

Parton Distribution Functions and Global Fitting

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2007 CTEQ Summer School

May 30 - June 7, 2007

Madison, Wisconsin

Outline - Lecture II

1. Treatment of Errors
 - Goodness of fit
 - Statistical errors
 - Systematic errors
 - What is *not* included
2. Overview of PDF results
3. Estimating PDF Errors
4. Outlook

Data Errors and Fitting

When performing global fits one needs a criterion for evaluating the “goodness of fit” for a particular set of PDFs. This is normally done by minimizing the chi square function. If only statistical errors are included then one has

$$\chi^2 = \sum_i \frac{(D_i - T_i)^2}{\sigma_i^2}$$

where D_i denotes the i^{th} data point with statistical error σ_i and T_i denotes the theory value for that point.

This approach works well when

- There is only one data set
- The data set is statistically limited, *i.e.*, the errors are not “too small”

- Experiments may also have some overall normalization uncertainty due, for example, to an uncertainty in the luminosity. The above expression can be modified to

$$\chi^2 = \sum_i \frac{(f_N D_i - T_i)^2}{\sigma_i^2} + \left[\frac{1 - f_N}{\sigma_N^{norm}} \right]^2$$

where f_N is the normalization parameter for the N^{th} data set (nominally equal to one) and σ_N^{norm} is the associated uncertainty in the normalization.

- This is useful when several data sets are being used in a fit
- This approach was the standard one used when most data sets were statistically limited, but it is not satisfactory today.
- Now, it is often necessary to include the effects of point-to-point systematic errors.

Suppose that a set of k systematic errors β are known for each of the data points in a particular set of data. Then an extension of the χ^2 function given previously is

$$\chi^2 = \sum_i \frac{(D_i - \sum_{j=1}^k \beta_{ij} s_j - T_i)^2}{\sigma_i^2} + \sum_{j=1}^k s_j^2$$

- The data points D_i are shifted by an amount reflecting the systematic errors β with the shifts given the the s_j parameters
- There is a quadratic penalty term for non-zero values of the shifts s_j .
- For a fixed set of theory parameters it is possible to analytically solve for the shifts s_j and, therefore, continually update them as the fit proceeds.
- Details may be found in D. Stump et al, Phys. Rev. D65:014012, 2002

Fitting multiple data sets

- Different data sets often have widely differing numbers of data points
- Significantly smaller(larger) than average errors can also affect the contribution to χ^2
- A particular data set may provide a significant constraint on a particular combination of PDFs, yet provide a relatively small contribution to the overall χ^2

Example: NA-51 provided *one point* yet it was the first direct measurement showing $\bar{d} \neq \bar{u}$

- One solution is to introduce a weight in the χ^2 function for each experiment. The weights can be adjusted to emphasize a particular experiment.

Multiple data sets (continued)

Generalize χ^2 to

$$\chi^2 = \sum_k w_k \chi_k^2 + \sum_k w_{N,k} \left[\frac{1 - f_N}{\sigma_N^{norm}} \right]^2$$

where the weights w_k and $w_{N,k}$ can be chosen to emphasize the contribution of a given experiment or normalization to the total chi-square. χ_k^2 represents the chi-square contribution of the k^{th} experiment and may - or may not - include systematic errors.

- Changing the weights in chi-square expression will alter the minimum found by the fitting procedure
- This implies that the minima found in global fits are not unique
- There are other factors, discussed in Lecture I, which also contribute to the non-uniqueness of the minima.

Overview of PDF results

I will use the CTEQ6M and 6.1M results to illustrate some key points of current global fits.

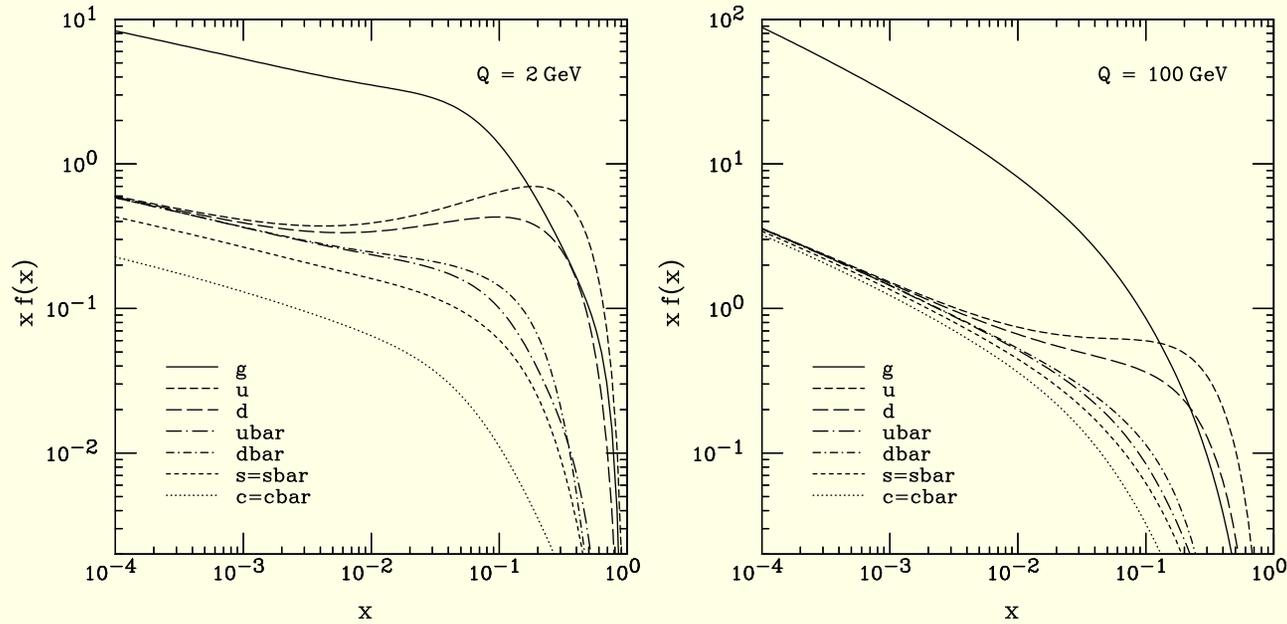
CTEQ6M: J. Pumplin et al, JHEP0207:012, 2002

CTE6.1M: D Stump et al., JHEP0310:046, 2003

Data sets included

- $\mu p, \mu d$ DIS: BCDMS, NMC,
- ep DIS: H1, ZEUS
- W lepton asymmetry: CDF
- $\nu, \bar{\nu}$ Fe: CCFR
- Hadronic μ pair production: E605, E866, NA-51
- Hadronic jet production: CDF, DØ

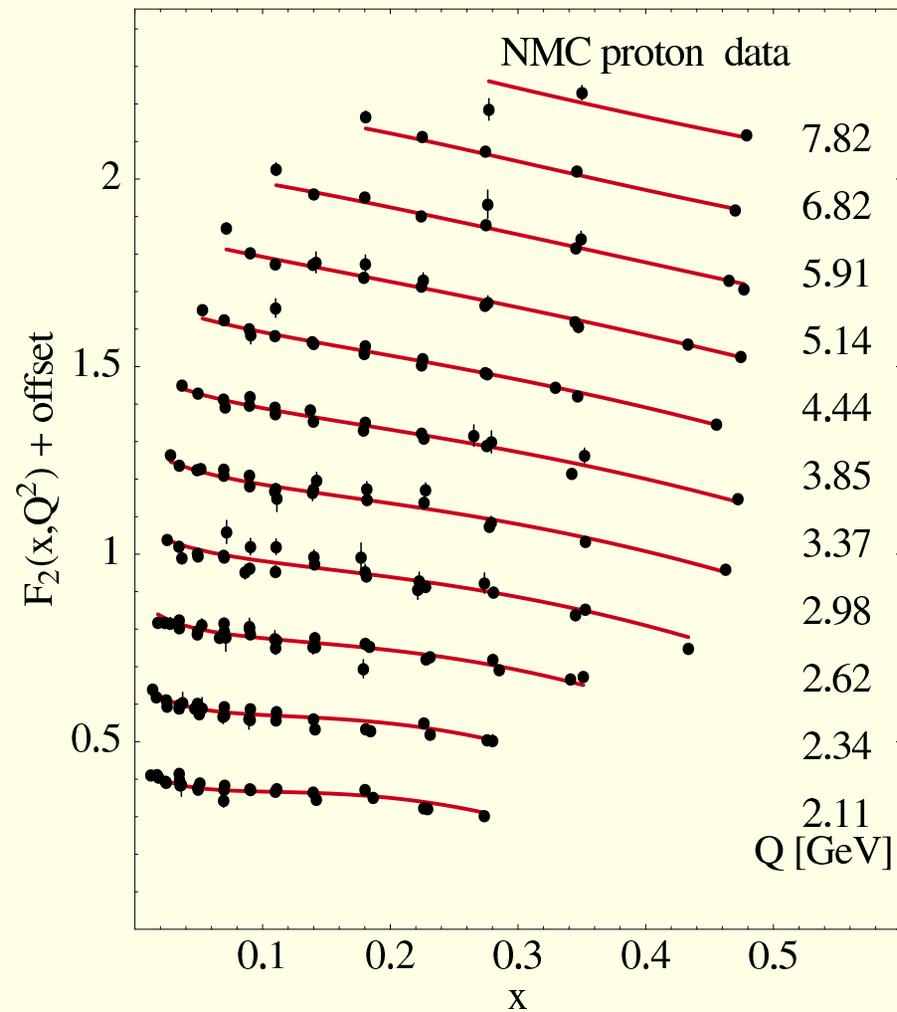
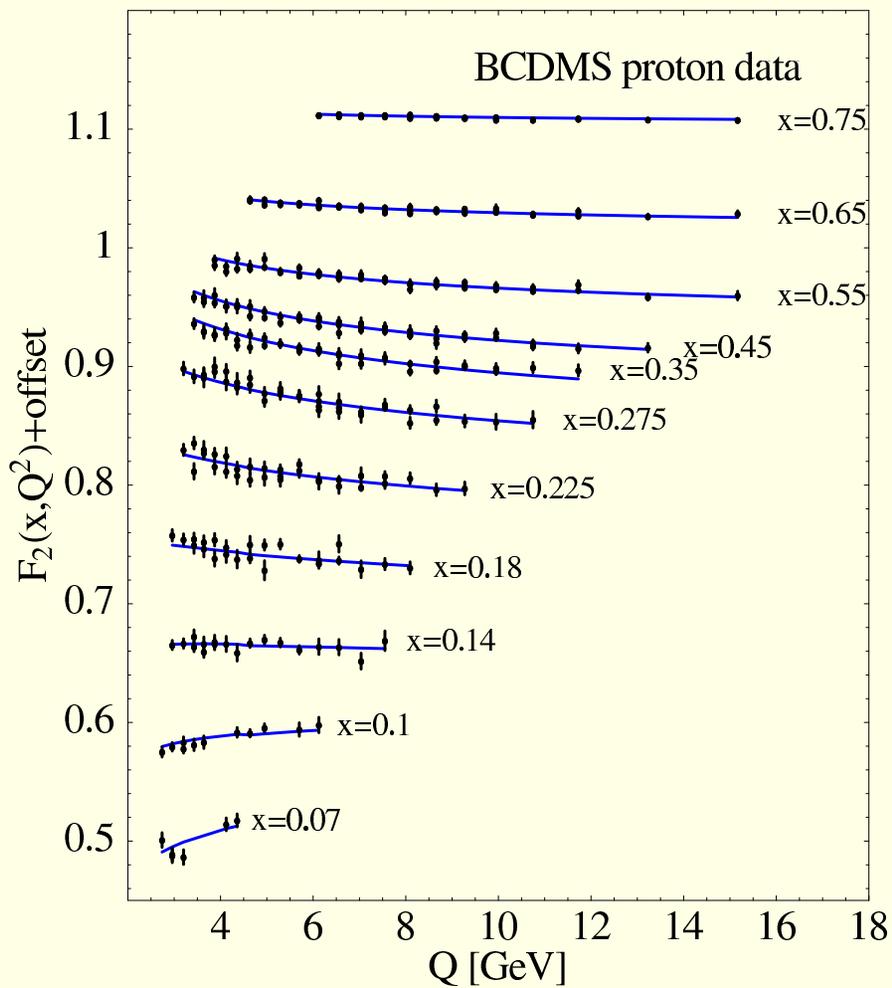
CTEQ6M PDFs



