

Treatment of correlated systematic errors

PDF4LHC August 2009

A M Cooper-Sarkar

Systematic differences combining ZEUS and H1 data

- In a QCD fit
- In a 'theory free' fit

Treatment of correlated systematic errors

$$\chi^2 = \sum_i \left[\frac{F_i^{\text{QCD}}(\mathbf{p}) - F_i^{\text{MEAS}}}{(\sigma_i^{\text{STAT}})^2 + (\Delta_i^{\text{SYS}})^2} \right]^2$$

Quadratic combination: errors on the fit parameters, \mathbf{p} , evaluated from $\Delta\chi^2 = 1$,

THIS IS NOT GOOD ENOUGH if experimental systematic errors are correlated between data points-

$$\chi^2 = \sum_i \sum_j [F_i^{\text{QCD}}(\mathbf{p}) - F_i^{\text{MEAS}}] V_{ij}^{-1} [F_j^{\text{QCD}}(\mathbf{p}) - F_j^{\text{MEAS}}]$$

$$V_{ij} = \delta_{ij}(\sigma_i^{\text{STAT}})^2 + \sum_\lambda \Delta_{i\lambda}^{\text{SYS}} \Delta_{j\lambda}^{\text{SYS}}$$

Where $\Delta_{i\lambda}^{\text{SYS}}$ is the correlated error on point i due to systematic error source λ

It can be established that this is equivalent to

$$\chi^2 = \sum_i \left[\frac{F_i^{\text{QCD}}(\mathbf{p}) - \sum_\lambda s_\lambda \Delta_{i\lambda}^{\text{SYS}} - F_i^{\text{MEAS}}}{(\sigma_i^{\text{STAT}})^2} \right]^2 + \sum s_\lambda^2$$

Where s_λ are systematic uncertainty fit parameters of zero mean and unit variance

This has modified the fit prediction by each source of systematic uncertainty

CTEQ, ZEUS, H1, MRST/MSTW have all adopted this form of χ^2 (MSTW still use some errors as quadratic) – but use it differently in the OFFSET and HESSIAN methods

How do experimentalists often proceed: OFFSET method

Perform fit without correlated errors ($s_\lambda = 0$) for central fit, and propagate statistical errors to the PDFs

$$\langle \sigma_q^2 \rangle = T \sum_j \sum_k \frac{\partial q}{\partial p_j} V_{jk} \frac{\partial q}{\partial p_k}$$

Where T is the χ^2 tolerance, $T = 1$.

1. Shift measurement to upper limit of one **of its systematic uncertainties** ($s_\lambda = +1$)
2. **Redo fit, record differences of parameters from those of step 1**
3. **Go back to 2, shift measurement to lower limit** ($s_\lambda = -1$)
4. **Go back to 2, repeat 2-4 for next source of systematic uncertainty**
5. **Add all deviations from central fit in quadrature (positive and negative deviations added in quadrature separately)**
6. **This method does not assume that correlated systematic uncertainties are Gaussian distributed**

A5

Fortunately, there are smart ways to do this – see extras

(Pascaud and Zomer LAL-95-05, Botje hep-ph-0110123)

Slide 3

A5

Cooper-Sarkar, 3/15/2004

HESSIAN method (covariance method)

Allow s_λ parameters to vary for the central fit. The total covariance matrix is then the inverse of a single Hessian matrix expressing the variation of χ^2 wrt both theoretical and systematic uncertainty parameters.

If we believe the theory why not let it calibrate the detector(s)? Effectively the theoretical prediction is not fitted to the central values of published experimental data, but allows these data points to move collectively according to their correlated systematic uncertainties

The fit determines the optimal settings for correlated systematic shifts such that the most consistent fit to all data sets is obtained. In a global fit the systematic uncertainties of one experiment will correlate to those of another through the fit. The resulting estimate of PDF errors is much smaller than for the Offset method for $\Delta\chi^2 = 1$

