PHYSICS AT THE TERA SCALE Helmholtz Alliance

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Extended Fits with Many Parameters

such as

Constrained Kinematic Fits

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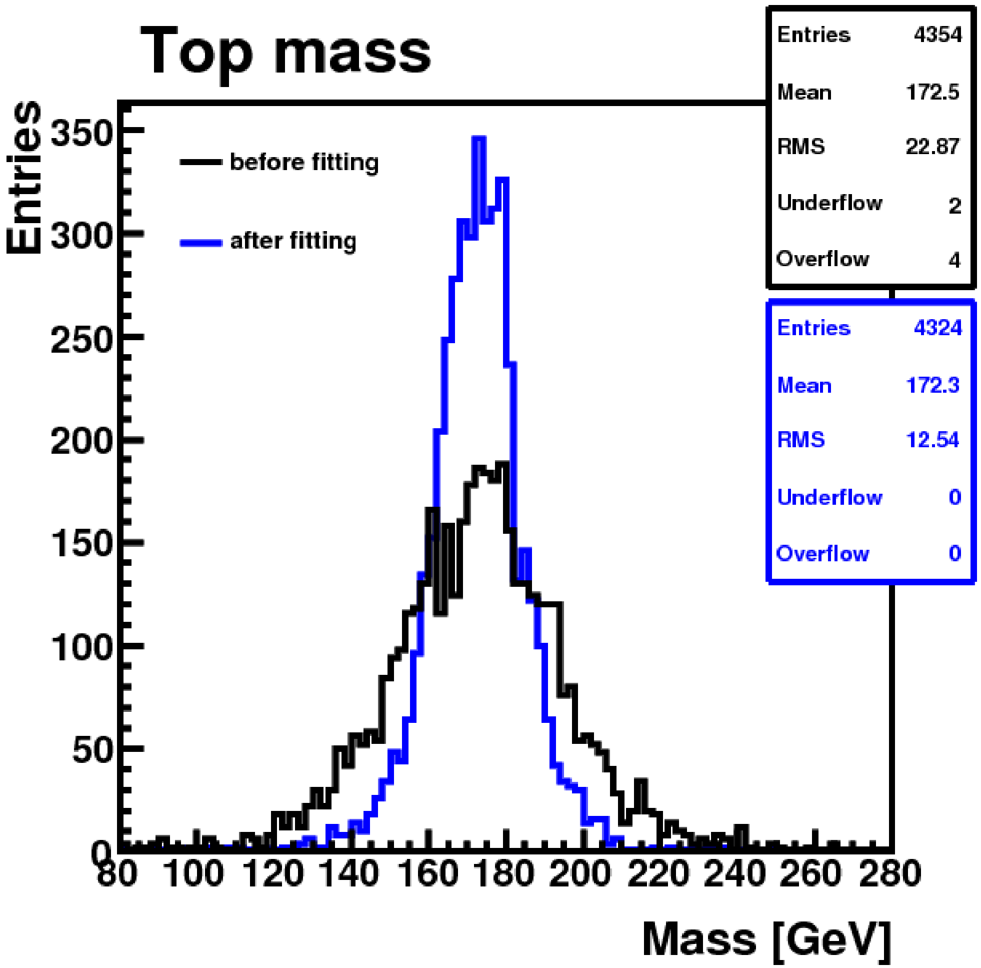
Fitting Workshop – DESY - 30th March ... 1st April 09

Outline

- *Short reminder*: least square fits
- Constrained fits with technique of Lagrangian Multipliers
- Linearization of minimization problems
- Kinematic fits:
  - mass constraints
  - momentum balance
  - unmeasured parameters
- Iterative algorithm and optimization
- Alternative method: minimization of cost function



Example: Improvement of top mass resolution using a kinematic fit

Reminder: Method of Least Squares

N **measurements:** y_i with **variances** σ_i^2

In case of statistically independent variables the **covariance matrix** is diagonal

$$V[y] = \begin{pmatrix} \sigma_1^2 & 0 & 0 & \cdots & 0 \\ 0 & \sigma_2^2 & 0 & \cdots & 0 \\ & \cdots & & & \\ 0 & 0 & 0 & \cdots & \sigma_N^2 \end{pmatrix} \quad V^{-1}[y] = \begin{pmatrix} 1/\sigma_1^2 & 0 & 0 & \cdots & 0 \\ 0 & 1/\sigma_2^2 & 0 & \cdots & 0 \\ & \cdots & & & \\ 0 & 0 & 0 & \cdots & 1/\sigma_N^2 \end{pmatrix}$$

Model $f_i(a_1 \ldots a_M)$ with M **free parameters** a_j

Normalized **residuals**

$$\chi^2 = \sum_{i=1}^{N} \frac{r_i^2}{\sigma_i^2} = \sum_{i=1}^{N} \frac{(y_i - f_i(\vec{a}))^2}{\sigma_i^2} = \sum_{i,j=1}^{N} (y_i - f_i(\vec{a}))^T V_{ij}^{-1}[y](y_j - f_j(\vec{a}))$$

The best fitting model parameters should minimize this expression

Reminder: Method of Least Squares

Minimization of χ^2: derivatives with respect to all model parameters a_i should vanish

$$\frac{d\chi^2}{da_i} \stackrel{!}{=} 0$$

Matrix notation for **linear models**

$$\vec{f} = A \cdot \vec{a}$$

→ Sum of residuals

$$\chi^2 = \vec{r}^{\,T} V^{-1}[y] \vec{r} = (\vec{y} - A \cdot \vec{a})^T V^{-1}[y] (\vec{y} - A \cdot \vec{a})$$

...

Normal equation: $$(A^T V^{-1}[y] A) \cdot \vec{a} = A^T V^{-1}[y] \vec{y}$$

Solution:

$$\begin{aligned} \vec{a}_{\text{estimate}} &= (A^T V^{-1}[y] A)^{-1} A^T V^{-1}[y] \vec{y} \\ V[\vec{a}_{\text{estimate}}] &= (A^T V^{-1}[y] A)^{-1} \end{aligned}$$

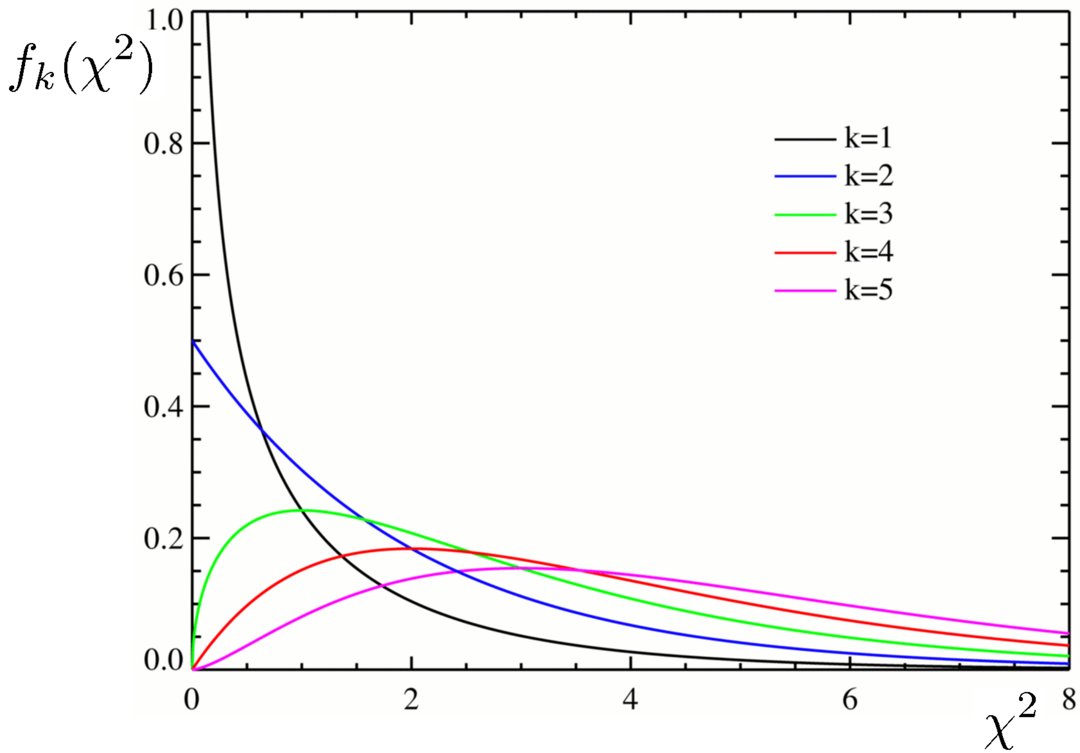
χ^2 Distribution & Degrees of Freedom

For N measurements with M fitted parameters,

$$\chi^2 = \sum_{i=1}^{N} \frac{r_i^2}{\sigma_i^2} = \sum_{i=1}^{N} \frac{(y_i - f_i(\vec{a}))^2}{\sigma_i^2}$$

is distributed according to a χ^2 distribution with $k = N - M$ degrees of freedom.

If we add P **constraints** between the fitted parameters (see later) the number of free parameters is reduced by P and the d.o.f. are increased: $\boldsymbol{k = N - M + P}$



Interpretation of Results

Pulls: normalized residuals with respect to true values

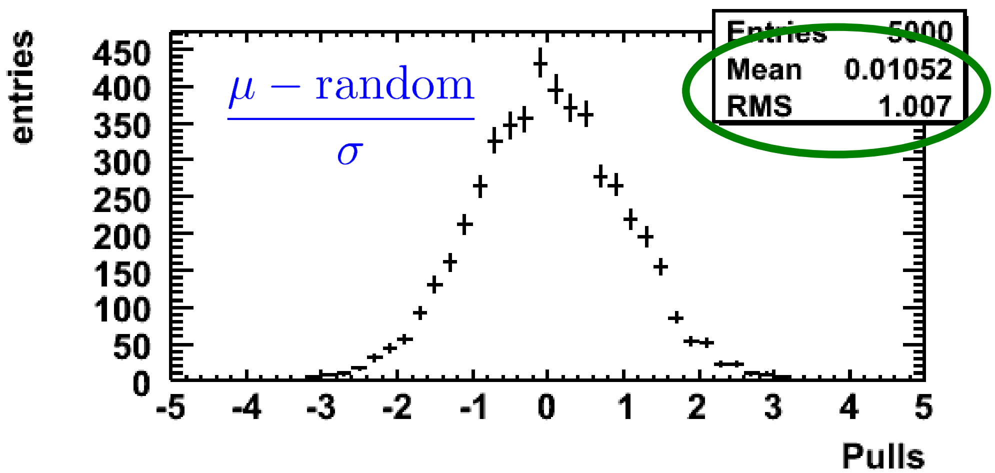
$$\text{pulls} = r_i = \frac{y_i^{\text{model}} - y_i^{\text{meas}}}{\sigma_i}$$

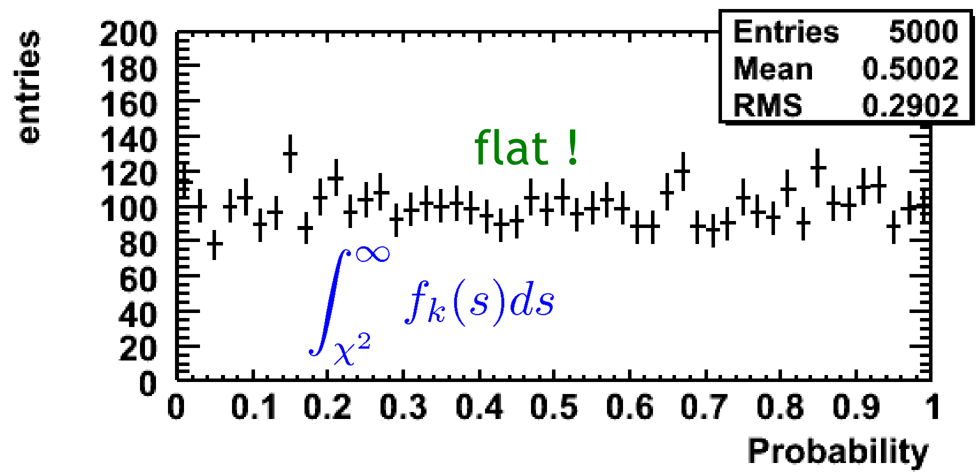
Properties of pulls for correct model:

- normal distributed with mean $\mu_r = 0$. If not → systematic errors of measurements.
- variance $\sigma_r = 1$. If large than 1 → errors are underestimated else overestimated.

