The NNPDF4.0 global analysis of the proton structure

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On behalf of the NNPDF Collaboration

Eur.Phys.J.C 82 (2022) 5, 428; arXiv:2109.02653

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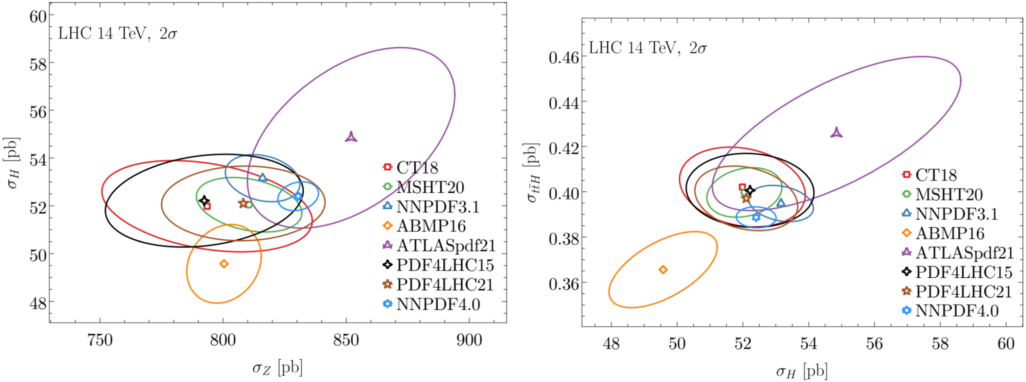
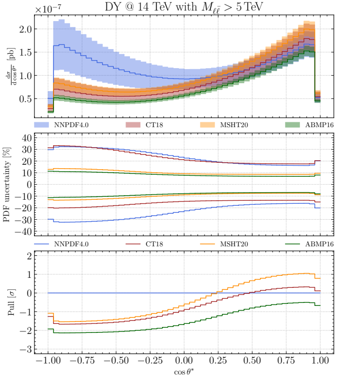
Status of modern PDF sets

PDF predictions are **consistent** but with **different uncertainties**

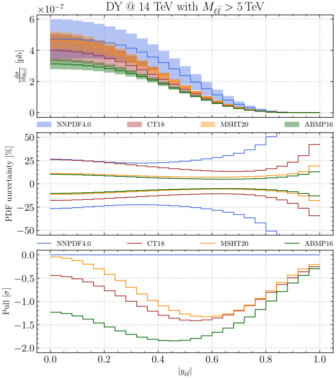


Data region: small NNPDF4.0 uncertainties

NC DY at high energies [R.D Ball et. al., in preparation]

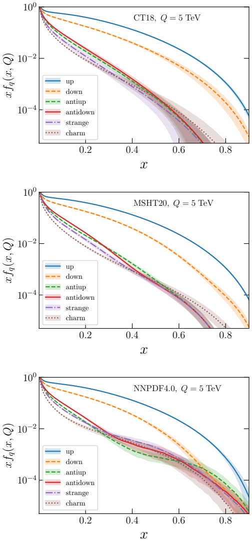


Rapidity



Collins-Soper frame angle

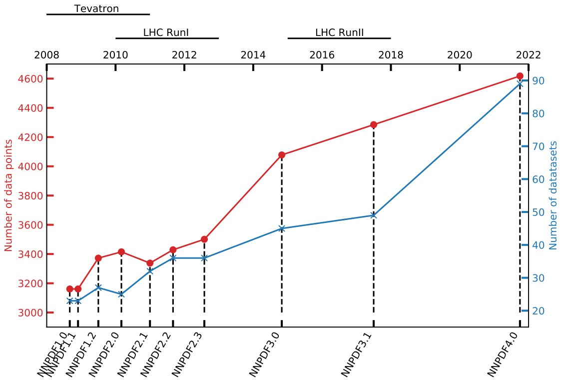
Extraplation region: large NNPDF4.0 uncertainties due to **flexibility** of the neural network