CTEQ have used this method with $\Delta\chi^2 \sim 100$ for 90%CL limits

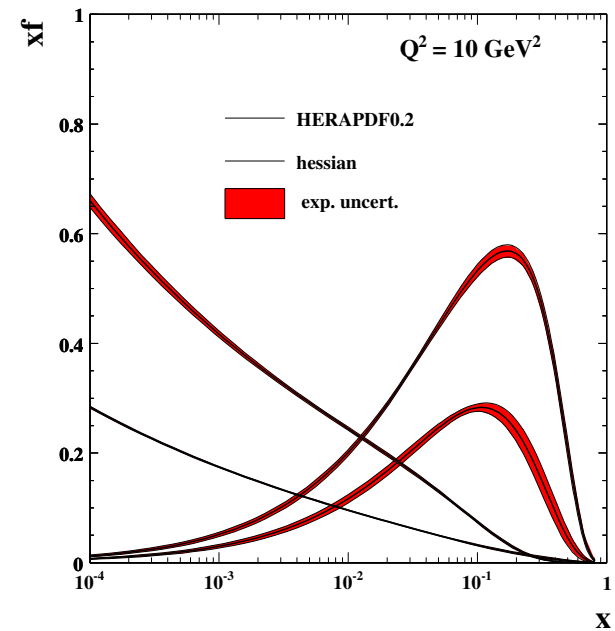
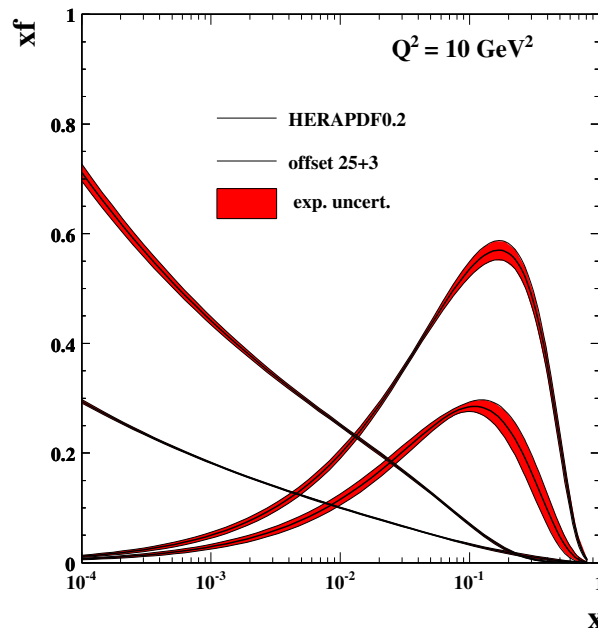
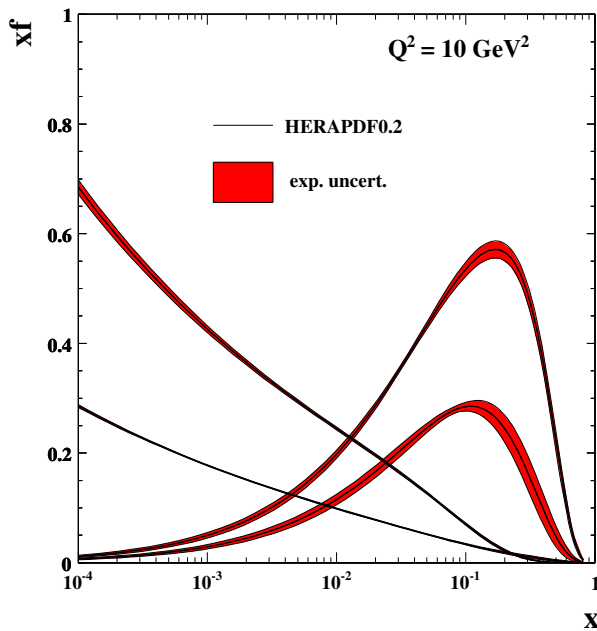
MRST have used $\Delta\chi^2 \sim 50$

H1, Alekhin have used $\Delta\chi^2 = 1$

Tolerances are now dynamic according to the eigenvector

It is not my purpose to justify these methods Just to compare them.

