Mathematical Modelling in the Natural Sciences SS21
Solutions to Exercises on Sheet 1

Exercises und Lecture Notes

Contents

Exercise 1: *Supersize Me*

Task

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

```
n = 30;
t = linspace(0,30,n);
p = 1.0;
m = 231.48 + (84-231.48)exp(-t/361.11) + p*randn(1,n);
```

Formulate a method for estimating the parameter ϕ 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 ℓ_2- or the ℓ_1-norm of the differences between simulated and measured data.

◦ Solution

A Matlab function for the solution to this initial value problem for a given value of `p` $(= \phi)$ is given as follows.

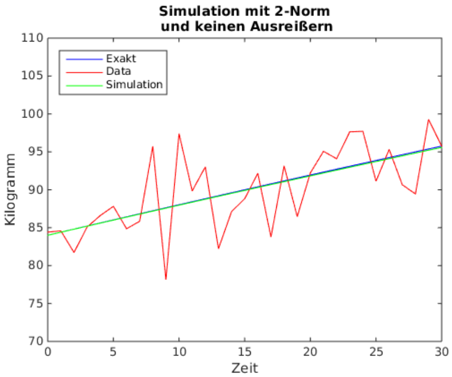
```
function m = super(p)

% for a given p in the ODE,
%     m' = (e/k) - (p/k)*m,  m(0) = m0
% compute the time course of the mass m over 30 days

% energy flow per day
    e = 5000;
% density kcal/kg
    k = 7800;

% ODE to solve is m' = dm(t,m)
    dm = @(t,m) (e/k) - (p/k)*m;

% initial mass
    m0 = 84;
% time points in which the solution should be output
    tpte = (0:30)';
% options
    opts = odeset('RelTol',1.0e-6);
% solution of the ODE
    [t,m] = ode45(dm,tpte,m0,opts);

end
```

This function is called from the following Matlab code to estimate a value of `p` $(= \phi)$ which fits the noise level `ns`.

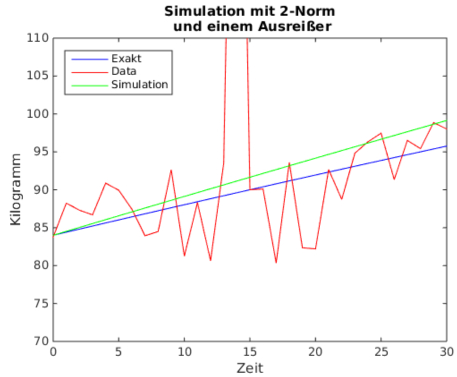
```
function S01Exp1

% determine the value of p in the ODE
%     m' = (e/k) - (p/k)*m,  m(0) = m0
% where the difference between the computed solution and simulated data
% is minimal in a chosen sense.

% energy outflow parameter, the target exact value
    pexact = 21.6;
```

```
% energy flow per day
    e = 5000;
% density, kcal/kg
    k = 7800;
% initial mass
    m0 = 84;
% time points in which the solution should be output
    tpte = (0:30)';
% exact solution of the ODE m' = (e/k) - (p/k)*m,  m(0) = m0
    mexact = (e/pexact) + (m0 - e/pexact)*exp(-tpte*pexact/k);
% noise in the data
    ns = 5;
% noisy solution, simulated data for the determination of p % with outlier
    mdata  = mexact + (ns*m0/100)*randn(31,1); %  mdata(15)=mdata(15)*2;

% objective function to minimize for the determination of p,
    f = @(p) norm(mdata - super(p),1);
% use 1-norm (here) or, say, the 2-norm

% initial value for the estimate of p
    p0 = 20;
% options for minimization
    opts = optimset('MaxFunEvals',1000,'TolX',1.0e-6);
% minimization for the determination of p
    p = fminsearch(f,p0,opts);

% results
    disp(['exact value = ',num2str(pexact)])
    disp(['noise level in daten = ',num2str(ns),'%'])
    disp(['estimated value = ',num2str(p)])

% grafical representation
    plot(tpte,mexact,'b',tpte,mdata,'r',tpte,super(p),'g')
    axis([0 30 70 110])
    xlabel('Time')
    ylabel('Kilogram')
    legend('Exact','Data','Simulation','Location','northwest')
    title(sprintf('Simulation with 2-Norm\n and no outlier'))
%   title(sprintf('Simulation with 2-Norm\n and one outlier'))
%   title(sprintf('Simulation with 1-Norm\n and one outlier'))

end
```

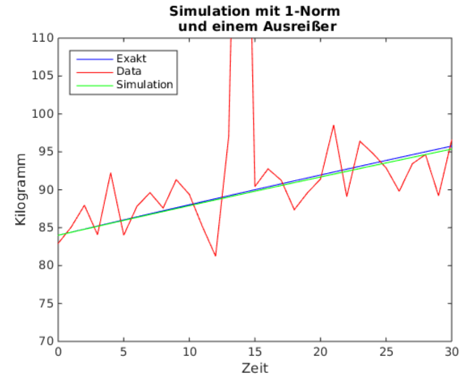
Results with `ns=5%` noise and with (a) ℓ_2-norm and no outliers, (b) ℓ_2-norm and one outlier, (c) ℓ_1-norm and one outlier are shown here with the estimated value of $\phi^\star$:



(a) $\phi^\star = 22.1$



(b) $\phi^\star = 11.6$



(c) $\phi^\star = 22.8$

• Exercise 2: *Supersize Me* Supplement

○ Task

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.

○ Solution

For the *Supersize Me!* model in the lecture notes the equilibrium satisfies

$$m^\star(\epsilon) = \epsilon/\phi$$

and therefore increases linearly with respect to ϵ. This is not realistic, since the efficiency of energy storage in the body presumably decreases as more energy is consumed. The next level of complexity for the relationship between the equilibrium $m^\star$ and the energy inflow ϵ is

$$m^\star(\epsilon) = \sqrt{\epsilon/\phi}$$

which is consistent with the new model,

$$m'(t) = \epsilon/\kappa - m^2(t)\phi/\kappa, \quad m(0) = m_0 = 84, \quad \epsilon = 5000, \quad \kappa = 7800.$$

The solution of this initial value problem is

$$m(t) = \sqrt{\frac{\epsilon}{\phi}} \tanh\left[\frac{\sqrt{\epsilon\phi}}{\kappa}t + \tanh^{-1}\left(m_0\sqrt{\frac{\phi}{\epsilon}}\right)\right]$$

