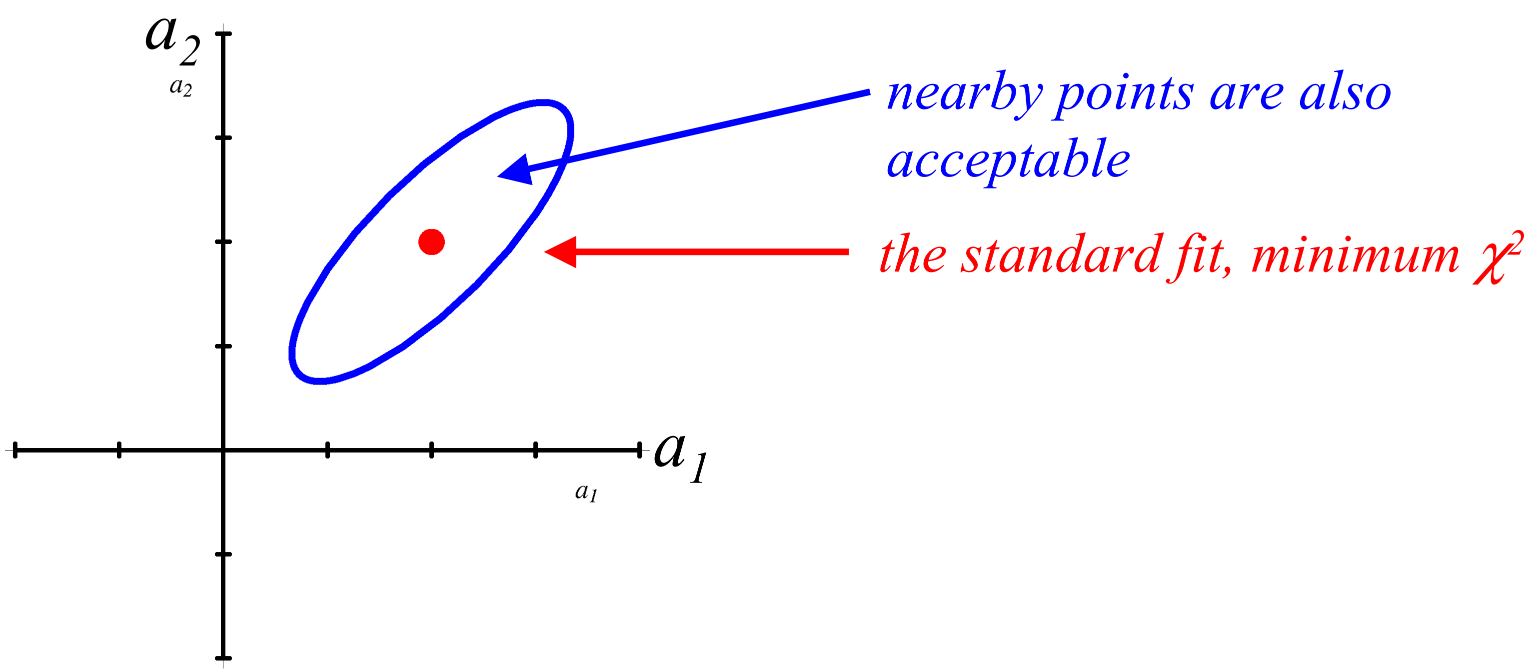
Uncertainty Analysis

(I) Methods

We continue to use χ^2_{global} as *figure of merit.* Explore the variation of χ^2_{global} in the neighborhood of the minimum.

