Tolerance in global PDF analysis

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Uncertainties in global PDF analysis

Theoretical errors

- *Examples:* input parameterisation form, neglected higher-order and higher-twist QCD corrections, electroweak corrections, choice of cuts, nuclear corrections, heavy flavour treatment.
- Difficult to quantify (\rightarrow talks by A. Guffanti, R. Thorne, S. Forte).

Experimental errors

- In principle there **should** be a well-defined procedure for propagating experimental uncertainties on the fitted data points through to the PDF uncertainties.
 - Hessian method: based on linear error propagation, produce eigenvector PDF sets suitable for use by the end user.

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 - **1** *Hessian method:* based on linear error propagation, produce eigenvector PDF sets suitable for use by the end user.
 - 2 Lagrange multiplier method: does not rely on linear error propagation, but requires access to global fit code.
 - **3** Neural networks: work in progress (\rightarrow talk by A. Guffanti).

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Traditional propagation of experimental uncertainties

• Assume χ^2_{global} is quadratic about the global minimum $\{a^0_i\}$:

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

where the Hessian matrix has components

$$H_{ij} = \left. \frac{1}{2} \frac{\partial^2 \chi^2_{\text{global}}}{\partial a_i \partial a_j} \right|_{\text{minimum}}$$

• Uncertainty on quantity $F(\{a_i\})$ from linear error propagation:

$$\Delta F = T \sqrt{\sum_{i,j} \frac{\partial F}{\partial a_i} C_{ij} \frac{\partial F}{\partial a_j}},$$

where $C \equiv H^{-1}$ is the covariance matrix, and $T = \sqrt{\Delta \chi^2_{\text{global}}}$ is the tolerance for the required confidence interval.

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Eigenvector PDF sets (pioneered by CTEQ)

• Convenient to diagonalise covariance (or Hessian) matrix:

$$\sum_{j} C_{ij} v_{jk} = \lambda_k v_{ik},$$

where λ_k is the *k*th eigenvalue and v_{ik} is the *i*th component of the *k*th orthonormal eigenvector ($k = 1, ..., N_{\text{parameters}}$).

• Expand parameter displacements from minimum in basis of rescaled eigenvectors $e_{ik} \equiv \sqrt{\lambda_k} v_{ik}$:

$$a_i-a_i^0=\sum_k e_{ik}z_k.$$

• Then can show that

$$\chi^2_{\text{global}} = \chi^2_{\text{min}} + \sum_k z_k^2,$$

i.e. $\sum_{k} z_{k}^{2} \leq T^{2}$ is the interior of a hypersphere of radius T

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Use of eigenvector PDF sets

• Produce eigenvector PDF sets S_k^{\pm} with parameters given by $a_i(S_k^{\pm}) = a_i^0 \pm t e_{ik},$

with t adjusted to give the desired $T = \sqrt{\Delta \chi^2_{\text{global}}}$.

• Then calculate uncertainties on a quantity F with

$$\Delta F = \frac{1}{2} \sqrt{\sum_{k} \left[F(S_k^+) - F(S_k^-) \right]^2},$$

or to account for asymmetric errors ($S_0 = \text{central PDF set}$):

$$(\Delta F)_{+} = \sqrt{\sum_{k} \left[\max(F(S_{k}^{+}) - F(S_{0}), F(S_{k}^{-}) - F(S_{0}), 0) \right]^{2}}$$

$$(\Delta F)_{-} = \sqrt{\sum_{k} \left[\max(F(S_0) - F(S_k^+), F(S_0) - F(S_k^-), 0) \right]^2}$$

• Correlations between two quantities \rightarrow talk by P. Nadolsky.

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Criteria for choice of tolerance $T = \sqrt{\Delta \chi^2_{ m globa}}$

Parameter-fitting criterion

- $T^2 = 1$ for 68% (1- σ) C.L., $T^2 = 2.71$ for 90% C.L.
- Appropriate if fitting consistent data sets with ideal Gaussian errors to a well-defined theory.
- In practice: minor inconsistencies between fitted data sets, and unknown experimental and theoretical uncertainties, so not appropriate for global PDF analysis.

Hypothesis-testing criterion

- Much weaker than the parameter-fitting criterion: treat eigenvector PDF sets as alternative hypotheses.
- Determine T^2 from the criterion that each data set should be described within its 90% C.L. limit.

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Hypothesis-testing criterion

- Much weaker than the parameter-fitting criterion: treat eigenvector PDF sets as alternative hypotheses.
- Determine T² from the criterion that each data set should be described within its 90% C.L. limit.