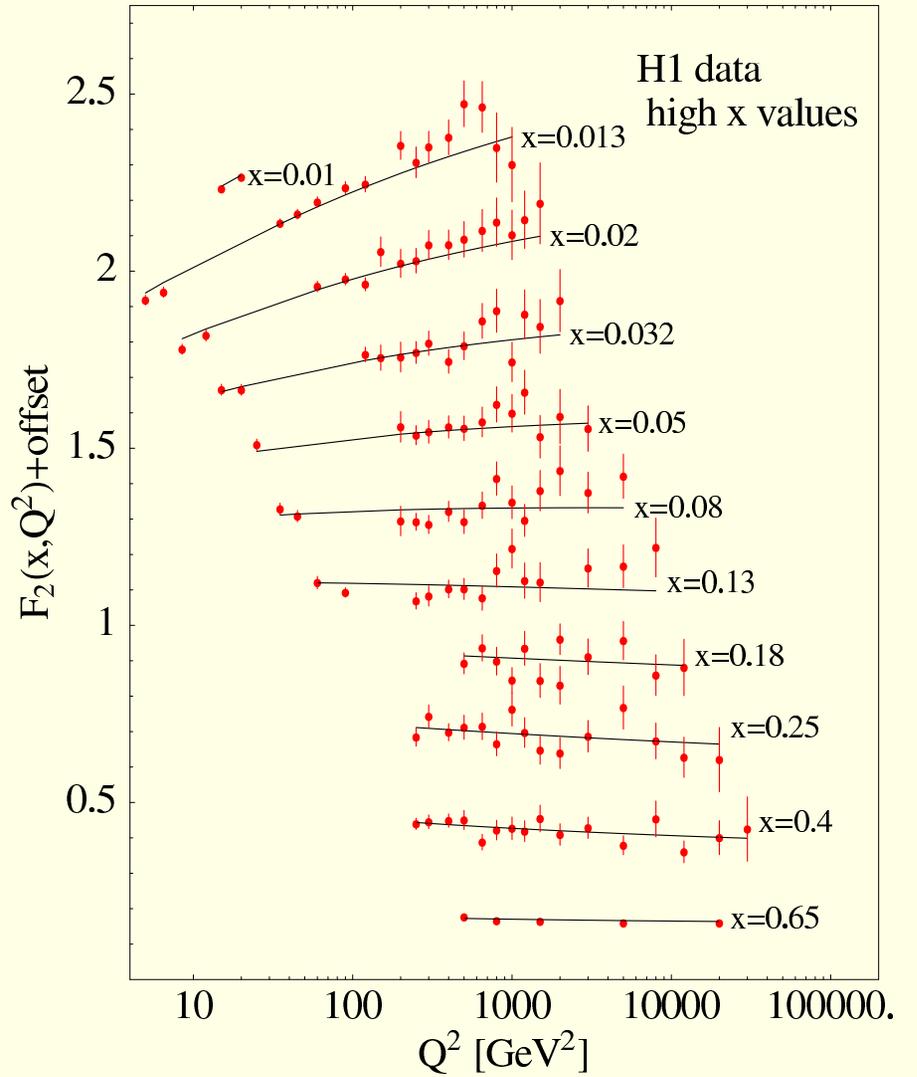
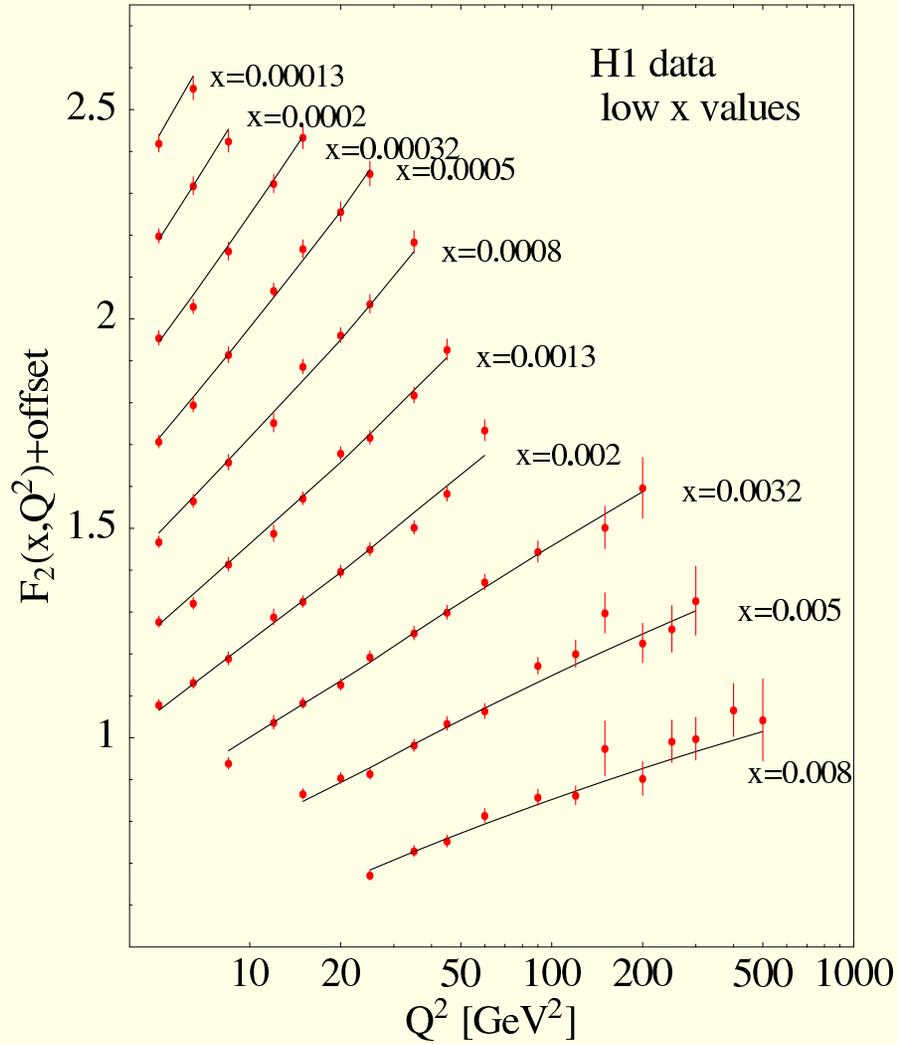
Some comments:

- Beware of extrapolating to values of x outside the range of fitted data (data cover $.00013 < x < 0.75$)
- Note the dominance of the gluon distribution at low values of x
- Note $\bar{d} > \bar{u}$ and $s = \bar{s} < \bar{d}, \bar{u}$
- Note the general decrease (increase) of the PDFs at large (small) values of x which follows from the DGLAP equations

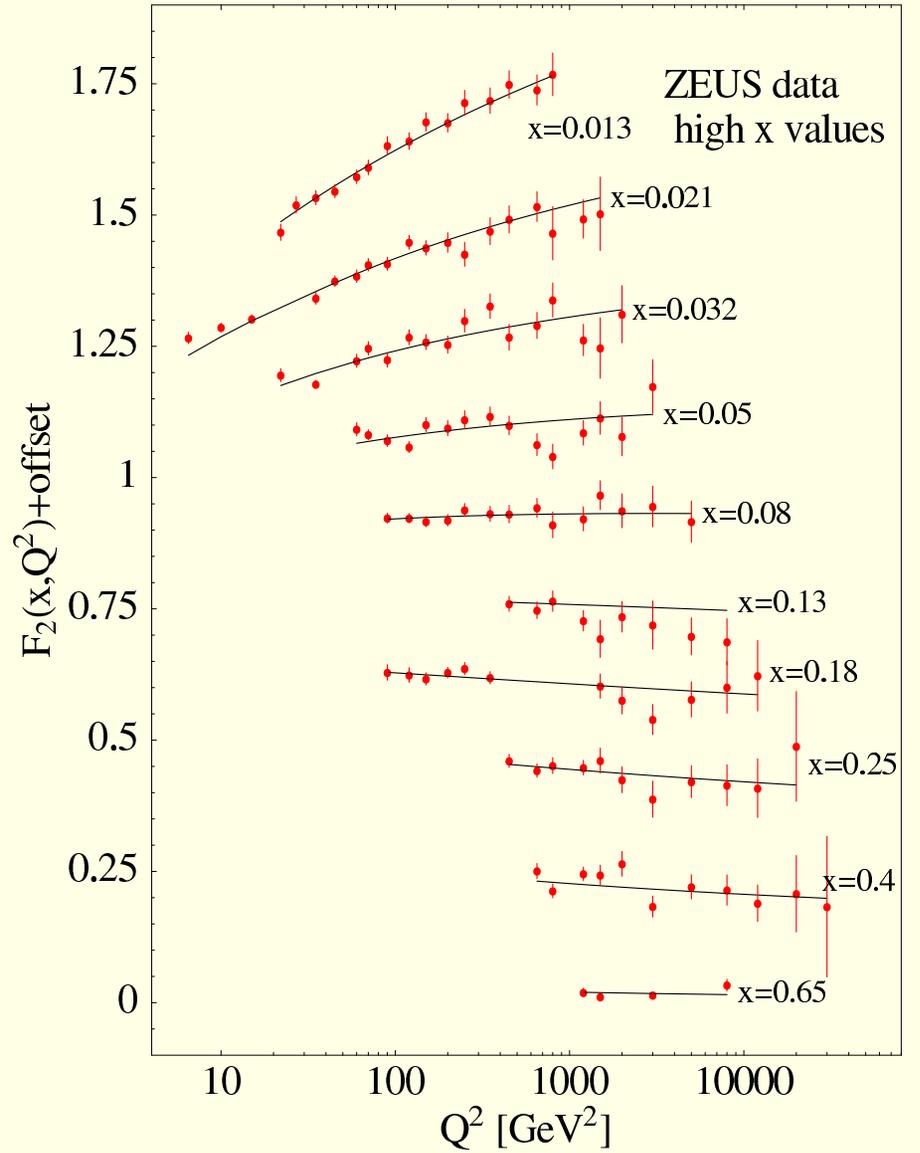
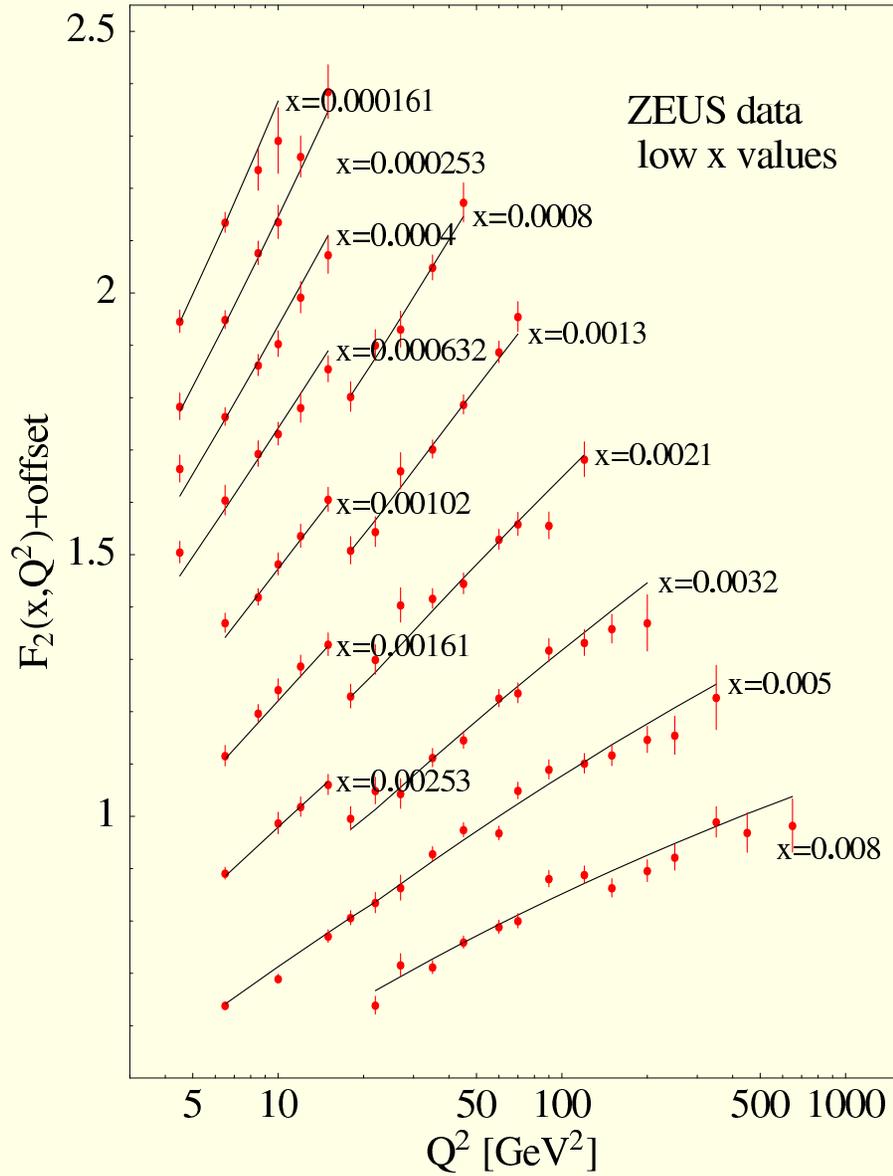
μp DIS data



