MSHT fit: Closure Test and Comparison of Approaches

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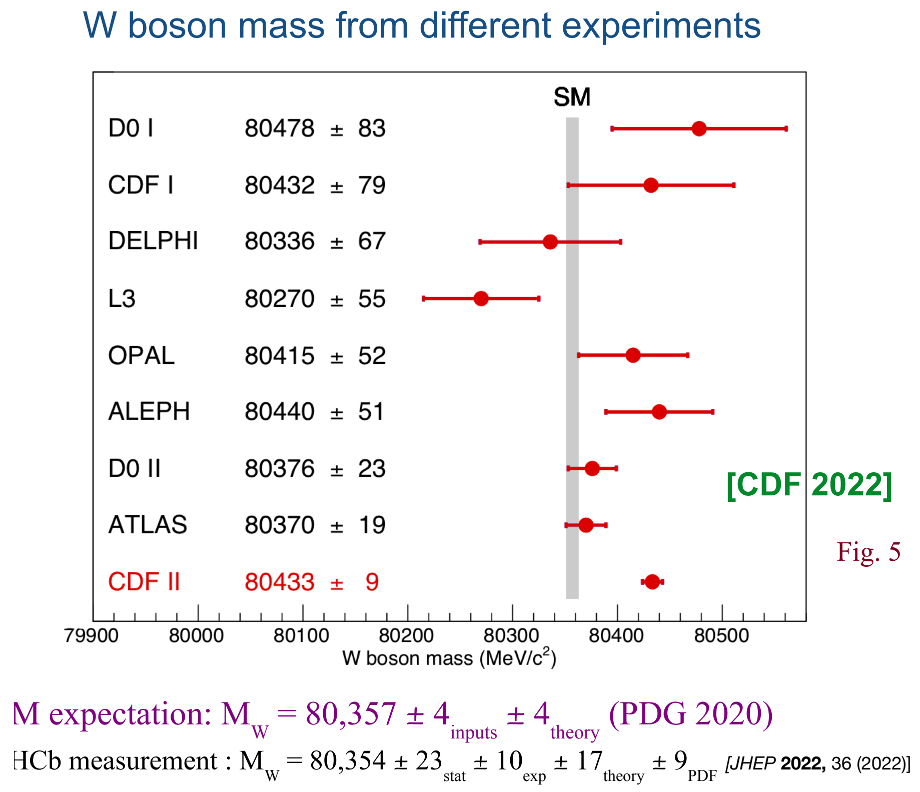
With Robert Thorne and Tom Cridge

UCL

Introduction

- Parton distribution functions (PDFs): a key ingredient in hadron collider physics.
- Knowledge of **PDFs** and their **uncertainties** a limiting factor in LHC precision and BSM searches.

W mass

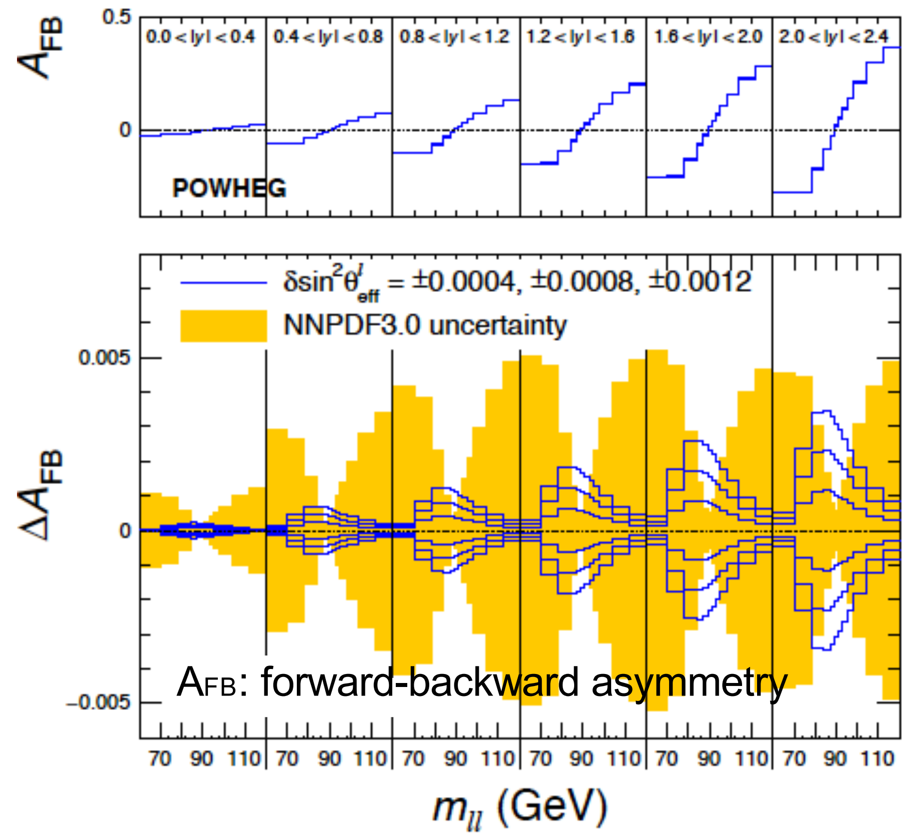


PDF unc. of CDF / ATLAS / LHCb: 3.9 / 8 / 9 MeV

$\sigma_{\rm PDF} \sim \sigma_{\rm tot}/2$

(up to)

$\sin^2\theta_W$

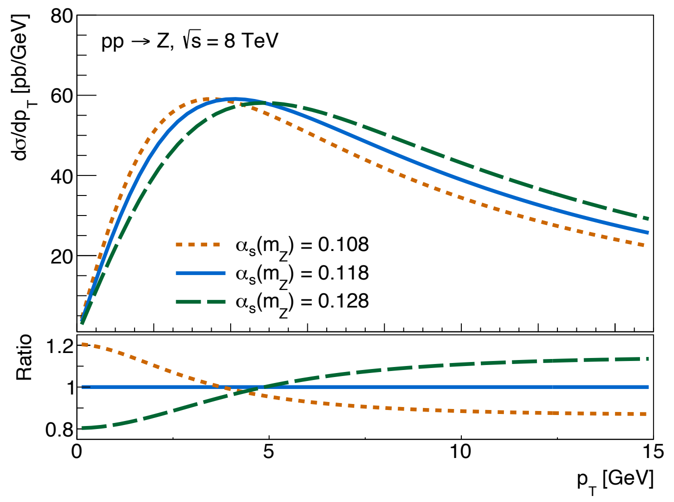


$\sin^2\theta^\ell_{\rm eff} = 0.23101 \pm 0.00036\,({\rm stat}) \pm 0.00018\,({\rm syst}) \pm 0.00016\,({\rm theo}) \pm 0.00031\,({\rm PDF})$

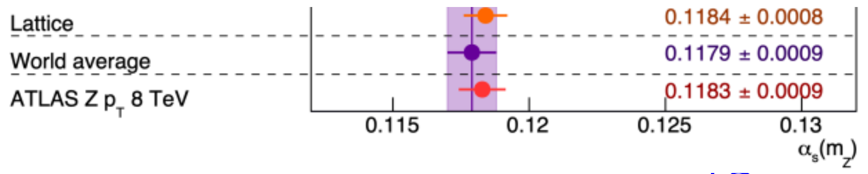
$\sigma_{\rm PDF} \sim \sigma_{\rm tot}/2$

4

α_S

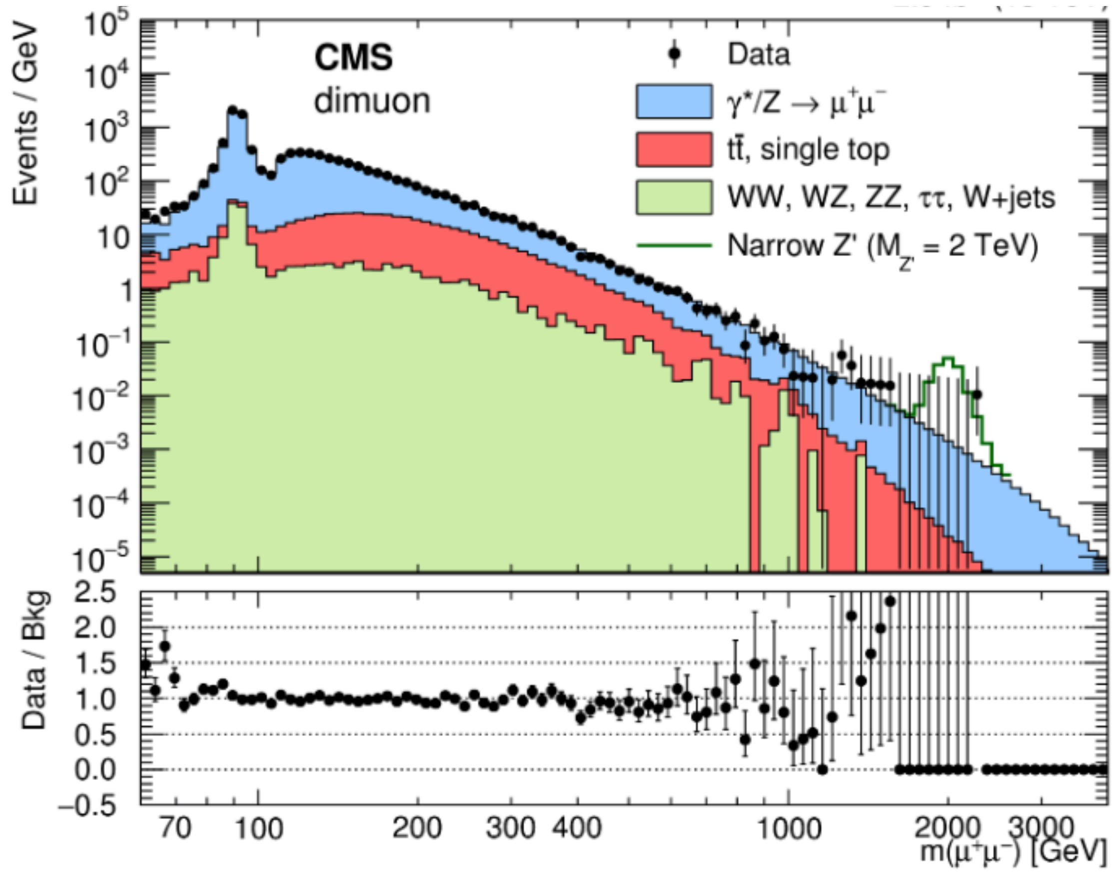


ATLAS, 2309.12986



$\sigma_{\rm PDF} \sim \sigma_{\rm tot}/2$

Disclaimer: will generally refer to papers by their arxiv number, even if published.



- The LHC is a BSM search machine. Often need PDFs here.
- High mass = high x , where PDFs are less well known. Key when looking for small/smooth deviations.

See my plenary talk on Monday!

- Accuracy and precision in PDF determinations essential.

Global PDF fits: parameterisation

- Two distinct methodologies on the market to parameterising PDFs: **Neural Nets** (NNPDF) or **Explicit Parameterisation** (CT, MSHT).

$$f_i(x,Q_0):\ A_f x^{a_f}(1-x)^{b_f}\times \begin{cases} \longrightarrow \sum_{i=1}^{n} \alpha_{f,i} P_i(y(x))\,, & \textbf{CT, MSHT...} \\ \searrow \mathrm{NN}_i(x) & \textbf{NNPDF} \end{cases}$$

✦ MSHT: **52** free parameters in terms of Chebyshev polynomials.

$$u_V(x,Q_0^2) = A_u(1-x)^{\eta_u}x^{\delta_u}\left(1+\sum_{i=1}^{6} a_{u,i}T_i(y(x))\right)$$

$$d_V(x,Q_0^2) = A_d(1-x)^{\eta_d}x^{\delta_d}\left(1+\sum_{i=1}^{6} a_{d,i}T_i(y(x))\right)$$

$$S(x,Q_0^2) = A_S(1-x)^{\eta_S}x^{\delta_S}\left(1+\sum_{i=1}^{6} a_{S,i}T_i(y(x))\right)$$

$$s_+(x,Q_0^2) = A_{s_+}(1-x)^{\eta_{s+}}x^{\delta_S}\left(1+\sum_{i=1}^{6} a_{s_+,i}T_i(y(x))\right)$$

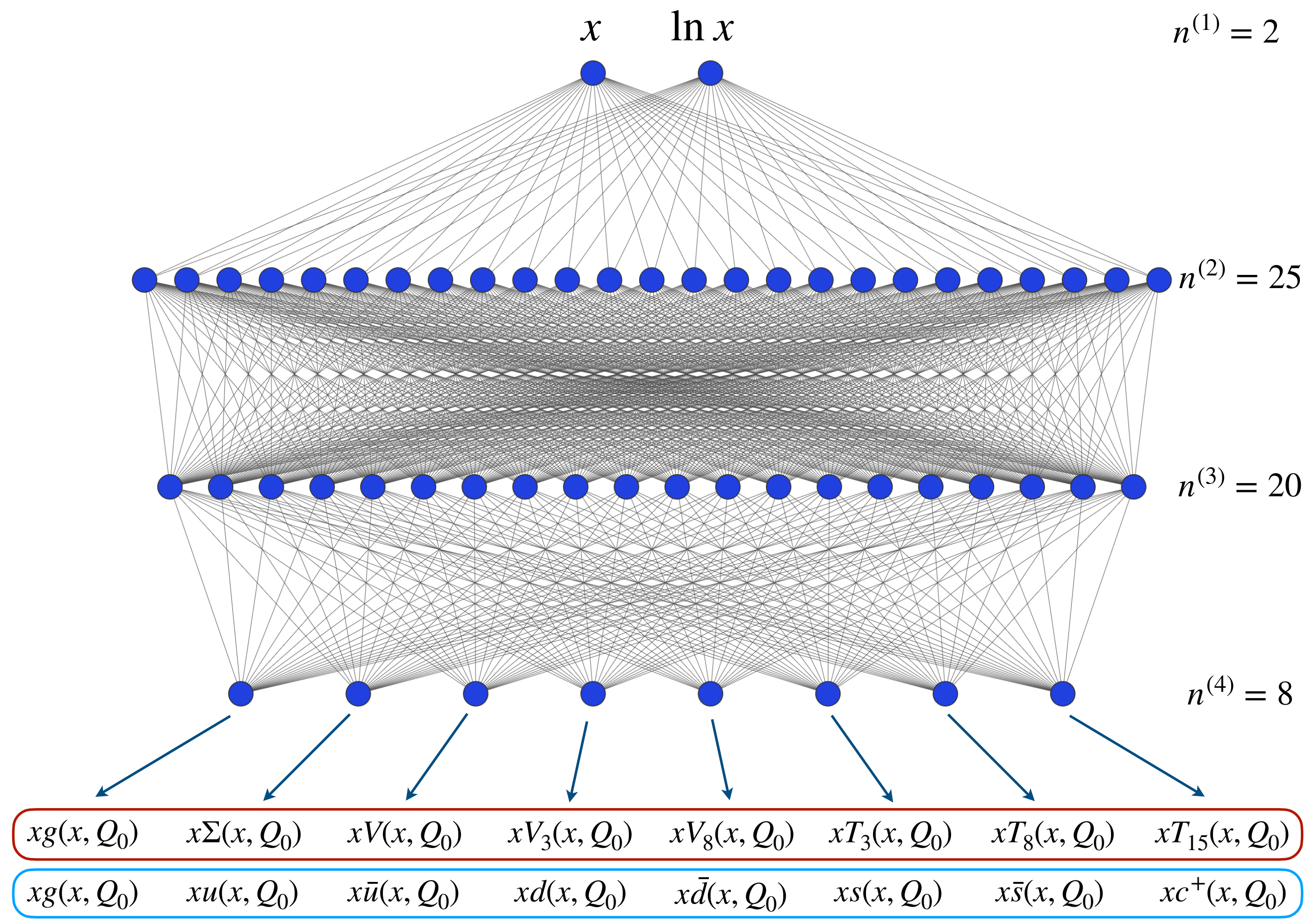
$$g(x,Q_0^2) = A_g(1-x)^{\eta_g}x^{\delta_g}\left(1+\sum_{i=1}^{4} a_{g,i}T_i(y(x))\right) + A_{g-}(1-x)^{\eta_{g-}}x^{\delta_{g-}}$$

$$s_-(x,Q_0^2) = A_{s_-}(1-x)^{\eta_{s-}}(1-x/x_0)x^{\delta_{s-}}$$

$$(\bar{d}/\bar{u})(x,Q_0^2) = A_\rho(1-x)^{\eta_\rho}\left(1+\sum_{i=1}^{6} a_{\rho,i}T_i(y(x))\right)$$

✦ Less flexible in general - need to be sure flexible enough! Allows direct handle on uncertainties in Hessian framework.

★ NNPDF: ***763*** free parameter Neural Net.



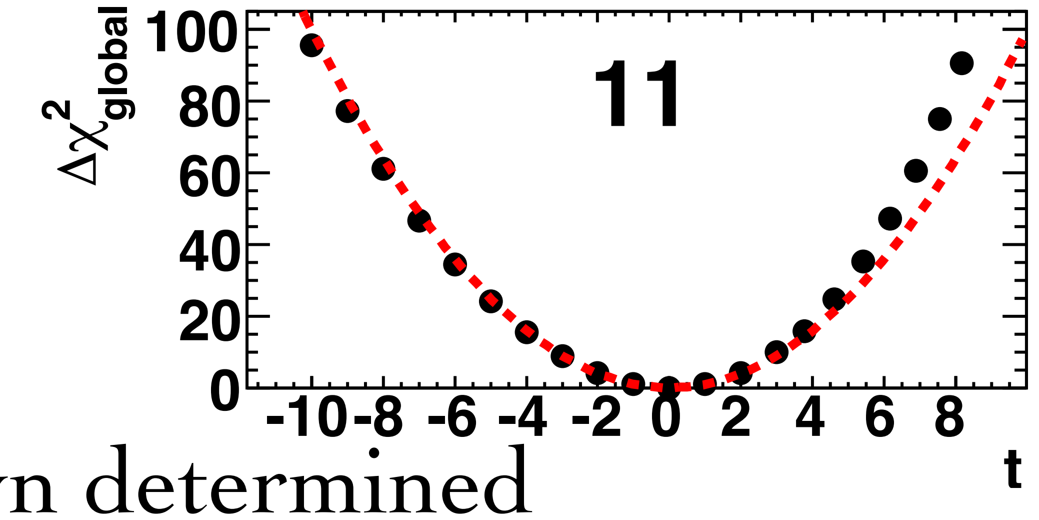
★ Increased flexibility, but needs robust optimisation + stopping (avoid over and under fitting).