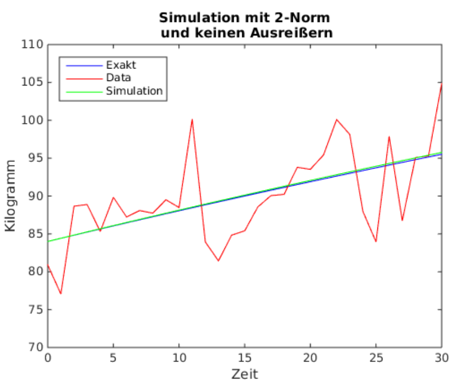
The Matlab code from the last example can be modified as follows for the new model.

```
% for a given p in the ODE,
%     m' = (e/k) - (p/k)*m^2,  m(0) = m0

...
```

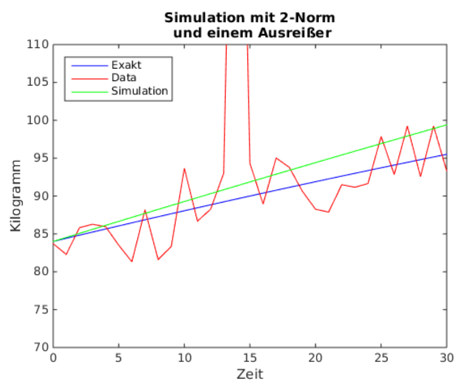
```
% ODE to solve is m' = dm(t,m)
    dm = @(t,m) (e/k) - (p/k)*m^2;

...

% energy outflow parameter, the target exact value
    pexact = 0.248;

...

% exact solution of the ODE m' = (e/k) - (p/k)*m,  m(0) = m0
    mexact = sqrt(e/pexact)*tanh(sqrt(e*pexact)*tpte/k ...
                                +atanh(m0*sqrt(pexact/e)));
```

where the exact value $\phi = 0.248$ corresponds to the final mass $m(30) = 95.5$. (Note that the value $\phi = 21.6$ for the the rule of thumb in the previous example is determined empirically in the same way.)

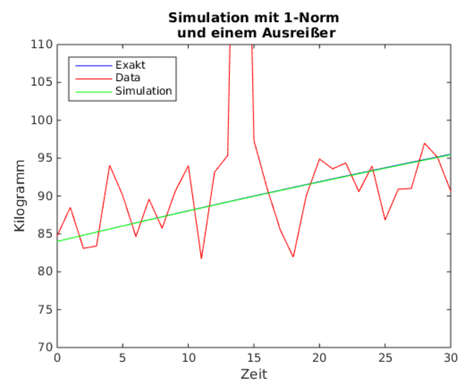
Results with `ns=5%` noise and with (a) ℓ_2-norm and no outliers, (b) ℓ_2-norm and one outlier, (c) ℓ_1-norm and one outlier are shown here with the estimated value of $\phi^\star$:



(a) $\phi^\star = 0.239$



(b) $\phi^\star = 0.118$



(c) $\phi^\star = 0.250$

- ## Exercise 3: Stochastic Discovery

◦ Task

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

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

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.

- **Solution**

That no treasures have been discovered at the time $t = 0$ corresponds to the initial state,

$$p_0(0) = 1, \quad p_1(0) = 0, \quad \dots \quad p_N(0) = 0, \quad \text{d.h. } p_i(0) = \delta_{i,0}.$$

A Matlab function for the solution to this system of ordinary differential equations is given as follows.

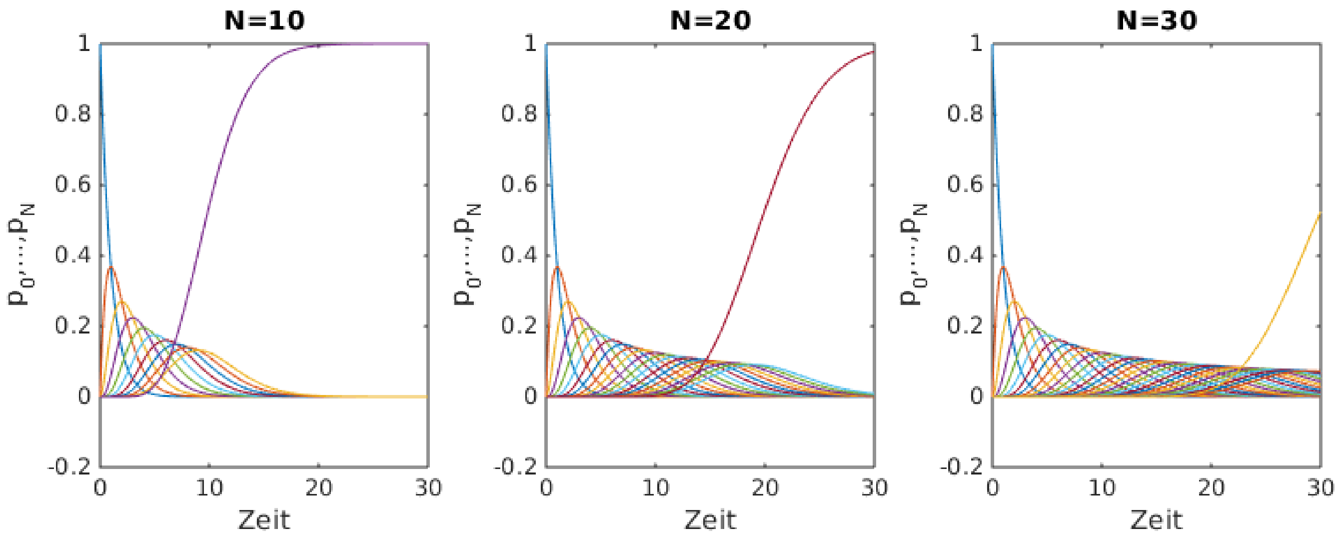
```
function [t,p] = treas(N,b,T)

% solve the system of ODEs
%    P'(t) = b*D*P(t),  P(t) = {p_{i+1}(t): i=0,N}
%    p_0(0) = 1, p_i(0) = 0, i=1,...,N

% coefficient matrix
    N1 = N+1;
    D  = spdiags(ones(N1,1),-1,N1,N1) ...
       - spdiags(ones(N1,1), 0,N1,N1);
    D(N1,N1) = 0;

% right side for the system
    dp = @(t,p) b*(D*p);

% solution time interval
    tpte = [0;T];
% options
    opts = odeset('RelTol',1.0e-6);
% initial conditions
    p0   = zeros(N1,1); p0(1) = 1;
% solution
    [t,p] = ode45(dp,tpte,p0,opts);

end
```

This is called from the following Matlab code to solve the system for various values of N.