First for the HERAPDF to the **combined HERA data** for which **correlated systematic errors are SMALL** relative to the statistical and uncorrelated errors



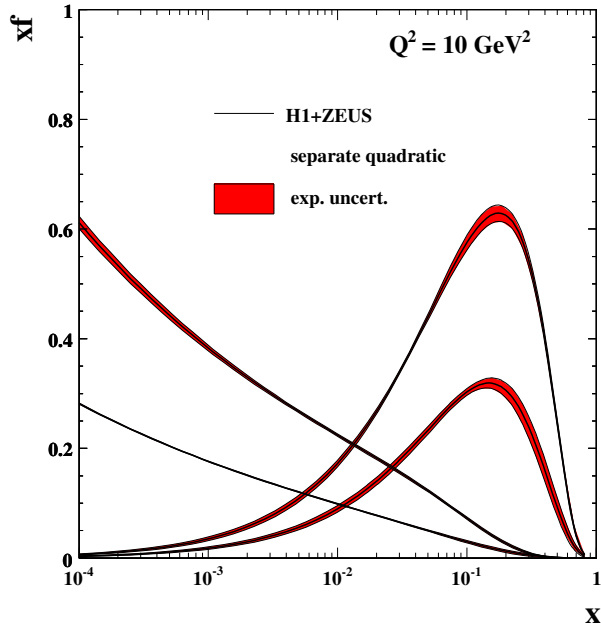
Quadratic

OFFSET

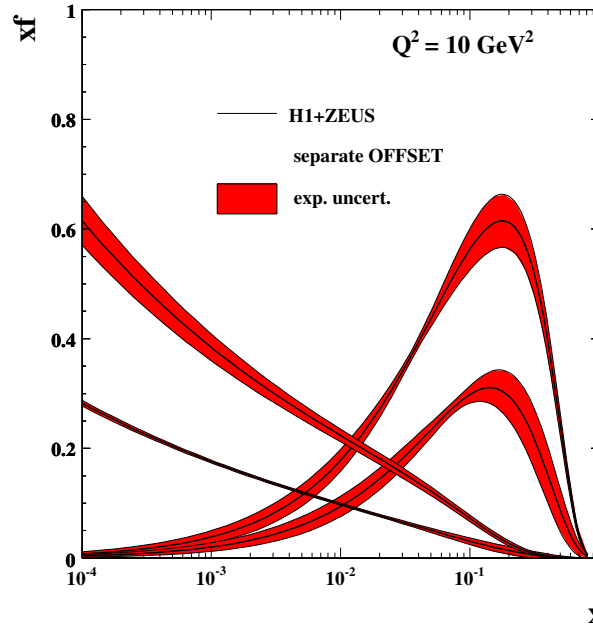
HESSIAN

For the HERAPDF with its small correlated systematic errors the treatment of these errors in the PDF fit gives only small differences in PDF central values and PDF uncertainty estimates

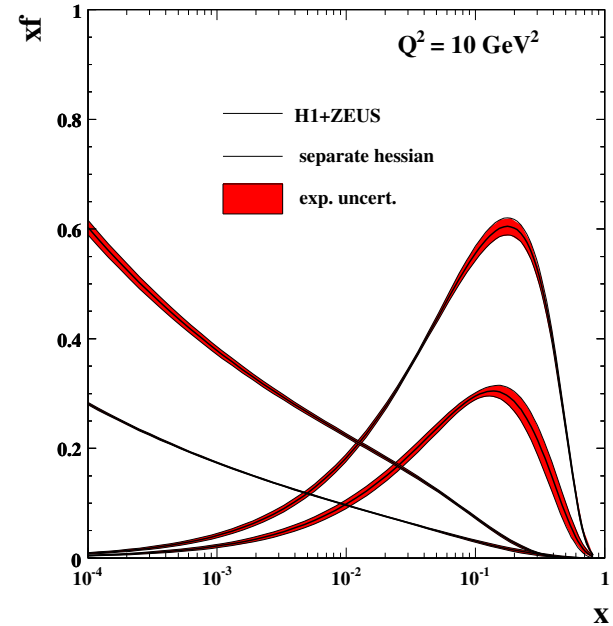
Secondly for the **separate ZEUS and H1 data** for which **correlated systematic errors are LARGE** relative to the statistical and uncorrelated errors for $Q^2 < 150$



