The rôle of parametrization in global analyses : The Fantômas project

CTEQ meeting

MSU

11/09/23

Aurore Courtoy

Instituto de Física

Universidad Nacional Autónoma de México (UNAM)

CONACYT

Consejo Nacional de Ciencia y Tecnología

dgapa

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Instituto de Física UNAM

Towards quantifying epistemic uncertainties in global PDF analyses

Mainly based on

“Testing momentum dependence of the nonperturbative hadron structure in a global QCD analysis” [Phys.Rev.D 103]

A.C. & Nadolsky

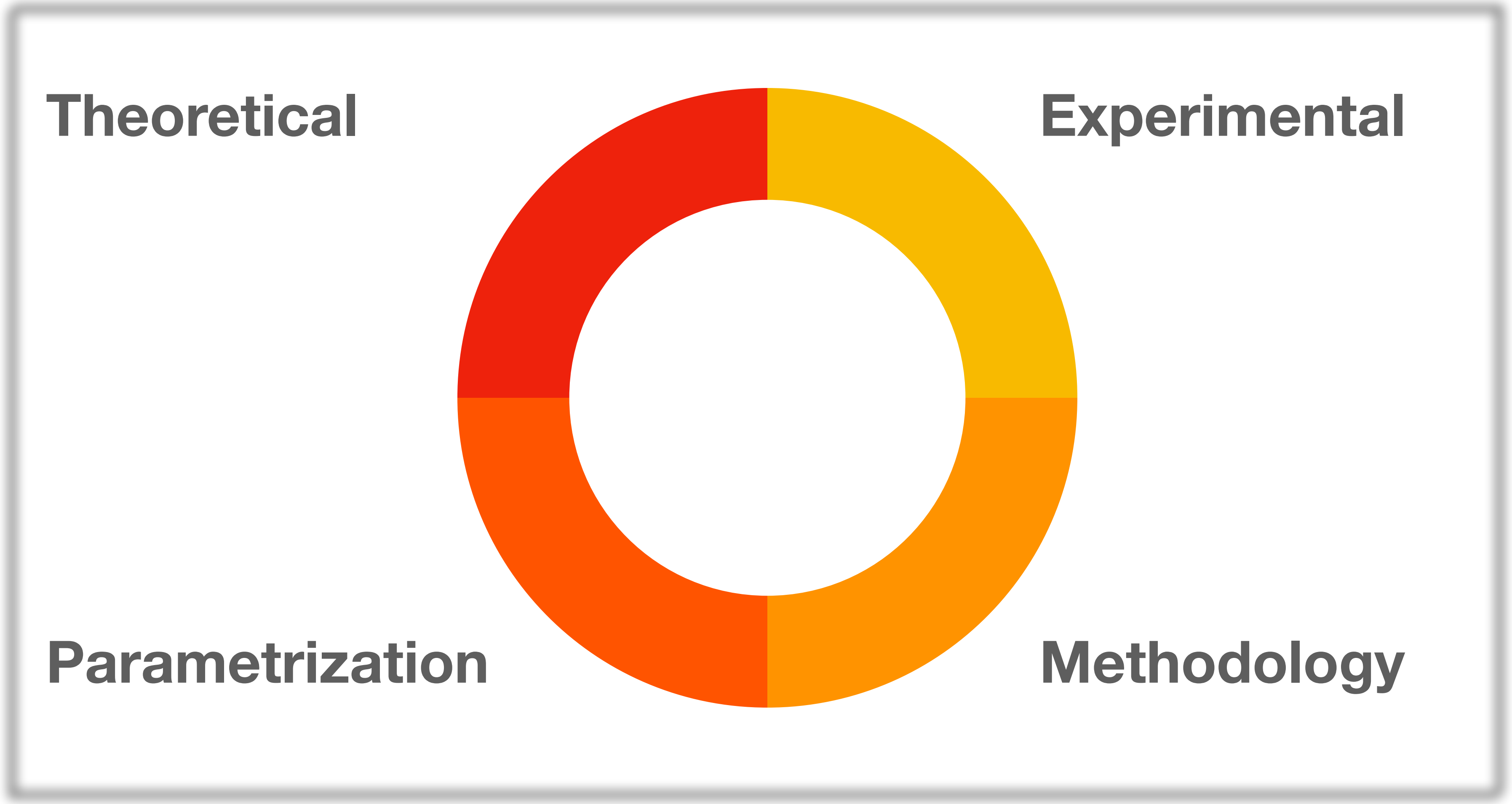
“Parton distributions need representative sampling” [Phys.Rev.D 107]

CTEQ-TEA collaboration

“An analysis of parton distributions in a pion with Bézier parametrizations ” [upcoming]

L. Kotz, A. Courtoy, P. Nadolsky, F. Olness, D.M. Ponce-Chávez

DIS23 proceedings [2309.00152]



Fantômas4QCD

Main idea: to quantify the rôle of parametrization form in global analyses.

Fantômas4QCD: Our new c++ code, Fantômas, automates series of fits using multiple functional forms.

Just like neural networks, these polynomial functional forms can approximate any arbitrary PDF shape.

This code facilitates unbiased estimates of parametrization dependence.

CONACYT
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I·ANQCD Network of Networks
Inter-American

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Fantômas team:

F. Olness, P. Nadolsky, D. M. Ponce-Chávez, L. Kotz, A. Courtoy

The shape of parton distributions

Low-energy QCD dynamics, encapsulated in PDFs, are learned from experimental data.

Classes of *first principle* constraints for x-dependence

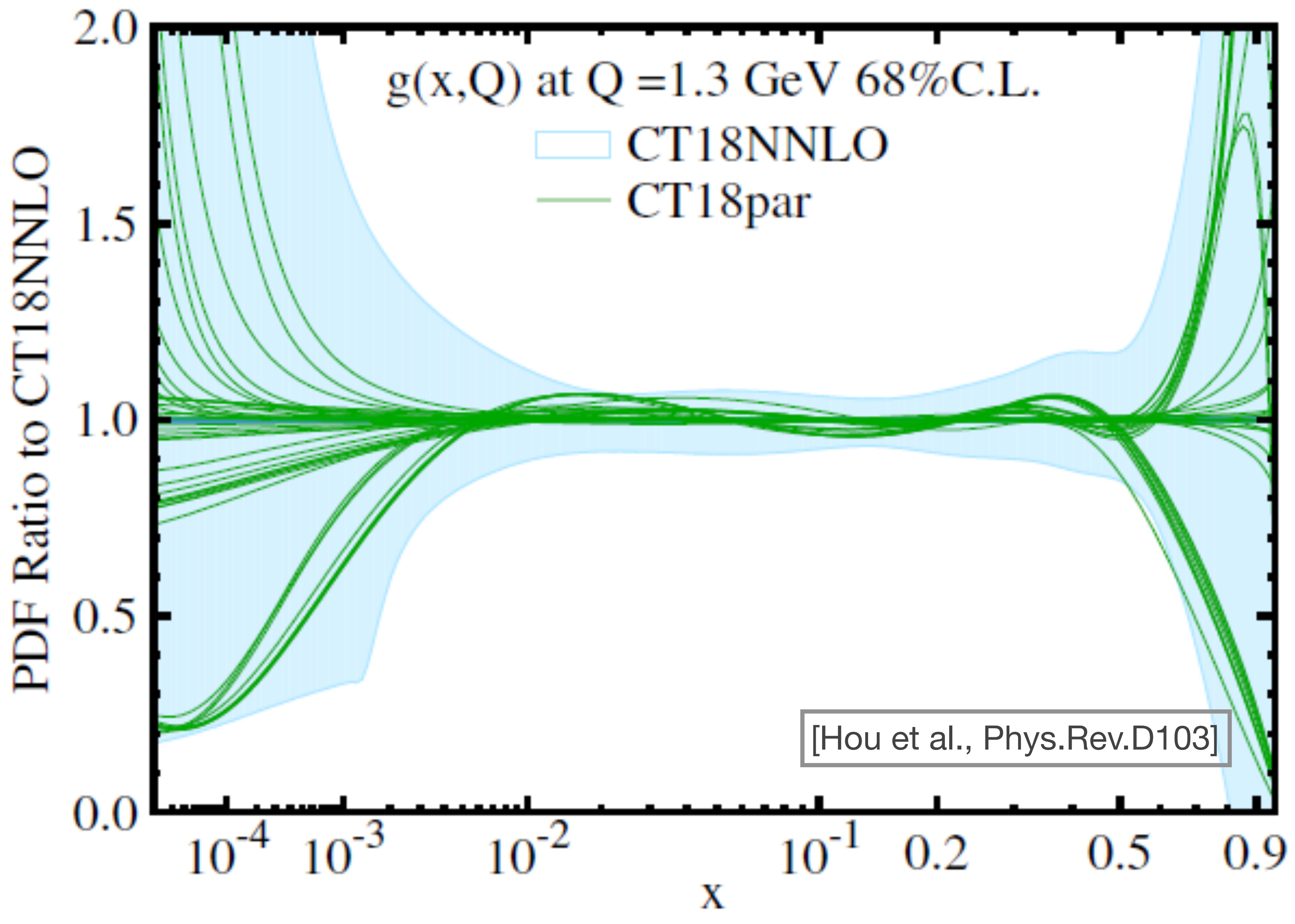
- positivity of cross sections
- support in $x \in [0,1]$
- end-point: $f(x=1)=0$
- sum rules: $< x >_n = \int_0^1 dx\, x^{n-1} f(x)$

