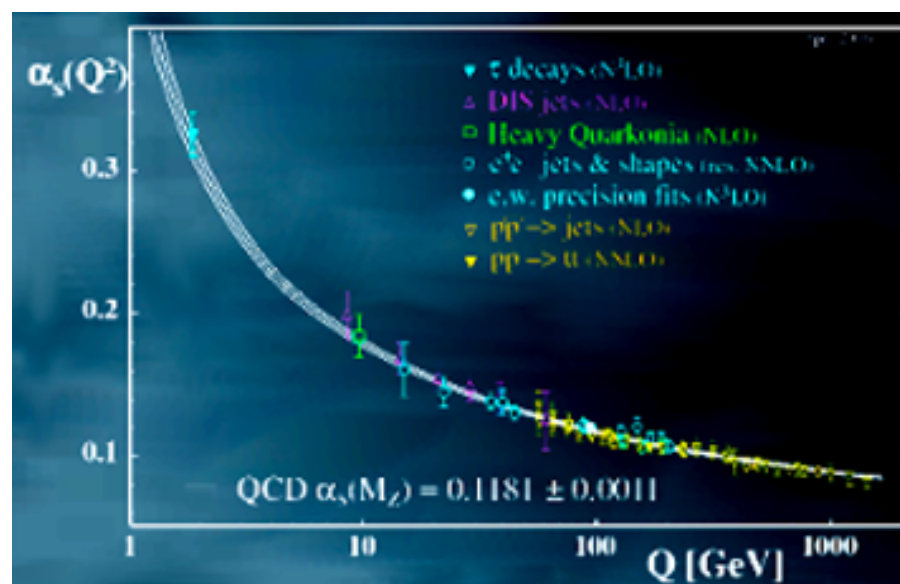


# Strong coupling fits from NNPDF global analyses

Juan Rojo, VU Amsterdam & Nikhef

alphas-2022 Workshop

February 1st 2022



$$\mathcal{L} = \frac{1}{4g^2} G_{\mu\nu}^a G_{\mu\nu}^a + \sum_j \bar{q}_j (i\gamma^\mu D_\mu + m_j) q_j$$

$$\text{where } G_{\mu\nu}^a \equiv \partial_\mu A_\nu^a - \partial_\nu A_\mu^a + if_{bc}^a A_\mu^b A_\nu^c$$

$$\text{and } D_\mu \equiv \partial_\mu + it^a A_\mu^a$$

# Outline

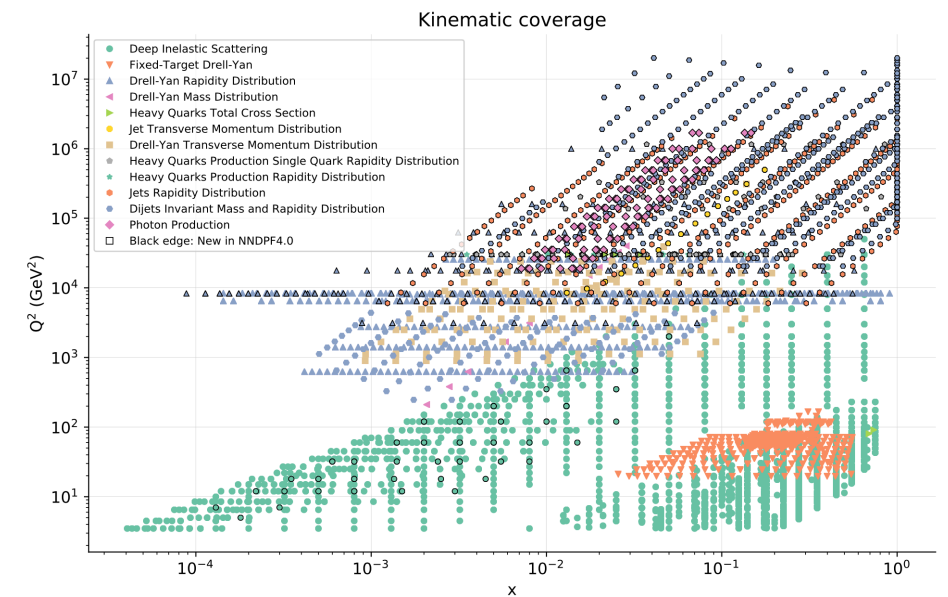
📌 The NNPDF4.0 global PDF analysis

📌 Strong coupling determination from NNPDF3.1

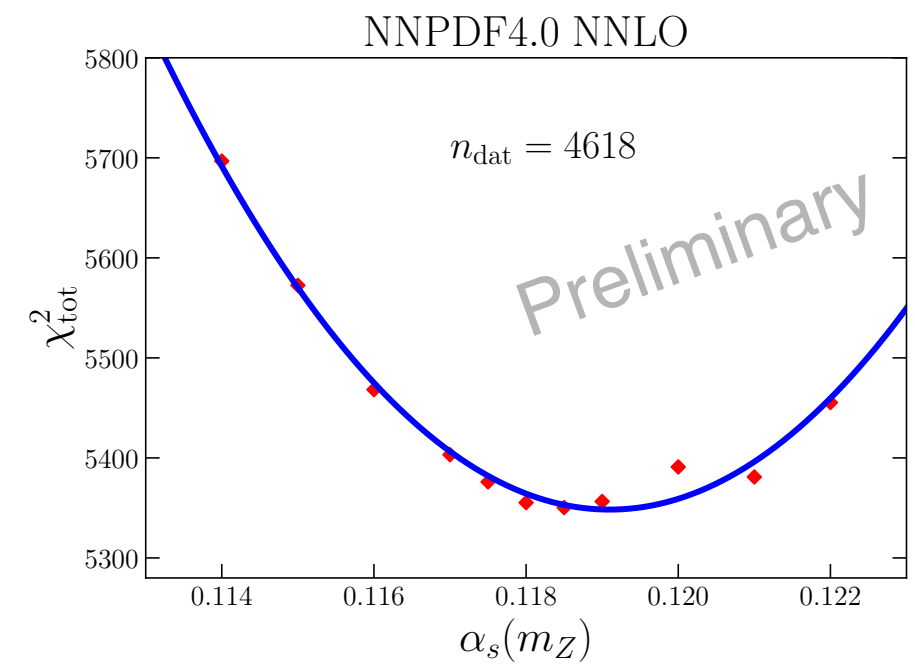
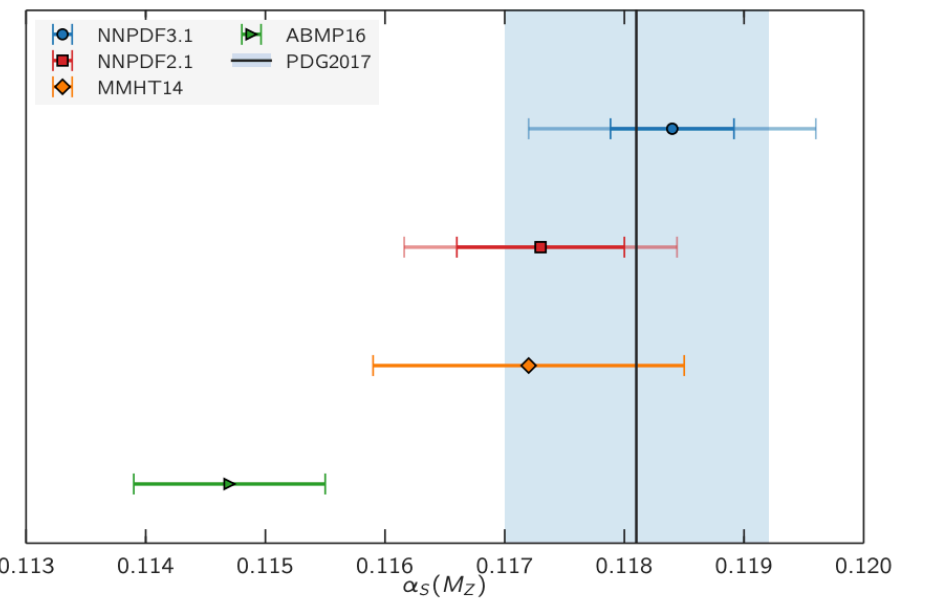
📌 Preliminary results based on NNPDF4.0

📌 The SimuNET strategy

NNPDF4.0: data set extension



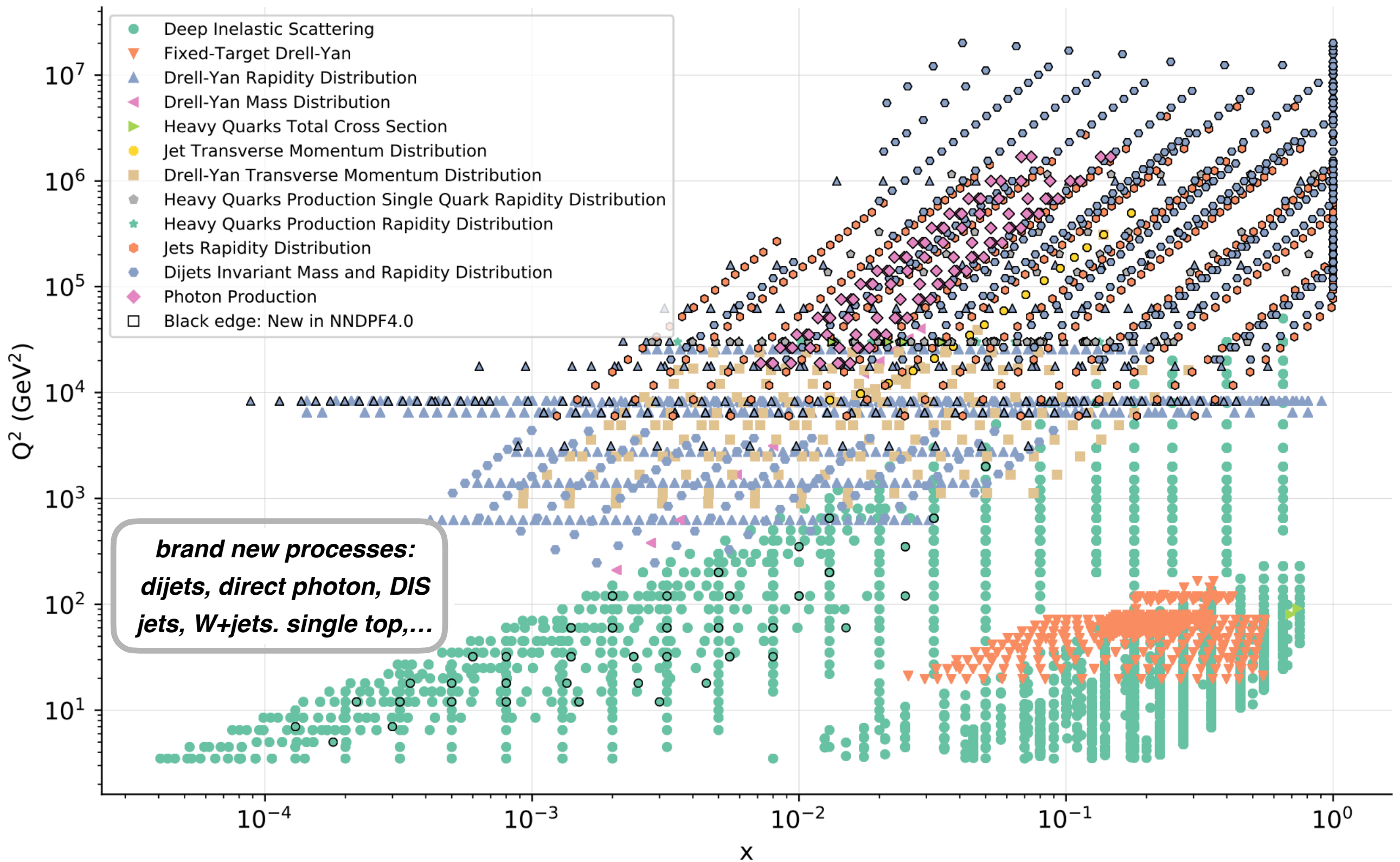
$\mathcal{O}(50)$  data sets investigated;  $\mathcal{O}(400)$  data points more in NNPDF4.0 than in NNPDF3.1



# **NNPDF4.0**

arXiv:2109.02653

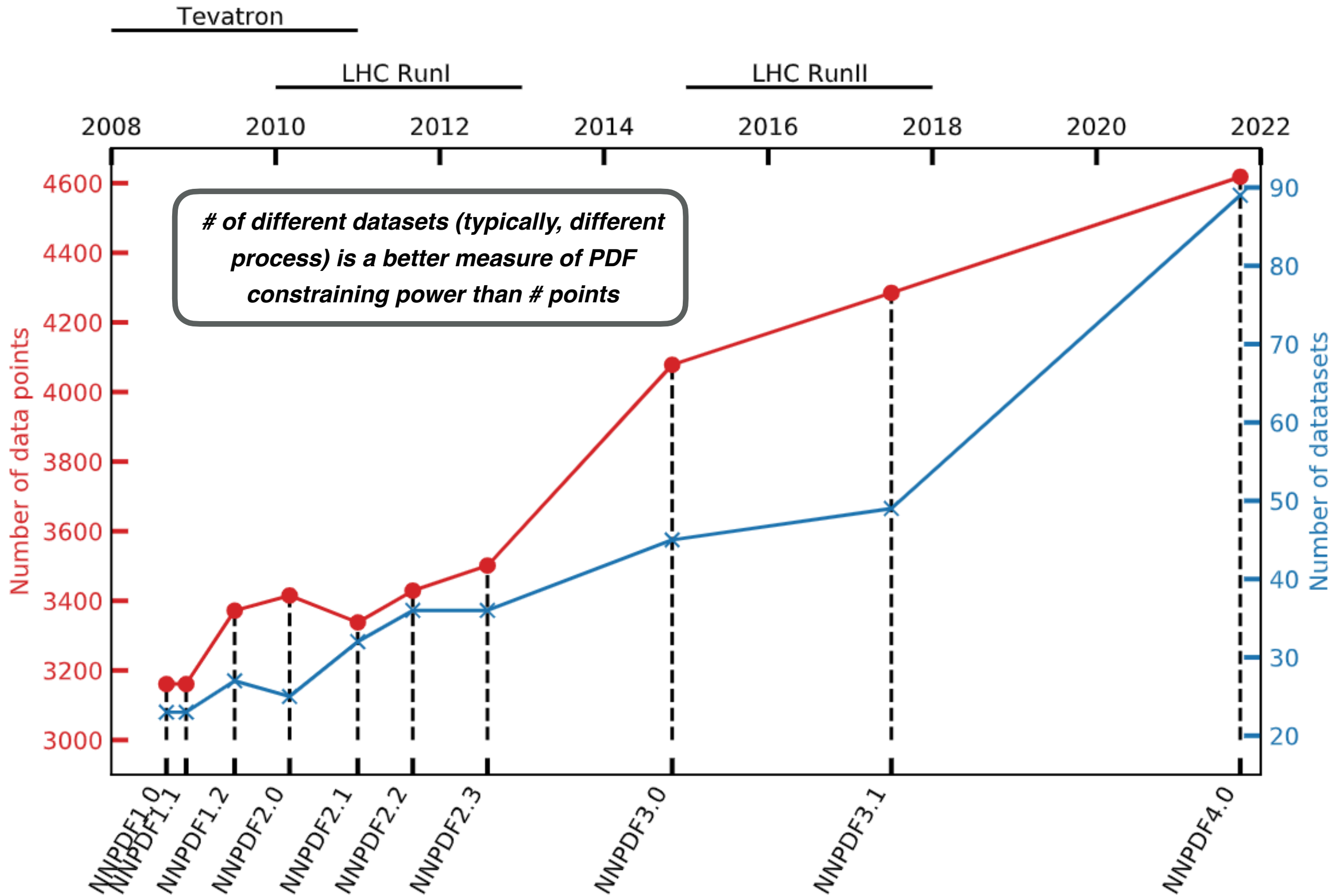
# The NNPDF4.0 dataset



$\mathcal{O}(50)$  data sets investigated;  $\mathcal{O}(400)$  data points more in NNPDF4.0 than in NNPDF3.1

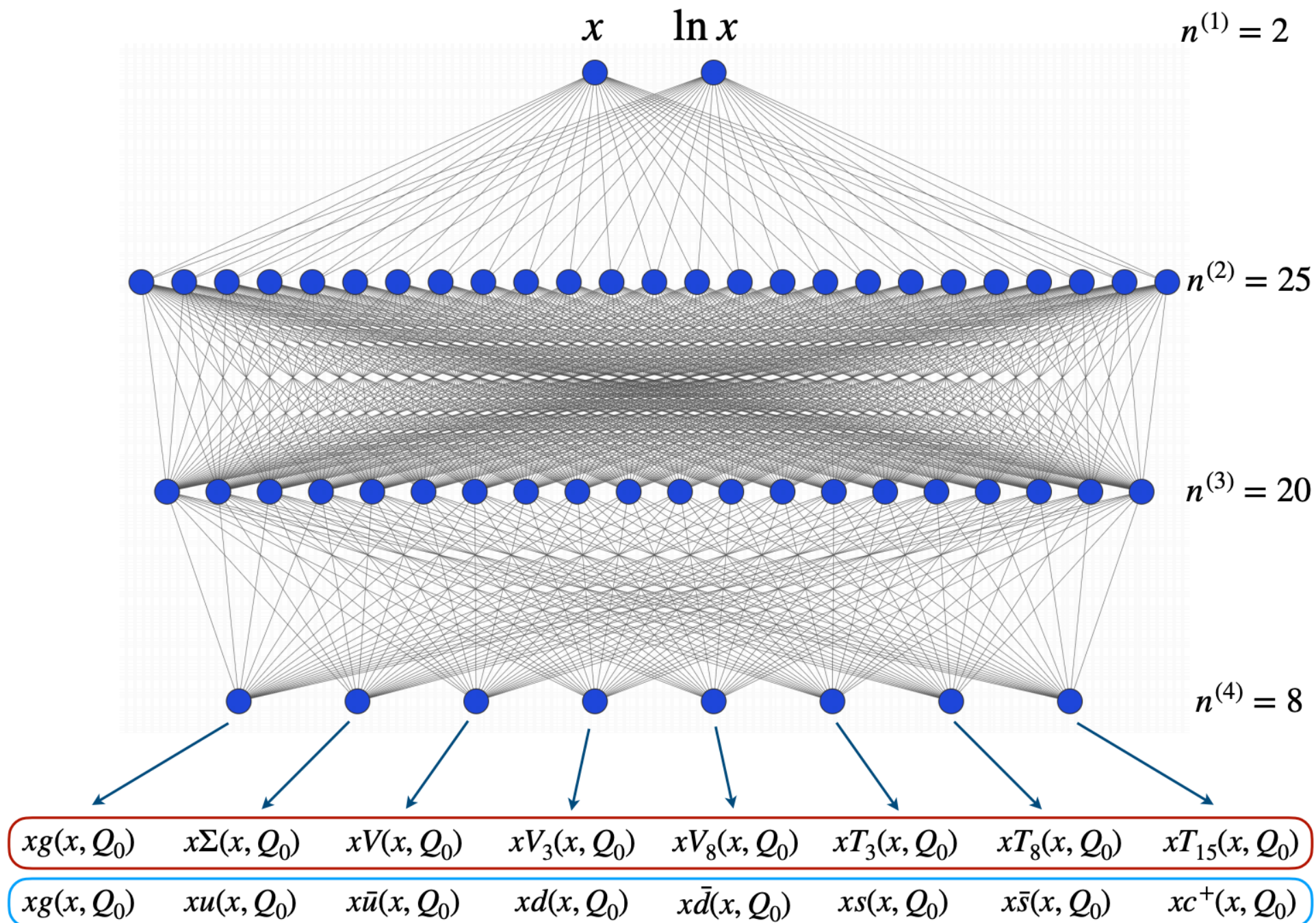


# From NNPDF1.0 to NNPDF4.0



# Improved fitting methodology

- ☑ **Stochastic Gradient Descent** via TensorFlow for NN training
- ☑ Automated model **hyperparameter optimisation**: NN architecture, minimiser, learning rates ...
- ☑ Validation with **future tests** (forecasting new datasets) and **closure tests** (data based on known PDFs)



