Statistical Data Analysis 2021/22
Lecture Week 8

London Postgraduate Lectures on Particle Physics

University of London MSc/MSci course PH4515

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www.pp.rhul.ac.uk/~cowan/stat_course.html

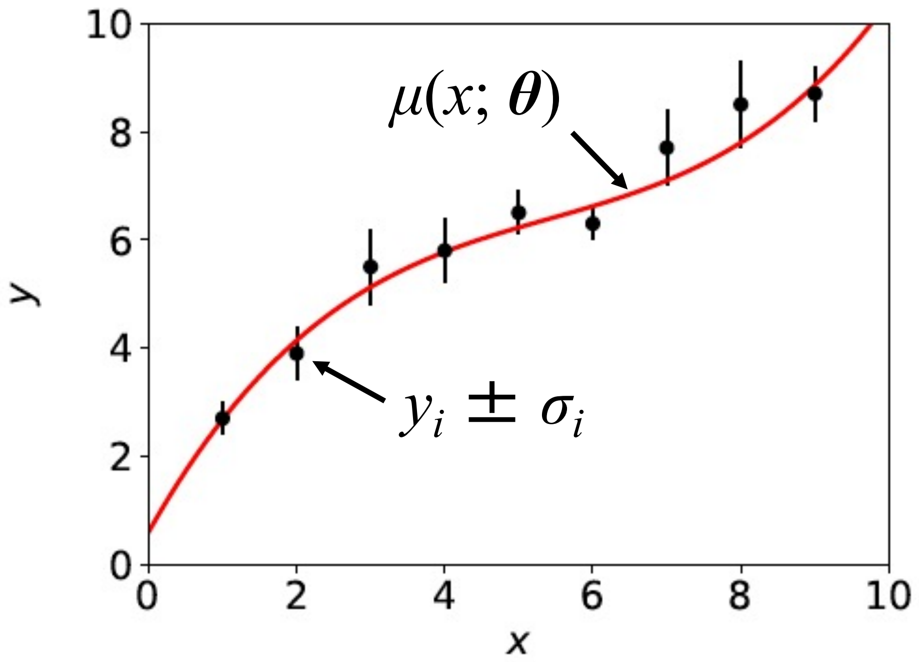
Statistical Data Analysis
Lecture 8-1

- Basic idea of curve fitting
- The method of Least Squares (LS)
- LS from maximum likelihood
- LS with correlated measurements

Curve fitting: basic idea

Consider N independent measured values y_i, $i = 1,.., N$.

Each y_i has a standard deviation σ_i, and is measured at a value x_i of a control variable x known with negligible uncertainty:



The goal is to find a curve $\mu(x; \boldsymbol{\theta})$ that passes “close to” the data points.

Suppose the functional form of $\mu(x; \boldsymbol{\theta})$ is given; goal is to estimate its parameters $\boldsymbol{\theta}$ (= “curve fitting”).

Minimising the residuals

If a measured value y_i has a small σ_i, we want it to be closer to the curve, i.e., measure the distance from point to curve in units of σ_i:

standardized residual of i^{th} point = $\dfrac{y_i - \mu(x_i;\boldsymbol{\theta})}{\sigma_i}$

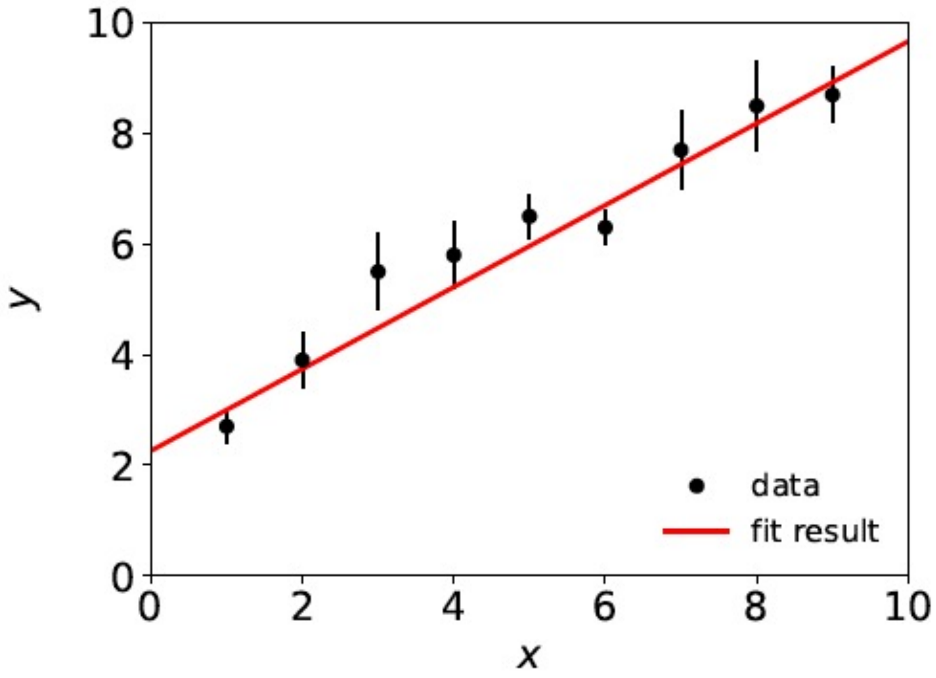
Idea of the method of Least Squares is to choose the parameters that give the minimum of the sum of squared standardized residuals, i.e., we should minimize the "chi-squared":

$$\chi^2(\boldsymbol{\theta}) = \sum_{i=1}^{N} \frac{(y_i - \mu(x_i;\boldsymbol{\theta}))^2}{\sigma_i^2}$$

Least squares estimators

The values that minimize $\chi^2(\boldsymbol{\theta})$ define the least-squares estimators for the parameters, e.g., here assuming

$$\mu(x;\theta_0,\theta_1) = \theta_0 + \theta_1 x$$



$$\hat{\theta}_0 = 2.258$$

$$\hat{\theta}_1 = 0.741$$

Gaussian likelihood function → LS estimators

Suppose the measurements $y_1, \ldots, y_N$, are independent Gaussian r.v.s with means $E[y_i] = \mu(x_i; \boldsymbol{\theta})$ and variances $V[y_i] = \sigma_i^2$, so the the likelihood function is

$$L(\boldsymbol{\theta}) = \prod_{i=1}^{N} \frac{1}{\sqrt{2\pi}\sigma_i} e^{-(y_i - \mu(x_i;\boldsymbol{\theta}))^2 / 2\sigma_i^2}$$

The log-likelihood function is therefore

$$\ln L(\boldsymbol{\theta}) = -\frac{1}{2} \sum_{i=1}^{N} \frac{(y_i - \mu(x_i;\boldsymbol{\theta}))^2}{\sigma_i^2} + \text{const.}$$

So maximizing the likelihood is equivalent to minimizing

$$\chi^2(\boldsymbol{\theta}) = \sum_{i=1}^{N} \frac{(y_i - \mu(x_i;\boldsymbol{\theta}))^2}{\sigma_i^2} = -2 \ln L(\boldsymbol{\theta}) + \text{const.}$$

The minimum of $\chi^2(\boldsymbol{\theta})$ defines the least squares (LS) estimators $\hat{\boldsymbol{\theta}}$.

ML $\leftrightarrow$ LS

So least-squares (LS) estimators same as maximum likelihood (ML) when the measurements are $y_i \sim$ Gauss($\mu(x_i; \boldsymbol{\theta})$, σ_i).

Note that the y_i here are independent but not identically distributed. Do not confuse this case with our previous example of an i.i.d. sample with $x_i \sim$ Gauss(μ, σ).

If the y_i are not Gaussian distributed the minimum of $\chi^2(\boldsymbol{\theta})$ still defines the LS estimators. But for most applications in practice the y_i are at least approximately Gaussian (a consequence of the Central Limit Theorem).

Often minimize $\chi^2(\boldsymbol{\theta})$, numerically (e.g. programs like curve_fit or MINUIT).

History

Least Squares fitting also called "regression"

F. Galton, *Regression towards mediocrity in hereditary stature*, The Journal of the Anthropological Institute of Great Britain and Ireland. 15: 246–263 (1886).

Developed earlier by Laplace and Gauss:

C.F. Gauss, *Theoria Motus Corporum Coelestium in Sectionibus Conicis Solem Ambentium*, Hamburgi Sumtibus Frid. Perthes et H. Besser Liber II, Sectio II (1809);

C.F. Gauss, *Theoria Combinationis Observationum Erroribus Minimis Obnoxiae*, pars prior (15.2.1821) et pars posterior (2.2.1823), Commentationes Societatis Regiae Scientiarium Gottingensis Recectiores Vol. V (MDCCCXXIII).

