Treatment of Correlated Systematic Uncertainties in the ZEUS QCD Fit

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Correlated Systematic Uncertainties

- "Conventional method" of calculating the χ^2

$$\chi^2 = \Sigma_i \frac{[F_i^{QCD}(p) - F_i^{MEAS}]^2}{(\sigma_i^{STAT})^2+(\Delta_i^{SYS})^2}$$

→ Errors on fit parameters, p, evaluated from $\Delta\chi 2 = 1$

- THIS IS NOT GOOD ENOUGH if experimental systematic uncertainties are correlated between data points
  → e.g. **Calorimeter energy scale/angular resolutions** can move events between x,Q^2 bins, thus changing the shape of exp. distributions

To take into account correlations between data points use:

$$\chi^2 = \Sigma_i \; \Sigma_j \; [\, F_i^{QCD}(p) - F_i^{MEAS}] \, V_{ij}^{-1} \, [\, F_j^{QCD}(p) - F_j^{MEAS}]$$

where the correlation matrix is: $V_{ij} = \delta_{ij}(\sigma_i^{STAT})^2 + \Sigma_\lambda \Delta_{i\lambda}^{SYS} \Delta_{j\lambda}^{SYS}$

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

Correlated Systematic Uncertainties

The general expression for the χ^2 can be shown to be equivalent to:

$$\chi^2 = \Sigma i \; \frac{[\, F_i^{QCD}(p) - \Sigma_\lambda \, s_\lambda \, \Delta_{i\lambda}^{SYS} - F_i^{MEAS}]^2}{(\sigma_i^{STAT})^2 + (\sigma_i^{UNC})^2} + \Sigma s_\lambda^{\,2}$$

→ where the s_λ are systematic uncertainty fit parameters (for each source of correlated uncertainty λ) of zero mean + unit variance

This has modified fit prediction by each source of systematic uncertainty

Two main approaches:

1. OFFSET METHOD :- used by Botje, ZEUS
2. HESSIAN METHOD :- used by H1, CTEQ

The Offset Method

1. Perform fit without correlated errors (s_λ = 0) for central fit
2. Shift measurement to upper limit of one of its systematic uncertainties (s_λ = +1)
3. Redo fit, record differences of parameters from those of step 1
4. Go back to 2, shift measurement to lower limit (s_λ = -1)
5. Go back to 2, repeat 2-4 for next source of systematic uncertainty
6. Add all deviations from central fit in quadrature (positive and negative deviations added separately)

This method does not assume that correlated systematic uncertainties are Gaussian distributed

Offset Method (as used in ZEUS fit)

Fortunately there are clever ways to perform an Offset (style) Method without having to perform the whole fit again for every ±1 variation in s_λ
→ Pascaud and Zomer LAL-95-05, Botje hep-ph-0110123

Define matrices:

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

→ M is Hessain matrix, evaluated theoretical parameters
→ C is a second Hessian matrix, expressing variation of χ^2 with theoretical and systematic uncertainty parameters

- Covariance matrix accounting for statistical errors is $V^p = M^{-1}$
- Covariance matrix accounting for correlated systematic uncertainties is $V^{ps} = M^{-1} C C^T M^{-1}$
- Total covariance matrix is $V^{tot} = V^p + V^{ps}$

Offset Method (as used in ZEUS fit)

Uncertainties on any distribution, F, which is a function of the theoretical parameters is:

$$\langle \sigma^2_F \rangle = T \; \Sigma_j \, \Sigma_k \frac{\partial F}{\partial p_j} V_{jk} \frac{\partial F}{\partial p_k}$$

where $V = V^p$, V^{ps}, V^{tot} for the calculation of uncorrelated, correlated or total uncertainties respectively and T is the χ^2 tolerance (T = 1 for 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

c.f. HESSIAN Method

- In contrast, the Hessian Method allows s_λ parameters to vary for the central fit
  - → total covariance matrix is inverse of single Hessian matrix expressing variation of χ^2 with both theoretical and syst. uncertainty parameters
  - → theoretical prediction is not simply fitted to central values of published experimental data but allows data points to move collectively according to correlated systematic uncertainties
    - Fit determines optimal settings for correlated systematic shifts so that most consistent fit to all data sets is obtained

      → theory is calibrating the detector(s)

BUT

→ Must be confident of theory to trust it for calibration and must be very confident of model choices made in setting boundary conditions to theory

→ Must check that $|s_\lambda|$ values are not >>1, so that data points are not shifted far outside their one standard deviation errors - Data inconsistencies!

