

## Week 7

## Deliverables

- Report 2: Section 3. Software for solving linear least squares problems.
- Report 2: The method of residuals for estimating parameters in absorption kinetics.

## Linear regression (linear least squares fitting)

Section 3 of Report Assignment 2 is about linear regression, that is, fitting a straight line to a set of data points. Examples 4.1, 4.2, and 4.5 of **LA** illustrate how you can use your solver for linear systems of equations to do linear regression.

- Create a MATLAB program called `lin_reg` that takes two vectors  $\mathbf{t}$  and  $\mathbf{y}$  as arguments and uses your solver for linear systems of equations (`Gauss_elim`) to do linear regression. (*Hint*: Set up the  $\mathbf{F}$  matrix and solve Equation 4.5 of **LA**.)
- Test your program by reproducing the linear least squares fit in Example 4.5 of **LA**.
- Test your program by using it to solve Problem 25 in Section 12.7.4 of **C**. (*Hint*: Compare to the solution in the back of the book.)

## Absorption kinetics

The final programming part of Report Assignment 2 is to implement the method of residuals for estimating parameters in absorption kinetics. This is the algorithm (1.–7.) described in the beginning of the report assignment.

If you would like to work on a simpler example before working on the algorithm (1.–7.), the following exercises provide a simpler example of parameter estimation in absorption kinetics. The goal is to measure how quickly the body eliminates a drug after intake. The following table describes how caffeine is eliminated in the human body.

$t$ (min)	$C_p$ ( $\mu\text{g/mL}$ )	$\ln C_p$
12	3.75	1.322
40	2.80	1.030
65	2.12	0.751
90	1.55	0.438
125	1.23	0.207
173	0.72	-0.329

- Plot in MATLAB how the plasma concentration of caffeine ( $C_p$ ) develops over time ( $t$ ). Do a normal plot and a semilog plot, where the  $C_p$ -axis uses the logarithmic scale.
- Find a linear least squares fit to the data points  $(t, \ln C_p)$  and write down the equation that describes how the plasma concentration of caffeine ( $C_p$ ) develops over time ( $t$ ).

If we let  $-k$  denote the slope of the line found in the linear least squares fit of this last exercise,  $k$  corresponds to the elimination rate in the report assignment.

Complete the algorithm (1.–7.) using your programs from Sections 1–3 of the report assignment (see the book appendix “Estimation of Absorption Kinetics from Plasma Concentration Data” for help). To test your implementation, use the data provided in the section of the report assignment called “Testing the Software”.

## Software design

If you have time to spare this week, try to draw a diagram that illustrates the design of your software for pharmacokinetics. This diagram should be handed in as a part of your Report 2 when it is in its final form. (*Hint:* You may find the “cross-reference information” provided by the `m2html` tool useful when drawing the diagram.)

## Curriculum

- LA** Chapter 4. *Linear Least Squares Problems*.
- P** Chapter 12. *From Programs to High-Quality Software*.
- LA** Section 3.2.3. *Google PageRank* (an example of math-based software).