Recent Progress on PDF Determination: NNPDF4.0 Updates

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OUTLINE OF THE TALK:

- 1. Introduction & Motivations
- 2. Approximate N₃LO (aN₃LO) PDFs
- 3. Theory Uncertainties in PDF Determination
- 4. PDF Determination with QED Corrections
- 5. Conclusions & Outlook





Introduction: NNPDF Landscape

Significant improvements on all 3 FRONTS for NNPDF4.0:

- Experiments: contains *O*(4500) datapoints, abundant LHC data from Run II, probe more processes and channels.
- Methodology: SGD for NN minimisation, Automated Optimisation of Hyperparameters, Methodology validation using Closure Tests/ Future Tests/Parametrisation Basis independence.
- **Theory:** NNLO QCD with **Electroweak** corrections and Nuclear Unc.



Tests passing DOI 10.5281/zenodo.7554886

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

The NNPDF collaboration determines the structure of the proton using Machine Learning methods. This is the main repository of the fitting and analysis frameworks. In particular it contains all the necessary tools to reproduce the NNPDF4.0 PDF determinations.

https://github.com/NNPDF/nnpdf





Introduction: Challenges

- incomplete knowledge of α_{s} .
- NC/CC DY processes requires N₃LO PDFs.
- determination of parton densities more accurate.
- accuracy/uncertainties on MHOUs & IHOUs.



Duhr, Mistlberger [arXiv:2111.10379]



What do we need for N3LO PDFs?

Several theory ingredients are required to achieve N3LO PDF fits:

O Splitting Functions/Anomalous Dimensions (AD) to evolve PDFs through the DGLAP equation

$$\gamma(\alpha_s) = \alpha_s \gamma^{(0)} + \alpha_s^2 \gamma^{(1)} + \alpha_s^3 \gamma^{(2)} + \alpha_s^4 \gamma^{(3)} + \cdots$$

O Matching Conditions/Transition Matrix Elements to change number of PDF flavours at heavy-quark matching scales

$$f_{\alpha}^{n_{f}+1}(x,Q^{2}) = \mathbf{A}_{\alpha\beta}^{(n_{f})}(x,Q^{2}/m_{h}^{2}) \otimes f_{\beta}^{n_{f}}(x,Q^{2}/m_{h}^{2})$$

O DIS Coefficient Functions to compute structure functions

$$F_{\alpha}(x,Q^2) = \sum_{\beta,\eta} \mathscr{C}_{\alpha,\beta,\eta}^{n_f+1}(x,Q^2) \otimes \mathbf{A}_{\eta\xi}^{(n_f)}(x,Q^2/m_h^2) \otimes \mathbf{A}_{\eta\xi}^{$$

O Hadronic Cross-Section k-factors

$$\Sigma(x) = \Sigma_0(x) + \Sigma_1(x) + \Sigma_2(x) + \Sigma_3(x) + \cdots$$

Several Pieces are still missing—>Need Reliable Approximations



What do we know about 4-Loop <u>Non-Singlet</u> AD?

The complete N₃LO Anomalous Dimensions are not known yet, but a lot of information is already available.

- The case of **NON-SINGLET** sector:
 - $\mathcal{O}(n_f^2)$ and $\mathcal{O}(n_f^3)$ terms are known **analytically** Davies, Vogt, Ruijl, Ueda, Vermaseren [arXiv:1610.07477]
 - $\mathcal{O}(n_f^0)$ and $\mathcal{O}(n_f)$ terms are known in the Large- N_c limit Moch, Ruijl, Ueda, Vermaseren, Vogt [arXiv:1707.08315]
 - **Small-N limit:** coefficients of logarithms at pole N = 0 are known 0 numerically Davies, Kom, Moch, Vogt [arXiv:2202.10362]

$$P_{\rm ns}(x) \supset \sum_{k=1}^{6} c_k \ln^k (1/x)$$

O Large-N limit: some coefficients and constant terms are known Henn, Korchemsky, Mistlberger [arXiv:1911:10174]; Duhr, Mistlberger, Vita [arXiv:2205:04493]

$$\gamma_{\rm ns}^{(3)}(N) \approx A_4 S_1(N) - B_4^+ C_4 \frac{S_1(N)}{N} - D_4 \frac{1}{N}$$

