Proton structure in the precision LHC era

Cameron Voisey
University of Cambridge

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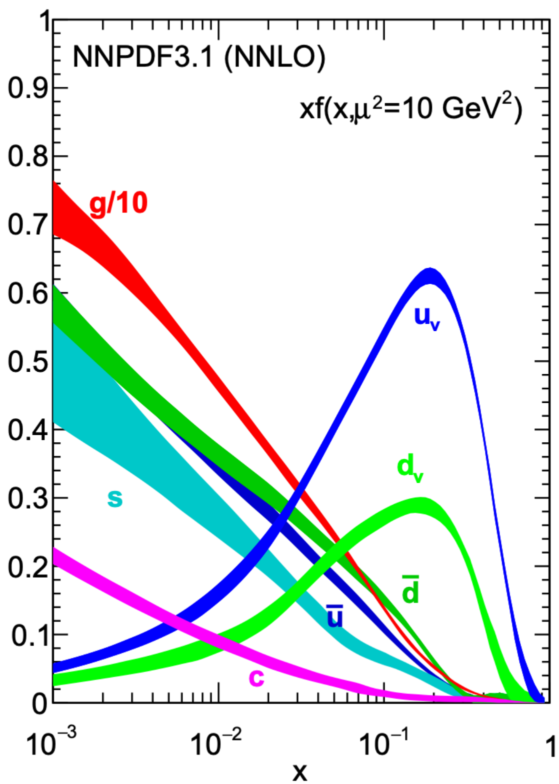
Outline

1. Proton structure (PDFs) and NNPDF
2. PDFs in the precision LHC era
3. New sources of uncertainty in PDF determinations
    - Approach I: The theoretical covariance matrix
    - Approach II: Monte Carlo scale uncertainties

What are PDFs?

$$\sigma_{p_1p_2\to X} = \sum_{a,b\in\{g,q,\bar{q}\}} \boxed{f_{p_1}\otimes f_{p_2}} \otimes \hat{\sigma}_{ab\to X}$$

PDFs



- **'Factorisation'** separates long and short distance behaviour
- Parton distribution functions (PDFs) represent the **distribution of quarks and gluons within the proton** for a given Bjorken-x and energy scale μ
- Proton structure is in **non-perturbative** regime: cannot use perturbation theory to calculate PDFs

How do we extract PDFs?

Data
cross sections and correlations (covariance matrix)
DIS, Drell-Yan
Top, Jets

Theory
NNLO predictions,
DGLAP evolution,
flavour scheme,
EW corrections, …

Methodology
Parametrisation,
error propagation,
minimisation

$$f_i(x, \mu^2) \pm \Delta_i(x, \mu^2)$$

The NNPDF approach

Guiding principles: introduce **minimal theoretical prejudice** into functional form of PDFs, and use **statistically sound error propagation**

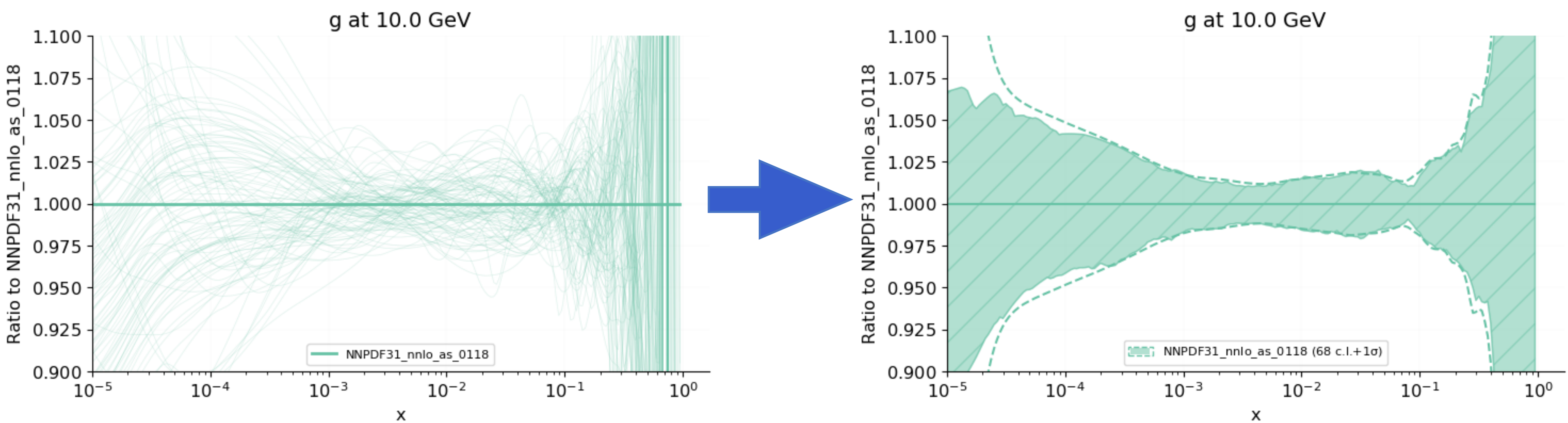
1. Generate N_{rep} **'data replicas'** by Monte Carlo sampling according to distribution of exp. data and their uncertainties, correlations (defined by cov_{exp})
2. For each data replica, parametrise PDFs with **Neural Networks**
3. Fit N_{rep} **'PDF replicas'** using χ^2 as a figure of merit with certain **algorithm**

$$\chi^2 = (\text{data} - \text{theory})^T(\text{cov}_{\text{exp}})^{-1}(\text{data} - \text{theory})$$

$$\text{cov}_{\text{exp,ij}} = \rho_{ij}\,\sigma_i\,\sigma_j$$

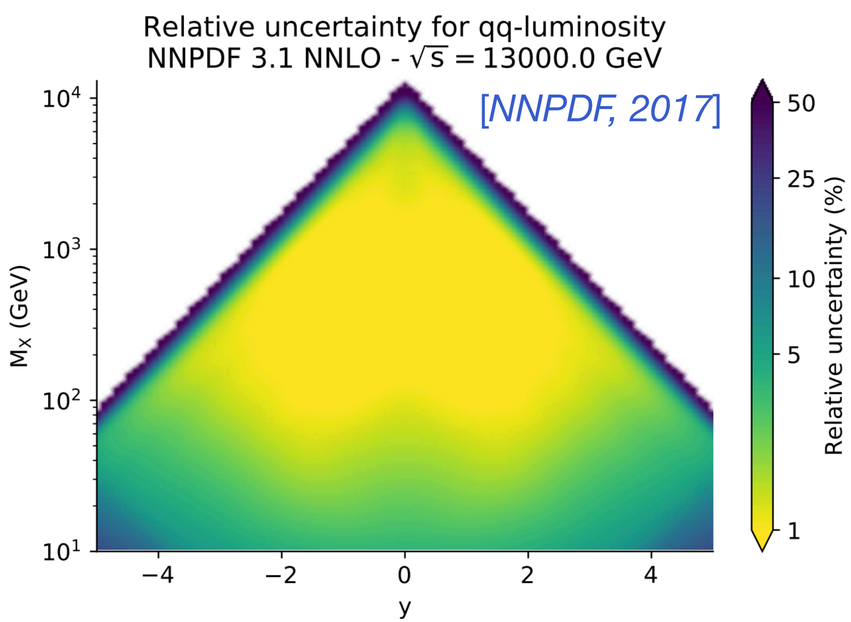
$\Rightarrow$ maximise agreement between data and theoretical predictions for each replica

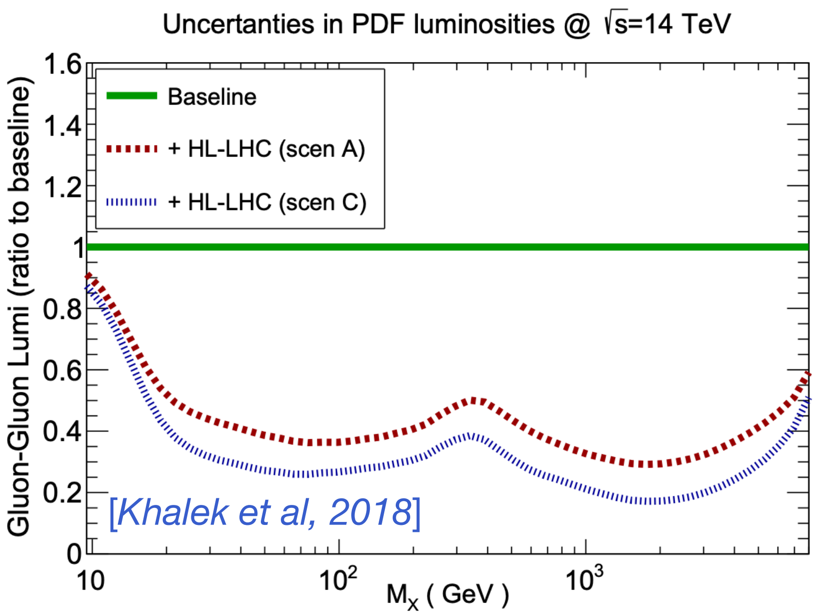
The NNPDF approach



- PDF uncertainties = **propagated experimental uncertainties**
- Methodological uncertainties under control (see ‘closure tests’)
- Uncertainties on theoretical predictions **not included**

State-of-the-art PDFs

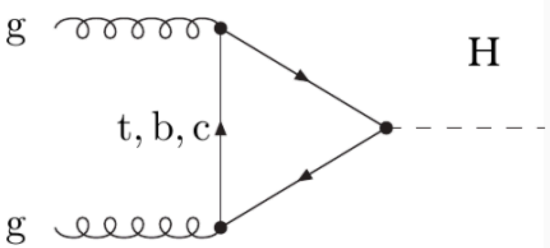


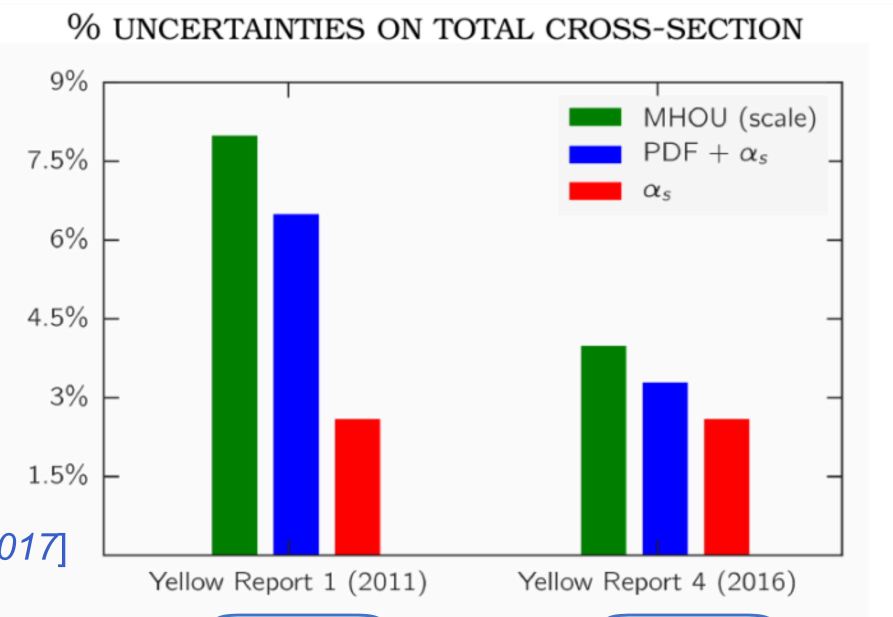


- PDFs now **high precision**: 1% uncertainty in data region
- Uncertainties will get **smaller** with HL-LHC
- PDFs are **precise**, but are they **accurate**?

Theoretical uncertainties at the LHC

Example: gluon-gluon fusion





[S. Forte, Lattice 2017]

NNLO N3LO

- **Missing higher-order uncertainties** (MHOUs) often dominant at LHC
- MHOUs are uncertainties due to **truncation** of series used in calculations, namely in **partonic cross sections** and **PDF evolution** (DGLAP equations)

Estimating MHOUs

Standard technique: **scale variations**

- Thinking behind method:

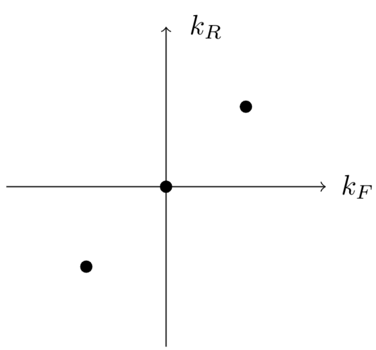
  1. μ_R, μ_F are **"unphysical"** scales that all-orders prediction cannot depend on
  2. Varying μ_R, μ_F in $O(\alpha_s^n)$ calculation generates $O(\alpha_s^{n+1})$ terms

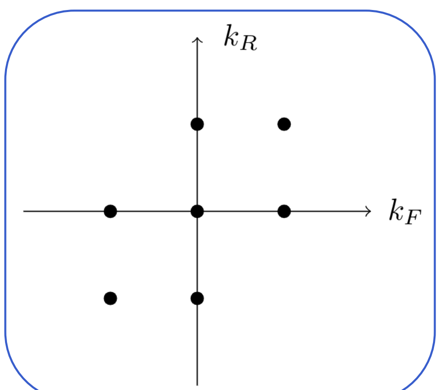
- Convention (for hadronic processes): vary μ_R in **partonic cross section** and μ_F in **PDF**, where

$$k_R, k_F \in \left(\frac{1}{2},\ 1,\ 2\right)$$

$$\boxed{k = \frac{\mu}{\mu_0}}$$

- Compute observable for different scale combinations and take **envelope**



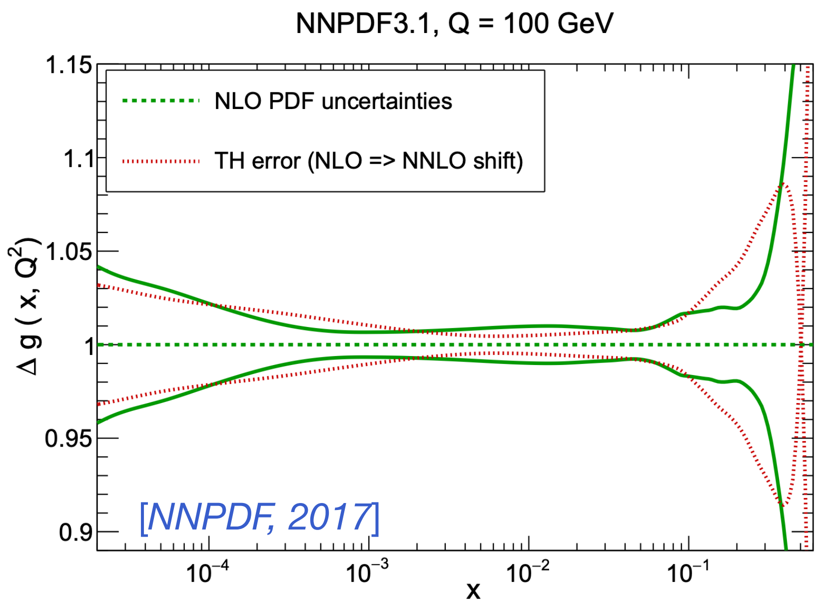


HXSWG recommendation

Missing higher-order uncertainties & PDFs

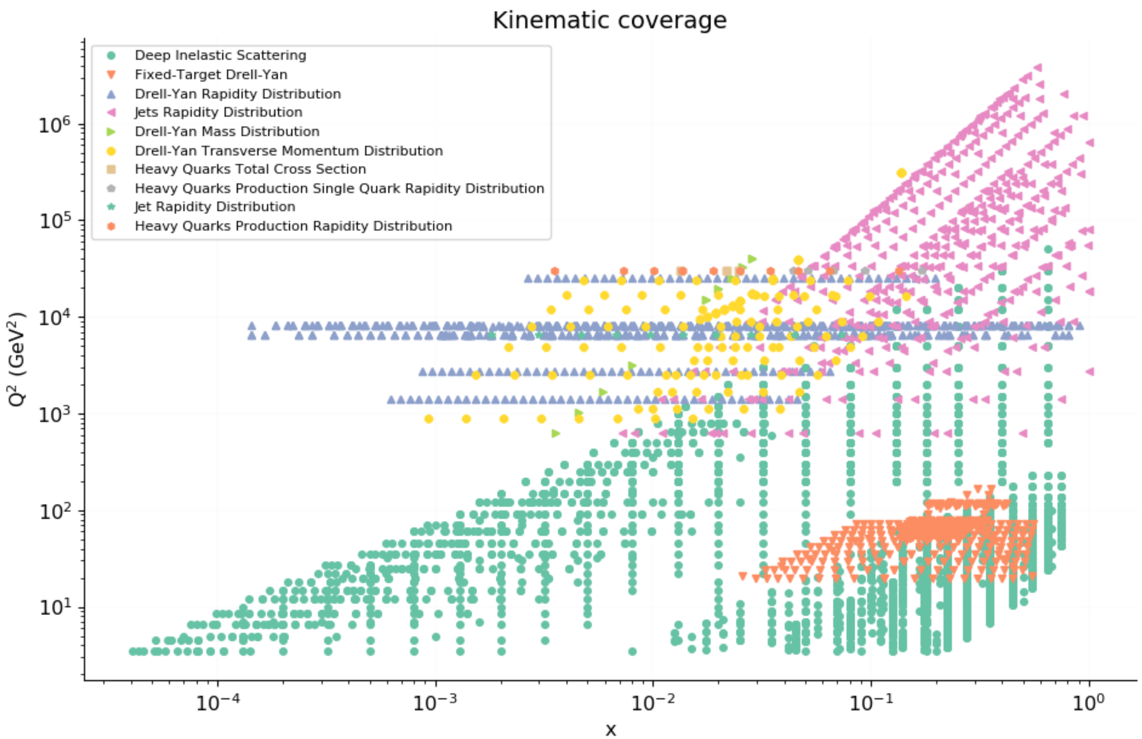
- Standard PDF fits use **fixed-order** partonic cross sections and **fixed-order** PDF evolution (**NNLO** for state-of-the-art PDFs)

What is the **potential impact** of MHOUs in PDF fits?