→ Must check that superficial changes of model choice (values of Q^2_0, form of parameterisation…) do not result in large changes of s_λ

Hessian Method 2 (as used by CTEQ)

- In practice, fitting many s_λ parameters can be cumbersome
  $\rightarrow$ CTEQ have given an analytic method

$$\chi^2 = \sum_i \frac{[\, F_i^{QCD}(p) \; - \; F_i^{MEAS}]^2}{(\sigma_i^{STAT})^2 + (\sigma_i^{UNC})^2} - B\, A^{-1} B$$

where

$$B_\lambda = \sum_i \Delta_{i\lambda}^{sys} \frac{[F_i^{\,QCD}(p) - F_i^{\,MEAS}]}{(\sigma_i^{STAT})^2 + (\sigma_i^{UNC})^2} \quad , A_{\lambda\mu} = \delta_{\lambda\mu} + \sum_i \frac{\Delta_{i\lambda}^{sys}\, \Delta_{i\mu}^{sys}}{(\sigma_i^{STAT})^2 + (\sigma_i^{UNC})^2}$$

$\rightarrow$ contributions to χ^2 from statistical and correlated sources can be evaluated separately

- Problem of large systematic shifts to data points becomes manifest at large $BA^{-1}B$ (correlated contribution to the χ^2)
  $\rightarrow$ small overall χ^2 can be obtained by the cancellation of two large numbers.

What can be done about this?

Could restrict data sets to those which are sufficiently consistent that these problems do not arise

$\rightarrow$ But lose information since partons need constraints from many different data sets – no one experiment has sufficient kinematic range / flavour infomation

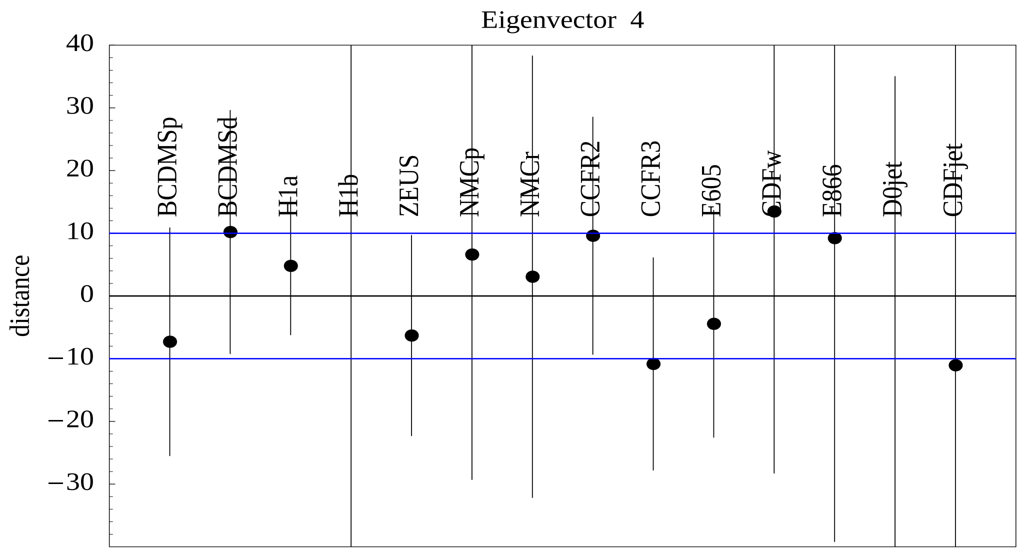
The CTEQ Approach

CTEQ suggest modification of χ^2 tolerance ($\Delta\chi^2 = 1$) with which errors are evaluated such that $\Delta\chi^2 = T^2$, and $T = 10$ (for CTEQ fit)

Why? Pragmatism

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 conditions for application of strict statistical criteria, namely Gaussian error distributions are also not met)

