Numerical Methods (2)

- Statistical Methods in Experimental Physics
  - W. T. Eadie, D. Drijard, F. E. James, M. Roos, B. Sadoulet
- Statistics for nuclear and particle Physics
  - Louis Lyon
- Probability and Statistics in Particle Physics
  - A. Frodesen, O. Skeggestad, H. Tofte
- Statistical Data Analysis
  - Glen Cowan
- Monte Carlo theory and practice
  - F. James
- Data Analysis Technique for High Energy Physics
  - M. Regler and R. Fruhwirth
- Statistical and Computational Methods in Data Analysis
  - Sigmund Brandt

Constrained Fits

In the general formulation of the least square problem, one can introduce a set of constraint equations which will modify the quality of measured quantities as well as unmeasured parameters significantly

Look at the general formulation of the Least Square problem

$\vec{m}$ variables measured in an experiment
$\vec{m}^0$ measurements of these variables
G_M the variance matrix
$\vec{x}$ unmeasured parameters
$f_i(\vec{x}, \vec{m}) = 0 \quad i = 1, \cdots, k$ a set of k constraint equations

The best estimates of measured and unknown quantities are obtained by minimising

$$\chi^2(m, x, \lambda) = (m - m_0)^\dagger G_M (m - m_0) + 2\lambda^\dagger f(x, m)$$

where λ = vector (of k components) of Lagrange multipliers

Fits with constraint relation

$$\frac{\partial \chi^2}{\partial m} = 0 = 2\left[(m - m_0)^\dagger G_M + \lambda^\dagger f_m(x, m)\right] \qquad \text{(A)}$$

$$\frac{\partial \chi^2}{\partial x} = 0 = 2\lambda^\dagger f_x(x, m) \qquad \text{(B)}$$

$$\frac{\partial \chi^2}{\partial \lambda} = 0 = 2f(x, m) \qquad \text{constraint equations} \qquad \text{(C)}$$

where

$$f_m = \frac{\partial f}{\partial m}$$

$$f_x = \frac{\partial f}{\partial x}$$

In general, the constraint relations are not linear in x, m

$\Rightarrow$ use iterative procedure

Start with an initial guess. Calculate values for the $(\nu + 1)$ th iteration using the results of the ν th iteration

Linearised constraint equation (C) $\Rightarrow$

$$f^{\nu+1} = 0 = f^\nu + f_x^\nu \left(x^{\nu+1} - x^\nu\right) + f_m^\nu \left(m^{\nu+1} - m^\nu\right) \qquad \text{(D)}$$

Fits with constraint relation

Equation (A) gives

$$\begin{aligned}
(m^{\nu+1}-m^0)^\dagger G_M &= -(\lambda^{\nu+1})^\dagger f_m^{\nu+1} \\
\Rightarrow \quad (m^{\nu+1}-m^0)^\dagger &= -(\lambda^{\nu+1})^\dagger f_m^{\nu+1} G_m^{-1} \\
\Rightarrow \quad m^{\nu+1}-m^0 &= -G_m^{-1}(f_m^{\nu+1})^\dagger \lambda^{\nu+1} \qquad \text{(A')}
\end{aligned}$$

Thus (D) becomes

$$f^\nu + f_x^\nu (x^{\nu+1}-x^\nu) + f_m^\nu \left[m^0 - m^\nu - G_M^{-1}(f_m^\nu)^\dagger \lambda^{\nu+1}\right] = 0 \qquad \text{(E)}$$

approximating $f^{\nu+1}$ with f^ν

Let

$$R = f^\nu + f_m^\nu (m^0 - m^\nu) \qquad \text{(F)}$$

$$S = f_m^\nu G_M^{-1} (f_m^\nu)^\dagger \qquad \text{(G)}$$

R, S depend on quantities known at iteration ν $\Rightarrow$

$$f_x^\nu (x^{\nu+1}-x^\nu) + R - S\lambda^{\nu+1} = 0$$

$$\begin{aligned}
\Rightarrow \quad \lambda^{\nu+1} &= S^{-1}\left[R + f_x^\nu (x^{\nu+1}-x^\nu)\right] \qquad \text{(H)} \\
&= S^{-1}R + S^{-1} f_x^\nu (x^{\nu+1}-x^\nu)
\end{aligned}$$