• For each eigenvector, plot location of the minimum for each data set and the 90% C.L. limits as the distance from the global minimum in units of $\sqrt{\Delta\chi^2_{\rm global}}$:



- A rough "average" over all eigenvectors gives $T = 10 \dots$
- ... But T = 10 exceeds the 90% C.L. limits of some data sets.



"We estimate $\Delta \chi^2 = 50$ to be a conservative uncertainty (perhaps of the order of a 90% confidence level or a little less than 2σ) due to the observation that **an increase of 50 in the global** χ^2 , which has a value $\chi^2 = 2328$ for 2097 data points, usually signifies that the fit to one or more data sets is becoming unacceptably poor. We find that an increase $\Delta \chi^2$ of 100 normally means that some data sets are very badly described by the theory."

- Fairly qualitative statements.
- \Rightarrow Study more quantitatively in new MSTW analysis.

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Data sets fitted in MSTW 2008 NLO (prel.) analysis

Data set	$\chi^2/N_{\rm pts.}$	Data set	$\chi^2/N_{\rm pts.}$
H1 MB 99 e ⁺ p NC	9 / 8	BCDMS $\mu p F_2$	182 / 163
H1 MB 97 e ⁺ p NC	42 / 64	BCDMS $\mu d F_2$	187 / 151
H1 low Q^2 96–97 e^+p NC	45 / 80	NMC $\mu p F_2$	121 / 123
H1 high Q ² 98–99 e ⁻ p NC	122 / 126	NMC $\mu d F_2$	103 / 123
H1 high Q^2 99–00 e^+p NC	132 / 147	NMC $\mu n/\mu p$	130 / 148
ZEUS SVX 95 e ⁺ p NC	35 / 30	E665 $\mu p F_2$	57 / 53
ZEUS 96–97 e ⁺ p NC	86 / 144	E665 $\mu d F_2$	53 / 53
ZEUS 98–99 e ⁻ p NC	54 / 92	SLAC ep F_2	30 / 37
ZEUS 99–00 e ⁺ p NC	62 / 90	SLAC ed F_2	40 / 38
H1 99–00 e ⁺ p CC	29 / 28	NMC/BCDMS/SLAC FL	38 / 31
ZEUS 99–00 e ⁺ p CC	38 / 30	E866/NuSea pp DY	227 / 184
H1/ZEUS ep $F_2^{ m charm}$	108 / 83	E866/NuSea <i>pd/pp</i> DY	15 / 15
H1 99–00 <i>e</i> + <i>p</i> incl. jets	19 / 24	NuTeV $\nu N F_2$	50 / 53
ZEUS 96–97 e ⁺ p incl. jets	29 / 30	CHORUS $\nu N F_2$	26 / 42
ZEUS 98–00 $e^{\pm}p$ incl. jets	16 / 30	NuTeV $\nu N xF_3$	40 / 45
DØ I pp̄ incl. jets	68 / 90	CHORUS $\nu N \times F_3$	31 / 33
CDF II <i>p</i> p̄ incl. jets	73 / 76	CCFR $\nu N \rightarrow \mu \mu X$	65 / 86
CDF II $W \rightarrow l \nu$ asym.	29 / 22	NuTeV $\nu N ightarrow \mu \mu X$	39 / 40
DØ II $W \rightarrow l\nu$ asym.	23 / 10	All data sets	2497 / 2723
DØ II Z rap.	19 / 28		
CDF II Z rap.	35 / 29	Red = Update to last MRST fit.	

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At input scale
$$Q_0^2 = 1$$
 GeV²:

$$\begin{aligned} xu_v &= A_u \, x^{\eta_1} (1-x)^{\eta_2} (1+\epsilon_u \sqrt{x}+\gamma_u x) \\ xd_v &= A_d \, x^{\eta_3} (1-x)^{\eta_4} (1+\epsilon_d \sqrt{x}+\gamma_d x) \\ xS &= A_S \, x^{\delta_5} (1-x)^{\eta_5} (1+\epsilon_S \sqrt{x}+\gamma_S x) \\ x\bar{d} - x\bar{u} &= A_\Delta \, x^{\eta_\Delta} (1-x)^{\eta_S+2} (1+\gamma_\Delta x+\delta_\Delta x^2) \\ xg &= A_g \, x^{\delta_g} (1-x)^{\eta_g} (1+\epsilon_g \sqrt{x}+\gamma_g x) + A_{g'} \, x^{\delta_{g'}} (1-x)^{\eta_{g'}} \\ xs + x\bar{s} &= A_+ \, x^{\delta_5} \, (1-x)^{\eta_+} (1+\epsilon_S \sqrt{x}+\gamma_S x) \\ xs - x\bar{s} &= A_- \, x^{\delta_-} (1-x)^{\eta_-} (1-x/x_0) \end{aligned}$$

- A_u , A_d , A_g and x_0 are determined from sum rules.
- 20 parameters allowed to go free for eigenvector PDF sets, cf. 15 for MRST eigenvector PDF sets.



