Fine Art of global fitting and Error Estimates

Jon Pumplin – 29 Sept 2003

Ringberg Workshop: New Trends in HERA Physics

High energy hadrons interact through their quark and gluon constituents. The interactions become weak at short distances due to the asymptotic freedom property of Quantum Chromodynamics, allowing perturbation theory to be applied to a rich variety of experiments.

The nonperturbative nature of the proton for single interactions is characterized by Parton Distribution Functions $f(Q,x)$ of momentum scale Q and light-cone momentum fraction x for each flavor. Evolution in Q is determined perturbatively by QCD renormalization group equations, so $f(Q,x)$ can be defined by functions $f(Q_0,x)$ of x at a fixed small Q_0. Those functions are measured by fitting a wide range of data.

Known and unknown systematic errors pose a challenge to global fitting.

Outline of talk

- Introduction to PDFs
- Handling correlated experimental errors
- Estimating uncertainties
- Eigenvector PDF sets
- Lagrange multipliers
- Reweighting experiments
- Bootstrap methods
- Application: Jet predictions
- Application: Strangeness asymmetry and NuTeV anomaly

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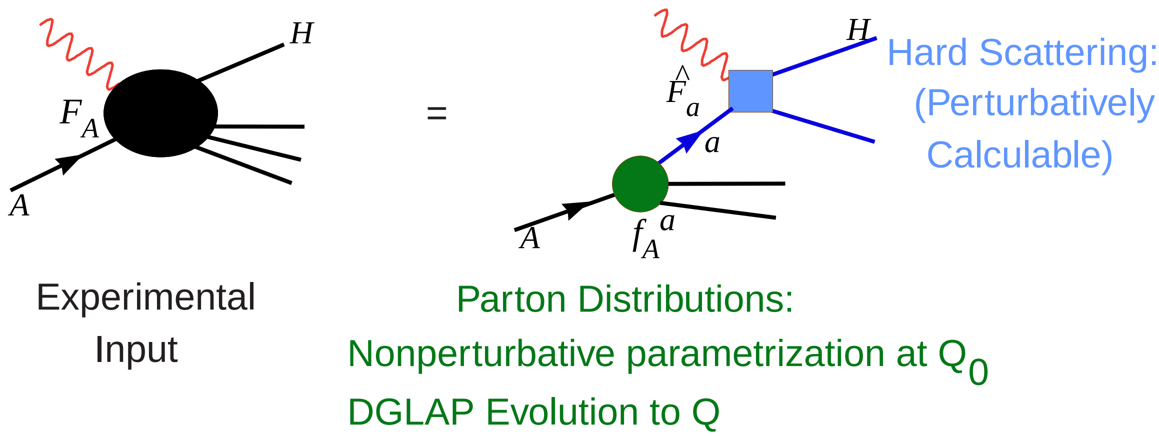
Global QCD analysis

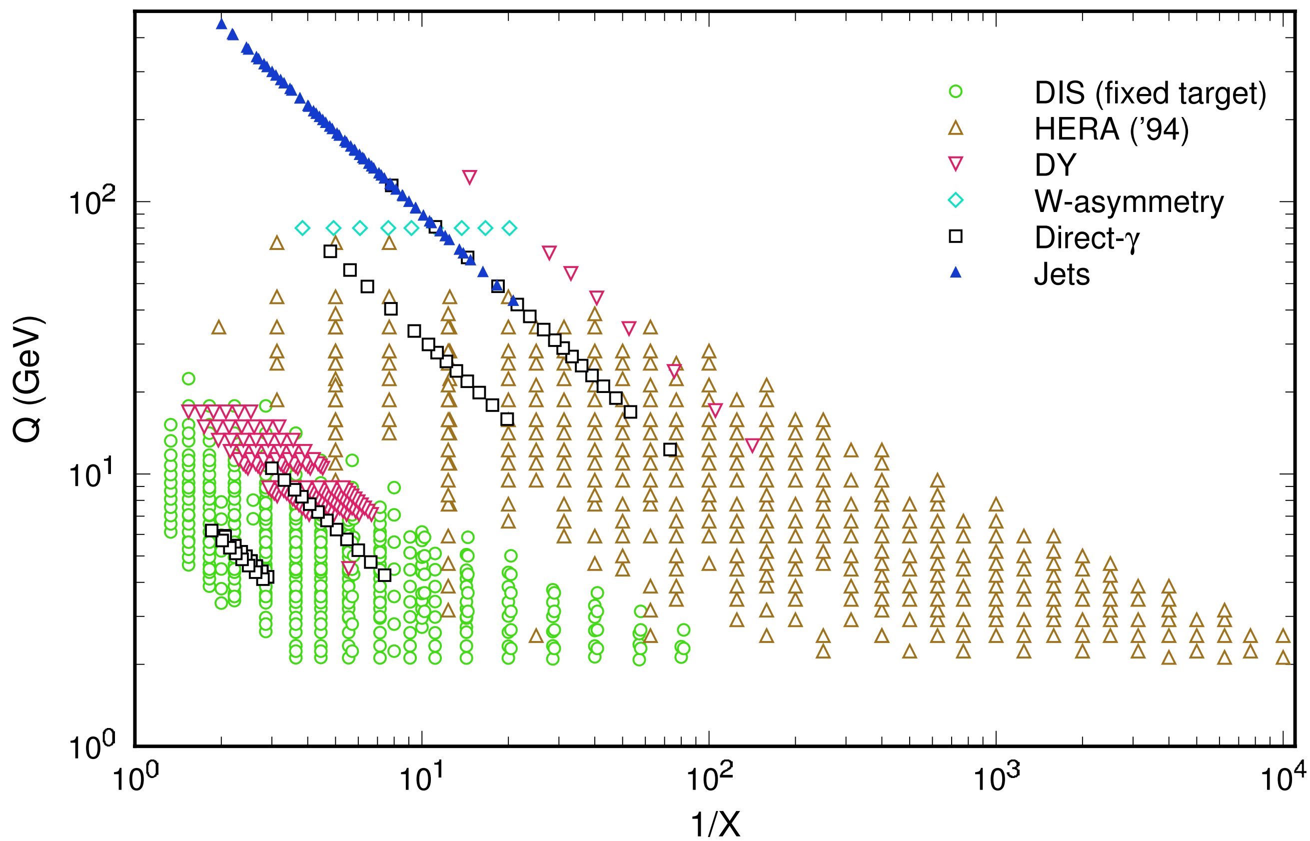
- Extract universal non-perturbative features of proton or nucleus from large variety of experiments
  - Factorization
    (Short distance and long distance separable)
  - Asymptotic Freedom
    (Hard scattering perturbatively calculable)
  - Renormalization Group Evolution in scale Q
    (PDFs characterized by functions of x at Q_0)
- Test consistency of QCD – overall and with individual experiments
- Make results available – needed by all experiments with hadron beams or targets: HERA, RHIC, Tevatron, LHC, non-accelerator
- Explore the range of uncertainties

Factorization Theorem

$$F_A^\lambda(x, \frac{m}{Q}, \frac{M}{Q}) = \sum_a f_A^a(x, \frac{m}{\mu}) \otimes \hat{F}_a^\lambda(x, \frac{Q}{\mu}, \frac{M}{Q}) + \mathcal{O}((\frac{\Lambda}{Q})^2)$$



Kinematic region covered by data



Data with a wide range of scales are tied together by the DGLAP renormalization group evolution equation.

Consistency or inconsistency between the different processes can be observed only by applying QCD to tie them together in a global fit.

HERA II, Tevatron run II (W, Z production), and LHC will dramatically extend the range and accuracy.

CTEQ6 Global analysis

Input from Experiment:

- ~ 2000 data points with $Q > 2\,\text{GeV}$ from e, μ, ν DIS; lepton pair production (DY); lepton asymmetry in W production; high p_T inclusive jets; $\alpha_s(M_Z)$ from LEP

Input from Theory:

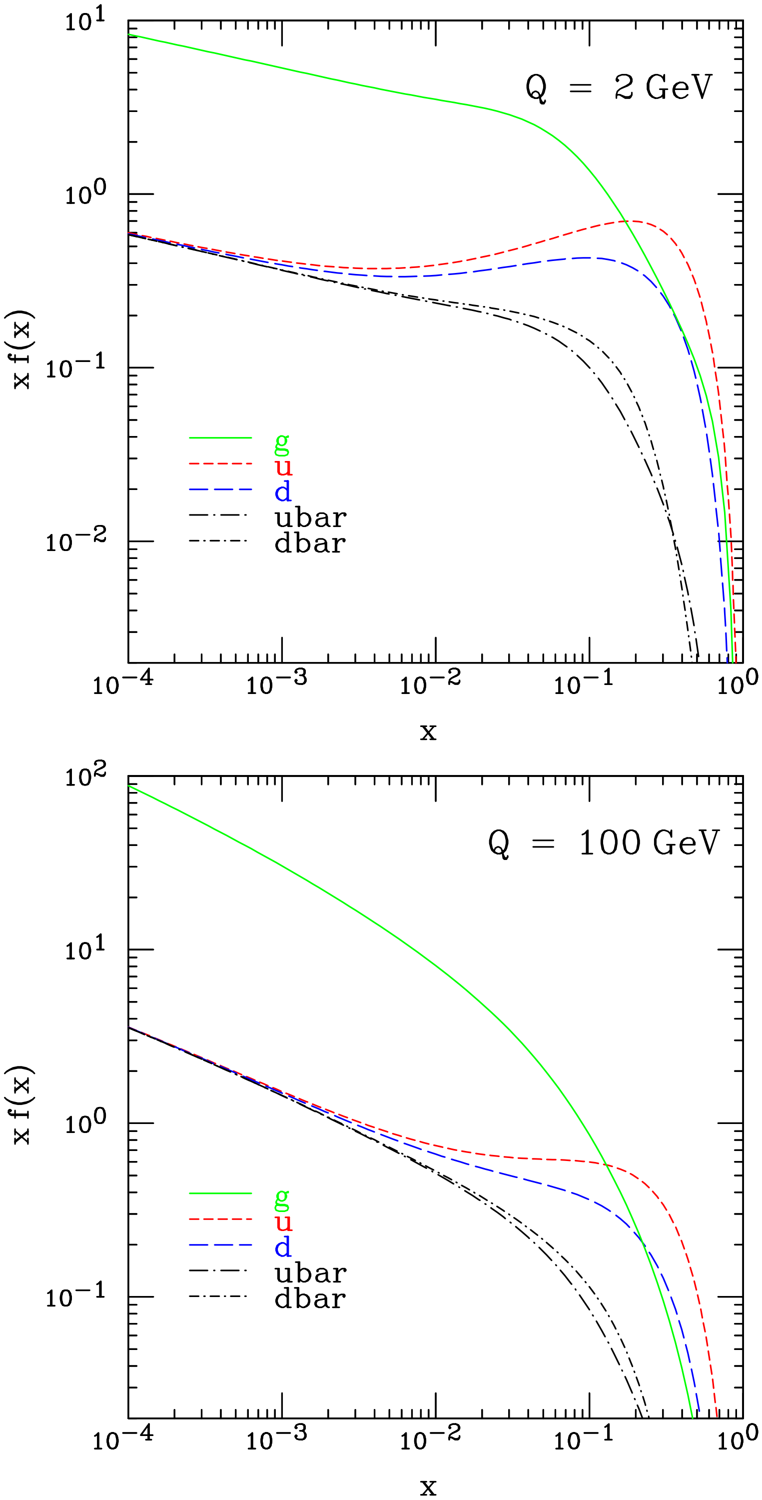
- NLO QCD evolution and hard scattering
- Parametrize at Q_0:
  $A_0\, x^{A_1}\,(1-x)^{A_2}\, e^{A_3 x}(1+A_4 x)^{A_5}$
- $s = \bar{s} = 0.4\,(\bar{u}+\bar{d})/2$ at Q_0; no intrinsic b or c

