Uncertainties in Parton Related Quantities

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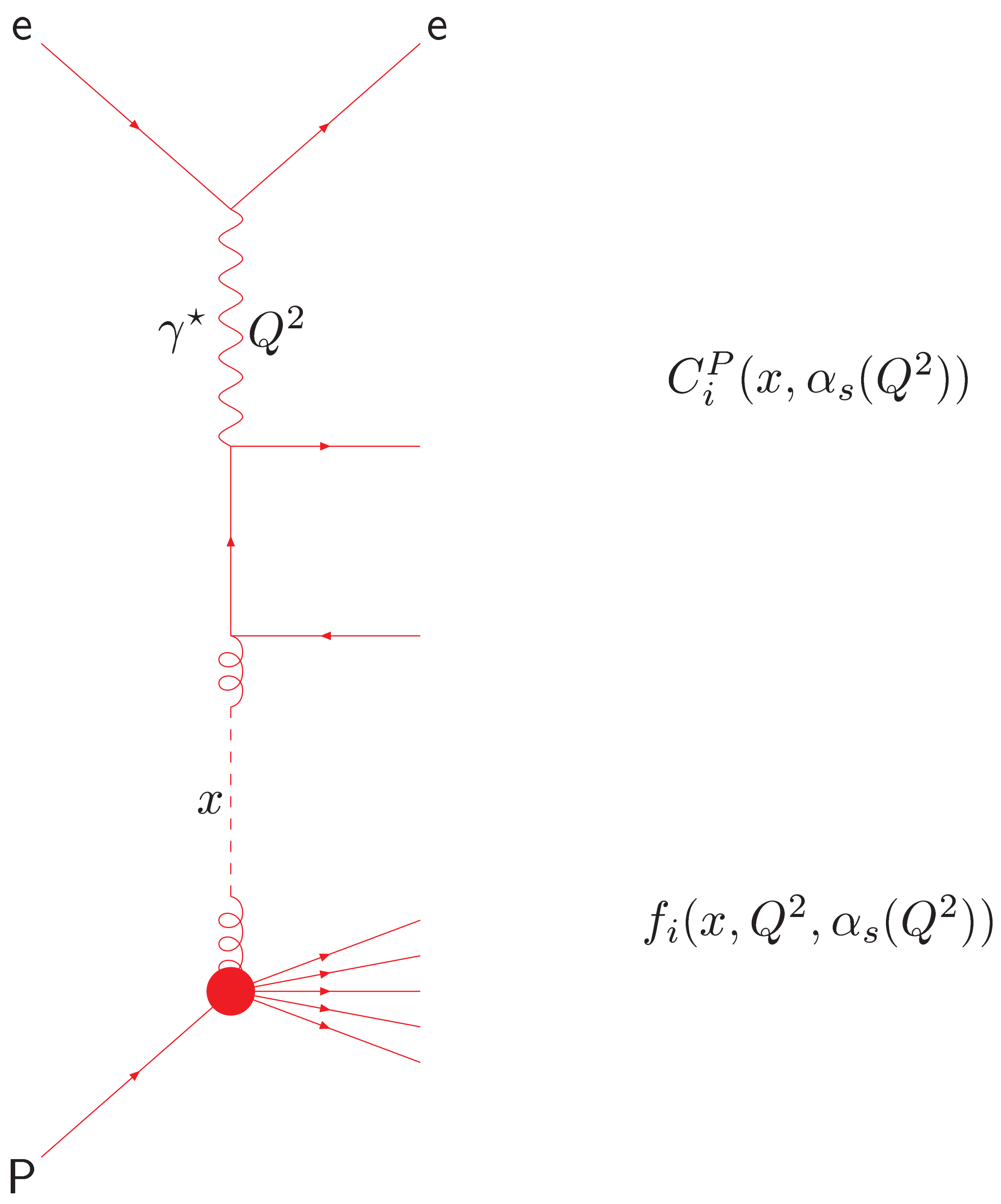
The fundamental quantities one requires in the calculation of scattering processes involving hadronic particles are the parton distributions. These can be derived from, and then used within, QCD. Using the **Factorization Theorem** it is possible to separate processes into nonperturbative parts which can be determined from experiment, and perturbative parts which can be calculated as a power-series in the strong coupling constant α_S.

Hadron scattering with an electron factorizes.



$\alpha_s(Q^2)$ – Strong Coupling

$x = \frac{2m\nu}{Q^2}$ – Momentum fraction of Parton (ν=energy transfer)

The cross-section for this process can be written in the factorized form

$$\sigma(ep \to eX) = \sum_i C_i^P(x, \alpha_s(Q^2)) \otimes f_i(x, Q^2, \alpha_s(Q^2))$$

where $f_i(x, Q^2, \alpha_s(Q^2))$ are the parton distributions, i.e the probability to find a parton of type i carrying a fraction x of the momentum of the hadron.

Corrections to above formula of size $\Lambda^2_{\rm QCD}/Q^2$ - Higher Twist. These can be associated with multi-parton correlation functions.

Because they depend on the nonperturbative way in which partons are bound into the hadron, these parton distributions are not calculable from first principles. However, they do evolve with Q^2 in a perturbative manner

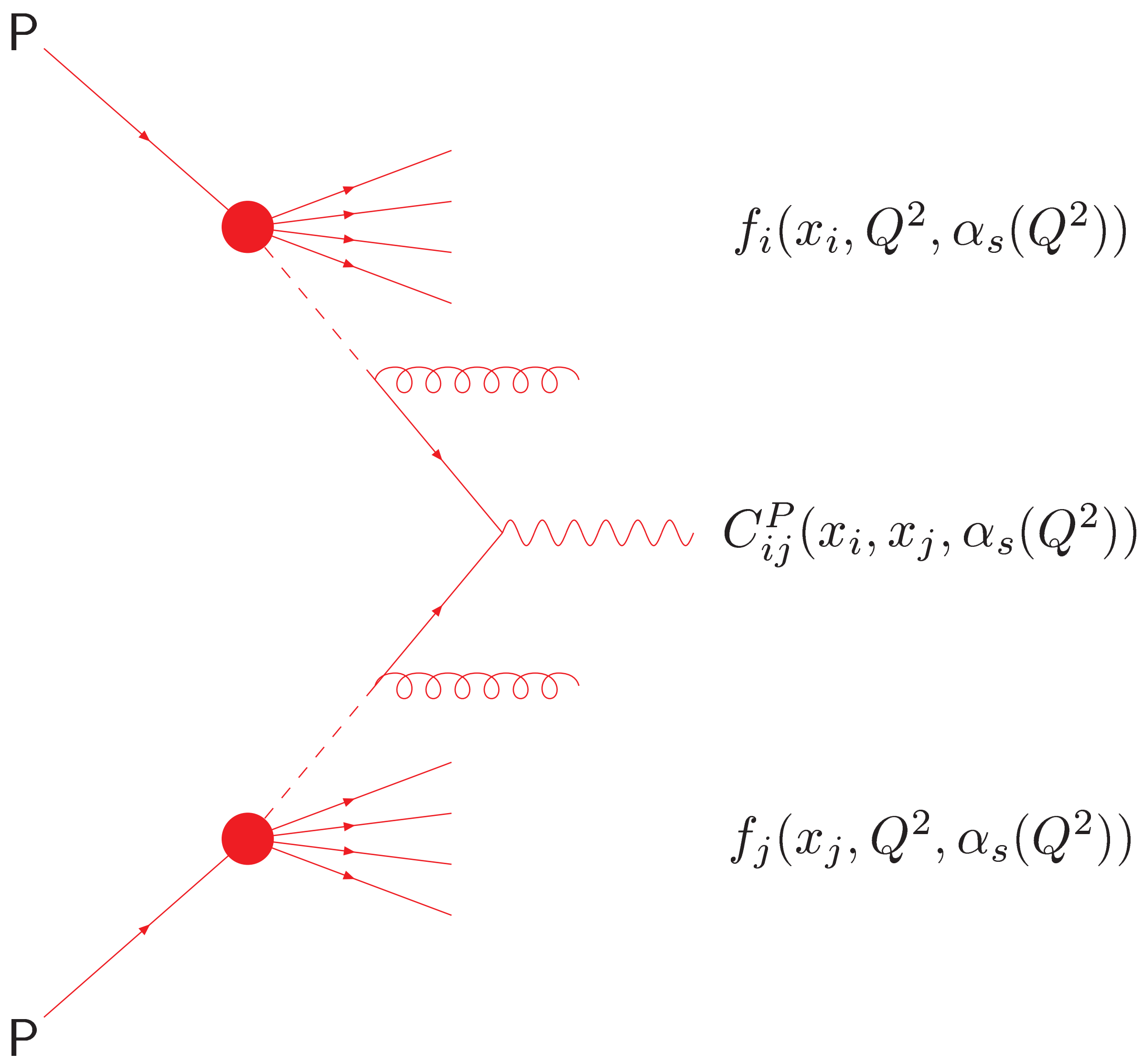
$$\frac{df_i(x, Q^2, \alpha_s(Q^2))}{d \ln Q^2} = \sum_i P_{ij}(x, \alpha_s(Q^2)) \otimes f_j(x, Q^2, \alpha_s(Q^2))$$

where the splitting functions $P_{ij}(x, Q^2, \alpha_s(Q^2))$ are calculable order by order in perturbation theory.

The coefficient functions $C_i^P(x, \alpha_s(Q^2))$ describing the hard scattering process are process dependent but are calculable as a power-series in the strong coupling constant $\alpha_s(Q^2)$.

$$C_i^P(x, \alpha_s(Q^2)) = \sum_k C_i^{P,k}(x)\alpha_s^k(Q^2).$$

Since the parton distributions $f_i(x, Q^2, \alpha_s(Q^2))$ are process-independent, i.e. **universal**, once they have been measured at one experiment, one can predict many other scattering processes.



Global fits to determine parton distributions use all available data - largely $ep \to eX$ (Structure Functions), and the most up-to-date QCD calculations to best determine **parton distributions** and their consequences. Currently use NLO–in–$\alpha_s(Q^2)$, i.e.

$$\begin{aligned} C_i^P(x,\alpha_s(Q^2)) &= C_i^{P,0}(x) + \alpha_S(Q^2)C_i^{P,0}(x). \\ P_{ij}(x,\alpha_s(Q^2)) &= \alpha_S(Q^2)P_{ij}^0(x) + \alpha_S^2(Q^2)P_{ij}(x). \end{aligned}$$

NNLO coefficient functions are known for some processes, e.g. structure functions, and NNLO splitting functions have considerable information, and may be known within a year or so. NNLO fits in near future.

Perturbation theory valid if $\alpha_s(Q^2) < 0.3$. Since running coupling constant $\alpha_s(Q^2)$

$$\alpha_s(Q^2) \approx \frac{4\pi}{(11 - 2/3N_f)\ln(Q^2/\Lambda^2_{QCD})}$$

where Λ_{QCD} is the scale of hadronic physics, i.e $\sim 150\mathrm{MeV}$, can use perturbation theory if $Q^2 > 2\mathrm{GeV}^2$. This cut should also remove influence of higher twists.

General procedure.

Start parton evolution at low scale $Q_0^2 \sim 1\mathrm{GeV}^2$, and evolve partons upwards using NLO DGLAP equations. Fit data for scales above $2-5\mathrm{GeV}^2$. In principle 11 different parton distributions to consider

$$u, \bar{u}, \quad d, \bar{d}, \quad s, \bar{s}, \quad c, \bar{c}, \quad b, \bar{b}, \quad g$$

$m_c, m_b \gg \Lambda_{\mathrm{QCD}}$ so heavy parton distributions determined perturbatively. Assume $s = \bar{s}$. Leaves 6 independent combinations. Relate s to $1/2(\bar{u}+\bar{d})$ and use

$$u_V = u - \bar{u}, \quad d_V = d - \bar{d}, \quad \mathrm{sea} = 2*(\bar{u}+\bar{d}+\bar{s}), \quad \bar{d}-\bar{u}, \quad g,$$

Input partons parameterized as, e.g.

$$xf(x, Q_0^2) = (1-x)^\eta (1 + \epsilon x^{0.5} + \gamma x) x^\delta.$$

For non-singlet combinations, valence quarks, $\bar{d}-\bar{u}$, δ expected to be ~ 0.5. For singlet combinations, sea and gluon, δ expected to be ~ 0.

