NNPDF4.0 uncertainties are faithful

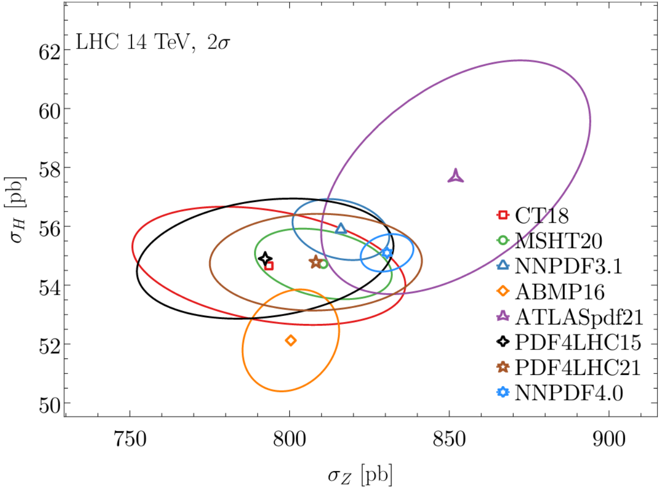
PDF4LHC meeting

Emanuele R. Nocera

on behalf of the NNPDF Collaboration

CERN - 23 November 2022

PDF uncertainties for the LHC Run III



[Figure taken from the Snowmass 2021 whitepaper: Proton structure at the precision frontier, arXiv:2203.13923]

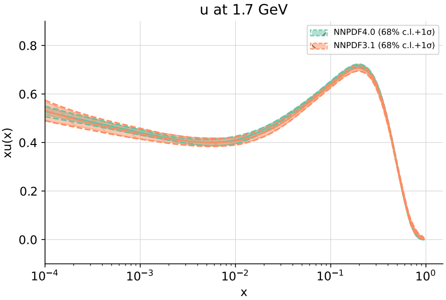
A statistically robust framework to estimate PDF uncertainties
is of paramount importance for precision and discovery LHC physics

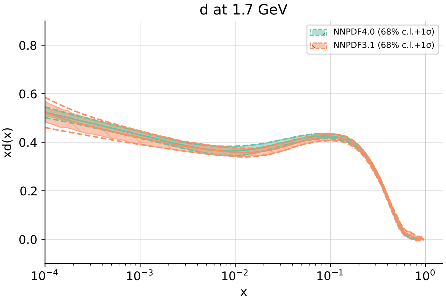
NNPDF4.0 uncertainties have been recently questioned

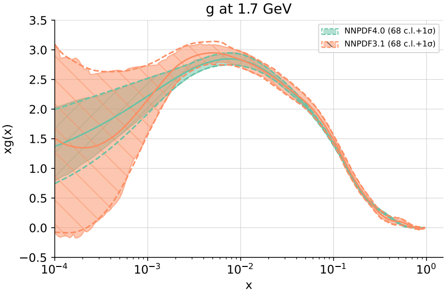
1. Understanding NNPDF4.0 uncertainties

[http://nnpdf.mi.infn.it/wp-content/uploads/2022/11/20221122_Paper.pdf]

From NNPDF3.1 to NNPDF4.0







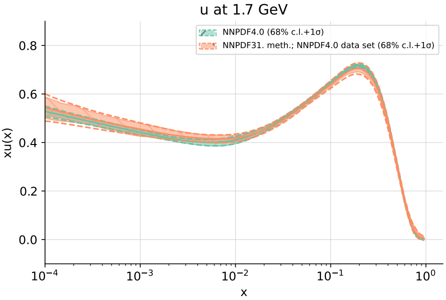
data set (N_{dat}) \ methodology	NNPDF3.1	NNPDF4.0
NNPDF3.1 (4092)	**1.19**	1.12
NNPDF4.0 (4618)	1.25	**1.15**

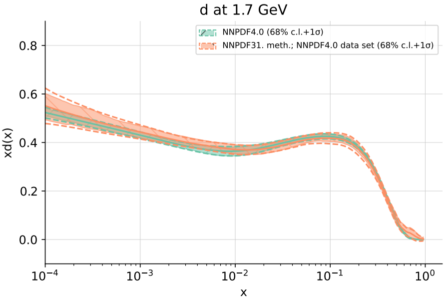
Consistency between PDF sets

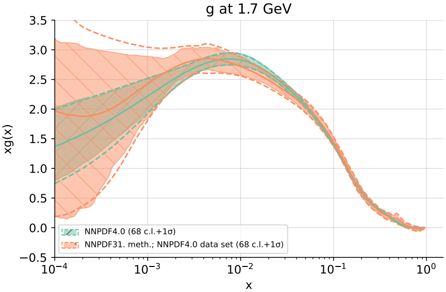
NNPDF4.0 more precise
(combination of data set and methodology)

NNPDF4.0 more accurate
(superiority of the NNPDF4.0 methodology)

