

Parton Distribution Functions for the LHC

Present Status & Uncertainty determination

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Ph. D. course on Particle Physics Phenomenology

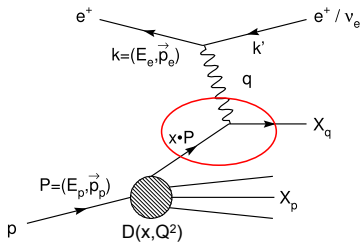
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October 4, 2011

What are Parton Distribution Functions?

Definition - Factorization

- Consider a process with one hadron in the initial state



- According to the **Factorization Theorem** we can write the cross section as

$$d\sigma = \sum_a \int_0^1 \frac{d\xi}{\xi} D_a(\xi, \mu^2) d\hat{\sigma}_a \left(\frac{x}{\xi}, \frac{\hat{s}}{\mu^2}, \alpha_s(\mu^2) \right) + \mathcal{O} \left(\frac{1}{Q^p} \right)$$



What are Parton Distribution Functions?

Definition - DGLAP equations

- The initial condition cannot be computed in Perturbation Theory (Lattice? In principle yes, but ...)
- ... but the energy scale dependence is governed by DGLAP evolution equations

$$\frac{\partial}{\ln Q^2} q^{NS}(\xi, Q^2) = P^{NS}(\xi, \alpha_s) \otimes q^{NS}(\xi, Q^2)$$
$$\frac{\partial}{\ln Q^2} \begin{pmatrix} \Sigma \\ g \end{pmatrix}(\xi, Q^2) = \begin{pmatrix} P_{qq} & P_{qg} \\ P_{gq} & P_{gg} \end{pmatrix}(\xi, \alpha_s) \otimes \begin{pmatrix} \Sigma \\ g \end{pmatrix}(\xi, Q^2)$$

- ... and the **splitting functions** P can be computed in PT and are known up to **NNLO**

(LO - Dokshitzer; Gribov, Lipatov; Altarelli, Parisi, 1977)

(NLO - Floratos, Ross, Sachrajda; Gonzalez-Arroyo, Lopez, Yndurain; Curci, Furmanski, Petronzio, 1981)

(NNLO - Moch, Vermaseren, Vogt, 2004)



Problem

Faithful estimation of errors on PDFs

- Single quantity: **1- σ error**
- Multiple quantities: **1- σ contours**
- Function: need an **"error band" in the space of functions**
(*i.e.* the probability density $\mathcal{P}[f]$ in the space of functions $f(x)$)

Expectation values are Functional integrals

$$\langle \mathcal{F}[f(x)] \rangle = \int \mathcal{D}f \mathcal{F}[f(x)] \mathcal{P}[f(x)]$$



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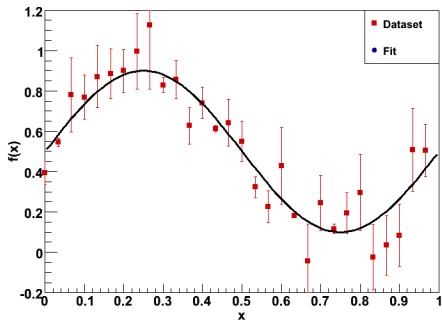
Expectation values are **Functional integrals**

$$\langle \mathcal{F}[f(x)] \rangle = \int \mathcal{D}f \mathcal{F}[f(x)] \mathcal{P}[f(x)]$$

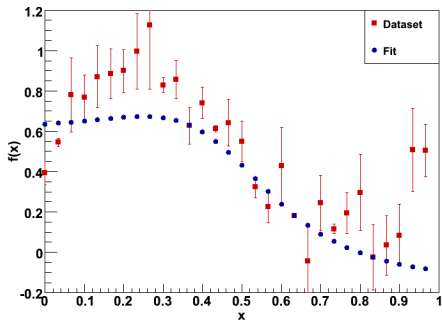
Determine a function from a finite set of data points



