Neural network approach to PDF fitting

The NNPDF Collaboration:
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Motivation

- The problem: parametrization of parton distributions from data.

- Shortcomings of standard approaches to pdf global fits:

  1. A priori bias introduced by the choice of a fixed functional form.

  2. Problems with estimation of uncertainties:

     – The pdf parametrization affects (in an unknown way) the representation of uncertainties.

     – Incompatible data, non gaussian errors $\rightarrow$ (arbitrary) Tolerance criteria.

  3. Correct implementation of error propagation: some methods use (not trustable) linear approximations.

- Very relevant problem: In parallel with the determination of best-fit PDFs an equally important front in global analysis has been opened ... the development of quantifiable uncertainties on the PDFs ... Much progress has been made, many useful results have been obtained, but there are no unambiguous conclusions, W.K. Tung, hep-ph/0410139

What is the problem?

- For a single quantity $\rightarrow$ 1 sigma errors

- For a pair of numbers $\rightarrow$ 1 sigma ellipse

- For a function $\rightarrow$ We need the probability measure $\mathcal{P}[f]$ in the space of functions $f(x)$

Expectation values $\rightarrow$ Functional integrals

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

The problem: Determine an infinite-dimensional object (a function) from finite set of data points.
$\rightarrow$ **Mathematically ill-posed** problem.

What is the problem?

Parton distributions $\rightarrow$ DIS structure functions

$$F(x, Q^2) = \sum_f C_f \left(\alpha_s \left(Q^2\right)\right) \otimes q_f(Q^2) + C_g \left(\alpha_s \left(Q^2\right)\right) \otimes g_f(Q^2)$$

- Trivial complication: disentangle quark flavors and gluon, evolution, deconvolution.

- Serious complication: determine error on pdfs $f(x)$, $f = q_i, g$

A (marginally) simpler problem: Determine the structure function $F(x, Q^2)$ with associated errors.

The NNPDF program: proceed in two steps:

1. Determination of structure functions: Done!

2. Determination of parton distributions: On the way ...

Step 1:
Determination of Structure Functions
(Completed)

The NNPDF Collaboration approach:

Use neural networks as unbiased universal interpolants to construct a probability measure in the space of structure functions $\mathcal{P}\left[F(x, Q^2)\right]$ from experimental data.

General strategy:

1. Monte Carlo sampling of data (Generation of replicas of experimental data) $\rightarrow$ Faithful representation of uncertainties

2. Neural network training over Monte Carlo replicas $\rightarrow$ Unbiased parametrization.

The probability measure $\mathcal{P}\left[F\right]$ contains all information from experimental data (central values, errors, correlations) with the only assumption of smoothness. Expectation values $\rightarrow$ Functional integrals over probability measure

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

$\mathcal{P}\left[F(x)\right]$ validated through statistical estimators.

1.- Monte Carlo sampling of experimental data

Generate N_{rep} Monte Carlo sets of 'pseudo-data', replicas of the original N_{dat} data points $F_i^{(exp)}$

$$F_i^{(art)(k)} \quad k = 1, \ldots, N_{rep}, \quad i = 1, \ldots, N_{dat}$$

using full information on experimental errors and correlations:

$$F_i^{(art)(k)} = \left(1 + r_N^{(k)}\sigma_N\right)\left[F_i^{(exp)} + r_i^s\sigma_i^{stat} + \sum_{l=1}^{N_{sys}} r^{l,(k)}\sigma_i^{sys,l}\right]$$

Size of set of replicas $\left\{F^{(art)(k)}\right\}$ large enough to reproduce central values, errors and correlations of exp. data.

Similar to the Bayesian Monte Carlo approach (Giele ,Kosower, Keller 01).

2.- Neural network replica training

Neural network: highly nonlinear mapping between input and output patterns, defined by its parameters (weights $\omega_{ij}^{(l)}$ and thresholds $\theta_i^{(l)}$)
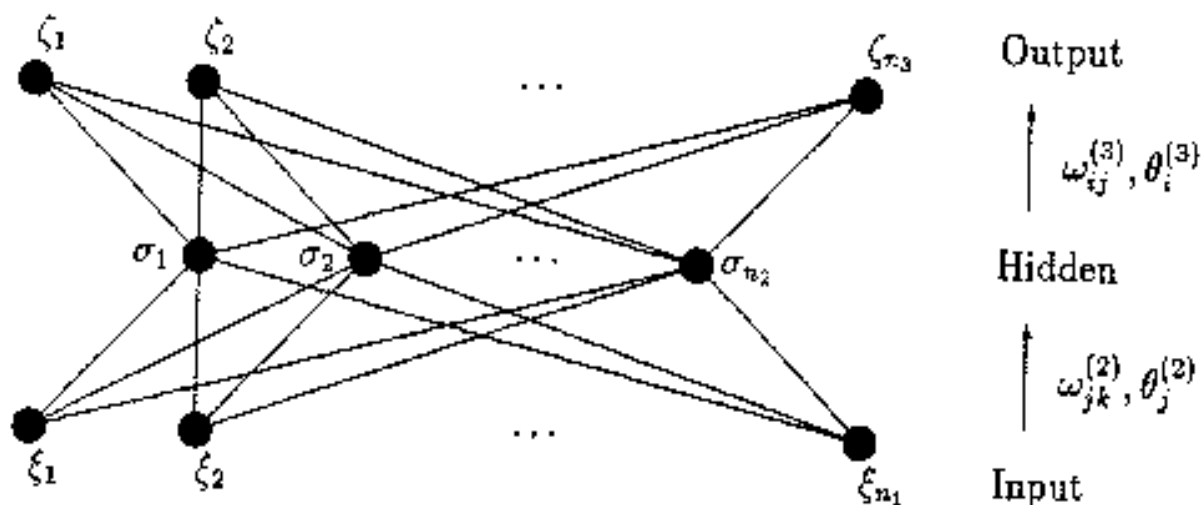
Neural networks are suitable to parametrize PDFs as