From NNPDF3.1 to NNPDF4.0







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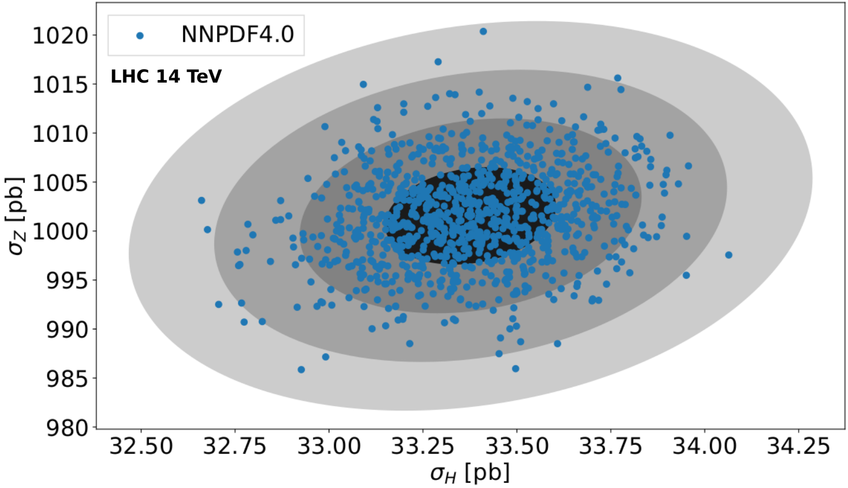
Importance sampling



$N_{\rm rep} = 100$ replicas are sufficient to reproduce mean values and uncertainties to 1%

Importance sampling is reproduced correctly (14 replicas out of 1000 vs 98.9% C.I.)

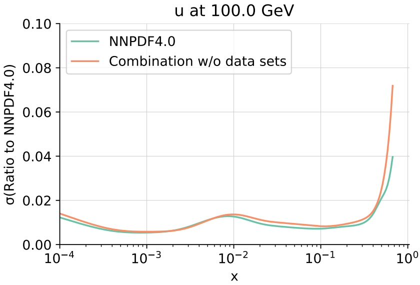
Outliers in the distribution of fitted replicas are good fits to unlikely fluctuations of the data

Combining Monte Carlo replicas

Each replica has the same statistical weight: one can construct combinations of ensembles
This feature is used, *e.g.*, to construct the PDF4LHC21 set [JPG 49 (2022), 080501]

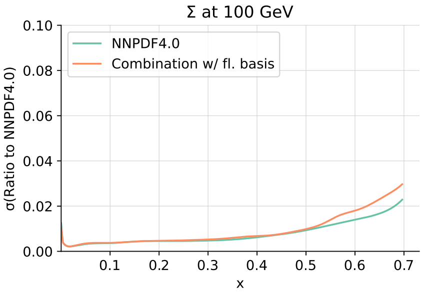
Data set variations

Data set	$N_{\rm dat}$	χ^2	n_σ
NMC σ^p	204	1.56	5.66
BCDMS F_2^p	333	1.41	5.29
HERA I+II	1145	1.20	4.79
HERA σ^c	37	2.03	4.43
E866 σ^p	89	1.56	3.74
ATLAS 7 TeV dijets	90	2.15	7.71
CMS 7 TeV dijets	54	1.81	4.20



Parametrisation basis variation

$$f_i \in \begin{cases} \{V, V_3, V_8, T_3, T_8, T_{15}, \Sigma, g\} \\ \{u, \bar{u}, d, \bar{d}, s, \bar{s}, c+\bar{c}, g\} \end{cases}$$