LS with correlated measurements

If the y_i follow a multivariate Gaussian with covariance matrix V,

$$f(\mathbf{y};\boldsymbol{\theta}) = \frac{1}{(2\pi)^{N/2}|V|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{y}-\boldsymbol{\mu}(\boldsymbol{\theta}))^T V^{-1}(\mathbf{y}-\boldsymbol{\mu}(\boldsymbol{\theta}))\right]$$

where $\boldsymbol{\mu}^{\mathrm{T}} = (\mu(x_1),\ldots,\mu(x_N))$, then maximizing the likelihood is equivalent to minimizing

$$\chi^2(\boldsymbol{\theta}) = (\mathbf{y}-\boldsymbol{\mu}(\boldsymbol{\theta}))^T V^{-1}(\mathbf{y}-\boldsymbol{\mu}(\boldsymbol{\theta}))$$

$$= \sum_{i,j=1}^{N} (y_i - \mu(x_i;\boldsymbol{\theta}))V_{ij}^{-1}(y_j - \mu(x_j;\boldsymbol{\theta}))$$

LS with correlated measurements (2)

For the special case of a diagonal covariance matrix, i.e., uncorrelated measurements. Then

$$V = \begin{pmatrix} \sigma_1^2 & 0 & \dots & 0 \\ 0 & \sigma_2^2 & 0 & \dots \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & \sigma_n^2 \end{pmatrix} \quad \rightarrow \quad V^{-1} = \begin{pmatrix} 1/\sigma_1^2 & 0 & \dots & 0 \\ 0 & 1/\sigma_2^2 & 0 & \dots \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & 1/\sigma_n^2 \end{pmatrix}$$

$V^{-1}{}_{ij} = \delta_{ij}/\sigma_i^2$, carry out one of the sums, $\chi^2(\boldsymbol{\theta})$ same as before:

$$\chi^2(\boldsymbol{\theta}) = \sum_{i,j=1}^{N} (y_i - \mu(x_i;\boldsymbol{\theta})) \frac{\delta_{ij}}{\sigma_i^2} (y_j - \mu(x_j;\boldsymbol{\theta})) = \sum_{i=1}^{N} \frac{(y_i - \mu(x_i;\boldsymbol{\theta}))^2}{\sigma_i^2}$$

Statistical Data Analysis
Lecture 8-2

- Finding the LS estimators
- The linear Least Squares problem
- Bias and variance of LS estimators

Recap of Least Squares

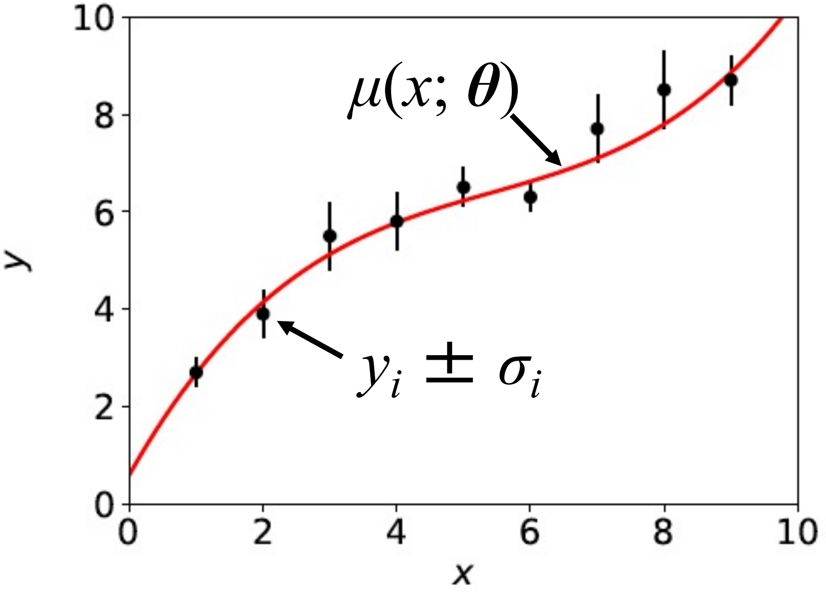
Measurements, $y_1, \ldots, y_N$

Standard deviations $\sigma_1, \ldots, \sigma_N$

or $V_{ij} = \mathrm{cov}[y_i, y_j]$

Control variable $x_1, \ldots, x_N$

Fit function $\mu(x_i; \boldsymbol{\theta}) = E[y_i]$



Estimate $\boldsymbol{\theta}$ by minimizing

$$\chi^2(\boldsymbol{\theta}) = \sum_{i=1}^{N} \frac{(y_i - \mu(x_i; \boldsymbol{\theta}))^2}{\sigma_i^2}$$

or

$$\chi^2(\boldsymbol{\theta}) = (\mathbf{y} - \boldsymbol{\mu}(\boldsymbol{\theta}))^T V^{-1} (\mathbf{y} - \boldsymbol{\mu}(\boldsymbol{\theta}))$$

Finding estimators in closed form

For a limited class of problem it is possible to find the LS estimators in closed form. An important example is when the function $\mu(x;\boldsymbol{\theta})$ is linear *in the parameters* $\boldsymbol{\theta}$, e.g., a polynomial of order M (note the function does not have to be linear in $\boldsymbol{x}$):

$$\mu(x;\boldsymbol{\theta}) = \sum_{n=0}^{M} \theta_n x^n$$

As an example consider a straight line (two parameters):

$$\mu(x;\boldsymbol{\theta}) = \theta_0 + \theta_1 x$$

We need to minimize:

$$\chi^2(\theta_0, \theta_1) = \sum_{i=1}^{N} \frac{(y_i - \theta_0 - \theta_1 x_i)^2}{\sigma_i^2}$$

Finding estimators in closed form (2)

Set the derivatives of $\chi^2(\boldsymbol{\theta})$ with respect to the parameters equal to zero:

$$\frac{\partial \chi^2}{\partial \theta_0} = \sum_{i=1}^{N} \frac{-2(y_i - \theta_0 - \theta_1 x_i)}{\sigma_i^2} = 0 \,,$$

$$\frac{\partial \chi^2}{\partial \theta_1} = \sum_{i=1}^{N} \frac{-2x_i(y_i - \theta_0 - \theta_1 x_i)}{\sigma_i^2} = 0 \,.$$

Finding estimators in closed form (3)

The equations can be rewritten in matrix form as

$$\begin{pmatrix} \sum_{i=1}^N \frac{1}{\sigma_i^2} & \sum_{i=1}^N \frac{x_i}{\sigma_i^2} \\ \sum_{i=1}^N \frac{x_i}{\sigma_i^2} & \sum_{i=1}^N \frac{x_i^2}{\sigma_i^2} \end{pmatrix} \begin{pmatrix} \theta_0 \\ \theta_1 \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^N \frac{y_i}{\sigma_i^2} \\ \sum_{i=1}^N \frac{x_i y_i}{\sigma_i^2} \end{pmatrix}$$

which has the general form

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \theta_0 \\ \theta_1 \end{pmatrix} = \begin{pmatrix} e \\ f \end{pmatrix}$$

Read off *a, b, c, d, e, f,* by comparing with eq. above.

Finding estimators in closed form (4)

Recall inverse of a 2 × 2 matrix:

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \qquad A^{-1} = \frac{1}{ad - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

Apply A^{-1} to both sides of previous eq. to find the estimators:

$$\hat{\theta}_0 = \frac{de - bf}{ad - bc},$$

$$\hat{\theta}_1 = \frac{af - ec}{ad - bc}.$$

Note estimators are linear functions of the measured y_i.

Linear LS Problem

Suppose the fit function is linear in the parameters $\boldsymbol{\theta}^{\mathrm{T}} = (\theta_1, \ldots, \theta_M)$,

$$\mu(x; \boldsymbol{\theta}) = \sum_{i=1}^{M} \theta_i a_i(x)$$

where the $a_i(x)$ are a set of linearly independent basis functions, and write $\boldsymbol{\mu}^{\mathrm{T}}(\boldsymbol{\theta}) = (\mu(x_1; \boldsymbol{\theta}), \ldots, \mu(x_N; \boldsymbol{\theta}))$.

Define $N \times M$ matrix $A_{ij} = a_j(x_i)$, so $\boldsymbol{\mu}(\boldsymbol{\theta}) = A\boldsymbol{\theta}$.

To find the LS estimators minimize:

$$\chi^2(\boldsymbol{\theta}) = (\mathbf{y} - \boldsymbol{\mu}(\boldsymbol{\theta}))^T V^{-1} (\mathbf{y} - \boldsymbol{\mu}(\boldsymbol{\theta}))$$

$$= (\mathbf{y} - A\boldsymbol{\theta})^T V^{-1} (\mathbf{y} - A\boldsymbol{\theta})$$

Linear LS Problem (2)

Set derivatives with respect to θ_i to zero,

$$\nabla \chi^2(\boldsymbol{\theta}) = -2(A^T V^{-1} \mathbf{y} - A^T V^{-1} A \boldsymbol{\theta}) = 0$$

$$\nabla = \left(\frac{\partial}{\partial \theta_1}, \ldots, \frac{\partial}{\partial \theta_M} \right)$$

Solve system of M linear equations to find the LS estimators,

$$\hat{\boldsymbol{\theta}} = (A^T V^{-1} A)^{-1} A^T V^{-1} \mathbf{y} \equiv B \mathbf{y}$$

Note that the estimators are linear functions of the measured y_i.