Fits with constraint relation

Put this back in (B) $\Rightarrow$

$$
\begin{aligned}
0 = \lambda^\dagger f_x &= \left[S^{-1}R + S^{-1}f_x^\nu\left(x^{\nu+1} - x^\nu\right)\right]^\dagger f_x^\nu \\
&= R^\dagger \left(S^{-1}\right)^\dagger f_x^\nu + \left(x^{\nu+1} - x^\nu\right)^\dagger \left(f_x^\nu\right)^\dagger \left(S^{-1}\right)^\dagger f_x^\nu \\
\Rightarrow \left(x^{\nu+1} - x^\nu\right)^\dagger \left(f_x^\nu\right)^\dagger \left(S^{-1}\right)^\dagger f_x^\nu &= -R^\dagger \left(S^{-1}\right)^\dagger f_x^\nu \\
\Rightarrow \left(f_x^\nu\right)^\dagger S^{-1} f_x^\nu \left(x^{\nu+1} - x^\nu\right) &= -\left(f_x^\nu\right)^\dagger S^{-1} R \\
\Rightarrow \left(x^{\nu+1} - x^\nu\right) &= -\left[\left(f_x^\nu\right)^\dagger S^{-1} f_x^\nu\right]^{-1} \left(f_x^\nu\right)^\dagger S^{-1} R \qquad \text{(I)}
\end{aligned}
$$

RHS of (I) is completely known at the iteration $\Rightarrow \quad x^{\nu+1}$

Substitute this in (H) $\Rightarrow \quad \lambda^{\nu+1}$

Substitute $\lambda^{\nu+1}$ in (A') $\Rightarrow \quad m^{\nu+1}$

So go from step to step choosing m, x, λ satisfying the constraint relations and minimising χ^2 simultaneously

Iterations stop when

- constraint relations are balanced at a level better than the required precision
- derivatives $\frac{\partial \chi^2}{\partial m}, \frac{\partial \chi^2}{\partial x}$ are sufficiently close to 0
- χ^2 change per iteration is small

Fits with constraint relation

Now $m^{\nu+1}, x^{\nu+1}$ can be expressed explicitly in terms of m_0, G_M^{-1}
Approximate to a linear relation

$$
\begin{aligned}
m^{\nu+1} &= g(m_0); \\
x^{\nu+1} &= h(m_0)
\end{aligned}
$$

Carry out error propagation

$$
\begin{aligned}
G^{-1}_{m^{\nu+1}} &= \frac{\partial g}{\partial m_0} G_M^{-1} \left(\frac{\partial g}{\partial m_0}\right)^\dagger \\
G^{-1}_{x^{\nu+1}} &= \frac{\partial h}{\partial m_0} G_M^{-1} \left(\frac{\partial h}{\partial m_0}\right)^\dagger
\end{aligned}
$$

and correlation between measured and unmeasured quantities

$$\left(\frac{\partial g}{\partial m_0}\right) G_M^{-1} \left(\frac{\partial h}{\partial m_0}\right)^\dagger$$

Now (A') $\Rightarrow$ $m^{\nu+1} = m^0 - G_M^{-1} \left(f_m^\nu\right)^\dagger \lambda^{\nu+1}$

So

$$
\begin{aligned}
\frac{\partial g}{\partial m_0} &= 1 - G_M^{-1} \left(f_m^\nu\right)^\dagger \frac{\partial \lambda^{\nu+1}}{\partial m_0} && \text{from (H)} \\
&= 1 - G_M^{-1} \left(f_m^\nu\right)^\dagger S^{-1} \left[\frac{\partial R}{\partial m_0} + f_x^\nu \frac{\partial}{\partial m_0}\left(x^{\nu+1} - x^\nu\right)\right] && \text{from (I)} \\
&= 1 - G_M^{-1} \left(f_m^\nu\right)^\dagger S^{-1} \left[\frac{\partial R}{\partial m_0} - f_x^\nu \left(f_x^{\nu\dagger} S^{-1} f_x^\nu\right)^{-1} f_x^{\nu\dagger} S^{-1} \frac{\partial R}{\partial m_0}\right] && \text{from (F)} \\
&= 1 - G_M^{-1} \left(f_m^\nu\right)^\dagger S^{-1} \left[f_m^\nu - f_x^\nu \left(f_x^{\nu\dagger} S^{-1} f_x^\nu\right)^{-1} f_x^{\nu\dagger} S^{-1} f_m^\nu\right]
\end{aligned}
$$

