



The inclusion of theory errors in NNPDF fits.

The NNPDF4.0MHOU and NNPDF4.0N3LO PDFs sets

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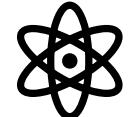
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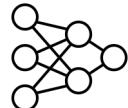
Outline.

||



PHYSICS

- How can we evaluate PDFs?
- What are theory errors?
- Why is it relevant to include them in a PDF fit?



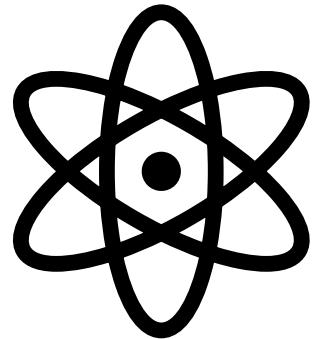
METHODOLOGY AND
VALIDATION

- How can we include MHOU in a NNPDF fit?
- Can we validate our estimation?
- What about N3LO?



RESULTS

- Does the fit quality improve upon inclusion of theory errors?
- What is the impact on the PDFs?
- What about pheno?

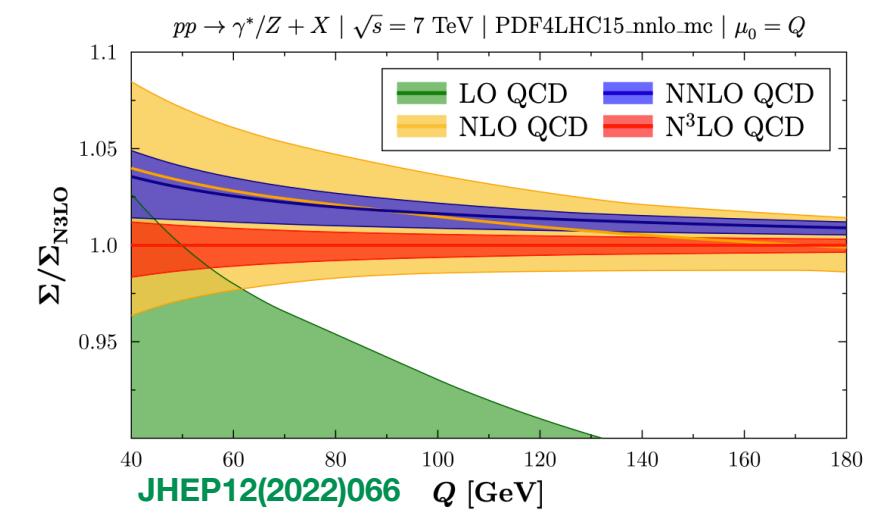
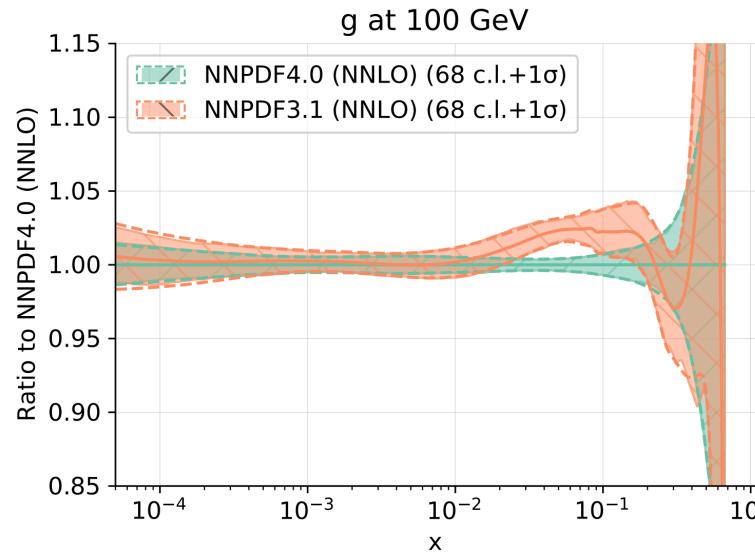
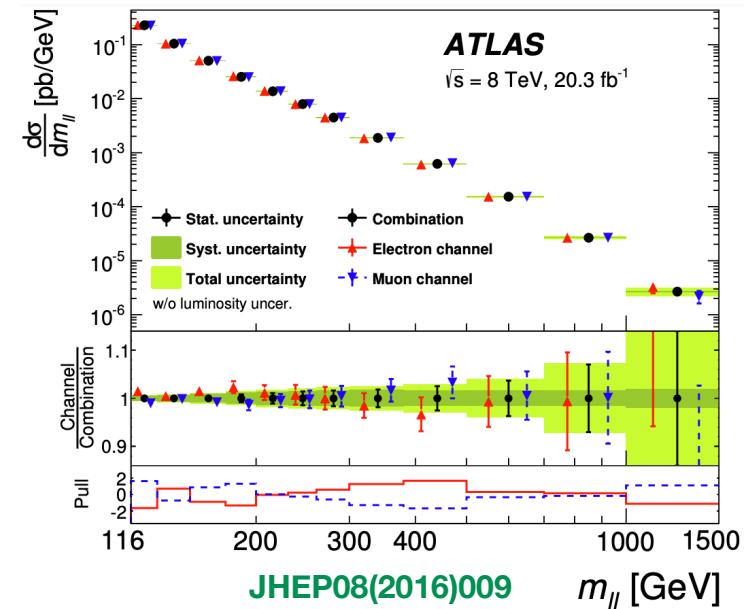
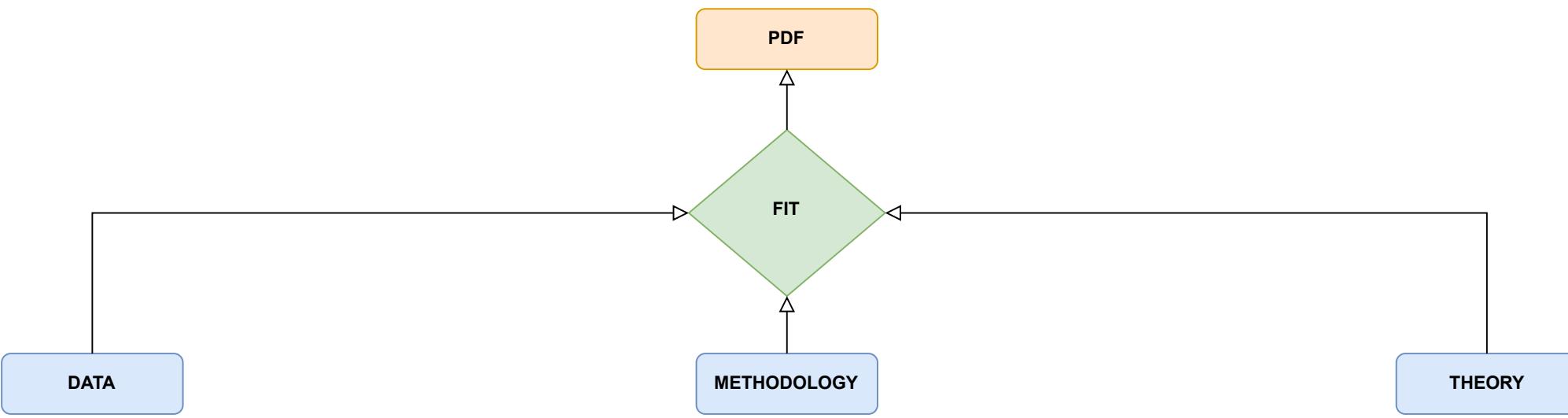


PHYSICS

- How can we evaluate PDFs?
- What are theory errors?
- Why is it relevant to include them in a PDF fit?

*“We are not strangers, only the introduction is missing”
(Jesus Apolinaris)*

Motivation.



PDF extraction.

Factorization theorem

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

Measured in experiments

computed in perturbation theory

unknown

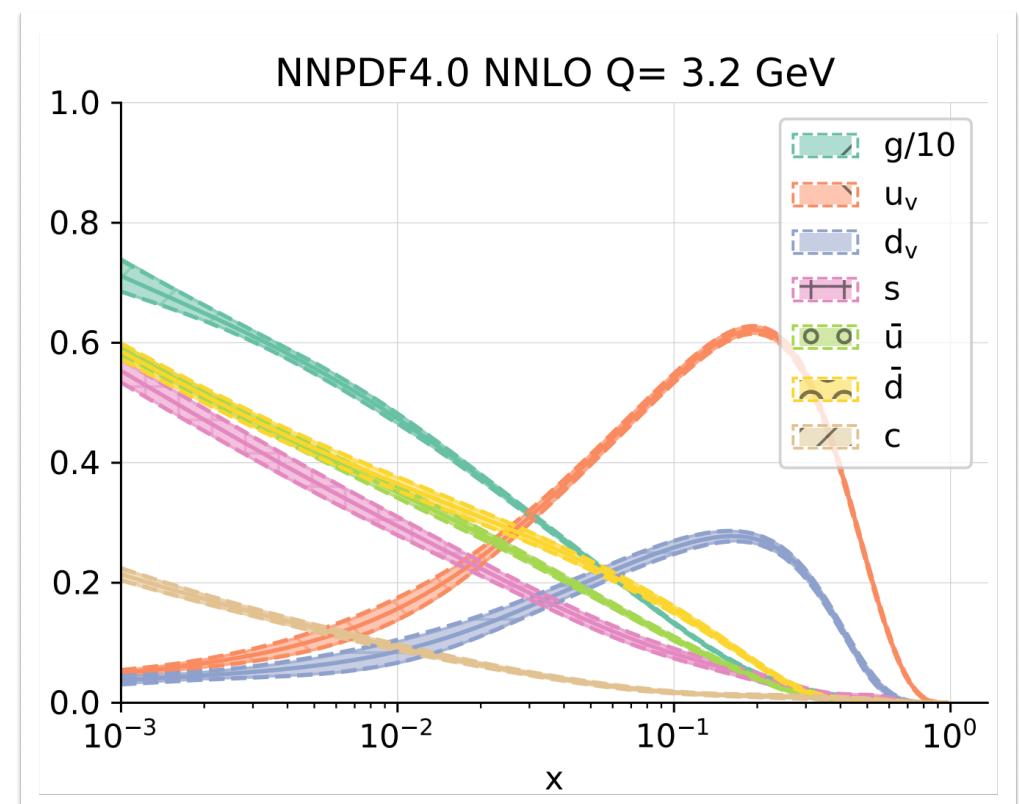
Inverse problem

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**

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

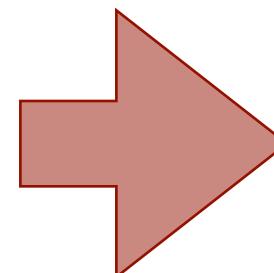


Theory errors.

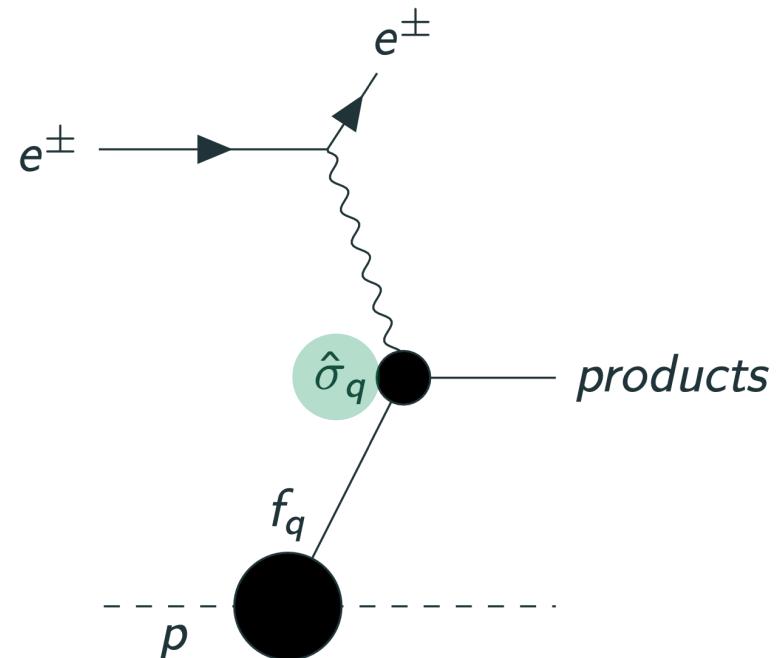
$$F(Q) = \hat{\sigma}(Q^2) \otimes E_{ij}(Q^2 \leftarrow Q_0^2) \otimes f_j(Q_0^2)$$

- **Partonic cross sections** are computed in perturbation theory
- **Anomalous dimensions** inside DGLAP operator are computed in perturbation theory

$$\begin{aligned}\hat{\sigma}^{NLO} &= \hat{\sigma}^{(0)} + \alpha_s \hat{\sigma}^{(1)} + \mathcal{O}(\alpha_s^2) \\ \gamma^{NLO} &= \alpha_s \gamma^{(0)} + \alpha_s^2 \gamma^{(1)} + \mathcal{O}(\alpha_s^3)\end{aligned}$$



Deep Inelastic Scattering (DIS)



MHOU
(Missing Higher Order Uncertainties)

How can we estimate them?

Theory errors: estimation.

Scale Variations

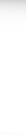
$$\bar{F}^{NLO}(\mu_f = \kappa_f Q, \mu_r = \kappa_r Q) - F^{NLO}(\mu_f = Q, \mu_r = Q) = \mathcal{O}(NNLO)$$



Factorization scale

Estimates **MHOU** of anomalous dimensions

$$E^{NLO}(Q \leftarrow Q_0) \rightarrow \bar{E}^{NLO}(Q \leftarrow Q_0, \kappa_f)$$



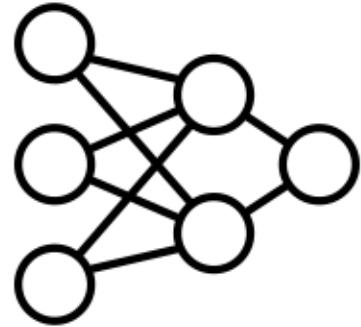
Renormalization scale

Estimates **MHOU** of partonic cross sections

$$\hat{\sigma}^{NLO}(Q) \rightarrow \bar{\sigma}(Q, \kappa_r)$$



$\kappa_f, \kappa_r \in (0.5, 2.0)$ is the most common choice

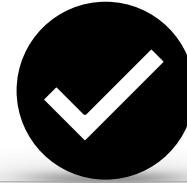


METHODOLOGY AND VALIDATION

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- What about N3LO?