Bias of LS estimators

By hypothesis $E[\boldsymbol{y}] = \boldsymbol{\mu} = A\boldsymbol{\theta}$ so for the linear problem, the LS estimators are unbiased:

$$E[\hat{\boldsymbol{\theta}}] = (A^T V^{-1} A)^{-1} A^T V^{-1} E[\mathbf{y}]$$

$$= (A^T V^{-1} A)^{-1} A^T V^{-1} \boldsymbol{\mu}$$

$$= (A^T V^{-1} A)^{-1} A^T V^{-1} A\boldsymbol{\theta} = \boldsymbol{\theta}$$

For the general nonlinear problem the LS estimators can have a bias.

Variance of LS estimators for linear problem

For the linear LS problem, the variance can be found using error propagation. Using

$$V_{ij} = \mathrm{cov}[y_i, y_j]$$

$$\hat{\boldsymbol{\theta}} = B\mathbf{y}$$

$$U_{ij} = \mathrm{cov}[\hat{\theta}_i, \hat{\theta}_j]$$

We find

$$U = BVB^T = (A^T V^{-1} A)^{-1}$$

Since the estimators are linear in the y_i, error propagation gives an exact result.

Variance of LS estimators for Gaussian data

If $y_i \sim$ Gauss, then we found $\ln L(\boldsymbol{\theta}) = -\frac{1}{2}\chi^2(\boldsymbol{\theta}) + \text{const.}$

To the extent this (approximately) holds, we can use

$$U_{ij}^{-1} = -E\left[\frac{\partial^2 \ln L}{\partial\theta_i \partial\theta_j}\right]$$

and so we estimate the inverse covariance matrix with

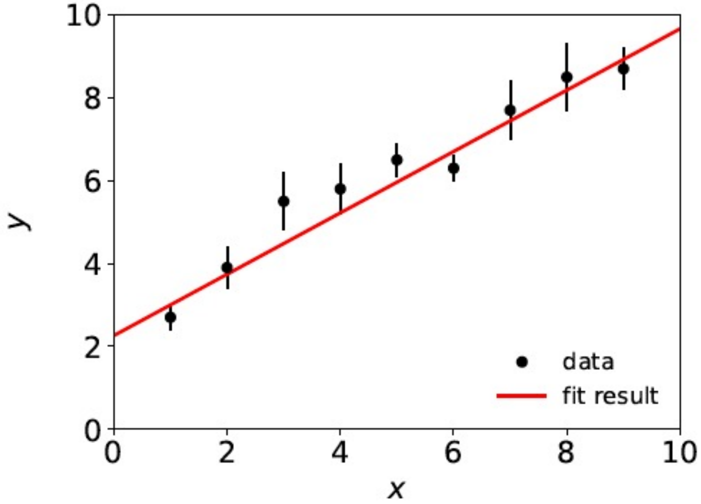
$$\widehat{U}_{ij}^{-1} = -\left.\frac{\partial^2 \ln L}{\partial\theta_i \partial\theta_j}\right|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}} = \frac{1}{2}\left.\frac{\partial^2 \chi^2}{\partial\theta_i \partial\theta_j}\right|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}}$$

and invert to estimate the covariance matrix U.

For Gaussian data with the linear LS problem, U is the minimum variance bound (the LS estimators are unbiased and efficient).

Covariance from derivatives of $\chi^2(\boldsymbol{\theta})$

This is what programs like **curve_fit** and **MINUIT** do (derivatives computed numerically). Example with straight-line fit gives:



$$\hat{\theta}_0 = 2.258$$

$$\hat{\theta}_1 = 0.741$$

$$U = \begin{pmatrix} 0.08537 & -0.01438 \\ -0.01438 & 0.003275 \end{pmatrix}$$

$$\sigma_{\hat{\theta}_0} = 0.29 \,,$$

$$\sigma_{\hat{\theta}_1} = 0.057 \,,$$

$$\mathrm{cov}[\hat{\theta}_0, \hat{\theta}_1] = -0.014 \,,$$

$$\rho = -0.86 \,.$$

The contour $\chi^2(\boldsymbol{\theta}) = \chi^2_{\min} + 1$

If $\mu(x; \boldsymbol{\theta})$ is linear in the parameters, then $\chi^2(\boldsymbol{\theta})$ is quadratic:

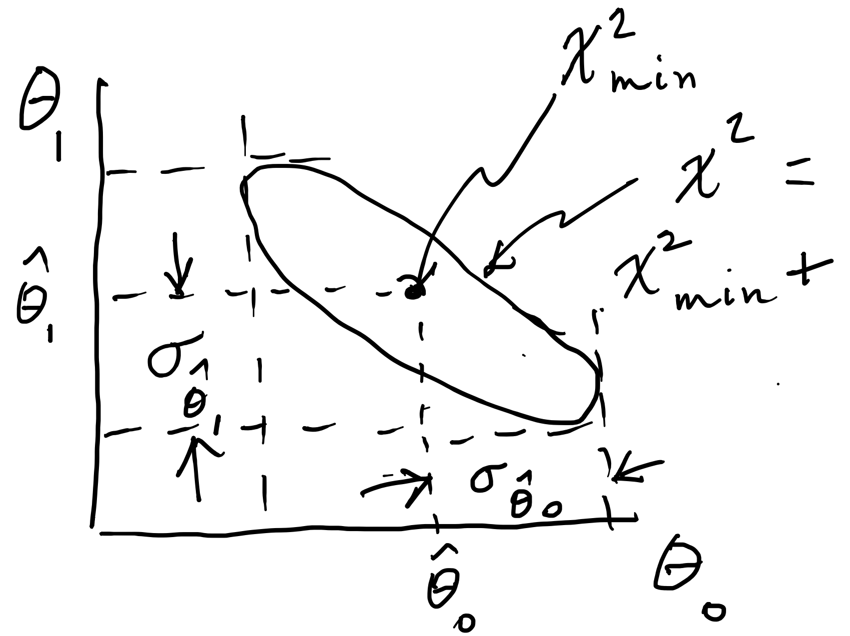
$$\chi^2(\boldsymbol{\theta}) = \chi^2(\hat{\boldsymbol{\theta}}) + \frac{1}{2} \sum_{i,j=1}^{M} \left. \frac{\partial^2 \chi^2}{\partial \theta_i \theta_j} \right|_{\boldsymbol{\theta} = \hat{\boldsymbol{\theta}}} (\theta_i - \hat{\theta}_i)(\theta_j - \hat{\theta}_j)$$

$$= \chi^2_{\min} + (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})^T U^{-1} (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})$$

Standard deviations from tangents to (hyper-) planes of

$$\chi^2(\boldsymbol{\theta}) = \chi^2_{\min} + 1$$

(corresponds to $\ln L(\boldsymbol{\theta}) = \ln L_{\max} - ½$)

