Data reduction and fitting

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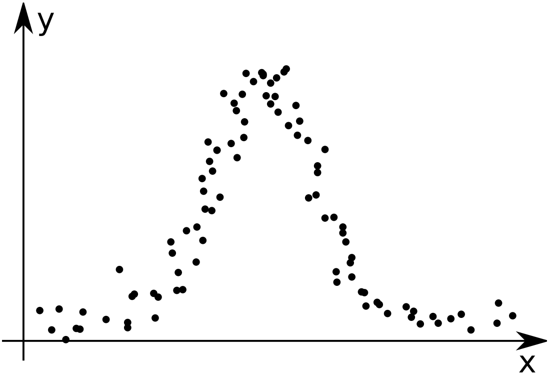
Lecture 07

Data reduction

- Typical modern experiment generates huge amount of data.
- there is no way for a human to comprehend such enormous amount of data



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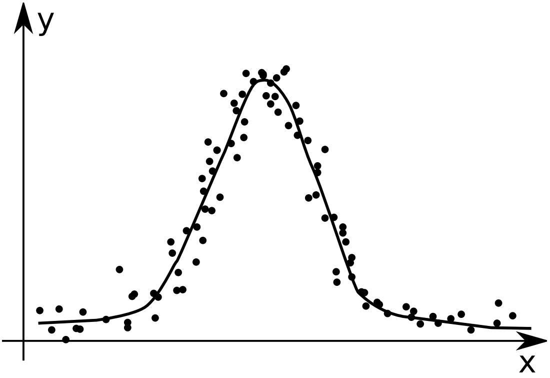


- to extract important parameters we need to post-process the data
- alternatively we want to check how our models reflect reality

Fitting

Someone measured the dependence of an experimental parameter y on another parameter x. We want to extract the unknown model parameters $p_1, p_2, p_3, \ldots = \vec{p}$ via fitting (i.e. finding the best $\vec{p}$) of the model function which depends on x and $\vec{p}$: $f(x, \vec{p})$.

In general x and y could be vectors i.e. multi-dimensional.

Example

- $\vec{x}$ has 2 coordinates: speed of a car and the weight of its load;
- y has the car fuel consumption and temperature.

For simplicity, **we will focus on the one dimensional case** for x and y

- we are given experimental points $x_i \to y_i$
- our model $x_i \to y_{f_i} = f(x_i, \vec{p})$

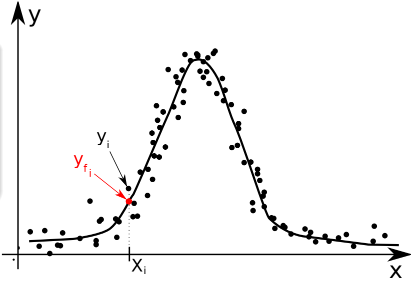
Goodness of the fit

We need to define some way to estimate the goodness of the fit.

Chi-squared test

$$\chi^2 = \sum_i (y_i - y_{f_i})^2$$

Differences of $(y_i - y_{f_i})$ are called residuals.



For a given set of $\{(x_i\, y_i)\}$ and f the goodness of the fit χ^2 depends only on parameters vector $\vec{p}$ of the model/fit function.

Our job is simple: find optimal $\vec{p}$ which minimizes χ^2 using any suitable algorithm. I.e., perform so called **the least square fit.**

Good fit should have the following properties

- the fit should use the smallest possible fitting parameters set
  - with enough fitting parameters you can make zero residuals fit but this is unphysical since all your data has uncertainties in the measurements
- residuals should be randomly scattered around 0
  - i.e. no visible trends of residuals vs x
- standard deviation or RMS residual $= \sqrt{\frac{1}{N}\sum_i^N (y_i - y_{f_i})^2}$ should be in order of the Δy (experimental uncertainty for y)
  - the above condition is often overlooked but you should keep your eyes on it. It also can give you actual estimate of the experimental error bars
- fit should be robust: new points must not change parameters much
- *Eugeniy's extra:* stay away from the high order polynomial fits.
  - line is good, parabola maybe
  - anything else only if there is a deep physical reason for it
  - besides, such fits are usually useless since every new data point usually drastically modifies the fit parameters.

Estimation of uncertainty for parameters

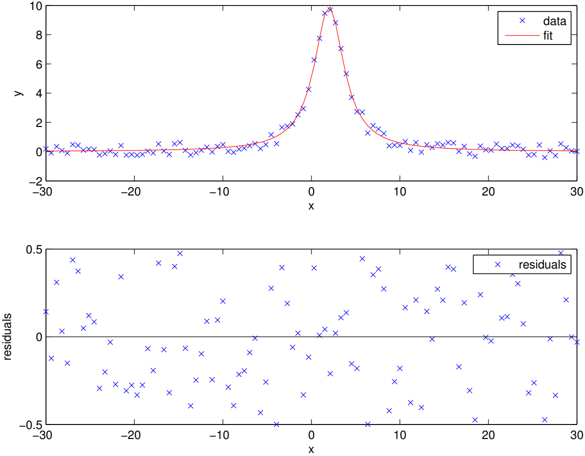
- Δp_i could be estimated by change of the χ^2,
- Δp_i: $\chi^2(p_1, p_2, p_3, \dots p_i + \Delta p_i, \dots) = 2\chi^2(p_1, p_2, p_3, \dots p_i, \dots)$

Practical realization

Have a look at 'fitter.m' where optimization of χ^2 is done with `fminsearch` matlab function.
See 'fitter_usage_example.m' for a particular usage example.

$$f(x,\vec{p}) = \frac{A}{1+\left(\frac{x-x_o}{\gamma}\right)^2}$$

$$\vec{p} = [A, x_o, \gamma] = [9.9444, 1.9936, 2.0354]$$



Matlab built-ins

- see `fit` from the Matlab curve fitting toolbox
  - more cumbersome to start using
  - provides parameters uncertainties
- see `lsqcurvefit` from the Matlab optimization toolbox

They are faster since they take an assumption that merit function is quadratic.

Matlab built-in fit usage example

```
%% built in fit function usage example

% load initial data file
data=load('data_to_fit.dat');
x=data(:,1); % 1st column is x
y=data(:,2); % 2nd column is y

% define the fitting function with fittype
% notice that it is quite human readable
% Matlab automatically treats x as independent variable
f=fittype(@(A,x0,gamma, x) A ./ (1 +((x-x0)/gamma).^2) )

% let's see did Matlab guess fit parameters right
coeffs = coeffnames(f)

% assign initial guessed parameters
% [A, x0, gamma] they are in the order of the appearance
% in the above fit function definition
pin=[3,3,1];

% We fit our data here
[fitobject,gof] = fit (x,y, f, 'StartPoint', pin)

disp('confidence interval/errorbars for  A, x0, and gamma');
ci = confint(fitobject)

% it is good idea to compare fit and data visually
builtin_fit_check(x,y, fitobject);
```