Prof. W. Gander **Masaryk University Fall 2014**

Least Squares

1. Determine the parameters a and b such that the function $f(x) = ae^{bx}$ fits the following data

x	30.0	64.5	74.5	86.7	94.5	98.9
y	4	18	29	51	73	90

Hint: If you fit $\log f(x)$ the problem becomes very easy!

Solution: Taking the logarithm of the function we get

$$\ln y = \ln a + bx.$$

With the unknown $c = \ln a$ the least squares problem becomes

$$\begin{pmatrix} 1 & 30.0 \\ 1 & 64.5 \\ 1 & 74.5 \\ 1 & 86.7 \\ 1 & 94.5 \\ 1 & 98.9 \end{pmatrix} \begin{pmatrix} c \\ b \end{pmatrix} \approx \begin{pmatrix} \ln 4 \\ \ln 18 \\ \ln 29 \\ \ln 51 \\ \ln 73 \\ \ln 90 \end{pmatrix}.$$

```
x=[30.0 , 64.5 , 74.5 , 86.7 , 94.5 , 98.9]';
y=[ 4    ,   18 ,   29 ,   51 ,    73 , 90]';
A = [ones(size(x)), x]
b=log(y);
p = A\b
a=exp(p(1))
b=p(2)
```

The solution is

$$b = 0.04524310648 \text{ and } c = 0.00789262406 \Rightarrow a = 1.00792752.$$

2. Consider the plane in $\mathbb{R}^3$ given by the equation

$$x_1 + x_2 + x_3 = 0.$$

Construct a matrix P which projects a given point on this plane. Hint: consider first the orthogonal complement of the plane.

Solution: The normal of the plane is $\mathbf{n} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$ and the orthogonal complement is therefore $Ax = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} x$. Because $\mathbb{R}^3 = \mathcal{R}(A) \oplus \mathcal{N}(A^\top)$ we have to compute the projector $P_{\mathcal{N}(A^\top)} = I - AA^+$.

$$A^+ = (A^\top A)^{-1} A^\top = \frac{1}{3}(1, 1, 1)$$

$$\Rightarrow \quad P = I - AA^{+} = I - \frac{1}{3}\begin{pmatrix}1 & 1 & 1\\ 1 & 1 & 1\\ 1 & 1 & 1\end{pmatrix} = \frac{1}{3}\begin{pmatrix}2 & -1 & -1\\ -1 & 2 & -1\\ -1 & -1 & 2\end{pmatrix}.$$

3. Given the matrix

$$A = \begin{pmatrix}1 & 2 & 6\\ 1 & 3 & 7\\ 1 & 4 & 8\\ 1 & 5 & 9\end{pmatrix}$$

Compute a Householder matrix P such that

$$PA = \begin{pmatrix}\sigma & x & x\\ 0 & x & x\\ 0 & x & x\\ 0 & x & x\end{pmatrix}$$

It is sufficient to determine σ and the Householder-vector $\mathbf{u}$.

Solution: $P = I - \mathbf{u}\mathbf{u}^\top$ with $\|\mathbf{u}\|_2 = \sqrt{2}$.

$$\mathbf{u} = \frac{\mathbf{x} - \sigma\mathbf{e}_1}{\sqrt{\|\mathbf{x}\|_2(|x_1| + \|\mathbf{x}\|_2)}}, \qquad \mathbf{x} = \begin{pmatrix}1\\1\\1\\1\end{pmatrix}, \qquad \sigma = -\|\mathbf{x}\|_2 = -2 \quad \text{(avoid cancellation)}$$

Thus

$$\mathbf{u} = \frac{1}{\sqrt{6}}\begin{pmatrix}3\\1\\1\\1\end{pmatrix}, \qquad P\mathbf{x} = \mathbf{x} - \mathbf{u}(\mathbf{u}^\top\mathbf{x}) = \begin{pmatrix}1\\1\\1\\1\end{pmatrix} - \frac{1}{\sqrt{6}}\begin{pmatrix}3\\1\\1\\1\end{pmatrix}\frac{6}{\sqrt{6}} = \begin{pmatrix}-2\\0\\0\\0\end{pmatrix}$$

4. Consider the plane in $\mathbb{R}^3$ given by the equation

$$2x_1 - 2x_3 = 0.$$

Construct a matrix $P \in \mathbb{R}^{3\times 3}$ which reflects a given point at this plane (computes the mirror image).

Solution: The normal vector of the plane is

$$\mathbf{u} = \begin{pmatrix}1\\0\\-1\end{pmatrix}$$

Since $\|\mathbf{u}\|_2 = \sqrt{2}$ the solution is given by the Householder matrix

$$P = I - \mathbf{u}\mathbf{u}^\top = I - \begin{pmatrix}1 & 0 & -1\\ 0 & 0 & 0\\ -1 & 0 & 1\end{pmatrix} = \begin{pmatrix}0 & 0 & 1\\ 0 & 1 & 0\\ 1 & 0 & 0\end{pmatrix}.$$

5. Let the measured points (t_k, y_k) for $i = k, \ldots, m$ be given. We want to fit the function $f(a, b) = ae^{bt}$ such that

$$\sum_{k=1}^{m} \left(ae^{bt_k} - y_k\right)^2 \longrightarrow \min$$

using the Gauss-Newton method. Write up the system of equations for the first iteration step.

Solution: We want to solve the nonlinear least squares problem $\mathbf{f}(\mathbf{x}) \approx 0$ where

$$f_i(\mathbf{x}) = x_1 e^{x_2 t_k} - y_k, \quad k = 1, \ldots, m$$

For Gauss-Newton we expand $\mathbf{f}(\mathbf{x} + \mathbf{h}) \approx \mathbf{f}(\mathbf{x}) + J\,\mathbf{h}$ with the Jacobian

$$J = \begin{pmatrix} \vdots & \vdots \\ \partial f_i / \partial x_1 & \partial f_i / \partial x_2 \\ \vdots & \vdots \end{pmatrix} = \begin{pmatrix} \vdots & \vdots \\ e^{x_2 t_k} & x_1 t_k e^{x_2 t_k} \\ \vdots & \vdots \end{pmatrix}.$$

The system of equations for the correction $\mathbf{h}$ is a linear least squares problem

$$\begin{pmatrix} e^{x_2 t_1} & x_1 t_1 e^{x_2 t_1} \\ \vdots & \vdots \\ e^{x_2 t_m} & x_1 t_m e^{x_2 t_m} \end{pmatrix} \begin{pmatrix} h_1 \\ h_2 \end{pmatrix} \approx - \begin{pmatrix} x_1 e^{x_2 t_1} - y_1 \\ \vdots \\ x_1 e^{x_2 t_m} - y_m \end{pmatrix}$$