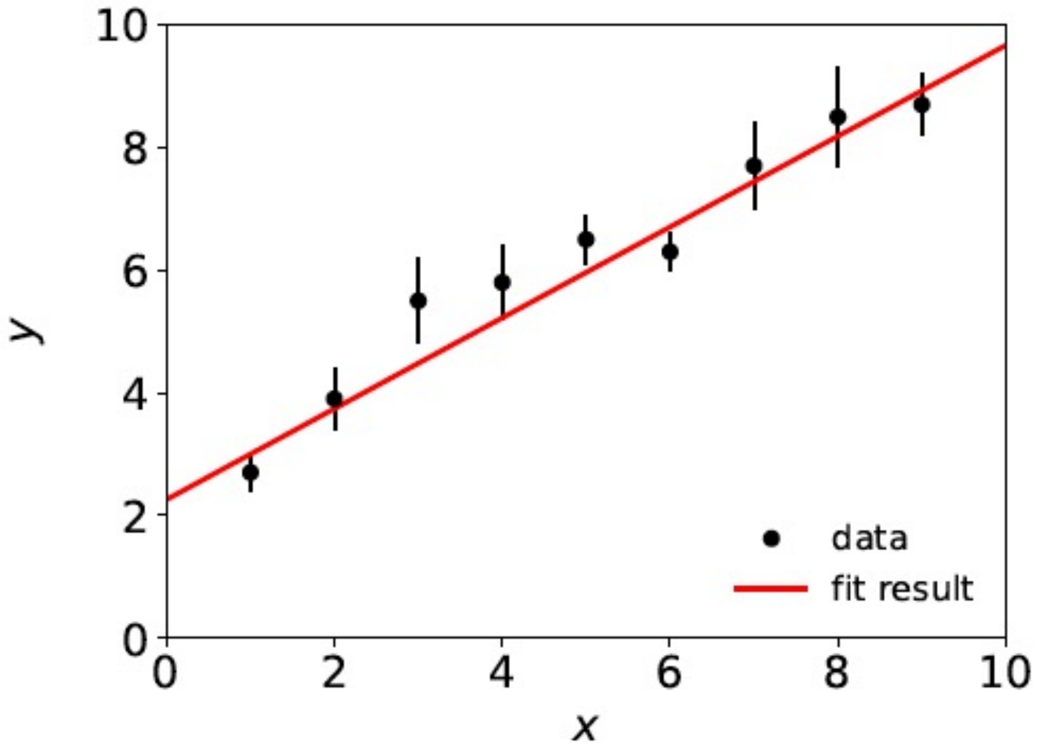


Statistical Data Analysis
Lecture 8-3

- Goodness of fit from $\chi^2_{\min}$
- Example of least-squares fit

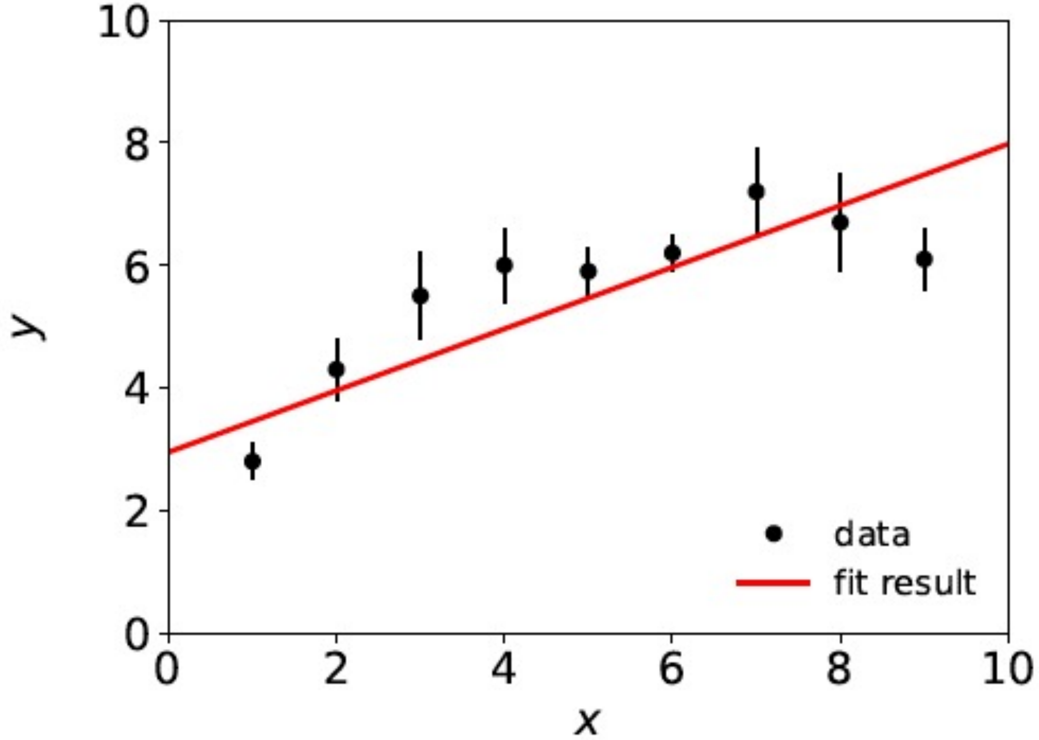
A “good” fit

In an earlier example we fitted data that were reasonably well described by a straight line:



A “bad” fit

But what if a straight-line fit looks like this:



Test hypothesized form of fit function with p-value, if this is below some (user-defined) threshold, reject the hypothesis and try some other function, e.g. a polynomial of higher order.

Goodness-of-fit from $\chi^2_{\min}$

The value of the χ^2 at its minimum is a measure of the level of agreement between the data and fitted curve:

$$\chi^2_{\min} = \sum_{i=1}^{N} \frac{(y_i - \mu(x_i; \hat{\boldsymbol{\theta}}))^2}{\sigma_i^2}$$

It can therefore be used as a goodness-of-fit statistic to test the hypothesized functional form $\mu(x; \boldsymbol{\theta})$.

The p-value of the hypothesized functional form is

$$p = \int_{\chi^2_{\min}}^{\infty} f(t; n_{\mathrm{d}})\, dt$$

= the probability, under assumption of $\mu(x; \boldsymbol{\theta})$, to get a $\chi^2_{\min}$ as high as the one we got or higher.

Distribution of $\chi^2_{\min}$

One can show that if the data follow $y \sim$ Gauss($\mu(x; \boldsymbol{\theta}),\sigma$), i.e., if the fit function is correct for some $\boldsymbol{\theta}$, then the statistic $t = \chi^2_{\min}$ follows the chi-square pdf,

$$f(t; n_{\mathrm{d}}) = \frac{1}{2^{n_{\mathrm{d}}/2}\Gamma(n_{\mathrm{d}}/2)} t^{n_{\mathrm{d}}/2-1} e^{-t/2}$$

where the number of degrees of freedom is

n_{d} = number of data points - number of fitted parameters

Note that the composite hypothesis with $E[y] = \mu(x; \boldsymbol{\theta})$ is only fully specified when we fix $\boldsymbol{\theta}$.

So the p-value is in principle a function of $\boldsymbol{\theta}$, and we should only reject $\mu(x; \boldsymbol{\theta})$ if $p \leq \alpha$ for all $\boldsymbol{\theta}$.

But here the pdf of our statistic $\chi^2_{\min}$ is independent of $\boldsymbol{\theta}$, so whatever we get for p holds for any $\boldsymbol{\theta}$.

The "chi-square per degree of freedom"

Recall also the chi-square pdf has an expectation value equal to the number of degrees of freedom, so

$\chi^2_{\rm min} \sim n_{\rm d}$ → fit is "good"

$\chi^2_{\rm min} \gg n_{\rm d}$ → fit is "bad"

$\chi^2_{\rm min} \ll n_{\rm d}$ → fit is better than what one would expect given fluctuations that should be present in the data.

Often this is done using the ratio $\chi^2_{\rm min}/n_{\rm d}$, i.e. fit is good if the "chi-square per degree of freedom" comes out not much greater than 1.

But, best to quote both $\chi^2_{\rm min}$ and $n_{\rm d}$, not just their ratio, since e.g.

$\chi^2_{\rm min} = 15,\ n_{\rm d} = 10 \rightarrow p\text{-value} = 0.13$

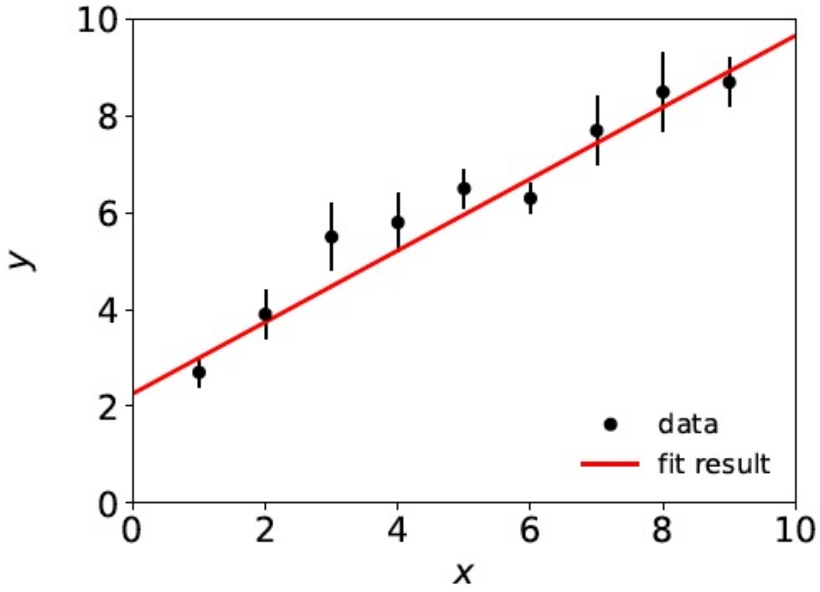
$\chi^2_{\rm min} = 150\ n_{\rm d} = 100 \rightarrow p\text{-value} = 0.00090$