If χ^2 follows a χ^2-distribution with k degrees of freedom → corresponding probability distribution is flat!

Example: normal distribution (μ = 1 and σ = 1) of random variable (one measurement $N = 1$, no fit parameter $M = 0$ and no constraint $P = 0$) → $k = 1$

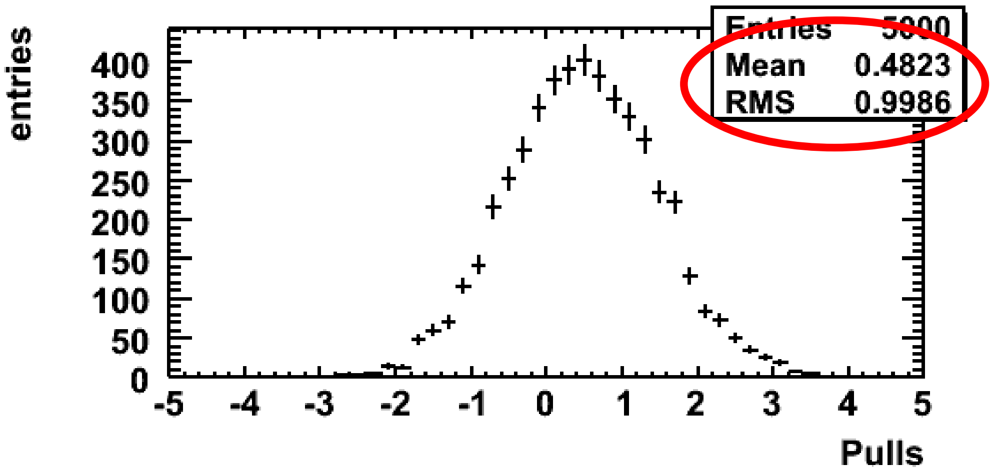


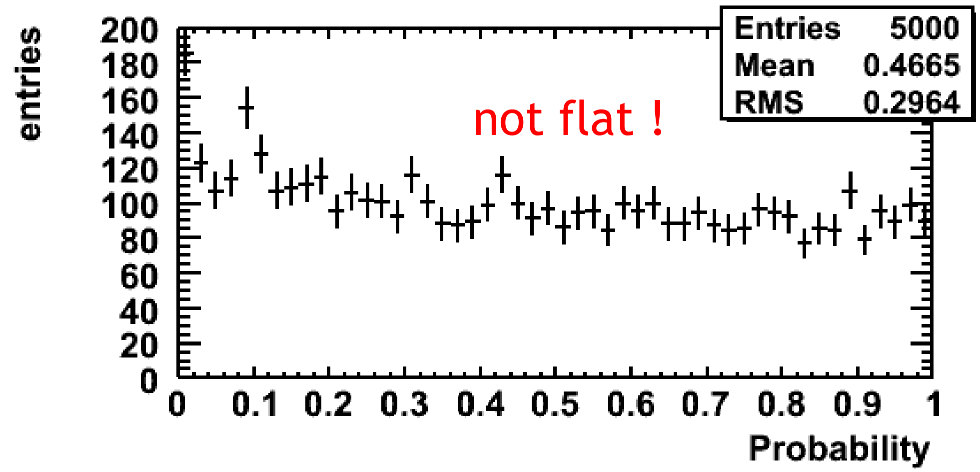


Example: Interpretation of Results

Incorrect model I: model value μ offset by +0.5 σ

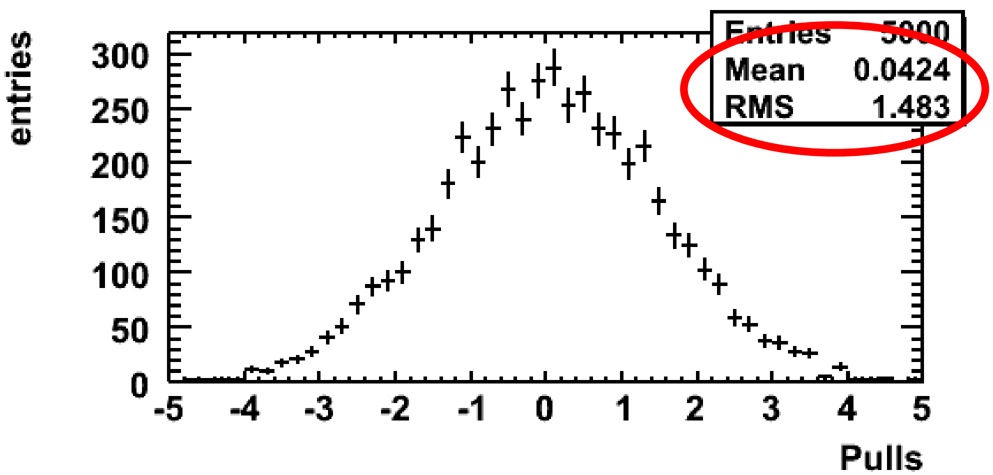
→ pulls shifted to the right, variance OK, probability rises at low values

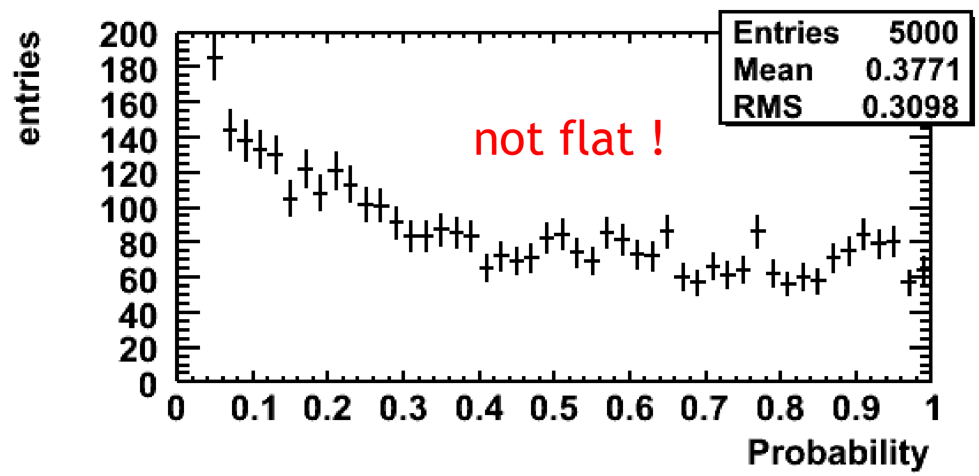




Incorrect model II: model error σ larger by factor 1.5

→ mean of pulls = 0, variance larger than 1, probability rises at low values





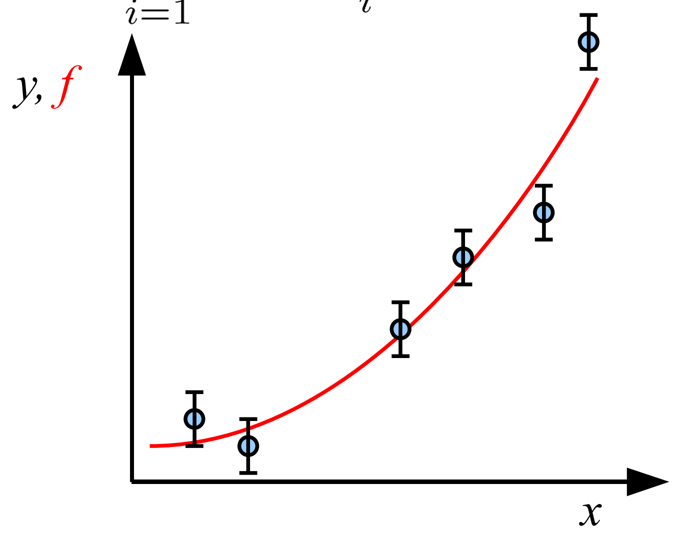
One Parameter for Each Measurement

Linear least squares: fit a function with few parameters to many measurements:

Example: Quadratic fit $f_i(\vec{a}) = a_0 + a_1 \cdot x_i + a_2 \cdot x_i^2 \to \chi^2 = \sum_{i=1}^{N} \frac{(y_i - f_i(\vec{a}))^2}{\sigma_i^2}$

Matrix form: $\vec{f} = A \cdot \vec{a}$

$$\begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \end{pmatrix} = \begin{pmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ & \cdots & \\ 1 & x_N & x_N^2 \end{pmatrix} \cdot \begin{pmatrix} a_0 \\ a_1 \\ a_2 \end{pmatrix}$$

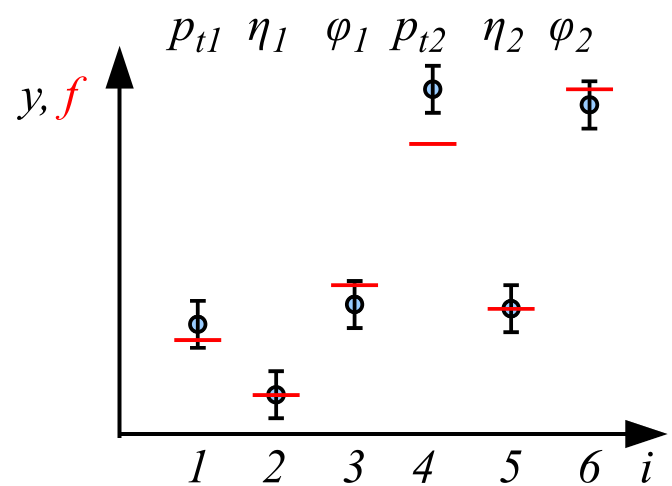


Now: One fit parameter for each measurement

$$f_i(\vec{a}) = a_i \to \chi^2 = \sum_{i=1}^{N} \frac{(y_i - a_i)^2}{\sigma_i^2}$$

Matrix form: $A = I$

$$\begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \end{pmatrix} = \begin{pmatrix} 1 & 0 & \cdots & \\ 0 & 1 & 0 & \vdots \\ \vdots & & \ddots & \\ & \cdots & & 1 \end{pmatrix} \cdot \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_N \end{pmatrix}$$



The solution of the unconstrained problem is trivial:

$$a_i = y_i$$

Problem: the model parameters are not entirely free but the model has to fulfill some special condition (constraint)