PDFs should be independent of **parametrisation basis!**

*evolution basis*

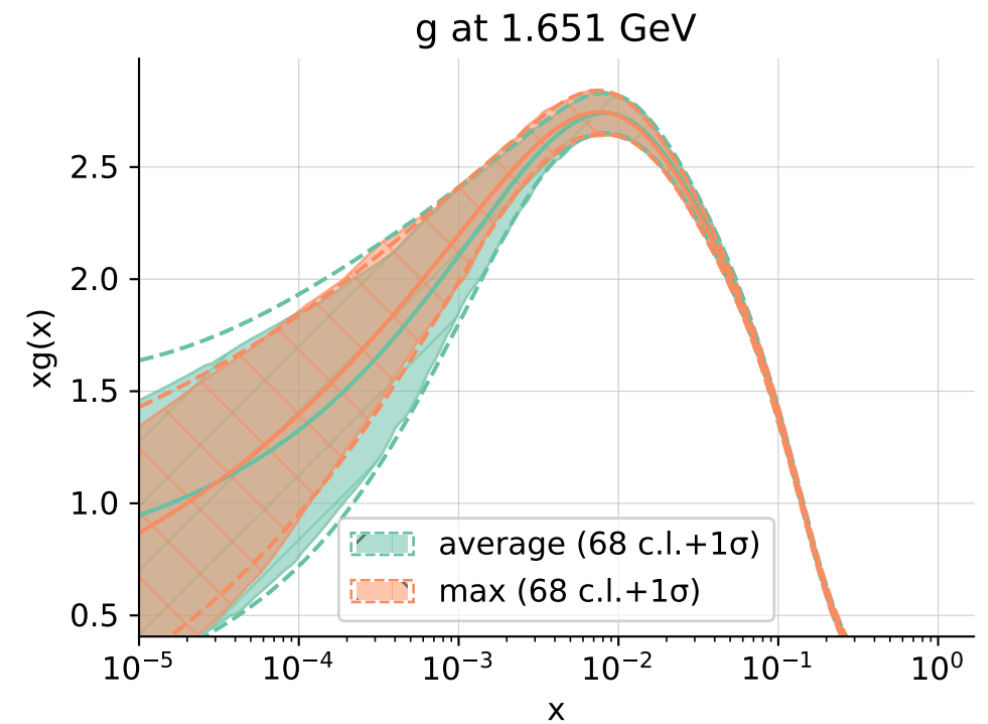
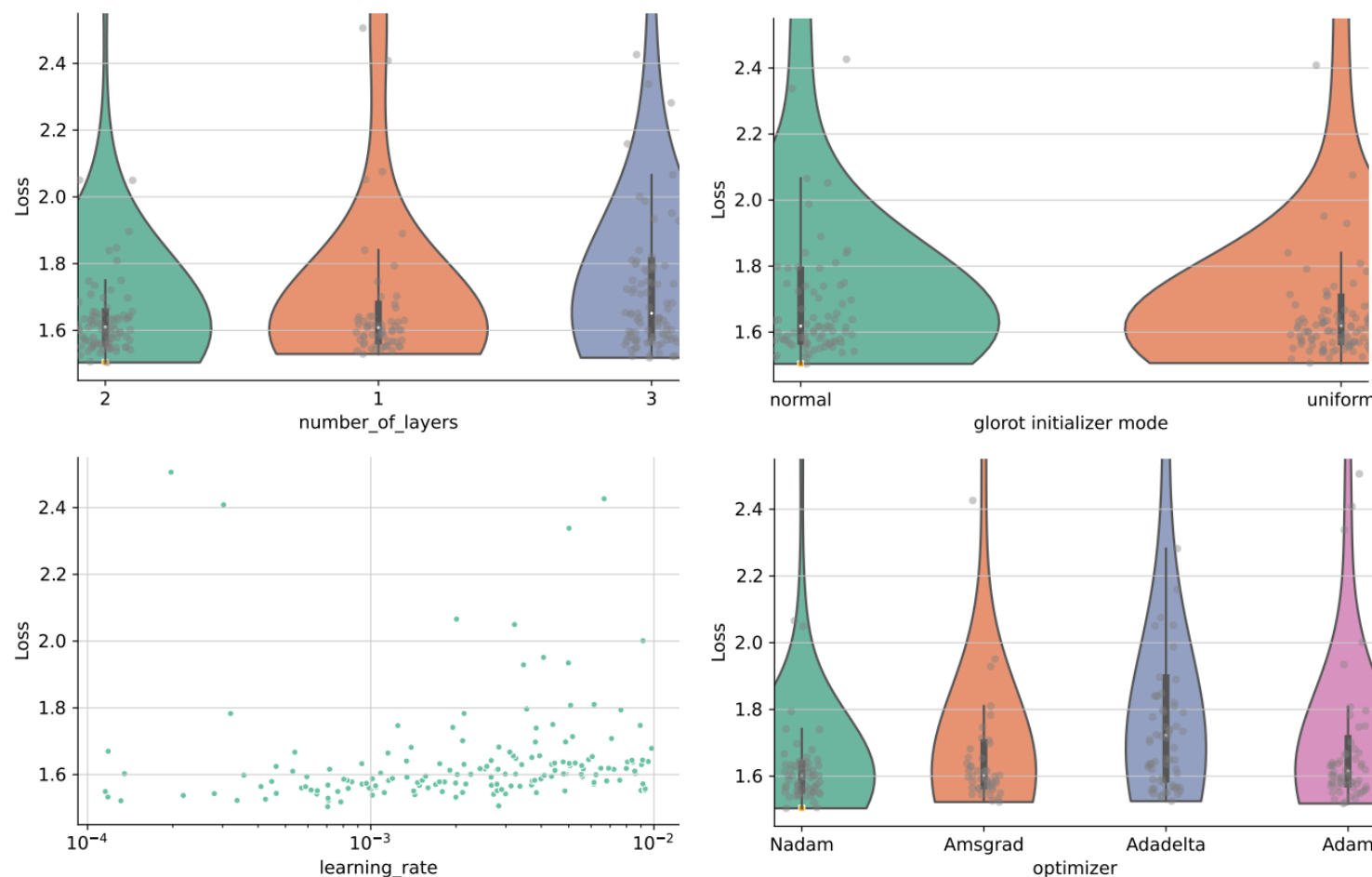
*flavor basis*

# Improved fitting methodology

- ☑ **Stochastic Gradient Descent** via TensorFlow for NN training
- ☑ Automated model **hyperparameter optimisation**: NN architecture, minimiser, learning rates ...
- ☑ Validation with **future tests** (forecasting new datasets) and **closure tests** (data based on known PDFs)

*ML model hyperparams*  $\hat{\theta} = \arg \min_{\theta \in \Theta} \left( \frac{1}{n_{\text{fold}}} \sum_{k=1}^{n_{\text{fold}}} \chi_k^2(\theta) \right)$

*Loss ("max")*  
 $L = \max(\chi_1^2, \chi_2^2, \chi_3^2, \dots, \chi_{n_{\text{fold}}}^2)$

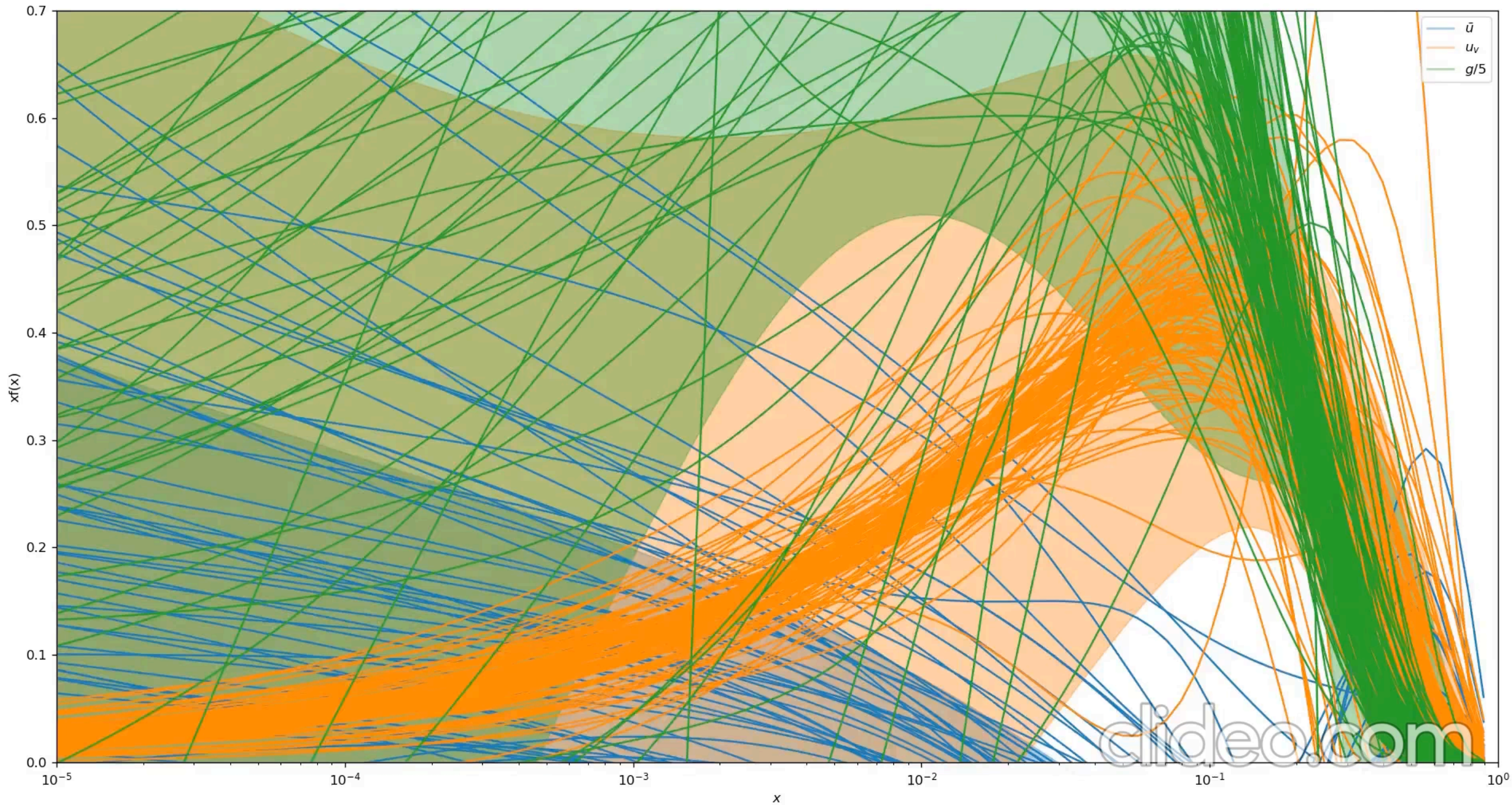


*Stability wrt hyperopt loss function*



# Improved fitting methodology

epoch 3



Illustrating the outcome of **SGD minimisation** (band: standard deviation over the MC replicas)



# Closure and future tests

## Closure tests

Generate **toy data** based on some known PDF, check *a posteriori* that the **true underlying law is reproduced** within errors

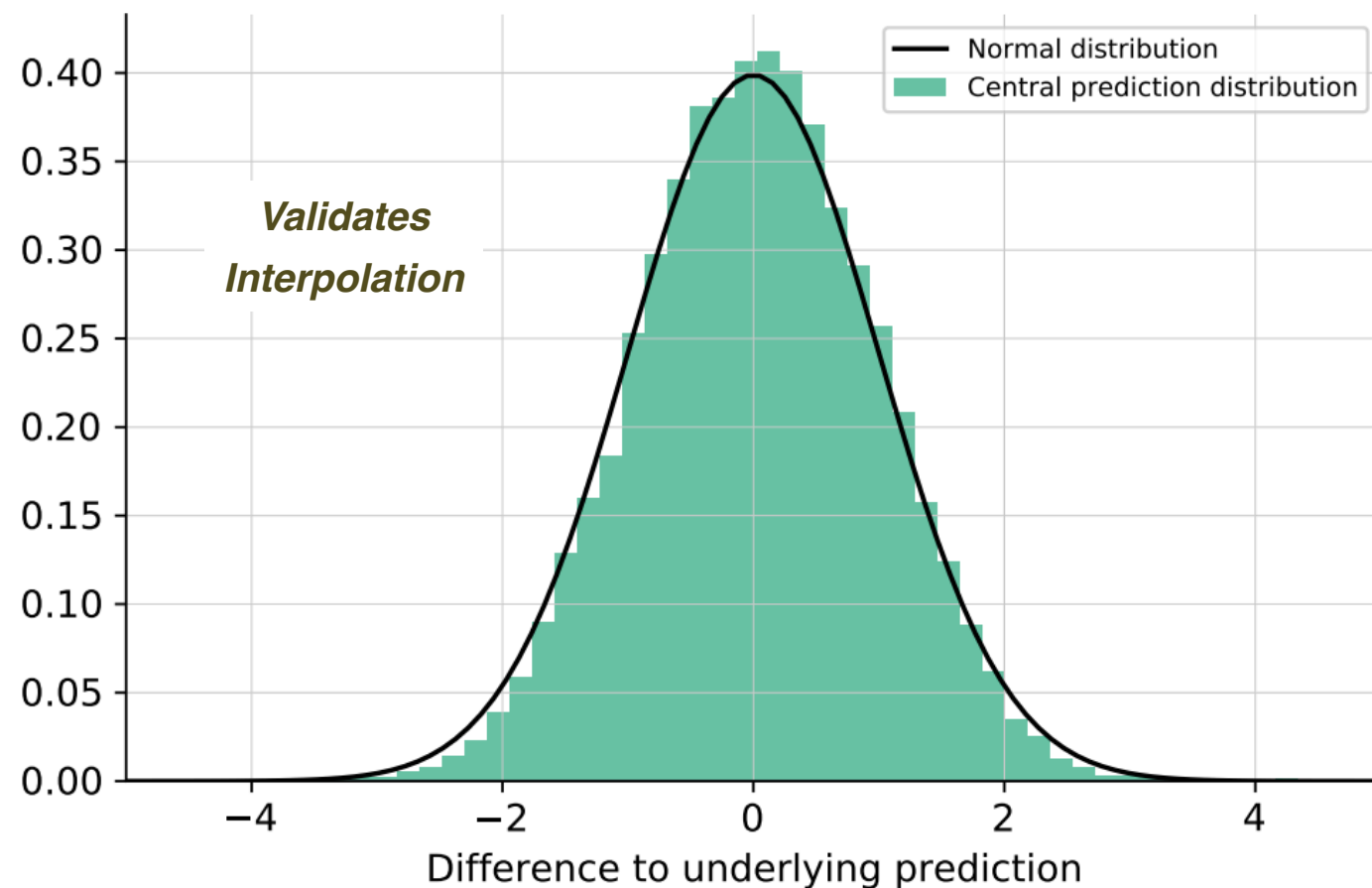
generate many toys

$$\delta_i^{(l)} \equiv \frac{\left( \mathbf{E}_\epsilon [g_i]^{(l)} - f_i \right)}{\sigma_i^{(l)}}$$