O Results for Even/Odd Mellin Moments are known Moch, Ruijl, Ueda, Vermaseren, Vogt [arXiv:1707.08315]

The dependence of $\gamma_{ii}^{(3)}$ on the number of active flavours can be expressed as follows:

$$\gamma_{ij}^{(3)} = \gamma_{ij}^{(3,0)} + n_f \gamma_{ij}^{(3,1)} + n_f^2 \gamma_{ij}^{(3,2)} + n_f^3 \gamma_{ij}^{(3,3)}$$

	n_f^0	n_f^1	n_f^2	n_f^3
$\gamma_{ns,-}^{(3)}$	\checkmark	\checkmark	\checkmark	\checkmark
$\gamma_{ns,+}^{(3)}$	\checkmark	\checkmark	\checkmark	\checkmark
$\gamma_{ns,s}^{(3)}$		\checkmark	\checkmark	



What do we know about 4-Loop <u>Singlet</u> AD?

The complete N₃LO Anomalous Dimensions are not known yet, but a lot of information is already available.

- The case of **SINGLET** sector:
 - O Leading Large- n_f contributions to $\mathcal{O}(n_f^3)$ terms are known analytically Davies, Vogt, Ruijl, Ueda, Vermaseren [arXiv:1610.07477]
 - Small-N limit: BFKL limits of $\gamma_{qg}^{(3)}$ and $\gamma_{gg}^{(3)}$ are known up to LL and NLL, respectively. Coefficients of logarithms at pole N = 1 are known numerically Bonvini and Marzani [arXiv:1805.06460]; Davies, Kom, Moch, Vogt [arXiv:2202.10362]

$$P_{\rm ns}(x) \supset \sum_{k=0}^{3} c_k \frac{\ln^k (1/x)}{x}$$

- **O Large-N limit:** Diagonal $(\gamma_{gg}^{(3)}, \gamma_{qq,ps}^{(3)})$ and Off-diagonal $(\gamma_{qg}^{(3)}, \gamma_{gq}^{(3)})$ need to be treated separately. Their coefficients in the expansion 1/N are known numerically Duhr, Mistlberger, Vita [arXiv:2205.04493]; Henn, Korchemsky, Mistlberger [arXiv:1911.10174]; Soar, Moch, Vermaseren, Vogt [arXiv:0912.0369]
- O Results for Even Mellin Moments are known Falcioni, Herzog, Moch, Vogt [arXiv:2302.07593]-[arXiv:2307.04158]; Moch, Ruijl, Ueda, Vermaseren, Vogt [arXiv:2111.15561]

The dependence of $\gamma_{ii}^{(3)}$ on the number of active flavours can be expressed as follows:

$$\gamma_{ij}^{(3)} = \gamma_{ij}^{(3,0)} + n_f \gamma_{ij}^{(3,1)} + n_f^2 \gamma_{ij}^{(3,2)} + n_f^3 \gamma_{ij}^{(3,3)}$$

	n_f^0	n_f^1	n_f^2	n_f^3
$\gamma_{gg}^{(3)}$	\checkmark	\checkmark	\checkmark	\checkmark
$\gamma^{(3)}_{gq}$	\checkmark	\checkmark	\checkmark	\checkmark
$\gamma^{(3)}_{qg}$		\checkmark	\checkmark	\checkmark
$\gamma^{(3)}_{qq,ps}$		\checkmark	\checkmark	\checkmark

Approximating N3LO Anomalous Dimensions

The approximation to the full $\gamma_{ij}^{(3)}$ is done in Mellin space for each power of n_f independently with the following steps:

- Select a basis function $G_1(N)$ for **leading** large-*N* contributions
- Select a basis function $G_2(N)$ for **leading** small-*N* contributions
- Select two basis functions $G_1(N), G_2(N)$ for subleading small- and large-*N* contributions
- Varying subleading G_{ℓ} bases to produce Candidates \longrightarrow IHOUs

 $G_1(N)$

 $G_2(N)$

 $\gamma_{qq,\mathrm{ps}}^{(3)}(N)$ $G_3(N)$

 $G_4(N)$



Approximating N3LO Anomalous Dimensions



Comparisons with MSHTaN3LO

N3LO DIS Coefficient Functions

Some of the perturbative ingredients to produce N3LO structure functions are not yet known.