ep DIS data



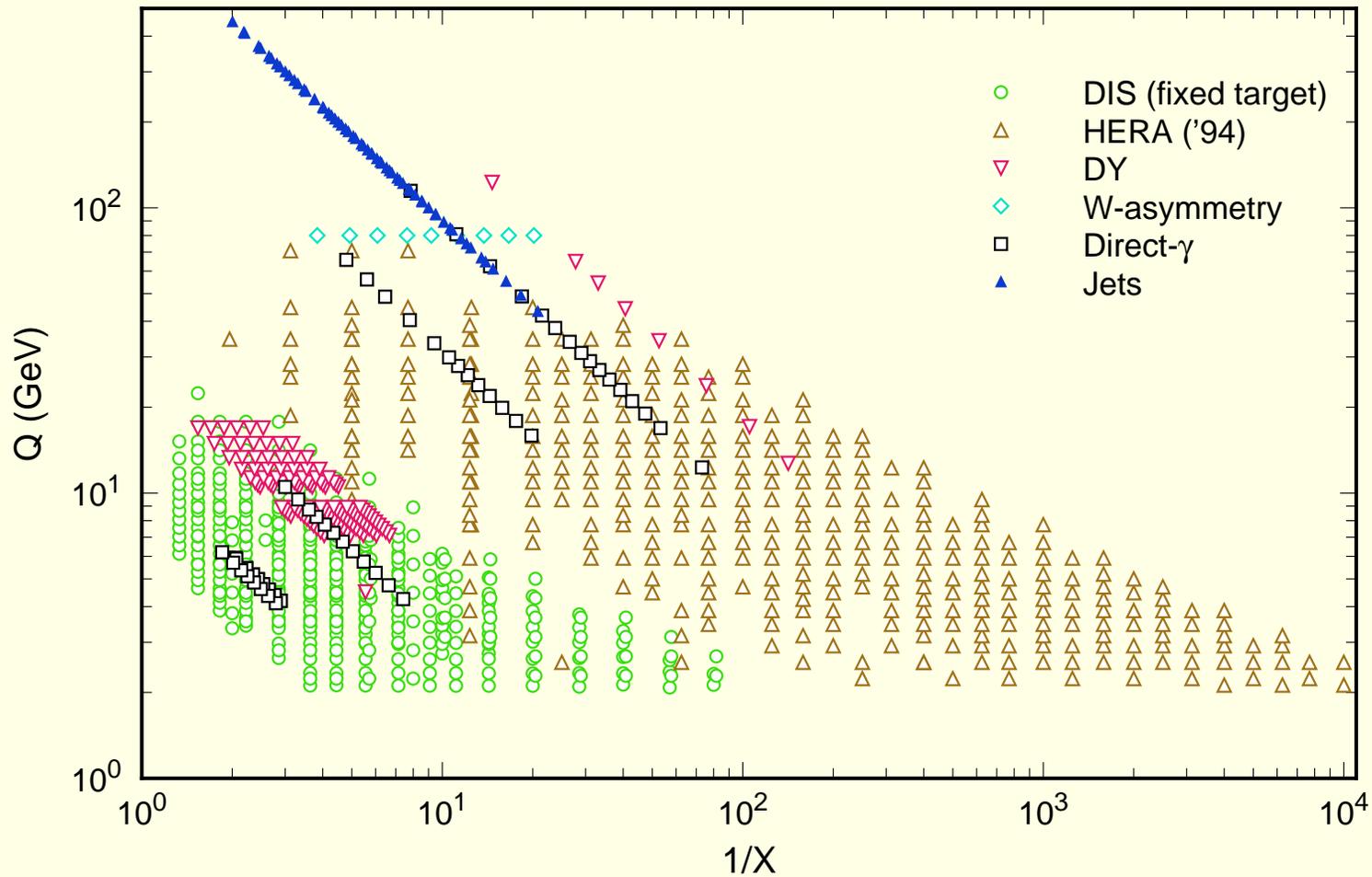
ep DIS data



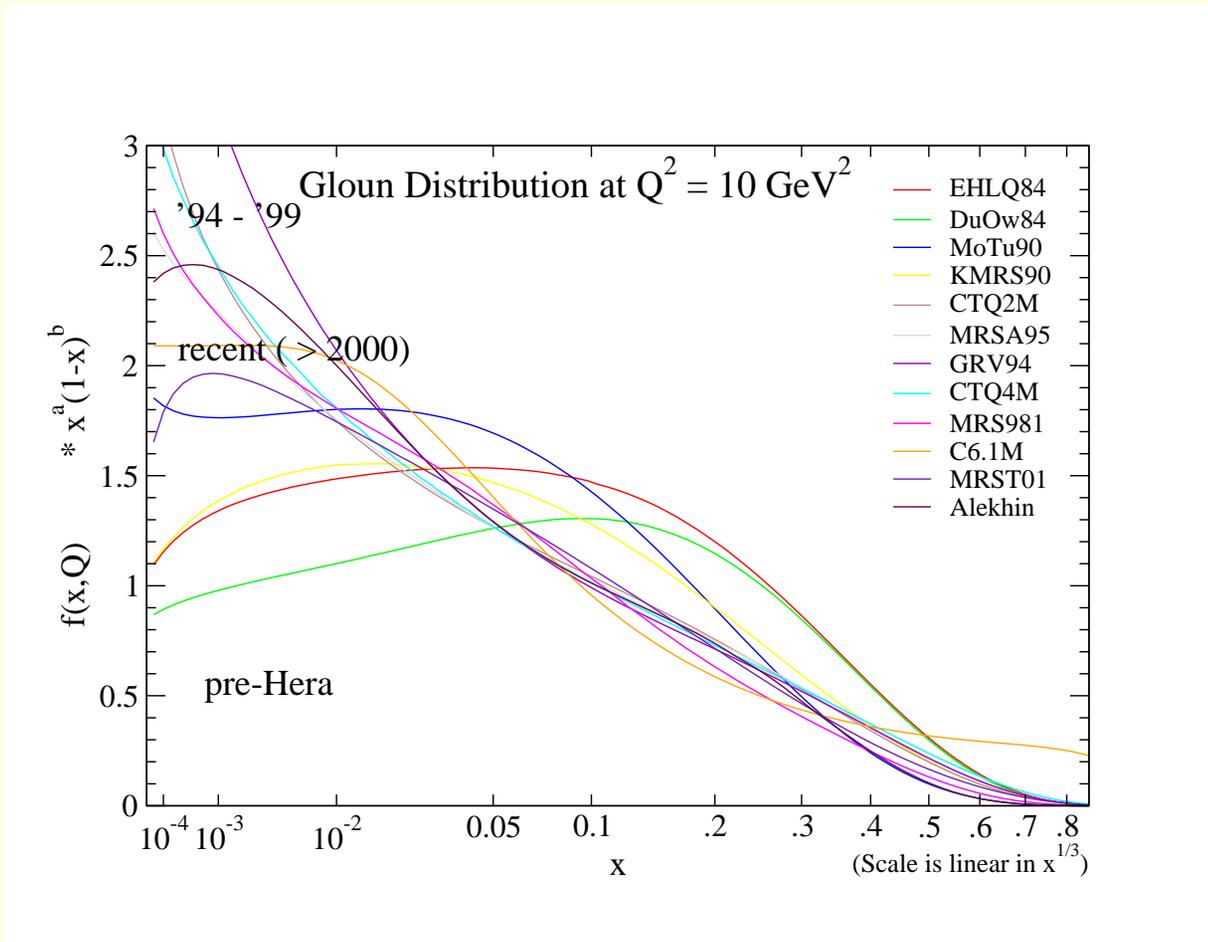
Some features not apparent from the figures

- DIS data provide strong constraints on the u and d distributions over the full range of x covered by the data
- The combination $4\bar{u} + \bar{d}$ is well constrained at small x
- The gluon is constrained at low values of x by the slope of the Q^2 dependence of F_2
- Need additional observables ...

Figure illustrating the kinematic coverage of current data

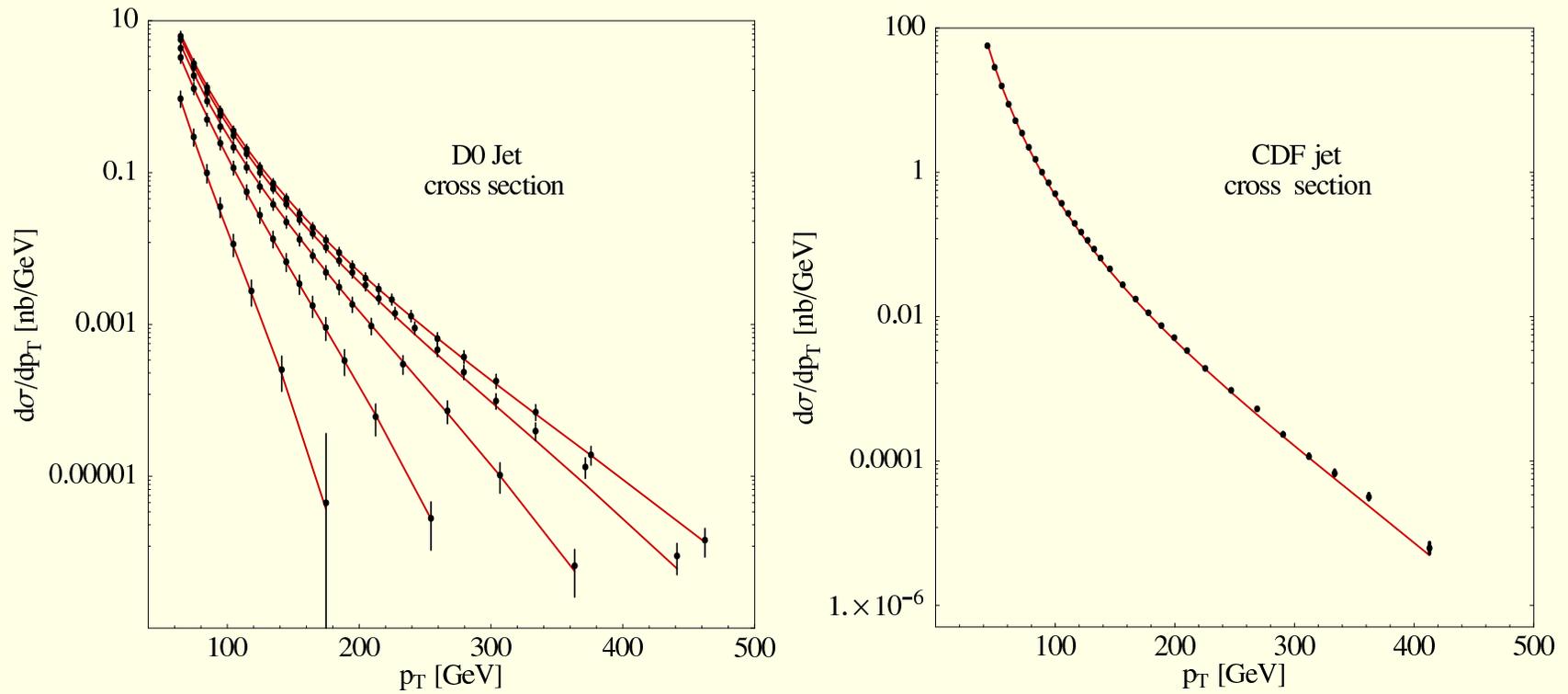


Pre-Hera data were limited to the lower left corner



- Comparison of various gluon distributions showing the effects of adding the HERA data
- There were no low- x data to constrain the gluon in the 1980s
- Illustrates the danger of extrapolating beyond the region where one has fit data.

High- E_T Jet Production



High- E_T jet data help constrain the gluon at large values of x

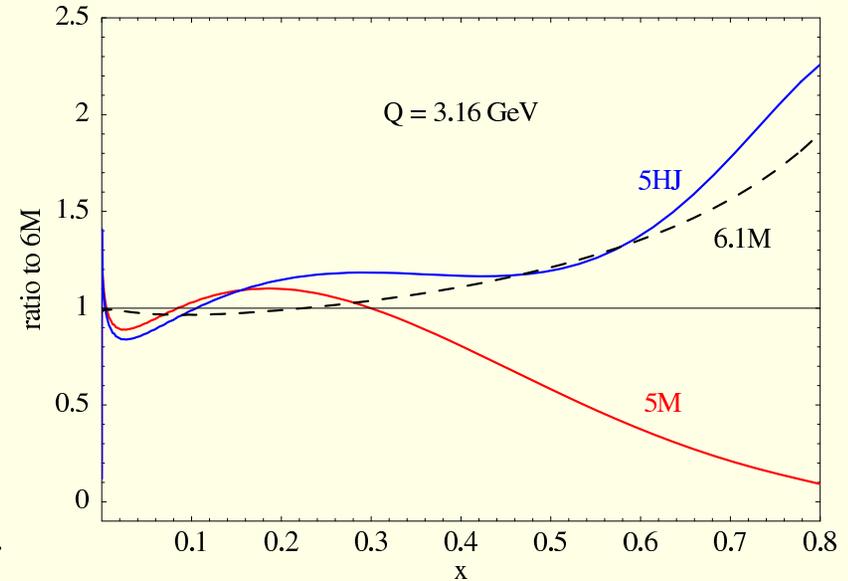
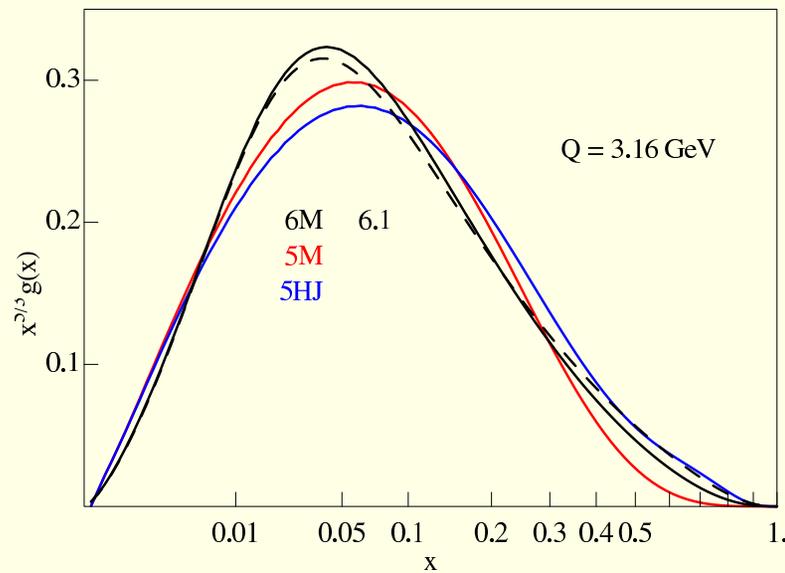
Some Kinematics

- The kinematics for the $2 \rightarrow 2$ subprocesses for the lowest order jet cross section sample x values of

$$x_{a,b} = \frac{E_T}{\sqrt{s}} (e^{\pm y_1} + e^{\pm y_2})$$

where $y_{1,2}$ are the jet rapidities

- Integrating over one of the jets smears out the ranges covered by $x_{a,b}$
- Basic effect is that as the jet rapidity grows, one x gets large and the other gets small.
- This allows one to probe the subprocess $gq \rightarrow gq$ and so one becomes sensitive to the gluon distribution



- Comparison of gluons from CTEQ5M, CTEQ5HJ, CTEQ6M, and CTEQ6.1M
- Gluon in the large- x region is constrained by the high- E_T jet data

Indications of $\bar{d} \neq \bar{u}$

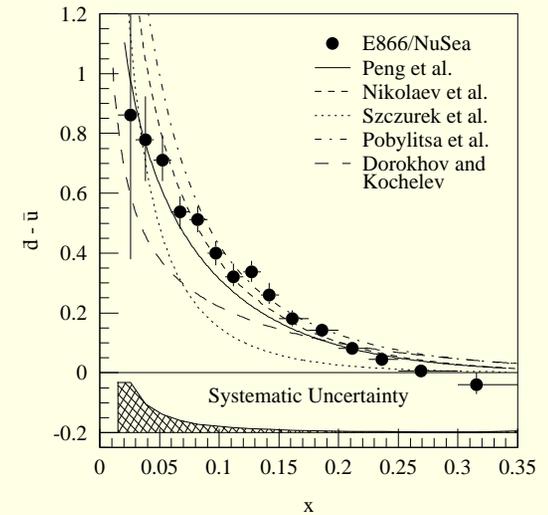
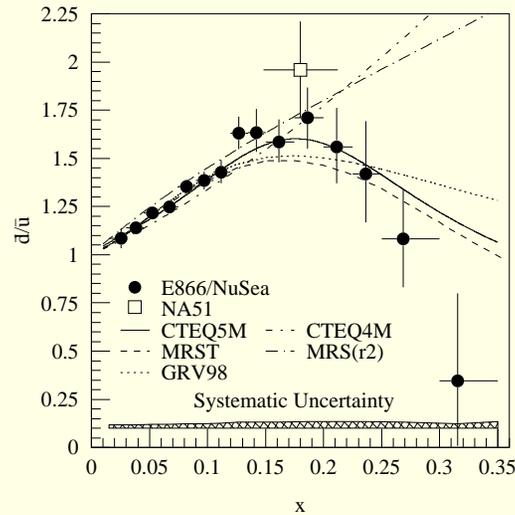
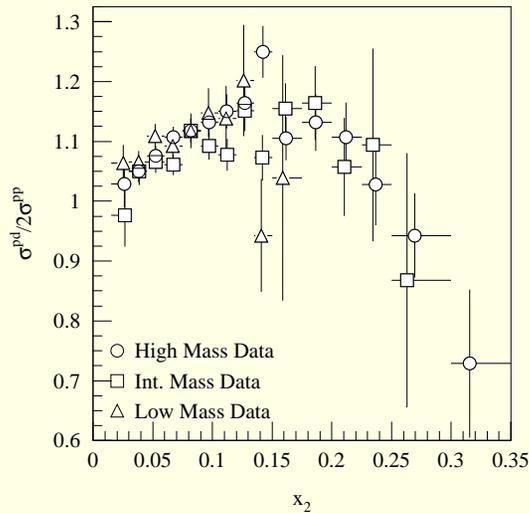
Gottfried Sum Rule

$$\begin{aligned} S_G &= \int_0^1 \frac{dx}{x} [F_2^p(x) - F_2^n(x)] \\ &= \frac{1}{3} + \frac{2}{3} \int_0^1 dx (\bar{u}(x) - \bar{d}(x)) \\ &= 0.235 \pm 0.026 \end{aligned}$$

$$\Rightarrow \bar{d} \neq \bar{u}$$

This result predated the NA-51 and E-866 results, but only suggested that $\bar{d} > \bar{u}$ with no indication of the x dependence.