Fixed Parameterisation PDFs

- Fixed parameterisation approach:

$$\chi^2_{\rm global} \sim \frac{(D_{\rm ata} - T_{\rm heory})^2}{\sigma^2} \qquad H_{ij} = \frac{1}{2}\frac{\partial^2 \chi^2_{\rm global}}{\partial a_i \partial a_j}\bigg|_{\rm min}$$

  - ✦ Find global minimum of χ^2 and evaluate eigenvectors of Hessian matrix at this point.
  - ✦ Parameter shifts corresponding to given $\Delta\chi^2$ criteria given in terms of these

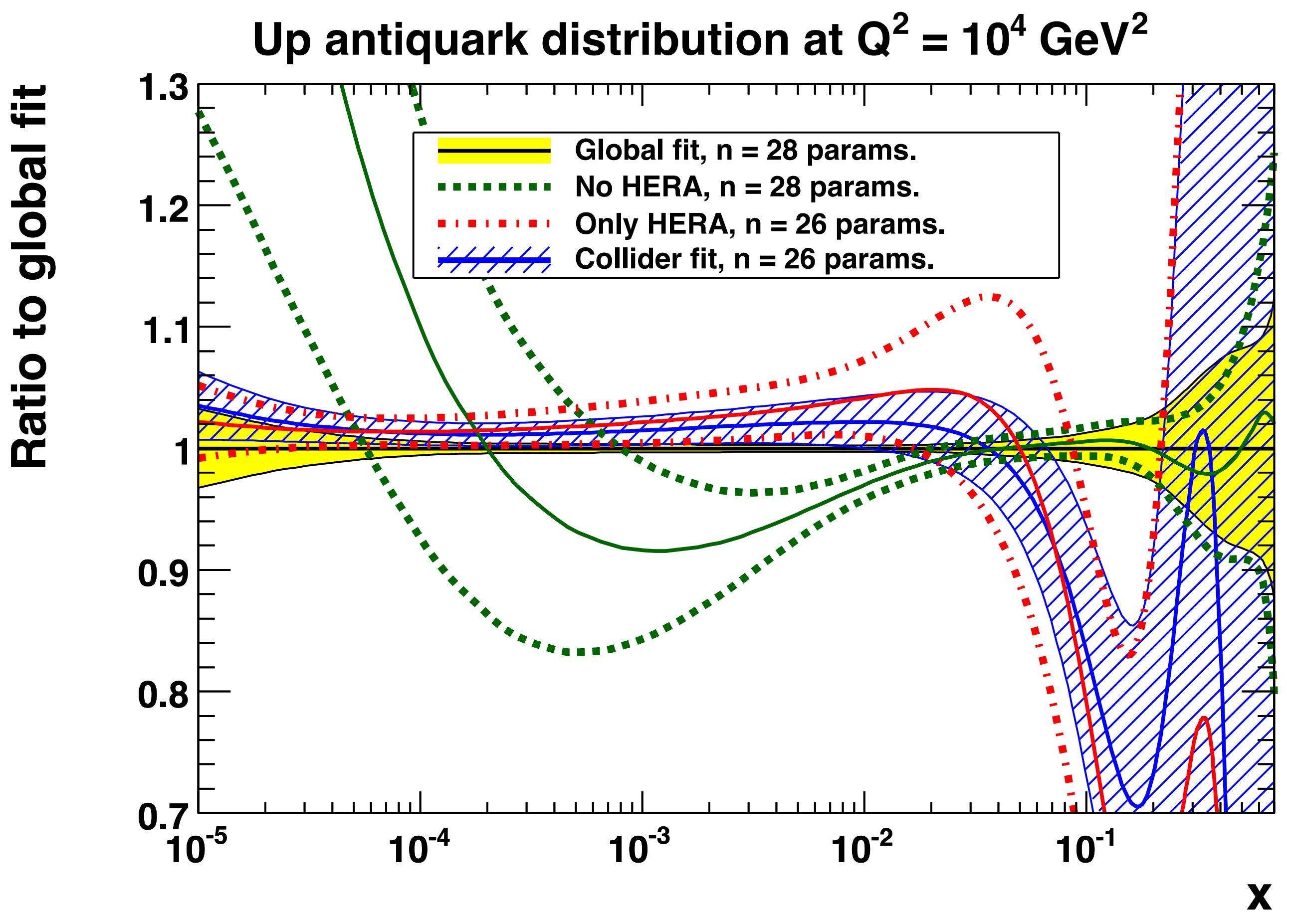


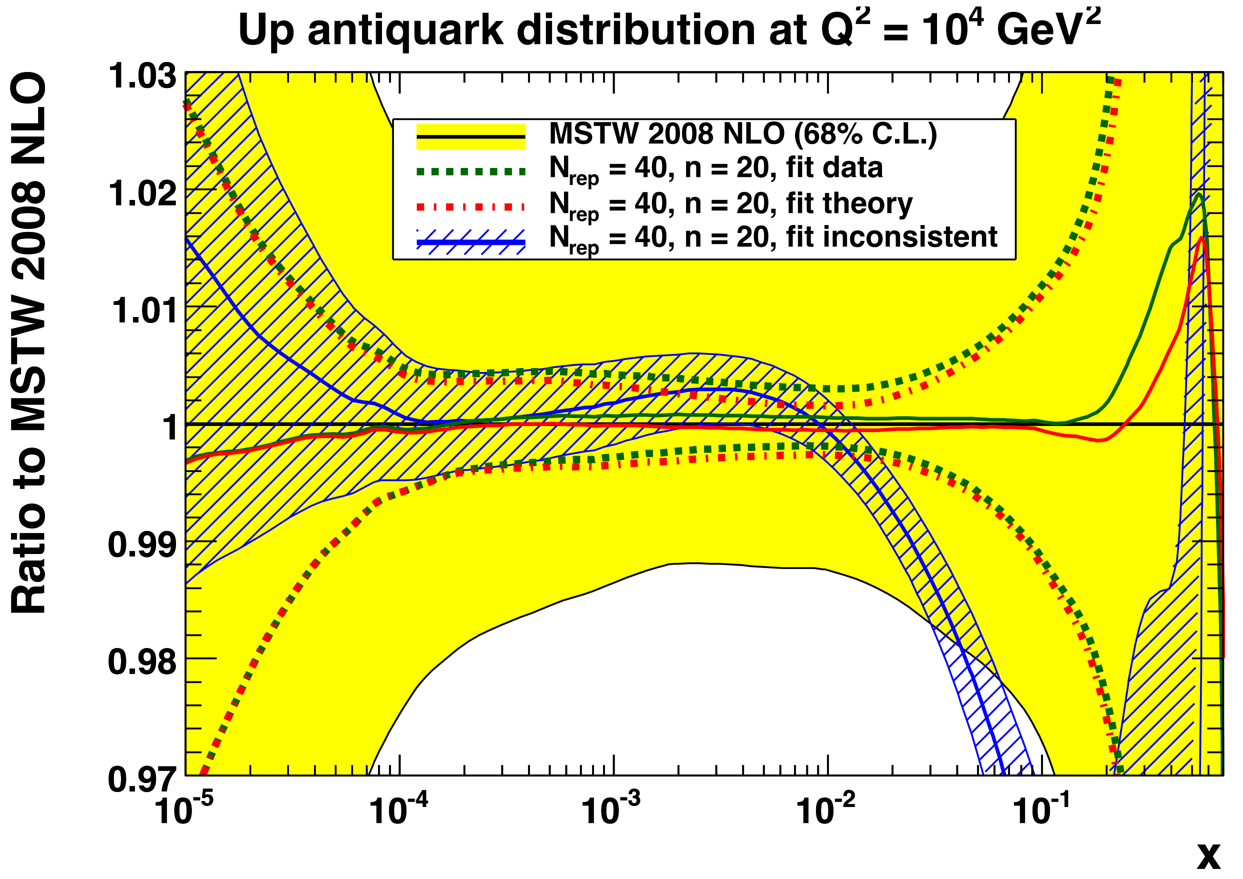
$$a_i(S_k^{\pm}) = a_i^0 \pm t\, e_{ik}, \qquad \text{with } t \text{ adjusted to give desired } T = \Delta\chi^2_{\rm global}$$

  - ✦ $T = 1$: `textbook' criteria for case where data matches theory perfectly up to known determined (Gaussian) errors, across entire global dataset ($N_{\rm pts} \sim 4000 - 5000$).

$$\frac{\chi^2}{N_{\rm pts}} \gg 1 + \sigma(N_{\rm pts}) \sim 1.02$$

- ✦ Expect to not be sufficient: fit quality poor by textbook standard, dataset tensions, theory incomplete…
- ✦ Backed up by evidence of e.g. fits to restricted datasets, or pseudodata with inconsistencies injected in.





$\longrightarrow$ Motivates an enlarged $T > 1$, either fixed or 'dynamic'.

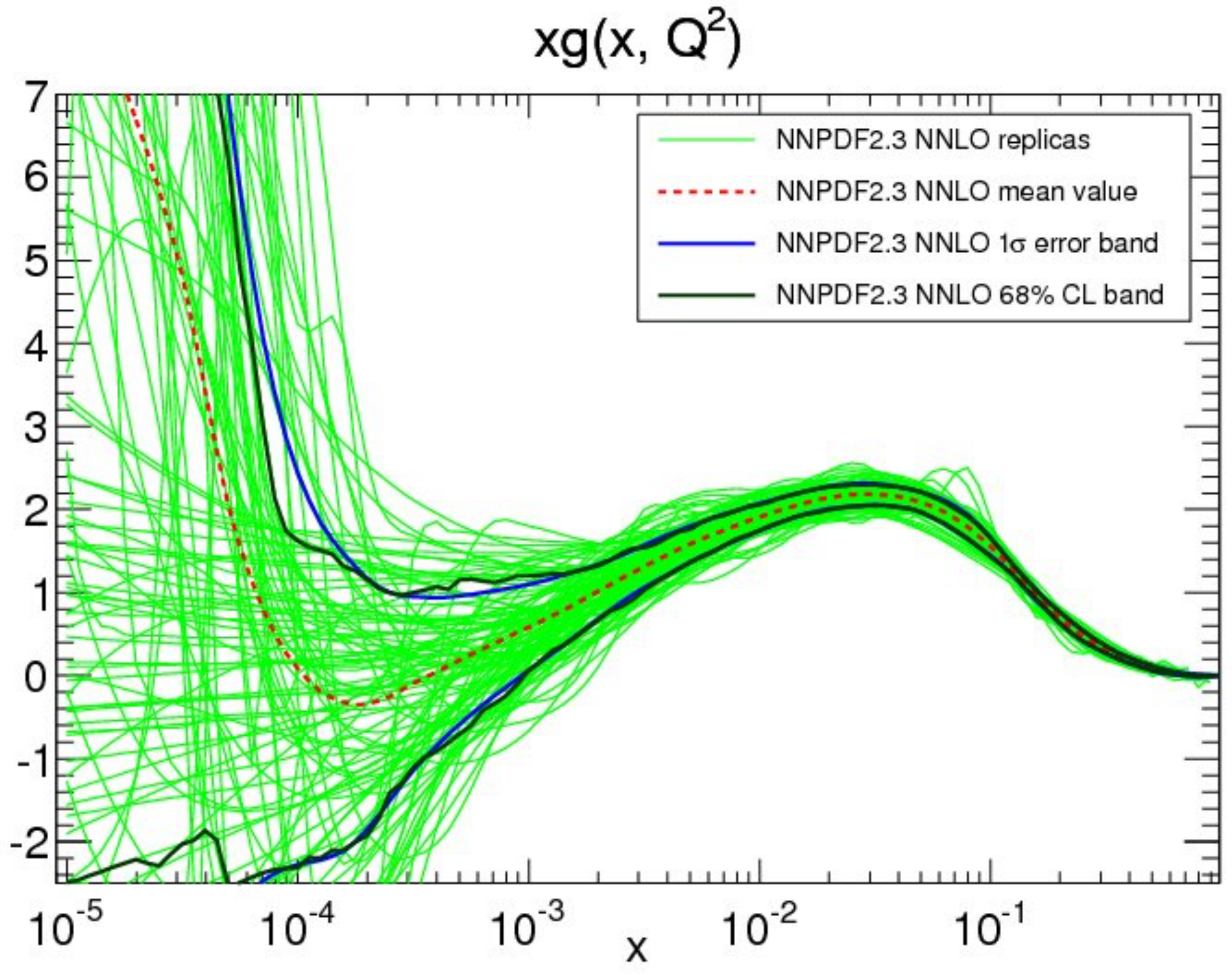
G. Watt and R. Thorne, arXiv:1205.4024

See also, J. Pumplin, arXiv:0909.0268

Neural Network PDFs

- Neural network approach:
  - ✦ Generate set of MC `replicas' by shifting data by errors.

    Each D_i gives f_i and from $\{f_i\} \Rightarrow$ PDF errors



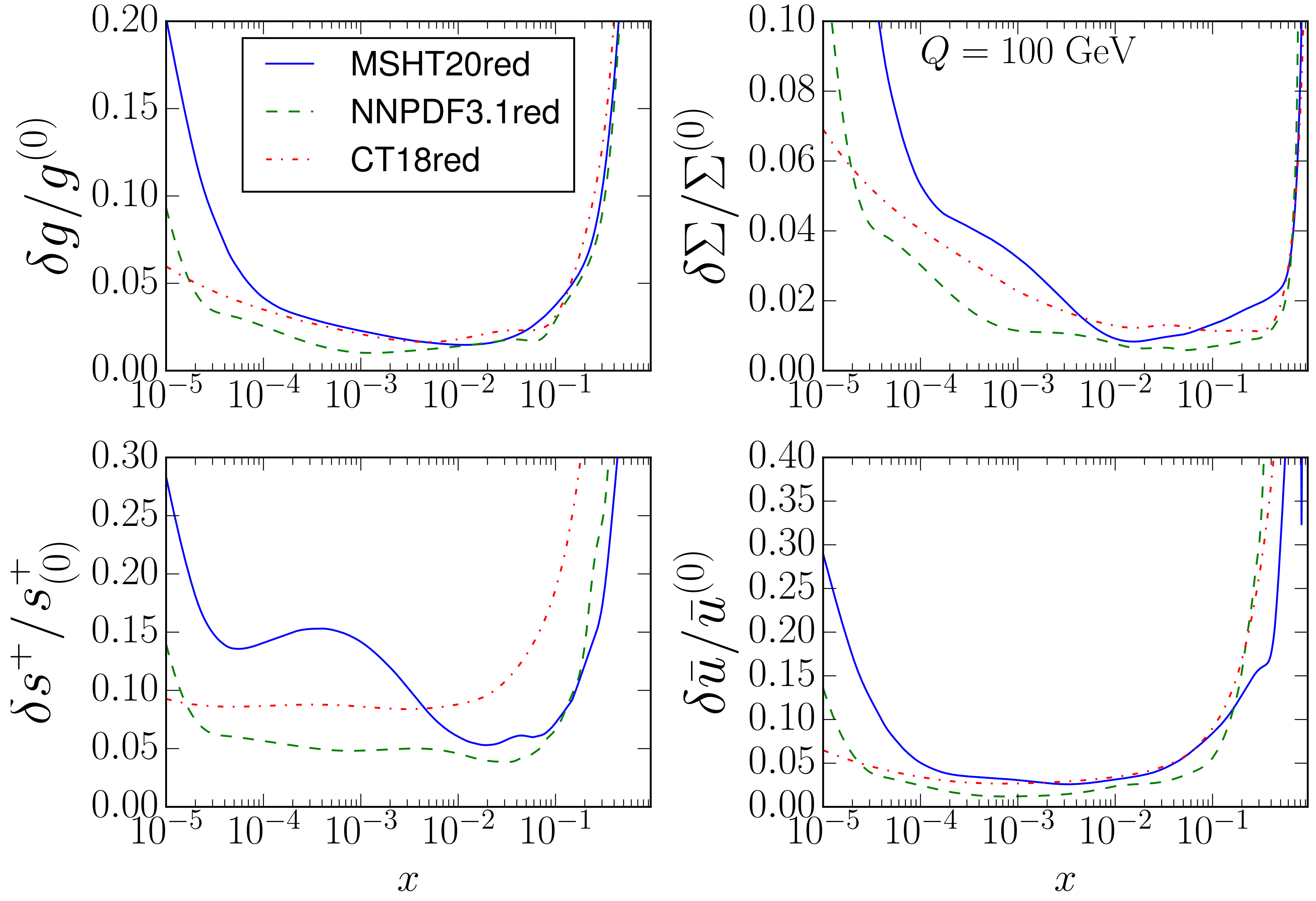
G. Watt and R. Thorne, arXiv:1205.4024

✦ Note not specific to NNs: can apply in fixed parameterisation as well: shown to be ~ equivalent to Hessian $\Delta\chi^2 = 1$ in that case.

✦ However, in NN approach direct correspondence is lost as Hessian approach does not apply.

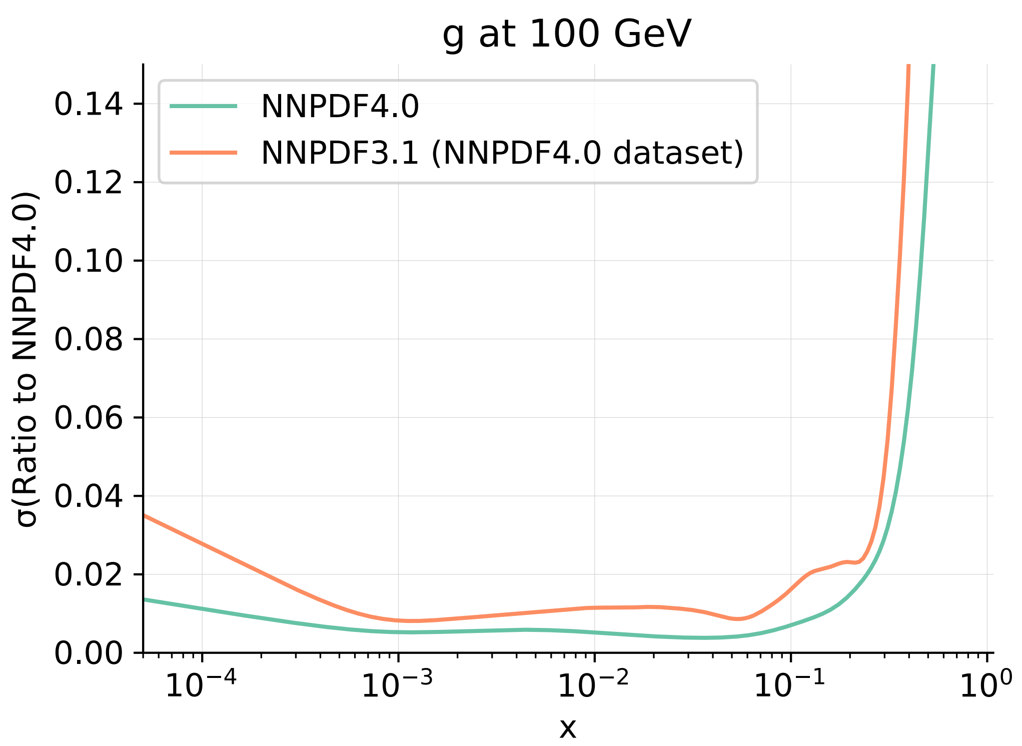
✦ Global fits give different errors in PDF4LHC21 benchmarking. NNPDF3.1 in general **smaller errors.**

