The inclusion of theory errors in PDF fitting

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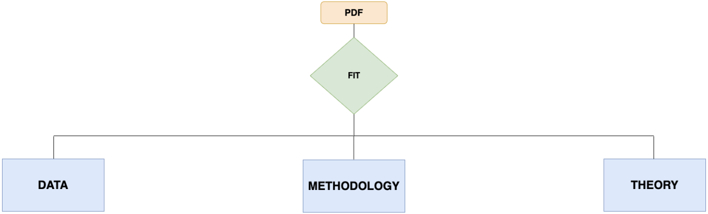
Machine Learning • PDFs • QCD

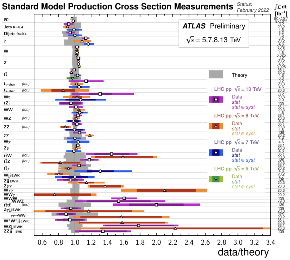
Outline

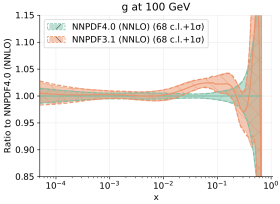
1. **Introduction and motivations**
   - What are theory errors?
   - How can we estimate them?
   - Why including them in a PDF fit is relevant?
2. **Methodology and validation**
   - How can we include MHOU in an NNPDF fit?
   - Can we validate our estimation?
3. **Results**

Introduction and motivations

Theory Errors: motivation







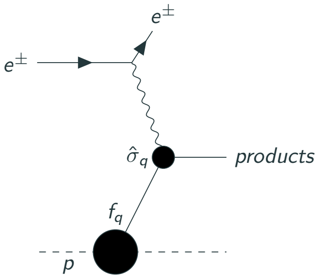
- Keep theory errors under control in PDFs determination.
- Missing higher order uncertainties (MHOU).

Theory Errors: definition of the problem

$$F(Q) = \overbrace{\hat{C}(Q)}^{\text{Coeff. funcs}} \otimes \overbrace{U(Q, Q_0)}^{\text{DGLAP op.}} \otimes \overbrace{f(Q_0)}^{\text{PDFs}}$$

- Coefficient functions are computed in perturbation theory.
- *Anomalous dimensions* inside DGLAP operator are computed in perturbation theory.

Deep Inelastic Scattering



$$\hat{C}_q^{\text{NLO}} = C^{(0)} + \alpha_s C^{(1)} + \overbrace{\mathcal{O}(\alpha_s^2)}^{\text{MHOU}}, \quad \gamma^{\text{NLO}} = \alpha_s \gamma^{(0)} + \alpha_s^2 \gamma^{(1)} + \overbrace{\mathcal{O}(\alpha_s^3)}^{\text{MHOU}}$$

Theory Errors: estimation

Scale variations

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

Thanks to **RGE**

- *Factorization* scale: estimates MHOU of anomalous dimensions.

$$U^{\text{NLO}}(Q, Q_0) \rightarrow \overline{U}^{\text{NLO}}(Q, Q_0, \kappa_f)$$

- *Renormalization* scale: estimates MHOU of coefficient functions.

$$C^{\text{NLO}}(Q) \rightarrow \overline{C}^{\text{NLO}}(Q, \kappa_r)$$

Methodology and validation

MHOU in an NNPDF fit: the theory covmat

Central fit

Experimental covariance matrix $\mathcal{C}$

- $\chi^2 \propto (D_i - T_i)\mathcal{C}_{ij}^{-1}(D_j - T_j)$.
- *Pseudodata* $\propto \mathcal{C}$.

MHOU fit

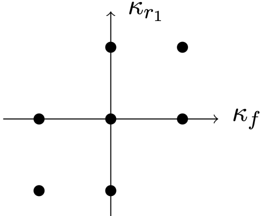
Theoretical covariance matrix $\mathcal{S}$

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

Constructing the theory covmat $\mathcal{S}$:

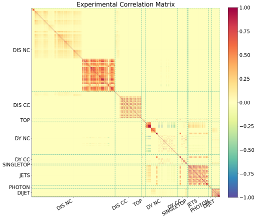
- $\mathcal{S}_{ij} = n_m \sum_{V_m} (\overline{F} - F)_{i_a} (\overline{F} - F)_{j_b}, \quad i, j \in$ datapoints
- Takes into account correlations between processes.
- MHOU affects relative weights of observables.

- $\kappa_f, \kappa_r \in (0.5, 1.0, 2.0)$
- 7 point prescription

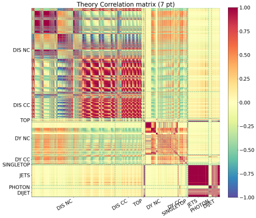


How does it look like?