Example: two measurements $y_1 = 1$ and $y_2 = 2$ with error $\sigma = 1$

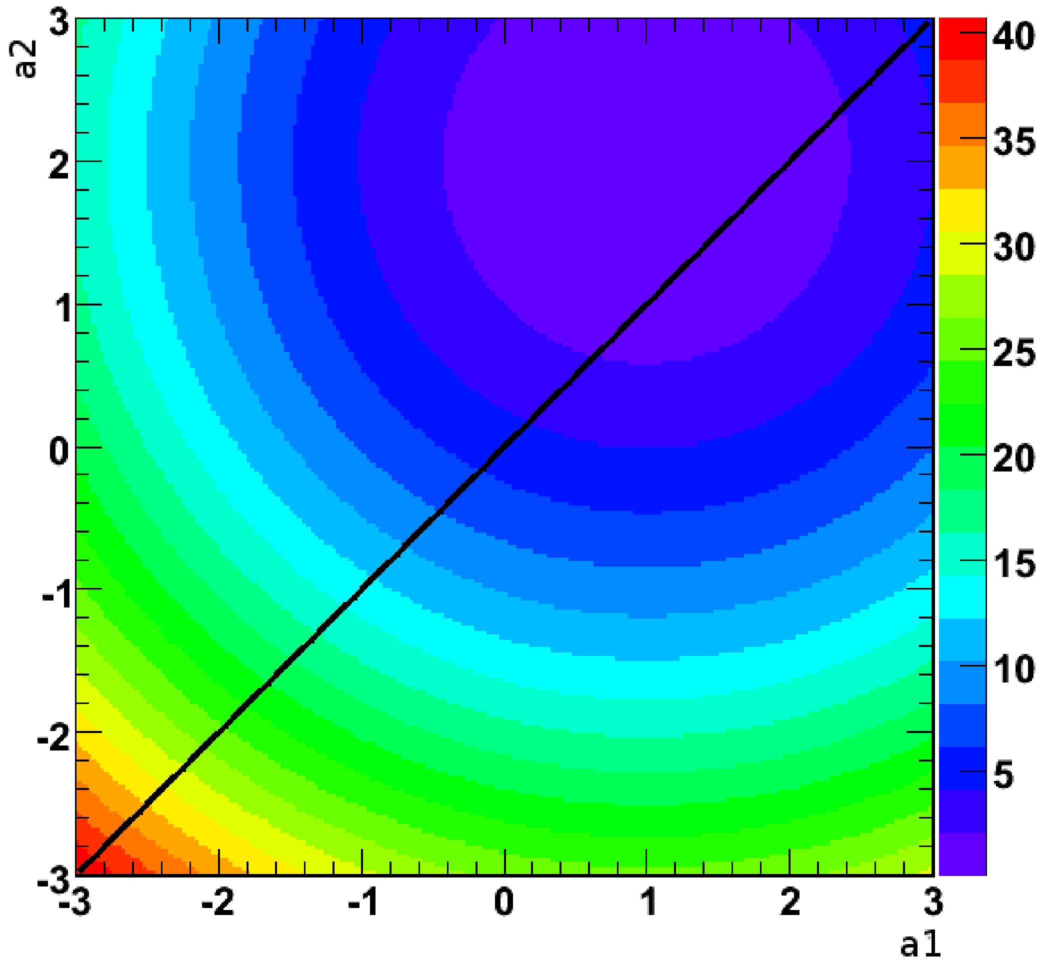
$$\chi^2 = (1 - a_1)^2 + (2 - a_2)^2$$

→ Minimum at $a_1 = 1$ and $a_2 = 2$

Wanted is the minimum for $a_1 = a_2$

$$a_1 - a_2 = 0$$

A widely used method to solve such a minimization problem with additional constraints is the **Method of Lagrangian Multipliers**



Method of Lagrangian Multipliers

The first step is to formulate each constraint as equation that equals zero

$$c(\vec{a}) \stackrel{!}{=} 0$$

Definition of a new function L for P constraints

$$L(\vec{y},\vec{a}) = \chi^2 + 2 \cdot \sum_{i=1}^{P} \lambda_i c_i(\vec{a})$$

with **Lagrangian Multipliers** λ_i

Partial derivative w.r.t. λ_i: $$\frac{\partial L}{\partial \lambda_i} = 2 \cdot c_i(\vec{a}) \stackrel{!}{=} 0$$

→ solution must fulfill the constraints!

Partial derivatives w.r.t. a_i:

$$\frac{\partial L}{\partial a_i} = \frac{\partial \chi^2}{\partial a_i} + 2 \cdot \sum_{j=1}^{P} \lambda_i \cdot \frac{\partial c_j}{\partial a_i} \stackrel{!}{=} 0 \rightarrow \nabla \chi^2 = -2 \cdot \sum_{j=1}^{P} \lambda_j \nabla c_j$$

→ for one constraint ($P = 1$): gradients of χ^2 function $\nabla\chi^2$ and of constraint function ∇c must be parallel !

→ χ^2 function has a local minimum on the constraint contour !

A Pictorial Representation

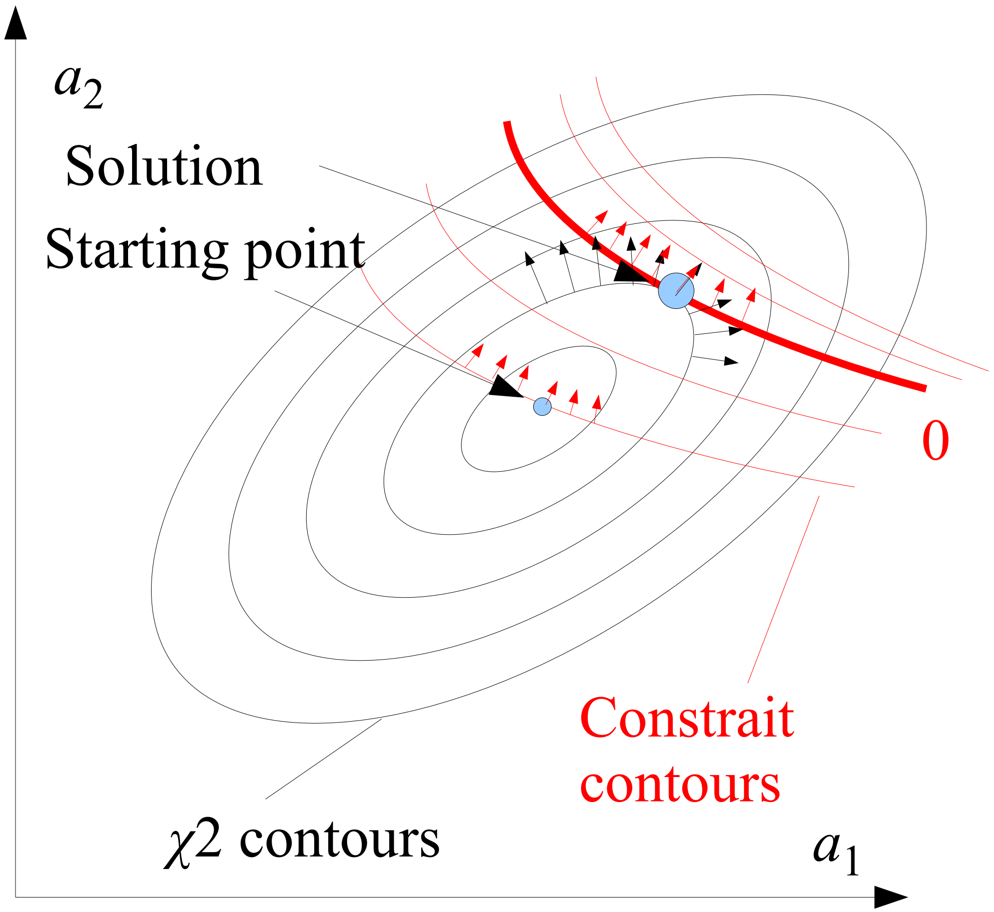
Visualization in 2D:

- Solution must lie on **zero contour** of the constraint

$$\frac{\partial L}{\partial \lambda} = 2 \cdot c(\vec{a}) \stackrel{!}{=} 0$$

- Constraint line must be parallel to χ^2 contour at solution, i.e. **gradients** of χ^2 and constraint must be **parallel**

$$\nabla \chi^2 = -2\lambda \nabla c$$



Example for 2 parameters a_1, a_2 and one constraint

Explicit Solution of the Example

Back to our problem: minimization of $\chi^2 = (1 - a_1)^2 + (2 - a_2)^2$

subject to the constraint $c(a_1, a_2) = a_1 - a_2 \stackrel{!}{=} 0$

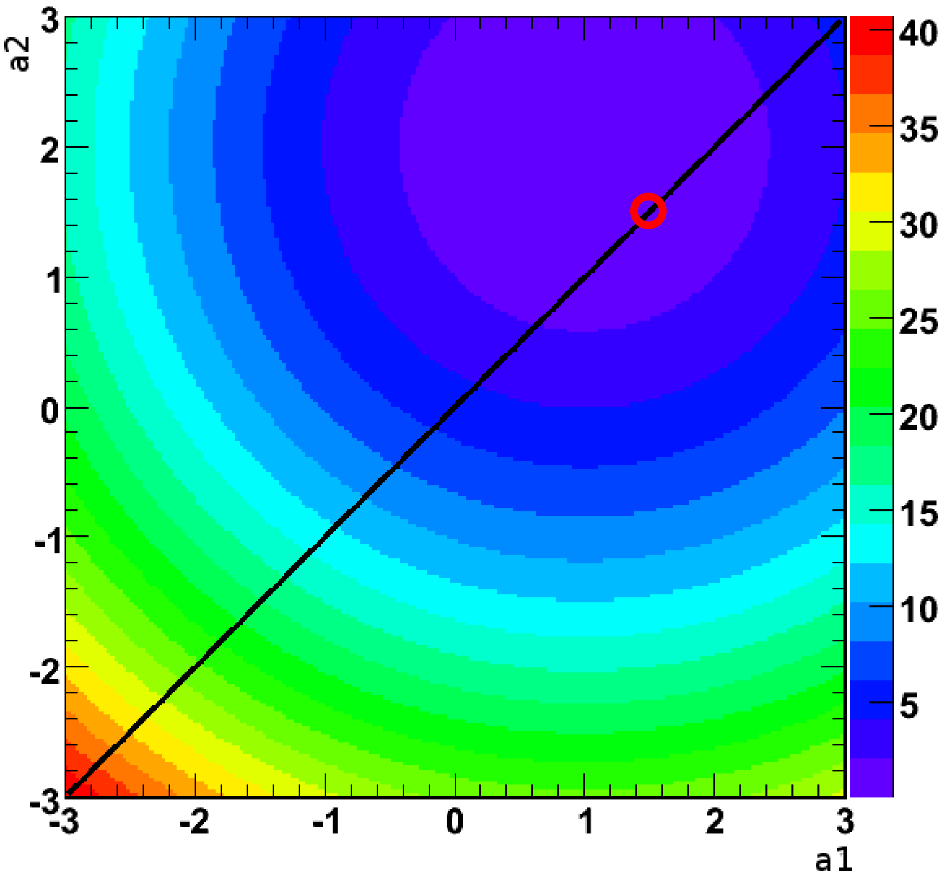
Definition of a Lagrange function $L(a_1, a_2) = (1 - a_1)^2 + (2 - a_2)^2 + 2 \cdot \lambda \cdot (a_1 - a_2)$

Partial derivatives have to vanish:

$$\frac{\partial L}{\partial a_1} = 2 \cdot (a_1 - 1) + 2 \cdot \lambda \quad = \quad 0 \qquad (1)$$

$$\frac{\partial L}{\partial a_2} = 2 \cdot (a_2 - 2) - 2 \cdot \lambda \quad = \quad 0 \qquad (2)$$

$$\frac{\partial L}{\partial \lambda} = a_1 - a_2 \quad = \quad 0 \qquad (3)$$



Add (1) and (2)

$$2 \cdot (a_1 - 1) + 2 \cdot (a_2 - 2) = 0$$

Insert (3)

$$2 \cdot (a_1 - 1) + 2 \cdot (a_1 - 2) = 0$$

Solution: $4 \cdot a_1 - 6 = 0 \rightarrow a_1 = a_2 = \frac{3}{2}$

Exercise 1: Energy Conservation

- A Z^0 decays in its rest frame into two massless particles with the opposite momentum (back to back) and same energy
- If the energies E_i of the particles are measured with an unknown uncertainty σ, this can be formulated as a constrained linear least square problem.
- Assuming perfect angular resolution this problem has only two parameters (E_i)

Login to the computer, open a shell or a browser and download the exercise material! In the shell type:

```
$> wget www.desy.de/~bmura/KinFitExercises.tar
```

- Unpack the downloaded archive:

```
$> tar xvf KinFitExercises.tar
```

- Change into the unpacked directory and run the setup script:

```
$> cd KinFitExercises
$> source setup.sh
```

- Do exercise 1a following the instructions on the exercise sheet!

