Missing higher order uncertainties in an NNPDF fit

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Outline

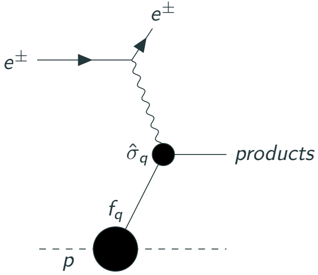
1. **Introduction and motivation**
    - What are missing higher order uncertainties?
    - How can we estimate them?
    - Why including them in a PDF fit is relevant?
2. **Methodology and validation**
    - How can we include MHOU in an NNPDF fit?
    - Can we validate our estimation?
3. **Results**

Introduction and motivation

Missing higher order uncertainties (MHOU)

$$F(Q) = \sum_q \big[\overbrace{U(Q, Q_0)}^{\text{DGLAP op.}} \overbrace{f_{q/p}(Q_0)}^{\text{PDFs}}\big] \otimes \overbrace{\hat{C}_q(Q)}^{\text{Coeff. funcs}}$$

Deep Inelastic Scattering



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

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

- Cannot be neglected in a PDF fit:
  - MHOU $\approx$ uncertainties of current PDF determinations.
  - MHOU affect relative weights of observables.

Scale variation as a probe of MHOU

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

- *Factorization* scale: estimates MHOU of anomalous dimensions [1].

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

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

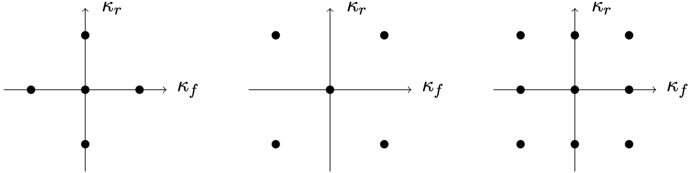
$$\overline{C}^{NNLO}(Q, \xi_R) = C^{(0)} + \alpha_s(\xi_R Q) C^{(1)} + \alpha_s^2(\xi_R Q)(C^{(2)} - \ln(\xi_R^2) \beta^{(0)} C^{(1)})$$

[1] *scheme B* arxiv:1906.10698

Methodology and validation

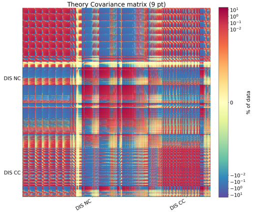
MHOU in NNPDF methodology

- Experimental covariance matrix $\mathcal{C}$ used in:
  - $\chi^2 = \frac{1}{N_{dat}} \sum^{N_{data}} (D_i - T_i)(\mathcal{C})^{-1}_{ij}(D_j - T_j)$
  - Data replica generation.
- Important to consider how MHOU correlate datapoints
- **Theory covariance matrix $\mathcal{S}$**
  - $\mathcal{C} \to \mathcal{C} + \mathcal{S}$ (under gaussianity hypothesis)
  - $S_{ij} = n_m \sum_{V_m} (\overline{F} - F)_{i_a} (\overline{F} - F)_{j_b}, \quad i, j \in$ datapoints
  - $a, b \in$ (**DIS CC**, **DIS NC**, **DY**, **Jets**, **Top**).
  - V_m : set of scale varied point in the given prescription with normalization n_m.

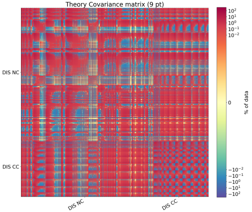


Theory covariance matrix (DIS CC + DIS NC)