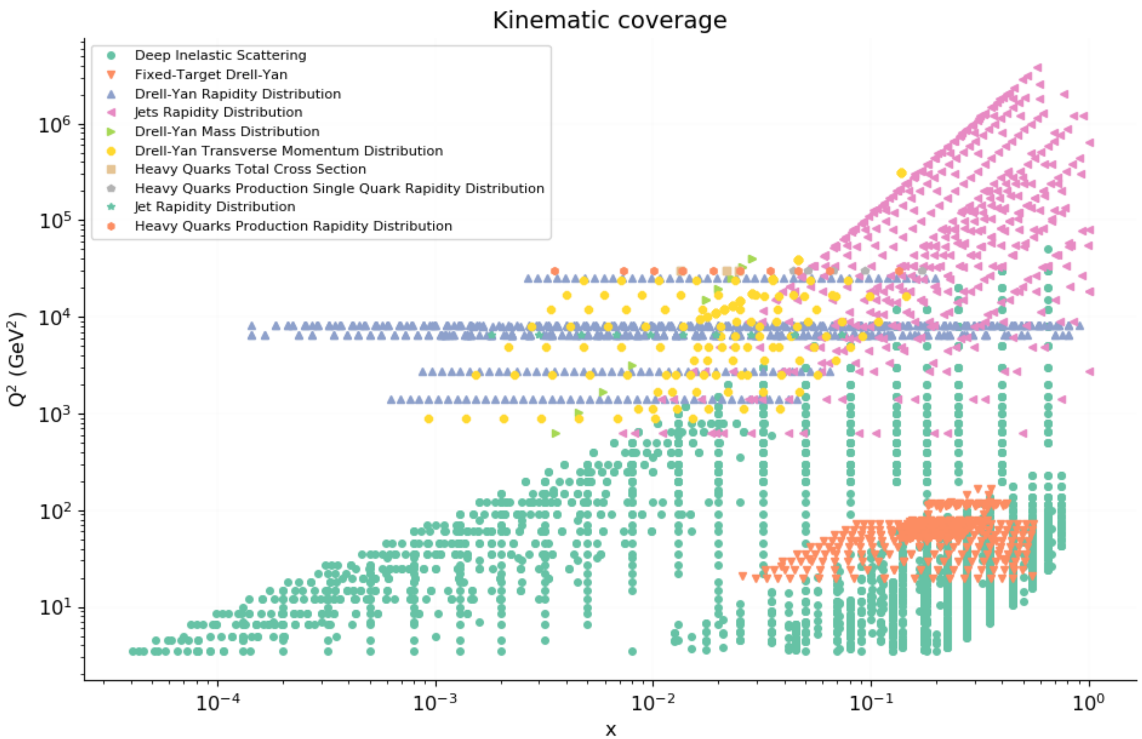


- **NNLO-NLO PDF shift** now of **same order** or **larger** than PDF uncertainties
- Should we worry about **accuracy** of PDFs? Looking forward: yes

PDF determinations



PDF determinations



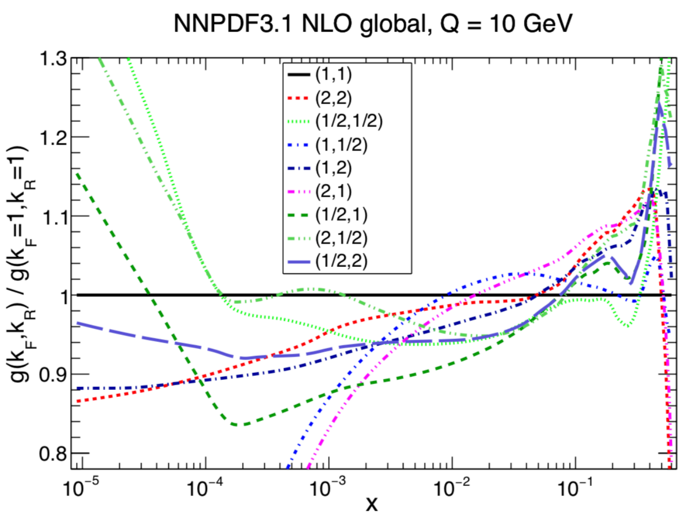
How to **extend** scale variation to **global PDF fits**?

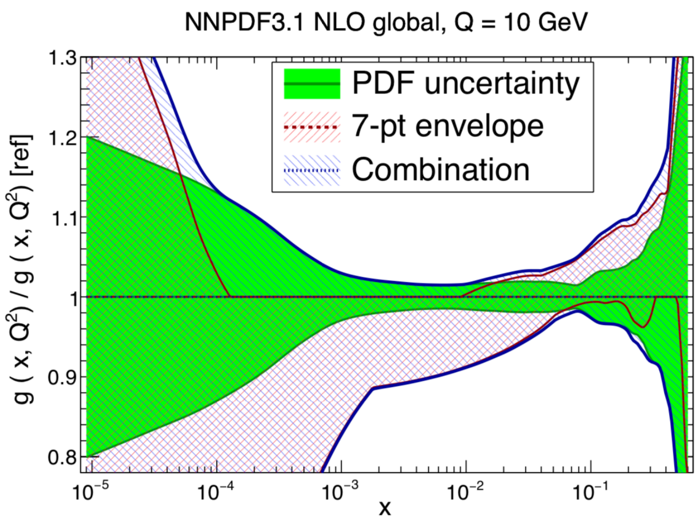
- **O(4000)** data points from **different processes**
- How to **correlate**? Common DGLAP evolution, different α_s dependence in partonic cross sections

PDF fits with varied scales

Starting point for estimating MHOUs:

- Produce PDF fits for **range of scale combinations**
- Define MHOUs band as **envelope of central values**





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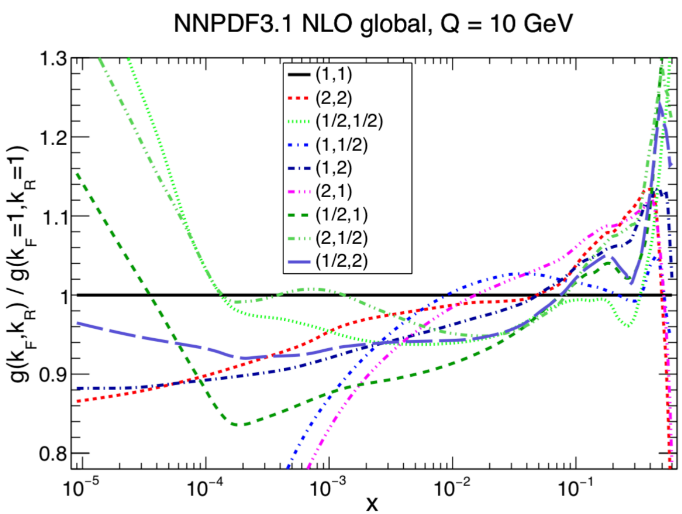

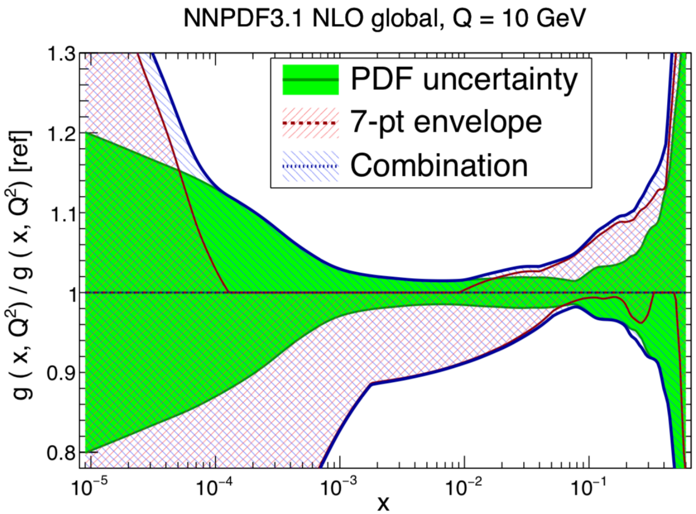

- **Neglects correlations** in scale variations
- MHOUs only **estimated**, not **included** in PDF uncertainties

Can we include MHOUs and their correlations in PDF uncertainties by accounting for them in **fitting methodology**?

Approach I:
The theoretical covariance matrix

arXiv: 1906.10698 - long paper
arXiv: 1905.04311 - summary paper

The theoretical covariance matrix

Experimental uncertainties propagated to PDFs via minimisation of figure of merit:

$$\chi^2 = (\text{data} - \text{theory})^T (\text{cov}_{\text{exp}})^{-1} (\text{data} - \text{theory})$$

Modify this to account for theory errors: *[R. D. Ball & A. Deshpande, 2018]*

$$\chi^2_{\text{tot}} = (\text{data} - \text{theory})^T (\text{cov}_{\text{exp}} + \text{cov}_{\text{th}})^{-1} (\text{data} - \text{theory})$$

Assumptions:

1. Theoretical uncertainties **independent** from experimental uncertainties

   → we are adding exp. and th. uncertainties in quadrature

2. Theoretical uncertainties are **Gaussianly distributed**

Applicable to other types of theoretical uncertainty, e.g. Monte Carlo, nuclear uncertainties *[R. D. Ball et al, 2018]*, …

A theoretical covariance matrix for MHOUs

Construct $\mathrm{cov}_{\mathrm{th}}$ from **scale variations** to estimate:

1. MHOU on each point
2. Correlations between points

i, j: data points

k: scale combinations

$$\mathrm{cov}_{\mathrm{th},ij} = \frac{1}{N}\sum_k \Delta_i^{(k)}\Delta_j^{(k)} \qquad \Delta_i^{(k)} = t_i(\mu_R,\mu_F) - t_i(\mu_{R,0},\mu_{F,0})$$

Choices:

0. Definition of covariance matrix
1. Range of scale variation
2. Number of scale combinations (3, 7, …)
3. Correlation between scales (same process, different processes)
4. Process categorisation
5. Type of scale variation

A theoretical covariance matrix for MHOUs

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Choices:

0. Definition of covariance matrix
1. Range of scale variation → $\frac{1}{2} \leq k_F, k_R \leq 2$
2. Number of scale combinations (3, 7, …)
3. Correlation between scales (same process, different processes)
4. Process categorisation
5. Type of scale variation

A theoretical covariance matrix for MHOUs

Construct $\mathrm{cov}_{\mathrm{th}}$ from **scale variations** to estimate:

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Choices:

0. Definition of covariance matrix
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2. Number of scale combinations (3, 7, …)
3. Correlation between scales (same process, different processes)
4. Process categorisation
5. Type of scale variation

How do we correlate scales in this multi-scale problem?

See next slides

A theoretical covariance matrix for MHOUs

Construct cov_{th} from **scale variations** to estimate:

1. MHOU on each point
2. Correlations between points

i, j: data points

k: scale combinations

$$\text{cov}_{\text{th,ij}} = \frac{1}{N}\sum_k \Delta_i^{(k)}\Delta_j^{(k)} \qquad \Delta_i^{(k)} = t_i(\mu_R, \mu_F) - t_i(\mu_{R,0}, \mu_{F,0})$$

Choices:

0. Definition of covariance matrix
1. Range of scale variation
2. Number of scale combinations (3, 7, …)
3. Correlation between scales (same process, different processes)
4. Process categorisation →
5. Type of scale variation

DIS neutral current

DIS charged current

Drell-Yan

Jets

Top

A theoretical covariance matrix for MHOUs

Construct cov_{th} from **scale variations** to estimate:

1. MHOU on each point
2. Correlations between points

i, j: data points

k: scale combinations

$$\text{cov}_{\text{th,ij}} = \frac{1}{N}\sum_k \Delta_i^{(k)}\Delta_j^{(k)} \qquad \Delta_i^{(k)} = t_i(\mu_R, \mu_F) - t_i(\mu_{R,0}, \mu_{F,0})$$

Choices:

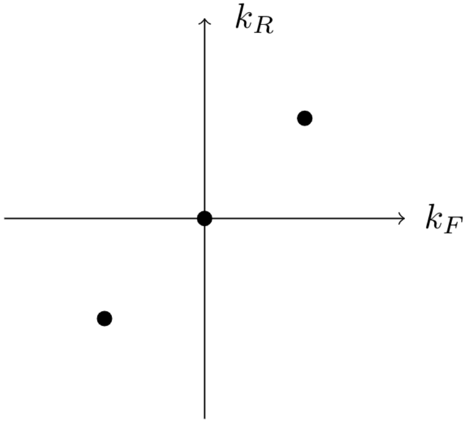
0. Definition of covariance matrix
1. Range of scale variation
2. Number of scale combinations (3, 7, …)
3. Correlation between scales (same process, different processes)
4. Process categorisation
5. Type of scale variation

- Vary μ_R in $\hat{\sigma}$
- Vary μ_F in PDF (scale at which PDF is evaluated)

Example: 3-pt theoretical covariance matrix

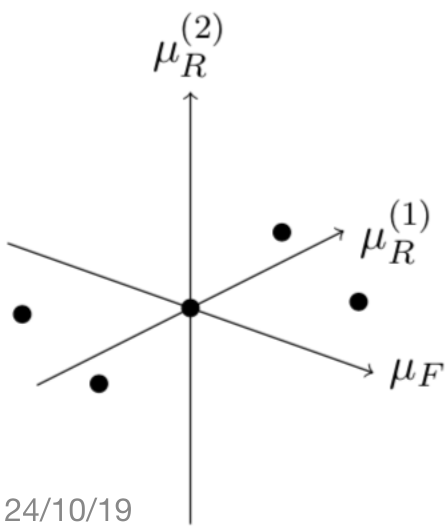
Assumptions: one μ_F in total, one μ_R per process

*i, j from **same process***



$$\text{cov}_{\text{th,ij}} = \frac{1}{2}\left\{\Delta_i(+,+)\Delta_j(+,+) + \Delta_i(-,-)\Delta_j(-,-)\right\}$$