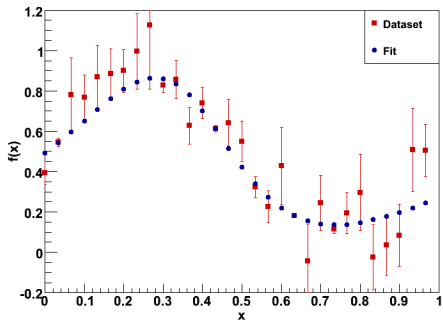
Proper Fitting avoiding Overlearning



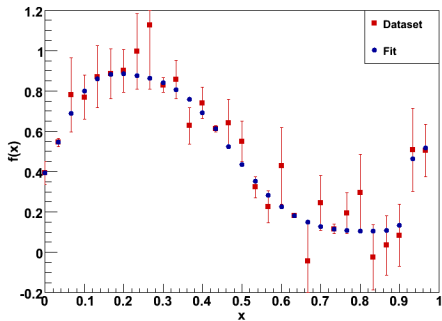
Proper Fitting avoiding Overlearning



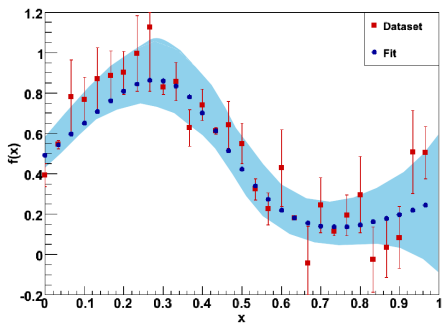
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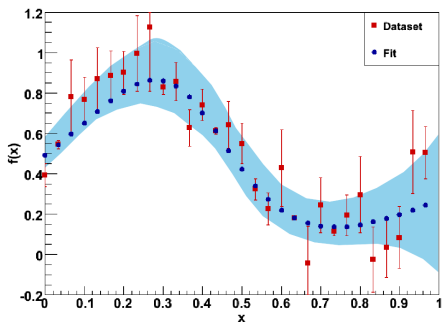
Proper Fitting avoiding Overlearning



Proper Fitting avoiding Overlearning



Proper Fitting avoiding Overlearning



- Need a **redundant parametrization** to avoid parametrization bias.
- Need a way of **stopping the fit before overlearning** sets in to avoid fitting statistical noise.
- Need a **reliable error estimation**.



DATA SET SELECTION



Choice of Dataset

Global vs. Restricted dataset

Restricted set Analyses

- **HERAPDF**: use only HERA DIS data
- **AB(K)M/JR**: use Fixed target DIS, HERA and Drell-Yan data
 - Focus on the most precise dataset(s)
 - Avoid possible incompatibilities
 - Limited flavour separation
 - Neglect important constraints (gluon at medium/large-x)

Global Analyses

- **CTEQ-TEA/MSTW/NNPDF**: HERA DIS, Fixed target DIS and Drell-Yan, Vector Boson and Inclusive jet production at colliders
 - Focus on completeness
 - Reliable flavour separation
 - Possible data incompatibilities



Choice of Dataset

Which data constrain which PDFs

H1, ZEUS: $F_2^{e^\pm p}(x, Q^2)$

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

NMC: $F_2^{\mu p}(x, Q^2), F_2^{\mu d}(x, Q^2), \frac{F_2^{\mu n}(x, Q^2)}{F_2^{\mu p}(x, Q^2)}$

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

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

CCFR, NuTeV, CHORUS: $F_{2,3}^{\nu(\bar{\nu})p}(x, Q^2)$

\Rightarrow q, \bar{q} at all x
 g at moderate and small x

E605, E702, E866: $pN \rightarrow \mu\bar{\mu} + X$

E605: Drell-Yan p, n asymmetry

CDF: W rapidity asymmetry

CDF, D0: Inclusive jet data

CCFR, NuTeV: Dimuon data

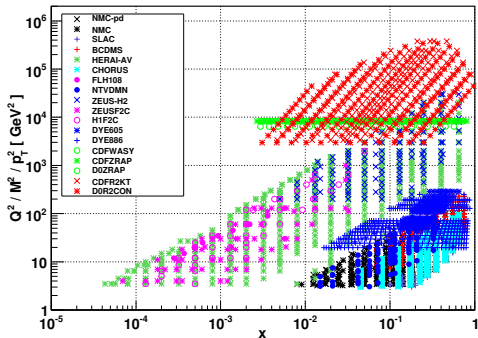
\Rightarrow $\bar{q}, (g)$
 \Rightarrow \bar{u}, \bar{d}
 \Rightarrow u/d ratio at high- x
 \Rightarrow g at high- x
 \Rightarrow s, \bar{s} sea



NNPDF 2.1

Dataset

NNPDF2.1 dataset



3338 data points

OBS	Data set
Deep Inelastic Scattering	
F_2^d / F_2^p	NMC-pd
F_2^p	NMC, SLAC, BCDMS
F_2^d	SLAC, BCDMS
σ_{NC}^{\pm}	HERA-I, ZEUS (HERA-II)
σ_{CC}^{\pm}	HERA-I, ZEUS (HERA-II)
F_L	H1
$\sigma_{\nu}, \sigma_{\bar{\nu}}$	CHORUS
dimuon prod.	NuTeV
F_2^c	ZEUS (99,03,08,09)
F_2^c	H1 (01,09,10)
Drell-Yan & Vector Boson prod.	
$d\sigma^{DY} / dM^2 dy$	E605
$d\sigma^{DY} / dM^2 dx_F$	E866
W asymm.	CDF
Z rap. distr.	D0/CDF
Inclusive jet prod.	
Incl. $\sigma^{(\text{jet})}$	CDF (k_T) - Run II
Incl. $\sigma^{(\text{jet})}$	D0 (cone) - Run II



PDF PARAMETRIZATION



PDF parametrization

Theoretical Requirements - QCD Sum Rules

- **Valence Sum Rules**

$$\int_0^1 [u(x, Q^2) - \bar{u}(x, Q^2)] dx = 2, \quad \int_0^1 [d(x, Q^2) - \bar{d}(x, Q^2)] dx = 1$$

$$\int_0^1 [s(x, Q^2) - \bar{s}(x, Q^2)] dx = 0$$

A proton has net quantum numbers of **2** up and **1** down quarks.