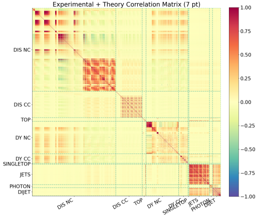
$\mathcal{C}^{\text{NLO}}$



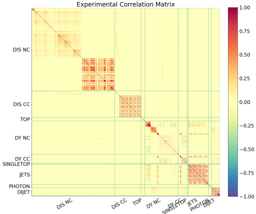
$\mathcal{S}^{\text{NLO}}$



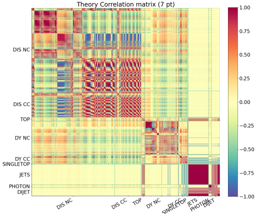
$\mathcal{C}^{\text{NLO}} + \mathcal{S}^{\text{NLO}}$



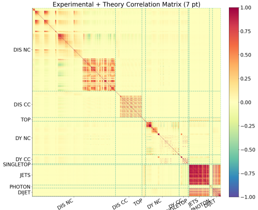
$\mathcal{C}^{\text{NNLO}}$



$\mathcal{S}^{\text{NNLO}}$



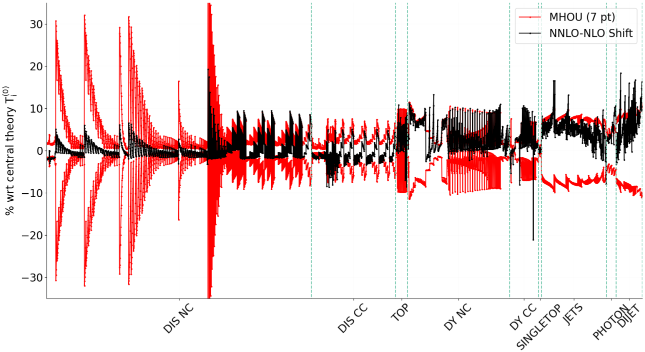
$\mathcal{C}^{\text{NNLO}} + \mathcal{S}^{\text{NNLO}}$



Is it reproducing the theory errors?

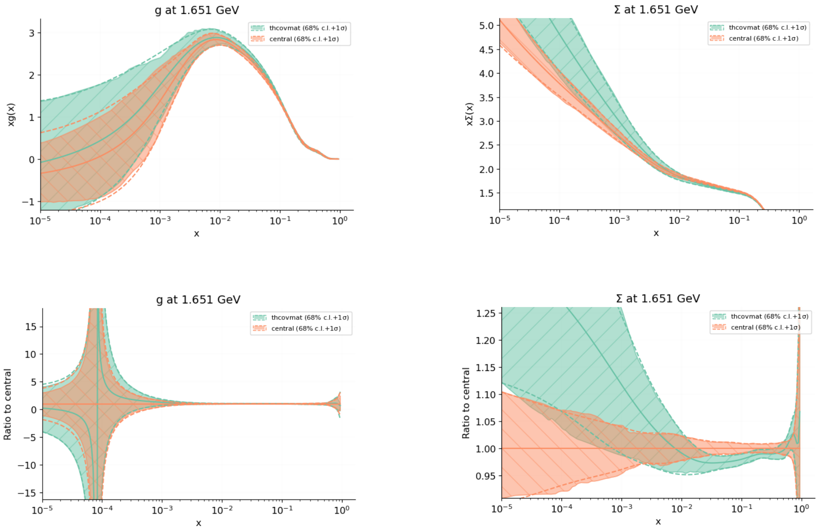
- Most of the predictions are currently known up to NNLO.

$$\left(\frac{\sqrt{\mathcal{S}_{ii}^{\text{NLO}}}}{F_i^{\text{NLO}}}\right) \times 100 \qquad \left(\frac{F_i^{\text{NNLO}} - F_i^{\text{NLO}}}{F_i^{\text{NLO}}}\right) \times 100$$

