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**

My Mathematica implementation of the solution is provided in `Ex5.1.m`. The notation somewhat follows the one of the Numerical Recipes, and to my mind the implementation is reasonably straightforward.

In the first case of the "wrong" model, even though the χ^2/n.d.f. is great, for the first three parameters, compared to their "true" values, deviations around two standard deviations or slightly larger are found.

For the correct model, the deviation of the first parameter turns out to be around 1σ, and for the other two parameters only half a σ. Also the global χ^2/n.d.f. for this fit is smaller than one and thus perfectly acceptable. Generally, one can also observe that some of the parameters display strong correlations.

EXERCISE 5.2: **Non-linear χ^2 fit**

For this example, no experimental uncertainties were available, and I adjusted them such that the global χ^2/n.d.f. for the fit is close to one. My Mathematica implementation of the solution is provided in `Ex5.2.m`. For this algorithm, maybe the replacements done in the Do-loop which performs the iteration over Newton's method is a little tricky, and should be discussed in some detail.

For this example, the physical significance of the parameters is very transparent, and the trial solution can be read off a plot of the data points. (Certainly, this is not true in the general case, and I intend to discuss doing general fits with MINUIT in my lecture.)

In my example solution, I perform 20 iterations and at first sight the fit does not change after the first 5. But if you look at the result with higher precision (for example with `?a` and `?chi2`), one observes that after a certain number of iterations, the solution fluctuates around the minimum and one cannot reach a higher precision. As for the stability, just play with the initial parameters.

The plot of data together with the fit is provided in `lorentz.ps`.