mean NN prediction      true central value

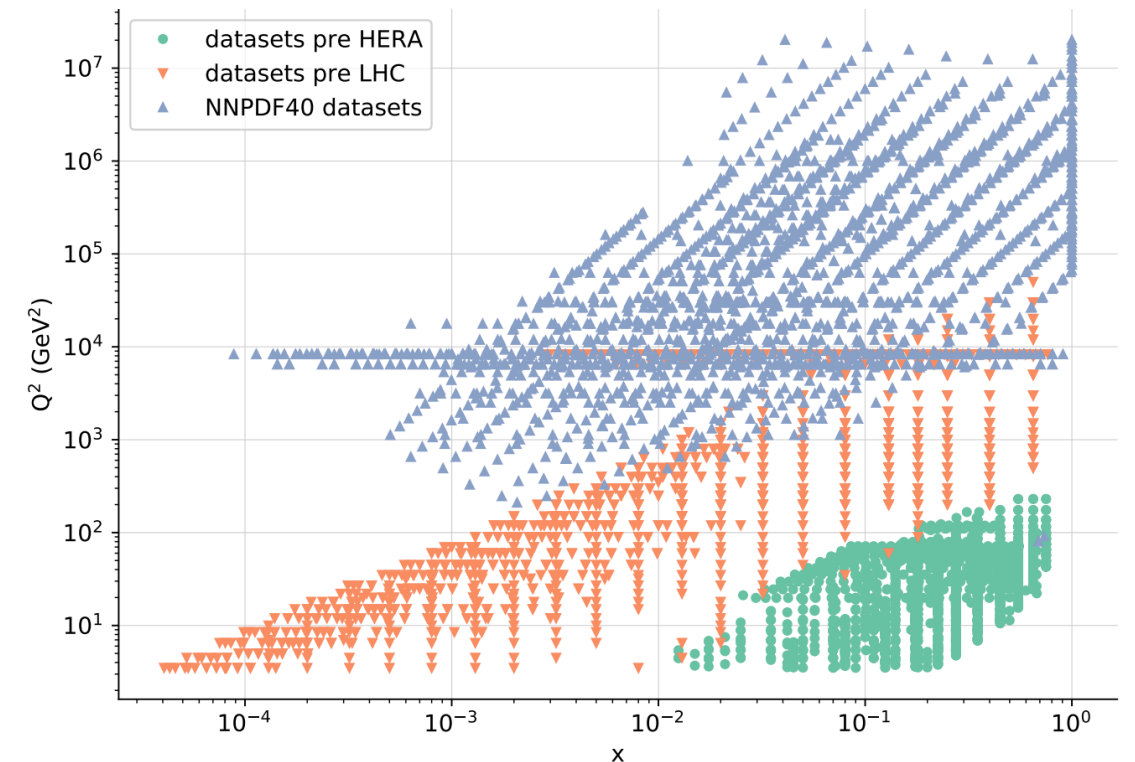
PDF uncertainty

data index



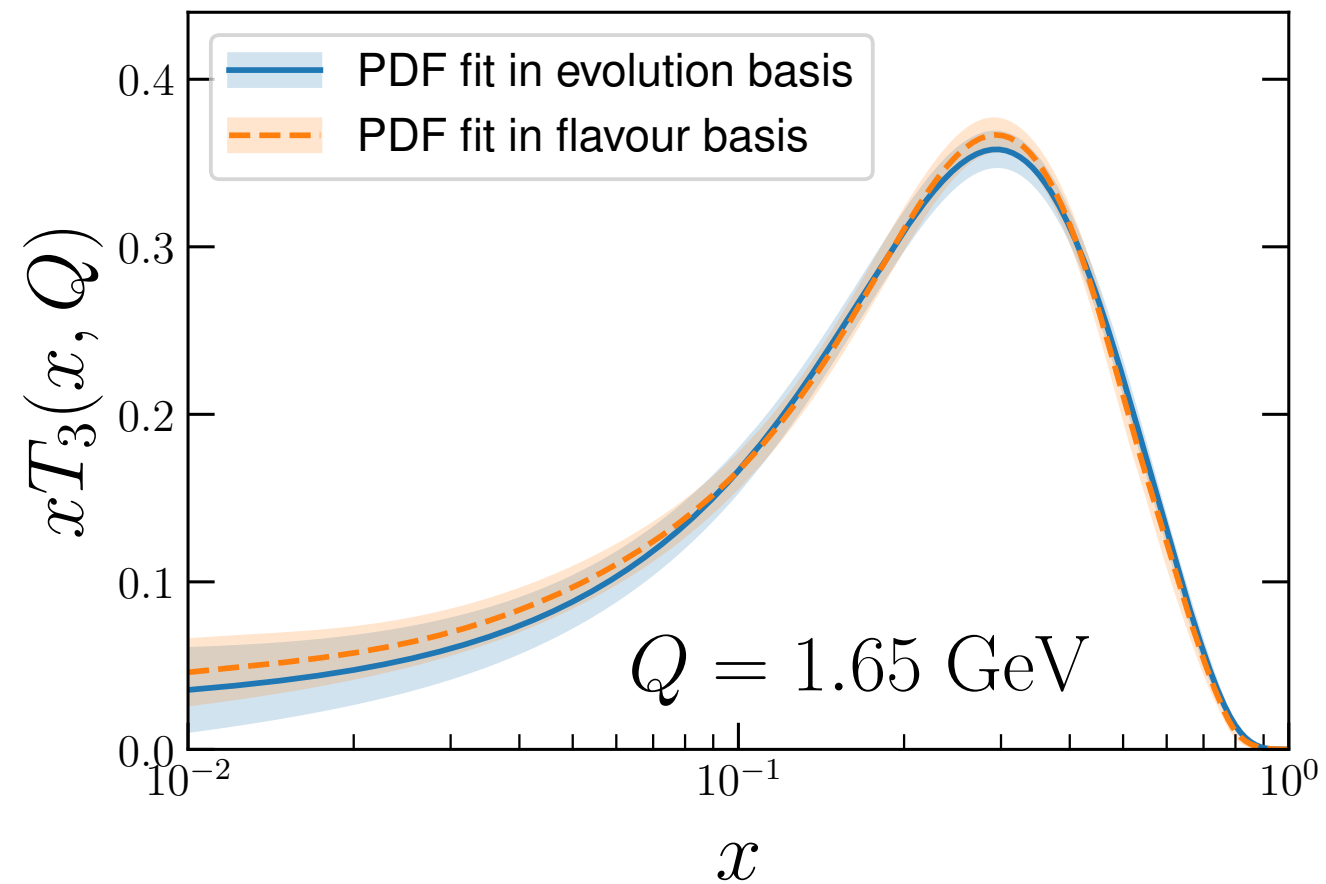
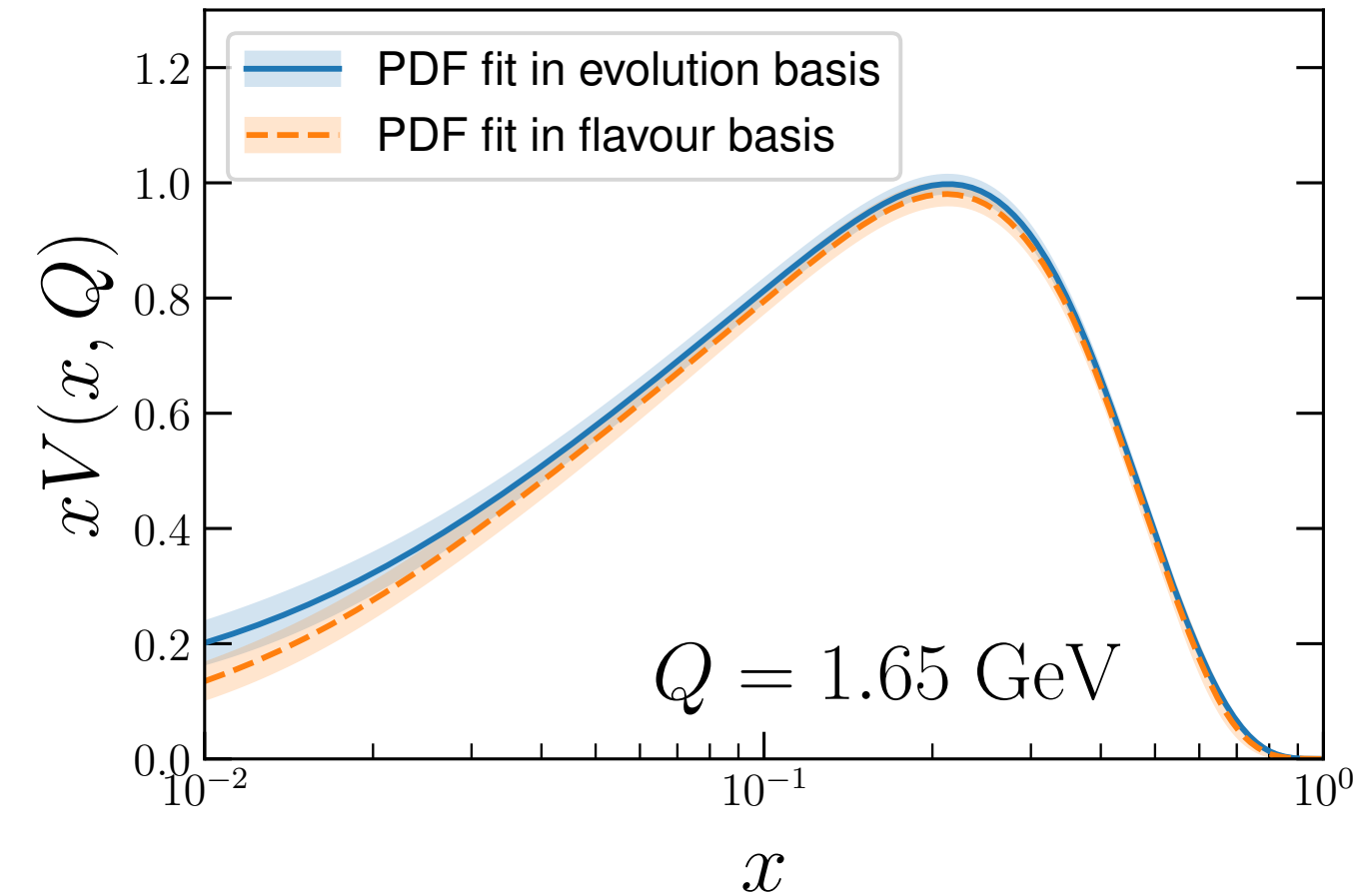
## Future tests

Fit data restricted to specific kinematic regions, then verify **successful extrapolation**



Process	$\chi^2_{\text{pre-HERA}}$	$\chi^2_{\text{pre-LHC}}$	$\chi^2_{\text{Global}}$
Fixed target NC DIS	1.05	1.18	1.23
Fixed target CC DIS	0.80	0.85	0.87
Fixed target Drell-Yan	0.92	1.27	1.59
HERA	27.20 (1.23)	1.22	1.20
Collider Drell-Yan (Tevatron)	5.52 (1.02)	0.99	1.11
Collider Drell-Yan (LHC)	18.91 (1.31)	2.63 (1.58)	1.53
Top quark production	20.01 (1.06)	1.30 (0.87)	1.01
Jet production	2.69 (0.98)	2.12 (1.10)	1.26

# Parametrisation basis independence



*evolution basis PDF parametrisation:*

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

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

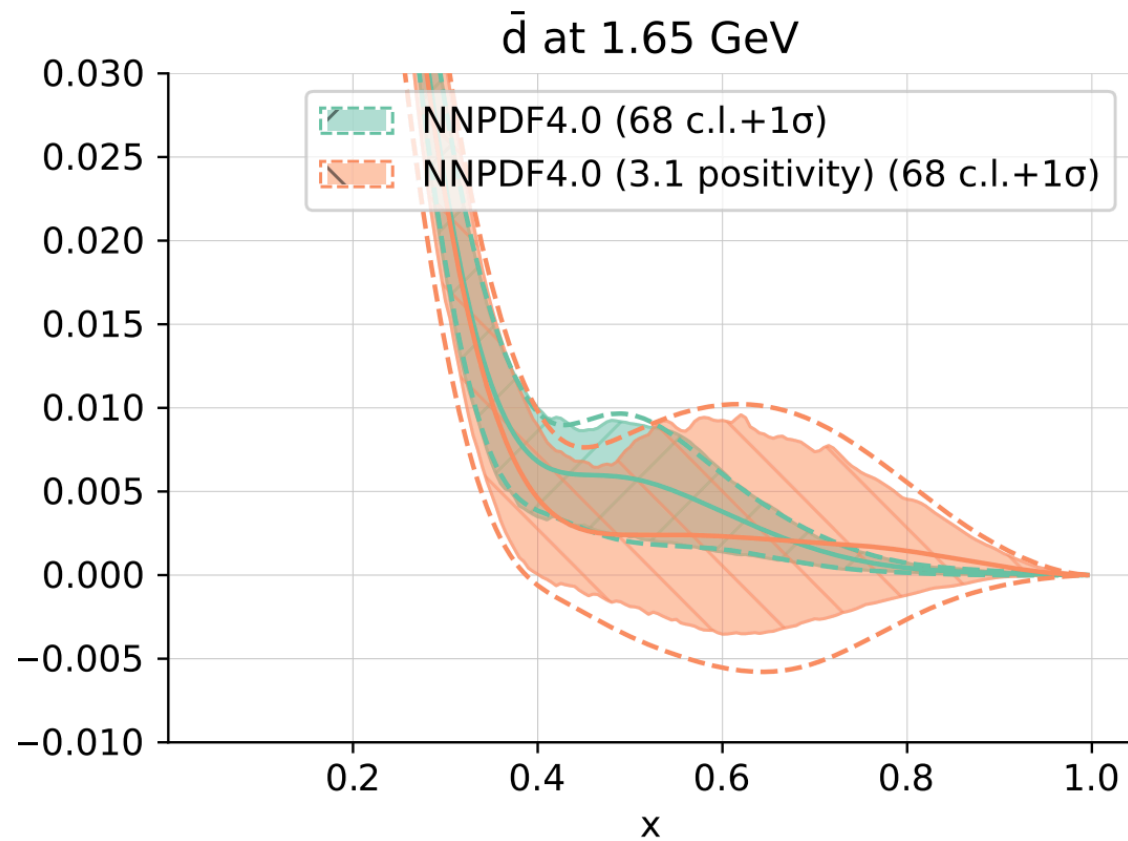
Radically different strategies to parametrize the **quark PDF flavour combinations** lead to identical results:  
ultimate test of **parametrisation independence**

*flavour basis PDF parametrisation:*

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

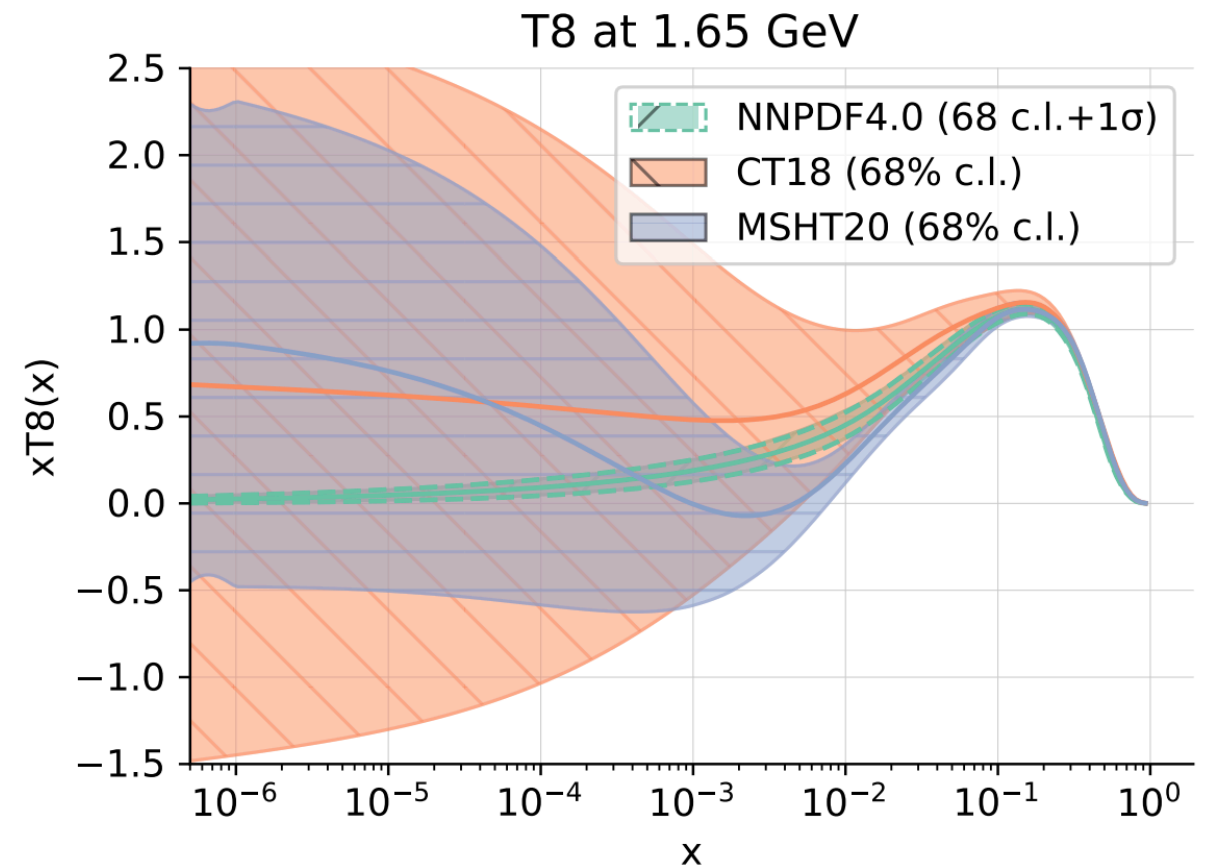
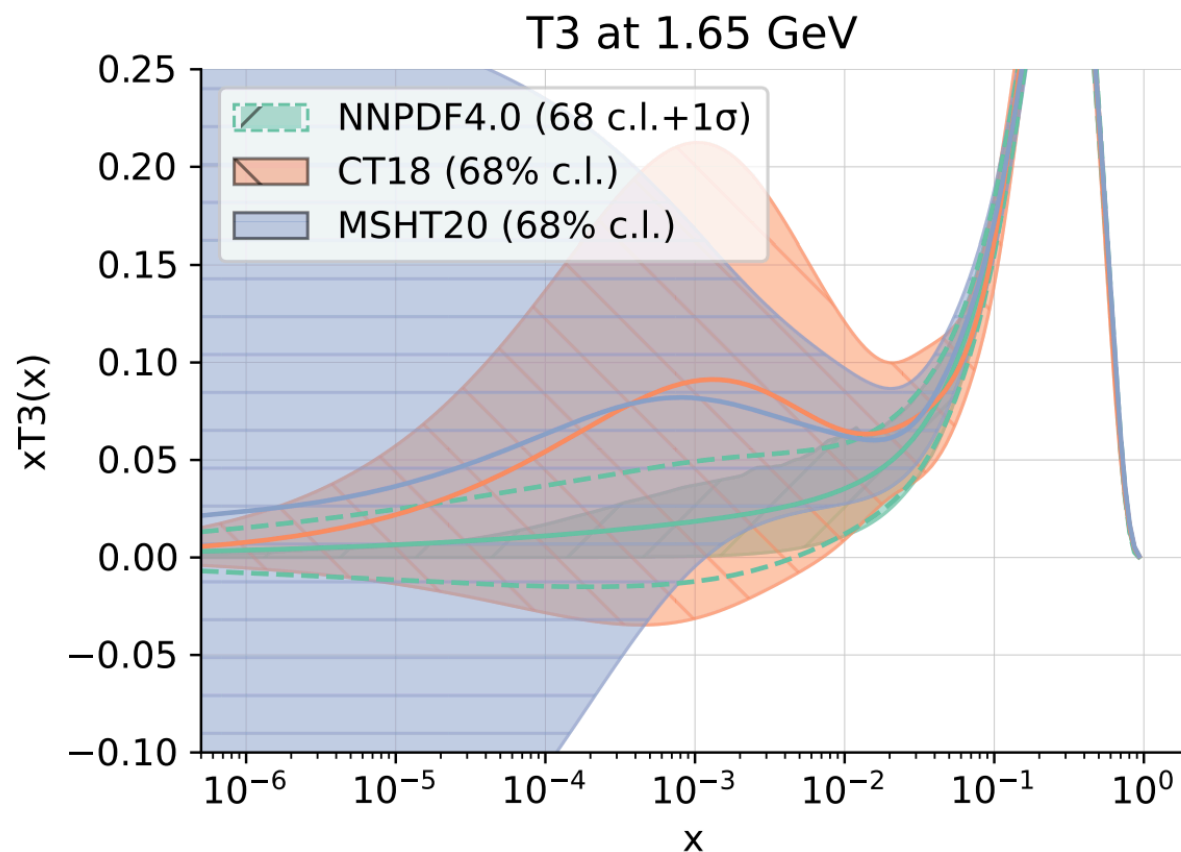
$$xT_3(x, Q_0) \propto (\text{NN}_u(x) + \text{NN}_{\bar{u}}(x) - \text{NN}_d(x) - \text{NN}_{\bar{d}}(x))$$

# Positivity and integrability



- MSbar PDFs have been shown to satisfy **positivity** requirements at all orders:  
**reduce large-x uncertainties**
- The non-singlet quark triplet and octet should be *integrable* (e.g. Gottfried sum rule): **reduce small-x uncertainties**

$$T_8 = (u + \bar{u}) + (d + \bar{d}) - 2(s + \bar{s})$$



# A ML open-source QCD fitting framework

zenodo Search Upload Communities j.rojo@vu.nl

September 1, 2021

Software Open Access

## NNPDF/nnpdf: An open-source machine learning framework for global analyses of parton distributions

Richard D. Ball; Stefano Carrazza; Juan M. Cruz-Martinez; Luigi Del Debbio; Stefano Forte; Tommaso Giani; Shayan Iranipour; Zahari Kassabov; Jose I. Latorre; Emanuele R. Nocera; Rosalyn L. Pearson; Juan Rojo; Roy Stegeman; Christopher Schwan; Maria Ubiali; Cameron Voisey; Michael Wilson

This version is used for producing all the publicly released fits for NNPDF4.0.

53 views 1 downloads  
See more details...