⇨ asymptotics usually ensured by a *carrier function*

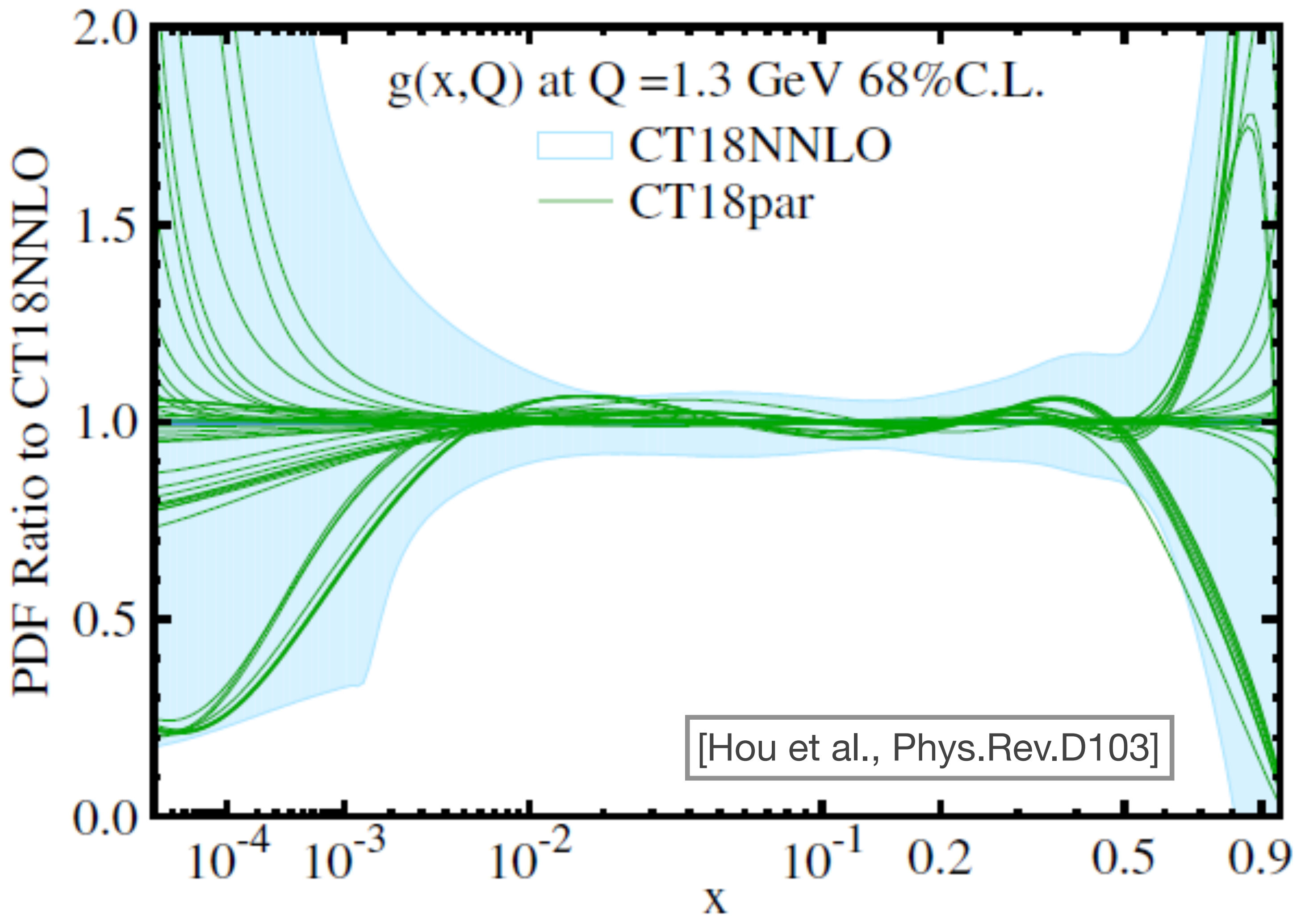
⇨ sum rules imposed through normalization

CT18 PDF (unpolarized proton PDF)

Hessian-based methodology
Inclusive of sampling bias/lack of knowledge
Tolerance criterion leads to cyan band



Rôle of parametrization and positivity



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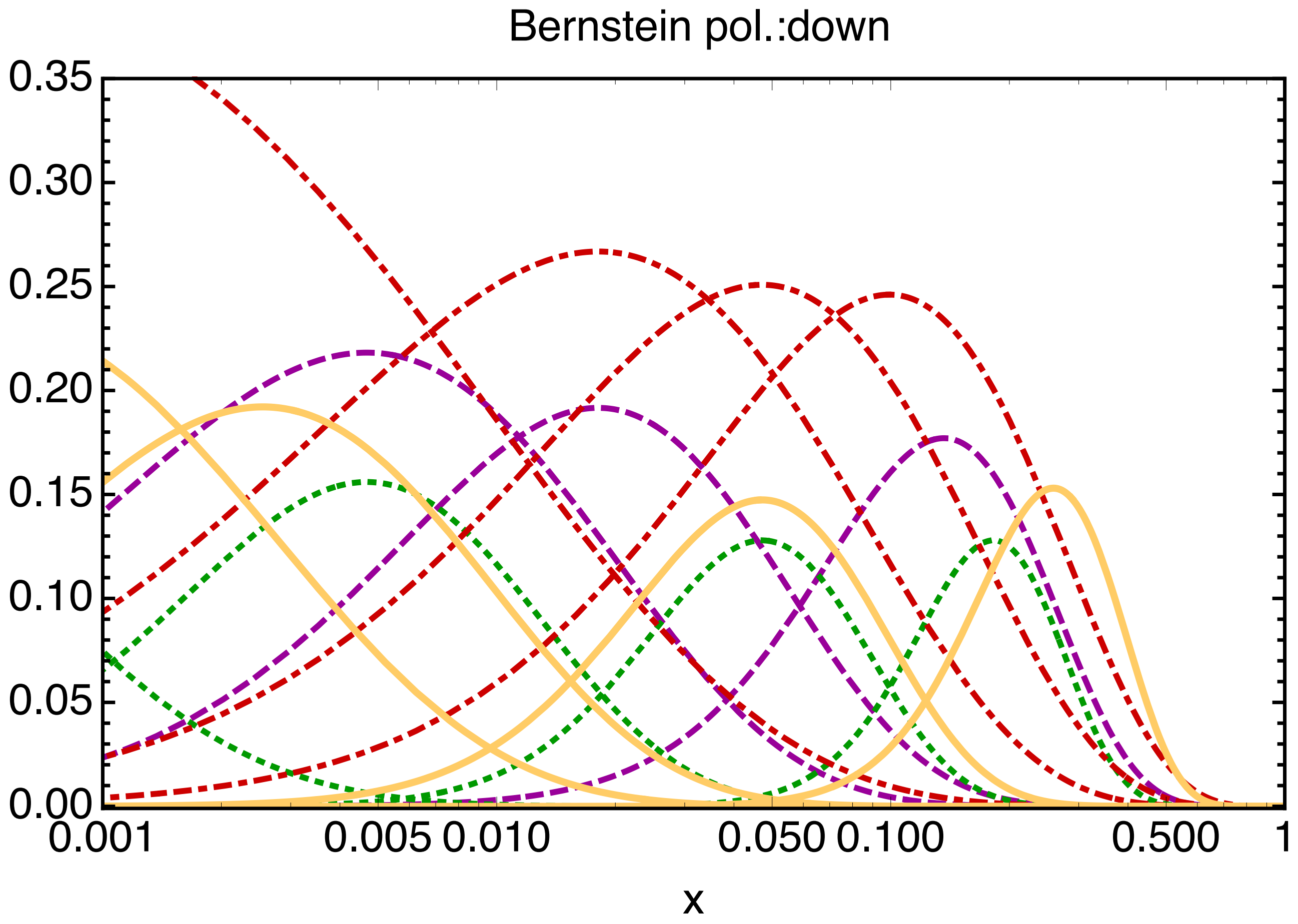