- **Momentum Sum Rule**

$$\sum_{a=q,\bar{q},g} \int_0^1 x f_a(x, Q^2) = 1$$

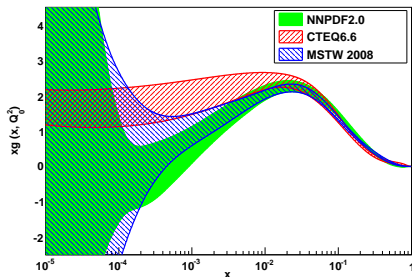
Momenta of all partons must add up to the proton momentum.



PDF parametrization

Theoretical Requirements - Positivity of Observables

- **Cross-sections must be positive**
 - Typically realized imposing PDF positivity
 - ... but remember: PDFs are not **P**robability **D**ensity **F**unctions (nor are they observables)
 - **No probabilistic interpretation** beyond Leading Order
 - Might result in excessive constraints on PDFs.



PDF parametrization

Standard Approach (CTEQ-TEA/MSTW/ABKM/HERAPDF)

- Introduce a simple functional form with enough free parameters

$$q(x, Q^2) = x^\alpha (1-x)^\beta P(x; \lambda_1, \dots, \lambda_n).$$

- "Theoretically motivated"-form
 - $x \rightarrow 0 : q \propto x^{a_1}$ - Regge-like behaviour
 - $x \rightarrow 1 : q \propto (1-x)^{a_2}$ - quark counting rules
 - $P(x; \lambda_1, \dots, \lambda_n)$: affects medium- x , just a convenient functional form



PDF parametrization

Standard Parametrization

Parton Distributions Combination

$$xU_V(x, Q^2) = A_U x^{\eta_1} (1-x)^{\eta_2} (1 + \epsilon_U \sqrt{x} + \gamma_U x)$$

$$xD_V(x, Q^2) = A_D x^{\eta_3} (1-x)^{\eta_4} (1 + \epsilon_D \sqrt{x} + \gamma_D x)$$

$$xS(x, Q^2) = A_S x^{\delta_S} (1-x)^{\eta_S} (1 + \epsilon_S \sqrt{x} + \gamma_S x)$$

$$x\Delta(x, Q^2) = A_\Delta x^{\eta_\Delta} (1-x)^{\eta_S+2} (1 + \gamma_\Delta + \delta_\Delta x^2)$$

$$xg(x, Q^2) = A_g x^{\delta_g} (1-x)^{\eta_g} (1 + \epsilon_g \sqrt{x} + \gamma_g x) + A_{g'} x^{\delta_{g'}} (1-x)^{\eta_{g'}}$$

$$x(s + \bar{s})(x, Q^2) = A_+ x^{\delta_S} (1-x)^{\eta_+} (1 + \epsilon_S \sqrt{x} + \gamma_S x)$$

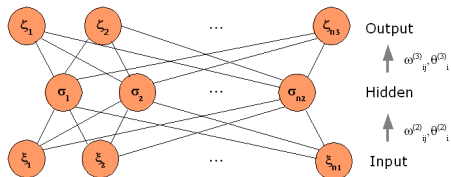
$$x(s - \bar{s})(x, Q^2) = A_- x^{\delta_-} (1-x)^{\eta_-} (1 + x/x_0)$$

29 parameters



PDF parametrization

The NNPDF Approach - Neural Networks



- Neural Networks are **non-linear** statistical tools.
- Any continuous function can be approximated with neural network with one internal layer and non-linear neuron activation function.
- **Efficient minimization algorithms** for complex parameter spaces.
- They provide a parametrization which is **redundant** and **robust** against variations.