- All Light Flavour Coefficient Functions both for NC and **CC** are known exactly Larin, Nogueira, Van Ritbergen, Vermaseren[arxiv:9605317]; Moch, Vermaseren, Vogt [arxiv:0411112], [arxiv:0504242]
- Some parts needed for the construction of **Heavy Flavour Coefficient Functions** are missing. Take the quark & gluon coefficient functions:

$$\mathscr{C}_{i}^{(3)} = \mathscr{C}_{i}^{(3,0)} + \mathscr{C}_{i}^{(3,1)} \ln\left(\frac{\mu^{2}}{m^{2}}\right) + \mathscr{C}_{i}^{(3,2)} \ln^{2}\left(\frac{\mu^{2}}{m^{2}}\right)$$

While $C_i^{(3,1)}$ and $C_i^{(3,2)}$ are known exactly $C_i^{(3,0)}$ can be constructed by combining known limits with some matching functions $f_1(x)$ and $f_2(z)$ that interpolate between the two limits:

 $\mathscr{C}_{i,\text{approx}}^{(3,0)}(z) = \mathscr{C}_{i,z\to 0}^{(3,0)}(z)f_1(z) + \mathscr{C}_{i,z\to z_{\text{max}}}^{(3,0)}(z)f_2(z)$

Matching Conditions & GM-VFNS

Predictions for structure valid for all Q^2 require matching Mass effects in the Machine Scheme with Log resummation in the Massless scheme.

In NNPDF, DIS structure functions are computed using the **FONLL** method:

$$\tilde{F}_{\alpha}(x,Q^2) = F_{\alpha}^{(n_f+1)}(x,Q^2) - F_{\alpha}^{(n_f,0)}(x,Q^2) + F_{\alpha}^{(n_f)}(x,Q^2)$$

PDFs defined in $(n_f + 1)$ and (n_f) are related via Matching **Conditions**:

$$f_{\alpha}^{n_f+1}(x,Q^2) = A_{\alpha i}^{(n_f)}(x,Q^2/m_h^2) \otimes f_i^{n_f}(x,Q^2)$$

The full entries of the Matching Condition matrix elements are **almost** completely known except for $a_{H,g}^{(3)}$ Ablinger, Behring, Blümlein, De Freitas, Goedicke, von Manteuffel, Schonwald [arXiv:2211.0546]; Ablinger, Behring, Blümlein, De Freitas, Hasselhuhn, von Manteuffel, Round, Schneider, Wißbrock. [arXiv:1406.4654]; Bierenbaum, Blümlein, Klein [arXiv:0904.3563]

[NNPDF] G. Magni, A. Barontini

Hadronic K-factors

https://github.com/jubaglio/n3loxs

- **Double Hadronic K-factors** are **much less known** than the other ingredients needed for (a)N3LO
- Various calculations are available at N₃LO but not useful for PDF fits: Higgs (ggF, VBF, VH) B. Mistlberger [arXiv:1802.00833]; A. Dreyer, A. Karlberg [arXiv:1606.00840], J. Baglio, C. Duhr, B. Mistlberger, R. Szafron [arXiv:2209.06138], Top N. Kidonakis, M. Guzzi, A. Toreno [arXiv: 2306.06166]
- In NNPDF, hadronic K-factors are computed using **n3loxs** for all NC/CC DY J. Baglio, C. Duhr, B. Mistlberger, R. Szafron [arXiv:2209.06138]:

Dataset: ATLASZHIGHMASS49FB

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IHOUs from N3LO Splitting Functions

How are higher-order uncertainties arising from the approximation of N₃LO splitting functions propagated into the PDF Fit?

Variation of the Basis functions used to parametrise $\tilde{\gamma}_{ij}$ generate N_{γ} variations. The spread of variation w.r.t. the Central Predictions is used to define a **Covariance Matrix**:

$$\operatorname{Cov}_{i,j}^{\mathrm{IHOU}} = \frac{1}{N_{\mathrm{var}} - 1} \sum_{k=1}^{N_{\mathrm{var}}} \left(T_{i,k} - \overline{T}_i \right) \left(T_{j,k} - \overline{T}_i \right)$$

Since theory uncertainties resulting from **IHOUs** are **independent** from experimental uncertainties, the two contributions can be added in Quadrature:

$$\operatorname{Cov}_{i,j} = \operatorname{Cov}_{i,j}^{\exp} + \operatorname{Cov}_{i,j}^{\operatorname{IHOU}}$$