Drell-Yan and \bar{d}/\bar{u}



- Towell et al., Phys. Rev.D64, 052002(2001)
- Let $R_{du}(x) = d(x)/u(x)$ and $\bar{R}_{du}(x) = \bar{d}(x)/\bar{u}(x)$
- For large x_1 and small x_2 (corresponding to large x_F) one can write the above cross section ratio in leading order as

$$\frac{\sigma_{pd}}{2\sigma_{pp}} \approx 1 + [\bar{R}_{du}(x_2) - 1] \frac{4 - R_{du}(x_1)}{8 + 2R_{du}(x_1)\bar{R}_{du}(x_2)}$$

- For large $x_1, d \ll u$ so one gets $\approx \frac{1}{2} (1 + \bar{R}_{du}(x_2))$

Why is $\bar{d} > \bar{u}$?

Pion Cloud argument

- Proton fluctuates into a neutron and a positive pion
- $p \rightarrow n\pi^+ \rightarrow p$
- At the quark level $uud \rightarrow (udd)(u\bar{d})$

$$\Rightarrow \bar{d} > \bar{u}$$

- This provides a simple model to motivate the breaking of the SU(2) symmetry of the sea quarks.

What about $s \neq \bar{s}$?

- Can get information utilizing the subprocesses

$$W^+ s \rightarrow c \text{ and } W^- \bar{s} \rightarrow \bar{c}$$

- The experimental signature involves muon pairs in the final state since the charm hadrons can decay semileptonically into states containing muons

$$c \rightarrow s \mu^+ \nu \text{ and } \bar{c} \rightarrow \bar{s} \mu^- \bar{\nu}$$

- So one sees

$$\nu N \rightarrow \mu^- c + X' \rightarrow \mu^- \mu^+ + X$$

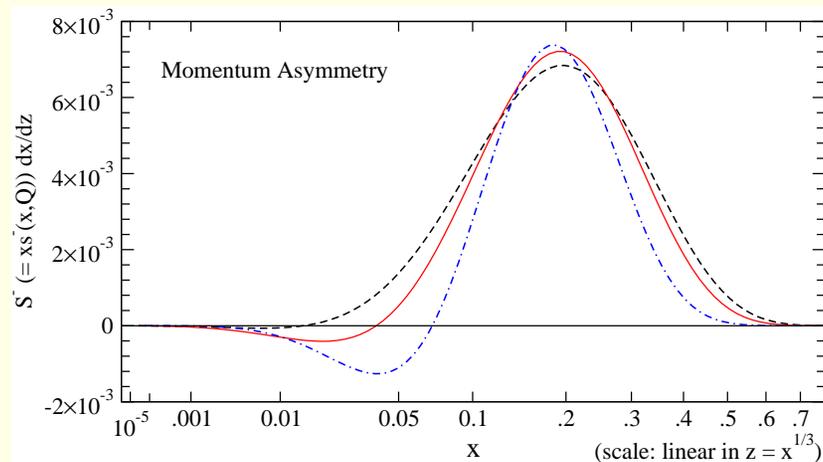
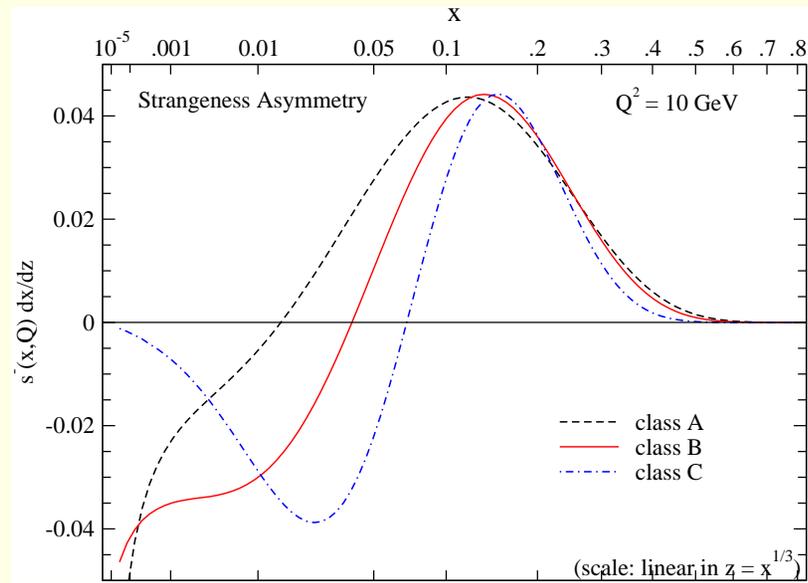
$$\bar{\nu} N \rightarrow \mu^+ \bar{c} + X' \rightarrow \mu^+ \mu^- + X$$

- Define number densities $s^\pm(x)$ and momentum densities $S^\pm(x)$

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

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

- Note: the strangeness number sum rule requires that $[s^-] = 0$ for all Q.
- This means that one must adopt a parametrization in which $s^-(x)$ has *at least* one zero



- Results from F. Olness et al., Eur. Phys. J.C40:145, 2005
- Scale expands the *low* – x region, Jacobian chosen so that the area under the curve represents the integral over x .

- The final result from this analysis is

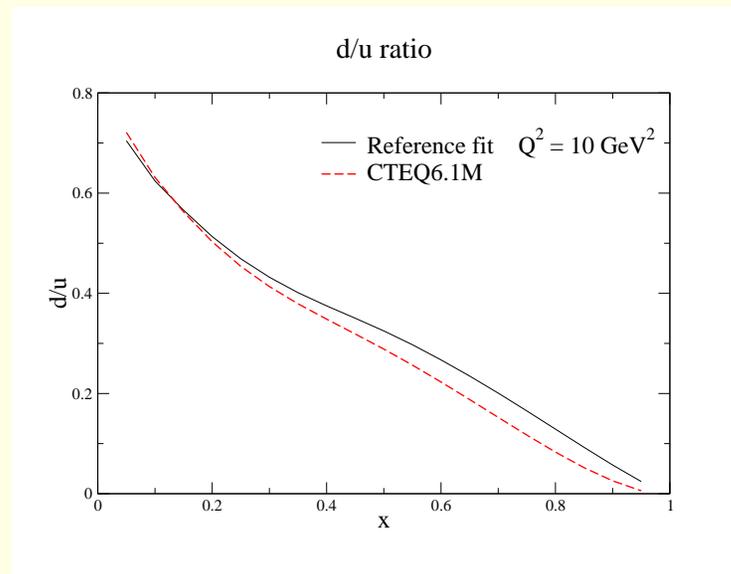
$$-0.001 < [S^-] < 0.004$$

- Consistent with s carrying slightly more momentum than \bar{s}
- Simple model: $p \rightarrow \Lambda K^+ \rightarrow p$
- At the quark level: $uud \rightarrow (uds)(u\bar{s})$
- Assumption is that the Λ carries most of the momentum of the proton and, hence, that the K^+ has a relatively smaller fraction of it
- Suggests $[S^-] > 0$

What about the valence quarks?

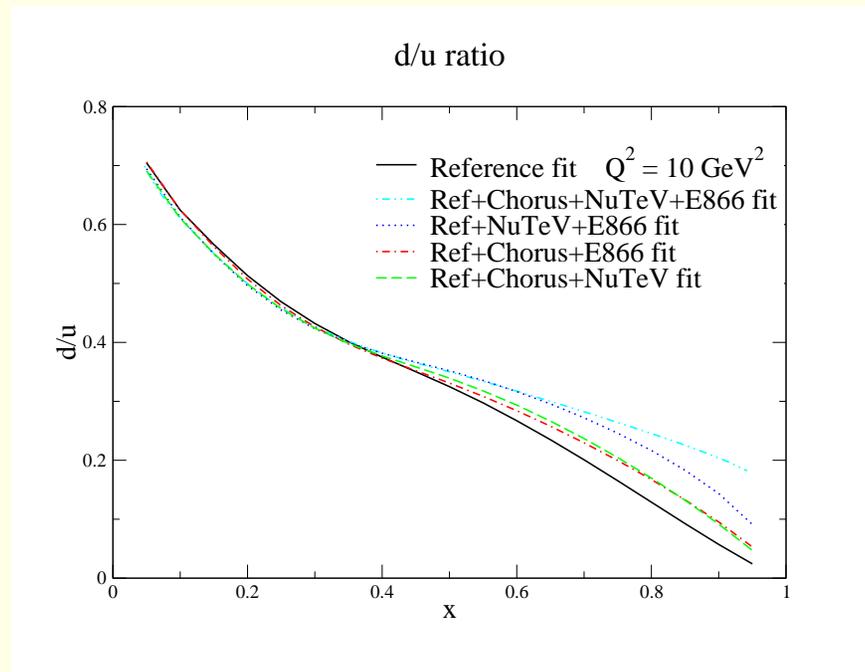
- Surely, they are well measured? well, yes and no,...
- Information on u and d quarks comes primarily from F_2^p and F_2^d in charged lepton DIS and F_2^N and xF_3^N measured in neutrino experiments.
- There are significant nuclear corrections in the neutrino experiments since heavy targets (iron, lead, ...) are typically used.
- There are even nuclear corrections associated with deuterium targets (see Wally Melnitchouk's lectures at the 2004 CTEQ Summer School for a good discussion)

- J.F. Owens et al., hep-ph/0702159, Phys. Rev.D75:054030(2007)
Recent analysis of the effects of adding new E-866, CHORUS, and NuTeV data into the global fits
- Figure shows the effect of including deuterium corrections in a CTEQ6.1M-based fit



- Shift in the medium-to-high- x region reflects the use of the deuterium corrections.
- d/u ratio changes but the χ^2 remains essentially unchanged
- Data are the same but the theory changes, so the PDFs change accordingly.

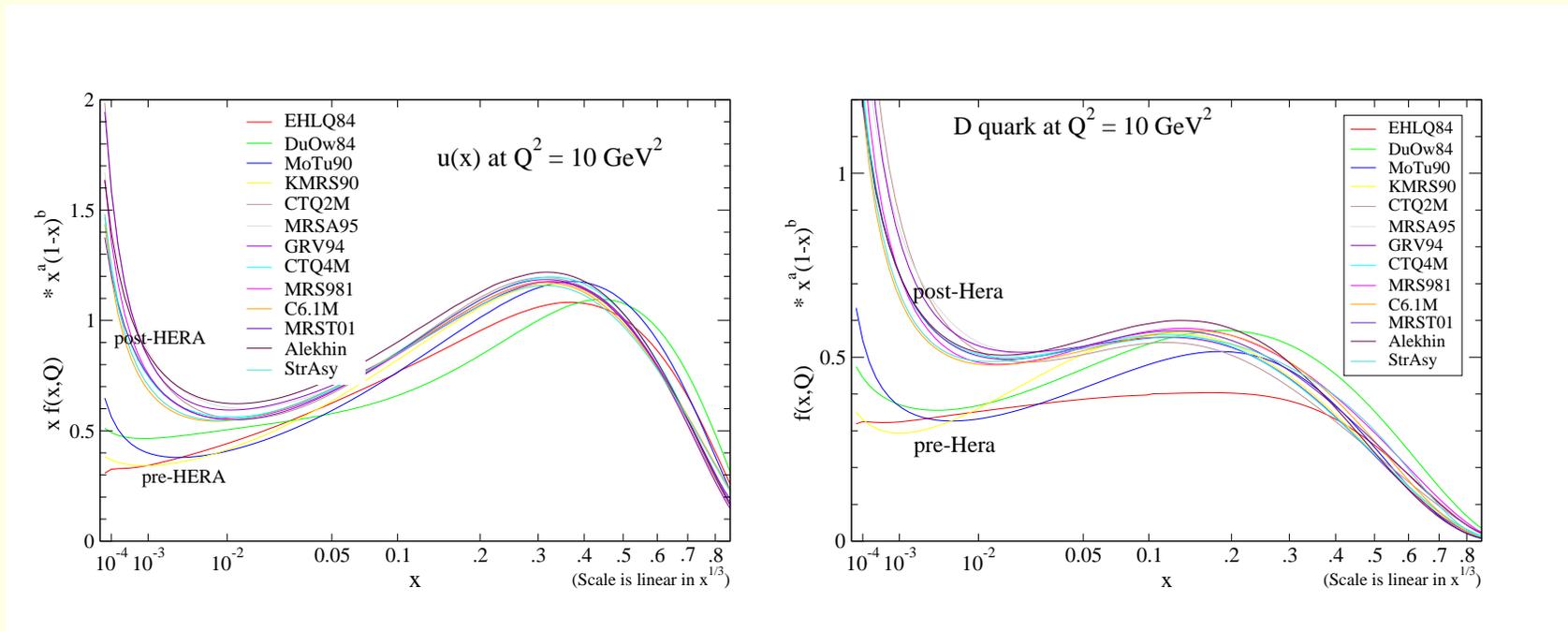
Analysis studied the effects of adding the E-866, CHORUS, and NuTeV data sets to the global fits. The short answer is that the E-866 data pulled the valence distributions down slightly at high- x while the NuTeV data pulled them higher. The tension between the two resulted in a severe spread of d/u values.