Construct effective $\chi^2_{\text{global}} = \sum_{\text{expts}} \chi^2_n$:

- χ^2_{global} includes the known systematic errors
- Minimizing χ^2_{global} yields "Best Fit" PDFs.
- Variation of χ^2_{global} in neighborhood of the minimum defines uncertainty limits.
- Estimate uncertainty as region of parameter space where $\chi^2 < \chi^2(\text{BestFit}) + T^2$ with $T \approx 10$.

(Quite different from Gaussian statistics because of unknown correlated systematic errors in theory and experiments – as measured by inconsistency between experiments).

Parton distributions at $Q = 2$ and 100 GeV



- Valence quarks dominate for $x \to 1$
- Gluon dominates for $x \to 0$, especially at large Q

χ^2 and Systematic Errors

The simplest definition

$$\chi_0^2 = \sum_{i=1}^{N} \frac{(D_i - T_i)^2}{\sigma_i^2} \qquad \left\{ \begin{array}{ll} D_i = & \text{data} \\ T_i = & \text{theory} \\ \sigma_i = & \text{“expt. error”} \end{array} \right.$$

is optimal for random Gaussian errors,

$$D_i = T_i + \sigma_i r_i \qquad \text{with} \qquad P(r) = \frac{e^{-r^2/2}}{\sqrt{2\pi}}.$$

With systematic errors,

$$D_i = T_i(a) + \alpha_i r_{\text{stat},i} + \sum_{k=1}^{K} r_k \beta_{ki} \,.$$

The fitting parameters are $\{a_\lambda\}$ (theoretical model) and $\{r_k\}$ (corrections for systematic errors).

Published experimental errors:

- α_i is the ‘standard deviation’ of the random uncorrelated error.

- β_{ki} is the ‘standard deviation’ of the k th (completely correlated!) systematic error on D_i.

To take into account the systematic errors, we define

$$\chi'^2(a_\lambda, r_k) = \sum_{i=1}^{N} \frac{\left(D_i - \sum_k r_k \beta_{ki} - T_i\right)^2}{\alpha_i^2} + \sum_k r_k^2,$$

and minimize with respect to $\{r_k\}$. The result is

$$\widehat{r}_k = \sum_{k'} \left(A^{-1}\right)_{kk'} B_{k'}, \qquad \text{(systematic shift)}$$

where

$$\begin{aligned} A_{kk'} &= \delta_{kk'} + \sum_{i=1}^{N} \frac{\beta_{ki}\beta_{k'i}}{\alpha_i^2} \\ B_k &= \sum_{i=1}^{N} \frac{\beta_{ki}\left(D_i - T_i\right)}{\alpha_i^2}. \end{aligned}$$

The $\widehat{r}_k$'s depend on the PDF model parameters $\{a_\lambda\}$. We can solve for them explicitly since the dependence is quadratic.

We then minimize the remaining $\chi^2(a)$ with respect to the model parameters $\{a_\lambda\}$.

- $\{a_\lambda\}$ determine $f_i(x, Q_0^2)$.

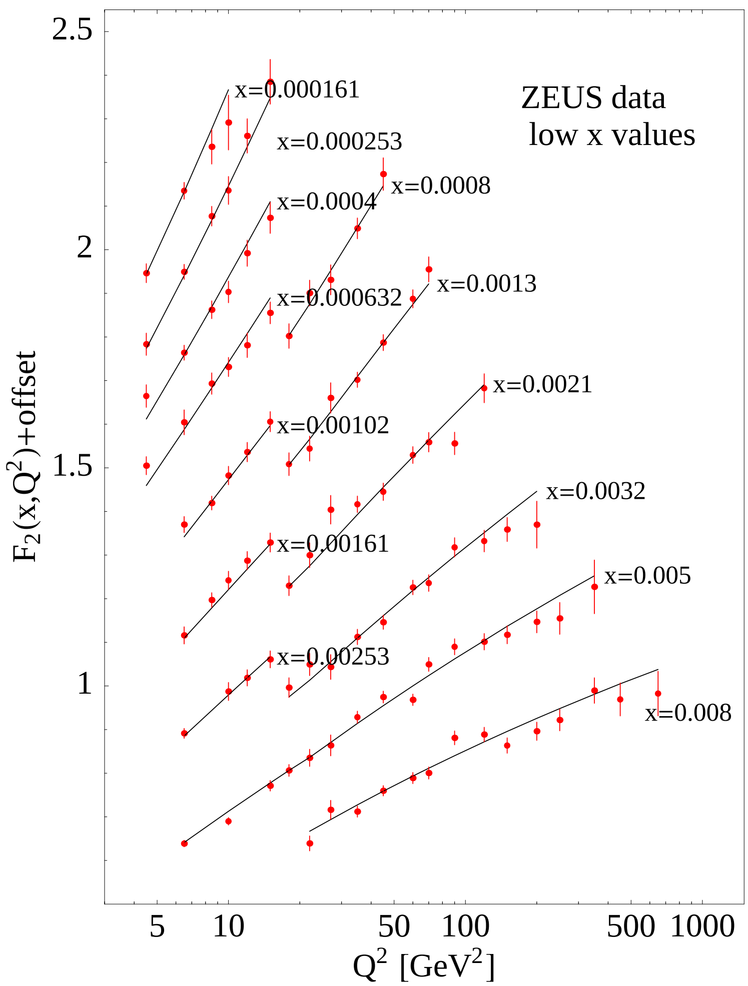
- $\{\widehat{r}_k\}$ are are the optimal "corrections" for systematic errors; i.e., systematic shifts to be applied to the data points to bring the data from different experiments into compatibility, within the framework of the theoretical model.

Comparison of CTEQ6M fit to data sets with correlated systematic errors

data set	N_e	χ_e^2	χ_e^2/N_e
BCDMS p	339	377.6	1.114
BCDMS d	251	279.7	1.114
H1a	104	98.59	0.948
H1b	126	129.1	1.024
ZEUS	229	262.6	1.147
NMC F2p	201	304.9	1.517
NMC F2d/p	123	111.8	0.909
DØ jet	90	69.0	0.766
CDF jet	33	48.57	1.472

Observe that $\chi^2/\mathrm{N}_{\mathrm{pt}}$ is close to 1.0 — but not as close as would be expected if we lived in the idealzed world of statistics.

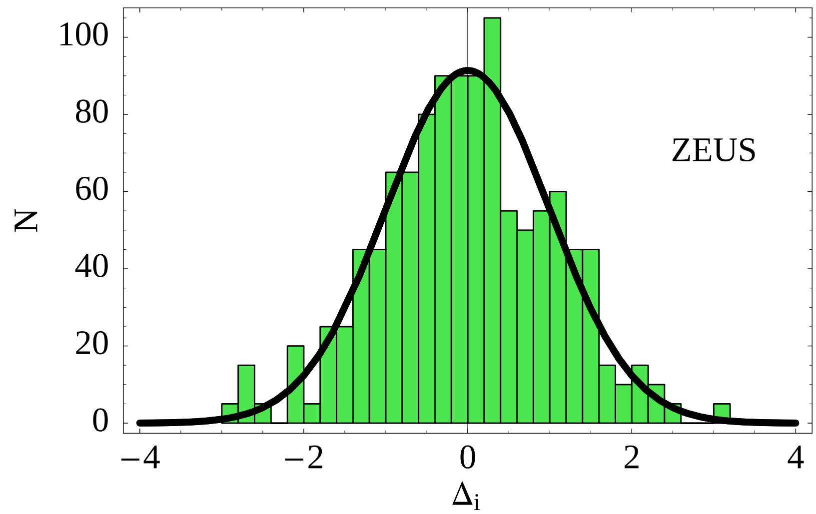
CTEQ6M fit to ZEUS data at low x



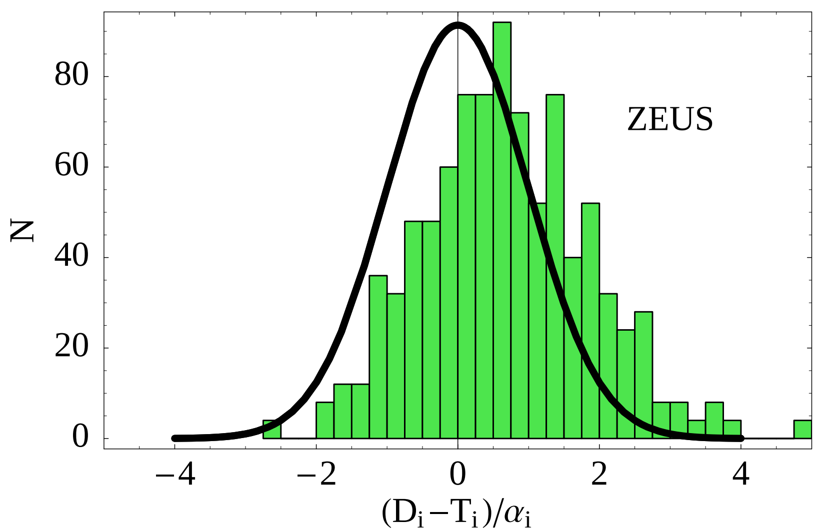
The data points include the estimated corrections for systematic errors. That is to say, the central values plotted have been shifted by an amount that is consistent with the estimated systematic errors, where the systematic error parameters are determined using other experiments via the global fit.

The error bars are statistical errors only.