Also define the singlet quark distribution

$$\Sigma = u_V + d_V + \mathrm{sea} + (c+\bar{c}) + (b+\bar{b})$$

Assuming isospin symmetry $p \to n$ leads to

$$d(x) \to u(x) \qquad u(x) \to d(x).$$

Various sum rules constraining parton inputs and conserved order by order in α_S for evolution.

$$\int_0^1 u_V(x)\,dx = 2 \qquad \int_0^1 d_V(x)\,dx = 1$$

i.e. conservation of number of valence quarks.

Also conservation of momentum carried by partons

$$\int_0^1 x\Sigma(x) + xg(x)\,dx = 1.$$

Important constraint on form of gluon which is only probed indirectly.

In determining partons need to consider that not only are there 6 different combinations of partons, but also wide distribution of x from 0.75 to 0.00003. Need many different types of experiment for full determination.

Data used

H1 $F_2^{e^+p}(x,Q^2)$ 1996-97 moderate Q^2 and 1996-97 high Q^2, and $F_2^{e^-p}(x,Q^2)$ 1998-99 high Q^2 small x.

ZEUS $F_2^{e^+p}(x,Q^2)$ 1996-97 small x wide range of Q^2.

NMC $F_2^{\mu p}(x,Q^2), F_2^{\mu d}(x,Q^2), (F_2^{\mu n}(x,Q^2)/F_2^{\mu p}(x,Q^2))$ medium x.

E665 $F_2^{\mu p}(x,Q^2), F_2^{\mu d}(x,Q^2)$ medium x.

BCDMS $F_2^{\mu p}(x,Q^2), F_2^{\mu d}(x,Q^2)$ large x.

SLAC $F_2^{\mu p}(x,Q^2), F_2^{\mu d}(x,Q^2)$ large x.

CCFR $F_2^{\nu(\bar{\nu})p}(x,Q^2), F_3^{\nu(\bar{\nu})p}(x,Q^2)$ large x , singlet, valence.

ZEUS $F_{2,c}^{e^+p}(x,Q^2)$ 1996-97 charm.

E605 $pN \to \mu\bar{\mu} + X$ large x sea.

E866 Drell-Yan asymmetry $\bar{u}, \bar{d}$ $\bar{d} - \bar{u}$.

CDF W-asymmetry u/d ratio at high x.

CDF Inclusive jet data high x gluon.

D0 Inclusive jet data high x gluon.

CCFR Dimuon data NuTev constrains strange sea.

Results.

Above procedure completely determines parton distributions at present. Total fit reasonably good, e.g CTEQ6.

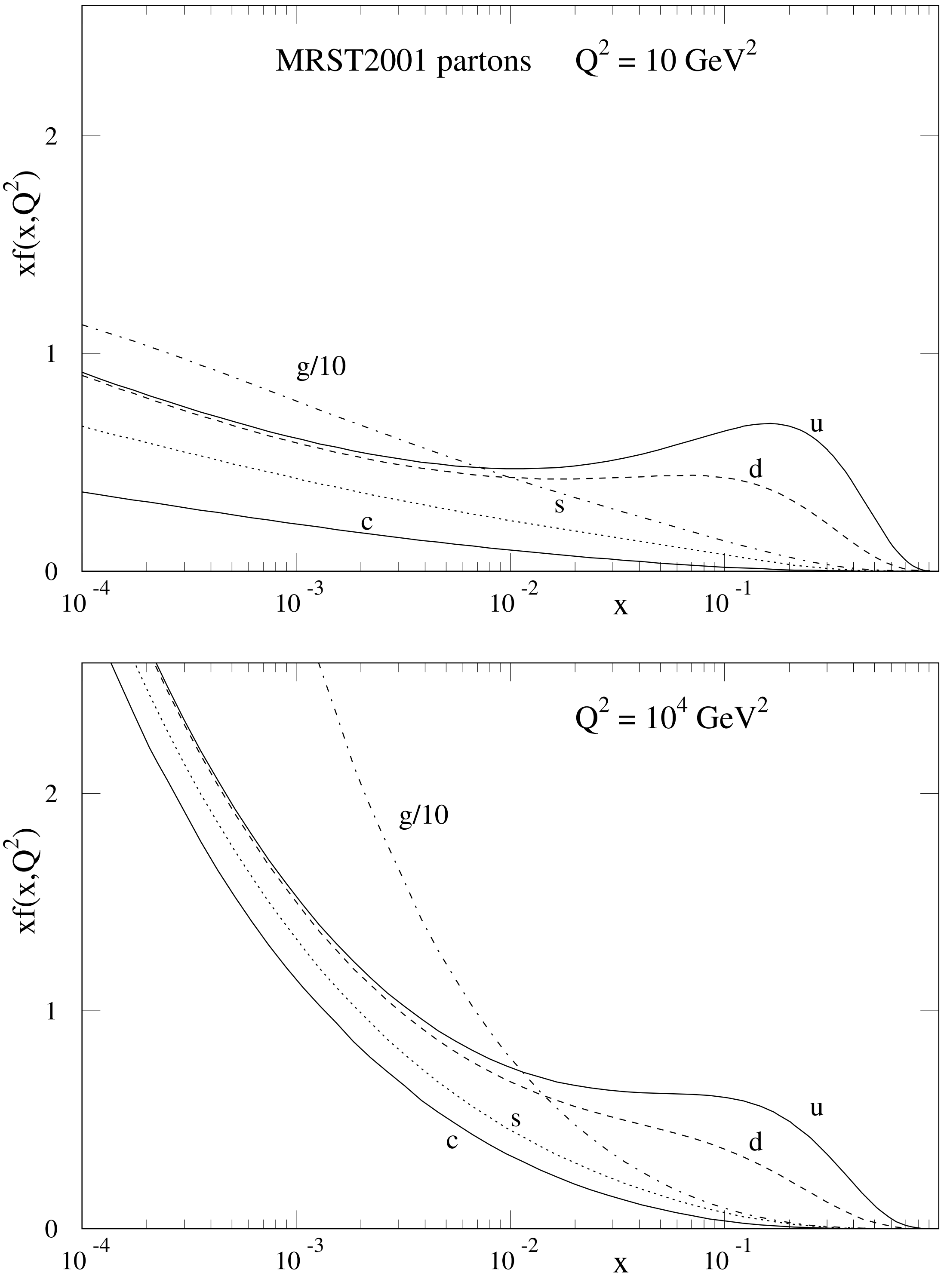
Data set	No. of data pts	χ^2
H1 ep	230	228
ZEUS ep	229	263
BCDMS μp	339	378
BCDMS μd	251	280
NMC μp	201	305
E605 (Drell-Yan)	119	95
D0 Jets	90	65
CDF Jets	33	49

And about 1 per point for smaller sets. $\alpha_S(M_Z^2)$ fixed at 0.118. Total $\chi^2 = 1954/1811$.

For MRST $\alpha_S(M_Z^2) = 0.119$. Compromise between different data sets. Total $\chi^2 = 2328/2097$ - but errors treated differently, and different data sets and cuts.

Some areas where theory perhaps needs to be improved.

Resulting partons over-leaf.



MRST2001 partons. CTEQ very similar.

Quality of fit.

Determined by χ^2 of fit to data. Various alternatives to calculating this.

Simplest - adding statistical and systematic errors in quadrature. Ignores correlations between data points. Should be improved (but sometimes perhaps not so bad?)

Covariance Matrix. The covariance matrix is constructed as

$$C_{ij} = \delta_{ij}\sigma^2_{i,stat} + \sum_{k=1}^{n} \rho^k_{ij}\sigma_{k,i}\sigma_{k,j},$$

where k runs over each source of correlated systematic error and ρ^k_{ij} are the correlation coefficients. The χ^2 is defined by

$$\chi^2 = \sum_{i=1}^{N}\sum_{j=1}^{N}(D_i - T_i(a))C^{-1}_{ij}(D_j - T_j(a)),$$

where N is the number of data points, D_i is the measurement and $T_i(a)$ is the theoretical prediction depending on parton input parameters a. Unfortunately this relies on inverting large matrices.

Minimization w.r.t. systematic errors. Here we incorporate the systematic errors into the theory prediction

$$f_i(a,s) = T_i(a) + \sum_{k=1}^{n} s_k \Delta_{ik},$$

where Δ_{ik} is the one-sigma correlated error for point i from source j. In this case the χ^2 is defined by

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{D_i - f_i(a,s)}{\sigma_{i,unc}} \right)^2 + \sum_{k=1}^{n} s_k^2,$$

where the second term constrains the values of s_k. This allows the data to move *en masse* relative to the theory, but assumes the correlated systematic errors are Gaussian distributed.

Can solve for each of the s_k analytically. Defining

$$B_k = \sum_{i=1}^{N} \frac{\Delta_{ik}(D_i - T_i(a))}{\sigma_{i,unc}^2}, \qquad A_{kl} = \delta_{kl} + \sum_{i=1}^{N} \frac{\Delta_{ik}\Delta_{il}}{\sigma_{i,unc}^2},$$

$$\frac{\partial \chi^2}{\partial s_k} = 0 \quad \rightarrow \quad s_i(a) = \sum_{l=1}^{n} (A^{-1})_{kl} B_l.$$

This leads to the χ^2 definition

$$\chi^2 = \sum_{i=1}^{N}\left(\frac{(D_i - T_i(a))}{\sigma_{i,unc}}\right)^2 - \sum_{k=1}^{n}\sum_{l=1}^{n} B_k (A^{-1})_{kl} B_l.$$

It can be shown that this is identical to the correlation matrix definition of χ^2, but it has the double advantage that smaller matrices need inverting and one sees the shift of data relative to theory explicitly.

However, are Gaussian correlated errors realistic? Is it valid to move data to compensate for the shortcomings of theory?

MRST find that for HERA data increments in χ^2 using this method are same as for adding in quadrature, and data moves towards theory rather than *vice versa* (sometimes in forbidden manner).

More sophisticated treatment is found to be essential for Tevatron jets where correlated systematic errors dominate. Used by all groups.

Parton Uncertainties - currently an issue attracting a lot of work. Number of approaches.

Hessian (Error Matrix) approach first used by H1 and ZEUS, recently extended by CTEQ.

$$\chi^2 - \chi^2_{min} \equiv \Delta\chi^2 = \sum_{i,j} H_{ij}(a_i - a_i^{(0)})(a_j - a_j^{(0)})$$

The Hessian matrix H is related to the covariance matrix of the parameters by

$$C_{ij}(a) = \Delta\chi^2 (H^{-1})_{ij}.$$

We can then use the standard formula for linear error propagation.

