NNPDF1.0: parton distribution functions with faithful errors

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DIS Parton distribution functions

Deep inelastic observables:

$$F_I(x,Q^2) = \sum_j C_{Ij}(x,\alpha_s(Q^2)) \otimes f_j(x,Q^2)$$

Scale-dependence of PDFs:

$$Q^{2} \frac{\partial}{\partial Q^{2}} f_{i}(x, Q^{2}) = \sum_{j} P_{ij}(x, \alpha_{s}(Q^{2})) \otimes f_{j}(x, Q^{2})$$
$$f_{i}(x, Q^{2}) = \sum_{j} \Gamma_{ij}(x, \alpha_{s}, \alpha_{s}^{0}) \otimes f_{j}(x, Q^{2})$$



Back to the observables:

$$F_{I}(x,Q^{2}) = \sum_{jk} C_{Ij}(x,\alpha_{s}) \otimes \Gamma_{jk}(x,\alpha_{s},\alpha_{s}^{0}) \otimes f_{k}(x,Q_{0}^{2})$$
$$= \sum_{j} K_{Ij}(x,\alpha_{s},\alpha_{s}^{0}) \otimes f_{j}(x,Q_{0}^{2})$$

Parton distributions for LHC



- different kinematics
- nonperturbative nucleon structure described by the same PDFs
- evolved to the relevant scales

LHC kinematics



- PDFs need to be extrapolated
- uncertainty in the extrapolation region
- uncertainty propagates into LHC physical observables
- important for modelling the QCD background at LHC
- necessity to develop PDFs with faithful errors

Partons with errors



given a set of data points, determine a set of functions with errors

data included in CTEQ5 parton fit



What's the problem? [Kosower 99]

- for a single quantity, we quote 1 sigma errors: value \pm error
- for a pair of numbers, we quote a 1 sigma ellipse
- for a function, we need an "error bar" in a space of functions

we must determine the probability density (measure) $\mathcal{P}[f_i(x)]$ in the space of parton distribution functions $f_i(x)$ (*i*=quark, antiquark, gluon)

EXPECTATION VALUE OF $\mathcal{F}[f_i(x)] \Rightarrow$ FUNCTIONAL INTEGRAL

$$\left\langle \mathcal{F}\left[f_{i}(x)\right] \right\rangle = \int \mathcal{D}f_{i} \mathcal{F}\left[f_{i}(x)\right] \mathcal{P}\left[f_{i}\right],$$

we must extract from the data a description of the probability distribution \mathcal{P}

The standard solution

- choose a parameterization at a reference scale
- evolve to desired scale & compute physical observables
- determine best-fit values of parameters
- determine error by propagation of error on parameters ('hessian method') or by parameter scans ('lagrange multiplier method')

problem projected onto the finite-dimensional space of parameters

Comparing global fits

\boldsymbol{W} production cross-section Tevatron

PDF set	xsec [nb]	PDF uncertainty
Alekhin	2.73	± 0.05
MRST2002	2.59	\pm 0.03
CTEQ6	2.54	± 0.10

[Thorne 03]

Alekhin vs. MRST/CTEQ \rightarrow W production xsect at tevatron do not agree within respective errors

Alekhin vs. MRST/CTEQ \rightarrow predictions for associate Higgs W production LHC do not agree within respective errors

Higgs production at LHC



[Djouadi and Ferrag 04]

Troubles with error bars

PDF4LHC workshop at CERN 08

- benchmark fits on reduced sets do not agree with global fits within errors
- incompatible experiments?
- Iack of generality in the parametrization?
- tolerance criterion $\Delta \chi^2 > 1$?



The Neural Monte Carlo

NNPDF collaboration (2004: Idd, Forte, Latorre, Piccione, Rojo; 2007: + Ball, Guffanti, Ubiali)

- Monte Carlo replicas $F_I^{(k)}(p_i)$ of the original dataset $F_I^{(\text{data})}(p_i)$ \Rightarrow representation of $\mathcal{P}[F_I(p_i)]$ at discrete set of points p_i
- train a neural net for each pdf on each replica, \rightarrow neural representation of the pdfs $f_i^{(net),(k)}$
- The set of neural nets is a representation of the probability density:

$$\left\langle \mathcal{F}\left[f_{i}\right]\right\rangle = \frac{1}{N_{rep}}\sum_{k=1}^{N_{rep}}\mathcal{F}\left[f_{i}^{(net)(k)}\right]$$