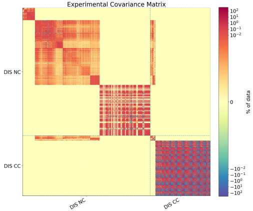
$\mathcal{S}^{\text{NLO}}$



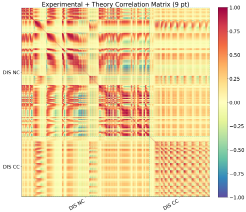
$\mathcal{S}^{\text{NNLO}}$



$\mathcal{C}$

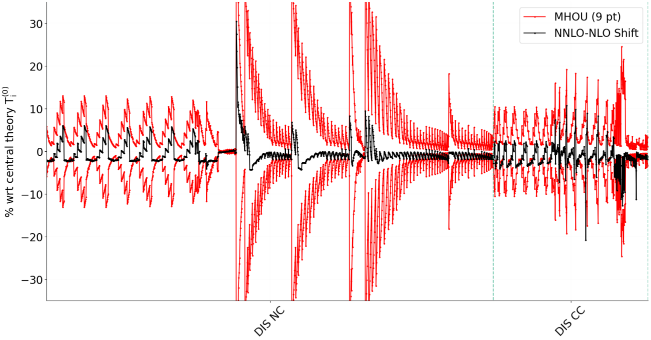


$\mathcal{C} + \mathcal{S}^{\text{NNLO}}$



Validation of the estimation

- Most of the predictions are currently known up to NNLO.
- Compare NNLO − NLO shifts with MHOU on NLO.

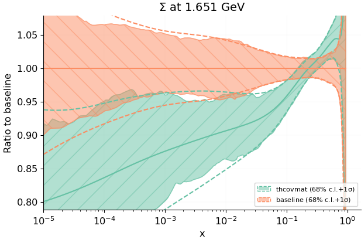


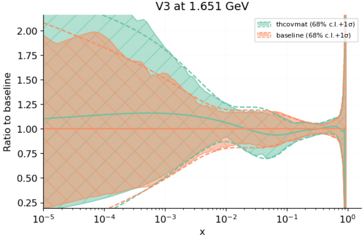
- Rather conservative but shape is predicted.

Results

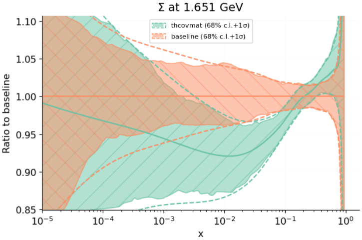
Uncertainties and central values change

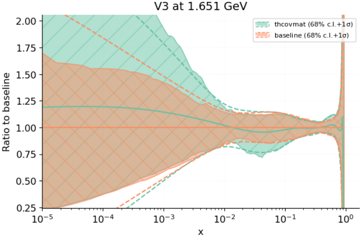
NLO





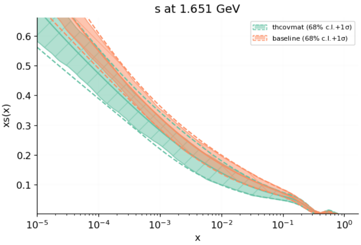
NNLO

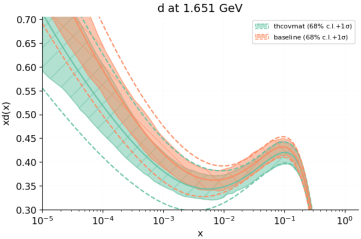




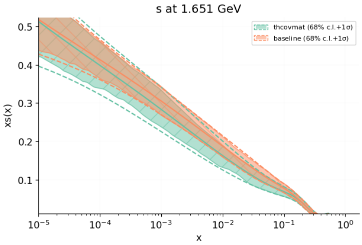
MHOU in NLO fit reproduce NNLO fit

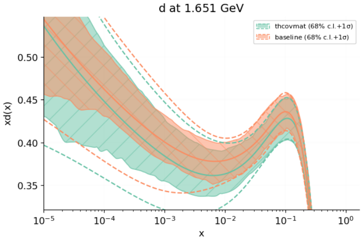
NLO





NNLO





Conclusions and outlook

- Including MHOU in a PDF fit is needed to have faithful uncertainties and central values.
- MHOU introduce correlations between datapoints that we need to take into account.
- Work in progress:
  - Extend the procedure beyond DIS.
  - Consider other possible grouping for the processes.
  - Consider other ways to estimate MHOU (see next talk by Marco...).

