

# HESSIAN vs OFFSET method

PDF4LHC February 2008

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Comparisons on using the SAME NLOQCD fit analysis

- in a global fit
- In a fit to just ZEUS data

Model dependence in Hessian and Offset fits- comparing ZEUS and H1

Systematic differences combining ZEUS and H1 data

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

## Treatment of correlated systematic errors

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

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  $\lambda$

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  $s_\lambda$  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  $\chi^2$  – but use it differently in the OFFSET and HESSIAN methods ...hep-ph/0205153**

## 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  $\chi^2$  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 (Pascaud and Zomer LAL-95-05, Botje hep-ph-0110123)

**Slide 3**

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**A5**

Cooper-Sarkar, 3/15/2004

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  $\chi^2$  wrt the theoretical parameters, accounting for the statistical errors, and C expresses the variation of  $\chi^2$  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  $\chi^2$  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  $s_\lambda$ , since it chooses to distrust that systematic uncertainties are Gaussian distributed.

## There are other ways to treat correlated systematic errors- HESSIAN method (covariance method)

**Allow  $s_\lambda$  parameters to vary for the central fit.** The total covariance matrix is then the inverse of a single Hessian matrix expressing the variation of  $\chi^2$  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  $\Delta\chi^2 = 100$  for 90%CL limits

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

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

Luckily there are also smart ways to do this:

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

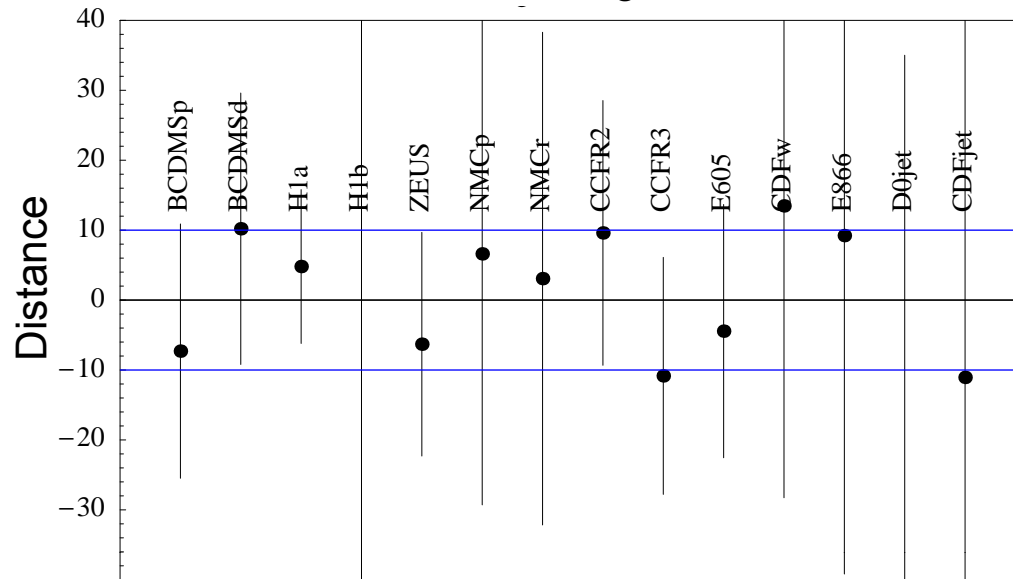
$$\chi^2 = \sum_i \frac{[F_i^{\text{QCD}}(p) - F_i^{\text{MEAS}}]^2}{(s_i^{\text{STAT}})^2} - \mathbf{B} \mathbf{A}^{-1} \mathbf{B}$$

where

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

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

illustration for eigenvector-4



WHY change the 

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  $\chi^2$  tolerance,  $\Delta\chi^2 = 1$ , with which errors are evaluated such that  $\Delta\chi^2 = T^2$ ,  $T = 10$ .