Systematic Error treatment works

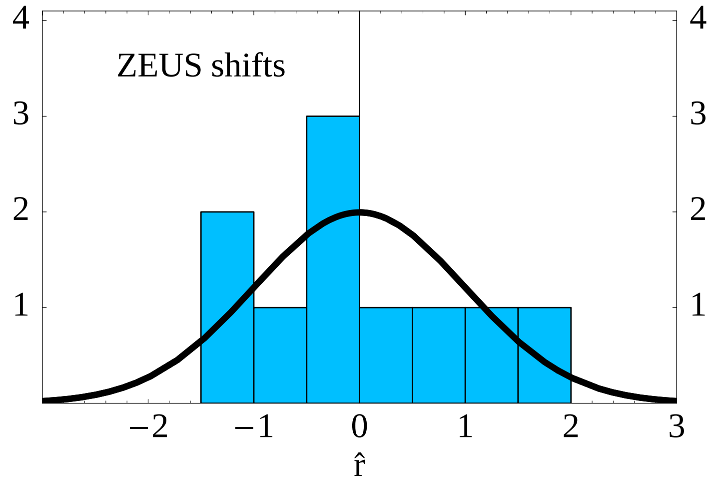


(a) Histogram of residuals for the ZEUS data. The curve is a Gaussian of width 1.

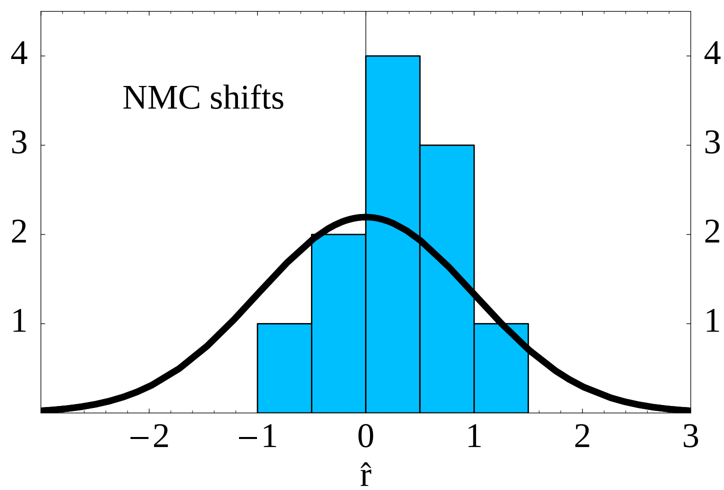


(b) Similar comparison without corrections for systematic errors on the data points.

Systematic shifts for the ZEUS data
(10 systematic errors)



Systematic shifts for the NMC data
(11 systematic errors)



Sources of uncertainty:

1. Experimental errors included in χ^2
2. Unknown experimental errors
3. Parametrization dependence
4. Higher-order corrections & Large Logarithms
5. Power Law corrections ("higher twist")

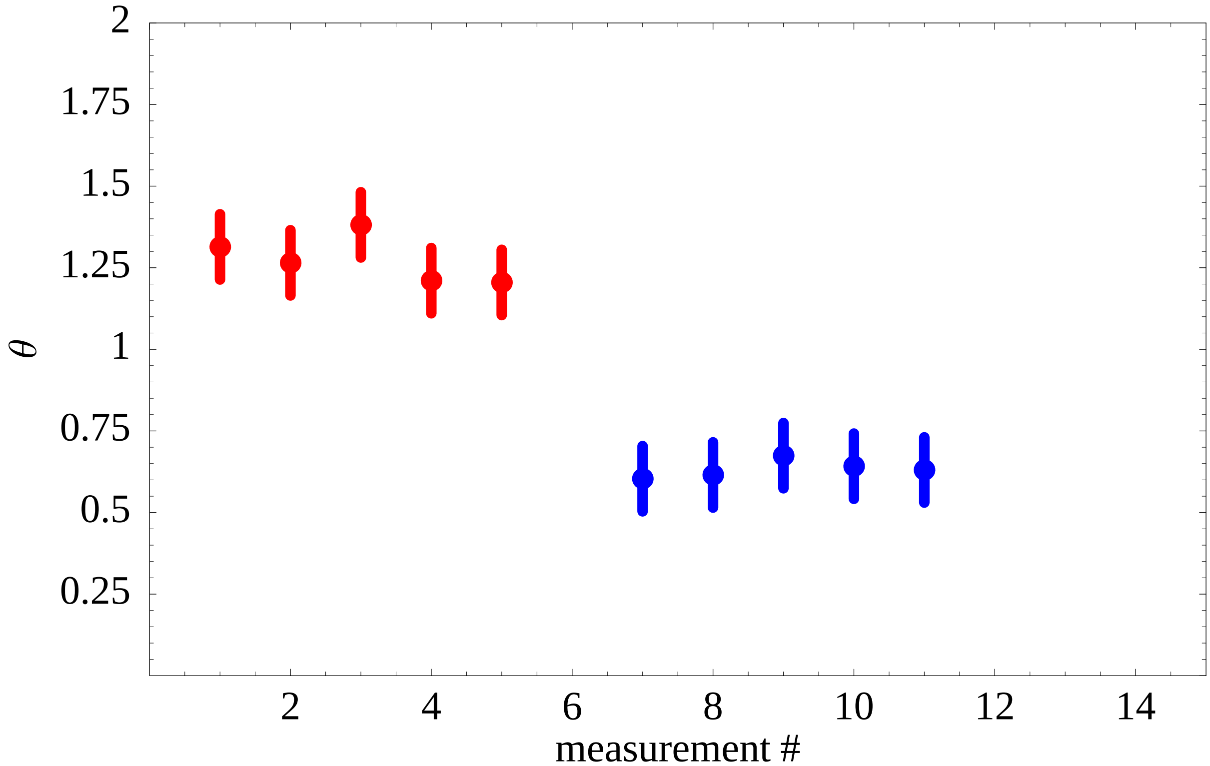
Fundamental difficulties:

1. Good experiments run until systematic errors dominate: the magnitude of remaining systematic errors involves guesswork.
2. Systematic errors of the theory and their correlations are even harder to guess.
3. Quasi–ill-posed problem: determine continuous functions from discrete data set
4. Some combinations of variables are unconstrained, e.g., $s - \bar{s}$ before NuTeV data.

Approach

Use "χ^2" as measure of fit, but vary weights of experiments to estimate range of acceptable fits, rather that relying on the classical $\Delta\chi^2 = 1$.

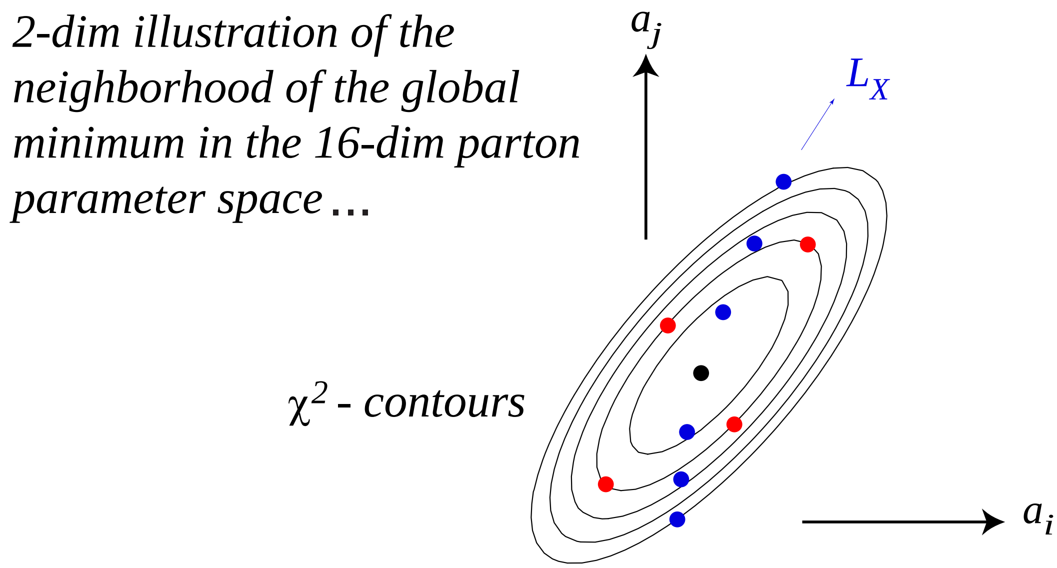
Essence of the Uncertainty Problem



Suppose the quantity θ is measured by two different experiments, or extracted using two different approximations to the True Theory.

What would you quote as the Best Fit and the Uncertainty?

MSU/CTEQ uncertainty methods



- Hessian Matrix Method: eigenvectors of error matrix yield 40 sets $\{S_i^{\pm}\}$ that are displaced "up" or "down" by $\Delta\chi^2 = 100$ from the best fit. Get error by sum of squares and construct extreme PDFs for any observable; or simply look at extremes from the 40 sets.

- Lagrange Multiplier Method: Track χ^2 as function of F (e.g. σ_W) by minimizing $\chi^2 + \lambda F$. Yields special-purpose PDFs that give extremes of σ_W, or $\langle y \rangle$ for rapidity distribution of W, or σ for $t\bar{t}$ production; or . . .

Hessian (Error Matrix) method

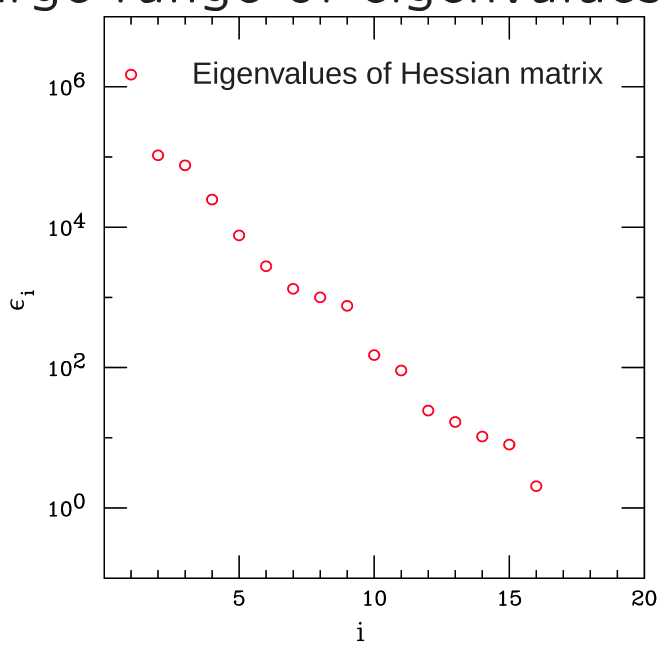
Classical error formulae

$$\Delta\chi^2 = \sum_{ij}(a_i - a_i^{(0)})(H)_{ij}(a_j - a_j^{(0)})$$

$$(\Delta F)^2 = \Delta\chi^2 \sum_{ij} \frac{\partial F}{\partial a_i} (H^{-1})_{ij} \frac{\partial F}{\partial a_j}$$

Hessian matrix H is inverse of error matrix.