PDF parametrization

Neural Networks ... just another basis of functions

Multilayer feed-forward networks

- Each neuron receives input from neurons in preceding layer and feeds output to neurons in subsequent layer
- Activation determined by **weights** and **thresholds**

$$\xi_i = g \left(\sum_j \omega_{ij} \xi_j - \theta_i \right)$$

- Sigmoid activation function

$$g(x) = \frac{1}{1 + e^{-\beta x}}$$



PDF parametrization

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A 1-2-1 NN:

$$\xi_1^{(3)}(\xi_1^{(1)}) = \frac{1}{1 + e^{\theta_1^{(3)} - \frac{\omega_{11}^{(2)}}{1 + e^{\theta_1^{(2)} - \xi_1^{(1)} \omega_{11}^{(1)}} - \frac{\omega_{12}^{(2)}}{1 + e^{\theta_2^{(2)} - \xi_1^{(1)} \omega_{21}^{(1)}}}}$$



PDF parametrization

NNPDF 2.1 Parametrization

Parton Distributions Combination

NN architecture

Singlet ($\Sigma(x)$)	\implies	2-5-3-1 (37 pars)
Gluon ($g(x)$)	\implies	2-5-3-1 (37 pars)
Total valence ($V(x) \equiv u_V(x) + d_V(x)$)	\implies	2-5-3-1 (37 pars)
Non-singlet triplet ($T_3(x)$)	\implies	2-5-3-1 (37 pars)
Sea asymmetry ($\Delta_S(x) \equiv \bar{d}(x) - \bar{u}(x)$)	\implies	2-5-3-1 (37 pars)
Total Strangeness ($s^+(x) \equiv (s(x) + \bar{s}(x))/2$)	\implies	2-5-3-1 (37 pars)
Strange valence ($s^-(x) \equiv (s(x) - \bar{s}(x))/2$)	\implies	2-5-3-1 (37 pars)

259 parameters



PDF UNCERTAINTIES



PDF Uncertainties

The Hessian Method

- The figure of merit to be minimized in the fit is the fully correlated χ^2

$$\chi^2 = \sum_{I,J=1}^{N_{dat}} (D_I - T_I(\{a\})) [(\text{cov})^{-1}]_{IJ} (D_J - T_J(\{a\}))$$

where D_k and T_k are the **data** and **theory** values for each data point

- Important to properly **account** for **correlated uncertainties**.
- Special care needed for **normalization uncertainties** (in general multiplicative uncertainties).

[R. D. Ball et al., arXiv:0912.2276]

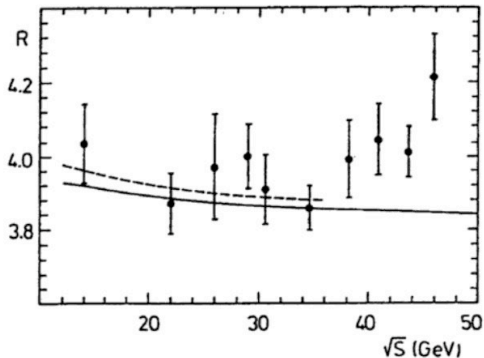


PDF Uncertainties

Normalization Uncertainties

m-COV

$R(e^+e^-)$
CELLO 1987



Dashed line: data below 36 GeV

Solid line: all data

D'Agostini 1994



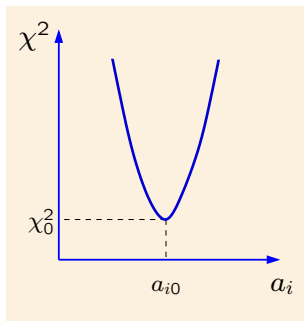
PDF Uncertainties

Multidimensional error Analysis

[P. Nadolsky, CTEQ School 2009]

Experimental observables Theoretical cross sections PDF parametrizations **Statistical aspects** Practical applications

Multi-dimensional error analysis



- Minimization of a likelihood function (χ^2) with respect to ~ 30 theoretical (mostly PDF) parameters $\{a_i\}$ and > 100 experimental systematical parameters



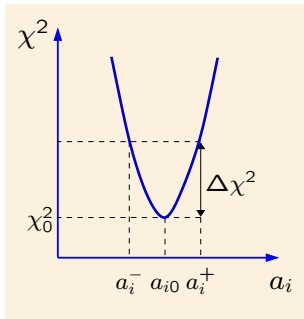
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- Establish a confidence region for $\{a_i\}$ for a given tolerated increase in χ^2
- In the ideal case of perfectly compatible Gaussian errors, 68% c.l. on a physical observable X corresponds to $\Delta\chi^2 = 1$ independently of the number N of PDF parameters

See, e.g., P. Bevington, K. Robinson, *Data analysis and error reduction for the physical sciences*



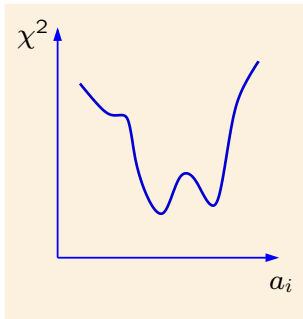
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Pitfalls to avoid

■ “Landscape”

- ▶ disagreements between the experiments

In the worst situation, significant disagreements between M experimental data sets can produce up to $N \sim M!$ possible solutions for PDF's, with $N \sim 10^{500}$ reached for “only” about 200 data sets