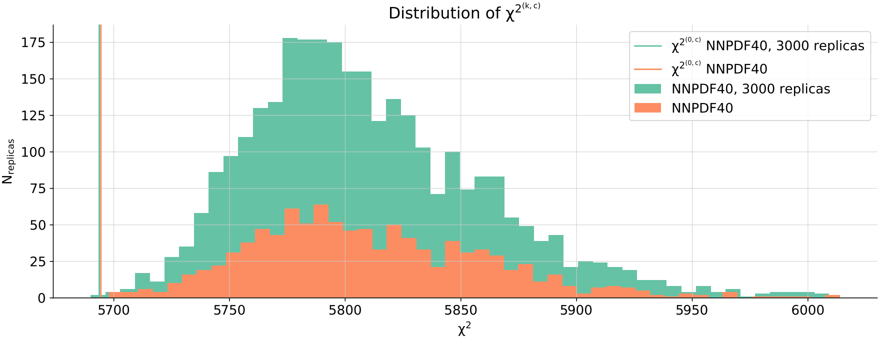


Defining the χ^2

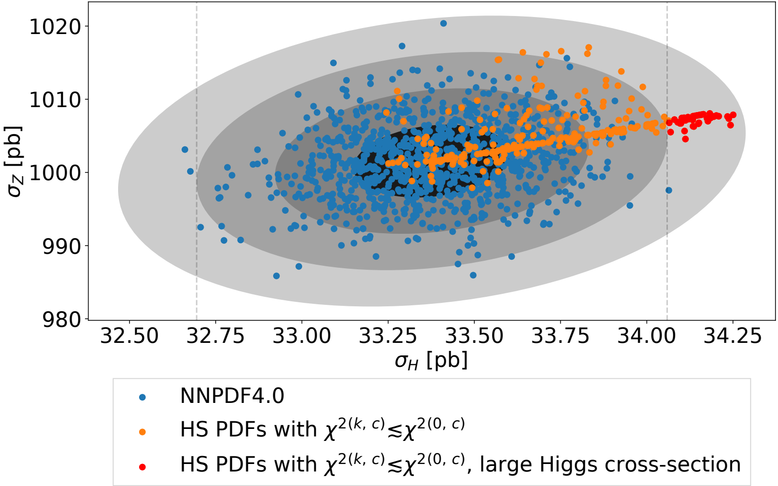
$$\chi^2 = \frac{1}{N_{\rm dat}} \sum_{i,j}^{N_{\rm dat}} \Delta_i \left(\mathrm{cov}_{t_0}^{-1}\right)_{ij} \Delta_j \qquad \begin{cases} \chi^{2(k)} & \Delta_i = T_i^{(k)} - D_i^{(k)} \\ \chi^{2(k,c)} & \Delta_i = T_i^{(k)} - D_i^{(c)} \\ \chi^{2(0,c)} & \Delta_i = T_i^{0} - D_i^{(c)} \end{cases}$$

t_0 used to avoid D'Agostini bias
[JHEP 05 (2010) 075]
[JHEP 04 (2013) 125]

$$(\mathrm{cov}_{t_0})_{ij} = \delta_{ij} s_i^{(\text{uncorr})}\, s_j^{(\text{uncorr})} + \sum_{m=1}^{N_{\rm norm}} \sigma_{i,m}^{(\rm norm)} \sigma_{j,m}^{(\rm norm)} T_i^{(0)} T_j^{(0)} + \sum_{l=1}^{N_{\rm corr}} \sigma_{i,l}^{(\rm corr)} \sigma_{j,l}^{(\rm corr)} D_i D_j,$$



Hopscotch PDFs [arXiv:2205.10444]



HS PDFs do not have statistical meaning in the same sense as replicas

$$\chi^{2(k,c)} - \chi^{2(0,c)} = -0.01 \qquad \sigma_{\chi^2} = \sqrt{2/N_{\rm dat}} \sim 0.02 \text{ (for } N_{\rm dat} \sim 4000)$$

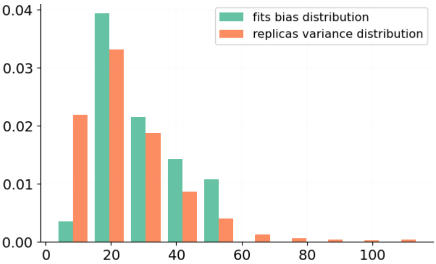
Closure tests [EPJ C77 (2017) 663; EPJ C82 (2022) 330]

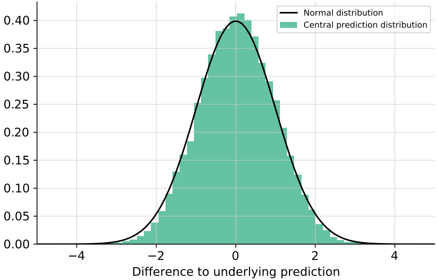
A test to validate PDF uncertainties in the data region

Fit PDFs to pseudodata generated
assuming a known underlying law

Define bias and variance
bias difference of central prediction and truth
variance uncertainty of replica predictions

If PDF uncertainty faithful, then
E[bias] = variance
25 fits, 40 replicas each



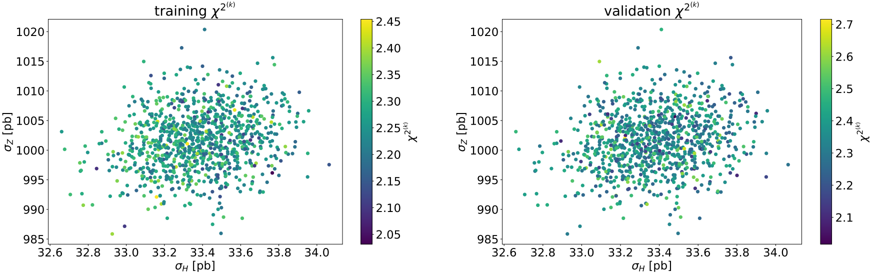


Can the NNPDF methodology find HS PDFs-like replicas?

Test 1

Are the value of the $\chi^{2(k)}$ similar
regardless of the values of predictions for the Z and H cross sections?

YES



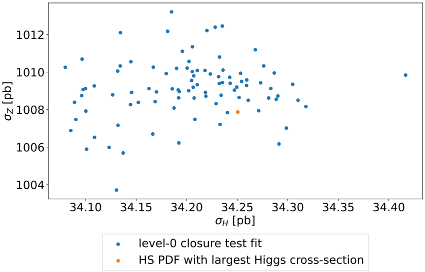
Can the NNPDF methodology find HS PDFs-like replicas?