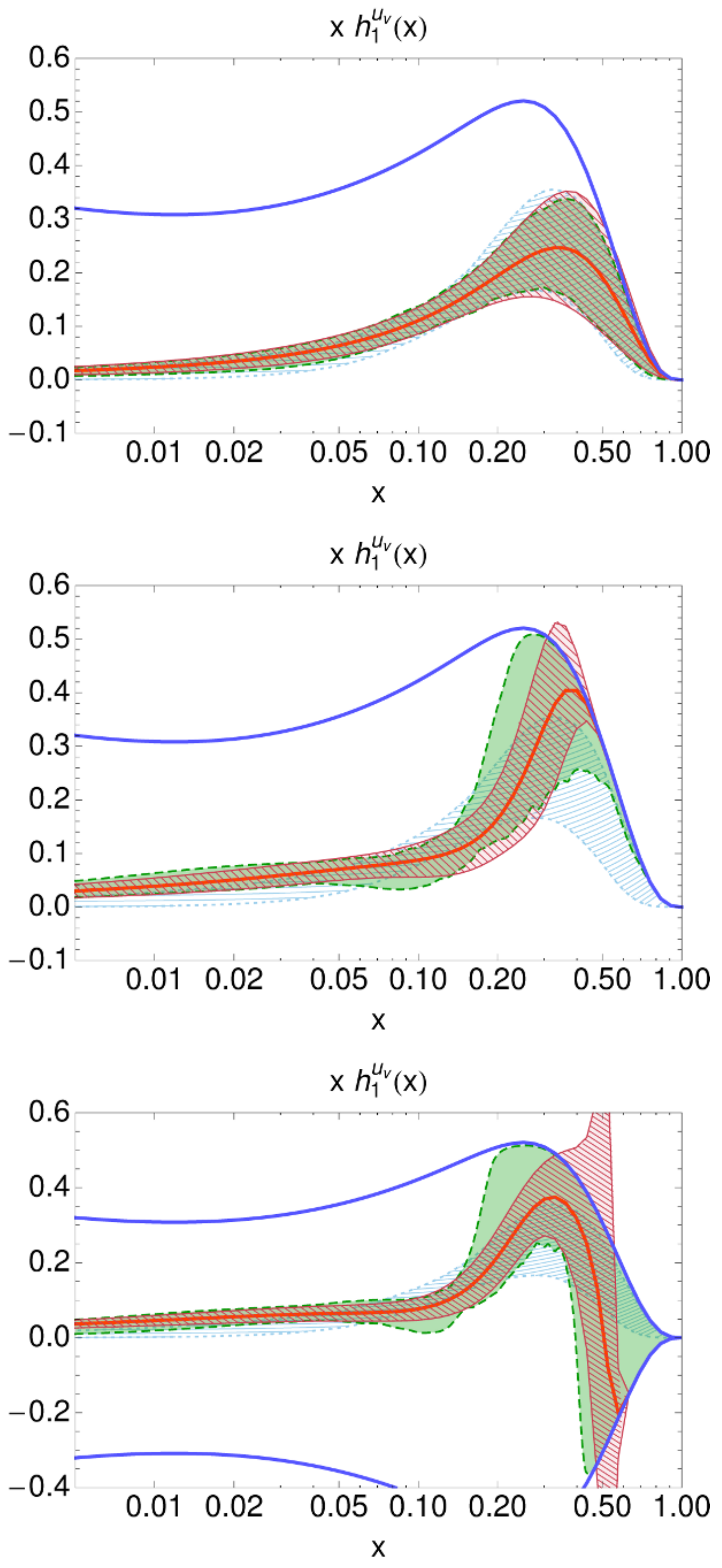
[Benel, AC & Ferro, EPJC 80 (2020)]

Mexico transversity PDF

Variation of Bernstein polynomials to span the x range.

Pavia transversity PDF

Hessian-based (with bootstrap) methodology
Variation on functional form (in early analyses).



[Bacchetta, AC & Radici, JHEP03 (2013)]

The shape of parton distributions

Low-energy QCD dynamics, encapsulated in PDFs, are learned from experimental data.