Final conclusion is that the nuclear corrections (for both deuterium and heavy targets) need to be understood better before definitive d/u studies can be made

PDF Error Analysis

Good old-fashioned way – plots lots of PDFs and look at the spread between the sets!



Figures from Wu-Ki Tung, hep-ph/0409145, showing a variety of PDF sets as they have evolved over the years.

- The previous method is *not* satisfactory because it is not systematic and it is not quantifiable.
- There are many sources of uncertainty in the PDFs, some of which we've touched on
 - Data set choice
 - Kinematic cuts
 - Parametrization choices
 - Treatment of heavy quarks, target mass corrections, and higher twist terms
 - Order of perturbation theory
 - Errors on the data
- Techniques have been developed to handle the last one
- The others require judgement and experience, but *are not* included in what are generally referred to as PDF errors.

Hessian Method

For a full discussion of the treatment of errors in fitting PDFs see the following references (and references therein):

1. Uncertainties of Predictions from Parton Distribution Functions I: the Lagrange Multiplier Method, D. Stump et al., Phys. Rev. D65:014012, 2002.
2. Uncertainties of Predictions from Parton Distribution Functions II: the Hessian Method, J. Pumplin et al., Phys. Rev. D65:014013, 2002.
3. New Generation of Parton Distributions with Uncertainties from Global QCD Analysis, J. Pumplin et al., JHEP 0207:012, 2002.
4. Dan Stump - PDF Lectures at the 2005 CTEQ Summer School

Basic idea is as follows:

Errors on data \rightarrow errors on PDF parameters \rightarrow uncertainty in theoretical predictions

Hessian Method (continued)

- PDF parameters denoted by $\{a_\mu\}$, $\mu = 1, \dots, d$
- As a byproduct of the fitting process, one obtains the Hessian $H_{\mu\nu}$

$$H_{\mu\nu} \equiv \frac{1}{2} \frac{\partial^2 \chi^2}{\partial a_\mu \partial a_\nu}$$

which is evaluated at the minimum of χ^2 .

- To estimate the error on some observable $X(a)$, taking into account only the experimental errors which entered into the calculation of χ^2 one uses the “Master Formula”

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

Comments

- Typically observe a large variation in the sensitivity of χ^2 to different observables. In practice, one uses the *eigenvectors* of $H_{\mu\nu}$ rather than the individual parameters.

$$(\Delta X)^2 = \frac{1}{4} \sum_{\mu=1}^d \left[X(S_{\mu}^{(+)}) - X(S_{\mu}^{(-)}) \right]^2$$

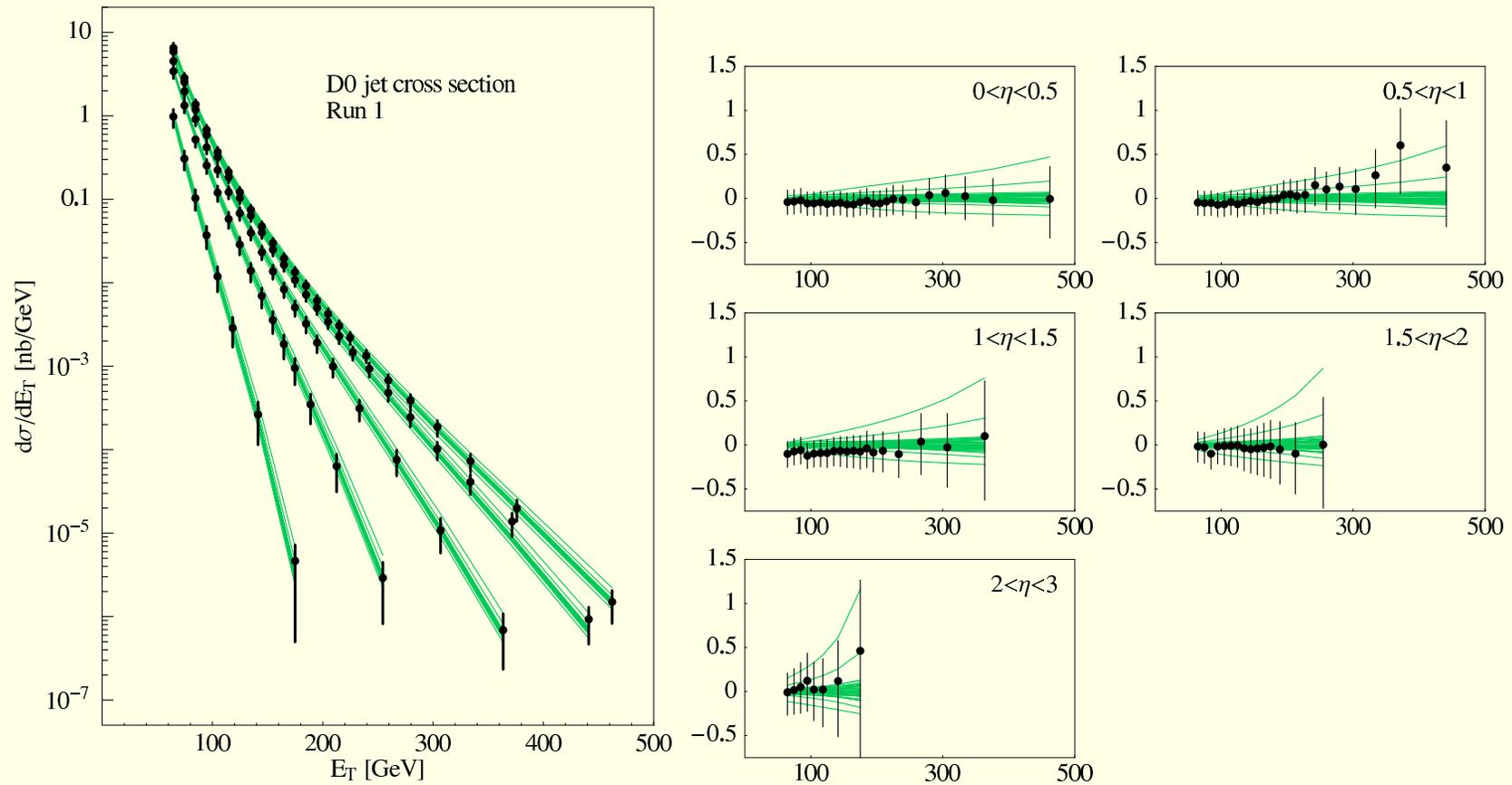
where $S_{\mu}^{(\pm)}$ denotes PDF sets with the parameters displaced along the \pm directions of the μ^{th} eigenvector by a distance corresponding to a tolerance $T = \sqrt{\Delta\chi^2}$

- CTEQ6M: Varied 20 parameters \Rightarrow “40 eigenvector basis sets”
- Can use the 40 sets to see the variations of some observable as the PDF parameters are varied in the allowed ranges

More Comments

- Critical quantity which determines the size of the error bands is the tolerance $T = \sqrt{\Delta\chi^2}$
- Usual choice, corresponding to gaussian errors on one experiment is $T = 1$
- The situation is made more complex by
 1. Systematic errors
 2. Multiple data sets
- For CTEQ6 an estimate of $T=10$ was used ($\Delta\chi^2 = 100$ for 2000 data points)
- Not a rigorous definition - based on how far the parameters could be varies while still yielding acceptable descriptions of all the data sets
- Different groups use different choices (and different choices of data sets)
- Must bear this in mind when comparing error estimates on PDFs from different groups

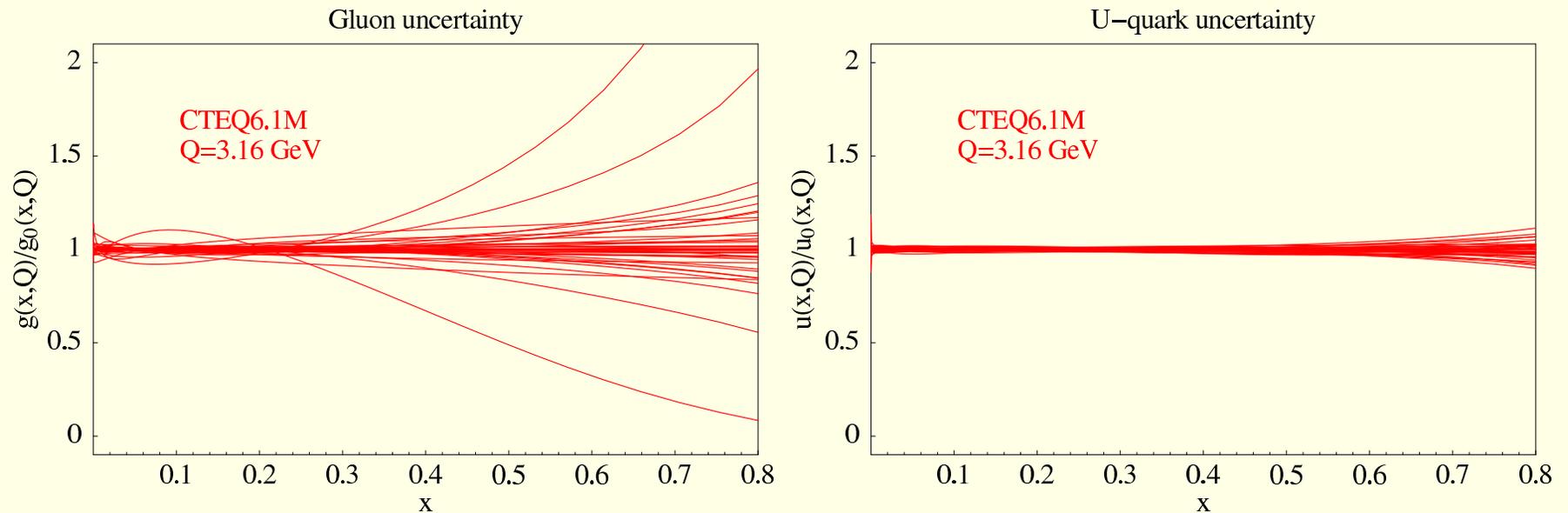
Large Example: High- E_T Jet Production



CTEQ6.1M compared to DØjet data (see D. Stump et al., JHEP 0310:046, 2003.)

High- E_T Jets (continued)

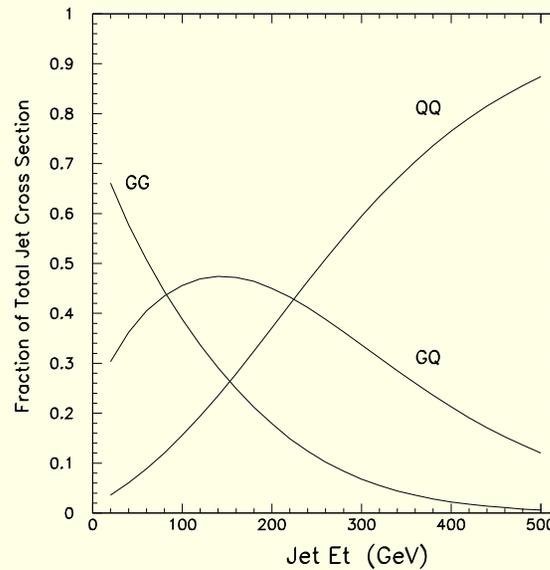
The 40 PDF sets can also be used to show the relative uncertainties of the PDFs themselves



Evident that the uncertainty is larger for the gluon than for the u quark, for example. Why is that?