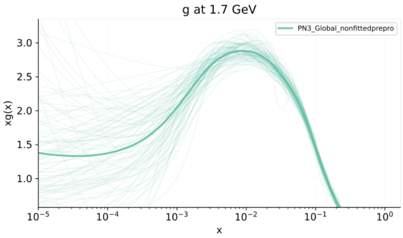
Thanks for your attention!

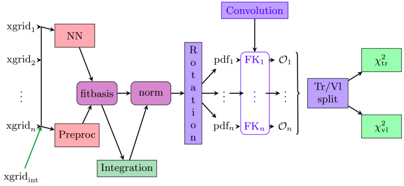
BACKUP SLIDES

The fitting problem: NNPDF methodology

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

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





How to include theory uncertainties in a fit

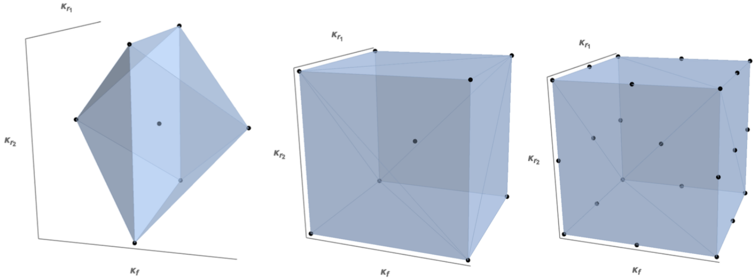
- Under gaussianity hypothesis

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

- 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:

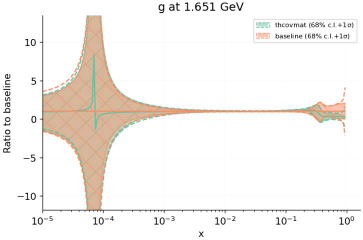
$$
\begin{aligned}
F(t,\kappa) &= C(t)\bar{f}(\alpha_s(t+\kappa),\kappa) \\
&= C(t)\big[1-\kappa\gamma(t+\kappa)+\dots\big]f(t+\kappa) \\
&= \hat{C}(t,\kappa)f(t+\kappa)
\end{aligned}
$$

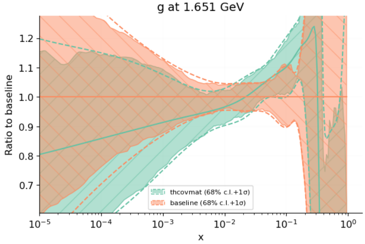
All these schemes are in principle equivalent but they can differ by subleading terms. Moreover, scheme A is not suited to be used for a fit because it requires the initial PDF to be refitted.

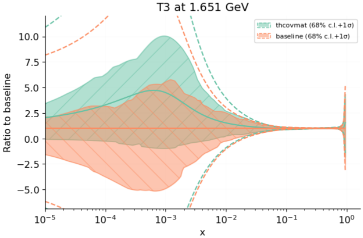
Uncertainties and central values change

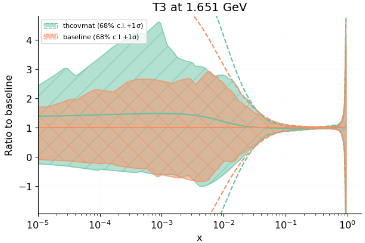
NLO

NNLO



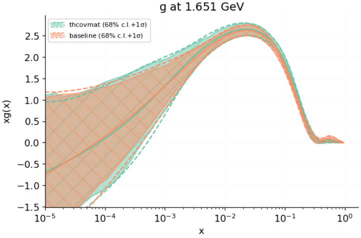


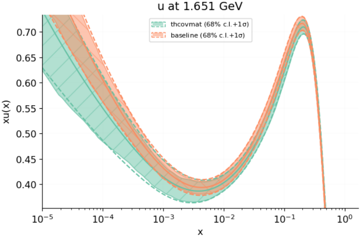




MHOU in NLO fit reproduce NNLO fit

NLO





NNLO