Uncertainty propagates from data and methodology to the PDF determination

I. assessment of uncertainty magnitude is key

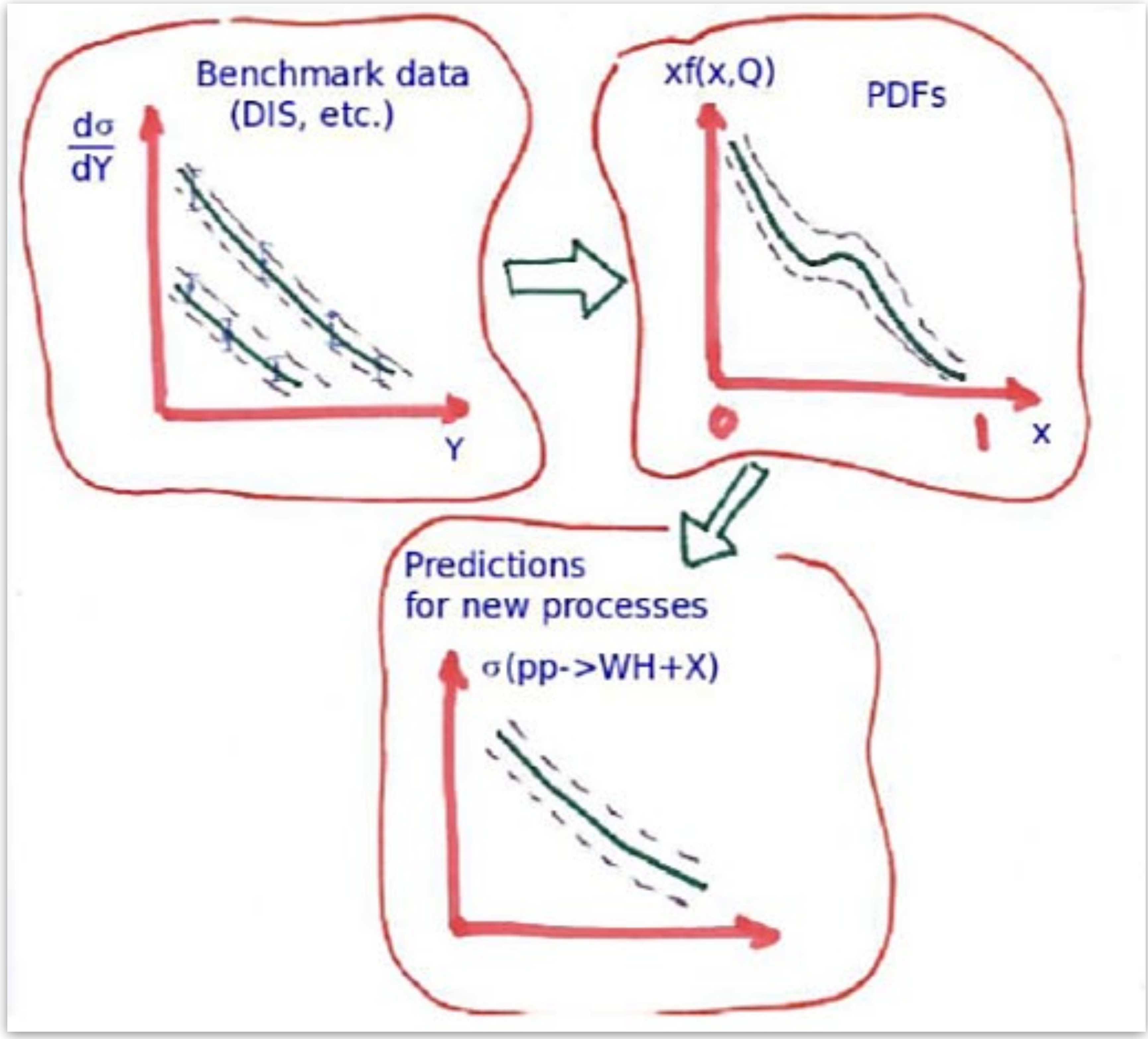
II. advanced statistical problem

III. evolving topic in the era of AI/ML

Epistemic vs. aleatory uncertainties

Uncertainty due to lack of knowledge —bias (may be reduced)

Statistical uncertainty propagated from experiments— irreducible



Hypothesis testing and parton distributions

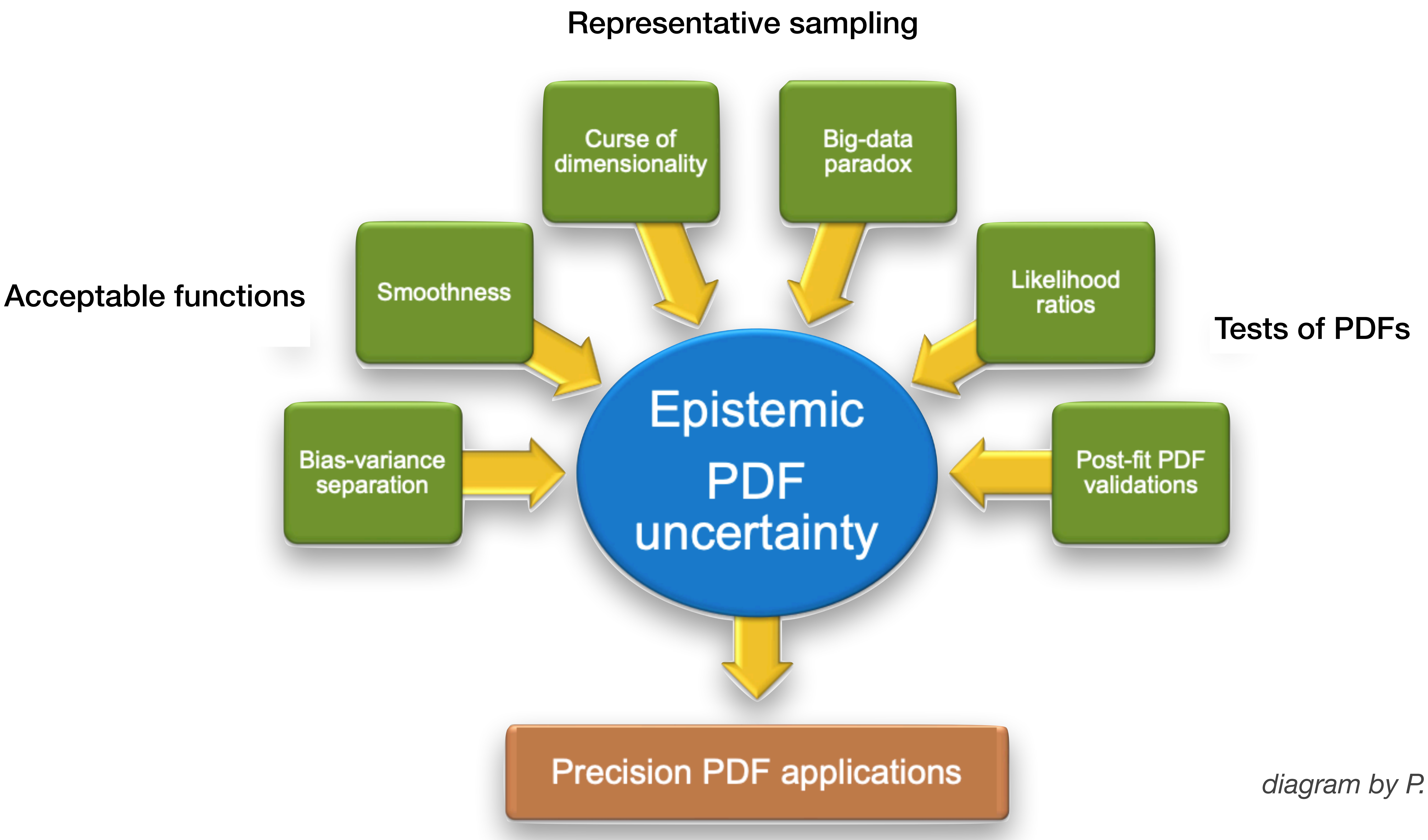


diagram by P. Nadolsky [DIS2023]

Epistemic uncertainties

How do we estimate the epistemic uncertainty of our analysis?

Global analyses in both Hessian and MC/ML approaches estimate experimental, theoretical, and epistemic uncertainties

The latter is due to methodological choices that

- can be estimated by sampling over analysis workflows, parametrization forms, analysis settings
- are associated with the prior probability

While challenging in general, such estimation is facilitated by several representative sampling techniques.

This talk focuses on sampling over parametrizations.