Fits with constraint relation

Similarly
$$\frac{\partial h}{\partial m_0} = \left[f_x^{\nu\dagger} S^{-1} f_x^{\nu}\right]^{-1} f_x^{\nu\dagger} S^{-1} f_m^{\nu}$$

Thus the variance becomes
$$\begin{aligned} G^{-1}_{m^{\nu+1}} &= G_M^{-1} - G_M^{-1} f_m^{\nu\dagger} S^{-1} f_m^{\nu} G_M^{-1} + \\ &\quad G_M^{-1} f_m^{\nu\dagger} S^{-1} f_x^{\nu} \left(f_x^{\nu\dagger} S^{-1} f_x^{\nu}\right)^{-1} f_x^{\nu\dagger} S^{-1} f_m^{\nu} G_M^{-1} \\ G^{-1}_{x^{\nu+1}} &= \left(f_x^{\nu\dagger} S^{-1} f_x^{\nu}\right)^{-1} \end{aligned}$$

And the correlation
$$C_{(mx)^{\nu+1}} = -G_M^{-1} f_m^{\nu\dagger} S^{-1} f_x^{\nu} \left(f_x^{\nu\dagger} S^{-1} f_x^{\nu}\right)^{-1}$$

So the overall correlation matrix becomes
$$\begin{pmatrix} G^{-1}_{m^{\nu+1}} & C_{(mx)^{\nu+1}} \\ C^{\dagger}_{(mx)^{\nu+1}} & G^{-1}_{x^{\nu+1}} \end{pmatrix}$$

The fit procedure reduces the variance on measured quantities but introduces some correlation among them where none existed initially

An Application

An experiment wants to measure the mass of one particle which is produced as a pair in electron-positron collisions and then each of them decays into a pair of objects

$$e^+e^- \rightarrow W^+W^-$$

$$\quad\quad\quad\quad |\quad |\_ \rightarrow q''\bar{q}'''$$

$$\quad\quad\quad\quad |\_ \rightarrow qq'$$

Measure the energies of the 4 jets coming from the 4 quarks and their angles. Jet directions are well measured but the energies are not so well measured. So try to utilise some of the known phenomena and see if this can help the measurements

- Energy and momentum are conserved in the particle production and decay processes
- The two W's have the same mass
- Since electrons and positrons collide head-on, the initial state momentum = 0 and initial state energy = $2E_{Beam}$

Here all quantities are measured with some precision $\Longrightarrow$ $\vec{x}$ has no entries

Application of Constrained Fit

Choose variables: $\vec{m} = E_i,\ \theta_i,\ \phi_i,\ \beta_i$

where $\beta_i = \dfrac{\sqrt{E_i^2 - m_i^2}}{E_i}$ for $i = 1, \cdots 4$

Constraint equations:

$$\sum_{i=1} E_i - 2E_{Beam} = 0 \qquad f_1$$

$$\sum_{i=1}^{4} \beta_i E_i \sin\theta_i \cos\phi_i = 0 \qquad f_2$$

$$\sum_{i=1}^{4} \beta_i E_i \sin\theta_i \sin\phi_i = 0 \qquad f_3$$

$$\sum_{i=1}^{4} \beta_i E_i \cos\theta_i = 0 \qquad f_4$$

$$(E_1 + E_2)^2 - (E_3 + E_4)^2 - (\beta_1 E_1 \sin\theta_1 \cos\phi_1 + \beta_2 E_2 \sin\theta_2 \cos\phi_2)^2 + (\beta_3 E_3 \sin\theta_3 \cos\phi_3 + \beta_4 E_4 \sin\theta_4 \cos\phi_4)^2 - (\beta_1 E_1 \sin\theta_1 \sin\phi_1 + \beta_2 E_2 \sin\theta_2 \sin\phi_2)^2 + (\beta_3 E_3 \sin\theta_3 \sin\phi_3 + \beta_4 E_4 \sin\theta_4 \sin\phi_4)^2 - (\beta_1 E_1 \cos\theta_1 + \beta_2 E_2 \cos\theta_2)^2 + (\beta_3 E_3 \cos\theta_3 + \beta_4 E_4 \cos\theta_4)^2 = 0 \qquad f_5$$

Application of Constrained Fits

Need to evaluate the derivatives:

f_1^m

$$\frac{\partial f_1}{\partial E_i} = 1$$
$$\frac{\partial f_1}{\partial \theta_i} = 0$$
$$\frac{\partial f_1}{\partial \phi_i} = 0$$
$$\frac{\partial f_1}{\partial \beta_i} = 0$$

f_2^m

$$\frac{\partial f_2}{\partial E_i} = \beta_i \sin\theta_i \cos\phi_i$$
$$\frac{\partial f_2}{\partial \theta_i} = \beta_i E_i \cos\theta_i \cos\phi_i$$
$$\frac{\partial f_2}{\partial \phi_i} = -\beta_i E_i \sin\theta_i \sin\phi_i$$
$$\frac{\partial f_2}{\partial \beta_i} = E_i \sin\theta_i \cos\phi_i$$

f_3^m

$$\frac{\partial f_3}{\partial E_i} = \beta_i \sin\theta_i \sin\phi_i$$
$$\frac{\partial f_3}{\partial \theta_i} = \beta_i E_i \cos\theta_i \sin\phi_i$$
$$\frac{\partial f_3}{\partial \phi_i} = \beta_i E_i \sin\theta_i \cos\phi_i$$
$$\frac{\partial f_3}{\partial \beta_i} = E_i \sin\theta_i \sin\phi_i$$

f_4^m

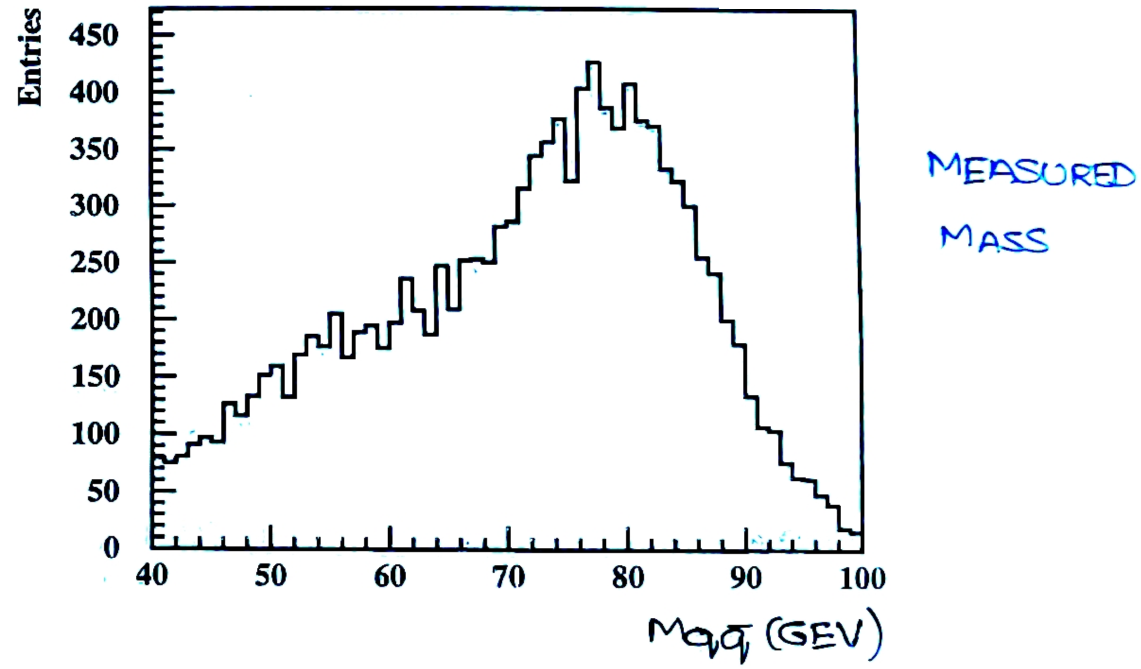
$$\frac{\partial f_4}{\partial E_i} = \beta_i \cos\theta_i$$
$$\frac{\partial f_4}{\partial \theta_i} = -\beta_i E_i \sin\theta_i$$
$$\frac{\partial f_4}{\partial \phi_i} = 0$$
$$\frac{\partial f_4}{\partial \beta_i} = E_i \cos\theta_i$$

