Introduction to Computational Physics

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(To be discussed on Friday, 13.6. and Monday, 16.6.)

EXERCISE 5.1: **General linear χ^2 fit**

Fit the data set given in `sinfit.dat` with a model that is polynomial up to cubic terms by implementing the solution to the general linear χ^2 fit into Mathematica. Calculate the corresponding one standard deviation errors, correlation coefficients and χ^2 for the fit.

Given the knowledge that the true model does not contain a quadratic term, refit the data with the corresponding model and calculate all parameters of the fit. Compare both fits with respect to the significance of their parameter estimates.

(N.B. Both data sets, `linearfit.dat` of exercise 4.2, and `sinfit.dat` of this exercise where generated from the model $f(x) = \sin(x/3) + 1/\pi$ with some (differing) statistical fluctuations.)

EXERCISE 5.2: **Non-linear χ^2 fit**

Fit the data set given in `lorentz.dat`, representing light emission by a gas, to the non-linear Lorentz model for the intensity as a function of the wave length λ:

$$I(\lambda) \;=\; B + \frac{I_0}{(1 + 4\,(\lambda - \lambda_0)^2/\Gamma^2)}\,.$$

Employ an implementation of Newtons algorithm in Mathematica, starting with the trial solution corresponding to the parameters:

$$\lambda_0 \;=\; 4358.4\,, \qquad \Gamma \;=\; 0.3\,, \qquad I_0 \;=\; 150\,, \qquad B \;=\; 25\,.$$

Investigate the stability of the algorithm while varying the parameters of the trial solution.

Plot the best fit together with the data.