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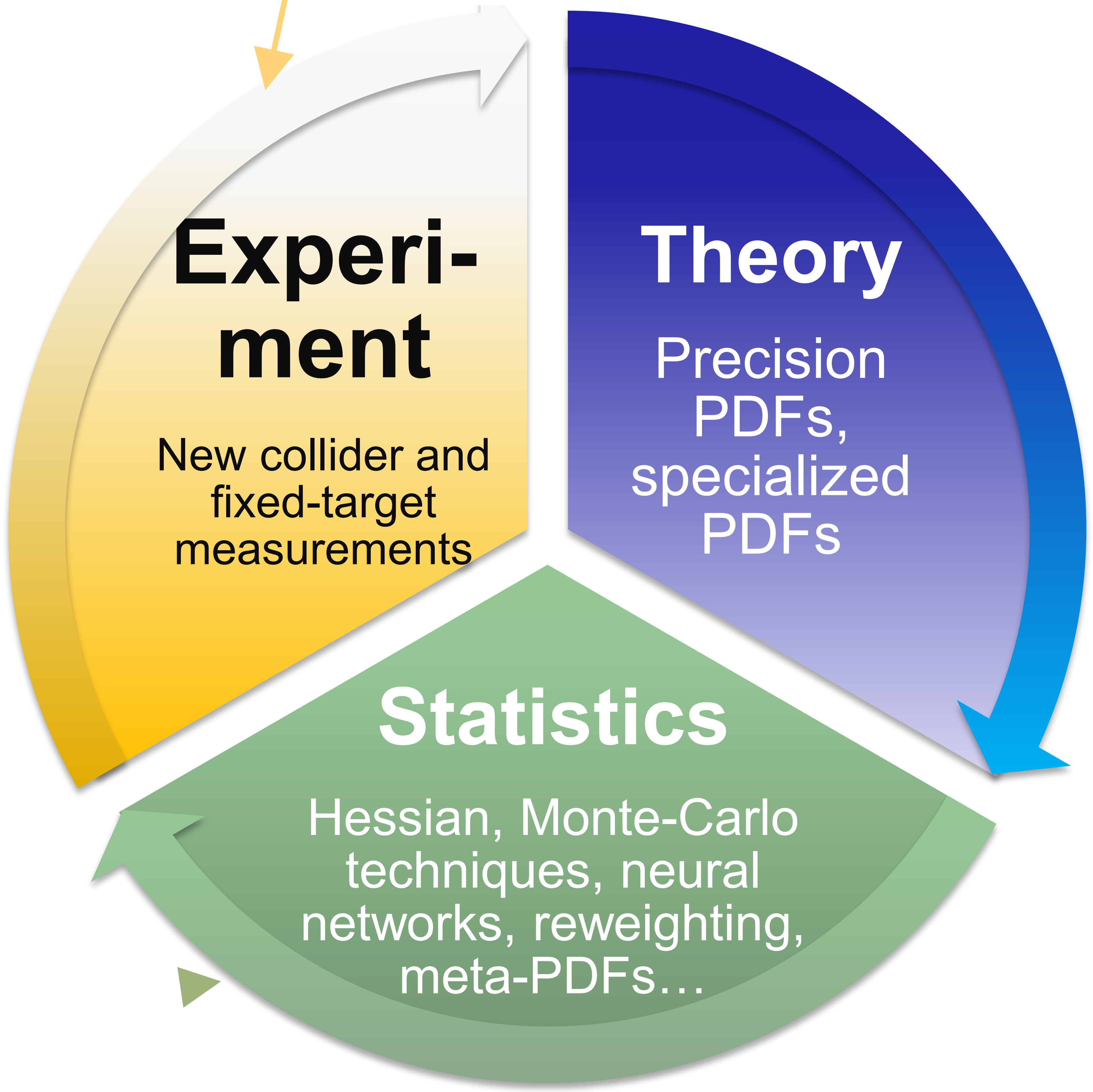

Bézier curve

Bézier curves are convenient for interpolating discrete data

The interpolation through Bézier curves is unique if the polynomial degree= (# points-1), there's a closed-form solution to the problem,

$$\mathcal{B}^{(n)}(x) = \sum_{l=0}^{n} c_l \ B_{n,l}(x)$$

with the Bernstein pol. $B_{n,l}(x) \equiv \binom{l}{n} x^l (1-x)^{n-l}.$

The Bézier curve can be expressed as a product of matrices:

- $\underline{T}$ is the vector of x^l
- $\underline{\underline{M}}$ is the matrix of binomial coefficients
- $\underline{C}$ is the vector of Bézier coefficient, c_l, to be determined

$$\mathcal{B} = \underline{T} \cdot \underline{\underline{M}} \cdot \underline{C},$$

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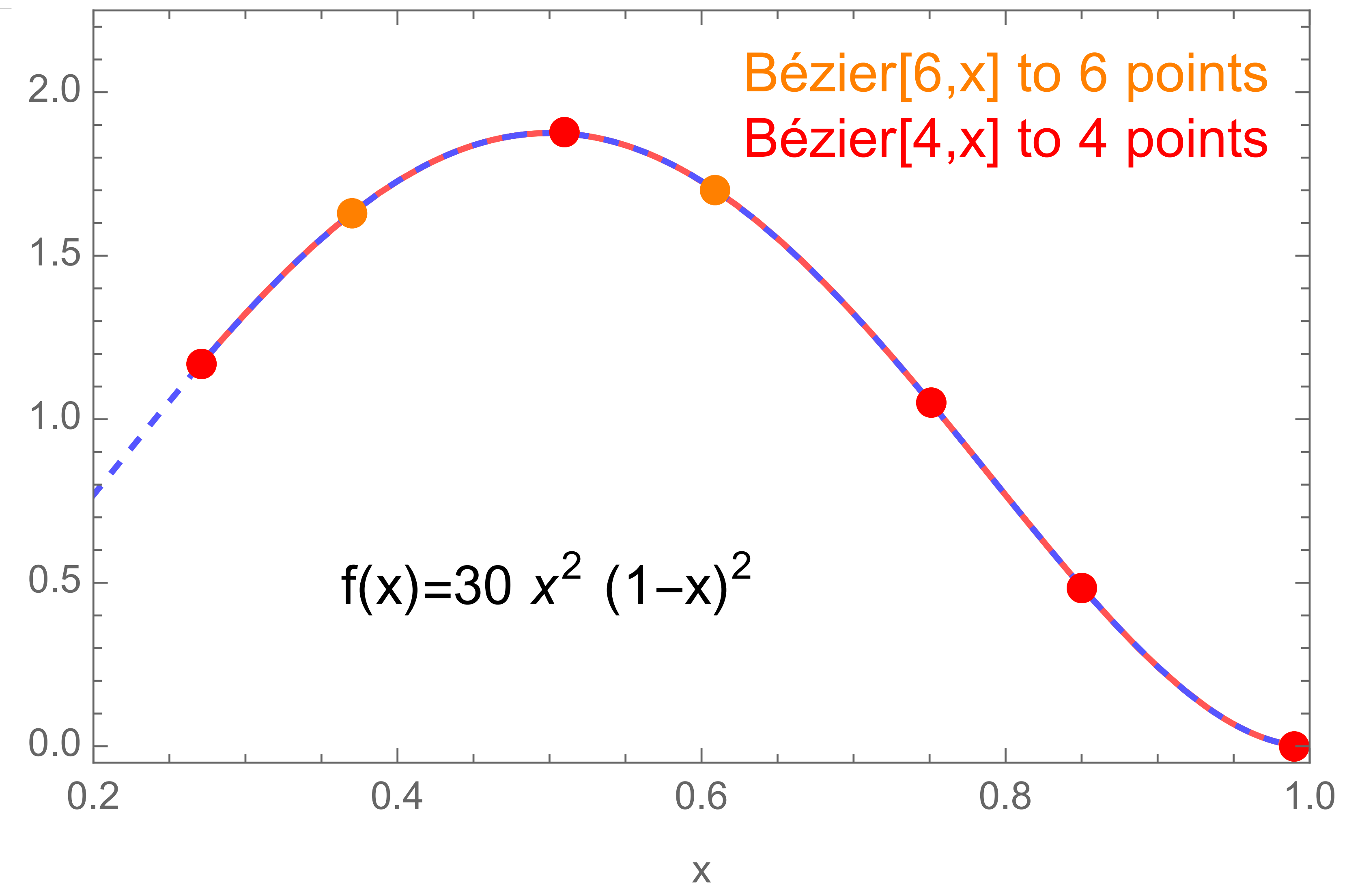
We can evaluate the Bézier curve at chosen **control points**, to get a vector of $\mathscr{B} \to \underline{P}$

$$\underline{P} = \underline{\underline{T}} \cdot \underline{\underline{M}} \cdot \underline{C}$$

$\underline{\underline{T}}$ is now a matrix of x^l expressed at the control points.