Exercise 1: Summary

- Extremum of

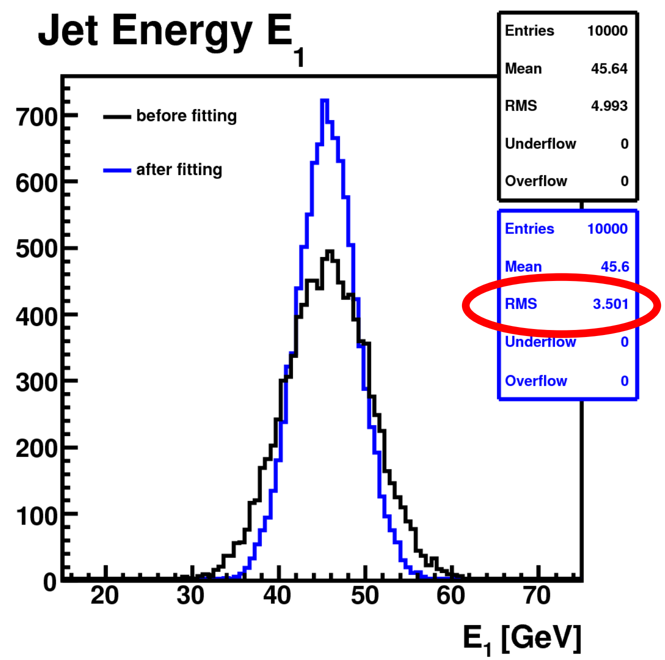
$$L(\vec{E}, \vec{a}) = \frac{(\hat{E}_1 - E_1)^2}{\sigma_1^2} + \frac{(\hat{E}_2 - E_2)^2}{\sigma_2^2} + 2 \cdot \lambda(E_1 + E_2 - M_Z)$$

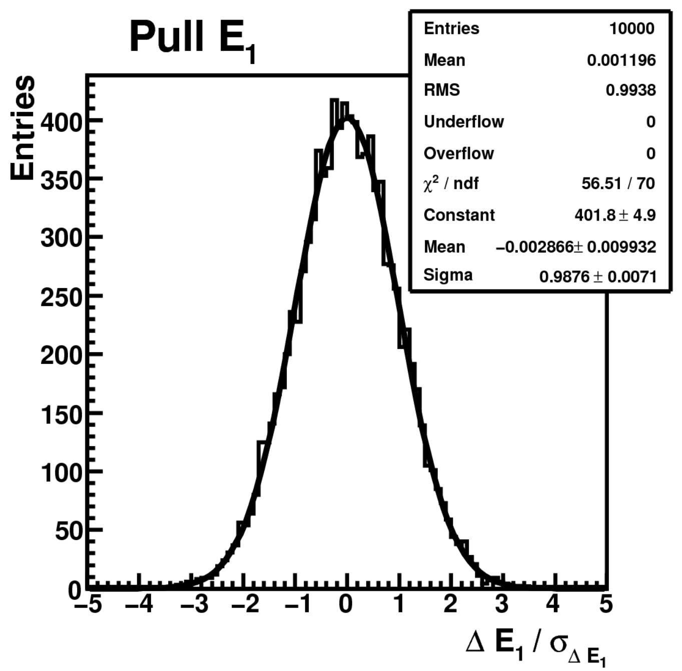
lies on diagonal in $E_1 - E_2$ plane defined by the constraint

- Solution is symmetric in E_1, E_2 if $\sigma_1 = \sigma_2$
- Energy resolution is improved as expected

$$\sigma_{\mathrm{fit}} = \sigma / \sqrt{2}$$

- Constraint fulfilled after fit
- Fit has **one** degree of freedom
- Perfectly gaussian input errors yield flat distribution of χ^2-probability and perfect pulls (normalized corrections to $E_{1/2}$)
- Sytematic shift of input energy is corrected by the fit





Non-linear Constraints

In our case: χ^2 is quadratic in a → derivatives are linear in a:

$$\chi^2 = (\vec{y}-\vec{a})^T V^{-1}[y](\vec{y}-\vec{a}) \rightarrow \frac{\partial \chi^2}{\partial \vec{a}} = -2 \cdot V^{-1}[y] \cdot (\vec{y}-\vec{a})$$

Constraint functions will in general be non-linear → make a Taylor expansion:

$$\vec{c}(\vec{a}) \approx \vec{c}(\vec{a^\star}) + \frac{\partial \vec{c}}{\partial \vec{a}} \cdot (\vec{a}-\vec{a^\star}) = \vec{c}(\vec{a^\star}) + A \cdot (\vec{a}-\vec{a^\star})$$

Full linearized Lagrange function:

$$L \approx (\vec{y}-\vec{a})^T V^{-1}[y](\vec{y}-\vec{a}) + 2 \cdot \vec{\lambda}^T \cdot \vec{c}(\vec{a^\star}) + 2 \cdot \vec{\lambda}^T \cdot A \cdot (\vec{a}-\vec{a^\star})$$

Partial derivatives:

$$\frac{\partial L}{\partial \vec{a}} = -2 \cdot V^{-1}[y] \cdot (\vec{y}-\vec{a}) + 2 \cdot A^T \cdot \vec{\lambda} \stackrel{!}{=} 0$$

$$\frac{\partial L}{\partial \vec{\lambda}} = 2 \cdot \vec{c}(\vec{a^\star}) + 2 \cdot A \cdot (\vec{a}-\vec{a^\star}) \stackrel{!}{=} 0$$

In matrix form:

$$\begin{pmatrix} V^{-1}[y] \cdot \vec{y} \\ A \cdot \vec{a^\star} - \vec{c}(\vec{a^\star}) \end{pmatrix} = \begin{pmatrix} V^{-1}[y] & A^T \\ A & 0 \end{pmatrix} \cdot \begin{pmatrix} \vec{a} \\ \vec{\lambda} \end{pmatrix}$$

→ Solve this equation to get a better solution, and iterate

Problems with Iterative Procedure

The main problem:

If local linear approximation of constraints is not very good, iterative procedure will make too large steps

→ new solution may not be better (or even worse) than the old one

→ no convergence !

Typical problems and ways to overcome/avoid them:

- How to define if a step improves solution → function of merit
- Step with unscaled length does not improve solution → step scaling
- Step rejected by "improvement criteria" (Maratos effect) → 2^{nd} order corrections
- Constraints are of completely different scales → scaling of constraints

Convergence

How to qualify if a step is an improvement or not?

If current parameters away from hyperplane of fulfilled constraints → ensure that each step reduces absolute values of constraints

If current parameters are (almost) fulfilling the constraints → ensure that objective function (e.g. χ^2) is reduced

Construct new **function of merit**:

$$m_\mu(\vec{a}) = \chi^2(\vec{a}) + \mu \cdot \sum_{i=1}^{P} |c_i(\vec{a})|$$

with $\mu > 0$ (good estimate for μ is $\max(\lambda_i)$)

One step is accepted if function of merit is reduced!

Convergence: two criteria have to be fulfilled

- Change of χ^2 becomes small: $\Delta\chi^2 = \chi^2(\vec{a}) - \chi^2(\vec{a} + \Delta\vec{a}) < \epsilon_1$
- Absolute sum of constraints becomes small: $\sum_{i=1}^{P} |c_i(\vec{a})| < \epsilon_2$

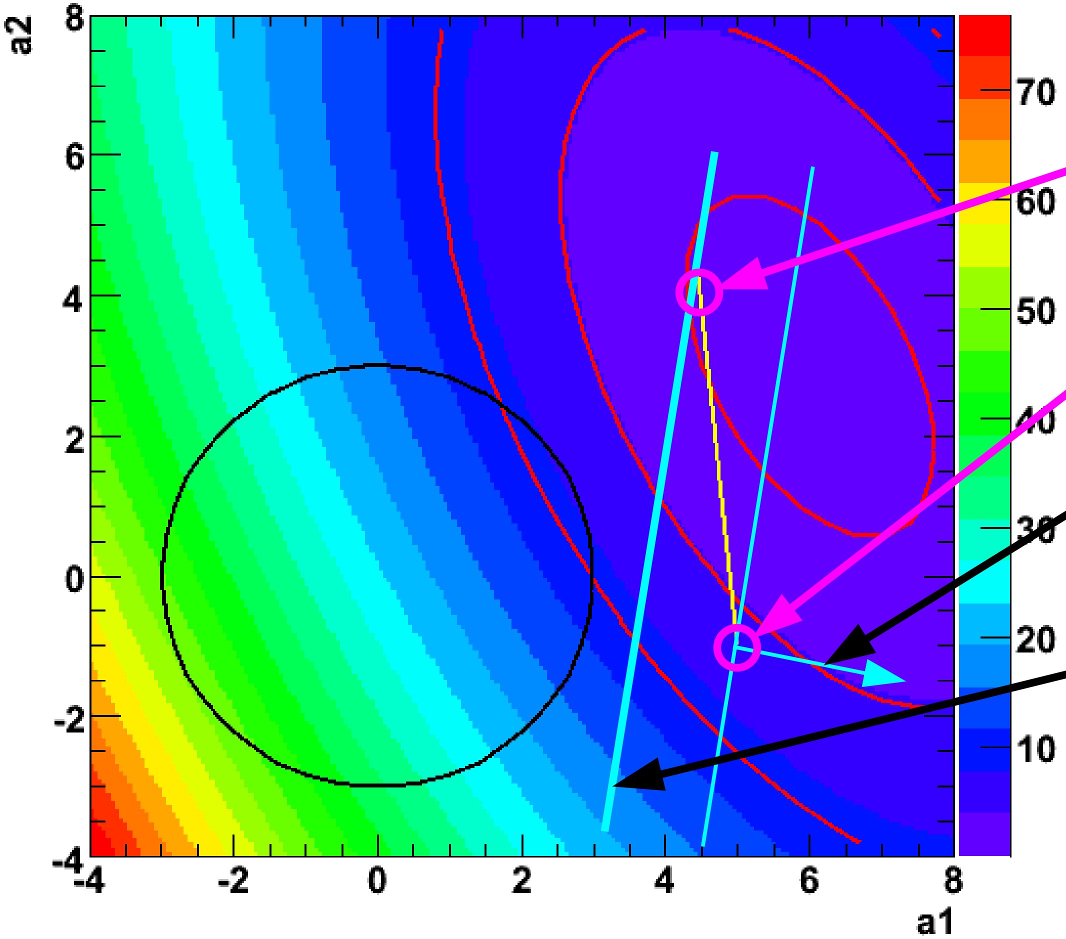
Iterative Solution

Example: find minimum of

$$\chi^2 = (a_1 - 6, a_2 - 3) \begin{pmatrix} 3 & -0.5\sqrt{3 \cdot 6} \\ -0.5\sqrt{3 \cdot 6} & 6 \end{pmatrix}^{-1} \begin{pmatrix} a_1 - 6 \\ a_2 - 3 \end{pmatrix}$$

subject to

$$c(a_1, a_2) = a_1^2 + a_2^2 - 9 \stackrel{!}{=} 0$$



Solution of linearized problem local minima of χ^2 on zero contour of linearized constraint