- Are the most unbiased prior.

- Robust, unbiased universal approximants

- Interpolate between data points with only assumption $\rightarrow$ smoothness.

2.- Neural network replica training

Perceptrons: feed-forward multilayer neural networks

$$\xi_i^{(l)} = g\left(\sum_{j=1}^{n_l-1} \omega_{ij}^{(l-1)} \xi_j^{(l-1)} - \theta_i^{(l)}\right) \quad g(x) = \frac{1}{1+e^{-\beta x}}$$

Choose redundant architecture → No smoothing bias

Neural network training (PDF fitting) → Minimization of covariance matrix error

$$\chi^{2(k)} = \frac{1}{N_{\text{dat}}} \sum_{i,j=1}^{N_{\text{dat}}} \left(F_i^{(\text{art})(k)} - F_i^{(\text{net})(k)}\right) \text{cov}_{ij}^{-1} \left(F_j^{(\text{art})(k)} - F_j^{(\text{net})(k)}\right)$$

Training method → Genetic Algorithms (highly nonlocal error function).
GA → extremely effective to find the global minimum, but slow convergence rate

Set of trained nets $\left\{ F^{(net)(k)}(x, Q^2) \right\} \equiv$ **Probability measure** $\mathcal{P}\left[F(x, Q^2) \right]$
$\rightarrow$ Compute observables with errors and correlations from weighted averages.

Ex.1 : Average and error of structure function for arbitrary (x, Q^2):

$$\left\langle F(x, Q^2) \right\rangle = \frac{1}{N_{rep}} \sum_{k=1}^{N_{rep}} F^{(net)(k)(x, Q^2)}$$
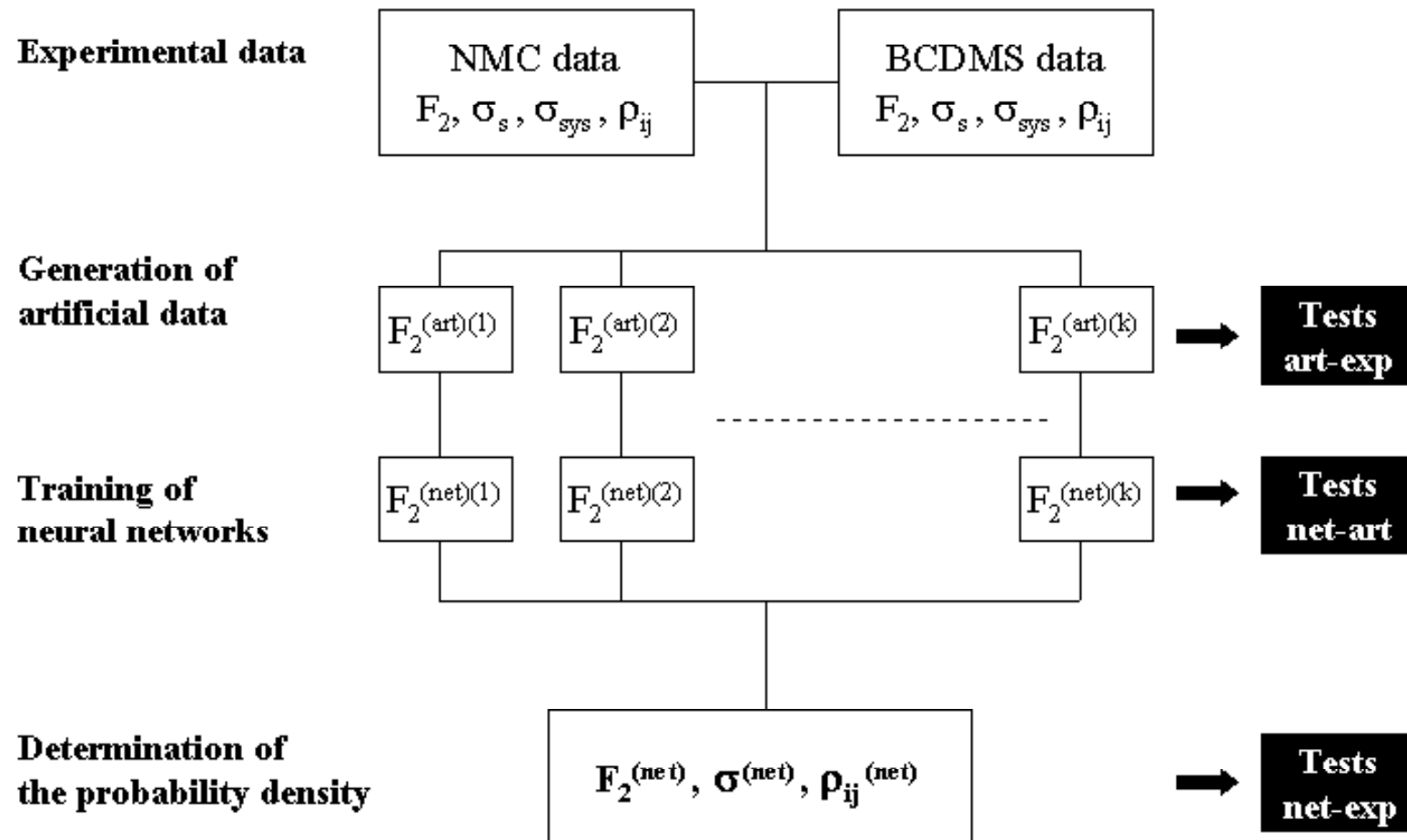
$$\sigma(x, Q^2) = \sqrt{\left\langle F(x, Q^2)^2 \right\rangle - \left\langle F(x, Q^2) \right\rangle^2}$$