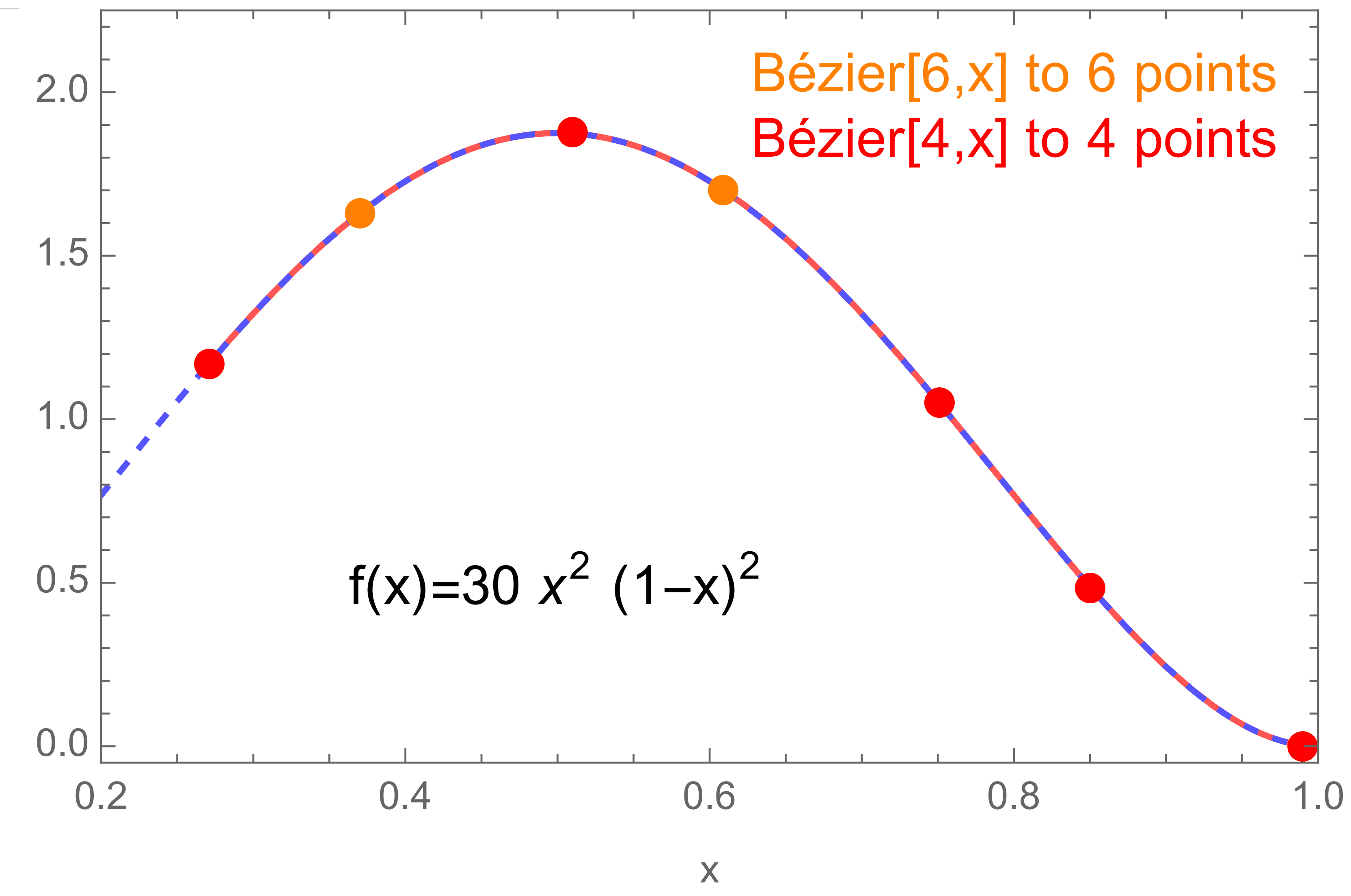
Bézier-curve methodology for global analyses



The orange/red points represent the control points, the number of which is related to the degree of the polynomial.

For simple functions, the interpolation is unique for any set of control points.

Bézier-curve methodology for global analyses



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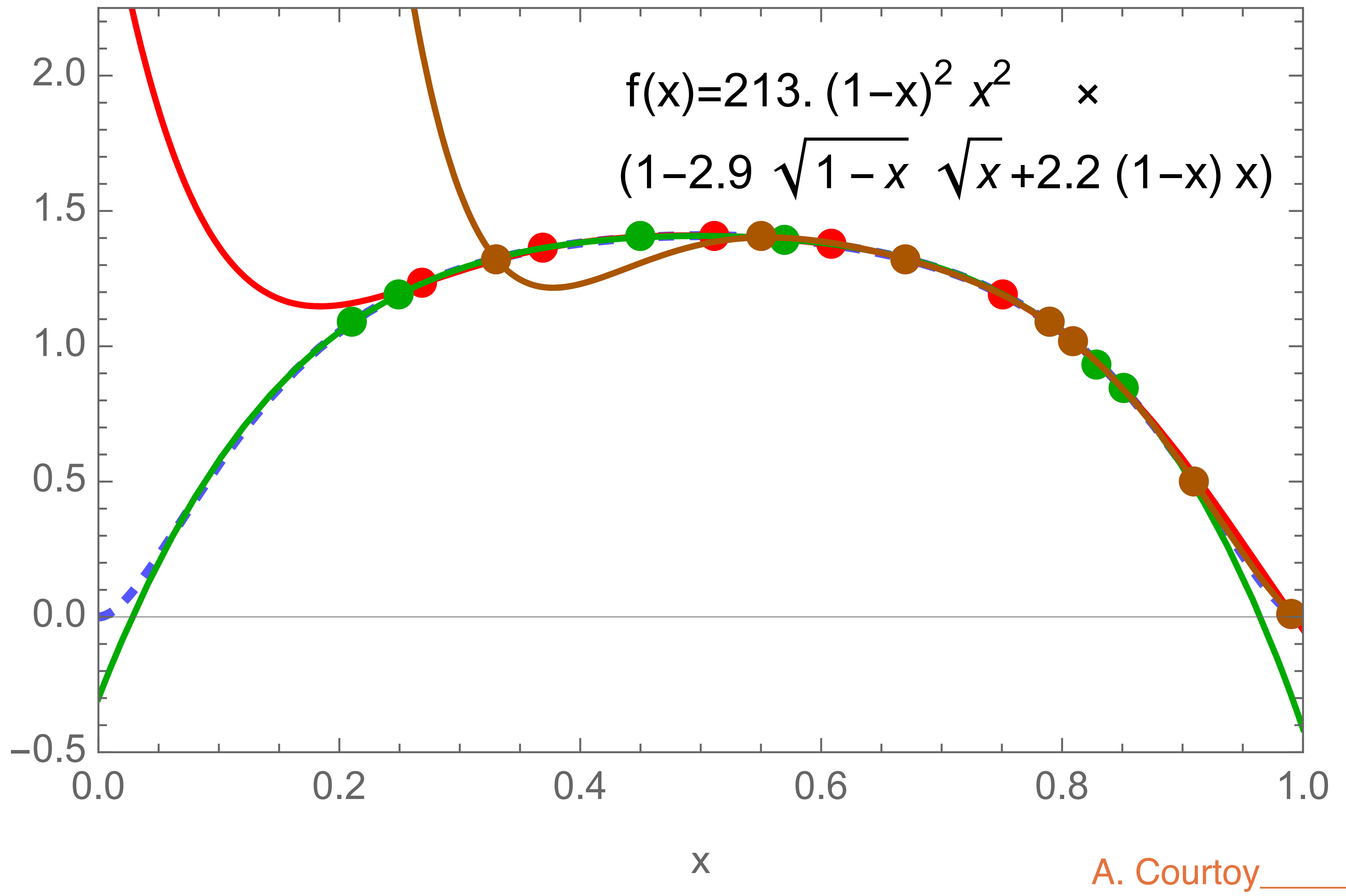


For more complex cases, the reconstructed function depends on the position and number of control points.

