NNPDF4.0

Neural networks techniques for parton distribution functions evaluation

Andrea Barontini on behalf of the NNPDF collaboration

Alpaca: modern algorithms in machine learning and data analysis: from medical physics to research with accelerators and in underground laboratories

20/11/2023

Based on: hep-ph:1907.05075,2109.02653,2208.08372,1906.10698,1509.00209

Machine Learning • PDFs • QCD

Outline

- The Physics
- The NNPDF framework
- Results and outlook

Outline

The Physics

The NNPDF framework

Results and outlook

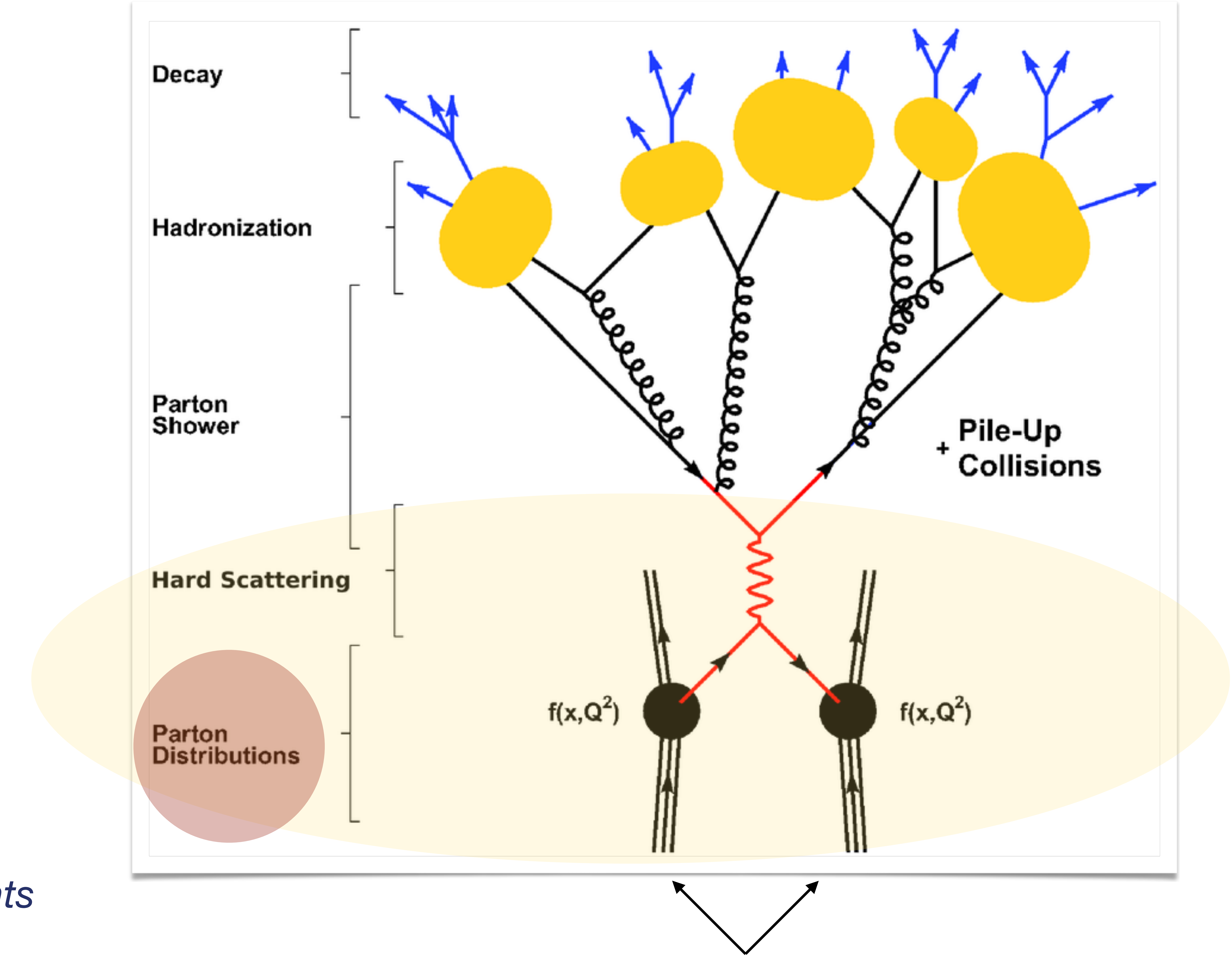
Describing a collision

The theoretical description of a **collision** involves several **QCD** (Quantum ChromoDynamics) ingredients

We are going to focus on

And, in particular, on Parton Distribution Functions **(PDFs)**

Describe the hadronic initial state in terms of their *partonic components*



Initial state = hadrons (protons, neutrons ,...)

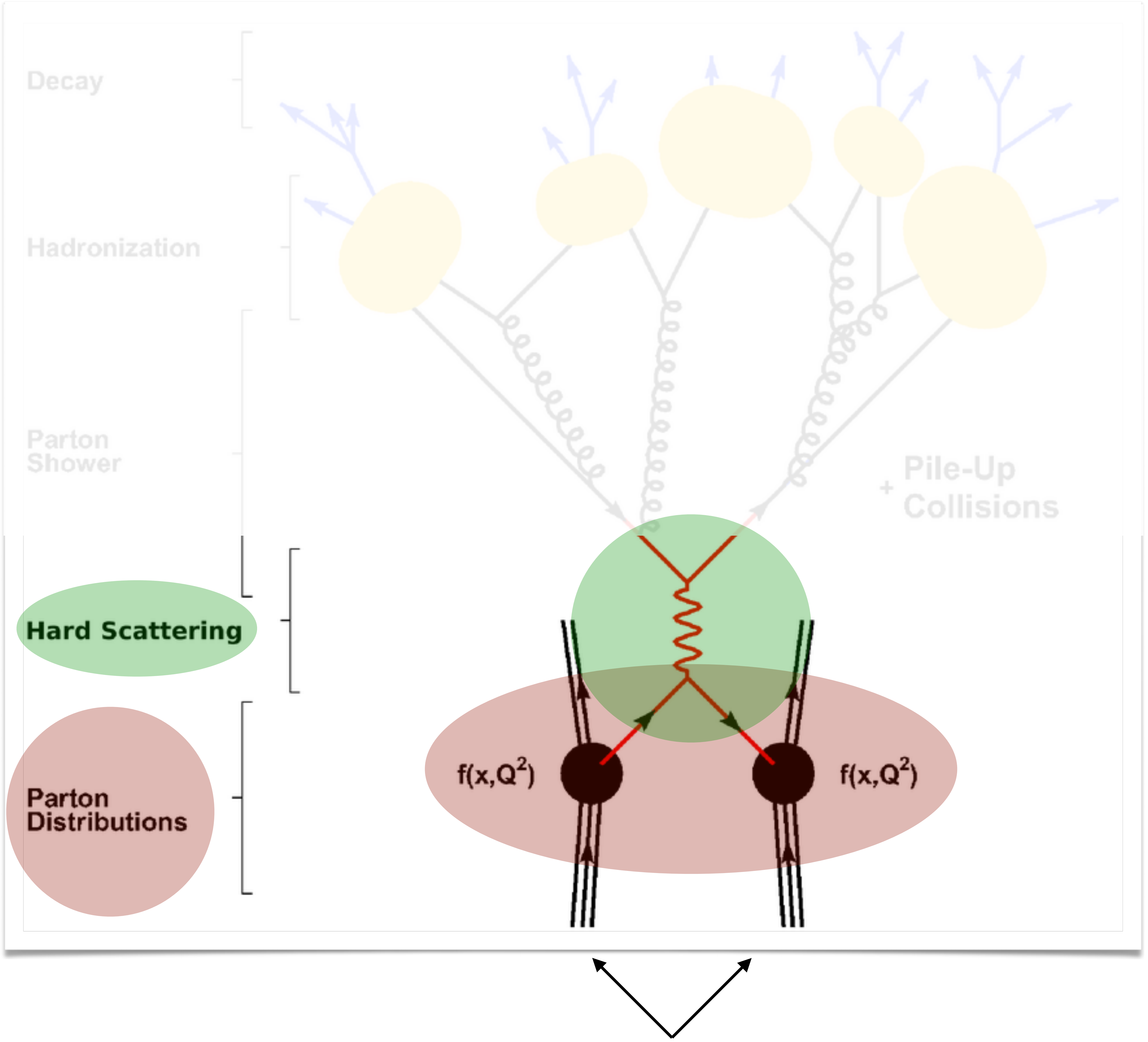
Factorization: divide and conquer

Thanks to **Factorization theorem**

PDFs

$$\sigma(x,Q^2) = \hat{\sigma}_{ij} \otimes f_i \otimes f_j = \int dz_1 dz_2 \hat{\sigma}(z_1,z_2,Q^2) f_i\left(\frac{x}{z_1},Q^2\right) f_j\left(\frac{x}{z_2},Q^2\right)$$

Partonic (hard) cross sections



- $\sigma(x,Q^2)$ is our **observable**
- Q^2 is the energy scale of the process
- $\hat{\sigma}(z_1,z_2,Q^2)$ can be computed in **perturbation theory**
- $f_{i/j}(x,Q^2)$ **cannot** be computed in perturbation theory

  (and they are **universal**)

BUT WHY??

Initial state = hadrons (protons, neutrons ,...)

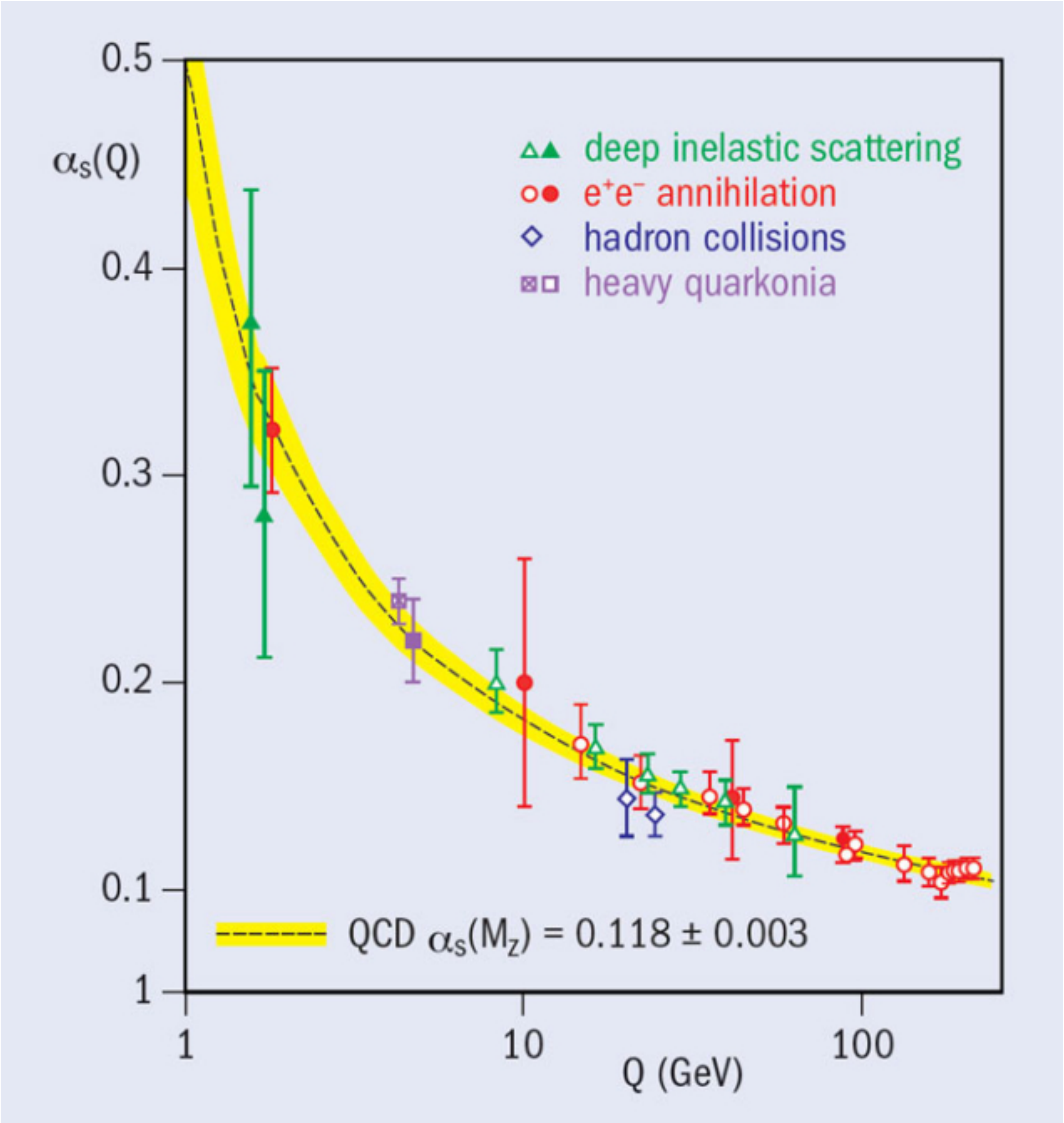
Asymptotic freedom

In **QCD** we are usually expand quantities in terms of the **strong coupling** $\alpha_s(Q^2)$ → (Notable counterexample is lattice QCD)

$$\hat{\sigma}^{NLO}(z_1, z_2, Q^2) = \hat{\sigma}^{(0)}(z_1, z_2, Q^2) + \alpha_s(Q^2)\hat{\sigma}^{(1)}(z_1, z_2, Q^2) + \mathcal{O}(\alpha_s^2)$$

$(NLO =$ Next-to-leading order)

But $\alpha_s(Q^2)$ is a decreasing function of the energy scale



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perturbative QCD
(pQCD)
from ~ 1 GeV

Partonic cross sections

Non perturbative QCD
below ~ 1 GeV

PDFs
(Mass of the proton ~ 0.938 GeV)

How can we extract them?

