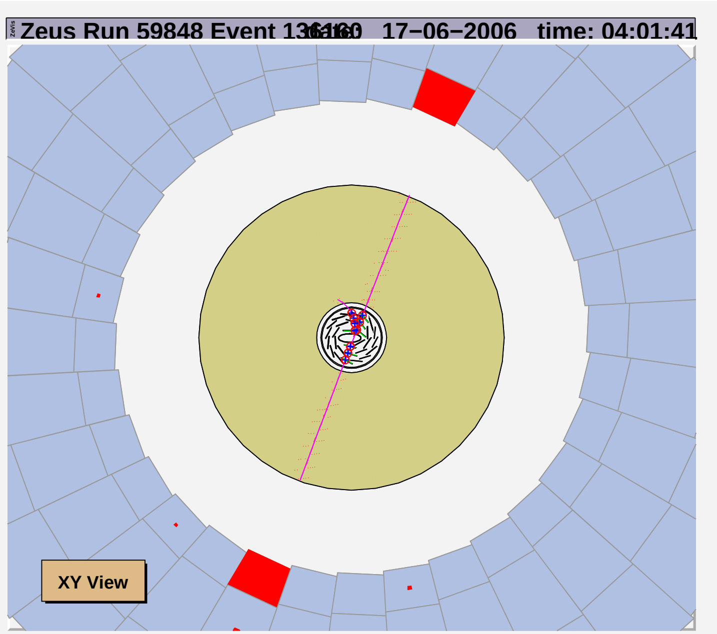
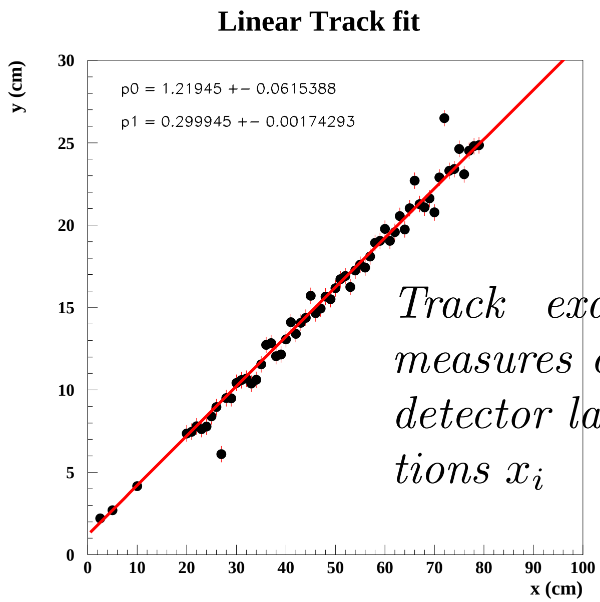
Linear Least square fit - introductory example

Example: Precise muon track fits for possible discovery $Z^* \to \mu^+\mu^-$





Track example: Detector measures coordinate y_i in n detector layers at fixed positions x_i

- Necessary conditions for linear least square fit:
  - Measurements with gaussian uncertainties
  - Linear model, here: $y = a_0 + a_1 x + a_2 x^2$
- Fit construction:
  - $\chi^2 = \sum_i \frac{\left[y_i - (a_0 + a_1 x + a_2 x^2)\right]^2}{\sigma_i^2}$
  - Determine a_0, a_1, a_2 by finding χ^2 total minimum (normal equations)
- Check consistency
  - χ^2 and fit probability
  - Outlier rejection
- Detailed error analysis
  - Parameter errors and correlations (error ellipses), track trajectory error band
  - Momentum calculation (error propagation)
- Possible Extensions:
  - Apply constraint fits to both tracks, e.g. $p_t(\mu^+) = p_t(\mu^-)$ $\to$ covered in session on extended fits
  - Analysis of obtained $\mu^+\mu^-$ mass spectrum containing background and possible signal events $\to$ covered in session on non-linear least square fits

Overview of Linear least square fit section

Part I	Part II	Part III
• Reminder of χ^2-fit method • Linear χ^2-fit examples (Constant, straight line, parabola, etc.) • **Fit of a constant (averaging measurements)** • One single measurement: χ^2_{min} and $\chi^2_{min}+1$, Hesse matrix • Exercise: Two measurements: perform fit by adding χ^2-parabolas • Averaging many measurements, results • Exercise: Compare weighted vs unweighted average	• **χ^2-fit-quality test:** Example: χ^2 of two measurements and known true value • χ^2-function for n degrees of freedom exercise: plot and study features of the χ^2-function vs n • χ^2-fit probability exercise: plot and study features of the χ^2-fit-probability • χ^2 for two measurements with unknown true value • Exercise: **Outlier rejection**, case world average of m_W, study how the rejection of certain measurements change the average and the χ^2-fit probability • Pulls of single measurements to the average • Averaging data with unknown errors • Upscaling of errors a la PDG to obtain reasonable χ^2	• General form of linear χ^2 • Solution by normal equations • General features: (Consistency, Unbiasedness, efficiency) • Normal equation solution for **straight line fit** • Exercise: Learn qualitative features of straight line fits, e.g. importance of lever arm • Exercise: Straight line fit and detailed error analysis (error ellipse, trajectory error band) • Exercise: **Parabola track fit**, complete analysis: *fit, outlier-rejection, parameter errors/correlation, trajectory uncertainty, **momentum calculation*** • Exercise: **Guessing the right fit function for smooth data (polynomial fit of background**

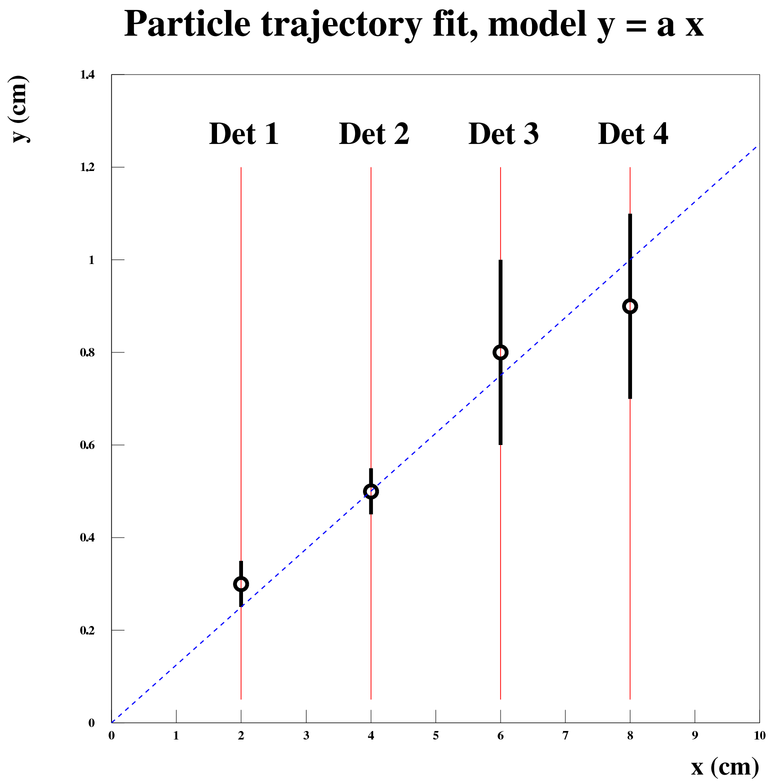
Lecture I on linear least square fits

Contents:

- Least square χ^2-fit method reminder
- Linear least square fits: definition and examples
- Fit of a constant: One, two and many measurements

Method of least squares fit - a reminder

Example problem: Particle trajectory measurement



general:
n-measurements
y_i with uncertainties σ_i
at fixed x_i
Modell: $y = f(x, a)$

$\Rightarrow$ how to determine a?

Idea: for the correct a one expects: $|y_i - f(x_i, a)| \leq \sigma_i$

i.e. curve describes data within measurement uncertainties

Method of least squares fit - a reminder

$\rightarrow \boxed{\chi^2 = \Sigma_{i=1}^{n} \frac{(y_i - f(x_i,a))^2}{\sigma_i^2}} \leftrightarrow$ Min. wrt a!