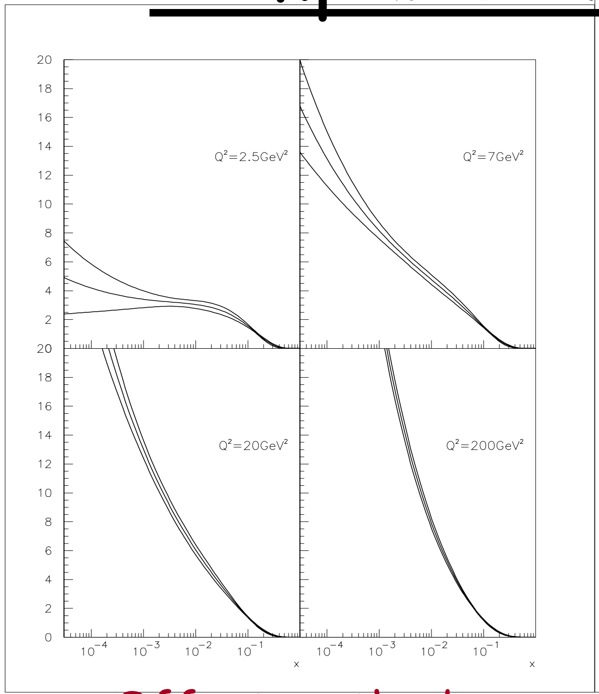
→ Don't want to lose constraints on PDFs by excluding data sets BUT the level of inconsistency between data sets must be reflected in the uncertainties



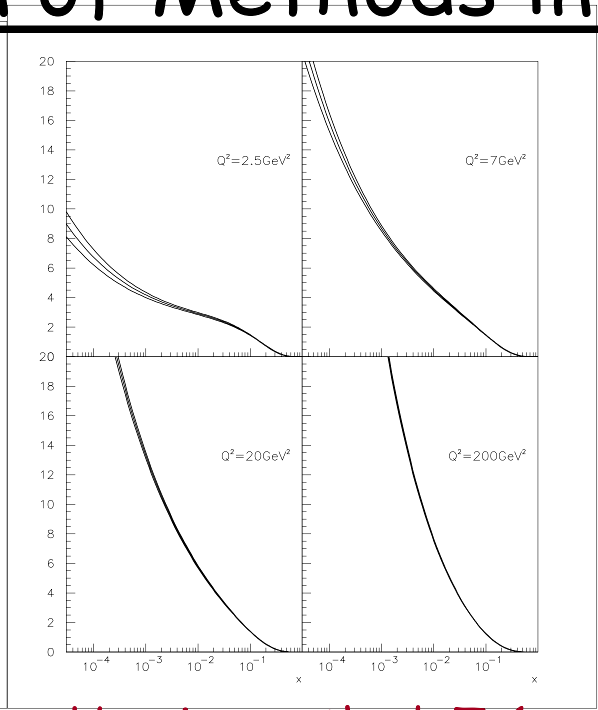
Size of tolerance T set by considering distances from χ^2 minima of individual data sets from global minimum for all parameters of the fit

N.B. MRST have also set larger tolerances (T=5) in recent fits

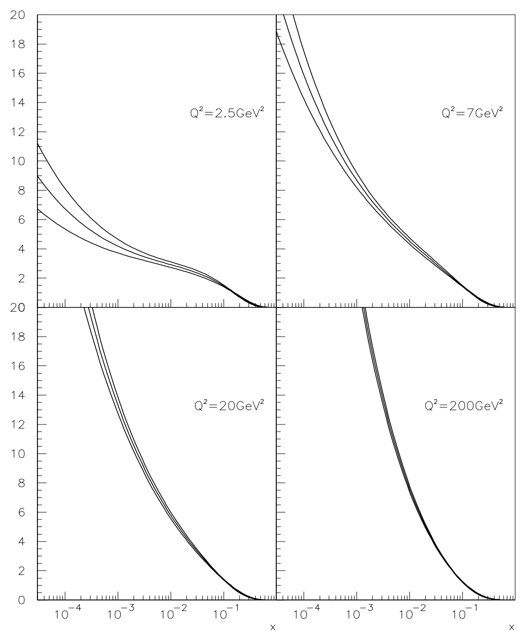
Comparison of Methods in ZEUS Fit



Offset method



Hessian method T=1



Hessian method T=7

Both methods have been tried in the ZEUS fit:

→ Hessian Method gives much smaller uncertainties than Offset if T=1

→ Comparable size error bands if tolerance is raised to T ~ 7

- similar ball park to CTEQ's chosen tolerance, T=10

N.B. This makes error band large enough to encompass reasonable variations of model choice since criterion for acceptability of alternative hypothesis (or model) is that the χ^2 lie within N ± $\sqrt{2N}$, where N is the number of degrees of freedom (for the ZEUS global fit $\sqrt{2N}$=50)

Model Uncertainties

We trust NLO QCD– but are we sure about every choice which goes into setting up the boundary conditions for QCD evolution ?
$\rightarrow$ form of parameterisation, starting scale Q_0^2, flavour structure of sea etc.

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 $Q^2{}_0$, 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 $N \pm\sqrt{2N}$.

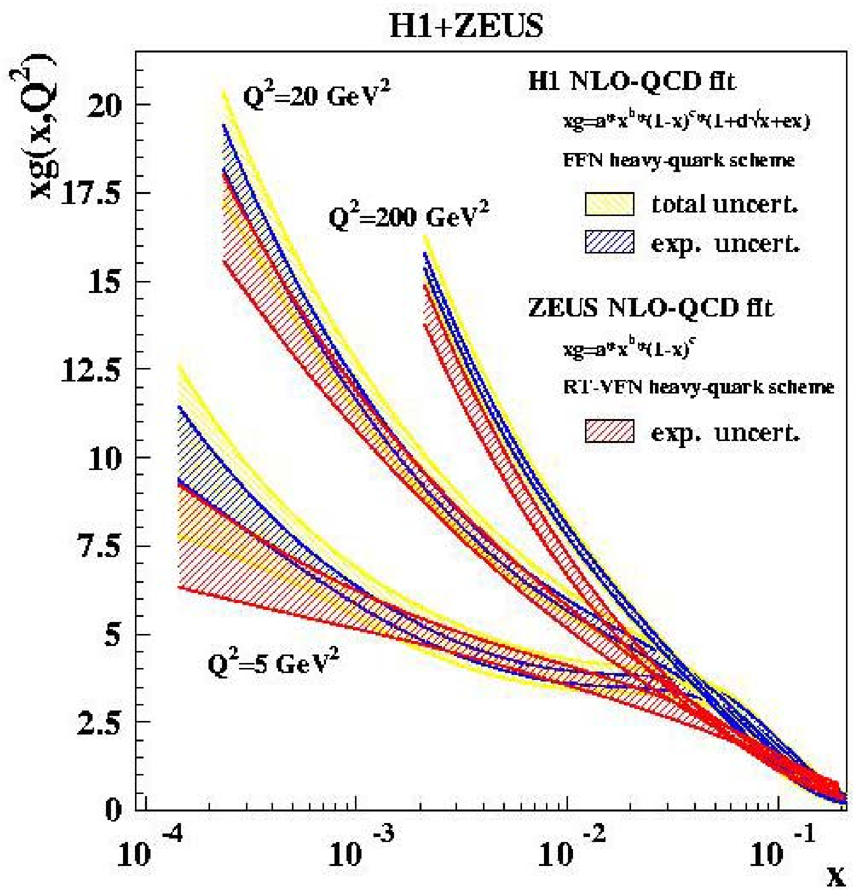
In this case the model error on the PDF parameters usually exceeds the experimental error on the PDF, if this has been evaluated using T=1, with the Hessian method.

Comparison of ZEUS/H1 Model Uncertainties

If the experimental errors have been estimated by the Hessian method with T=1, then the model errors are usually larger. Use of restricted data sets also results in larger model errors. Hence total error (model + experimental) can end up being in the same ball park as the Offset Method, (or the Hessian method with T ~ 7-10).