*i, j from **different processes***



$$\text{cov}_{\text{th,ij}} = \frac{1}{4}\left\{(\Delta_i(+,+) + \Delta_i(-,-))(\Delta_j(+,+) + \Delta_j(-,-))\right\}$$

where

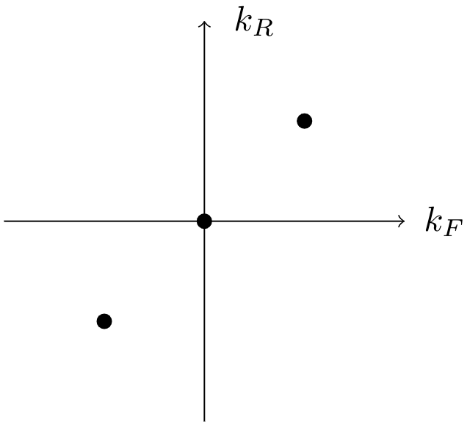
$$\Delta_i(+,+) = t_i(k_F = 2,\ k_R = 2) - t_i(k_F = 1,\ k_R = 1)$$

$$\Delta_i(-,-) = t_i\left(k_F = \frac{1}{2},\ k_R = \frac{1}{2}\right) - t_i(k_F = 1,\ k_R = 1)$$

Example: 3-pt theoretical covariance matrix

Assumptions: one μ_F in total, one μ_R per process

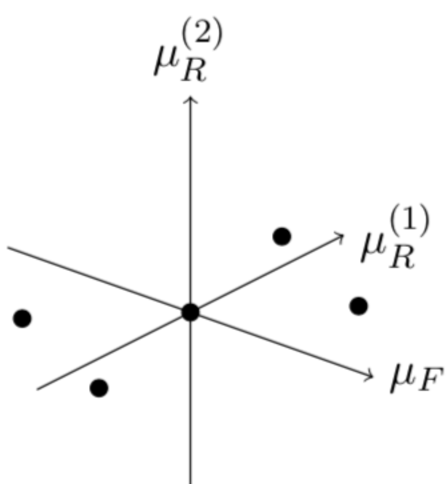
i, j from ***same process***



$$\text{cov}_{\text{th},ij} = \frac{1}{2}\{\Delta_i(+,+)\Delta_j(+,+) + \Delta_i(-,-)\Delta_j(-,-)\}$$

μ_F, μ_R fully correlated

i, j from ***different processes***



$$\text{cov}_{\text{th},ij} = \frac{1}{4}\{(\Delta_i(+,+) + \Delta_i(-,-))(\Delta_j(+,+) + \Delta_j(-,-))\}$$

μ_F, μ_R fully uncorrelated

$\Rightarrow$ missing μ_F correlation

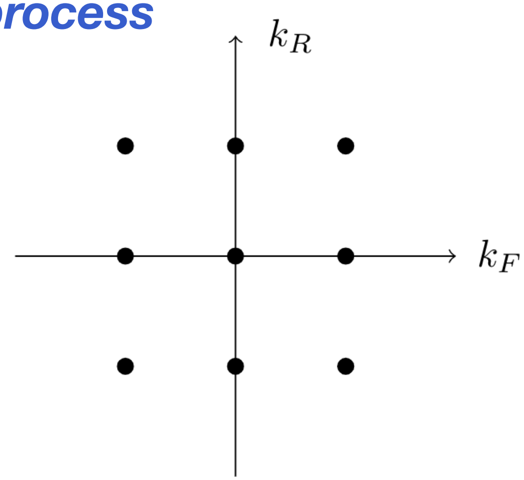
where

$$\Delta_i(+,+) = t_i(k_F = 2,\ k_R = 2) - t_i(k_F = 1,\ k_R = 1)$$

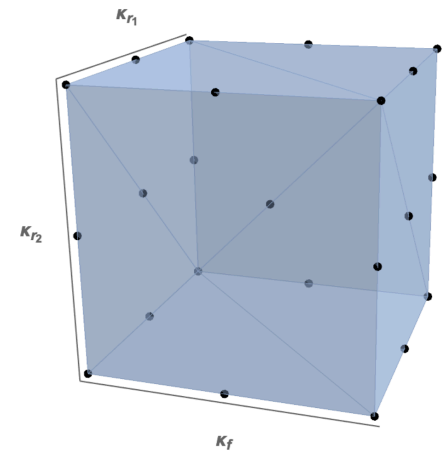
$$\Delta_i(-,-) = t_i\left(k_F = \frac{1}{2},\ k_R = \frac{1}{2}\right) - t_i(k_F = 1,\ k_R = 1)$$

More complex scale combinations: 9-pt

i, j from ***same process***



i, j from ***different processes***

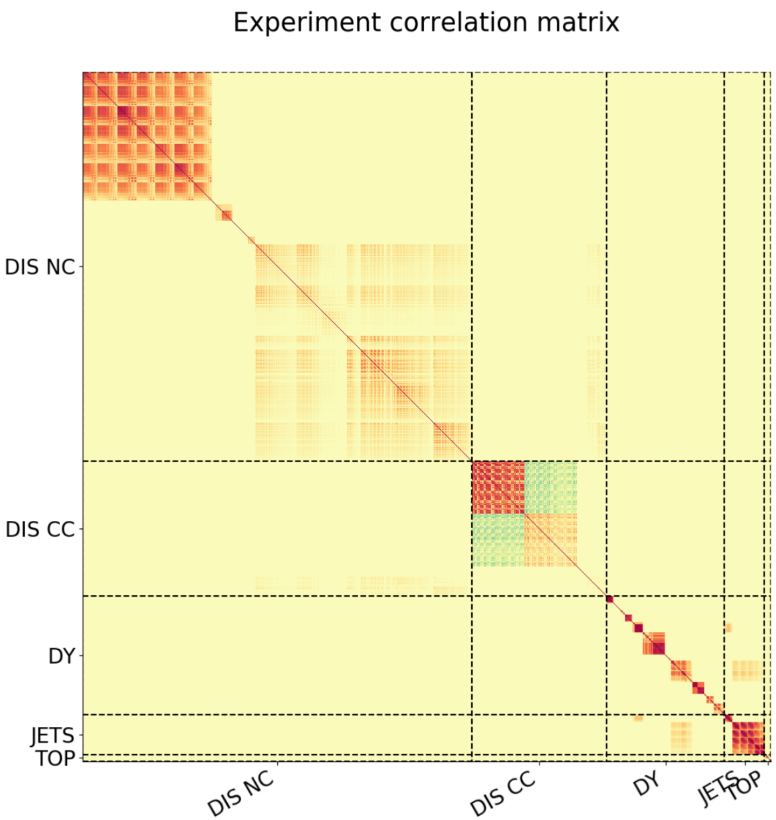


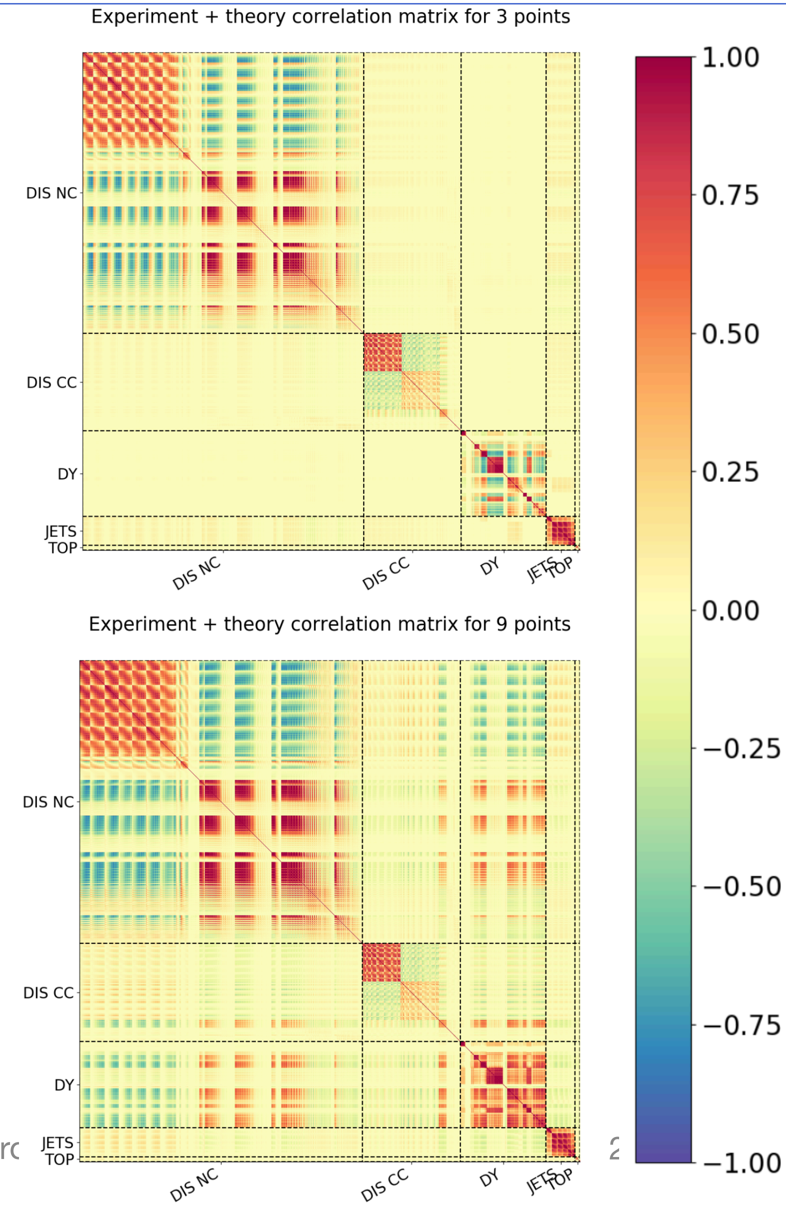
The more complex scale combination allows us to define **more complex correlation structure**:

- same process: μ_F, μ_R fully correlated
- different processes: μ_F fully correlated, μ_R fully uncorrelated

We expect this to produce a more **accurate** correlation structure, since we account for common DGLAP evolution, and different α_s dependence in partonic cross sections

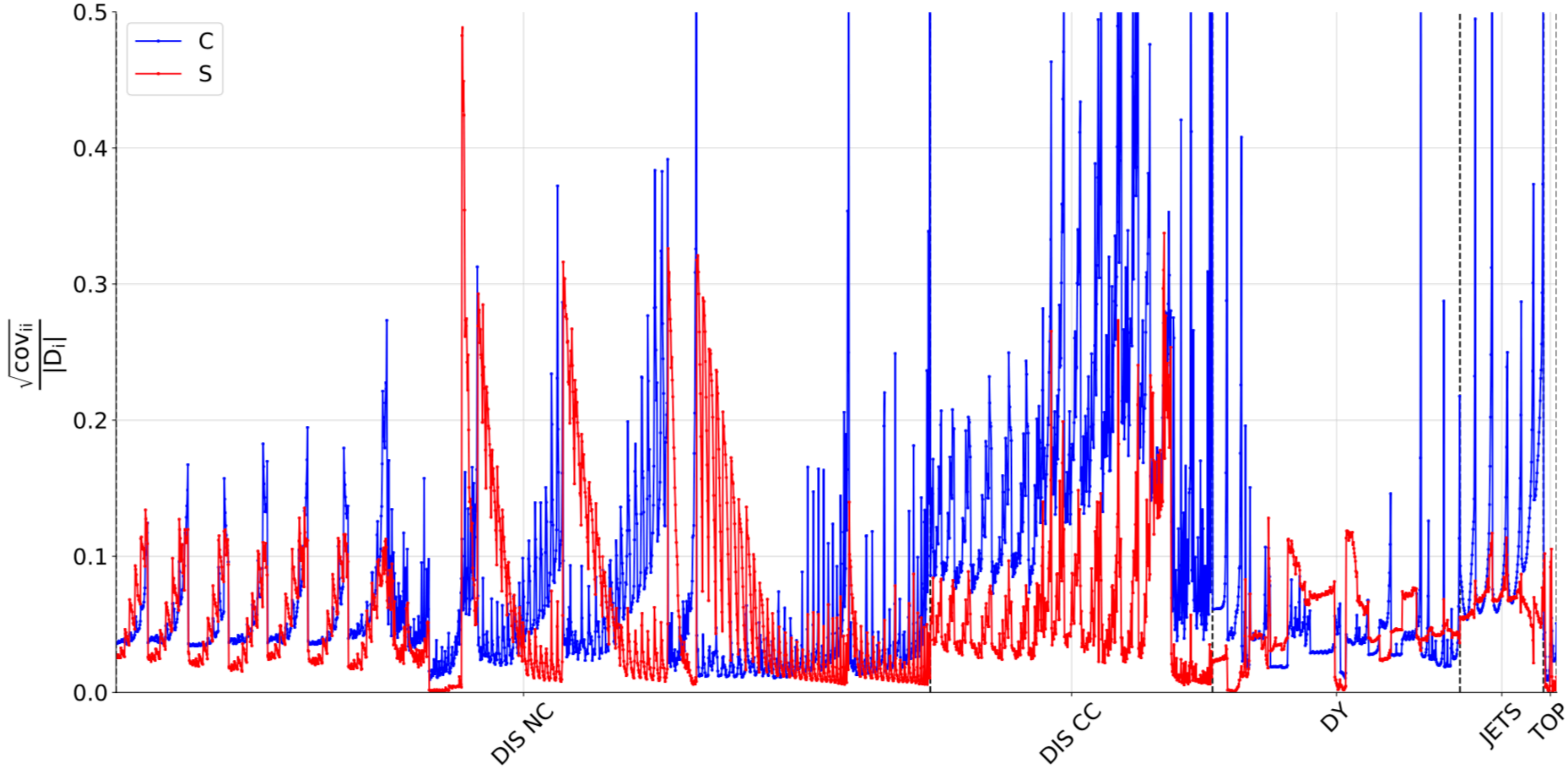
A theoretical covariance matrix for MHOUs





How can we **validate** and **compare** our theory covariance matrices?

Validation



We can compare **MHOU per point**, but this only tests diagonal elements of theoretical covariance matrix

→ We want to test **full covariance matrix**: MHOU per point + correlations

Validation: uncertainties + correlations

- We validate $\mathrm{cov}_{\mathrm{th}}$ against exact result: **NNLO-NLO shift**

- $\mathrm{cov}_{\mathrm{th}}$ is **positive semi-definite** (eigenvalues > 0 or 0)
- Eigenvalue of covariance matrix is variance in direction of eigenvector
- Eigenvalue = 0 $\Rightarrow$ no variance/**shift** predicted by $\mathrm{cov}_{\mathrm{th}}$ in direction of eigenvector
- Define **angle**, θ, of matrix as angle between shift and proportion of shift that is contained within **non-zero eigenvectors**

$$0^\circ \leq \theta \leq 90^\circ$$

$\theta = 0^\circ$: $\mathrm{cov}_{\mathrm{th}}$ predicts variation in same directions as shift

Validation: uncertainties + correlations

3-pt

Per **data set**: $0.14^\circ \leq \theta \leq 73.5^\circ$

Per **process**:

Process	Angle, θ
DIS NC	54°
DIS CC	36°
DY	39°
Jets	24°
Top	12°

Global: $\theta = 52^\circ$

Validation: uncertainties + correlations

3-pt

Per **data set**: $0.14^\circ \leq \theta \leq 73.5^\circ$

Per **process**:

Process	Angle, θ
DIS NC	54°
DIS CC	36°
DY	39°
Jets	24°
Top	12°

Global: $\theta = 52^\circ$

9-pt

Per **data set**: $0.00^\circ \leq \theta \leq 24.6^\circ$

Per **process**:

Process	Angle, θ
DIS NC	32°
DIS CC	16°
DY	22°
Jets	14°
Top	3°

Global: $\theta = 26^\circ$

Validation: uncertainties + correlations

3-pt / **9-pt**

Per **data set**: $0.14^\circ \leq \theta \leq 73.5^\circ$ (3-pt); $0.00^\circ \leq \theta \leq 24.6^\circ$ (9-pt)

Per **process**:

3-pt:

Process	Angle, θ
DIS NC	54°
DIS CC	36°
DY	39°
Jets	24°
Top	12°

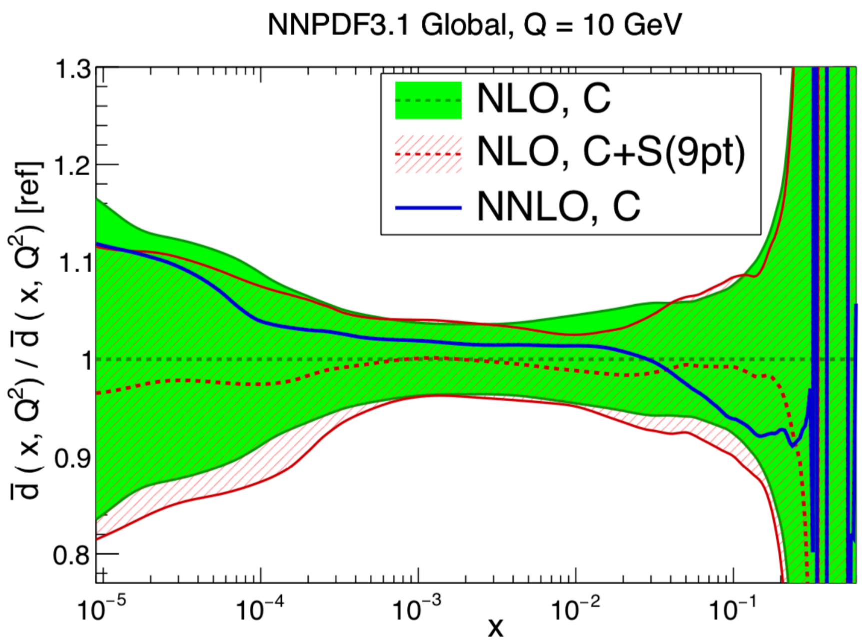
9-pt:

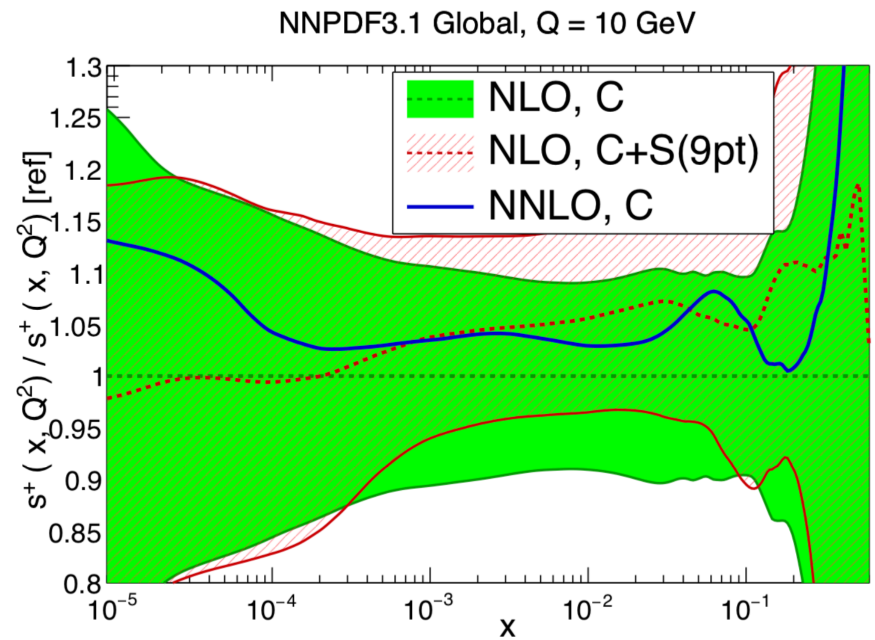
Process	Angle, θ
DIS NC	32°
DIS CC	16°
DY	22°
Jets	14°
Top	3°

Global: $\theta = 52^\circ$ (3-pt); $\theta = 26^\circ$ (9-pt)

9-pt does best $\rightarrow$ use this for our PDF fits

Results: PDF fits with $\mathrm{cov}_{\mathrm{th}}$

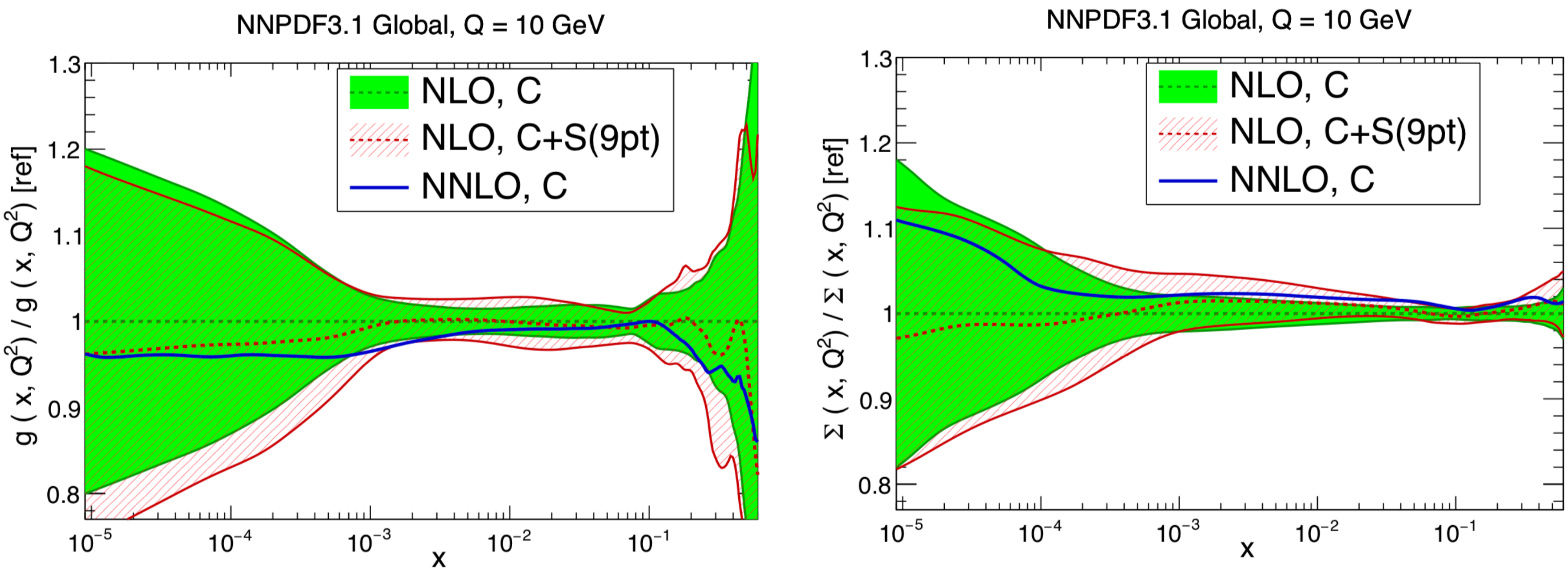




- We use $\mathrm{cov}_{\mathrm{th}}$ in both MC **sampling** (replica generation) and **fitting** (χ^2)
- Overall **small increase** in uncertainties (if at all): **tensions relieved**

$\Rightarrow$ Increase in PDF uncertainties counteracted by change of data set weighting in fit: addition of MHOUs leads to **better fit**

Results: PDF fits with cov_{th}



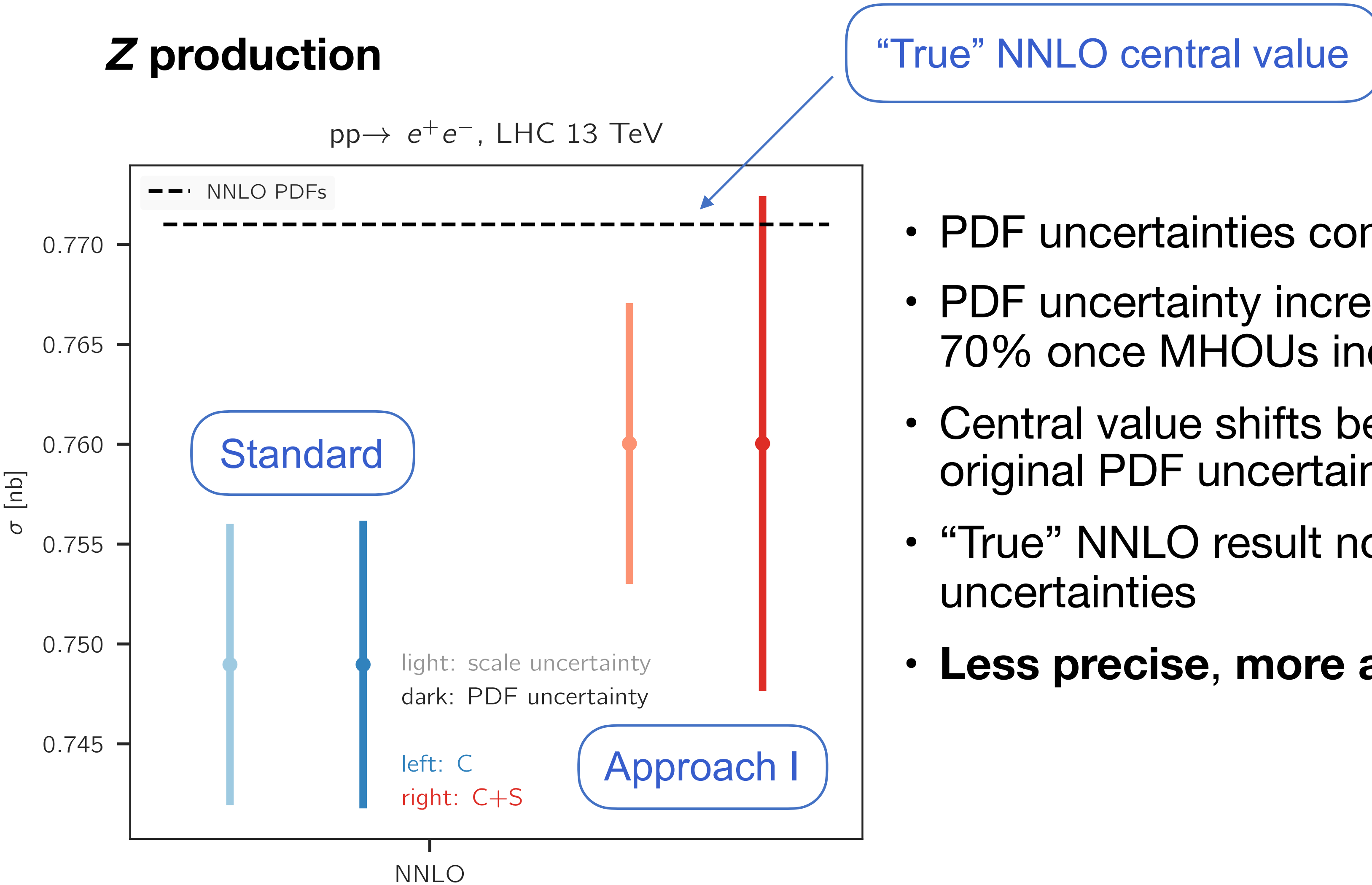
If NNLO-NLO shift is large compared to standard NLO PDF uncertainty:

- PDF uncertainty increases with addition of cov_{th}
- Shift contained within PDF uncertainty when MHOUs accounted for

$\Rightarrow$ **More reliable PDF uncertainties**

Results: Impact at the LHC

***Z* production**

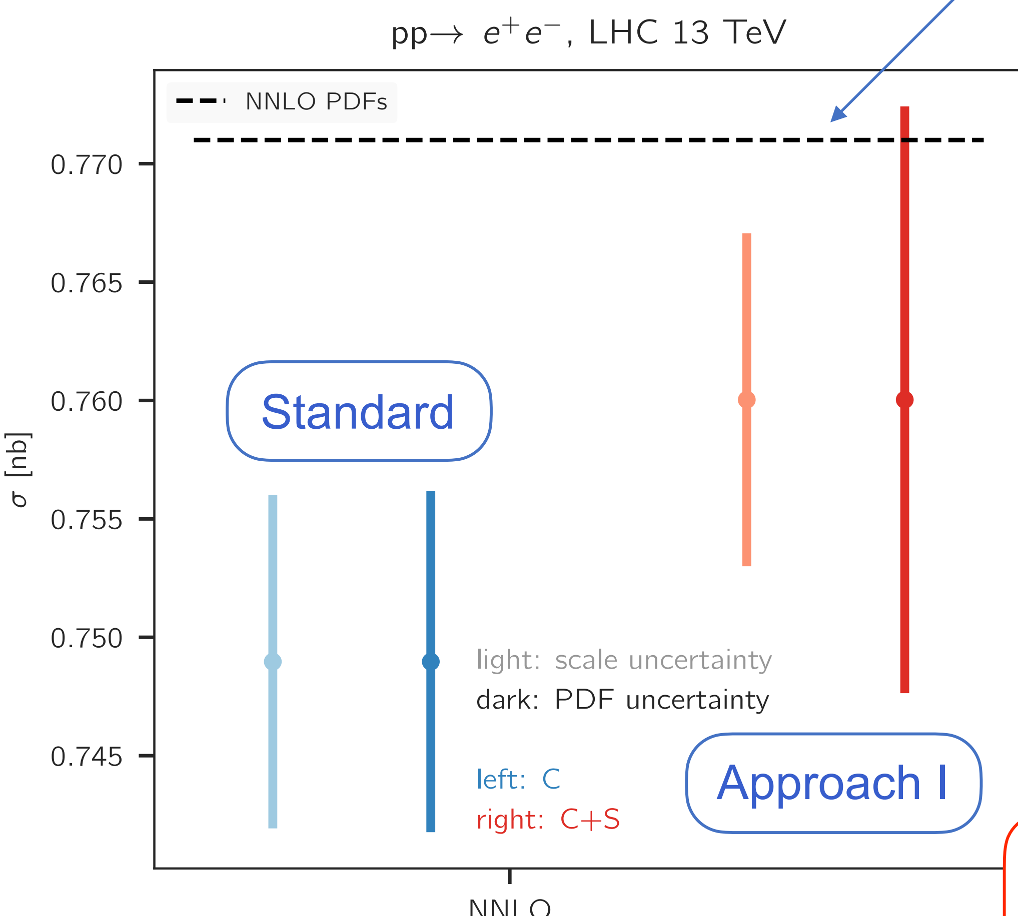


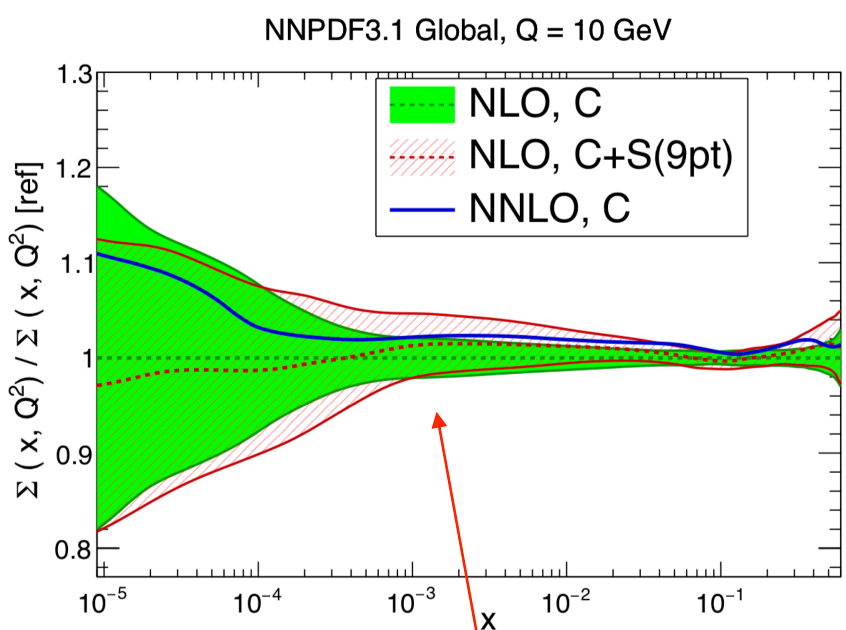
- PDF uncertainties compatible
- PDF uncertainty increases by 70% once MHOUs included
- Central value shifts beyond original PDF uncertainty
- "True" NNLO result now within uncertainties
- **Less precise, more accurate**