large-x PDFs

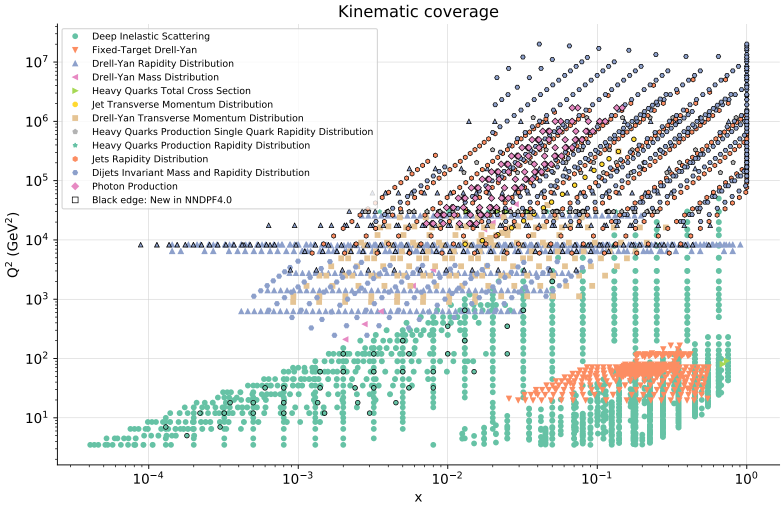
Data

Data from NNPDF1.0 to NNPDF4.0



The number of datasets – normally corresponding to different processes – is generally more relevant than the number of datapoints

Experimental data in NNPDF4.0



More than 4000 datapoints!

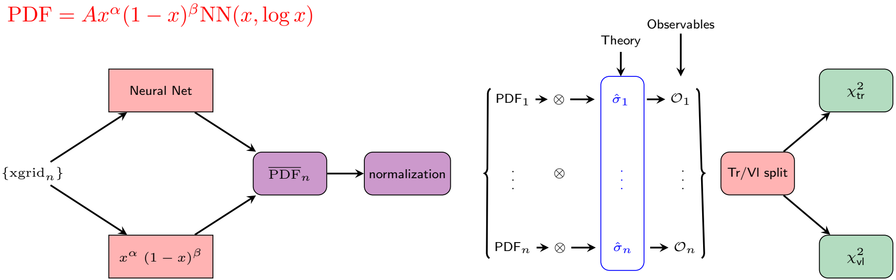
New processes:

- direct photon
- single top
- dijets
- W+jet
- DIS jet

Methodology

The NNPDF4.0 model

See EPJ C79 (2019) 676



- Modular `Python` codebase
- Freedom to use external libraries (default: `TensorFlow`)

Automated model selection

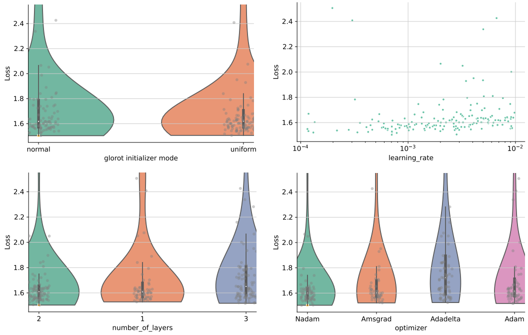
NNPDF aims to minimize sources of bias in the PDF:

- Functional form → Neural Network
- Model parameters → **Hyperoptimization**

Scan over thousands of hyperparameter combinations and select the best one

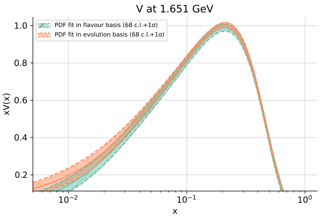
k-fold cross-validation: used to define the reward function based on a **test dataset**

Objective function:
$L = \mathrm{mean}(\chi_1^2, \chi_3^2, \chi_2^2, \ldots, \chi_k^2)$

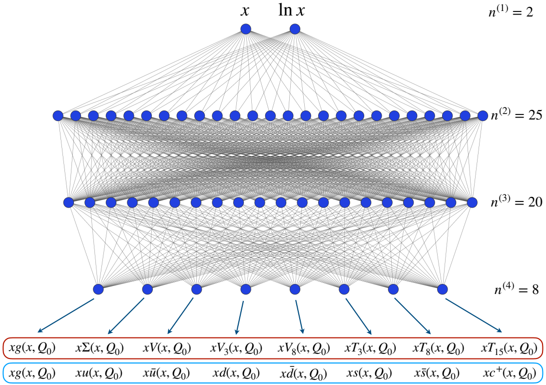


Further methodological improvments

- Improved implementation of physical constraints
  - PDF **positivity**
  - **Integrability** of non-singlet distributions
- Extended validation of PDFs
  - Explicit check of **basis independence**
  - **Test uncertainties** using closure and future test