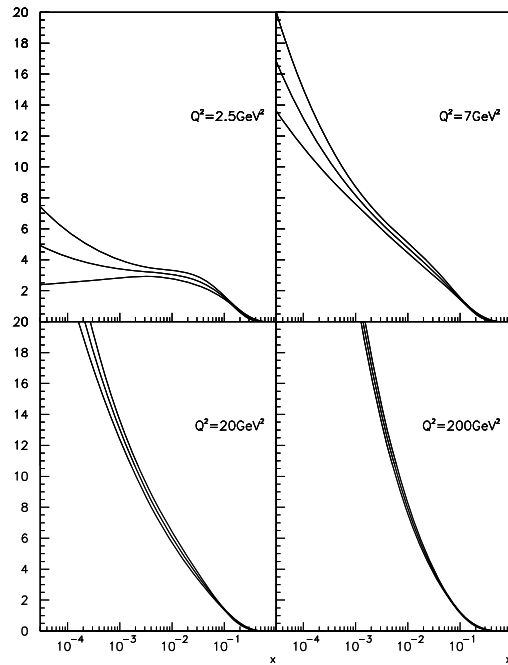
Why? Pragmatism. The size of the tolerance  $T$  is set by considering the distances from the  $\chi^2$  minima of individual data sets from the global minimum for all the eigenvector combinations of the parameters of the fit.

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.

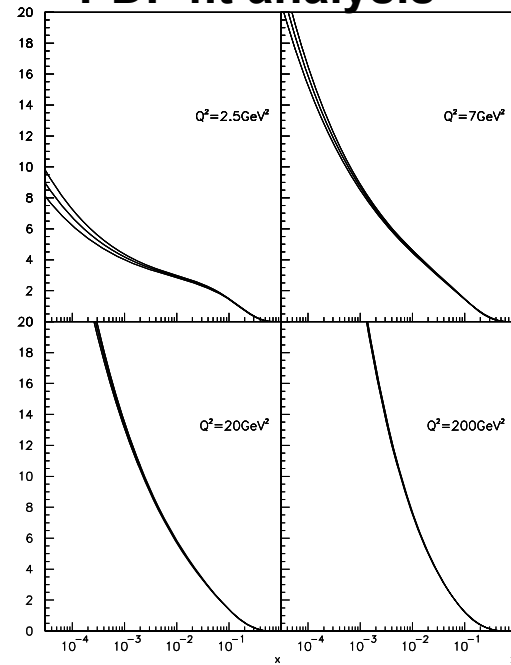
One does not wish to lose constraints on the PDFs by dropping data sets, but the level of inconsistency between data sets must be reflected in the uncertainties on the PDFs.



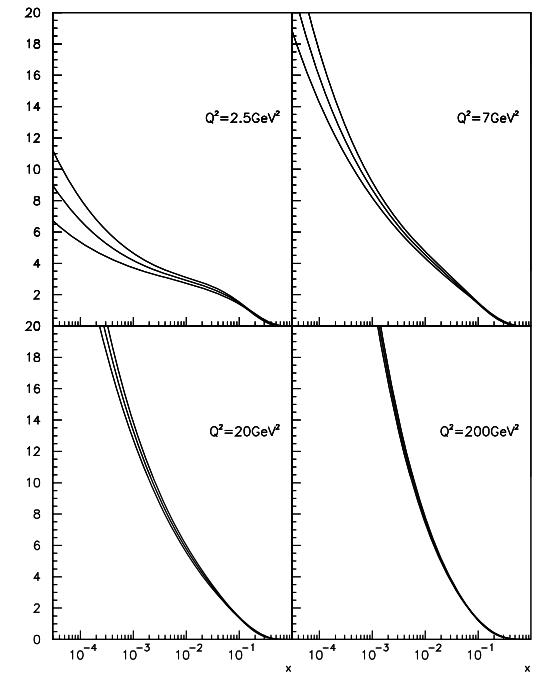
# Compare gluon PDFs for HESSIAN and OFFSET methods for the ZEUS global PDF fit analysis



Offset method



Hessian method  $T^2=1$



Hessian method  $T^2=50$

The Hessian method gives comparable size of error band as the Offset method, when the tolerance is raised to  $T^2 \sim 50$  – (similar ball park to CTEQ,  $T^2=100$ )