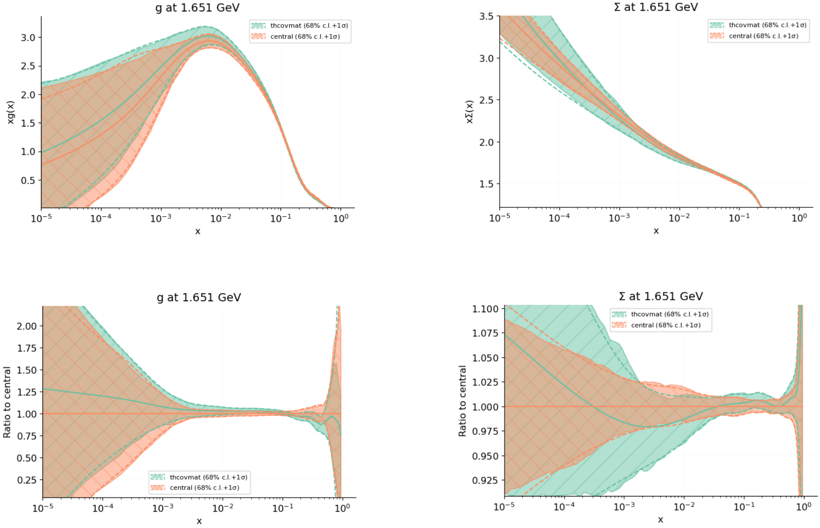


Results

Both central values and uncertainties change: NLO



Both central values and uncertainties change: NNLO

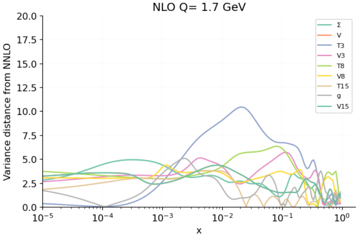


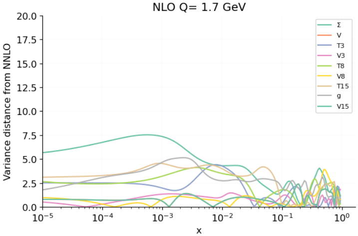
Uncertainties seem to be less affected than central values

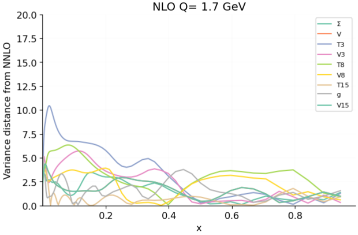
The perturbative convergence improves

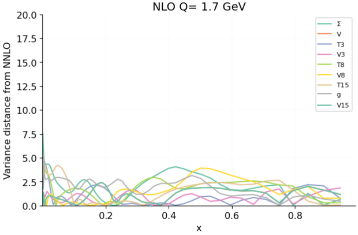
Central fit

MHOU fit

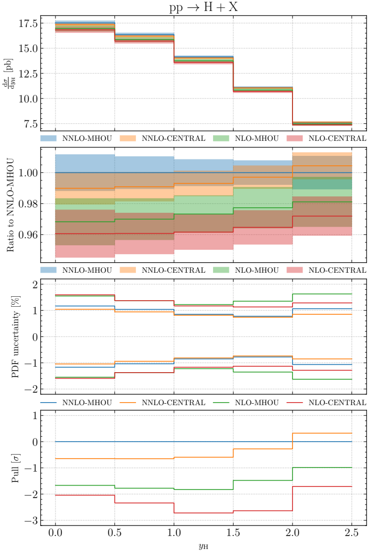


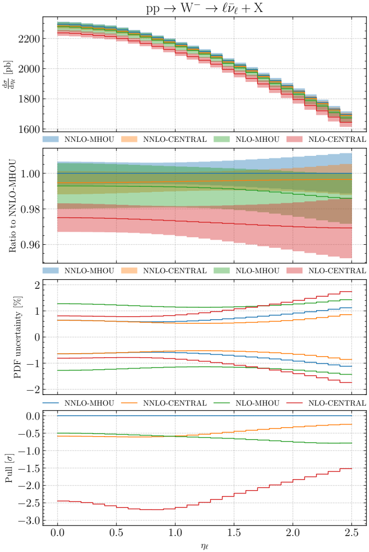






Phenomenology improvements





Conclusion

- Thanks to *scale variation* it is possibile to estimate MHOU while, using the theory covmat formalism, it is possible to include them in an PDF fit.
- Including MHOU in a PDF fit is necessary to have faithful uncertainties and central values.
- The perturbative convergence from NLO to NNLO improves when including MHOU in the fit.

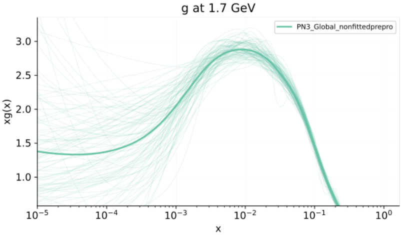
Thanks for your attention!