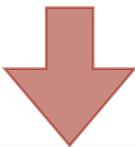
“Truth has nothing to do with the conclusion, and everything to do with the methodology”
(Stefan Molyneux)

MHOU in a PDF fit: the *theory covmat*.



How to use it

- Experimental and theoretical uncertainties enter in a symmetric way in the figure of merit used for PDF determination.
- The theory covariance matrix S describes theoretical uncertainties and correlations.
- Include it both in figure of merit and in pseudodata generation.



FIT WITHOUT THEORY ERRORS

$$\chi^2 \propto (D_i - T_i)C_{ij}^{-1}(D_j - T_j)$$

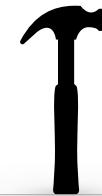
$$Pseudodata\ replica \propto C$$

FIT WITH THEORY ERRORS

$$\chi^2 \propto (D_i - T_i)(C + S)_{ij}^{-1}(D_j - T_j)$$

$$Pseudodata\ replica \propto C + S$$

MHOU in a PDF fit: the *theory covmat*.



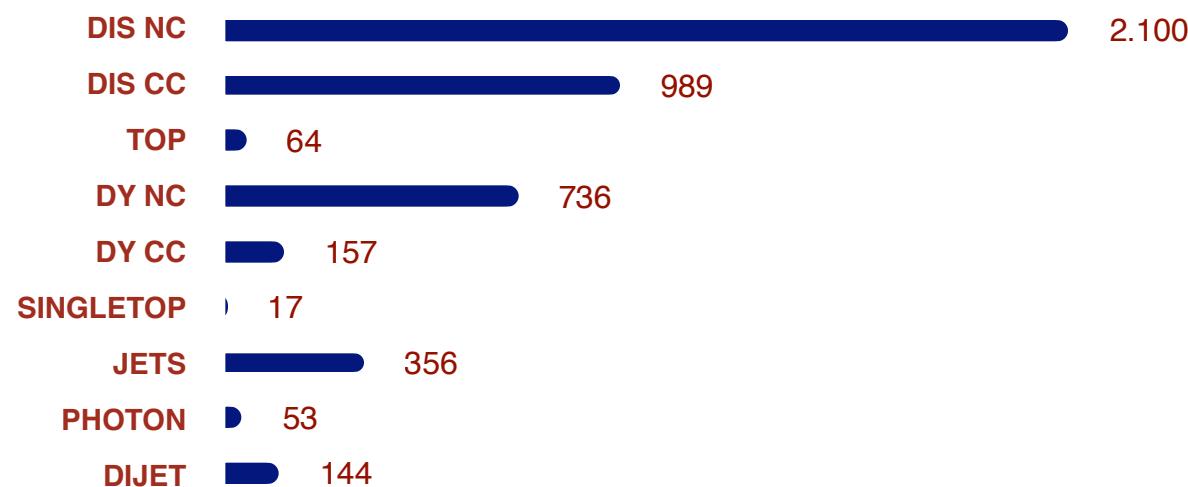
How to construct it



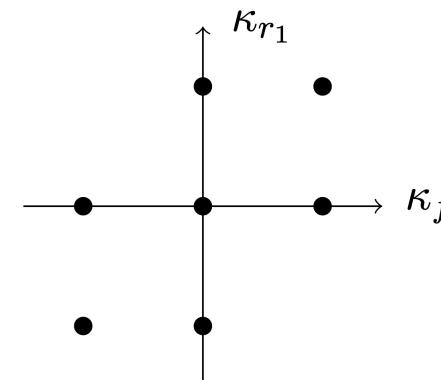
$$S_{ij} = n_m \sum_{V_m} \left(\bar{F}(\kappa_f, \kappa_{r_a}) - F \right)_{i_a} \left(\bar{F}(\kappa_f, \kappa_{r_b}) - F \right)_{j_b}$$

→ Factorization scale **correlates** all the points

→ Renormalization scale **correlates** points belonging to the same process

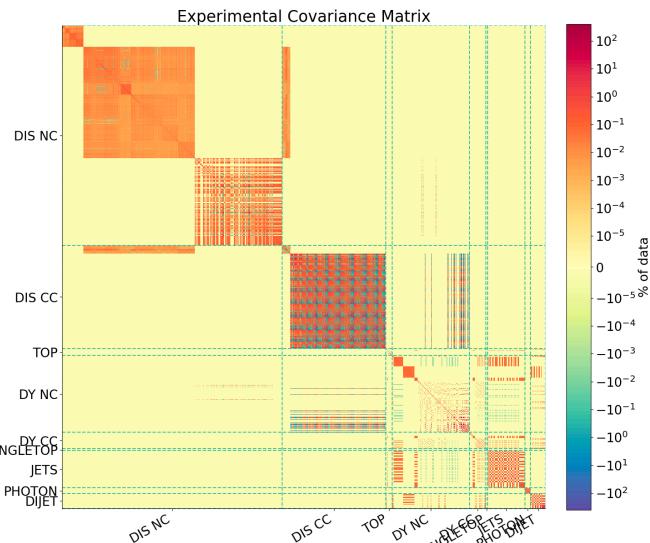


7 points

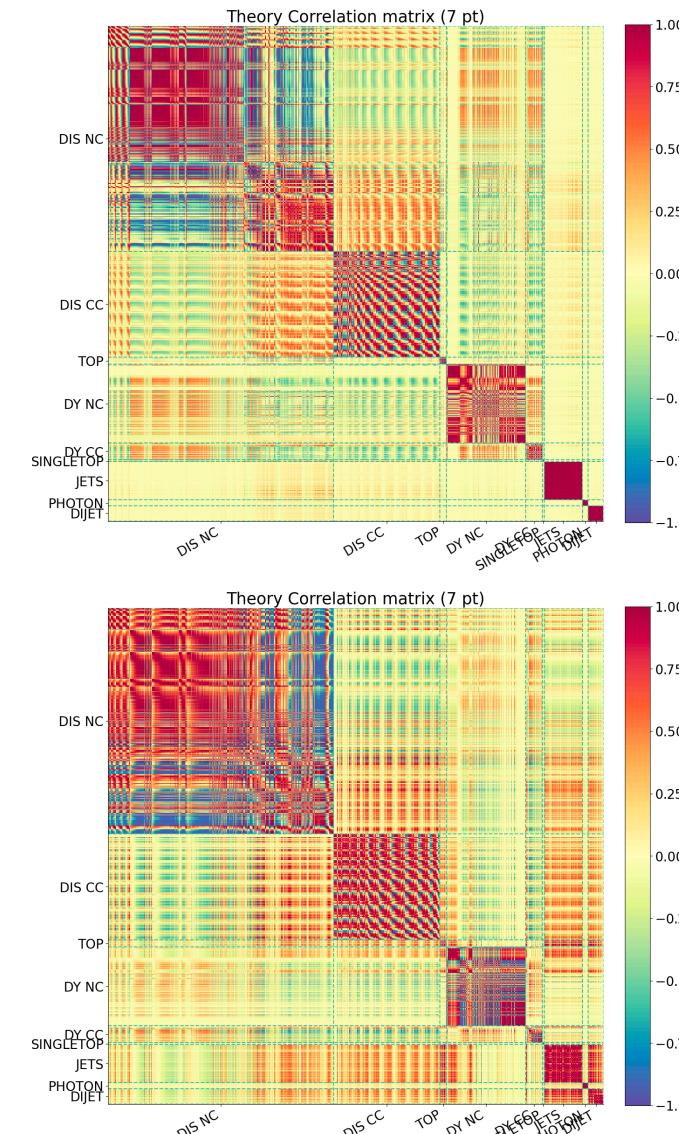


How do they look like?

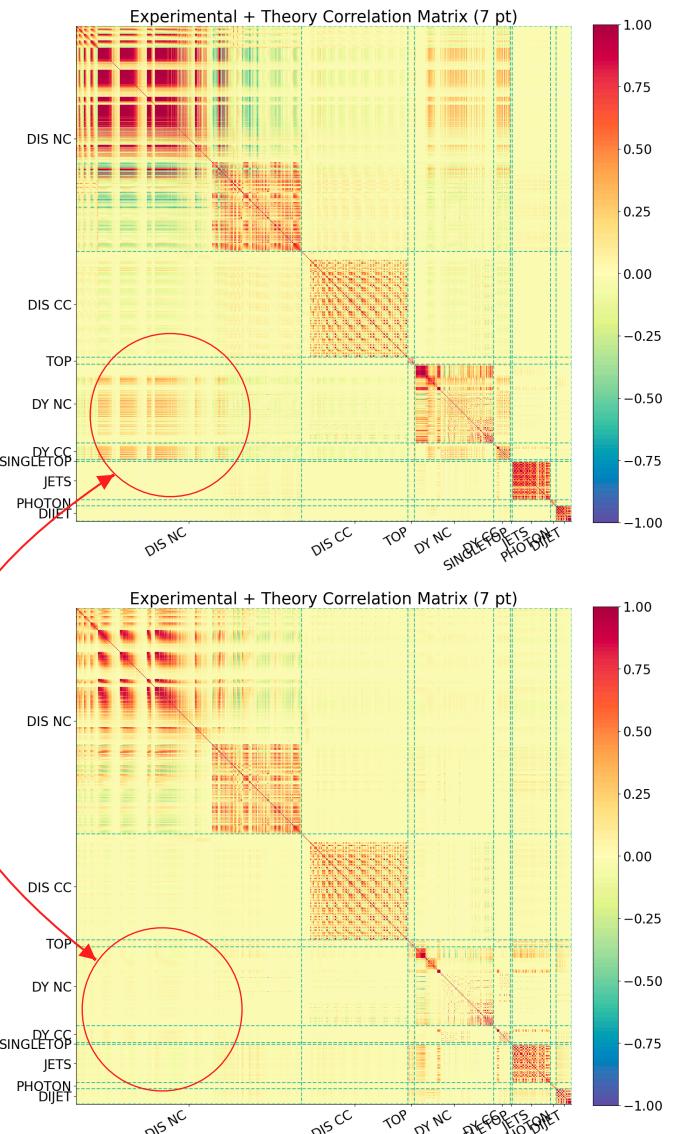
↓
 C



↓
 S

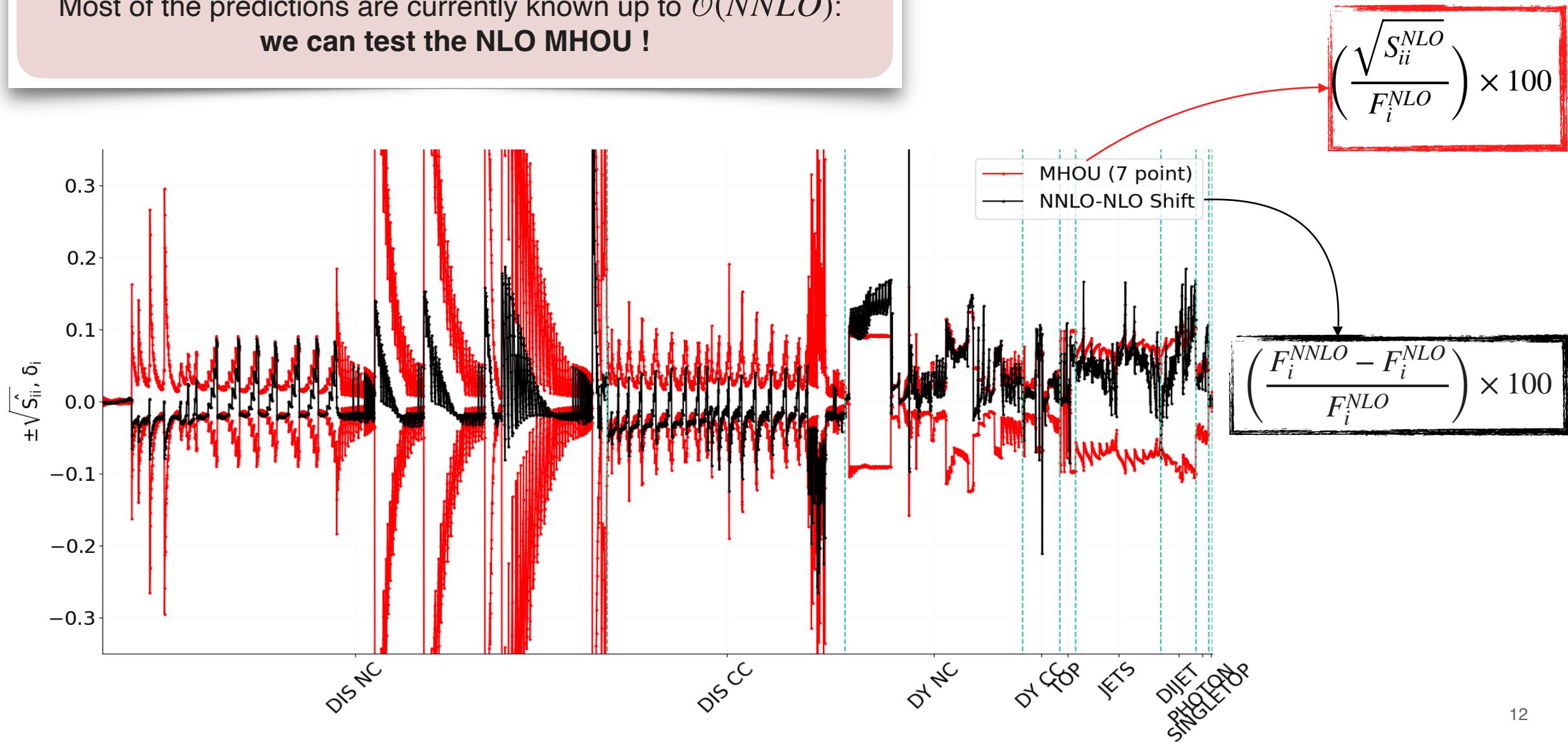


↓
 $C + S$



Validation: is it reproducing the known NNLO?

Most of the predictions are currently known up to $\mathcal{O}(NNLO)$:
we can test the NLO MHOU !