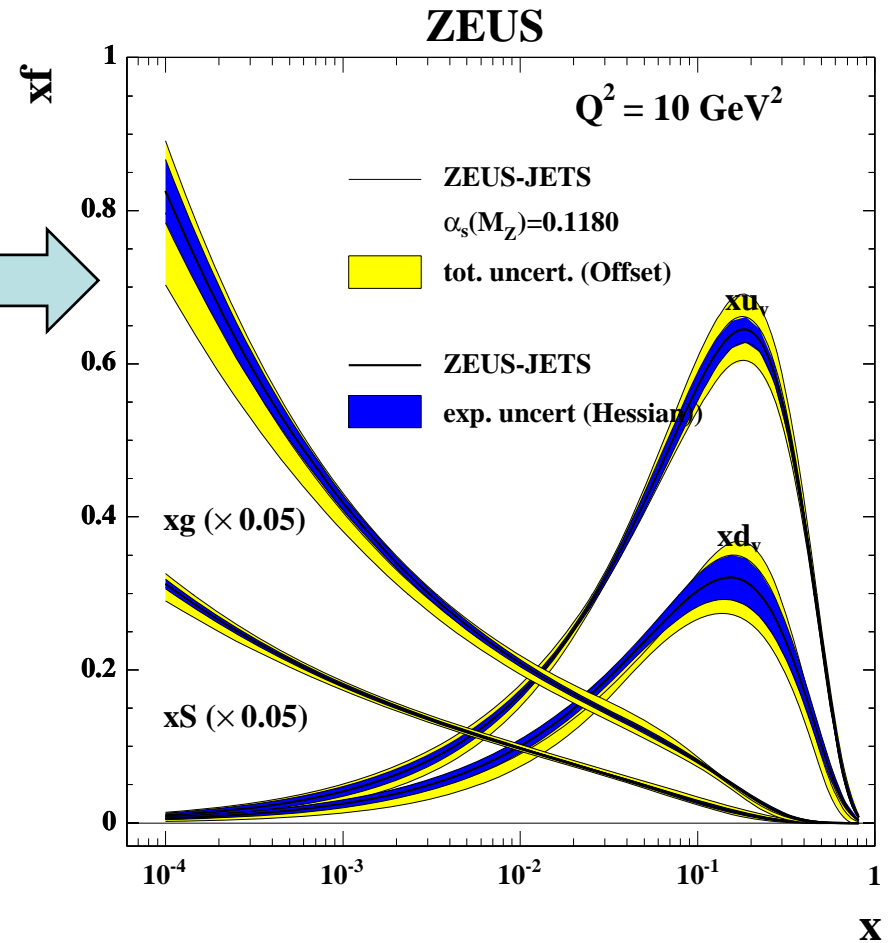
**BUT this was not just an effect of having many different data sets of differing levels of compatibility in this fit**

Comparison of Hessian and Offset methods for ZEUS-JETS FIT 2005 which uses only ZEUS data

For the gluon and sea distributions the Hessian method still gives a much narrower error band. A comparable size of error band to the Offset method, is again achieved when the tolerance is raised to  $T^2 \sim 50$ .

Note this is not a universal number  $T^2 \sim 5$  is more appropriate for the valence distributions.

It depends on the relative size of the systematic and statistical experimental errors which contribute to the distribution



## Model dependence is also important when comparing Hessian and Offset methods

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  $\chi^2$  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  $\chi^2$  change for these different hypotheses often exceeds  $\Delta\chi^2=1$ , while remaining acceptably within the range  $N \pm \sqrt{2N}$ .**