Results: Impact at the LHC

Z production

"True" NNLO central value

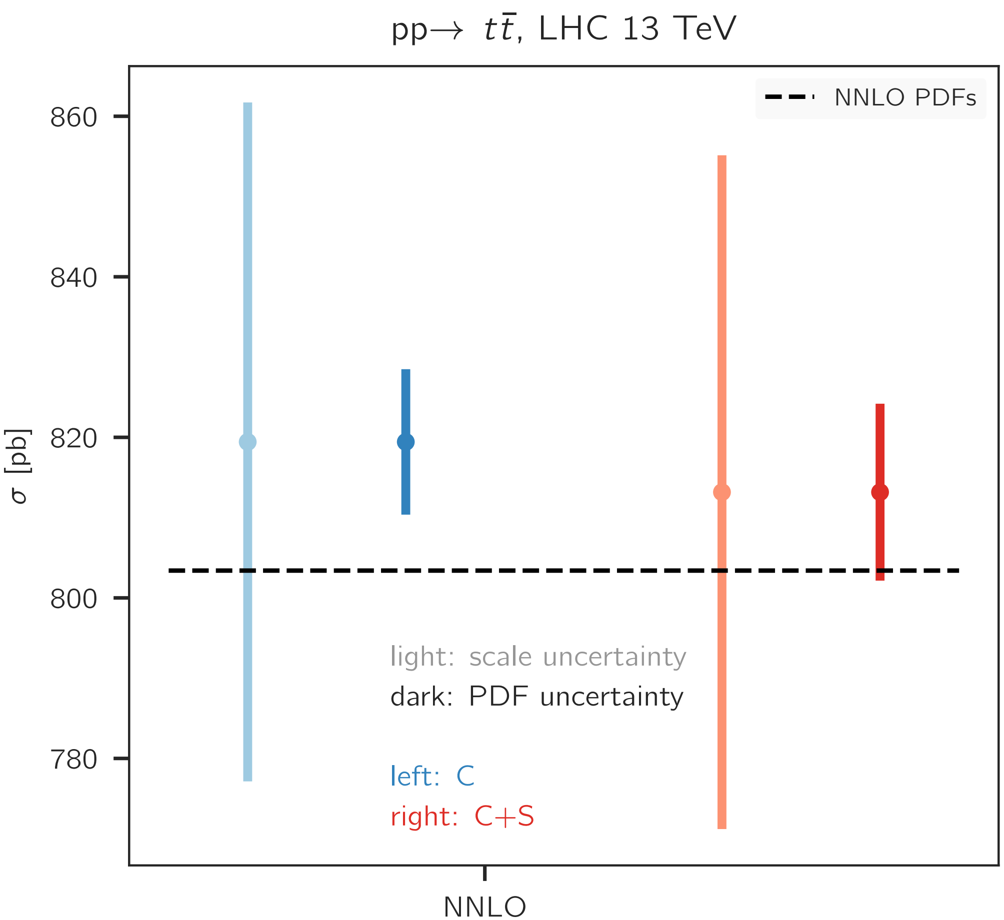




Relevant quantity:
Light sea quark PDFs down to $x \sim 10^{-3}$

Results: Impact at the LHC

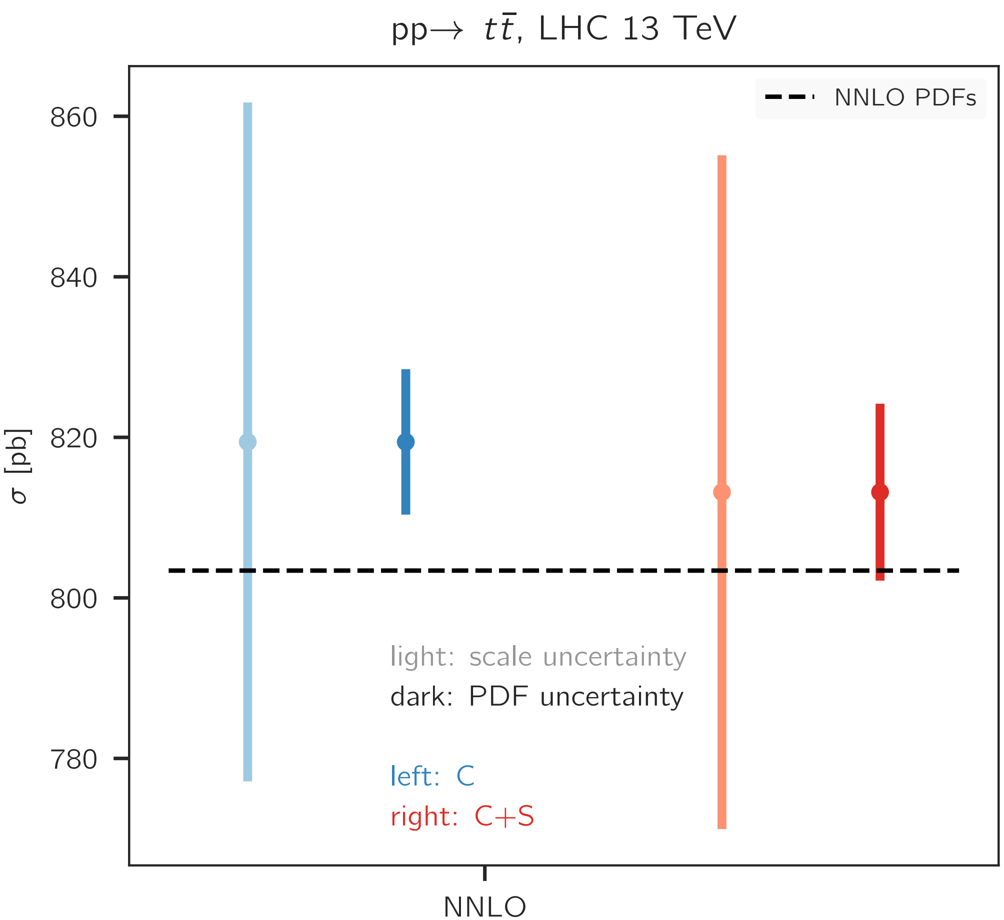
Top pair production

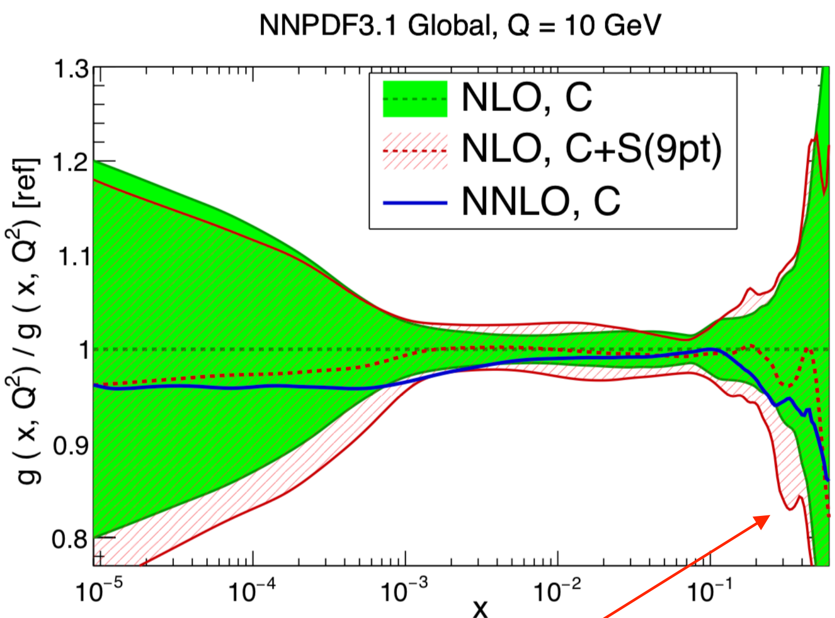


- PDF uncertainty increases by 20% once MHOUs included
- Central value shifts by amount comparable to original PDF uncertainty
- Again, "true" NNLO result now within uncertainties
- Slightly **less precise, more accurate**

Results: Impact at the LHC

Top pair production





Relevant quantity:
Gluon PDF at $x \sim 0.3$

Approach I: Conclusions

- Systematically including MHOUs in PDFs is now important, and will become crucial
- A new framework for including MHOUs in PDFs has been developed, based on **fitting with a theory covariance matrix**
- This is **validated** against **NNLO-NLO shift**
- Using this we have produced the **first PDF fits including MHOUs**, which are **more consistent** with NNLO PDFs than standard NLO fits
- Framework is applicable to **all sources of theoretical uncertainty**

Shortcomings of the approach

- **Black-box approach**: user of PDFs has no choice over the prescription used to include MHOUs
    - Effect of scale variations integrated into PDF replicas

- **Missing correlation** when combining PDFs with partonic cross sections:
    - For processes not included in fit (e.g. Higgs), missing μ_F correlation
    - For processes included in fit (e.g. $t\bar{t}$), missing μ_F, μ_R correlation

Approach II:
Monte Carlo scales uncertainties

Monte Carlo scale uncertainties

Idea: sample from the space of scale variations for each PDF replica

Overcomes two issues with envelope approach:

1. μ_R no longer has to be the same for all processes
2. We define a **probability density** for the PDFs by Monte Carlo sampling

Overcomes two issues with the theory covariance matrix approach:

1. No longer a “black-box”: the user can **resample** the replicas
2. Can keep track of **correlation** between scales in observable (e.g. Higgs cross section) and scales in PDFs

Monte Carlo scale uncertainties

Idea: sample from the space of scale variations for each PDF replica

- Split data into N_p processes, assign one μ_F (fully correlated approx.) and N_p renormalisation scales to theory predictions for each replica
- Vary these scales. Again, $k_F, k_R \in \left(\frac{1}{2}, 1, 2\right)$
- Build set of N_{rep} replicas where **scale info. is recorded** (in LHAPDF files)

$\Rightarrow$ Experimental uncertainties and MHOUs propagated to PDFs

E.g. rep_1: $k_F = 1,\ k_{R,\text{DIS NC}} = \frac{1}{2},\ k_{R,\text{jets}} = 2,\ \ldots$

rep_2: $k_F = 2,\ k_{R,\text{DIS NC}} = 2,\ k_{R,\text{jets}} = 1,\ \ldots,$ etc.

Monte Carlo scale uncertainties

- There are then 3^{N_p+1} scale combinations (729 for $N_p = 5$)
- Given $N_{\rm rep} = 100$ for a normal PDF fit (~ 1 day per replica), impractical to fit same no. of replicas for each scale combination

$\Rightarrow$ Define **probability distribution** for sampling scale combinations

Monte Carlo scale uncertainties

- There are then 3^{N_p+1} scale combinations (729 for $N_p = 5$)
- Given $N_{\text{rep}} = 100$ for a normal PDF fit (~ 1 day per replica), impractical to fit same no. of replicas for each scale combination

$\Rightarrow$ Define **probability distribution** for sampling scale combinations

Define: $\boxed{P(\mu = \xi) = \sum_{\text{all reps where } \mu=\xi} P(\omega)}$, where $\omega \in (\mu_F, \mu_{R,1}, \ldots, \mu_{R,N_p})$

Define: $\boxed{P(\mu_1 = \xi_1 \,|\, \mu_2 = \xi_2) = \frac{1}{P(\mu_2 = \xi_2)} \sum_{\text{all reps where } \mu_1=\xi_1,\ \mu_2=\xi_2} P(\omega)}$

Sampling model - symmetries

1. For one process, probability invariant under exchange of μ_F and μ_R

$$P(\mu_F = \xi) = P(\mu_{R,i} = \xi) \qquad \forall\ i = 1, \ldots, N_p$$

Sampling model - symmetries

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$$P(\mu_F = \xi) = P(\mu_{R,i} = \xi) \qquad \forall\ i = 1, \ldots, N_p$$

2. Conditional probabilities symmetric

$$P(\mu_F = \xi_x \,|\, \mu_{R,i} = \xi_y) = P(\mu_{R,i} = \xi_x \,|\, \mu_F = \xi_y) \qquad \forall\ i = 1, \ldots, N_p$$

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3. Probability symmetric under flipping of upper and lower variations

$$P(\mu_F = 2,\ \mu_{R,1} = 1,\ \mu_{R,2} = \frac{1}{2}, \ldots) = P(\mu_F = \frac{1}{2},\ \mu_{R,1} = 1,\ \mu_{R,2} = 2, \ldots)$$

Sampling model - symmetries

4. Renormalisation scales are not directly dependent on each other

$$P(\mu_{R,i} = \xi_i \,|\, \mu_F = \xi_F, \mu_{R,j} = \xi_j) = P(\mu_{R,i} = \xi_i \,|\, \mu_F = \xi_F)$$

$$\forall\ i, j = 1, \ldots, N_p$$

Sampling model - symmetries

4. Renormalisation scales are not directly dependent on each other

$$P(\mu_{R,i} = \xi_i \,|\, \mu_F = \xi_F, \mu_{R,j} = \xi_j) = P(\mu_{R,i} = \xi_i \,|\, \mu_F = \xi_F)$$

$$\forall\ i, j = 1, \ldots, N_p$$

5. Symmetry between renormalisation scales

$$P(\mu_{R,i} = \xi) = P(\mu_{R,j} = \xi)$$

$$\forall\ i, j = 1, \ldots, N_p$$

$$P(\mu_{R,i} = \xi \,|\, \mu_F = \xi_\mu) = P(\mu_{R,j} = \xi \,|\, \mu_F = \xi_\mu)$$

Monte Carlo scale uncertainties

- μ_R variations independent so we write:

$$P(\mu_F = \xi_F, \ldots, \mu_{R,N_p} = \xi_{R,N_p}) = \underbrace{P(\mu_F = \xi_F)}_{3} \prod_{i=1}^{N_p} \underbrace{P(\mu_{R,i} = \xi_{R,i} \mid \mu_F = \xi_F)}_{9}$$

- Four normalisation constraints:

$$\sum_{\xi \in \frac{1}{2},1,2} P(\mu = \xi) = 1 \qquad \sum_{\xi \in \frac{1}{2},1,2} P(\mu = \xi \mid \mu_F = \xi_F) = 1 \qquad 12 \to 8$$

- Symmetry when flipping upper and lower variations: 4 more $\quad 8 \to 4$
- Symmetry when flipping μ_F and μ_R in probability: 1 more $\quad 4 \to 3$

Free parameters

Under the symmetries of the model, there are just **three free parameters**

$$a \equiv \frac{P(k_F = 1)}{P(k_F = 2)} = \frac{P(k_F = 1)}{P(k_F = \frac{1}{2})}$$

$$b \equiv \frac{P(k_R = 1 \,|\, k_F = 1)}{P(k_R = 2 \,|\, k_F = 1)} = \frac{P(k_R = 1 \,|\, k_F = 1)}{P(k_R = \frac{1}{2} \,|\, k_F = 1)}$$

$$c \equiv \frac{P(k_R = 2 \,|\, k_F = 2)}{P(k_R = \frac{1}{2} \,|\, k_F = 2)} = \frac{P(k_R = \frac{1}{2} \,|\, k_F = \frac{1}{2})}{P(k_R = 2 \,|\, k_F = \frac{1}{2})}$$

Interpretation:

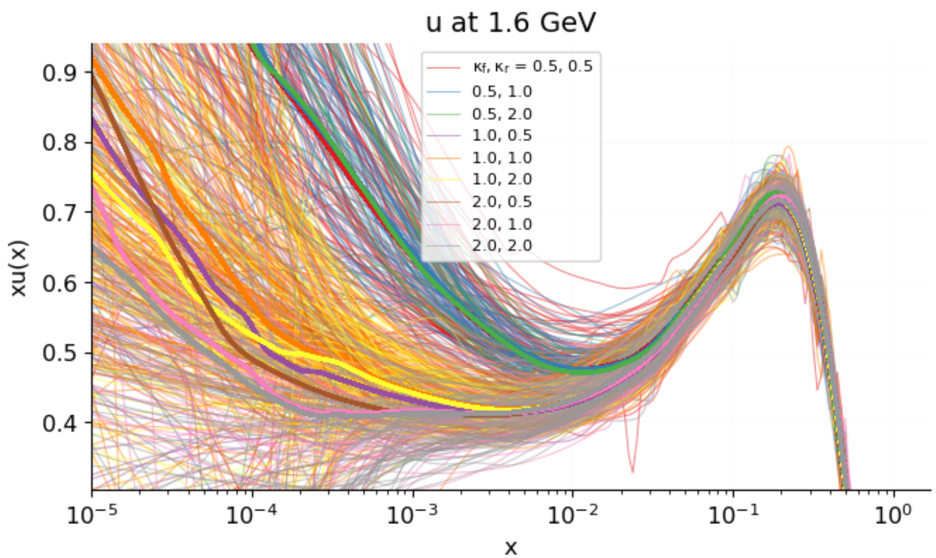
- If μ_F and μ_R are totally **independent** then $a = b$, $c = 1$
- If μ_F and μ_R are fully **correlated** then $b, c \to \infty$