Missing Higher Order Uncertainties (MHOUs)

For a given observable \mathcal{O} , MHOUs are commonly estimated by varying the unphysical scales in the Parton evolutions and in the partonic cross-sections:

$$\mathcal{O}\left(\alpha_{s}\left(\mu^{2}\right),\frac{Q^{2}}{\mu_{F}^{2}},\frac{Q^{2}}{\mu_{R}^{2}}\right) = \mathcal{L}\left(\alpha_{s}\left(\mu_{F}^{2}\right),\frac{Q^{2}}{\mu_{F}^{2}}\right) \mathcal{O}\left(\alpha_{s}\left(\mu_{R}^{2}\right),\frac{Q^{2}}{\mu_{R}^{2}}\right)$$

Variation of Factorisation Scale $\kappa_F = Q^2/\mu_R^2$ estimates MHOUs from Anomalous Dimensions in the evolution while variation of **Renormalisation Scale** $\kappa_R = Q^2/\mu_R^2$ estimates MHOUs from partonic cross-sections.

Similar to **IHOUs**, **MHOUs** can be added as a nuisance parameter to the Covariance Matrix NNPDF [arxiv:1906.10698], [arxiv:2105.05114]

$$\operatorname{Cov}_{i,j} = \operatorname{Cov}_{i,j}^{\exp} + \operatorname{Cov}_{i,j}^{\operatorname{MHOU}}, \quad \operatorname{Cov}_{i,j}^{\operatorname{MHOU}} = \frac{1}{N_{\operatorname{var}} - 1} \sum_{k=1}^{N_{\operatorname{var}}} \left(S_{i,k} - \bar{S}_i \right) \left(S_{j,k} - \bar{S}_j \right)$$

7-point scale variation prescription is used. Points belonging to the same process are CORRELATED by κ_R -variation while κ_F correlates all the points.

Missing Higher Order Uncertainties (MHOUs)

$$\left(\frac{\sqrt{\text{Cov}_{ii,\text{NLO}}^{MHOU}}}{\mathcal{O}_i^{MHOU}}\right) \times 100$$

$$\left(\frac{\mathcal{O}_i^{\text{NNLO}} - \mathcal{O}_i^{\text{NLO}}}{\mathcal{O}_i^{\text{NLO}}}\right) \times 10$$

Good consistency between MHOUs & NNLO-NLO Shifts

NNLO MHOU Correlation Matrices

by experimental Covariance Matrix

[NNPDF] A. Barontini

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Impacts of MHOUs on PDFs

Compare Perturbative Convergence

Phenomenological Impacts of MHOUs

[NNPDF] C. Schwan & A. Barontini

- NLO-MHOU predictions are closer to NNLO than pure NLO.
- Very good agreement between NNLO and NNLO-MHOU.
- MHOUs improve perturbative convergence from NLO to NNLO.
- NLO vs. NNLO exhibit the largest Uncertainty Pull.

NNPDF4.0@aN3LO PDFs with MHOUs

u at 1.651 GeV

PDF Determination with QED

PDF Fits with QED Effects

- Photon PDF $\gamma(x, Q^2)$ can no longer be neglected as determination of parton densities become more accurate $\alpha \sim \mathcal{O}(\alpha_{\rm s}^2) \sim \mathcal{O}(1\%).$
- **LuxQED**: γ -PDF can be computed perturbatively using as inputs structure functions A.V. Manohar, P. Nason, G.P. Salam, G. Zanderighi [arXiv:1607.04266]—[arXiv:1708.01256]; NNPDF3.1 [arXiv:1712.07053]; MSHT20 [arXiv: 2111.05357]

Two main changes are required to account for QED effects in PDF fits:

Modified QCD \otimes QED DGLAP Evolution:

$$\mu^{2} \frac{df_{i}\left(N,\mu^{2}\right)}{d\mu^{2}} = \sum_{j} \gamma_{ij}\left(N,\alpha_{s}\left(\mu^{2}\right),\alpha\left(\mu^{2}\right)\right) f_{j}\left(N,\mu^{2}\right)$$