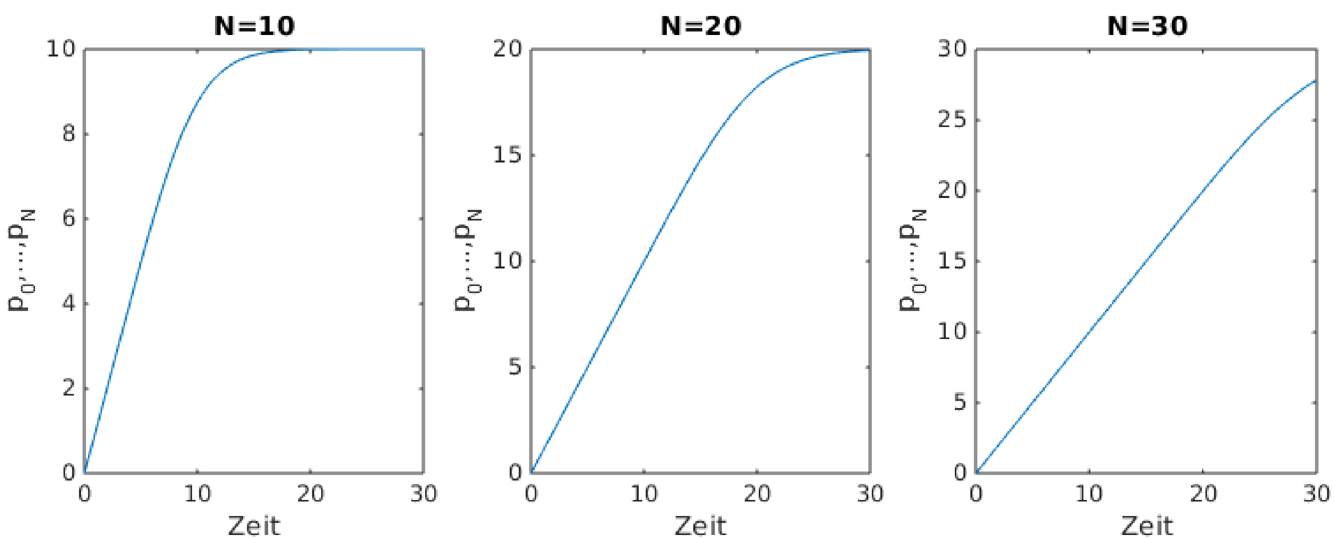
```
function S01Exp3

    b = 1;
    T = 30;

    N = 10;
    [t1,p1] = treas(N,b,T);
    N = 20;
    [t2,p2] = treas(N,b,T);
    N = 30;
    [t3,p3] = treas(N,b,T);

    h1 = figure(1); close(h1); h1 = figure(1);
    set(h1,'Position',[10 10 900 300]);
```

```
    subplot(1,3,1)
    plot(t1,p1)
    xlabel('Zeit'); ylabel('p_0,...,p_N'); title('N=10')
    subplot(1,3,2)
    plot(t2,p2)
    xlabel('Zeit'); ylabel('p_0,...,p_N'); title('N=20')
    subplot(1,3,3)
    plot(t3,p3)
    xlabel('Zeit'); ylabel('p_0,...,p_N'); title('N=30')

    h2 = figure(2); close(h2); h2 = figure(2);
    set(h2,'Position',[10 10 900 300]);
    subplot(1,3,1)
    plot(t1,p1*(0:10)')
    xlabel('Zeit'); ylabel('p_0,...,p_N'); title('N=10')
    subplot(1,3,2)
    plot(t2,p2*(0:20)')
    xlabel('Zeit'); ylabel('p_0,...,p_N'); title('N=20')
    subplot(1,3,3)
    plot(t3,p3*(0:30)')
    xlabel('Zeit'); ylabel('p_0,...,p_N'); title('N=30')

end
```

Results for $\beta = 1$, $T = 30$ and for $N = 10, 20, 30$ are given first in terms of the following probabilities $\{p_i(t) : t \in [0, T]\}_{i=0}^N$



and then in terms of the expected values $\{E(t) : t \in [0, T]\}$, $E(t) = \sum_{i=0}^N ip_i(t)$,



In each case $p_i(t)$ reaches a maximum later than $p_{i-1}(t)$ for $1 \leq i \leq N - 1$. Toward the end of the time interval $p_N(t)$ approaches 1, but for N ever larger, $p_N(t)$ approaches 1 ever later. If the system were infinity large (i.e., $N \to \infty$), then $p_i(t) \to 0$, $t \to \infty$, would hold for every $i \geq 0$. For N ever larger the curve $E(t)$ is ever closer to βt.

• Exercise 4: PCA and ICA

○ Task

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_c, $K = \frac{1}{4} Y_c Y_c^\top$, V and $\Lambda = \text{diag}\{\lambda_i\}$ with $KV = V\Lambda$ and $Y_s = \Lambda^{-\frac{1}{2}} V^\top Y_c$. Plot Y and Y_s.

(b) Show that the sphered data satisfy $\frac{1}{4} Y_s Y_s^\mathrm{T} = I$. 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 $J(\theta) = \mathcal{K}^2(\boldsymbol{u}(\theta) Y_s)$ where $\mathcal{K}$ is the kurtosis. Using this plot, determine the value θ^* which maximizes J. Set $X_c = U(\theta^*) Y_s$. 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.,

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

○ Solution

∗ Part (a) Principle Components

The averaged data are

$$\bar{Y} = \tfrac{1}{4} Y \mathbf{1} = \begin{bmatrix} (0+1+2+3)/4 \\ (0+1+1+2)/4 \end{bmatrix} = \begin{bmatrix} 1.5 \\ 1.0 \end{bmatrix}, \quad \mathbf{1} \in \mathbb{R}^4$$

The centered data are

$$Y_z = Y - \bar{Y} \mathbf{1}^\top = \begin{bmatrix} -1.5 & -0.5 & +0.5 & +1.5 \\ -1.0 & 0.0 & 0.0 & 1.0 \end{bmatrix}$$

The covariance matrix is

$$K = \tfrac{1}{4} Y_z Y_z^\top = \begin{bmatrix} 1.25 & 0.75 \\ 0.75 & 0.50 \end{bmatrix}$$

The eigenspace decomposition of the covariance matrix is

$$KV = V\Lambda, \quad V = \begin{bmatrix} +0.5257 & -0.8507 \\ -0.8507 & -0.5257 \end{bmatrix}, \quad \Lambda = \begin{bmatrix} 0.0365 & 0 \\ 0 & 1.7135 \end{bmatrix}$$

The sphered data are

$$Y_s = \Lambda^{-\frac{1}{2}} V^\top Y_z = \begin{bmatrix} 0.3249 & -1.3764 & 1.3764 & -0.3249 \\ 1.3764 & 0.3249 & -0.3249 & -1.3764 \end{bmatrix}, \quad \text{die erfüllen} \quad \frac{1}{4} Y_s Y_s^\top = I$$