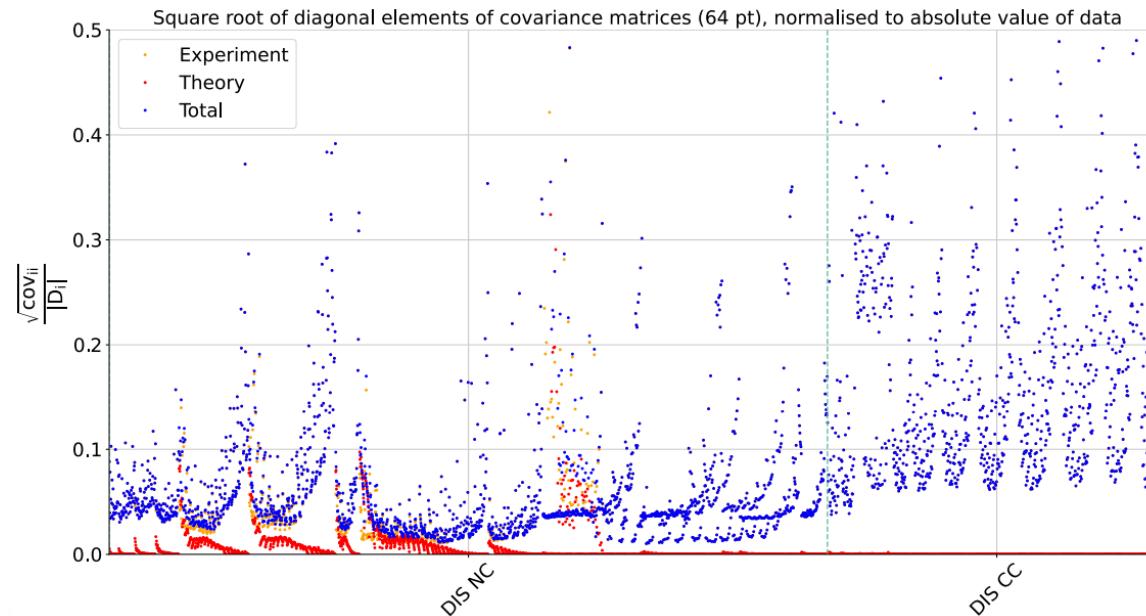
- Not all the ingredients (*coefficient functions, anomalous dimensions,...*) are available at N3LO yet



Incomplete Higher Order Uncertainties (IHOU)



- *Splitting functions @ N3LO*
- *Massive DIS coeff. functions @ N3LO*



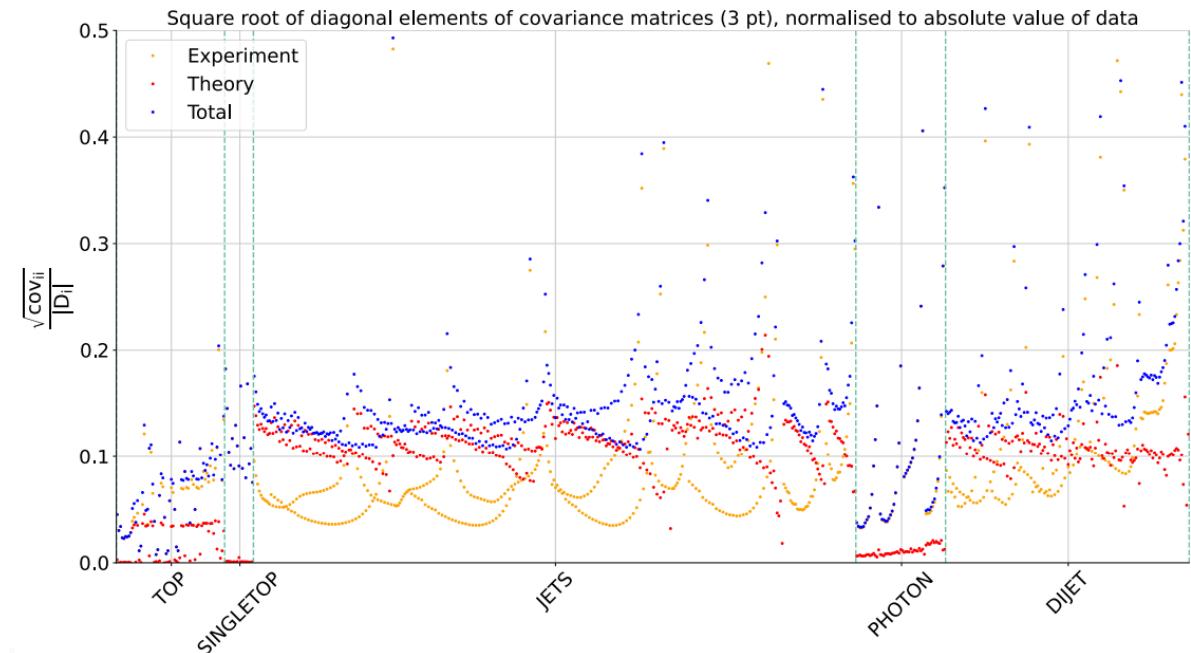
IHOU have a larger effect on the **small-x, low-Q** DIS data



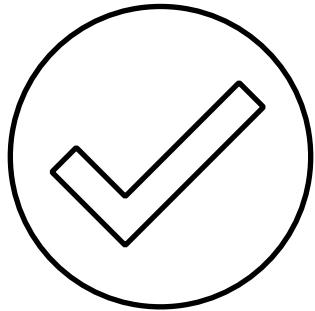
Missing Higher Order Uncertainties (MHOU)



- *NNLO MHOU for all data but DIS*



MHOU are included when ME @ N3LO are not available

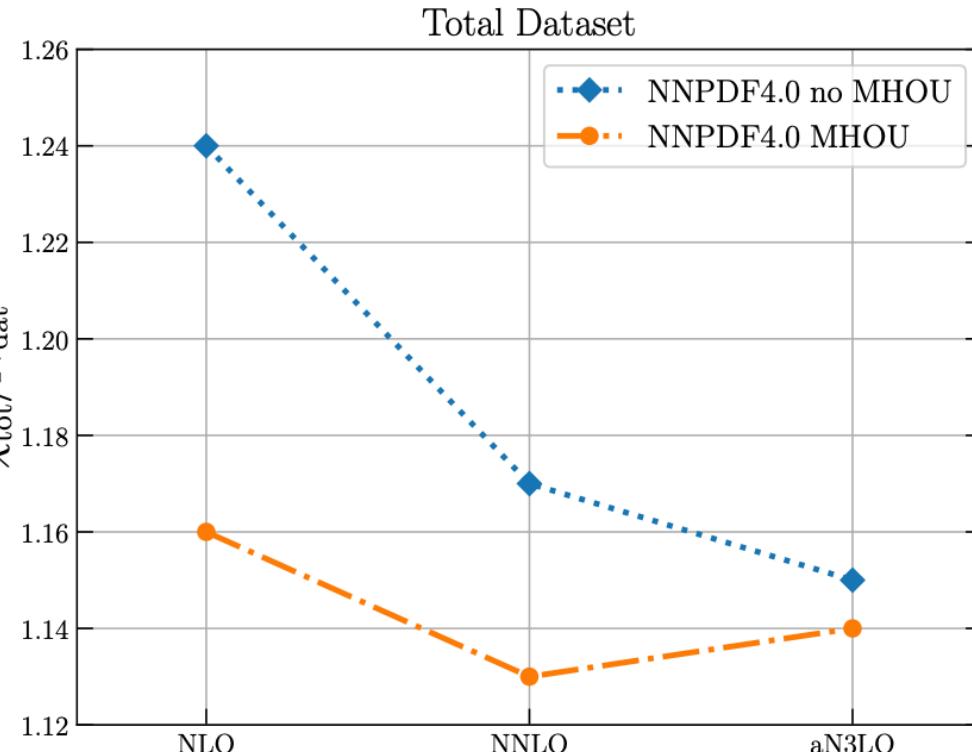


RESULTS

- Does the fit quality improve upon inclusion of theory errors?
- What is the impact on the PDFs?
- What about pheno?

"We're always, by the way, in fundamental physics, always trying to investigate those things in which we don't understand the conclusions. After we've checked them enough, we're okay"
(Richard P. Feynman)

Fit quality.

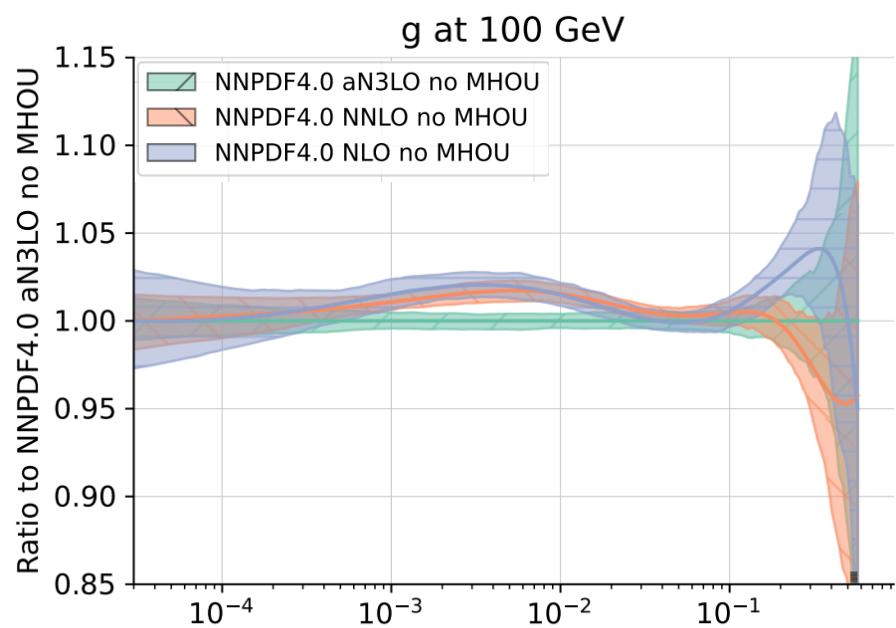


- The χ^2 of the fit with MHOU is much more flat as a function of the perturbative order
- The N3LO fit quality is the same irrespective of whether MHOU are included or not.

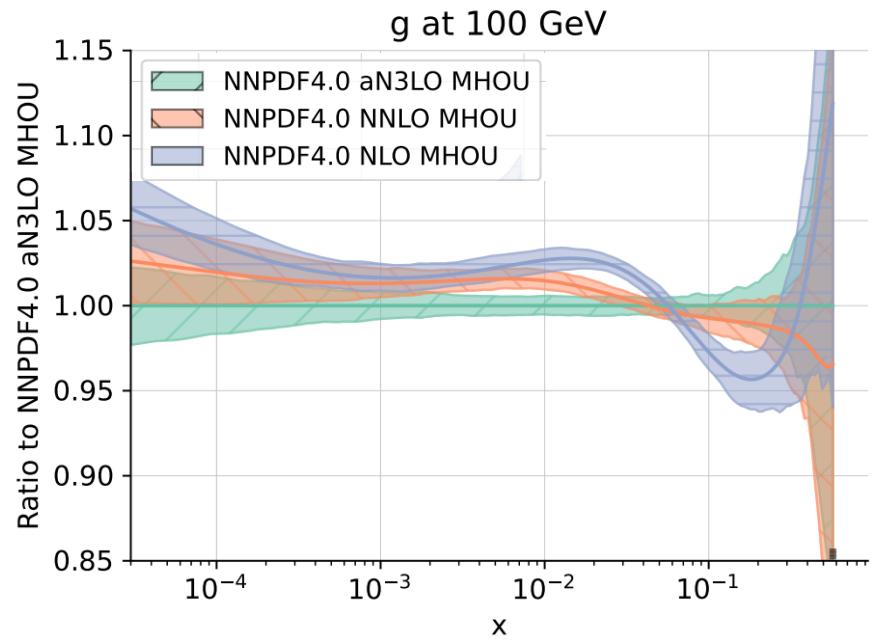
Dataset	χ^2	NLO			NNLO			aN ³ LO		
		N_{dat}	no MHOU	MHOU	N_{dat}	no MHOU	MHOU	N_{dat}	no MHOU	MHOU
DIS NC		1980	1.30	1.22	2100	1.22	1.20	2100	1.22	1.20
DIS CC		988	0.92	0.87	989	0.90	0.90	989	0.91	0.92
DY NC		667	1.49	1.32	736	1.20	1.15	736	1.17	1.16
DY CC		193	1.31	1.27	157	1.45	1.37	157	1.37	1.36
Top pairs		64	1.90	1.24	64	1.27	1.43	64	1.23	1.41
Single-inclusive jets		356	0.86	0.82	356	0.94	0.81	356	0.84	0.83
Dijets		144	1.55	1.81	144	2.01	1.71	144	1.78	1.67
Prompt photons		53	0.58	0.47	53	0.76	0.67	53	0.72	0.68
Single top		17	0.35	0.34	17	0.36	0.38	17	0.35	0.36
Total		4462	1.24	1.16	4616	1.17	1.13	4616	1.15	1.14

PDF comparison.