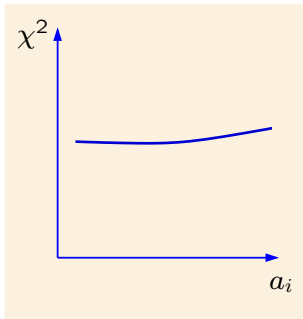
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Pitfalls to avoid

- Flat directions
 - ▶ unconstrained combinations of PDF parameters
 - ▶ dependence on free theoretical parameters, especially in the PDF parametrization
 - ▶ impossible to derive reliable PDF error sets



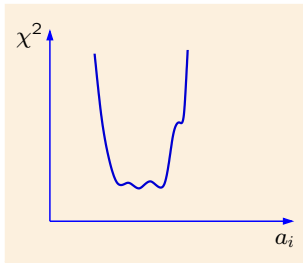
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The actual χ^2 function shows

- a well pronounced global minimum χ_0^2
- weak tensions between data sets in the vicinity of χ_0^2 (mini-landscape)
- some dependence on assumptions about flat directions



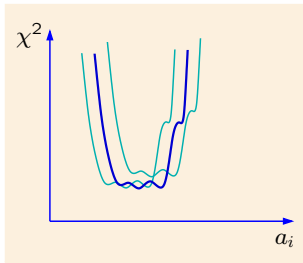
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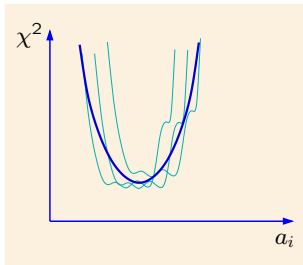
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The likelihood is approximately described by a quadratic χ^2 with a revised tolerance condition $\Delta\chi^2 \leq T^2$



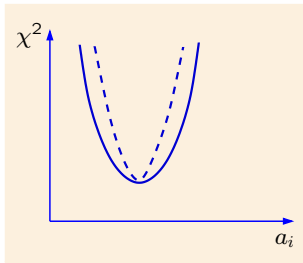
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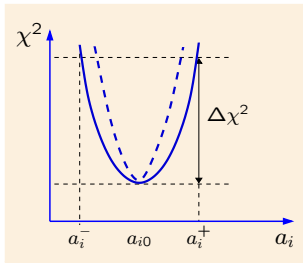
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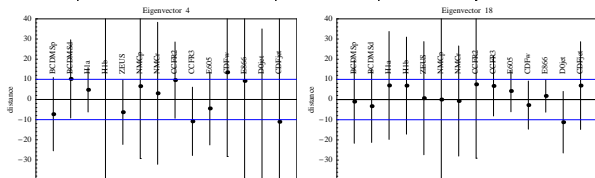
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CTEQ6 tolerance criterion (2001)

Acceptable values of PDF parameters must agree at $\approx 90\%$ c.l. with all experiments included in the fit, *for a plausible range of assumptions about the PDF parametrization, scale dependence, experimental systematics, ...*



Can be crudely approximated (but does not have to) by assuming $T \approx 10$ for all PDF parameters

A somewhat stricter variant of this criterion is applied in the MSTW'08 analysis



PDF Uncertainties

The Hessian Method

- Used by most PDF fitters (CTEQ, MSTW, ABKM, HERAPDF).
- Given an observable which depends on a set of parameters $\{z\}$

$$X(\{z\}) = X_0 + z_i \partial_i X(\{z\})$$

the variance is given by

$$\sigma_X^2 = \sigma_{ij} \partial_i X \partial_j X$$

with σ_{ij} being the covariance matrix in parameter space.

- **Diagonalization:** choose the z_i as eigenvectors of σ_{ij} with unit eigenvalues so that

$$\sigma_X^2 = |\vec{\nabla} X|^2$$

- Relies on **linear error propagation**, i.e. **Gaussian approximation**



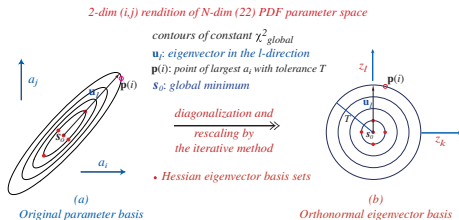
PDF Uncertainties

The Hessian Method

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Tolerance hypersphere in the PDF space



A hyperellipse $\Delta\chi^2 \leq T^2$ in space of N physical PDF parameters $\{a_i\}$ is mapped onto a filled hypersphere of radius T in space of N orthonormal PDF parameters $\{z_i\}$



PDF Uncertainties

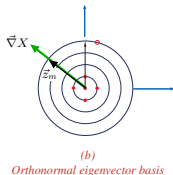
The Hessian Method

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Tolerance hypersphere in the PDF space