$\Rightarrow$ determine a from $\frac{d\chi^2}{da} = 0$

$\rightarrow \boxed{\chi^2 = \Sigma_{i=1}^{n} \frac{(y_i - f(x_i,a))}{\sigma_i^2} \cdot \frac{df(x_i,a)}{da} = 0}$

Most general not analytically solvable.
$\Rightarrow$ use iterative (numerical) methods
(MINUIT, Mathematica)

Method of least squares fit - a reminder

Most general case

- y_i, y_j correlated meas. with covariance V_{ij}
- m fitparms $\vec{a}$

$$\rightarrow \boxed{\begin{aligned} \chi^2 &= \Sigma_{i,j=1}^{n}(y_i - f(x_i,\vec{a}))V_{ij}^{-1}(y_i - f(x_i,\vec{a})) \\ &= (\vec{y} - \vec{f}(\vec{a}))^t V^{-1}(\vec{y} - \vec{f}(\vec{a})) \end{aligned}}$$

Linear least square fits

$\vec{y}$ Vektor of n meas. $\begin{pmatrix} y_1(x_1) \\ . \\ y_n(x_n) \end{pmatrix}$ with Cov. Matrix V

$\vec{a}$ Vektor of m fitparms $\begin{pmatrix} a_1 \\ . \\ a_m \end{pmatrix}$

Modell for $\vec{y} :\; = A\,\vec{a}$

Watch out: linear in $\vec{a}$, *but not necessarily in* x.

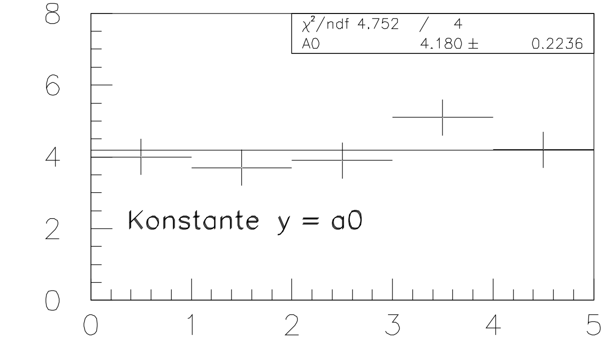
Example fct $= ae^{-x}$, i.e. model for y_i: $= e^{-x_i}\,a$

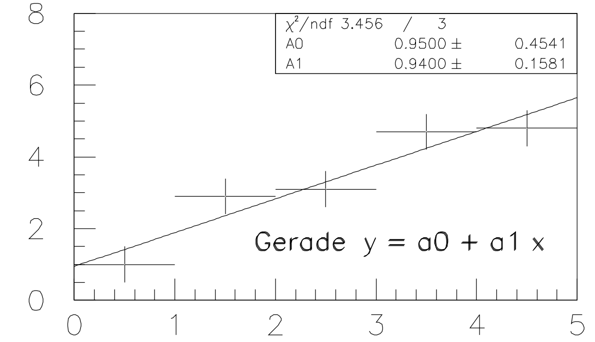
$$\boxed{\chi^2 = (\vec{y} - A\,\vec{a})^t\, V^{-1}\, (\vec{y} - A\,\vec{a})}$$

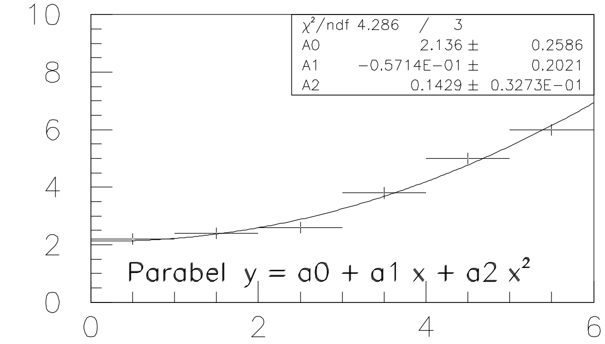
$\longrightarrow$ to be minimised w.r.t $\vec{a}$

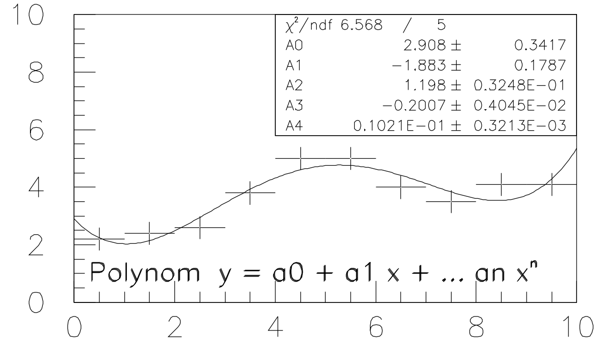
Examples for linear least square fits

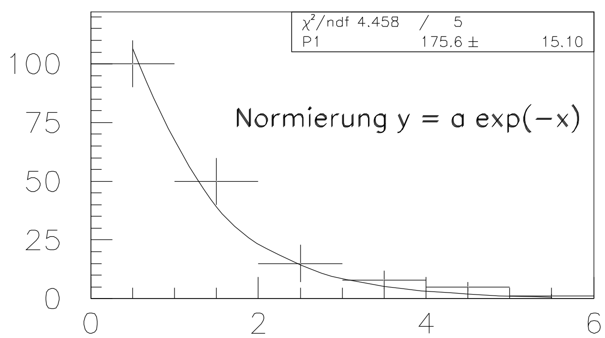
Attention: Linear means that y depends linearly on the fitparameters a_i.











Fit of a constant

Example: Averaging of n different measurements $a_i \pm \sigma_i$ of an observable a (e.g. $a = \alpha_s(m_Z)$)

$$\chi^2 = \Sigma_i^n \frac{(a_i - a)^2}{\sigma_i^2}$$

"Idiot example" of one single measurement $a_1 \pm \sigma_1$:

$$\chi^2 = \frac{(a_1 - a)^2}{\sigma_1^2}$$

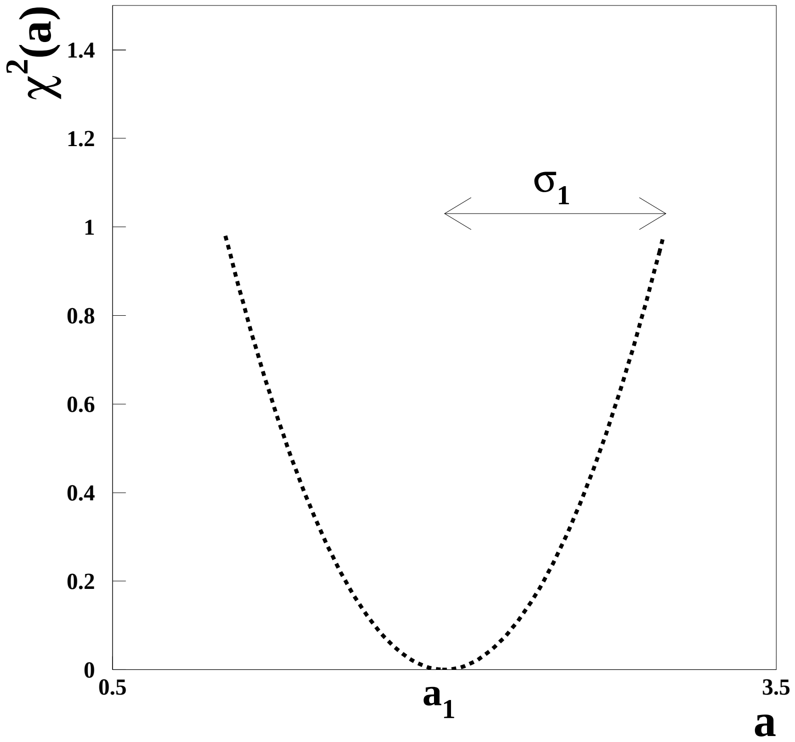
$$Min.\chi^2 : \quad \frac{d\chi^2}{da} = 0 \;\rightarrow\; \text{Estimated value} \quad \hat{a} = a_1;\ \sigma_{\hat{a}} = \sigma_1$$

Fit of a constant

Continuing example of one single meas.: Probability density p for true value of a (*inverse probability*):

$$p \sim e^{-\chi^2/2} = e^{-\frac{(a-\hat{a})^2}{2\sigma_{\hat{a}}^2}}$$

Important general relation: $\sigma_{\hat{a}} = \left[-\frac{d^2\chi^2}{da^2}_{|a=\hat{a}} \right]^{-1/2}$



$$\chi^2(\hat{a} + \sigma_{\hat{a}}) = 1$$

Generalisation to any one parameter fit

Taylor expansion of χ^2 around estimated value $\hat{a}$:

$$\chi^2 = \chi^2(\hat{a}) + \frac{d\chi^2}{da}_{|a=\hat{a}} \cdot (a - \hat{a}) + \frac{1}{2}\,\frac{d^2\chi^2}{da^2}_{|a=\hat{a}} \cdot (a - \hat{a})^2 + \ldots$$

$$= \chi^2(\hat{a}) + H \cdot (a - \hat{a})^2 \quad \text{with} \quad H = \frac{1}{2}\,\frac{d^2\chi^2}{da^2}_{|a=\hat{a}} \quad \text{Hesse matrix}$$