No need of linear approximations in error propagation.

Ex.2 : Correlations between (arbitrary) pairs of points:

$$\left\langle F(x_1, Q_1^2) F(x_2, Q_2^2) \right\rangle = \frac{1}{N_{rep}} \sum_{k=1}^{N_{rep}} F^{(net)(k)}(x_1, Q_1^2) F^{(net)(k)}(x_2, Q_2^2)$$
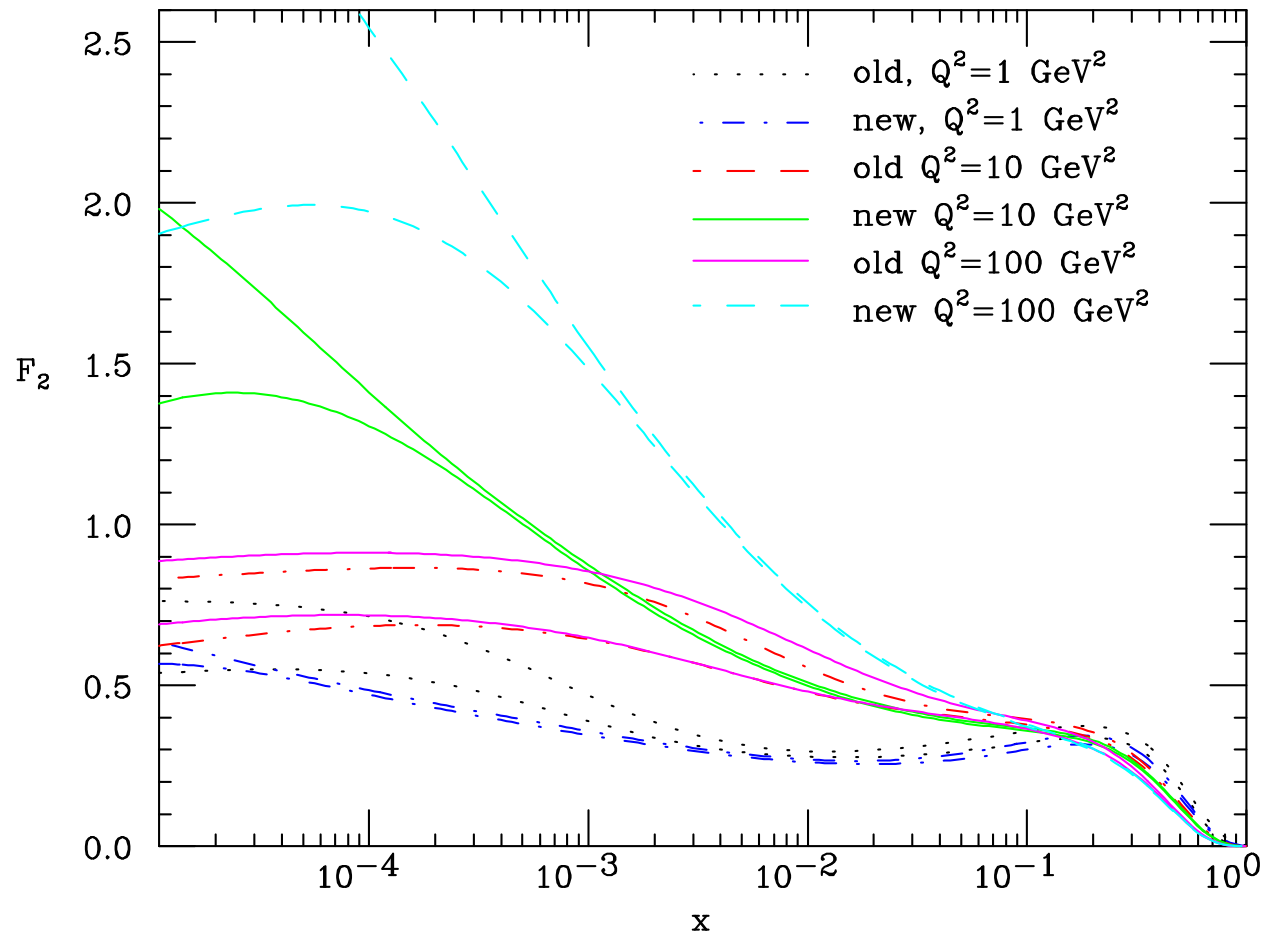
Summary of the NNPDF strategy