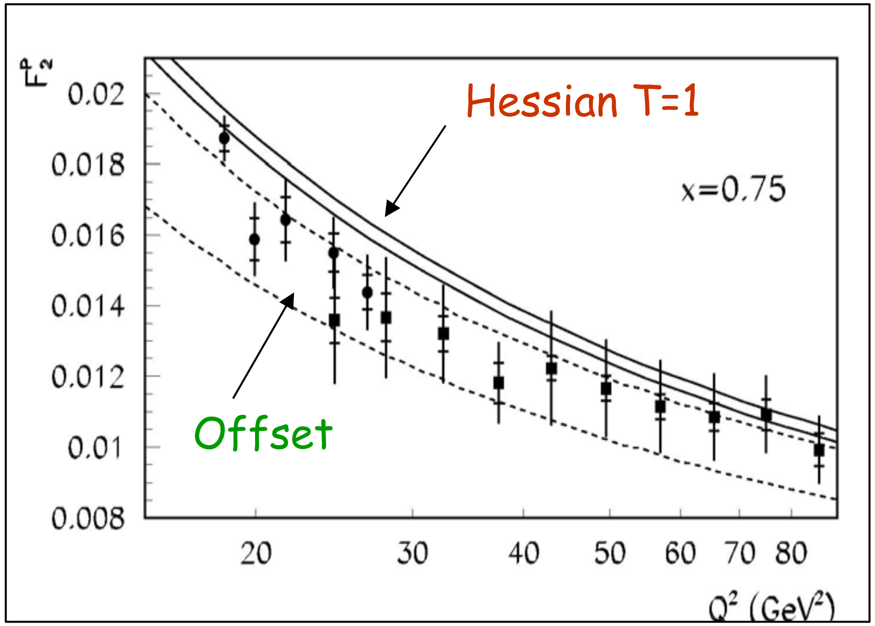
Comparison of ZEUS (Offset) and H1 (Hessian, T=1) gluon distributions

Yellow band (total error) of H1 comparable to red band (total error) of ZEUS



Hessian Versus Offset Methods

Five reasons why ZEUS choose to use Offset Method as opposed to Hessian Method



1. Alekhin's plot hep-ph-0011002

2. Compare the conventional χ^2 evaluated by adding systematic and statistical uncertainties in quadrature

Expt.	Data points	χ^2/d.p. hessian	χ^2/d.p. offset
ZEUS 96/7	242	1.37	0.83
NMC D+p	436	1.33	1.11
BCDMS	305	0.95	0.89

Results from the ZEUS-S fit

Hessian Versus Offset Methods

3. s_λ parameters are estimated as different for same data set when different combinations of data/models are used
   → different calibration of detector according to model

4. Estimates of s_λ made by Hessian method for ZEUS and H1 data pull the data points apart- not electronic

5. Hessian is best used when systematic errors are not large compared to statistical – Zarnecki, not electronic

ZEUS s_λ	CTEQ6 fit	ZEUS-fit
1	1.67	-0.36
2	-0.67	1.17
3	-1.25	1.20
4	-0.44	0.40
5	0.00	0.32
6	-1.07	0.39
7	1.28	-1.40
8	0.62	0.20
9	-0.40	0.04
10	0.21	-0.06

Extras …

What is Available?

http://www-pnp.physics.ox.ac.uk/~cooper/zeus2002.html
or from Durham HEPDATA : http://durpdg.dur.ac.uk/hepdata

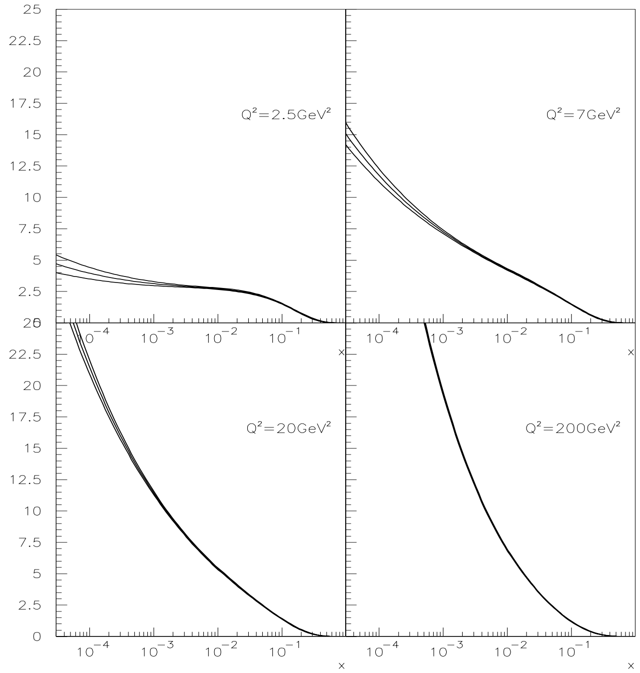
1. PDF grids: u_v, d_v, Sea, Gluon, plus Sea flavour break up into u, d, s, c, b and also (new) d/u
2. Structure function grids: F_2(e-), F_L(em) F_2^{charm}, F_2(NC), F_L(NC) and xF_3(NC)
3. Reduced cross section grids: σ(NCe+), σ(NCe-), σ(CCe+), σ(NCe-)
4. Programme gluon_grid.f to show how to use these grids