MC sampling of exp data



$$F_{I,p}^{(\text{art})(k)} = S_{p,N}^{(k)} F_{I,p}^{(\text{exp})} \left(1 + \sum_{l=1}^{N_c} r_{p,l}^{(k)} \sigma_{p,l} + r_p^{(k)} \sigma_{p,s} \right) , \ k = 1, \dots, N_{\text{rep}} ,$$

where

$$S_{p,N}^{(k)} = \prod_{n=1}^{N_a} \left(1 + r_{p,n}^{(k)} \sigma_{p,n} \right) \prod_{n=1}^{N_r} \sqrt{1 + r_{p,n}^{(k)} \sigma_{p,n}}.$$

Monte Carlo errors

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- for each replica (k) we fit one set of PDFs
- the ensemble of fitted replicas represents the probability distribution in the space of PDFs
- statistical properties of any function of the PDFs can be computed using standard methods:

$$\begin{aligned} \langle \mathcal{F}[f(x)] \rangle &= \frac{1}{N_{\rm rep}} \sum_{k=1}^{N_{\rm rep}} \mathcal{F}[f^{(k)(\rm net)}(x)] \\ \sigma_{\mathcal{F}[f(x)]} &= \sqrt{\langle \mathcal{F}[f(x)]^2 \rangle - \langle \mathcal{F}[f(x)] \rangle^2} \\ [f_a(x_1, Q_1^2), f_b(x_2, Q_2^2)] &= \frac{\langle f_a(x_1, Q_1^2) f_b(x_2, Q_2^2) \rangle - \langle f_a(x_1, Q_1^2) \rangle \langle f_b(x_2, Q_2^2) \rangle}{\sigma_a(x_1, Q_1^2) \sigma_b(x_2, Q_2^2)} \end{aligned}$$

Experimental data

OBS	Data set	OBS	S Data set	
F_2^p	NMC	σ_{NC}^{-}	ZEUS	
	SLAC		H1	
	BCDMS	σ_{CC}^+	ZEUS	
F_2^d	SLAC		H1	
	BCDMS	σ_{CC}^{-}	ZEUS	
σ_{NC}^+	ZEUS		H1	
	H1	$\sigma_ u,\sigma_{ar u}$	CHORUS	
F_2^d/F_2^p	NMC-pd	F_L	H1	



- Kinematical cuts: $Q^2 > 2 \text{ GeV}^2$ $W^2 = Q^2(1-x)/x > 12.5$ GeV^2
- \sim **3000** points.

Neural Networks?



Determination of the probability density

each PDF at the reference scale is parametrised by one NN:

$$f_i(x, Q_0^2) = N_i(x)$$

NN is a non–linear mapping:

$$N_i: \mathbb{R}^n \to \mathbb{R}^m$$

Some details about Neural Networks



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

... just another set of basis functions!

eg, a 1-2-1 NN:
$$\xi_1^{(3)}(\xi_1^{(1)}) = \frac{1}{1 + \exp[\theta_1^{(3)} - \frac{\omega_{11}^{(2)}}{1 + e^{\theta_1^{(2)} - \xi_1^{(1)}\omega_{11}^{(1)}}} - \frac{\omega_{12}^{(2)}}{1 + e^{\theta_2^{(2)} - \xi_1^{(1)}\omega_{21}^{(1)}}}]$$

Thm: any function can be represented by a sufficiently big neural network

Basis set

- Each independent PDF at the initial scale $Q_0^2 = 2 \text{GeV}^2$ is parameterized by an individual NN.
- Little constraint on strange \rightarrow Flavor Assumptions:
 - Symmetric strange sea $s(x) = \bar{s}(x)$
 - Strange sea proportional to non-strange sea $\bar{s}(x) = \frac{C}{2}(\bar{u}(x) + \bar{d}(x))$ (C = 0.5)
 - Intrinsic heavy quarks contributions neglected.
- Parametrization of (4+1) combinations of PDFs at $Q_0^2 = 2 \text{ GeV}^2$:

Singlet : $\Sigma(x)$	$\longmapsto \mathrm{NN}_{\Sigma}(x)$	2-5-3-1 37 pars
Gluon: g(x)	$\longmapsto \mathrm{NN}_g(x)$	2-5-3-1 37 pars
Total valence : $V(x) \equiv u_V(x) + d_V(x)$	$x) \longmapsto \mathrm{NN}_V(x)$	2-5-3-1 37 pars
Non-singlet triplet : $T_3(x)$	$\longmapsto \mathrm{NN}_{T3}(x)$	2-5-3-1 37 pars
Sea asymmetry : $\Delta_S(x) \equiv \bar{d}(x) - \bar{u}(x)$	$(x) \longmapsto \mathrm{NN}_{\Delta}(x)$	2-5-3-1 <mark>37</mark> pars