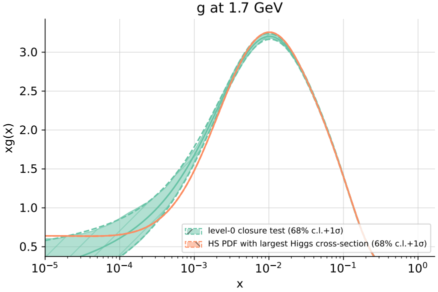
Test 2

Can we fit HS PDFs if these are used as truth in a closure test level-0?

YES

$$\langle \chi^{2(k)} \rangle_{\rm tr} = 0.03 \pm 0.01 \qquad \langle \chi^{2(k)} \rangle_{\rm val} = 0.04 \pm 0.02$$



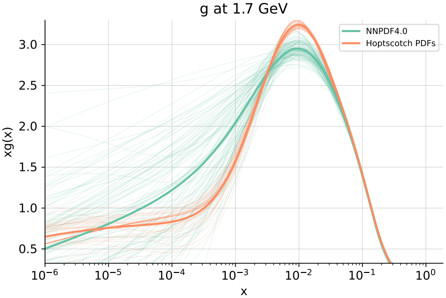


Yet HS PDFs look different w.r.t. NNPDF replicas:
they must have a feature which is not data-driven

Why are HS-PDFs-like replicas unlikely in NNPDF sets?

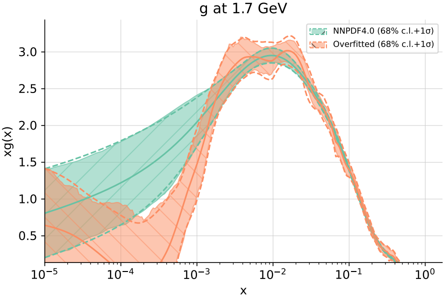
Observation 1

A comparison between NNPDF replicas and HS PDFs reveals a peculiar kink in HS PDFs



Observation 2

An overfitted gluon can be obtained with $\chi^{2(0,c)}$ smaller than NNPDF4.0 by $0.08 \times N_{\rm dat}$



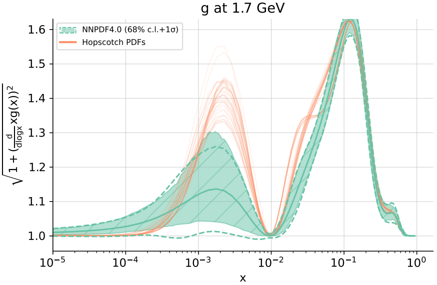
Is the kink peculiar to HS PDFs a sign of overfitting?

Why are HS-PDFs-like replicas unlikely in NNPDF sets?

Metric 1: Kinetic Energy

$$\mathrm{KE} = \sqrt{1 + \left(\frac{d}{d\ln x} x f(x, Q^2)\right)^2}$$

A measure of PDF wiggliness:
the higher the KE, the longer the curve that joins two fixed points



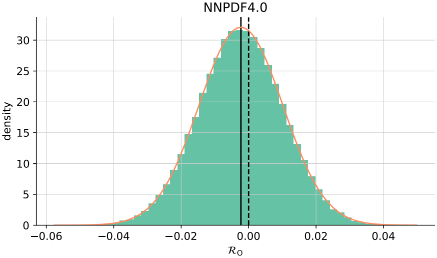
Why are HS-PDFs-like replicas unlikely in NNPDF sets?

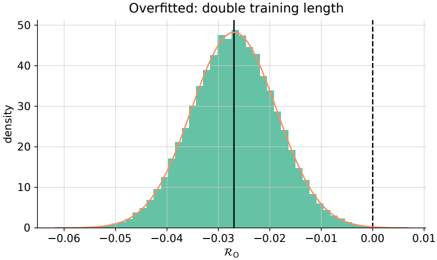
Metric 2: Overfit metric

$$\mathcal{R}_O = \chi^2_{\rm val}\left[T^{(k)}, D^{(k)}\right] - \overline{\chi^2_{\rm val}}\left[T^{(k)}, D^{(k)}\right]$$

$$\overline{\chi^2_{\rm val}}\left[T^{(k)}, D^{(k)}\right] \equiv \frac{1}{N}\sum_{k'=1}^{N} \chi^2_{\rm val}\left[T^{(k)}, D^{(k')}\right]\Big|_{\rm fixed\,mask}$$

A measure of PDF overfitting:
for each replica, there is a different fluctuation and training/validation split (mask)
if $\mathcal{R}_O < 0$ the replica is overfitted, *i.e.* it contains information specific to D^k