* **Part (b) Projections**

In general it holds that

$$\begin{aligned}\tfrac{1}{n}Y_\mathrm{s}Y_\mathrm{s}^\top &= \tfrac{1}{n}(\Lambda^{-\frac{1}{2}}V^\top Y_\mathrm{z})(\Lambda^{-\frac{1}{2}}V^\top Y_\mathrm{z})^\top = \Lambda^{-\frac{1}{2}}V^\top(\tfrac{1}{n}Y_\mathrm{z}Y_\mathrm{z}^\top)V\Lambda^{-\frac{1}{2}}\\ &= \Lambda^{-\frac{1}{2}}V^\top KV\Lambda^{-\frac{1}{2}} = \Lambda^{-\frac{1}{2}}V^\top(V\Lambda V^\top)V\Lambda^{-\frac{1}{2}}\\ &= \Lambda^{-\frac{1}{2}}(V^\top V)\Lambda(V^\top V)\Lambda^{-\frac{1}{2}} = \Lambda^{-\frac{1}{2}}\Lambda\Lambda^{-\frac{1}{2}} = I.\end{aligned}$$

For a $\boldsymbol{w} \in \mathbb{R}^2$ with $\|\boldsymbol{w}\|_{\ell_2} = 1$ the projections $\boldsymbol{p} = \boldsymbol{w}\boldsymbol{y}_\mathrm{p}^\top$ of the sphered data Y_s onto the $\boldsymbol{w}$-axis satisfy

$$0 = \boldsymbol{w}^\top(\boldsymbol{p} - Y_\mathrm{s}) = (\boldsymbol{w}^\top\boldsymbol{w})\boldsymbol{y}_\mathrm{p}^\top - \boldsymbol{w}^\top Y_\mathrm{s} = \boldsymbol{y}_\mathrm{p}^\top - \boldsymbol{w}^\top Y_\mathrm{s}.$$

Thus $\boldsymbol{p} = \boldsymbol{w}\boldsymbol{w}^\top Y_\mathrm{s}$ holds, and the coordinates of these points on the $\boldsymbol{w}$-axis are

$$\boldsymbol{y}_\mathrm{p} = \boldsymbol{w}^\top Y_\mathrm{s}$$

The mean and variance of these values are

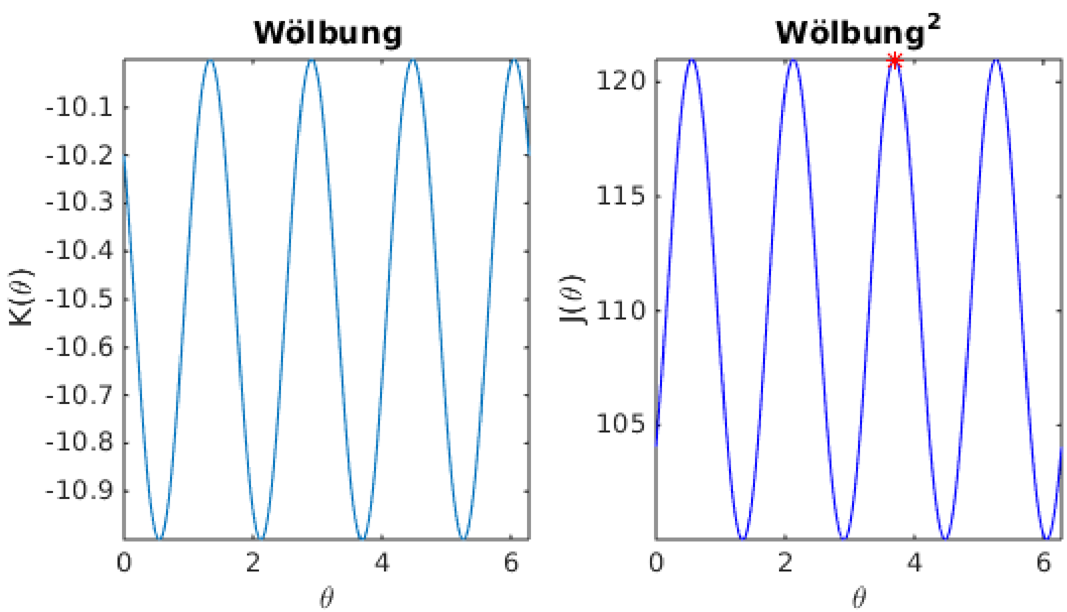
$$\tfrac{1}{4}\boldsymbol{y}_\mathrm{p}\mathbf{1} = \tfrac{1}{4}\boldsymbol{w}^\top Y_\mathrm{s}\mathbf{1} = \tfrac{1}{4}\boldsymbol{w}^\top(\Lambda^{-\frac{1}{2}}V^\top Y_\mathrm{z})\mathbf{1} = \tfrac{1}{4}\boldsymbol{w}^\top\Lambda^{-\frac{1}{2}}V^\top[(Y - \bar{Y}\mathbf{1}^\top)\mathbf{1}] = \boldsymbol{w}^\top\Lambda^{-\frac{1}{2}}V^\top[\tfrac{1}{4}Y\mathbf{1} - \bar{Y}] = 0$$

respectively

$$\tfrac{1}{4}\boldsymbol{y}_\mathrm{p}\boldsymbol{y}_\mathrm{p}^\top = \tfrac{1}{4}(\boldsymbol{w}^\top Y_\mathrm{s})(\boldsymbol{w}^\top Y_\mathrm{s})^\top = \boldsymbol{w}^\top(\tfrac{1}{4}Y_\mathrm{s}Y_\mathrm{s})^\top)\boldsymbol{w} = \boldsymbol{w}^\top\boldsymbol{w} = 1.$$

* **Part (c) Independent Components**

The graphical representation of the functions $\mathcal{K}(\theta) = \mathcal{K}(\boldsymbol{u}(\theta)Y_\mathrm{s})$ respectively $J(\theta) = \mathcal{K}^2(\boldsymbol{u}(\theta)Y_\mathrm{s})$ are