PDF extraction

Let’s look at the **Factorization theorem** from another prospective

unknown

$$\sigma(x, Q^2) = \hat{\sigma}_{ij} \otimes f_i \otimes f_j = \int dz_1 dz_2 \hat{\sigma}(z_1, z_2, Q^2) f_i\left(\frac{x}{z_1}, Q^2\right) f_j\left(\frac{x}{z_2}, Q^2\right)$$

Inverse problem

Measured in experiments

computed in perturbation theory

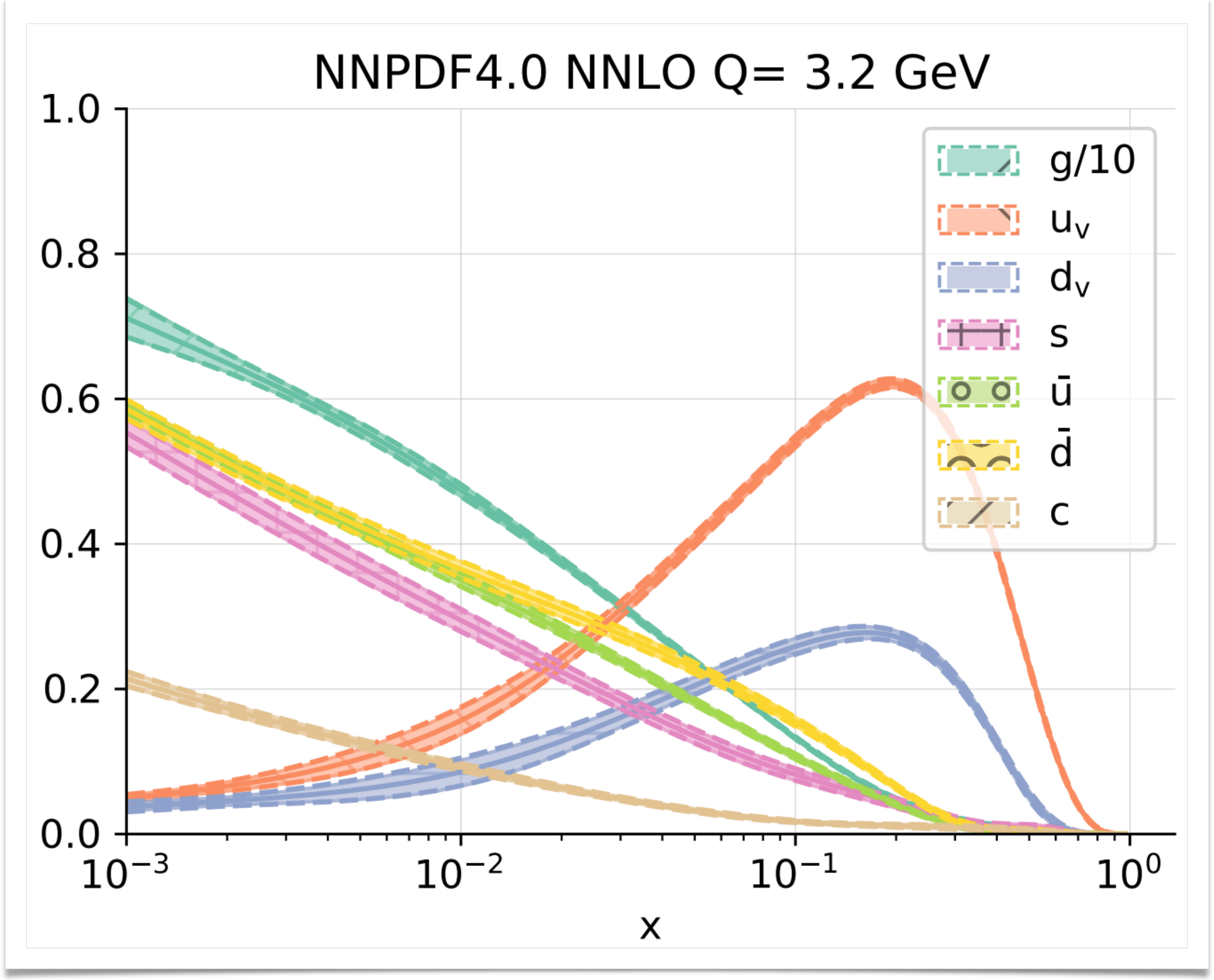
Also, **DGLAP equations** allow us to compute the PDFs at all scale Q^2, once known at a certain scale Q_0^2

$$f_i(Q^2) = E_{ij}(Q^2 \leftarrow Q_0^2) f_j(Q_0^2)$$

PDFs are then just a set of **unknown functions**

$$f_i : [0,1] -> \mathbb{R}$$

$f_i(x) \sim$ probability of extracting parton i from the proton with momentum fraction x



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Inverse problems

Number of datapoints is **finite**[1] while function space is **infinite-dimensional**

Fitting PDFs is always an **under-determined** problem

ASSUMPTIONS

Fixed parametrization

- Reduce the number of parameters
- Assumptions = choice of the parameters to be fitted

Neural Network

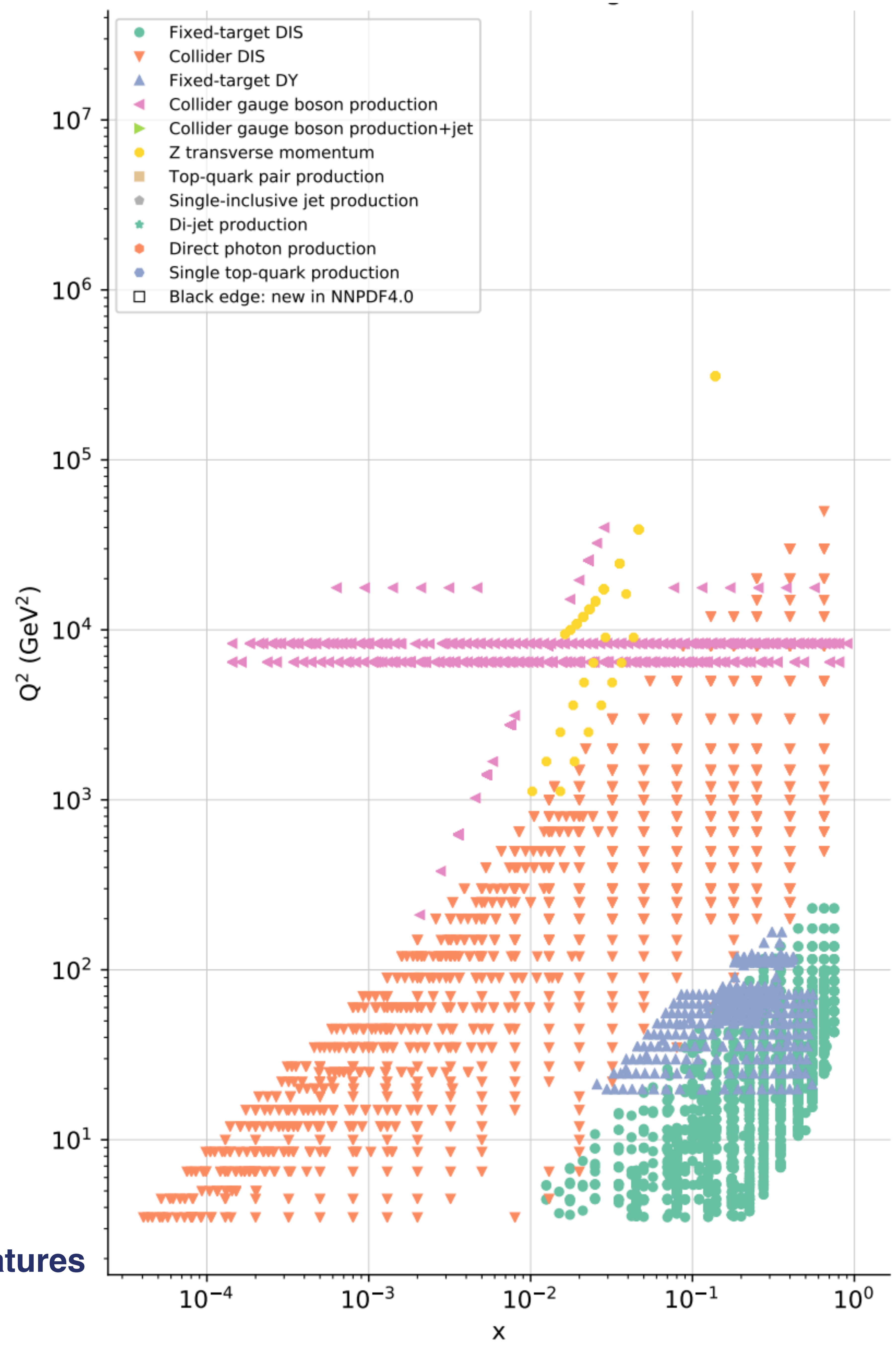
NNPDF choice

- Applies a **regularization**
- Assumptions = encoded in the network (and not only…)

Which is better?

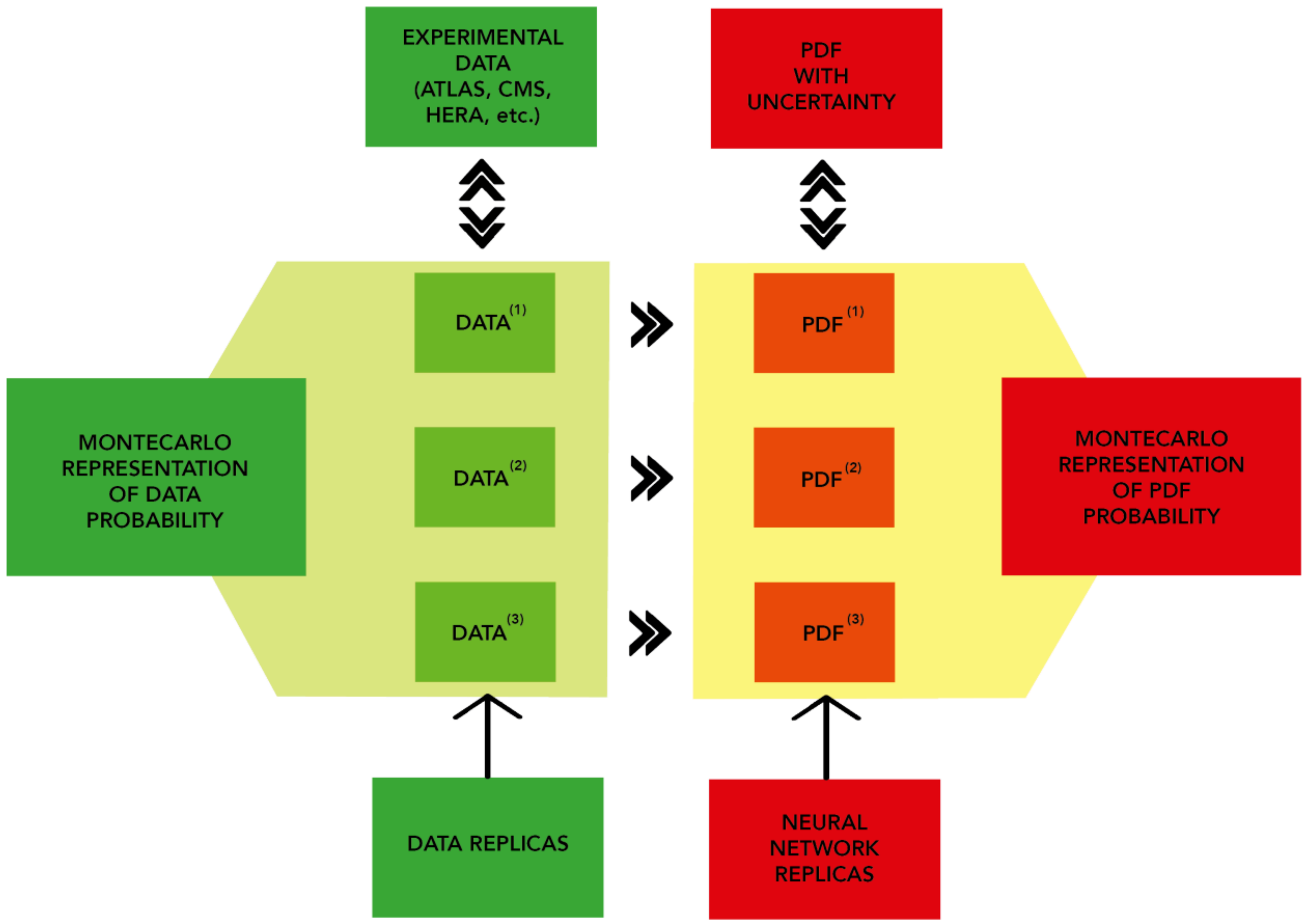
- Needs theoretical insight on PDFs shape
- Can be biased by human prejudice

- Needs theoretical insight on more **abstract features**
- Human prejudice effect can be minimized