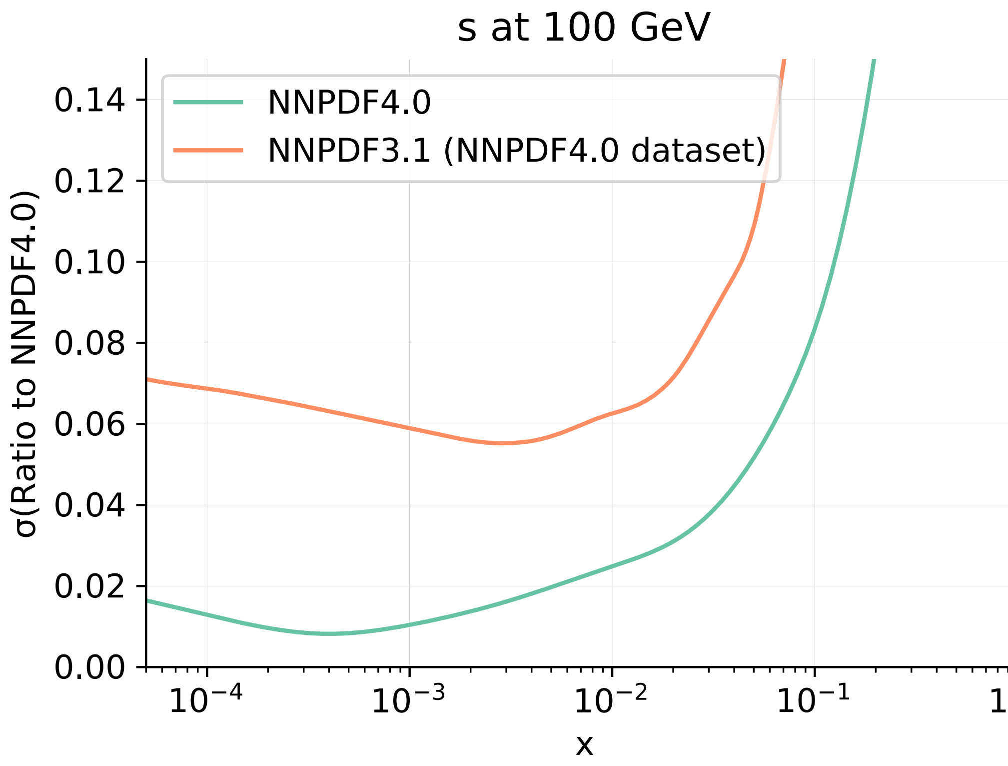
Benchmark = similar data/settings



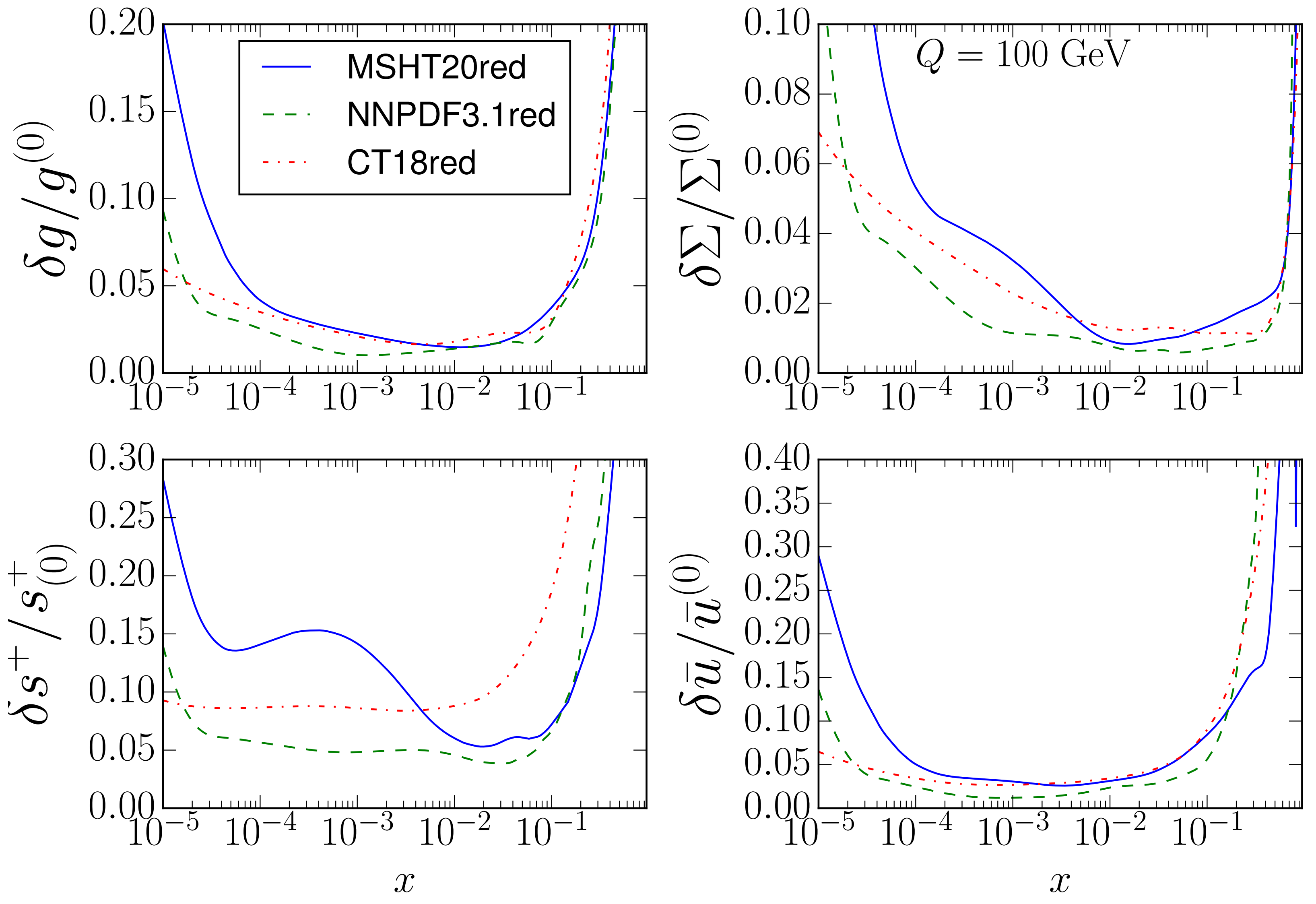
PDF4LHC21, arXiv:2203.05506

✦ And **4.0 methodology** gives further errors reduction.





Aims of Talk



- Suggests three possibilities:

  1. **NNPDF4.0** uncertainty not conservative enough (**too small**).
  2. **MSHT (CT)** uncertainty too conservative (**too large**).
  3. **MSHT (CT)** fit less accurate, due to parameterisation inflexibility, and hence enlarged errors needed (**less precise**).

- Or some combination of the three. Finding out which clearly important for LHC precision.
- In this talk I will present results that aim to address this issue. In particular will show:

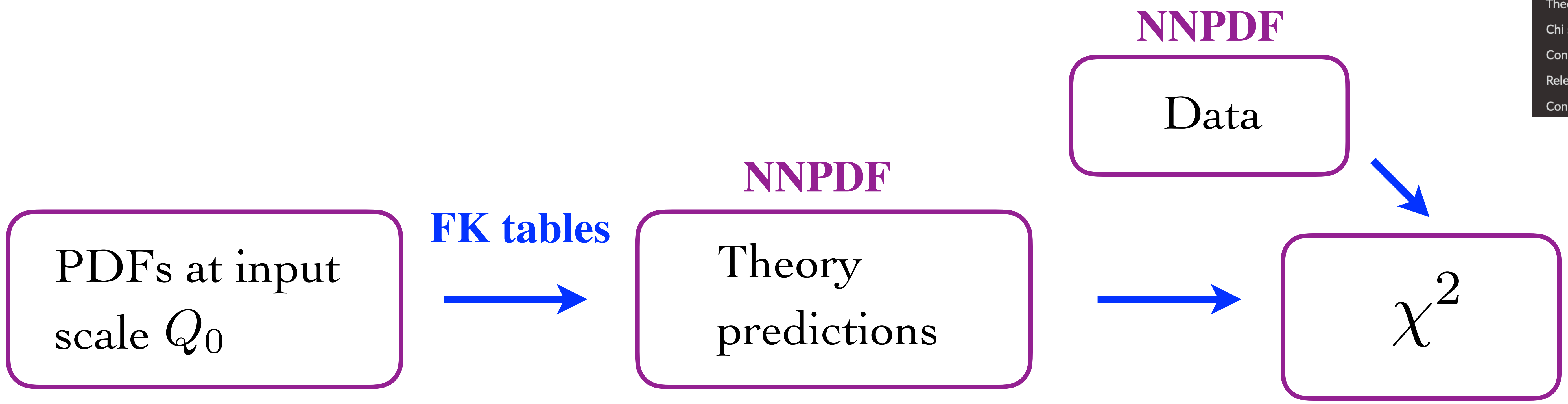
  ⋆ **First** global **closure test** of fixed parameterisation (MSHT) approach: is parameterisation flexible enough to give faithful description of global pseudodata?

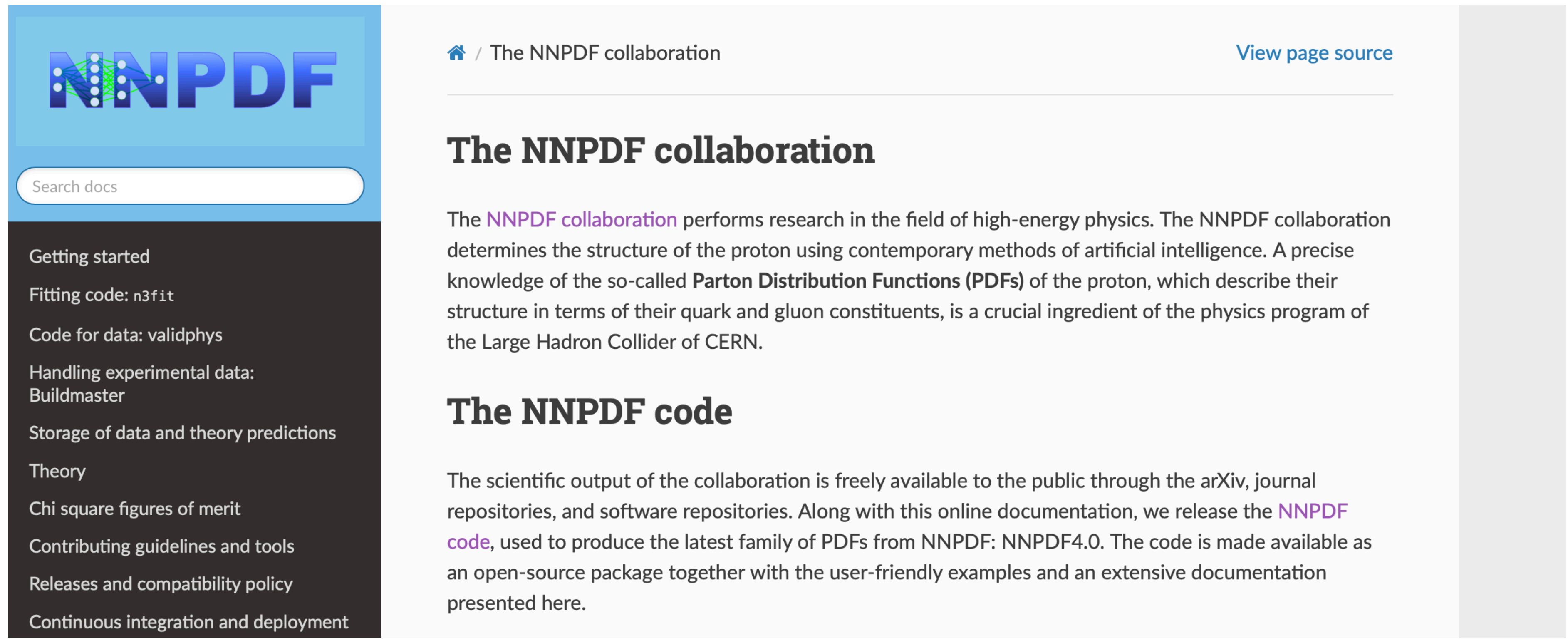
  ⋆ **First** completely direct **comparison** between fixed parameterisation (MSHT) and NN approaches. How do these compare in full global fit?

- Study is ongoing, so all slides can be viewed as if they have a `**preliminary**' label on them!

Global Closure - set up

- How best to set up a global closure test? Will make use of publicly available NNPDF fitting code.
- Provides python libraries to load NNPDF dataset and theory predictions, given PDF set. More precisely gives:

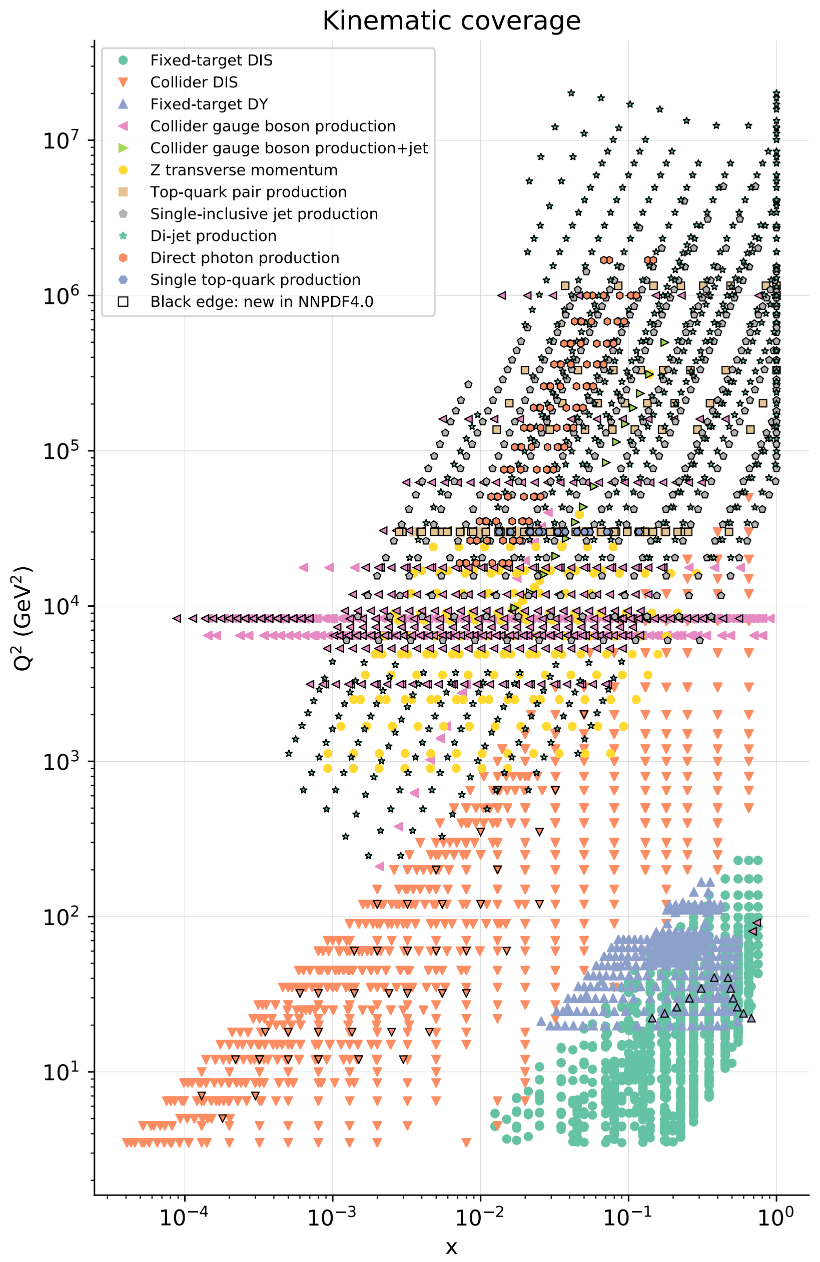




https://docs.nnpdf.science/

- Given arbitrary PDF set (grid of $\{f_i\}$ at $\{x_i\}$ and Q_0) can evaluate theory predictions + fit quality.
- This allows us to evaluate corresponding fit quality with a (MSHT) fixed parameterisation, but to NNPDF data/theory - **only difference** is **input parameterisation.** From above module can also build up optimizer in usual way to give best fit, Hessian errors etc.
- Will use for closure tests (though not essential) - but setting things up in this way will allow direct comparison at level of full fit.

Global Closure Test



NNPDF, arXiv:2109.02653

Always NNLO

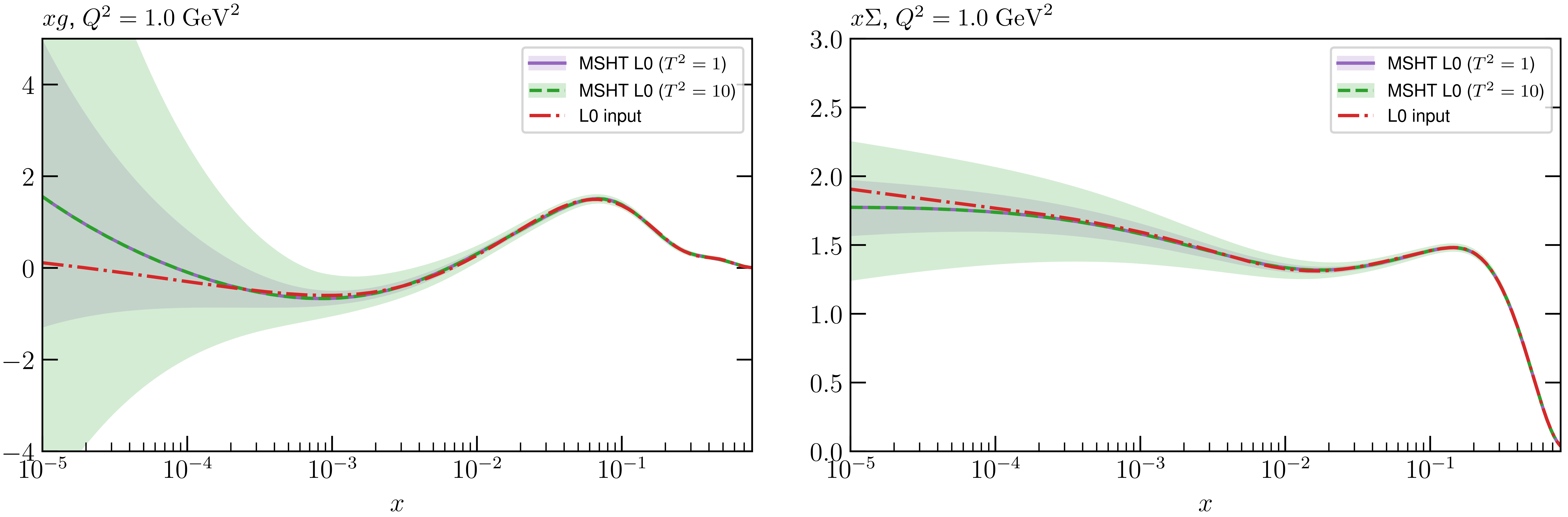
- For direct comparison will consider perturbative charm - NNPDF4.0pch set as input.
- Then generate unshifted pseudodata for 4.0 global dataset ($N_{\rm pts} = 4627$). In principle exact agreement possible, with $\chi^2 = 0$. But will propagate data errors via Hessian approach, so ~ Level 0 + 2 (but not 1 yet).
- Then perform fit with default MSHT parameterisation. What do we find?

	χ^2	$\chi^2/N_{\rm pts}$
Fit quality:	2.4	0.0005

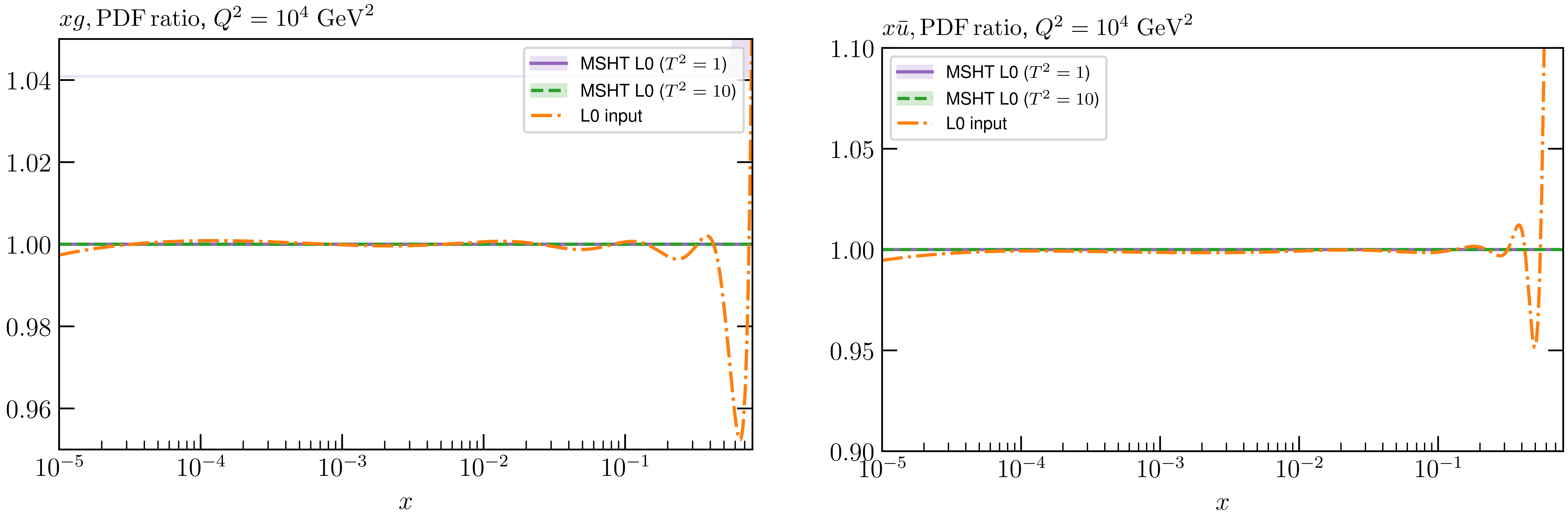
- **Remarkably good!** In fact lower than reported result of NNPDF L0 closure test.

		3.1 meth.	**4.0 meth.**
L. Del Debbio, T. Giani and M. Wilson, arXiv:2111.05787	$\chi^2/N_{\rm pts}$	0.012	0.002

- **Caveat**: only one input set, may well be different (not quite as good) for others. Trend should be similar.
- But apparently no issue with parameterisation inflexibility in this case. But what about PDFs?