Thus the *inverse probability density* is

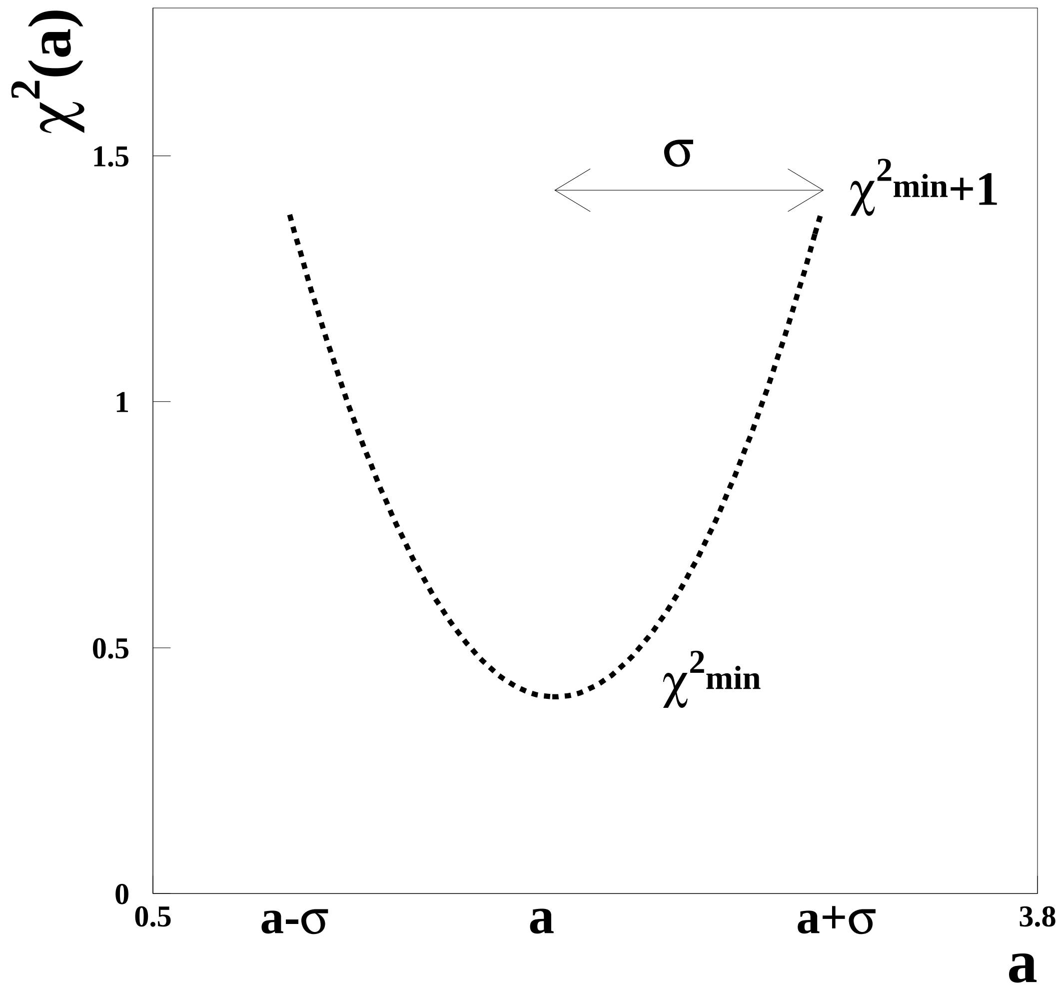
$$p(a|\hat{a}) \sim e^{-\frac{\chi^2(\hat{a})}{2}} \cdot e^{-\frac{1}{2}\,H\cdot(\hat{a}-a)^2)}$$

$\longrightarrow$ gaussian distribution around $\hat{a}$ with width $\sigma = H^{-1/2}$

Generalisation to any one parameter fit

$$\chi^2(a) = \chi^2(\hat{a}) + \frac{(a-\hat{a})^2}{\sigma^2}$$

$$\rightarrow \quad \chi^2(a \pm 1\sigma) = \chi^2(\hat{a}) + 1 = \chi^2_{min} + 1$$

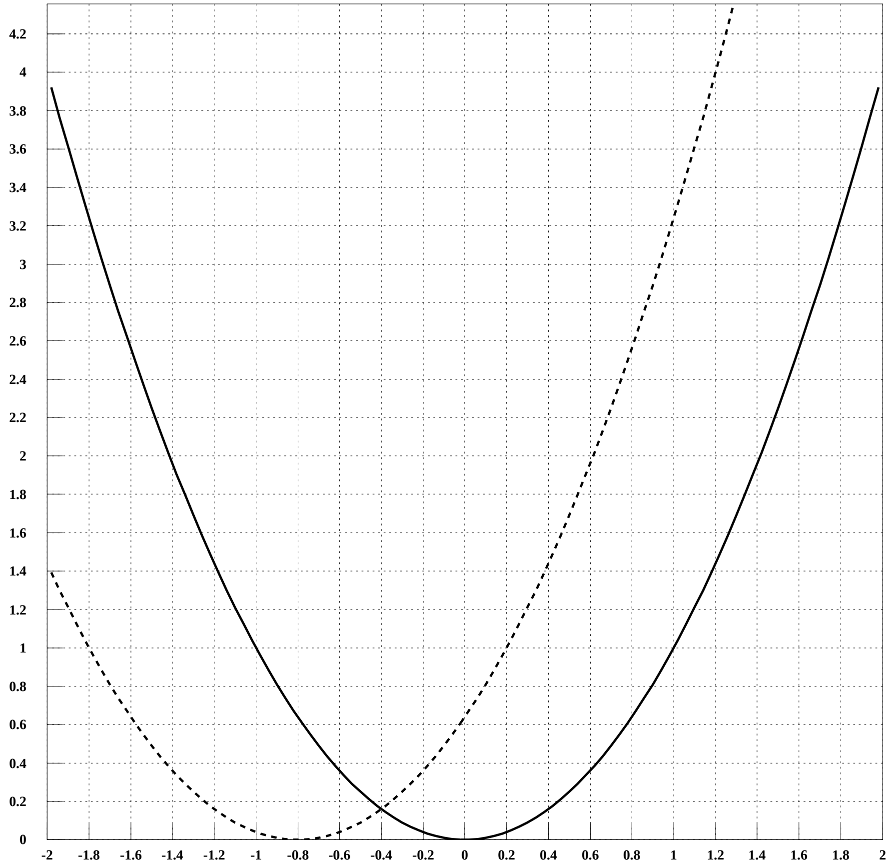


→ Read error directly from χ^2 curve

Mini-exercise Averaging of two meas. via χ^2 parabolas

Two measurements y_1, y_2 of the same quantity a can be represented by their χ^2 parabolas: $\chi_i^2 = (y_i - a)^2/\sigma_i^2; \quad i = 1, 2$

- **draw for the example below the total χ^2, i.e. the sum of the two parabolas**
- **Read off the value $\hat{a}$ (where the total χ^2 is minimal)**
- **Estimate the error of $\hat{a}$ from the points where $\chi^2 = \chi^2_{min} + 1$**



Averaging several measurements

n measurements $y_i \pm \sigma_i$ of the same quantity $y \longrightarrow$ what is the best way to average?