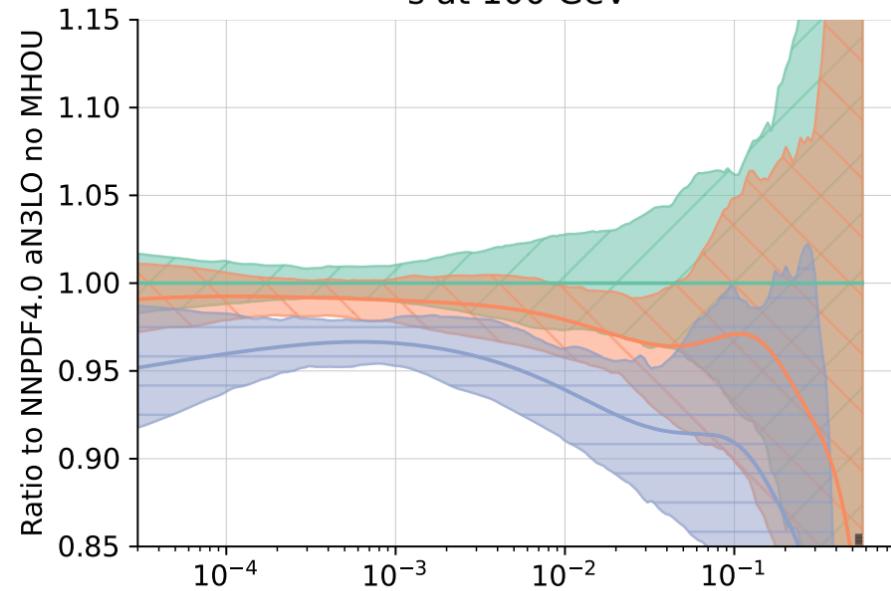
noMHOU



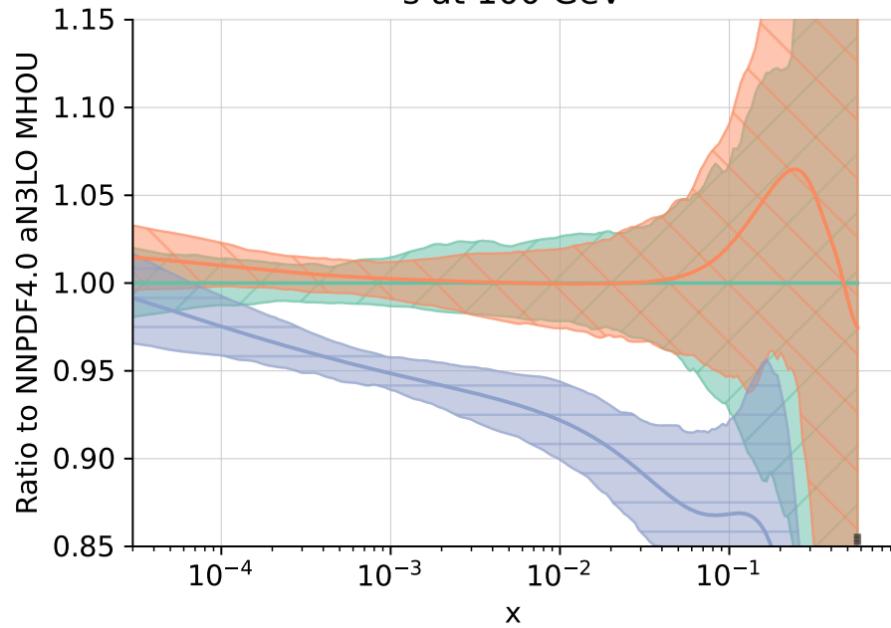
MHOU



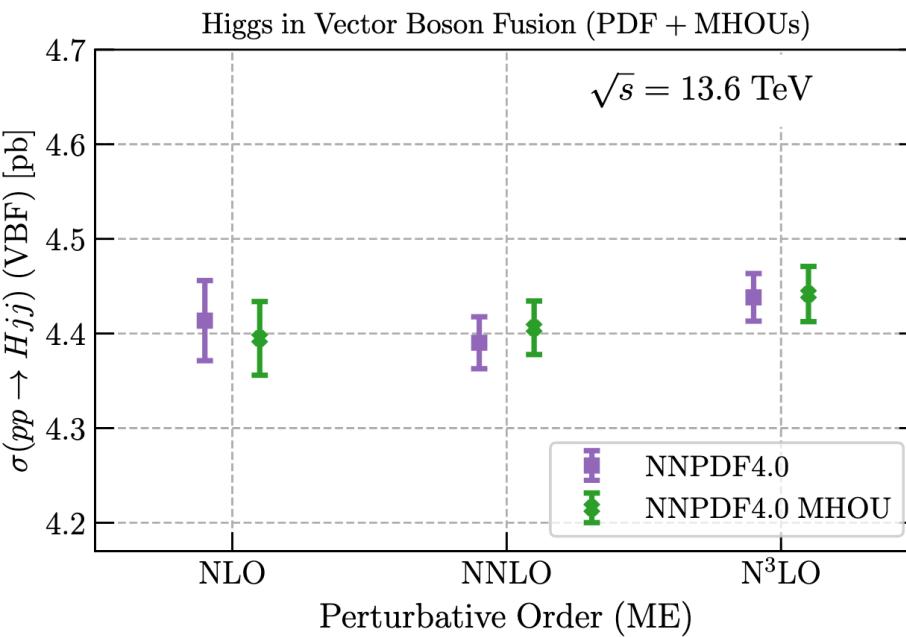
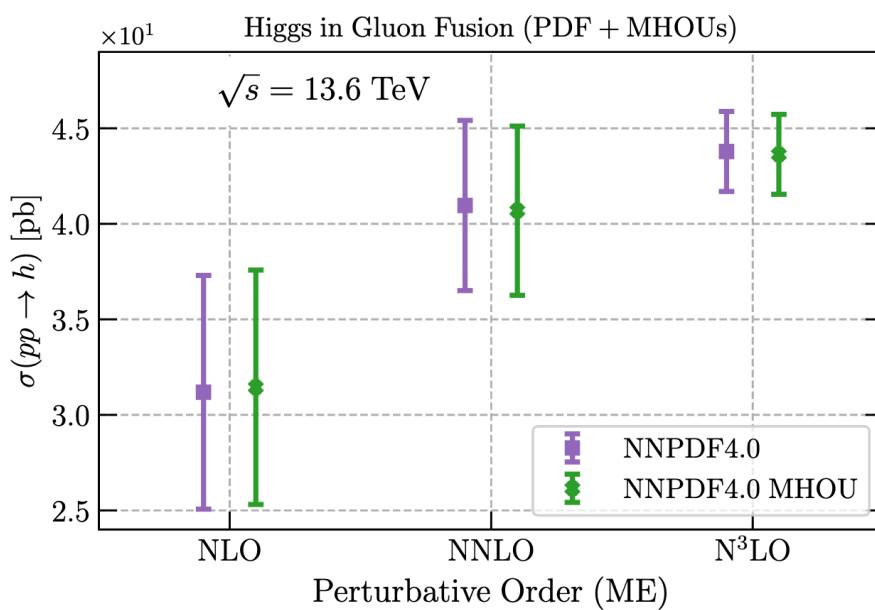
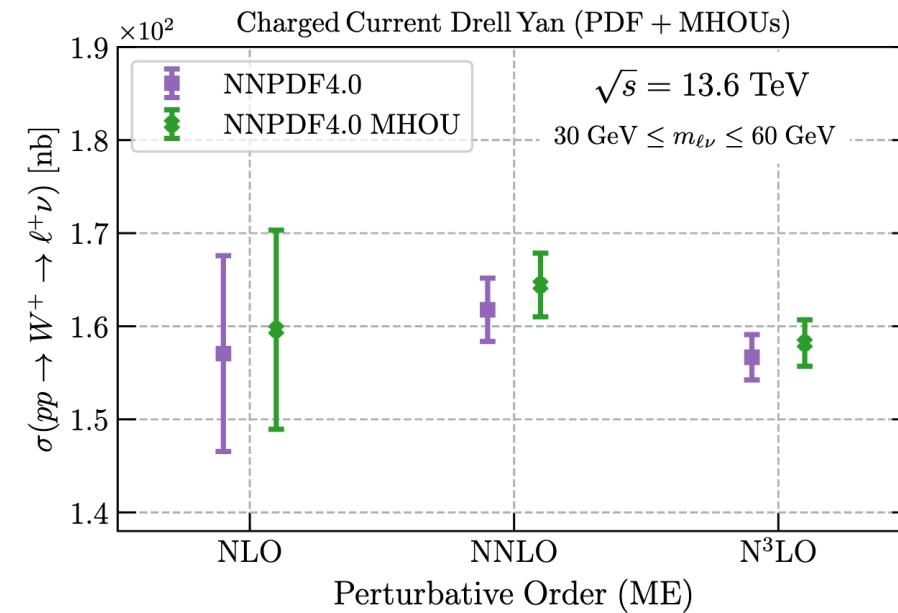
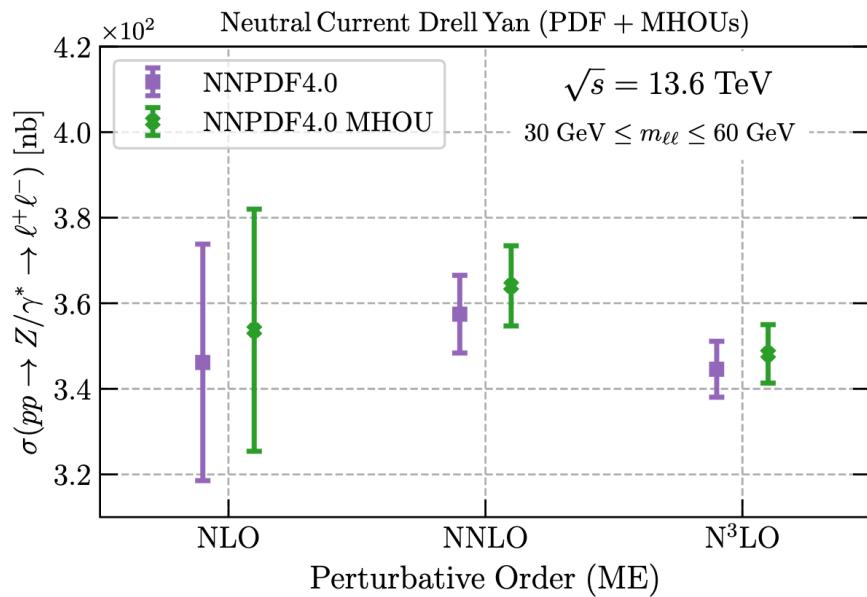
s at 100 GeV



s at 100 GeV



Perturbative convergence.



Conclusions and outlooks.

- Thanks to *scale variations* it is possible to estimate MHOU while, thanks to the theory covmat formalism, it is possible to include such estimation in a PDF fit.
- Including MHOU in a PDF fit is necessary to have faithful uncertainties and central values.
- The perturbative convergence from NLO to N3LO improves once theory errors are accounted for.

Thanks for your attention!



BACKUP

Describing a collision.

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

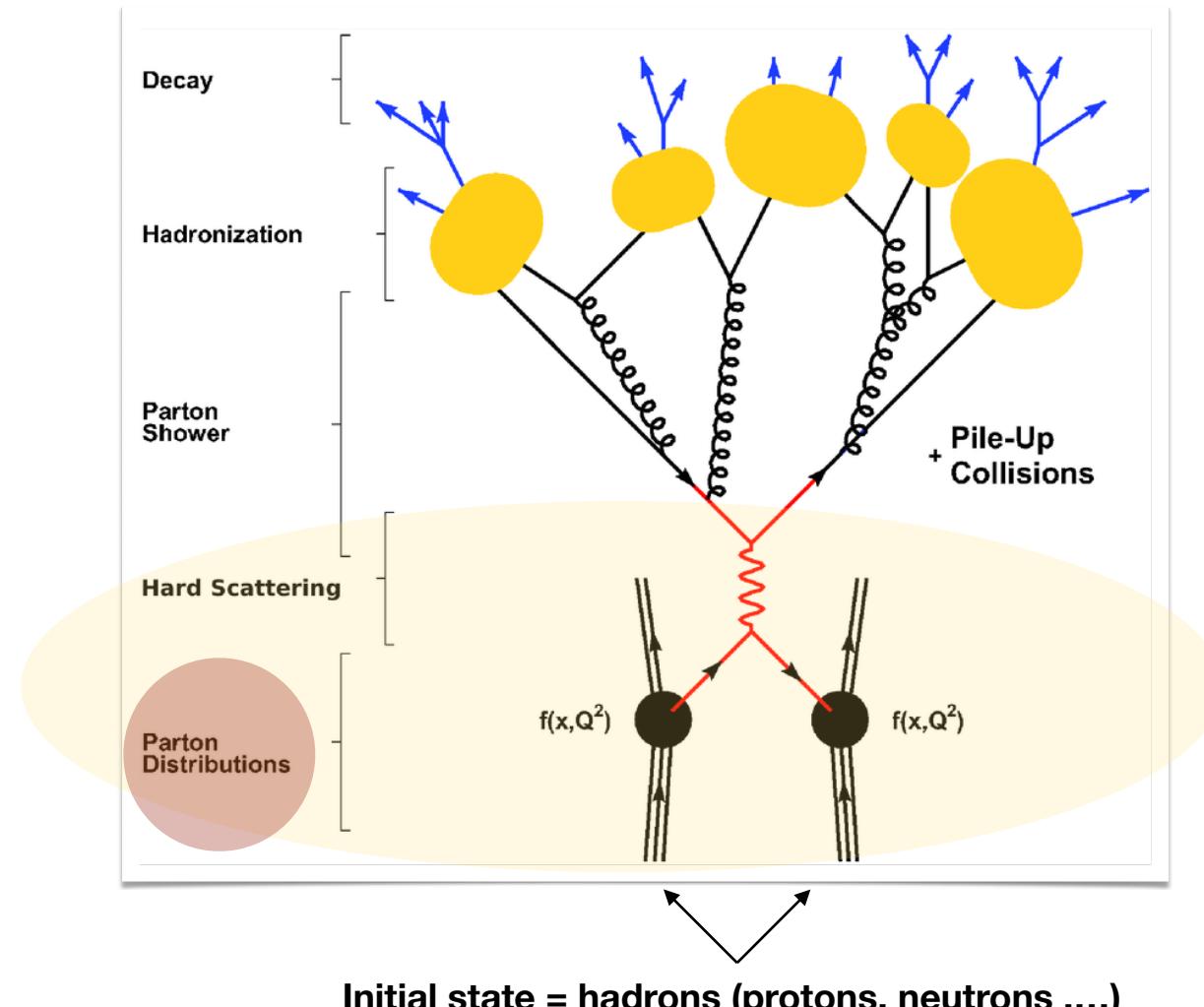


We are going to focus on

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



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



Describing a collision.

