Mathematical Modelling in the Natural Sciences
SS19, Exercises, Sheet 2

Solutions to be presented on 18. March 2019

1. For given data,
$$Y = \begin{bmatrix} 0 & 1 & 2 & 3 \\ 0 & 1 & 1 & 2 \end{bmatrix}$$
   (a) carry out PCA to determine Y_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_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 $\|\hat{\boldsymbol{w}}\|_{\ell_2} = 1$, they 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 θ^* 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_c are statistically independent, i.e.,
$$P(x = \alpha \ \&\ y = \beta) = P(x = \alpha) \cdot P(y = \beta).$$
   Solved by Mr. Habring.

   Bonus: Apply PCA to compress the data,
   `http://imsc.uni-graz.at/keeling/manuskripten/dcemri.mpg`
   down to 10 principal components and thereby denoise the image sequence. Hint: The article
   `http://imsc.uni-graz.at/keeling/manuskripten/pcaica.pdf`
   may be helpful.

2. 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 `http://imsc.uni-graz.at/thaller/lehre/mpt/skriptum.pdf`, and don't forget to verify the conditions of the Buckingham Pi Theorem.) Solved by Mr. Haberl.

3. 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 κ_2/κ_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 κ_2/κ_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. Solved by Mr. Habring.