- First look: encouraging results! In more detail…



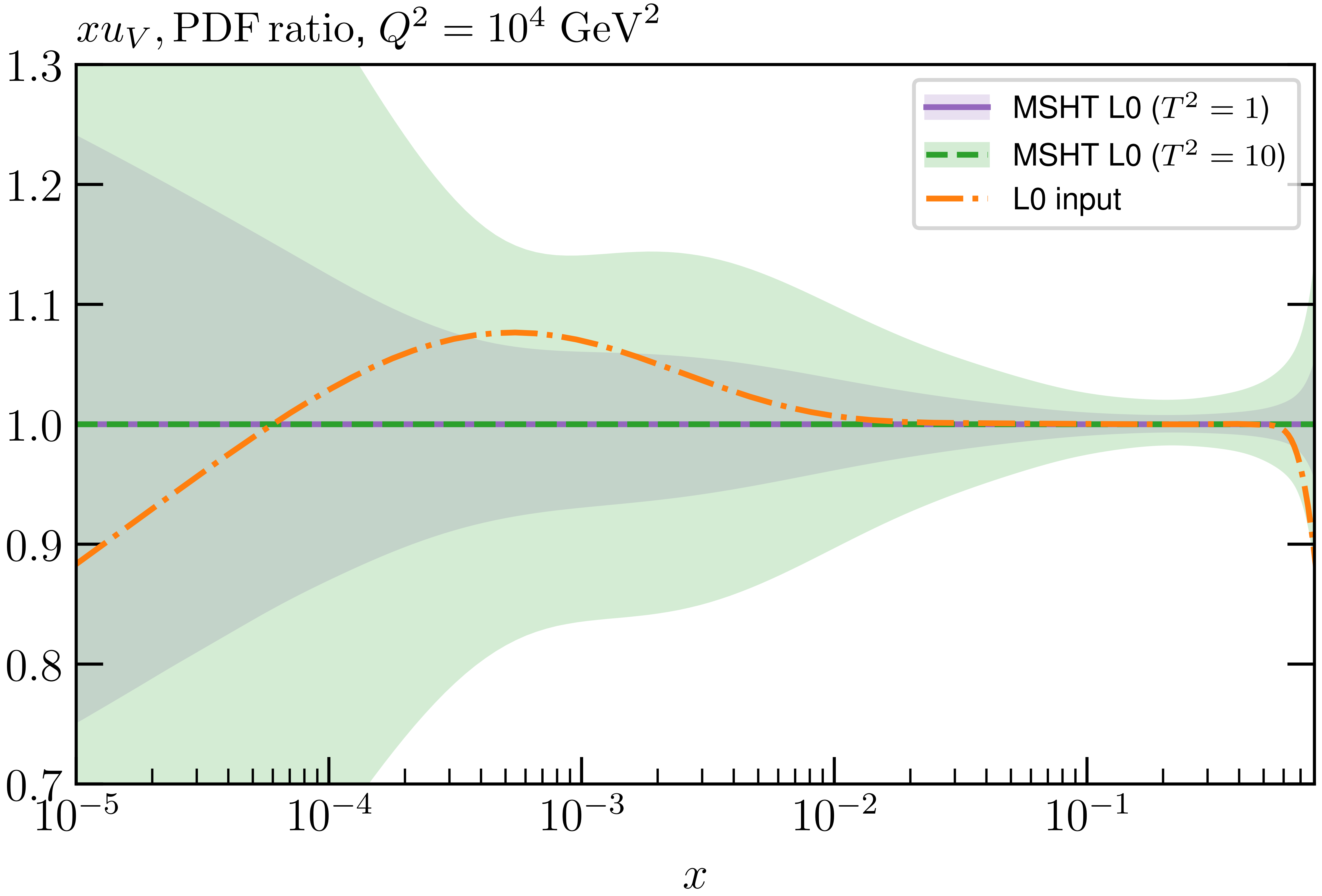
- Ratio of (NNPDF4.0pch) L0 input to fit result, including PDF uncertainties with $T^2 = 1$ and 10 that come from the closure test fit. Latter is ~ result of dynamic tolerance used in MSHT20 (checked here).

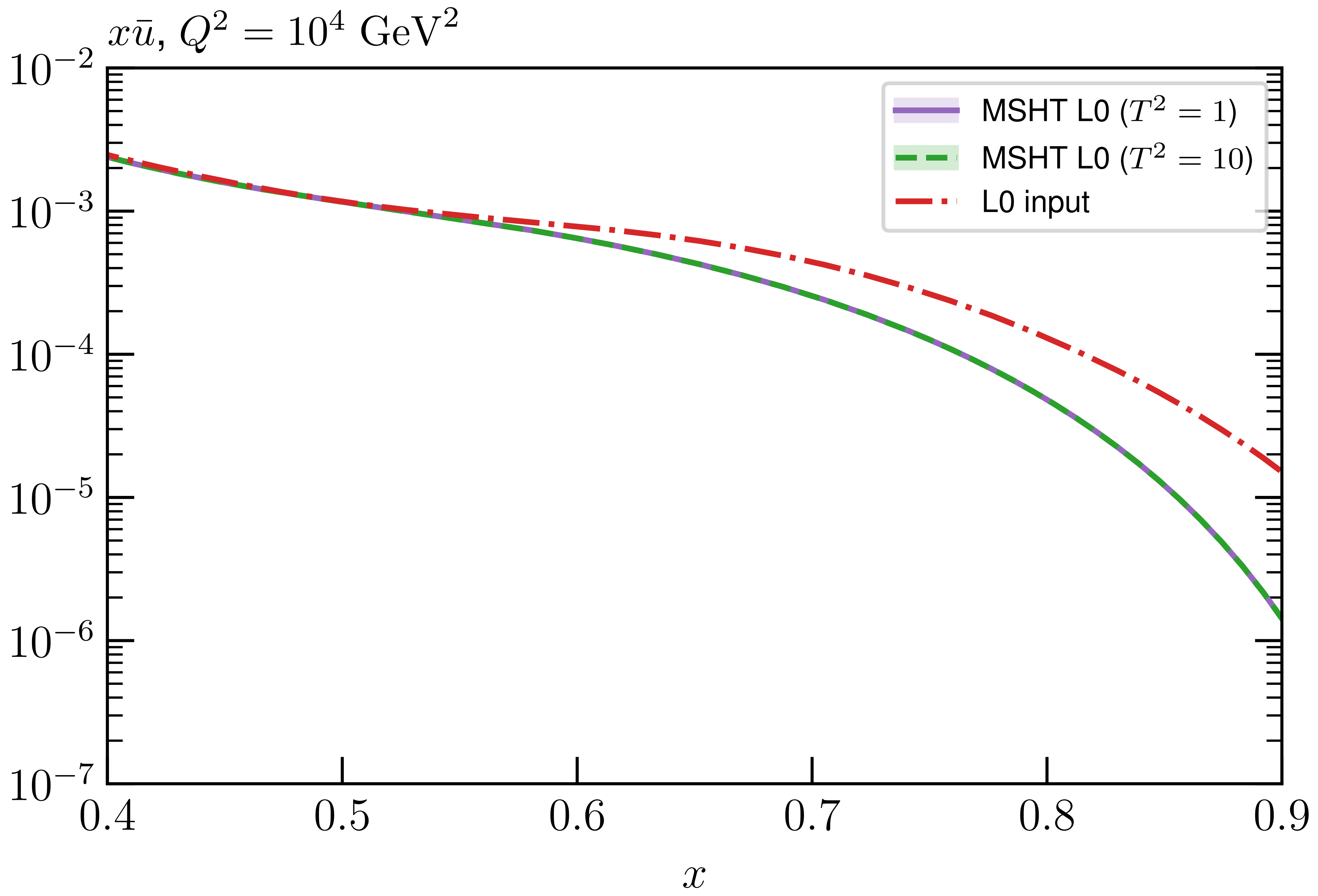
Similar results for other quarks - see backup

★ **Deviation** in general (in data region) **per mille** level and well within the $T^2 = 1$ uncertainties.

★ More precisely, deviation is ~ 10% or less of $T^2 = 1$ uncertainty, and a factor of $\sim 2 - 5$ lower a a fraction of the $T^2 = 10$ uncertainty.

$\longrightarrow$ In **data region** L0 input PDF matched very well, and much better than $T^2 = 1$ uncertainties. **No evidence** that the increased tolerance is driven by **parameterisation inflexibility** for MSHT.





- In less well constrained regions deviation larger, e.g for u_V, d_V at low and high x and the $\overline{u}, \overline{d}$ at high x .
- Hence in extrapolation region L0 input not always consistent within uncertainties
- As ~ outside data region not inconsistent (errors driven by data), but indicates more conservative error definition in these regions may be desirable (as tends to happen in NN approach).
- Though arguably no 'right' answer in true extrapolation region (too conservative vs. over-conservative).

- So far only considered L0 test, though L1 underway. Would not expect to change picture dramatically.

Comparison to NNPDF uncertainties

- Can do first comparison of **MSHT** vs. **NNPDF** PDF **uncertainties**. Not completely direct as MSHT is in closure test, and NNPDF result of full fit. But theory and underlying datasets same. Find:

★ Quark flavour decomposition: $\sigma(\text{NNPDF}) \sim \sigma(\text{MSHT}, T^2 = 1)$

★ Gluon (singlet at intermediate x): $\sigma(\text{MSHT}, T^2 = 1) \lesssim \sigma(\text{NNPDF}) \lesssim \sigma(\text{MSHT}, T^2 = 10)$

MSHT, $T^2 = 1$
MSHT, $T^2 = 10$
NNPDF4.0pch

- With rather similar overall trends with x .
- Exception at high x where NNPDF uncertainty becomes larger.

Full fit: comparison

- Can also consider result of fit to real data entering NNPDF4.0 fit. To restate: exactly **same data and theory**, with **only difference** from PDF input **parameterisation**.
- Will in addition consider case where positivity is imposed at PDF (and cross section) level, as in NNPDF fit, for $x_i \in \{5 \cdot 10^{-7}, 0.9\}$. Not something that is done in MSHT fits!

	NNPDF4.0 pch	MSHT fit	MSHT fit (w positivity)
$\chi^2_{t_0}$	5928.3 (1.282)	5736.7 (1.240)	5837.8 (1.262)

$$\Delta\chi^2_{t_0}: \quad -191.6\,(-0.04) \quad -90.5\,(-0.02)$$

$\longrightarrow$ Fit quality with **MSHT** parameterisation is **significantly better** than result of central NNPDF set.

- **Positivity** clearly plays significant role - completely dominated by low x gluon. Indeed removing it from pure NNPDF fit gives O(100) improvement. But **not the only difference** here.

Integrability checked and not issue: Backup

- Improvement spread across fixed target, HERA DIS (without positivity) and LHC DY data.
- Do not expect central replica $\chi^2_{\text{rep},0}$ to be absolute minimum of χ^2 but difference too large for this. Overfitting seems unlikely given fixed parameterisation, though not impossible?

See Backup

PDFs

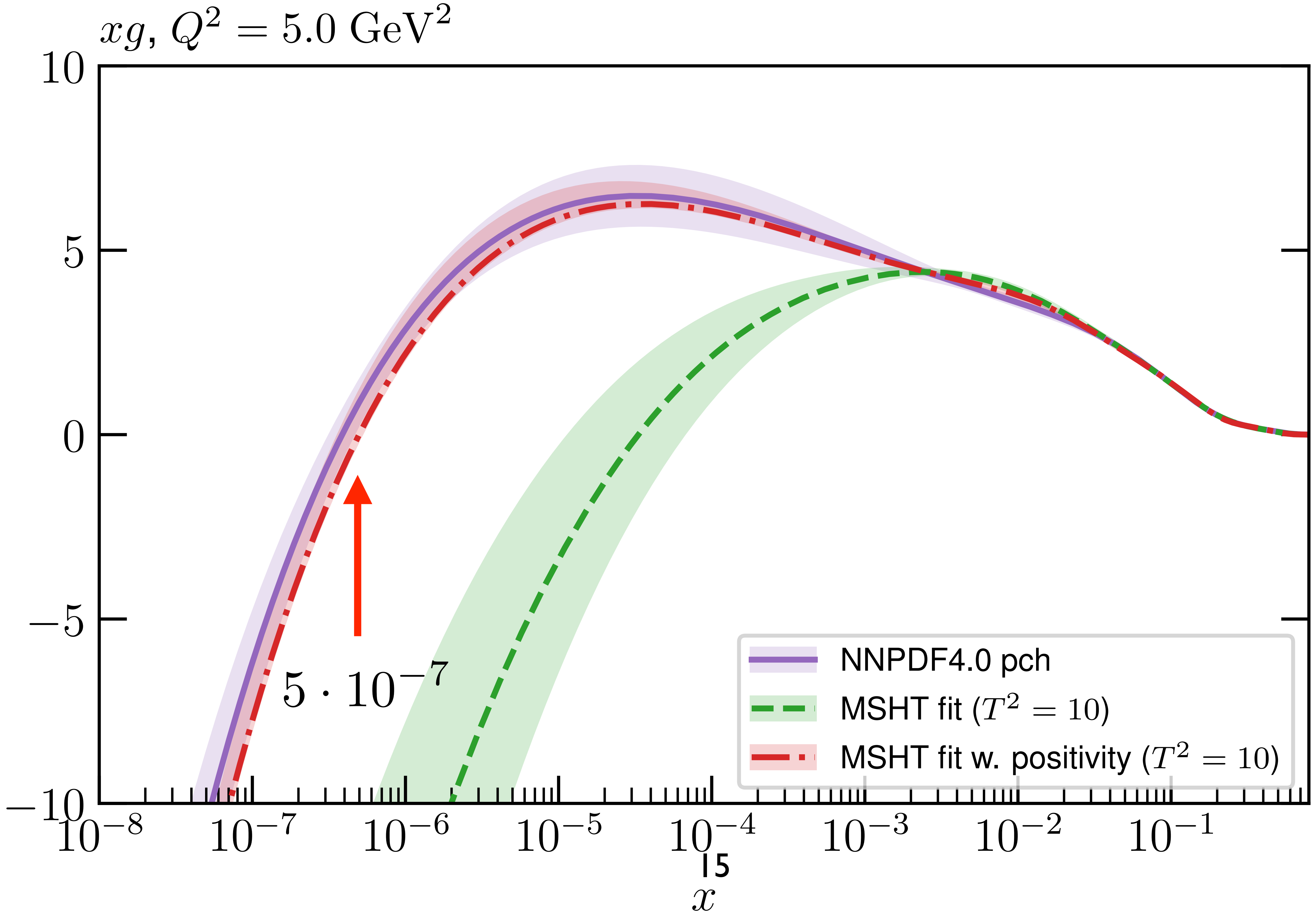
- Comparing PDFs, see clear effect of positivity at low x: driven by known fact that default result prefers gluon to be negative at low x, Q^2. Trend also seen if positivity removed from pure NNPDF fit.
- Imposing **positivity** gives much better agreement at low x , but clear **difference** in flavour decomposition **remains**.
- Notable that qualitatively this follows trend of using flavour rather than evolution basis (though difference larger and not identical). **See Backup**

NNPDF4.0pch MSHT (pos) $T^2 = 10$ MSHT, $T^2 = 10$

Candido et al., arXiv:2308.00025

Positivity?

- General arguments for imposing strict positivity on PDFs outside of current data region rely on perturbative stability. Not clear for (very) low gluon - sensitivity to resummation etc.
- More imporantly - **all cases** are actually **negative** at low x! Notable that the NNPDF gluon still prefers to be as negative as possible, i.e. just below the minimum x_i value where positivity imposed. Driving fit in undesirable way?



Comparison to NNPDF uncertainties

- Can do same comparison of MSHT vs. NNPDF PDF uncertainties but now in global fit. Completely like-for-like. Results very similar to closure test comparison:

★ Quark flavour decomposition: $\sigma(\text{NNPDF}) \sim \sigma(\text{MSHT}, T^2 = 1)$

★ Gluon (singlet at intermediate x): $\sigma(\text{MSHT}, T^2 = 1) \lesssim \sigma(\text{NNPDF}) \lesssim \sigma(\text{MSHT}, T^2 = 10)$

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MSHT, $T^2 = 10$
NNPDF4.0pch