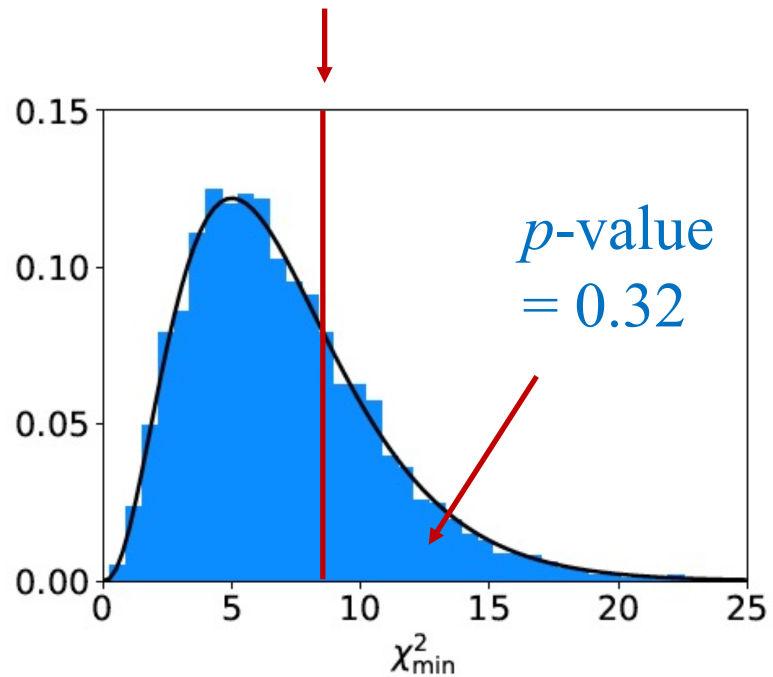
p-value for the "good" fit

$N = 9$ data points, $m = 2$ fitted parameters,

$\chi^2_{\min} / n_{\mathrm{dof}} = 8.2/7 = 1.2$

$\chi^2_{\min} = 8.2$





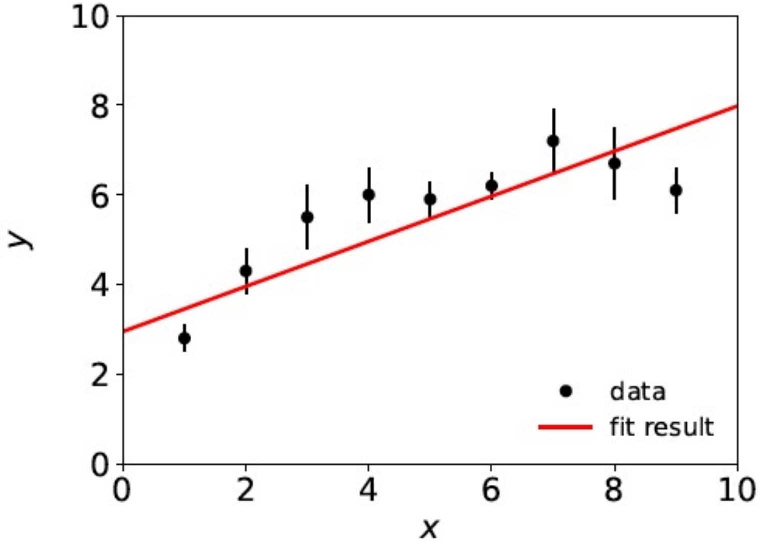
If the straight-line hypothesis is true, expect equal or worse agreement almost 1/3 of the time (i.e. our result is not unusual).

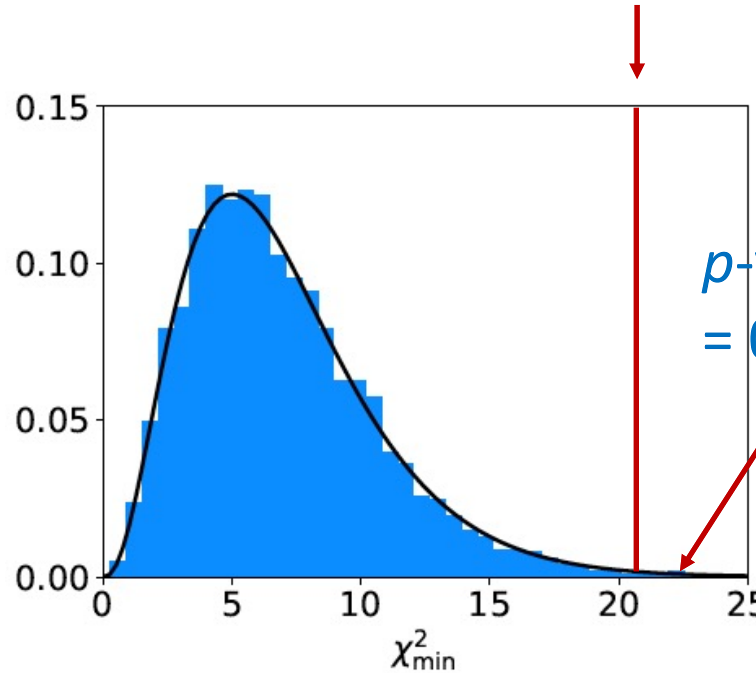
p-value for the "bad" fit

$N = 9$ data points, $m = 2$ fitted parameters,

$\chi^2_{\min} / n_{\text{dof}} = 20.9/7 = 3.0$

$\chi^2_{\min} = 20.9$





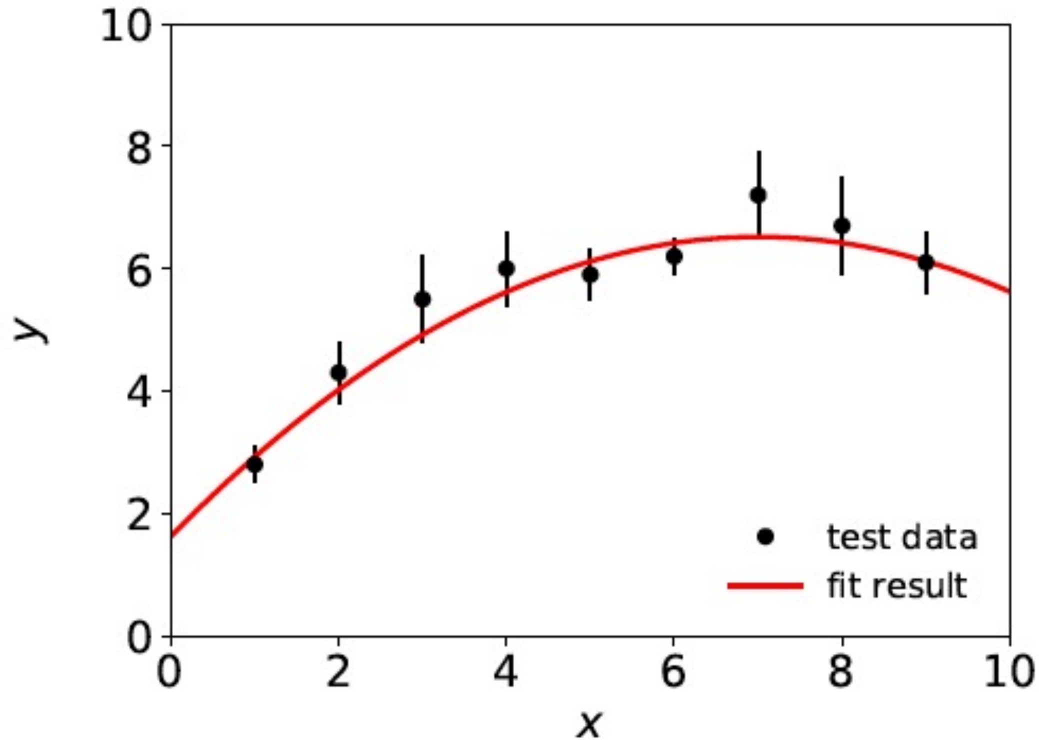
p-value = 0.0039

So is the straight-line hypothesis correct? It could be, but if so we would expect a $\chi^2_{\min}$ as high as observed or higher only 4 times out of a thousand.

A better fit

If we decide the agreement between data and hypothesis is not good enough (exact threshold is a subjective choice), we can try a different model, e.g., a 2nd order polynomial:

$$f(x;\boldsymbol{\theta}) = \theta_0 + \theta_1 x + \theta_2 x^2$$



$\chi^2_{\min} = 3.5$ for $n_{\mathrm{dof}} = 6$

$\chi^2_{\min} / n_{\mathrm{dof}} = 0.58$

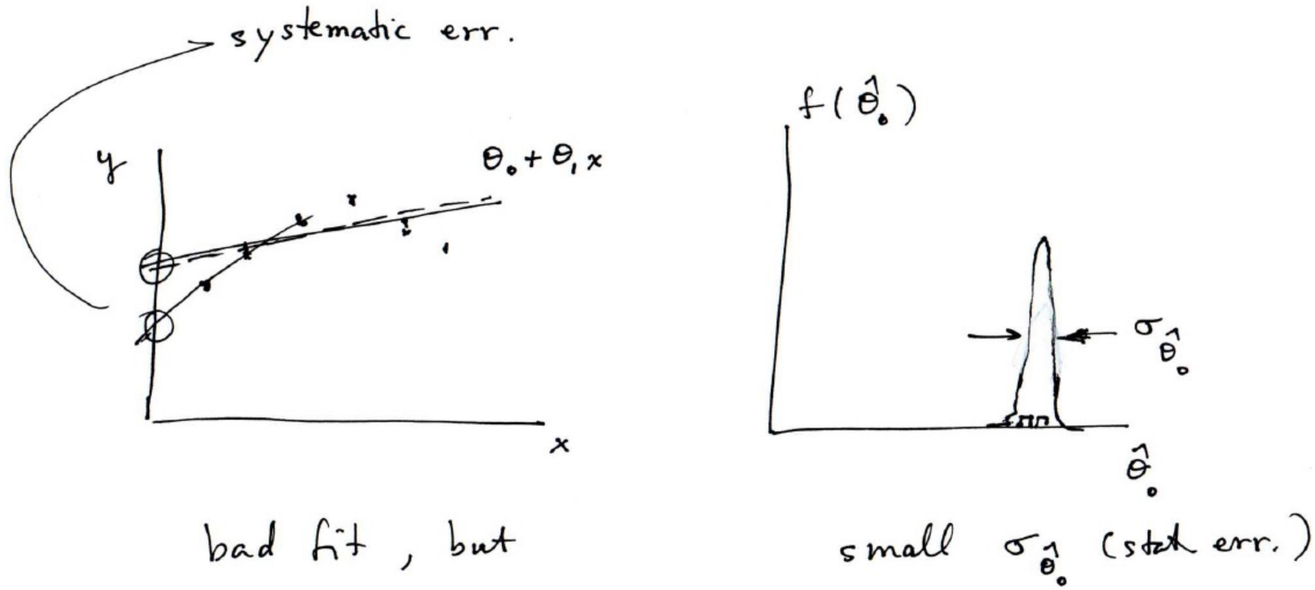
p-value $= 0.75$

Goodness-of-fit vs. statistical errors

If the fit is “bad”, something is “wrong” and you may expect large statistical errors for the fitted parameters. This is not the case.