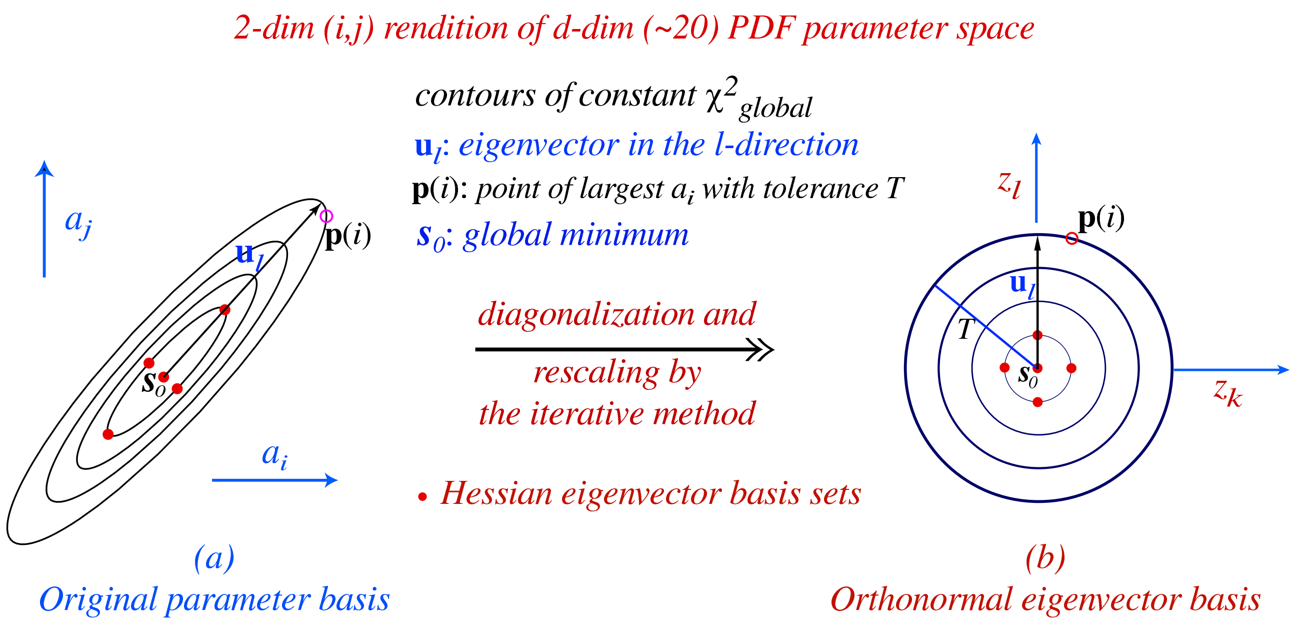
$$(\Delta F)^2 = \Delta\chi^2 \sum_{i,j} \frac{\partial F}{\partial a_i}(H)^{-1}_{ij}\frac{\partial F}{\partial a_j},$$

This has been used to find partons with errors by Alekhin and $H1$, each with restricted data sets. (See also Blümlein and Böttcher for spin structure functions.)

Problematic due to extreme variations in $\Delta\chi^2$ in different directions in parameter space.

Solved by finding and rescaling eigenvectors of H leading to diagonal form

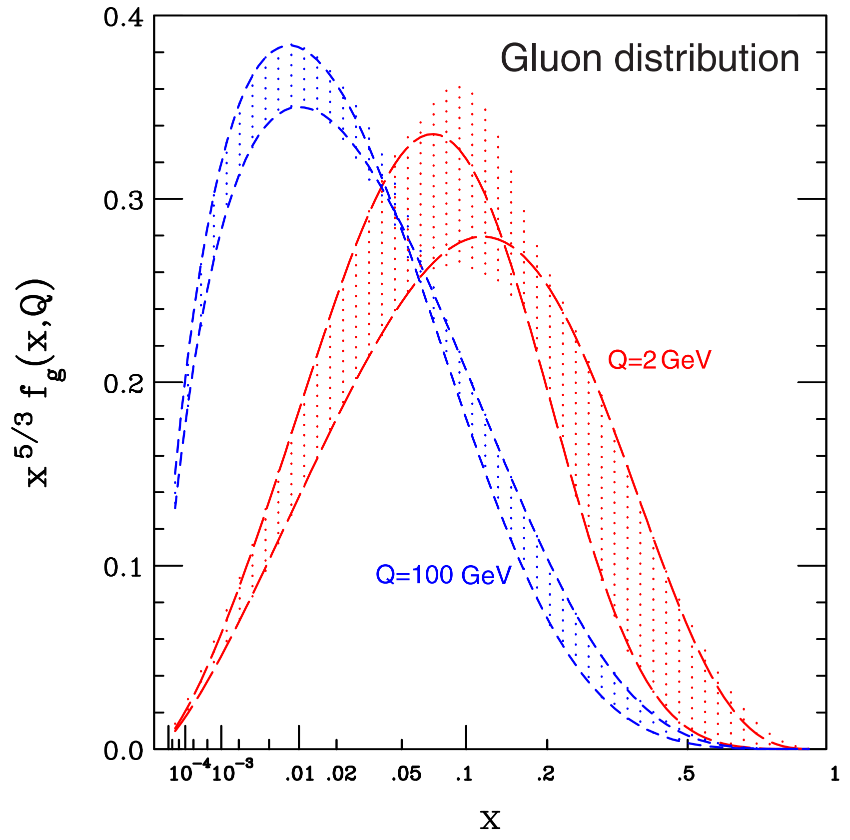
$$\Delta\chi^2 = \sum_i z_i^2$$

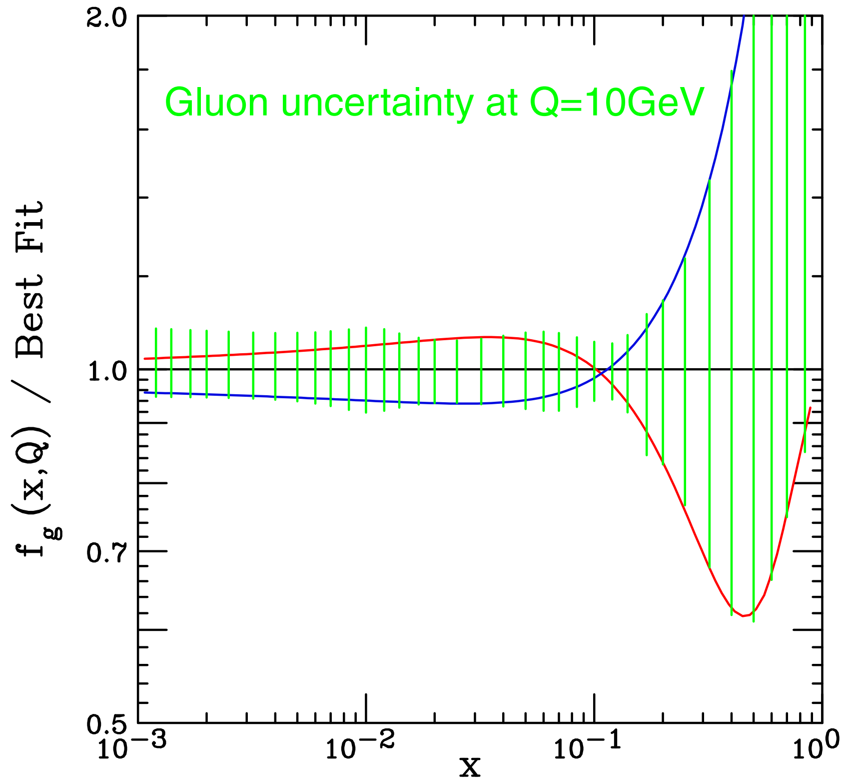


Implemented by CTEQ. Uncertainty on physical quantity then given by

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

where $S_i^{(+)}$ and $S_i^{(-)}$ are PDF sets displaced along eigenvector direction by given $\Delta\chi^2$. Art in choosing "correct" $\Delta\chi^2$ given complication of errors in full fit. CTEQ choose $\Delta\chi^2 \sim 100$.





Results of CTEQ Hessian approach for gluon uncertainty.

Offset method. Best fit obtained by minimizing

$$\chi^2 = \sum_{i=1}^{N} \left(\frac{(D_i - f_i(a,s))}{\sigma_{i,unc}} \right)^2,$$

i.e. best fit and parameters a_0 obtained from only uncorrelated errors. Forces theory to be close to unshifted data. Quality of fit then estimated by adding in quadrature. Systematic errors on a_i determined by letting each $s_k = \pm 1$ and add deviation in quadrature. Replaced by calculating 2 Hessian matrices

$$M_{ij} = \frac{\partial^2 \chi^2}{\partial a_i \partial a_j} \qquad V_{ij} = \frac{\partial^2 \chi^2}{\partial a_i \partial s_j},$$

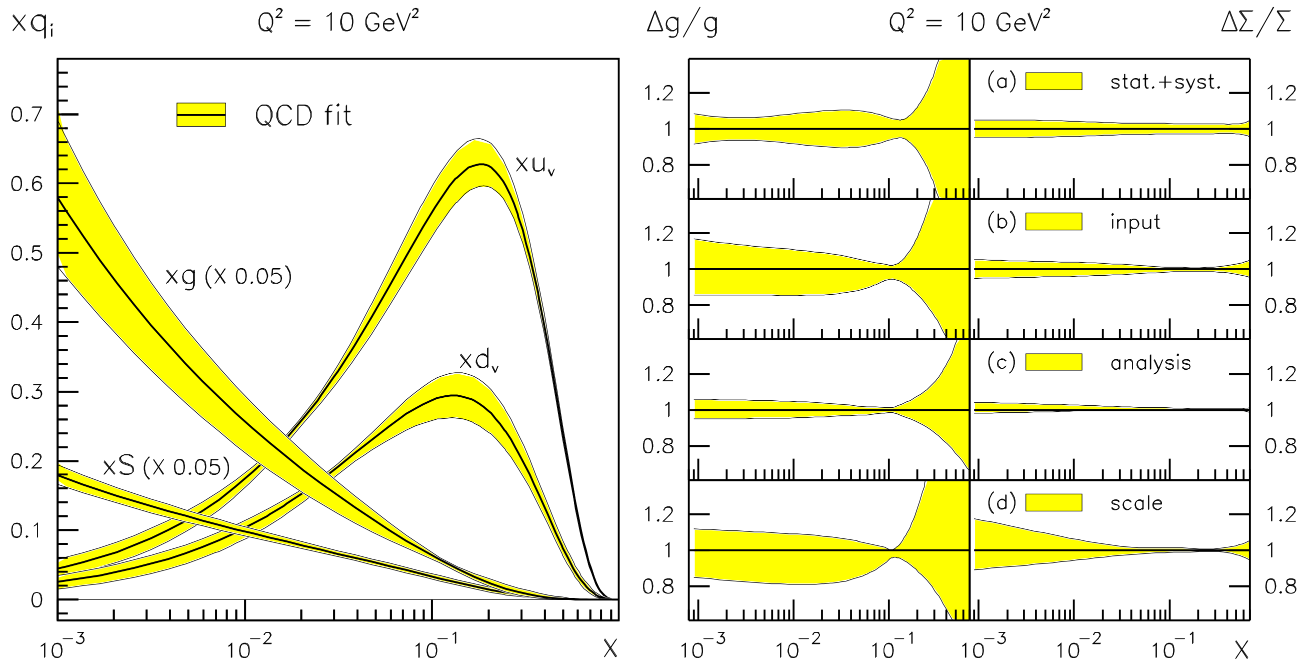
and defining covariance matrices

$$C_{stat} = M^{-1} \qquad C_{sys} = M^{-1} V V^T M^{-1}$$

$$C_{tot} = C_{stat} + C_{sys}.$$

Used by early H1 fits (Zomer and Pascaud) and by ZEUS (Botje) (DIS (and E866) data only).

$\rightarrow$ bigger uncertainty for same $\Delta\chi^2$.



Parton densities and their errors extracted by fits by Botje.