• Deviations from ideal quadratic behaviour (red dashed lines) for higher eigenvector numbers.

Tolerance in global PDF analysis

Fractional change in χ^2 for each data set

MSTW 2008 NLO PDF fit (prel.) Eigenvector number 1



- Plot $(\chi^2 \chi_0^2)/\chi_0^2$ versus the distance along a particular eigenvector.
- Define 90% C.L. region for each data set as

 $(\chi^2 - \chi_0^2)/\chi_0^2 < (\xi_{90} - \xi_{50})/\xi_{50}.$

 $\xi_{\rm 90}$ is the 90th percentile of the χ^2 -distribution with $N_{\rm pts.}$ d.o.f. $\xi_{\rm 50}\simeq N_{\rm pts.}$ is the most probable value.

• Similarly for the 68% C.L.

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Fractional change in χ^2 for each data set

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• Eigenvector direction sensitive to low-x gluon distribution.

ZEUS ep 99-00 σ H1/ZEUS ep F



• Eigenvector direction sensitive to low-x gluon distribution.



• Eigenvector direction sensitive to strange quark asymmetry.





Eigenvector direction sensitive to many parton flavours.





• Eigenvector direction sensitive to high-x gluon distribution.

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Contribution to PDF uncertainty from single eigenvector

MSTW 2008 NLO PDF fit (prel.)

Fractional contribution to uncertainty from eigenvector number 1



MSTW 2008 NLO PDF fit (prel.)

Fractional contribution to uncertainty from eigenvector number 6

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At input scale

 $Q_0^2 = 1 \text{ GeV}^2$

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Contribution to PDF uncertainty from single eigenvector

MSTW 2008 NLO PDF fit (prel.)

Fractional contribution to uncertainty from eigenvector number 11

0.8 0.6 0.4 0.2 0 xg xu, 0.6 0.2 0.: -0.2 -0.4 -0.6 -0.2 -0.4 -0.4 10 10.3 10 10 10** 10'1 $xS = 2x\overline{u} + 2x\overline{d} + xS + x\overline{S}$ 0.8 0.6 0.4 0.2 0 xd, 0.6 -0.2 -0.2 -0. -0.4 -0.4 10 10 10 10* 10 $\mathbf{x}\Delta = \mathbf{x}\overline{\mathbf{d}} - \mathbf{x}\overline{\mathbf{u}}$ xs + xs 0.8 0.6 0.4 0.2 0.6 0.0 0.: -0.2 -0.4 -0.2 10 10 10 10 xs - x5 0.8 0.6 0.4 0.2 0 At input scale $Q_0^2 = 1 \text{ GeV}^2$ -0.2 -0.4 -0.6 10 10 10

MSTW 2008 NLO PDF fit (prel.)

Fractional contribution to uncertainty from eigenvector number 19



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 Tolerance vs. eigenvector number





Eigenvector number

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Tolerance vs. eigenvector number

MSTW 2008 NLO PDF fit (prel.)



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Summary

- CTEQ and MRST have so far used a fixed value of the tolerance $T = \sqrt{\Delta \chi^2_{\rm global}}$ in producing eigenvector PDF sets.
- Propose **dynamic** determination of tolerance: different for each eigenvector of the Hessian/covariance matrix.
- In general 90% C.L. given by $T \sim \sqrt{50}$. Close to MRST value. CTEQ tolerance ($T = \sqrt{100}$) too large?
- Smaller tolerance for some eigenvectors, e.g. strange quarks.

Outlook

- Will provide LO, NLO, NNLO (+ modified LO for MCs) PDFs, each with 40 additional eigenvector PDF sets.
- Will provide stand-alone FORTRAN, C++, MATHEMATICA interpolation code (in addition to inclusion in LHAPDF).
- Timescale: \sim few weeks for publication and public release.

Appendix

MSTW 2008 NLO (prel.) compared to MRST 2001 NLO