The statistical errors say how much the parameter estimates fluctuate when repeating the experiment, under assumption of the hypothesized fit function. This is not the same as the degree to which the function can describe the data.

If the hypothesized $\mu(x; \boldsymbol{\theta})$ is not correct, the fitted parameters will have some systematic uncertainty – a more complex question that we will take up later.



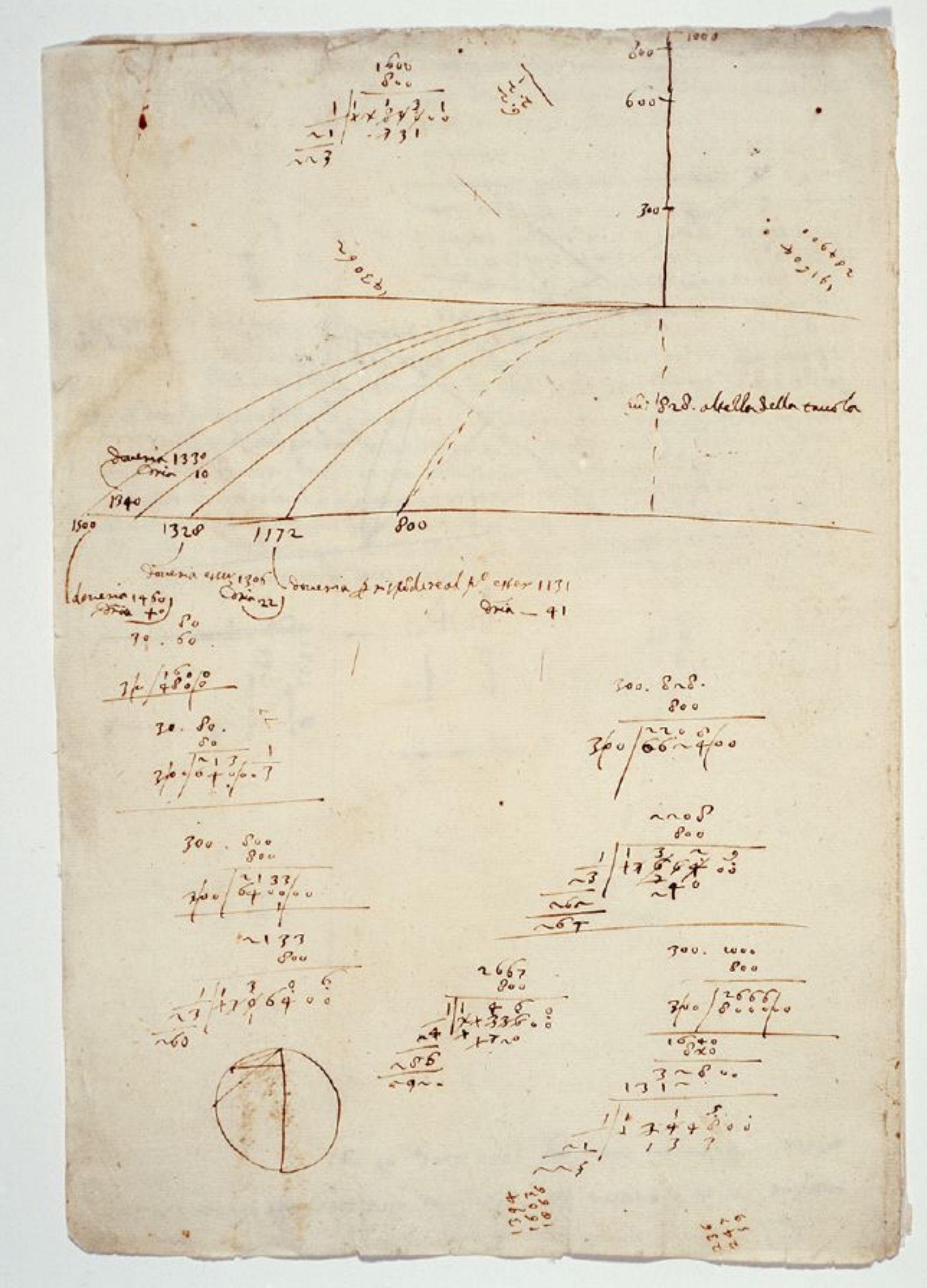
Statistical Data Analysis
Lecture 8-4

- Example of a least-squares fit
- Least squares to combine measurements

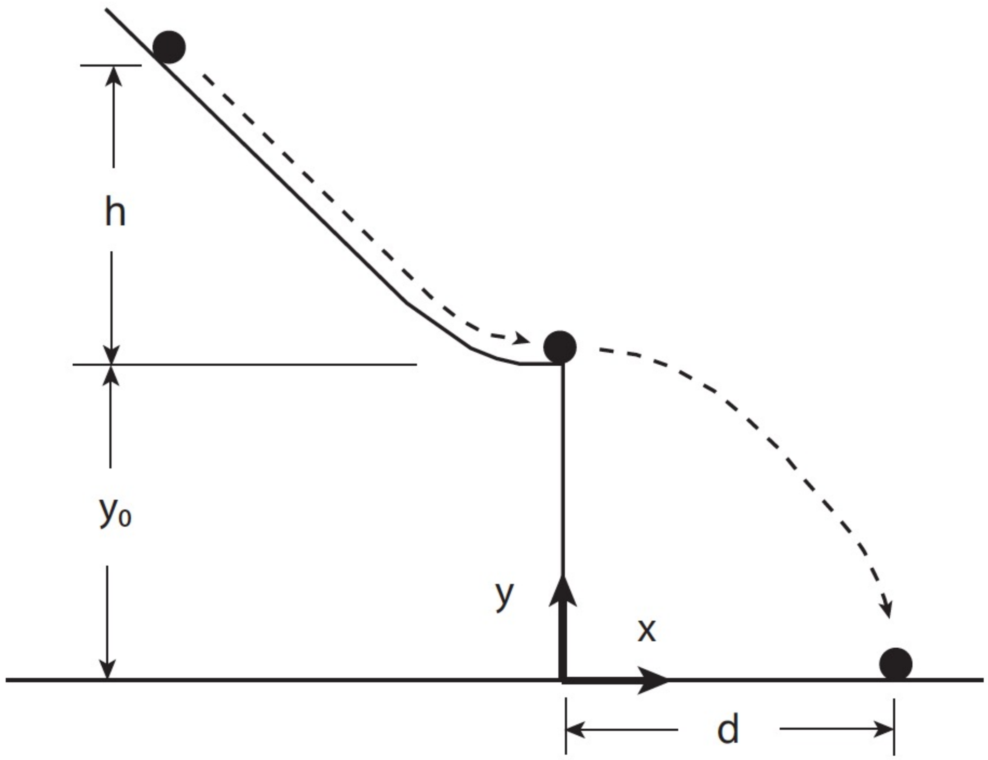
Ball and ramp data from Galileo

Galileo Galilei, Manuscript *f*.116, Biblioteca Nazionale Centrale di Firenze, www.bncf.firenze.sbn.it

In 1608 Galileo carried out experiments rolling a ball down an inclined ramp to investigate the trajectory of falling objects.



Ball and ramp data from Galileo



Units in punti
(approx. 1 mm)

h	d
1000	1500
828	1340
800	1328
600	1172
300	800

Suppose h is set with negligible uncertainty, and d is measured with an uncertainty σ = 15 punti.

Analysis of ball and ramp data

What is the correct law that relates *d* and *h*?