Gluon PDF

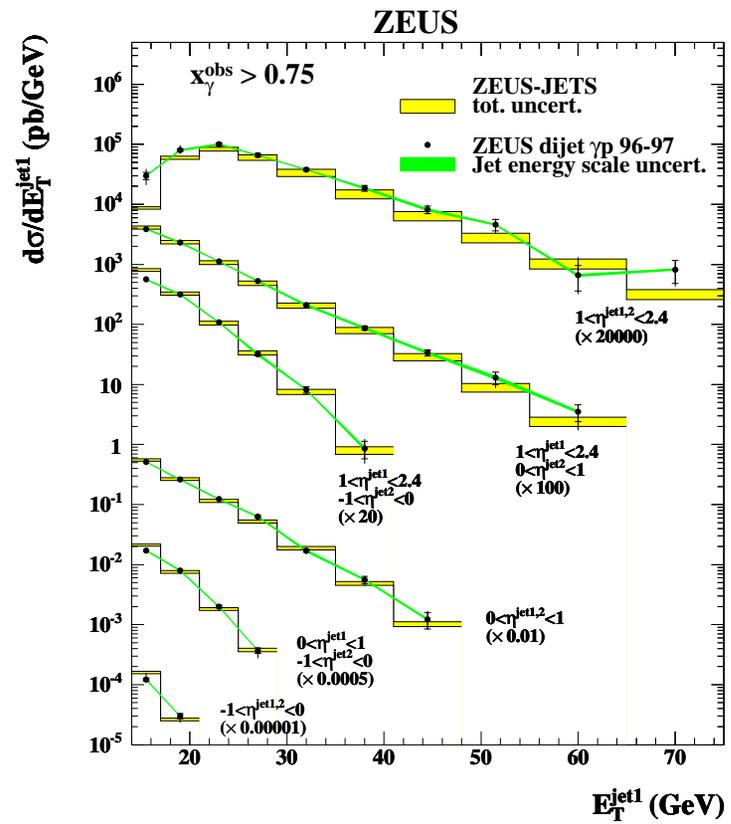
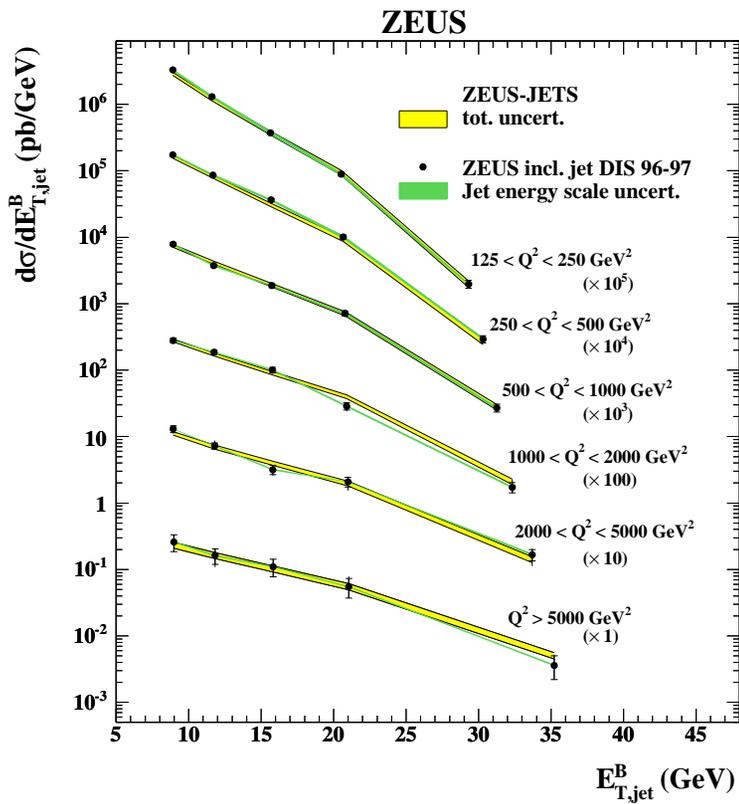
- Would like a process which is proportional to the gluon PDF at lowest order
- First thought might be **direct photon production** - $\mathcal{O}(\alpha\alpha_s)$ subprocesses are $q\bar{q} \rightarrow \gamma g$ and $qg \rightarrow \gamma q$
- Second choice would be **high- E_T jets** - $\mathcal{O}(\alpha_s^2)$ subprocesses are $qq \rightarrow qq, qg \rightarrow qg,$ and $gg \rightarrow gg$
- Can also use jet data from DIS processes – LO subprocesses are $\gamma^* q \rightarrow gq$ and $\gamma^* g \rightarrow q\bar{q}$
- Will say more about direct photons shortly, but look at the jets first.



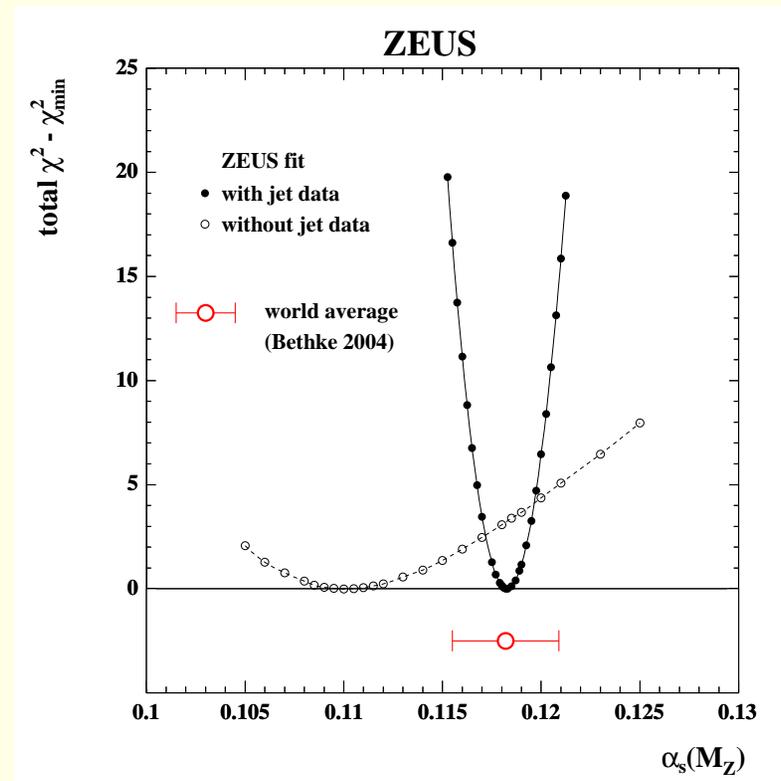
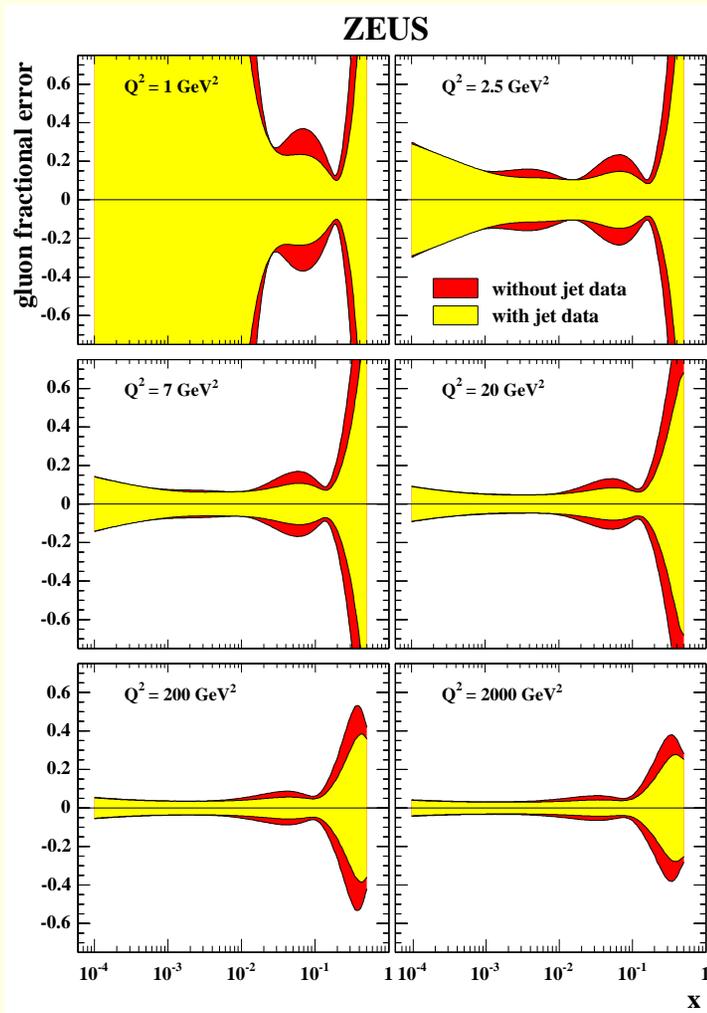
- Quark contributions dominate over the gluon subprocesses in the high- E_T region
- Range in $x_T = 2E_T/\sqrt{s}$ extends to about 0.5
- Sensitivity to higher x values is from the DGLAP equations - high x , low Q region feeds down to low x , high Q
- In current global fits the high- x gluon is constrained almost entirely by the High- E_T jet data
- Powerful, yet somewhat indirect constraint

Gluon PDF from DIS

- Low- x gluon PDF is constrained by the scaling violations in DIS
- Momentum sum rule connects the low- x and high- x behavior
- Include DIS jet data and dijet photoproduction data
- As noted previously, there is sensitivity to the gluon PDF in the lowest order subprocesses for jet DIS and photoproduction
- Data can also constrain α_s and break the correlation between α_s and the gluon shape.
 - A factor of α_s accompanies the gluon distribution in the DGLAP equations
 - A larger (smaller) α_s can be compensated by a smaller (larger) gluon contribution
- ZEUS PDF fits show a reduction in the error on the gluon distribution when DIS neutral current jet data and dijet photoproduction data are included in a global fit



Figures show jet data on the left and dijet photoproduction data on the right



The yellow bands show the reduction in the gluon uncertainty from adding the jet data to the fits. The figure on the right shows the reduction in the uncertainty on α_s .

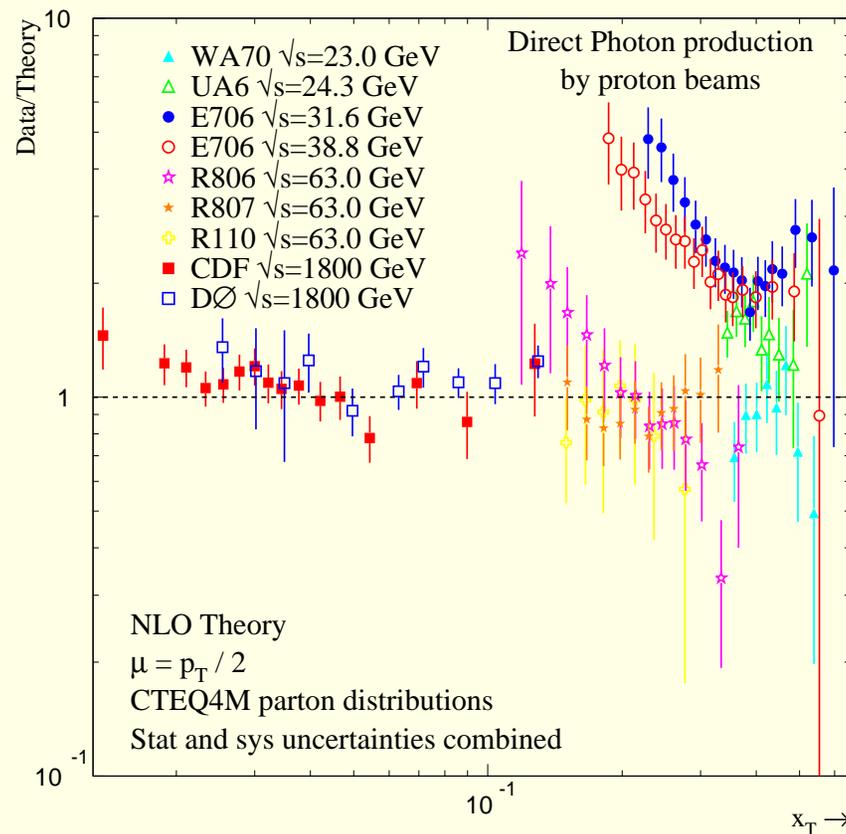
- The DIS jet data show promise for helping to constrain the gluon PDF
- The previous results used only ZEUS data and so were limited in their sensitivity to flavor decomposition
- Moreover, the error bands in the large- x region are comparable to those estimated in CTEQ6.1M
- It would be interesting to do a global fit including the DIS jet data

Next

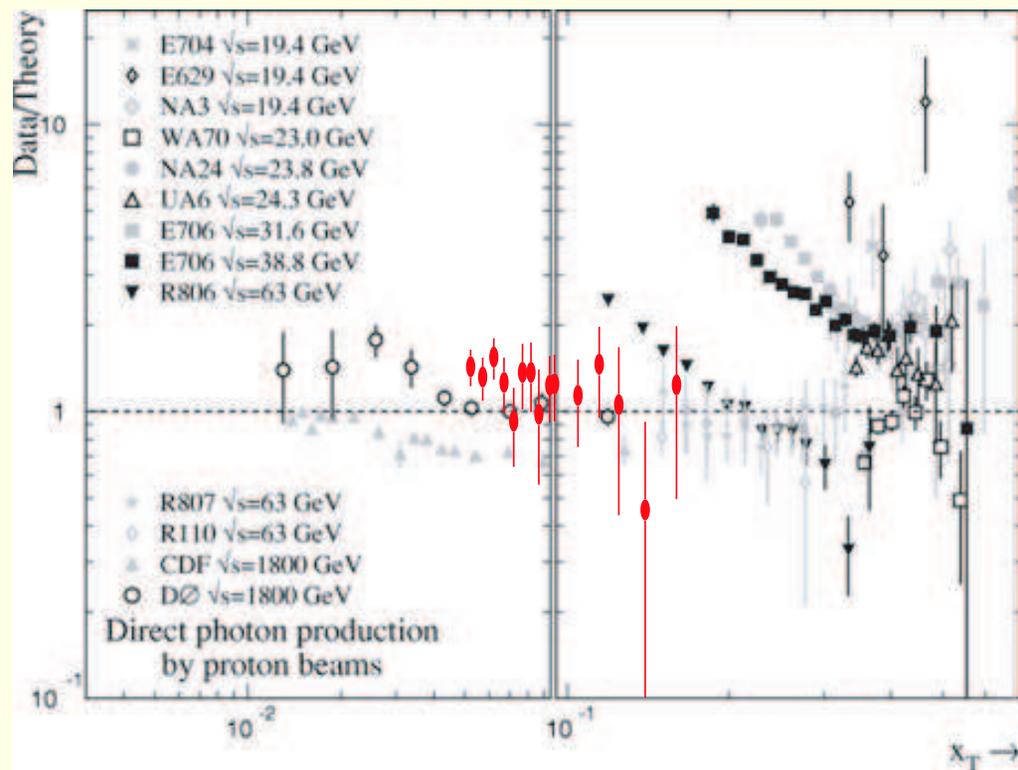
We used to include direct photon data in the global fits, but no longer do so. Whatever happened to direct photons?