where a red $*$ marks the maximum. The maximizing value for $J(\theta)$ is

$$\theta^\star = 3.6945$$

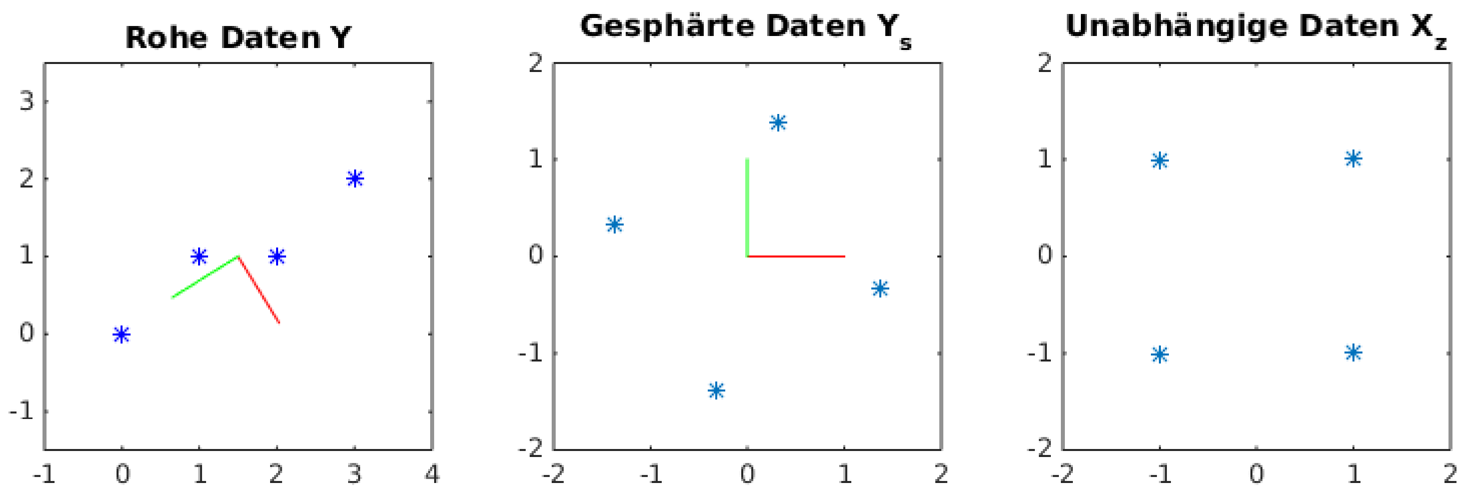
and the maximally independet data are

$$X_\mathrm{z} = U(\theta^\star)Y_\mathrm{s} = \begin{bmatrix} -1 & +1 & -1 & +1 \\ -1 & -1 & +1 & +1 \end{bmatrix}$$

where each column satisfies the following with equal probability,

$$P(x = \alpha \& y = \beta) = P(x = \alpha) \cdot P(y = \beta), \quad x, y = \pm 1.$$

The graphical representation of the data Y, Y_s and X_z is



These results are computed with the following Matlab Code.

```
Y=[0 1 2 3;0 1 1 2];
Yq = Y*ones(4,1)/4;
Yz = Y-Yq*ones(1,4);
K  = Yz*Yz'/4;
[V,D] = eig(K);
Ys = D^(-1/2)*V'*Yz;
f = @(t) sum(([cos(t),sin(t)]*Ys).^4)/4-3*sum(([cos(t),sin(t)]*Ys).^2)^2/4;
n = 1001;
th = linspace(0,2*pi,n);
fh = zeros(1,n);
for i=1:n
   fh(i) = f(th(i));
end
ih = find(fh.^2 == max(fh.^2),1);
tt = th(ih);
Xz = [cos(tt),sin(tt);-sin(tt),cos(tt)]*Ys;

h2 = figure(2); close(h2); h2 = figure(2);
set(h2,'Position',[10 10 600 300]);
subplot(1,2,1)
plot(th,fh)
xlabel('\theta')
ylabel('K(\theta)')
```

```
axis tight
title('Wlbung')
subplot(1,2,2)
plot(th,fh.^2,'b',tt,max(fh.^2),'r*')
xlabel('\theta')
ylabel('J(\theta)')
axis tight
title('Wlbung^2')

h1 = figure(1); close(h1); h1 = figure(1);
set(h1,'Position',[10 10 900 300]);

subplot(1,3,1)
plot(Y(1,:),Y(2,:),'b*', ...
     [Yq(1),Yq(1)+V(1,1)],[Yq(2),Yq(2)+V(1,2)],'r', ...
     [Yq(1),Yq(1)+V(2,1)],[Yq(2),Yq(2)+V(2,2)],'g')
axis([-1 4 -1.5 3.5])
pbaspect([1 1 1])
title('Rohe Daten Y')

subplot(1,3,2)
plot(Ys(1,:),Ys(2,:),'*',[0,1],[0,0],'r',[0,0],[0,1],'g')
axis([-2 2 -2 2])
pbaspect([1 1 1])
title('Gesphrte Daten Y_s')

subplot(1,3,3)
plot(Xz(1,:),Xz(2,:),'*')
axis([-2 2 -2 2])
pbaspect([1 1 1])
title('Unabhngige Daten X_z')
```

• Exercise 5: Dimensional Analysis

◦ Task

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.)

◦ Solution

∗ Part (a) Stone

The $n = 6$ involved quantities are

G_1	v	impact velocity	LZ^{-1}
G_2	h	height of the stone	L
G_3	m_S	mass of the stone	M
G_4	m_E	mass of the Earth	M
G_5	g	acceleration on Earth surface	LZ^{-2}
G_6	τ	fall time of the stone	Z

with respect to the $r = 3$ base quantities g_1 = length (L), g_2 = time (Z) und g_3 = mass (M). The 2., 3. and 6. columns of the matrix

$$A = \underbrace{\begin{bmatrix} 1 & 1 & 0 & 0 & 1 & 0 \\ -1 & 0 & 0 & 0 & -2 & 1 \\ 0 & 0 & 1 & 1 & 0 & 0 \end{bmatrix}}_{G_1\ G_2\ G_3\ G_4\ \ G_5\ G_6} \begin{matrix} g_1 \\ g_2 \\ g_3 \end{matrix}$$

are clearly linearly independet, and so the matrix A has rank $r = 3$. According to the Buckingham Pi theorem $n - r = 3$ dimensionless combinations $\{\Pi_1, \Pi_2, \Pi_3\}$ of the derived quantities $\{G_1, \ldots, G_6\}$ are sought, where $\Phi(G_1, \ldots, G_6) = 1$ may be rewritten as $\Psi(\Pi_1, \Pi_2, \Pi_3)$. One choses very simply,

$$\Pi_3 = m_\mathrm{S}/m_\mathrm{E}$$

since this can be estimated with a constant, namely $\Pi_3 \approx 0$. Yet 2 more are sought which are independent of this one. Simply trying possibilities, one writes v and supplements it with other quantities until the product is dimensionless,

$$\Pi_1 = v\tau h^{-1}.$$

Since acceleration on the Earth surface is constant, the following can be estimated with a constant,

$$\Pi_2 = g\tau v^{-1}.$$

The quantitites Π_1 and Π_2 are of course not uniquely determined. The desired physical relationship should describe the impact velocity. It is of the form

$$v = F(h, m_\mathrm{S}, m_\mathrm{E}, g, \tau)$$

where the function F is still unknown. Since the vectors

$$\begin{aligned} \Pi_1 : \ \boldsymbol{\lambda}_1 &= (1, -1, 0, 0, 0, 1) \\ \Pi_2 : \ \boldsymbol{\lambda}_2 &= (-1, 0, 0, 0, 1, 1) \\ \Pi_3 : \ \boldsymbol{\lambda}_3 &= (0, 0, 1, -1, 0, 0) \end{aligned}$$

are linearly independent, the Buckingham Pi theorem can be used to replace the relation in F with a relation involving the dimensionless quantities,

$$\Pi_1 = f(\Pi_2, \Pi_3)$$

i.e.,

$$v\tau h^{-1} = f(g\tau v^{-1}, m_\mathrm{S}/m_\mathrm{E})$$

or

$$v = h\tau^{-1} f(g\tau v^{-1}, m_\mathrm{S}/m_\mathrm{E})$$

where the function f is still unknown. Yet the mass of the Earth is very large and with $g \approx$ constant, it follows that $v/\tau \approx g$. There results approximately

$$\Pi_2 = g\tau v^{-1} \approx 1, \quad \Pi_3 = m_{\mathrm{S}}/m_{\mathrm{E}} \approx 0.$$