[1] ~4600 datapoints in NNPDF4.0

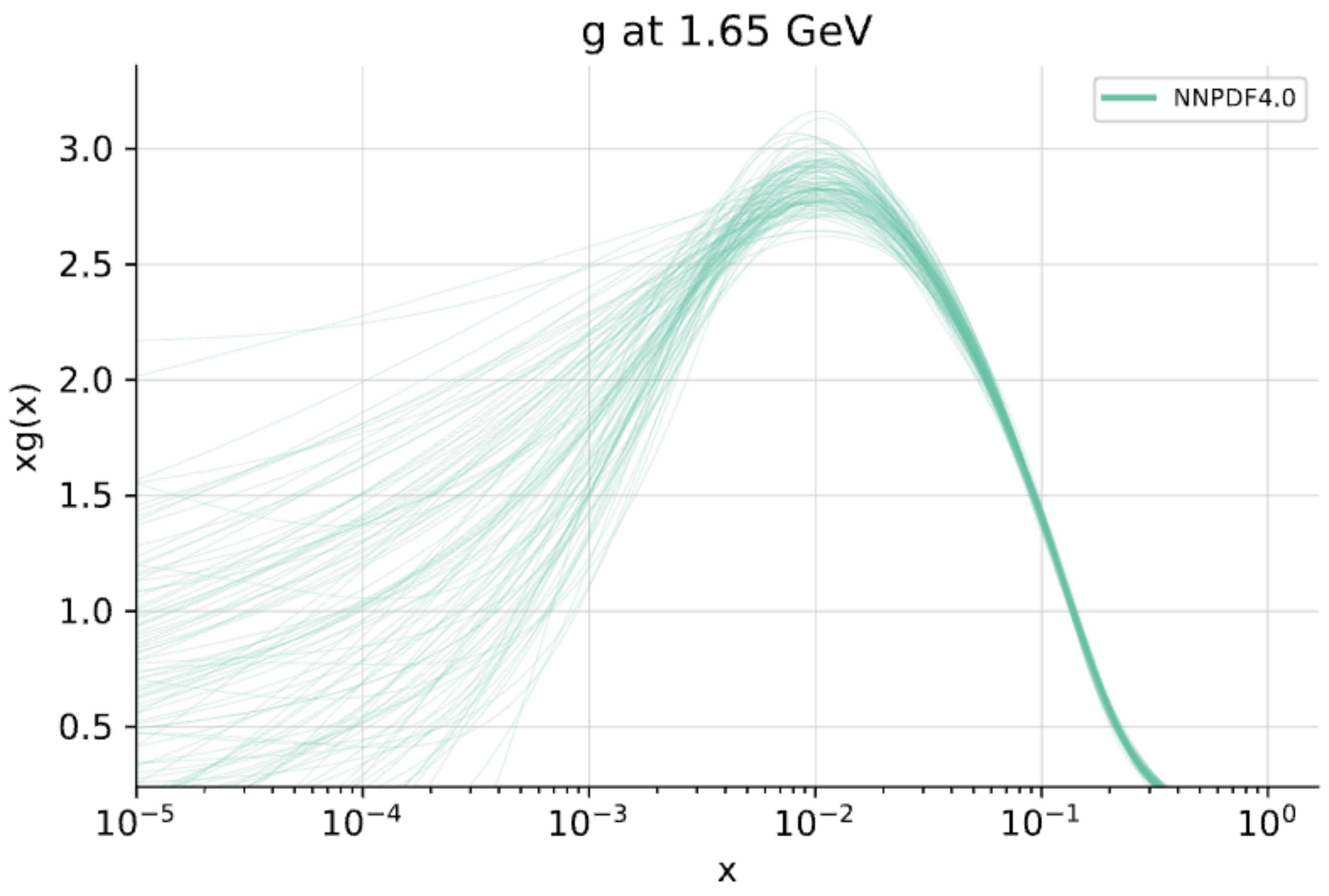
Propagating uncertainties: data to PDFs

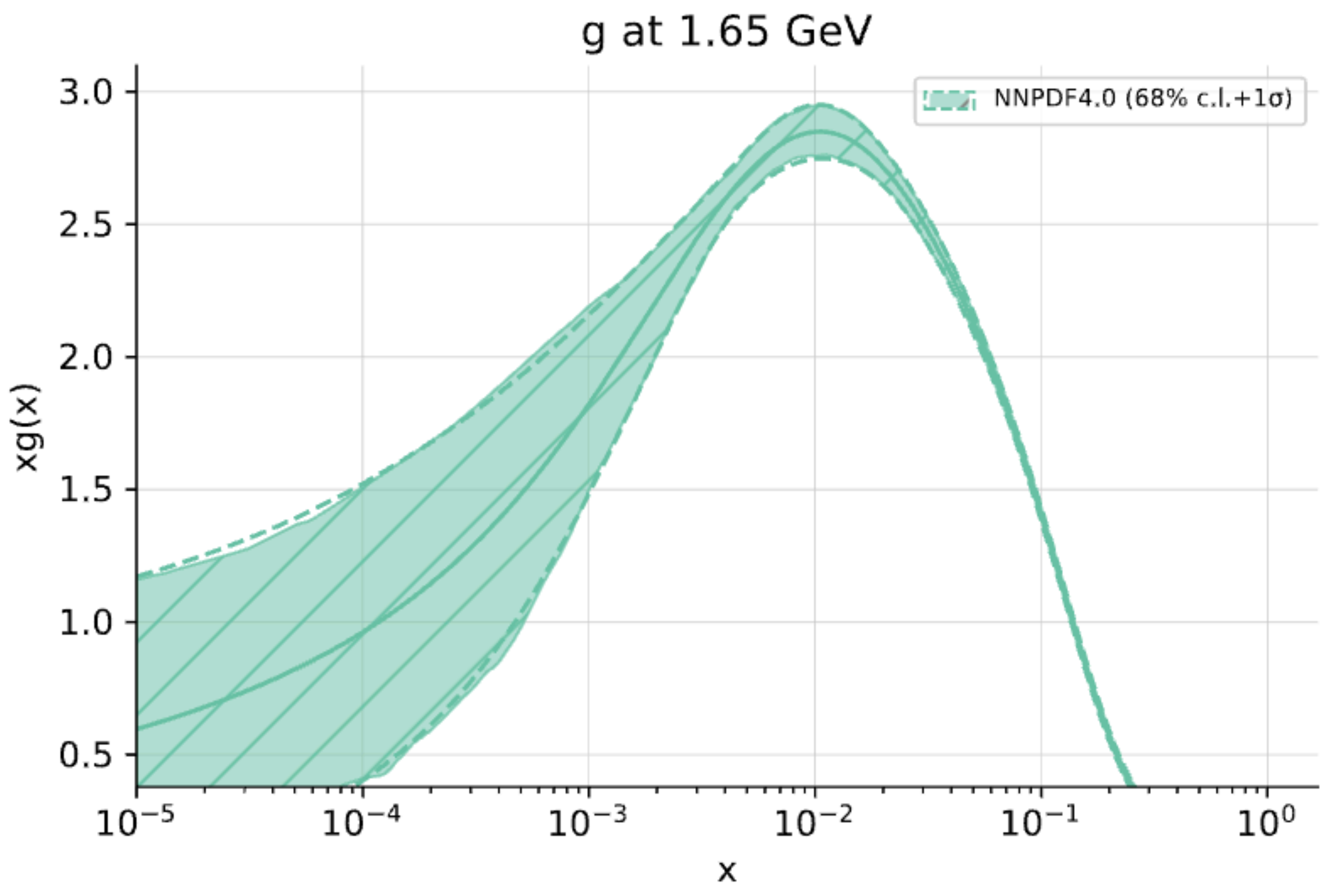


NNPDF adopt a **Monte Carlo** approach

1. Start with the original dataset D and its **covariance matrix** C
2. Generate N_{rep} **pseudodata** D_i according to C
3. Fit a **Neural Network NN$_i$** to each of the pseudodata replica
4. Deliver the full set of replicas

PDFs uncertainties are given by the distribution of the Monte Carlo set





NB: Another possibility is the Hessian approach. The two methods can be converted one in the other (hep-ph:1505.06736)

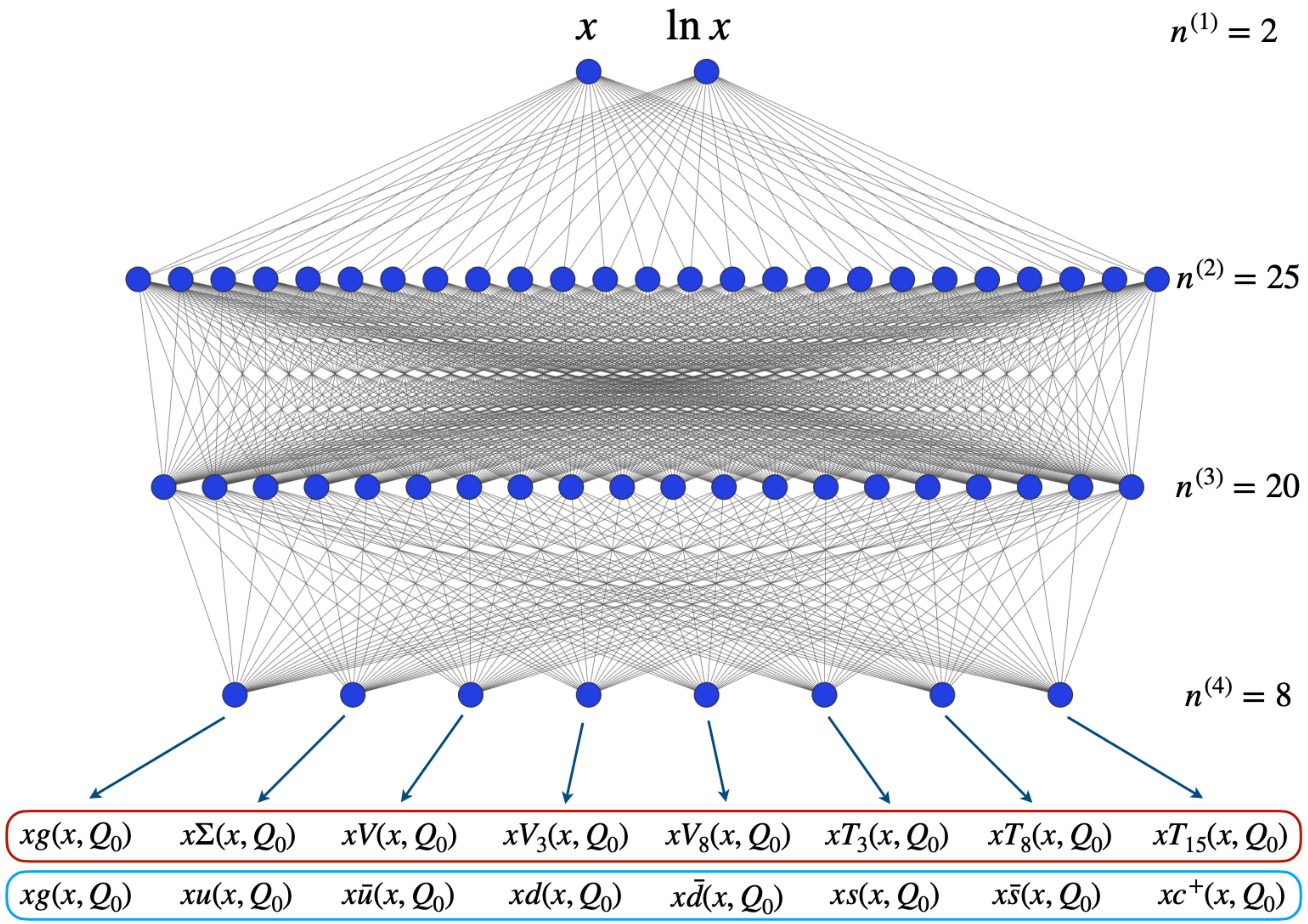
The Neural Network

Architecture: 2-25-20-8
Activation functions: hyperbolic; linear for the last layer
Preprocessing: $A_k x^{-\alpha_k}(1-x)^{\beta_k}$
Optimizer: Adadelta
Physics assumptions:

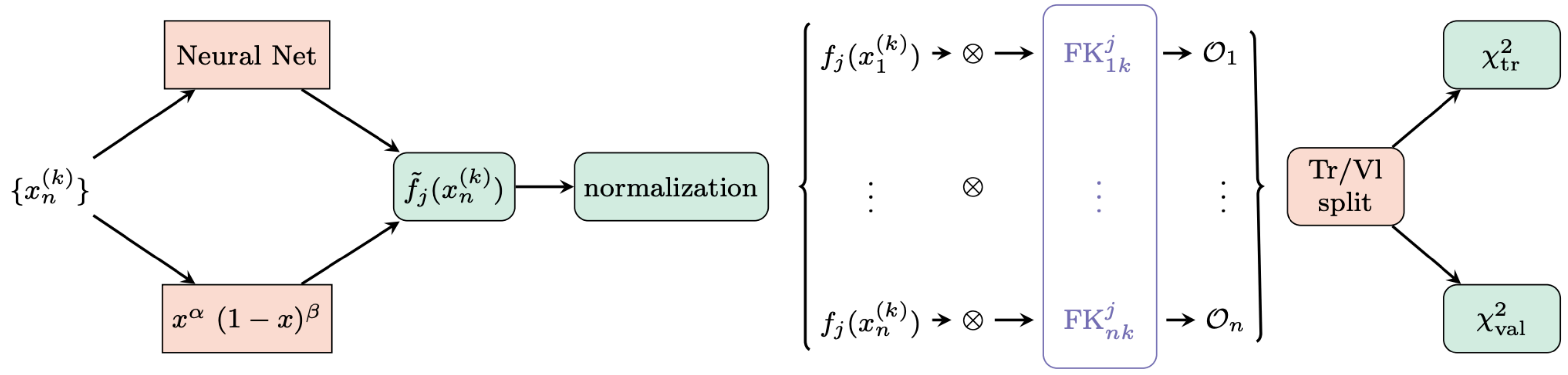
→ **Sum Rules** $\int_0^1 dx V(x,Q) = 3$