(Why is $\frac{1}{n}\Sigma y_i$ not the best? $\longrightarrow$ measurements with large errors get too much weight and can spoil the average!)

$$\chi^2 = \Sigma_{i=1}^{n} \frac{(y_i - a)^2}{\sigma_i^2}$$

$$\frac{d\chi^2}{da} = 0 = \Sigma_{i=1}^{n} \frac{-2(y_i - a)}{\sigma_i^2} = -2\Sigma_{i=1}^{n} \frac{y_i}{\sigma_i^2} + 2a\Sigma_{i=1}^{n} \frac{1}{\sigma_i^2}$$

$$\longrightarrow \quad \boxed{\hat{a} \;=\; \Sigma_{i=1}^{n} \frac{y_i}{\sigma_i^2} / \Sigma_{i=1}^{n} \frac{1}{\sigma_i^2}}$$

Averaging several measurements

$\rightarrow$ Single measurements contribute with weight $G_i = \frac{1}{\sigma_i^2}$;

Define $G_s := \Sigma_{i=1}^n G_i$;   Hesse Matrix $H = 1/2 \frac{d^2\chi^2}{da^2} = G_s$

$$\rightarrow \quad \boxed{\hat{a} \;=\; \frac{1}{\Sigma_{i=1}^n G_i} \cdot \Sigma_{i=1}^n G_i y_i = \frac{1}{G_s} \cdot \Sigma_{i=1}^n G_i y_i}$$

Error on $\hat{a}$:

$$\boxed{\begin{aligned} \sigma_{\hat{a}}^2 &= \Sigma_{i=1}^n \left(\frac{d\hat{a}}{dy_i}\right)^2 \cdot \sigma_i^2 = \Sigma_{i=1}^n \left(\frac{G_i}{G_s}\right)^2 \cdot \sigma_i^2 \\ &= \frac{1}{G_s^2} \cdot \Sigma_{i=1}^n G_i = \frac{1}{G_s} = \frac{1}{\Sigma_{i=1}^n 1/\sigma_i^2} \end{aligned}}$$

In short

$$\boxed{\hat{a} = \frac{\Sigma_{i=1}^n y_i/\sigma_i^2}{\Sigma_{i=1}^n 1/\sigma_i^2} \;\pm\; \frac{1}{\sqrt{\Sigma_{i=1}^n 1/\sigma_i^2}}}$$

Mini-exercise Gain from weighted average

Die totale Teilchenrate aus einer Quelle soll gemessen werden. Um die Quelle herum ist ein hermetischer Detektor gebaut. Die eine Hälfte des Detektors misst

$$N_1 = 100 \pm 10$$

Die andere Hälfte des Detektors ist sehr ineffizient und misst (effizienzkorrigiert!)

$$N_2 = 100 \pm 100$$

Schätzen Sie die Gesamtrate N mit den folgenden zwei Methoden:

1. $\hat{N} = N_1 + N_2$
2. Multipliziere N_1 und N_2 jeweils mit Faktor 2 (beide Hälften 'sehen' ja 50%!) $\rightarrow$ separate Messungen:
   - Erste Messung: $N = 200 \pm 20$
   - Zweite Messung $N = 200 \pm 200$

   $\rightarrow$ Bilde das gewichtete Mittel beider Messungen als Schätzwert $\hat{N}$.

$\rightarrow$ **Bestimmen Sie für beide Verfahren den Fehler auf $\hat{N}$ (Formeln s. Vorlesung!)**

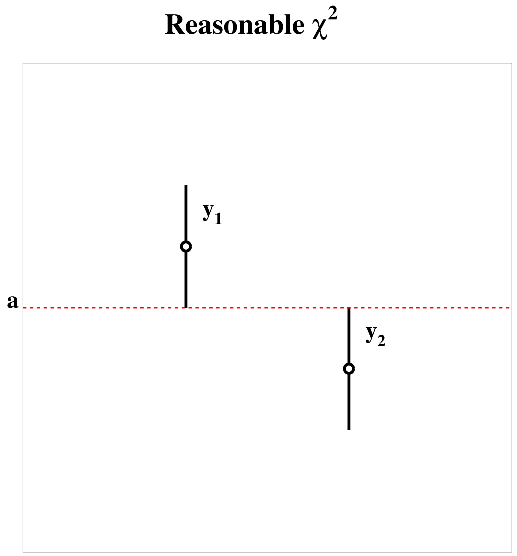
Lecture II on linear least square fits

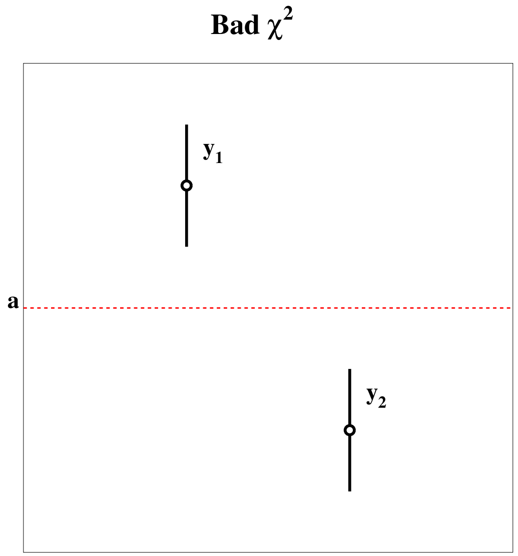
Contents:

- Consistency of measurements $\rightarrow$ χ^2 fit quality test
- Outlier rejection

Consistency of measurements

Example: Two measurements y_1 and y_2 with errors σ_1 and σ_2; the true value a is known, are the meas. consistent with a?:





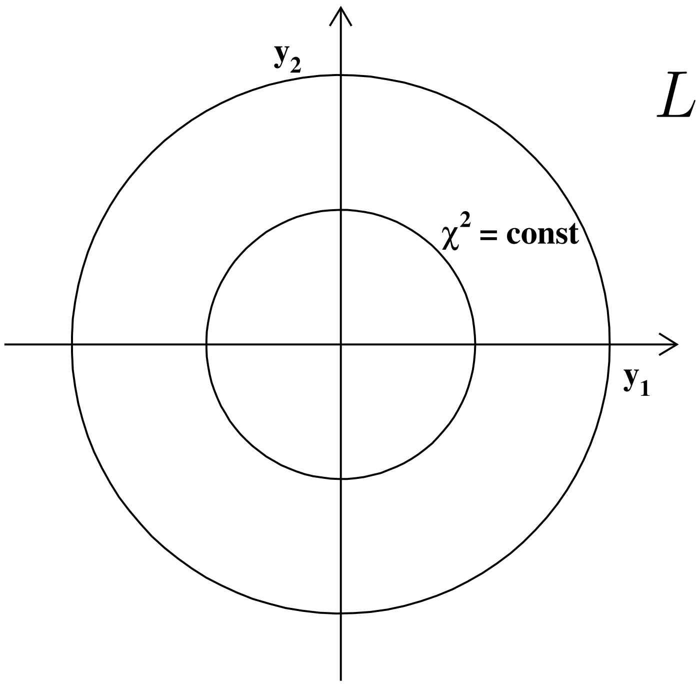
$$\chi^2 = \frac{(y_1 - a)^2}{\sigma_1^2} + \frac{(y_2 - a)^2}{\sigma_2^2} = 2$$

$$\chi^2 = 8$$

$\longrightarrow \chi^2$ is a measure of the consistency

Consistency of measurements

Expected prob. density for $\vec{y} = (y_1, y_2)$ (for case $a = 0; \sigma_1 = \sigma_2 = \sigma$):



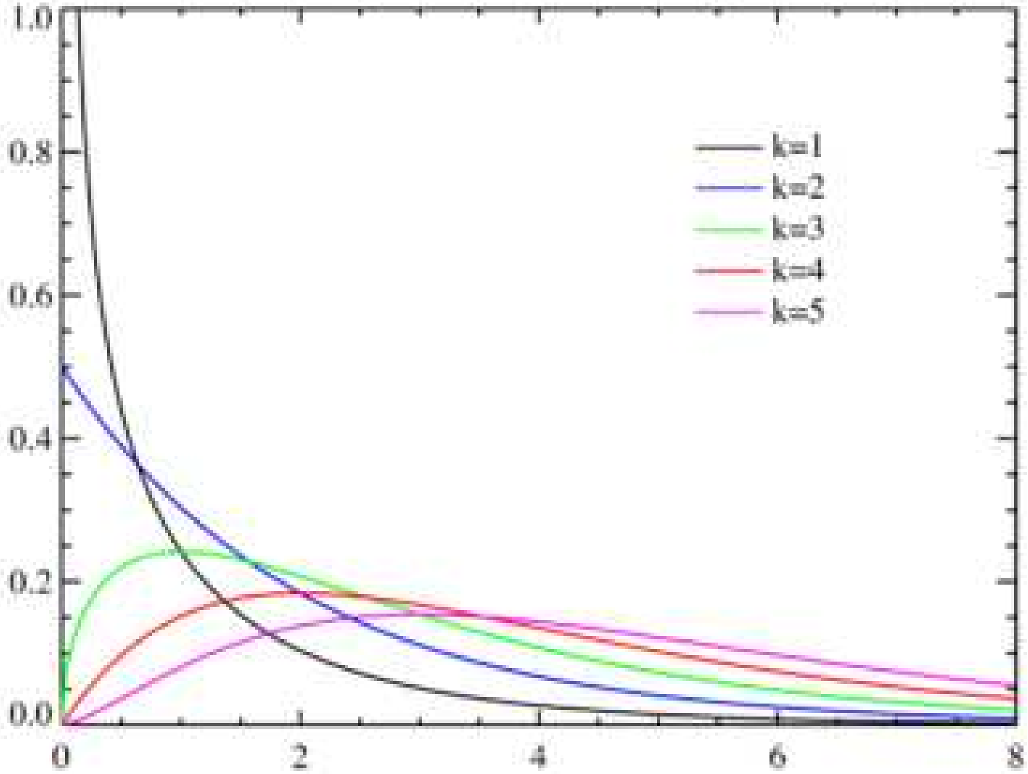
$$L(\vec{y}, a) \propto e^{-y_1^2/2} e^{-y_2^2/2} \sim e^{-\chi^2/2}$$