Direct application fails because of extreme differences in variation of χ^2 for different directions in parameter space ("steep" and "flat" directions), as shown by large range of eigenvalues of H:



Convergence problems in the minimization are solved by an iterative method that finds and rescales the eigenvectors of H, leading to a diagonal form

$$\Delta\chi^2 = \sum_i z_i^2$$

$$(\Delta F)^2 = \sum_i \left(F(S_i^{(+)}) - F(S_i^{(-)}) \right)^2$$

where $S_i^{(+)}$ and $S_i^{(+)}$ are PDF sets that are displaced along the eigenvector directions.

The eigenvector PDF sets are published, along with the Best Fit, for estimating PDF uncertainties of predictions.

New ways to measure consistency of fit

(Work in progress with John Collins)

Key idea: In addition to the

Hypothesis-testing criterion: $\Delta\chi^2 \sim \sqrt{2N}$

use the stronger

Parameter-fitting criterion: $\Delta\chi^2 \sim 1$

Parameters here are relative weights assigned to

various experiments, or to results obtained using various experimental methods. Examples:

- Plot minimum χ_i^2 vs. $\chi^2_{\mathrm{tot}} - \chi_i^2$, where χ_i^2 is one of the experiments, or all data on nuclei, or all data at low Q^2,...

or

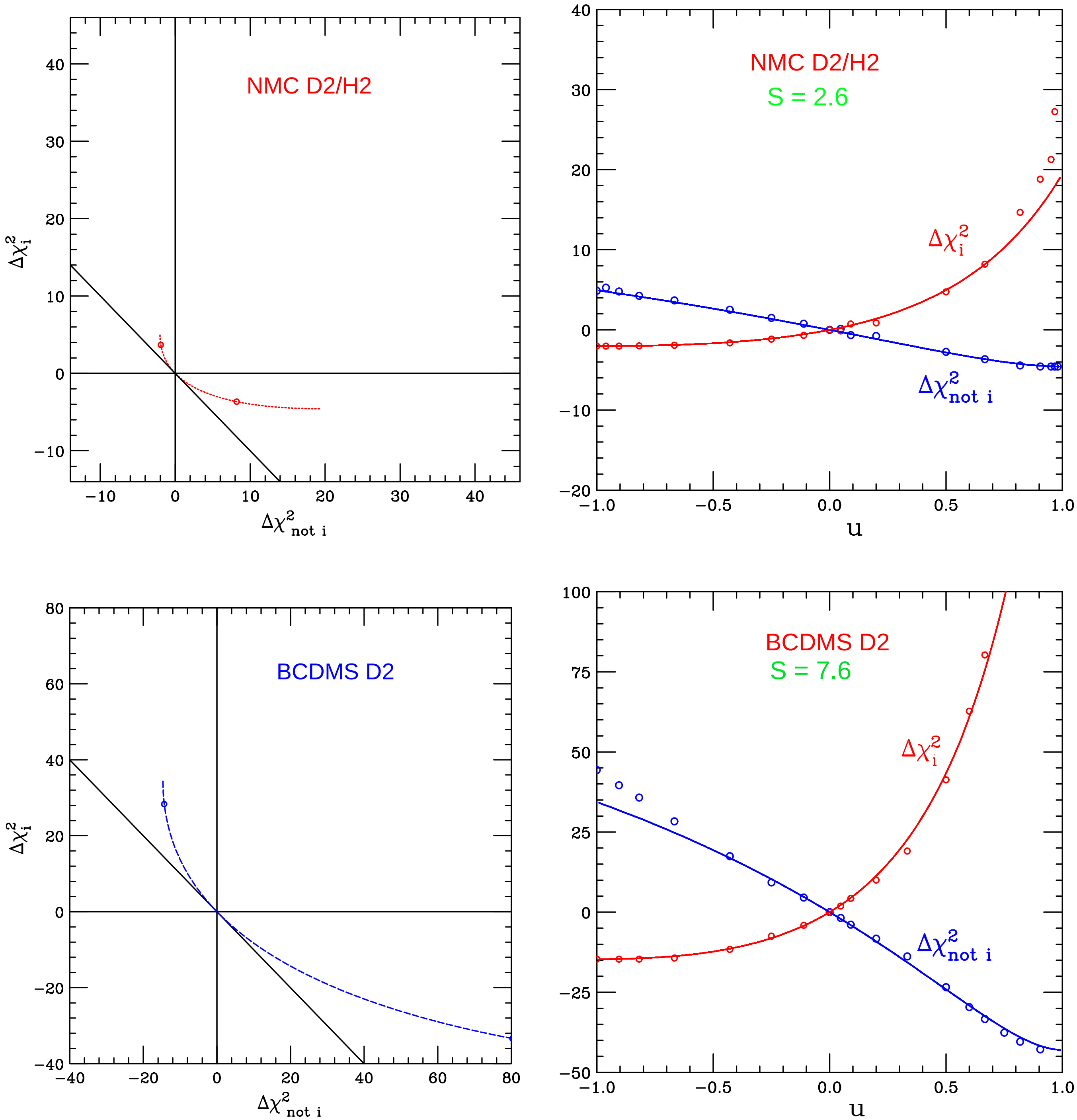
- Plot both as function of Lagrange multiplier u where $(1-u)\chi_i^2 + (1+u)(\chi^2_{\mathrm{tot}} - \chi_i^2)$ is the quantity minimized.

Can obtain quantitative results by fitting to a model with a single common parameter p:

$$\chi_i^2 = A + \left(\frac{p}{\sin\theta}\right)^2 \quad \Rightarrow \quad p = 0 \pm \sin\theta$$

$$\chi^2_{\mathrm{not}\ i} = B + \left(\frac{p-S}{\cos\theta}\right)^2 \quad \Rightarrow \quad p = S \pm \cos\theta$$

These differ by $S \pm 1$, i.e., by S "standard deviations"



Fits to 8 of the experiments in the CTEQ5 analysis

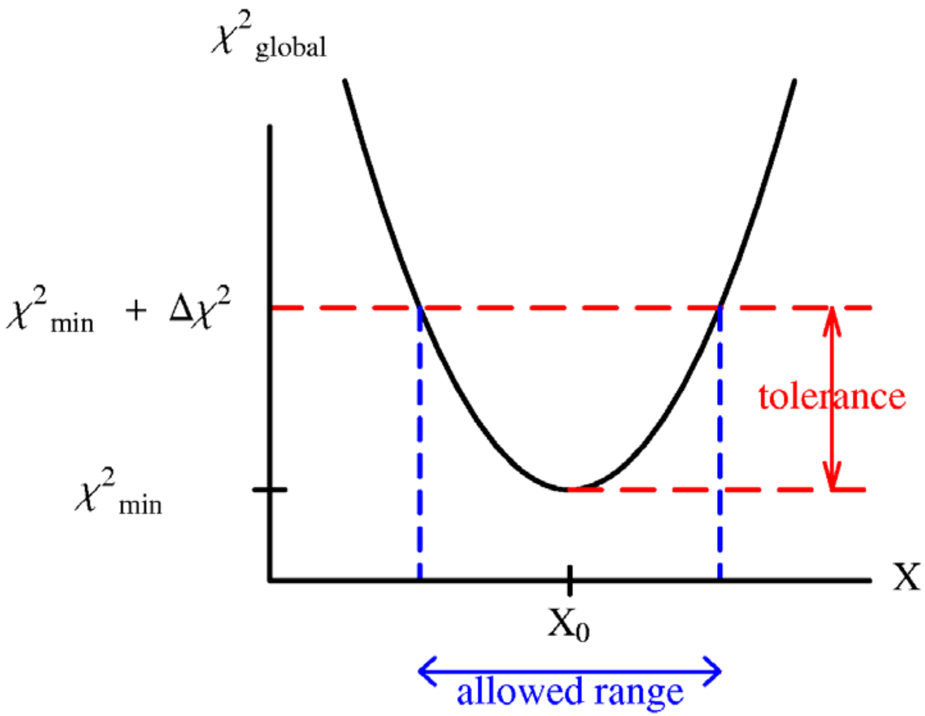
Expt	1	2	3	4	5	6	7	8
S	2.7	3.3	3.3	4.2	5.3	7.6	7.4	8.3
$\tan\phi$	0.56	0.54	0.99	0.86	0.71	1.14	0.65	0.39

Lessons from these *reweighting* studies

• Global analysis requires compromises – the PDF model that gives the best fit to one set of data does not give the best fit to others. This is not surprising because there are systematic differences between the experiments.

• The scale of acceptable changes of χ^2 must be large. Adding a new data set and refitting may increase the χ^2's of other data sets by amounts >> 1.

The question of tolerance



X : any variable that depends on PDF's

X_0 : the prediction in the standard set

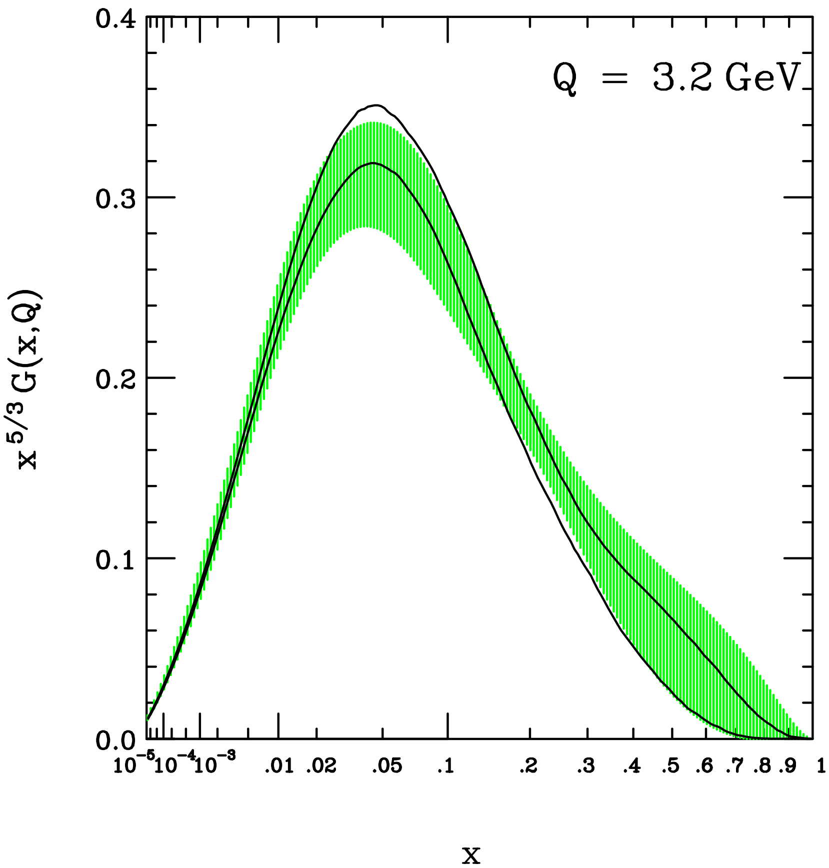
$\chi^2(X)$: curve of constrained fits

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?