Thanks to **Factorization theorem**

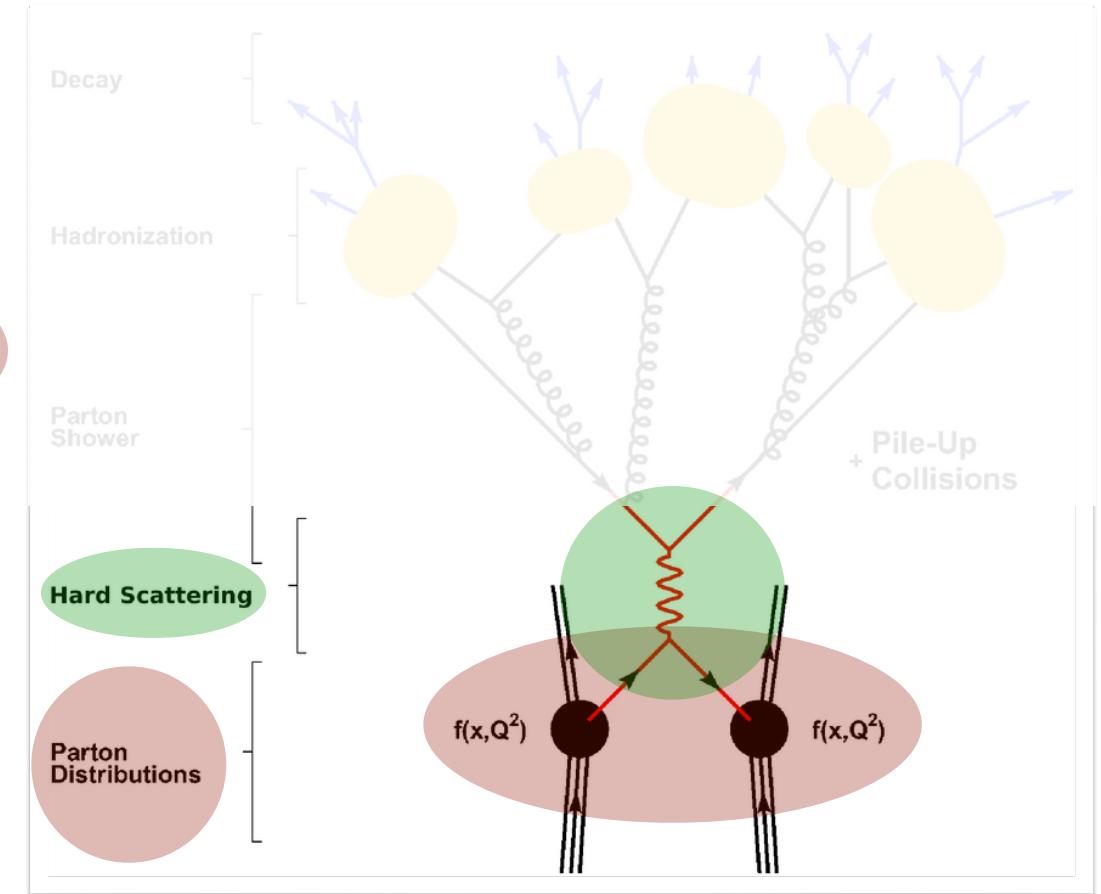
$$\sigma(x, Q^2) = \hat{\sigma}_{ij} \otimes f_i \otimes f_j = \int dz_1 dz_2 \hat{\sigma}(z_1, z_2, Q^2) f_i\left(\frac{x}{z_1}, Q^2\right) f_j\left(\frac{x}{z_2}, Q^2\right)$$

Partonic (hard) cross sections

PDFs

- $\sigma(x, Q^2)$ 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**
NLO, NNLO, ...
- $f_{ilj}(x, Q^2)$ **cannot** be computed in perturbation theory
(and they are **universal**)

↓
Non perturbative objects



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 →



perturbative QCD
(pQCD)
from ~ 1 GeV

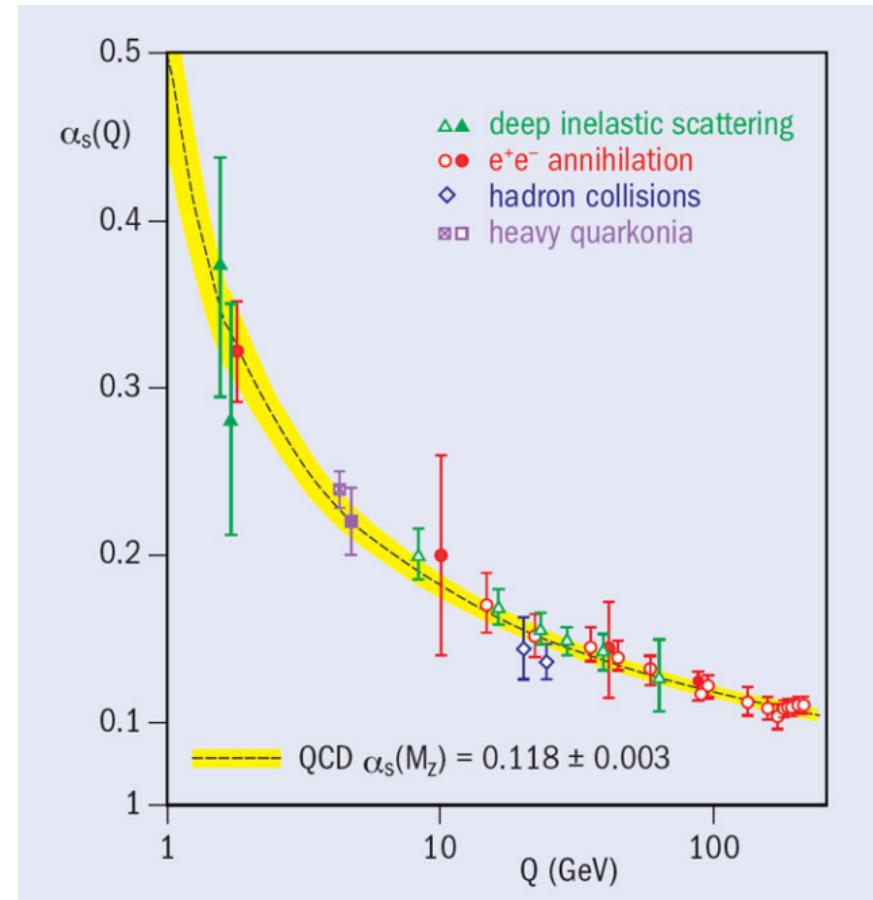
Non perturbative
QCD
below ~ 1 GeV



Partonic cross sections

PDFs
(Mass of the proton ~ 0.938 GeV)

How can we extract them?



Inverse problems.

Number of datapoints is **finite** 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

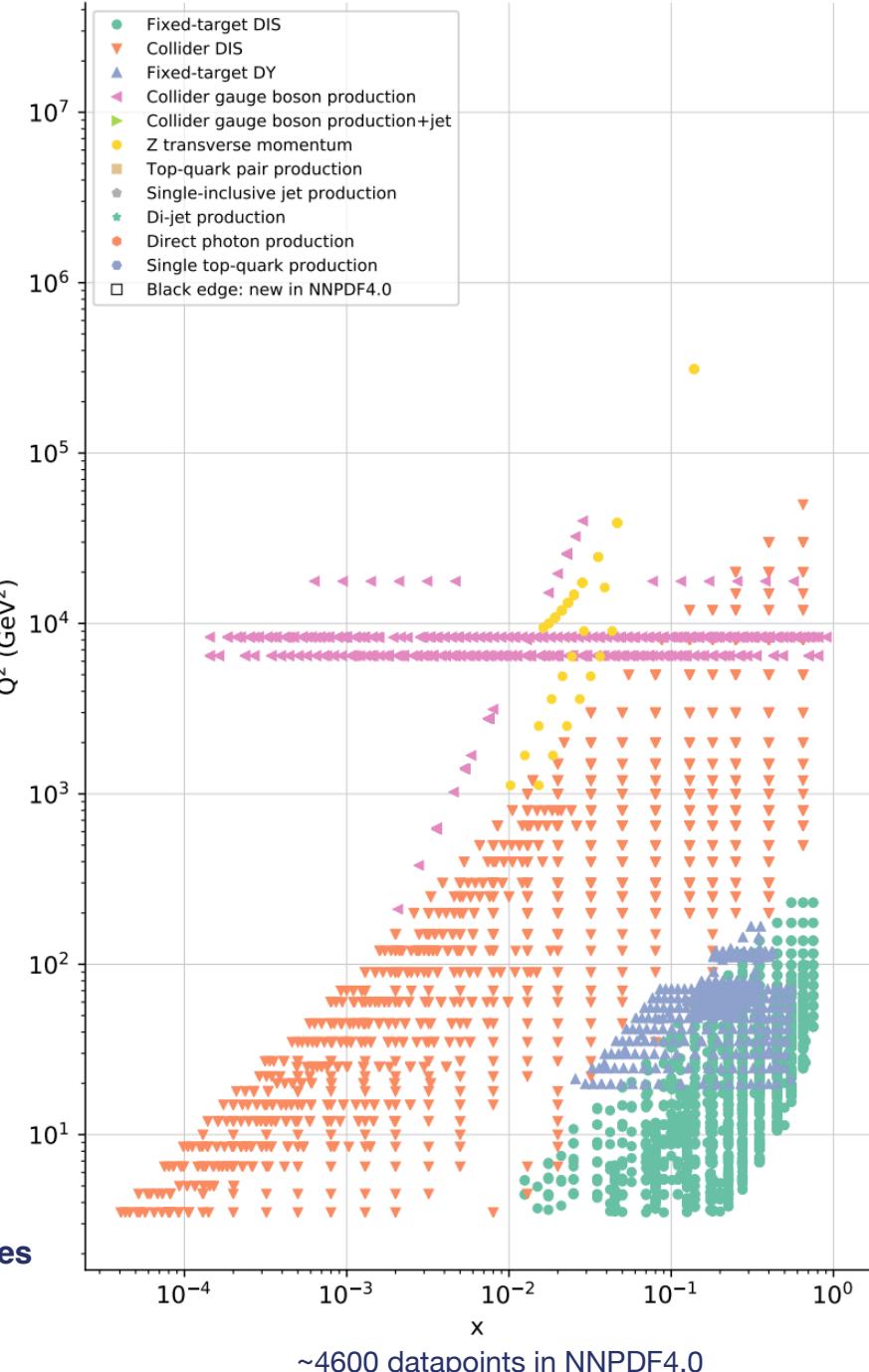
- Applies a **regularization**
- Assumptions = encoded in the network (and not only...)



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

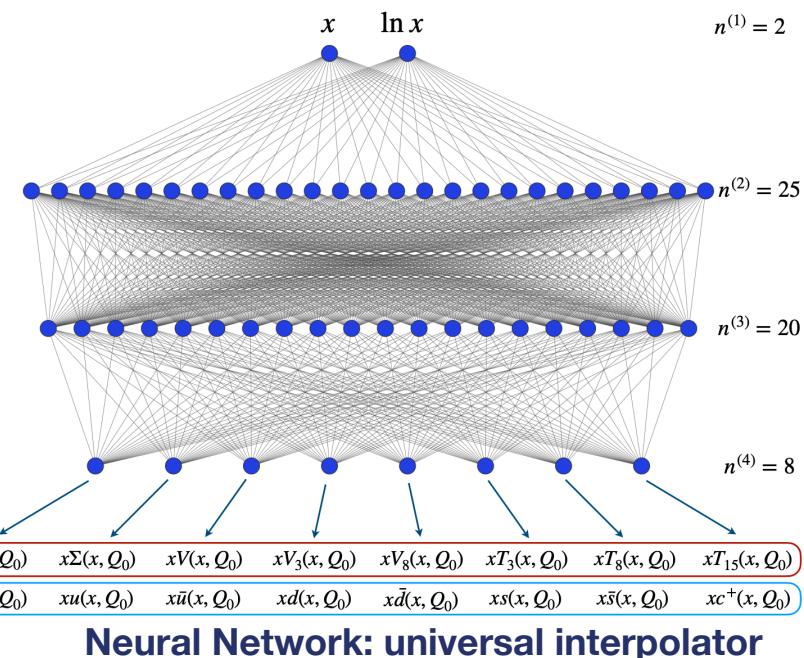


Parametrization: the Neural Network.

$$f(x) = A_k x^{-\alpha_k} (1 - x)^{\beta_k} \mathbf{NN}(x)$$

Architecture: 2-25-20-8

Activation functions: hyperbolic; linear for the last layer

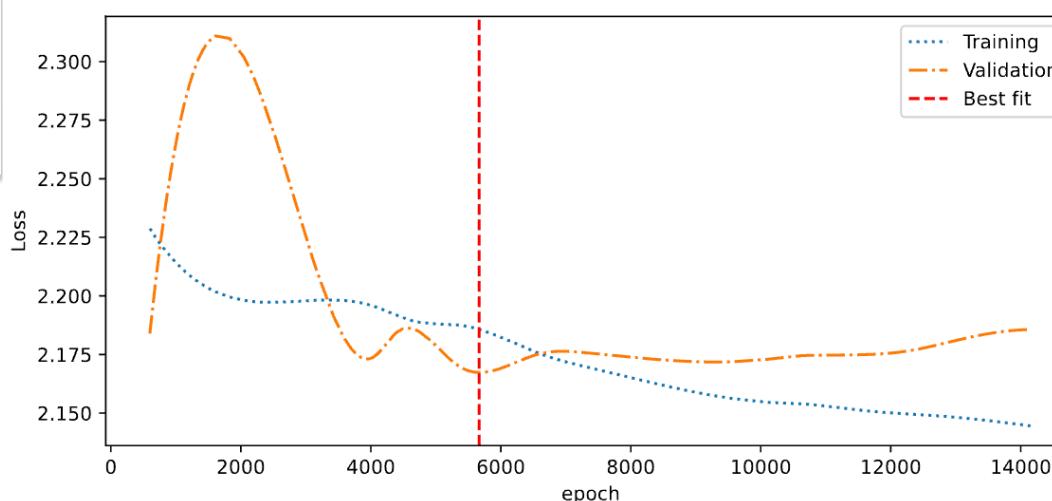


Avoid fitting the noise (**overfitting**)

