NNPDF: Neural Networks, Monte Carlo techniques and Parton Distribution Functions

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on behalf of the **NNPDF Collaboration**:
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HiX2010

3rd International Workshop on Nucleon Structure at Large Bjorken *x*

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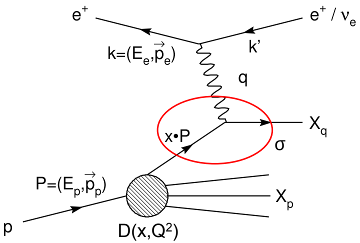
What are Parton Distribution Functions?

- 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?

- The **absolute value** of PDFs at a given x and Q^2 **cannot be computed** in QCD Perturbation Theory
  (Lattice? In principle yes, but ...)
- ... but the **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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Determine a function from a finite set of data points

Solution

Standard Approach

- Introduce a simple functional form with enough free parameters

$$q(x, Q_0^2) = x^\alpha (1-x)^\beta P(x; \lambda_1, ..., \lambda_n).$$

- Fit parameters minimizing χ^2.

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Open problems:

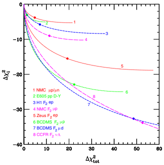
- **Error propagation** from data to parameters and from parameters to observables is **not trivial**.
- **Theoretical bias** due to the chosen **parametrization** is difficult to assess.

Shortcomings of the Standard approach

What is the meaning of a one-σ uncertainty?

- Standard $\Delta\chi^2 = 1$ criterion is **too restrictive** to account for large discrepancies among experiments.

[Collins & Pumplin, 2001]



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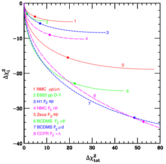
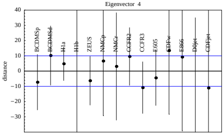


- Introduce a **TOLERANCE** criterion, i.e. take the envelope of uncertainties of experiments to determine the $\Delta\chi^2$ to use for the global fit (CTEQ).



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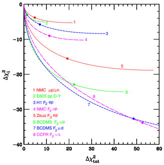

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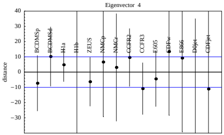
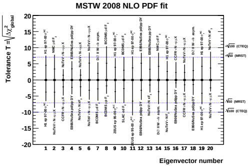


- Make it **DYNAMICAL**, i.e. determine $\Delta\chi^2$ separately for each hessian eigenvector (MSTW).

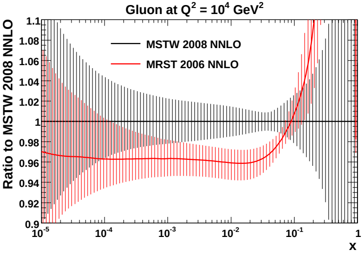


Shortcomings of the Standard approach

What determines PDF uncertainties?

- Uncertainties in standard fits often increase when adding new data to the fit.
- Need of extending the parametriztion in order to accomodate the new data

Smaller high-x gluon (and slightly smaller α_S) results in larger small-x gluon – now shown at NNLO.



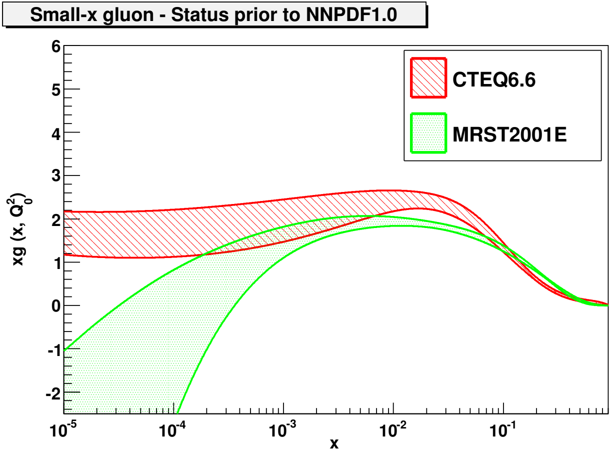
Larger small-x uncertainty due to extrat free parameter.