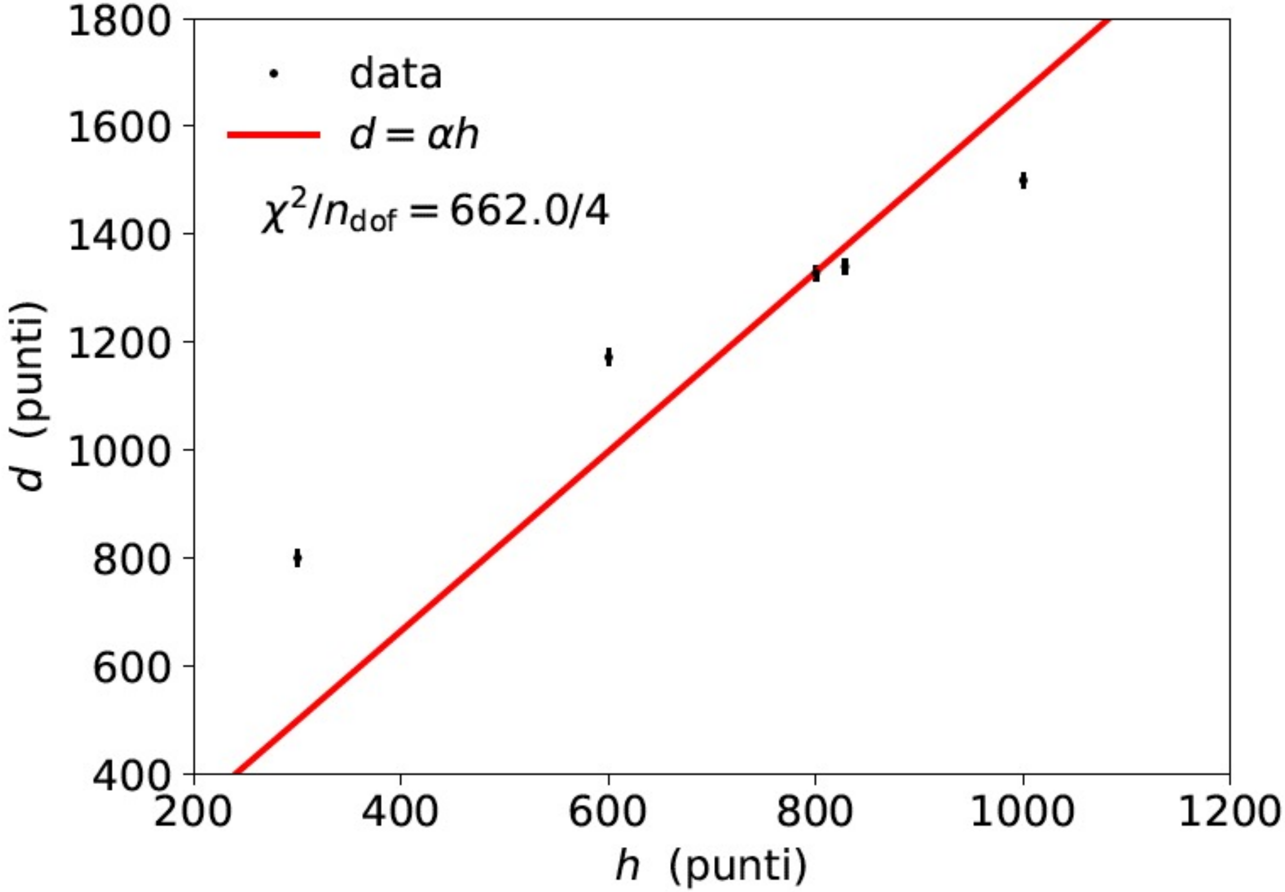
Try different hypotheses:

$$d = \alpha h$$

$$d = \alpha h + \beta h^2$$

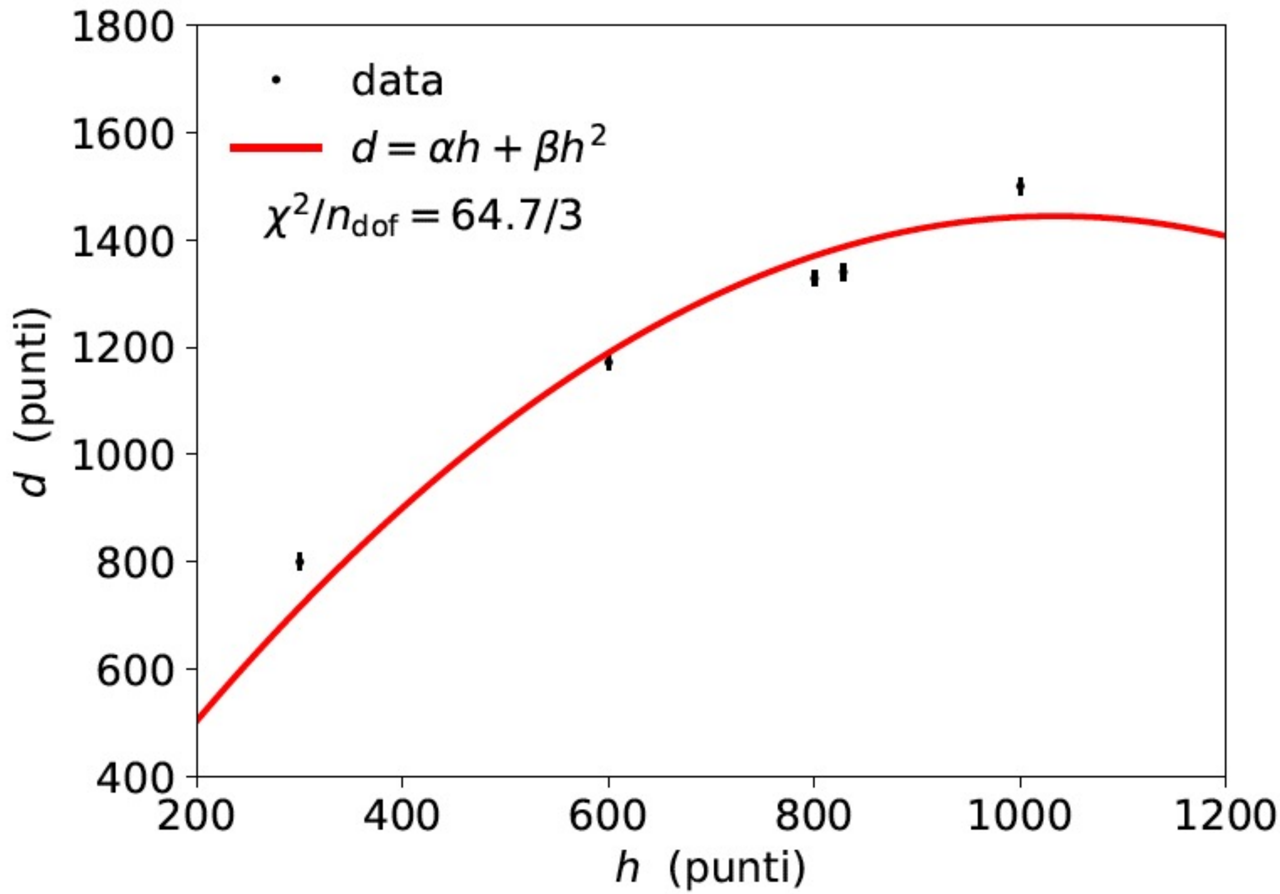
$$d = \alpha h^\beta$$

$$d = \alpha h$$

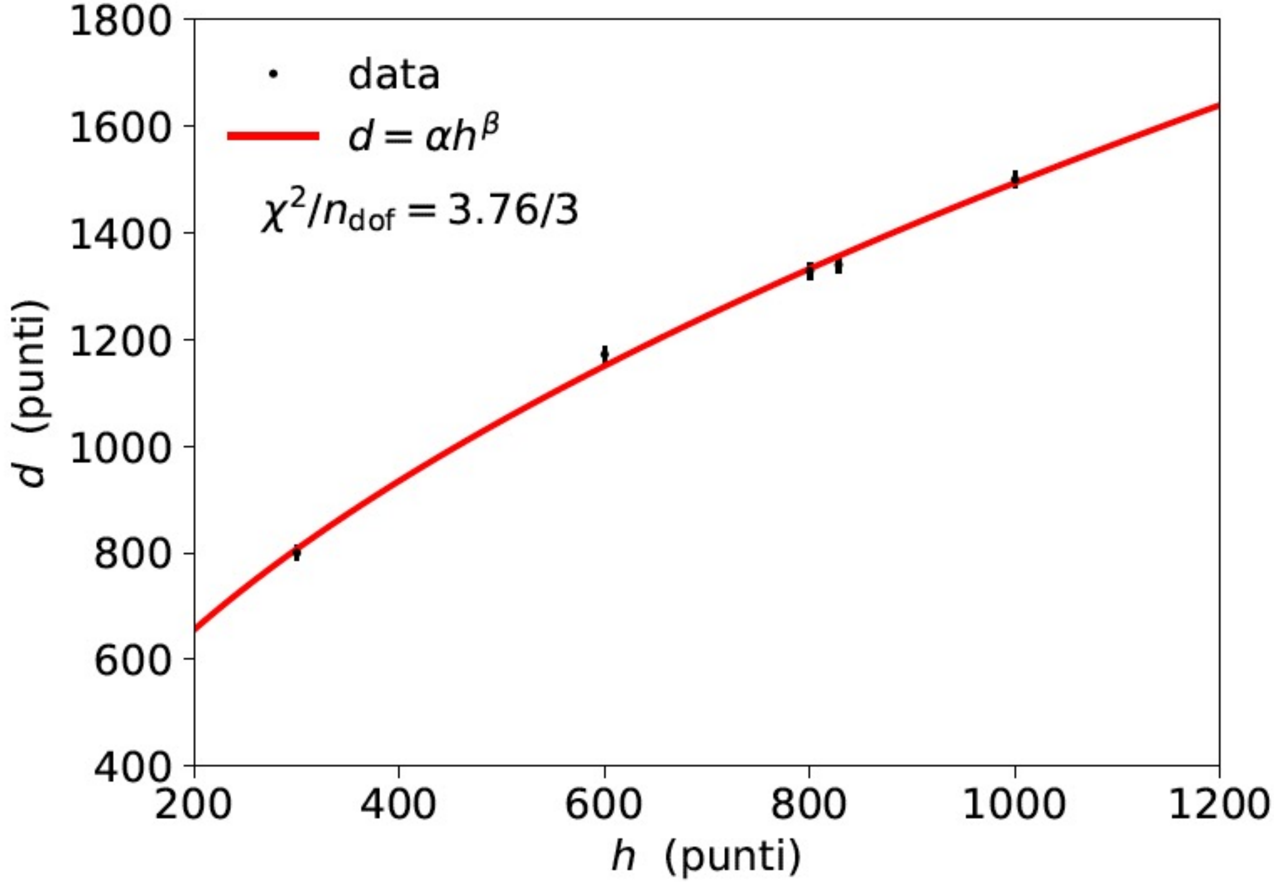


data
$d = \alpha h$
$\chi^2/n_{\rm dof} = 662.0/4$
1800
1600
1400
1200
1000
800
600
400
200
400
600
800
1000
1200
d (punti)
h (punti)

$$d = \alpha h + \beta h^2$$



$$d = \alpha h^{\beta}$$



Summary of ball-and-ramp analysis

function	$\chi^2_{\min}$	$n_{\rm dof}$	p-value	α	$\sigma_{\hat{\alpha}}$	β	$\sigma_{\hat{\beta}}$	ρ
$d = \alpha h$	662.0	4	5.9×10^{-142}	1.663	0.0090			
$d = \alpha h + \beta h^2$	64.7	3	5.7×10^{-14}	2.793	0.047	−0.001351	0.000055	−0.9816
$d = \alpha h^{\beta}$	3.76	3	0.29	43.8	4.8	0.511	0.017	−0.9988