Trafo $L(\vec{y}, a) \longrightarrow$ prob. density $f(\chi^2)$

General result for n measurements: χ^2 fct. for n-degrees of freedom

$$\rightarrow f(\chi^2, n) = \frac{1}{\Gamma(n/2) 2^{n/2}} \cdot (\chi^2)^{n/2-1} \cdot e^{-\chi^2/2}$$

χ^2-function for n degrees of freedom



$$f(\chi^2, n) = \frac{1}{\Gamma(n/2)2^{n/2}} \cdot (\chi^2)^{n/2-1} \cdot e^{-\chi^2/2}$$

with $\Gamma(n/2) = \int_0^\infty dt e^{-t} t^{n/2-1}$

$$\boxed{\begin{array}{l} \int_0^\infty f(\chi^2, n) d\chi^2 = 1 \\ \langle \chi^2 \rangle = n \\ V(\chi^2) = 2n;\ \sigma(\chi^2) = \sqrt{2n} \\ \rightarrow \langle \chi^2/n \rangle = 1 \\ \sigma(\chi^2/n) = \sqrt{2/n} \end{array}}$$

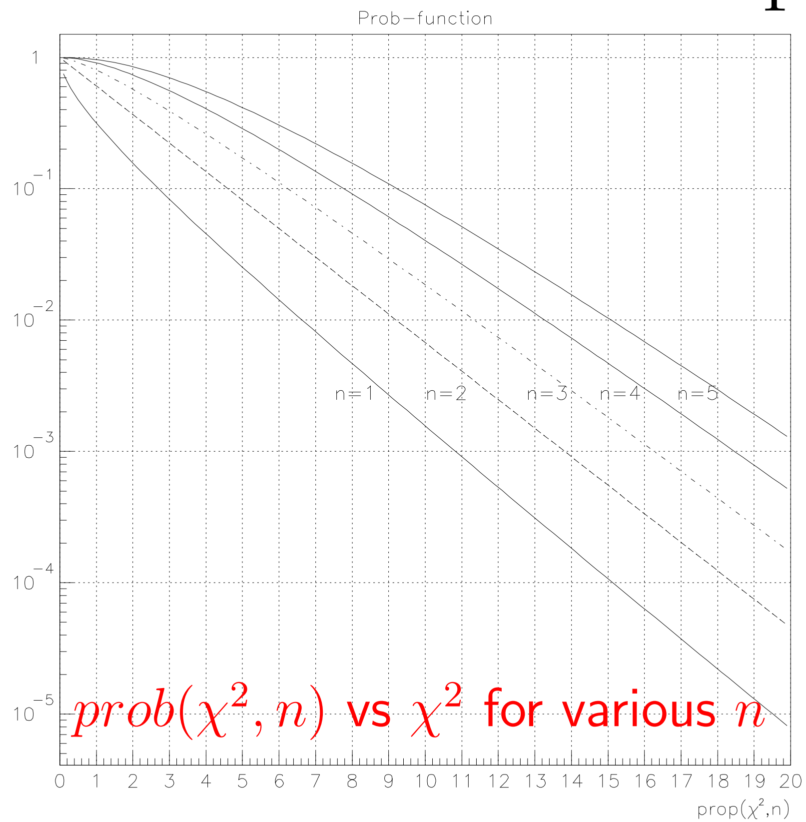
χ^2-fit probability

Common measure for consistency of measurements:

Probability that for repeated experiments a $\chi^2 \geq \chi^2_{actual}$ is observed

$$prob(\chi^2, n) = \int_{\chi^2}^{\infty} f(\chi^2, n) d\chi^2 \quad \text{subst. } t = \chi^2/2$$

$$= \frac{1}{\Gamma(n/2)} \cdot \int_{\chi^2/2}^{\infty} dt\, e^{-t}\, t^{n/2-1}$$



$prob(\chi^2, n)$ vs χ^2 for various n

Add plot of expected flat distribution

χ^2 for two measurements with unknown true value

Until now the true value of a was assumed to be known, now replace by estimated $\hat{a}$;

Example of two measurements:

$$\chi^2_{min} = \frac{(y_1 - \hat{a})^2}{\sigma_1^2} + \frac{(y_2 - \hat{a})^2}{\sigma_2^2}$$

Using the weighted average for $\hat{a}$ and with $G_i := 1/\sigma_i^2 \longrightarrow$

χ^2 for two measurements with unknown true value

$$
\begin{aligned}
\chi^2_{min} &= G_1 \cdot \left(y_1 - \frac{(G_1 y_1 + G_2 y_2)}{G_1 + G_2} \right)^2 + G_2 \cdot \left(y_2 - \frac{(G_1 y_1 + G_2 y_2)}{G_1 + G_2} \right)^2 \\
&= G_1 \cdot \left(\frac{(G_2 y_1 - G_2 y_2)}{G_1 + G_2} \right)^2 + G_2 \cdot \left(\frac{(G_1 y_2 - G_1 y_1)}{G_1 + G_2} \right)^2 \\
&= \frac{G_1 G_2^2}{(G_1 + G_2)^2} (y_1 - y_2)^2 + \frac{G_2 G_1^2}{(G_1 + G_2)^2} (y_1 - y_2)^2 \\
&= \frac{G_1 G_2 (G_1 + G_2)}{(G_1 + G_2)^2} \cdot (y_1 - y_2)^2 = \frac{G_1 \cdot G_2}{G_1 + G_2} \cdot (y_1 - y_2)^2 \\
&= \frac{1}{1/G_1 + 1/G_2} \cdot (y_1 - y_2)^2 = \boldsymbol{\frac{1}{\sigma_1^2 + \sigma_2^2} \cdot (y_1 - y_2)^2}
\end{aligned}
$$

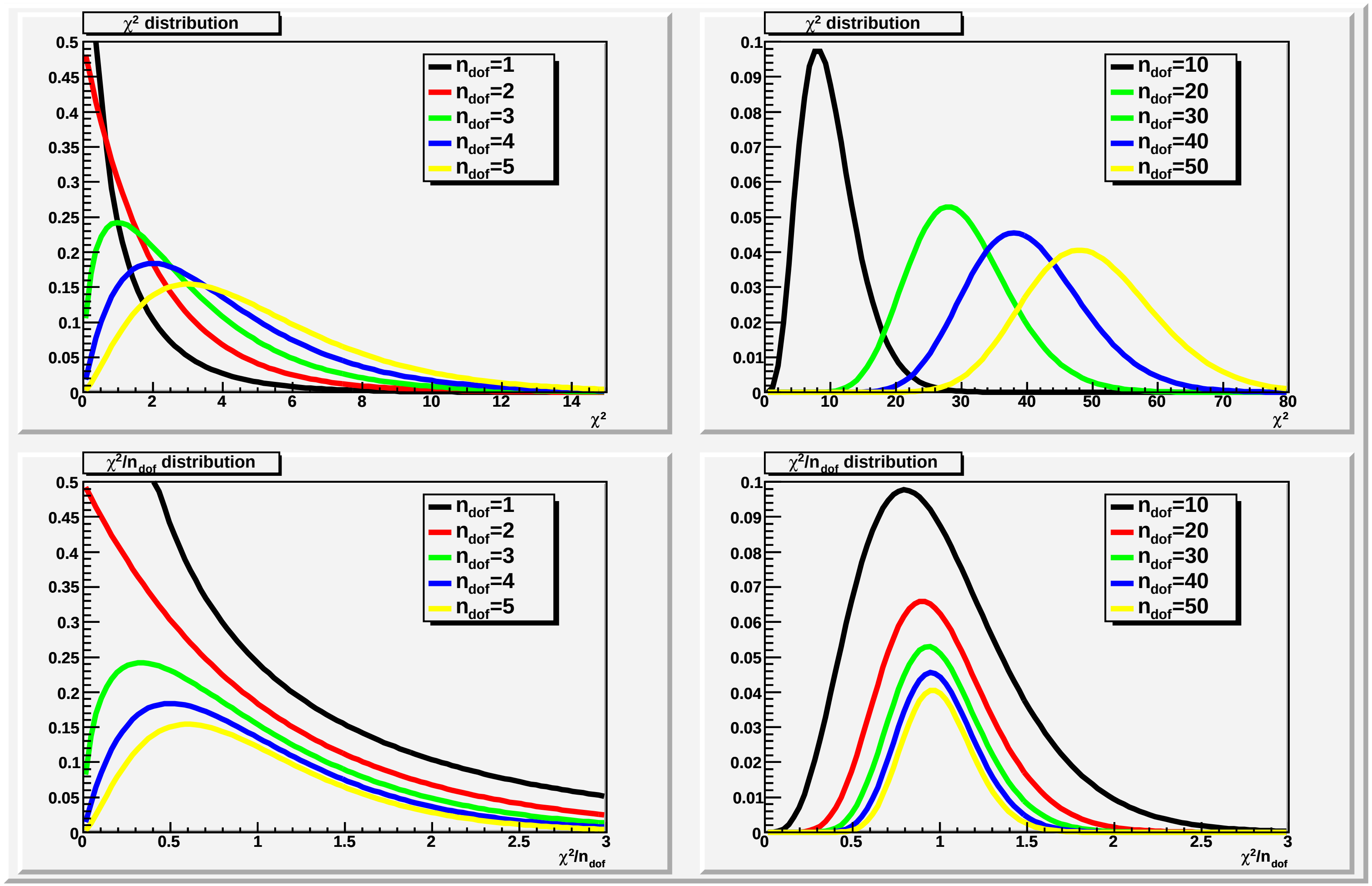
Observable $\Delta = \frac{y_1 - y_2}{\sqrt{\sigma_1^2 + \sigma_2^2}}$ follows (obviously) gauss distribution $\sim e^{-\frac{\Delta^2}{2}}$