→ **PDF positivity**

→ **Integrability**



Neural Network: universal interpolator



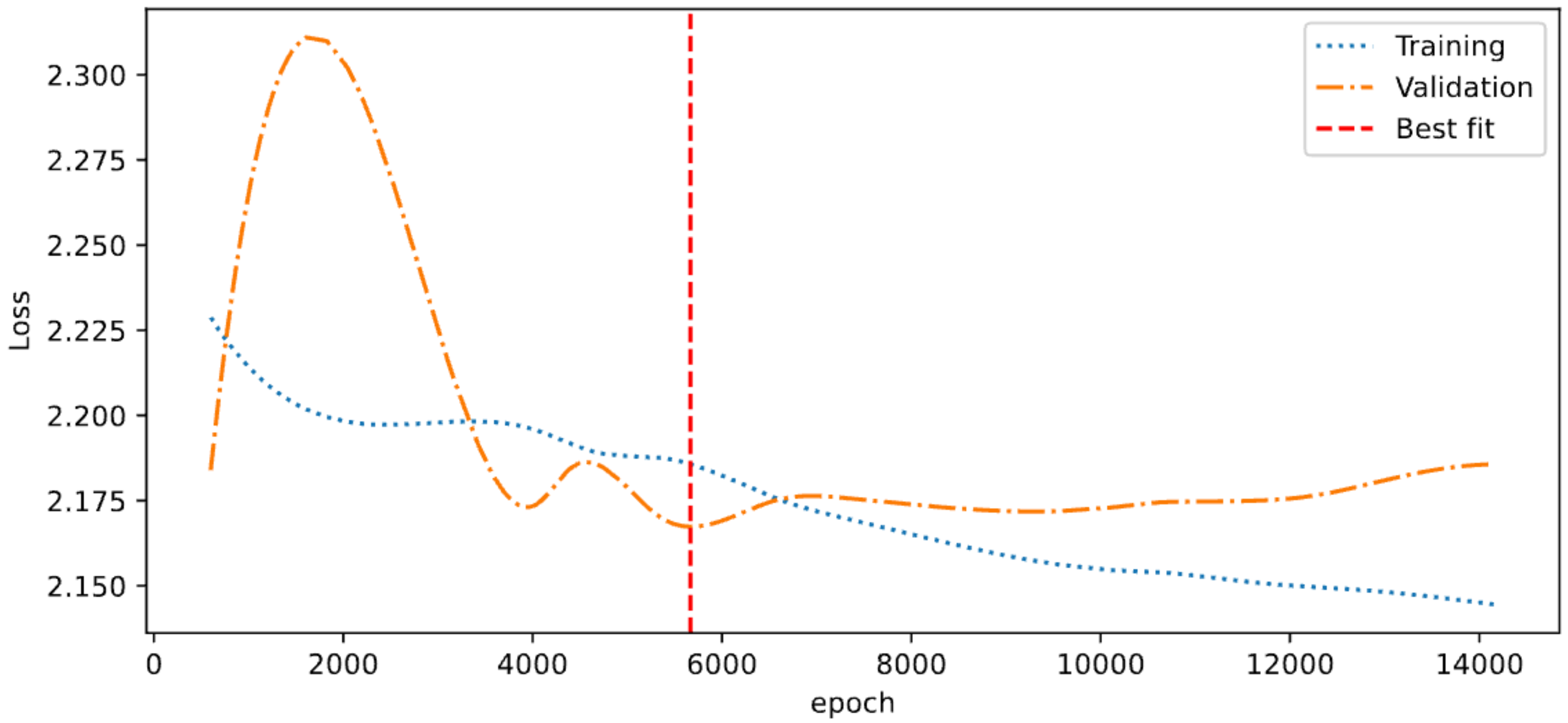
The Neural Network: training

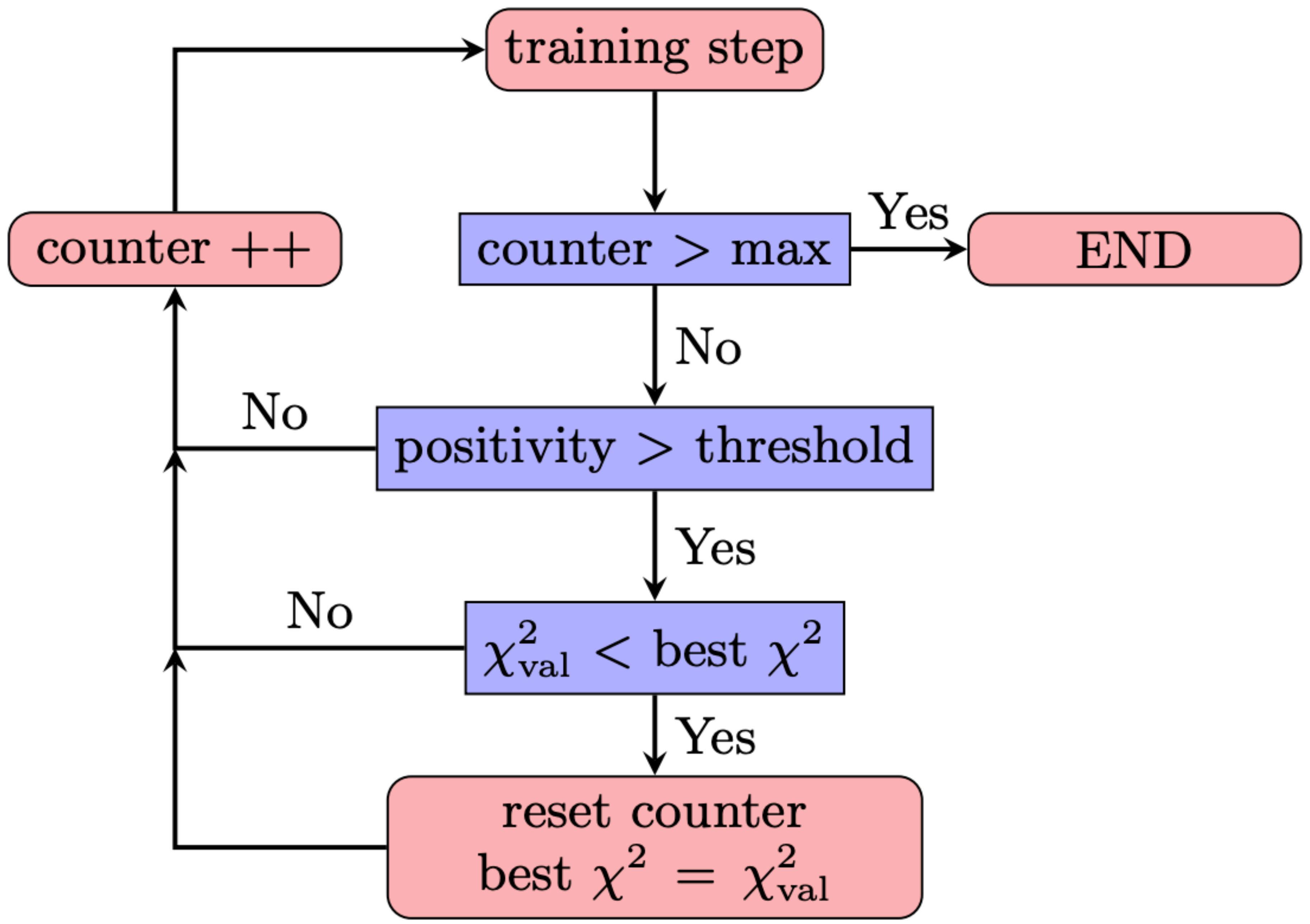
Avoid **overfitting** (fitting the noise)

Cross-validation

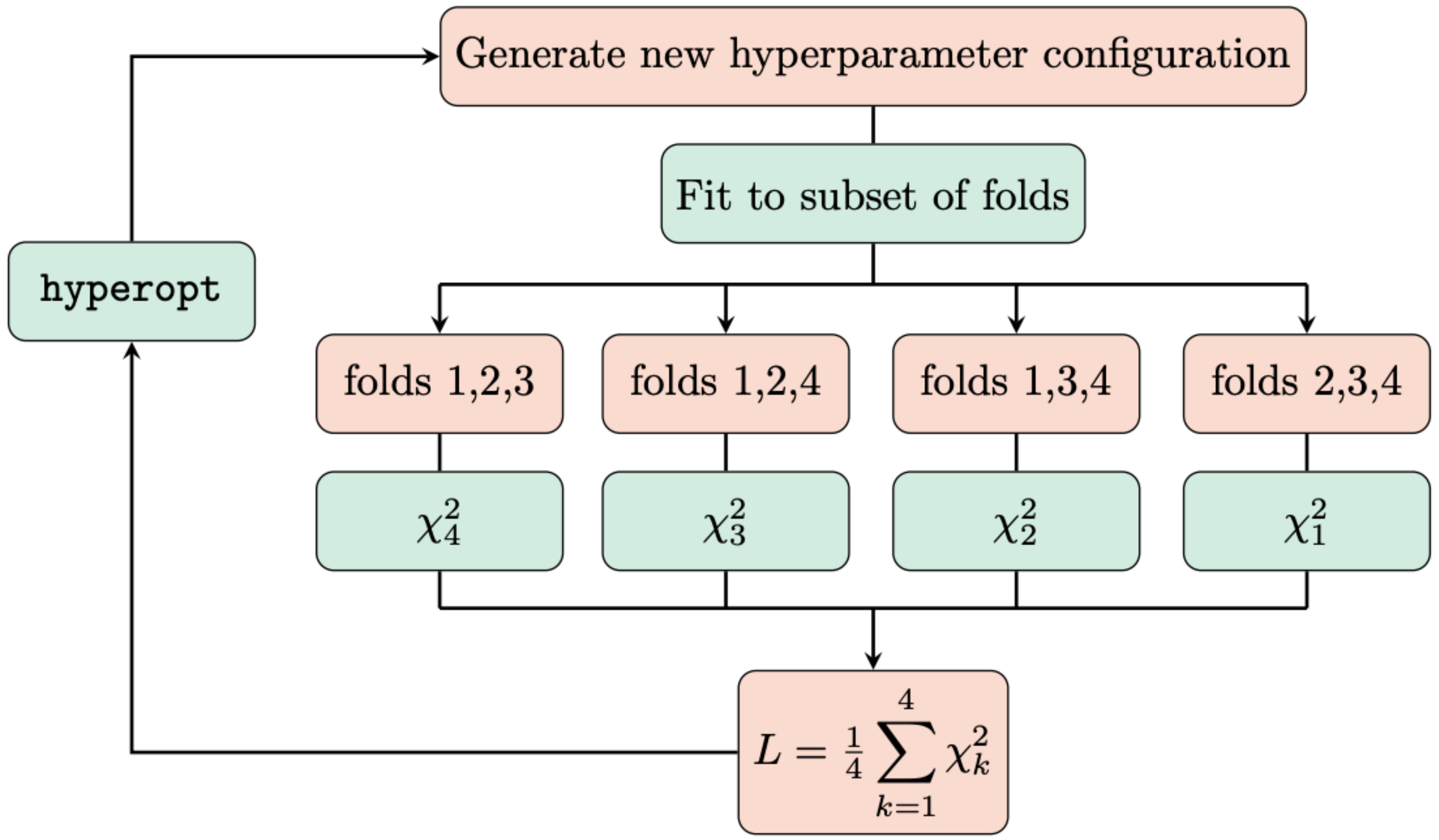
Stopping

1. Divide data into **training** and **validation**
2. Minimize training χ^2
3. Stop if validation χ^2 no longer improves





Automated model selection



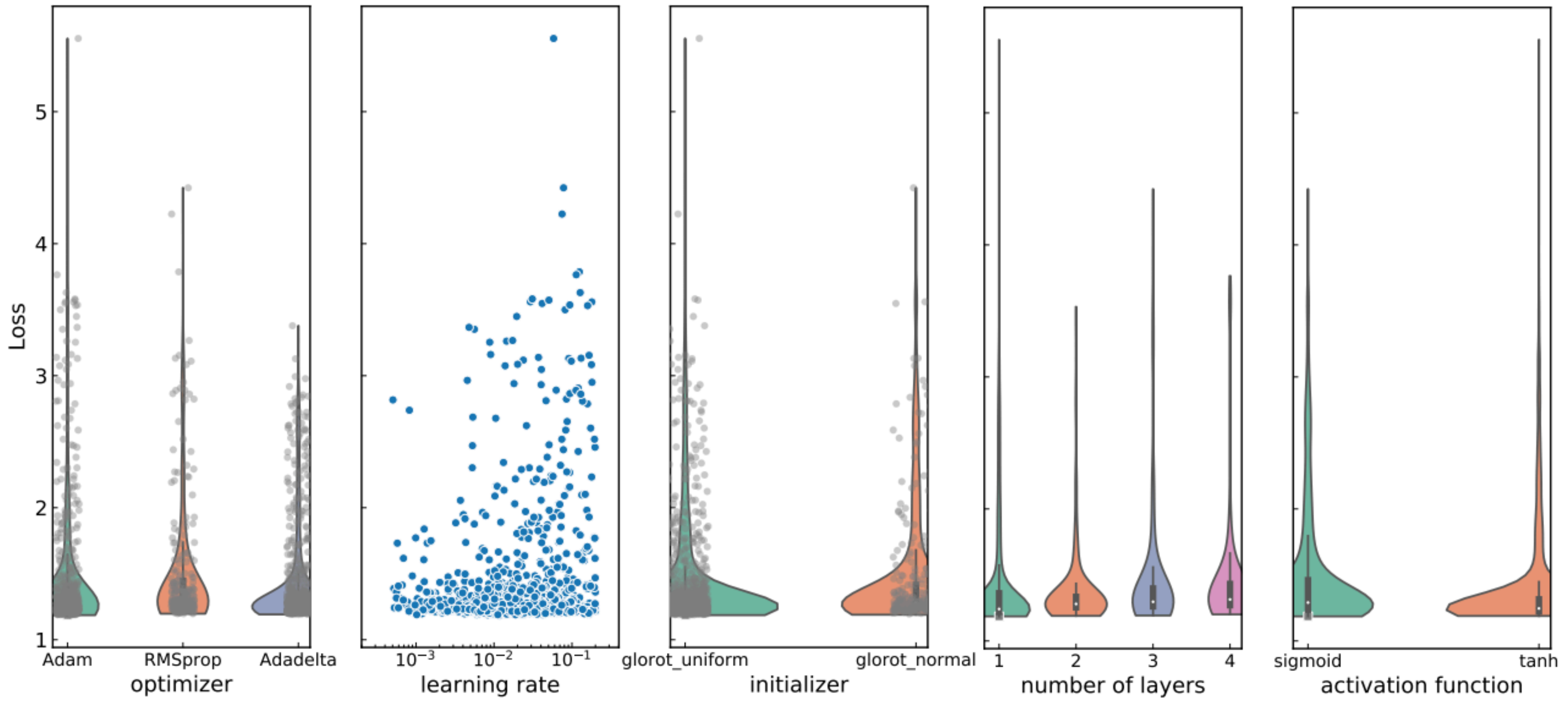
Minimize sources of **bias** in the PDFs:

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

Idea is to scan over a large enough hyperparameter space and select the best set

Best → best χ^2 on a **test dataset** (never seen by the NN)

NB: Still requires some human input (more on this later)



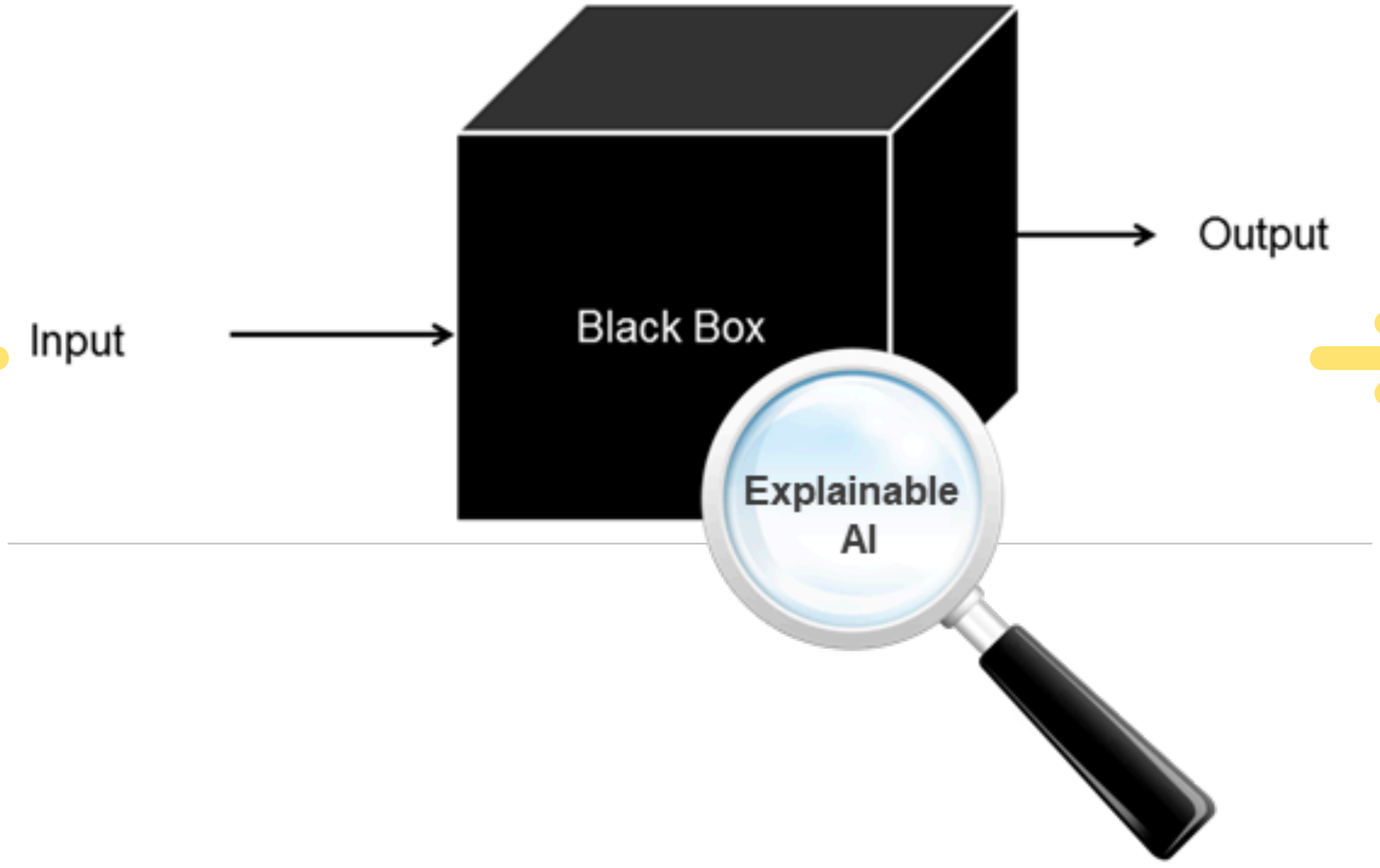
Can we trust our results?

Downside of Neural Networks:
we lack a **full analytical insight** on the process

NN is often considered to be a **black box**

Tests a priori (WIP)

- Test internal features of the NN
- "Analytical" approach



Tests a posteriori

- Test properties of the results
- Empirical approach

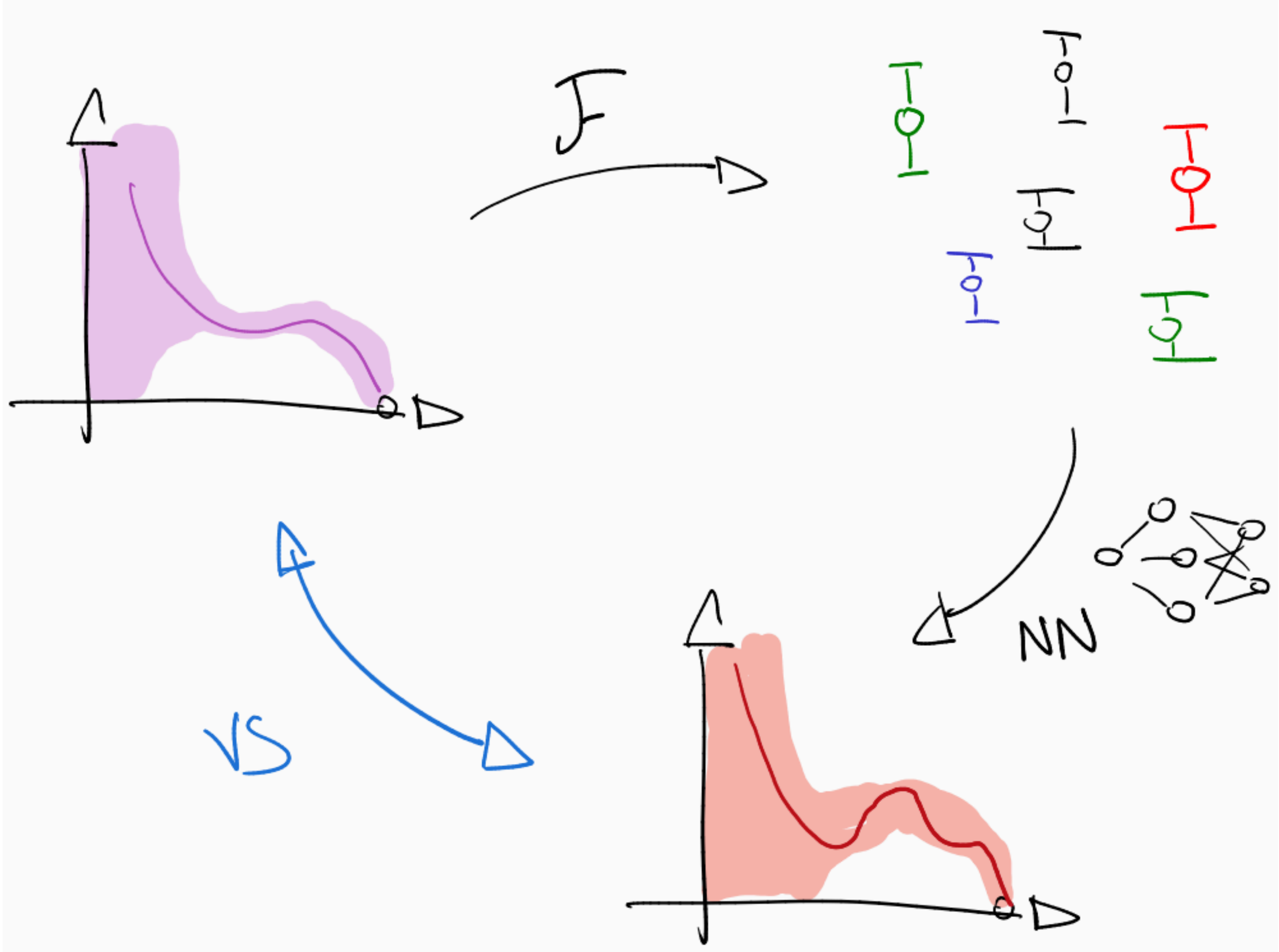
Focus on these!

Closure and future tests

Closure test

Test the algorithm in a controlled environment where the **"truth" is known**

1. Choose a PDF as underlying truth
2. Generate central fake data (**LEVEL 0**)
3. Generate smeared fake data with the experimental covariance matrix (**LEVEL 1**)
4. Generate and fit pseudodata replica (**LEVEL 2**)
5. Compare the results with known distribution