Direct Photon Production

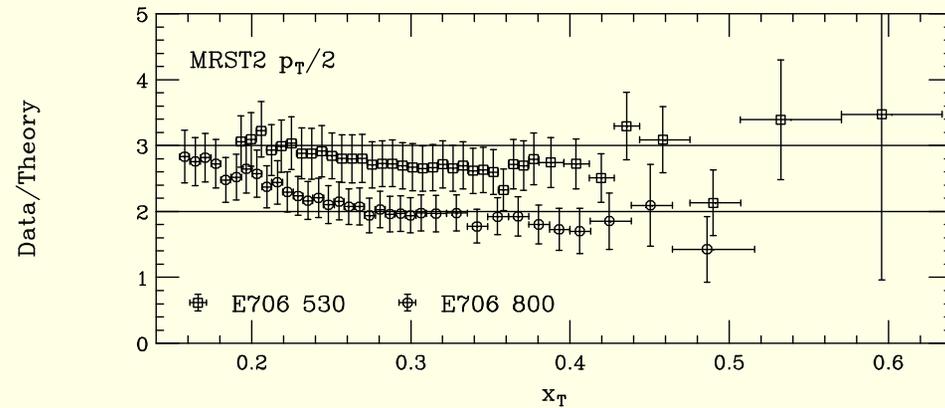
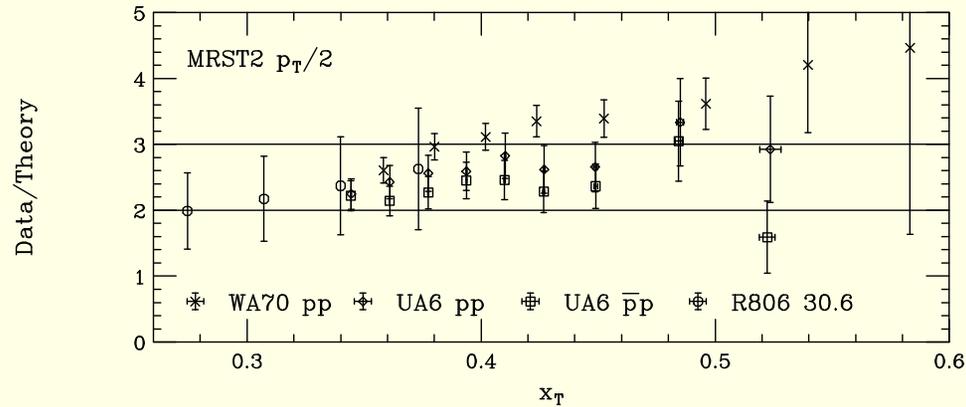
- Early candidate process for constraining the gluon PDF
- NLO calculations available by mid 1980's
- Fixed target experiments covered the range of x_T out to about 0.6
- But, when it came to global fits it seemed that there was a problem



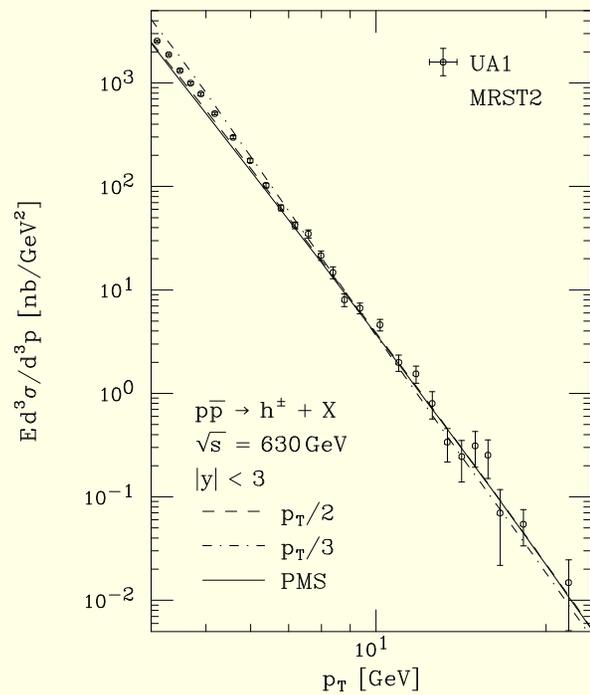
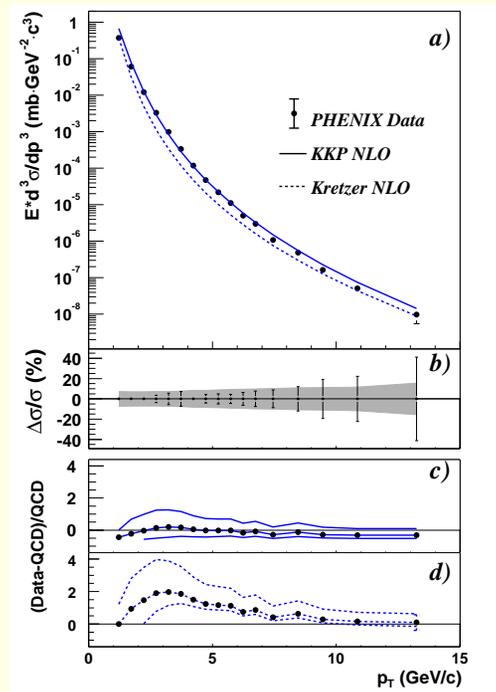
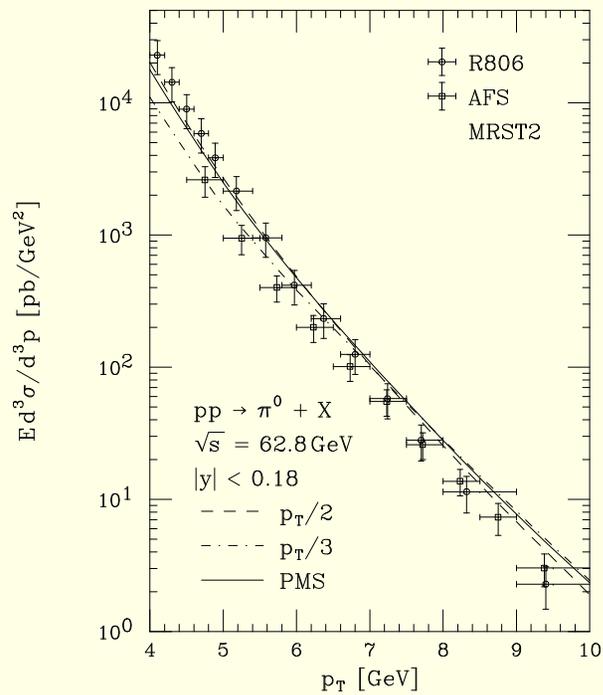
But, new PHENIX data confirmed that the situation gets better at higher energies



Meanwhile, a related problem existed with inclusive π^0 production



Data/Theory values were between 2-3 at fixed target energies, yet the agreement got better as one went up in energy.



Need a mechanism to get agreement with the fixed target regime without ruining the agreement at higher energies

Soft Gluon Resummation

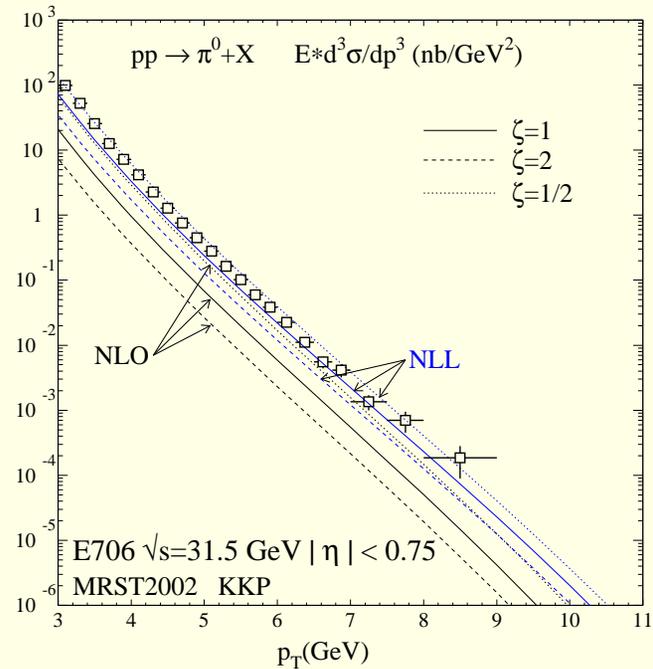
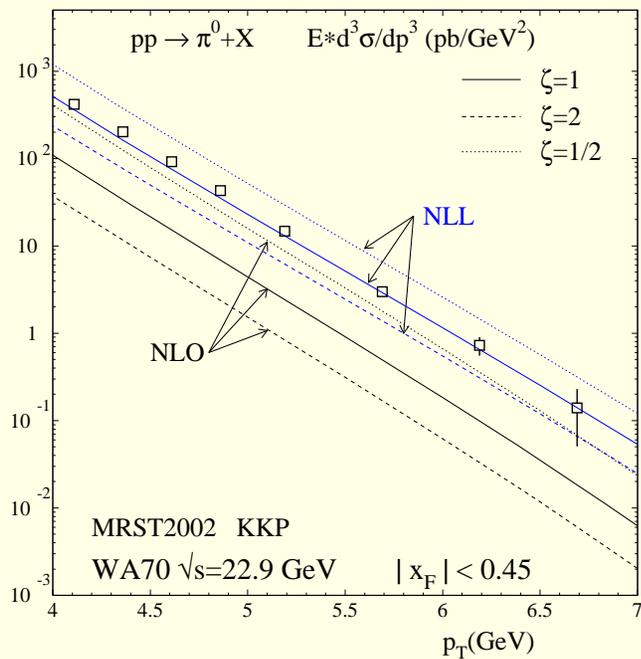
- Vogelsang and de Florian (hep-ph/0501258, Phys. Rev. D71:114004, 2005 and hep-ph/0506150, Phys. Rev. D72:014014, 2005) – possible explanation of both problems
- High- x_T π^0 production forces the fragmentation variable z towards one (trigger bias)

$$E \frac{d\sigma}{d^3p}(AB \rightarrow h + X) = \sum_{a,b,c} \int dx_a dx_b dz_c G_{a/A}(x_a) G_{b/B}(x_b) D_{h/c}(z_c) \frac{\hat{s}}{\pi z_c^2} \frac{d\sigma}{d\hat{t}}(ab \rightarrow c) \delta(\hat{s} + \hat{t} + \hat{u})$$

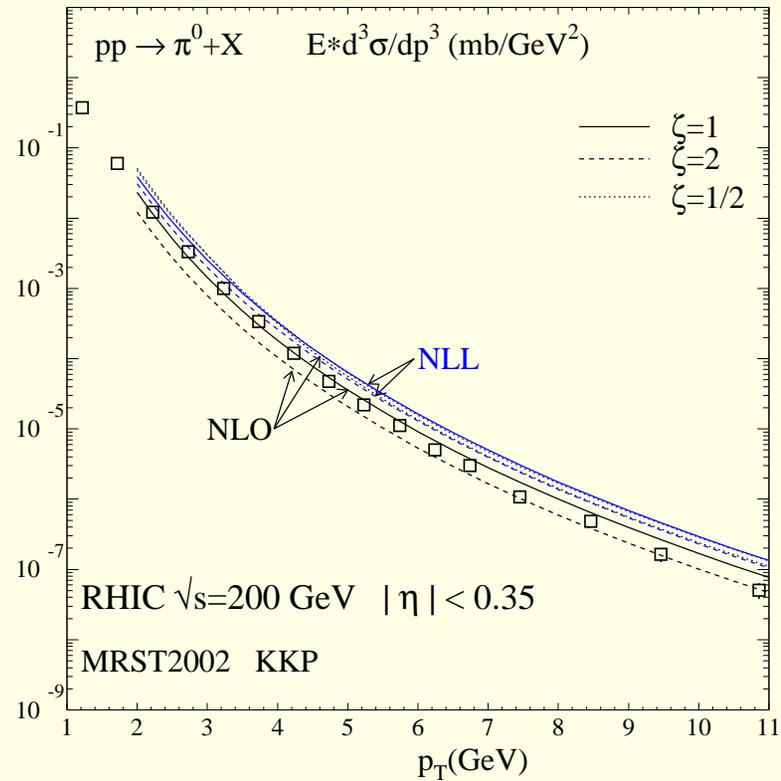
where \hat{s} , \hat{t} , and \hat{u} denote Mandelstam variables at the parton level.

- To get a high- p_T hadron it is more efficient to go to high z_c and lower parton-parton center-of-mass energy $\sqrt{\hat{s}}$ than to go to higher $\sqrt{\hat{s}}$ and lower z_c . This is referred to as trigger bias.

- As $z_c \rightarrow 1$ the phase space for the radiation of additional gluons is limited.
- This leads to large logarithmic corrections $\sim \log(1 - z_c)$
- Soft gluon resummation is a method for summing these large logarithmic contributions
- Vogelsang and de Florean showed that one could describe the fixed target π^0 data without ruining the good agreement found at higher energies
- At higher energies x_T is smaller, the trigger bias effect is reduced, and the resummation effects are smaller



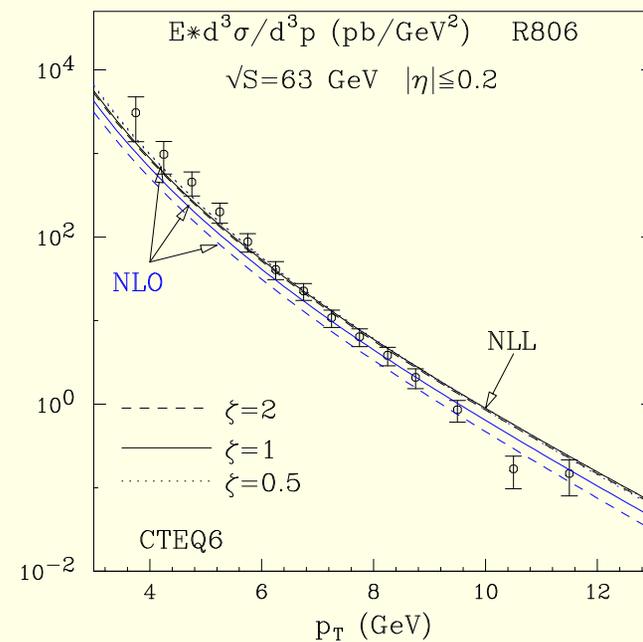
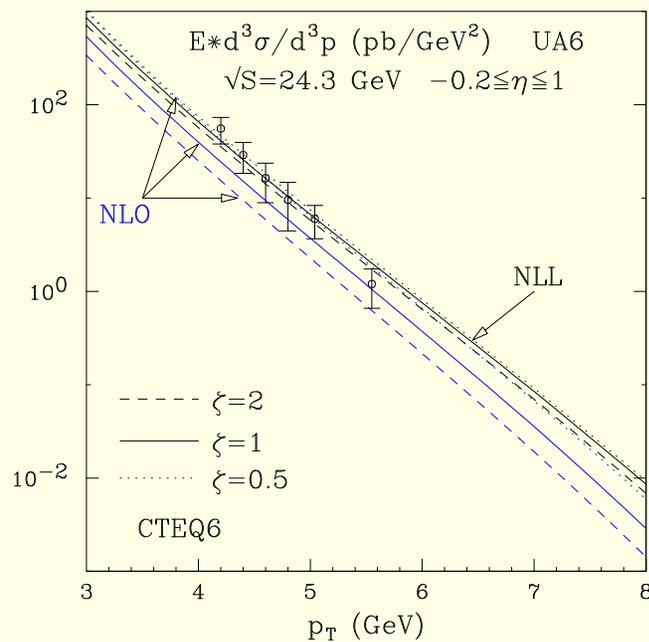
- Blue curves include the resummation corrections properly matched to an existing NLO calculation in order to avoid double counting.
- Note the reduced scale dependence of the resummed results.