Statistical Bootstrap method

Generate random weights for each of the 16 experiments in global fit by $\frac{dP}{dW_i} = e^{-W_i}$. Find best fit for each set of weights. Repeat 200 times and take the central 90 % at each x as the measure of uncertainty range. Shows sizable uncertainty with no *ad hoc* assumption such as $\Delta\chi^2 = 100$.



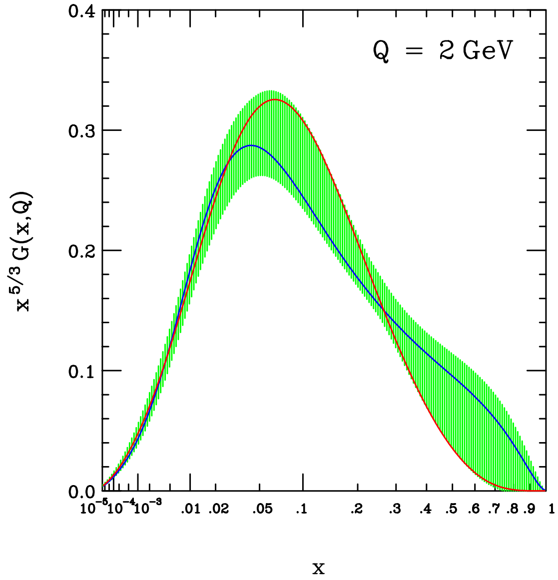
Traditional statistical bootstrap (Efron and Tibshirani) uses integer weights $0 - 16$ defined by random selection; this continuum method is similar but avoids zero weights.

Summary of Uncertainty Methods

Consistent estimates of the uncertainty ranges are found using several different methods:

- "Hessian Method" – eigenvectors of the error matrix
- "Lagrange Multiplier Method" – variation of χ^2
- systematic reweighting of experiments
- random reweighting (statistical bootstrap)

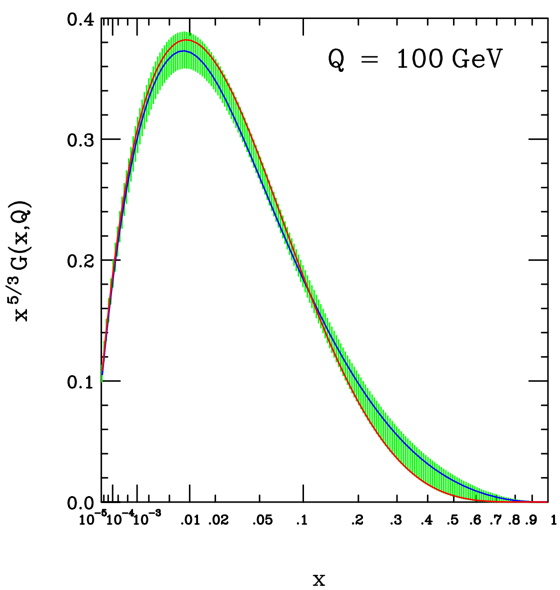
Uncertainty of Gluon distribution



Red: Weight 50 for CDF Jet Blue: Weight 50 for DØ Jet

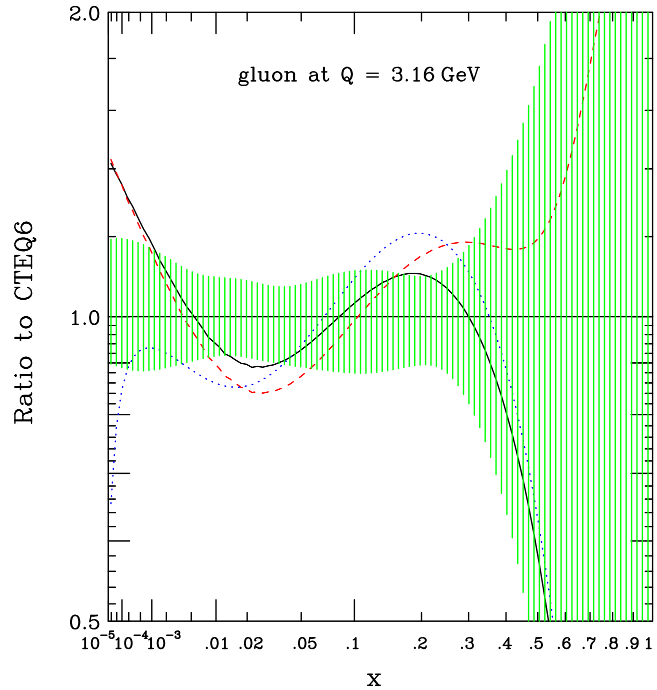
Consistency check: Estimated uncertainty is comparable to the difference between nominally similar experiments.

Area under curve is proportional to momentum fraction carried by gluon – strongly constrained by DIS data. Hence the envelope itself is not an allowed solution.



Convergent Evolution: Uncertainty smaller at large Q

Fractional uncertainty of gluon



Uncertainty bands (envelope of possible fits) for the gluon distribution at $Q^2 = 10\,\mathrm{GeV}^2$.

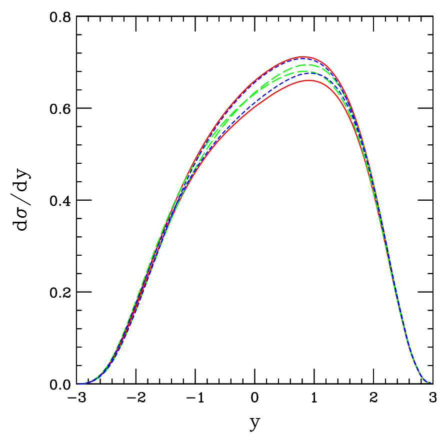
Curves show CTEQ5M1 (solid), CTEQ5HJ (dashed), MRST2001 (dotted)
Differences between these are comparable to the estimated uncertainty(?!

Uncertainties of quark distributions are much smaller than this because DIS measurements see the quark charge in leading order.

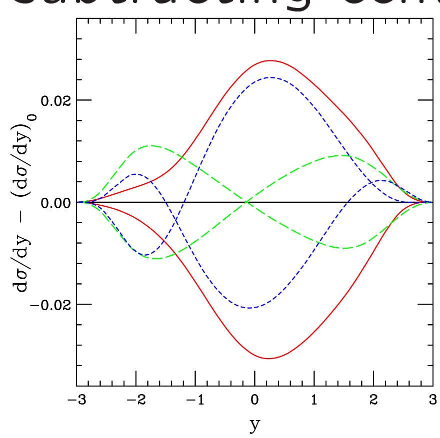
Application: W rapidity distribution

Our methods allow us to calculate the extreme predictions due to PDF uncertainty for whatever quantity is of experimental interest.

For example, extremes of σ_W, $\langle y \rangle$, $\langle y^2 \rangle$ for W production at FNAL – relevant for M_W measurement:

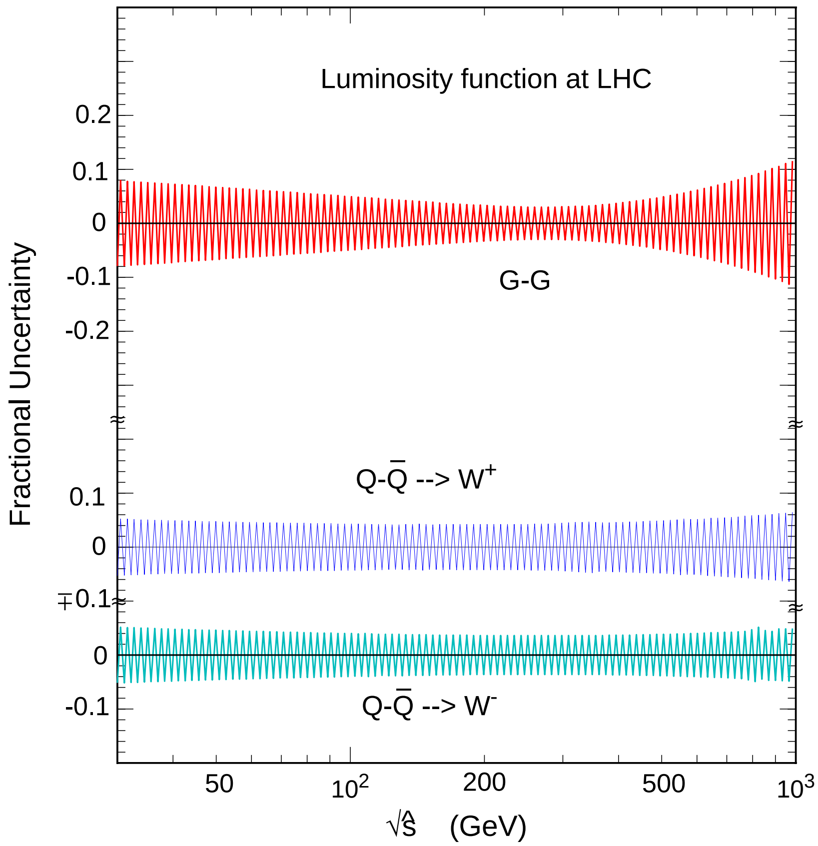


Same curves after subtracting central values:



Important for measuring W mass at FNAL.