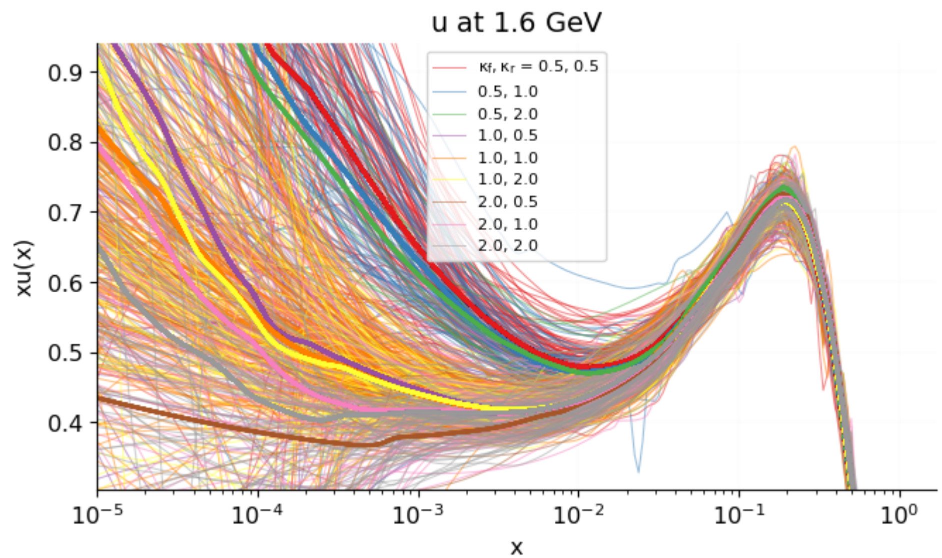
Preliminary results: PDFs

$a = 2, b = \dfrac{10}{3}, c = 9$

DIS CC

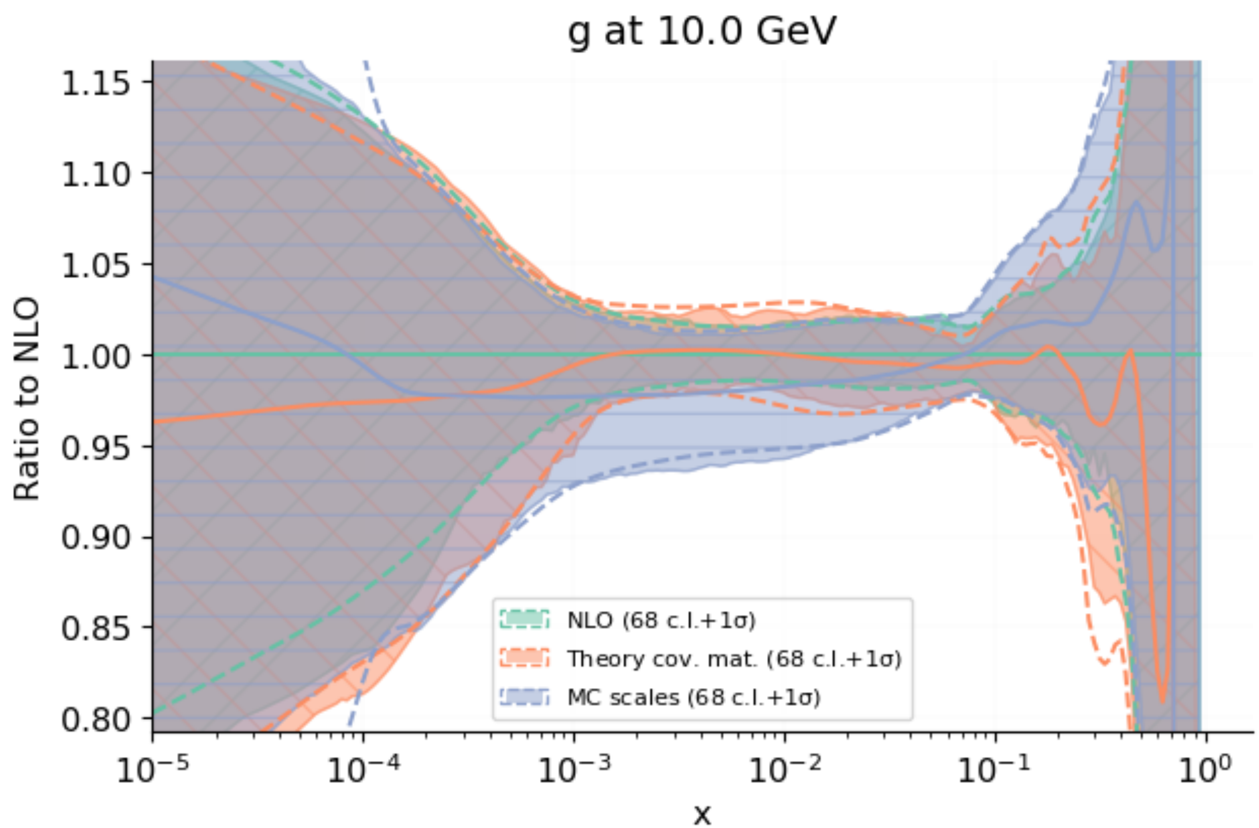
Jets





- We can plot PDF replicas and analyse the **scale dependence for each process**
- E.g. here $\mu_F = 0.5$ leads to enhancement of the u distribution below 0.05
- Can ask new questions: e.g. do certain scale choices for certain processes lead to bad fits?

Preliminary results: PDFs



$$a = 2$$
$$b = \frac{10}{3}$$
$$c = 9$$

- **Compatible PDFs** with theory cov. mat. and MC scales approaches
- MC scales leads to **larger uncertainties** in data regions → effect of MHOU not 'integrated out' in MC scale approach

Computing cross sections

‘**Default**’ predictions:

- Whatever scale choices in partonic cross section, convolute with all PDF replicas

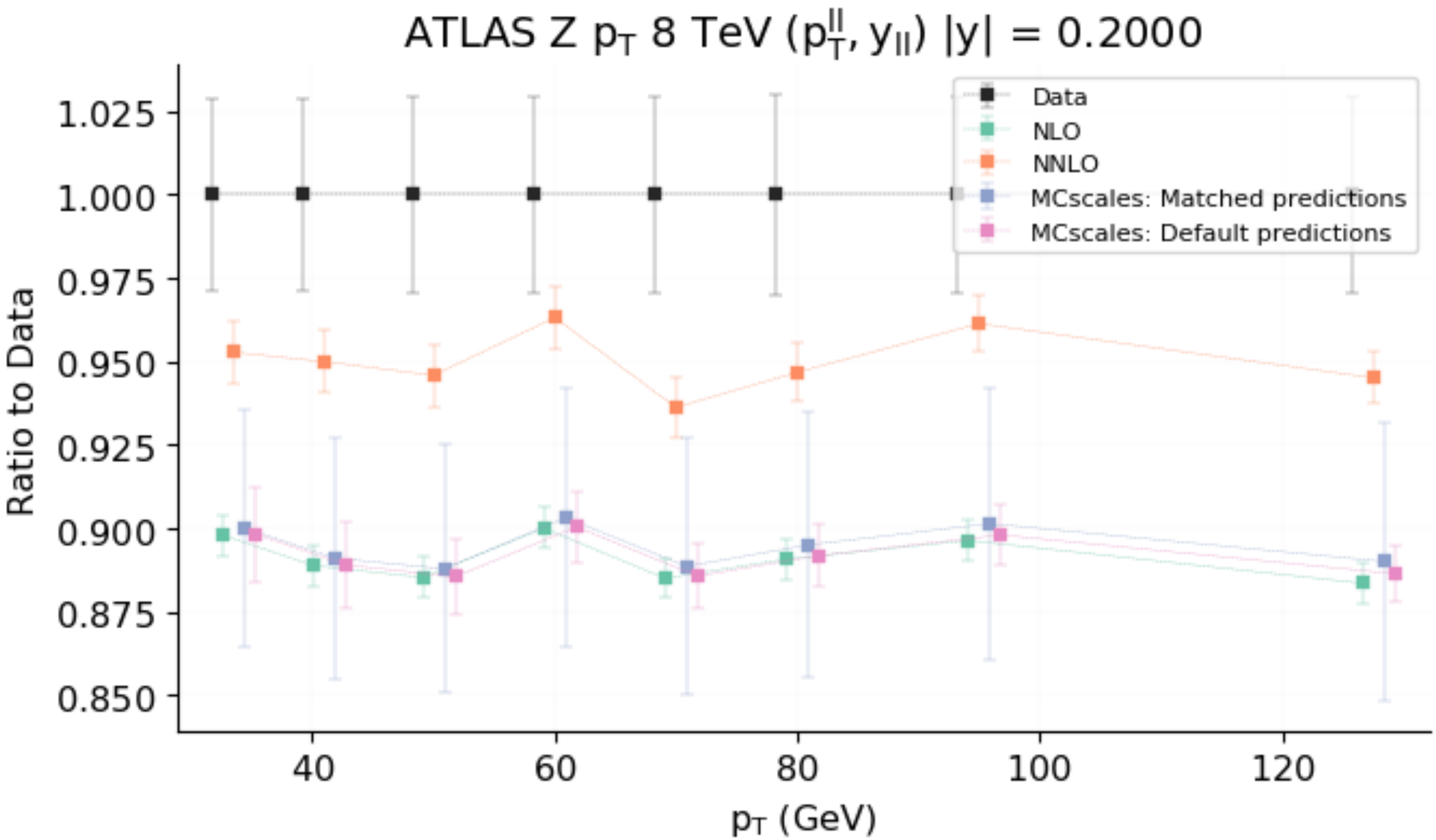
‘**Matched**’ predictions:

- Combine pieces in **correlated** way
- Convolute PDF replicas with partonic cross section at **same scales**
- Generate combined scale variation, PDF (inc. MHOU) uncertainty

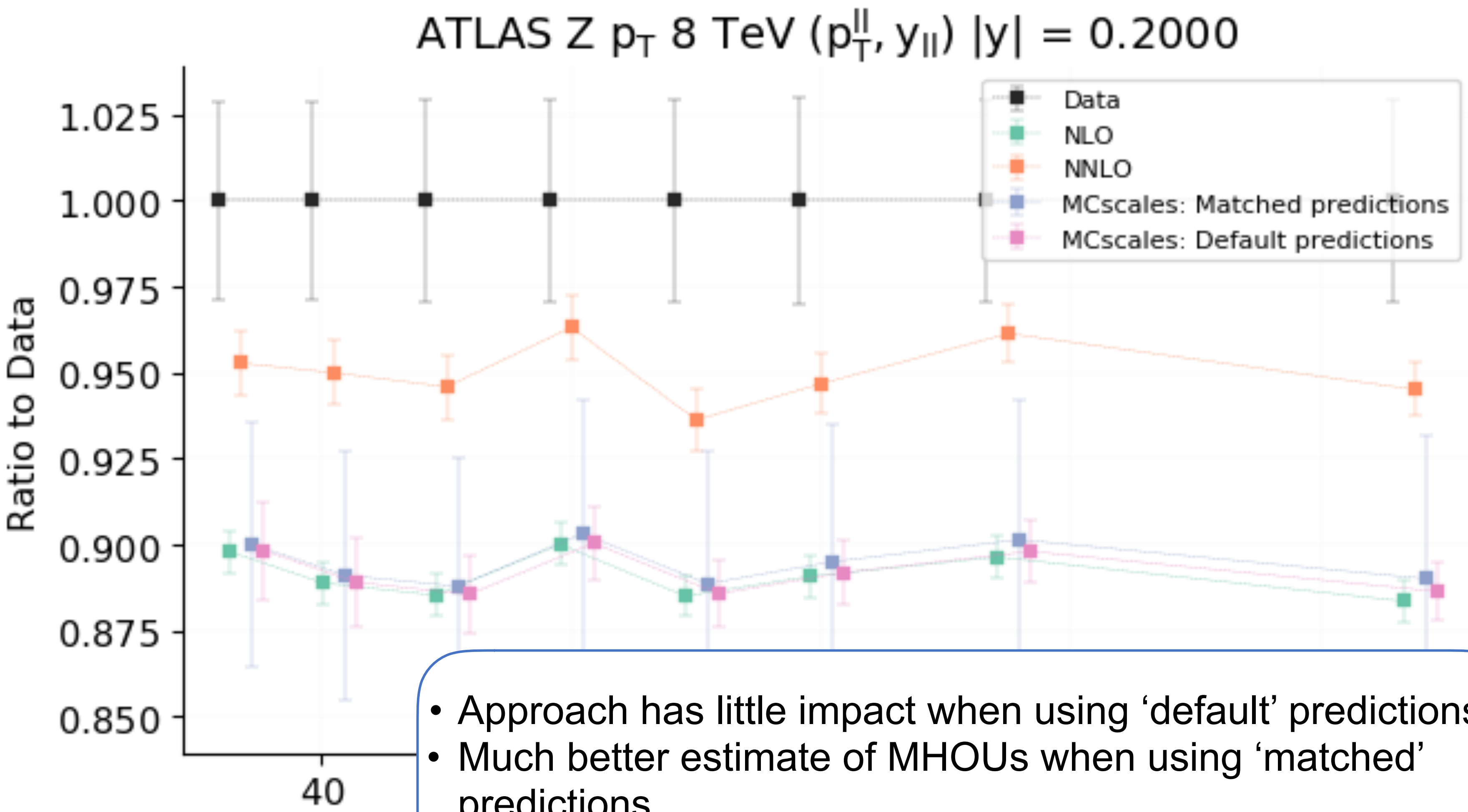
$$\sigma(\mu_{F,\mathrm{top}}, \mu_{R,\mathrm{top}}) = \hat{\sigma}(\mu_R = \mu_{R,\mathrm{top}}) \otimes f^{(k)}(\mu_F = \mu_{F,\mathrm{top}}, \mu_R = \mu_{R,\mathrm{top}})$$

$$\sigma(\mu_{F,\mathrm{Higgs}}, \mu_{R,\mathrm{Higgs}}) = \hat{\sigma}(\mu_R = \mu_{R,\mathrm{Higgs}}) \otimes f^{(k)}(\mu_F = \mu_{F,\mathrm{Higgs}})$$