Starting parameters

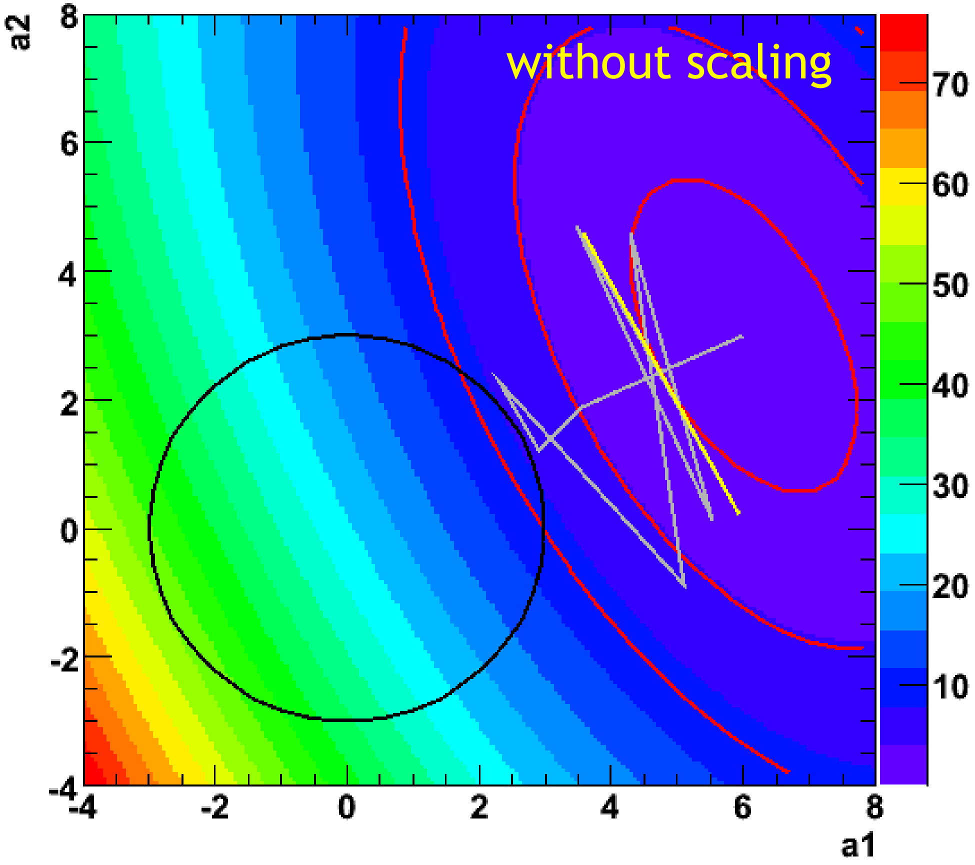
Local gradient of constraint

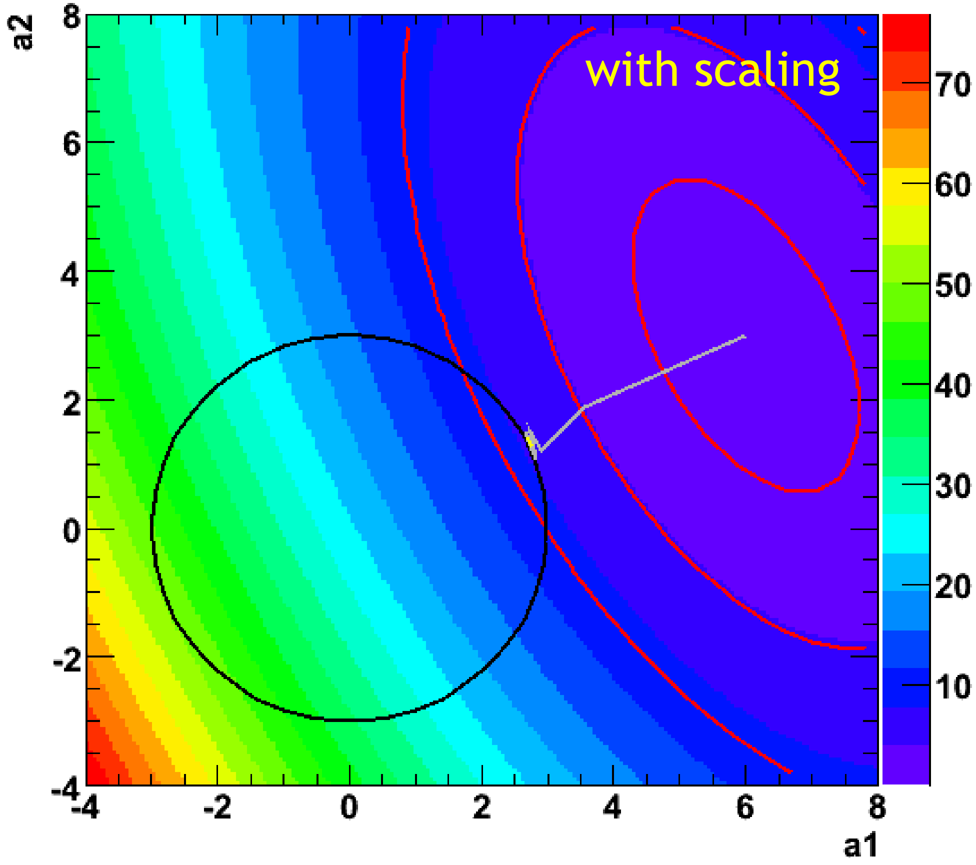
Zero contour of linearized constraint

Solution of problem:
If step does not "improve" solution, make smaller step!

Scaling of Step Length

For non-linear problems step after linearization does not improve solution (no reduction of function of merit) → **scale step length with α** (e.g. $\alpha = 0.5$)





Application in High Energy Physics

Possible applications of constrained fits:

- Vertex constrained track fits
- Tracker Alignment
- Kinematic fits ...

Kinematic Fits:

- If measured jets are decay products of heavy particles → invariant mass of added 4-vectors should equal the mass of decaying particle
- Different parametrizations of final state momenta possible (see next slide)
- In general the measurements have to be shifted within their uncertainty to fulfill the constraint (problem can be formulated as constrained non-linear least square fit)

Example for 2 jets from W decay:

Cartesian parametrization:

$$m_W^2 - ((E_1 + E_2)^2 - (p_{x,1} + p_{x,2})^2 - (p_{y,1} + p_{y,2})^2 - (p_{z,1} + p_{z,2})^2) \stackrel{!}{=} 0$$

Advantage: simple calculation of derivatives, quadratic constraints

Disadvantage: measurements of different jet momentum components are correlated (some off-diagonal elements of the covariance matrix are non-zero)

Different parametrization (here for massless jets):

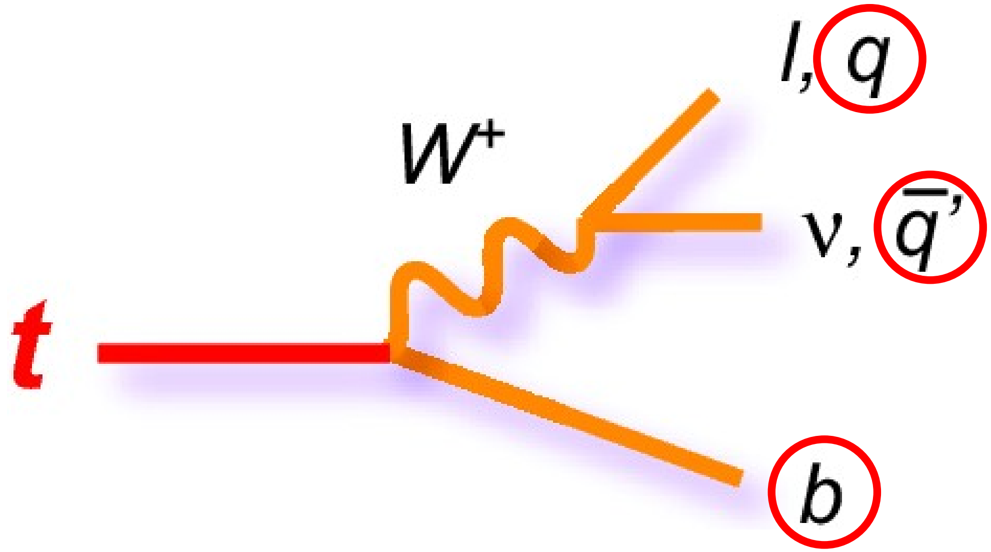
$$m_W^2 - \left(\left(\sum_{i=1}^{2} p_t \cosh \eta \right)^2 - \left(\sum_{i=1}^{2} p_t \cos \phi \right)^2 - \left(\sum_{i=1}^{2} p_t \sin \phi \right)^2 - \left(\sum_{i=1}^{2} p_t \sinh \eta \right)^2 \right) \stackrel{!}{=} 0$$

Advantage: measurements are independent (covariance matrix diagonal)

Disadvantage: highly non-linear constraints, derivatives more complicated

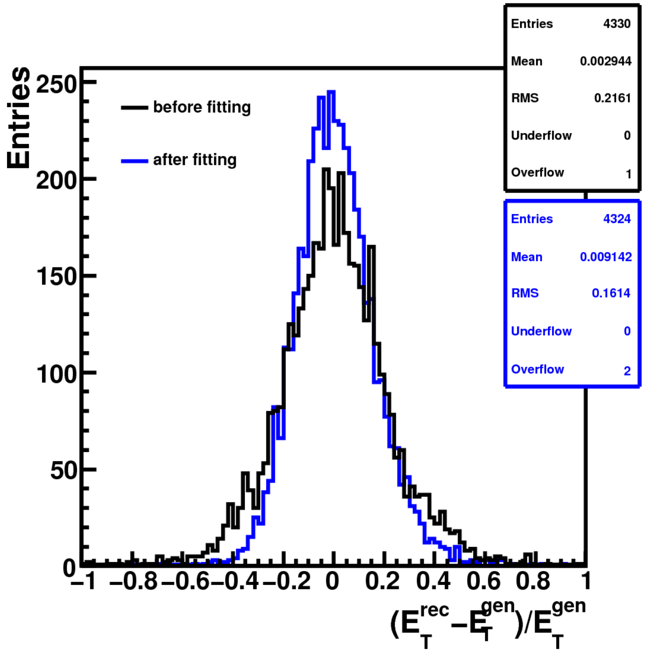
Exercise 2: W- and Top-Mass Constraint

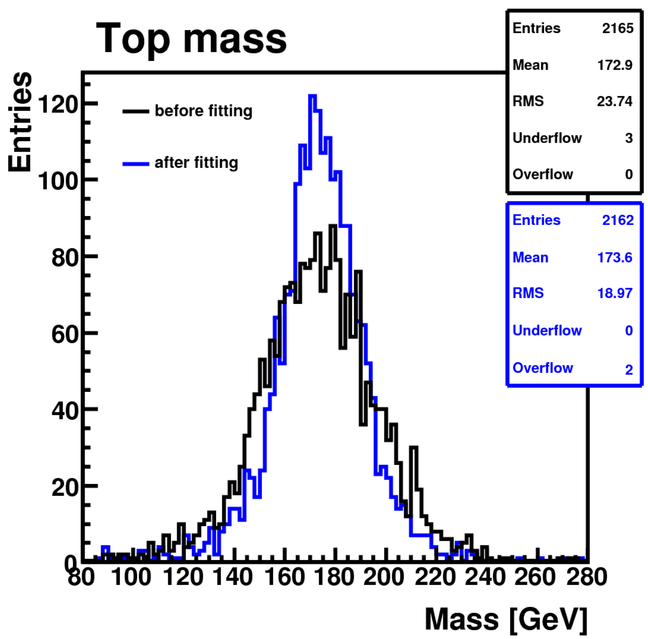
- Reconstruction of an hadronic top decay
- Measured parameters: one b jet and two W jets = 9 parameters
- Mass constraints:
  - One W-mass constrained
  - Use known top mass in addition