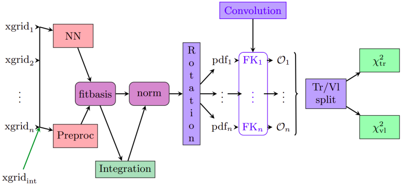
BACKUP SLIDES

The fitting problem: NNPDF methodology

- Neural Network used to provide an unbiased functional form
  - $f_i = A_i x^{\alpha_i}(1-x)^{\beta_i} NN_i(x, \log x)$
- Minimization of the *loss function*

$$\chi^2 = \sum_{ij}^{N_{\rm dat}} (D-P)_i C^{-1}_{ij} (D-P)_j \quad C = \text{experimental covariance matrix}$$





Theory Errors: estimation

Scale variations

$$\overline{F}^{\text{NLO}}(\mu_F = \xi_F Q, \mu_R = \xi_R Q) - F^{\text{NLO}}(\mu_F = Q, \mu_R = Q) = \mathcal{O}(\text{NNLO})$$

Thanks to **RGE**

- *Factorization* scale: estimates MHOU of anomalous dimensions.

$$\overline{U}^{\text{NLO}}(Q, Q_0, \xi_F) = \left[1 + \alpha_s(\xi_F Q) \ln(\xi_F^2) \gamma^{(0)}\right] U^{\text{NLO}}(Q, Q_0)$$

- *Renormalization* scale: estimates MHOU of coefficient functions.

$$\overline{C}^{\text{NNLO}}(Q, \xi_R) = C^{(0)} + \alpha_s(\xi_R Q) C^{(1)} + \alpha_s^2(\xi_R Q)(C^{(2)} + \ln(\xi_R^2) \beta^{(0)} C^{(1)})$$

How to include theory uncertainties in a fit

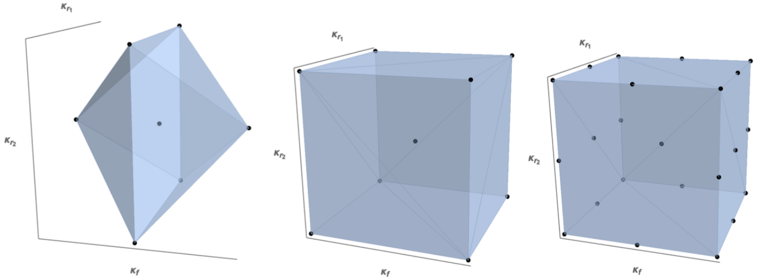
- Under gaussianity hypothesis

$$P(T|D) \propto \exp(-\frac{1}{2}(D_i - T_i)(C+S)^{-1}_{ij}(D_j - T_j))$$

- C, S : experimental and theoretical covariance matrices $\rightarrow$ **just sum them in quadrature**.
- T_i : theory predictions, D_i : datapoints.
- In the fit, the covariance matrix is used in:
  - $\chi^2 = \frac{1}{N_{dat}} \sum^{N_{data}} (D_i - T_i)(C+S)^{-1}_{ij}(D_j - T_j)$.
  - Pseudodata generation.

Theory covariance for different processes

- For each point of the theory covariance matrix, we need to consider at most two renormalization scales (plus the usual factorization scale).
- So we need only to change normalization factor as $N_m = n_m/d_m$, where d_m counts the degeneracy given by the irrelevant renormalization scale variations.



Different factorization scale-variations schemes

Let's define $t = \ln\left(Q^2/\Lambda^2\right)$ and $\kappa = \ln\left(\mu^2/Q^2\right)$. Then

- **Scheme A**: The renormalization scale of the anomalous dimensions is directly varied in the evolution:
  $\bar{\gamma}(\alpha_s(t+\kappa),\kappa) = \alpha_s(t+\kappa)\gamma_0 + \alpha_s^2(t+\kappa)(\gamma_1 + \kappa\beta_0\gamma_0) + \dots$
- **Scheme B**: The scale-varied anomalous dimensions are expanded and factorized out from the exponential:

$$\exp\left(\int^{t+\kappa} dt'\bar{\gamma}\right) = \left[1 + \kappa\gamma(t+\kappa) + \dots\right]\exp\left(\int^{t+\kappa} dt'\gamma\right)$$

so that

$$\bar{f}(\alpha_s(t+\kappa),\kappa) = \left[1 + \kappa\gamma(t+\kappa) + \dots\right]f(t+\kappa)$$

Different factorization scale-variations schemes

- **Scheme C**: The scale-dependent terms are factorized into the coefficient function:

$$
\begin{aligned}
F(t,\kappa) &= C(t)\bar{f}(\alpha_s(t+\kappa),\kappa) \\
&= C(t)\big[1+\kappa\gamma(t+\kappa)+\ldots\big]f(t+\kappa) \\
&= \hat{C}(t,\kappa)f(t+\kappa)
\end{aligned}
$$

All these schemes are in principle equivalent but they can differ by subleading terms. Moreover, scheme A is not suited to be used for a fit because it requires the initial PDF to be refitted.