Thus it is assumed

$$f(\Pi_2, \Pi_3) = f(g\tau v^{-1}, m_{\mathrm{S}}/m_{\mathrm{E}}) \overset{\Pi_2,\Pi_3 \to (1,0)}{\longrightarrow} k \quad \text{(constant)}.$$

It follows

$$v = kh/\tau$$

where the constant can be estimated with $k \approx 2$ through experimentation.

∗ Part (b) Atom Bomb

The $n = 9$ involved quantities are

G_1	E	energy of the atomic bomb	$\mathrm{ML^2Z^{-2}}$
G_2	t	time since the ignition	Z
G_3	R	radius of the fireball	L
G_4	ρ_{A}	outside air density	$\mathrm{ML^{-3}}$
G_5	ρ_{I}	inside air density	$\mathrm{ML^{-3}}$
G_6	p_{A}	outside air pressure	$\mathrm{ML^{-1}Z^{-2}}$
G_7	p_{I}	inside air pressure	$\mathrm{ML^{-1}Z^{-2}}$
G_8	T_{A}	outside air temperature	T
G_9	T_{I}	inside aire temperature	T

with respect to $r = 4$ base quantities g_1 = length (L), g_2 = time (Z), g_3 = mass (M) and g_4 = temperature (T). The 1., 2., 3. and 9. columns of the matrix

$$A = \underbrace{\begin{bmatrix} 2 & 0 & 1 & -3 & -3 & -1 & -1 & 0 & 0 \\ -2 & 1 & 0 & 0 & 0 & -2 & -2 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \end{bmatrix}}_{G_1 \; G_2 \; G_3 \; G_4 \; G_5 \; G_6 \; G_7 \; G_8 \; G_9} \begin{matrix} g_1 \\ g_2 \\ g_3 \\ g_4 \end{matrix}$$

are clearly linearly independet, and so the matrix A has ranke $r = 3$. According to the Buckingham Pi theorem $n - r = 5$ dimensionless combinations $\{\Pi_1, \Pi_2, \Pi_3\}$ of the derived quantities $\{G_1, \ldots, G_6\}$ are sought, where $\Phi(G_1, \ldots, G_6) = 1$ may be rewritten as $\Psi(\Pi_1, \Pi_2, \Pi_3)$. One choses very simply,

$$\Pi_3 = \rho_{\mathrm{A}}/\rho_{\mathrm{I}}, \quad \Pi_4 = p_{\mathrm{A}}/p_{\mathrm{I}}, \quad \Pi_5 = T_{\mathrm{A}}/T_{\mathrm{I}}$$

since this can be estimated with a constant, namely $\Pi_3, \Pi_4, \Pi_5 \approx 0$. Yet 2 more are sought which are independent of these. Simply trying possibilities, one writes E and supplements it with other quantities until the product is dimensionless,

$$\Pi_1 = E(\rho_{\mathrm{A}}^{-1} R^5 t^2).$$

Compared with p_{A} and t, E und ρ_{I} are large, and therefore

$$\Pi_2 = t^6 p_{\mathrm{A}}^5 E^{-2} \rho_{\mathrm{I}}^{-3}$$

can be well estimated with a constant, $\Pi_2 \approx 0$. The quantitites Π_1 and Π_2 are of course not uniquely determined. The desired physical relationship should describe the energy. It is of the form

$$E = F(t, R, \rho_\mathrm{A}, \rho_\mathrm{I}, p_\mathrm{A}, p_\mathrm{I}, T_\mathrm{A}, T_\mathrm{I})$$

where the function F is still unknown. Since the vectors

$$\begin{array}{rcl} \Pi_1: \boldsymbol{\lambda}_1 &=& (1,2,-5,-1,0,0,0,0,0) \\ \Pi_2: \boldsymbol{\lambda}_2 &=& (-2,6,0,0,-3,5,0,0,0) \\ \Pi_3: \boldsymbol{\lambda}_3 &=& (0,0,0,1,-1,0,0,0,0) \\ \Pi_4: \boldsymbol{\lambda}_4 &=& (0,0,0,0,0,1,-1,0,0) \\ \Pi_5: \boldsymbol{\lambda}_4 &=& (0,0,0,0,0,0,0,1,-1) \end{array}$$

are linearly independent, the Buckingham Pi theorem can be used to replace the relation in F with a relation involving the dimensionless quantities,

$$\Pi_1 = f(\Pi_2, \Pi_3, \Pi_4, \Pi_5)$$

i.e.,

$$E(\rho_\mathrm{A}^{-1} R^5 t^2) = f(t^6 p_\mathrm{A}^5 E^{-2} \rho_\mathrm{I}^{-3}, \rho_\mathrm{A}/\rho_\mathrm{I}, p_\mathrm{A}/p_\mathrm{I}, T_\mathrm{A}/T_\mathrm{I})$$

or

$$E = (\rho_\mathrm{A} R^{-5} t^{-2}) f(t^6 p_\mathrm{A}^5 E^{-2} \rho_\mathrm{I}^{-3}, \rho_\mathrm{A}/\rho_\mathrm{I}, p_\mathrm{A}/p_\mathrm{I}, T_\mathrm{A}/T_\mathrm{I})$$

where the function f is still unknown. Yet through

$$\Pi_2, \Pi_3, \Pi_4, \Pi_5 \approx 0$$

it is assumed that f can be estimated with a constant,

$$f(\Pi_2, \Pi_3, \Pi_4, \Pi_5) = f(t^6 p_\mathrm{A}^5 E^{-2} \rho_\mathrm{I}^{-3}, \rho_\mathrm{A}/\rho_\mathrm{I}, p_\mathrm{A}/p_\mathrm{I}, T_\mathrm{A}/T_\mathrm{I}) \stackrel{\Pi_2,\Pi_3,\Pi_4,\Pi_5 \to 0}{\longrightarrow} k \quad \text{(constant)}.$$

