Uncertainty Analysis

(I) Methods
We continue to use $\chi^2_{\text{global}}$ as figure of merit. Explore the variation of $\chi^2_{\text{global}}$ in the neighborhood of the minimum.

The Hessian method

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

nearby points are also acceptable
the standard fit, minimum $\chi^2$
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 $\chi^2_{\text{global}}$ 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 $H_{\mu\nu}$.

diagonalize

rescale

which converges to a good complete set of eigenvectors of $H_{\mu\nu}$.
Classical error formula for a variable $X(a)$

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

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

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

$S^{(+)}_\mu$ and $S^{(-)}_\mu$ denote PDF sets displaced from the standard set, along the ± directions of the $\mu^{\text{th}}$ 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

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

\( \lambda : \text{Lagrange multiplier} \)

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

Hence we obtain a curve of \( \chi^2_{\text{global}} \) 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 $\theta$ with normal errors $\{\sigma_i\}$

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

Estimate $\theta$ by minimization of $\chi^2$,

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

The mean of $\theta_{\text{combined}}$ is $\theta_{\text{true}}$, the SD is $\Delta \theta_c = \left(\sum_i 1 / \sigma_i^2\right)^{-1/2}$ 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 \( \theta \) by minimization of \( \chi'^2 \)

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

( \( s \) : systematic shift, \( \theta \) : observable)

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

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” $\beta_{ij}$ may be inaccurate.
- We trust our *physics judgement* instead.
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

<table>
<thead>
<tr>
<th>Method</th>
<th>$\Delta \chi^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>CTEQ6</td>
<td>$\Delta \chi^2 = 100$</td>
</tr>
<tr>
<td>ZEUS</td>
<td>$\Delta \chi^2 = 50$ (effective)</td>
</tr>
<tr>
<td>MRST01</td>
<td>$\Delta \chi^2 = 20$</td>
</tr>
<tr>
<td>H1</td>
<td>$\Delta \chi^2 = 1$</td>
</tr>
<tr>
<td>Alekhin</td>
<td>$\Delta \chi^2 = 1$</td>
</tr>
<tr>
<td>GKK</td>
<td>not using $\chi^2$</td>
</tr>
</tbody>
</table>
To judge the PDF uncertainty, we return to the individual experiments.

Lumping all the data together in one variable – $\Delta \chi^2_{\text{global}}$ – 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

$$\Delta \chi'^2 \bigg|_{\text{fixed norms}} \gg 1$$

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 $\chi^2$ in which the normalization factors are continually optimized as the $\{a_\mu\}$ vary.