Available in  
**GitHub**  
Indexed in  
**OpenAIRE**

Preview

nnpdf-4.0.3.zip

The previewer is not showing all the files

- NNPDF-nnpdf-1229126
  - .ciscrpts
    - build-deploy-linux.sh 1.1 kB
    - build-deploy-osx.sh 966 Bytes
    - deploy-documentation.sh 878 Bytes
  - .github
    - workflows
      - rules.yml 3.4 kB
  - .gitignore 5.0 kB
  - .pylintrc 15.1 kB
  - .travis.yml 3.6 kB
  - CMakeLists.txt 9.2 kB

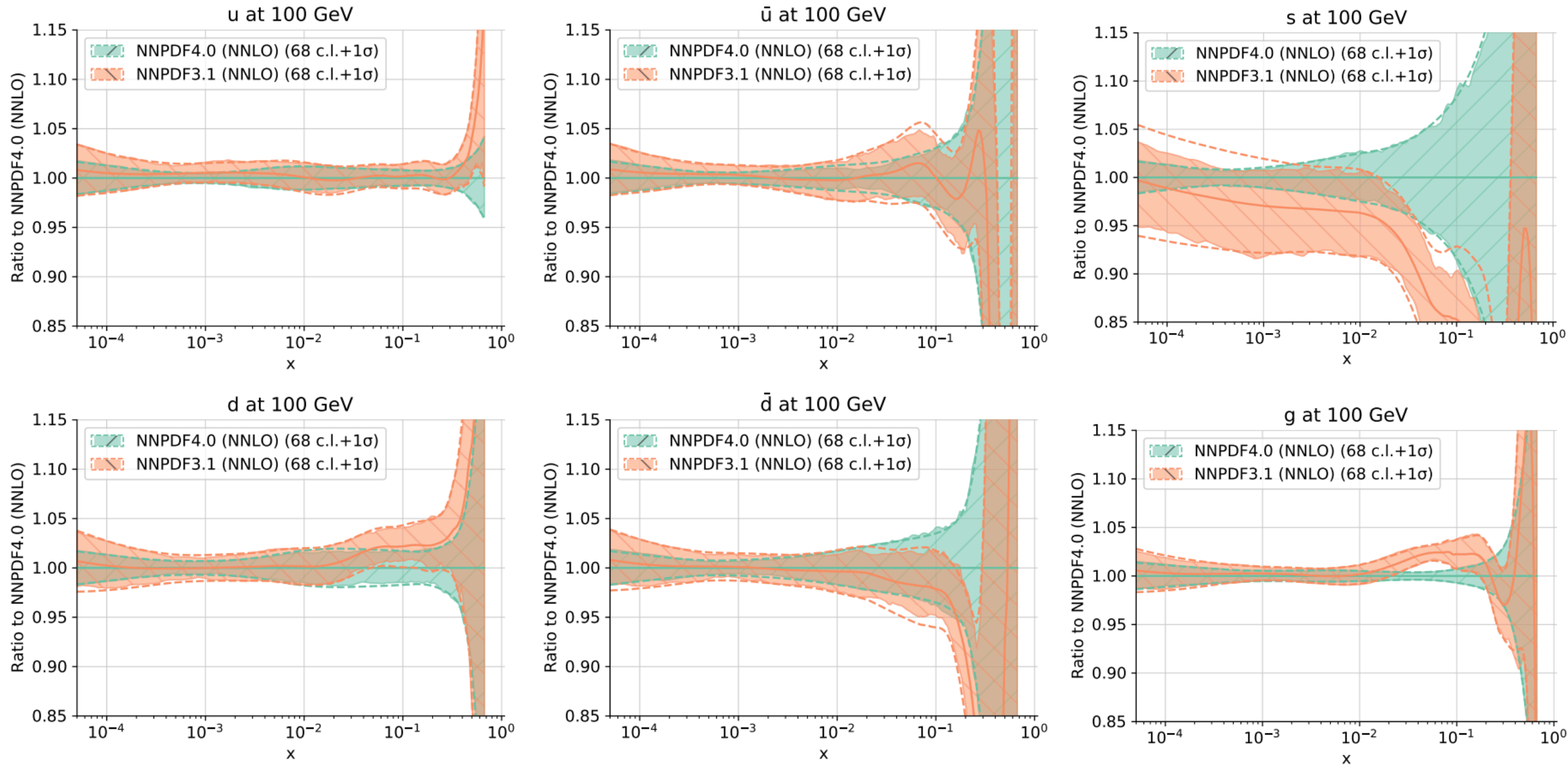
Publication date:  
September 1, 2021

DOI:  
DOI 10.5281/zenodo.5362229

The full **NNPDF machine learning fitting framework** has been publicly released open source, together with extensive documentation and user-friendly examples



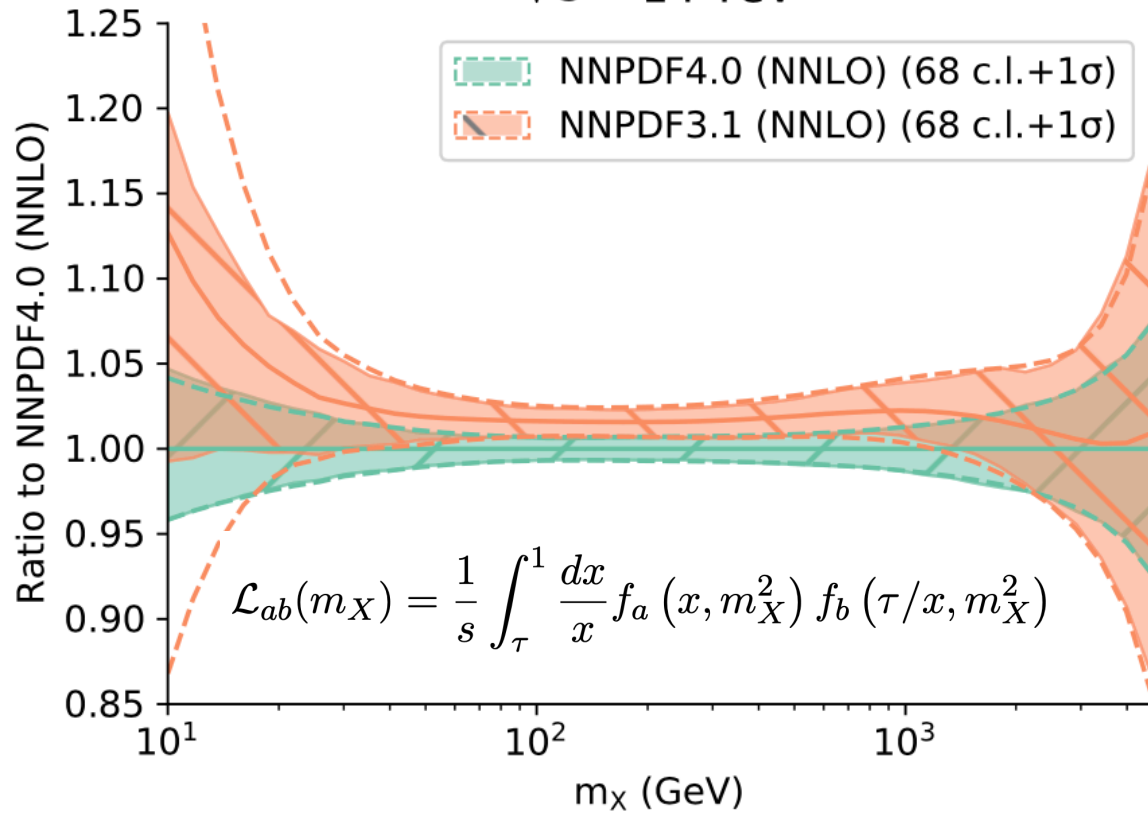
# Comparison with NNPDF3.1



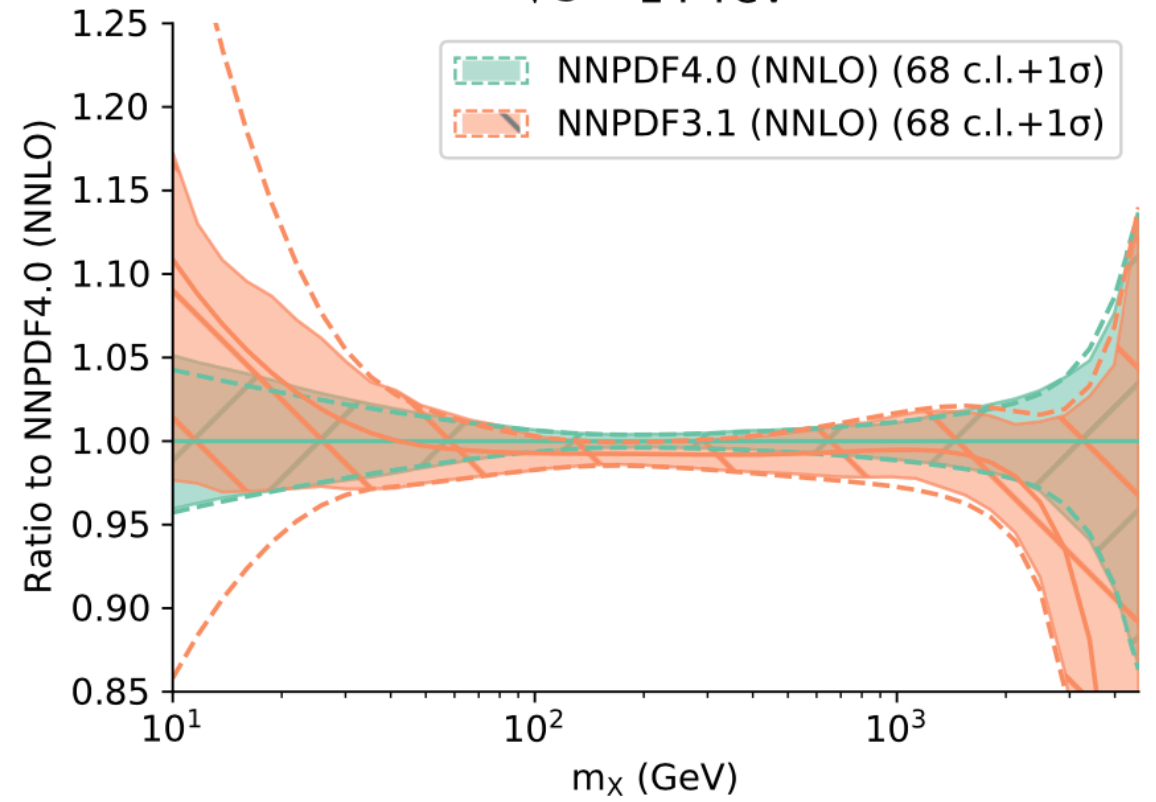
- 🎯 **Good agreement** with NNPDF3.1 within uncertainties, with NNPDF4.0 being more precise
- 🎯 Differences can be traced back to the **impact of specific datasets** (e.g. dijets for large- $x$  gluon) or improvements in **theory calculations** (e.g. NNLO corrections in dimuon DIS for strangeness)

# Comparison with NNPDF3.1

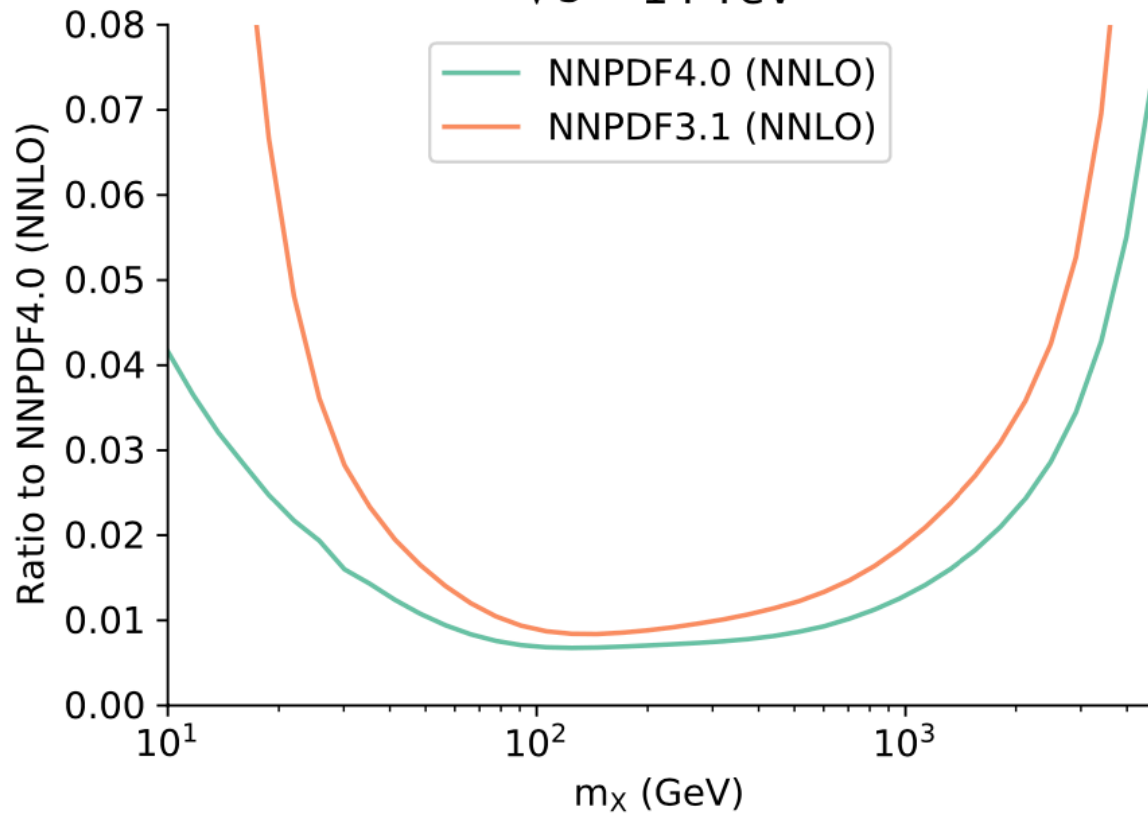
gg luminosity  
 $\sqrt{s} = 14$  TeV



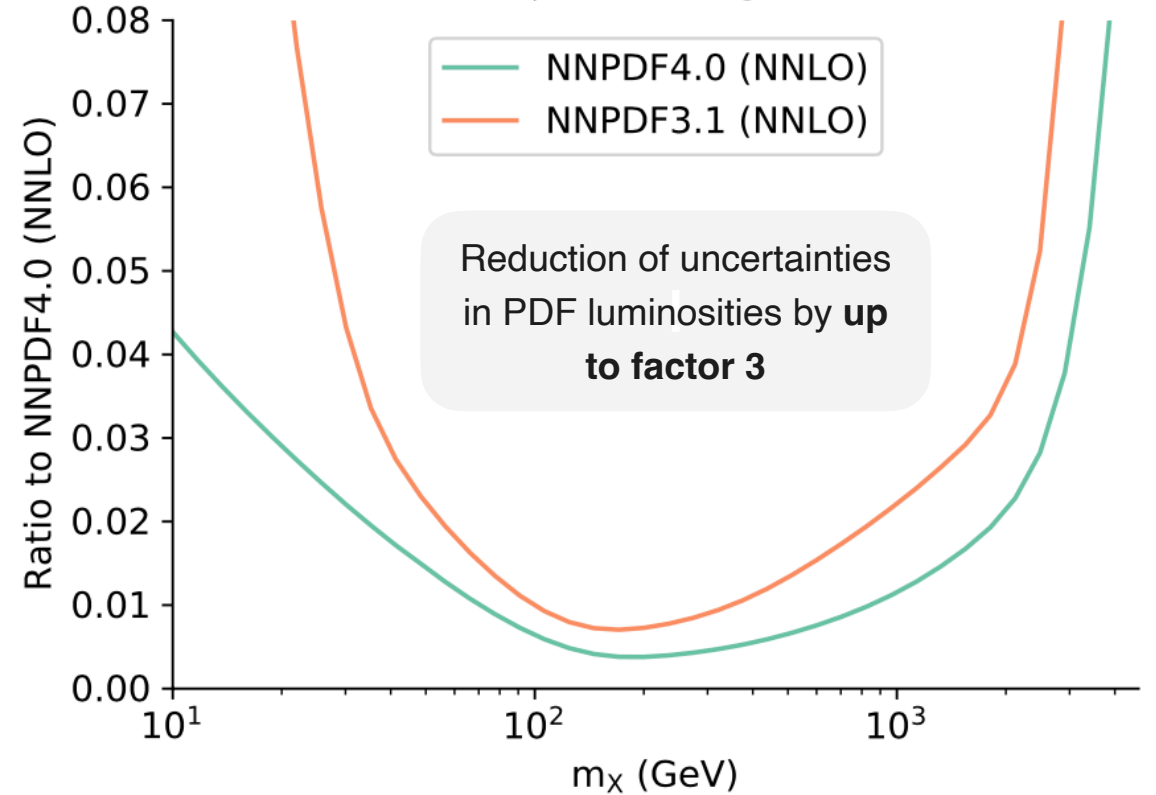
q $\bar{q}$  luminosity  
 $\sqrt{s} = 14$  TeV



gg luminosity uncertainty  
 $\sqrt{s} = 14$  TeV



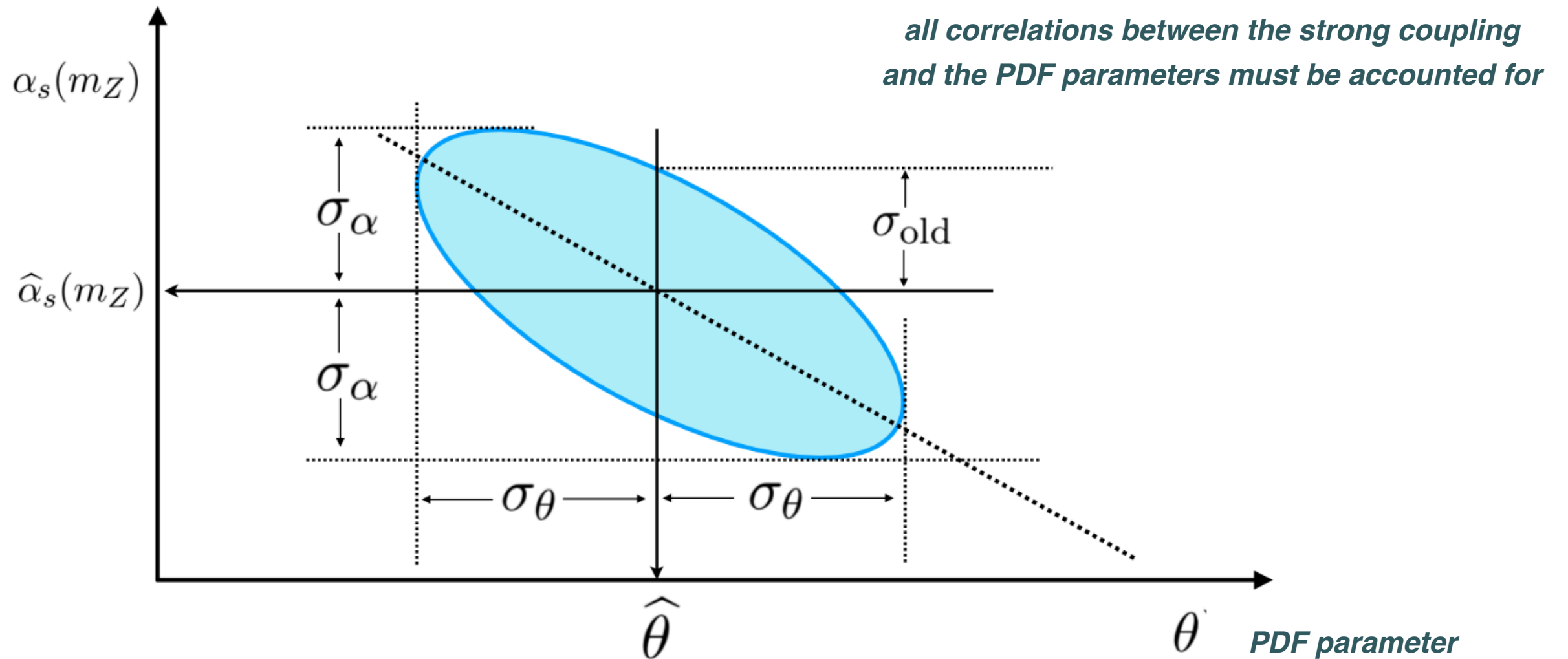
q $\bar{q}$  luminosity uncertainty  
 $\sqrt{s} = 14$  TeV