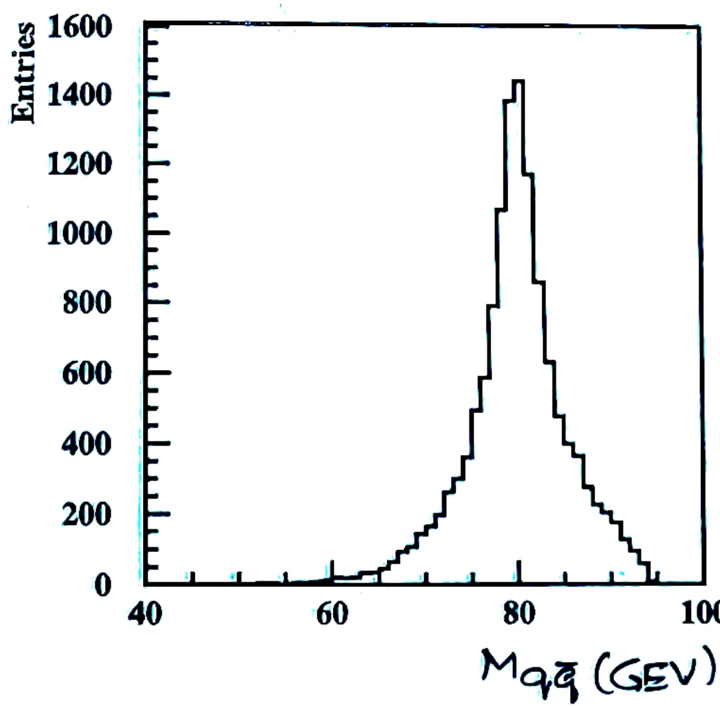
f_5^m

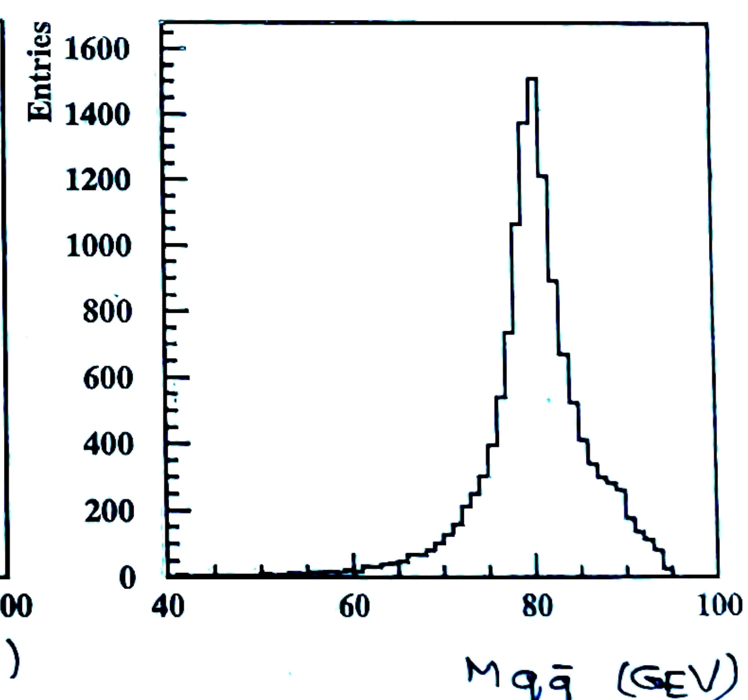
Num

Results from the fits

Measurement was done with data using $\sqrt{s} =$ 189 GeV







After 4C fit

$$\sum_i \vec{p_i} = 0$$

$$\sum_i E_i = 2E_{Beam}$$

After 5C fit

$$m_{12} = m_{34}$$

Kinematic Fit (Example)

Measurement of three angles of a triangle