$\rightarrow \chi^2 = \Delta^2$ follows <u>1-dim</u> χ^2 distr.!

$\rightarrow$ One degree of freedom "sacrificed" for determination of $\hat{a}$.

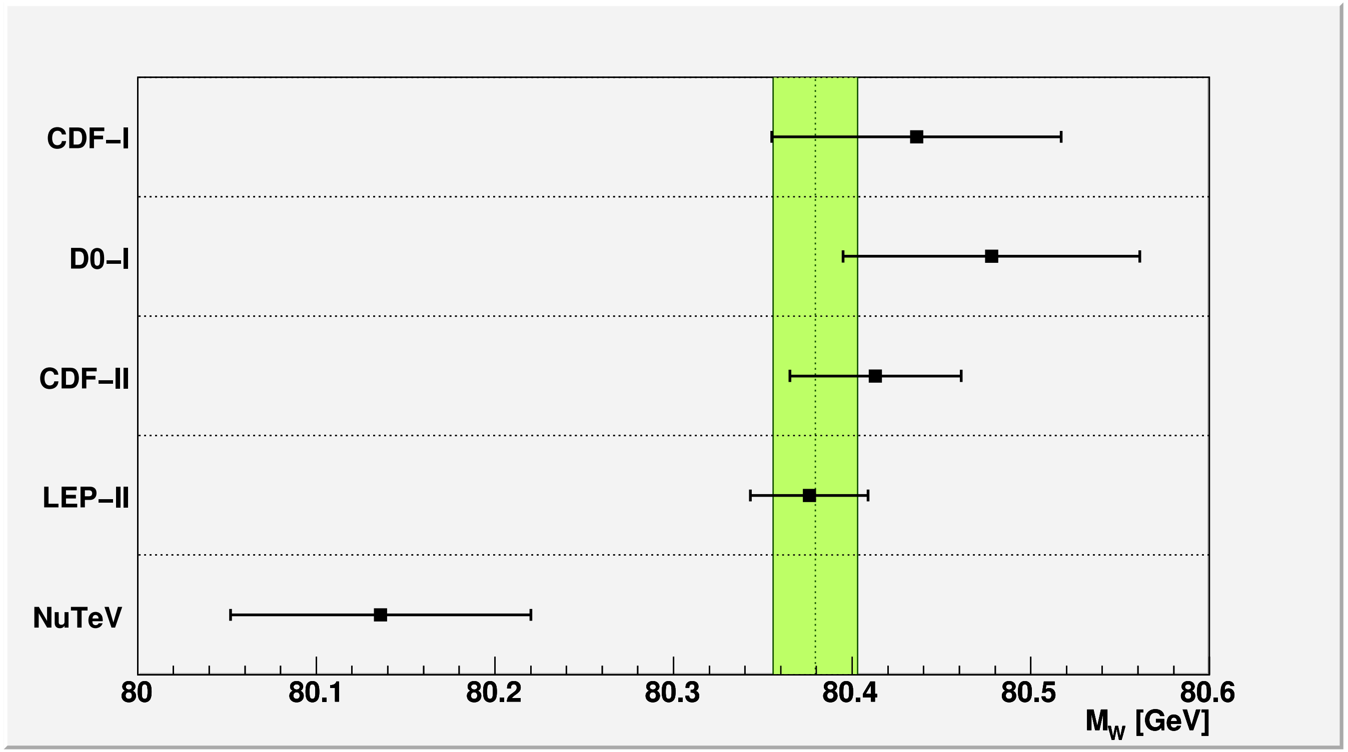
General: n-measurements with one unknown a $\rightarrow$ follows χ^2 distribution with $n-1$ degrees of freedom

Mini-exercise Plot χ^2 curves with computer



see $/afs/desy.de/user/m/mgoebel/public/StatisticsWS/ChiSquareDistribution.C$

Mini-exercise Outlier rejection



see $/afs/desy.de/user/m/mgoebel/public/StatisticsWS/AverageMW.C$

Tasks: Determined weighted average, thi χ^2_{min} and fit-probability, see what happens if one takes out the value with the largest deviation from the mean, etc.

Lecture III on linear least square fits

Contents:

- General solution (normal equations) of linear least square fits
- Straight line fits ... and other fit examples

Solution via normal equations

Linear fit $\longrightarrow$ determines estimator for $\vec{a}$

$$\chi^2 = (\vec{y} - A\vec{a})^t V^{-1} (\vec{y} - A\vec{a})$$

$$Min.\chi^2 \ \longrightarrow \ \frac{d\chi^2}{d\vec{a}} = 0$$

$$\longrightarrow \ -2A^t V^{-1}(\vec{y} - A\vec{a}) = 0$$

$$\longrightarrow \ A^t V^{-1} A\vec{a} = A^t V^{-1}\vec{y}$$

Side remark: why can't we just set: $\vec{y} = A\vec{a}$??? Because $\vec{y}$ has dimension n and $\vec{a}$ has dimension m !!! Solution:

$$\boxed{\begin{aligned} \vec{a} &= (A^t V^{-1} A)^{-1} A^t V^{-1} \vec{y} \\ &= H^{-1} A^t V^{-1} \vec{y} \\ &= U A^t V^{-1} \vec{y} \\ &\quad \text{with } U = H^{-1} = Cov(a) \end{aligned}}$$

Normal equations

To be xchecked: Properties of linear least square fits

1. consistency: $\lim_{N\to\infty} \hat{\vec{a}} = \vec{a}$ (follows from next point)
2. Unbiasedness: $\langle \hat{\vec{a}} \rangle = \langle B\vec{y} \rangle = B \langle \vec{y} \rangle = B\,A\,\vec{a} = (A^t\,V^{-1}\,A)^{-1}\,A^t\,V^{-1}\,A\,\vec{a} = \vec{a}$
   $\longrightarrow$ unbiased!
3. Efficiency: Gauss-Markov-Theorem:

For randomly distributed $\vec{y}$ the linear least square fit is the most efficient estimator

   (Proof e.g. in Blobel/Lohrmann book)
4. For measurements $\vec{y}$ with gaussian errors and if $\vec{y} = A\vec{a}$ is the correct model, then χ^2 follows a χ^2-distribution with N-m degrees of freedom (with N = number of data points and m = number of fit parameters)