# Alphas from NNPDF3.1

**arXiv:1802.03398**

# Correlated Monte Carlo replicas



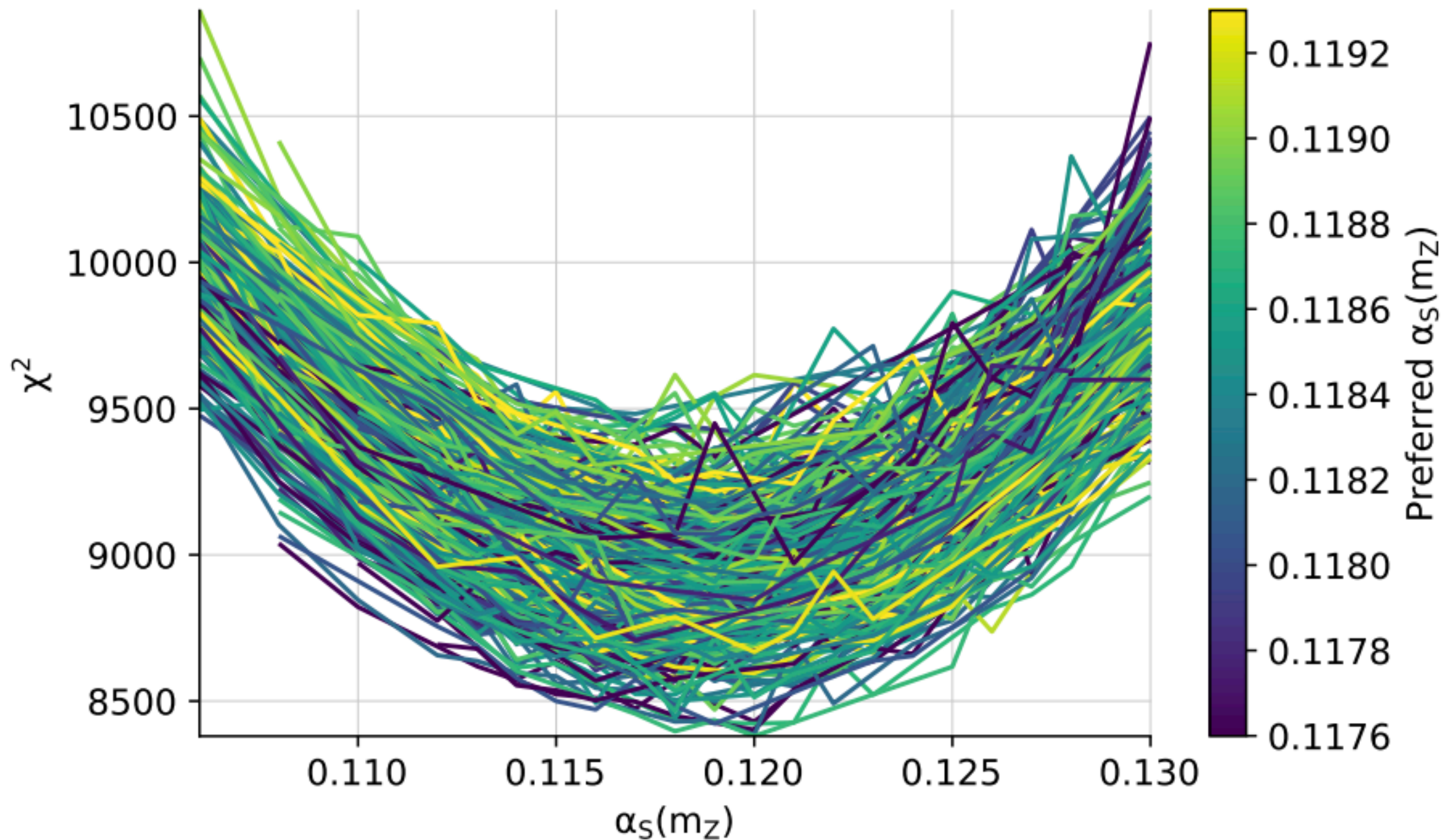
- Most used method to extract alphas from global PDF fit is repeating analysis for a range of alphas values and then **fitting a parabolic curve**
- Within a Monte Carlo fit such as NNPDF, such parabolic fit misses part of the correlations between PDF parameters, since **the underlying data is unchanged**
- Solution is to generate **correlated Monte Carlo replicas** to fully account for this effect

*c-replicas: identical settings except for alphas value*



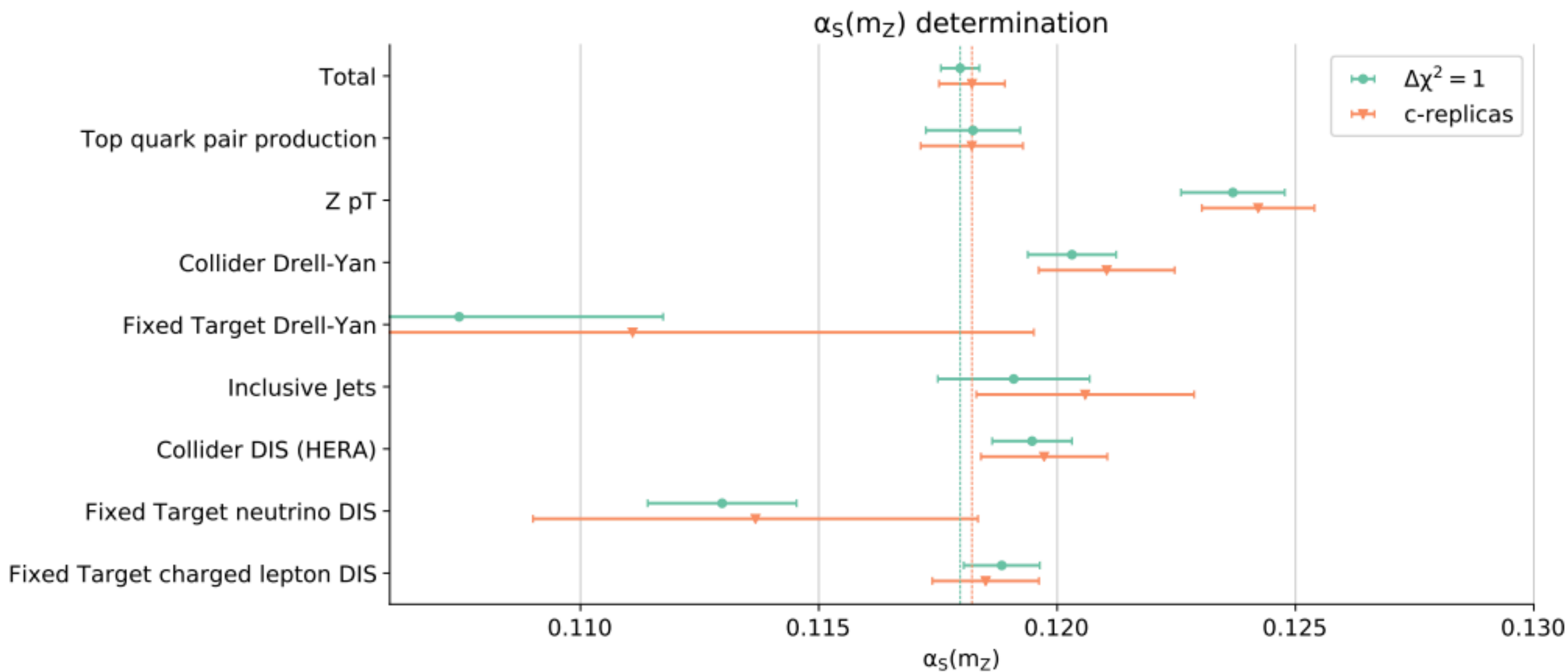
# Correlated Monte Carlo replicas

$\alpha_s(m_Z)$  distribution at NNLO



*Distribution of 400 correlated replicas fitted to the NNPDF3.1 dataset*

# Impact of correlated Monte Carlo replicas



Within a Monte Carlo determination, neglecting correlations between replicas **underestimates the PDF uncertainty** on the strong coupling by up to a factor 2

# Process sensitivity

	NLO	NNLO
Fixed-target charged lepton DIS	973	973
Fixed-target neutrino DIS	908	908
Collider DIS (HERA)	1221	1211
Fixed Target Drell-Yan	189	189
Collider Drell-Yan	378	388
Inclusive jets	164	164
$Z p_T$	120	120
Top quark pair production	26	26
<b>Total</b>	<b>3979</b>	<b>3979</b>

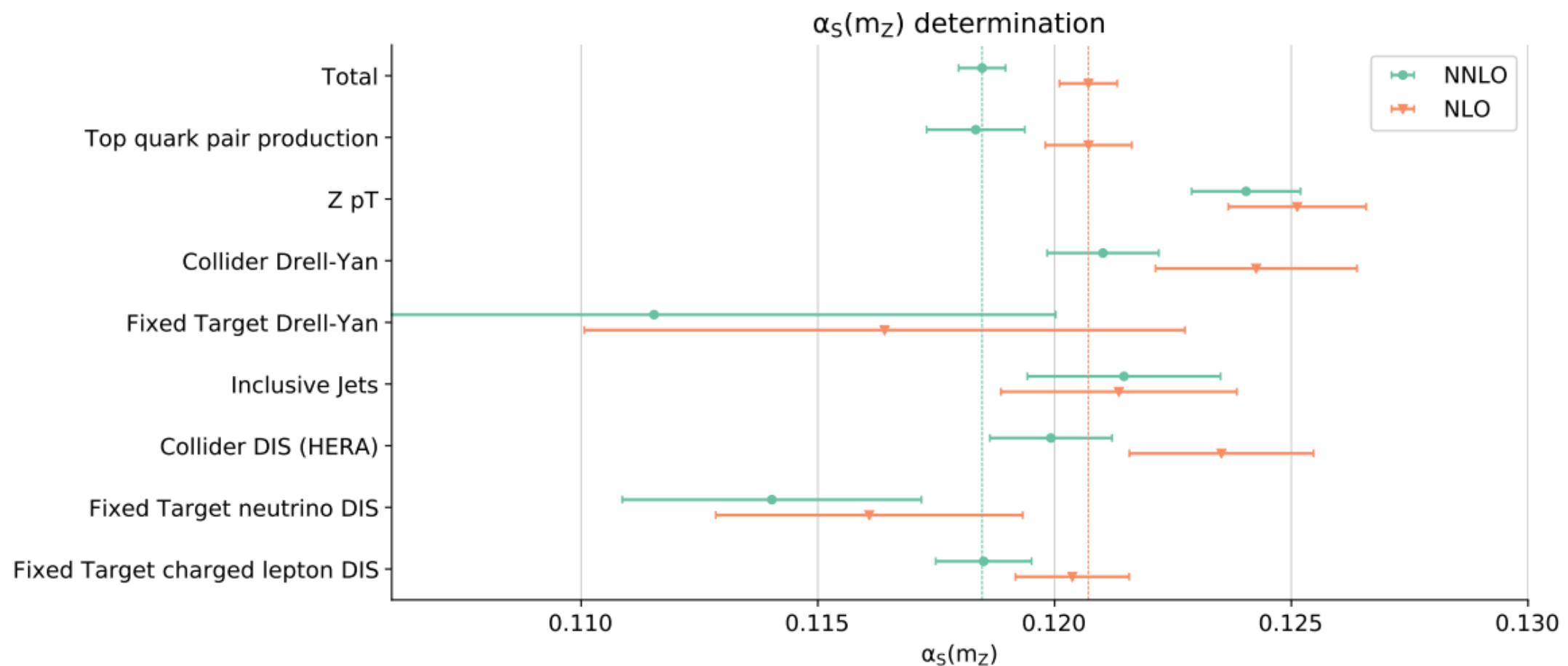
Estimate **pull from different process** by comparing alphas fits from the partial chi2s for specific datasets

Important caveats when (mis)interpreting these results as the **“preferred alphas value”** from a specific process type

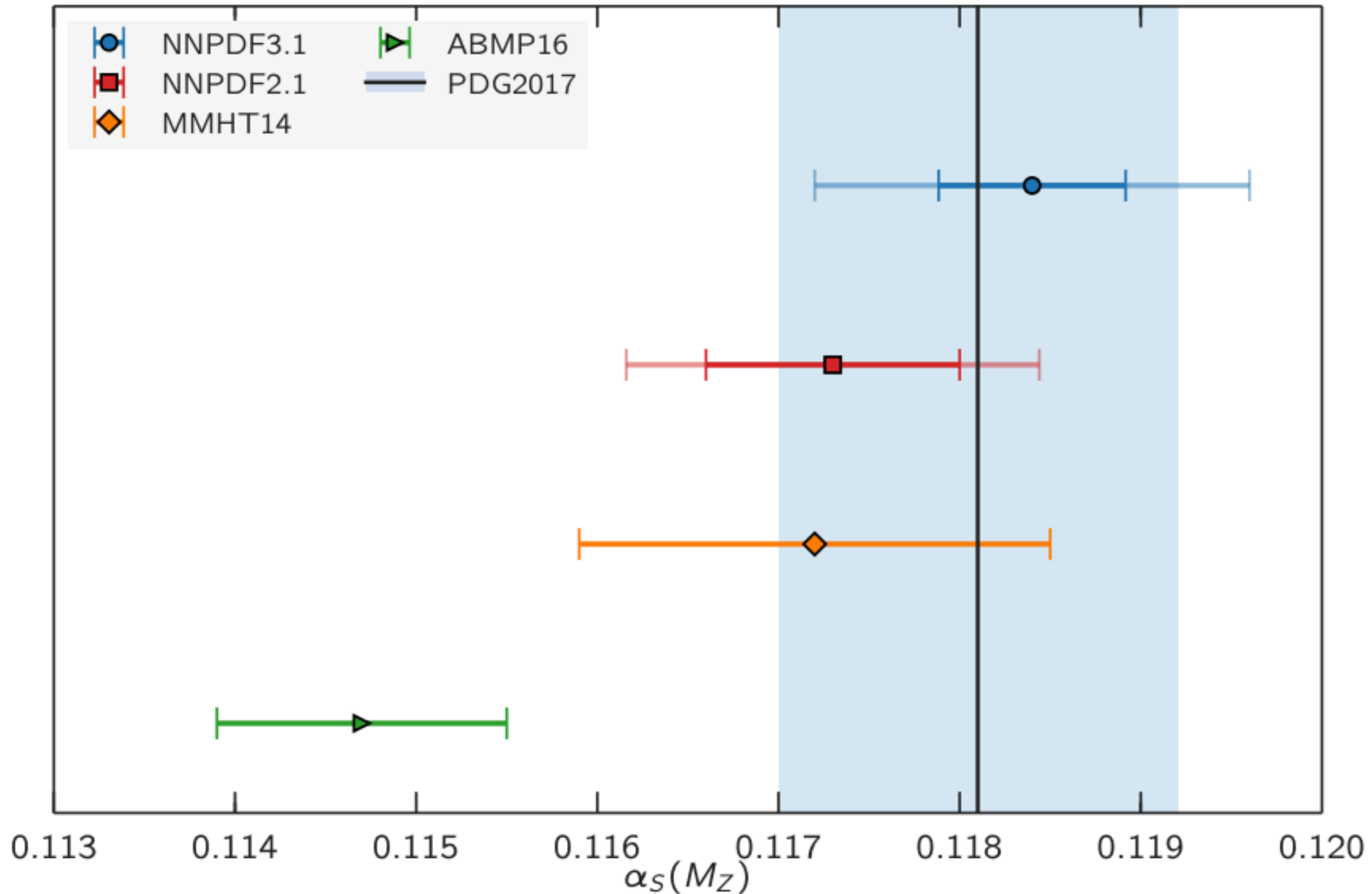
Why  $\alpha_s$  Cannot be Determined from Hadronic Processes without Simultaneously Determining the Parton Distributions

[2001.04986](#) [hep-ph]

Stefano Forte<sup>1</sup> and Zahari Kassabov<sup>2</sup>



# NNPDF3.1-based results



$$\alpha_s^{\text{NNLO}}(m_Z) = 0.1185 \pm 0.0005^{\text{exp}} \pm 0.0001^{\text{meth}} \pm 0.0011^{\text{th}} = 0.1185 \pm 0.0012 (1\%),$$

*Good agreement with PDG average and previous NNPDF determinations*

*Precision limited by MHOU, here estimated as half the (NNLO-NLO) shift*

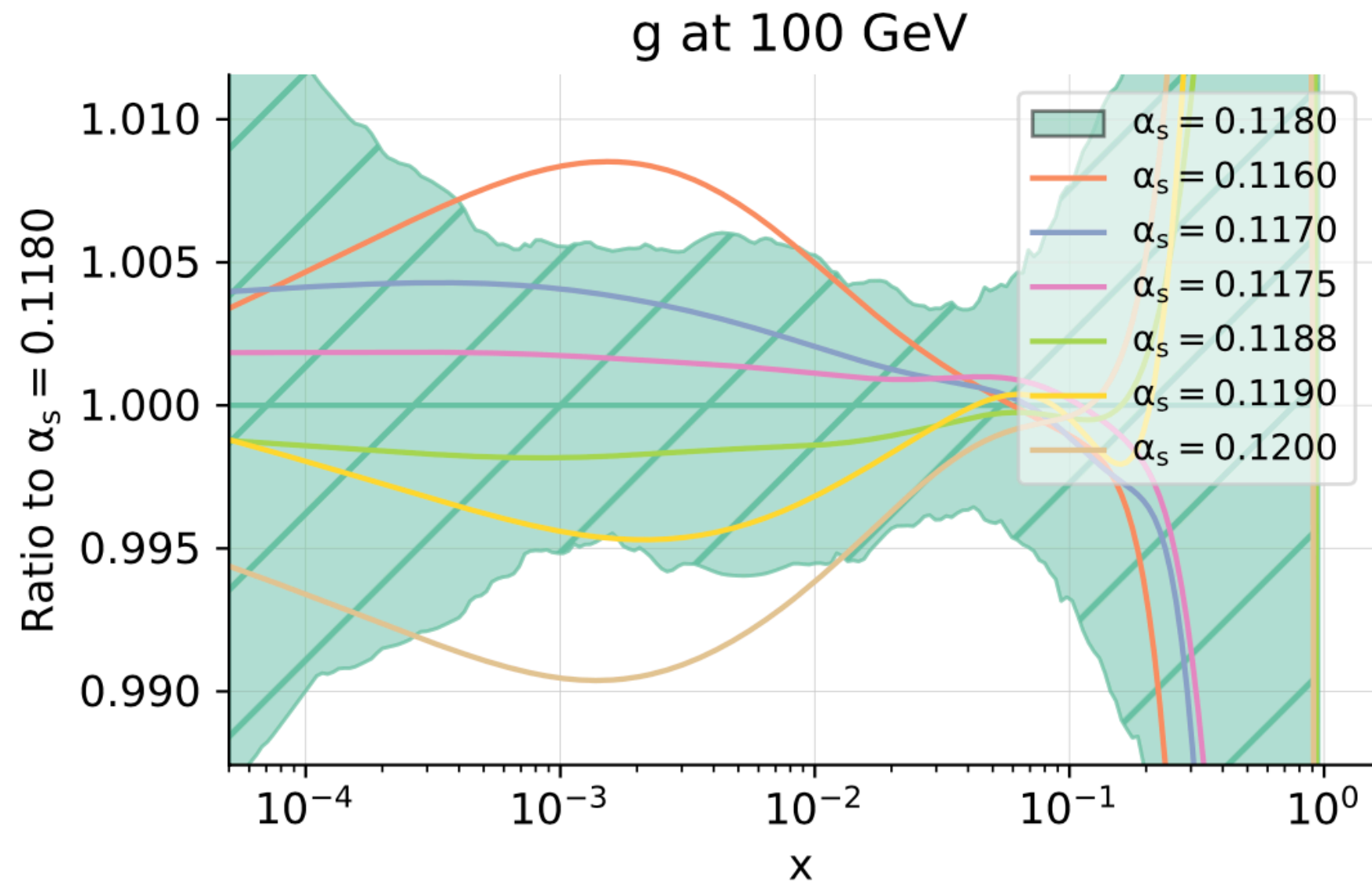


# Alphas from NNPDF4.0

*work in progress, preliminary results!*

# Settings

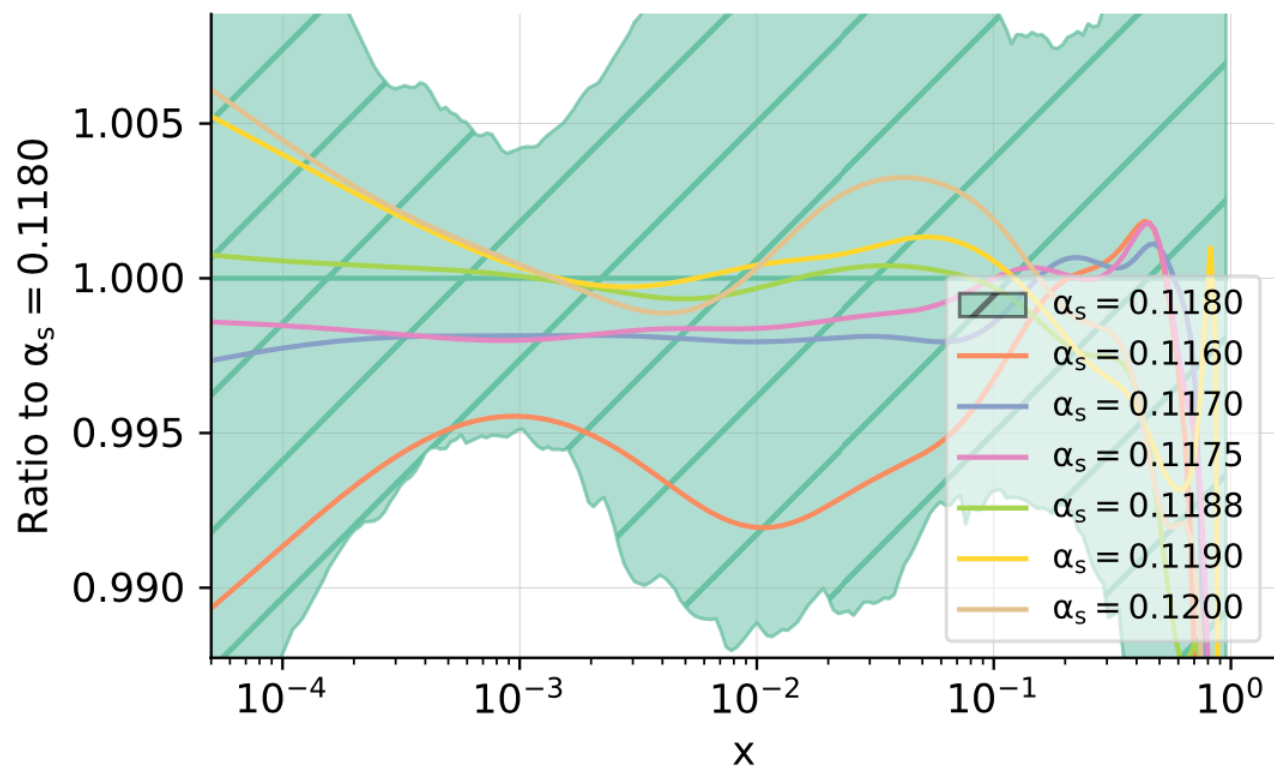
- 2 batches of correlated replicas, **200 replicas** for each alphas value
- Scan the region between **alphas=0.114** to **alphas=0.122**
- Denser coverage near the expected (PDG) minimum
- This talk: results from **parabolic fits**, results based on correlated replicas WIP