Quadratic



OFFSET

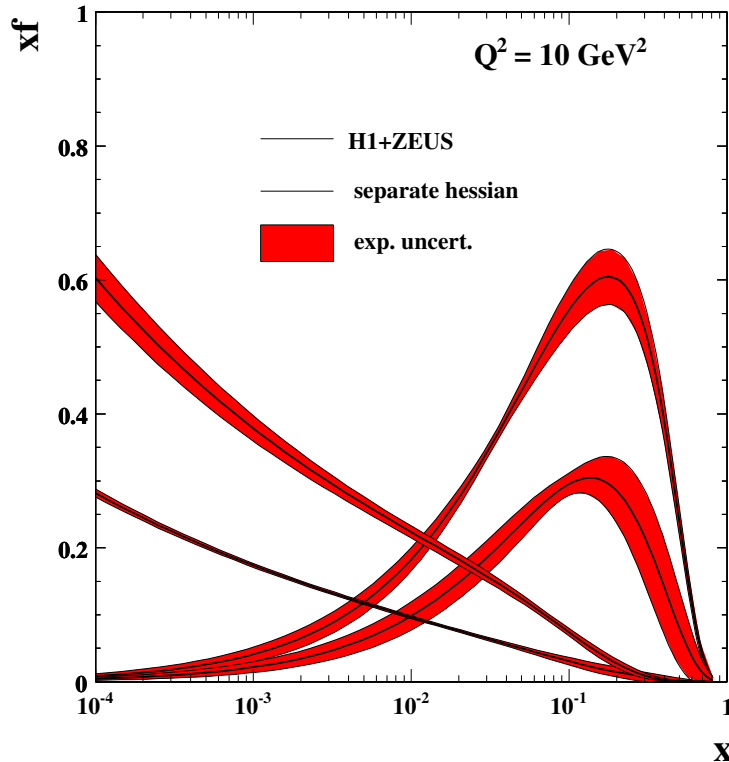


HESSIAN

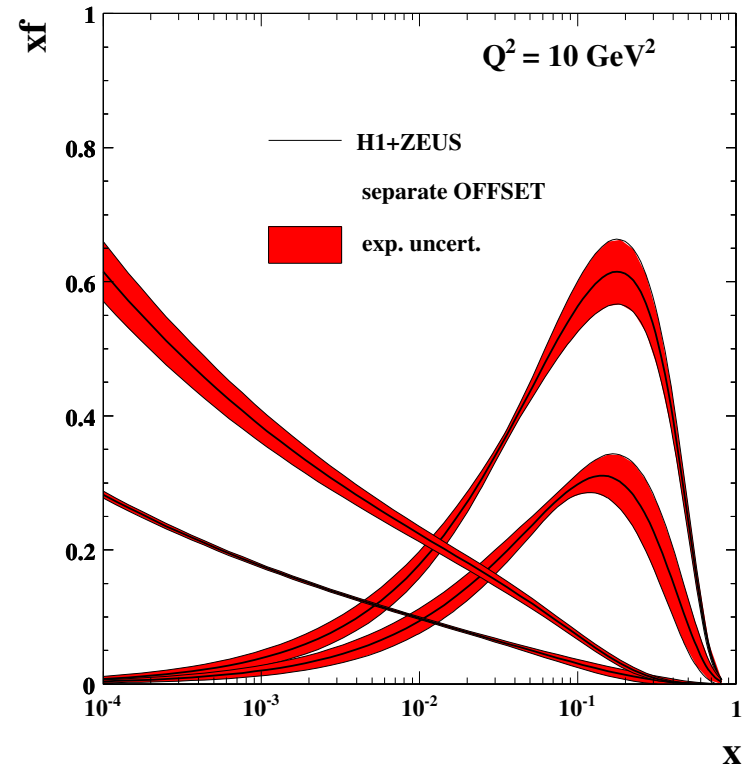
When fitting to data with large correlated systematic errors the treatment of these errors in the PDF fit gives significant differences in PDF central values and PDF uncertainty estimates