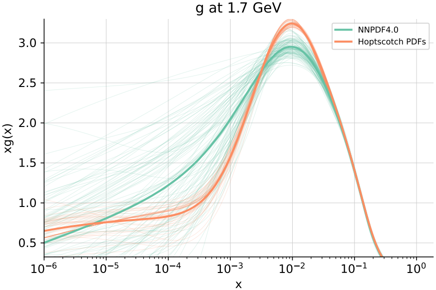


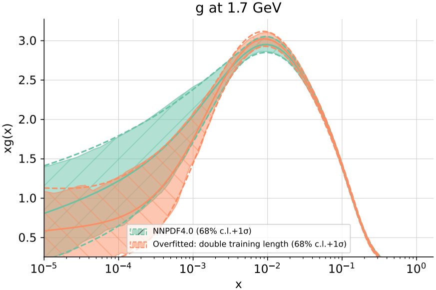
$\mathcal{R}_O = -0.001 \pm 0.013$ (NNPDF4.0) $\quad$ $\mathcal{R}_O = -0.027 \pm 0.001$ (overfitted NNPDF4.0)

Why are HS-PDFs-like replicas unlikely in NNPDF sets?

Conclusion

The NNPDF4.0 methodology can produce overfitted PDFs that look like HS PDFs





HS PDFs are not found by the default NNDPF4.0 methodology
because they would correspond to overfitted replicas

2. NNPDF4.0 extrapolation uncertainties: A_{FB}

[arXiv:2209.08115]

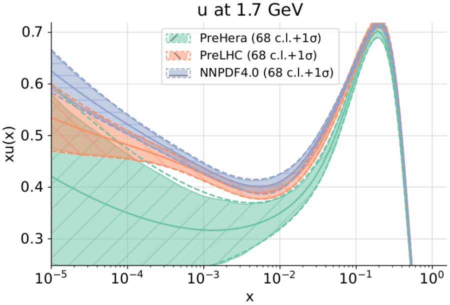
Future tests [Acta Phys.Polon. B52 (2021) 243]

A test to validate PDF uncertainties in the extrapolation regions

Test PDF uncertainties on data sets
not included in a given PDF fit
that cover unseen kinematic regions

Data set	NNPDF4.0	pre-LHC	pre-HERA
pre-HERA	1.09	1.01	0.90
pre-LHC	1.21	1.20	23.1
NNPDF4.0	1.29	3.30	23.1

Only exp. cov. matrix



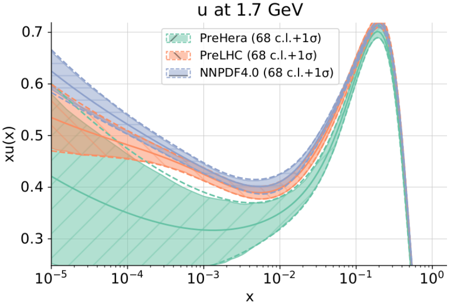
Future tests [Acta Phys.Polon. B52 (2021) 243]

A test to validate PDF uncertainties in the extrapolation regions

Test PDF uncertainties on data sets
not included in a given PDF fit
that cover unseen kinematic regions

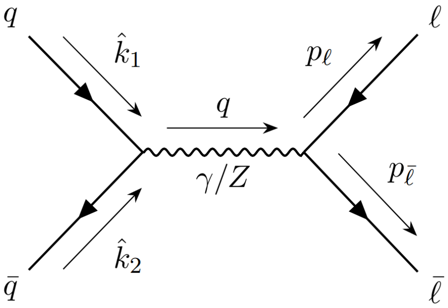
Data set	NNPDF4.0	pre-LHC	pre-HERA
pre-HERA			0.86
pre-LHC		1.17	1.22
NNPDF4.0	1.12	1.30	1.38

Exp+PDF cov. matrix



The Drell-Yan forward-backward asymmetry

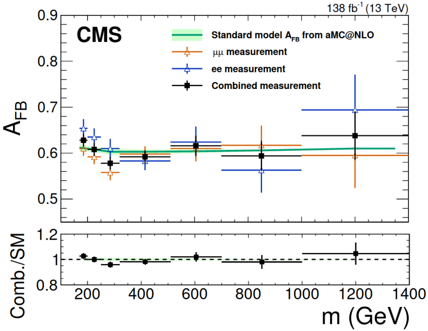
$$A_{\rm fb}(\cos\theta) \equiv \frac{\frac{d\sigma}{d\cos\theta}(\cos\theta) - \frac{d\sigma}{d\cos\theta}(-\cos\theta)}{\frac{d\sigma}{d\cos\theta}(\cos\theta) + \frac{d\sigma}{d\cos\theta}(-\cos\theta)}$$

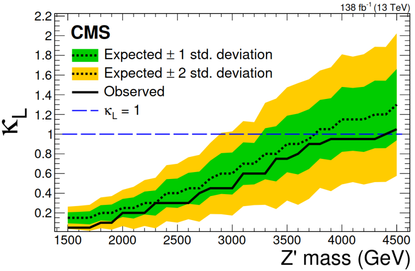


$A_{\rm fb}$ sensitive to chiral BSM couplings

Exp. uncertainties cancel out in the ratio

PDF uncertainties may be large
(large-x extrapolation region)





