\frac{1}{4} Y_\mathrm{s} Y_\mathrm{s}^\mathrm{T} = I$. Show that when the sphered data are projected onto an arbitrary axis $\hat{\boldsymbol{w}} \in \mathbb{R}^2$ with $\|\hat{\boldsymbol{w}}\|_{\ell_2} = 1$, the projected data have the variance 1.

   (c) For $\theta \in [0, 2\pi]$ define $\boldsymbol{u} = (\cos(\theta), \sin(\theta))$, $\boldsymbol{u}^\perp = (-\sin(\theta), \cos(\theta))$ and $U(\theta) = (\boldsymbol{u}(\theta); \boldsymbol{u}^\perp(\theta))$. Plot $J(\theta) = \mathcal{K}^2(\boldsymbol{u}(\theta) Y_\mathrm{s})$ where $\mathcal{K}$ is the kurtosis. Using this plot, determine the value $\theta^*$ which maximizes $J$. Set $X_\mathrm{c} = U(\theta^*) Y_\mathrm{s}$. Assume that the columns of $Y$ have equal probability, and show that the coordinates $(x, y)$ of columns of the resulting $X_\mathrm{c}$ are statistically independent, i.e.,

$$P(x = \alpha \;\&\; y = \beta) = P(x = \alpha) \cdot P(y = \beta).$$

Bonus: Apply PCA to compress these data down to 10 principal components and thereby denoise the image sequence. Hint: This article may be helpful.

5. With dimensional analysis derive the third Kepler Law: *The squares of the orbital periods of two planets are proportional to the cubes of their semi-major axes.* (Hint: See page 35 in the script, and don't forget to verify the conditions of the Buckingham Pi Theorem.)

6. The chemical reaction

$$kA + lB \underset{\kappa_2}{\overset{\kappa_1}{\rightleftharpoons}} mC + nD$$

is given with the following parameters:

$$k = 2, \quad l = 1, \quad m = 2, \quad n = 1$$

$$[A](0) = 2, \quad [B](0) = 2, \quad [C](0) = 2, \quad [D](0) = 1.$$

Determine the initial value problem

$$x'(t) = f(x(t); \kappa_1, \kappa_2), \quad x(0) = x_0$$

where

$$[A](t) = [A](0) - kx(t), \quad [B](t) = [B](0) - lx(t)$$

$$[C](t) = [C](0) + mx(t), \quad [D](t) = [D](0) + nx(t).$$

Rewrite the equation $f(x^*; \kappa_1, \kappa_2) = 0$ in the form,

$$\kappa_2/\kappa_1 = r(x^\star)$$

giving a relationship between equilibria and the quotient $\kappa_2/\kappa_1$. (Note that the condition $\kappa_2/\kappa_1 > 0$ implies, through the form of $r$, that an equilibrium must satisfy $x^\star > -1$.) Show that any equilibrium $x^\star$ with $r'(x^\star) < 0$ is (locally asymptotically) stable, while any equilibrium $x^\star$ with $r'(x^\star) > 0$ is unstable. (Hint: It holds that $f'(x^\star; \kappa_1, \kappa_2)/\kappa_1 = 4r'(x^\star)(1 + x^\star)^3$.) Derive a corresponding potential landscape $p(x, \kappa_2/\kappa_1)$, where $f(x; \kappa_1, \kappa_2)/\kappa_1 = -p_x(x, \kappa_2/\kappa_1)$. For various values of $\kappa_2/\kappa_1$, plot $f(x; \kappa_1, \kappa_2)$ and $p(x, \kappa_2/\kappa_1)$ in the interval $0 \le x \le 3$ to demonstrate the associated hysteresis graphically.