Clearly the best fit suggests $d \sim h^{1/2}$, and this is exactly what Newton's laws predict!

Using LS to combine measurements

Use LS to obtain weighted average of N measurements of λ:

$$y_i = \text{result of measurement } i,\ i = 1, \ldots, N;$$

$$\sigma_i^2 = V[y_i], \text{ assume known;}$$

$$\lambda = \text{true value (plays role of } \theta) \quad = E[y_i] \text{ for all } i$$

For uncorrelated y_i, minimize

$$\chi^2(\lambda) = \sum_{i=1}^{N} \frac{(y_i - \lambda)^2}{\sigma_i^2},$$

Set $\frac{\partial \chi^2}{\partial \lambda} = 0$ and solve,

$$\rightarrow \quad \hat{\lambda} = \frac{\Sigma_{i=1}^{N} y_i/\sigma_i^2}{\Sigma_{j=1}^{N} 1/\sigma_j^2} \qquad V[\hat{\lambda}] = \frac{1}{\Sigma_{i=1}^{N} 1/\sigma_i^2}$$

Combining correlated measurements with LS

If $\mathrm{cov}[y_i, y_j] = V_{ij}$, minimize

$$\chi^2(\lambda) = \sum_{i,j=1}^{N} (y_i - \lambda)(V^{-1})_{ij}(y_j - \lambda) ,$$

$$\rightarrow \quad \hat{\lambda} = \sum_{i=1}^{N} w_i y_i , \qquad w_i = \frac{\sum_{j=1}^{N} (V^{-1})_{ij}}{\sum_{k,l=1}^{N} (V^{-1})_{kl}}$$

$$V[\hat{\lambda}] = \sum_{i,j=1}^{N} w_i V_{ij} w_j$$

LS $\hat{\lambda}$ has zero bias, minimum variance (Gauss–Markov theorem).

Example: averaging two correlated measurements

Suppose we have y_1, y_2, and $V = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}$

$$\rightarrow \quad \hat{\lambda} = w y_1 + (1-w) y_2, \quad w = \frac{\sigma_2^2 - \rho\sigma_1\sigma_2}{\sigma_1^2 + \sigma_2^2 - 2\rho\sigma_1\sigma_2}$$

$$V[\hat{\lambda}] = \frac{(1-\rho^2)\sigma_1^2\sigma_2^2}{\sigma_1^2 + \sigma_2^2 - 2\rho\sigma_1\sigma_2} = \sigma^2$$

The increase in inverse variance due to 2nd measurement is

$$\frac{1}{\sigma^2} - \frac{1}{\sigma_1^2} = \frac{1}{1-\rho^2}\left(\frac{\rho}{\sigma_1} - \frac{1}{\sigma_2}\right)^2 > 0$$

$\rightarrow$ 2nd measurement can only help.

Negative weights in LS average

If $\rho > \sigma_1/\sigma_2, \rightarrow w < 0,$

$\rightarrow$ weighted average is not between y_1 and y_2 (!?)

Cannot happen if correlation due to common data, but possible for shared random effect; very unreliable if e.g. ρ, σ_1, σ_2 incorrect.

See example in SDA Section 7.6.1 with two measurements at same temperature using two rulers, different thermal expansion coefficients:

average is outside the two measurements; used to improve estimate of temperature.

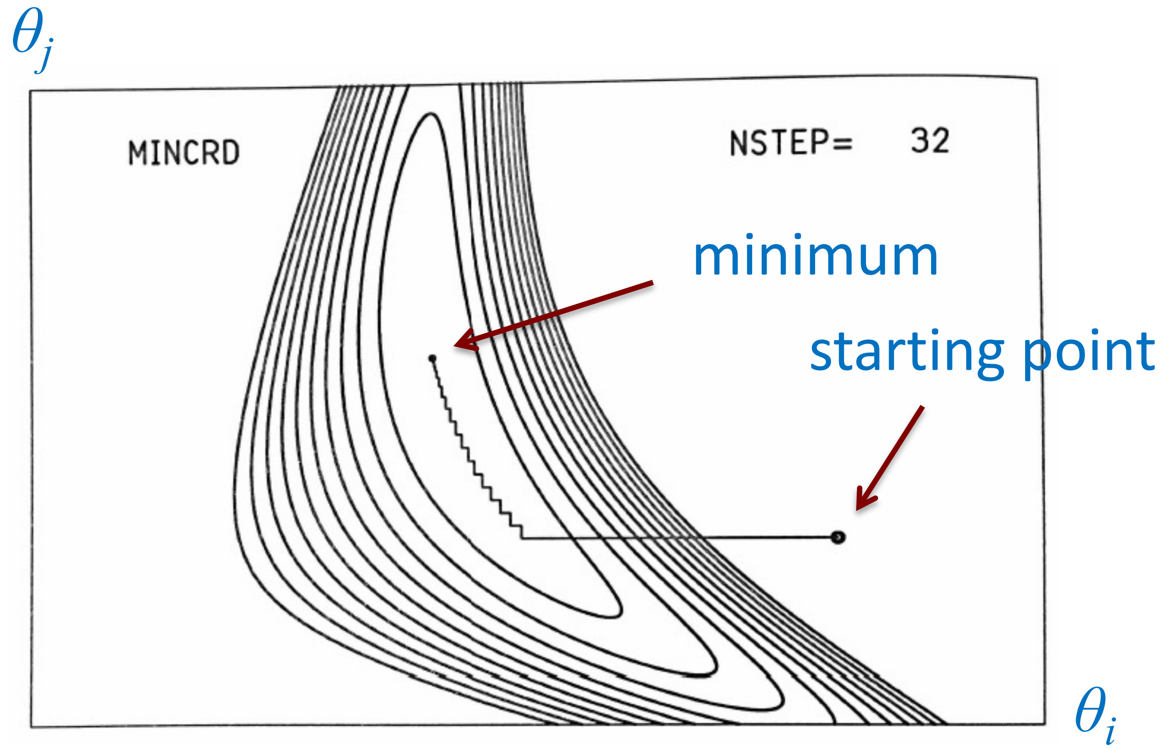
Extra slides

Finding LS estimators numerically

Start at a given point in the parameter space and move around according to some strategy to find the point where $\chi^2(\boldsymbol{\theta})$ is a minimum.

For example, alternate minimizing with respect to each component of $\boldsymbol{\theta}$:

Many strategies possible, e.g., steepest descent, conjugate gradients, ... (see Brandt Ch. 10).



Siegmund Brandt, Data Analysis: Statistical and Computational Methods for Scientists and Engineers 4th ed., Springer 2014

Fitting the parameters with Python

The routine routine **curve_fit** from **scipy.optimize** can find LS estimators numerically. To use it you need:

```
import numpy as np
from scipy.optimize import curve_fit
```

We need to define the fit function $\mu(x; \boldsymbol{\theta})$, e.g., a straight line:

```
def func(x, *theta):
    theta0, theta1 = theta
    return theta0 + theta1*x
```

Fitting the parameters with Python (2)

The data values (x_i, y_i, σ_i) need to be in the form of NumPy arrays, e.g,

```
x   = np.array([1.0, 2.0, 3.0, 4.0, 5.0, 6.0, 7.0, 8.0, 9.0])
y   = np.array([2.7, 3.9, 5.5, 5.8, 6.5, 6.3, 7.7, 8.5, 8.7])
sig = np.array([0.3, 0.5, 0.7, 0.6, 0.4, 0.3, 0.7, 0.8, 0.5])
```

Start values of the parameters can be specified:

```
p0 = np.array([1.0, 1.0])
```

To find the parameter values that minimize $\chi^2(\boldsymbol{\theta})$, call **curve_fit**:

```
thetaHat, cov = curve_fit(func, x, y, p0, sig, absolute_sigma=True)
```

Returns estimators and covariance matrix as NumPy arrays.

Need **absolute_sigma=True** for the fit errors (cov. matrix) to have desired interpretation.