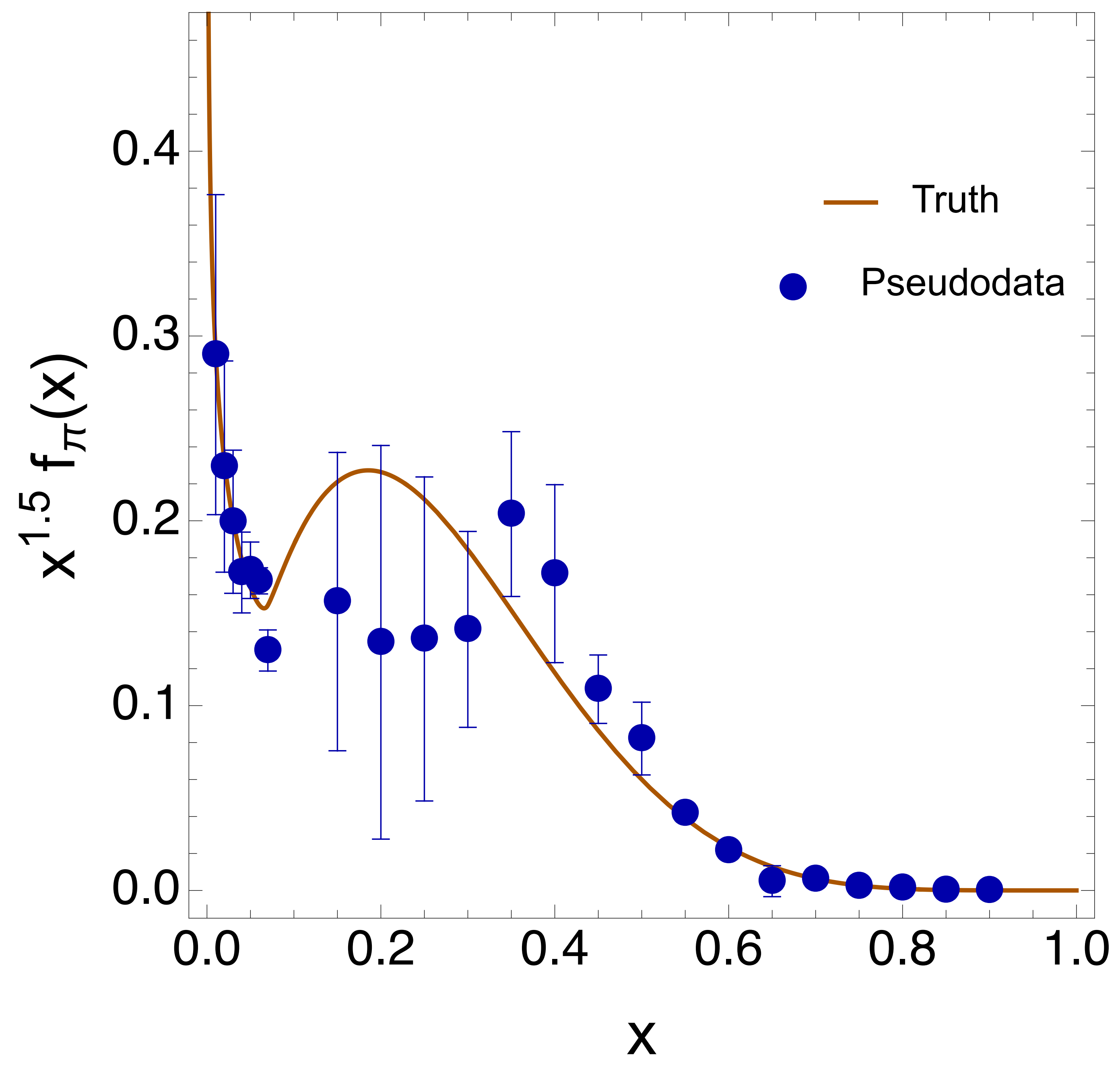
Global analyses can exploit this property to generate many functional forms.

⇒ polynomial mimicry

Bézier-curve methodology for global analyses — toy model

Fantômas4QCD program

➪ $\mathscr{B}$ can modulate the PDFs in flexible ways at intermediate x using a set of free and fixed control points



$$x\, q(x, Q_0^2) = A'_q\, x^{B_q} (1-x)^{C_q} \times \left(1 + \mathcal{B}^{(N_m)}(x^{\alpha_x}, Q_0^2; \underline{v})\right)$$

with $\underline{v} = \{\underline{C}, \underline{P}\}$

$$\underline{P} = \underline{\underline{T}} \cdot \underline{\underline{M}} \cdot \underline{C}$$

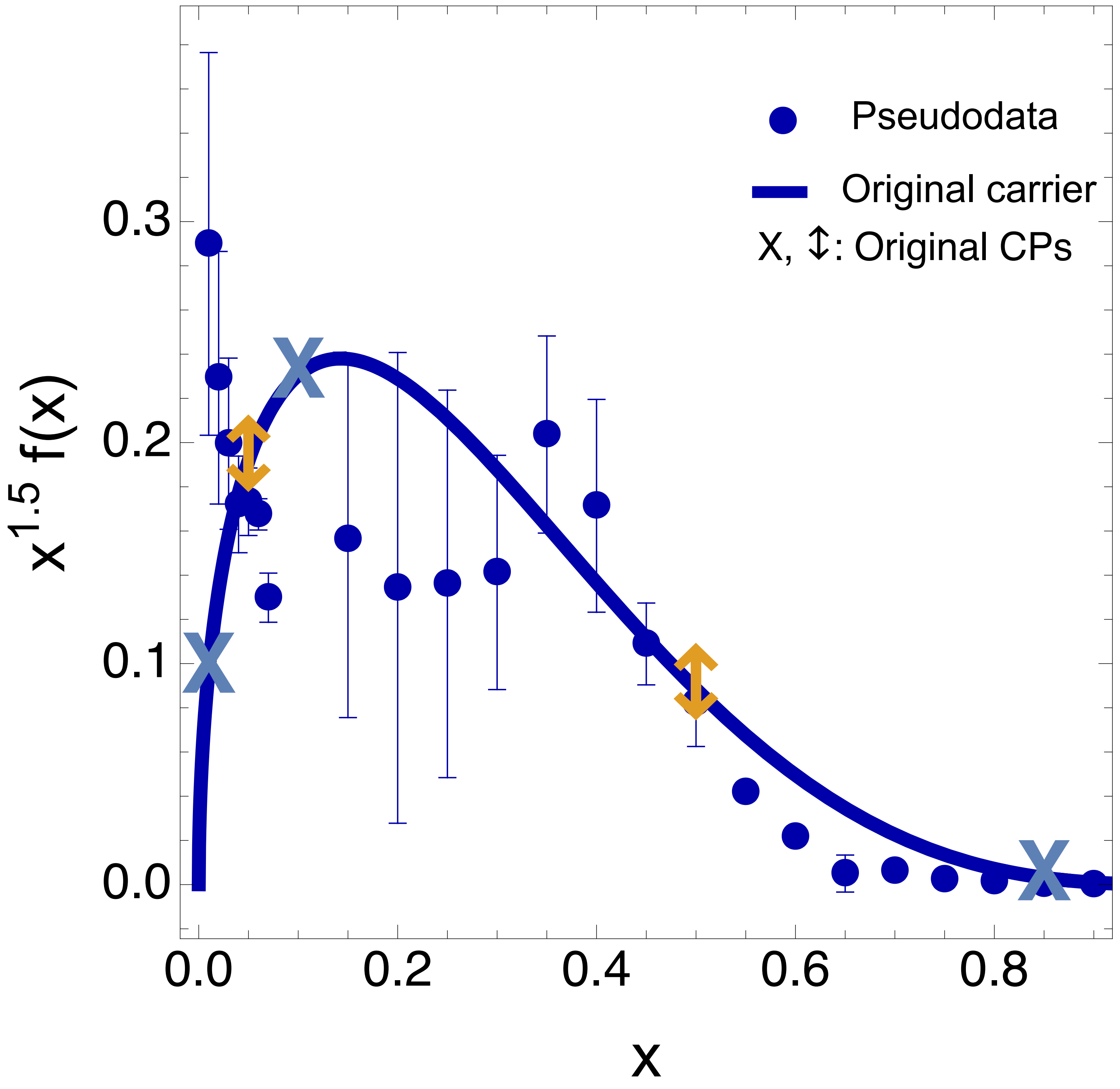
Classical fit: determines the vector $\underline{C}$