[R. Thorne, PDF4LHC]

PDF4LHCMSTW 24

Shortcomings of the standard approace

What determines PDF uncertainties? Parmetrization bias?



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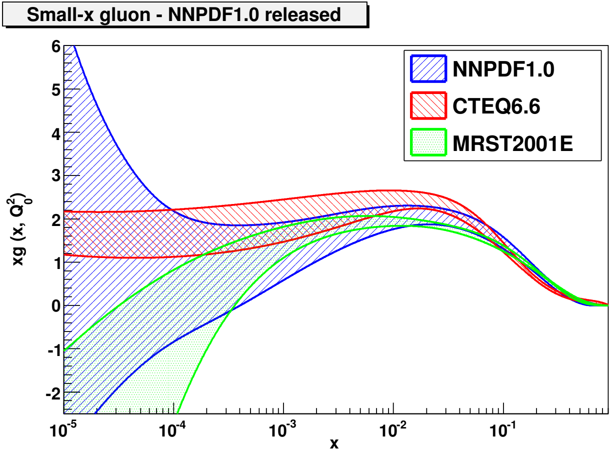

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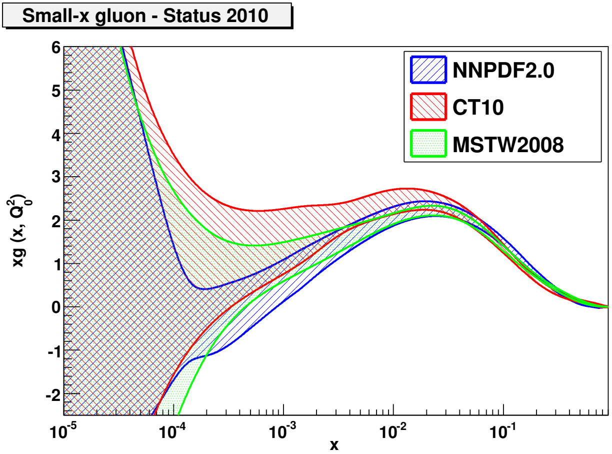


NNPDF Methodology

Main Ingredients

- **Monte Carlo** determination of errors
  - No need to rely on linear propagation of errors
  - Possibility to test for the impact of non gaussianly distributed errors
  - Possibility to test for non-gaussian behaviour in fitted PDFs ($1 - \sigma$ vs. 68% CL)
- **Neural Networks**
  - Provide an **unbiased** parametrization
- **Stopping based on Cross Validation**
  - Ensures proper fitting avoiding overlearning

NNPDF Methodology

... in a Nutshell

- Generate N_{rep} **Monte-Carlo replicas** of the experimental data (sampling of the probability density in the space of data)
- Fit a set of Parton Distribution Functions on each replica (sampling of the probability density in the space of PDFs)
- **Expectation values** for observables are **Monte Carlo integrals**

$$\langle \mathcal{F}[f_i(x,Q^2)] \rangle = \frac{1}{N_{rep}} \sum_{k=1}^{N_{rep}} \mathcal{F}\left(f_i^{(net)(k)}(x,Q^2) \right)$$

... the same is true for errors, correlations, etc.

NNPDF Methodology

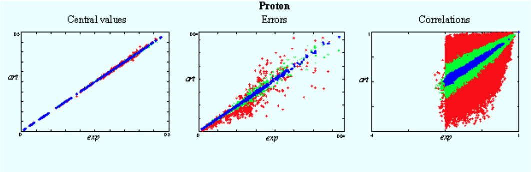
Monte Carlo replicas generation

- 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

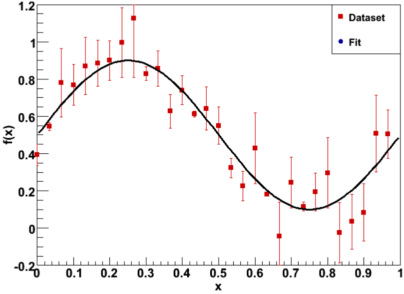
- Validate Monte Carlo replicas against experimental data (statistical estimators, faithful representation of errors, convergence rate increasing N_{rep})