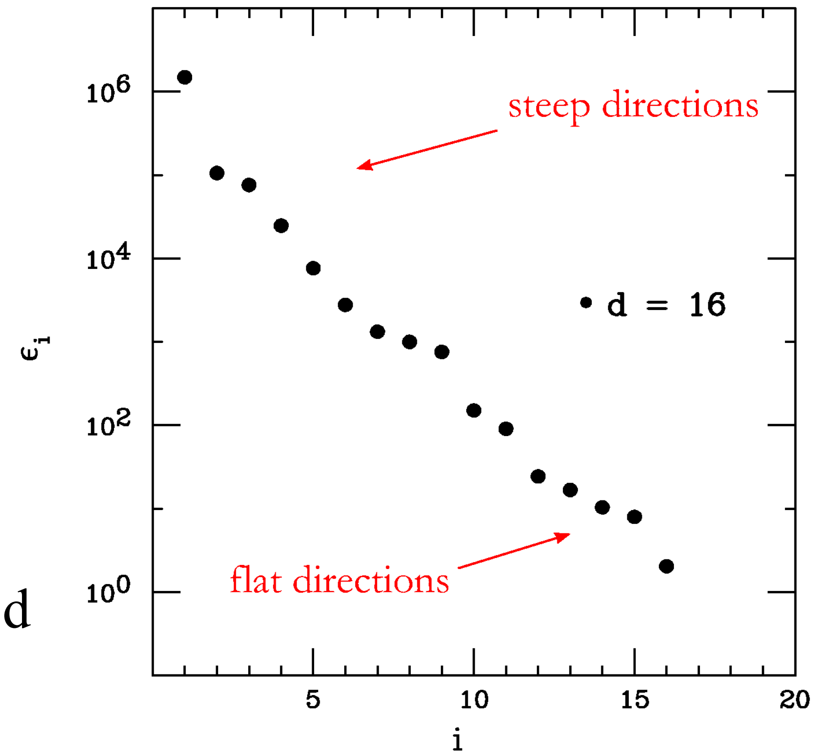


The Hessian method

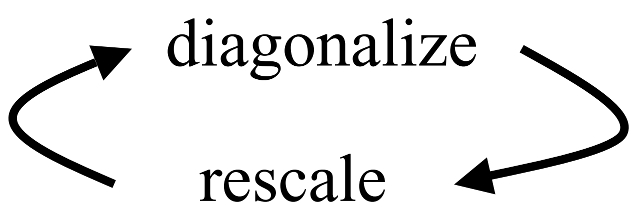
$$H_{\mu\nu} \equiv \frac{1}{2} \frac{\partial^2 \chi^2}{\partial a_\mu \partial a_\nu}\bigg|_0 \qquad (\mu, \nu = 1\ 2\ 3 \ldots d)$$

The numerical computation of $H_{\mu\nu}$ by finite differences is nontrivial:

• the eigenvalues of $H_{\mu\nu}$ vary over many orders of magnitude,
• computation of χ^2_{global} is subject to small numerical errors leading to discontinuities as a function of $\{a_\mu\}$.



The finite step size must be direction dependent. We devised an iterative method



which converges to a good complete set of eigenvectors of $H_{\mu\nu}$.

“Master Formula”

Classical error formula for a variable $X(a)$

$$(\Delta X)^2 = \Delta\chi^2 \sum_{\mu,\nu} \frac{\partial X}{\partial a_\mu} \left(H^{-1}\right)_{\mu\nu} \frac{\partial X}{\partial a_\nu}$$

Obtain better convergence using eigenvectors of $H_{\mu\nu}$

$$(\Delta X)^2 = \sum_{\mu=1}^{d} \left[X\left(S_\mu^{(+)}\right) - X\left(S_\mu^{(-)}\right) \right]^2$$

$S_\mu^{(+)}$ and $S_\mu^{(-)}$ denote PDF sets displaced from the standard set, along the ± directions of the μ^{th} eigenvector, by distance $T = \sqrt{(\Delta\chi^2)}$ in parameter space.

(available in the LHAPDF format : 2d alternate sets)

The Lagrange Multiplier Method

… for analyzing the uncertainty of PDF-dependent predictions.

The fitting function for *constrained fits*

$$F(a_\mu, \lambda) = \chi^2_{\text{global}}(a_\mu) + \lambda X(a_\mu)$$

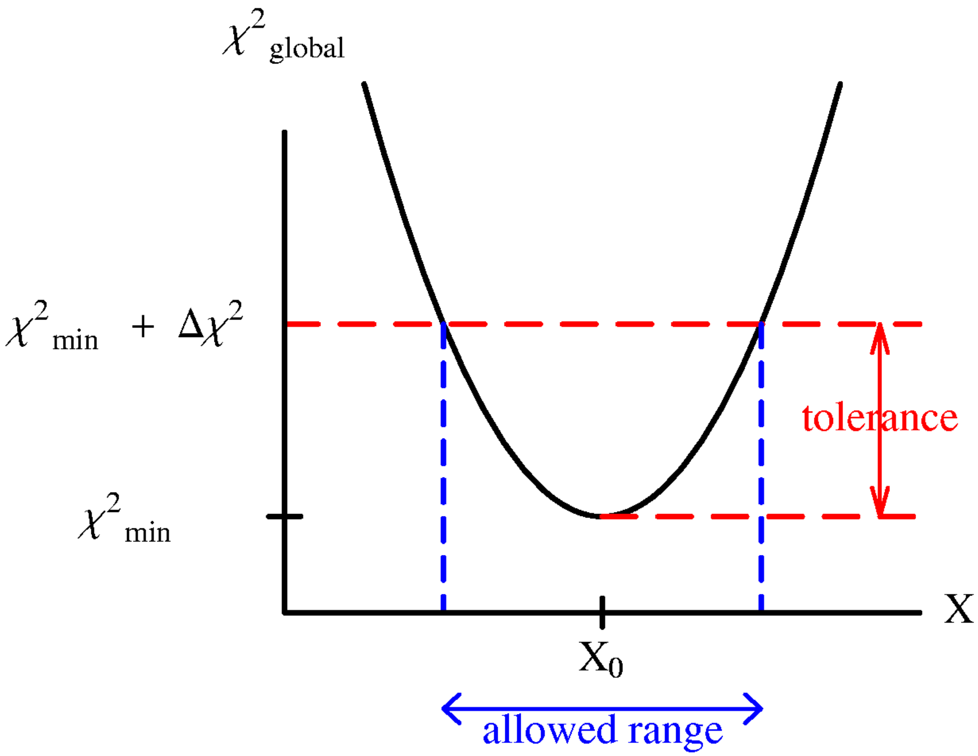
λ : Lagrange multiplier

Minimization of F [w.r.t $\{a_\mu\}$ and λ] gives the best fit for the value $X(a_{\min,\mu})$ of the variable X.

controlled by the parameter λ

Hence we obtain a curve of χ^2_{global} versus X.