Basis independence



$$f_i\left(x, Q_0\right) = x^{-\alpha_i}(1-x)^{\beta_i}\mathrm{NN}_i(x)$$

Validation

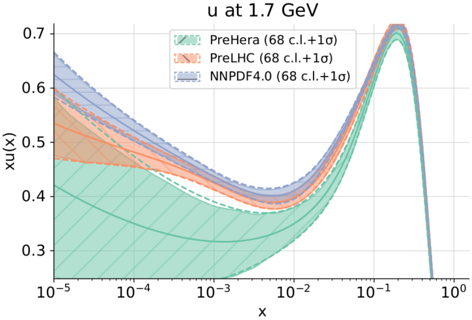
Future tests

See Acta Phys.Polon.B 52 (2021) arxiv:2103.08606

χ^2/N (only exp. covmat)

(dataset)	NNPDF4.0	pre-LHC	pre-Hera
pre-HERA	1.09	1.01	0.90
pre-LHC	1.21	1.20	**23.1**
NNPDF4.0	1.29	**3.30**	**23.1**

1. Take a historic dataset
   e.g. pre-HERA or pre-LHC
2. Perform fit
3. Compare predictions to “future” data



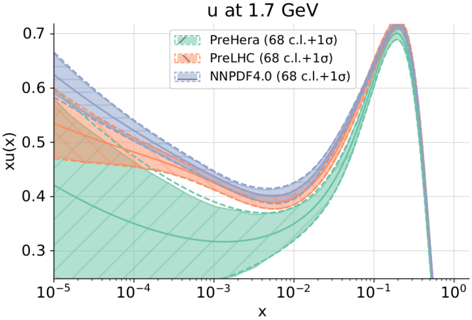
Future tests

See Acta Phys.Polon.B 52 (2021) arxiv:2103.08606

χ^2/N (exp. and PDF covmat)

(dataset)	NNPDF4.0	pre-LHC	pre-Hera
pre-HERA			0.86
pre-LHC		1.17	**1.22**
NNPDF4.0	1.12	**1.30**	**1.38**

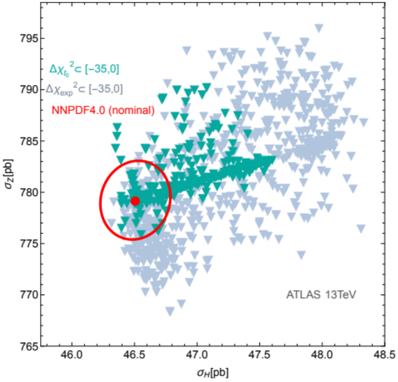
1. Take a historic dataset
   e.g. pre-HERA or pre-LHC
2. Perform fit
3. Compare predictions to "future" data



The total uncertainty increases, and accommodates for difference between predictions and new data.

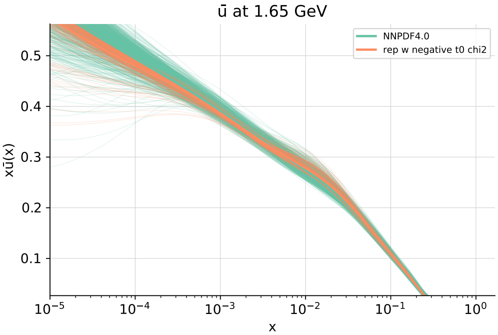
Sampling for solutions

Is the sampling of the PDF uncertainty of an experimental observable truly representative of all acceptable solutions?



arXiv:2205.10444, A. Courtoy et. al.

- A "hopscotch scan" to search for solutions with equal or better χ^2
- All solutions fall within the NNPDF4.0 distribution



Open-source code

The open-source NNPDF code

The full NNPDF code has been made **public** along with user friendly **documentation**

This includes: fitting, hyperoptimization, theory, data processing, visualization

It is possible to reproduce all results of NNPDF4.0 and more!

Eur.Phys.J.C 81 (2021) 10, 958
`https://github.com/NNPDF/nnpdf`
`https://docs.nnpdf.science`

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`https://github.com/NNPDF/nnpdf`
`https://docs.nnpdf.science`

Thank you!

Backup

Experimental data in NNPDF4.0

- 44 new datasets included
- 323 more data points in NNPDF4.0 than in NNPDF3.1
- New data is mostly from the LHC RUN II