Previous work

- S. Forte, L. Garrido, J. I. Latorre and A. Piccione, "Neural network parametrization of deep-inelastic structure functions," JHEP **0205** (2002) 062 [arXiv:hep-ph/0204232].
  $\rightarrow$ Determination of F_2^p, F_2^d, F_2^{NS} from NMC and BCDMS data

- L. Del Debbio, S. Forte, J. I. Latorre, A. Piccione and J. Rojo [NNPDF Collaboration], "Unbiased determination of the proton structure function F_2^p with faithful uncertainty estimation" , arXiv:hep-ph/0501067.
  $\rightarrow$ Determination of F_2^p from all available data (including HERA)
  $\rightarrow$ Incoporates data from 13 experiments in very different kinematical regions.

Source code, driver program and graphical web interface for F_2 plots and numerical computations available

http://sophia.ecm.ub.es/f2neural

Comparing old and new fits of $F_2^p(x, Q^2)$

Legend:
- old, $Q^2 = 1$ GeV^2
- new, $Q^2 = 1$ GeV^2
- old $Q^2 = 10$ GeV^2
- new $Q^2 = 10$ GeV^2
- old $Q^2 = 100$ GeV^2
- new $Q^2 = 100$ GeV^2

Features:

- Compatibility old & new
- Extrapolation
- Faithful uncertainty est.

Step 2
Determination of Parton Distributions
(preliminary results)

The neural network approach to pdf fitting

Same strategy as with structure functions + Altarelli-Parisi evolution

1. Monte Carlo sampling of structure functions data → Faithful estimation of uncertainties

2. Parametrize parton distributions with neural networks → Unbiased parametrization.

3. Evolution of parton distributions to experimental data scale and training over Monte Carlo replica sample.

The probability measure $\mathcal{P}[q]$ contains all information from experimental data (central values, errors, correlations) with the only assumption of smoothness.

The neural network approach to pdf fitting

Expectation values $\rightarrow$ Functional integrals over probability measure

$$\langle \mathcal{F}[q(x)] \rangle = \int \mathcal{D}q \mathcal{F}[q(x)] \mathcal{P}[q(x)] = \frac{1}{N_{rep}} \sum_{k=1}^{N_{rep}} \mathcal{F}\left(q^{(net)(k)}(x)\right)$$

Monte Carlo sampling $\rightarrow$ Compute correlations between pairs of different parton distributions at different points:

Ex. : Correlation of quark pdf $q_f(x)$ and gluon pdf $g(x)$

$$\langle q_f(x_1)g(x_2) \rangle = \frac{1}{N_{\mathrm{rep}}} \sum_{k=1}^{N_{\mathrm{rep}}} q_f^{(net)(k)}(x_1, Q_0^2) g^{(net)(k)}(x_2, Q_0^2)$$

$\rightarrow$ Extremely important for computation of physical processes

Example $\rightarrow$ Correlation between u and d quark pdfs.

Strategies in PDF global fits

The standard approach:

1.- PDFs parametrized by functional forms $q(x, Q_0^2) = x^\alpha (1-x)^\beta P(x)$

2.- Uncertainties: representation as ranges in parameters, estimation with different methods (offset, Hessian, Lagrange multiplier,..)

3.- Error propagation (sometimes) in linearized approximation, depends on parametrization.

The NNPDF approach:

1.- PDFs $q(x, Q_0^2)$ parametrized by neural networks. $\rightarrow$ no bias due to functional form.

2.- Monte Carlo sampling of experimental data $\rightarrow$ Faithful representation of errors and correlations.

3.- Monte Carlo sampling of experimental data $\rightarrow$ Exact error propagation.

Parton distribution evolution

PDFs parametrized by a neural network $\rightarrow$ Mellin inversion of N-space evolution kernel (no complex neural networks):

$$q(N, Q^2) = q(N, Q_0^2) \Gamma\left(N, \alpha_s\left(Q^2\right), \alpha_s\left(Q_0^2\right)\right)$$

$$\Gamma\left(x, \alpha_s\left(Q^2\right), \alpha_s\left(Q_0^2\right)\right) \equiv \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} x^{-N} \Gamma\left(N, \alpha_s\left(Q^2\right), \alpha_s\left(Q_0^2\right)\right)$$

$\Gamma(x)$ is a distribution, diverges at $x = 1$.