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

Proper Fitting avoiding Overlearning

- Let's see how proper fitting works in a toy model



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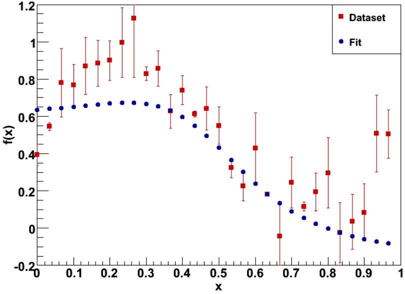

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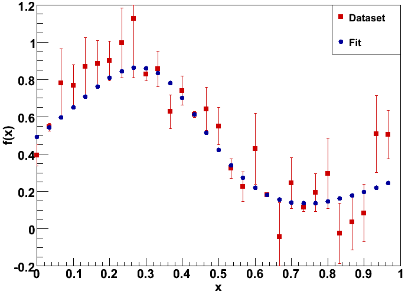

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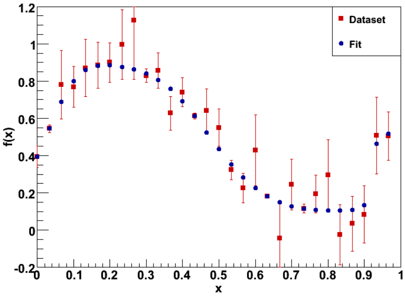

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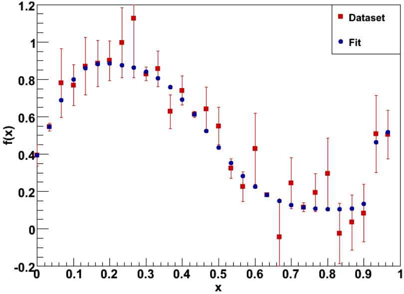

- Need a **redundant parametrization** to avoid parametrization bias.
- Need a way of **stopping the fit before overlearning** sets in to avoid fitting statistical noise.

Neural Networks

... a suitable basis of functions

- We use **Neural Networks** as **functions** to represent **PDFs at the starting scale**
- We employ **Multilayer Feed-Forward** Neural Networks trained using a **Genetic Algorithm**
- Activation determined by weights and thresholds

$$\xi_i = g\left(\sum_j \omega_{ij}\xi_j - \theta_i\right) , \qquad g(x) = \frac{1}{1+e^{-\beta x}}$$

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Ex.: 1-2-1 NN:

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

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- They provide a parametrization which is **redundant** and **robust** against variations

Neural Networks

Stopping criterion

Stopping criterion based on Training-Validation separation

- Divide the data in two sets: Training and Validation
- Minimize the χ^2 of the data in the Training set
- Compute the χ^2 for the data in the Validation set
- When Validation χ^2 stops decreasing, **STOP** the fit

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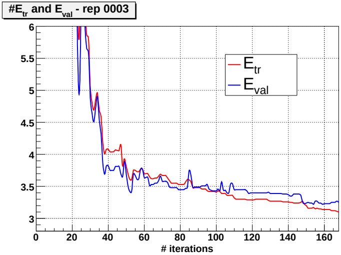
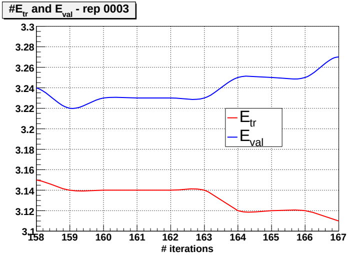
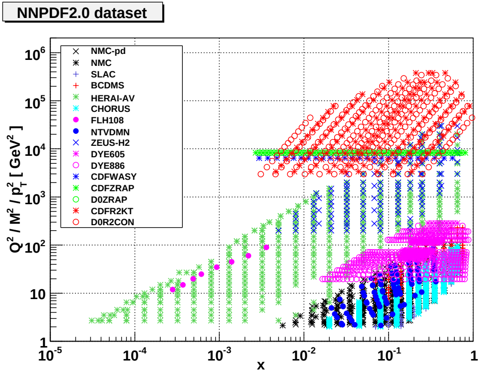