It follows

$$E = k \rho_\mathrm{A} R^{-5} t^{-2}$$

where the constant k must be estimated through experimentation. With a video of the explosion, the data $\{(t_n, R_n)\}_{n=1}^N$ (fireball radius vs. time) are available. Through

$$R^5 = \left(\frac{E}{\rho_\mathrm{A} k}\right) t^2 \quad \text{oder} \quad R(t) = \gamma t^{2/5}$$

the constant

$$\gamma = \left(\frac{E}{\rho_\mathrm{A} k}\right)^{\frac{1}{5}} \quad \text{is so estimated:} \quad \gamma \approx \frac{1}{N} \sum_{n=1}^N R_n t_n^{-2/5}.$$

One carrys out a sufficiently similar experiment, in which a known about of explosive mit known energy E_0 is ignited. For this it is assumed that the above constant k is again the same. For the course of the controlled explosion the data $\{(t_0, R_0)_m\}_{m=1}^M$ (fireball radius vs. time) are measured and the constant is calculated,

$$\gamma_0 = \left(\frac{E_0}{\rho_\mathrm{A} k}\right)^{\frac{1}{5}} \quad \text{so abgeschätzt:} \quad \gamma_0 \approx \frac{1}{M} \sum_{m=1}^M (R_0 t_0^{-2/5})_m.$$

It follows that the sought energy E is given through $k = E/(\rho_\mathrm{A}\gamma^5) = E_0/(\rho_\mathrm{A}\gamma_0^5)$ or

$$E = E_0(\gamma/\gamma_0)^5.$$

∗ **Part (c) Kepler's Law**

(The solution in the lectures notes of Prof Thaler should be supplemented with the confirmation that the prerequisites of the Buckingham Pi theorem are satisfied.) First the list of $n = 6$ involved quantities is:

G_1	τ	orbital period	Z
G_2	G	gravitational constant	$\mathrm{M}^{-1}\mathrm{L}^3\ \mathrm{Z}^{-2}$
G_3	m_S	mass of the sun	M
G_4	m_P	mass of the planet	M
G_5	r	length of the major axis	L
G_6	e	eccentricity	1

with respect to the $r = 3$ base quantities g_1 = length (L), g_2 = time (Z) and g_3 = mass (M). According to Keplers first law the planet trajectories are ellipses. Therefore the eccentricity is included in the list. The eccentricity e of an ellipse is the distance from the center to the focus divided by the length of the major axis, so it is dimensionless. The 1., 3. and 5. columns of the matrix

$$A = \underbrace{\begin{bmatrix} 0 & 3 & 0 & 0 & 1 & 0 \\ 1 & -2 & 0 & 0 & 0 & 0 \\ 0 & -1 & 1 & 1 & 0 & 0 \end{bmatrix}}_{G_1\ G_2\ G_3\ G_4\ G_5\ G_6} \begin{matrix} g_1 \\ g_2 \\ g_3 \end{matrix}$$

are clearly linearly independent, so the matrix A has ranke $r = 3$. According to the Buckingham Pi theorem, $n - r = 3$ dimensionless combinations $\{\Pi_1, \Pi_2, \Pi_3\}$ of the derived quantities Größen $\{G_1, \ldots, G_6\}$ are sought, where $\Phi(G_1, \ldots, G_6) = 1$ may be rewritten as $\Psi(\Pi_1, \Pi_2, \Pi_3)$. One choses very simply,

$$\Pi_2 = e, \quad \Pi_3 = m_\mathrm{P}/m_\mathrm{S}$$

since this can be estimated with a constant, namely $\Pi_2, \Pi_3 \approx 0$. Yet another is sought which is independent of these. Simply trying possibilities, one writes G and supplements it with other quantities until the product is dimensionless,

$$\Pi_1 = G m_\mathrm{S} \tau^2 r^{-3}$$

This choice for Π_1 is of course not uniquely determined. The desired physical relationship should describe the orbital period. It is of the form

$$\tau = F(G, m_\mathrm{P}, m_\mathrm{S}, r, e)$$

where the function F is still unknown. Since the vectors

$$\begin{aligned} \Pi_1 : \ \boldsymbol{\lambda}_1 &= (2, 1, 1, 0, -3, 0) \\ \Pi_2 : \ \boldsymbol{\lambda}_2 &= (0, 0, 0, 0, 0, 1) \\ \Pi_3 : \ \boldsymbol{\lambda}_3 &= (0, 0, -1, 1, 0, 0) \end{aligned}$$

are linearly independent, the Buckingham Pi theorem can be used to replace the relation in F with a relation involving the dimensionless quantities,

$$\Pi_1 = f(\Pi_2, \Pi_3)$$

i.e.,

$$G m_\mathrm{S} \tau^2 r^{-3} = f(e, m_\mathrm{P}/m_\mathrm{S})$$

or

$$\tau^2 = r^3 G m_S f(e, m_P/m_S)$$

where the function f is still unknown. One considers that in real planetary systems the eccentricity of the orbits is very small, and the mass of the sun is very large, so it is a good approximation that

$$\Pi_2 = e \approx 0, \quad \Pi_3 = m_P/m_S \approx 0.$$

So it is assumed that

$$f(\Pi_2, \Pi_3) = f(e, m_P/m_S) \overset{\Pi_2,\Pi_3 \to 0}{\longrightarrow} k \quad \text{(constant)}.$$

This assumption should not be taken for granted. An arbitrary function f need not to be continuous or even bounded near a chosen point. In physics one simply often tries to push an argument as far as possible with very few assumptions. There now results

$$\tau^2 = k G m_S r^3.$$

Thus the square of the orbital time is proportional to the third power of the distance to the sun. Since the constant of proportionality $k/(G m_S)$ can be assumed to be independent of the planet considered, there results the third Kepler law when the ratio τ_1^2/τ_2^2 is considered for two planets. By solving Newton's equations for planetary systems, there results for the function f,

$$f(e, m_P/m_S) = 4\pi^2.$$

So the eccentricity and the mass of the planet are not even involved, and the correct formula is,

$$\tau^2 = 4\pi^2 G m_S r^3.$$

It is noteworthy that this formula has been found without computational expense. The method requires only an informed understanding of physics, since this is necessary to identify the relevant physical quantities. If m_S were taken, e.g., to be the mass of Sirius and r were taken to be the distance between the planet and the center of the galaxy, then the result may reflect correct dimensions and yet be senseless and physically incorrect.

• Exercise 6: Chemical Reactions

○ Task

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.