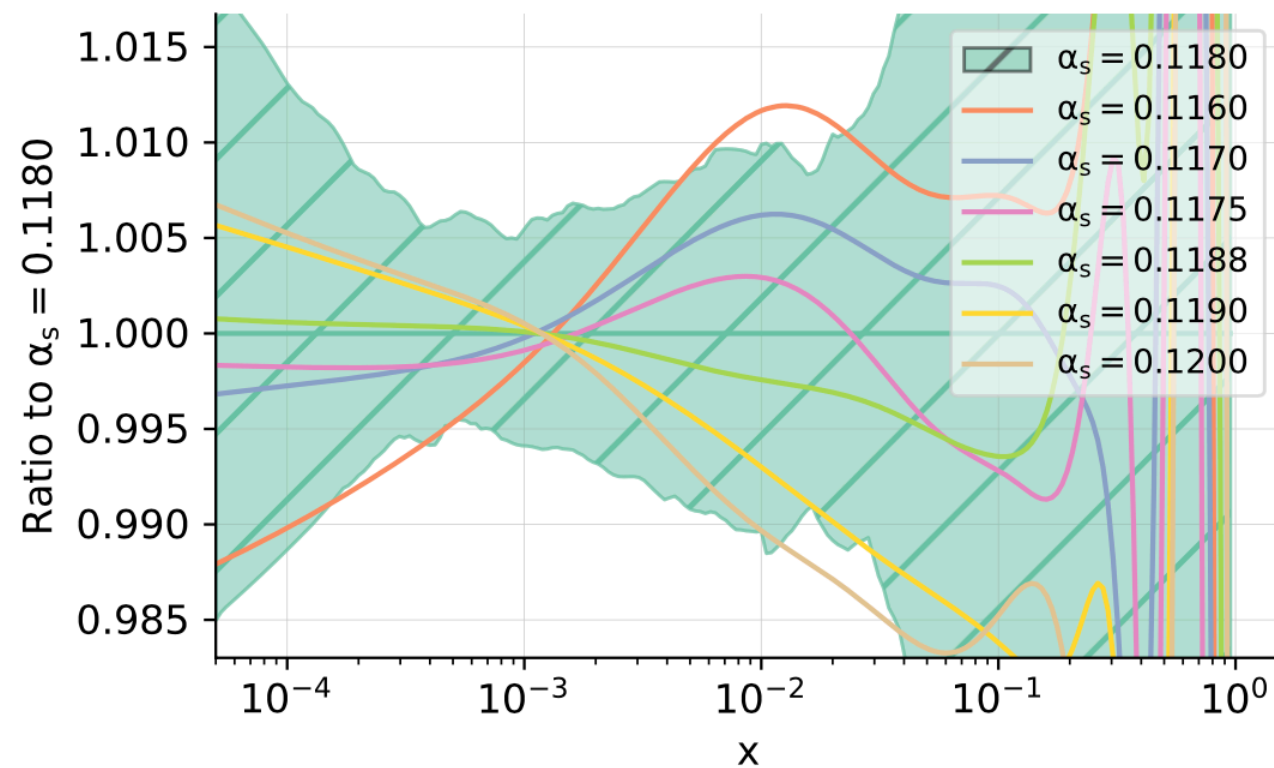
*gluon PDF is (anti-)  
correlated to alphas at  
large (small) x*

# Settings

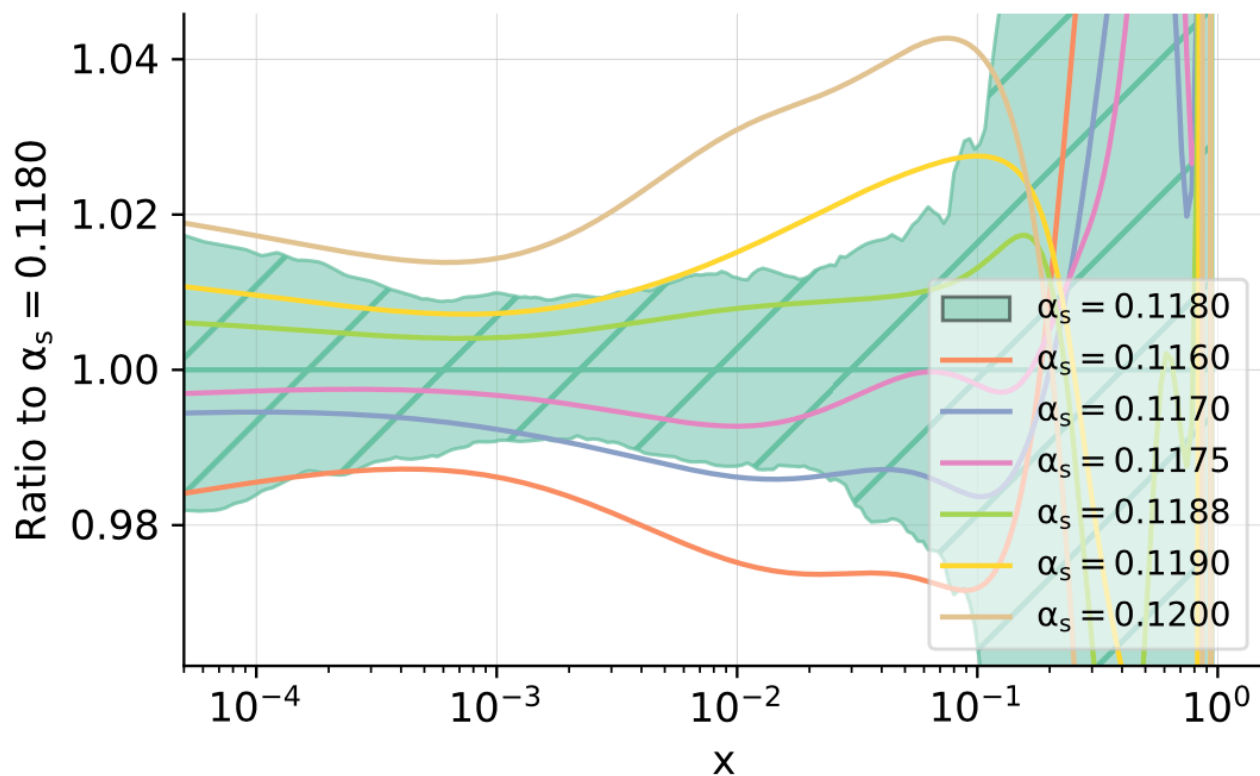
u at 100 GeV



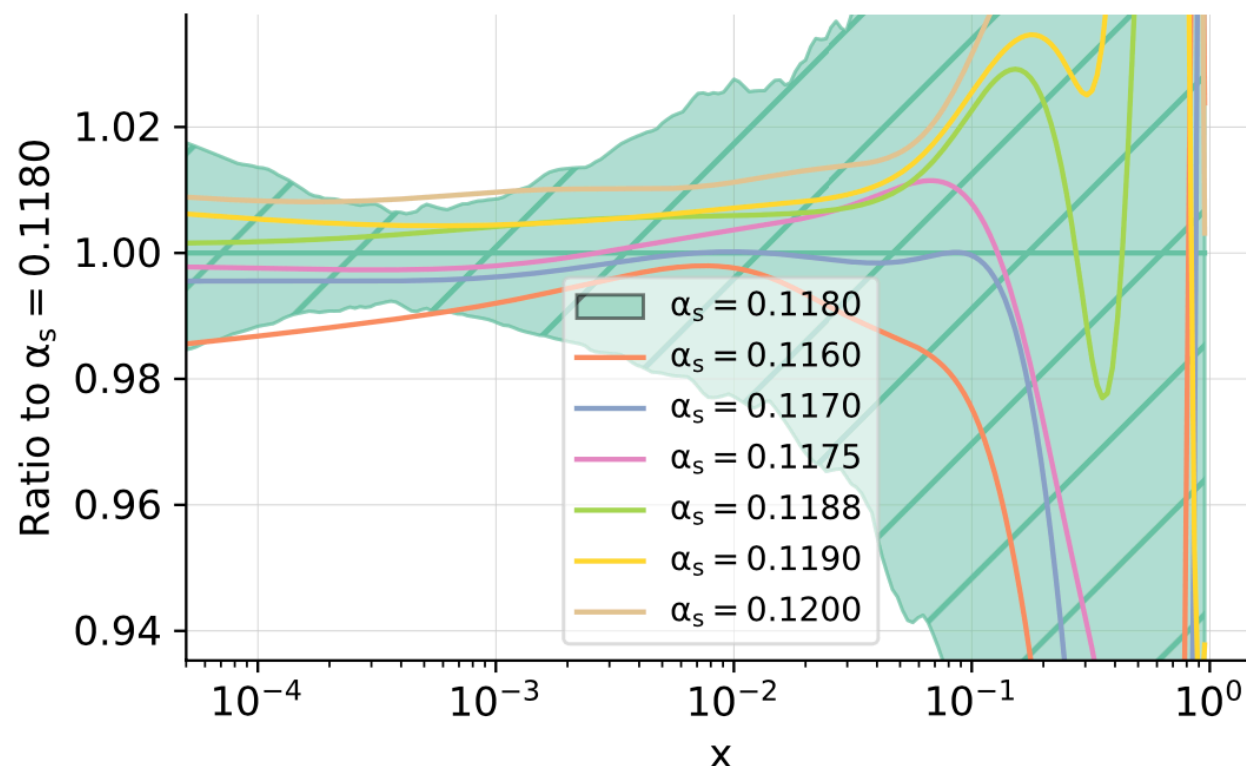
$\bar{u}$  at 100 GeV



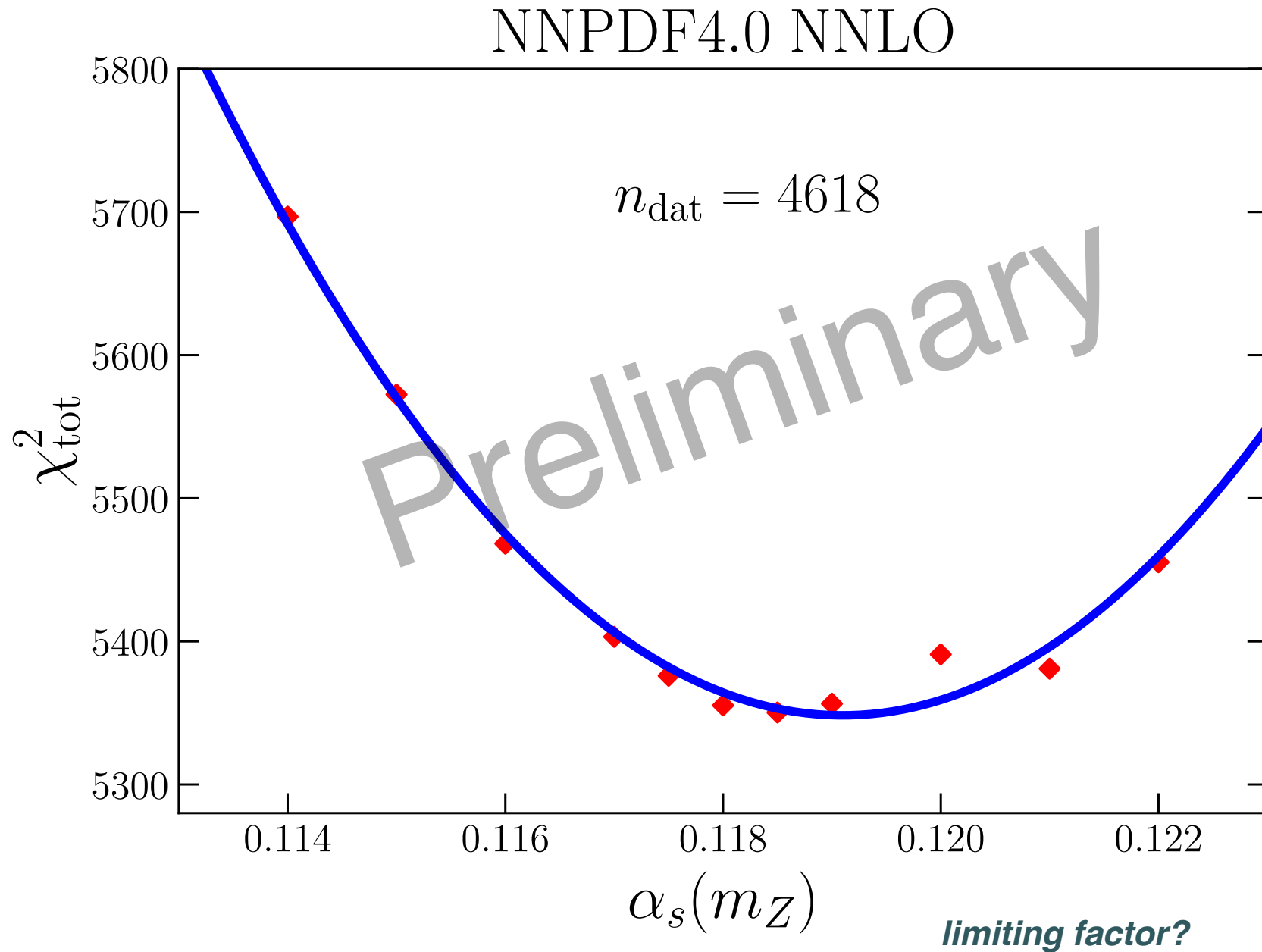
c at 100 GeV



s at 100 GeV



# Results

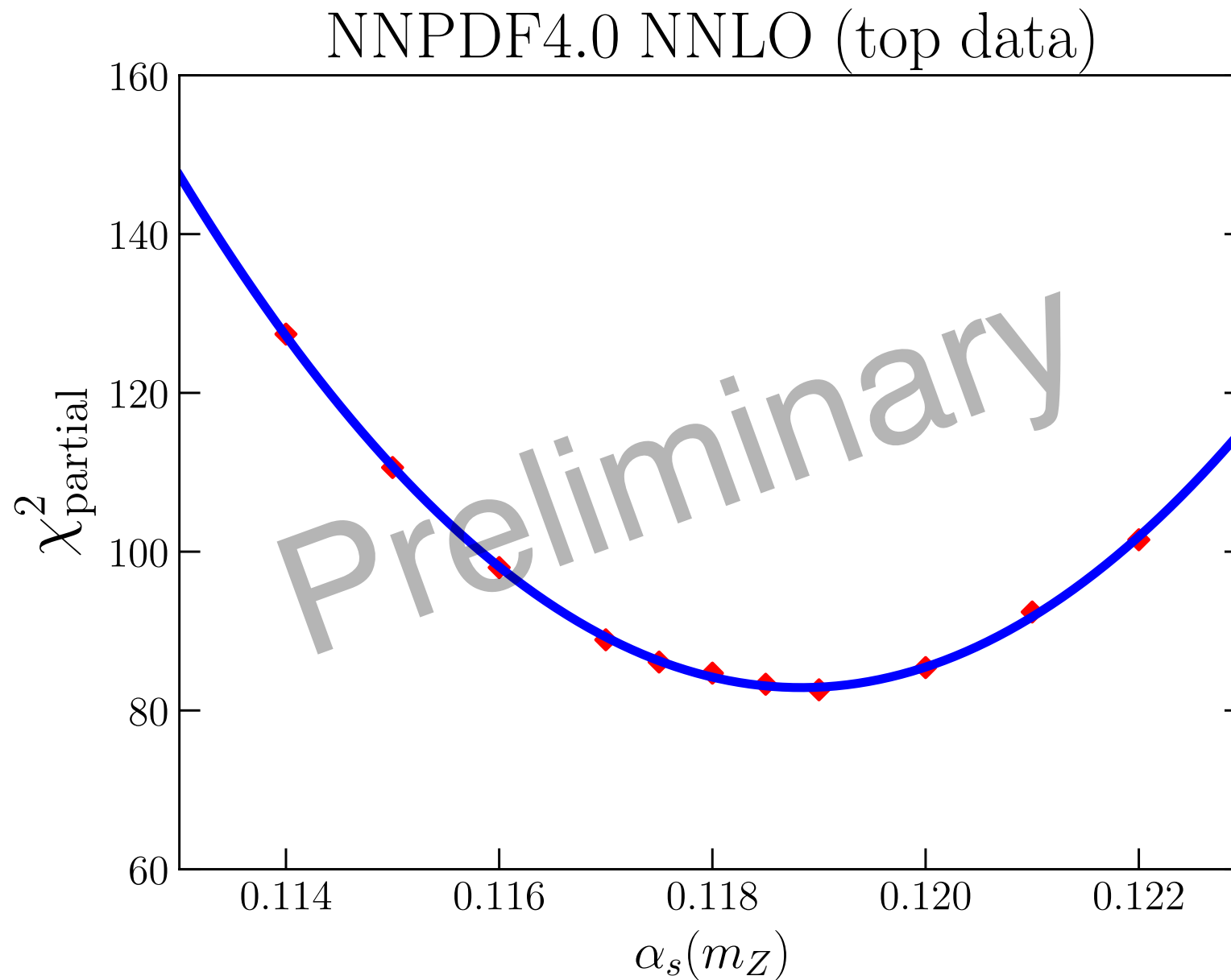


$$\alpha_s(m_Z) = 0.1191 \pm 0.0003_{\text{pdf}} \pm (?)_{\text{meth}} \pm (?)_{\text{mhou}} \quad \text{NNPDF4.0, parabolic fit}$$

$$\alpha_s(m_Z) = 0.1185 \pm 0.0005_{\text{pdf}} \pm 0.0001_{\text{meth}} \pm 0.0011_{\text{mhou}} \quad \text{NNPDF3.1 correlated replicas}$$