NNPDF 2.0

Dataset



3415 data points

(for comparison MSTW08 includes 2699 data points)

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

NNPDF 2.0

Technical improvements

- The fit is carried at **NLO** QCD, in the **Zero-Mass Variable Flavour Number Scheme**
- Fast DGLAP evolution based on higher-order interpolating polynomials
- Improved treatment of normalization errors (t_0 method)
  - For details see [R. D. Ball et al., arXiv:0912.2276]
- Improvements in training/stopping
  - Target Weighted Training
  - Improved stopping for avoiding under-/over-learning
- All details given in [R. D. Ball et al., arXiv:1002.4407]

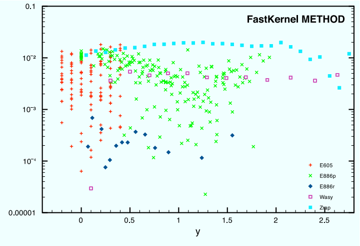
NNPDF 2.0

FastKernel

- NLO computation of hadronic observables too slow for parton global fits.
- MSTW08 and CTEQ include Drell-Yan NLO as (local) K factors rescaling the LO cross section
- K-factor depends on PDFs and it is not always a good approximation.

* NNPDF2.0 includes full NLO calculation of hadronic observables.
* Use available fastNLO interface for jet inclusive cross-sections.[hep-ph/0609285]
* Built up our own **FastKernel** computation of DY observables.

$$\int_{x_{0,1}}^{1} dx_1 \int_{x_{0,2}}^{1} dx_2\, f_a(x_1) f_b(x_2) C^{ab}(x_1, x_2) \rightarrow \sum_{\alpha,\beta=1}^{N_x} f_a(x_{1,\alpha}) f_b(x_{2,\beta}) \int_{x_{0,1}}^{1} dx_1 \int_{x_{0,2}}^{1} dx_2\, \mathcal{I}^{(\alpha,\beta)}(x_1, x_2) C^{ab}(x_1, x_2)$$



- DGLAP evol. and double convolution improved
  - Use high-orders polynomial interpolation
  - Precompute all Green Functions

A truly NLO analysis

NNPDF 2.0

Parametrization

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

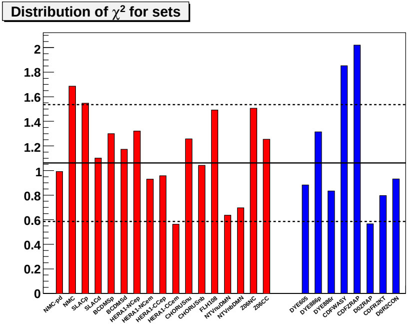
259 parameters
Standard fits have $\sim$ 25 parameters in total

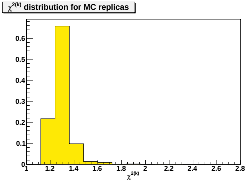
No change in the parametrization from NNPDF1.2 ... despite substantial **enlargement of the dataset**

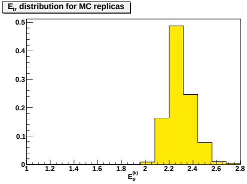
NNPDF 2.0

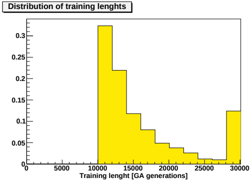
General features of the fit

$\chi^2_{\rm tot}$	1.21
$\langle E \rangle \pm \sigma_E$	2.32 ± 0.10
$\langle E_{\rm tr} \rangle \pm \sigma_{E_{\rm tr}}$	2.29 ± 0.11
$\langle E_{\rm val} \rangle \pm \sigma_{E_{\rm val}}$	2.35 ± 0.12
$\langle {\rm TL} \rangle \pm \sigma_{\rm TL}$	16175 ± 6257
$\langle \chi^{2(k)} \rangle \pm \sigma_{\chi^2}$	1.29 ± 0.09