Mixed QCD \otimes QED Sum Rules:

$$\int_{0}^{1} dx \left(x\Sigma + xg + x\gamma \right) = 1$$

★ Orders Included

***** Orders Not Included

Determination of *γ* **PDF**

Parton density functions and γ -PDF are determined such that they satisfy the following Sum Rule:

$$\int_{0}^{1} dx \left(x\Sigma \left(x, Q^{2} \right) + xg \left(x, Q^{2} \right) + x\gamma \right)$$

Where $\gamma(x, Q^2)$ is computed iteratively during the fit using structure function inputs:

$$x\gamma(x,\mu^{2}) = \frac{2}{a_{em}(\mu^{2})} \int_{x}^{1} \frac{dz}{z} \left\{ \int_{\frac{m_{p}^{2}x^{2}}{(1-z)}}^{\frac{\mu^{2}}{(1-z)}} \frac{dQ^{2}}{Q^{2}} a_{em}^{2}(Q^{2}) \left[-z^{2}F_{L}(x) + \left(zP_{\gamma q}(z) + \frac{2x^{2}m_{p}^{2}}{Q^{2}} \right) F_{2}(x/z,Q) \right] \right\}$$

While $\gamma(x, Q^2)$ depends on the PDFs through the structure functions, it affects their determination.

Because photons couple differently to up-like and down-like quarks

 \Leftrightarrow

QCD©QED Evolution is more difficult to Diagonalise

$$\mu^{2} \frac{d}{d\mu^{2}} \begin{pmatrix} g \\ \gamma \\ \Sigma \\ \Sigma_{\Delta} \end{pmatrix} = -\Gamma_{s} \begin{pmatrix} g \\ \gamma \\ \Sigma \\ \Sigma_{\Delta} \end{pmatrix}, \quad \mu^{2} \frac{d}{d\mu^{2}} \begin{pmatrix} V \\ V_{\Delta} \end{pmatrix} = \Gamma_{V} \begin{pmatrix} V \\ V_{\Delta} \end{pmatrix}, \quad \mu^{2} \frac{d}{d\mu^{2}} f_{ns,\pm}^{u/d} = \left(\gamma_{ns,\pm} + \tilde{\gamma}_{ns,\pm}^{u/d}\right) f_{ns,\pm}^{u/d}$$

$$f_{ns,\pm}^{u} = \begin{cases} u^{\pm} - c^{\pm} \\ u^{\pm} + c^{\pm} - 2t^{\pm} \end{cases}, \quad f_{ns,\pm}^{d} = \begin{cases} d^{\pm} - s^{\pm} \\ d^{\pm} + s^{\pm} - 2b^{\pm} \end{cases}, \quad \Sigma_{\Delta} = \frac{n_{d}}{n_{u}} \sum_{i=1}^{n_{u}} u_{i}^{+} - \sum_{i=1}^{n_{d}} d_{i}^{+} \quad V_{\Delta} = \frac{n_{d}}{n_{u}} \sum_{i=1}^{n_{u}} u_{i}^{-} - \sum_{i=1}^{n_{d}} d_{i}^{-}$$

Mixed QCD \otimes QED Evolution

NNPDF4.0QED uses a so called **Unified Evolution Basis** n_f active quarks are split into n_u and n_f flavors ($n_f = n_u + n_d$)

NNLO QCD & QED PDFs

 γ at 100 GeV

[NNPDF] E. Nocera

Phenomenological Impacts of QCD & QED PDFs

Non-negligible corrections in highinvariant mass and high-p_T regions

[NNPDF] C. Schwan & N. Laurenti

Conclusions & Outlook

- More precise and accurate PDF central values AND uncertainties are vital for precision and beyond the Standard Model Physics.
- Inclusion of **Electroweak corrections** is becoming more relevant \leftarrow **QED corrections & photon** γ **-PDF**

Stay tuned for new NNPDF4.0 releases:

- NNLO PDFs with Faithful estimation of MHO uncertainties ⇒ NNPDF4.0 MHOU
- **PDF** determination with QED \implies **NNPDF4.0 QED**
- Approximate N3LO PDF determination \implies NNPDF4.0 aN3LO

Backup Slides

A new Toolchain for PDF predictions

arXiv:2302.12124

aN3LO PDFs: Perturbative Stability

aN3LO PDFs: Luminosities

MHOUs: closer look at CovMat

QCD©QEDEvolution

Scale Dependence of γ **-PDF**