- Note reduced enhancement at RHIC energy compared to the previous fixed target results

Photons can also be produced via processes involving photon fragmentation functions (see my photon lectures at previous CTEQ summer schools, for example)

Resummation also enhances the photon fragmentation component at fixed target energies

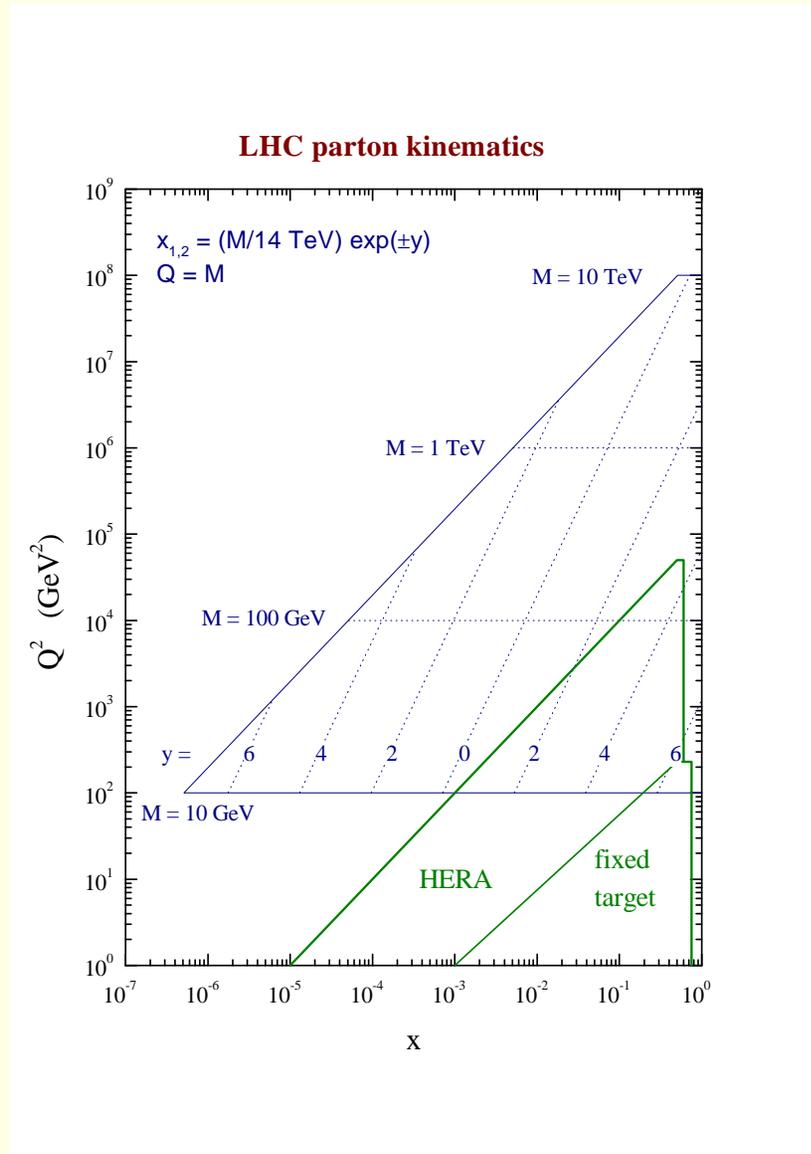


Effect is less pronounced at higher energies - retains good agreement at RHIC and TeVatron energies

Bottom line on threshold resummation

- Provides reduced scale dependence
- Provides an enhancement in the fixed target regime, but the effect is much smaller at higher energies
- Can improve the agreement with some fixed target experiments without adversely affecting the agreement at higher energies
- Global fits are currently done with a much better treatment of correlated systematic errors
- It would be interesting to do a global fit to direct photon data using resummed perturbation theory and including systematic errors.
- Perhaps this old problem could be put to rest!

A Look Ahead



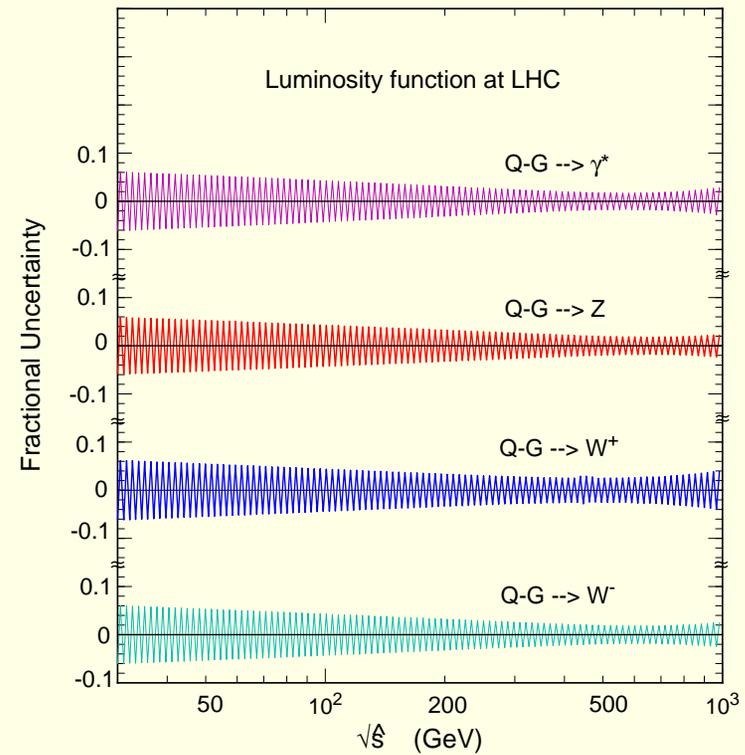
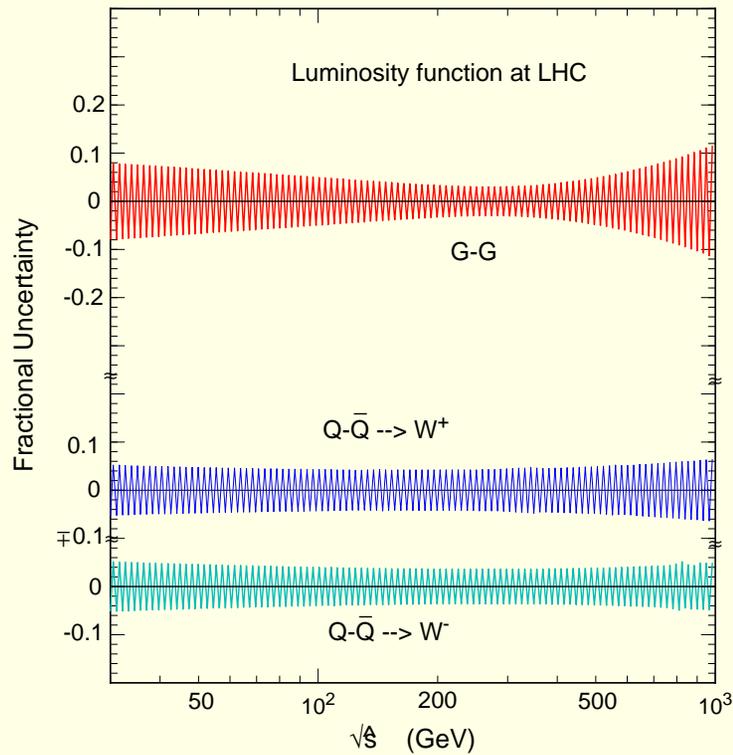
Kinematics of particle production at the LHC (hep-ph/0507015, Thorne et al.)

- Illustrates wide kinematic range over which pdf's must be known
- PDF technology will be driven by the needs of the LHC

Example – W production

- PDFs probed in the range of $x \approx M_W/\sqrt{s} \approx .006$
- Knowledge of sea quarks is important
- Can study the uncertainty bands on the luminosity functions

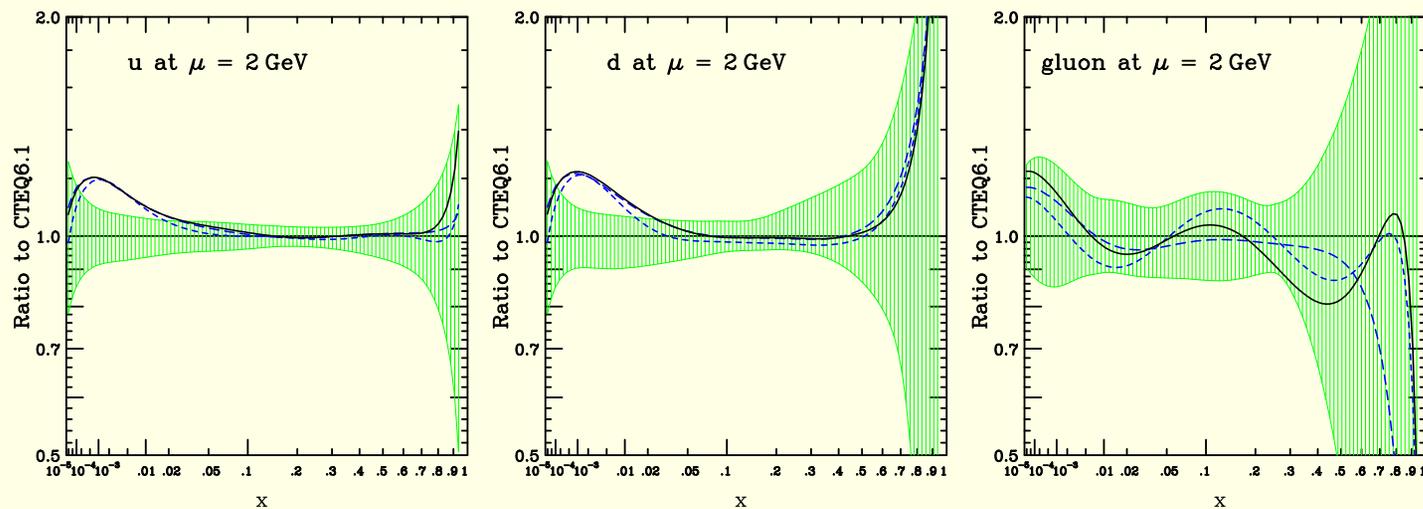
$$\begin{aligned}
 L(\hat{s}, s) &= \sum_{a,b} C_{ab} \int dx_a dx_b G_a(x_a, Q) G_b(x_b, Q) \delta(\hat{s} - x_a x_b s) \\
 &= \sum_{a,b} C_{ab} \int_{\hat{s}/s}^1 dx_a \frac{1}{x_a s} G_a(x_a, Q) G_b\left(\frac{\hat{s}}{x_a s}, Q\right)
 \end{aligned}$$



- Luminosity error bands from CTEQ6M
- $Q\bar{Q}$ band for W production shows about $\pm 5\%$ for $\hat{s} \approx M_W^2$
- CTEQ6M used the ZM-VFNS for treating the heavy quarks

W production (continued)

- Recent CTEQ6.5M global fit (hep-ph/0611254) used the VFNS with quark masses retained as summarized in Lecture I
- Formalism suppresses the heavy quark contributions relative to the zero mass case in the low- x , low- Q region
- Causes the u and d quark PDFs to increase relative to the ones from CTEQ6.1M to make up the difference since the data haven't changed



W production (continued)

- Differences persist to higher values of Q
- W production at the LHC is dominated by low- x u and d PDFs (since $u \approx \bar{u}, d \approx \bar{d}$ at low values of x)
- Causes an increase in the W cross section of $\Delta\sigma_W/\sigma_W = 8\%$
- This exceeds the estimate implied by the luminosity error band shown earlier
- Lesson is that the error bands can not account for a change in the theory!
- Likewise, the error bands that are typically quoted do not take into account the effects of the various choices and conventions discussed in Lecture I.
- The error bands only represent the propagation of experimental errors in the context of a given set of choices and conventions.

Prospective New Developments and CTEQ Projects

- Knowledge of PDFs at much smaller value of x will be needed for LHC predictions
 - Need to include final HERA cross section data in the global fits
- Extension of fitting package to NNLO
 - NNLO technology has been implemented in one evolution code and work is underway to include it in others
 - NNLO hard scattering cross sections are also becoming available
 - NNLO promises reduced scale dependence and better theoretical accuracy
- Impact of the treatment of heavy quark effects is still being evaluated
 - Affects fits at lower energies
 - Evolution can lead to changes in predictions at LHC energies

CTEQ Projects (continued)

- $(s - \bar{s})$
 - LO analysis completed - showed allowed range for $s - \bar{s}$
 - Extension to full NLO underway in conjunction with members of NuTeV
- Further study of d/u
 - Include new CDF and DØ W asymmetry data
 - Further study the role of deuterium corrections
 - Impact of final E-866 data
- Include above developments in a new CTEQ7 set

Concluding Comments for Lecture II _v

- You have seen an overview of how experimental errors are treated in the global fits
- The method for estimating the PDF error bands has been presented along with some cautionary words concerning the interpretation and use of these estimates
- Some examples of recent global fits have been described along with the potential impact on LHC physics
- Some current and future projects have been discussed

There is still much to be done in the area of global fits and the determination of PDFs!