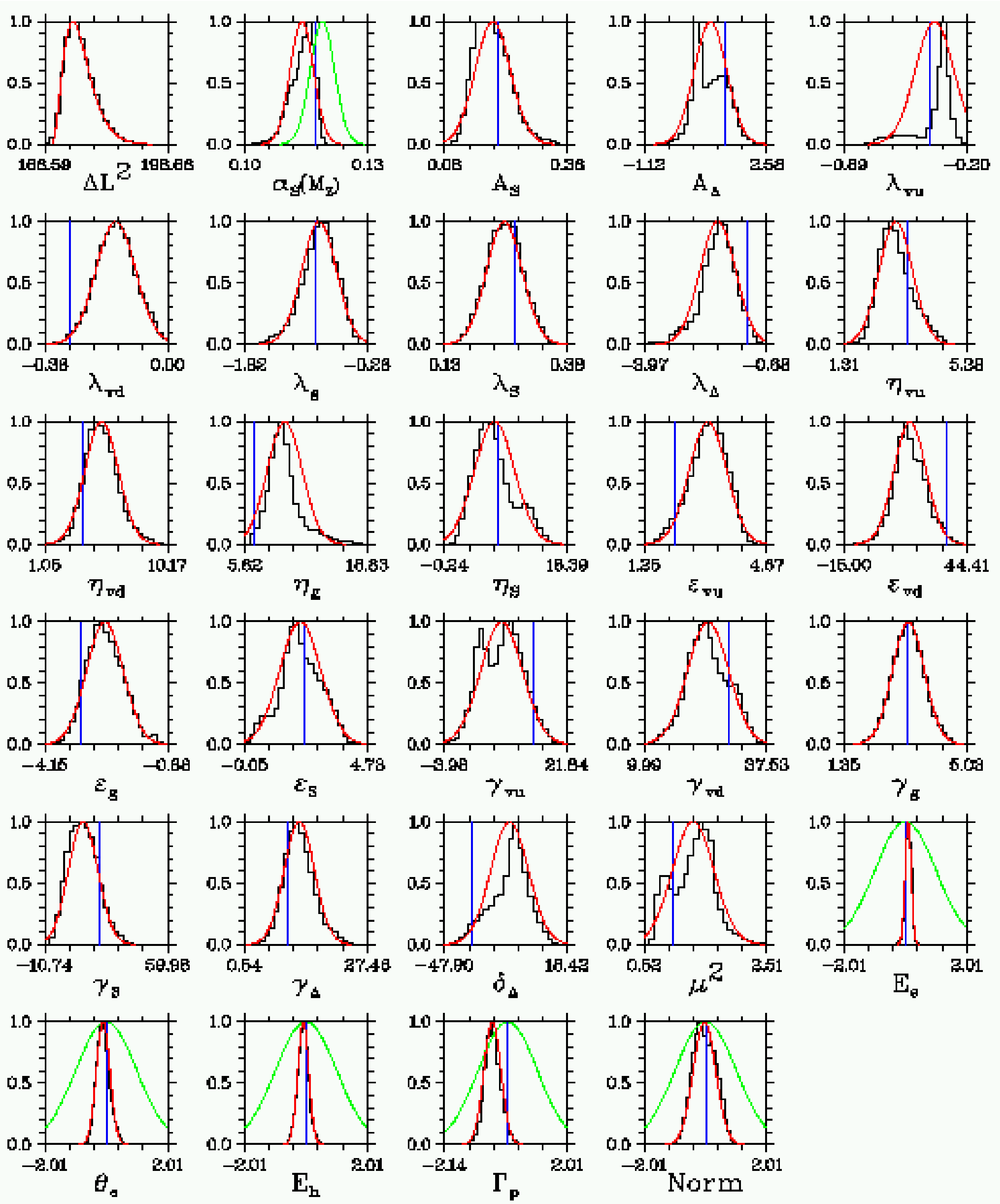
Statistical Approach (Giele, Keller and Kosower) constructs an ensemble of distributions labeled by $\mathcal{F}$ each with probability $P(\{\mathcal{F}\})$. Mean μ_O and deviation σ_O of observable O then given by

$$\mu_O = \sum_{\{\mathcal{F}\}} O(\{\mathcal{F}\})P(\{\mathcal{F}\}), \quad \sigma_O^2 = \sum_{\{\mathcal{F}\}} (O(\{\mathcal{F}\}) - \mu_O)^2 P(\{\mathcal{F}\}).$$

While this is statistically correct, and does not rely on the approximation of linear propagation errors in calculating observables, it is inefficient and in practice they generate N_{pdf} different distributions with unit weight but distributed according to $P(\{\mathcal{F}\})$ where N_{pdf} can be made as small as 100. Then

$$\mu_O = \frac{1}{N_{pdf}} \sum_{1}^{N_{pdf}} O(\{\mathcal{F}\}), \quad \sigma_O^2 = \frac{1}{N_{pdf}} \sum_{1}^{N_{pdf}} (O(\{\mathcal{F}\}) - \mu_O)^2.$$

Can incorporate full information about measurements and their error correlations in the calculation of $P(\{\mathcal{F}\})$.



H1 set of parton parameters from GKK approach. Red curve Gaussian approx and blue line MRST value. Green curve for α_S is LEP result. Gaussian approx often not good. Also shows potential complications.

Currently uses only proton DIS data sets in order to avoid complicated uncertainty issues such as shadowing effects for nuclear targets.

Using strict confidence limits it is difficult to obtain consistency between many different DIS experiments. Also lack of important data sets leads to “unusual” values for some parameters. Shows that this is a complicated game.

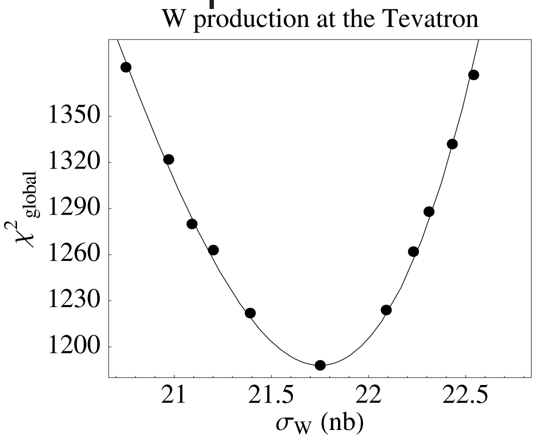
However, previous plots show that the Gaussian approx is often not good. Also shows potential complications for simplistic approaches.

Very attractive but ambitious large-scale project with a lot of work still to be done.

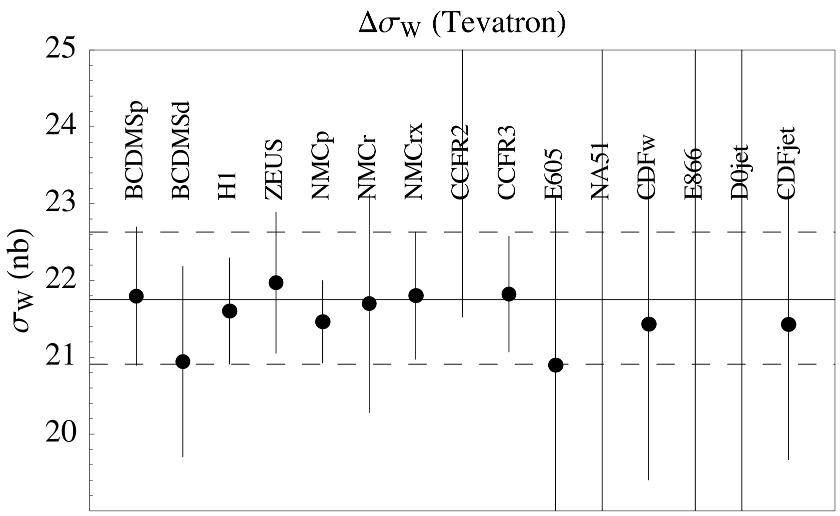
Can also look at uncertainty on a given physical quantity using Lagrange Multiplier method, first suggested by CTEQ and also used by MRST, i.e. perform fit while constraining value of some physical quantity. Minimize

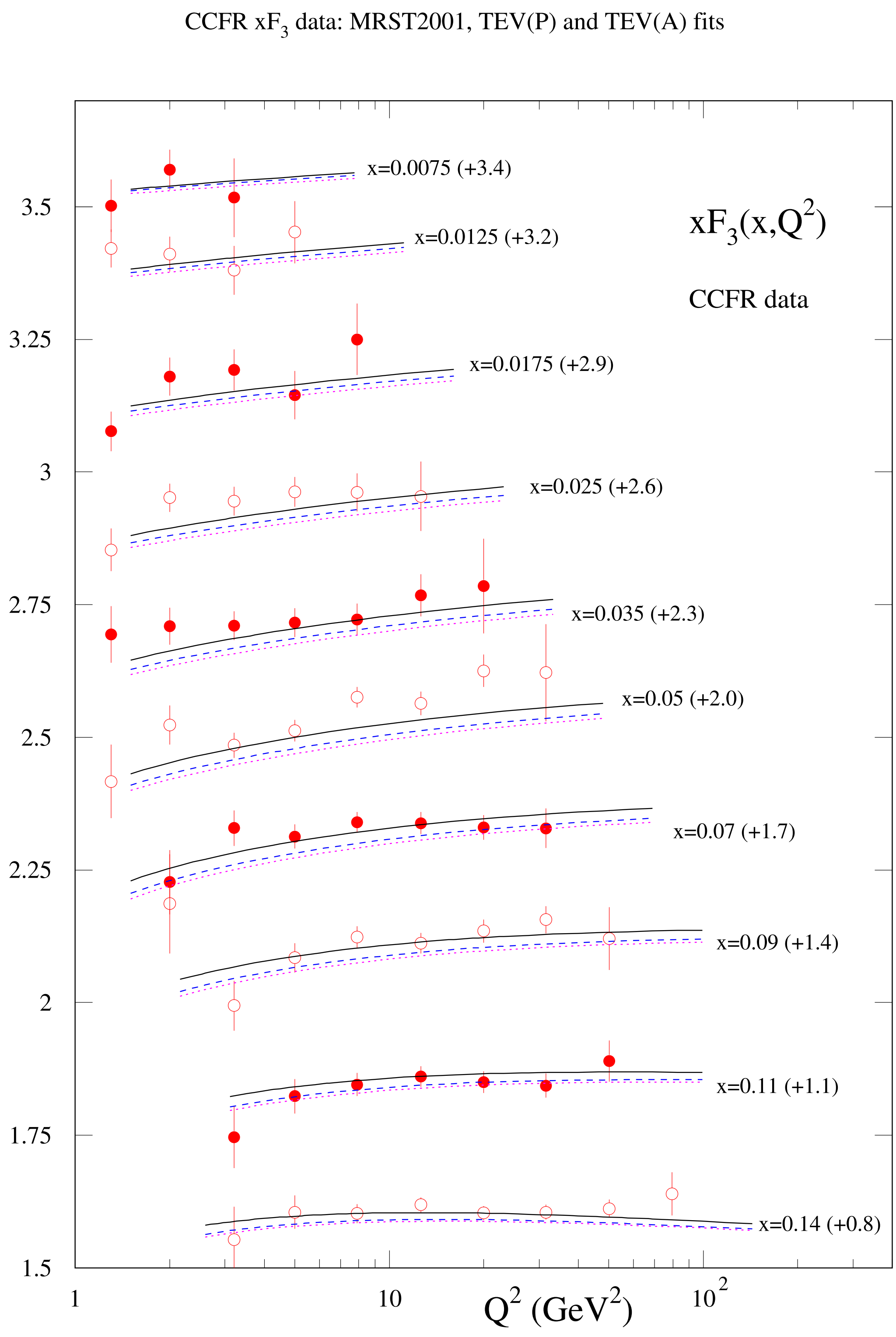
$$\Psi(\lambda, a) = \chi^2_{global}(a) + \lambda F(a)$$

for various values of λ. Give set of best fits for particular values of parameter $F(a)$ without relying on Gaussian approx for χ^2. Useful example W cross-section at Tevatron.



Uncertainty then determined by deciding allowed range of $\Delta\chi^2$. Can also look at range of allowed variation in $F(a)$ for each of the experiments in the global fit. Checks if total $\Delta\chi^2$ is coming specifically from one region.





Deterioration in fit to CCFR $F_3(x, Q^2)$ data (most sensitive indicator) for decrease in $\sigma_W(\mathrm{Tev})$ obtained by MRST.

Results.

Once again, no unique prescription for deciding when a fit is actually acceptable or not. Use global χ^2 only or look at individual sets. What are criteria for limit for acceptable fit globally, or for one experiment?