Exercise 2: Summary

- Jet energy resolution is improved in the fit
- Top mass peak becomes narrower and top mass resolution is improved
- Jet η and ϕ resolution not significantly changed as the assumed uncertainties are small
- Small peak at small χ^2-probability: e.g. from events far from the assumed W-mass
- χ^2 follows curve for **two** d.o.f in case of second constraint (2b)
- Pulls slightly distorted in such a more "realistic" scenario

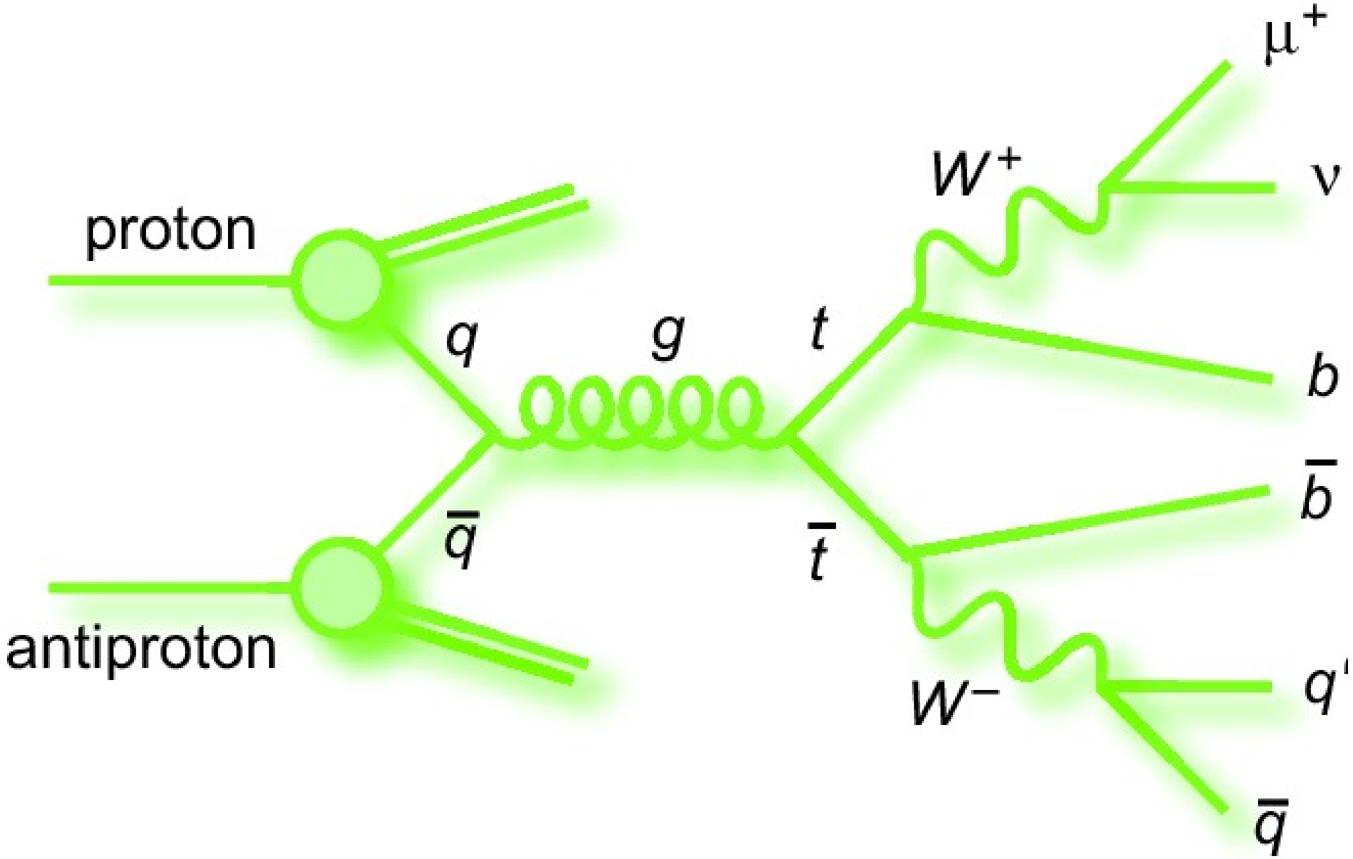




Kinematic Fits of Whole Events

If a whole event is fitted the momentum balance can be used as **additional two constraints** (if the initial state has small transverse momentum)

In case of hard initial state radiation (ISR) the momentum balance of the hard process is broken → the ISR jets have to be taken into account



Example: semileptonic $t\bar{t}$ events

Unmeasured Parameters

General Problem:

- N measurements $\vec{y}$ and parameters $\vec{a}$ as before
- Unmeasurable particles (e.g. ν) → M additional unmeasured parameters $\vec{b}$
- P constraints $\vec{c}(\vec{a},\vec{b}) = 0$
- $P > M$ → over constrained problem

Kinematic fit can be used to reconstruct unmeasured particle

Linearized function L:

$$L \approx (\vec{y}-\vec{a})^T V^{-1}[y](\vec{y}-\vec{a}) + 2\vec{\lambda}^T(\vec{c}(\vec{a^\star},\vec{b^\star}) + A\cdot(\vec{a}-\vec{a^\star}) + B\cdot(\vec{b}-\vec{b^\star}))$$

with Jacobian A of constraints $\vec{c}$ with respect to **measured** parameters $\vec{a}$

and Jacobian B of constraints $\vec{c}$ with respect to **unmeasured** parameters $\vec{b}$

and

$$\vec{c}(\vec{a},\vec{b}) \approx \vec{c}(\vec{a^\star},\vec{b^\star}) + A\cdot(\vec{a}-\vec{a^\star}) + B\cdot(\vec{b}-\vec{b^\star})$$

where all derivatives and function values are evaluated at starting values $\vec{a^\star}$ and $\vec{b^\star}$

Unmeasured Parameters (cont.)

Vanishing derivatives: Overall $N+P+M$ coupled equations

$$\begin{pmatrix} V^{-1}[y]\cdot\vec{y} \\ 0 \\ A\cdot\vec{a^\star}+B\cdot\vec{b^\star}-\vec{c}(\vec{a^\star},\vec{b^\star}) \end{pmatrix} = \begin{pmatrix} V^{-1}[y] & 0 & A^T \\ 0 & 0 & B^T \\ A & B & 0 \end{pmatrix}\cdot\begin{pmatrix} \vec{a} \\ \vec{b} \\ \vec{\lambda} \end{pmatrix}$$

with solution $\vec{a}$ and $\vec{b}$ which are new approximation of solution

→ The matrix which has to be inverted has a special structure

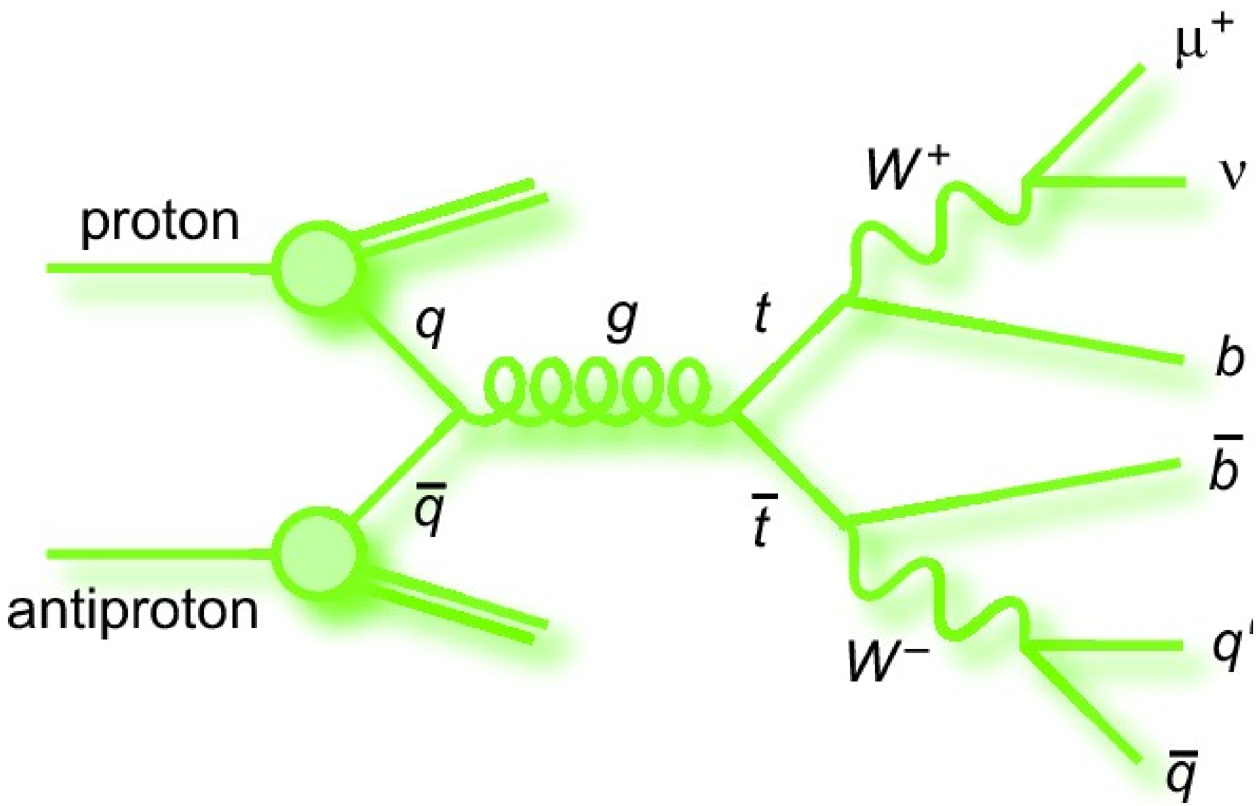
→ Special algorithms make use of this structure which can save lots of computing resources (depending of the size of the problem)

Exercise 3: Full Reconstruction of $t\bar{t}$

Reconstruction of hadronic and semileptonic $t\bar{t}$ events

a) Both tops decay hadronically: Perform fit requiring an equal top mass on both branches.

b) Semi-leptonic decay: Count parameters and find possible setup for an over-constrained fit