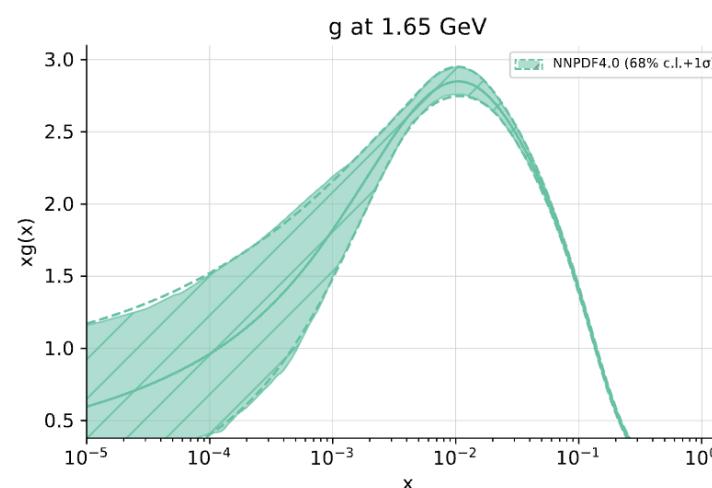
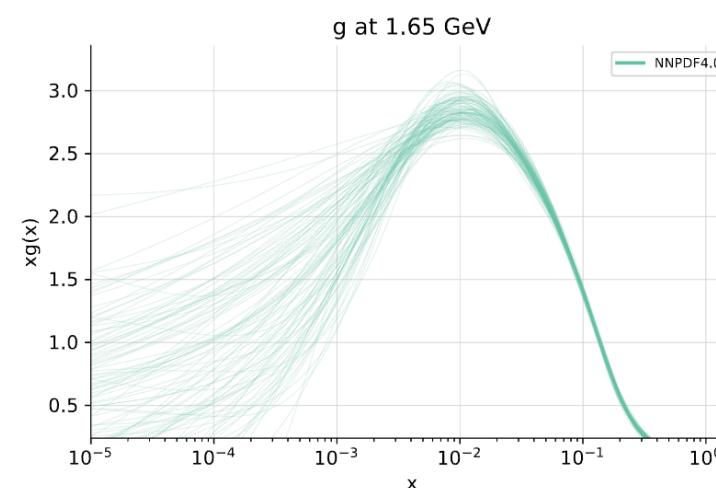
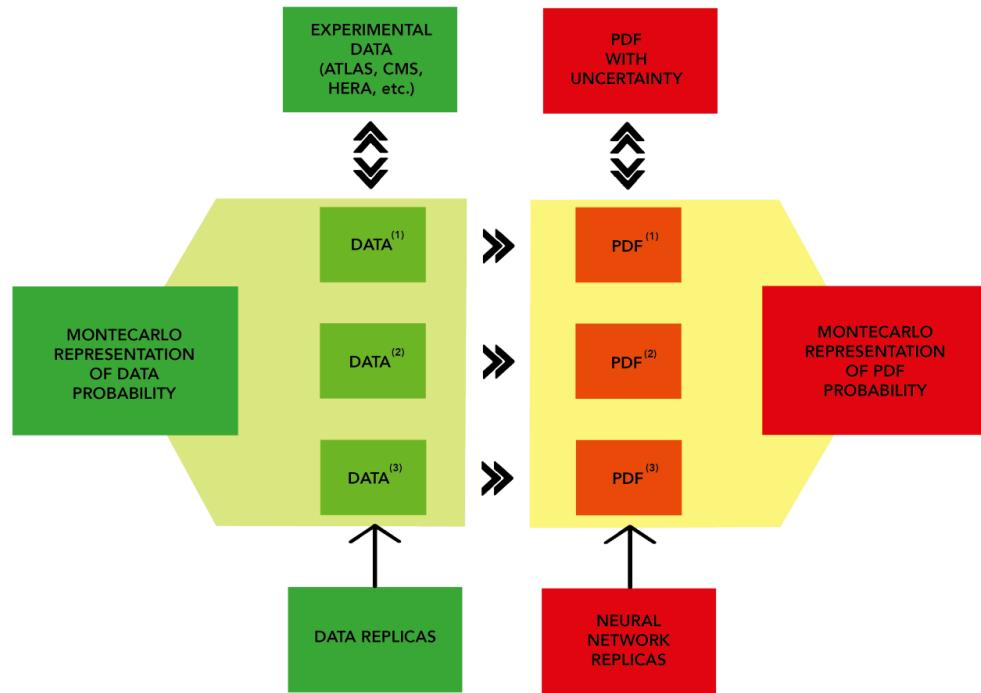
Cross-validation

1. Divide data **D** into **training** set and **validation** set
2. Minimize training χ^2
3. Stop if validation χ^2 no longer improves
4. Take best validation χ^2

Stopping



Propagating uncertainties: data to PDF.



NNPDF adopts 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

Automated model selection

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

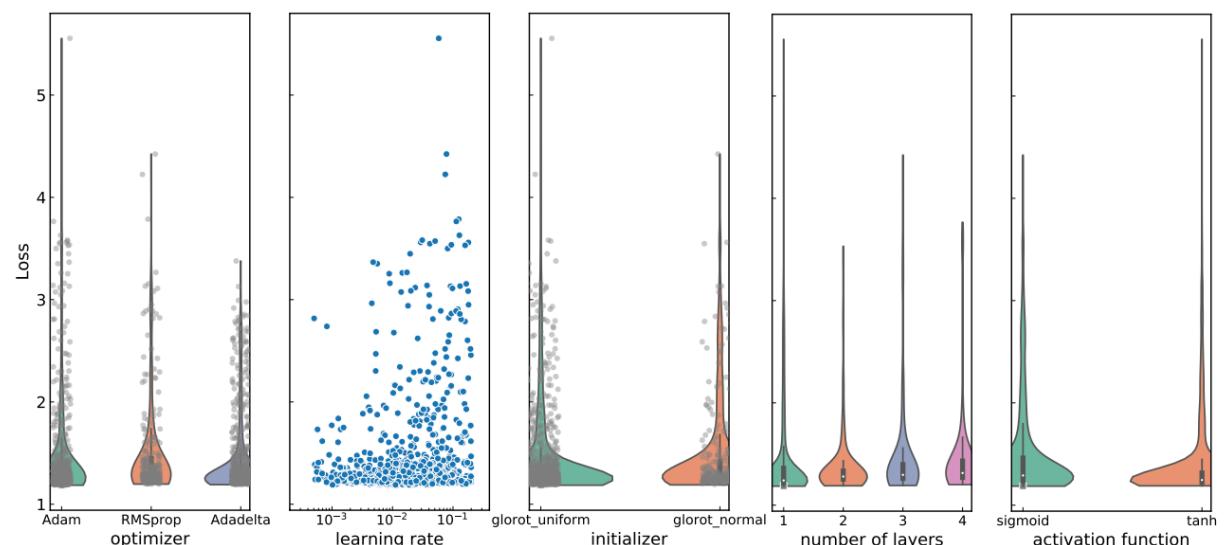
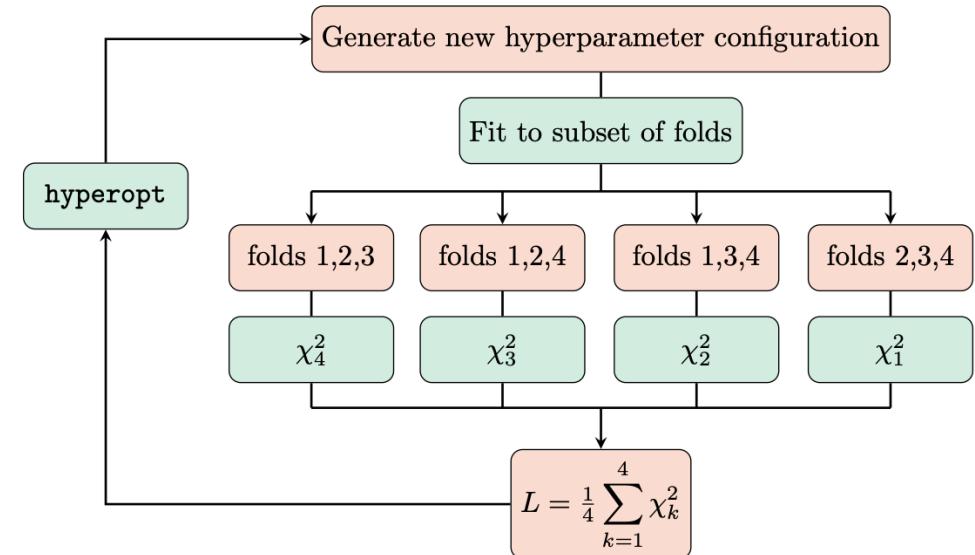
- Functional form → Neural Network
- Model parameters → **Hyperoptimization**



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)



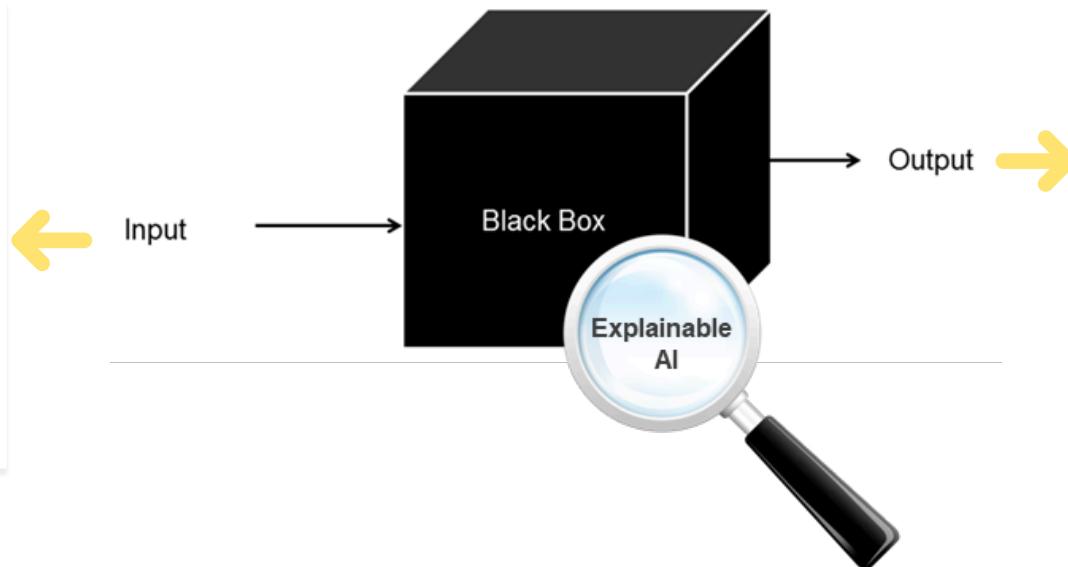
NB: Still requires some human input (more on this later)

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!

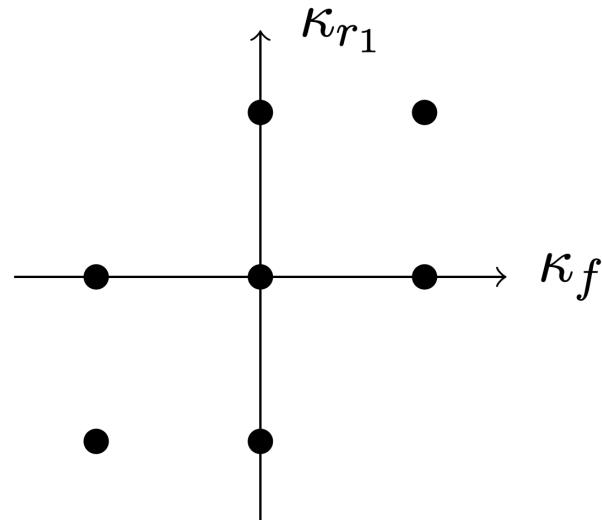
More on the construction: point prescriptions.

Depending on how many (κ_f, κ_r) points among the 9 possible points, one has a different **point prescription**

$$\Delta_{i_a}^{(\pm,0);(\pm,0)} = (\bar{F}(\kappa_f, \kappa_{r_a}) - F)_{i_a} \rightarrow + \rightarrow \kappa_{f,r} = 2.0 \quad - \rightarrow \kappa_{f,r} = 0.5 \quad 0 \rightarrow \kappa_{f,r} = 1.0$$

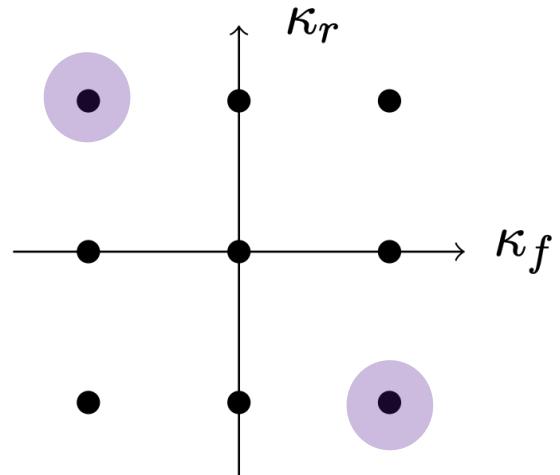
7 points

$$S_{i,j} = \frac{1}{3} [\Delta_i^{+0} \Delta_j^{+0} + \Delta_i^{-0} \Delta_j^{-0} + \Delta_i^{0+} \Delta_j^{0+} \\ + \Delta_i^{0-} \Delta_j^{0-} + \Delta_i^{++} \Delta_j^{++} + \Delta_i^{--} \Delta_j^{--}]$$



9 points

$$S_{i_1,j_2} = \frac{1}{4} [\Delta_i^{+0} \Delta_j^{+0} + \Delta_i^{-0} \Delta_j^{-0} + \Delta_i^{0+} \Delta_j^{0+} + \Delta_i^{0-} \Delta_j^{0-} \\ + \Delta_i^{++} \Delta_j^{++} + \Delta_i^{+-} \Delta_j^{+-} + \Delta_i^{-+} \Delta_j^{-+} + \Delta_i^{--} \Delta_j^{--}]$$