NOTE the fit formalism, parametrization etc is the same as for the HERAPDF fit. The OFFSET method gives largest errors and covers the **difference between the valence PDFs** of the other two

For the **separate ZEUS and H1 data** for which **correlated systematic errors are LARGE** relative to the statistical and uncorrelated errors



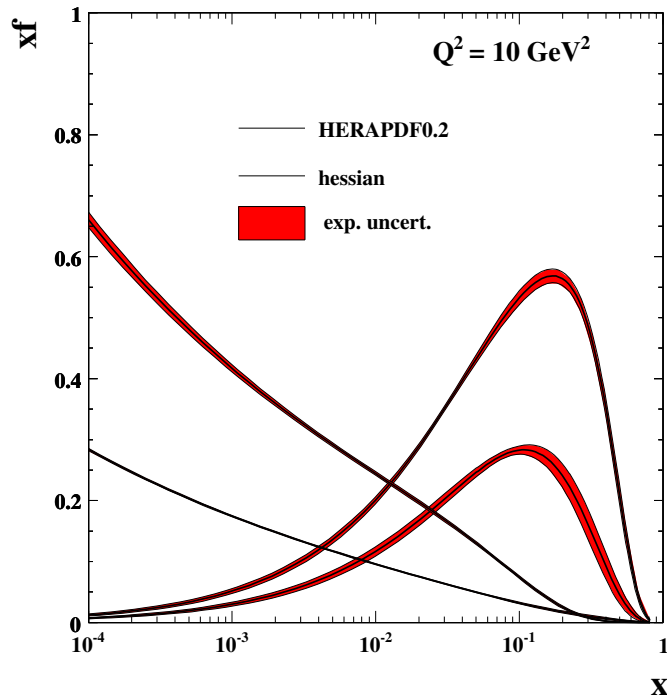
HESSIAN with increased χ^2 tolerance



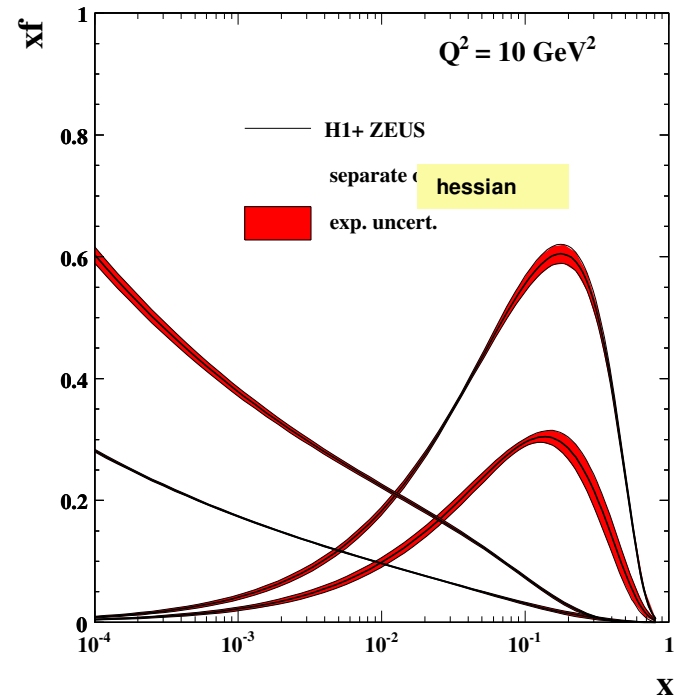
OFFSET

Applying an increased tolerance to the HESSIAN fit results in similar sized errors to those of the OFFSET method for $\Delta\chi^2 \sim 10$

Now compare Hessian fitting to the HERA combined data to Hessian fitting to separate H1 and ZEUS data sets.



HESSIAN PDF fit to HERA combined data



HESSIAN PDF fit to H1 and ZEUS separately

A comparable experimental error results BUT the shapes of the gluon and valence are significantly different. For the PDF fit to the HERA combined data the systematic error parameters of the separate data sets were already shifted in the fit which combined the data. The PDF fit does not make further significant shifts. For the separate H1 and ZEUS data the systematic error parameters of the separate data sets are shifted in the PDF fit itself.