Application: Uncertainties of luminosity functions at LHC



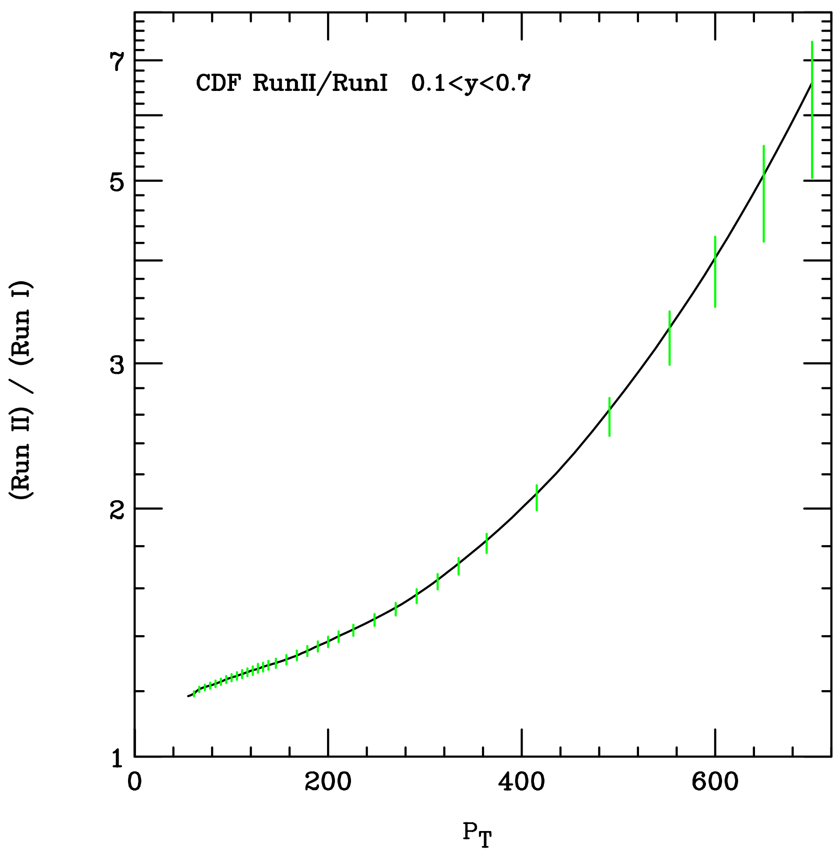
- One component of the uncertainty in predicting the Higgs production cross section at LHC is an uncertainty of 8 % due to PDF uncertainty.

Application: Inclusive jet ratio

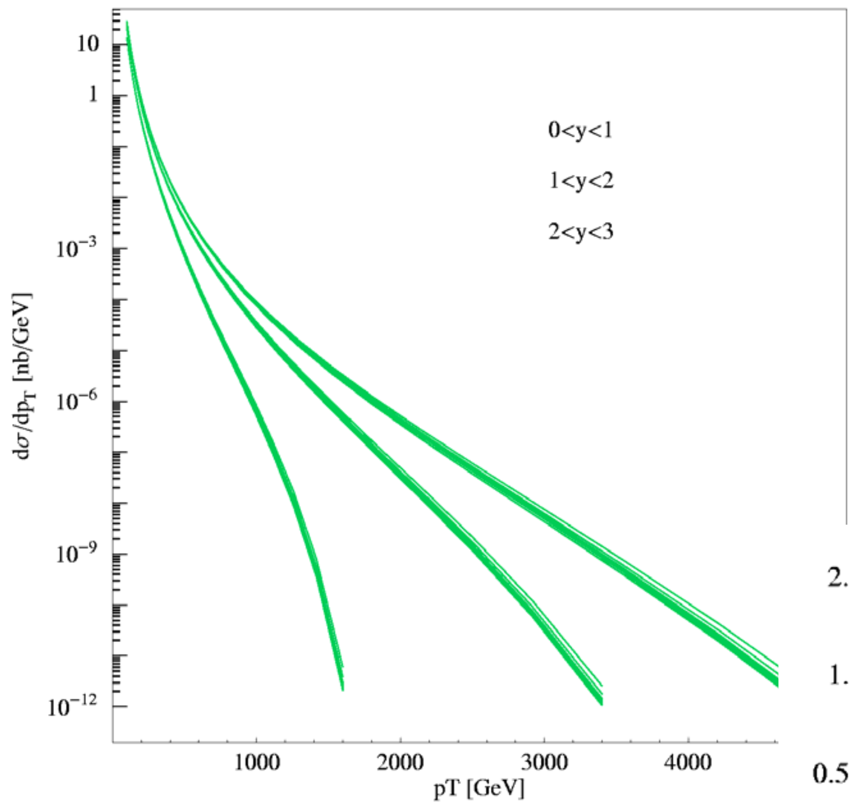
Inclusive jet energy dependence

$$\frac{\frac{d\sigma}{dP_T}(1.96\ \text{TeV})}{\frac{d\sigma}{dP_T}(1.80\ \text{TeV})}$$

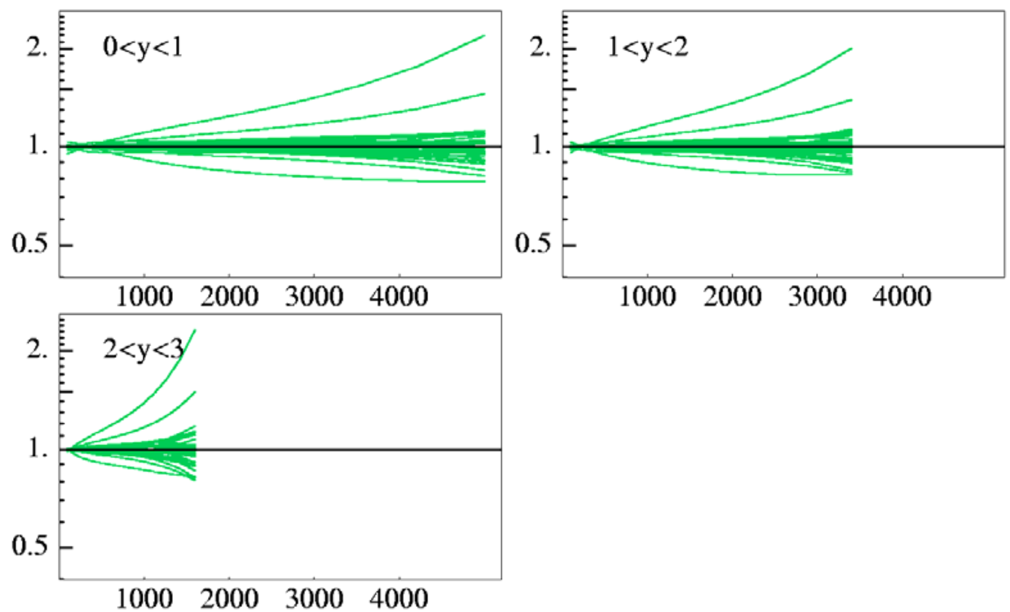
between Tevatron Run I and Run II offers a sensitive test of QCD and a probe for quark substructure, because many systematic errors cancel. Right now it is an important check on the experimental jet "energy scale" calibration.



Prediction and uncertainty range from CTEQ6.1



The inclusive jet cross section versus pT for 3 rapidity bins at the LHC. Predictions of all 40 eigenvector basis sets are superimposed.



Strangeness Asymmetry and NuTeV

Background:

- CCFR–NuTeV measurements of dimuon production in ν, $\bar{\nu}$ scattering (on Fe) (2001)
- NuTeV measurement of the Weinberg angle via Paschos-Wolfenstein ratio (2002)

$$\frac{\sigma^{\nu}_{NC} - \sigma^{\bar{\nu}}_{NC}}{\sigma^{\nu}_{CC} - \sigma^{\bar{\nu}}_{CC}} \cong \frac{1}{2} - \sin^2\theta_W$$

3.1 σ discrepancy with world average:

$$\begin{aligned} \sin^2\theta_W &= 0.2277 \pm 0.0016 \quad \text{[NuTeV]} \\ \sin^2\theta_W &= 0.2227 \pm 0.0004 \quad \text{[LEP EWWG]} \end{aligned}$$

Recent development: CTEQ Global analysis with $s(x) \neq \bar{s}(x)$, including the dimuon data

- Preliminary report at Lepton-Photon 2003: $s(x) > \bar{s}(x)$ at large x may remove some or all of the anomaly.
- Much further work in progress: previous global fits assumed $s(x) = \bar{s}(x) = \kappa\,[\bar{u}(x) + \bar{d}(x)]$ at Q_0.
- More experiments sensitive to s, $\bar{s}$ would help.

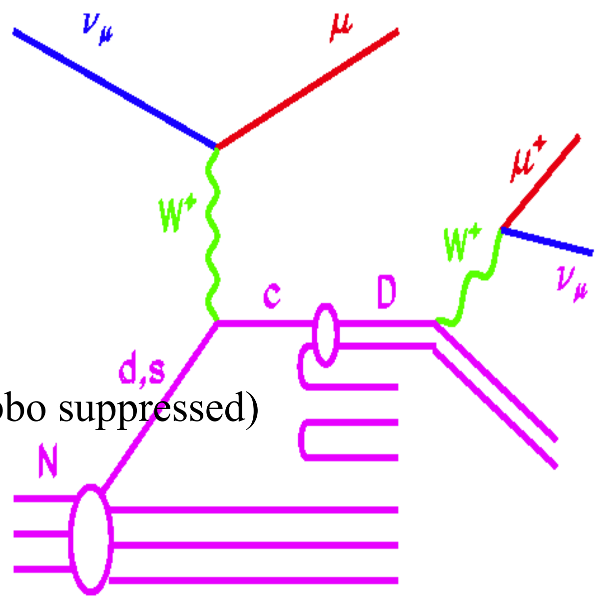
Corrections to R$^-$

$$R^- = \frac{1}{2} - s^2_W - \left(\underbrace{\delta N \frac{\int x(u_v - d_v)dx}{\int x(u_v + d_v)dx}}_{\text{neutron excess}} + \underbrace{\frac{\int x(s - \bar{s})dx}{\int x(u_v + d_v)dx}}_{\text{strange asymmetry}} \right) \left[1 - \frac{7}{3} s^2_W + \underbrace{\frac{4\alpha_s}{9\pi} \left(\frac{1}{2} - s^2_W \right)}_{\text{NLO correction (NuTeV : LO)}} \right]$$

These corrections have been under close scrutiny by many authors, in particular BPZ (Barone et.al) and Davidson et.al.

Kulagin
hep-ph/0301045

Strangeness Structure of the Nucleon: Dimuon Production in $\nu, \bar{\nu}$ Scattering



(*d* is Cabibbo suppressed)

\# of events:

di-muon	NuTeV	CCFR	Combined
Neutrino	5012	5030	10042
Anti-Nu	1458	1060	2518

* High stats & high precision data
* Best constraints on strange quark

$$\frac{d\sigma^{+}_{\mu^\pm \mu^\mp}}{dx\ dy} = \int d\Gamma\, d\Omega\ \frac{d\sigma_{\mu^\mp c}}{dx\ dy\ d\Gamma} \otimes D_c(\Gamma) \otimes \Delta_c(\Omega)\Big|_{E_{\mu^\pm} > 5\ GeV}$$

Di-muon cross-section

Charm Production cross-section

Fragmentation Function

Decay Distribution

Modeling needed to compare theory with data.