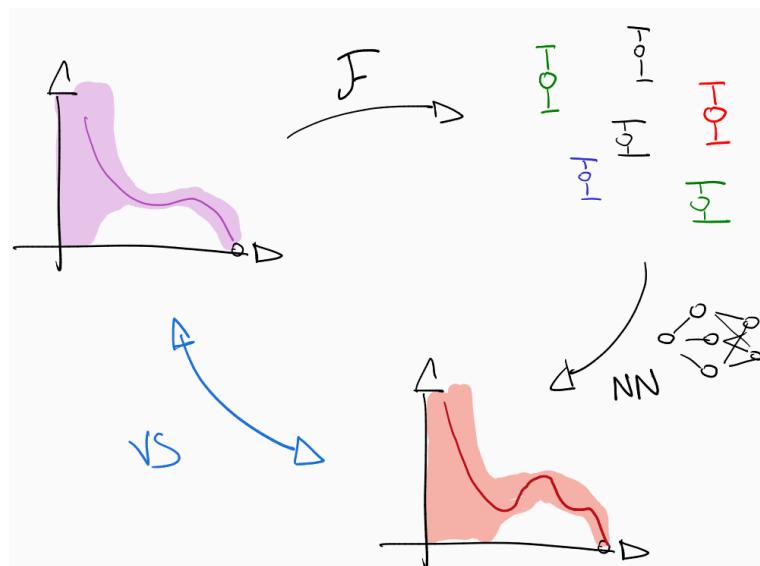


Closure and future tests

Closure test

Test the algorithm in a controlled environment where the “truth” is known

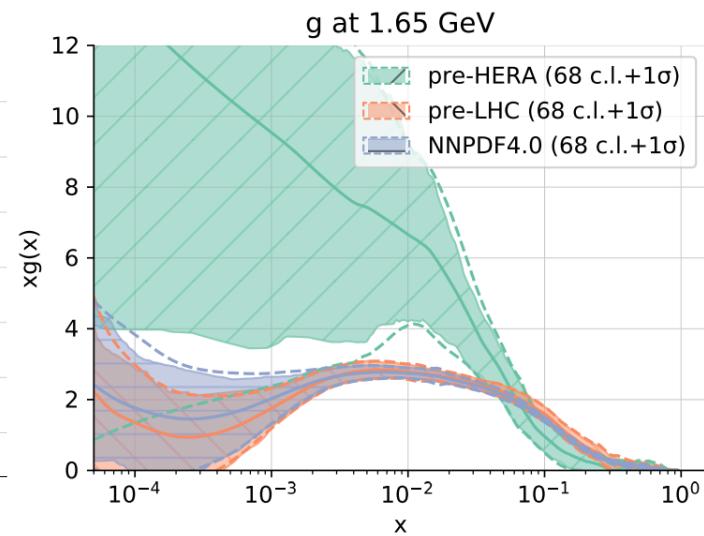
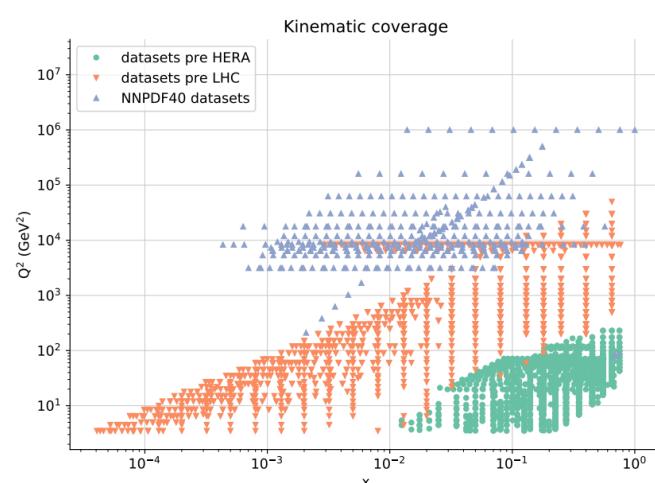
1. Choose a PDF as underlying truth
2. Generate central fake data (**LEVEL 0**)
3. Generate smeared fake data with the experimental covariance matrix (**LEVEL 1**)
4. Generate and fit pseudodata replica (**LEVEL 2**)
5. Compare the results with known distribution



Future test

What about data you have not seen yet?

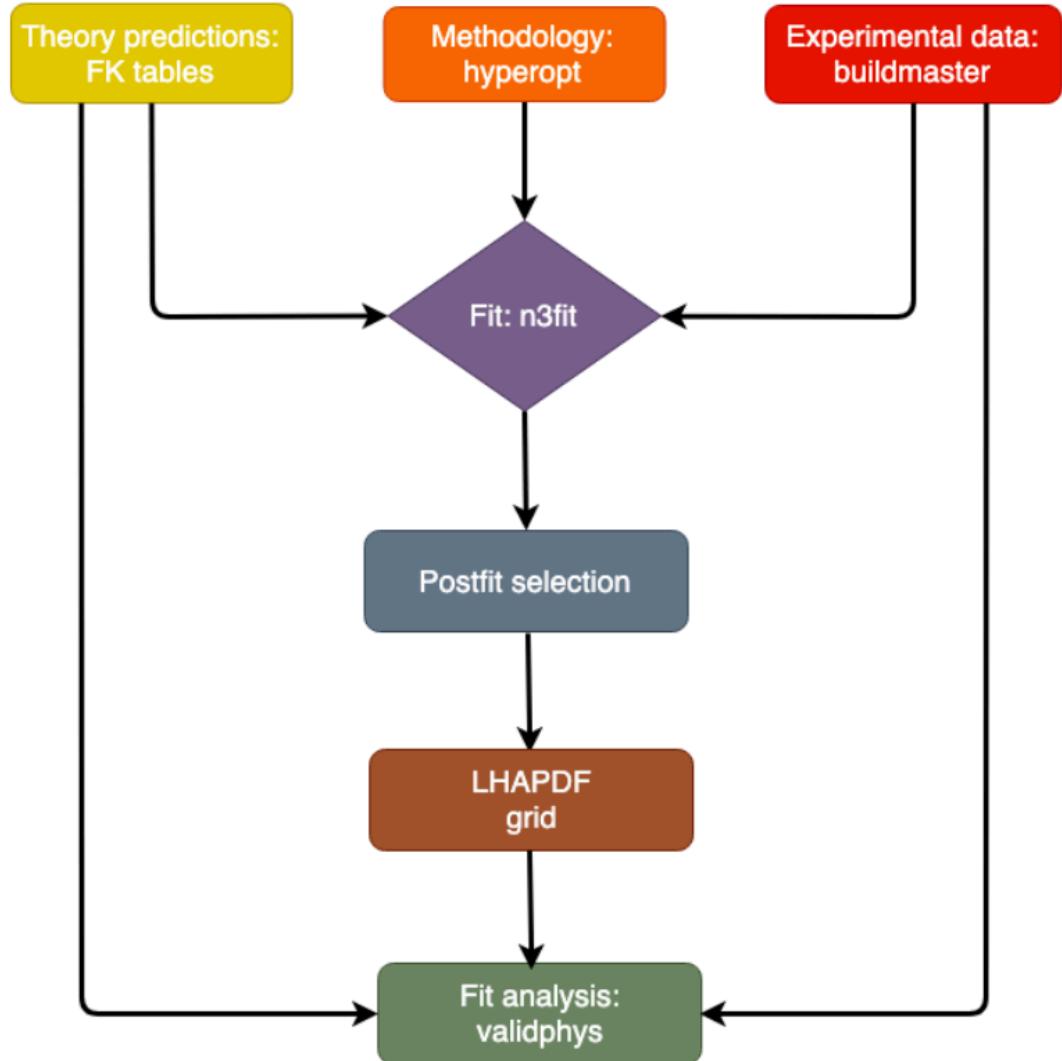
- Traveling in time is not possible but I know **history!**
- Divide the dataset **chronologically** and perform a fit for each set:
yesterday's extrapolation region is today's data region



The NNPDF code is open-source

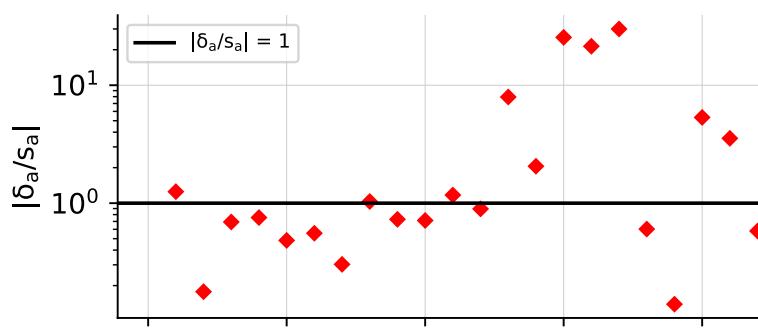
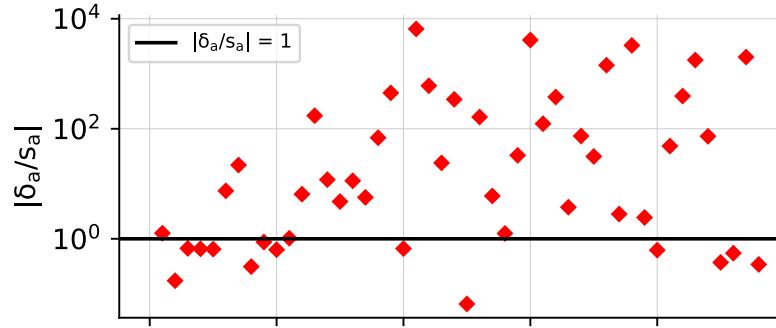
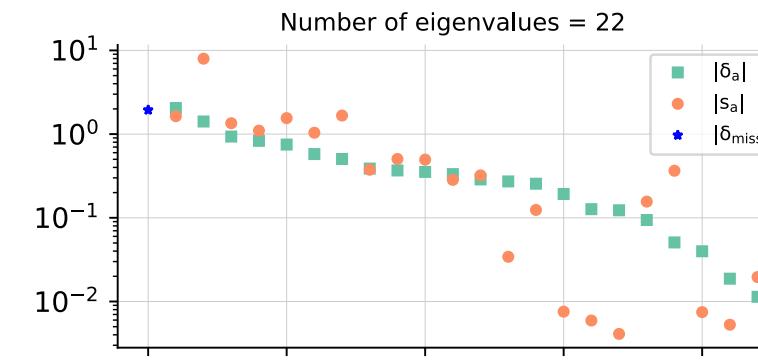
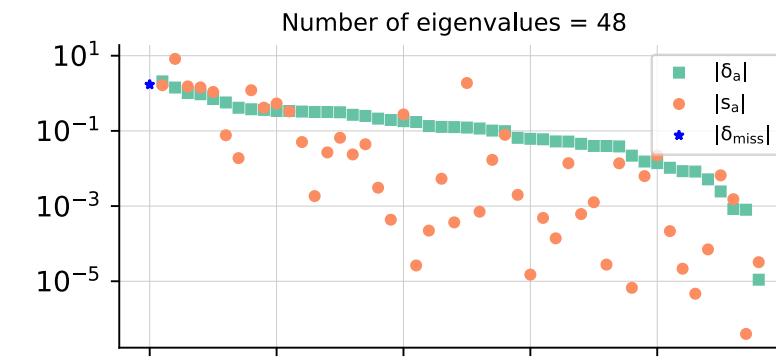
The full NNPDF code has been made **public** along with **user friendly documentation**

-  <https://github.com/NNPDF/nnpdf>
-  <https://docs.nnpdf.science/>



Validation: comparing point prescriptions.

$$\delta_i = \left(\frac{F_i^{NNLO} - F_i^{NLO}}{F_i^{NLO}} \right) \rightarrow \delta^\alpha = \sum_{i=1}^{N_D} \delta_i e_i^\alpha \rightarrow \delta_i^S = \sum_{\alpha=1}^{N_{sub}} \delta^\alpha e_i^\alpha \rightarrow \theta = \arccos\left(\frac{|\delta^S|}{|\delta|}\right) \rightarrow \delta_i^{miss} = \delta_i - \delta_i^S$$



Where e^α are the **eigenvectors** of the theory covariance matrix with eigenvalue $\lambda^\alpha = (s^\alpha)^2$ such that $s^\alpha > 0$

Good agreement for the **largest eigenvalues** with both prescriptions.

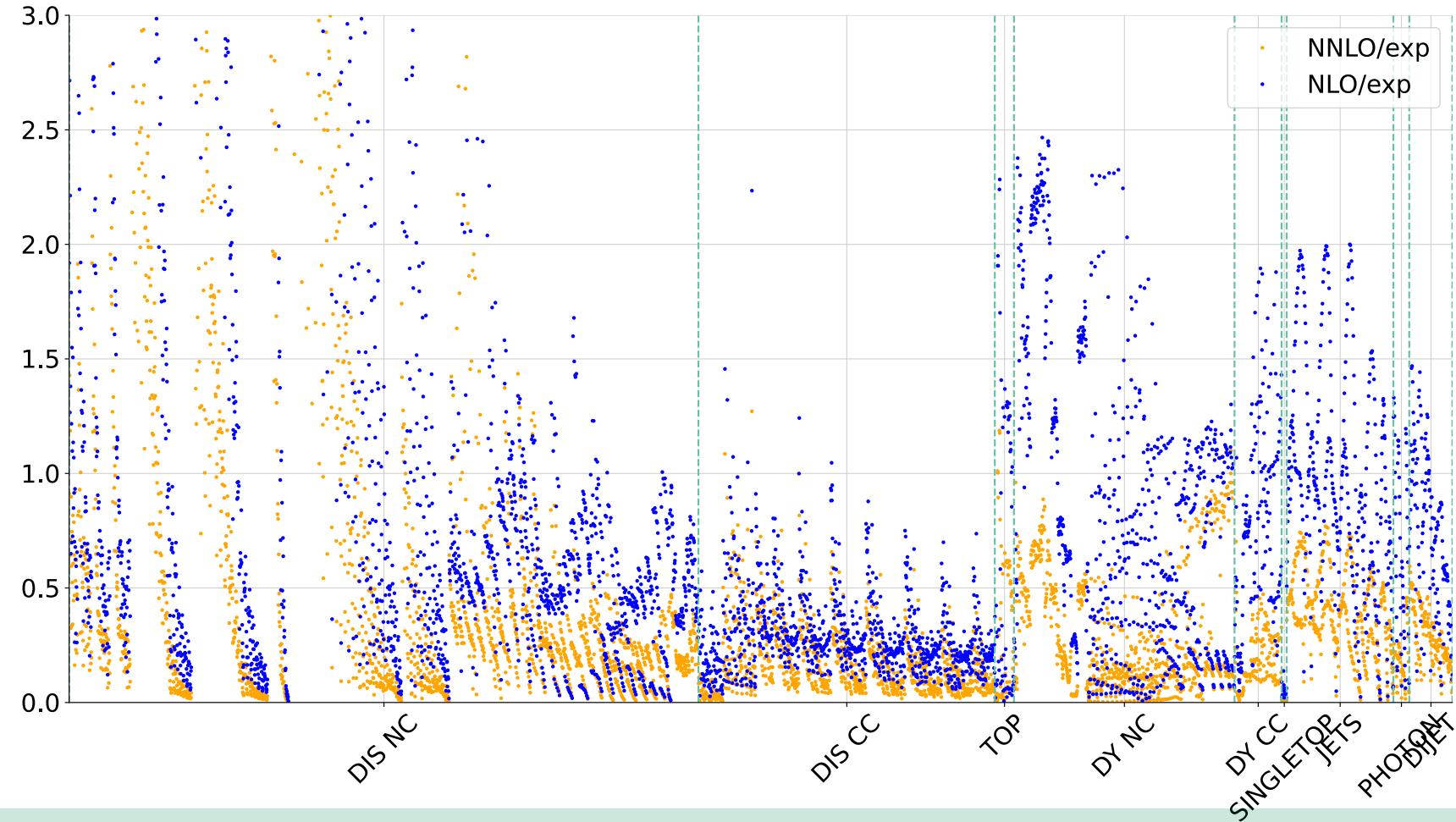
9 pts prescription **underestimates** the size of the shift for smaller eigenvalues

