Worksheet: PARAMETER ESTIMATION (17. July 2012)
Lecture "Computational Systems Biology", Dr. Jürgen Pahle

1) Comprehension questions
a) How does the particle swarm optimisation algorithm work?
b) Which is better for parameter estimation, the Levenberg-Marquardt method or genetic algorithms?
c) How can you populate your model with parameter values?
d) What is overfitting? How can you detect it?
e) The model you want to fit has structural non-identifiabilities. A colleague recommends you to increase the sampling frequency from one per five minutes to one per minute to help with parameter estimation. Another colleague gives you the advice to get a better mass spectrometer for measuring. What do you think?
f) What are the no free lunch theorems of optimisation (and, thus, also of parameter estimation)?
g) What can happen if you do not scale/weight the residuals in your fitting function appropriately?

2) In the following we will, again, use model number 23 by Rohwer and Botha (2011) in the Biomodels.net database (see exercises on sensitivities and MCA, and on optimisation). Please use the data file SucroseData.csv that can be downloaded from the course webpage. It contains data from several steady state experiments. Try to fit the model to the data using COPASI. Remark: define plots as needed, and also consider that the data file contains information on both dependent and independent "variables".