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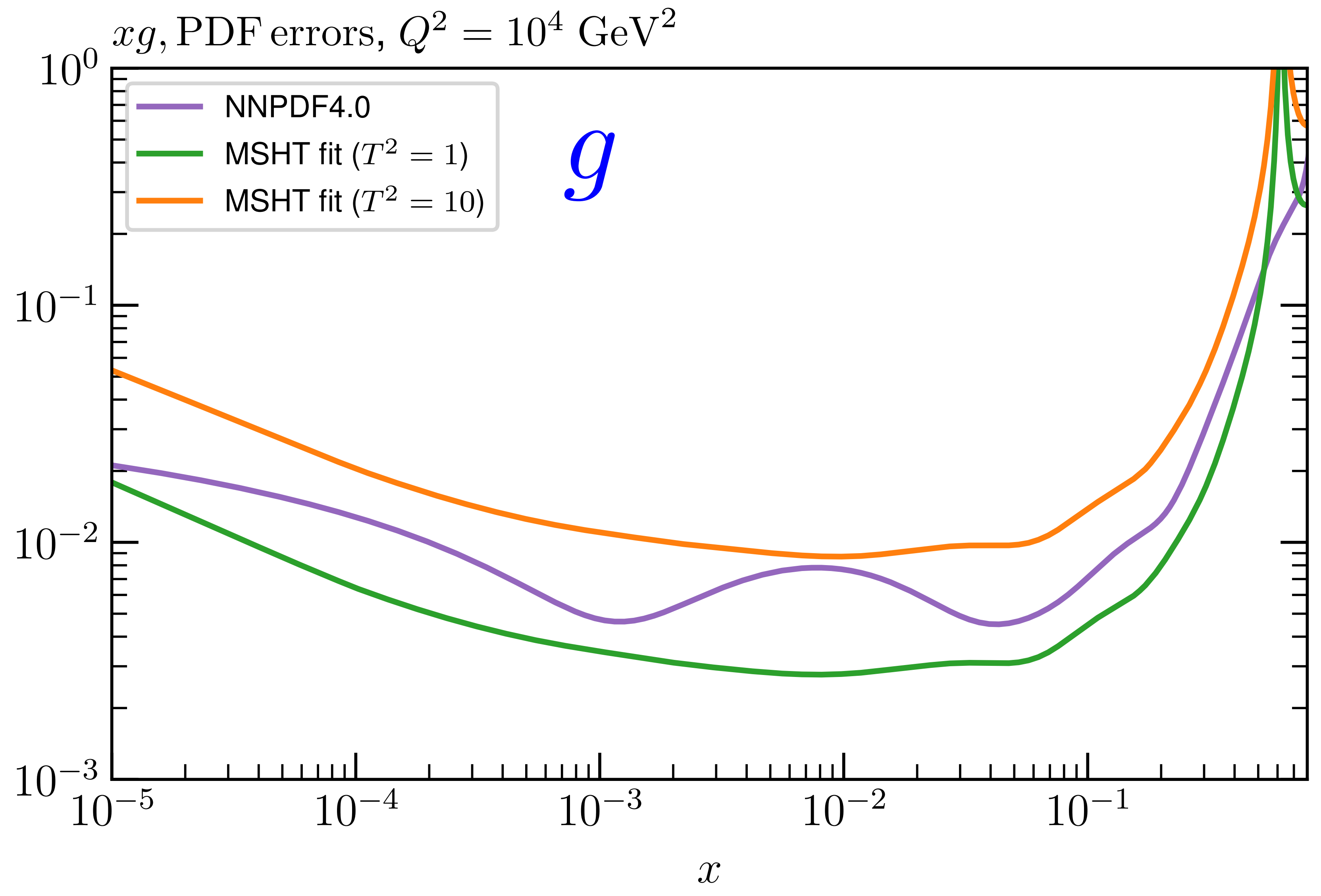
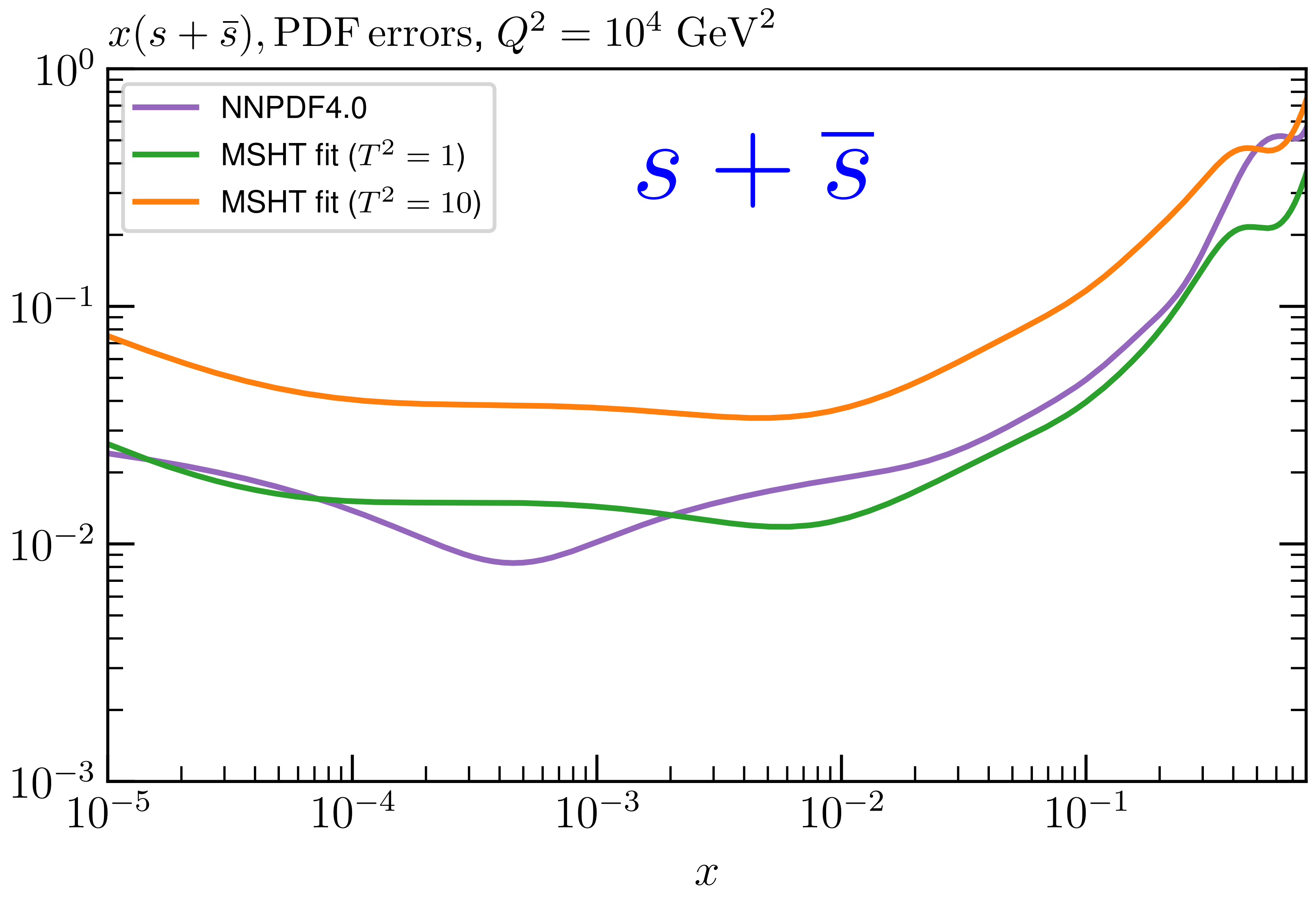
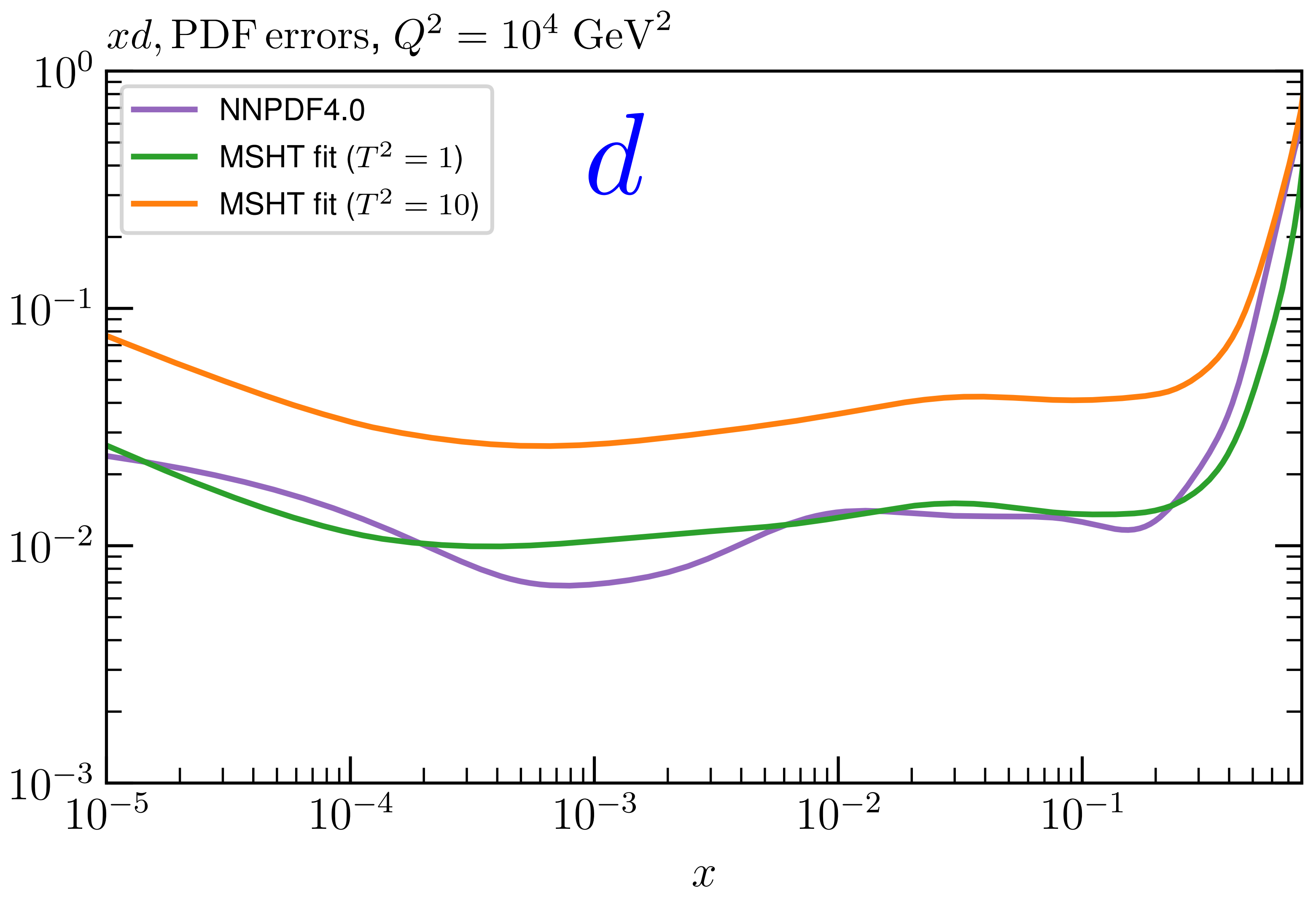


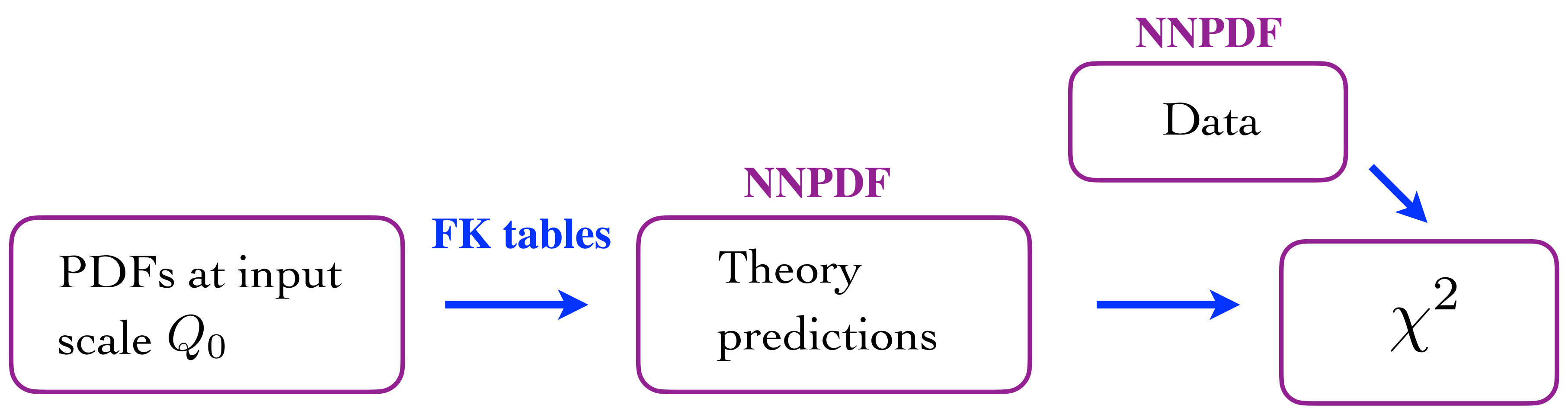




Full fit with fitted charm

- Readily extend previous study to include **fitted charm**. NNPDF theory inputs change accordingly, while PDFs parametrised at $Q_0 = 1.65\,\text{GeV}\,(> m_c)$ rather than 1 GeV, and parameterise charm:

$$xc_+(x,Q_0) = A_{c_+} x^{\delta_{c+}} (1-x)^{\eta_{c+}} \left(1 + \sum_{i=1}^{6} a_{c,i} T_i(y(x))\right)$$
$$xc_-(x,Q_0) = 0$$



- Find:

	NNPDF4.0	MSHT fit	MSHT fit (w positivity)
$\chi^2_{t_0}$	5692.1 (1.233)	5645.2 (1.222)	5651.0 (1.224)

$\Delta\chi^2_{t_0}$: $-46.9\,(0.011)$ $-41.1\,(0.009)$

⟶ Fit quality with **MSHT** parameterisation again **better** than result of central NNPDF set, albeit by less than in perturbative charm case.

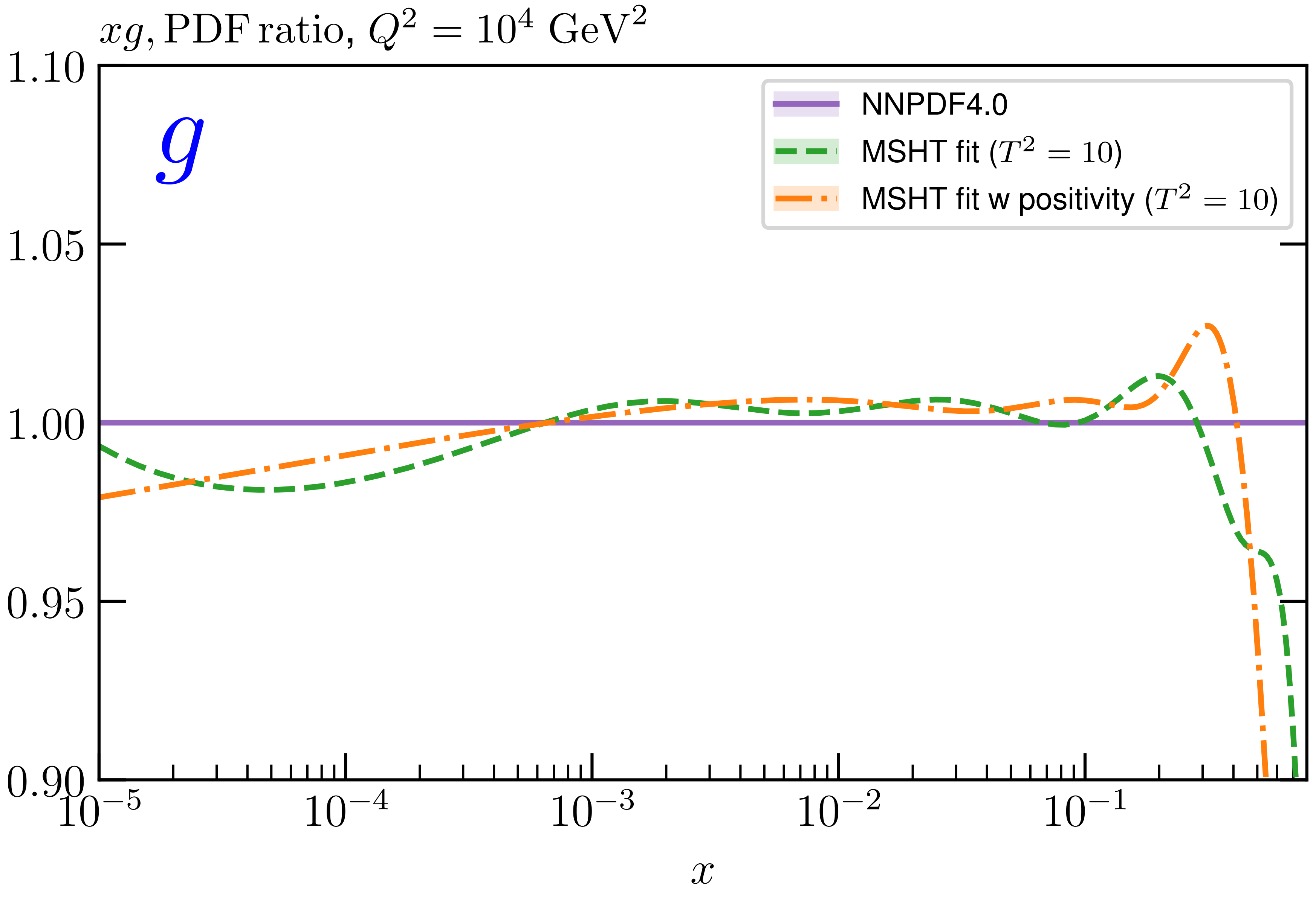
- Improvement spread across fixed target and LHC DY data.
- Role of **positivity** now **marginal** (confirmed with direct NNPDF fit).

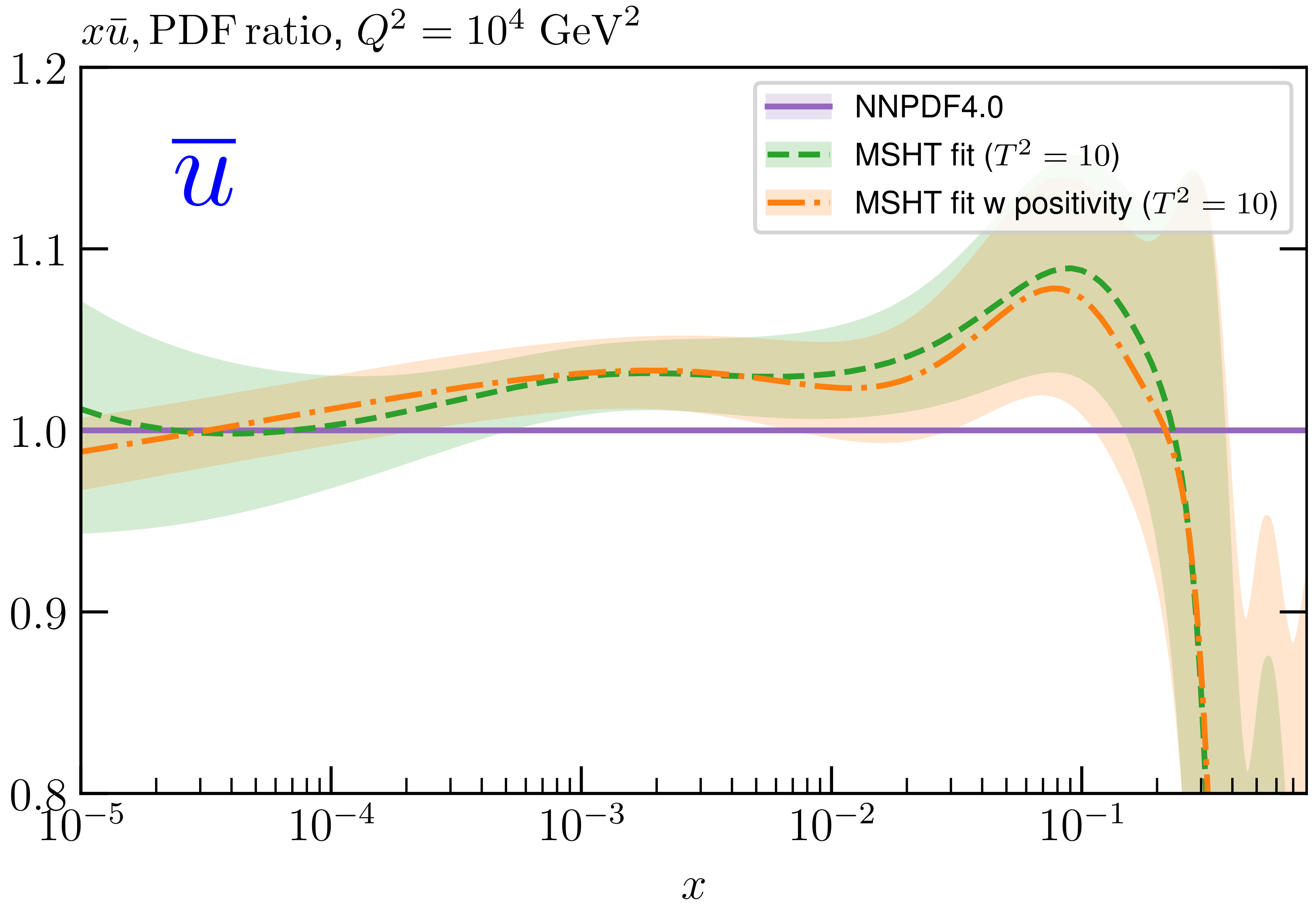
Integrability checked and not issue: Backup

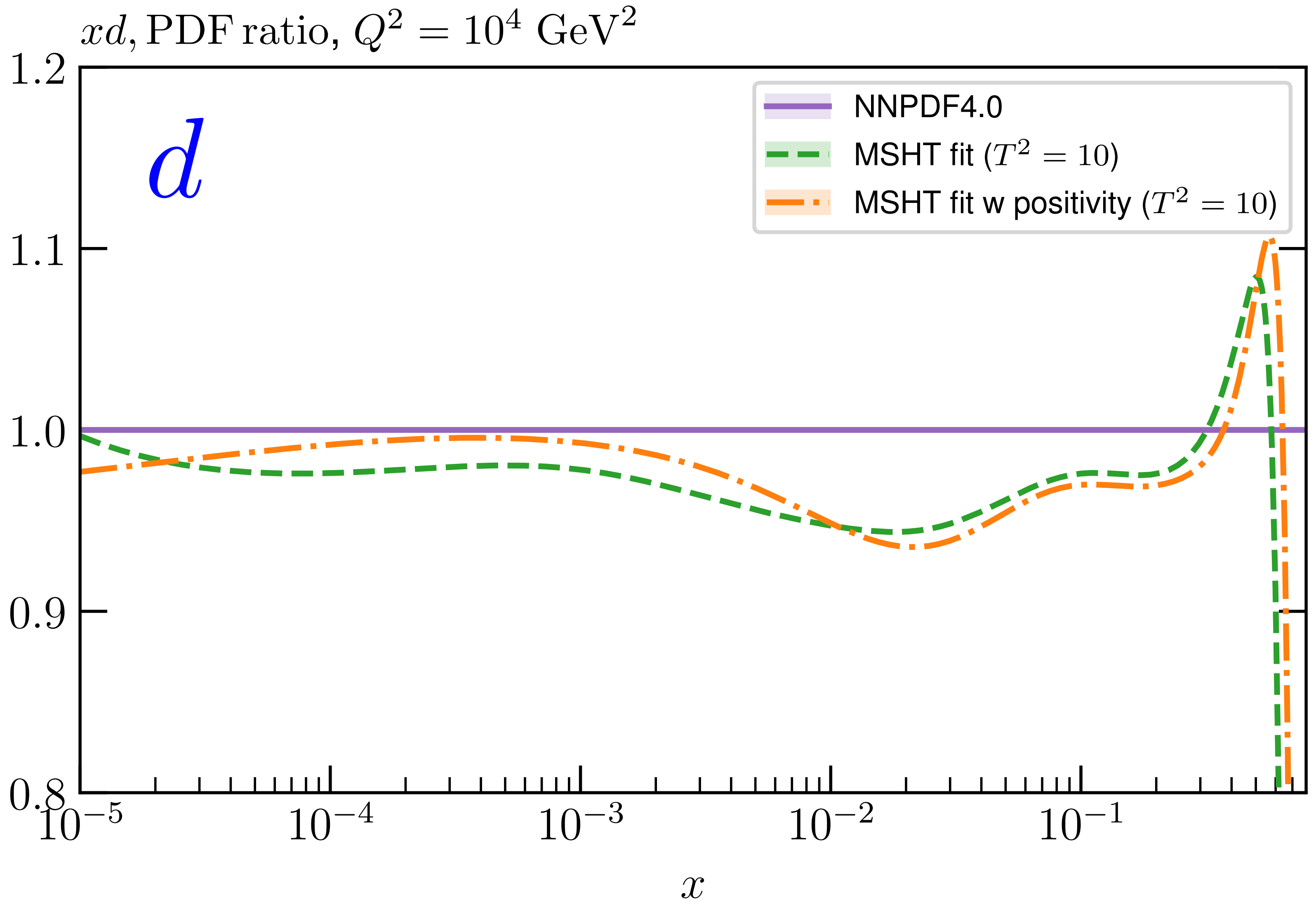
PDFs

- Confirm that role of **positivity** now **marginal**. Also seen if positivity removed from pure NNPDF fit.
- Difference less than in p. charm case, but **clear difference** in **flavour decomposition** remains.
- Again qualitatively this follows trend of using flavour rather than evolution basis (though difference larger and not identical). **See Backup**
- Show $T^2 = 10$ for concreteness and fact that there is reasonable (not perfect) agreement within these not relevant factor, given fit quality is better for MSHT sets.