Regulating the $\Gamma(x)$ distribution $\rightarrow$ PDF evolution equation:

$$q(x, Q^2) = q(x, Q_0^2) \int_x^1 \Gamma(y) dy + \int_x^1 \frac{dy}{y} \Gamma(y) \left(q\left(\frac{x}{y}, Q_0^2\right) - y q(x, Q_0^2) \right)$$

Details of PDF evolution (I)

- At higher orders $\rightarrow$ Wilson coefficients $C(N, \alpha_s\left(Q^2\right))$ through a modified evolution factor

$$\tilde{\Gamma}\left(x, \alpha_s\left(Q^2\right), \alpha_s\left(Q_0^2\right)\right) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} x^{-N} C(N, \alpha_s\left(Q^2\right)) \Gamma\left(N\right)$$

- Mellin transform inversion of evolution factor $\Gamma(N)$ with Fixed Talbot algorithm (very efficient).

- Evolution formalism benchmarked against the Les Houches parton distribution evolution benchmark results, (G. Salam, A. Vogt, hep-ph/0204316)

Details of PDF evolution (II)

- During pdf fitting (neural network training) only $\Gamma(x)$ is required
  Compute $\Gamma(x)$ and its integral

$$\gamma(x) = \int_0^x dy\, \Gamma(y)$$

  before the fit (hard numerical task) and interpolate them.

- Interpolation of $\Gamma(x)$ non trivial ($\Gamma(x)$ is a distribution, diverges at $x = 1$)
  $\rightarrow$ Benchmark evolution with interpolated $\Gamma(x)$.

- Much faster evolution with interpolated $\Gamma(x)$.

- Resulting formalism: Fast and efficient parton evolution.

The nonsinglet parton distribution

First application of the method:

$\rightarrow$ Determination of the nonsinglet parton distribution $q_{NS}(x, Q_0^2)$ from the NS structure function $F_2^{NS}(x, Q^2)$.

At Leading Order:

$$F_2^{NS}(x, Q^2) \equiv 2\left(F_2^p - F_2^d\right)(x, Q^2) = \frac{x}{6}\left(u + \bar{u} - d - \bar{d}\right)(x, Q^2) \equiv xq_{NS}(x, Q^2)$$

In the NS sector $\int_0^1 dx \Gamma(x) = 1$ to all orders $\rightarrow$ Simplified evolution equations

$$q_{NS}(x, Q^2) = q_{NS}(x, Q_0^2) + \int_x^1 \frac{dy}{y} \Gamma(y) \left(q_{NS}\left(\frac{x}{y}, Q_0^2\right) - yq_{NS}(x, Q_0^2)\right)$$
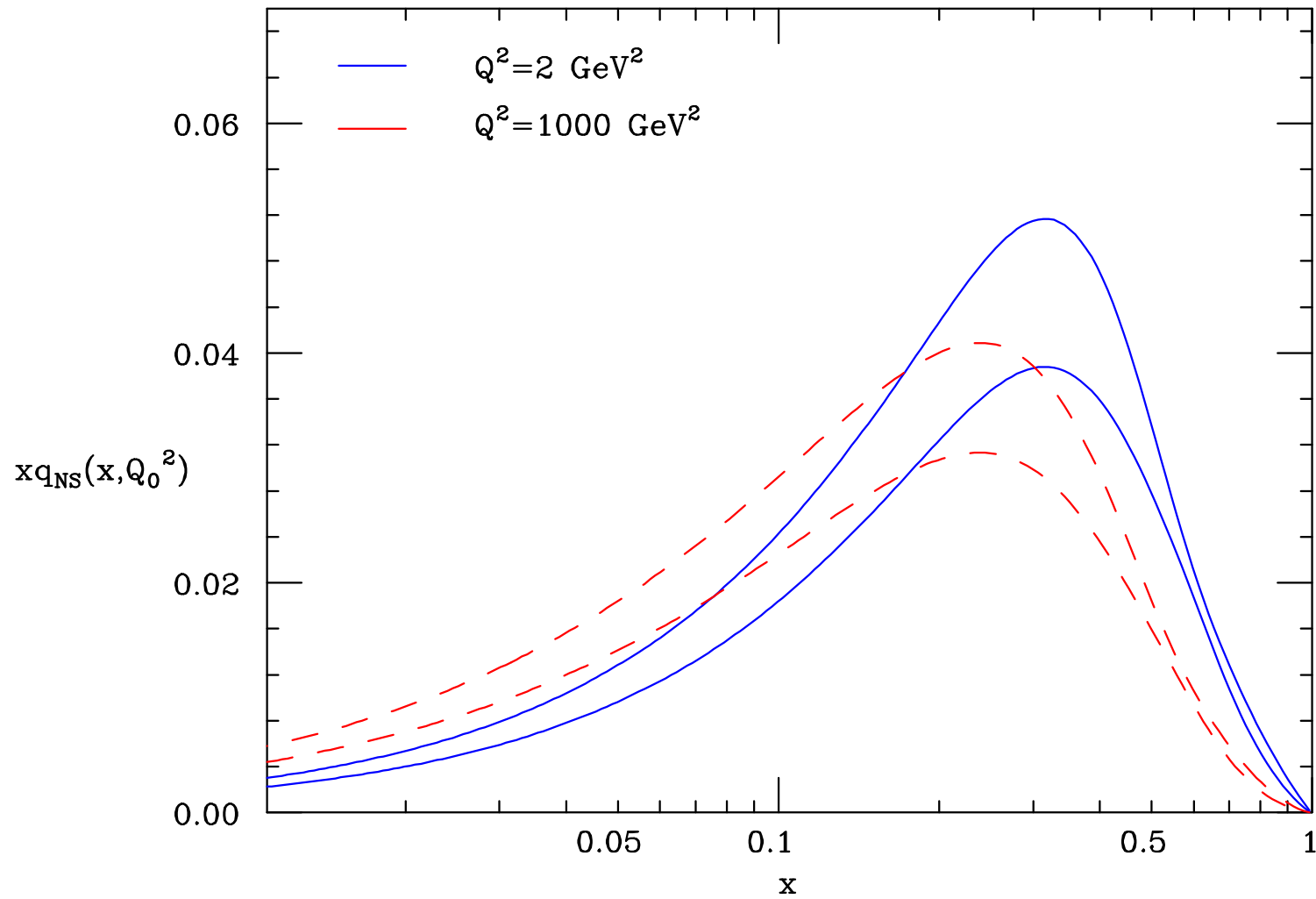
$$-q(x, Q_0^2) \int_0^x \Gamma(y) dy$$