*Good consistency with previous determination*

# Results



$$\alpha_s(m_Z) = 0.1196 \pm 0.0007_{\text{pdf}} \pm (?)_{\text{meth}} \pm (?)_{\text{mhou}}$$

*NNPDF4.0, parabolic fit*

*Consistency with global fit results*

Note that this is the alphas value extracted from the **partial chi2 contribution from top quark data** in the global fit, this is **not** the value of the strong coupling preferred by top data



# SimuNET

A new generation of simultaneous fits to LHC data  
using deep learning

---

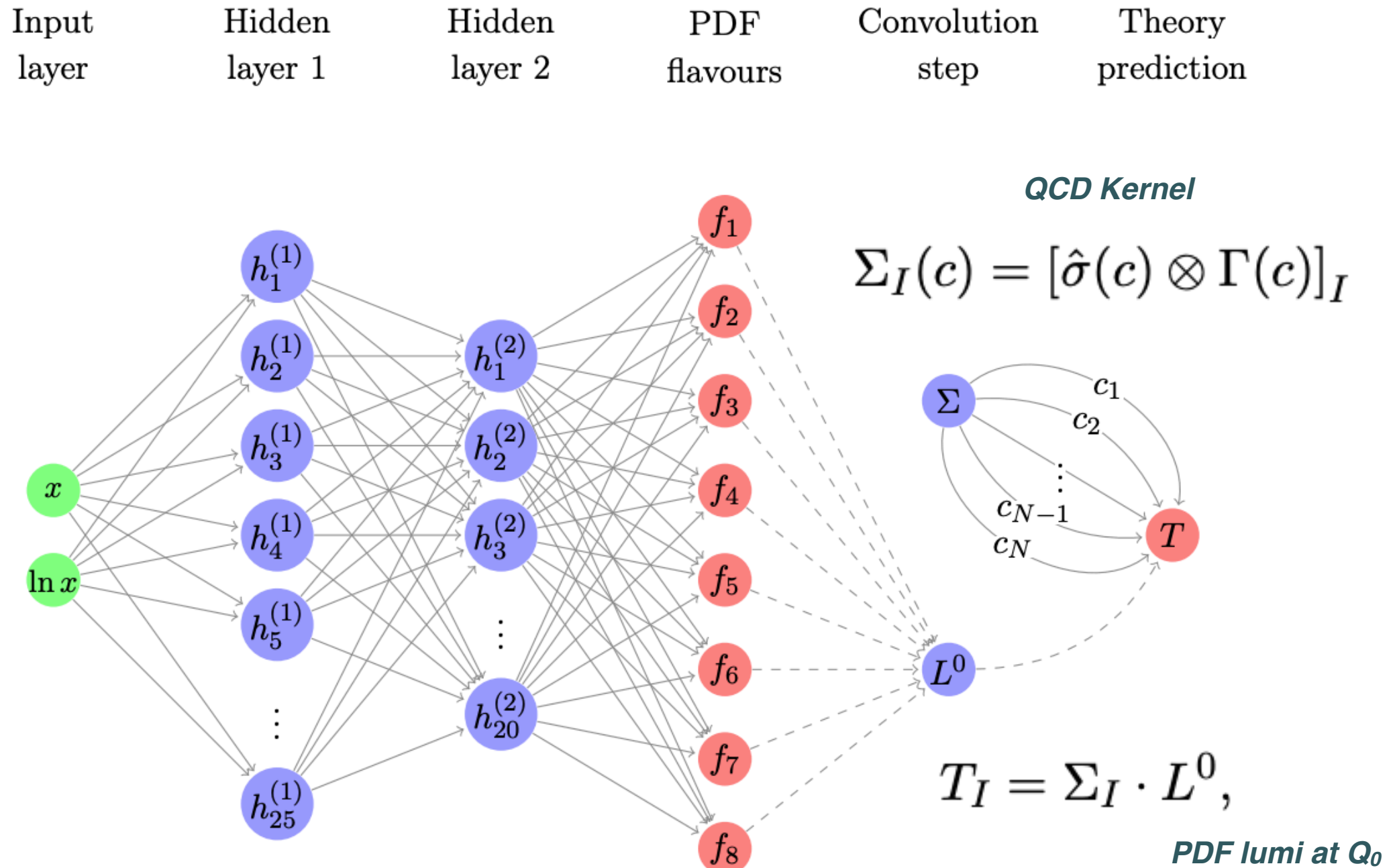
**arXiv:2201.07240**

**Shayan Iranipour, Maria Ubiali**

*DAMTP, University of Cambridge, Wilberforce Road, Cambridge, CB3 0WA, United Kingdom*

*E-mail: [s.iranipour@damtp.cam.ac.uk](mailto:s.iranipour@damtp.cam.ac.uk), [m.ubiali@damtp.cam.ac.uk](mailto:m.ubiali@damtp.cam.ac.uk)*

# The SimuNET approach

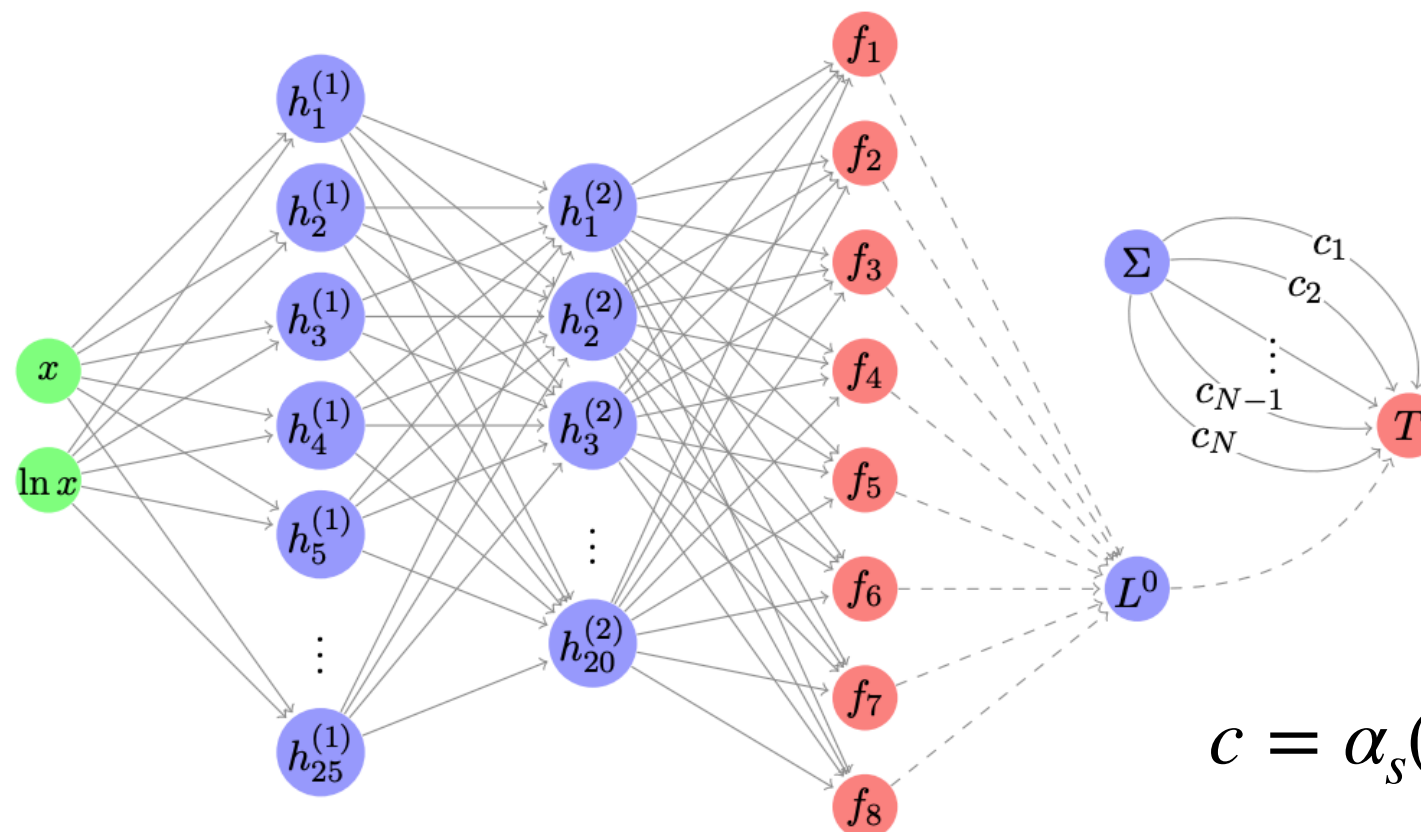


Extend the NNPDF4.0 architecture with an **extra convolutional layer** that depends on SM (or BSM) parameters, e.g. alphas,  $m_c$ , or EFT Wilson coefficients

*Simultaneous minimisation of the figure of merit wrt to PDF and SM/BSM parameters*

# The SimuNET approach

Input layer	Hidden layer 1	Hidden layer 2	PDF flavours	Convolution step	Theory prediction
----------------	-------------------	-------------------	-----------------	---------------------	----------------------



$$c = \alpha_s(m_Z) \quad c^* = 0.118$$

$$K = \hat{\sigma}_0 \otimes \Gamma_0 + (c - c^*)(\hat{\sigma}_1 \otimes \Gamma_0 + \hat{\sigma}_0 \otimes \Gamma_1) + \dots$$

$$\equiv K_0 + (c - c^*)K_1 + \dots$$

**Linear expansion** of the QCD kernels in the strong coupling

*Alternatively, element-wise interpolation in alphas of the FK table elements*

*Work in progress, stay tuned!*

# Summary and outlook

- 📍 The global NNPDF4.0 fit achieves **high accuracy** in an unprecedentedly broad kinematic range, thanks so its **extensive dataset** combined with **deep-learning optimisation models**
- 📍 It is hence suitable to be deployed for the **simultaneous determination of PDFs and (B)SM parameters**, such as the strong coupling constant
- 📍 Several complementary techniques under consideration: parabolic fits, correlated replicas, the SimuNet approach, ....
- 📍 Limiting factor in alphas extractions from global fits is **robust estimate of MHOU**, which requires estimating also the **MHOUs associated to the PDFs**

*Theory Covariance  
Matrix approach,  
NNPDF 19*

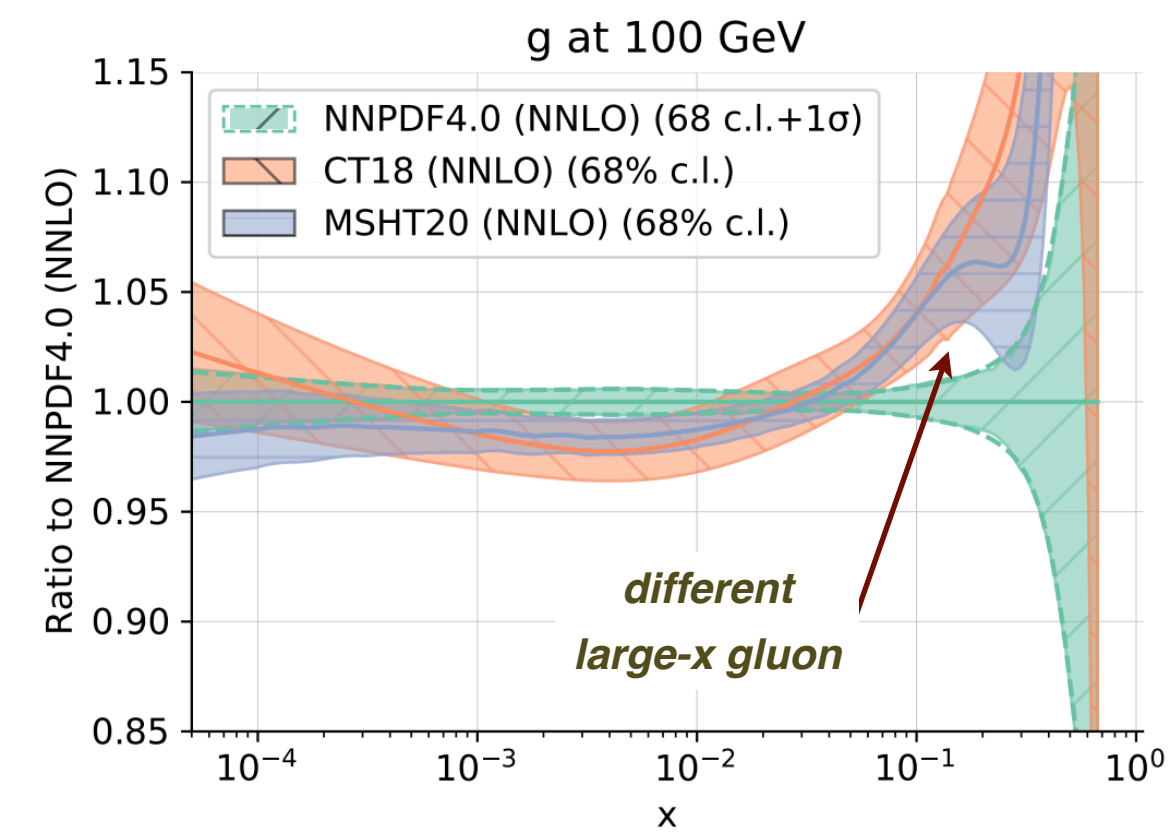
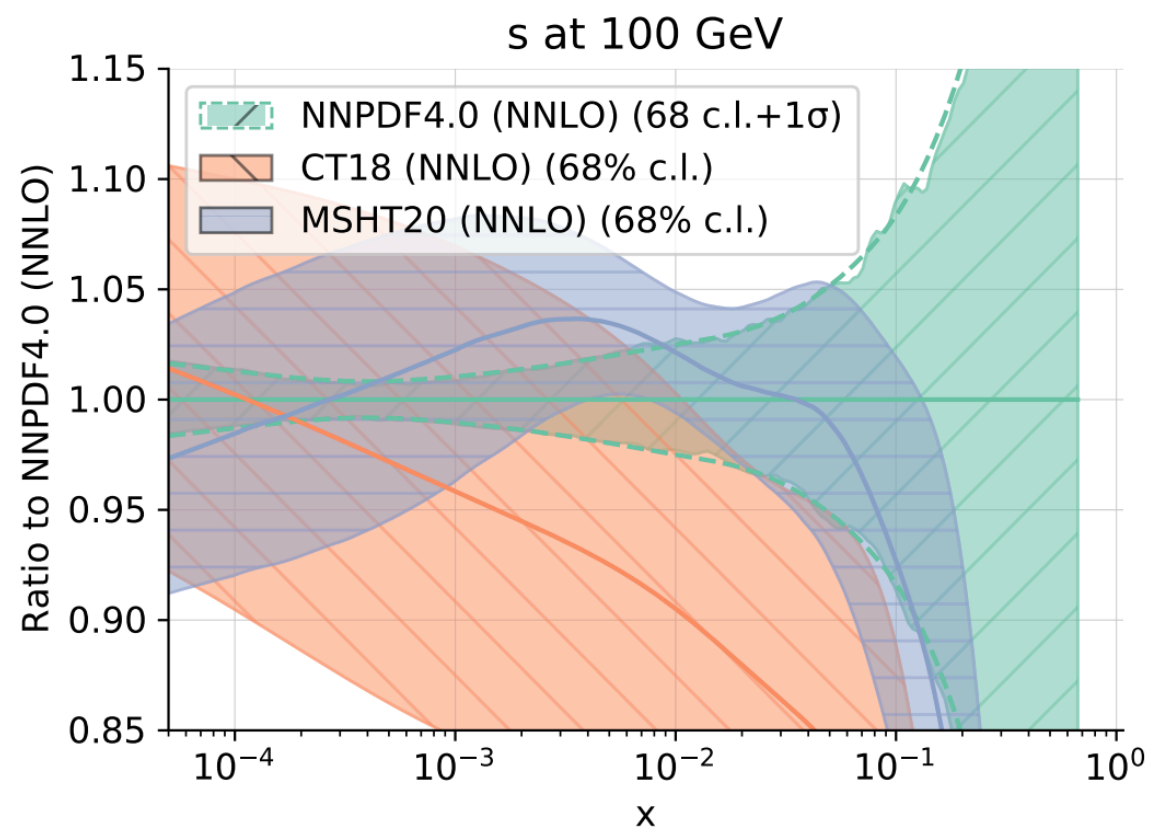
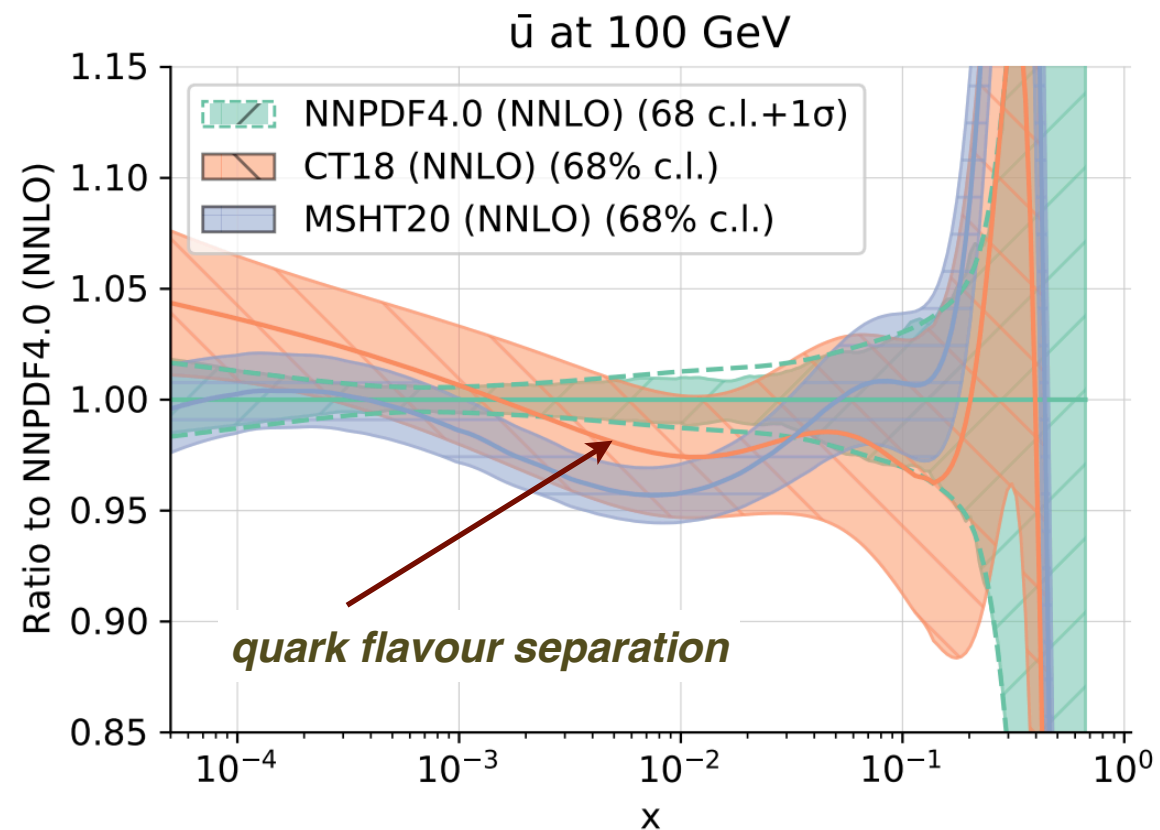
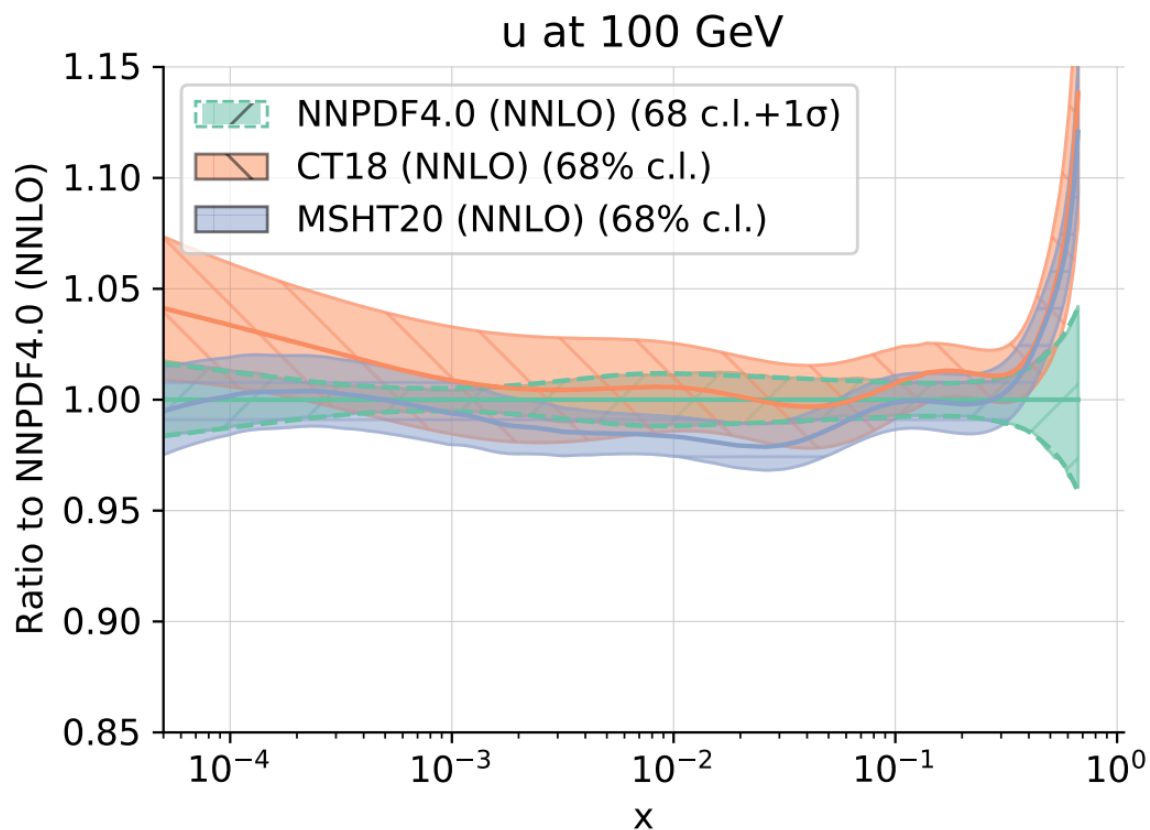
**Stay tuned!**