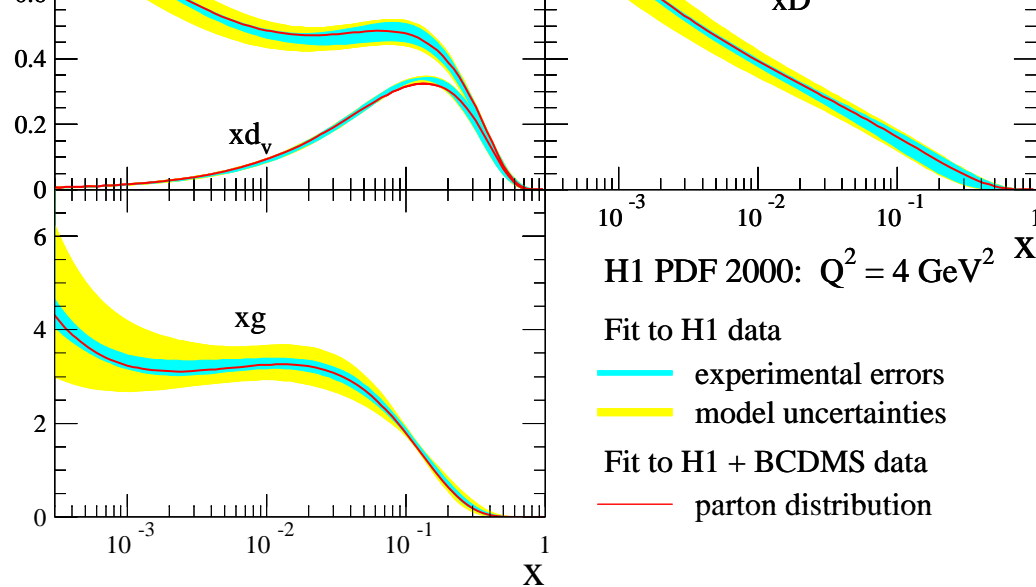
The model uncertainty on the PDFs generally exceeds the experimental uncertainty, if this has been evaluated using  $T=1$ , with the Hessian method.

Compare ZEUS-JETS 2005 and H1 PDF2000

both of which use restricted data sets,

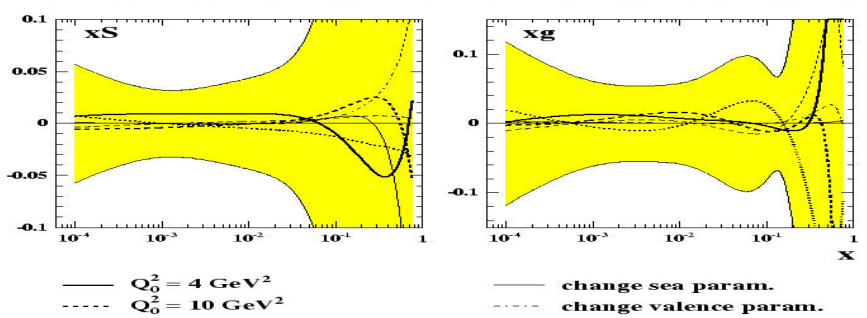
both use  $\Delta\chi^2=1$

but with OFFSET and HESSIAN methods respectively



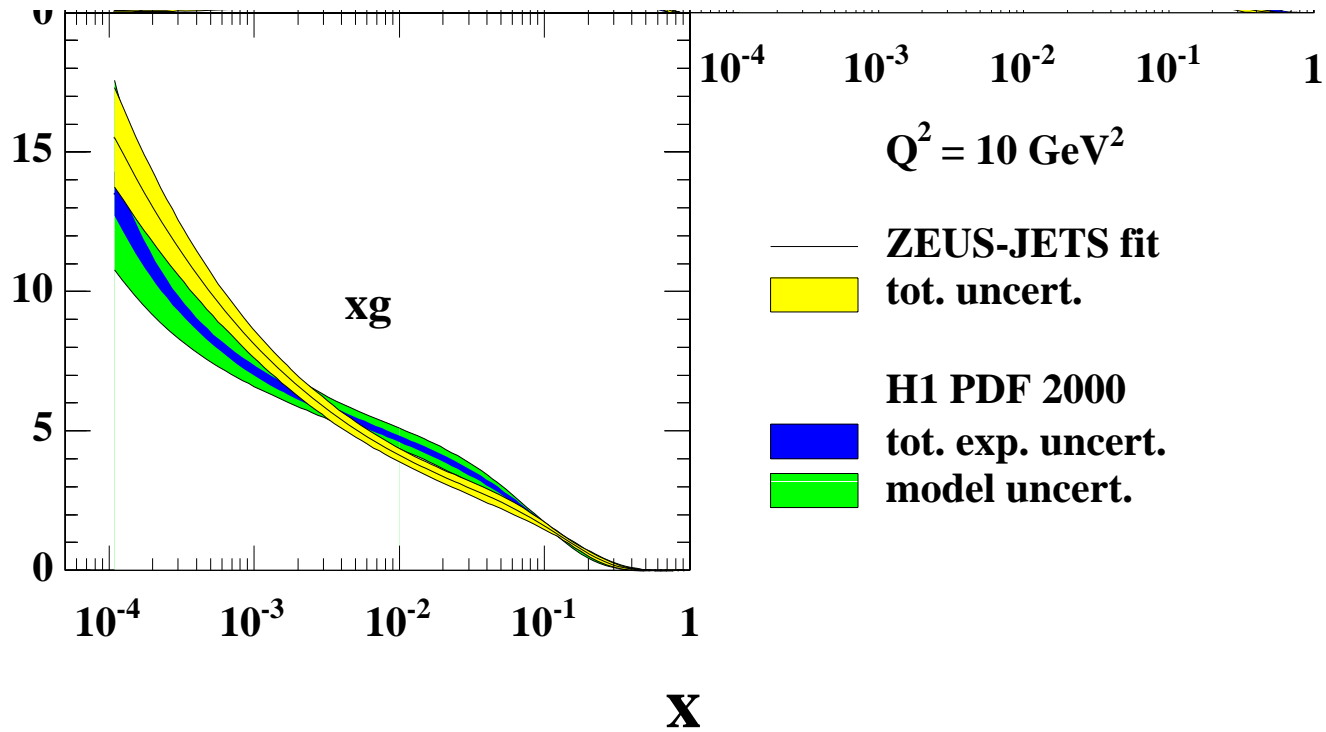
For the H1 analysis model uncertainties are larger than the HESSIAN experimental uncertainties because each change of model assumption can give a different set of systematic uncertainty parameters,  $s\lambda$ , and thus a different estimate of the shifted positions of the data points.