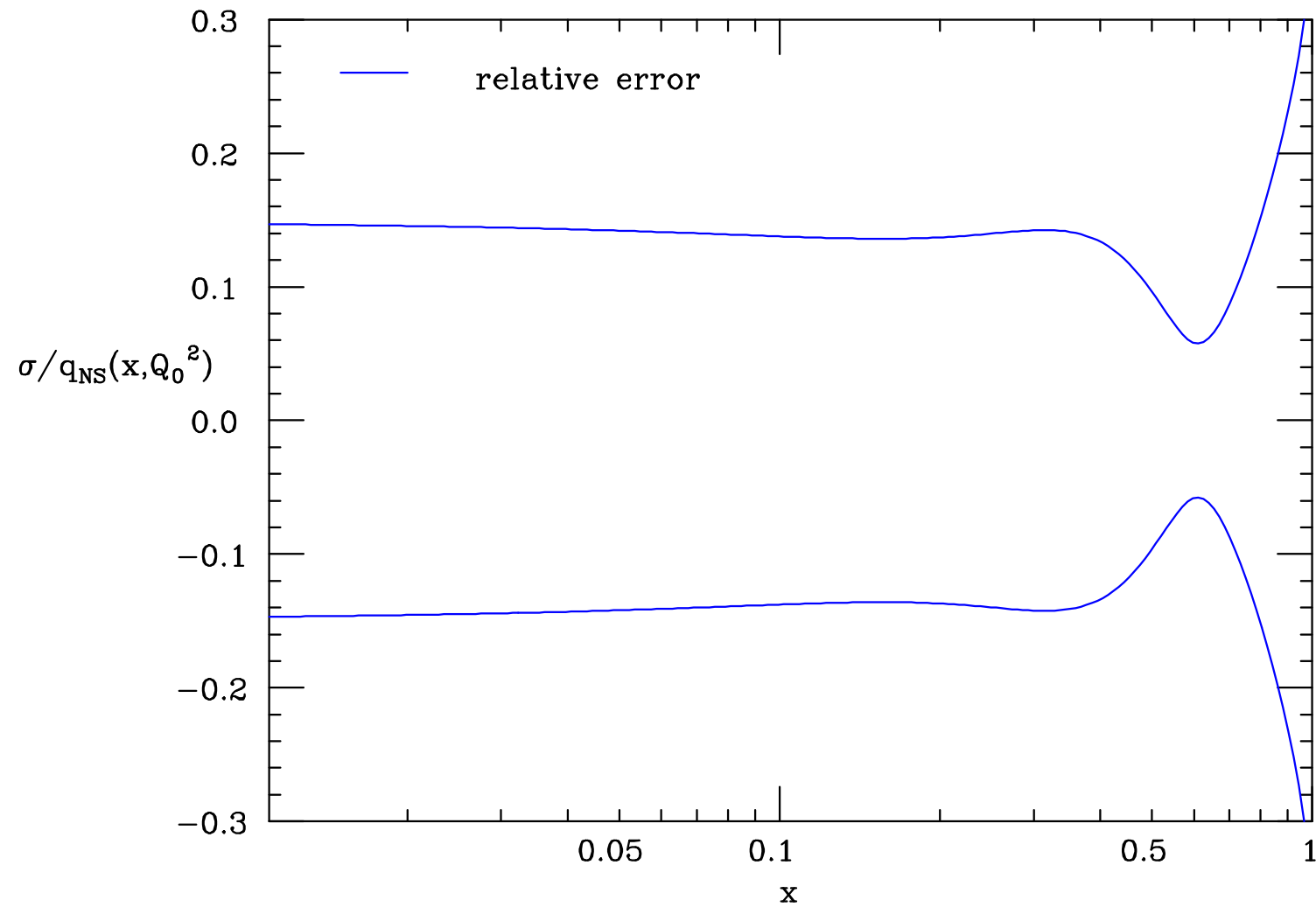where $q_{NS}(x, Q_0^2)$ is parametrized by a neural network.