Data set	Ref.	NNPDF3.1	NNPDF4.0	ABMP16	CT18	MSHT20
ATLAS W,Z 7 TeV ($\mathcal{L}=35$ pb^{-1})	[51]	✓	✓	✓	✓	✓
ATLAS W,Z 7 TeV ($\mathcal{L}=4.6$ fb^{-1})	[52]	✓	✓	✗	(✓)	✓
ATLAS low-mass DY 7 TeV	[53]	✓	✓	✗	(✓)	✗
ATLAS high-mass DY 7 TeV	[54]	✓	✓	✗	(✓)	✓
ATLAS W 8 TeV	[79]	✗	(✓)	✗	✗	✓
ATLAS DY 2D 8 TeV	[78]	✗	✓	✗	✗	✓
ATLAS high-mass DY 2D 8 TeV	[77]	✗	✓	✗	(✓)	✓
ATLAS $\sigma_{W,Z}$ 13 TeV	[81]	✗	✓	✓	✗	✗
ATLAS W+jet 8 TeV	[93]	✗	✓	✗	✗	✓
ATLAS Z p_T 7 TeV	[260]	(✓)	✗	✗	(✓)	✗
ATLAS Z p_T 8 TeV	[63]	✓	✓	✗	✓	✓
ATLAS $W+c$ 7 TeV	[83]	✗	✓	✗	(✓)	✗
ATLAS $\sigma^{\rm tot}_{tt}$ 7, 8 TeV	[65]	✓	✓	✓	✗	✗
ATLAS $\sigma^{\rm tot}_{tt}$ 7, 8 TeV	[261–266]	✗	✗	✓	✗	✗
ATLAS $\sigma^{\rm tot}_{tt}$ 13 TeV ($\mathcal{L}=3.2$ fb^{-1})	[66]	✓	✗	✓	✗	✗
ATLAS $\sigma^{\rm tot}_{tt}$ 13 TeV ($\mathcal{L}=139$ fb^{-1})	[134]	✗	✓	✗	✗	✗
ATLAS $\sigma^{\rm tot}_{tt}$ and Z ratios	[267]	✗	✗	✗	✗	(✓)
ATLAS $t\bar{t}$ lepton+jets 8 TeV	[67]	✓	✓	✗	✓	✓
ATLAS $t\bar{t}$ dilepton 8 TeV	[89]	✗	✓	✗	✗	✓
ATLAS single-inclusive jets 7 TeV, R=0.6	[73]	✓	(✓)	✗	✓	✓
ATLAS single-inclusive jets 8 TeV, R=0.6	[86]	✗	✓	✗	✗	✗
ATLAS dijets 7 TeV, R=0.6	[148]	✗	✓	✗	✗	✗
ATLAS direct photon production 8 TeV	[100]	✗	(✓)	✗	✗	✗
ATLAS direct photon production 13 TeV	[101]	✗	✓	✗	✗	✗
ATLAS single top R_t 7, 8, 13 TeV	[94,96,98]	✗	✓	✓	✗	✗
ATLAS single top diff. 7 TeV	[94]	✗	✓	✗	✗	✗
ATLAS single top diff. 8 TeV	[96]	✗	✓	✗	✗	✗

Data set	Ref.	NNPDF3.1	NNPDF4.0	ABMP16	CT18	MSHT20
CMS W asym. 7 TeV ($\mathcal{L}=36$ pb^{-1})	[268]	✗	✗	✗	✗	✓
CMS Z 7 TeV ($\mathcal{L}=36$ pb^{-1})	[269]	✗	✗	✗	✗	✓
CMS W electron asymmetry 7 TeV	[55]	✓	✓	✗	✓	✓
CMS W muon asymmetry 7 TeV	[56]	✓	✓	✓	✓	✗
CMS Drell-Yan 2D 7 TeV	[57]	✓	✓	✗	(✓)	✓
CMS Drell-Yan 2D 8 TeV	[270]	(✓)	✗	✗	✗	✗
CMS W rapidity 8 TeV	[58]	✓	✓	✓	✓	✓
CMS W,Z p_T 8 TeV ($\mathcal{L}=18.4$ fb^{-1})	[271]	✗	✗	✗	(✓)	✗
CMS Z p_T 8 TeV	[64]	✓	✓	✗	(✓)	✗
CMS $W+c$ 7 TeV	[76]	✓	✓	✗	(✓)	✓
CMS $W+c$ 13 TeV	[84]	✗	✓	✗	✗	(✓)
CMS single-inclusive jets 2.76 TeV	[75]	✓	✗	✗	✗	✓
CMS single-inclusive jets 7 TeV	[147]	✓	(✓)	✗	✓	✓
CMS dijets 7 TeV	[74]	✗	✓	✗	✗	✗
CMS single-inclusive jets 8 TeV	[87]	✗	✓	✗	✓	✓
CMS 3D dijets 8 TeV	[149]	✗	(✓)	✗	✗	✗
CMS $\sigma^{\rm tot}_{tt}$ 5 TeV	[88]	✗	✓	✗	✗	✗
CMS $\sigma^{\rm tot}_{tt}$ 7, 8 TeV	[146]	✓	✓	✗	✗	✗
CMS $\sigma^{\rm tot}_{tt}$ 8 TeV	[272]	✗	✗	✗	✗	✓
CMS $\sigma^{\rm tot}_{tt}$ 5, 7, 8, 13 TeV	[68, 273–281]	✗	✗	✓	✗	✗
CMS $\sigma^{\rm tot}_{tt}$ 13 TeV	[69]	✓	✓	✓	✗	✗
CMS $t\bar{t}$ lepton+jets 8 TeV	[70]	✓	✓	✗	✗	✓
CMS $t\bar{t}$ 2D dilepton 8 TeV	[90]	✗	✓	✗	✓	✓
CMS $t\bar{t}$ lepton+jet 13 TeV	[91]	✗	✓	✗	✗	✗
CMS $t\bar{t}$ dilepton 13 TeV	[92]	✗	✓	✗	✗	✗
CMS single top $\sigma_t+\sigma_{\bar{t}}$ 7 TeV	[95]	✗	✓	✓	✗	✗
CMS single top R_t 8, 13 TeV	[97,99]	✗	✓	✓	✗	✗
CMS single top 13 TeV	[282, 283]	✗	✗	✗	✗	(✓)