$$\chi^2 = \frac{(\theta_1 - \theta_{10})^2}{\sigma_1^2} + \frac{(\theta_2 - \theta_{20})^2}{\sigma_2^2} + \frac{(\theta_3 - \theta_{30})^2}{\sigma_3^2} + 2\,\lambda(\theta_1 + \theta_2 + \theta_3 - 180^\circ)$$

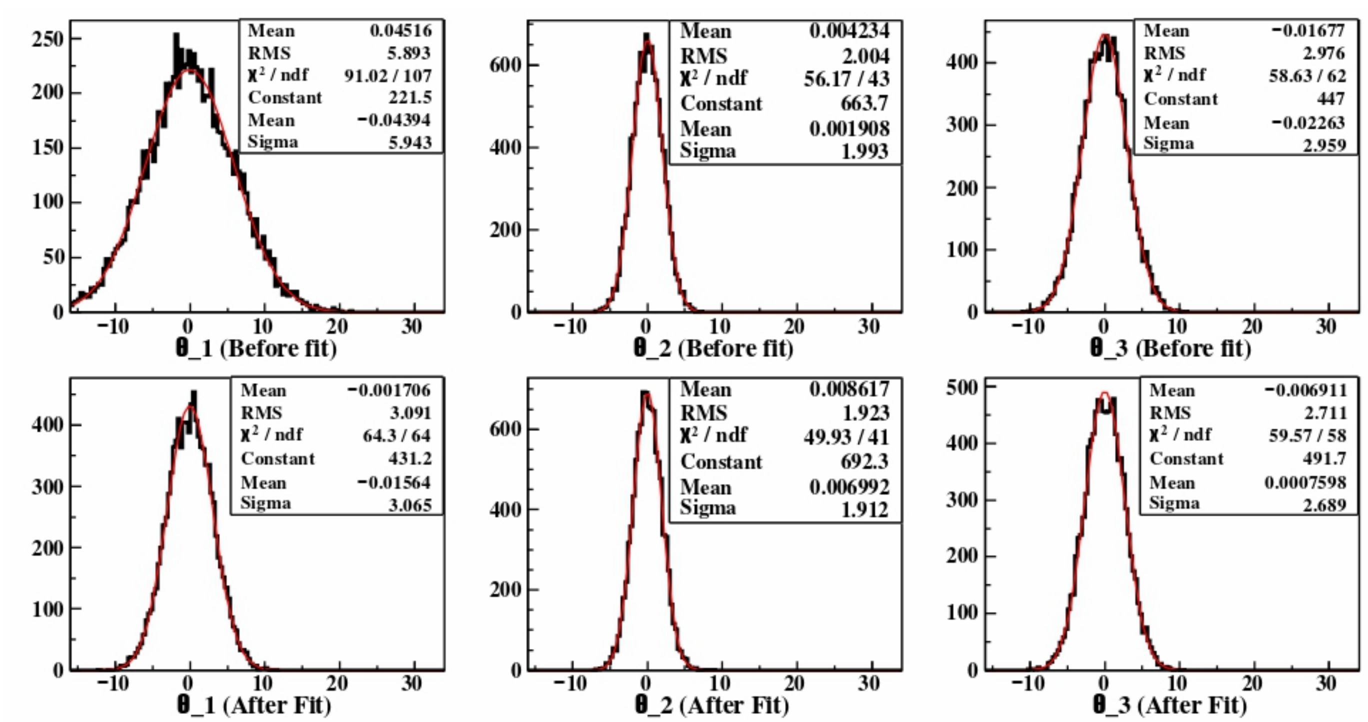
$$\frac{1}{2}\frac{\partial \chi^2}{\partial \theta_i} = \frac{(\theta_i - \theta_{i0})}{\sigma_i^2} + \lambda = 0 \rightarrow \theta_i = \theta_{i0} + \lambda \cdot \sigma_i^2$$