Details of the fit

- Experimental data: $F_2^{NS}(x, Q^2)$ from the NMC and BCDMS Collaborations: 347 points.

- Kinematical cuts: $Q^2 \geq 9$ GeV^2, $W^2 \geq 6.25$ GeV^2

- Only assumption $\rightarrow q_{NS}(x = 1, Q_0^2) = 0$, implemented adding artificial data points $F_2^{NS}(x = 1, Q^2) = 0$.

- Sample of 100 replicas trained during 900 GA generations. ($\sim$ 4 hours CPU time per replica)

- Neural network architecture: 2-2-2-1.

- Strong coupling $\alpha_s\left(Q^2\right)$ determined from world average value:

$$\alpha_s\left(M_Z^2\right) = 0.118$$

Results: $q_{NS}(x, Q_0^2)$ **NNPDF at Leading Order**

$Q^2 = 2$ GeV^2

$Q^2 = 1000$ GeV^2

$xq_{NS}(x, Q_0{}^2)$

0.06

0.04

0.02

0.00

0.05

0.1

0.5

1

x

Results: Relative error in $q_{NS}(x, Q_0^2)$

Legend: relative error

Y-axis: $\sigma/q_{NS}(x, Q_0{}^2)$ — values: 0.3, 0.2, 0.1, 0.0, −0.1, −0.2, −0.3