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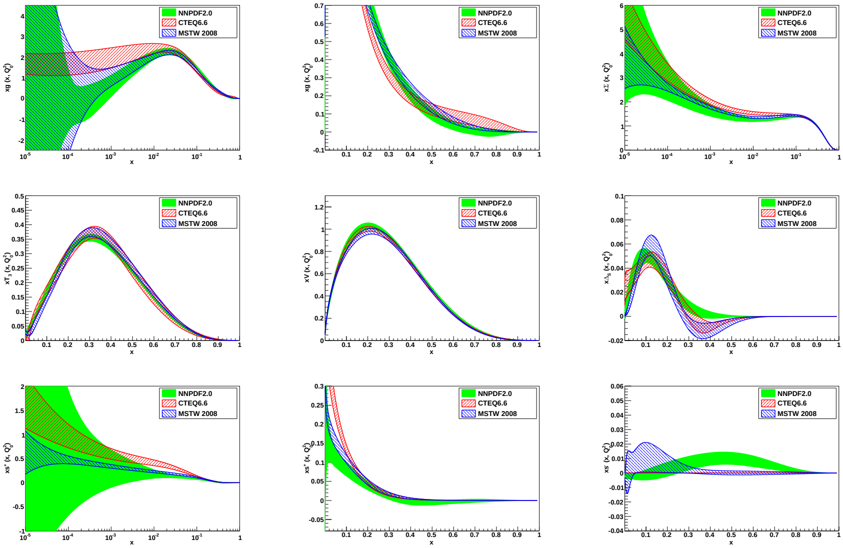
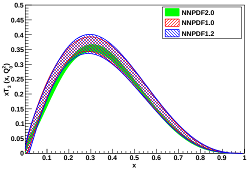
Partons - Comparison to other global fits



NNPDF2.0

Results - Partons - A couple of upshots

- **Reduction of uncertainties** with respect to older NNPDF sets due to **inclusion of new data**



NNPDF2.0

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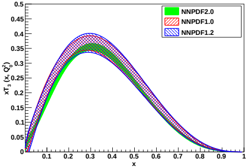
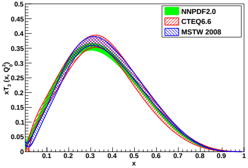


- **Uncertainties** on PDFs **competitive** with results from other groups ...



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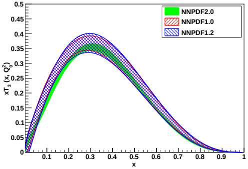

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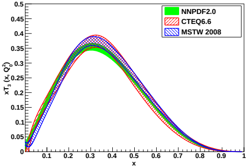
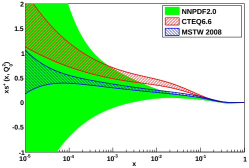


- ... but still retain **unbiasedness** in regions where there are little or no experimental constraints



PDF Uncertainties and Correlations

A practitioner's guide to NNPDF predictions

Central Value

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

Standard Deviation

$$\sigma_{\mathcal{F}} = \left(\frac{1}{N_{\rm N_{set}}} \sum_{k=1}^{N_{\rm set}} \left(\mathcal{F}[\{q^{(k)}\}] - \langle \mathcal{F}[\{q\}] \rangle \right)^2 \right)^{1/2}$$

Correlation

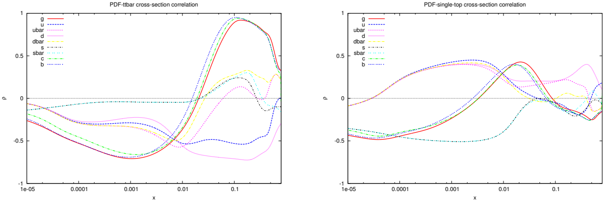
$$\rho \equiv \cos[\varphi(\mathcal{F},\mathcal{G})] = \frac{< \mathcal{F}\,\mathcal{G} >_{\rm rep} - < \mathcal{F} >_{\rm rep} < \mathcal{G} >_{\rm rep}}{\sqrt{< \mathcal{F}^2 >_{\rm rep} - < \mathcal{F} >^2_{\rm rep}}\sqrt{< \mathcal{G}^2 >_{\rm rep} - < \mathcal{G} >^2_{\rm rep}}}$$