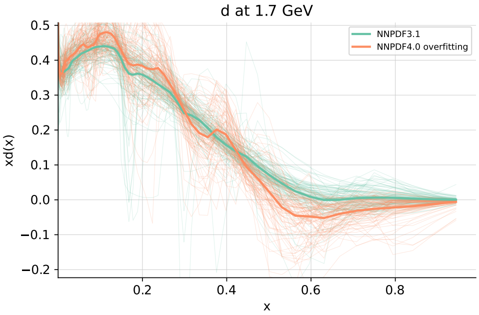
Data set	Ref.	NNPDF3.1	NNPDF4.0	ABMP16	CT18	MSHT20
LHCb Z 7 TeV ($\mathcal{L}=940$ pb^{-1})	[59]	✓	✓	✗	✗	✓
LHCb $Z\to ee$ 8 TeV ($\mathcal{L}=2$ fb^{-1})	[61]	✓	✓	✓	✓	✓
LHCb W 7 TeV ($\mathcal{L}=37$ pb^{-1})	[284]	✗	✗	✗	✗	✓
LHCb $W,Z\to\mu$ 7 TeV	[60]	✓	✓	✓	✓	✓
LHCb $W,Z\to\mu$ 8 TeV	[62]	✓	✓	✓	✓	✓
LHCb $W\to e$ 8 TeV	[80]	✗	(✓)	✗	✗	✗
LHCb $Z\to\mu\mu, ee$ 13 TeV	[82]	✗	✓	✗	✗	✗

Performance benefit - time per replica

	NNPDF3.1	NNPDF4.0 (CPU)	NNPDF4.0 (GPU)
Fit timing per replica	15.2 h	38 min	6.6 min
Speed up factor	1	24	140
RAM use	1.5 GB	6.1 GB	NA

Hyperoptimization: the reward function

Choosing as the hyperoptimization target the χ^2 of fitted data results in overfitting.



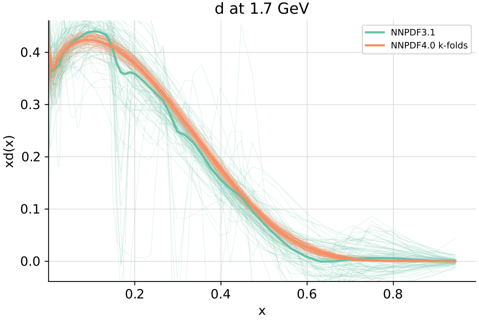
Hyperoptimization: the reward function

Choosing as the hyperoptimization target the χ^2 of fitted data results in overfitting.

We solve this using **k-fold cross-validation**:

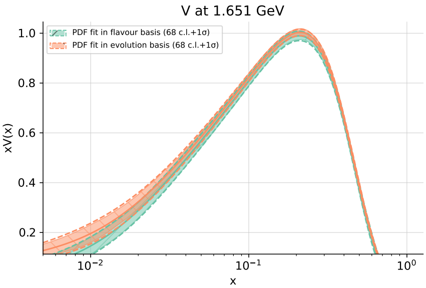
1. Divide the data into k representative subsets
2. Fit $k-1$ sets and use k-th as test set
   $\Rightarrow$ k values of χ^2_{test}
3. Optimize the average χ^2_{test} of the k test sets

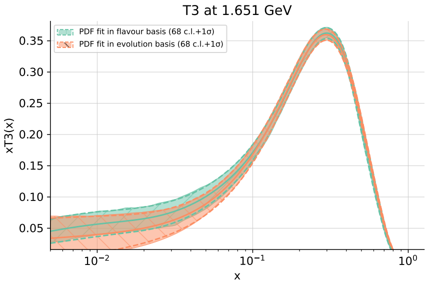
$\Rightarrow$ The hyperoptimization target is not based on data that entered the fit.