Using particular criteria CTEQ use $\Delta\chi^2 = 100$ (same as for Hessian approach). Obtain for $\alpha_S = 0.118$

$$\Delta\sigma_W(\mathrm{LHC}) \approx \pm 4\% \quad \Delta\sigma_{\mathrm{W}}(\mathrm{Tev}) \approx \pm 5\%$$

$$\Delta\sigma_H(\mathrm{LHC}) \approx \pm 5\%.$$

Procedure also used by MRST for a wider range of data, and using $\Delta\chi^2 \sim 50$. Find for $\alpha_S = 0.119$

$$\Delta\sigma_W(\mathrm{Tev}) \approx \pm 1.2\% \quad \Delta\sigma_{\mathrm{W}}(\mathrm{LHC}) \approx \pm 2\%$$

$$\Delta\sigma_H(\mathrm{Tev}) \approx \pm 4\% \quad \Delta\sigma_{\mathrm{H}}(\mathrm{LHC}) \approx \pm 2\%.$$

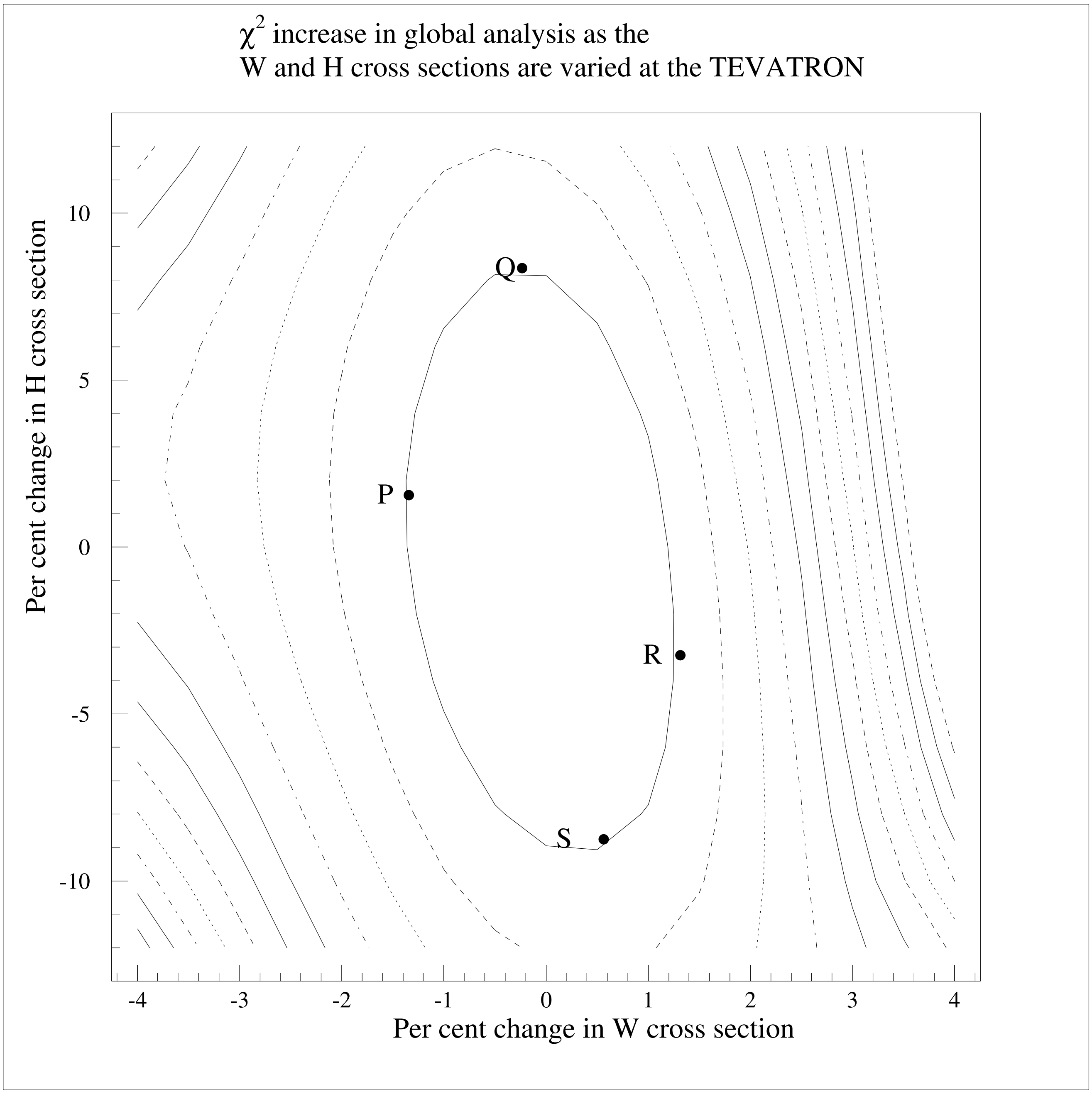
If α_S also varies $\Delta\sigma_W$ quite stable but $\Delta\sigma_H$ almost doubles.

Can repeat for other processes.

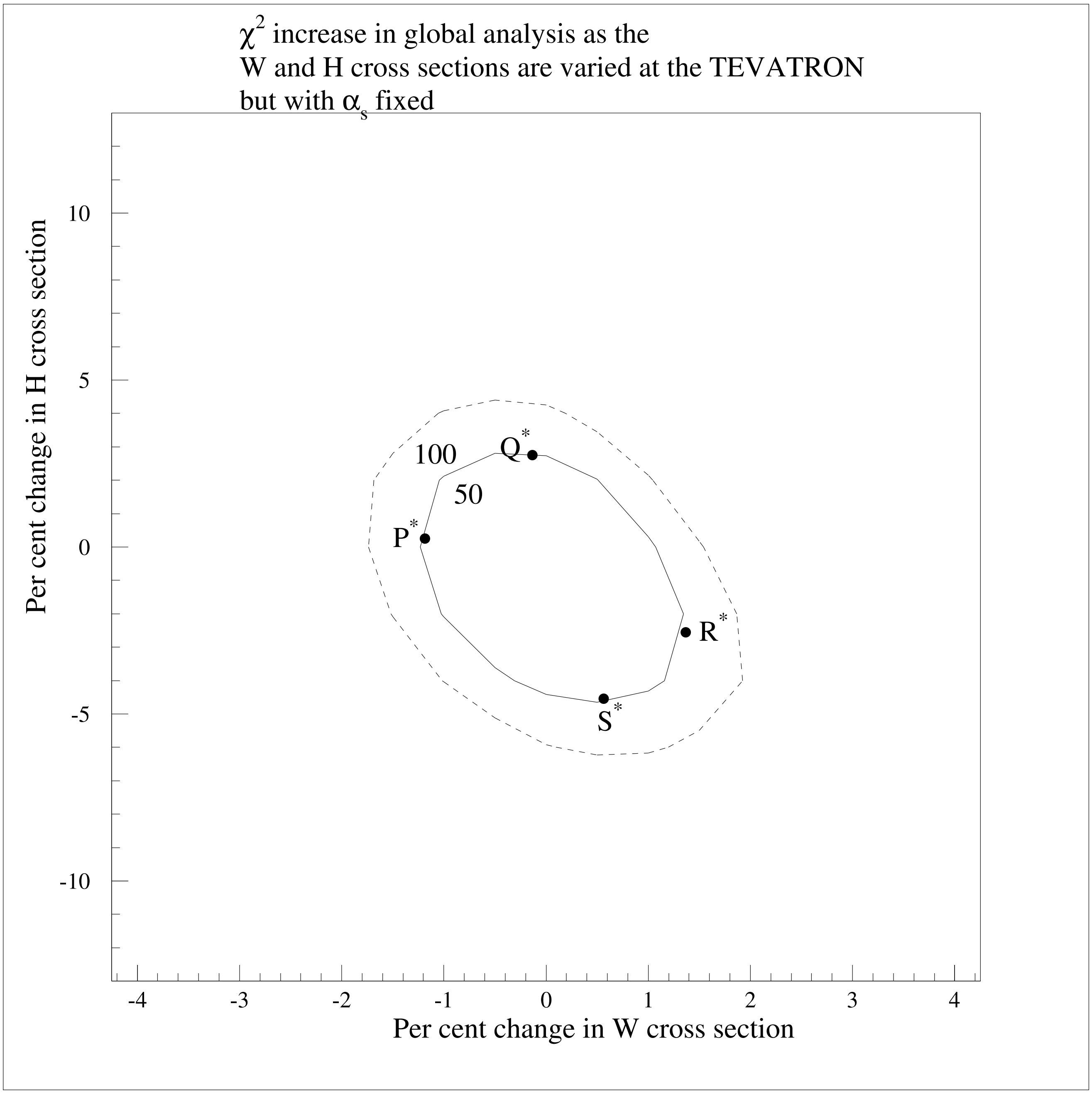
- HERA charged current data sensitive to very high x quarks
- Tevatron jet data sensitive to high x gluon.
- ....

Hence conclude that uncertainty due to experimental errors rather small, however they are dealt with. Only more than few % for quantities determined by high x gluon.

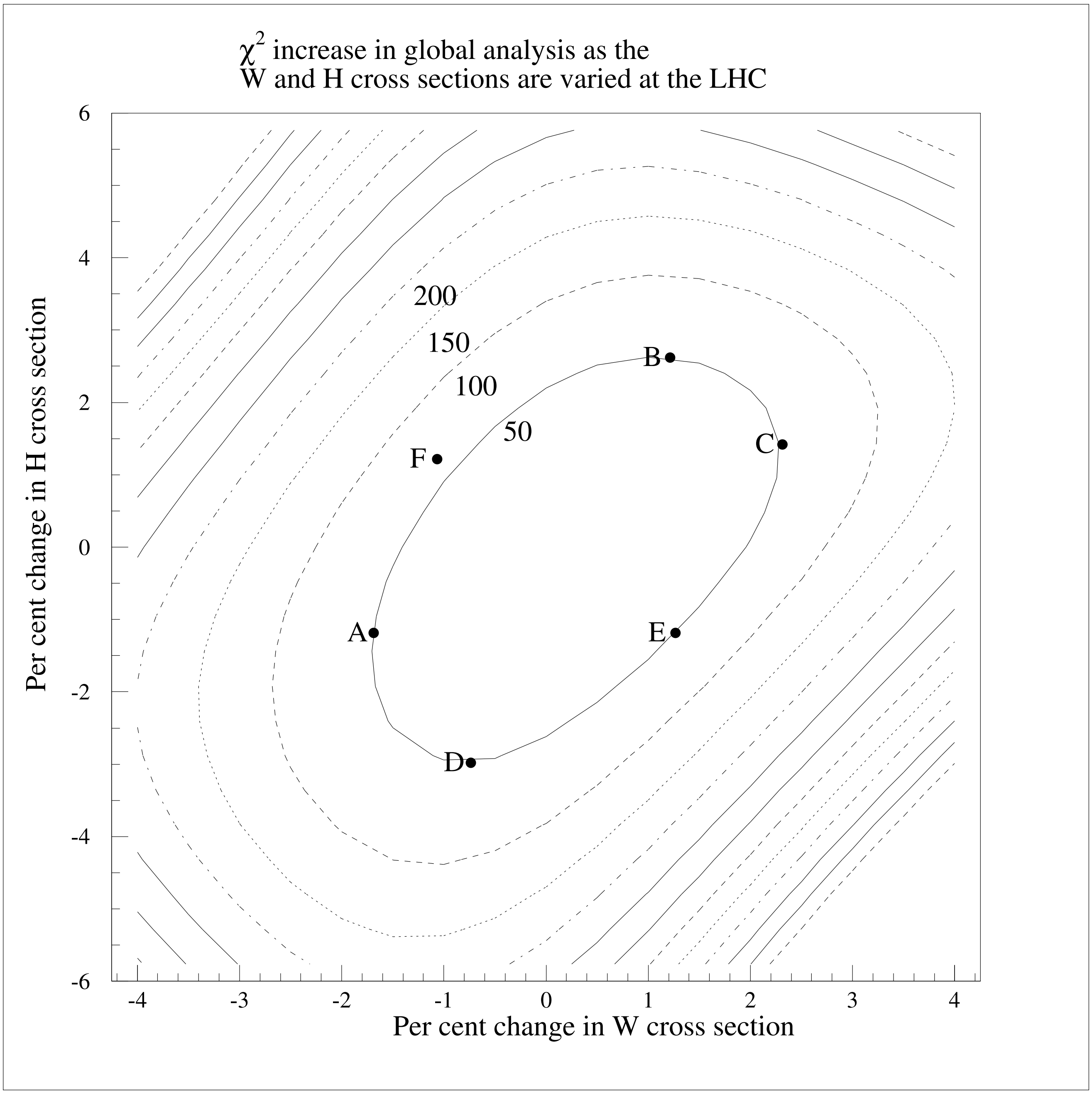
χ^2-plot for W and Higgs production at the Tevatron α_S free.