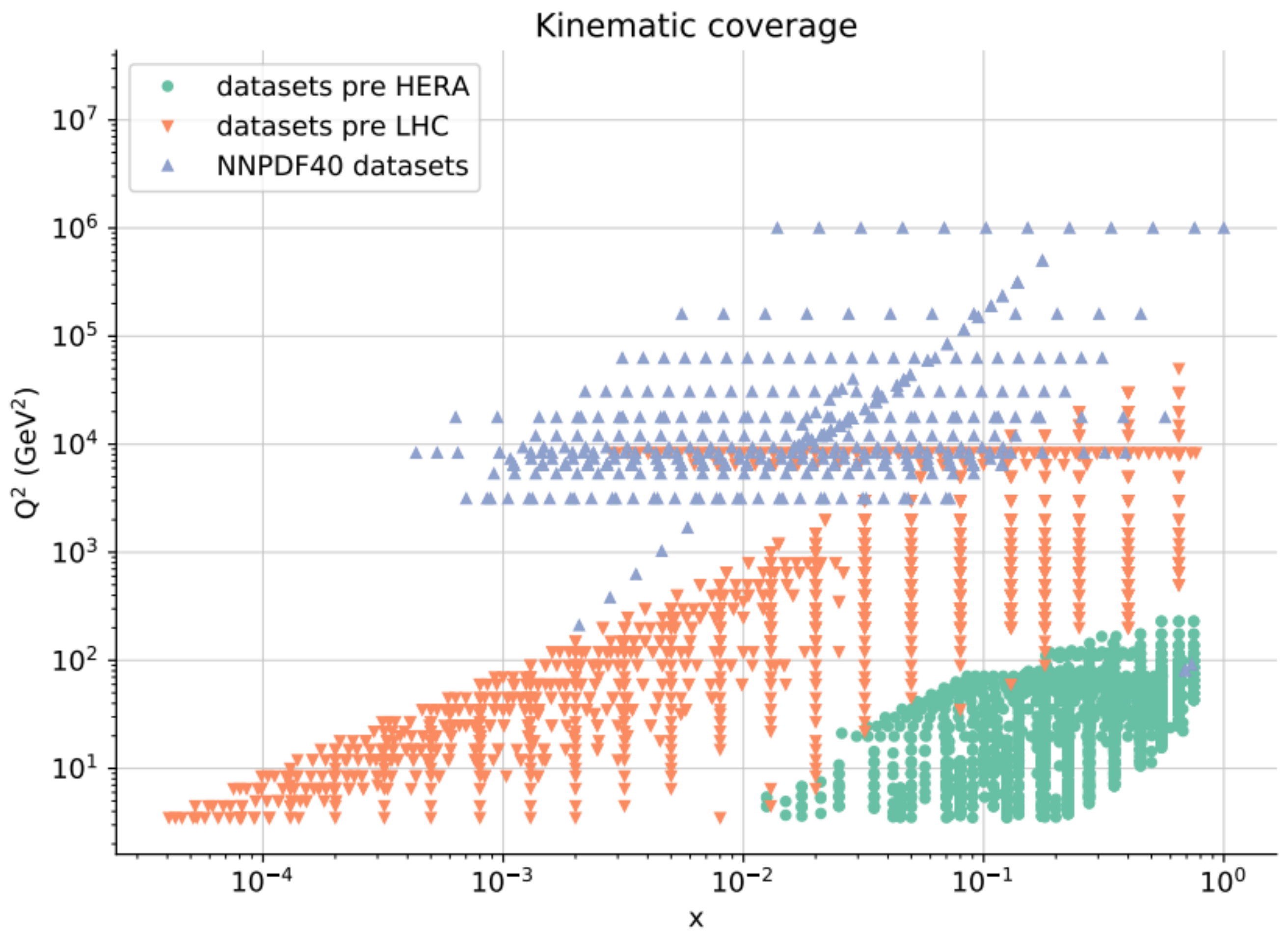


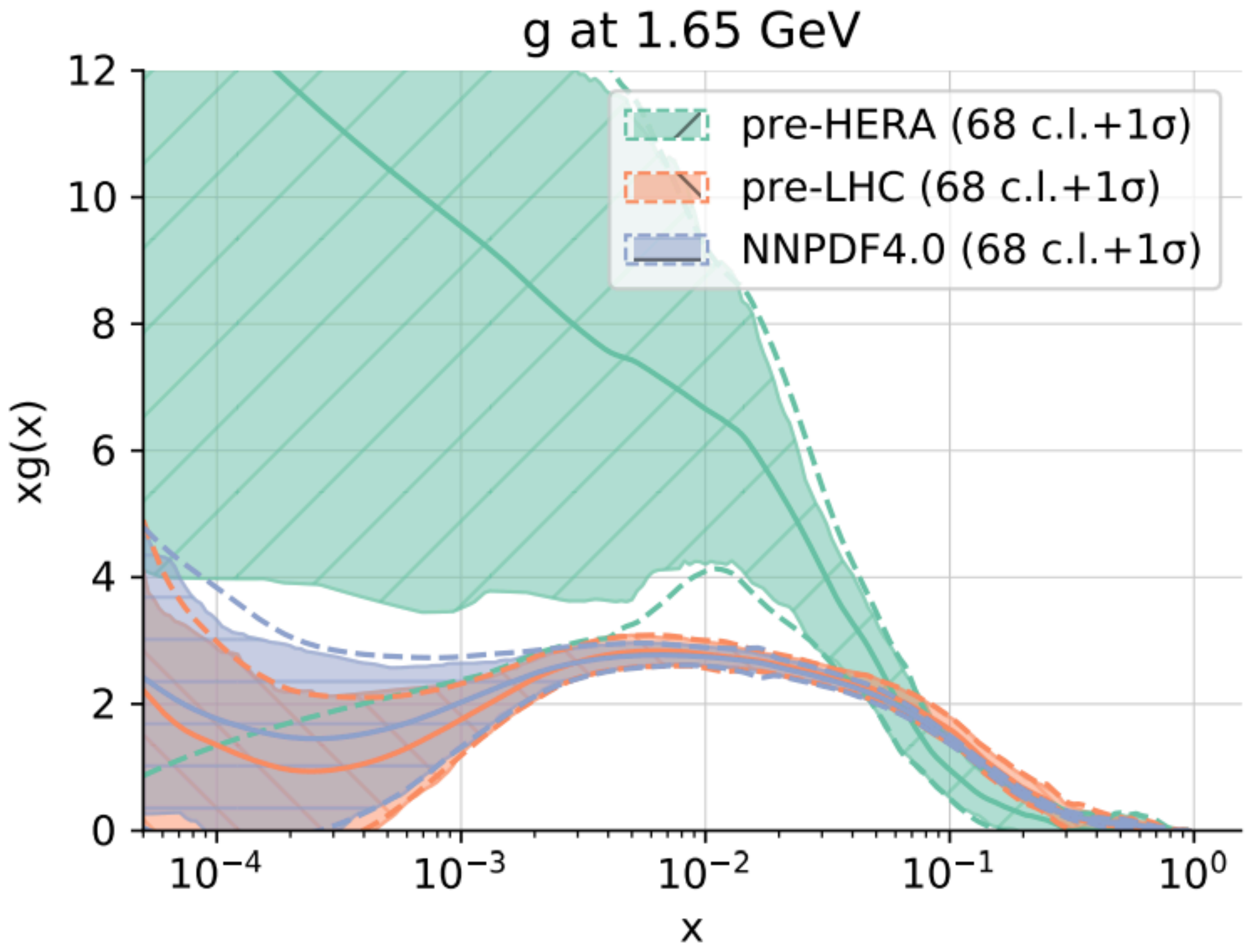
Future test

What about data you have not seen yet?

Traveling in time is not possible but I know **history!**

Divide the dataset **chronologically** and perform a fit for each set: **yesterday's extrapolation region is today's data region**



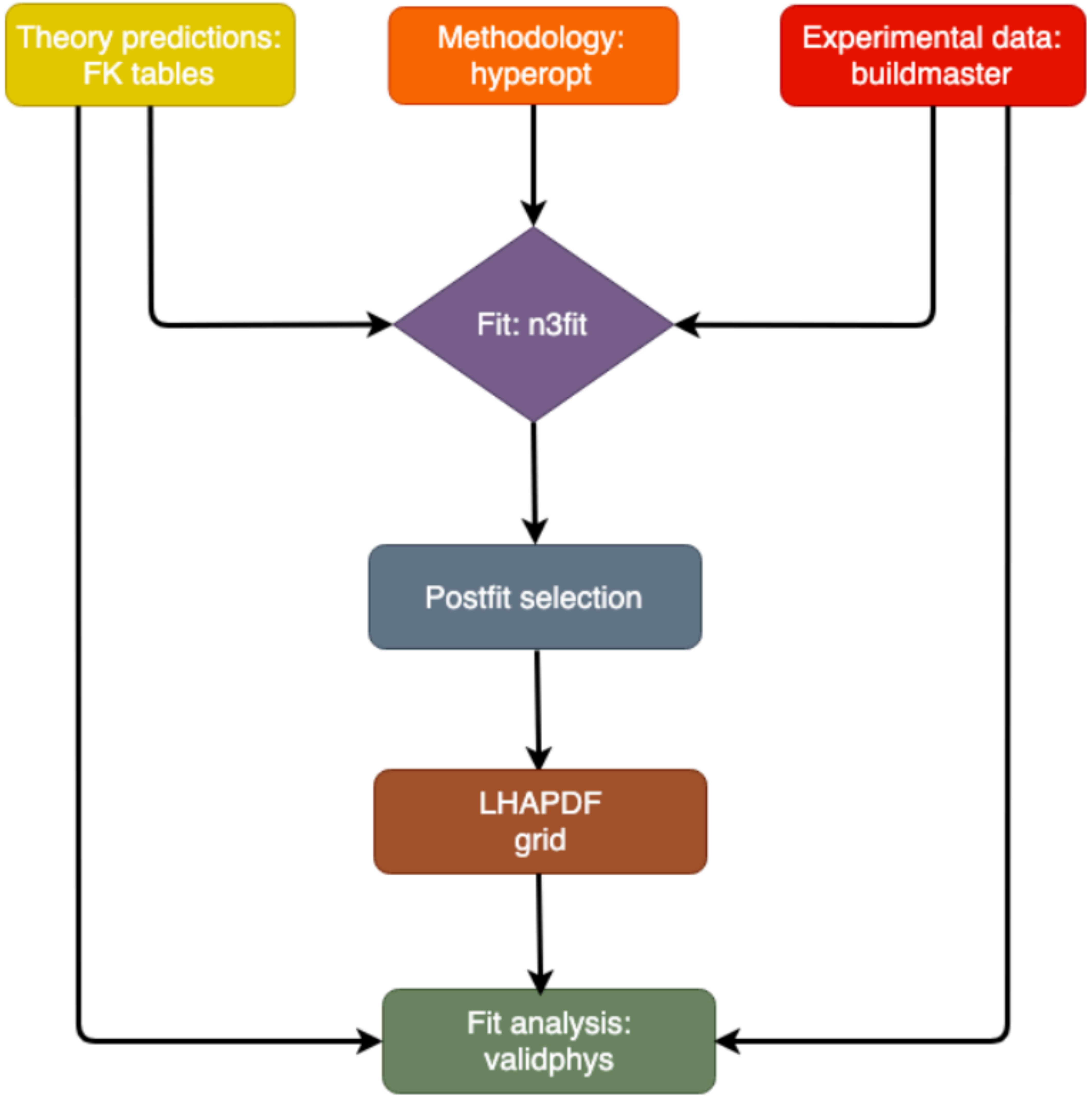


The NNPDF code is open-source

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

https://github.com/NNPDF/nnpdf

https://docs.nnpdf.science/



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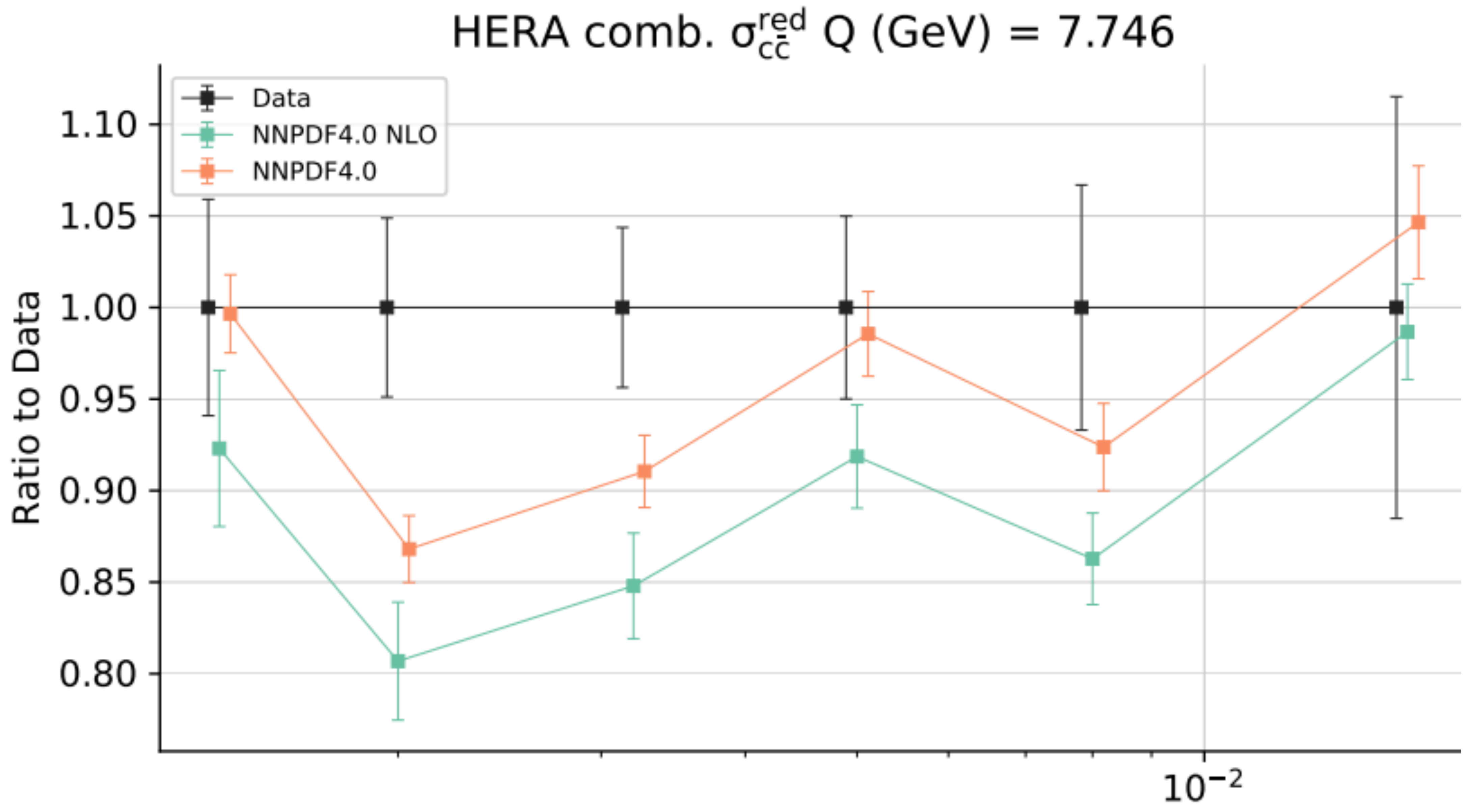
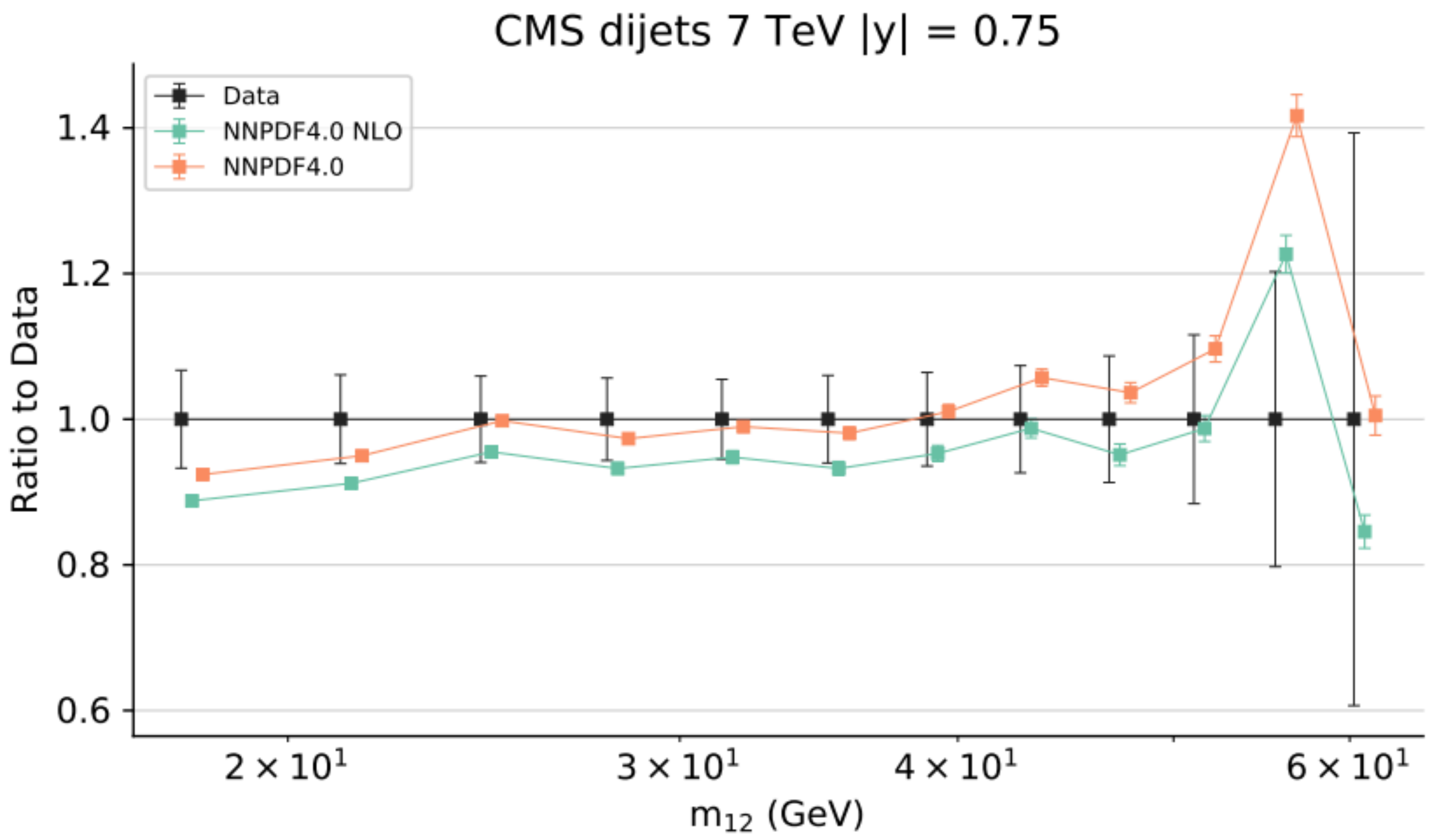
Fit quality: PDFs