When you put the separate data sets into a PDF fit it floats the systematic parameters of the data sets to different values than the 'theory free' combination fit. Representative examples below

Fitted systematics

Combination fit

NLO QCD PDF fit

20	zd1_e_eff	0.2940	1.2284
21	zd2_e_theta_a	0.6286	-0.8520
22	zd3_e_theta_b	-0.0871	-1.40265
23	zd4_e_escale	0.4240	-0.0090
24	zd5_had1	0.6210	-0.9657
25	zd6_had2	-0.1757	-0.4113
26	zd7_had3	-0.0167	0.6413
51	h1670e8	0.4860	0.5295
52	h1670e9	-0.3290	-0.0793
53	h1670e10	1.0718	-0.7934
54	h1670e11	0.0833	0.8154
55	h1670e12	-0.5428	1.2503
56	h1670e13	0.0820	0.0484
62	h195-00e10	-1.1148	1.6024
63	h195-00e11	-0.0917	0.3942
64	h195-00e12	-0.5950	0.8569
65	h195-00e13	0.2882	-0.2562
66	h195-00e14	-0.1547	-1.3632
67	h195-00e15	-0.4395	0.4583
68	h195-00e16	0.1103	-1.2396
69	h195-00e17	0.5173	-1.8413

Agreement on
Systematic shift

BAD

GOOD

Middling

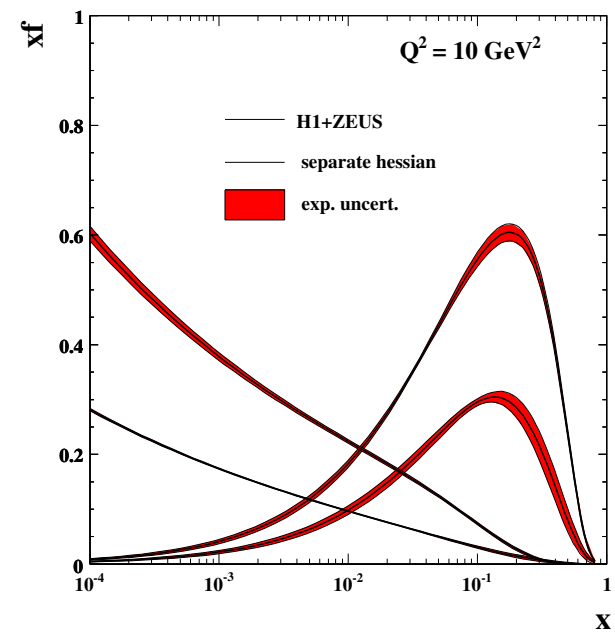
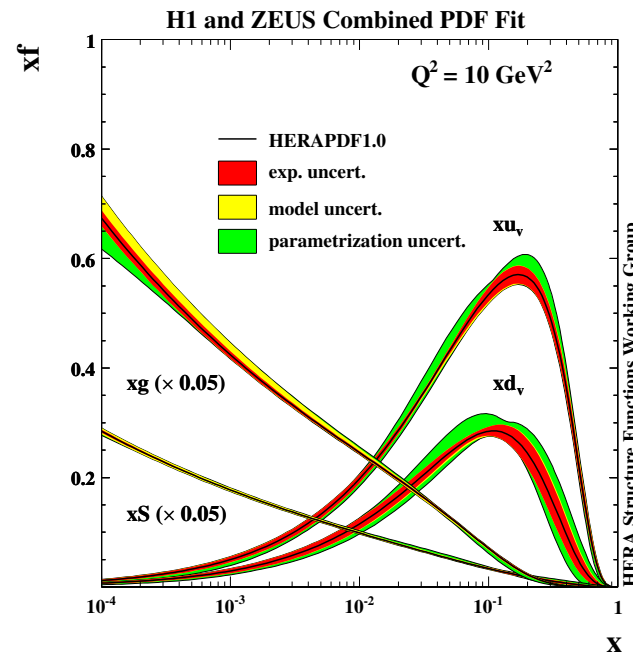
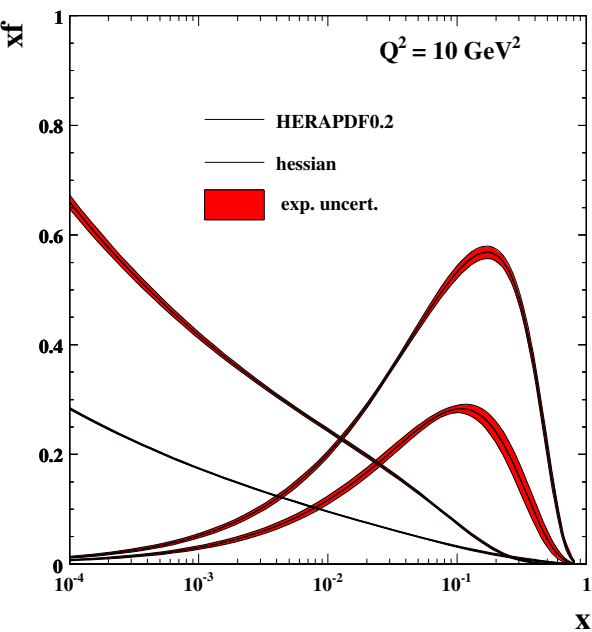
So whereas you might think that the QCD PDF fits are already doing the job of combining the HERA data- they are not getting the same answer as the HERA combination fit.