PDF induced correlations

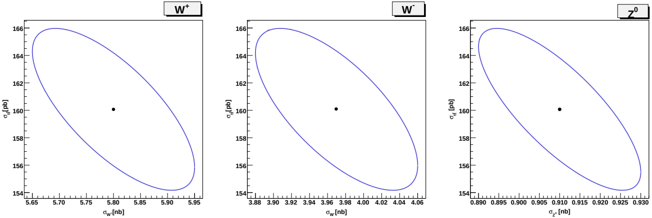
Ex.: Top-quark studies within the NNPDF framework

[J. Rojo and AG, arXiv:1008.4671]

- It is easy to compute **correlations** among **PDFs and observables**



- ... or **pairs of observbles**



Reweighting PDFs

Assessing the impact of new data on PDF fits

- Inspired by Giele and Keller [hep-ph/9803393]
- The N_{rep} replicas of a NNPDF fit give the probability density in the space of PDFs
- **Expectation values** for observables are **Monte Carlo integrals**

$$\langle \mathcal{F}[f_i(x,Q^2)] \rangle = \frac{1}{N_{rep}} \sum_{k=1}^{N_{rep}} \mathcal{F}\left(f_i^{(net)(k)}(x,Q^2) \right)$$

(... the same is true for errors, correlations, etc.)

- We can **assess the impact** of including **new data** in the fit updating the probability density distribution.

Reweighting PDFs

Assessing the impact of new data on PDF fits

- According to **Bayes Theorem** we have

$$\mathcal{P}_{\rm new}(\{f\}) = \mathcal{N}_\chi \mathcal{P}(\chi^2|\{f\}) P_{\rm init}(\{f\}) , \quad \mathcal{P}(\chi^2|\{f\}) = [\chi^2(y,\{f\})]^{\frac{n_{dat}}{2}-1} e^{-\frac{\chi^2(y,\{f\})}{2}}$$

- **Monte Carlo integrals** are now **weighted sums**

$$\langle \mathcal{F}[f_i(x,Q^2)]\rangle = \sum_{k=1}^{N_{rep}} w_k \mathcal{F}\left(f_i^{(net)(k)}(x,Q^2)\right)$$

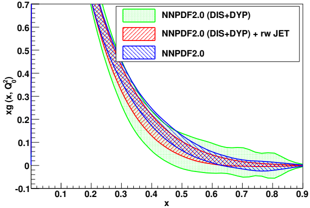
where the **weights** are

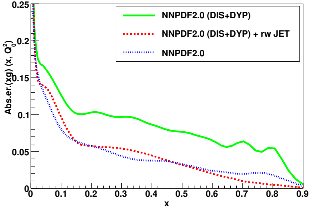
$$w_k = \frac{[\chi^2(y,f_k)]^{\frac{n_{dat}}{2}-1} e^{-\frac{\chi^2(y,f_k)}{2}}}{\sum_{i=1}^{N_{\rm rep}} [\chi^2(y,f_i)]^{\frac{n_{dat}}{2}-1} e^{-\frac{\chi^2(y,f_i)}{2}}}$$

Reweighting PDFs

Proof-of-concept: Inclusive Jet data, reweighting vs. refitting

- Use **DIS+DY-fit** as **prior** probability distribution
- Add Tevatron Inclusive Jet data through refitting and through reweighting
- **Reweighting** and **refitting** yield **statistically equivalent** results