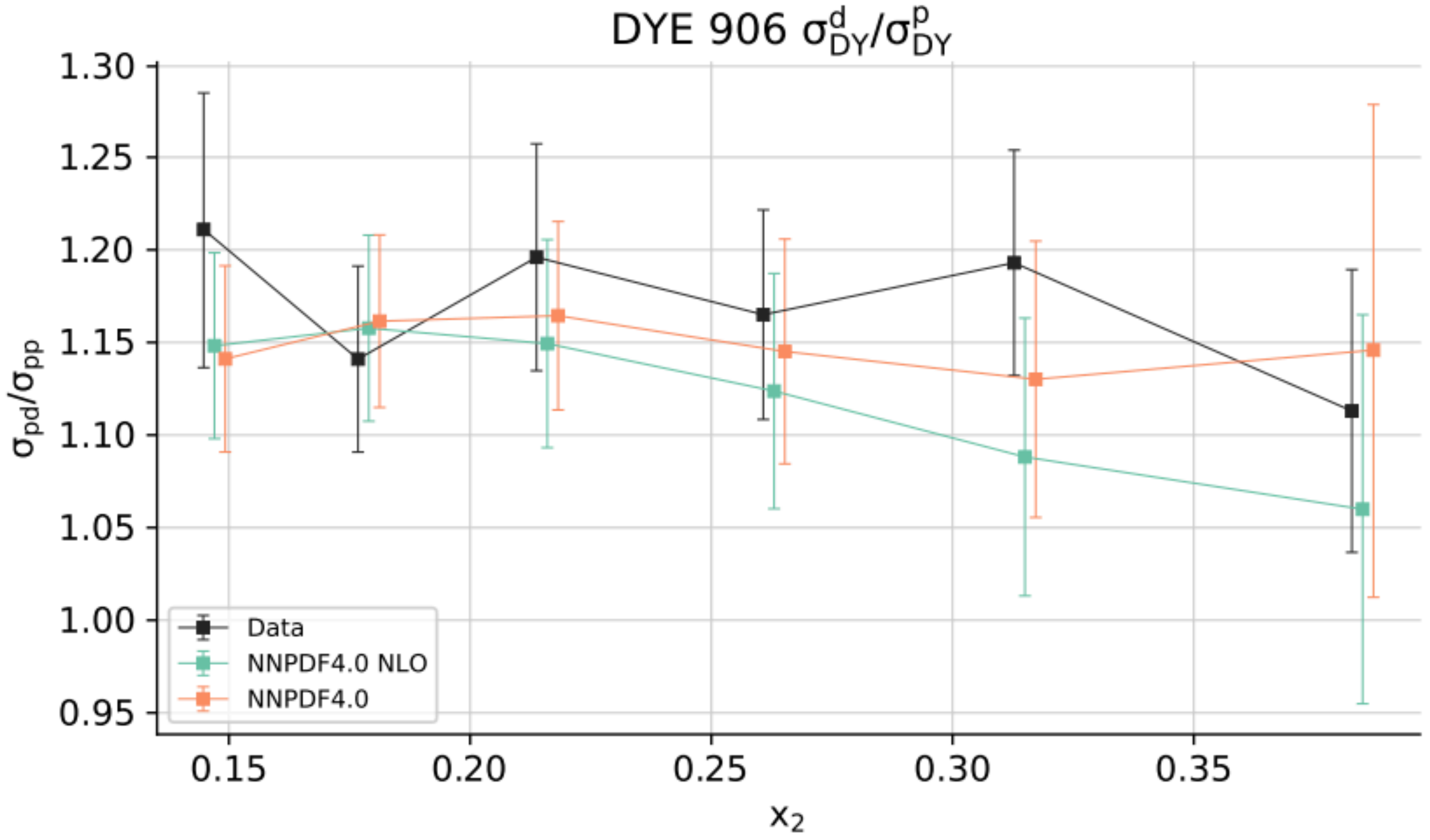
The fit quality clearly **improves** with the perturbative order (LO < NLO < NNLO)

Fit quality: predictions vs data

Also the description of the data clearly **improves** from NLO to NNLO





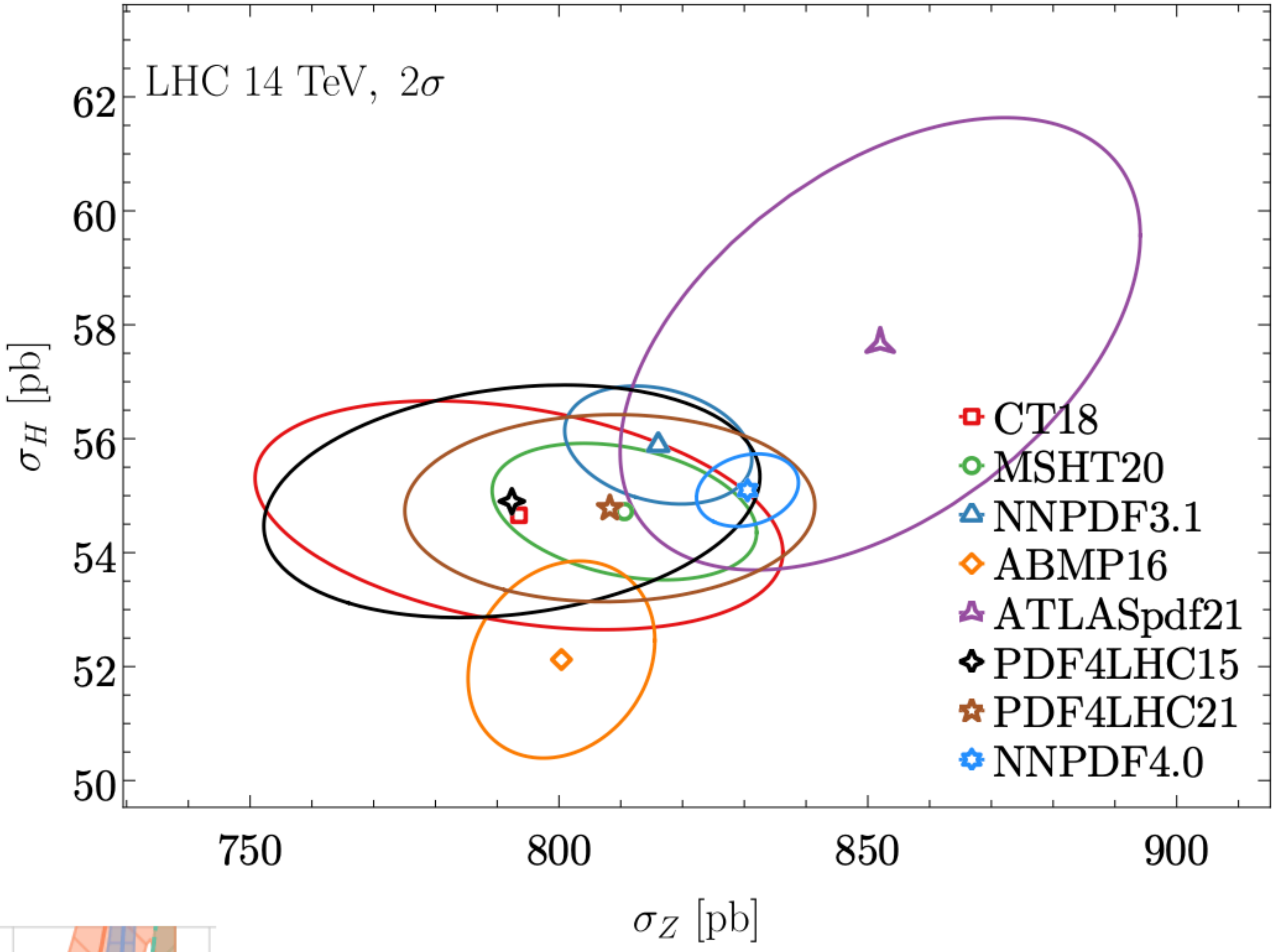


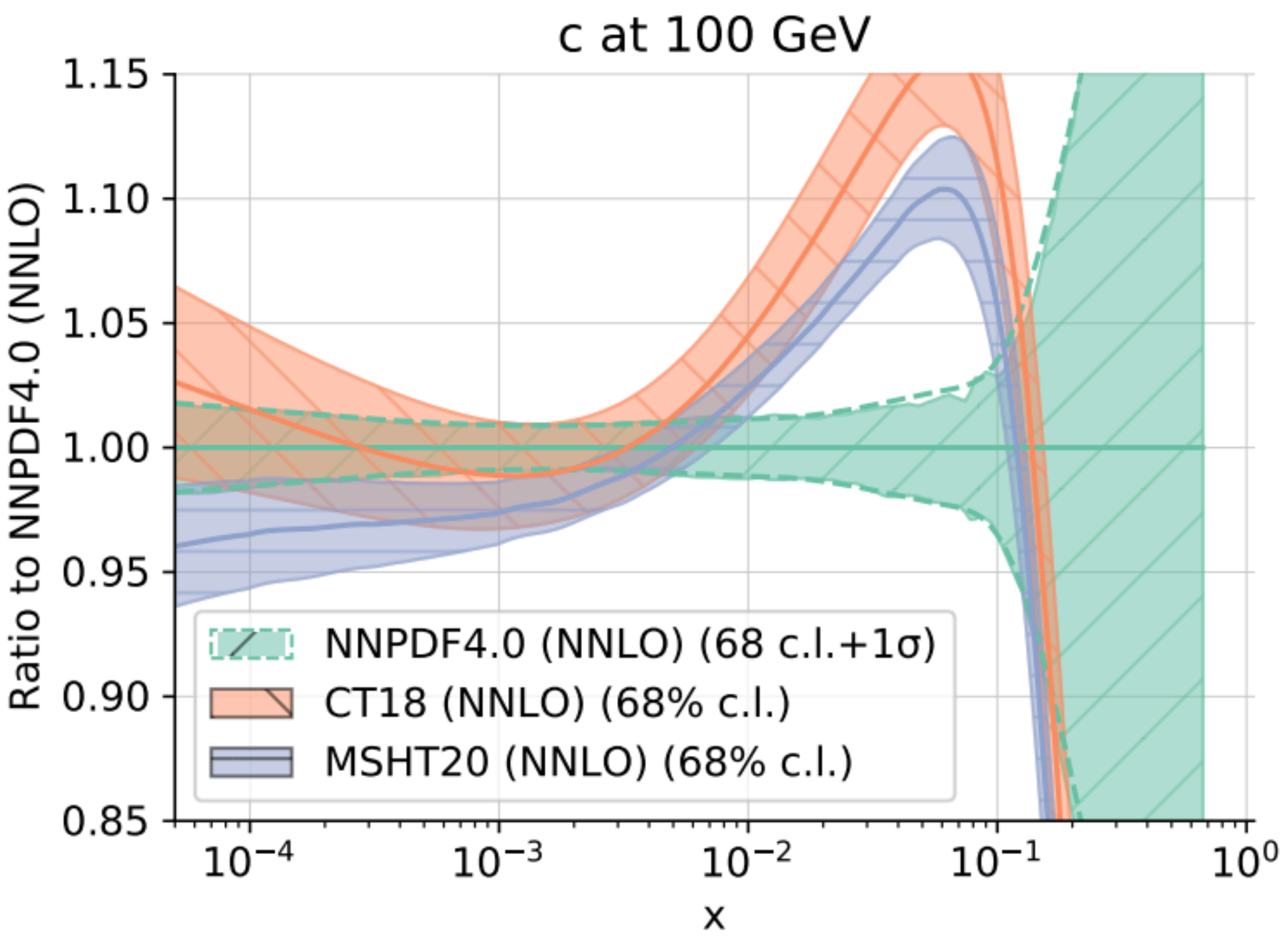
Comparison to other methodologies

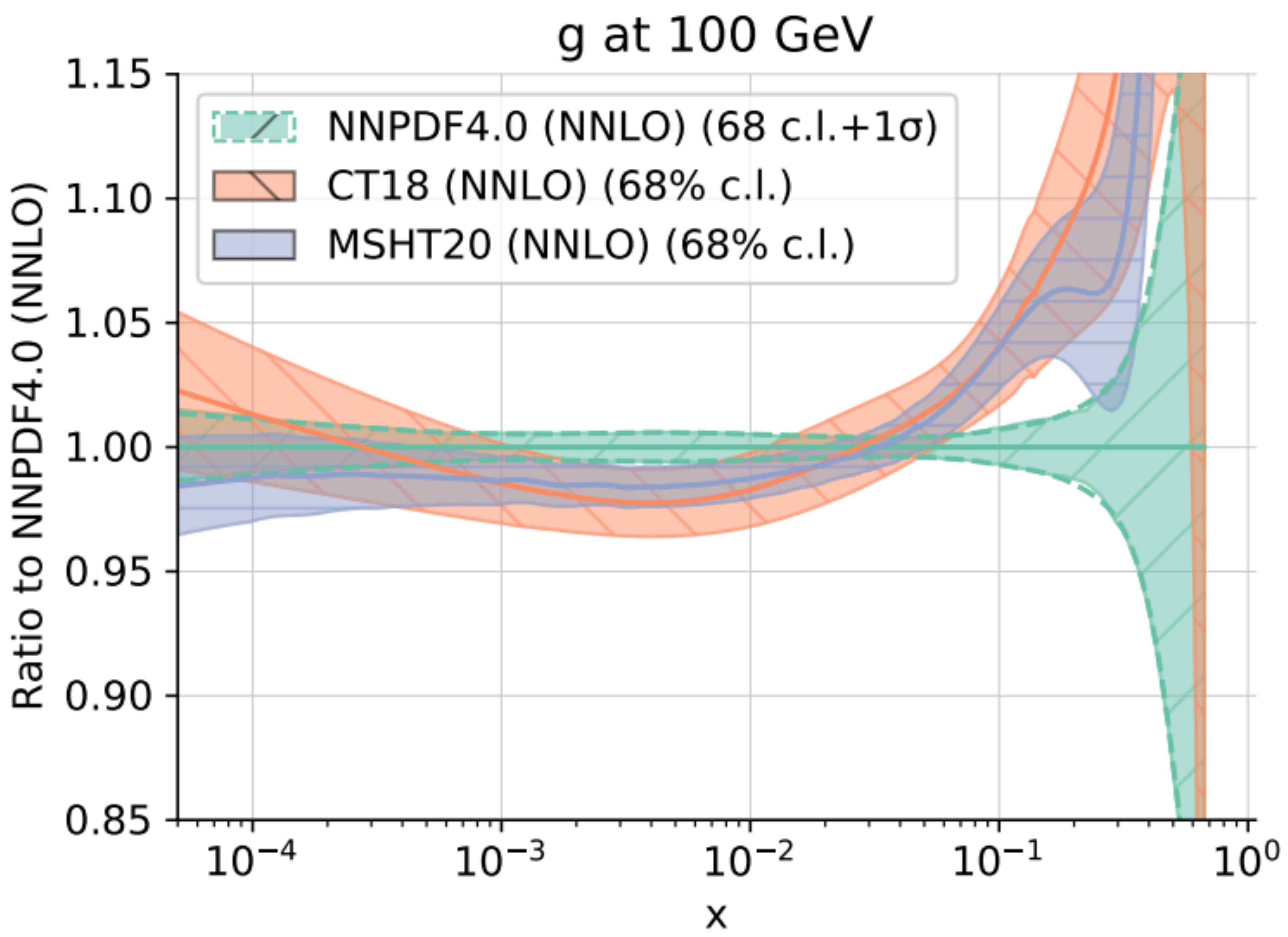
The agreement among different PDF fitting group is rather good