- No overfitting
- Compared to NNPDF3.1:
  - Increased stability
  - Reduced uncertainties

Parametrization basis independence





Evolution Basis:

$$xV(x, Q_0) \propto \mathrm{NN}_V(x)$$

$$xT_3(x, Q_0) \propto \mathrm{NN}_{T_3}(x)$$

Flavour Basis:

$$xV(x, Q_0) \propto (\mathrm{NN}_u(x) - \mathrm{NN}_{\bar{u}}(x) + \mathrm{NN}_d(x) - \mathrm{NN}_{\bar{d}}(x) + \mathrm{NN}_s(x) - \mathrm{NN}_{\bar{s}}(x))$$

$$xT_3(x, Q_0) \propto (\mathrm{NN}_u(x) + \mathrm{NN}_{\bar{u}}(x) - \mathrm{NN}_d(x) - \mathrm{NN}_{\bar{d}}(x))$$

Different strategies to parametrize the quark PDF flavour combinations leave the uncertainties essentially unchanged

Closure test

See Eur.Phys.J.C 82 (2022); arxiv:2111.05787

Closure test of a known input assumption

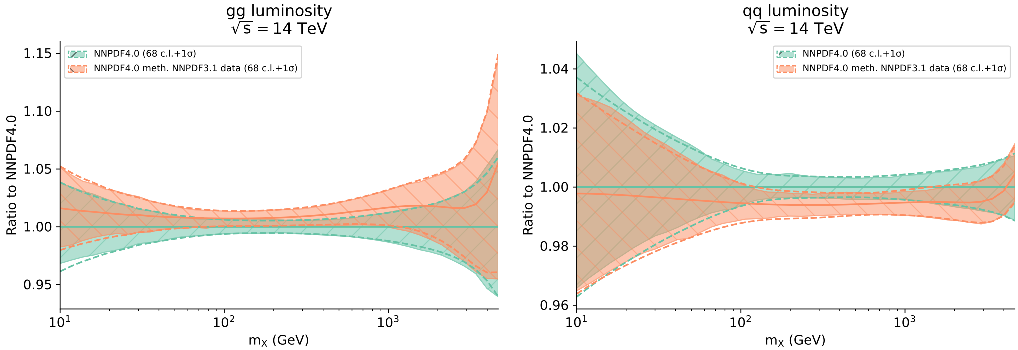
1. Assume a "true" underlying PDF (e.g. a single PDF replica)
2. Produce data distributed according to the experimental covariance matrices
3. Perform a fit to this data

Examples of statistical estimators:

- **Bias**: squared difference between central value and true observable
  Variance: variance of the model predictions
  Faithful uncertainties require $E[\text{bias}] = \text{variance}$
- Is truth within one sigma in 68% of cases?

$\sqrt{\text{bias}/\text{variance}}$	$\xi_{1\sigma}^{(\text{data})}$
1.03 ± 0.05	0.68 ± 0.02

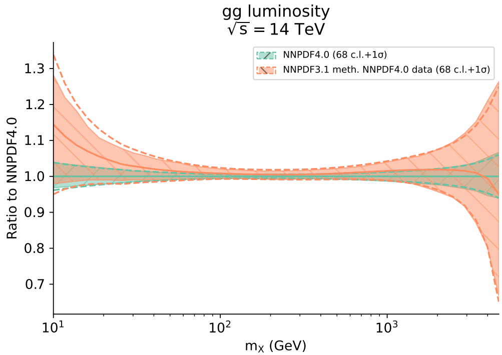
Impact of the new data

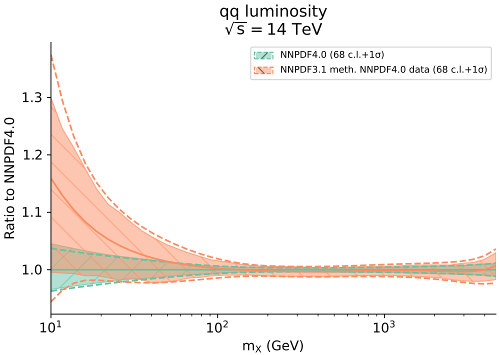


Individual datasets have a limited impact, but collectively they result in:

- Moderate reduction of PDF uncertainties
- Shifts in central value at the one-sigma level

Impact of the new fitting methodology



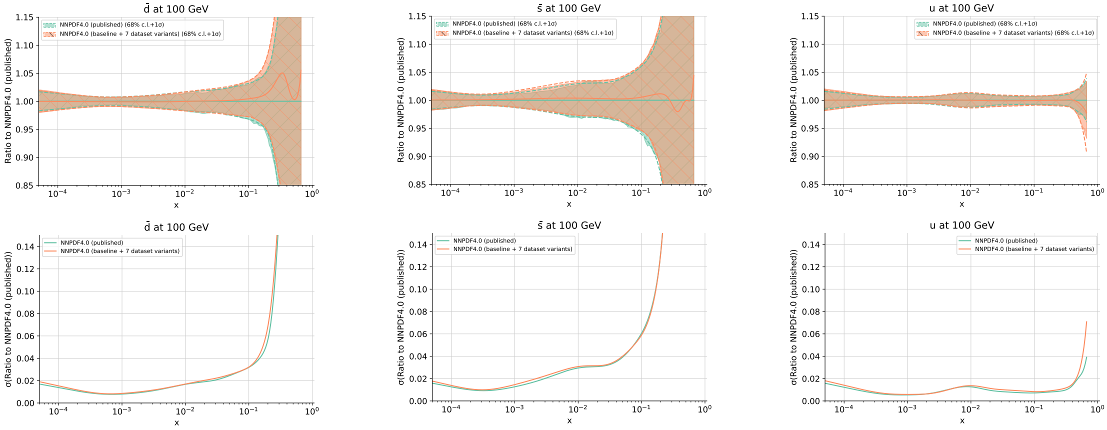


- Significant reduction of PDF uncertainties
- Good agreement between the central values

> PDF uncertainties are validated using closure tests and future tests
> Validation tests successful for both NNPDF4.0 and NNPDF3.1

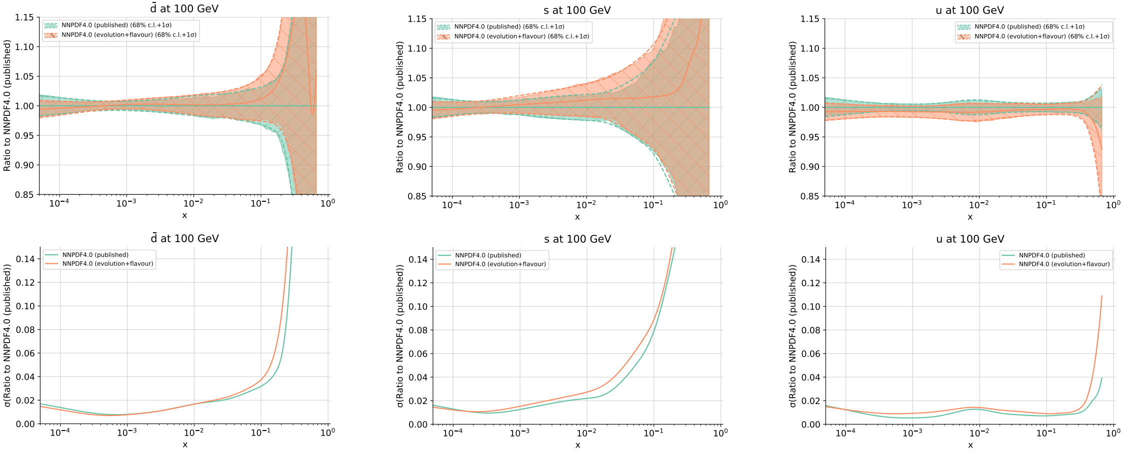
The (negligible) impact of datasets with tension

Excluding datasets with large $(\chi^2 - 1)/\sigma_{\chi^2}$ one at a time and combining the resulting PDFs following the conservative PDF4LHC15 prescription shows stability at the level of statistical fluctuations.