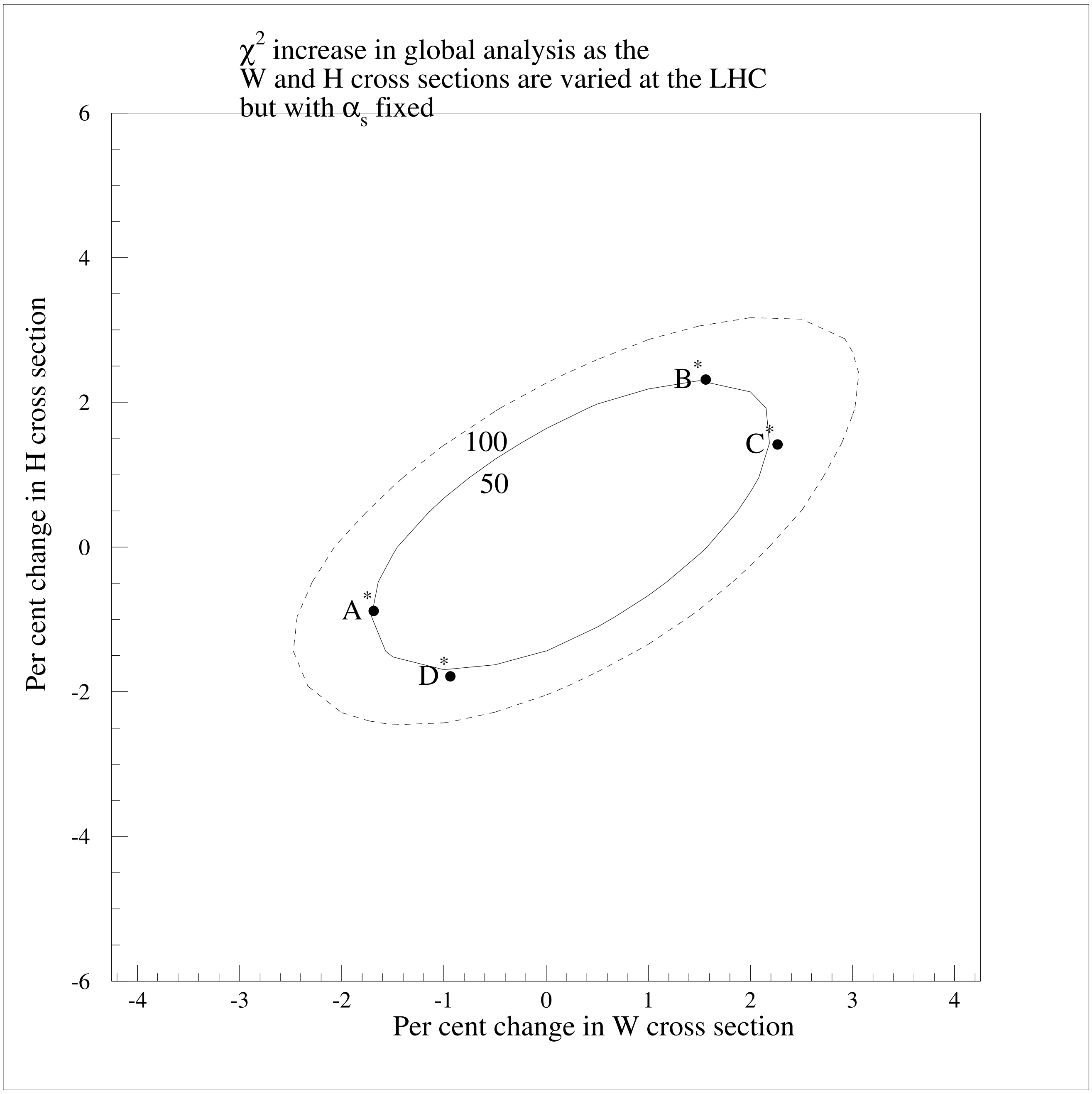
χ^2-plot for W and Higgs production at the Tevatron α_S fixed.



χ^2-plot for W and Higgs production at the LHC α_S free.



χ^2-plot for W and Higgs production at the LHC α_S fixed.



However, also need to consider effect of assumptions made during fit.

Cuts made on data, data sets fit, parameterization for input sets, form of strange sea, heavy flavour prescription, assumption of no isospin violation, strong coupling, constraint on large x gluon ......

Many can be as important as experimental errors on data used (or more so).

Vital to consider theoretical errors. These include ....

- higher orders (NNLO)

- small x $(\alpha_s^n \ln^{n-1}(1/x))$

- large x $(\alpha_s^n \ln^{2n-1}(1-x))$

- low Q^2 (higher twist)

Note renormalization/factorization scale variation is **not** reliable in general.

Note - renormalization/factorization scale variation is **not** reliable. e.g., at large x

$$C_{2,q}^{1,NS}(x,\mu^2) \sim \alpha_S(\mu^2)\frac{\ln(1-x)}{(1-x)_+}$$

$$C_{2,q}^{n,NS}(x,\mu^2) \sim \alpha_S^n(\mu^2)\frac{\ln^{2n-1}(1-x)}{(1-x)_+}$$

The scale variation of $C_{2,q}^{1,NS}(x,\mu^2)$ does not give an indication of these higher power $\ln(1-x)$ terms.

Similarly at small x

$$P_{qg}^1 \sim \alpha_S(\mu^2) \qquad\qquad P_{qg}^2 \sim \frac{\alpha_s(\mu^2)}{x}$$

$$P_{qg}^n \sim \frac{\alpha_S^n(\mu^2)\ln^{n-2}(1/x)}{x}$$

and scale variations of P_{qg}^1, P_{qg}^2 never give an indication of these terms.

In order to investigate true theoretical error must consider some way of performing correct large and small x resummations, and/or use what we already know about NNLO. Implies some quantities acquire large higher order corrections.

Alternatively use empirical approach of investigating in detail the effect of cuts on the fit quality.

In order to investigate real quality of fit and regions with problems we try varying kinematic cuts on data.

Procedure - change W^2_{cut}, Q^2_{cut} and x_{cut}, re-fit and see if quality of fit to remaining data improves and/or input parameters change dramatically.

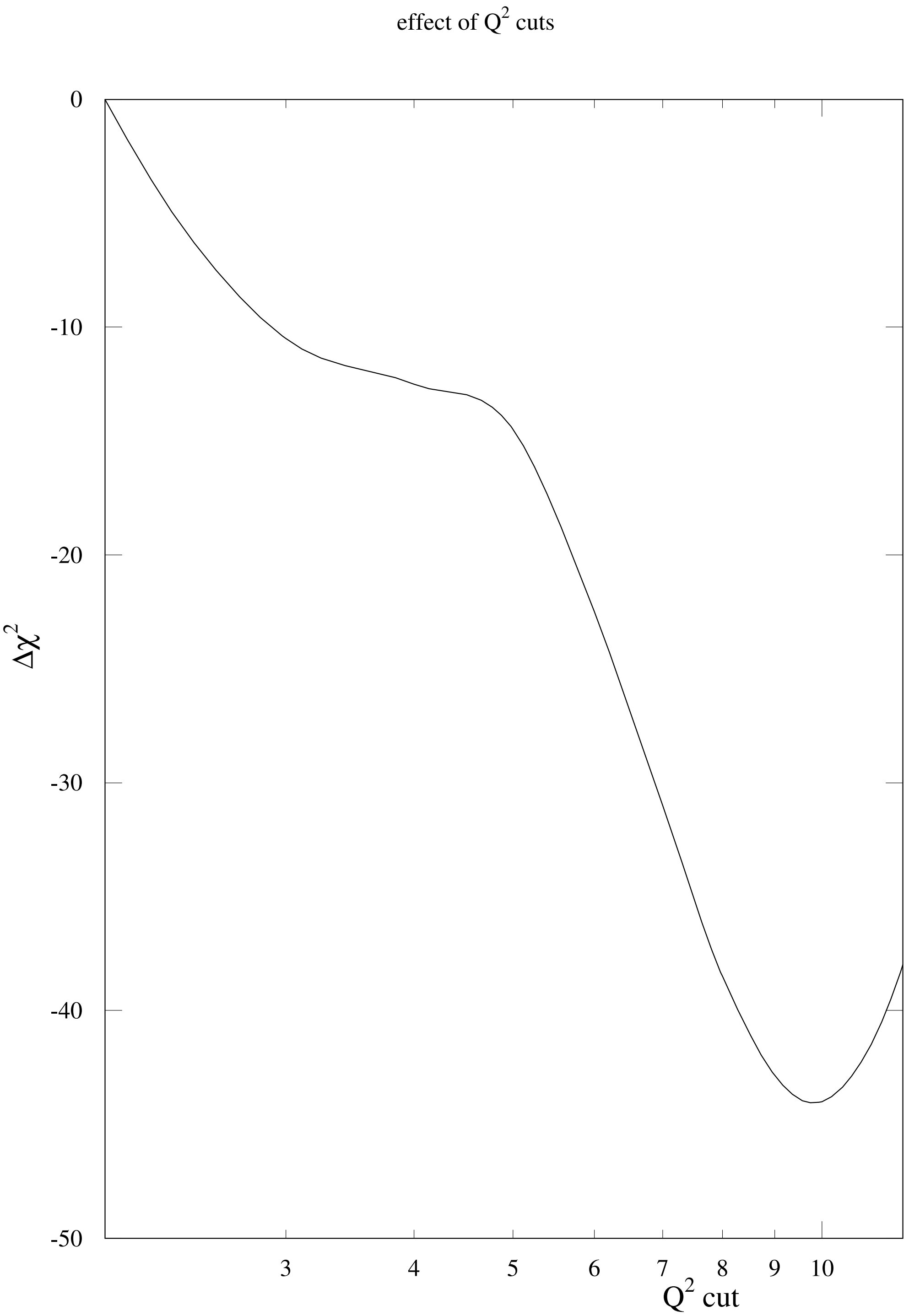
Similar to Collins and Pumplin suggestion in terms of data sets rather than region of parameter space.

Continue until quality of fit and partons stabilize.

For W^2_{cut} raising from $12.5\mathrm{GeV}^2$ has no effect.

Raising Q^2_{cut} from $2\mathrm{GeV}^2$ to $3\mathrm{GeV}^2$ very small effect - $\Delta\chi^2 = 11$ input gluon slightly more negative. Slow continuous improvement for higher Q^2 up to $> 12\mathrm{GeV}^2$ - suggests higher orders not higher twist.

Improvement in χ^2 with Q^2 cut for refit compared to default fit.



Raising x_{cut} from 0 to 0.0002 to 0.001 to 0.005 continuous improvement - $\Delta\chi^2 = 56$, $\delta_- \to 0.5$ and $\alpha_S(M_Z^2) \to 0.118$.

Stability reached at $x = 0.005$. At each step moderate x gluon becomes more positive. Gluon outside range negative, but unknown theory could cure this (quite plausible).

At $x_{cut} = 0.005$, the fit to jets is much improved, i.e. high E_T problem largely cured.