↓

However, NNPDF (3.1 and 4.0) has **smaller uncertainties** than the other groups → **effect of the NN**







Outlook: WIP and future projects

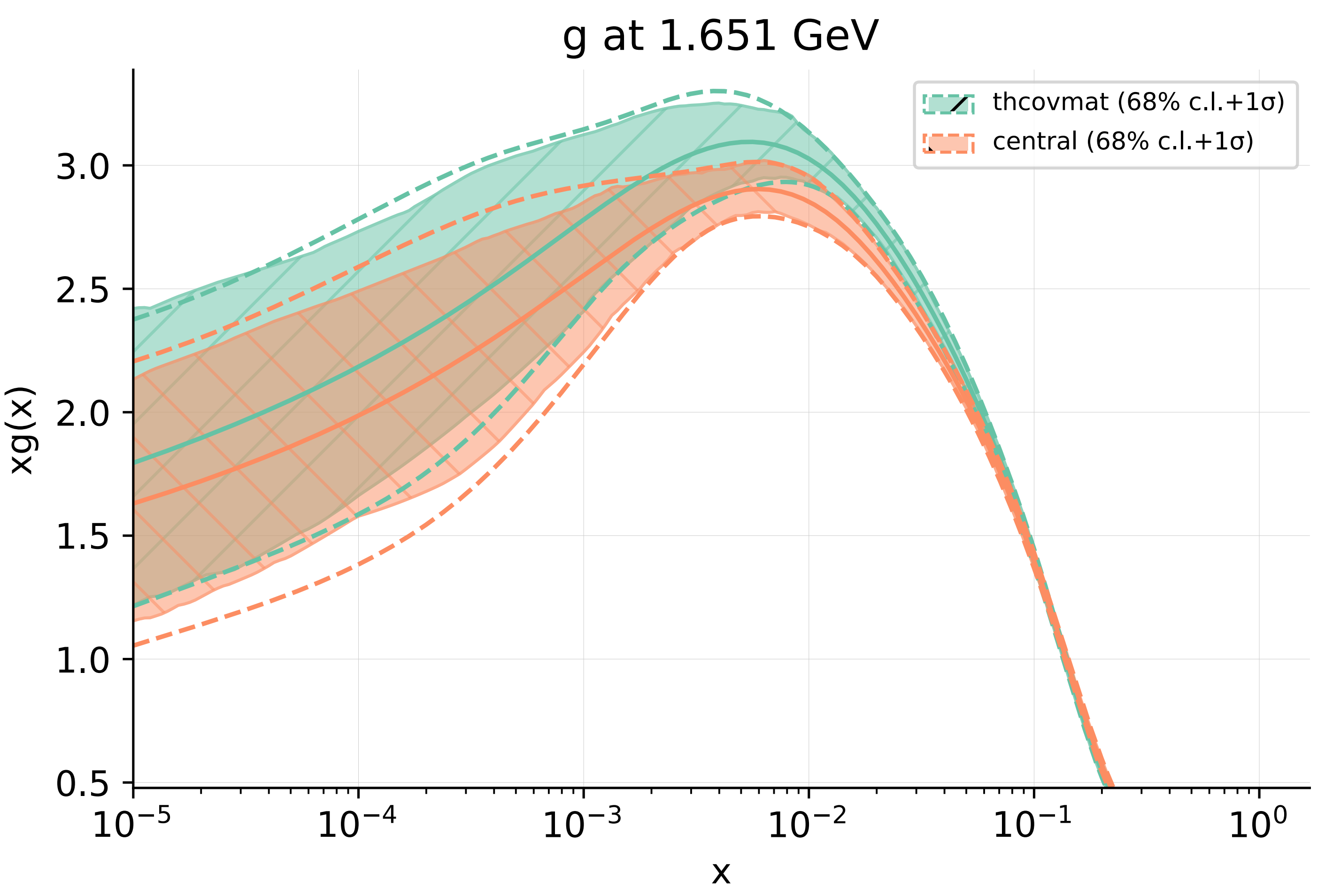
Physics projects

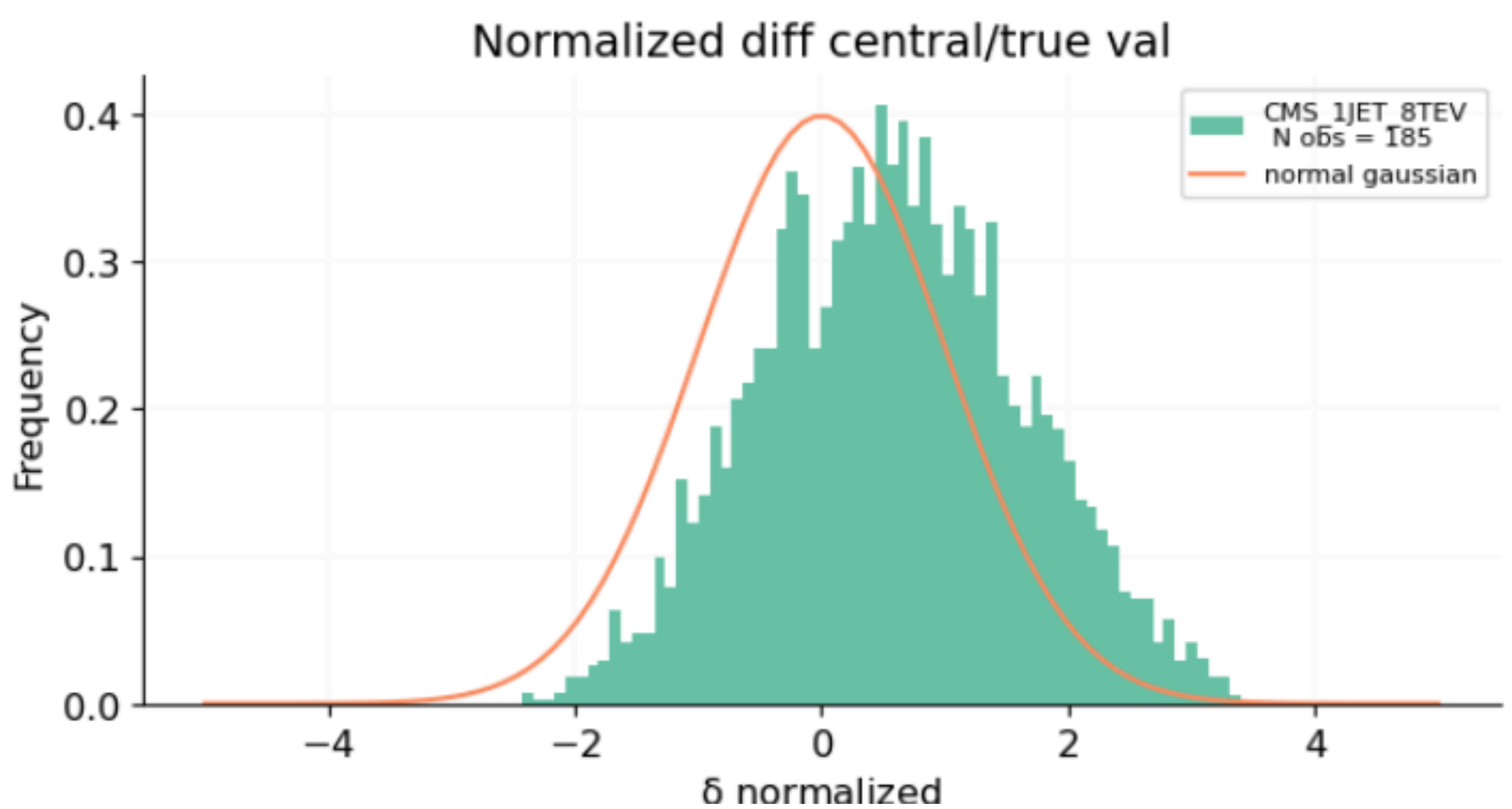
- Fit with theoretical uncertainties
- Fit with photon induced effects
- Fit at N3LO perturbative order

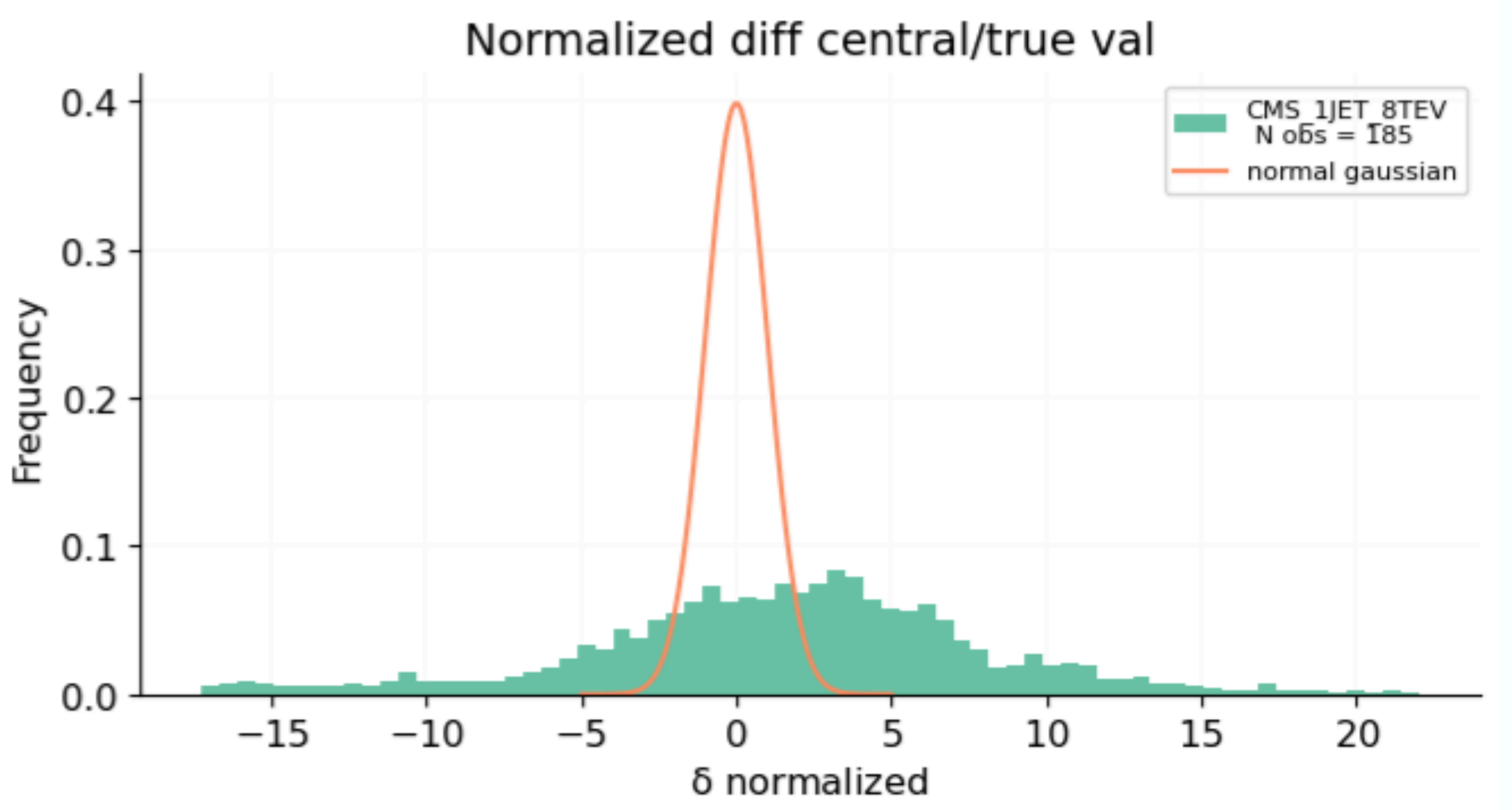
Methodology projects

- Bayesian fit
- New overfitting metrics for hyperopt
- Closure tests with inconsistent data

Preliminary results!







Conclusions

- Using neural networks techniques for PDF evaluation has led to several successes
- The comparison with other PDF fitting groups has shown that using NN techniques it is possible to obtain results with smaller uncertanties, while keeping them reliable
- For the future, it will be important to focus on explainability and improvements of the methodology

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