2-dim (i,j) rendition of N-dim (22) PDF parameter space



PDF error for a physical observable X is given by

$$\Delta X = \vec{\nabla} X \cdot \vec{z}_m = |\vec{\nabla} X| = \frac{1}{2} \sqrt{\sum_{i=1}^N (X_i^{(+)} - X_i^{(-)})^2}$$



PDF Uncertainties

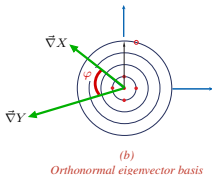
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Correlation cosine for observables X and Y :

$$\cos \varphi = \frac{\vec{v}_X \cdot \vec{v}_Y}{\Delta X \Delta Y} = \frac{1}{4 \Delta X \Delta Y} \sum_{i=1}^N \left(X_i^{(+)} - X_i^{(-)} \right) \left(Y_i^{(+)} - Y_i^{(-)} \right)$$



PDF Uncertainties

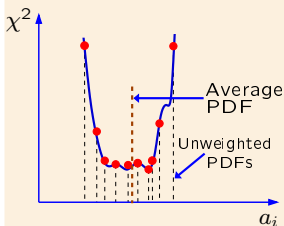
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Confidence intervals in global PDF analyses

Monte-Carlo sampling of the PDF parameter space



A very general approach that

- realizes stochastic sampling of the probability distribution

(Alekhin; Giele, Keller, Kosower; NNPDF)

- can parametrize PDF's by flexible neural networks (NNPDF)

- does not rely on smoothness of χ^2 or Gaussian approximations



PDF Uncertainties

The Monte Carlo Method

- Used by NNPDF (and old Fermi and Alekhin sets).
- Generate N_{rep} Monte Carlo **replicas of the data** (Monte Carlo in the space of parameters is not a smart idea, because of flat directions)
- Fit a set of PDFs to each replica, the **ensemble of replicas** gives the **probability density** in the space of PDFs
- You get a set of N_{rep} replicas, compute central values, standard deviations, correlations as you would do for any Monte Carlo ensemble:

$$\langle \mathcal{F}[\{q\}] \rangle = \frac{1}{N_{rep}} \sum_{k=1}^{N_{rep}} \mathcal{F}[\{q^{(k)}\}]$$

$$\sigma_{\mathcal{F}} = \sqrt{\frac{N_{rep}}{N_{rep} - 1} (\langle \mathcal{F}[\{q\}]^2 \rangle - \langle \mathcal{F}[\{q\}] \rangle^2)}$$



PDF Uncertainties

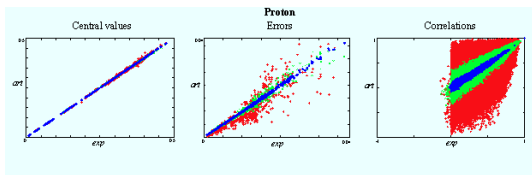
The Monte Carlo Method in practice

- **Generate artificial data** according to distribution

$$O_i^{(art)(k)} = (1 + r_N^{(k)} \sigma_N) \left[O_i^{(exp)} + \sum_{p=1}^{N_{sys}} r_p^{(k)} \sigma_{i,p} + r_{i,S}^{(k)} \sigma_S^i \right]$$

where r_i are univariate (gaussian) random numbers

- **Validate** Monte Carlo **replicas** against experimental data (statistical estimators, faithful representation of errors, convergence rate increasing N_{rep})



- $\mathcal{O}(1000)$ **replicas** needed to reproduce **correlations to percent accuracy**



PDF Uncertainties

Hessian vs. Monte Carlo

- **Q:** Are the two methods equivalent?

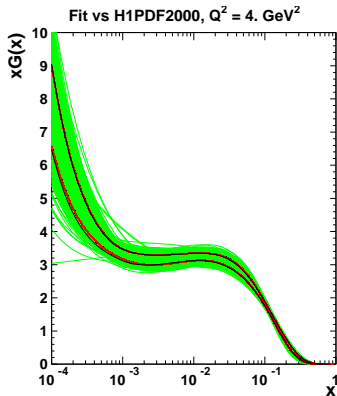
A: Hessian and MC method give the same results in the linear error propagation approximation

- **Q:** Nice, but what about in the real world?

A: [arXiv:0901.2504](https://arxiv.org/abs/0901.2504), pg. 41

- **Q:** Wait a minute, you assumed gaussian errors ...