Preliminary results: cross sections

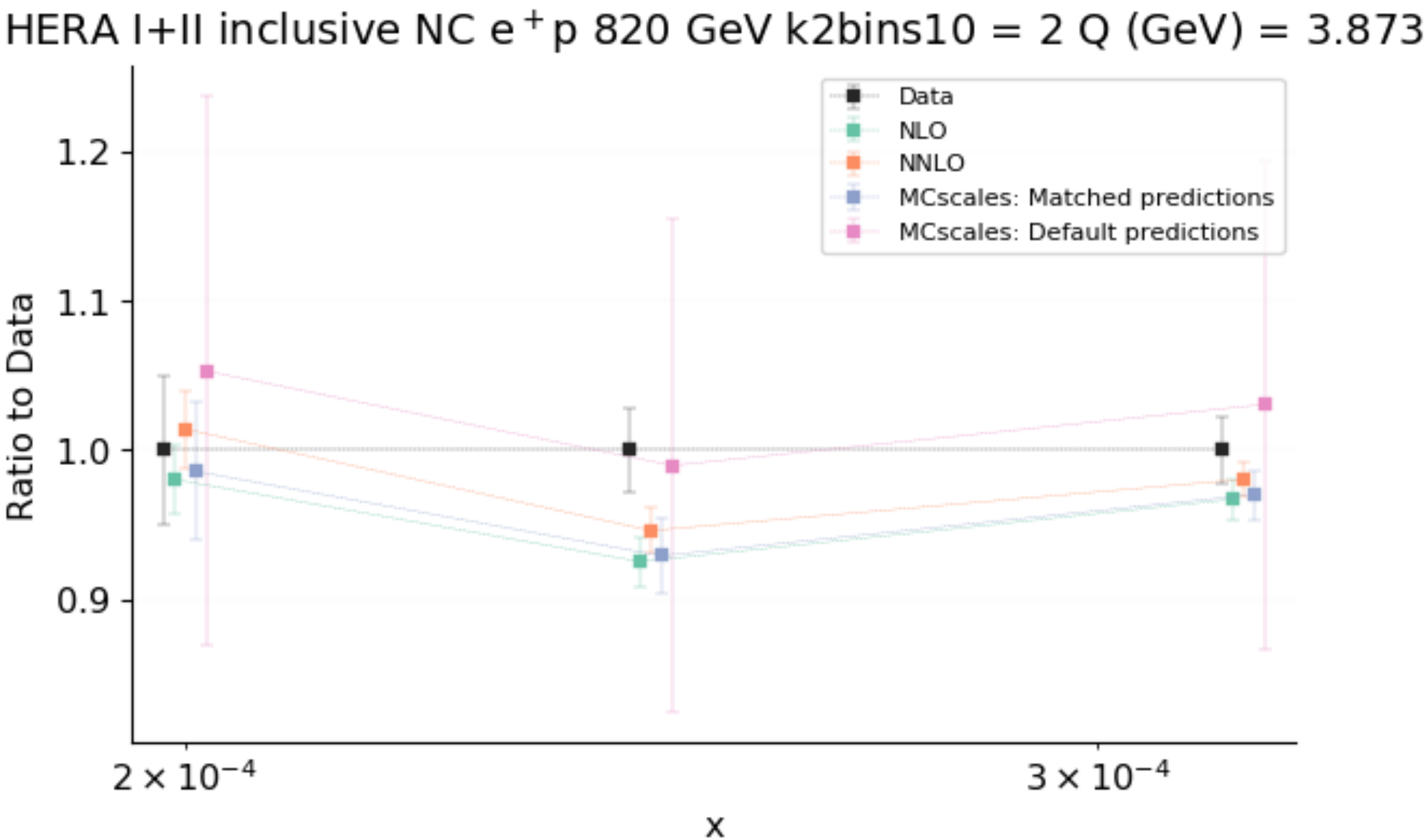


Preliminary results: cross sections

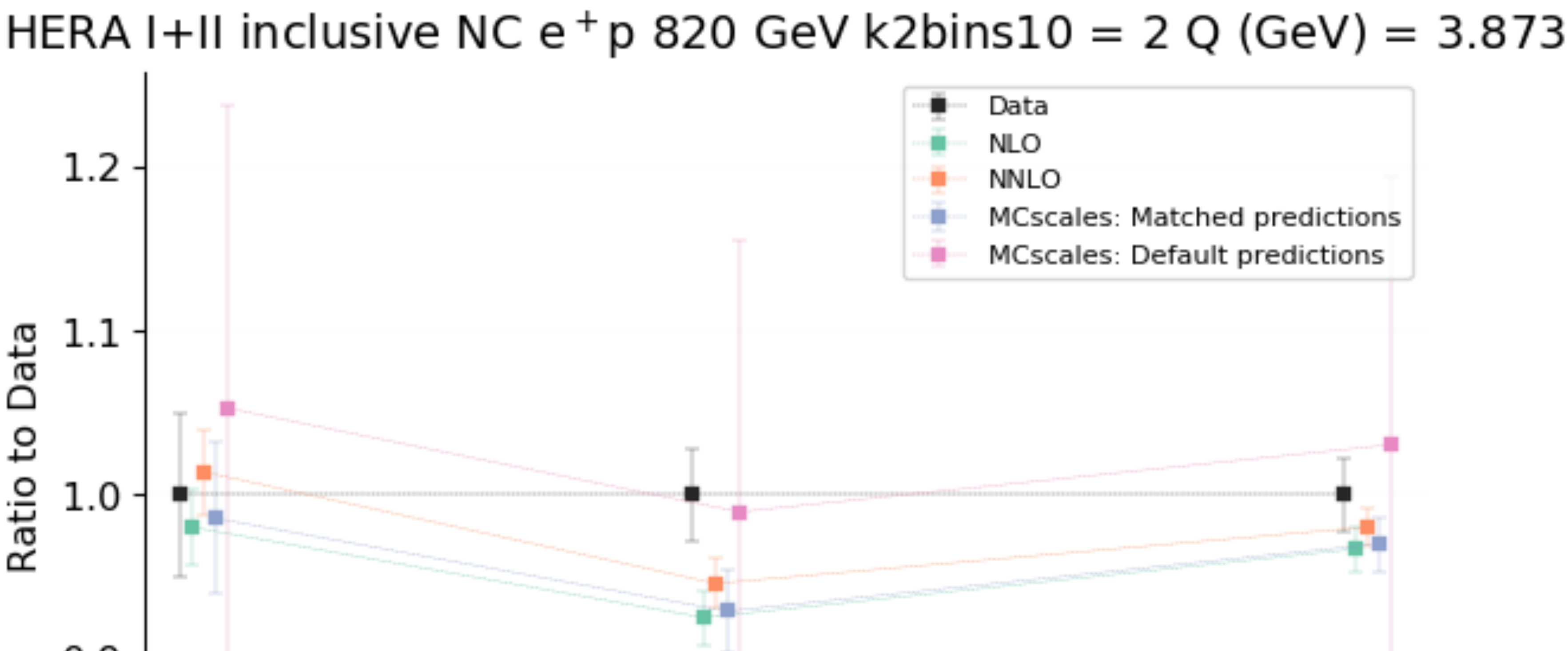


- Approach has little impact when using 'default' predictions
- Much better estimate of MHOUs when using 'matched' predictions
- **Correlation of scales has big impact**

Preliminary results: cross sections



Preliminary results: cross sections



- Situation is reversed w.r.t. Z production (matched predictions reduce PDF uncertainty)
- Matched predictions again give reasonable results, while default predictions do not
- **Correlation of scales has big impact**

Future work

- Develop MC scales approach by e.g. studying impact of choices of a, b, c
- Study differences between two approaches. Do they give similar results?

Refine each approach:

- Study impact of **process categorisation**
- **Decorrelate** μ_F by having independent variations for different PDFs (singlet vs non-singlet evolution)
- Produce **global NNLO fits with MHOUs** included - will be most state-of-the-art PDFs available

Thank you for listening!

Extra slides

Theoretical covariance matrix

- Theory is perturbative expansion to some order : $t_p = \sum_{m=0}^{p} c_m$
- Standard case: $P(d|t_p) \propto \exp\Big(-\frac{1}{2} \underbrace{(d-t_p)^T \mathrm{cov}_{\mathrm{exp}}^{-1} (d-t_p)}_{\chi^2_{\mathrm{exp}}} \Big)$
- Bayes' theorem: $P(t_p|d) = \frac{P(d|t_p)P(t_p)}{P(d)} \propto P(d|t_p)P(t_p)$
- Assume Gaussian theory prior:

$$P(t_p) = \prod_{m=0}^{p} P(c_m) \quad \text{where} \quad P(c_m) \propto \exp\Big(-\frac{1}{2} \underbrace{c_m^T \mathrm{cov}_{\mathrm{th},m}^{-1} c_m}_{\chi^2_{\mathrm{th}}} \Big)$$

- Assume MHOUs due to O(α^{p+1}) terms only → marginalise these terms:

$$P(t_p|d) \propto \int dc_{p+1} P(d|c_{p+1}) P(t_{p+1})$$

$$\propto \exp\Big(-\frac{1}{2} \underbrace{(d-t_p)^T (\mathrm{cov}_{\mathrm{exp}} + \mathrm{cov}_{\mathrm{th}})^{-1} (d-t_p)}_{\chi^2_{\mathrm{tot}}} \Big)$$

- Include higher order terms by induction

THEORY COVARIANCE MATRICES
SUBTLETIES I: DEFINITION

"STANDARD" DEFINITION OF SCALE VARIATION:
USE RG INVARIANCE OF PHYSICAL OBSERVABLE

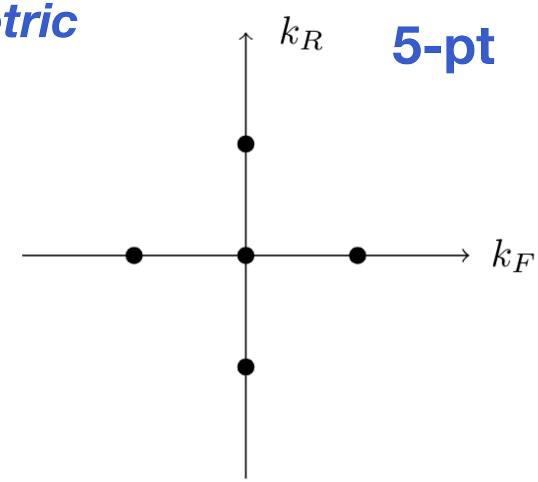
- HADRONIC (HXSWG...): $\sigma(Q^2) = \sum_{ij} \hat\sigma_{ij}\left(\frac{Q^2}{\mu_F^2}, \frac{Q^2}{\mu_R^2}, \alpha_s(\mu_R^2)\right) f_i(\mu_F^2) f_j(\mu_F^2)$
  - FACTORIZATION: $f_i({\mu'_F}^2) = \left(1 + P_0 \ln \frac{{\mu'_F}^2}{{\mu'_F}^2}\right) f_i(\mu_F^2)$
  - RENORMALIZATION: $\alpha({\mu'}_r^2)\left(1 - \beta_0 \alpha \mu_R^2 \ln \frac{{\mu'_R}^2}{{\mu'_R}^2}\right)$
  - μ_F DEP IN PDF, μ_R DEP IN $\hat\sigma$
- DIS (Virchaux-Milsztajn, MRS, PEGASUS, APFEL,...):
  $F(Q^2) = \sum_i C_i\left(\frac{Q^2}{\mu_F^2}, \frac{Q^2}{\mu_R^2}, \alpha_s(Q^2)\right) f_i(\mu_F^2, \mu_R^2)$
  - FACTORIZATION: AS ABOVE
  - RENORMALIZATION: LET $\alpha(\mu_F^2) \to \alpha(\mu_R^2)$ IN EVOLUTION EQUATION
  - BOTH μ_R, μ_F VARIED IN PDF
- DIFFERENCE DIFFERENT NNLO TERMS GENERATED AT NLO
  "ADDITIVE" VS. "MULTIPLICATIVE"
  - DIS NLO $\ln \frac{\mu_R}{\mu_F}$, HADRONIC $\ln \frac{\mu_R}{Q} \ln \frac{\mu_F}{Q}$
  - DIS NLO $\beta_0 P_1$ TERMS, HADRONIC $\beta_0 + P_1$

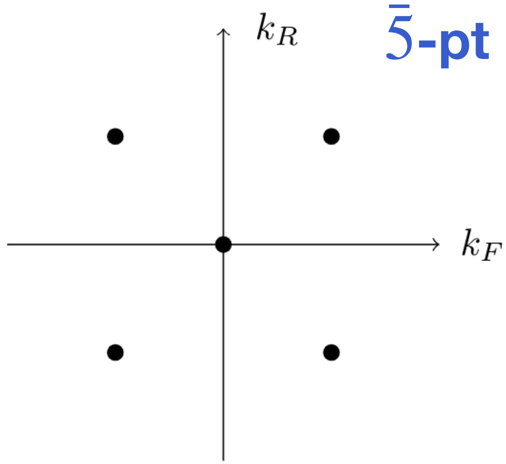
$\Rightarrow$ ADOPT A COMMON PRESCRIPTION

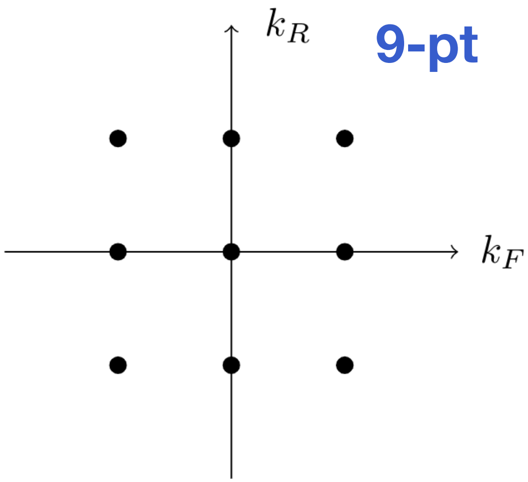
[credit: *S. Forte, 2018*]