M. Goncharov et al., NuTeV Collaboration PRD 64:110226 (2001)

CCFR-NuTeV Analysis of Strange Quarks and the Weinberg Angle Measurement

- Ingredients to the CCFR-NuTeV dimuon analysis:
  - Data on $\nu N, \bar{\nu} N \longrightarrow \mu^+ \mu^- + X$
  - Fragmentation functions

    Peterson, Schlatter, Schmitt, Zerwas '83 ; Collins, Spiller '85

    heavy quark fragmentation: Cacciari, Greco '97
  - Buras-Gaemer /CTEQ/GRV non-strange partons
  - Strange distributions assumed given by

$$
\begin{aligned}
s(x,Q^2) &= \kappa_\nu \frac{\bar{u}(x,Q^2) + \bar{d}(x,Q^2)}{2} (1-x)^{\alpha_\nu} \\
\bar{s}(x,Q^2) &= \kappa_{\bar{\nu}} \frac{\bar{u}(x,Q^2) + \bar{d}(x,Q^2)}{2} (1-x)^{\alpha_{\bar{\nu}}}
\end{aligned}
$$

- $\Rightarrow$ Gave parameters κ and α, but no actual plots of $s(x,Q)$, …

Strangeness Asymmetry according to NuTeV

- For implication on NuTeV anomaly, the key is the Strangeness Asymmetry. Define:

$$[s^{\pm}] \equiv \int_0^1 s^{\pm}(x)\,dx \equiv \int_0^1 [s(x) \pm \bar{s}(x)]\,dx$$

and the corresponding momentum fractions:

$$[S^{\pm}] \equiv \int_0^1 S^{\pm}(x)\,dx \equiv \int_0^1 x[s(x) \pm \bar{s}(x)]\,dx$$

In particular, it is $[S^{-}]$ that enters the P-W ratio correction term.

CCFR-NuTeV claimed $[S^{-}] \sim -0.0027$ opposite to direction that would decrease the anomaly.

"CTEQ" Global Analysis

- Almost the same ingredients as CTEQ6 analysis
- Add CCFR-NuTeV dimuon data (and a few more)
- Allow a non-symmetric strangeness sector:

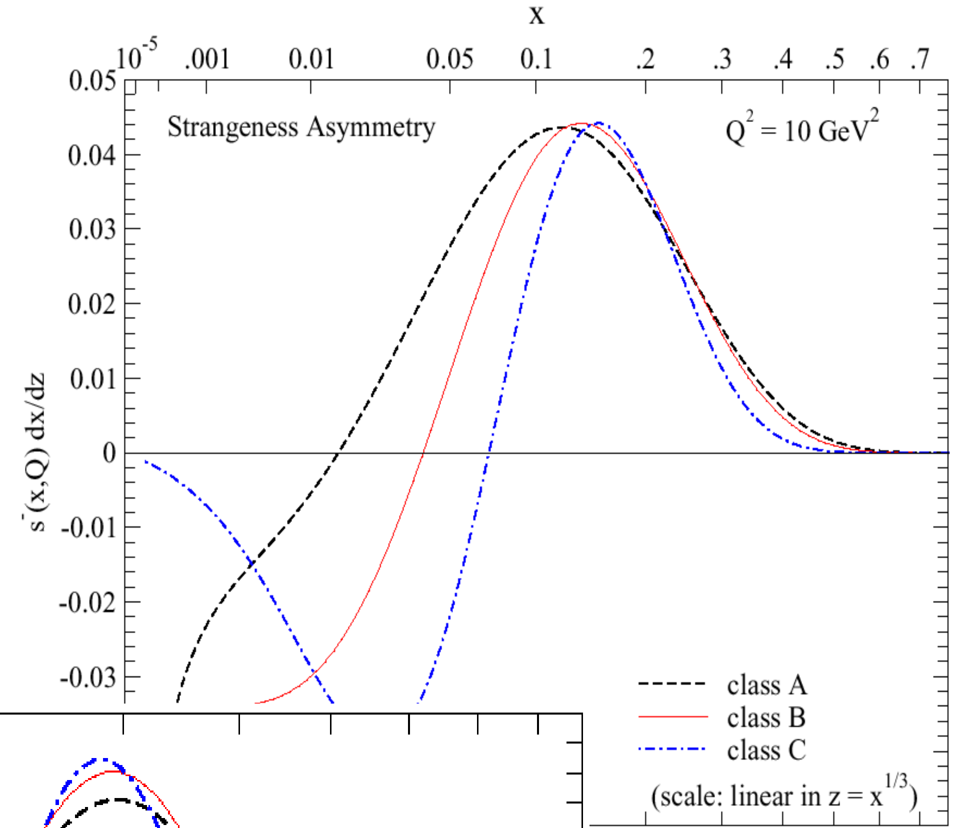
Parametrization of the Strangeness sector (at some $Q=Q_0$)

$$
\begin{aligned}
s^+(x,Q_0) &= A_0\, x^{A_1}(1-x)^{A_2} P_+(x;A_3,A_4,\ldots) \\
s^-(x,Q_0) &= s^+ \tanh[a\, x^b (1-x)^c P_-(x;x_0,d,e,\ldots)]
\end{aligned}
$$

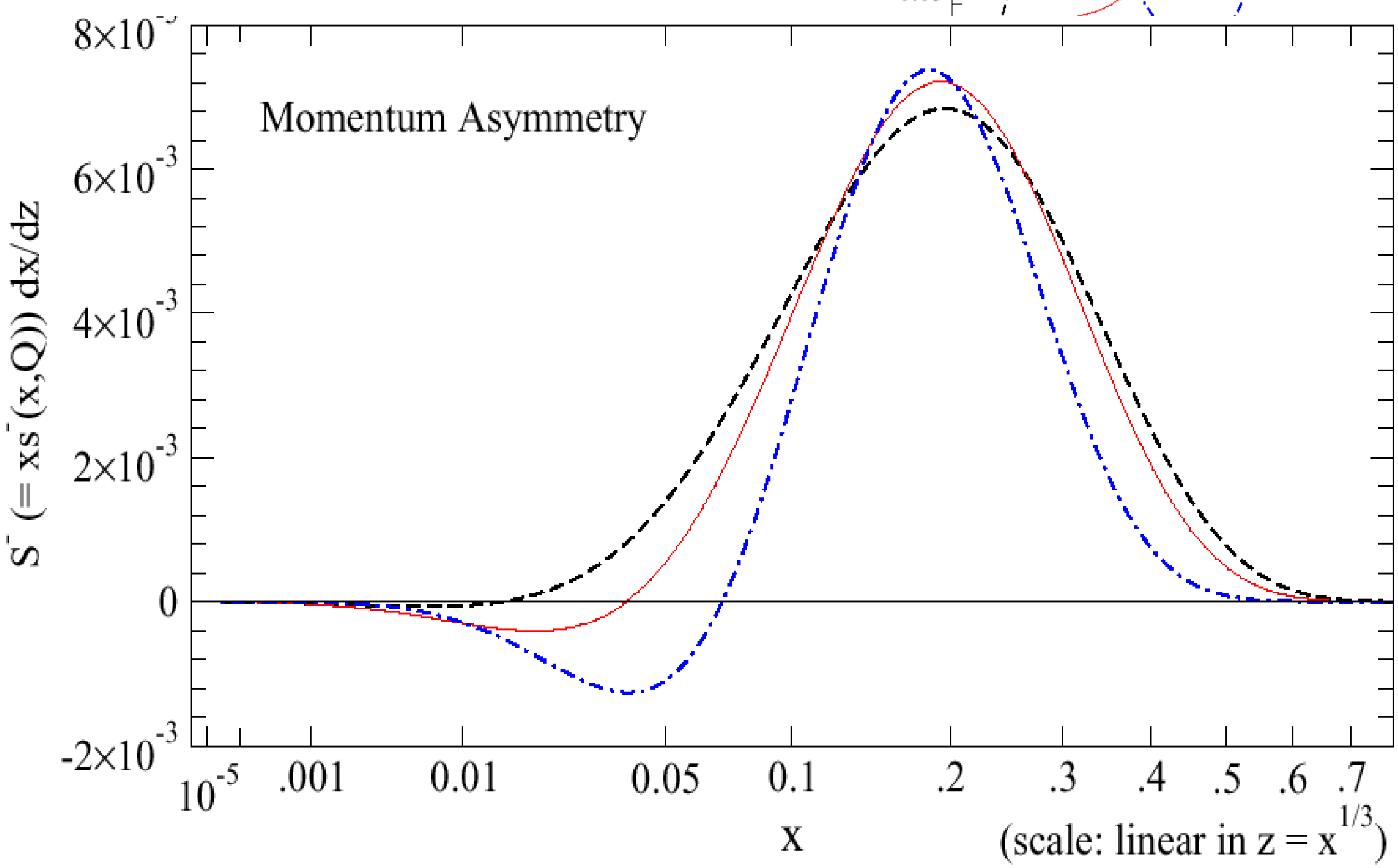
$$
P_-(x) = (1 - \frac{x}{x_0} + dx^2 + ex^3 + \ldots)
$$

Where x_0 is to be determined by the condition $[s-] = 0$.