$$\frac{1}{2}\frac{\partial \chi^2}{\partial \lambda} = (\theta_1 + \theta_2 + \theta_3 - 180^\circ) = 0$$

$$\lambda = \frac{180^\circ - (\theta_{10} + \theta_{20} + \theta_{30})}{(\sigma_1^2 + \sigma_3^2 + \sigma_3^2)}$$

$$\theta_i = \theta_{i0} + \lambda \cdot \sigma_i^2 = \theta_{i0} + \frac{1}{3}[180^\circ - (\theta_{10} + \theta_{20} + \theta_{30})]$$

For same errors in all three measurements, error on corrected angles are $(2/3) \times \sigma$.



Kinematic Fit (Example)

Simple calculation, because the function was linear in the variables. But, in general kinematic fitting becomes an iterative procedure.

Improvement of P_{π^0} in the reconstruction of the mass of π^0 from two photons

- Measured parameters (y) : $E_1, \theta_1, \phi_1, E_2, \theta_2$ and ϕ_2
- Constraint : $2\,\mathrm{E_1}\,\mathrm{E_2}\,(1 - \cos\theta_{12}) - \mathrm{m}_{\pi^0}^2 = \mathrm{f(y)} - \mathrm{m}_{\pi^0}^2 = 0,$ with $\cos\theta_{12} = \sin\theta_1\,\sin\theta_2\,\cos(\phi_1 - \phi_2) + \cos\theta_1\,\cos\theta_2$

$$\chi^2 = \sum_{i=1}^{6} \frac{(y_i - y_{i0})^2}{\sigma_{y_i}{}^2} + \frac{(f(y) - m_{\pi^0}^2)^2}{\sigma_{\pi^0}{}^2}$$

$$\frac{\partial\chi^2}{\partial y_i} = 2\frac{y_i - y_{i0}}{\sigma_{y_i^2}} + 2\frac{\partial f}{\partial y_i}\,\frac{(f(y) - m_{\pi^0}^2)}{\sigma_{\pi^0}{}^2} = 0$$

$$\frac{Dy_i}{\sigma_{y_i}^2} = -\frac{\partial f}{\partial y_i}\,\frac{(f(y_0) + \frac{\partial f}{\partial y_i}\,Dy_i - m_{\pi^0}^2)}{\sigma_{\pi^0}{}^2}$$

In matrix notation,

$$V^{-1} \cdot Dy = B^T \cdot (m_{\pi^0}^2 - f(y_0) - B \cdot Dy)/\sigma_{\pi^0}^2$$

$$(V^{-1} + B^T \cdot B/\sigma_{\pi^0}^2) \cdot Dy = B^T \cdot (m_{\pi^0}^2 - f(y_0))/\sigma_{\pi^0}^2$$

$$Dy = (V^{-1} + B^T \cdot B/\sigma_{\pi^0}^2)^{-1} \cdot B^T \cdot (m_{\pi^0}^2 - f(y_0))/\sigma_{\pi^0}^2$$