	DIS NC	DIS CC	TOP	DY NC	DY CC	SINGLETOP	JETS	PHOTON	DIJET	TOTAL
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However 9 pts prescription performs better in terms of the **angles** θ

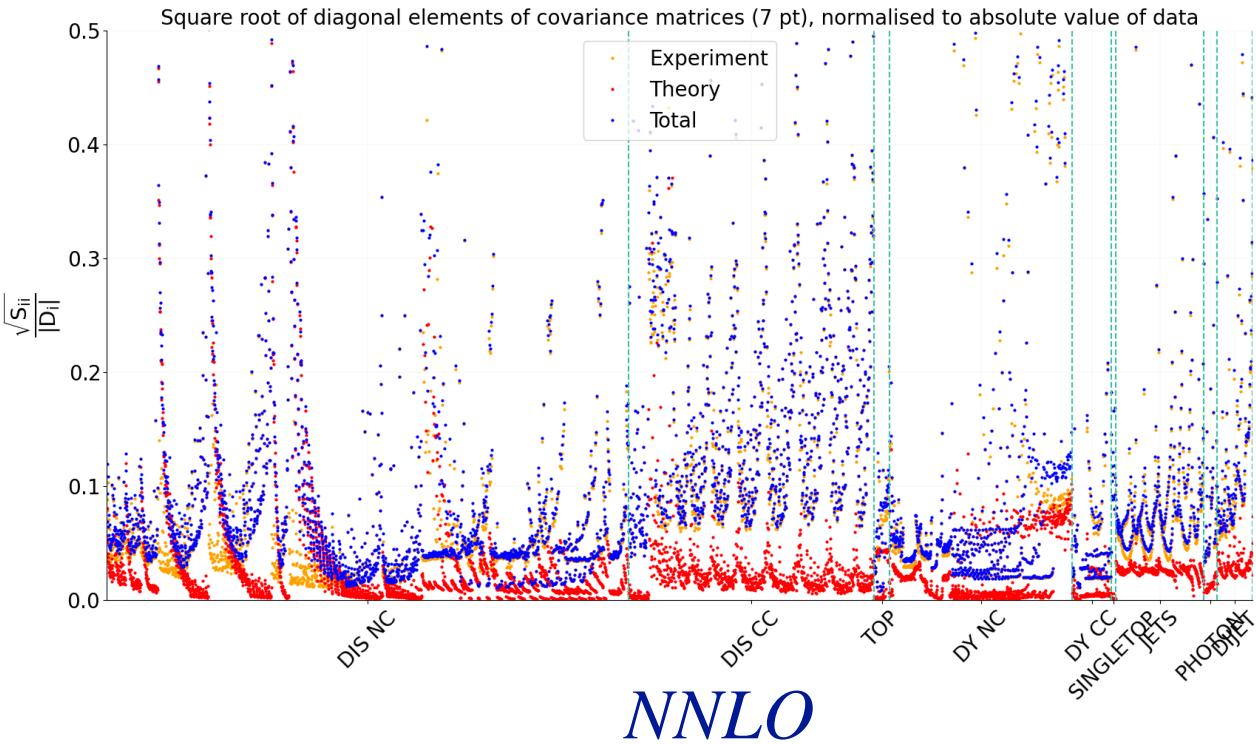
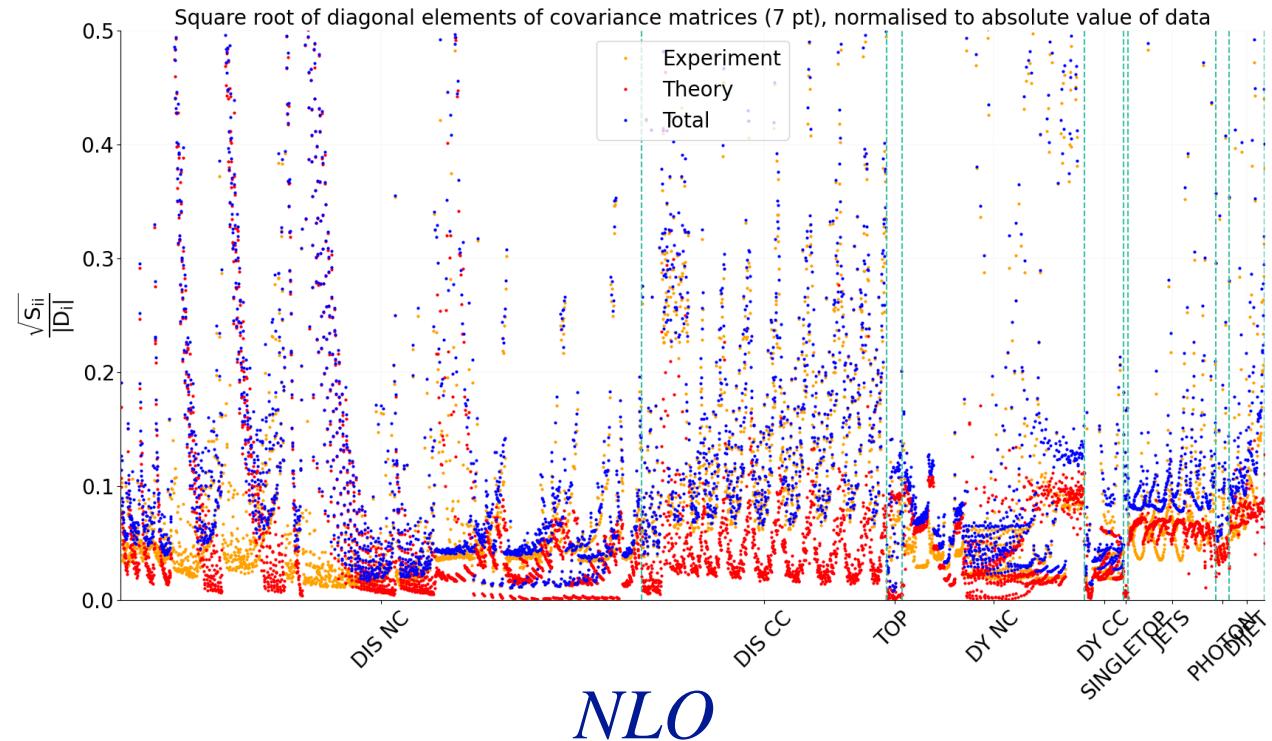
Prescription	N_{sub}	$\theta [{}^\circ]$									
7-point	22	39	18	24	23	38	14	15	12	32	
9-point	48	37	15	20	23	34	12	13	7	28	

Diagonal elements.



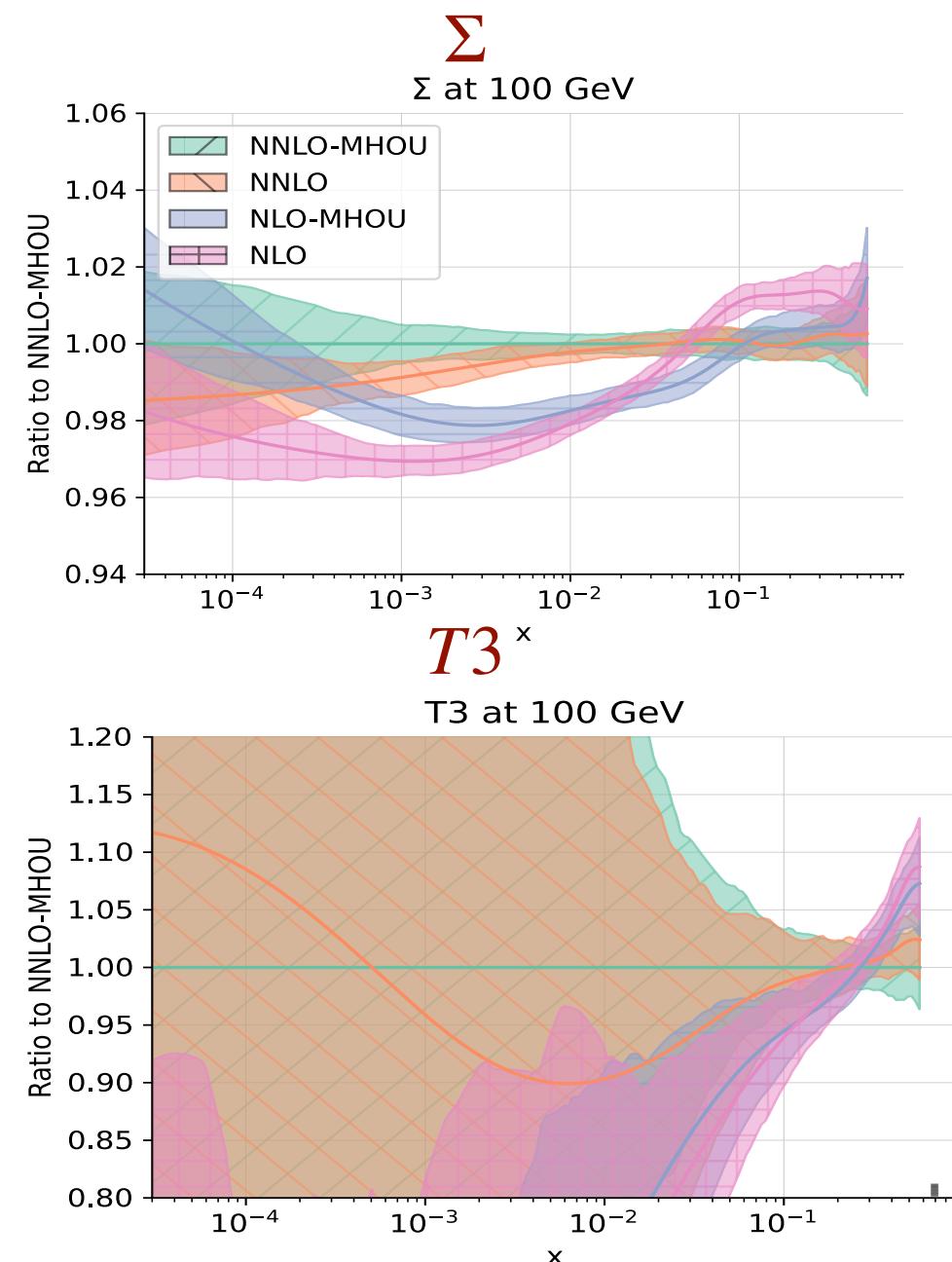
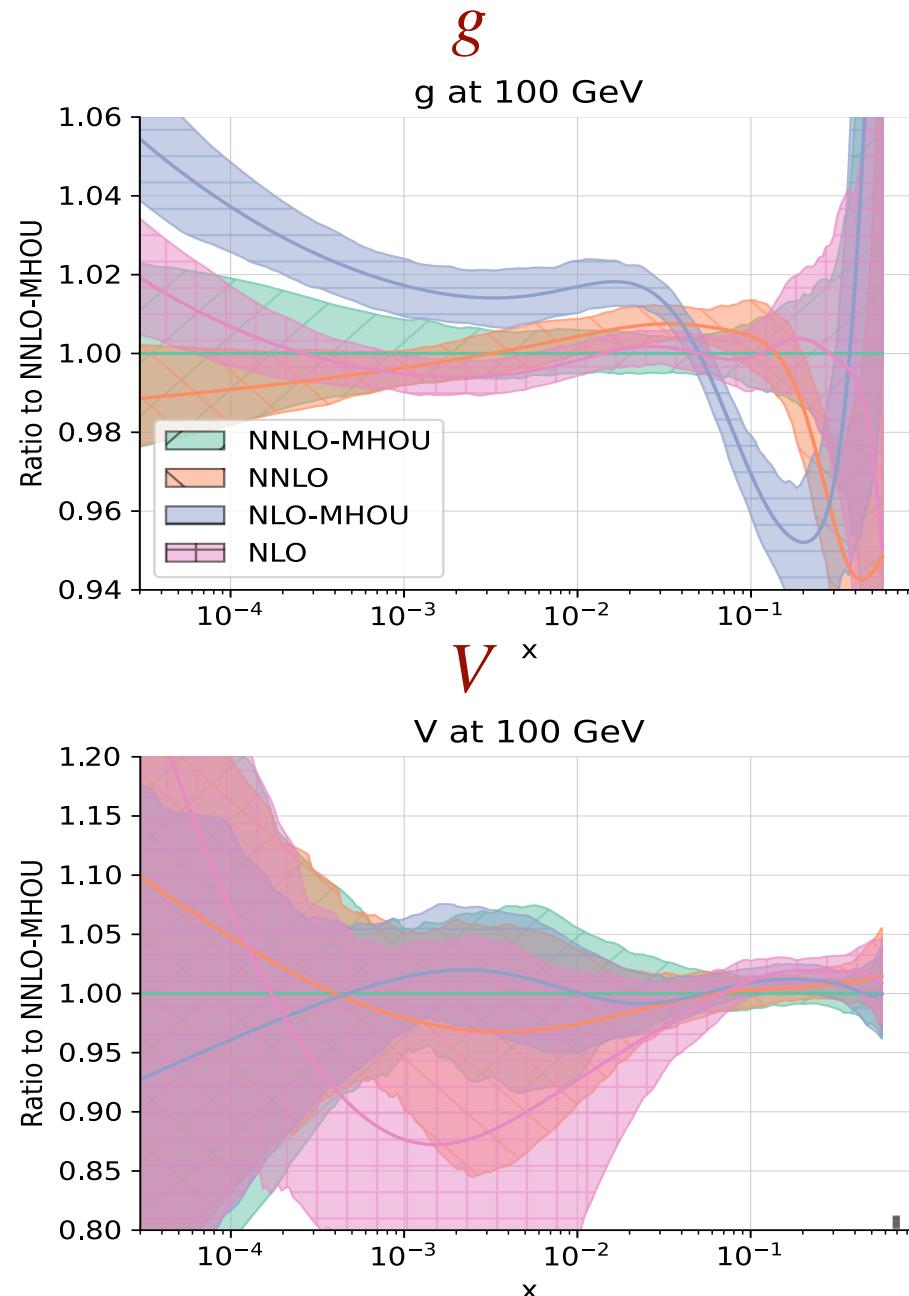
At **NNLO** theory errors are clearly subdominant, while at **NLO** they are of the same size of experimental errors

Diagonal elements.



At **NNLO** theory errors are clearly subdominant, while at **NLO** they are of the same size of experimental errors

PDF comparison.



PDF uncertainties.