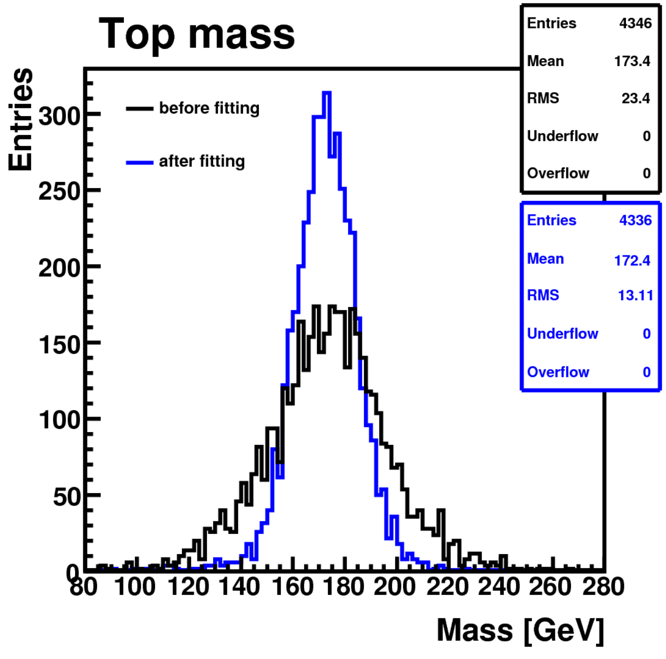


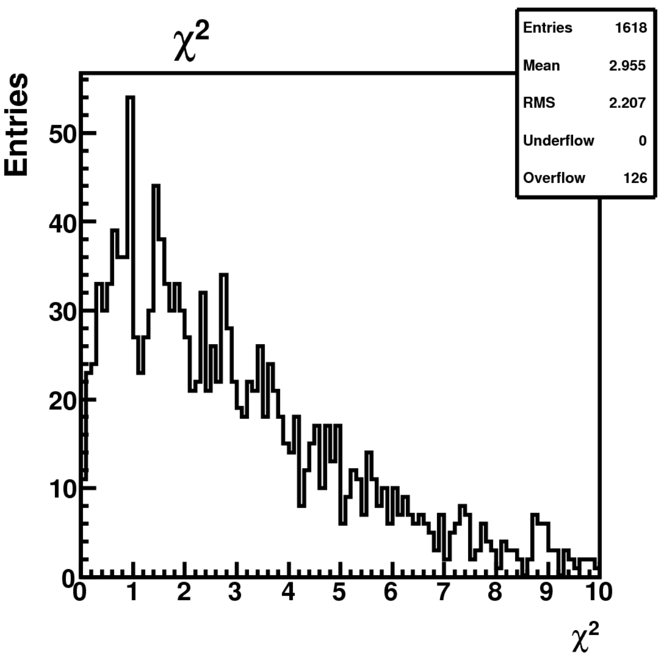
Exercise 3a: Summary

- Both tops decaying hadronically:

  $2 \times W$-mass + equal top-mass = **3 constraints**
- Same mass constraint brings gain in top mass width and resolution w.r.t. exercise 2a
- Energy resolution of jets profits from the fit as before
- χ^2 as for **three** d.o.f. but some events accumulate at low fit probability

(**Remember:** No combinatorics included here!)



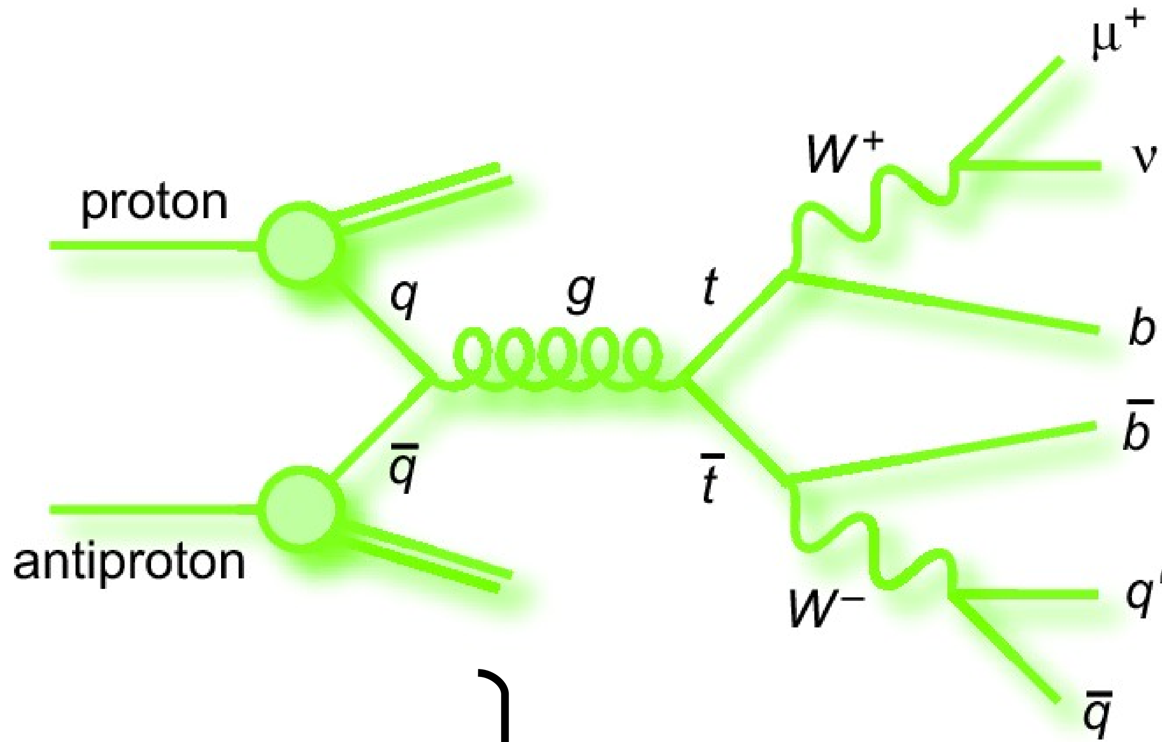


Exercise 3b: Summary

- Reconstruction of semileptonic $t\bar{t}$ events
- Measured parameters:
  - Two b jets
  - Two W jets
  - One lepton

  $\}$ 15 parameters
- Unmeasured parameters:
  - One neutrino = 3 parameters
- Mass constraints:
  - Two $\times$ W mass
  - Two $\times$ p_T momentum balance
  - Zero, one (equality of two masses) or two $\times$ top mass

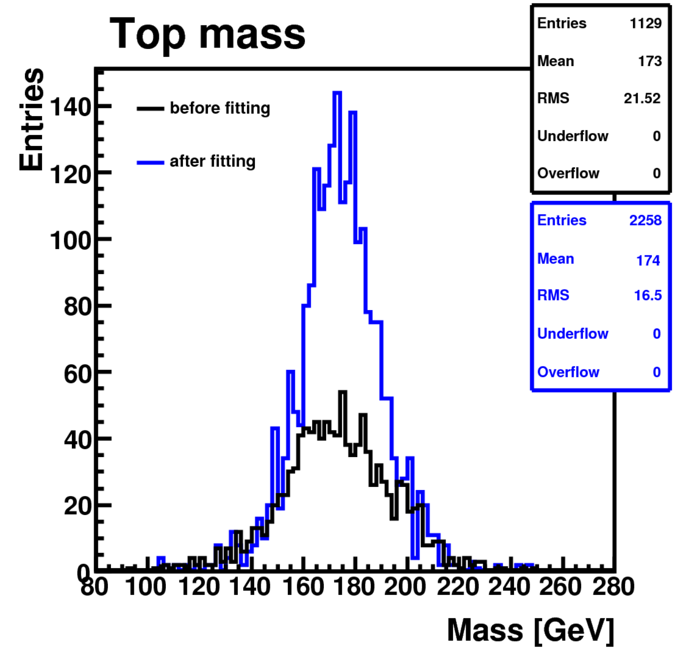
  $\}$ 4 … 6 constraints

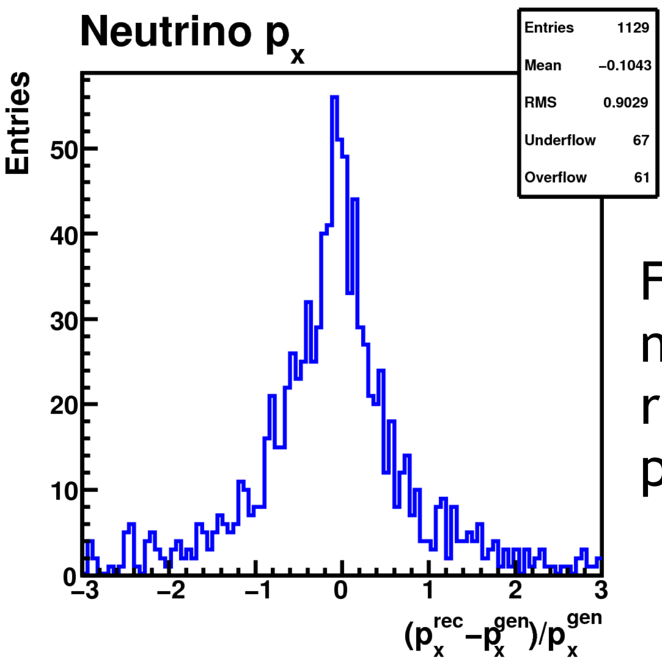


→ **Need at least four constraints for kinematic fit!**

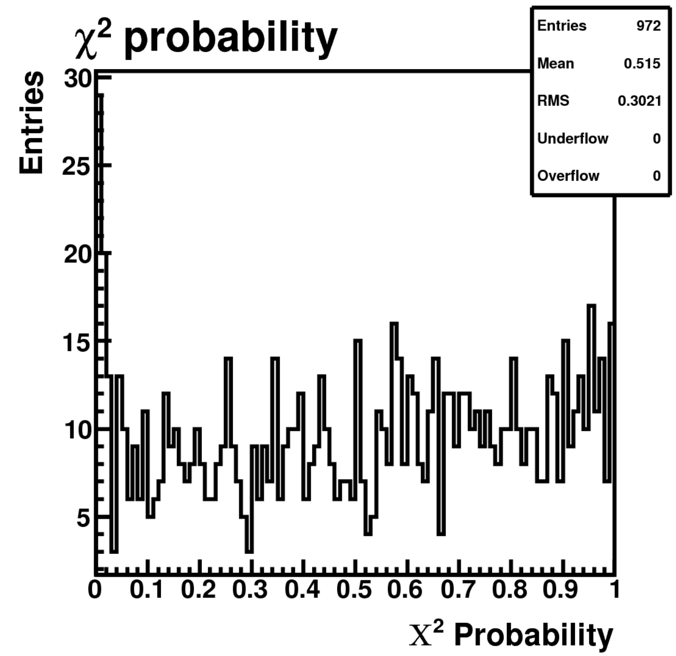
Exercise 3b: Summary

- Use 2 $\times$ W-mass + p_T-balance + equal top-mass = 5 constraints
- For some events fit does not converge!
- Top mass reconstruction: good improvement by the fit
- Neutrino momentum (p_x, p_y, p_z) reconstructed with some width