[JHEP 08 (2022) 063]

Anatomy of the asymmetry

Scattering angle in the partonic CM frame

Measure $\cos\theta^* = \text{sign}(y_{\ell\bar\ell})\cos\theta$: w.r.t. direction of Z

$$\cos\theta \equiv \frac{p_\ell^+ p_{\bar\ell}^- - p_\ell^- p_{\bar\ell}^+}{m_{\ell\bar\ell}\sqrt{m_{\ell\bar\ell}^2 + p_{\mathrm{T},\ell\bar\ell}^2}}, \quad p^\pm = p^0 \pm p^3$$

At LO: direction of parton with largest x

LO cross section

$$\frac{d^3\sigma}{dm_{\ell\bar\ell}\,dy_{\ell\bar\ell}\,d\cos\theta^*} = \frac{\pi\alpha^2}{3m_{\ell\bar\ell}s}\left((1+\cos^2(\theta^*))\sum_q S_q\mathcal{L}_{S,q}(m_{\ell\bar\ell},y_{\ell\bar\ell}) + \cos\theta^*\sum_q A_q\mathcal{L}_{A,q}(m_{\ell\bar\ell},y_{\ell\bar\ell})\right)$$

Symmetric and antisymmetric luminositites

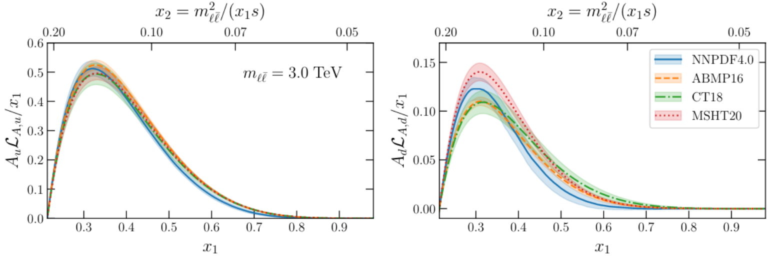
$$\mathcal{L}_{S,q}(m_{\ell\bar\ell},y_{\ell\bar\ell}) \equiv f_q(x_1,m_{\ell\bar\ell}^2)f_{\bar q}(x_2,m_{\ell\bar\ell}^2) + f_q(x_2,m_{\ell\bar\ell}^2)f_{\bar q}(x_1,m_{\ell\bar\ell}^2)$$
$$\mathcal{L}_{A,q}(m_{\ell\bar\ell},y_{\ell\bar\ell}) \equiv \text{sign}(y_{\ell\bar\ell})\left[f_q(x_1,m_{\ell\bar\ell}^2)f_{\bar q}(x_2,m_{\ell\bar\ell}^2) - f_q(x_2,m_{\ell\bar\ell}^2)f_{\bar q}(x_1,m_{\ell\bar\ell}^2)\right]$$
$$x_1 = \frac{m_{\ell\bar\ell}}{\sqrt{s}}\exp(y_{\ell\bar\ell}) \qquad x_2 = \frac{m_{\ell\bar\ell}}{\sqrt{s}}\exp(-y_{\ell\bar\ell}) \qquad x_1x_2 = \frac{m_{\ell\bar\ell}}{\sqrt{s}}$$

Integrate over $m_{\ell\bar\ell}$ and $y_{\ell\bar\ell}$

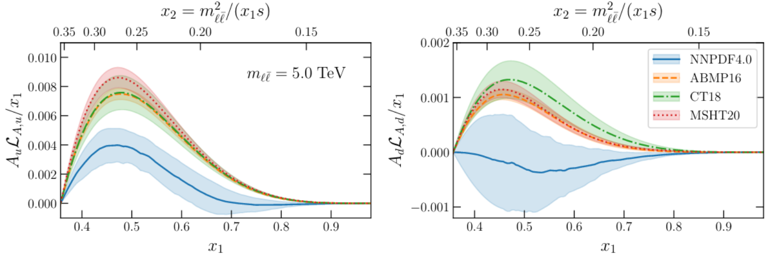
$$A_{\text{fb}}(\cos\theta^*) = \frac{\cos\theta^*}{1+\cos^2(\theta^*)}\frac{g_A}{g_{S,q'}} \qquad g_{A,S} \propto \int \frac{dm_{\ell\bar\ell}}{m_{\ell\bar\ell}}\frac{dx_1}{x_1}\mathcal{L}_{\mathcal{A},\mathcal{S}}(m_{\ell\bar\ell},x_1)$$