185 parameters

Normalization and sum rules

$$\begin{split} \Sigma(x,Q_0^2) &= (1-x)^{m_{\Sigma}} x^{-n_{\Sigma}} \mathrm{NN}_{\Sigma}(x) ,\\ V(x,Q_0^2) &= A_V (1-x)^{m_V} x^{-n_V} \mathrm{NN}_V(x) ,\\ T_3(x,Q_0^2) &= (1-x)^{m_{T_3}} x^{-n_{T_3}} \mathrm{NN}_{T_3}(x) ,\\ \Delta_S(x,Q_0^2) &= A_{\Delta_S} (1-x)^{m_{\Delta_S}} x^{-n_{\Delta_S}} \mathrm{NN}_{\Delta_S}(x) ,\\ g(x,Q_0^2) &= A_g (1-x)^{m_g} x^{-n_g} \mathrm{NN}_g(x) . \end{split}$$

- Polynomial Preprocessing → Training Efficiency
- Normalization \rightarrow Fixed by valence and momentum sum rules

$$\int_{0}^{1} dx \, x \left(\Sigma(x) + g(x) \right) = 1$$
$$\int_{0}^{1} dx \left(u(x) - \bar{u}(x) \right) = 2$$
$$\int_{0}^{1} dx \left(d(x) - \bar{d}(x) \right) = 1.$$

Evolution



Observables are a convolution over x of PDFs and Coefficient Functions:

$$F_I(x,Q^2) = \sum_j C_{Ij}(x,\alpha_s) \otimes f_j(x,Q^2) = \sum_{j,k} C_{Ij}(x,\alpha_s) \otimes \Gamma_{jk}(x,\alpha_s,\alpha_s^0) \otimes f_k(x,Q_0^2)$$

Kernels for a physical observable

 F_2 proton structure function

$$F_2^p = x\{\frac{5}{18}C_{2,q}^s \otimes \Sigma + \frac{1}{6}C_{2,q} \otimes (T_3 + \frac{1}{3}(T_8 - T_{15}) + \frac{1}{5}(T_{24} - T_{35})) + \langle e_q^2 \rangle C_{2,g} \otimes g\}$$

$$F_2^p = x\{K_{F2,\Sigma} \otimes \Sigma_0 + K_{F2,g} \otimes g_0 + K_{F2,+} \otimes \left(T_{3,0} + \frac{1}{3}(T_{8,0} - T_{15,0})\right)\}$$

In Mellin space

$$K_{F2,\Sigma} = \frac{5}{18}C_{2,q}^{s}\Gamma_{S}^{qq} + \frac{1}{30}C_{2,q}(\Gamma_{S}^{24,q} - \Gamma_{S}^{35,q}) + \langle e_{q}^{2}\rangle C_{2,g}\Gamma_{S}^{gq}$$

$$K_{F2,g} = \frac{5}{18}C_{2,q}^{s}\Gamma_{S}^{qg} + \frac{1}{30}C_{2,q}(\Gamma_{S}^{24,g} - \Gamma_{S}^{35,g}) + \langle e_{q}^{2}\rangle C_{2,g}\Gamma_{S}^{gg}$$

$$K_{F2,+} = \frac{1}{6}C_{2,q}\Gamma_{NS}^{+}$$

Theoretical errors

- Higher perturbative orders \rightarrow NLO fit
- Heavy quark treatment → Zero Mass Variable Flavor Number scheme. quarks are radiatively generated at thresholds. [Thorne,Tung, arXiv:0809.0714]
- Target Mass Corrections included and factorized into the hard kernels.

$$\begin{aligned} \tau &= 1 + \frac{4M_N^2 x^2}{Q^2} \\ \widetilde{F}_2(\xi, Q^2) &= \frac{x^2}{\tau^{3/2}} \frac{F_2(\xi, Q^2)}{\xi^2} + 6\frac{M_N^2}{Q^2} \frac{x^3}{\tau^2} I_2(\xi, Q^2) \\ I_2(\xi, Q^2) &= \int_{\xi}^1 \frac{dz}{z^2} F_2(z, Q^2). \end{aligned}$$