Point prescriptions

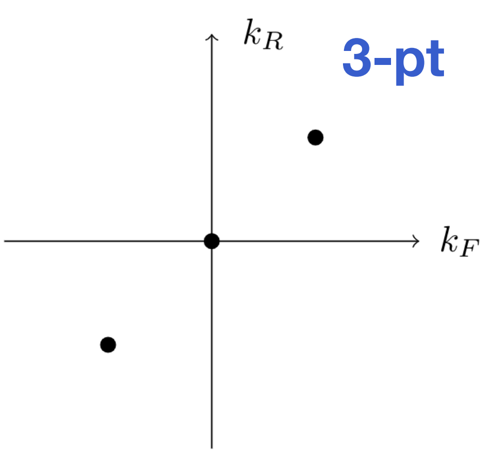
Symmetric

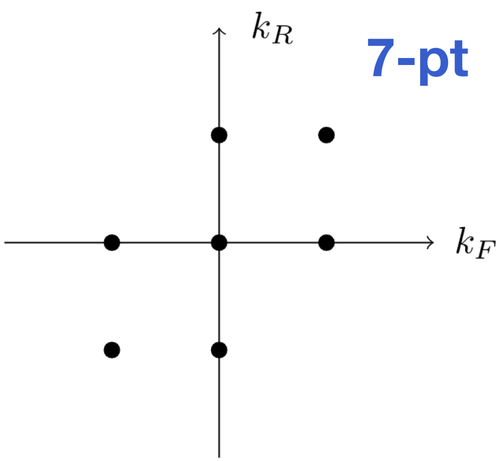






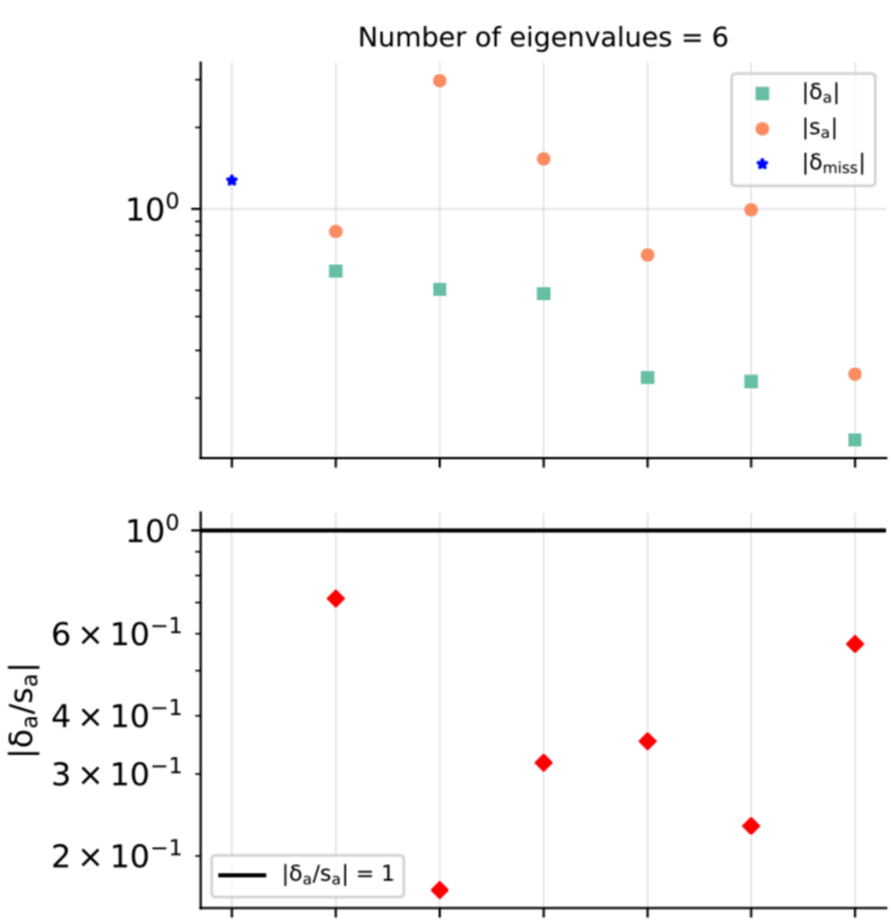
Asymmetric



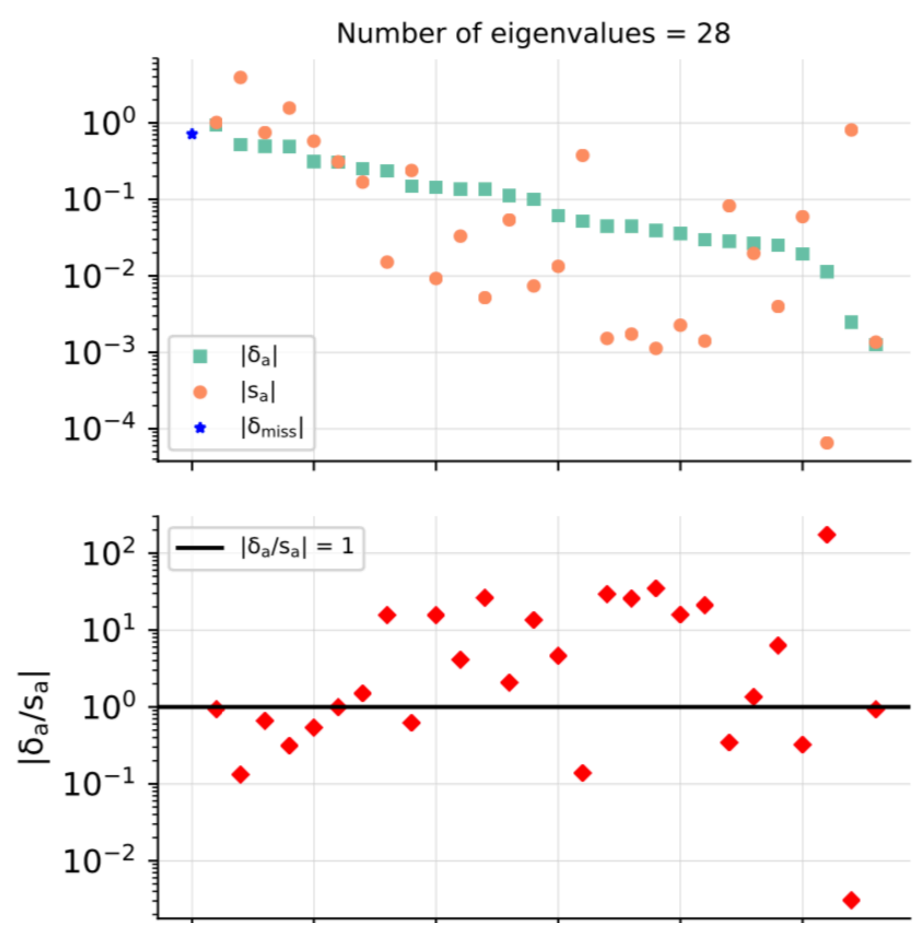


Validation: size of uncertainties

3-pt



9-pt



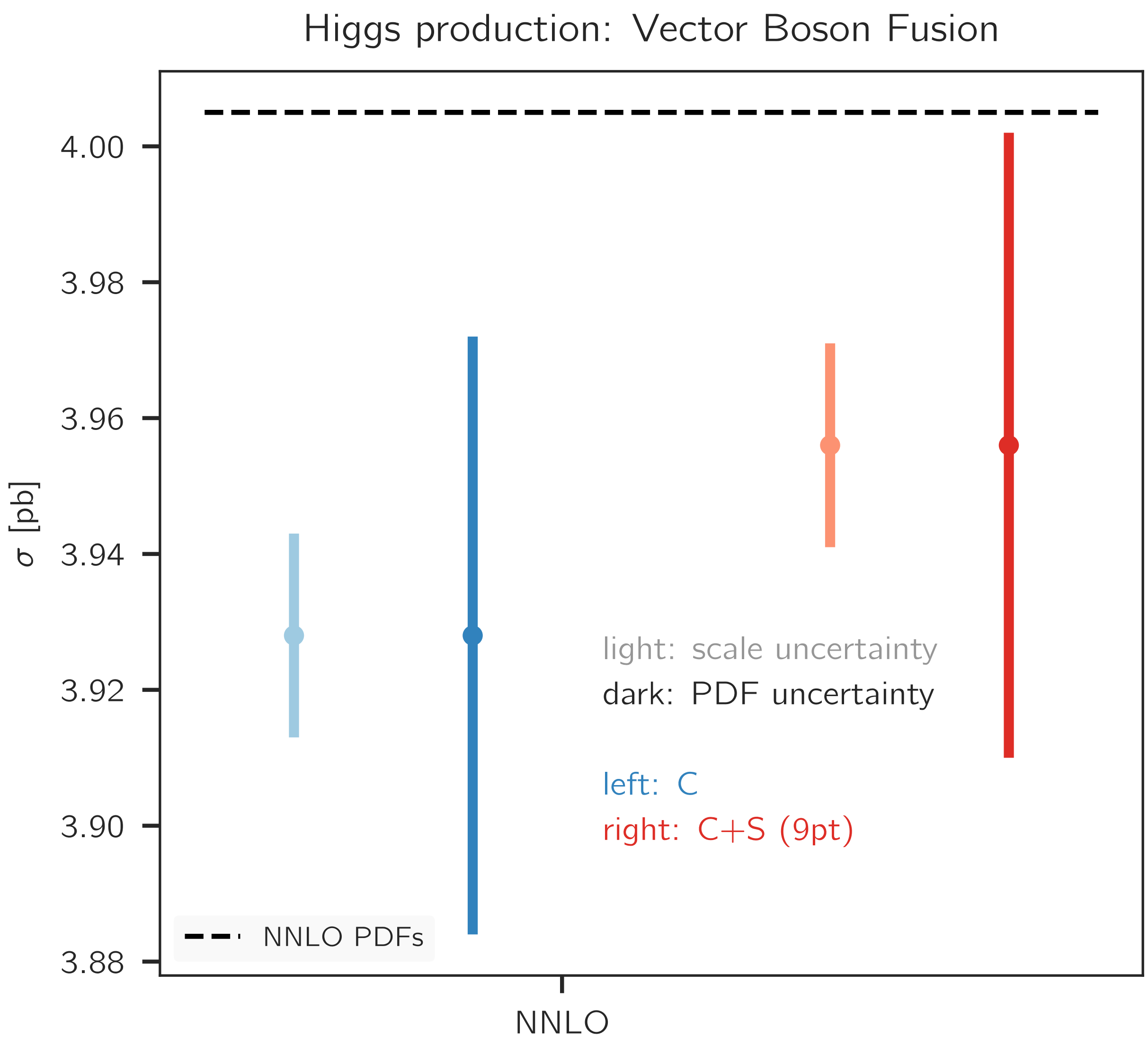
Results: Impact at the LHC

- Now do this comparison at level of **observable predictions**
- Recommended method for combining partonic cross section with PDFs: **proceed as normal**

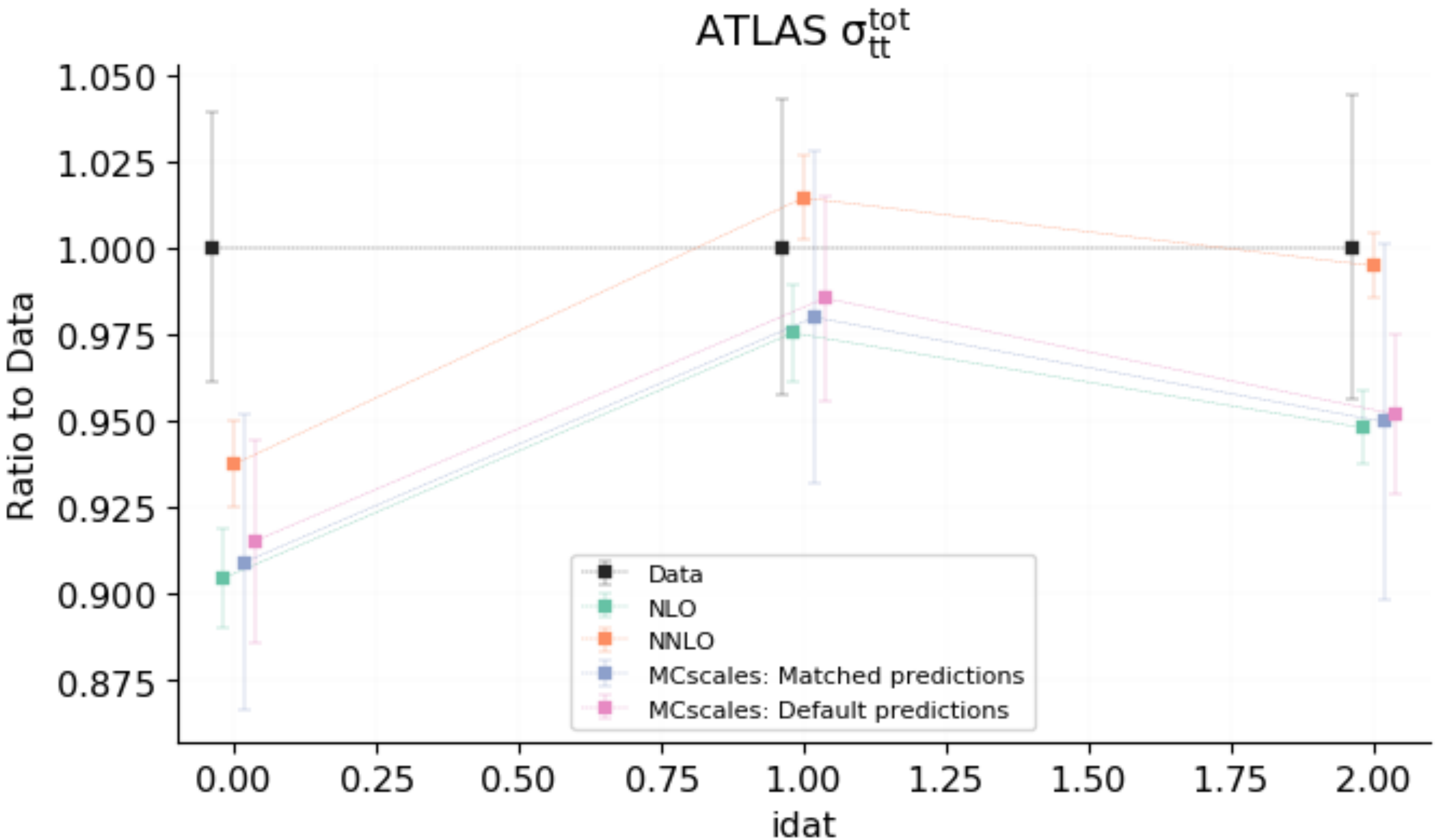
1. Use DGLAP evolution with central scale choice (μ_F variation accounted for elsewhere)
2. Compute PDF uncertainty as normal, by convoluting all PDF replicas with partonic cross section at central scales: this now includes MHOUs
3. Estimate MHOU on partonic cross section by using scale variations, can e.g. use a point prescription

How does our treatment of MHOUs impact **precision** and **accuracy** of predictions?

Results: Impact at the LHC



Preliminary results: cross sections



Data set and cuts

The following datasets are included in both `NNPDF31_nlo_as_0118_1000` and `190302_ern_nlo_central_163_global`:

- HERA I+II inclusive NC e^+p 920 GeV
- NMC p
- LHCb Z 940 pb
- CMS W rapidity 8 TeV
- D0 Z rapidity
- HERA I+II inclusive CC e^+p
- CDF Z rapidity
- ATLAS low-mass DY 2011
- CMS $\sigma_{tt}^{\rm tot}$
- HERA I+II inclusive NC e^+p 820 GeV
- CHORUS $\sigma_{CC}^{\bar\nu}$
- ATLAS W, Z 7 TeV 2011
- ATLAS HM DY 7 TeV
- ATLAS $\sigma_{tt}^{\rm tot}$
- BCDMS d
- BCDMS p
- LHCb $W, Z \to \mu$ 8 TeV
- CMS W asymmetry 840 pb
- HERA I+II inclusive NC e^+p 575
- NuTeV $\sigma_c^{\bar\nu}$
- HERA I+II inclusive NC e^+p 460
- D0 $W \to e\nu$ asymmetry
- HERA I+II inclusive CC e^-p
- D0 $W \to \mu\nu$ asymmetry
- NMC d/p
- HERA $\sigma_c^{\rm NC}$
- SLAC d
- CMS Drell-Yan 2D 7 TeV 2011
- LHCb $W, Z \to \mu$ 7 TeV
- LHCb $Z \to ee$ 2 fb
- ATLAS $t\bar{t}$ rapidity y_t
- NuTeV σ_c^{ν}
- SLAC p
- ATLAS Z p_T 8 TeV (p_T^{ll}, M_{ll})
- CHORUS σ_{CC}^{ν}
- ATLAS Z p_T 8 TeV (p_T^{ll}, y_{ll})
- CMS jets 7 TeV 2011
- CMS $t\bar{t}$ rapidity $y_{t\bar{t}}$
- HERA I+II inclusive NC e^-p
- CMS Z p_T 8 TeV (p_T^{ll}, y_{ll})
- CMS W asymmetry 4.7 fb
- ATLAS W, Z 7 TeV 2010
- ATLAS jets 2011 7 TeV

Changes to cuts:

$$Q^2_{\rm min} = 3.49 \to 13.96\ \mathrm{GeV}^2$$

Intersection of NLO, NNLO cuts

The following datasets are included in `NNPDF31_nlo_as_0118_1000` but not in `190302_ern_nlo_central_163_global`:

- ATLAS jets 2.76 TeV
- CMS $W + c$ ratio
- DY E886 $\sigma^p_{\rm DY}$
- ATLAS jets 2010 7 TeV
- CMS jets 2.76 TeV
- HERA H1 F_2^b
- DYE 866 $\sigma^d_{\rm DY}/\sigma^p_{\rm DY}$
- CMS $W + c$ total
- DY E605 $\sigma^p_{\rm DY}$
- CDF Run II k_t jets
- HERA ZEUS F_2^b

Data removed:

- Fixed target Drell-Yan
- Bottom structure function
- Jets without exact NNLO theory
- W+charm

Correlating scale variations between PDFs and predictions

How to use these PDFs consistently in theoretical predictions?

Consider a situation when all data is at one scale. Let us only have evolution uncertainties, i.e. turn off uncertainties in hard cross sections

We have three scales:

- Q_0 : fitting scale of PDFs
- $Q_{\rm data}$: scale of data
- $Q_{\rm pred.}$: scale of prediction

$\rightarrow$

We have two evolutions:

$Q_0 \to Q_{\rm data}$

$Q_0 \to Q_{\rm pred.}$

1. Q_0 is kept fixed. There is no dependence on Q_0 because for a sufficiently flexible parameterisation changes in Q_0 are absorbed by fit
2. We vary $Q_{\rm data}$ in fits (in a correlated way among data points)
3. One varies $Q_{\rm pred.}$ when making a prediction for an observable

Correlating scale variations between PDFs and predictions

How are Q_{data} and $Q_{\text{pred.}}$ correlated?

- In our procedure Q_{data} and $Q_{\text{pred.}}$ variations will necessarily be uncorrelated - necessary consequence of delivering universal PDFs
- For points where $Q_{\text{data}} = Q_{\text{pred.}} \neq Q_0$, the variations are fully correlated and we overestimate uncertainty by factor of $\sqrt{2}$
- In global fit overestimate due to missing correlation will be between 1 and $\sqrt{2}$, but likely to be closer to 1
- **Importantly**: if one neglects either variation, one will **in general** underestimate MHOUs
- Better to have a conservative estimate of uncertainties than to underestimate them
- Same for coefficient function: if estimating μ_R uncertainty for process included in fit, we will miss correlations $\Rightarrow$ larger uncertainty than in ideal scenario
- **Not a double counting.** Instead, a problem of **missing correlation**