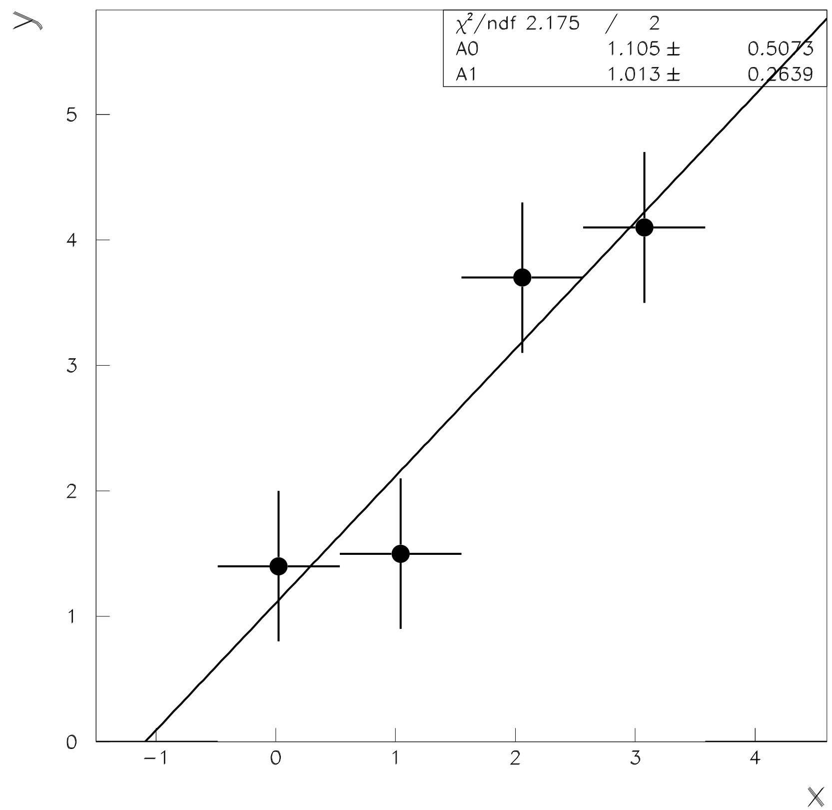
Straight line fit

Model: $y = a_0 + a_1 x$

Example: All y_i have the same uncertainty

$$V = \begin{pmatrix} \sigma^2 & & 0 \\ & . & \\ 0 & & \sigma^2 \end{pmatrix}$$

$$\chi^2 = \sum_{i=1}^{n} \frac{(y_i - a_0 - a_1\, x_i)^2}{\sigma^2}$$



Matrix notation: $\vec{y} = A\vec{a}$; $\quad A = \begin{pmatrix} 1 & x_1 \\ . & . \\ 1 & x_n \end{pmatrix}, \quad A^T = \begin{pmatrix} 1 & \dots & 1 \\ x_1 & \dots & x_n \end{pmatrix}$

$$\hat{\vec{a}} = \begin{pmatrix} \hat{a}_0 \\ \hat{a}_1 \end{pmatrix} = (A^T V^{-1} A)^{-1} A^T V^{-1} \vec{y}; \qquad V^{-1} = \begin{pmatrix} 1/\sigma^2 & & 0 \\ & . & \\ 0 & & 1/\sigma^2 \end{pmatrix}$$

Straight line fit

$$\hat{\vec{a}} = \sigma^2 (A^T A)^{-1} \cdot \frac{1}{\sigma^2} A^T \cdot \vec{y} = (A^T A)^{-1} A^T \cdot \vec{y}$$

$$= \begin{pmatrix} \sum_i 1 & \sum_i x_i \\ . & . \\ \sum_i x_i & \sum_i x_i^2 \end{pmatrix}^{-1} \cdot \begin{pmatrix} \sum_i y_i \\ \sum_i x_i y_i \end{pmatrix} = \begin{pmatrix} N & N\overline{x} \\ N\overline{x} & N\overline{x^2} \end{pmatrix}^{-1} \cdot \begin{pmatrix} N\overline{y} \\ N\overline{xy} \end{pmatrix}$$

$$= \begin{pmatrix} 1 & \overline{x} \\ \overline{x} & \overline{x^2} \end{pmatrix}^{-1} \cdot \begin{pmatrix} \overline{y} \\ \overline{xy} \end{pmatrix} = \frac{1}{\overline{x^2} - \overline{x}^2} \begin{pmatrix} \overline{x^2} & -\overline{x} \\ -\overline{x} & 1 \end{pmatrix} \begin{pmatrix} \overline{y} \\ \overline{xy} \end{pmatrix} = \frac{1}{V[x]} \cdot \begin{pmatrix} \overline{x^2}\,\overline{y} - \overline{x}\,\overline{xy} \\ -\overline{x}\,\overline{y} + \overline{xy} \end{pmatrix}$$

Covariance matrix:

$$U = \begin{pmatrix} \sigma_{a_0}^2 & cov(a_0, a_1) \\ cov(a_0, a_1) & \sigma_{a_1}^2 \end{pmatrix} = (A^t V^{-1} A)^{-1} = \frac{\sigma^2}{NV[x]} \begin{pmatrix} \overline{x^2} & -\overline{x} \\ -\overline{x} & 1 \end{pmatrix}$$

Mini exercise: straight line track-fit with N det.

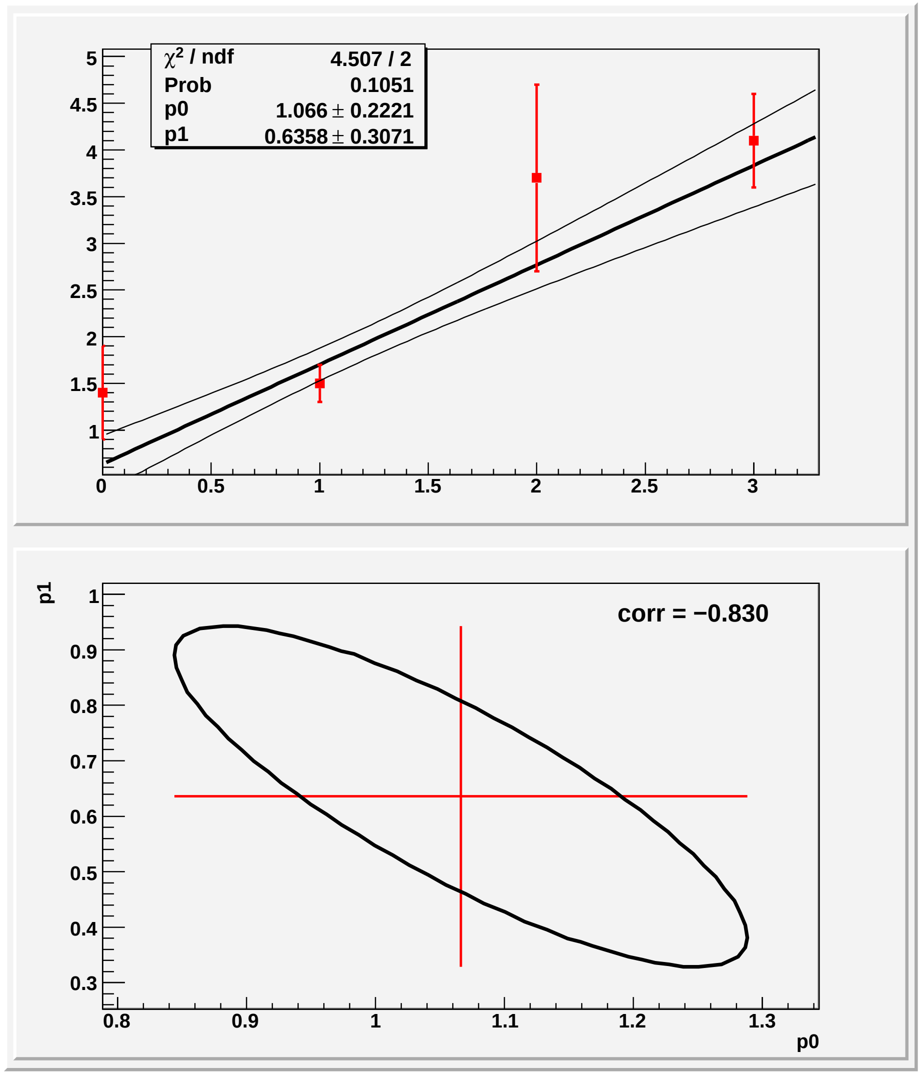
Using the above formulas - determine the improvements on the track slope error σ_{a_1} by:

a) Doubling the number of detector layers within the same interval in x

b) Distributing the detector layers over an interval in x twice as large

c) Buying detectors with measurement uncertainties reduced by a factor two

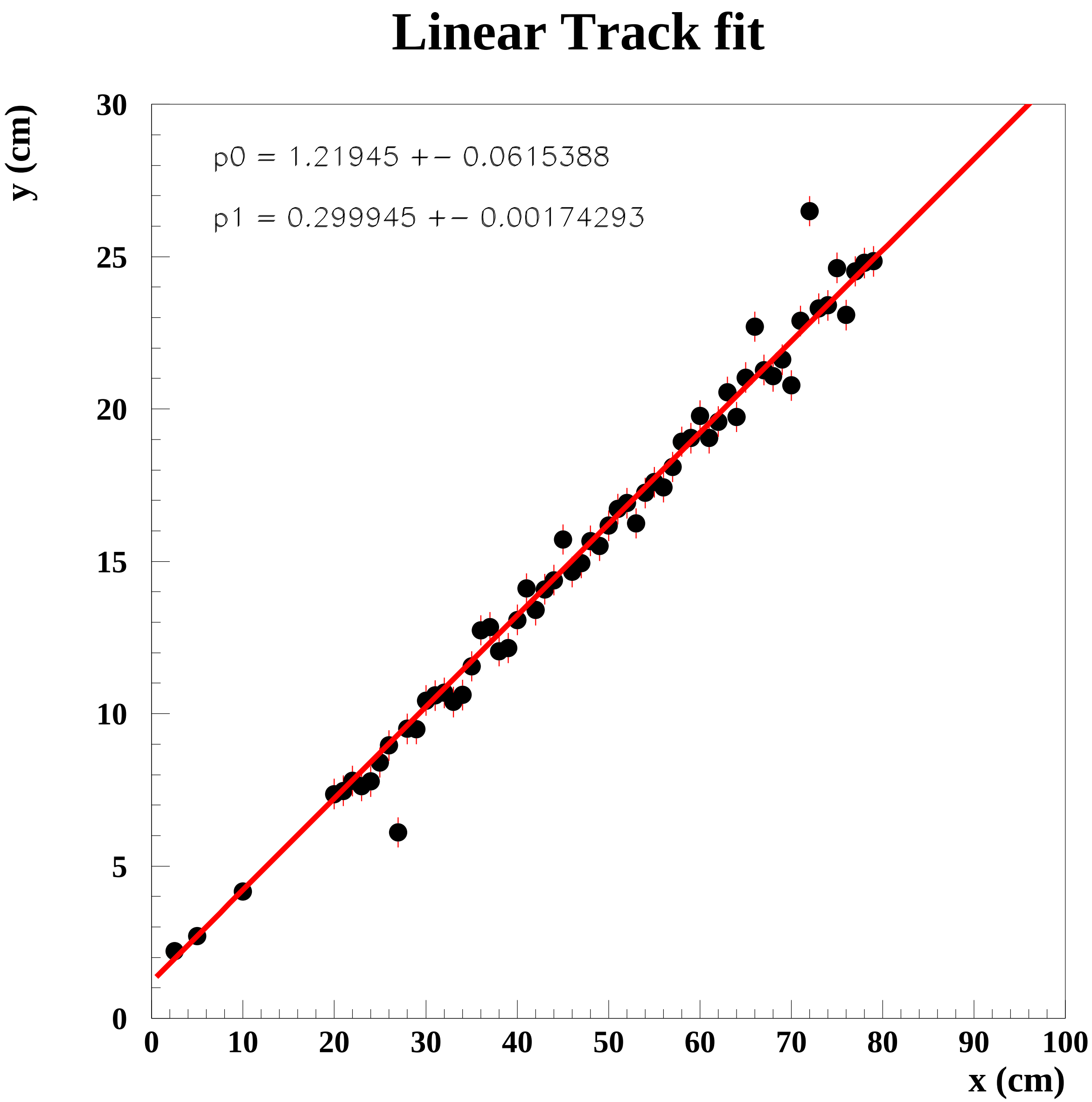
Mini-exercise Straight-line fit example



Tasks: Do the fit, plot the error ellipse, get the 1-sigma band, judge fit quality, etc.

see $/afs/desy.de/user/m/mgoebel/public/StatisticsWS/StraightLineFit.C$

Mini-exercise Real Trackfit in Si + driftchamber



Tasks: Do the straight line fit, plot the error ellipse, get the 1-sigma band, judge fit quality, reject outliers!, fit with parabola, determine momentum and error, extension: add vertex constraint

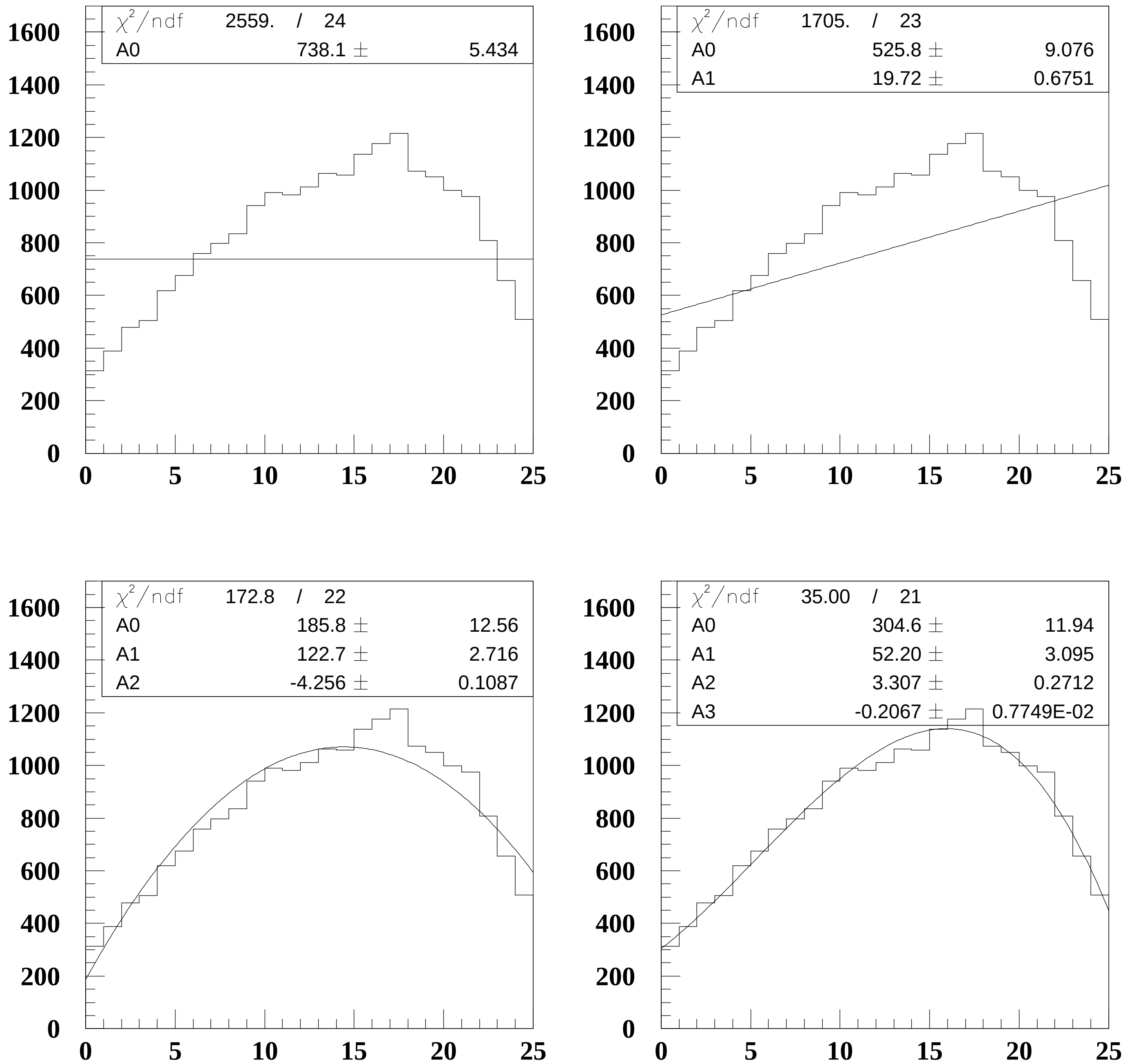
Mini-exercise: Find best data parametrisation

The plots on the next two pages show χ^2-fits of the same data distribution with eight different parametrisations (polynomials of different orders). Which parametrisation is the most reasonable one? Try to judge using the following three criteria:

1. optically, how well the curves fit the data
2. a reasonable parametrisation should lead to $\chi^2/ndf \approx 1$.
3. choose only a more complicated parametrisation if a significant improvement of χ^2/ndf can be achieved

$\longrightarrow$ Try to find your personal favorite.

Mini-exercise: Find best data parametrisation



Mini-exercise: Find best data parametrisation