At LO, the effective coupling is determined by the luminosity

Symmetric and antisymmetric PDF luminositites

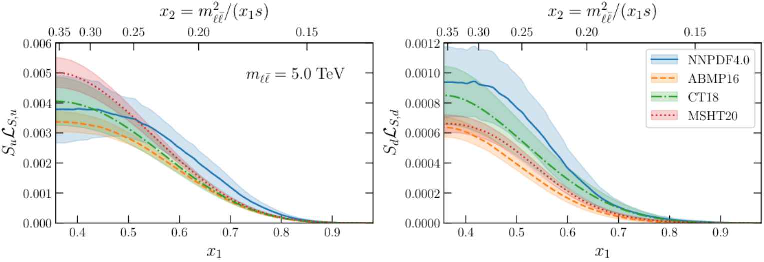


Antisymmetric luminosities look valence-like at $m_{\ell\bar{\ell}} = 3$ TeV; agreement across PDF sets

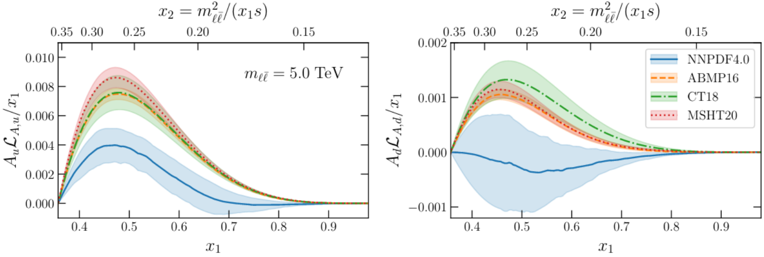


Antisymmetric luminosities differ for $m_{\ell\bar{\ell}} = 5$ TeV across PDF sets
NNPDF4.0 uncertainties are the largest

Symmetric and antisymmetric PDF luminositites



Symmetric luminosities agree across PDF sets at $m_{\ell\bar{\ell}} = 5$ TeV



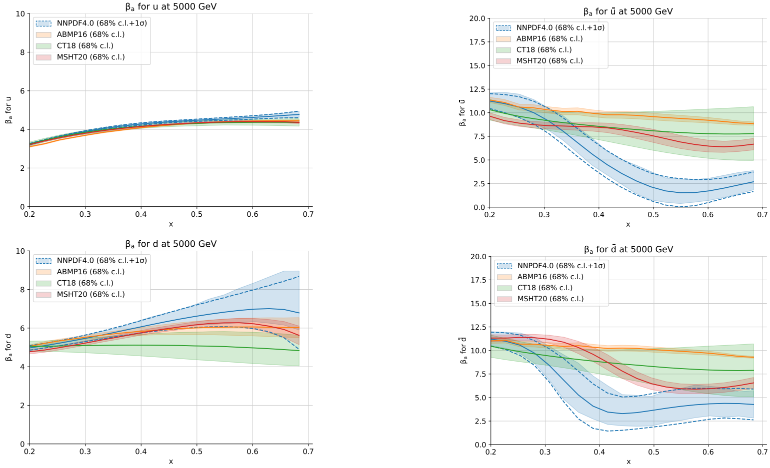
Antisymmetric luminosities differ for $m_{\ell\bar{\ell}} = 5$ TeV across PDF sets
NNPDF4.0 uncertainties are the largest

Positive or negative asymmetry?

$\mathcal{L}_{A,q}$ depends on q, $\bar{q}$ relative decrease rate $\mathcal{L}_{A,q} = f_q(x_2) f_{\bar{q}}(x_2) \left[\frac{f_q(x_1)}{f_q(x_2)} - \frac{f_{\bar{q}}(x_1)}{f_{\bar{q}}(x_2)} \right]$

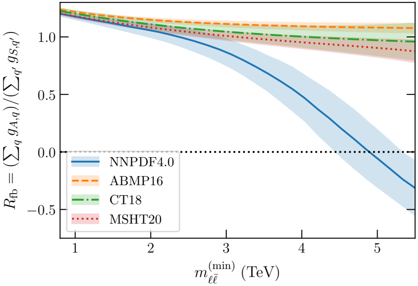
A_{fb} is sensitive to these rates at large x; at high mass, no hierarchy between x_1 and x_2

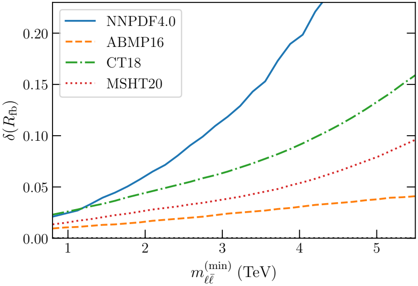
This decrease can be quantified by asymptotic exponents $\beta_{a,q} = \frac{\partial \ln |x f_q(x,Q)|}{\partial \ln(1-x)}$



Positive or negative asymmetry?

$$A_{\mathrm{fb}}(\cos\theta^*) \overset{\mathrm{LO}}{=} \frac{\cos\theta^*}{1+\cos^2(\theta^*)}\frac{g_A}{g_{S,q'}} \qquad g_{A,S} \propto \int \frac{dm_{\ell\bar{\ell}}}{m_{\ell\bar{\ell}}}\frac{dx_1}{x_1}\mathcal{L}_{\mathcal{A},\mathcal{S}}(m_{\ell\bar{\ell}}, x_1)$$