# Extra Material



# Comparison between global fits

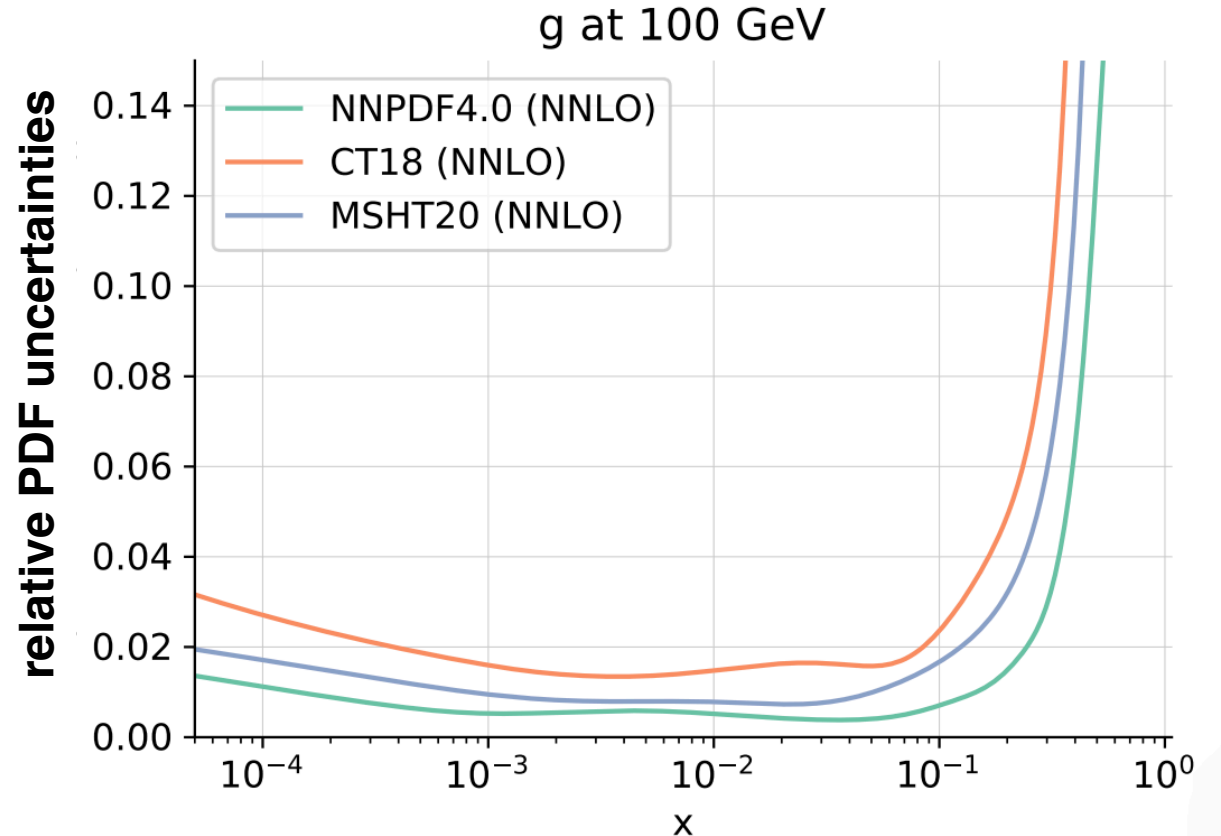
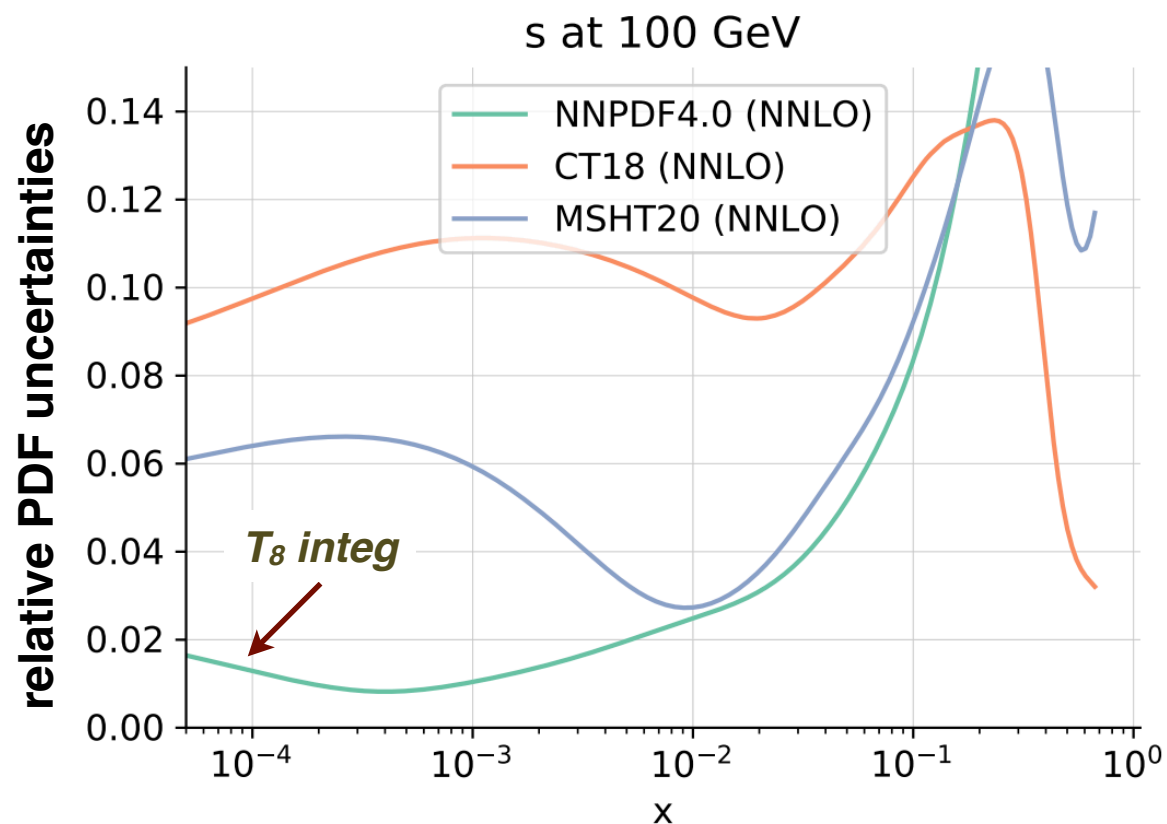
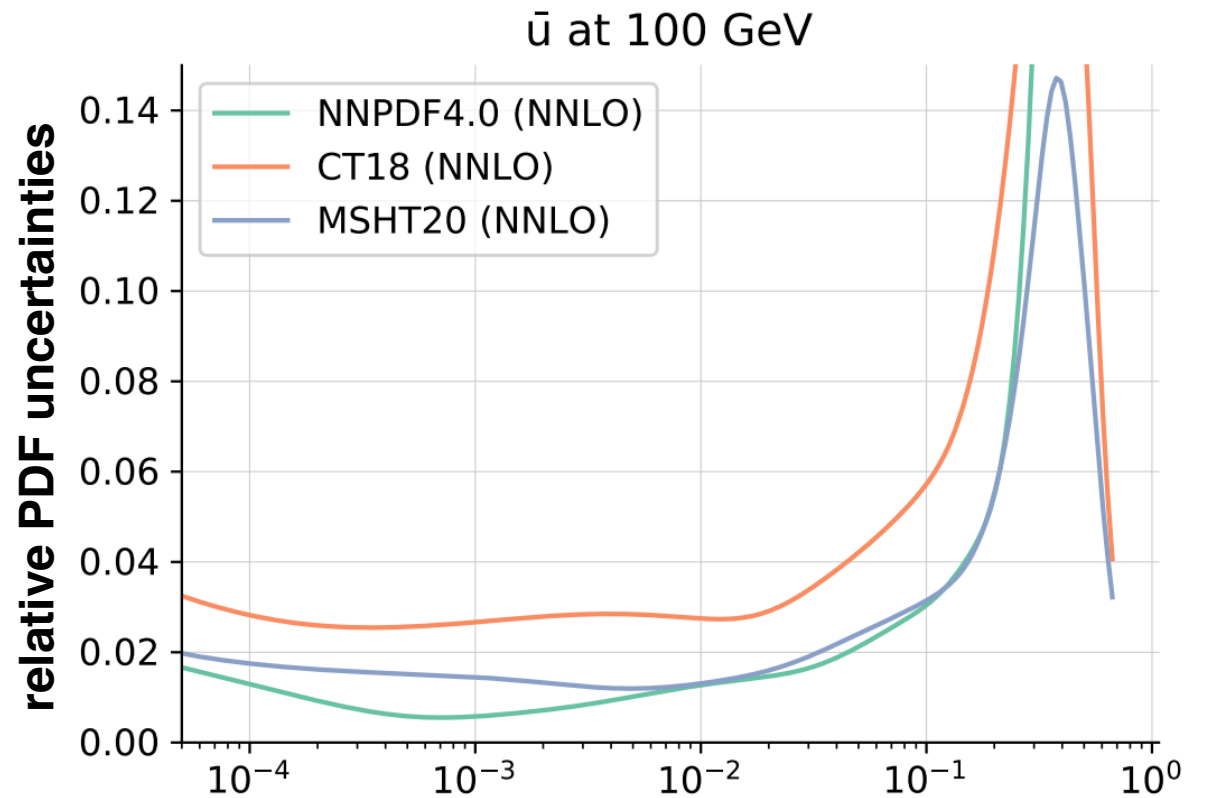
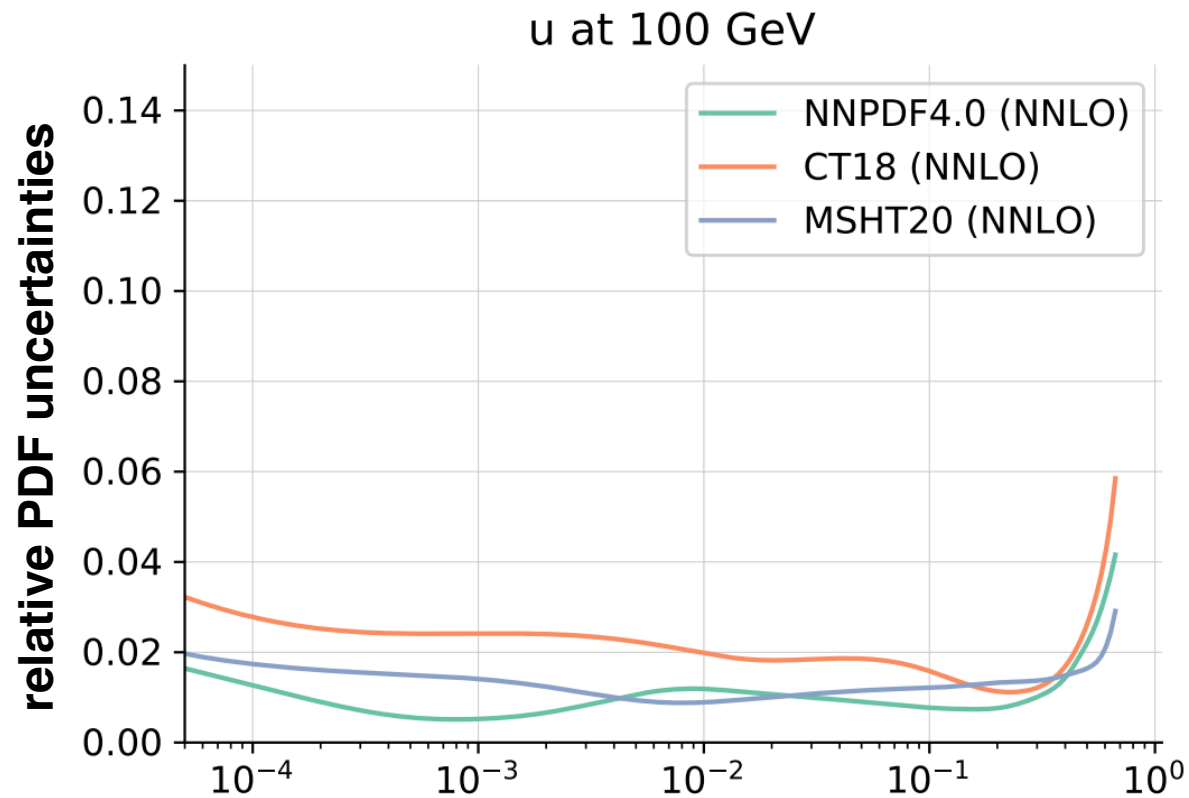
reasonable agreement with CT18, and MSHT20, different pattern of PDF uncertainties



# Comparison between global fits

different **pattern of PDF uncertainties** ...

$$\delta_{\text{PDF}}(\text{CT}) \gtrsim \delta_{\text{PDF}}(\text{MSHT}) \gtrsim \delta_{\text{PDF}}(\text{NNPDF})$$



# Comparison between global fits

... follows pattern of input datasets

$$\delta_{\text{PDF}}(\text{CT}) \gtrsim \delta_{\text{PDF}}(\text{MSHT}) \gtrsim \delta_{\text{PDF}}(\text{NNPDF})$$

Data set	Ref.	NNPDF3.1	NNPDF4.0	ABMP16	CT18	MSHT20
ATLAS $W, Z$ 7 TeV ( $\mathcal{L} = 35 \text{ pb}^{-1}$ )	[51]	✓	✓	✓	✓	✓
ATLAS $W, Z$ 7 TeV ( $\mathcal{L} = 4.6 \text{ fb}^{-1}$ )	[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	[259]	(✓)	✗	✗	(✓)	✗
ATLAS $Z$ $p_T$ 8 TeV	[63]	✓	✓	✗	✓	✓
ATLAS $W + c$ 7 TeV	[83]	✗	✓	✗	(✓)	✗
ATLAS $\sigma_{tt}^{\text{tot}}$ 7, 8 TeV	[65]	✓	✓	✓	✗	✗
ATLAS $\sigma_{tt}^{\text{tot}}$ 7, 8 TeV	[260–265]	✗	✗	✓	✗	✗
ATLAS $\sigma_{tt}^{\text{tot}}$ 13 TeV ( $\mathcal{L} = 3.2 \text{ fb}^{-1}$ )	[66]	✓	✗	✓	✗	✗
ATLAS $\sigma_{tt}^{\text{tot}}$ 13 TeV ( $\mathcal{L} = 139 \text{ fb}^{-1}$ )	[134]	✗	✓	✗	✗	✗
ATLAS $\sigma_{tt}^{\text{tot}}$ and $Z$ ratios	[266]	✗	✗	✗	✗	(✓)
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 ( $\mathcal{L} = 36 \text{ pb}^{-1}$ )	[267]	✗	✗	✗	✗	✓
CMS $Z$ 7 TeV ( $\mathcal{L} = 36 \text{ pb}^{-1}$ )	[268]	✗	✗	✗	✗	✓
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	[269]	(✓)	✗	✗	✗	✗
CMS $W$ rapidity 8 TeV	[58]	✓	✓	✓	✓	✓
CMS $W, Z$ $p_T$ 8 TeV ( $\mathcal{L} = 18.4 \text{ fb}^{-1}$ )	[270]	✗	✗	✗	(✓)	✗
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 $\sigma_{tt}^{\text{tot}}$ 5 TeV	[88]	✗	✓	✗	✗	✗
CMS $\sigma_{tt}^{\text{tot}}$ 7, 8 TeV	[146]	✓	✓	✗	✗	✗
CMS $\sigma_{tt}^{\text{tot}}$ 8 TeV	[271]	✗	✗	✗	✗	✓
CMS $\sigma_{tt}^{\text{tot}}$ 5, 7, 8, 13 TeV	[68,272–280]	✗	✗	✓	✗	✗
CMS $\sigma_{tt}^{\text{tot}}$ 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	[281,282]	✗	✗	✗	✗	(✓)

Data set	Ref.	NNPDF3.1	NNPDF4.0	ABMP16	CT18	MSHT20
LHCb $Z$ 7 TeV ( $\mathcal{L} = 940 \text{ pb}^{-1}$ )	[59]	✓	✓	✗	✗	✓
LHCb $Z \rightarrow ee$ 8 TeV ( $\mathcal{L} = 2 \text{ fb}^{-1}$ )	[61]	✓	✓	✓	✓	✓
LHCb $W$ 7 TeV ( $\mathcal{L} = 37 \text{ pb}^{-1}$ )	[283]	✗	✗	✗	✗	✓
LHCb $W, Z \rightarrow \mu$ 7 TeV	[60]	✓	✓	✓	✓	✓
LHCb $W, Z \rightarrow \mu$ 8 TeV	[62]	✓	✓	✓	✓	✓
LHCb $W \rightarrow e$ 8 TeV	[80]	✗	(✓)	✗	✗	✗
LHCb $Z \rightarrow \mu\mu, ee$ 13 TeV	[82]	✗	✓	✗	✗	✗

✓ in baseline dataset  
 ✗ not considered  
 (✓) impact assessed but excluded from baseline