NNPDF4.0pch   MSHT (pos) $T^2 = 10$ MSHT, $T^2 = 10$

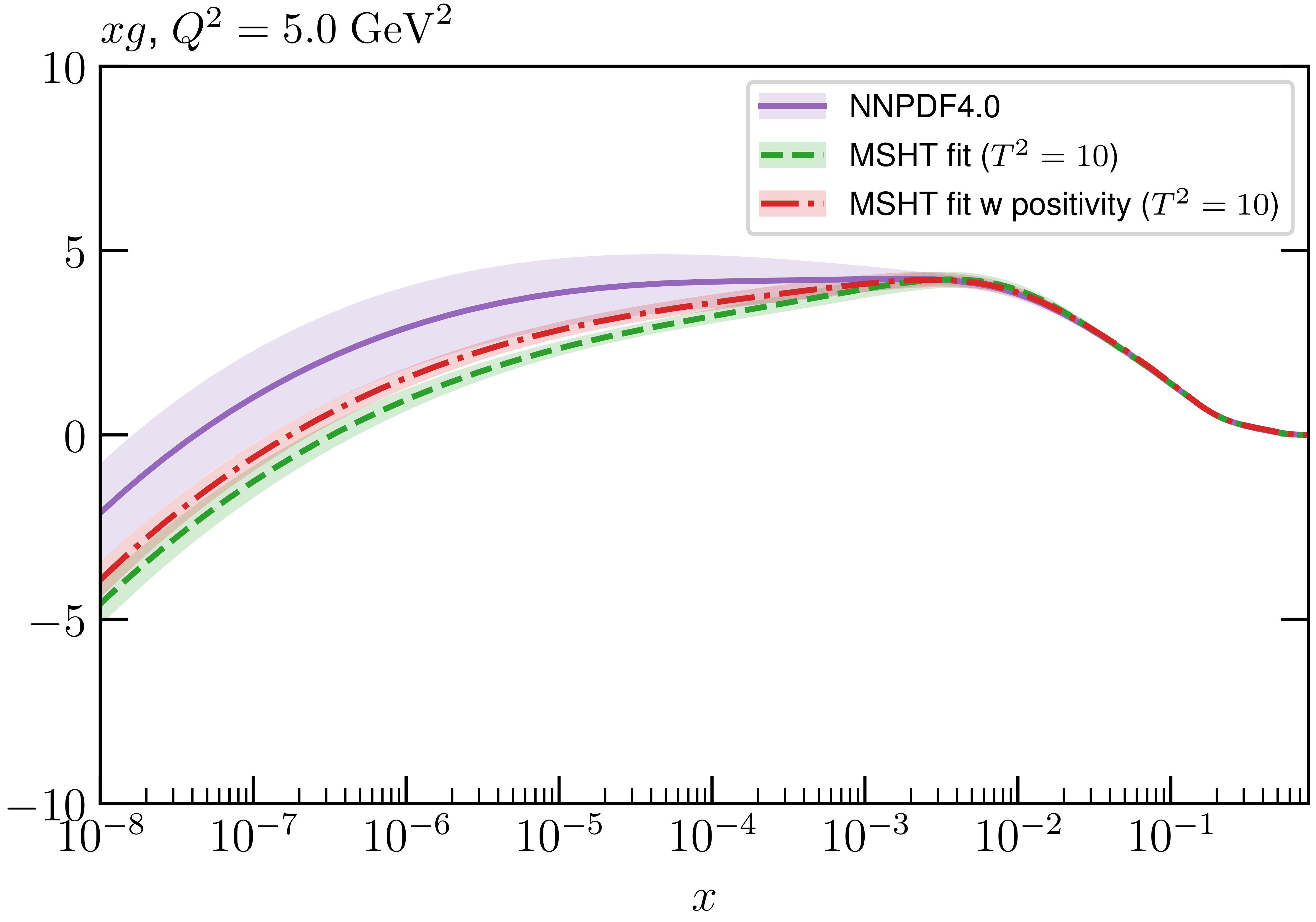






Positivity?

- With fitted charm tendency for preferred gluon to be negative reduced and pushed to lower x : why positivity requirement plays minor role - also seen in direct NNPDF fit.
- Not clear why this is (under investigation) but given intrinsic charm is expected to be high x phenomena might be concern?



Comparison to NNPDF uncertainties

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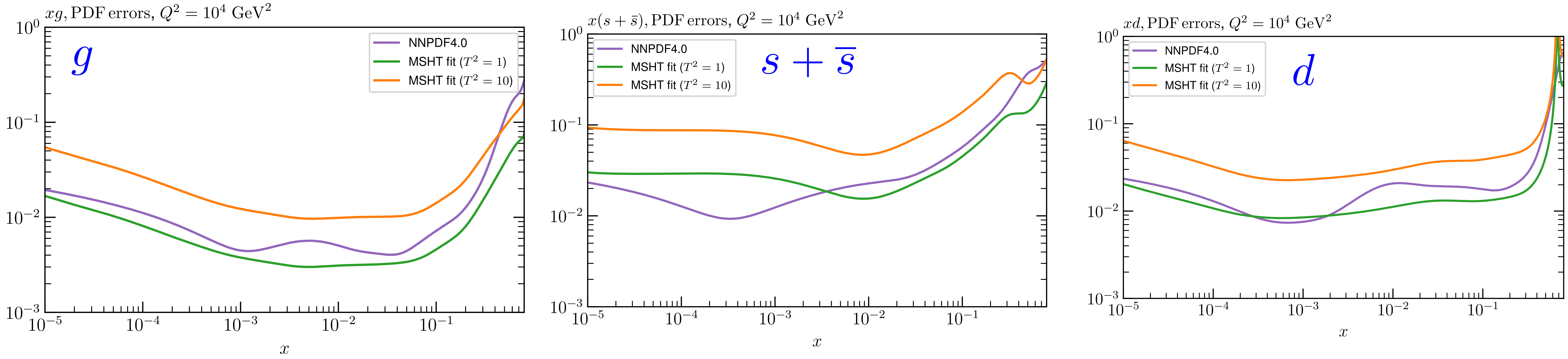
MSHT, $T^2 = 1$
MSHT, $T^2 = 10$
NNPDF4.0

  - With rather similar overall trends with x .
  - Exception at high x where NNPDF uncertainy can become larger.
  - Some trend for gluon to be a little closer to $T^2 = 1$ case.



Cross Sections

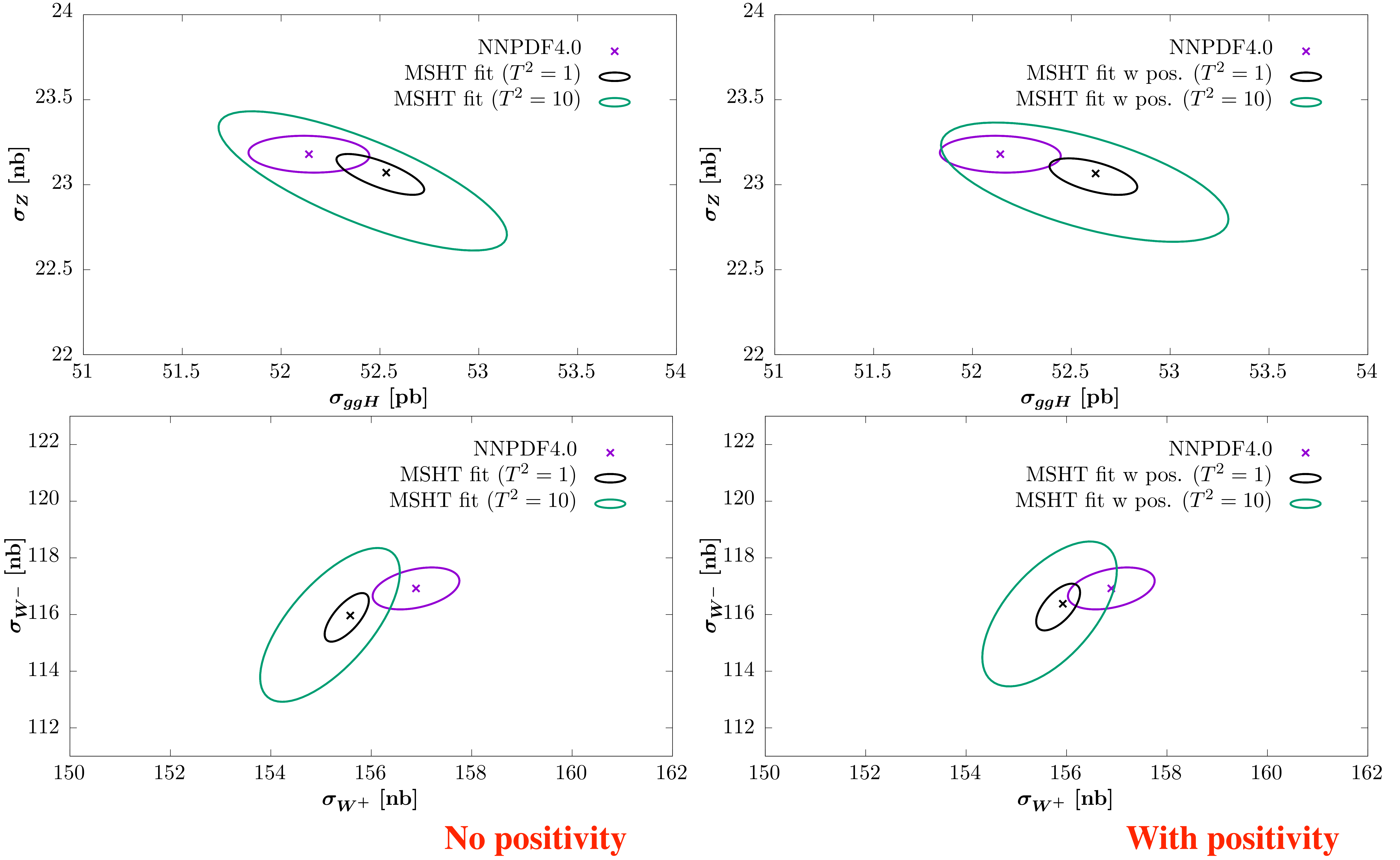
- Consider ggH, and W, Z cross sections (14 TeV) in fitted charm case:

n3loxs

MSHT, $T^2 = 10$ MSHT ($T^2 = 1$) NNPDF4.0

★ NNPDF uncertainties ~ MSHT ($T^2 = 1$) but **significantly smaller** than $T^2 = 10$

★ NNPDF and MSHT fit basically consistent within $T^2 = 1$ uncertainties but not relevant factor given fit qualities.



p. charm: Backup

Summary

- In this talk I have presented:

  ★ **First** global **closure test** of fixed parameterisation (MSHT) approach: is parameterisation flexible enough to give faithful description of global pseudodata?

  ✦ **Yes**: no issue in passing (unfluctuated) global closure test.

  ★ **First** completely direct **comparison** between fixed parameterisation (MSHT) and NN approaches. How do these compare in full global fit?

  ✦ At level of errors $\sigma(\mathrm{NNPDF}) \sim \sigma(\mathrm{MSHT}, T^2 = 1)$ in general with some exceptions - gluon larger though less than $T^2 = 10$ (MSHT20 default).

  ✦ At level of PDFs, surprisingly find fit quality is **lower** in **MSHT** fixed parameterisation case, and outside of NNPDF uncertainties. Reason for this is currently unclear. Positivity clearly important in p. charm case, but not only source (PDF basis?).

Summary

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2. MSHT uncertainty too conservative (too large).
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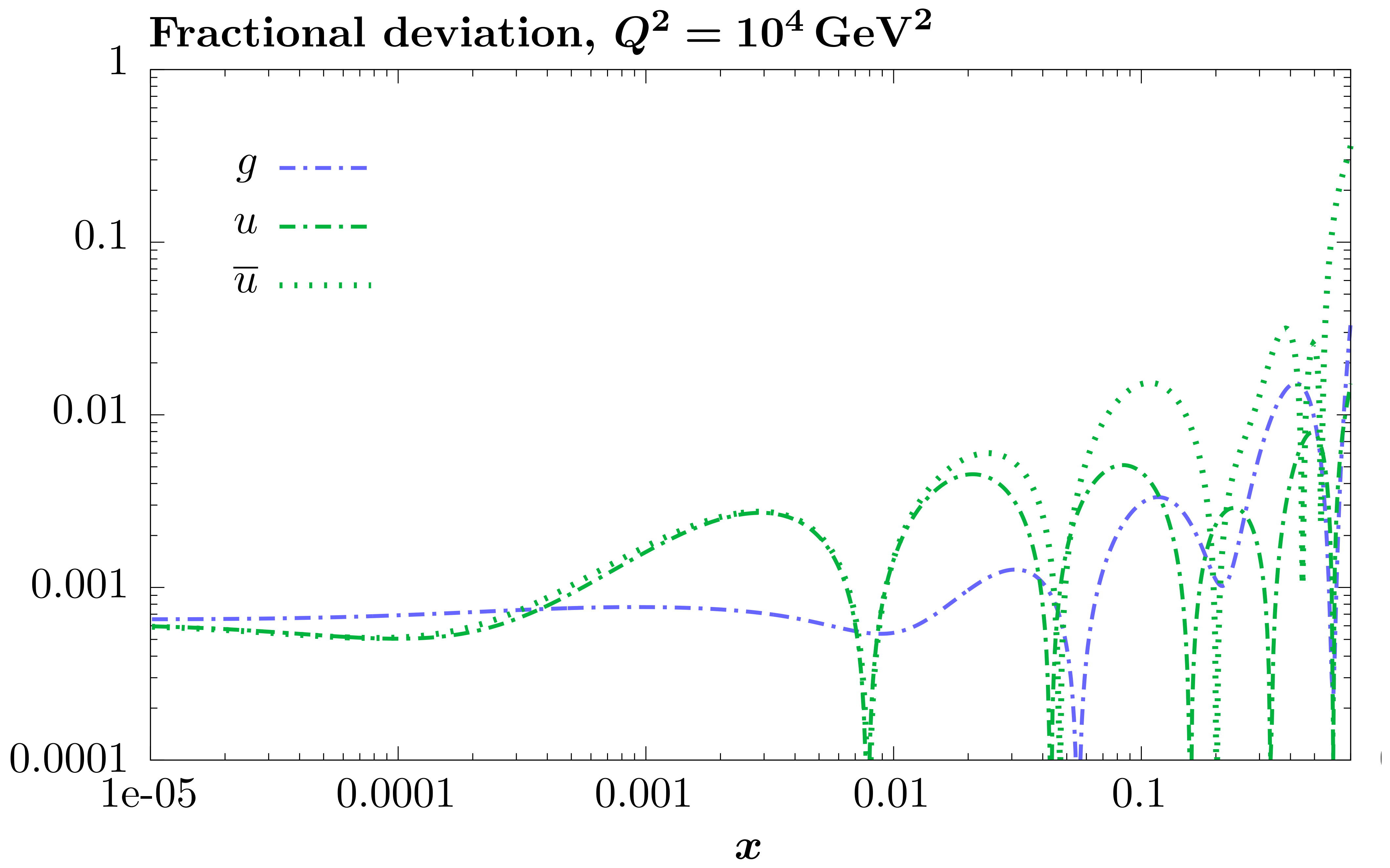
- Put together, this implies that **either 1 or 2 is true** (or both). This study has not addressed which, though question of tolerance discussed elsewhere, but either way suggests more work needed.
- **Future steps:** extend to L1 closure, look again at question of tolerance in closure test framework…

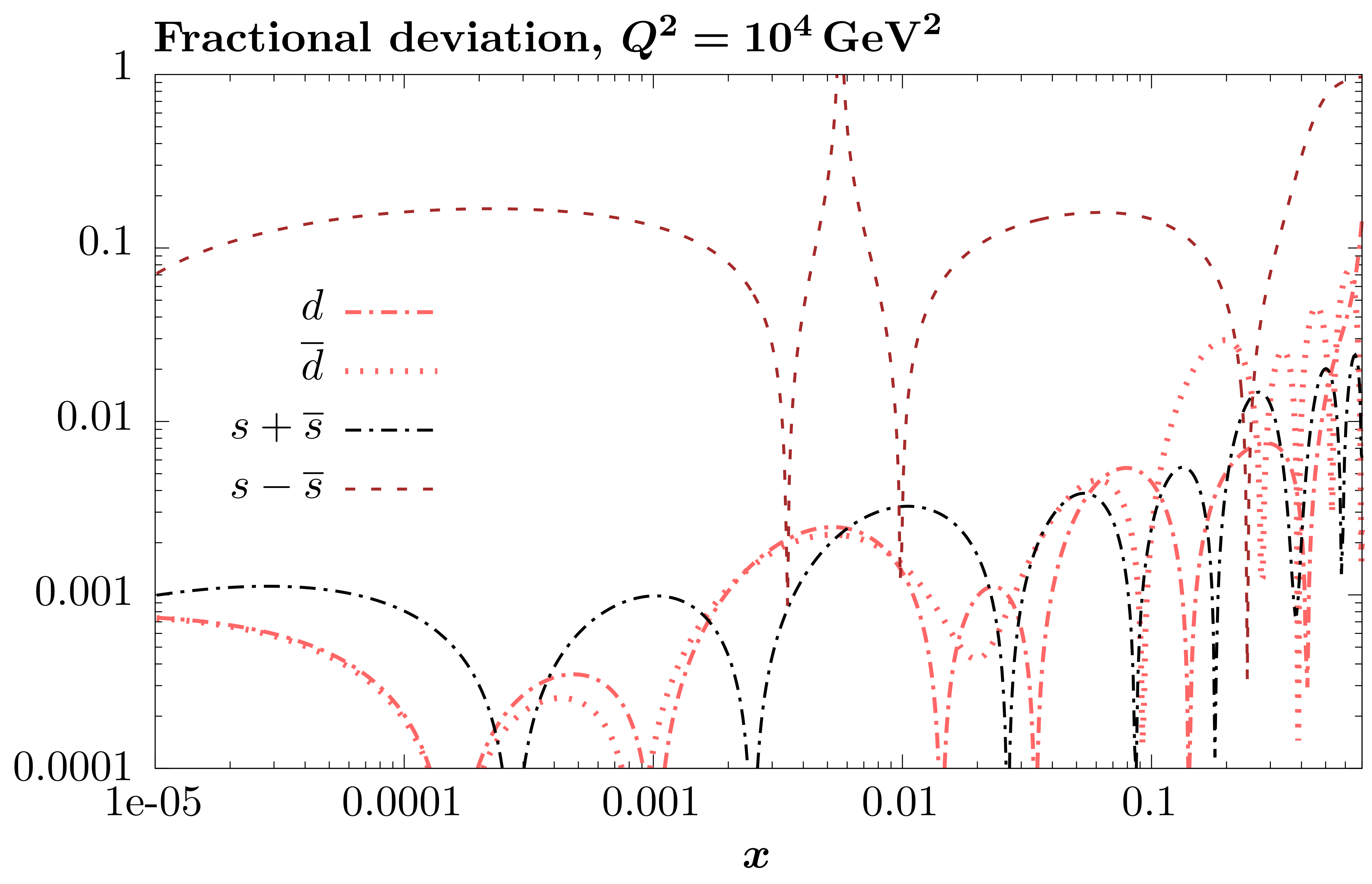
Backup

Closure test - warm up

Similar study: A.D. Martin et al., arXiv:1211.1215

- Before considering global closure test, consider related question. Given PDF-level pseudodata, how closely can MSHT parameterisation match it Basic point: for LHC precision aim for sub-1% agreement.
- 500 PDF points logarithmically in $x \in \{10^{-5}, 0.99\}$ scattered by 1% uncertainty, for $u_V, d_V, S, s_+, s_-, g, \bar{d}/\bar{u}$
- Take NNPDF4.0 (p. charm) as input and plot fractional deviation. Find this is $\ll 0.01$ for most of the x region. Biggest deviations at high x and for s_- (as expected - MSHT parameterisation limited at moment).





- Encouraging, but rather artificial - really want to see how deviation compares in data region of global fit.