X-axis: x — values: 0.05, 0.1, 0.5, 1
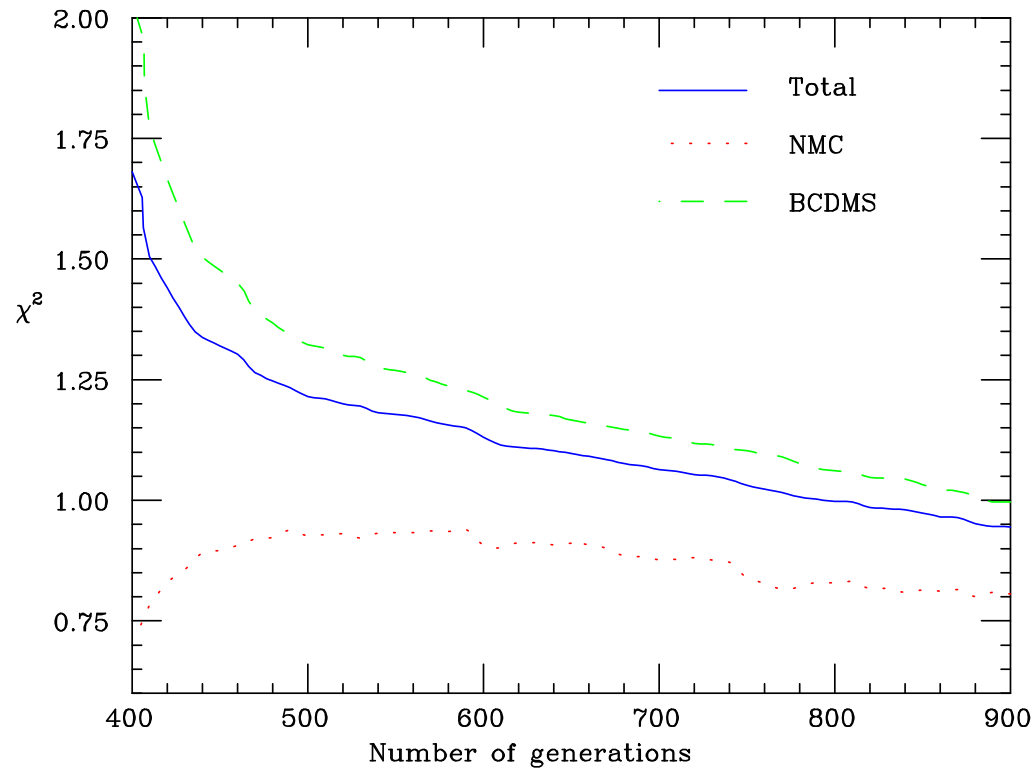
Results: NNPDF F_2^{NS} vs. data
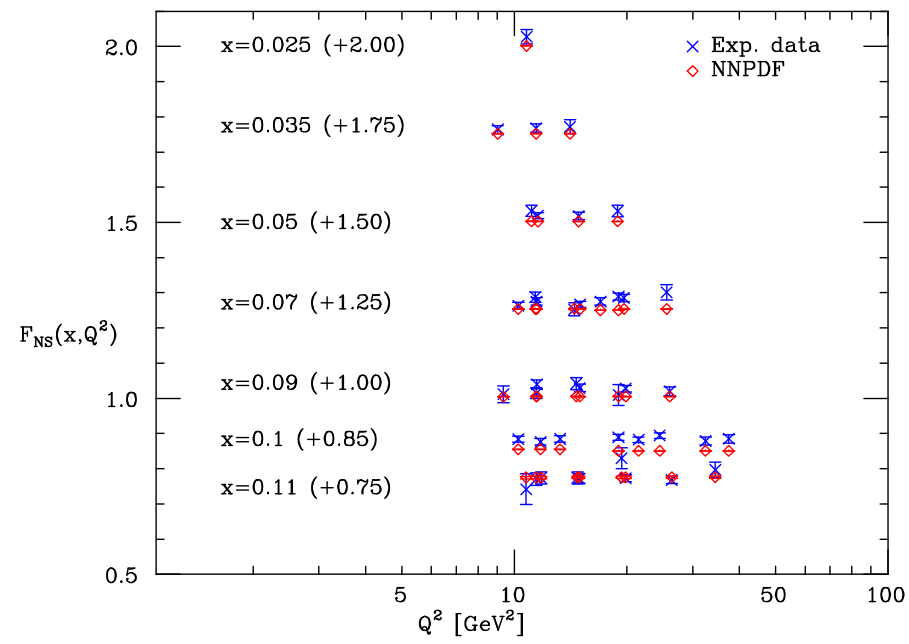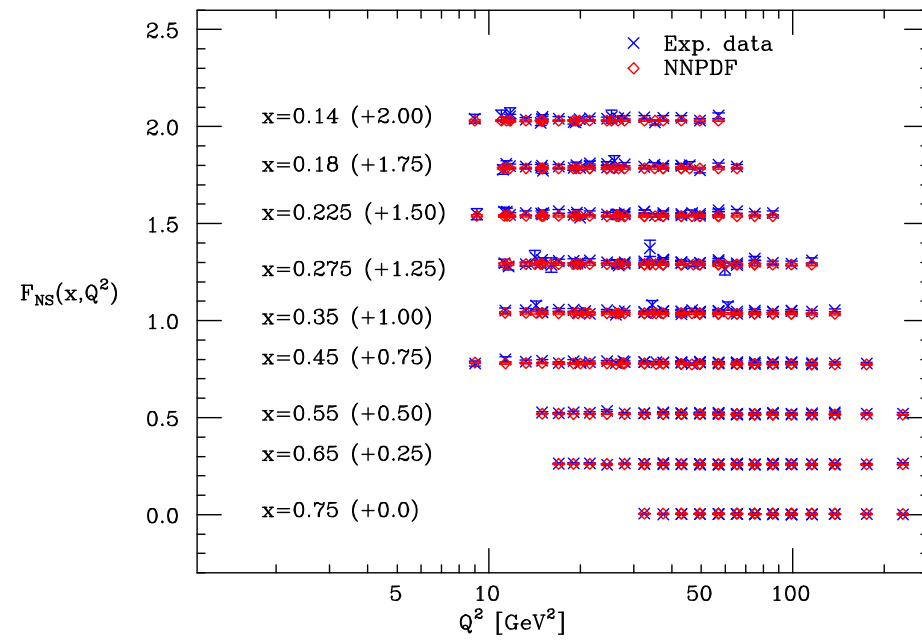
Results: χ^2 during the training

$$\chi^2 = \frac{1}{N_{\mathrm{dat}}} \sum_{i,j=1}^{N_{\mathrm{dat}}} \left(\left\langle F_i^{(\mathrm{net})} \right\rangle_{\mathrm{rep}} - F_i^{(\mathrm{exp})} \right) \left(\mathrm{cov}^{-1} \right)_{ij} \left(\left\langle F_j^{(\mathrm{net})} \right\rangle_{\mathrm{rep}} - F_j^{(\mathrm{exp})} \right) ,$$

Details of the training

Experiment	χ^2
Total	0.99
NMC	0.85
BCDMS	1.05

Summary

- Unbiased determination of structure functions with faithful estimation of uncertainties.

- Successful implementation of neural parton fitting

  1. Determination of nonsinglet parton distribution at LO with fully correlated uncertainties from $F_2^{NS}(x, Q^2)$.

  2. Full NLO and NNLO nonsinglet fits before end of HERA-LHC Workshop.

Outlook

- Construct full set of NNPDF parton distributions from all available data.

- Estimate impact of theoretical uncertainties.

- Assess impact of uncertainties of PDFs for relevant observables at LHC.

- Perform a benchmark set of pdfs, to compare the different fitting programs (CTEQ,MRST, Alekhin) (proposed by S. Alekhin).

- Make formalism compatible with standard interfaces (LHAIPDF, PDFLIB) $\rightarrow$ NNPDF partons available for use in Monte Carlo generators.