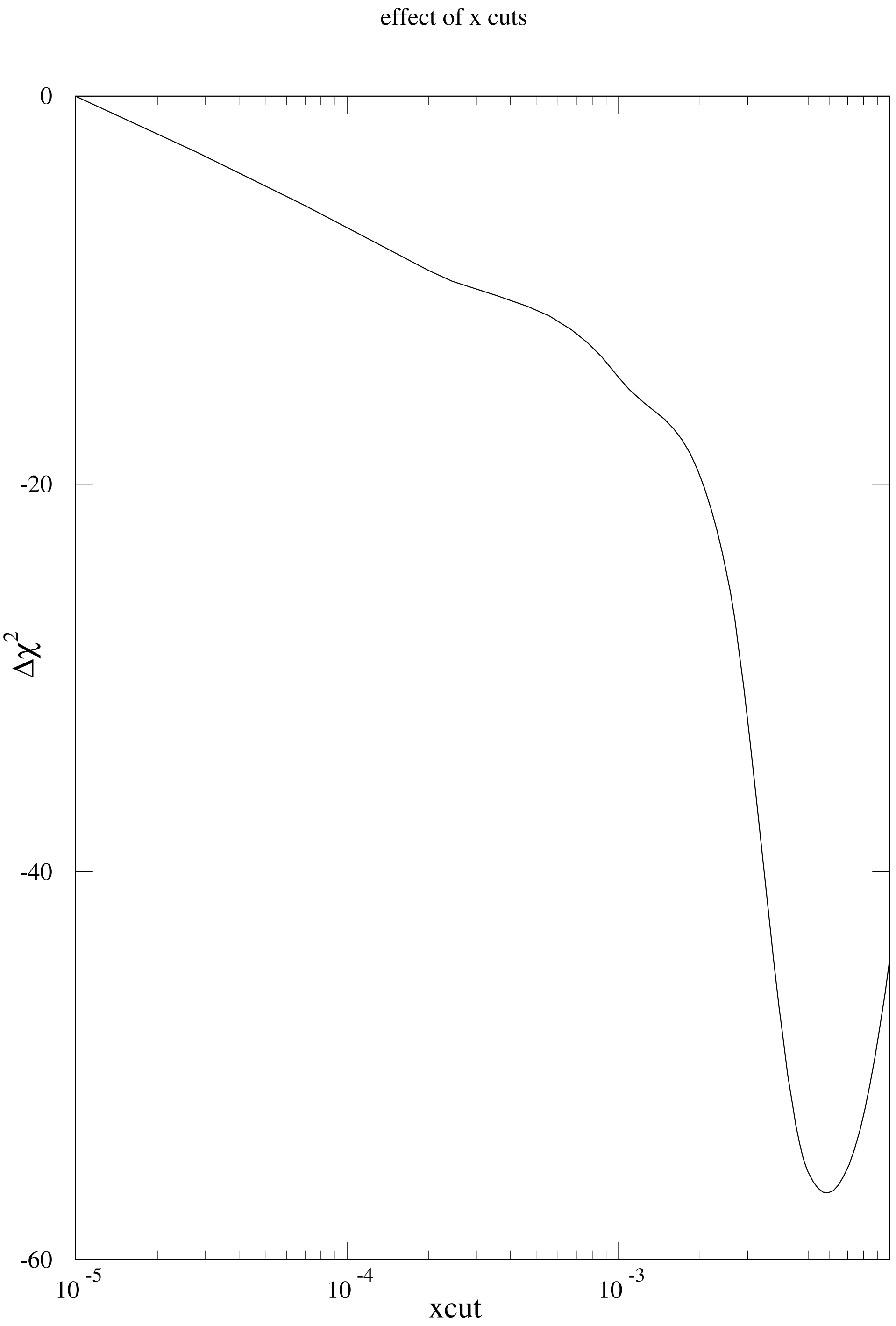
Data set	No. of data pts	MRST	$x_{cut} = 0.005$
H1 ep	287	296	274
ZEUS ep	141	131	143
NMC μp	125	134	121
NMC μd	125	100	88
Jets	113	170	151

Little tension between data sets. When $x_{cut} = 0.005$ raising Q^2 does not improve fit.

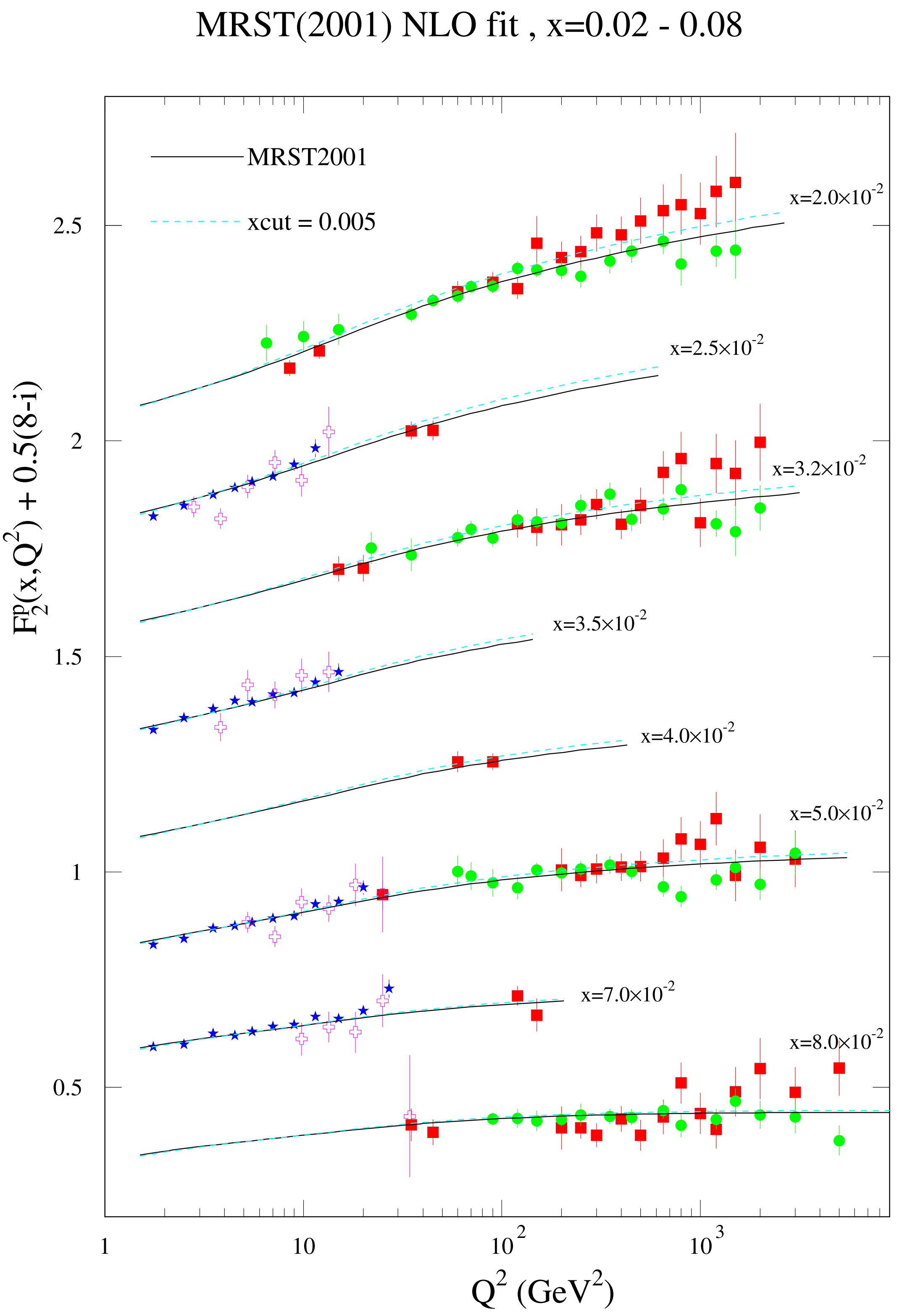
Predictions for Tevatron cross-sections still safe. Large change compared to default fit. Well outside limit set by experimental errors!

LHC predictions not available.

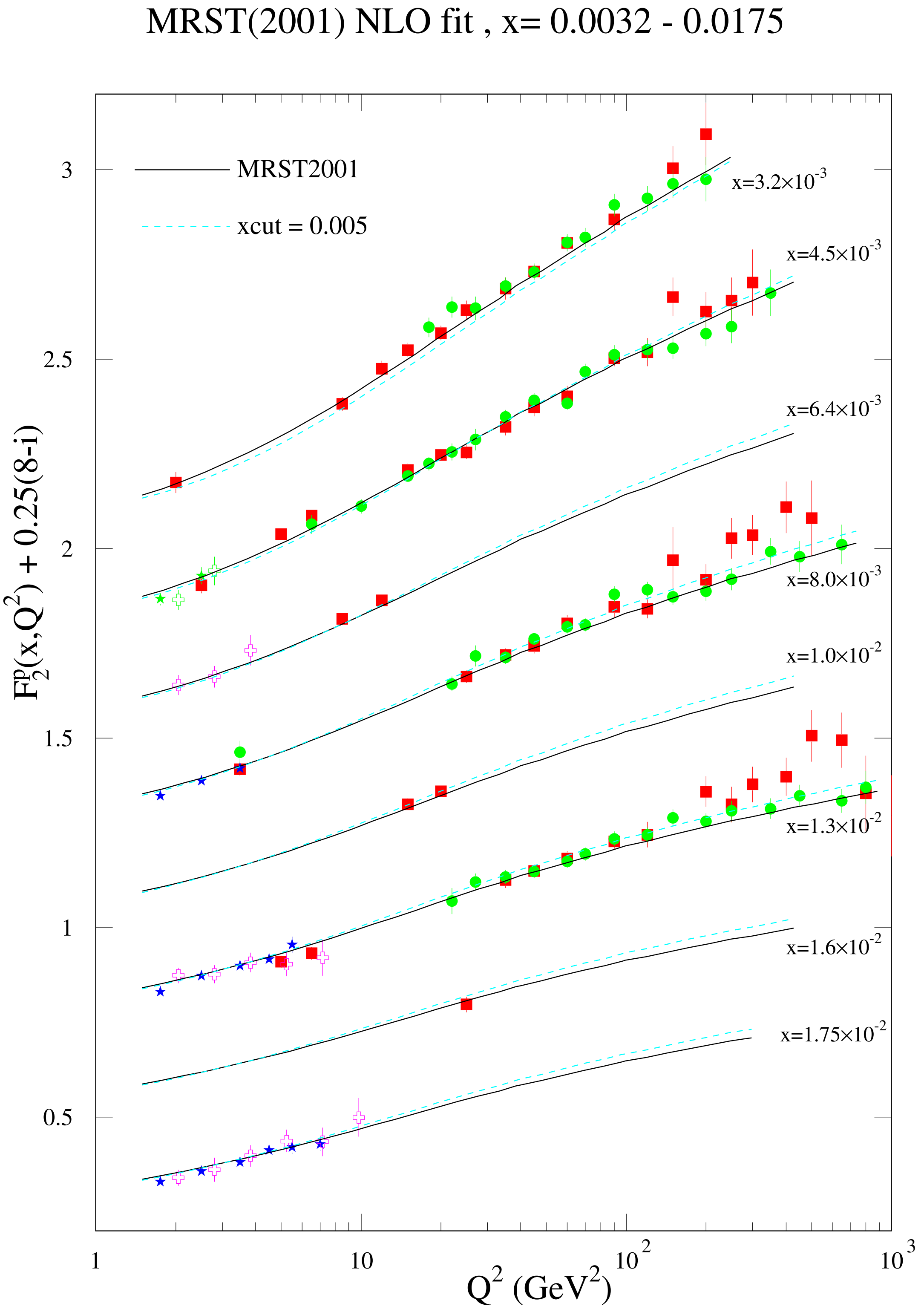
Improvement in χ^2 with x cut.