The question of tolerance



X : any variable that depends on PDF's

X_0 : the prediction in the standard set

$\chi^2(X)$: curve of constrained fits

For the specified tolerance ($\Delta\chi^2 = T^2$) there is a corresponding range of uncertainty, $\pm \Delta X$.

What should we use for T?

Estimation of parameters in Gaussian error analysis would have

$$T = 1$$

We do not use this criterion.

Aside: The familiar ideal example

Consider N measurements $\{\theta_i\}$ of a quantity θ with normal errors $\{\sigma_i\}$

$$dP = \frac{e^{-r^2/2}}{\sqrt{2\pi}}$$

$$\theta_i = \theta_{\text{true}} + \sigma_i r_i$$

Estimate θ by minimization of χ^2,

$$\chi^2(\theta) = \sum_{i=1}^{N} \frac{(\theta_i - \theta)^2}{\sigma_i^2} \quad \Rightarrow \quad \theta_{\text{combined}} = \frac{\sum_i \theta_i / \sigma_i^{\,2}}{\sum_i 1/\sigma_i^{\,2}}$$

The mean of θ_{combined} is θ_{true} , the SD is $\Delta\theta_c = \left(\sum_i 1/\sigma_i^2 \right)^{-1/2}$

$(= \sigma / \sqrt{N})$

and

$$\chi^2(\theta_c \pm \Delta\theta_c) - \chi^2(\theta_c) = 1.$$

The proof of this theorem is straightforward. It does not apply to our problem because of systematic errors.

Add a systematic error to the ideal model…

$$\theta_i = \theta_{\text{true}} + \sigma_i r_i + \beta_i \tilde{r}$$

(for simplicity suppose $\beta_i = \beta$)

Estimate θ by minimization of χ'^2

$$\chi'^2(\theta, s) = \sum_{i=1}^{N} \frac{(\theta_i - \beta_i s - \theta)^2}{\sigma_i^2} + s^2$$

(s : systematic shift, θ : observable)

$$\theta_{\text{combined}} = \frac{\sum_i \theta_i / \sigma_i^2}{\sum_i 1/\sigma_i^2} \quad \text{and} \quad (\Delta\theta_c)^2 = \frac{1}{\sum_i 1/\sigma_i^2} + \beta^2$$

($= \sigma^2/N + \beta^2$)

Then, letting $\chi^2(\theta) \equiv \chi'^2[\theta, s_0(\theta)]$, again

$$\chi^2(\theta_c \pm \Delta\theta_c) - \chi^2(\theta_c) = 1.$$

Still we do not apply the criterion $\Delta\chi^2 = 1$!

Reasons

- We keep the normalization factors fixed as we vary the point in parameter space. The criterion $\Delta\chi^2 = 1$ requires that the systematic shifts be continually optimized versus $\{a_\mu\}$.
- Systematic errors may be nongaussian.
- The published "standard deviations" β_{ij} may be inaccurate.
- We trust our *physics judgement* instead.

To judge the PDF uncertainty, we return to the individual experiments.

Lumping all the data together in one variable – $\Delta\chi^2_{global}$ – is too constraining.

Global analysis is a compromise. All data sets should be fit *reasonably* well -- that is what we check. As we vary $\{a_\mu\}$, does any experiment *rule out* the displacement from the standard set?

In testing the goodness of fit, we keep the normalization factors (i.e., optimized luminosity shifts) fixed as we vary the shape parameters.

End result

$$\Delta\chi'^2 \Big|_{\text{fixed norms}} >> 1$$

e.g., ~100 for ~2000 data points.

This does not contradict the $\Delta\chi^2 = 1$ criterion used by other groups, because that refers to a *different* χ^2 in which the normalization factors are continually optimized as the $\{a_\mu\}$ vary.

Some groups *do* use the criterion of $\Delta\chi^2 = 1$ for PDF error analysis.

Often they are using limited data sets – e.g., an experimental group using only their own data. Then the $\Delta\chi^2 = 1$ criterion may underestimate the uncertainty implied by systematic differences between experiments.

An interesting compendium of methods, by R. Thorne

CTEQ6	$\Delta\chi^2 = 100$ (fixed norms)
ZEUS	$\Delta\chi^2 = 50$ (effective)
MRST01	$\Delta\chi^2 = 20$
H1	$\Delta\chi^2 = 1$
Alekhin	$\Delta\chi^2 = 1$
GKK	not using χ^2