A: [arXiv:0901.2504](https://arxiv.org/abs/0901.2504), pg. 42



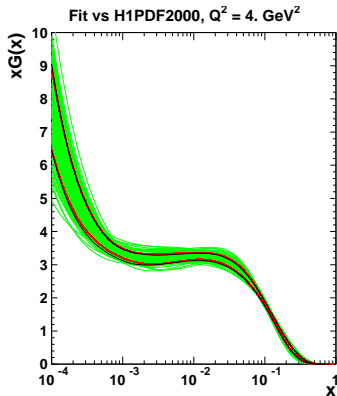
[S. Glazov and V. Radescu]



PDF Uncertainties

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[S. Glazov and V. Radescu]



PDF fits status



The present status of PDF fits

The PDF sets Matrix

	Dataset	Pert. Order	Heavy Flavours	α_S	Param.	Uncert.
ABKM09	DIS (FT, HERA) Drell-Yan (FT)	NLO NNLO	FFN (BMSN)	fitted	6 indep. PDF Polynomial (25 param.)	Hessian ($\Delta\chi^2 = 1$)
CT10	DIS (FT, HERA) Drell-Yan (FT, Tev) Jets (Tevatron)	LO NLO	GM-VFNS (S-ACOT)	external	6 indep. PDF Polynomial (26 param.)	Hessian ($\Delta\chi^2 = 100$)
JR09	DIS (FT, HERA) Drell-Yan (FT) Jets (Tevatron)	NLO NNLO	FFN VFN	fitted	5 indep. PDF Polynom. (15 param.)	Hessian ($\Delta\chi^2 = 1$)
HERAPDF1.5	DIS (HERA)	NLO NNLO	GM-VFNS (TR)	external	5 indep. PDF Polnom. (14 param.)	Hessian ($\Delta\chi^2 = 1$)
MSTW08	DIS (FT, HERA) Drell-Yan (FT, Tev) Jets (HERA, Tev)	LO NLO NNLO	GM-VFNS (TR)	fitted	7 indep. PDF Polynom. (20 param.)	Hessian ($\Delta\chi^2 \sim 25$)
NNPDF2.1	DIS (FT, HERA) Drell-Yan (FT, Tev) Jets (Tevatron)	LO NLO NNLO	GM-VFNS (FONLL)	external	7 indep. PDF Neural Netw. (259 param.)	Monte Carlo

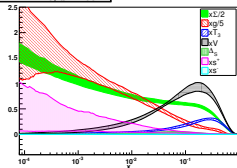


The present status of PDF fits

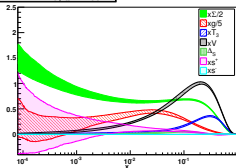
PDFs ... a family portrait

- At the starting scale (2 GeV^2) ...

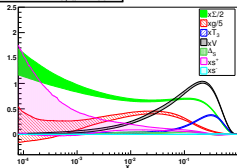
NNPDF2.1 LO, $Q^2 = 2 \text{ GeV}^2$



NNPDF2.1 NLO, $Q^2 = 2 \text{ GeV}^2$



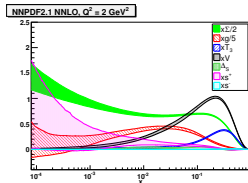
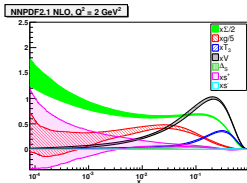
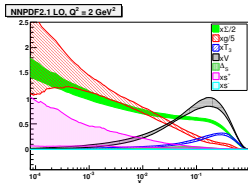
NNPDF2.1 NNLO, $Q^2 = 2 \text{ GeV}^2$



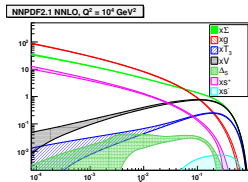
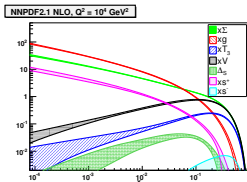
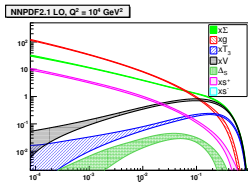
The present status of PDF fits

PDFs ... a family portrait

- At the starting scale (2 GeV^2) ...



- ... and at the typical EW scale (100 GeV^2)

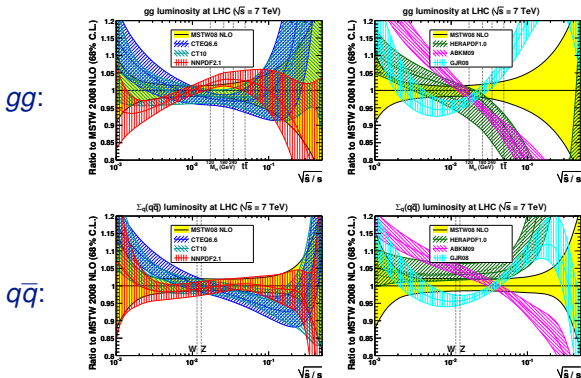


The present status of PDF fits

Comparison between Parton Luminosities

- When trying to understand **differences between PDF** sets it is useful to look at **parton luminosities**