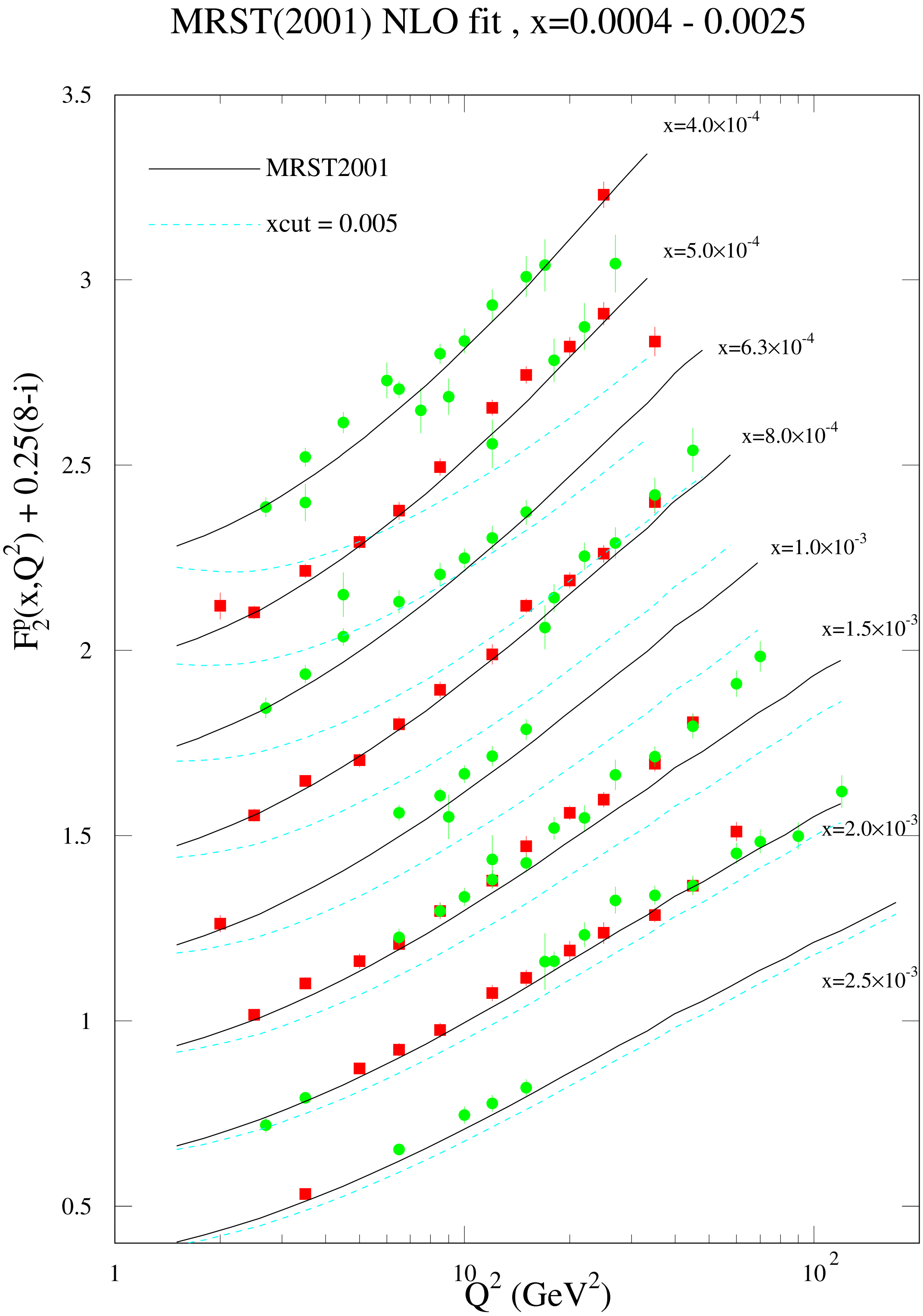
Comparison of MRST(2001), $x_{cut} = 0.005$ and resummed fit.



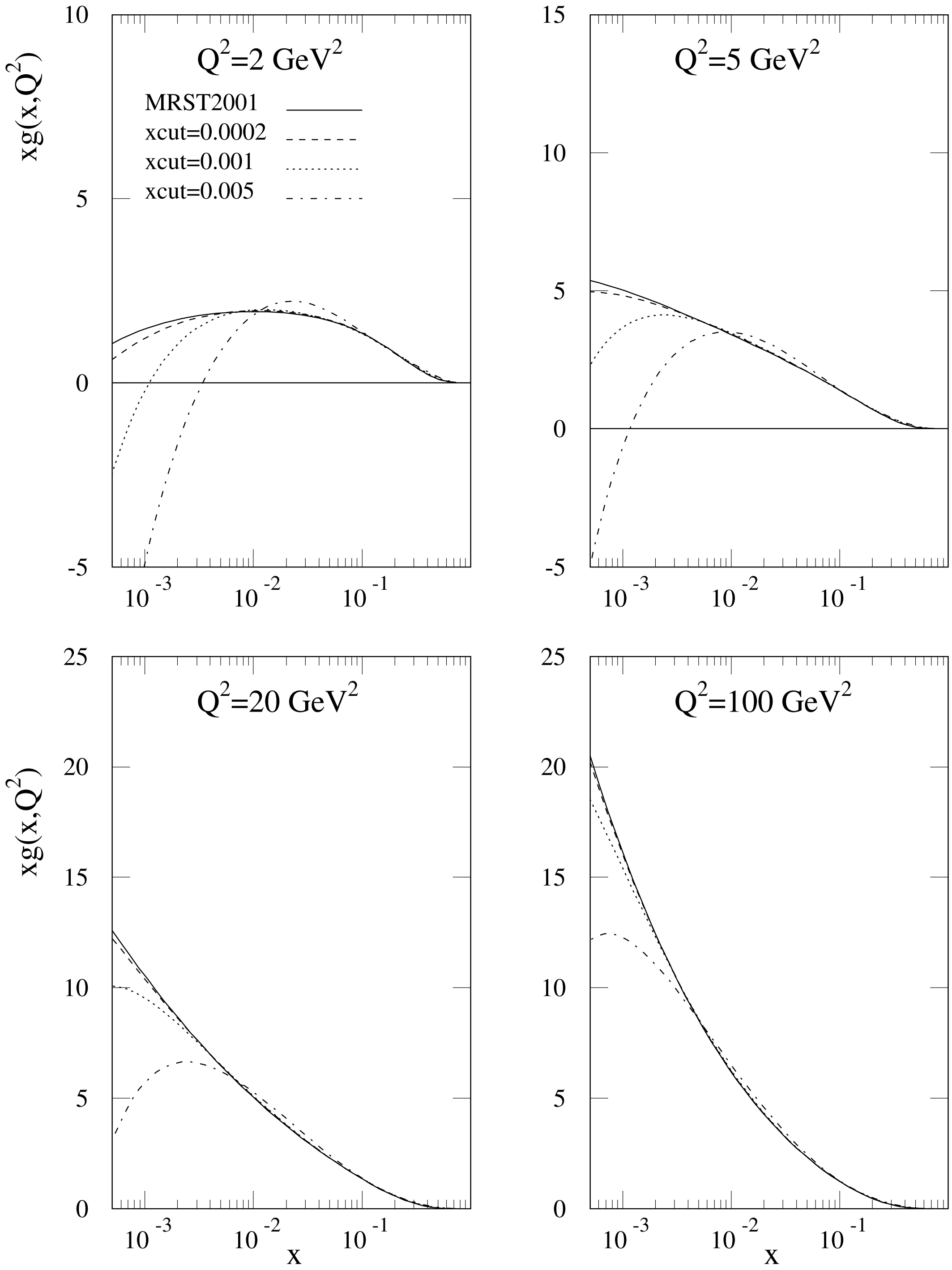
Comparison of MRST(2001), $x_{cut} = 0.005$ and resummed fit.



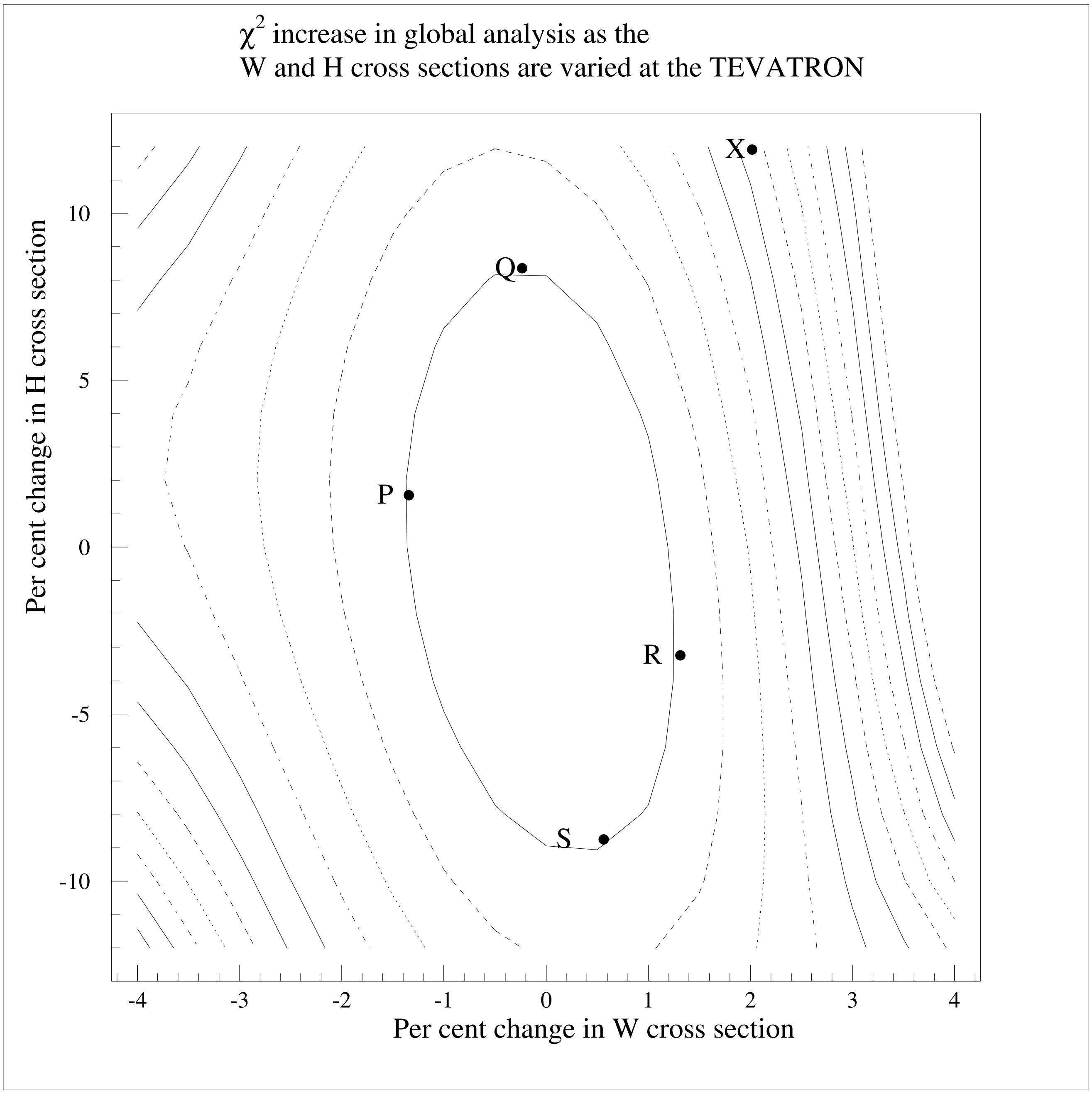
Comparison of MRST(2001), $x_{cut} = 0.005$ and resummed fit.



Comparison of gluons obtained when x_{cut} is varied.



χ^2-plot for W and Higgs production at the Tevatron α_S free, with prediction for fit with only data with $x < 0.005$ in the fit marked by **X**.



Conclusions

One can perform global fits to all up-to-date data over wide range of parameter space. Fit fairly good - some slight worries:

Various ways of looking at uncertainties due to errors on data alone. Much good work on this topic recently. No totally preferred approach - all have pros and cons. Useful to concentrate on W (and Z) and Higgs cross-sections as measure of uncertainties. Errors rather small using all approaches $\sim 1-5\%$. Methods can be applied in same manner to other quantities.

Uncertainties from this source rather small. Uncertainty from input assumptions e.g. $\alpha_S(M_Z^2)$, cuts on data, parameterizations ..., comparable and potentially larger.

Errors from higher orders/resummation potentially large in some regions of parameter space, and from correlations between partons feed into all regions (small x gluon influences large x gluon). For some/many processes theory probably the dominant source of uncertainty at present. Systematic study needed. Much harder than uncertainties due to errors. Just beginning.