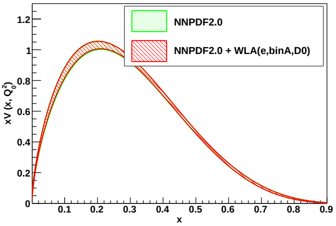


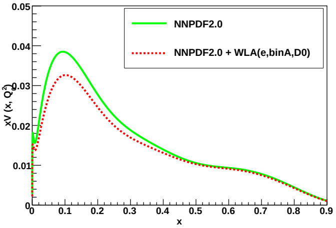


Reweighting PDFs

Reweighting real data: W lepton asymmetry

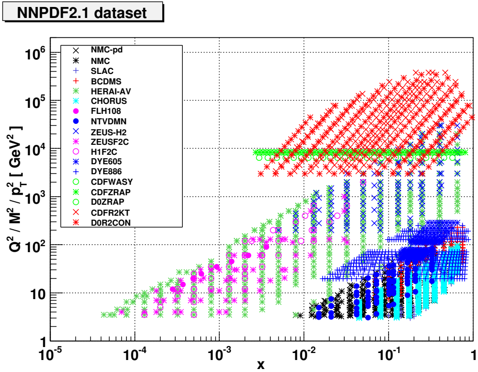
- In the NNPDF2.0 fit we only included CDF W asymmetry data
- We evaluated W electron asymmetry with NNPDF20 1000 replicas set using **DYNNLO** [Catani et al., arXiv:0903.2120].
- .. and included D0 W electron asymmetry data points through reweighting.
- Main impact on reduction of middle-x Valence uncertainty.
- **No** need of **refitting**





NNPDF 2.1

Dataset



3554 data points

Deep Inelastic Scattering	
F_2^d / F_2^p	NMC-pd
F_2^p	NMC, SLAC, BCDMS
F_2^d	SLAC, BCDMS
$\sigma_{NC}^{\pm}$	HERA-I, ZEUS (HERA-II)
$\sigma_{CC}^{\pm}$	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.	
$d\sigma^{\rm DY}/dM^2 dy$	E605
$d\sigma^{\rm DY}/dM^2 dx_F$	E866
W asymm.	CDF
Z rap. distr.	D0/CDF

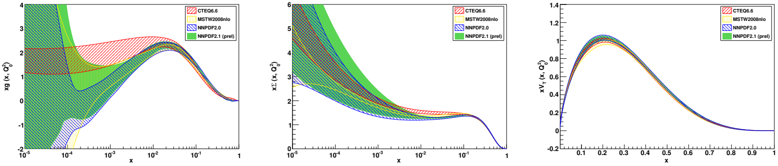
Inclusive jet prod.	
Incl. $\sigma^{\rm (jet)}$	CDF (k_T) - Run II
Incl. $\sigma^{\rm (jet)}$	D0 (cone) - Run II

- We adopt the **FONLL-A** General Mass-Variable Flavour Number Scheme

  (M. Cacciari, M. Greco and P. Nason, (1998))

  (S. Forte, P. Nason E. Laenen and J. Rojo, (2010))

- **Preliminary** results for partons



- Small- and medium-x **gluon** and **Singlet** are most sensitive, **Non-Singlet** combinations **mostly unaffected**
- Effect of improved heavy flavour treatment is within **one-σ**, both on PDFs and LHC Standard Candles
- **Fixed-**(3- and 4-)**Flavour Number Scheme** PDFs will also be released

Conclusions

- The **NNPDF methodology** based on using **Monte Carlo** techniques and **Neural Networks** is well suited to address problems of standard fits.
- **NNPDF2.0** is the first **global NNPDF fit**
  - Exact inclusion of NLO corrections
  - **No** sign of **strong tension** among different datasets
- NNPDF sets are **available** within the **LHAPDF** interface.
- **Reweighting** technique allows to study impact of **new data without refitting**
- Next steps:
  - Improved treatment of Heavy Flavour contributions (FONLL)
  - Inclusion of higher order contributions (NNLO QCD/EW effects)
  - Study the impact of theoretical uncertainties (α_S, quark masses ...)
  - Inclusion of resummation (small-/large-x) effects