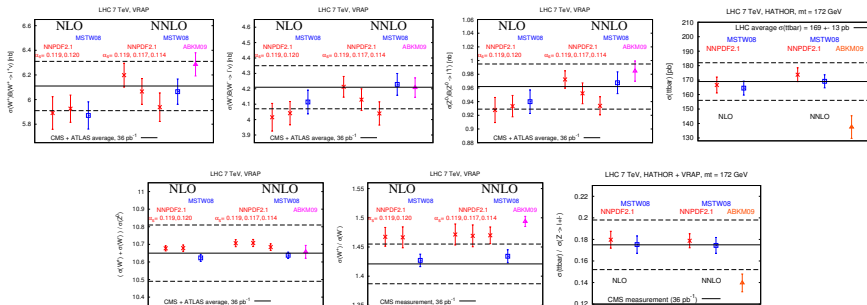
$$\Phi_{ij}(M_X^2) = \frac{1}{s} \int_{\tau}^1 \frac{x_1}{x_1} f_i(x_1, M_X^2) f_j(\tau/x_1, M_X^2)$$



The present status of PDF fits

Comparisons to LHC data

- Predictions for **LHC Standard Candles** compared to **LHC data**



- LHC data will soon be precise enough to distinguish between different predictions.

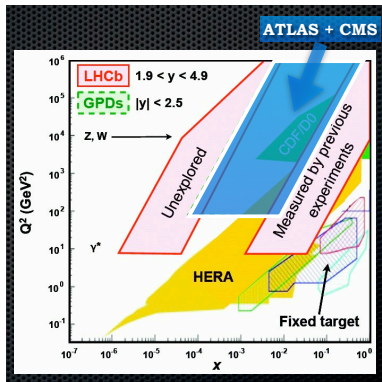


The present status of PDF fits

W lepton asymmetry data at the LHC

$$A_W^l = \frac{\sigma(pp \rightarrow W^+ \rightarrow l^+ \nu_l) - \sigma(pp \rightarrow W^- \rightarrow l^- \bar{\nu}_l)}{\sigma(pp \rightarrow W^+ \rightarrow l^+ \nu_l) + \sigma(pp \rightarrow W^- \rightarrow l^- \bar{\nu}_l)}$$

- **ATLAS**: muon charge asymmetry (31pb^{-1}) [ArXiv:1103:2929]
- **CMS**: muon charge asymmetry (36pb^{-1}) [ArXiv:1103:3470]

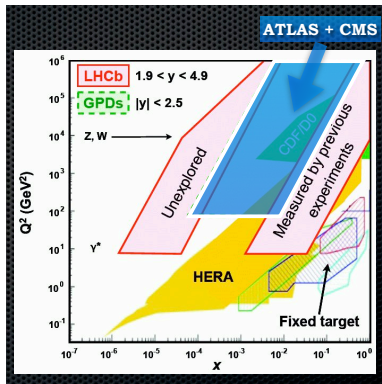


The present status of PDF fits

W lepton asymmetry data at the LHC

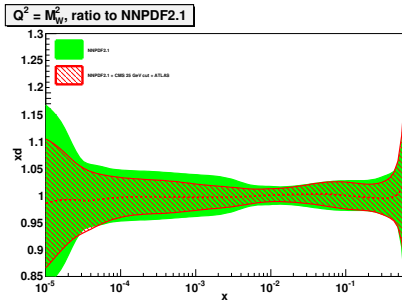
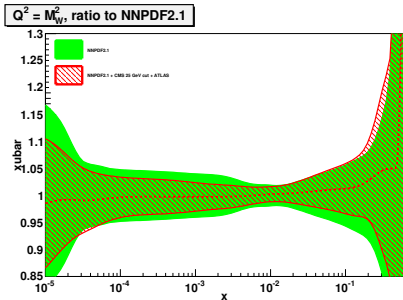
$$A'_W \sim \frac{u(x_1, M_W^2) \bar{d}(x_2, M_W^2) - d(x_1, M_W^2) \bar{u}(x_2, M_W^2)}{u(x_1, M_W^2) \bar{d}(x_2, M_W^2) + d(x_1, M_W^2) \bar{u}(x_2, M_W^2)}$$

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The present status of PDF fits

First constraints on PDFs from LHC



- ATLAS and CMS data compatible with data included in global analysis
- The provide important constraint to PDFs in the small medium- x region
- Significant uncertainty reduction for light (anti-)flavour distributions



The present status of PDF fits

... the data we would love to have from the LHC

- Medium- and large- x **gluon**
 - Prompt photons
 - Inclusive Jets
 - t -quark distributions (p_{\perp}, y) (?)
- **Light flavour separation** at medium- & small- x
 - Low-mass Drell-Yan
 - High-mass W production
 - Z rapidity distribution
 - $W(+jets)$ asymmetry
- **Strangeness & Heavy Flavours**
 - $W + c$
 - $Z + c, \gamma + c$
 - $Z + b$