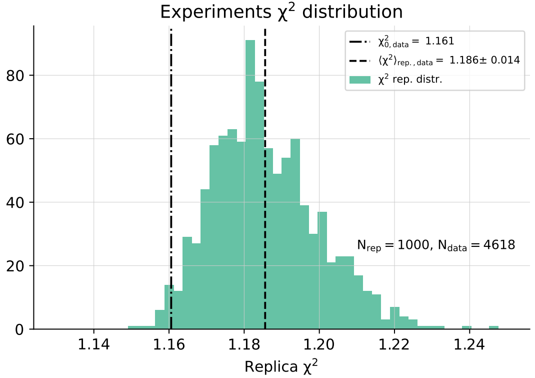
Envelope of fits with different parametrization bases

Different strategies to parametrize the PDF flavour combinations lead to the same result

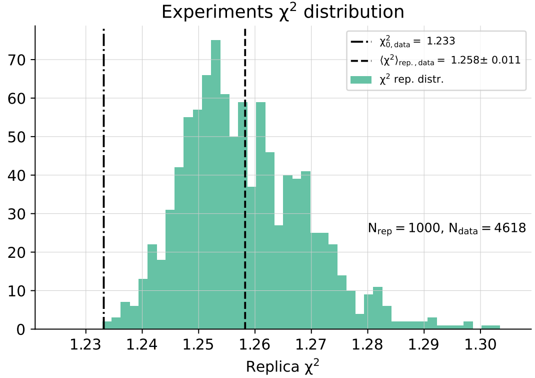


Understanding the χ^2 distribution

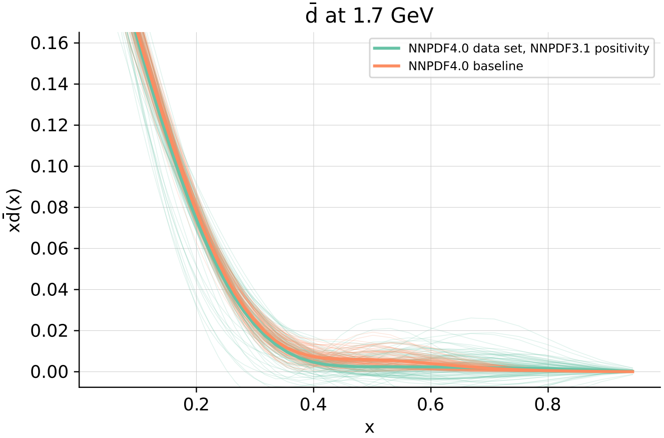
Experimental χ^2



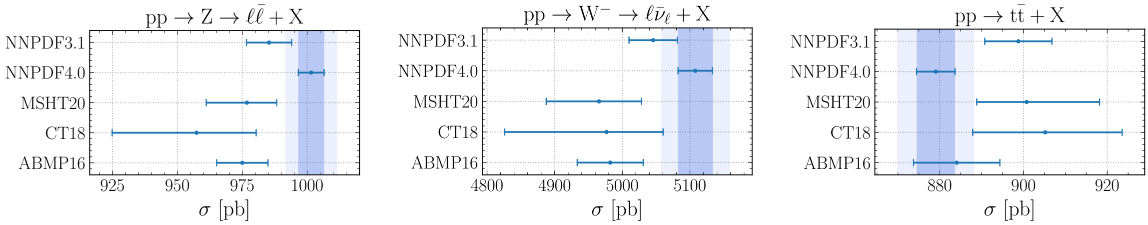
t_0 χ^2



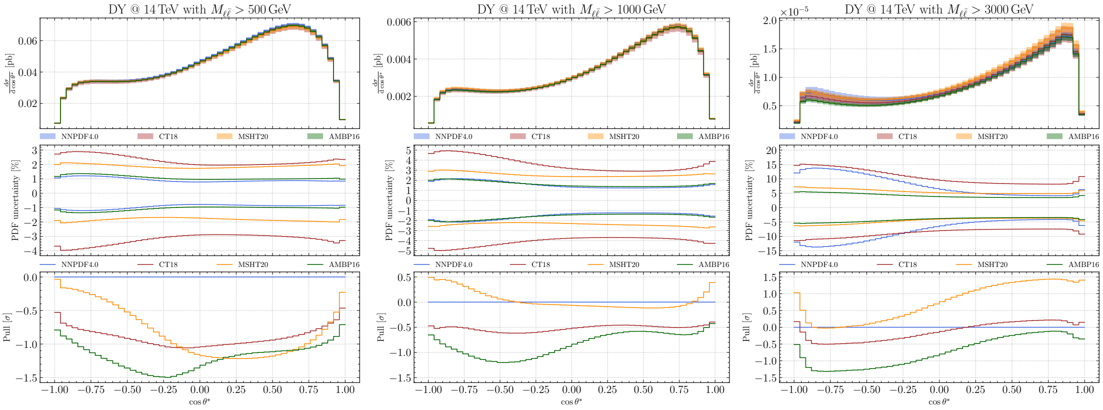
Impact of positivity on the PDFs



More implications for phenomenology



Small M_{ll}



Small uncertainties in the data region