MSHT parameterisation

$$u_V(x,Q_0^2) = A_u(1-x)^{\eta_u}x^{\delta_u}\left(1+\sum_{i=1}^{6}a_{u,i}T_i(y(x))\right)$$

$$d_V(x,Q_0^2) = A_d(1-x)^{\eta_d}x^{\delta_d}\left(1+\sum_{i=1}^{6}a_{d,i}T_i(y(x))\right)$$

$$S(x,Q_0^2) = A_S(1-x)^{\eta_S}x^{\delta_S}\left(1+\sum_{i=1}^{6}a_{S,i}T_i(y(x))\right)$$

$$s_+(x,Q_0^2) = A_{s_+}(1-x)^{\eta_{s+}}x^{\delta_S}\left(1+\sum_{i=1}^{6}a_{s_+,i}T_i(y(x))\right)$$

$$g(x,Q_0^2) = A_g(1-x)^{\eta_g}x^{\delta_g}\left(1+\sum_{i=1}^{4}a_{g,i}T_i(y(x))\right) + A_{g-}(1-x)^{\eta_{g-}}x^{\delta_{g-}}$$

$$s_-(x,Q_0^2) = A_{s_-}(1-x)^{\eta_{s-}}(1-x/x_0)x^{\delta_{s-}}$$

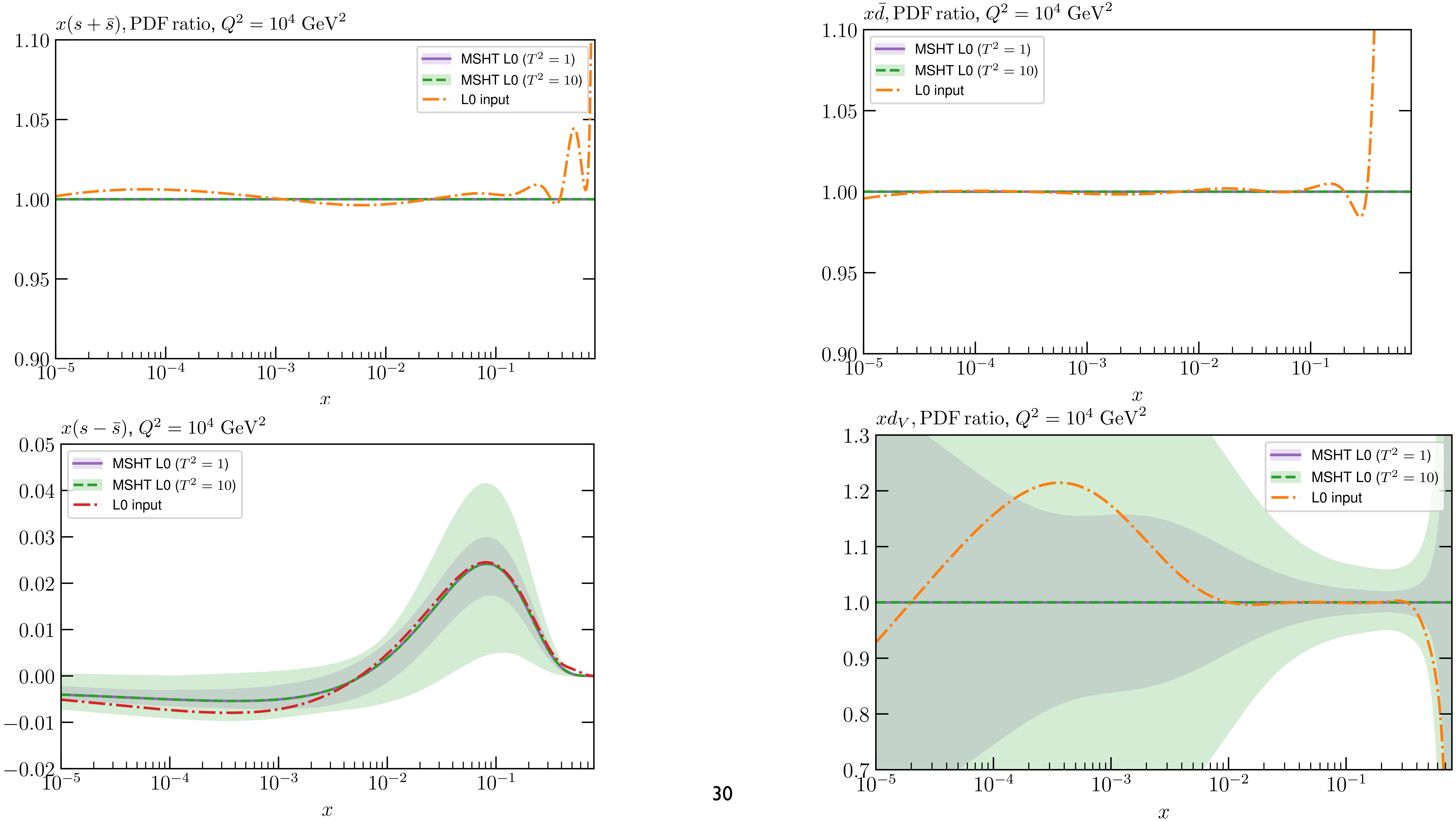
$$(\bar{d}/\bar{u})(x,Q_0^2) = A_\rho(1-x)^{\eta_\rho}\left(1+\sum_{i=1}^{6}a_{\rho,i}T_i(y(x))\right)$$

$$y(x) = 1-2\sqrt{x}$$

$$S(x) = 2(\bar{u}(x)+\bar{d}(x))+s(x)+\bar{s}(x)$$

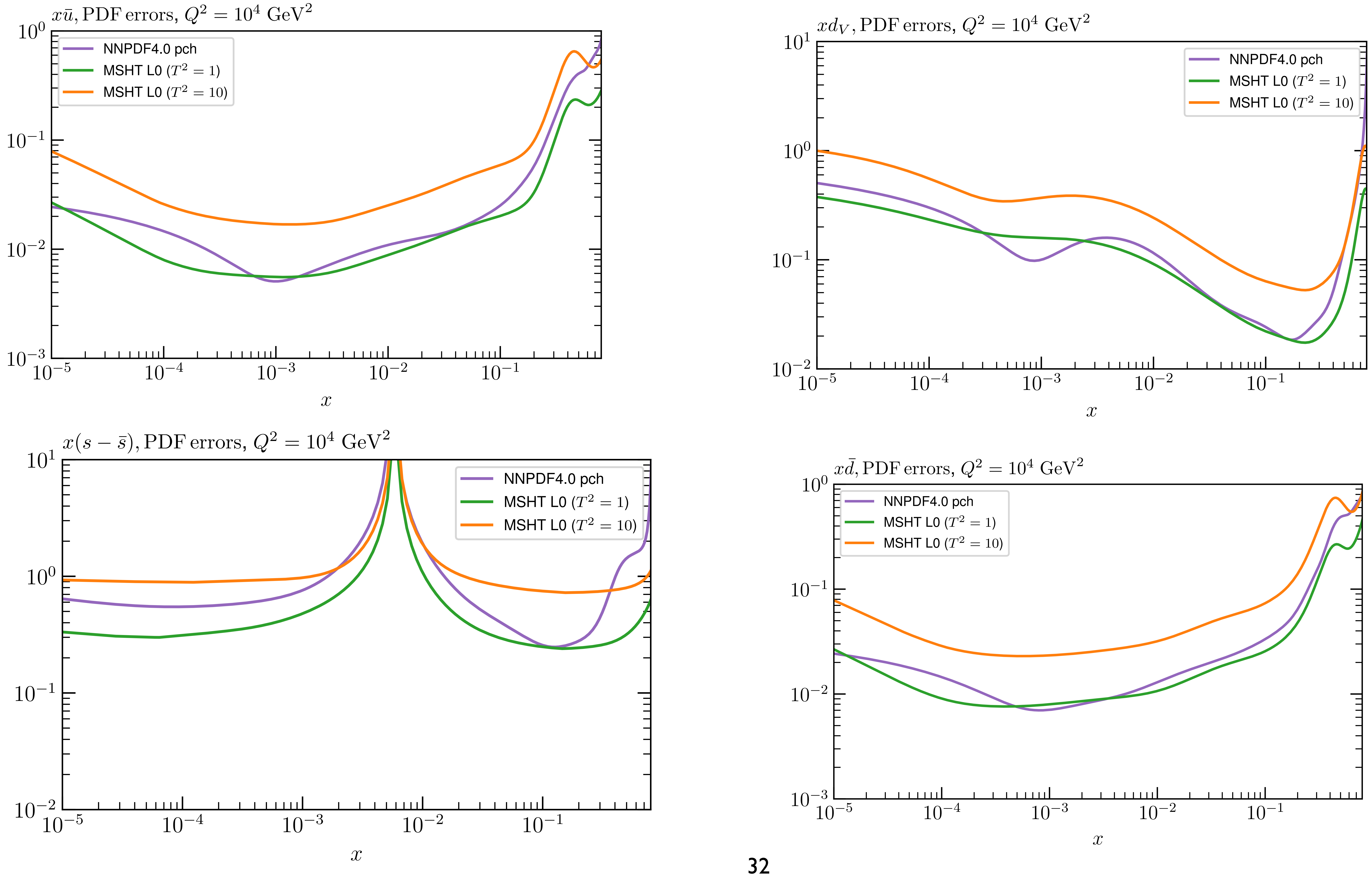
T_i: Chebyshev Polynomials

Global Closure PDFs



xd, $Q^2 = 10^4$ GeV^2
MSHT L0 ($T^2 = 1$)
MSHT L0 ($T^2 = 10$)
L0 input
xu, $Q^2 = 10^4$ GeV^2
MSHT L0 ($T^2 = 1$)
MSHT L0 ($T^2 = 10$)
L0 input
$x\bar{d}$, $Q^2 = 10^4$ GeV^2
MSHT L0 ($T^2 = 1$)
MSHT L0 ($T^2 = 10$)
L0 input
$x(s+\bar{s})$, $Q^2 = 10^4$ GeV^2
MSHT L0 ($T^2 = 1$)
MSHT L0 ($T^2 = 10$)
L0 input
xg, $Q^2 = 10^4$ GeV^2
MSHT L0 ($T^2 = 1$)
MSHT L0 ($T^2 = 10$)
L0 input
x

Comparison to NNPDF errors - Closure



Positivity

- We take:

$$\chi^2_{\rm tot} \to \chi^2_{\rm tot} + \sum_{k=1}^{8} \Lambda_k \sum_{i=1}^{n_i} \mathrm{Elu}_\alpha \left(-\tilde{f}_k \left(x_i, Q^2\right)\right) \,, \qquad \text{with} \qquad \Lambda_k = 10^3$$

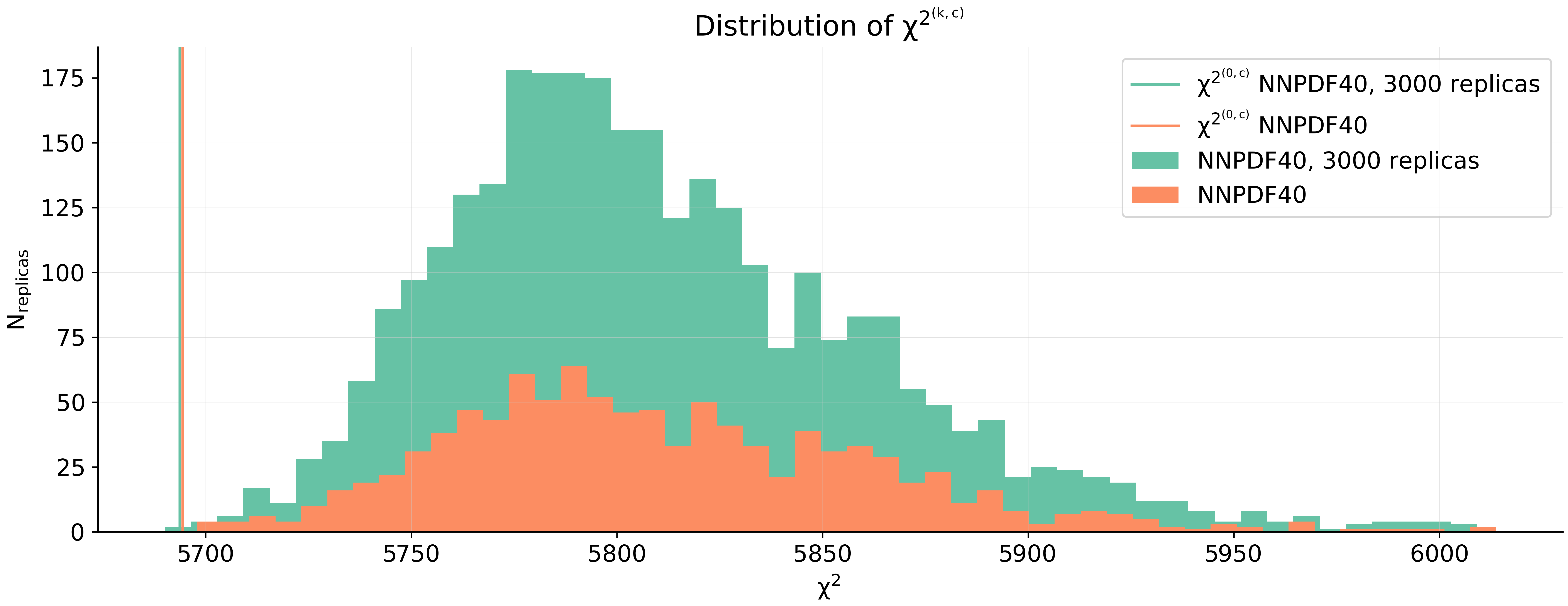
$$x_i \in \{5 \cdot 10^{-7}, 0.9\}$$

See NNPDF, arXiv:2109.02653

$$\mathrm{Elu}_\alpha\left(t\right) = \begin{cases} t & \text{if} \quad t > 0 \\ \alpha\left(e^t - 1\right) & \text{if} \quad t < 0 \end{cases} \,,$$

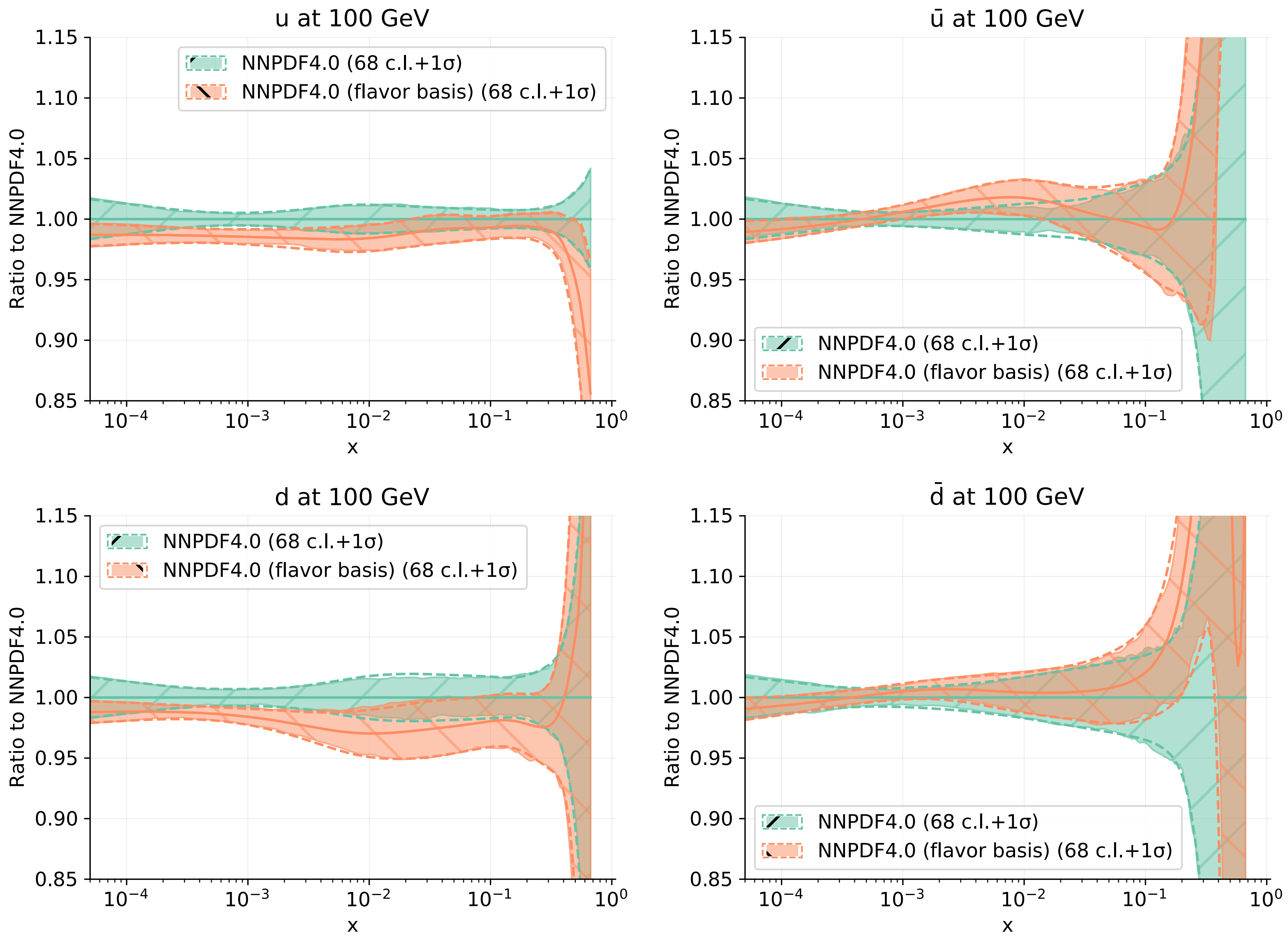
- And similarly for cross section constraints.