◦ **Solution**

The initial value problem for the reaction is

$$x'(t) = f(x), \quad x(0) = 0$$

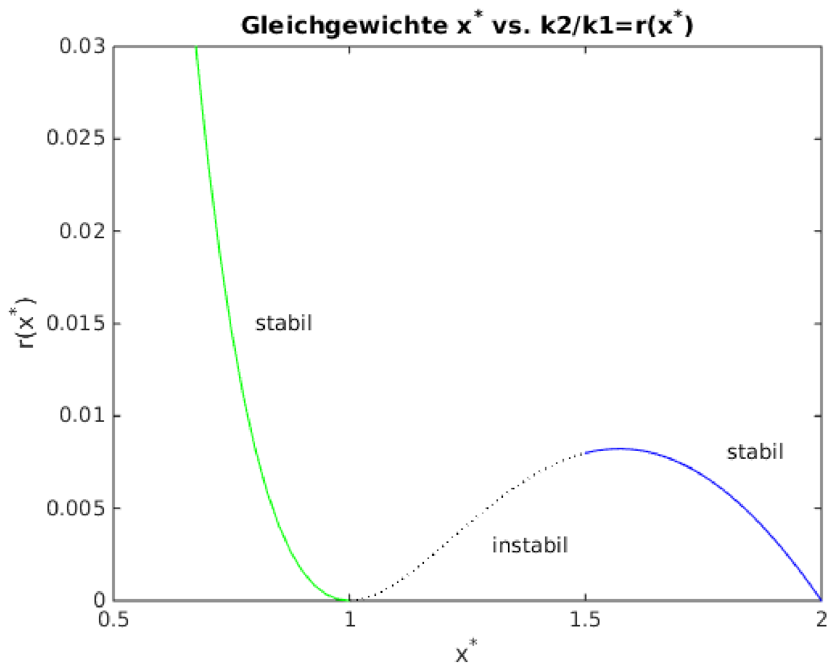
where

$$f(x) = \kappa_1(2 - 2x)^2(2 - x) - \kappa_2(1 + x)(2 + 2x)^2.$$

An equilibrium $x^\star$ for the reaction satisfies $f(x^\star) = 0$ or

$$0 < \frac{\kappa_2}{\kappa_1} = \frac{(1 - x^\star)^2(2 - x^\star)}{(1 + x^\star)^3} =: r(x^\star) \quad \text{für } x^\star \in (-1, 2)$$

where $r(x)$ has the following graphical representation.



It remains to show that the equilibrium states $x^\star$ satisfying

$$r'(x^\star) < 0$$

are (locally asymptotically) stable, while the equilibrium states $x^\star$ satisfying

$$r'(x^\star) > 0$$

are unstable. Due to the calculation

$$r'(x) = \frac{-11 + 18x - 7x^2}{(1+x)^4} = \frac{(x-1)(11-7x)}{(1+x)^4}$$

it follows

$$r'(x) < 0, \quad x \in (-1,1) \cup (11/7, +\infty) \quad \text{and} \quad r'(x) > 0, \quad x \in (1, 11/7)$$

Due to the calculation

$$f'(x) = -4\left[3\kappa_2(1+x)^2 + \kappa_1(5 - 8x + 3x^2)\right] = -4\left[3\frac{\kappa_2}{\kappa_1}(1+x)^2 + (5 - 8x + 3x^2)\right]\kappa_1$$

it follows with $\kappa_2/\kappa_1 = r(x^\star)$,

$$\frac{f'(x^\star)}{4\kappa_1} = 3r(x^\star)(1+x^\star)^2 + (5 - 8x^\star + 3x^{\star 2}) = \frac{-11 + 18x^\star - 7x^{\star 2}}{(1+x^\star)} = r'(x^\star)(1+x^\star)^3$$

and the claimed stability follows:

$$f'(x^\star) < 0, \quad x^\star \in (-1,1) \cup (11/7, +\infty) \quad \text{und} \quad f'(x^\star) > 0, \quad x^\star \in (1, 11/7)$$

With

$$p(x, R) = -8x + 10x^2 - 16x^3/3 + x^4 + R(1+x)^4$$

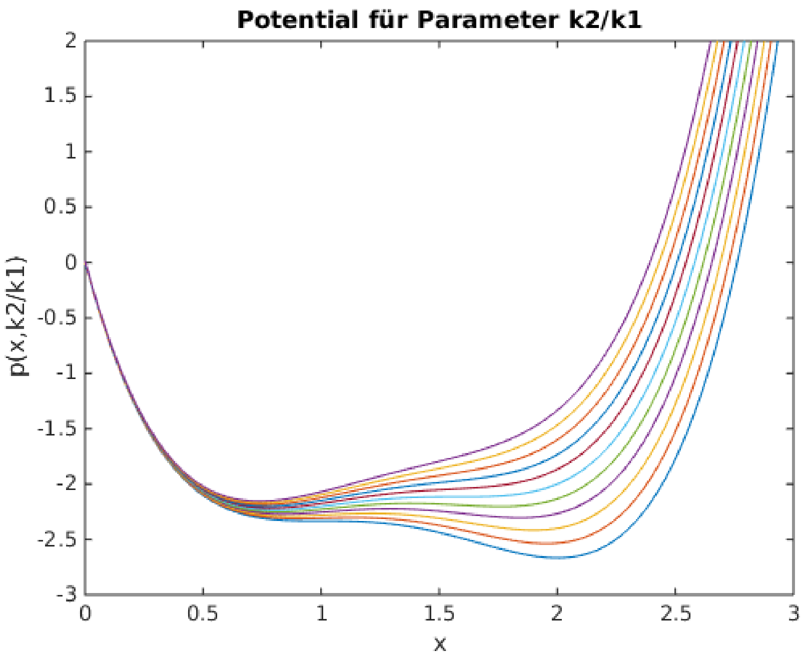
follows

$$f(x)/\kappa_1 = -p_x(x, \kappa_2/\kappa_1)$$

and p is a potential for the function f. For the values

$$R = \frac{2k}{10} \cdot r(11/7) = \frac{2k}{10} \cdot \max_{1 \le x \le 2} r(x), \quad k = 0, \ldots, 10$$

the potential landscape appears as follows,



where the index k increases through these curves from the bottom to the top. The deepest point at the left corresponds to a stable equilibrium $x^\star > 11/7$ where $r'(x^\star) < 0$ holds. The highest point in the middle corresponds to an unstable equilibrium $x^\star \in (1, 11/7)$ where $r'(x^\star) > 0$ holds. As R increases from 0 to $2 \cdot r(11/7)$, the solution remains at the equilibrium in the right valley, as long as it is a valley, even if the left valley is deeper. As soon as the deep point to the right is no longer in a valley, the equilibrium jumps into the valley to the left. On the other hand, as R decreases from $2 \cdot r(11/7)$ to 0, the solution remains at an equilibrium in the left valley, as long as it is a valley, even if the right valley is deeper. As soon as the deep point to the left is no longer in a valley, the equilbrium jumps into the valley to the right. In this way the system exhibits hysteresis.