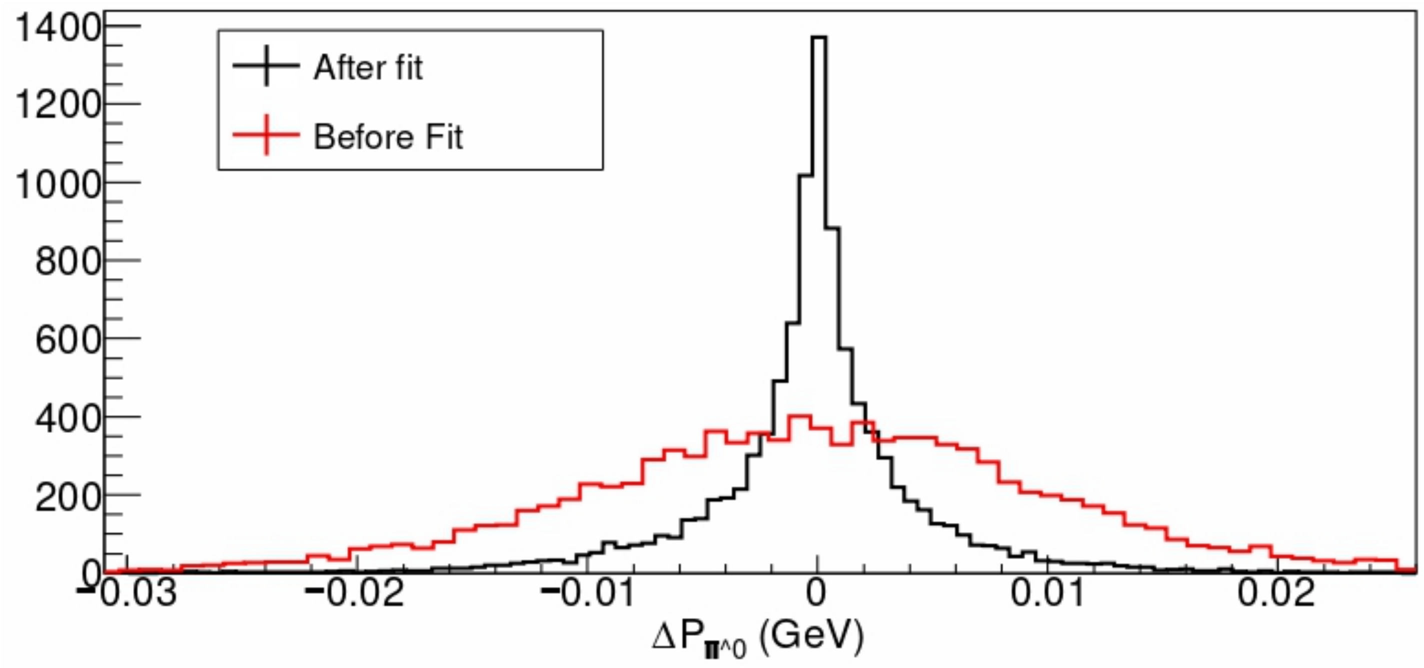
With an iterative procedure, recalculate parameters, until the change in m_π and χ^2 is lower than a certain value (e.g., $1.e^{-5}$).

Error on the fitted mass,

$$\sigma_{\pi^0}^2 = V \cdot \left[I - B^T \cdot \left(B \cdot V \cdot B^T\right)^{-1} \cdot B \cdot V\right]$$

Derive this expression

Results from Kinematic Fit



Numerical r

Kinematic Fit (Problem)

Kinematic fit

http://www.phys.ufl.edu/~avery/fitting.html

Assume the following decay chains of $\bar{B}$ meson

$$\begin{aligned} \overline{B}^0 \rightarrow\ & D^{*+}\pi^- \\ & D^{*+} \rightarrow D^0\pi^+ \\ & \qquad D^0 \rightarrow K^-\pi^+\pi^0 \\ & \qquad\qquad \pi^0 \rightarrow \gamma\gamma \end{aligned}$$

Several kinematic constraints may be applied to improve mass resolution of $\overline{B}^0$, e.g. and example from B-factory,

1. Mass of $\gamma\gamma$ to M_{π^0} (Mass constraint)
2. the $K^-\pi^+\pi^0$ mass is equal to M_{D^0}
3. K^- and π^+ from D^0 decay intersect single space point (vertex constraint)
4. Inv mass of $D^0\pi^+$ is equal to $M_{D^{*+}}$
5. Slow π^+ from D^+ decay and fast π^+ from $\overline{B}^0$ decay come from same space point
6. Energies of final state particles is the energy of beam (in CM frame)