Taking Mellin transforms with respect to ξ , defines a new target mass corrected coefficient function

$$\widetilde{C}_{2,j}(N,\alpha_s,\tau) = \frac{(1+\tau^{1/2})^2}{4\tau^{3/2}} \left(1 + \frac{3\left(1-\tau^{-1/2}\right)}{N+1}\right) C_{2,j}(N,\alpha_s)$$

Training strategy



- unbiased basis of functions, parametrized by a large number of parameters
- genetic algorithms for minimization
- might accomodate statistical fluctutations of the data
- optimal training, beyond which the fit is just adjusting to statistical fluctutations
- dynamical stopping by cross validation
- for each replica divide the data randomly into training and validation
- minimization performed on the training set only
- when the training χ^2 still decreases while the validation χ^2 stops decreasing \rightarrow STOP

Dynamical stopping



Ensemble of replicas



- individual replicas fluctuate significantly
- averages are smooth as the number of replicas is increased

PDFs uncertainties

Monte Carlo prescription (NNPDF)

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

HEPDATA prescription (CTEQ and MRST/MSTW)

$$\sigma_{\mathcal{F}} = \frac{1}{2C_{90}} \left(\sum_{k=1}^{N_{\text{set}}/2} \left(\mathcal{F}[\{f^{(2k-1)}\}] - \mathcal{F}[\{f^{(2k)}\}] \right)^2 \right)^{1/2}, \quad C_{90} = 1.64485$$

 C_{90} accounts for the fact that the upper and lower parton sets correspond to 90% confidence levels rather than to one- σ uncertainties.

HEPDATA* prescription (Alekhin)

$$\sigma_{\mathcal{F}} = \left(\sum_{k=1}^{N_{\text{set}}} \left(\mathcal{F}[\{f^{(k)}\}] - \mathcal{F}[\{f^{(0)}\}]\right)^2\right)^{1/2}.$$

The NNPDF1.0 parton set



The NNPDF1.0 parton set









Relative uncertainties



- comparable uncertainty in the data region
- BUT larger uncertainties in the extrapolation

PDFs correlations

Correlations between u - u and g - g (Q=85GeV) [nadolsky 08]



 $\rho\left[f_a(x_1, Q_1^2)f_b(x_2, Q_2^2)\right] = \frac{\langle f_a(x_1, Q_1^2)f_b(x_2, Q_2^2)\rangle_{\rm rep} - \langle f_a(x_1, Q_1^2)\rangle_{\rm rep}\langle f_b(x_2, Q_2^2)\rangle_{\rm rep}}{\sigma_a(x_1, Q_1^2)\sigma_b(x_2, Q_2^2)}$

Distance between MC ensembles.

- Stability of the NNPDF parton set can be assessed by using standard statistical tools.
- Distances between two probability distributions: $\left\{f_{ik}^{(1)} = f_k^{(1)}(x_i, Q_0^2)\right\}$

$$\langle d[f] \rangle = \sqrt{\left\langle \frac{\left(\langle f_i \rangle_{(1)} - \langle f_i \rangle_{(2)} \right)^2}{\sigma^2 [f_i^{(1)}] + \sigma^2 [f_i^{(2)}]} \right\rangle_{\text{pts}}}$$

• where:

$$\langle f_i \rangle_{(1)} \equiv \frac{1}{N_{\rm rep}^{(1)}} \sum_{k=1}^{N_{\rm rep}^{(1)}} f_{ik}^{(1)} ,$$

$$\sigma^{2}[f_{i}^{(1)}] \equiv \frac{1}{N_{\rm rep}^{(1)}(N_{\rm rep}^{(1)}-1)} \sum_{k=1}^{N_{\rm rep}^{(1)}} \left(f_{ik}^{(1)} - \langle f_{i} \rangle_{(1)}\right)^{2}$$

• For statistically equivalent PDF sets: $\langle d[f] \rangle \sim \langle d[\sigma_f] \rangle \sim 1$