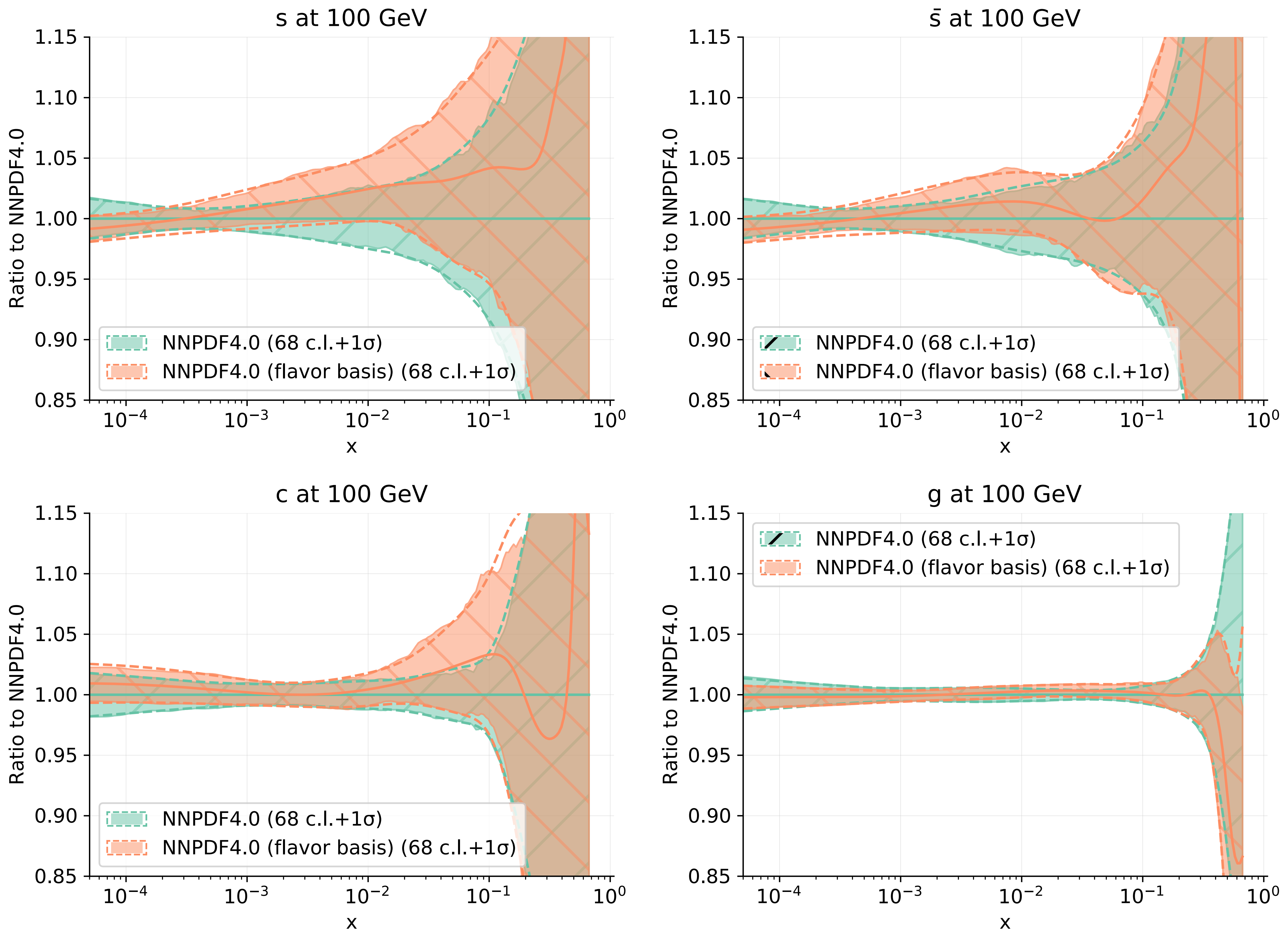
NNPDF chi^2 spread



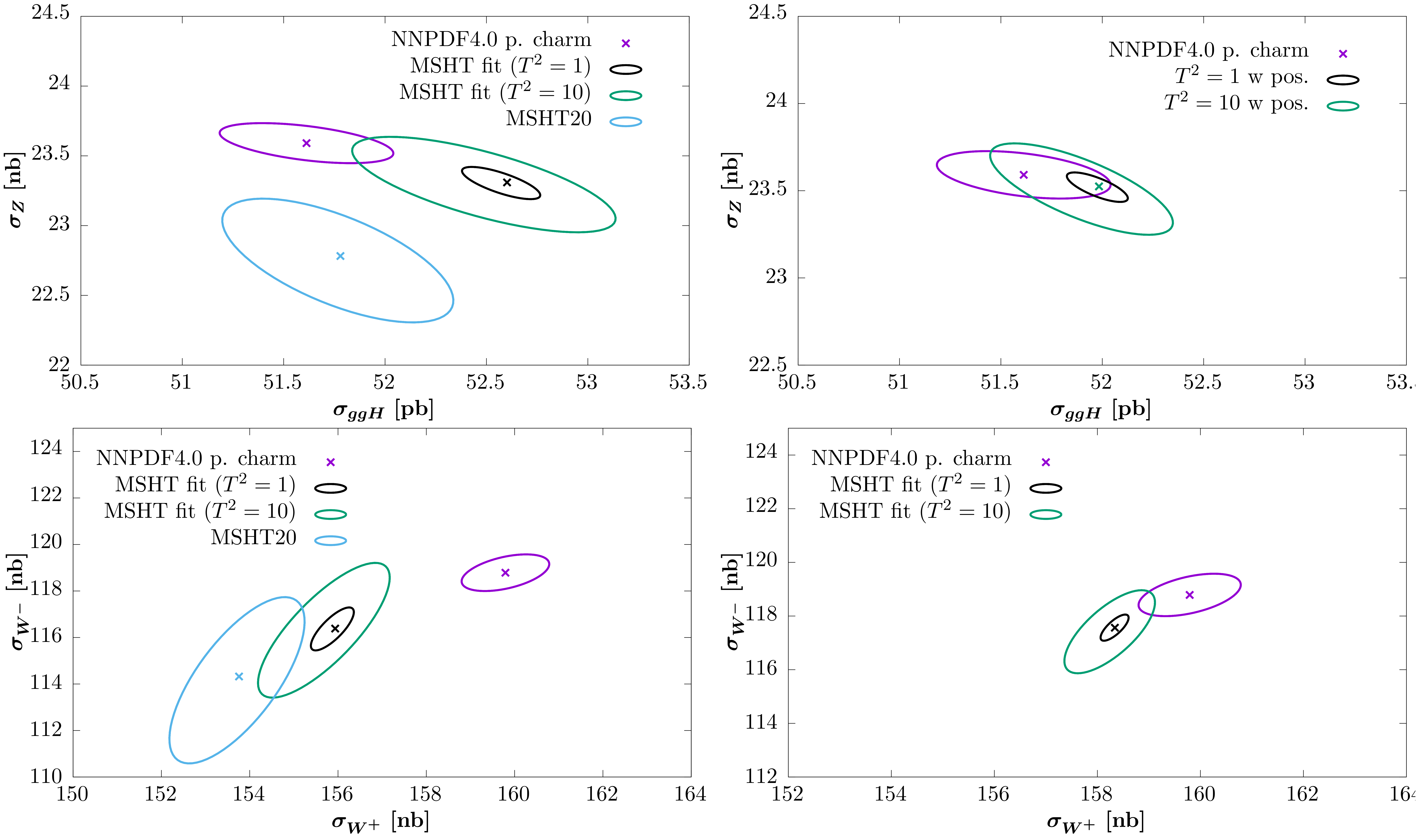
- In general do not expect central replica $\chi^2_{\mathrm{rep},0}$ to be absolute minimum of χ^2 in NN approach due to overfitting regularization and statistical nature of replica ensemble. However former seems ruled out here (fixed parameterization) and latter should only give a handful of points lower.

NNPDF flavour basis

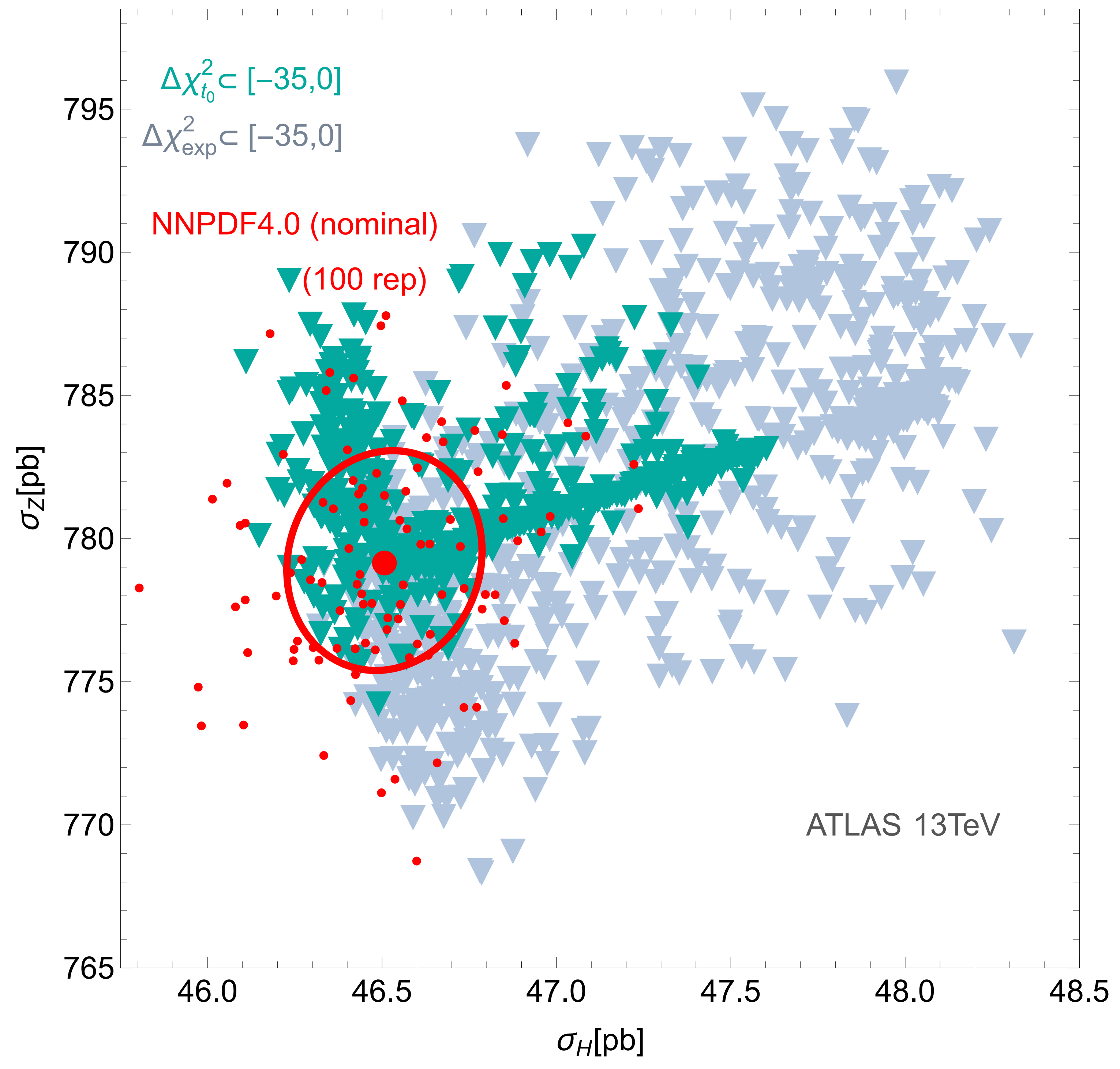




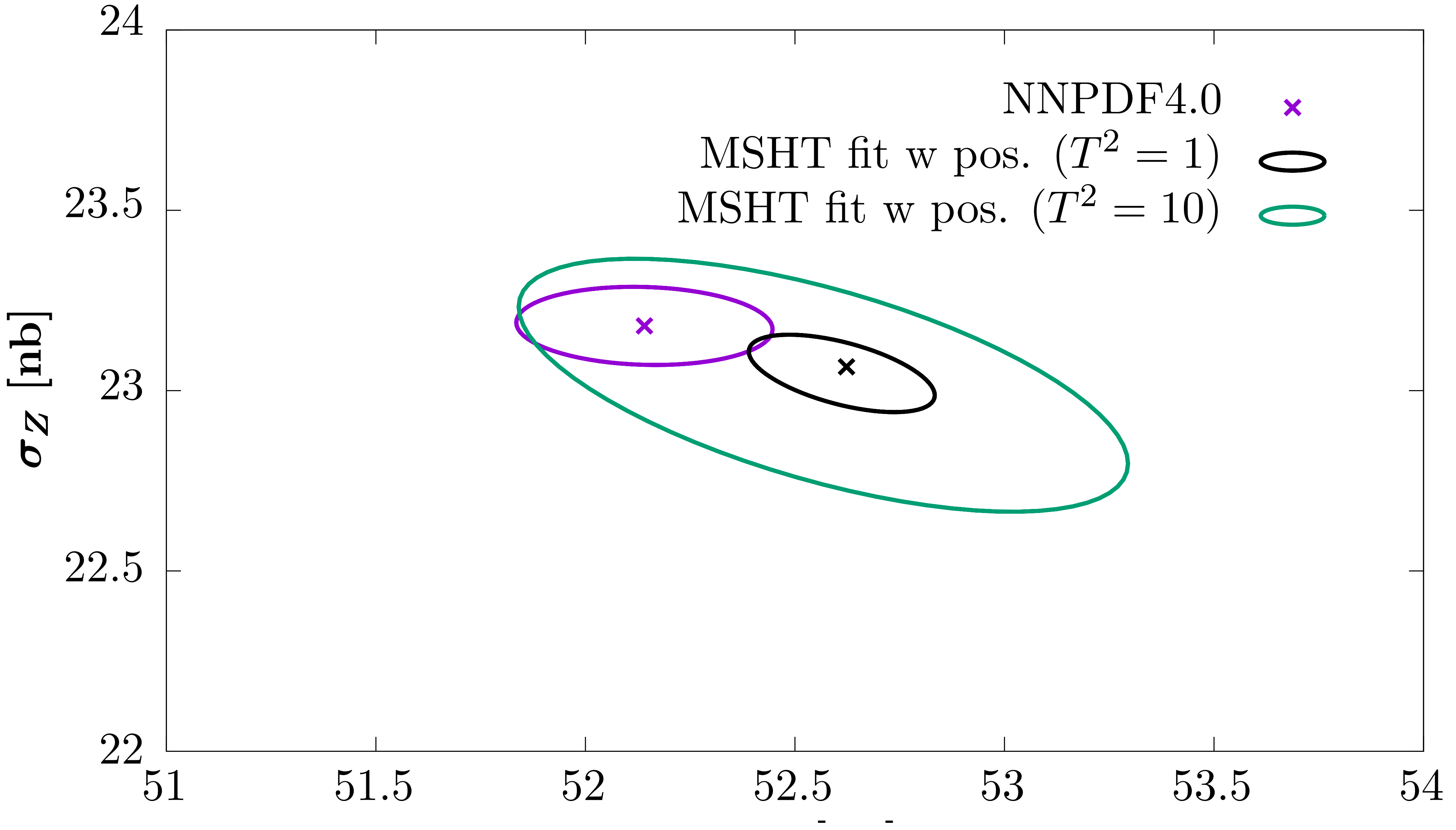
Cross Sections - p. charm



Comparison to hopscotch



A. Courtoy et al., arXiv: 2205.10444

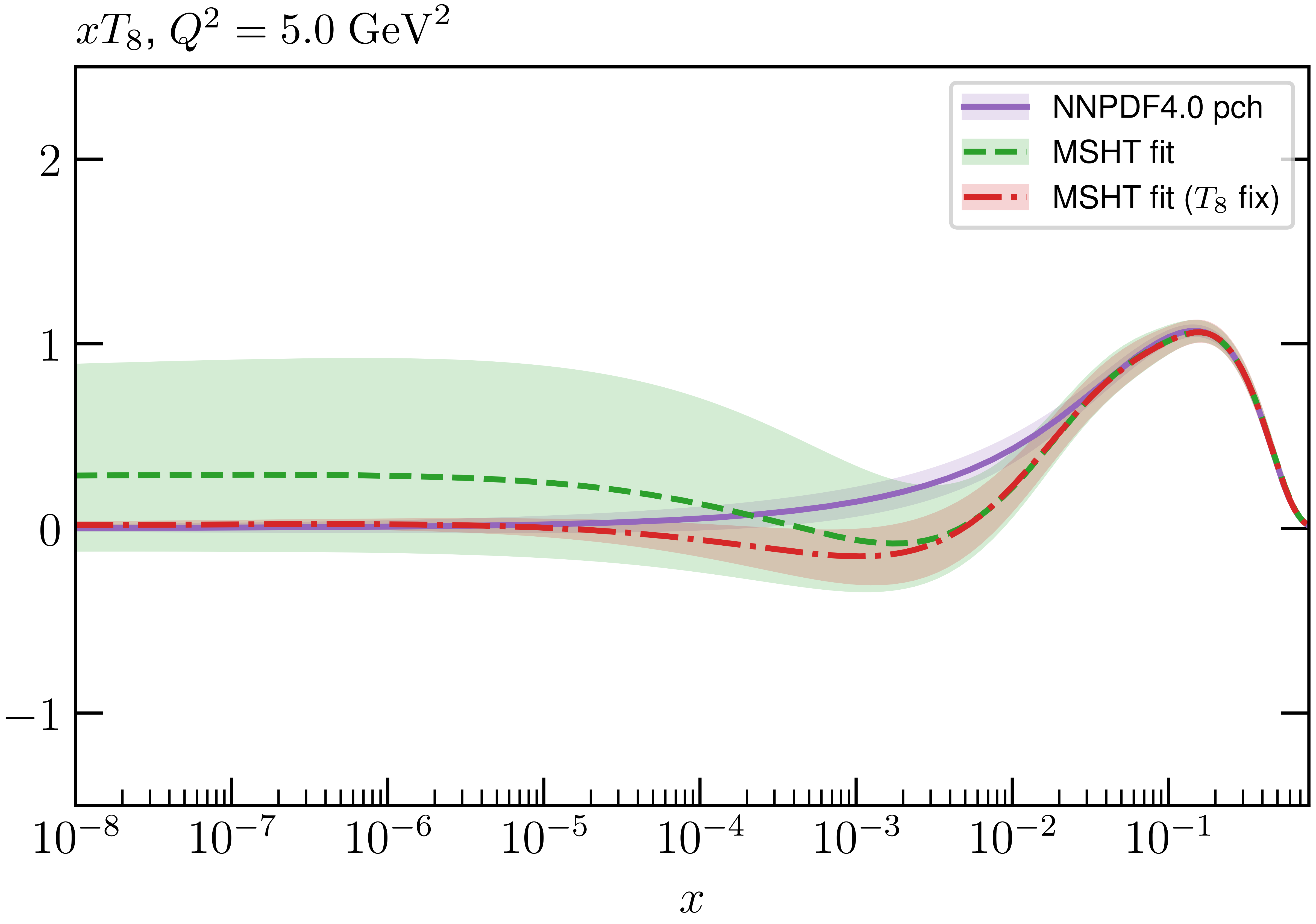


Integrability

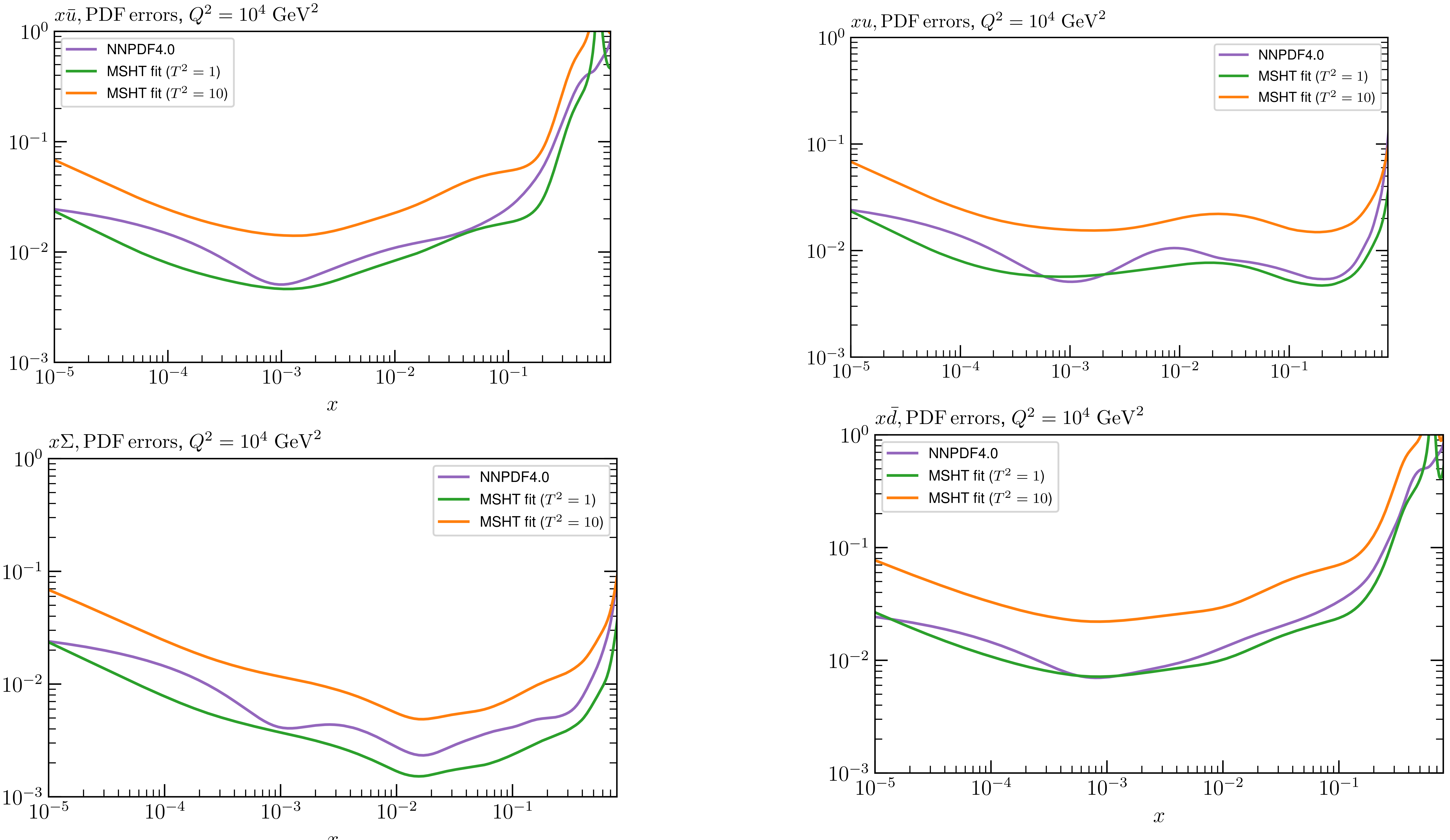
$$\lim_{x\to 0} x f_k(x,Q) = 0\,, \quad \forall\, Q\,, \qquad f_k = T_3,\, T_8\,.$$

$$\chi^2_{\rm tot} \to \chi^2_{\rm tot} + \sum_k \Lambda_k^{(\rm int)} \sum_{i=1}^{n_i} \left[x f_k \left(x_{\rm int}^{(i)}, Q_i^2 \right) \right]^2 \,, \qquad x_{\rm int}^{(i)} = 10^{-9},\, 10^{-8},\, 10^{-7}. \qquad \Lambda_k^{(\rm int)} = 100$$

- Biggest deviation from this for MSHT is for the T_8 combination.
- In MSHT fixed parameterisation can impose that this vanishes at low x by simply fixing strangeness normalization.
- Gives ~ same fit quality for p. charm, and ~ 3 points worse for fitted.



Uncertainties - p. charm



Uncertainties - fitted charm