Preliminary Results



positive [S^-] case

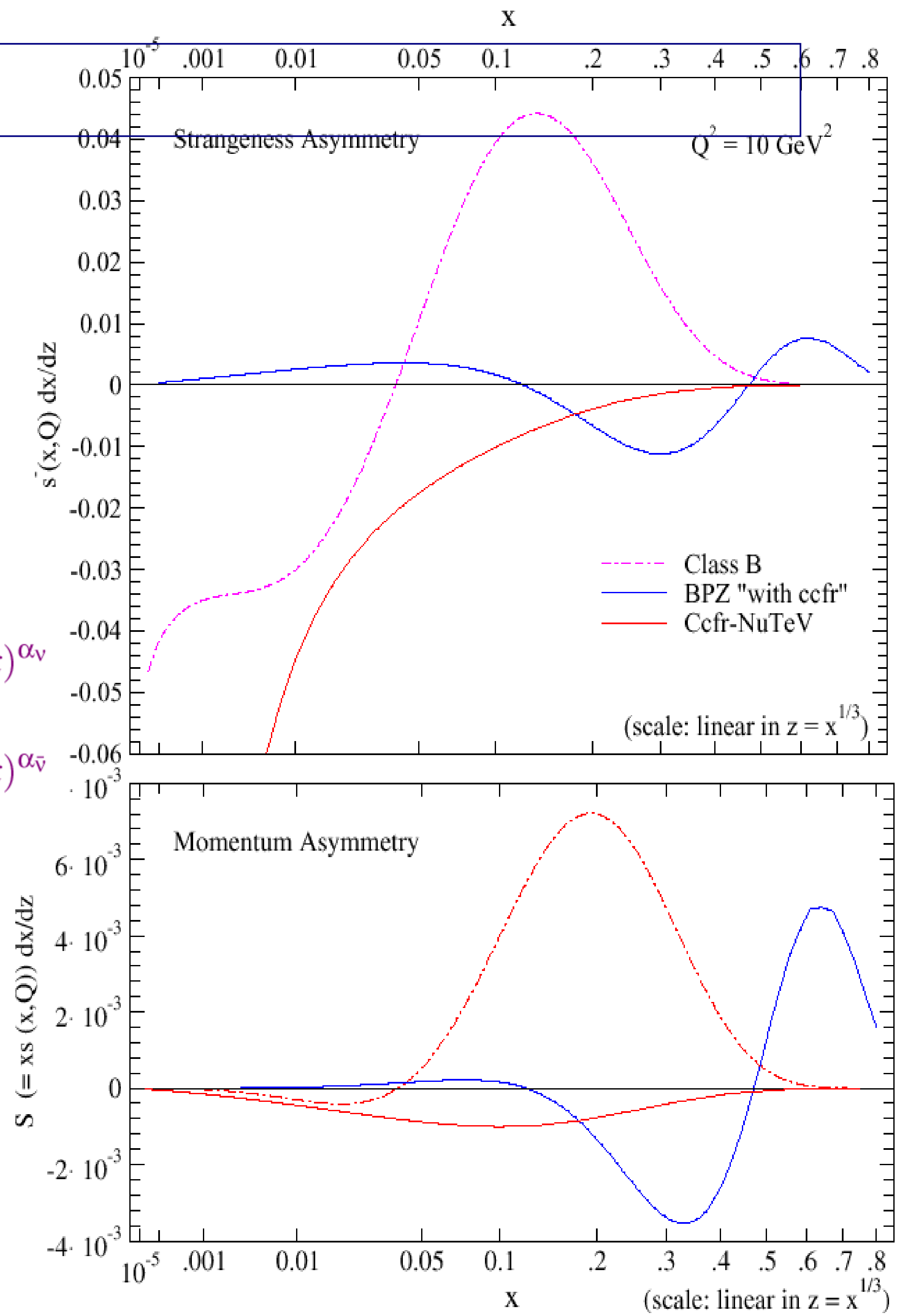


Negative [S-] case: flipped.

Central flaw of NuTeV analysis: “CCFR ansatz”:

$$s(x,Q^2) = \kappa_\nu \frac{\bar{u}(x,Q^2)+\bar{d}(x,Q^2)}{2}(1-x)^{\alpha_\nu}$$

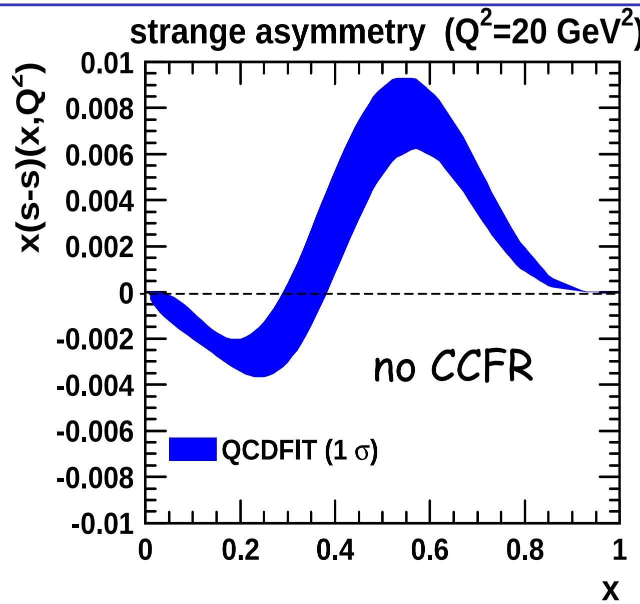
$$\bar{s}(x,Q^2) = \kappa_{\bar{\nu}} \frac{\bar{u}(x,Q^2)+\bar{d}(x,Q^2)}{2}(1-x)^{\alpha_{\bar{\nu}}}$$

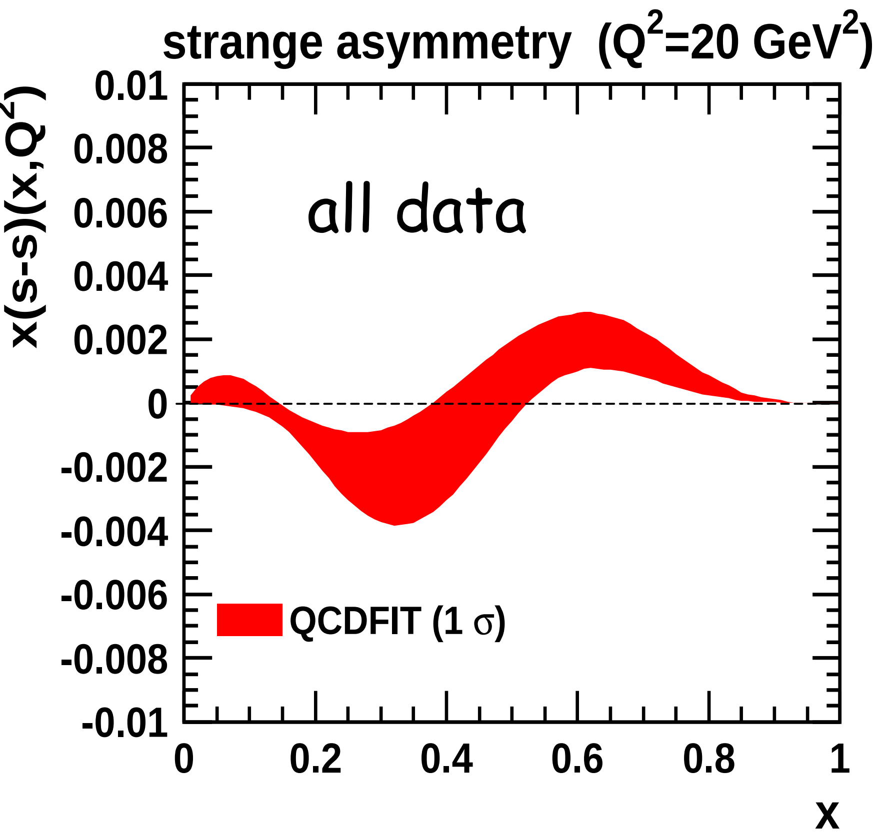


Results on the strange sea asymmetry from BPZ

without CCFR, same asymmetry as in previous studies

$$\int_0^1 (xs - x\bar{s})\,dx = 1.8 \pm 0.5 \times 10^{-3}$$



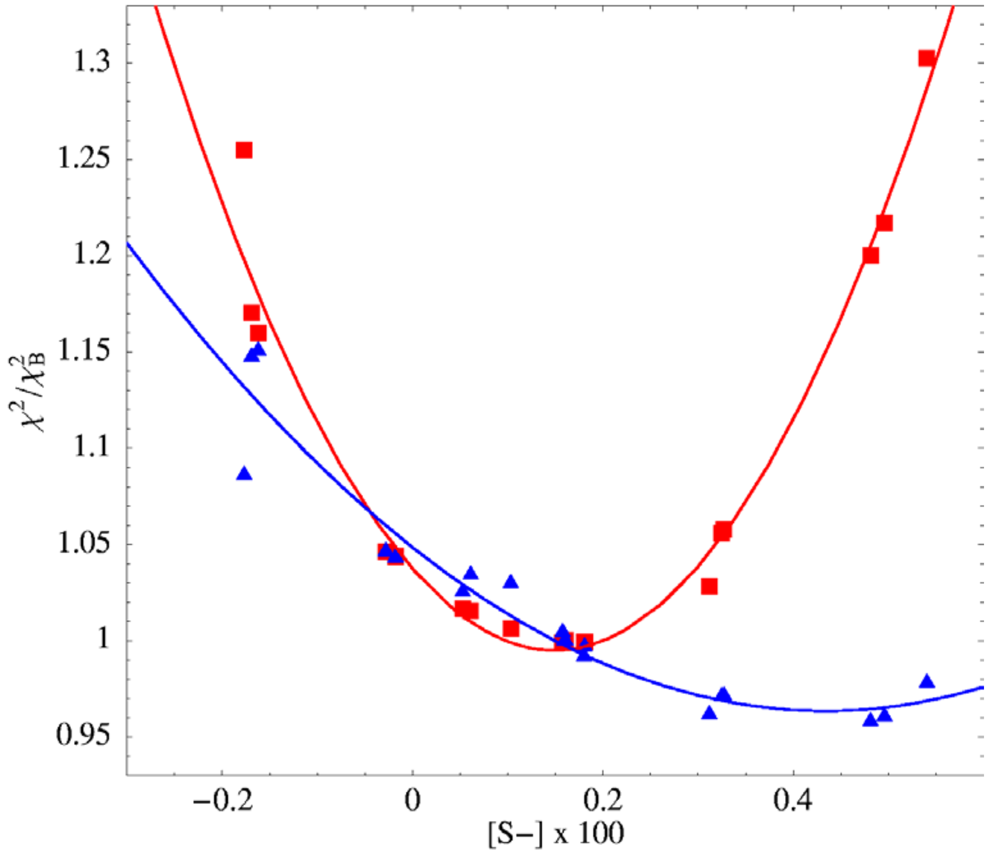


using all data sets, the asymmetry is strongly reduced

$$\int_0^1 (xs - x\bar{s})\,dx = 1.8 \pm 3.8 \times 10^{-4}$$

momentum asymmetry is compatible with zero

Figure 2.
Correlation between χ^2 values and [S^-]



Red: dimuon cross section

Blue: other data sensitive to $s - s_{bar}$ (F3)

Outlook – I

- Parton Distribution Functions are a necessary infrastructure for precision Standard Model studies and New Physics searches at hadron colliders and experiments using hadron targets.
- PDFs of the proton are increasingly well measured.
- Useful tools are in place to estimate the uncertainty of PDFs and to propagate those uncertainties to physical predictions. There is adequate agreement between various methods for estimating the uncertainty.
- The "Les Houches Accord" interface makes it easy to handle the large number of PDF solutions that are needed to characterize uncertainties. [hep-ph/0204316]

Outlook – II

- Improvements in the treatment of heavy quark effects are in progress, and together with neutrino experiments they will allow improved flavor differentiation.
- PDFs summarize fundamental nonperturbative physics of the proton – a challenge to be computed! (Moments of meson PDFs have been done on lattice.)
- Other non-perturbative methods, e.g. for $s(x) - \bar{s}(x)$?
- HERA and Fermilab run II data will provide the next major experimental steps forward, followed by LHC.
- Theoretical improvements such as resummation to use direct photon and W transverse momentum data will be useful.
- In view of possible isospin breaking, and the importance of nuclear shadowing & anti-shadowing effects, HERA measurements on deuterons would be highly welcome.