Stability under variation of the parametrization



	Data	Extrapolation	
$\Sigma(x,Q_0^2)$	$5 10^{-4} \le x \le 0.1$	$10^{-5} \le x \le 10^{-4}$	
$\langle d[f] angle$	0.98	1.25	
$\langle d[\sigma] angle$	1.14	1.34	
$g(x,Q_0^2)$	$5 10^{-4} \le x \le 0.1$	$10^{-5} \le x \le 10^{-4}$	
$\langle d[f] angle$	1.52	1.15	
$\langle d[\sigma] angle$	1.16	1.07	
$T_3(x,Q_0^2)$	$0.05 \le x \le 0.75$	$10^{-3} \le x \le 10^{-2}$	
$\langle d[f] angle$	1.00	1.11	
$\langle d[\sigma] angle$	1.76	2.27	
$V(x,Q_0^2)$	$0.1 \le x \le 0.6$	$310^{-3} \le x \le 310^{-2}$	
$\langle d[f] angle$	1.30	0.90	
$\langle d[\sigma] angle$	1.10	0.98	
$\Delta_S(x,Q_0^2)$	$0.1 \le x \le 0.6$	$310^{-3} \le x \le 310^{-2}$	
$\langle d[f] angle$	1.04	1.91	
$\langle d[\sigma] angle$	1.44	1.80	

Stability under change of architecture of the nets:

37 pars \rightarrow 31 pars

Independence on the parametrization!

HERA-LHC benchmark

Benchmark PDF fit to a reduced consistent set of DIS data [hep-ph/0511119]



3163 data \longrightarrow **773** data

HERA-LHC benchmark

Comparison between collaborations and between benchmark/global partons. $u(x,Q^2 = 2 \text{GeV}^2)$: MRST data region



HERA-LHC benchmark

Comparison between collaborations and between benchmark/global partons. $u(x, Q^2 = 2 \text{GeV}^2)$: MRST extrapolation region



HERA-LHC benchmark

- benchmark partons and global partons do not agree within error!
- note that PDFs input parametrization, flavor assumptions and statistical treatment $(\Delta \chi^2_{\text{global}} = 50, \Delta \chi^2_{\text{bench}} = 1)$ are tuned to data.
- not satisfactory especially to predict the behaviour of PDFs in the extrapolation region (LHC)

HERA-LHC benchmark

Comparison between collaborations and between benchmark/global partons. $u(x,Q^2=2{
m GeV}^2)$: data region



HERA-LHC benchmark

Comparison between collaborations and between benchmark/global partons. $u(x, Q^2 = 2 \text{GeV}^2)$: extrapolation region



HERA-LHC benchmark

- NNPDF1.0 is consistent with MRST global fit.
- NNPDFbench is consistent with NNPDF1.0 and MRST.
- Same parametrization and flavour assumption.
- Same statistical treatment.
- Underestimation of the error in the standard approach.

Comparison with present experimental data



LHC standard candle processes

- All quantities have been computed at NLO with MCFM [http://mcfm.fnal.gov]
- Quoted uncertainties are the 1σ bands due to the PDF uncertainty only.

	$\sigma_{W^+} \mathcal{B}_{l^+ \nu_l}$	$\Delta \sigma_{W^+} / \sigma_{W^+}$	$\sigma_Z \mathcal{B}_{l+l}$	$\Delta \sigma_Z / \sigma_Z$
NNPDF1.0	11.83 ± 0.26	2.2%	1.95 ± 0.04	2.1%
CTEQ6.1	11.65 ± 0.34	2.9%	1.93 ± 0.06	3.1%
MRST01	11.71 ± 0.14	1.2%	1.97 ± 0.02	1.0%
CTEQ6.5	12.54 ± 0.29	2.3%	2.07 ± 0.04	1.9%



Conclusions

- Standard approaches with fixed parametrization tend to underestimate uncertainties unless experimental errors are inflated by essentially arbitrary amount.
- Monte Carlo ensemble
 - Any statistical property of PDFs can be calculated using standard statistical methods.
 - ^o No need of any tolerance criterion.
- The Neural Network parametrization
 - Small uncertainties come from an underlying physical law, not from parametrization bias.
 - ^o Inconsistent data or underestimated uncertainties do not require a separate treatment and are automatically signalled by a larger value of the χ^2 .
- The first NNPDF parton set [arXiv:0808.1231] is available on the common LHAPDF interface [http://projects.hepforge.org/lhapdf].

Outlook

- Inclusion of hadronic data to
 - $^{\circ}$ improve the accuracy of gluon at large x (jets)
 - ^o determine the light antiquark sea asymmetry (Drell-Yan)
 - ^o allow for a direct determination of the strange distribution (dimuon data)
- More accurate treatment of Heavy Quark thresholds.
- LO parton set in view of its use in Monte Carlo generators.
- More sophisticated theoretical treatment: NNLO parton distributions, large and small x resummation corrections should also be considered.
- Study of the impact of PDFs uncertainties on LHC phenomenology