As the scale increases, larger x is probed

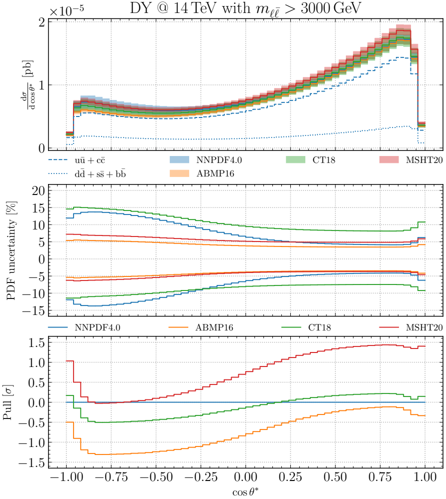
ABMP16, CT18 and MSHT20:
approximately scale independent

NNPDF: the coupling depends on the scale, larger uncertainty

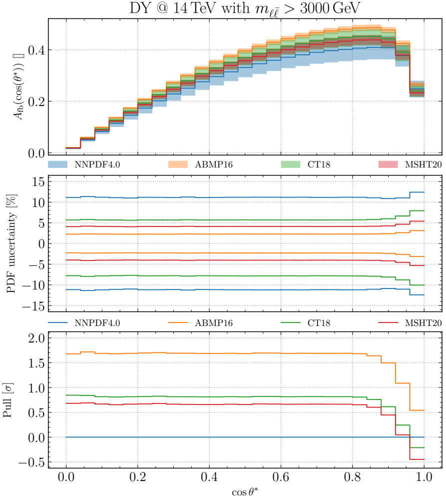
Expectation: for NNPDF4.0, A_{fb} vanishes at large $m_{\ell\bar{\ell}}$

The Drell-Yan forward-backward asymmetry at the LHC

angular distribution



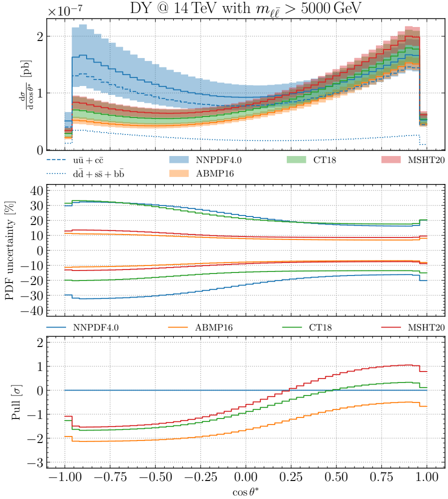
asymmetry



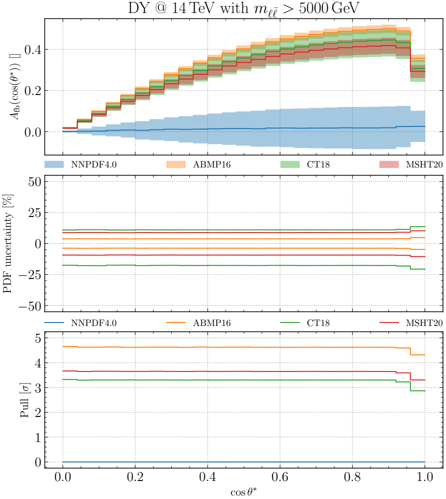
$M_{Z'} \geq 3$ TeV, data region: predictions from all PDF sets agree
NNPDF uncertainties similar, if not larger than other PDF sets

The Drell-Yan forward-backward asymmetry at the LHC

angular distribution



asymmetry



$M_{Z'} \geq 5$ TeV, extrapolation region: CT, MSHT and ABMP predictions unchanged
NNPDF asymmetry disappears, uncertainties increase

3. Conclusion

Summary

NNPDF4.0 uncertainties are statistically faithful

They are completely validated by closure and future tests

The increasing accuracy and precision of NNPDF4.0 is rooted in data and methodology

Hopscotch PDFs do not have statistical meaning in the same sense as NNPDF replicas

Hopscotch PDFs are not found by the default NNPDF4.0 methodology
because they would correspond to overfitted replicas

NNPDF4.0 uncertainties remain largely unconstrained in the high-mass discovery region

Fixed-parametrisation PDF sets are comparatively over restrictive
(overconstrained extrapolation and underestimated uncertainties)

Future Drell-Yan measurements are important to constrain PDFs more

Summary

NNPDF4.0 uncertainties are statistically faithful

They are completely validated by closure and future tests

The increasing accuracy and precision of NNPDF4.0 is rooted in data and methodology

Hopscotch PDFs do not have statistical meaning in the same sense as NNPDF replicas

Hopscotch PDFs are not found by the default NNPDF4.0 methodology
because they would correspond to overfitted replicas

NNPDF4.0 uncertainties remain largely unconstrained in the high-mass discovery region

Fixed-parametrisation PDF sets are comparatively over restrictive
(overconstrained extrapolation and underestimated uncertainties)

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Thank you