5. Central PDF set for ZMVFN/ FFN/ RTVFN heavy flavour schemes -plus corresponding eigenvector PDF sets so that you could make all these calculations (and more) yourself straight from the PDF parameters WITH ERRORS.
6. These eigenvector sets are available separately for
   a. statistical plus uncorrelated systematic errors,
   b. correlated systematic errors
   c. and total errors.
7. Programmes gluon.f, qcd_results.f to show you how use eigenvector PDF sets

8. Central PDF set plus covariance matrices if you want to do it the hard way. These are also available for ZMVFN/ FFN/ RTVFN and uncorrelated plus correlated errors as well as total errors

HERA data: NC 96/7 CC94-97 NC 98/9 CC 98/9

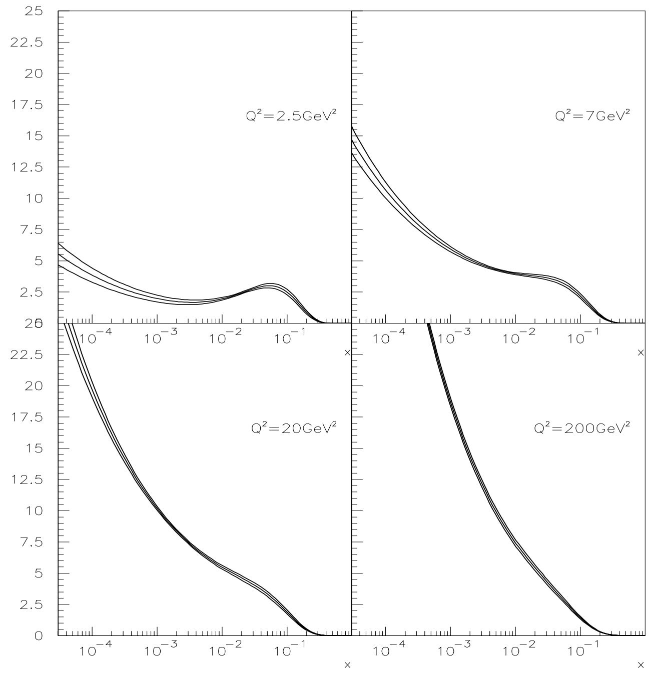
statistical errors only (ZMVFN scheme)



ZEUS only gluon:

p3 = 5.8 ±4.2   p5 = -0.56 ± 15.

(p2 valence = 0.61 ± 0.14)



H1 only gluon:

p3 = 14.5 ± 0.6   p5 = 48.2 ± 3.6

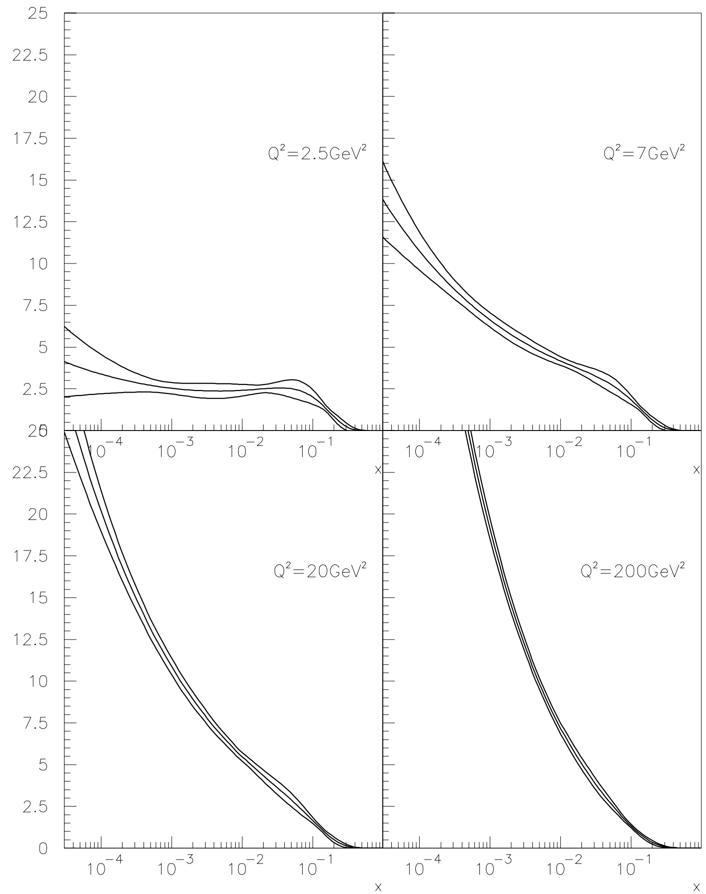
(p2 valence = 0.89 ± 0.03)