Model dependence is also important

The statistical criterion for parameter error estimation within a particular hypothesis is $\Delta\chi^2 = T^2 = 1$. But for judging the acceptability of an hypothesis the criterion is that χ^2 lie in the range $N \pm \sqrt{2N}$, where N is the number of degrees of freedom

There are many choices, such as the form of the parametrization at Q_0^2 , the value of Q_0^2 itself, the flavour structure of the sea, etc., which might be considered as superficial changes of hypothesis, but the χ^2 change for these different hypotheses often exceeds $\Delta\chi^2=1$, while remaining acceptably within the range $N \pm \sqrt{2N}$.

The model uncertainty on the PDFs generally exceeds the experimental uncertainty, if this has been evaluated using $T=1$, with the Hessian method.



Compare HESSIAN fitting to HERA combined data

To Hessian fitting to HERA combined data PLUS model and param. errors

To HESSIAN fitting to H1 and ZEUS separately

The differences between fitting the combination and fitting the separate data sets are covered by the model and param uncertainties- and would also be covered by a larger $\Delta\chi^2$ tolerance

BUT we are trying our best to get it right and to define clearly where the uncertainties come from

extras

Fortunately, there are smart ways to do this (Pascaud and Zomer LAL-95-05)

Define matrices $M_{jk} = \frac{1}{2} \frac{\partial^2 \chi^2}{\partial p_j \partial p_k}$ $C_{j\lambda} = \frac{1}{2} \frac{\partial^2 \chi^2}{\partial p_j \partial s_\lambda}$

Then M expresses the variation of χ^2 wrt the theoretical parameters, accounting for the statistical errors, and C expresses the variation of χ^2 wrt theoretical parameters and systematic uncertainty parameters.

Then the covariance matrix accounting for statistical errors is $V^p = M^{-1}$ and the covariance matrix accounting for correlated systematic uncertainties is $V^{ps} = M^{-1} C C^T M^{-1}$. The total covariance matrix $V^{tot} = V^p + V^{ps}$ is used for the standard propagation of errors to any distribution F which is a function of the theoretical parameters

$$\langle \sigma_F^2 \rangle = T \sum_j \sum_k \frac{\partial F}{\partial p_j} V_{jk}^{tot} \frac{\partial F}{\partial p_k}$$

Where T is the χ^2 tolerance, $T = 1$ for the OFFSET method.

This is a conservative method which gives predictions as close as possible to the central values of the published data. It does not use the full statistical power of the fit to improve the estimates of s_λ , since it chooses to distrust that systematic uncertainties are Gaussian distributed.