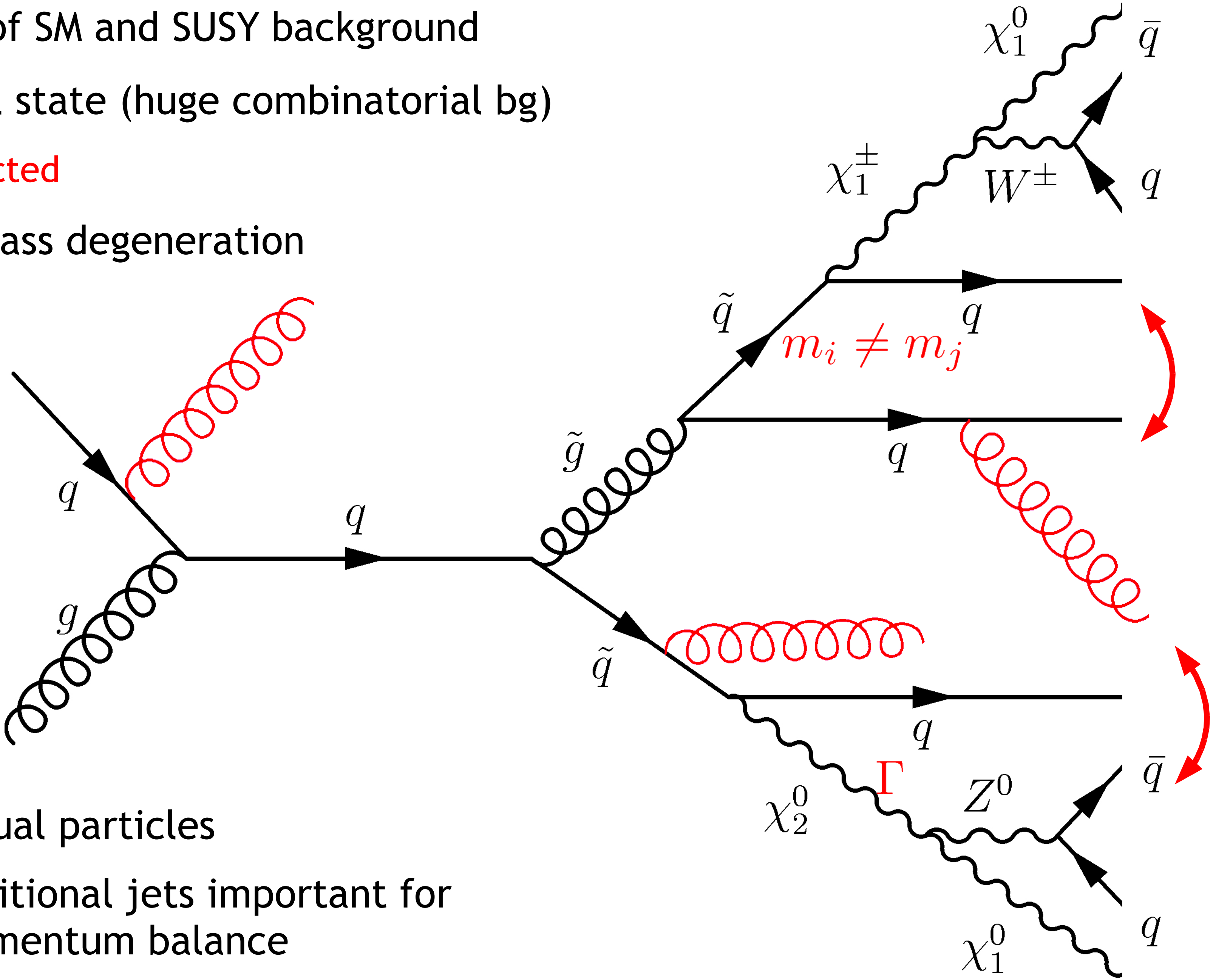


Fit probability for **two** d.o.f.: not ideally distributed, reflects complexity of the problem



Example: SUSY Events - Potential Problems

- Suppression of SM and SUSY background
- 7 jets in final state (huge combinatorial bg)
  - all reconstructed
- No perfect mass degeneration



- Width of virtual particles
- +FSR
- +ISR

} additional jets important for momentum balance

Jet Combinatorics

In case of many jets there are a lot of possible jet combinatorics

Example: *full hadronic $t\bar{t}$ events with 6 jets, two W jet pairs and two identical cascade branches*

Without information from b-tagging this leads to

$$\frac{6!}{2\cdot 2}\cdot\frac{1}{2} = 90$$

combinations. With b-tagging:

$$2\cdot\frac{4!}{2\cdot 2}\cdot\frac{1}{2} = 6$$

Another example: *full hadronic SUSY event with 7 jets, two W jet pairs and different cascades* → 1260 combinations !

Finite Width of Constraining Mass

If a mass of a constraint has a non-negligible width

→ Add a new parameter x to the model

x is scaling factor of constraining mass → new constraint has the form:

$$(x \cdot m)^2 - M_{\mathrm{inv}}^2(\vec{a}, \vec{b}) \stackrel{!}{=} 0$$

The new parameter is treated as a new measurement per event with a variance according to the mass width:

$$\sigma_x^2 = \frac{\Gamma_m^2}{m^2}$$

→ A new χ^2 term:

$$\chi_x^2 = \frac{(x-1)^2}{\sigma_x^2}$$

Problems of Non-Linear Least Squares

General problems:

- Fit can converge at local (and not global) minimum
- Non linear problems can suffer from "Maratos effect"

Alternative: Formulation of constraints as additional χ^2 term → "cost function"

Interpretation of cost function as χ^2: all correlations have to be taken into account, e.g.

$$\left(\frac{M_{\text{inv}}(j_1, j_2, j_3) - M}{\sigma}\right)^2$$

with

$$\sigma^2 = \sum_{i=1}^{N_m} \left(\frac{\partial M_{\text{inv}}}{\partial i}\right)^2 \cdot \sigma_i^2 + \Gamma_m^2$$

Minimize cost function: many possible algorithms (gradient, simplex, LBFGS, simulated annealing, genetic algorithm ...)

In general this quadrature is not advised, but the procedure might be useful for finding good starting values of the unmeasured fit parameters

Remark: 2nd Order Corrections

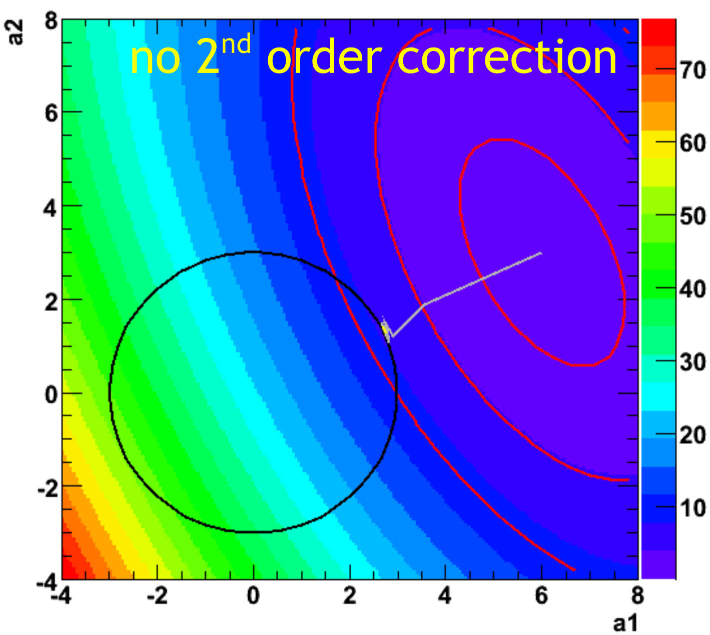
If constraints non-linear → one could suffer from Maratos effect, i.e. a step $\Delta\vec{a}_k$ calculated from the linearized problem might not improve the merit function → significant slow down of convergence

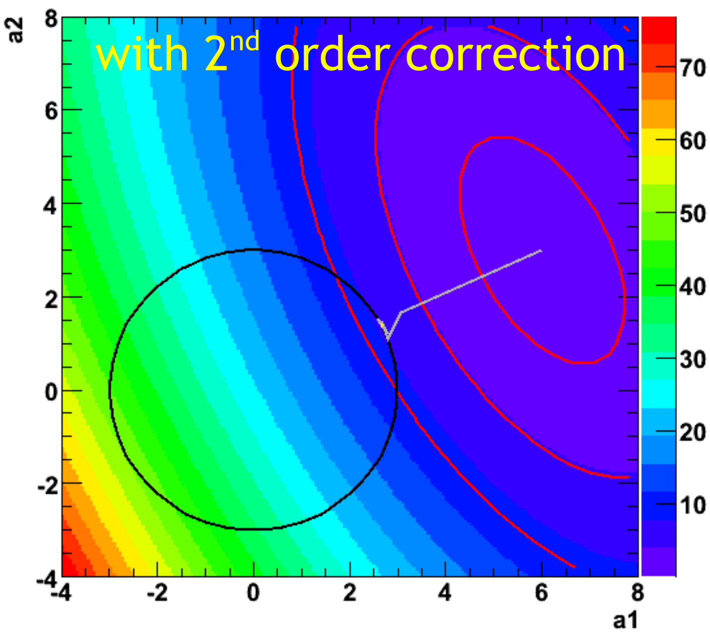
The following correction will reduce the merit function at least near the solution:

$$\Delta\vec{a'}_k = A_k^T(A_k A_k^T)^{-1}\vec{c}(\vec{a}_k + \Delta\vec{a}_k)$$

where $\Delta\vec{a}_k$ is the step, $\vec{c}(\vec{a})$ the constraints and A the Jacobian of $\vec{c}$

This step is only tried once, since back tracking make no sense ($\Delta\vec{a}_k$ is not steepest descent at $\vec{a}_k + \Delta\vec{a'}_k$)





In this example “only” small improvement of convergence with 2nd order correction

Remark: Scaling of Constraints

If objective function χ^2 has to be minimized, subject to a number of constraints which are not fulfilled at starting parameters, it's possible that constraint values are of completely different magnitude!

Function of merit might be dominated by one single constraint

$$m_\mu(\vec{a},\vec{b}) = \chi^2(\vec{a},\vec{b}) + \mu \cdot \sum_{i=1}^{P} |c_i(\vec{a},\vec{b})| \approx \chi^2(\vec{a},\vec{b}) + \mu \cdot |c_k(\vec{a},\vec{b})|$$

For optimal performance of iterative algorithm → **scaling of constraint to same order of magnitude**

Example: invariant mass constraint in cascade decay

$$m(j_1+j_2)^2 - m_1^2 = 0 \quad \text{and} \quad m(j_1+j_2+j_3)^2 - m_2^2 = 0$$

with $m_1 \ll m_2$

Squared mass difference of larger mass m_2 is dominant → normalize by expected uncertainty of constraint, e.g. $\Delta m_2^2 \approx 2m_2$

Remark: Inequality Constraints

Constraints can also be described by inequalities, e.g. if a parameter is restricted to positive values

Two possibilities:

- **Variable transformation:** mapping from finite to infinite parameter space, e.g. with trigonometric functions. Often this introduces more problems, e.g. additional saddle point or numeric uncertainties
- **Modification of Lagrangian multiplier method:** separation in active and non-active constraints → not simple

Summary

- (Constrained) kinematic fits provide a powerful tool for event reconstruction. They can be used for:
  - Improvement of resolutions of measurements
  - Improvement of mass resolutions
  - Reconstruction of unknown parameters, like neutrino momenta
- Output is a χ^2 which can be interpreted in terms of probabilities and can be used for event hypothesis classification
- Non linear problems have to be solved iteratively. The modification of the algorithm to achieve convergence is the hardest part!
- Minimization of scalar cost function might be useful to get good starting values of unmeasured parameter

Literature

Books:

- V. Blobel and E. Lohrmann: ***Statistische und numerische Methoden der Datenanalyse*** (Teubner Studienbücher, 1998)
- J. Nocedal and S. J. Wright: ***Numerical Optimization***, 2nd Edition (Springer, 2006)
- L. Lyons: ***Statistics for nuclear and particle physicists*** (Cambridge Univ. Press 1986)