The gluons really are very different even when exactly the same analysis is performed

Combine ZEUS and H1

Allow free relative normalisations
→ ZEUS 96/7 norm 0.986
→ H1 96/7norm 1.013

With Offset errors we achieve a reasonable compromise – but because of data differences/ incompatibility(?) the combination does not have much smaller errors than ZEUS alone



With statistical plus Offset Method correlated errors

Eigenvector PDF sets- a better way to store the results of the fits
see http://www-pnp.physics.ox.ac.uk/~cooper/zeus2002.html

- **The errors on the PDF parameters are given by the error matrices V_{ij}** and are propagated to quantities of interest like parton distributions, structure functions and reduced cross-sections via
- $\Delta F^2=\sum_{ij} \partial F/\partial p_i V_{ij} \partial F/\partial p_j$
- This would clearly be easier if V were diagonalised

- **Diagonalising the error matrix of the fit has various further benefits**
- **It tells you if you have a stable fit- are the eigenvalues all positive?**
- **It tells you if you NEED all the parameters you are using**
- **It tells you which parameters are constrained best**

- The results of the fit are then summarised in one central PDF set and 2 * N_{pdf} parameter sets for the errors, where N_{pdf} is the number of PDF parameters

These parameter sets are obtained by moving up(+) or down(-) along the i=1,Npdf eigenvector directions by the corresponding error. These moves are propagated back to the original PDF parameters to create new PDF sets- **(Si+) (Si-).** The error on a derived quantity is then obtained from

$$\Delta F^2= \tfrac{1}{2}\sum_I (F(Si+) - F(Si-))$$

The ZEUS fits are well-behaved. It has been the experience of CTEQ and MRST- that along some eigenvector directions the χ2 increases very slowly- leading to asymmetries and the breakdown of the quadratic approximation for **χ2**. ZEUS has avoided this by not assuming that we can determine more parameters than we actually can!

The form of our parametrisation is

xq(x) = p1 x p2 (1-x) p3 (1+p5x)

Examining the eigenvectors and eigenvalues of the total error matrix of the ZEUS-Only (12 param.) and the ZEUS-S (13 param.) fits shows that

The best determined parameters are p2 for the sea and the gluon –i.e the low –x behaviour of the Sea and Glue as determined by the ZEUS data – and the next best determined is p1 for the sea. These parameters dominate the first 3 eigenvectors. A combination of parameters which is 90% p2 Sea and 4% p2 Glue and 4% p1 Sea, with negligible amounts of the other PDF parameters, is BETTER determined than either of these parameters separately. The eigenvalues for the ZEUS-S and ZEUS-O fits are fairly similar

p2 for the valence parameters is also moderately well determined, through the number sum rules, for both fits

The next best determined parameters are p3 for the u and d-valence –i.e. the high-x valence parameters, but the eigenvalues are larger for the ZEUS-O than for the ZEUS-S fit, reflecting the fact that the fixed target data is still making a more precise measurement. However the 5th and 6th eigenvectors are more purely dominated by these parameters for the ZEUS-O fit so that statistical improvement should be significant

The remainder of the parameters p3, p5 for the glue and sea, and p5 for the valence are very much mixed into the eigenvectors. They are clearly much better detrmined in the ZEUS-S fit with fixed target data