For the H1 fit  $\sqrt{2N} \sim 35$



For the ZEUS analysis model uncertainties are smaller than the OFFSET experimental uncertainties because  $s\lambda$

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ZEUS/H1 published fits comparison including model uncertainties gives similar total uncertainty

## QCD fits to both ZEUS and H1 data

One can make an NLOQCD fit to both data sets using the Hessian method

OR one can combine the data sets using the Hessian method with no theoretical assumption- other than that the data measure the same 'truth'

The systematic shift parameters as determined by these two fits are quite different.

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systematic shift $s_\lambda$	QCDfit ZEUS+H1	'theory free' ZEUS+H1
zd1_e_eff	1.65	-0.41
zd3_e_theta_b	-1.26	-0.29
zd4_e_escale	-1.04	1.05
zd6_had2	-0.85	0.01
zd7_had3	1.05	-0.73
h2_Ee_Spacal	-0.51	0.63
h8_H_Scale_L	-0.26	-0.99
h9_Noise_Hca	1.00	-0.43
h11_GP_BG_LA	-0.36	1.44

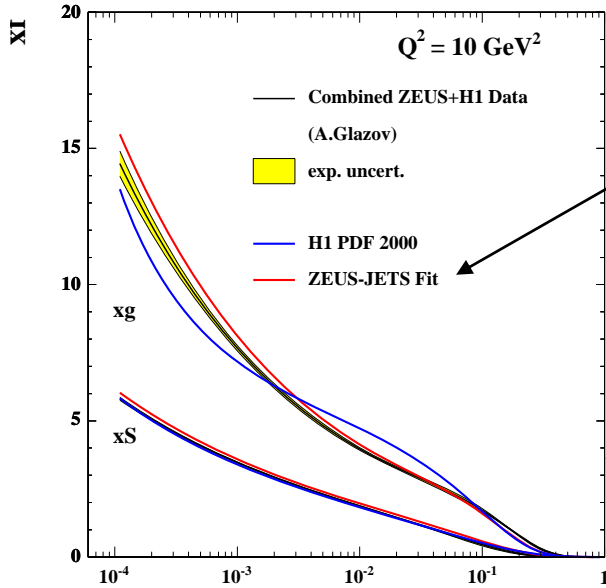
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What then is the optimal setting for these parameters?