Luckily there are also smart ways to do perform the Hessian method

CTEQ have given an analytic method CTEQ hep-ph/0101032, hep-ph/0201195

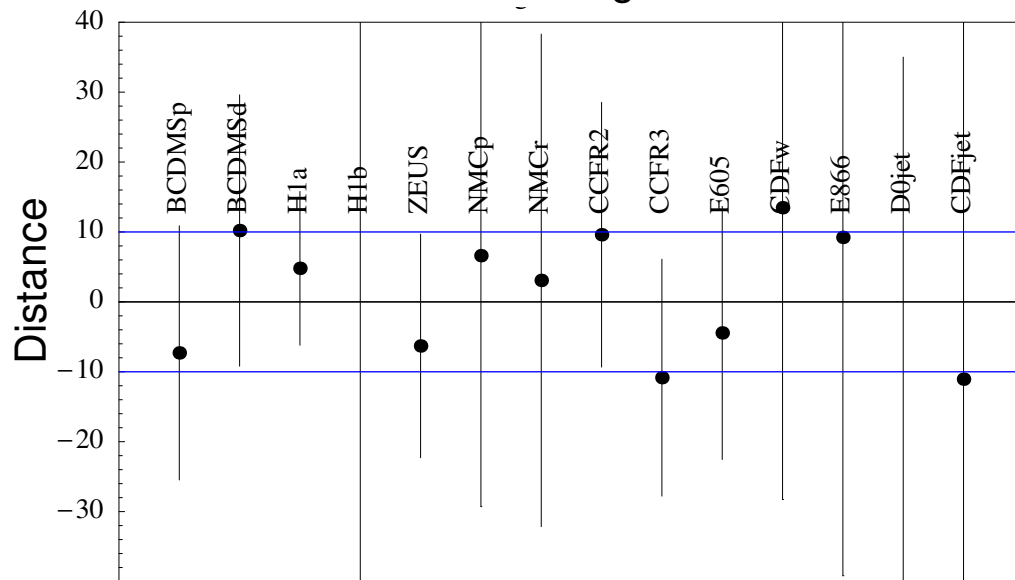
$$\chi^2 = \sum_i \frac{[F_i^{\text{QCD}}(\mathbf{p}) - F_i^{\text{MEAS}}]^2}{(s_i^{\text{STAT}})^2} - \mathbf{B} \mathbf{A}^{-1} \mathbf{B}$$

where

$$\mathbf{B}_\lambda = \sum_i \frac{\Delta_{i\lambda}^{\text{sys}} [F_i^{\text{QCD}}(\mathbf{p}) - F_i^{\text{MEAS}}]}{(s_i^{\text{STAT}})^2}, \quad \mathbf{A}_{\lambda\mu} = \delta_{\lambda\mu} + \sum_i \frac{\Delta_{i\lambda}^{\text{sys}} \Delta_{i\mu}^{\text{sys}}}{(s_i^{\text{STAT}})^2}$$

such that the contributions to χ^2 from statistical and correlated sources can be evaluated separately.

illustration for eigenvector-4



WHY change the χ^2 tolerance?

CTEQ6 look at eigenvector combinations of their parameters rather than the parameters themselves. They determine the 90% C.L. bounds on the distance from the global minimum from $\int P(\chi_e^2, N_e) d\chi_e^2 = 0.9$ for each experiment

This leads them to suggest a modification of the χ^2 tolerance, $\Delta\chi^2 = 1$, with which errors are evaluated such that $\Delta\chi^2 = T^2$, $T = 10$.

Why? Pragmatism. The size of the tolerance T is set by considering the distances from the χ^2 minima of individual data sets from the global minimum for all the eigenvector combinations of the parameters of the fit.

All of the world's data sets must be considered acceptable and compatible at some level, even if strict statistical criteria are not met, since the conditions for the application of strict statistical criteria, namely Gaussian error distributions are also not met.

One does not wish to lose constraints on the PDFs by dropping data sets, but the level of inconsistency between data sets must be reflected in the uncertainties on the PDFs.