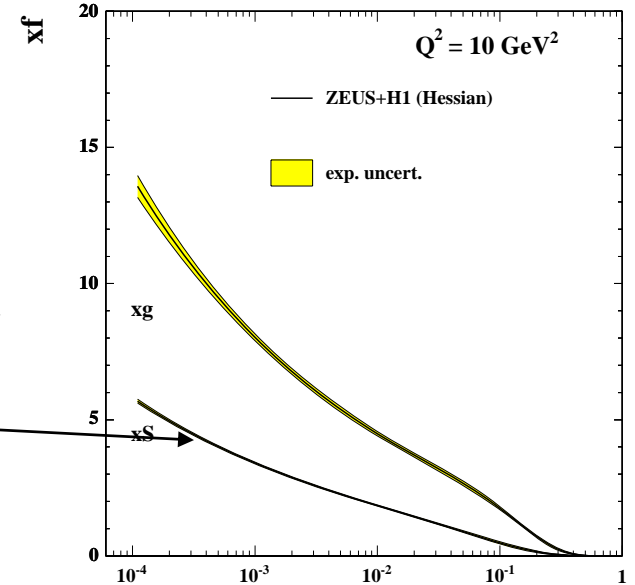
One can also make an NLOQCD fit to the combined data set

The QCDfit to the combined HERA data set gives different central values from the QCDfit to the separate data sets

# QCD PDF fit to the H1 and ZEUS combined data set

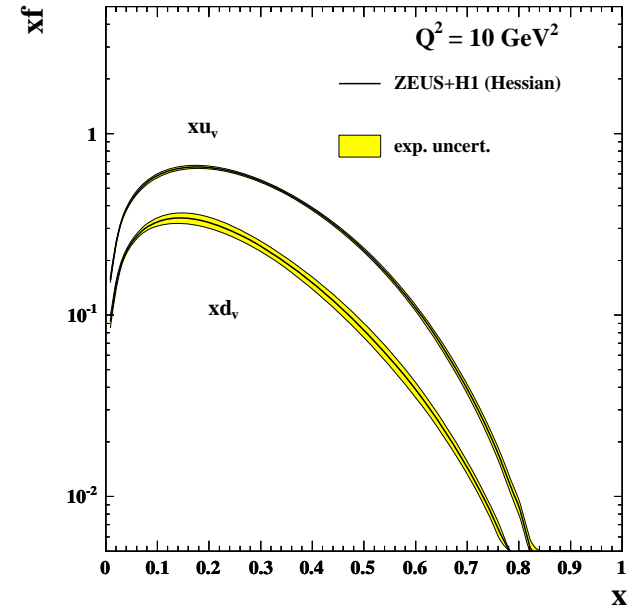
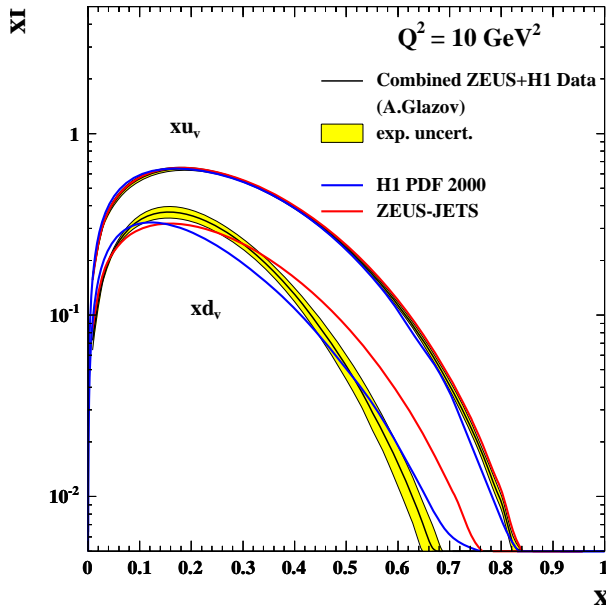


# QCD PDF fit to H1 and ZEUS separate data sets



The central values of the PDFs are rather different particularly for gluon and dv because the systematic shifts determined by these fits are different

NOTE: this is very preliminary and there is no model uncertainty applied



## Summary

OFFSET method is non Bayesian and non-optimal in terms of using the full statistical power of the fit to set the systematic shifts  $s\lambda$

BUT it does produce uncertainty estimates compatible with those of the HESSIAN method with increased tolerance  $T^2 \sim 50-100$

The uncertainty estimates are also generous enough to encompass a large variety of model dependent uncertainties

Systematic shifts set by the Hessian method depend on the theoretical input of the fit- this makes experimentalists feel uncomfortable