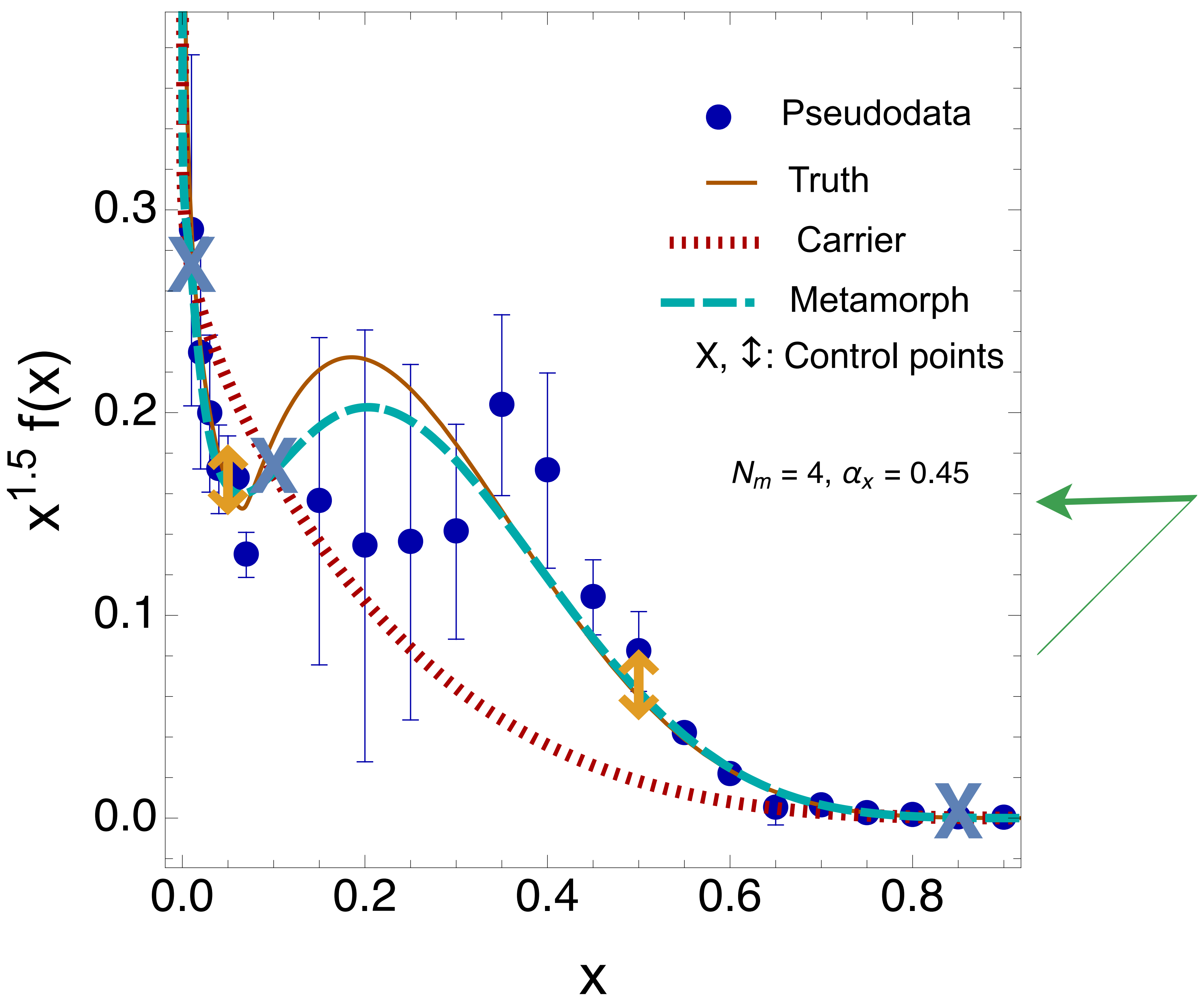
`metamorph` fit: determines the vector $\underline{P}$

➤ We parametrize the Bézier coefficients as the shifts of the position of the **control points:**

$$P_i = \mathcal{B}(x_i) \to P'_i = \mathcal{B}(x_i) + \delta\mathcal{B}(x_i)$$

Bézier-curve methodology for global analyses — toy model





Shift of the control points $(\delta D_q, \ldots)$ replace free parameters

N_m= degree of polynomial can vary

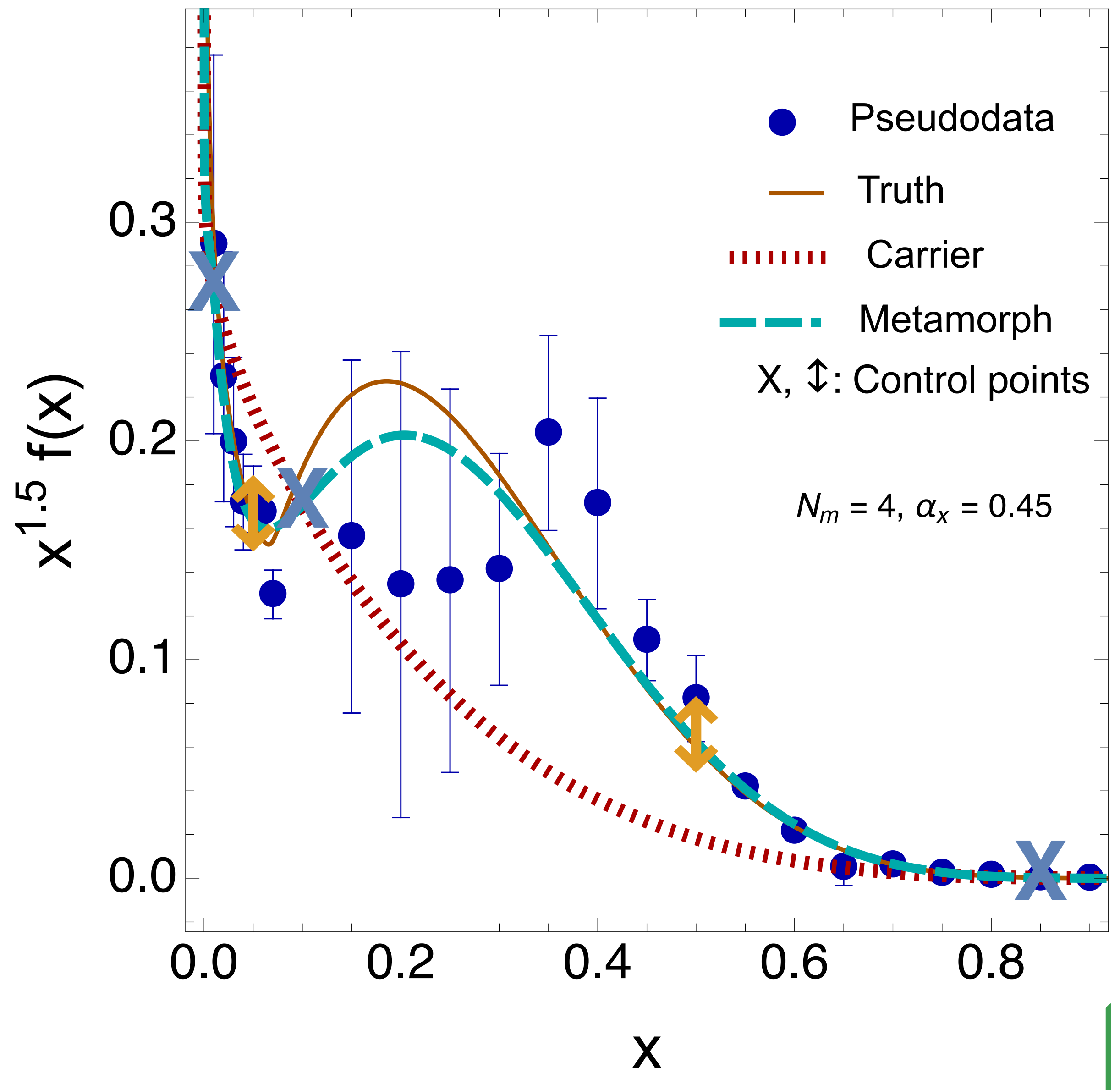
$\delta B_q \,\&\, \delta C_q$ allow the carrier to vary

α_x can vary

`metamorph` fit:

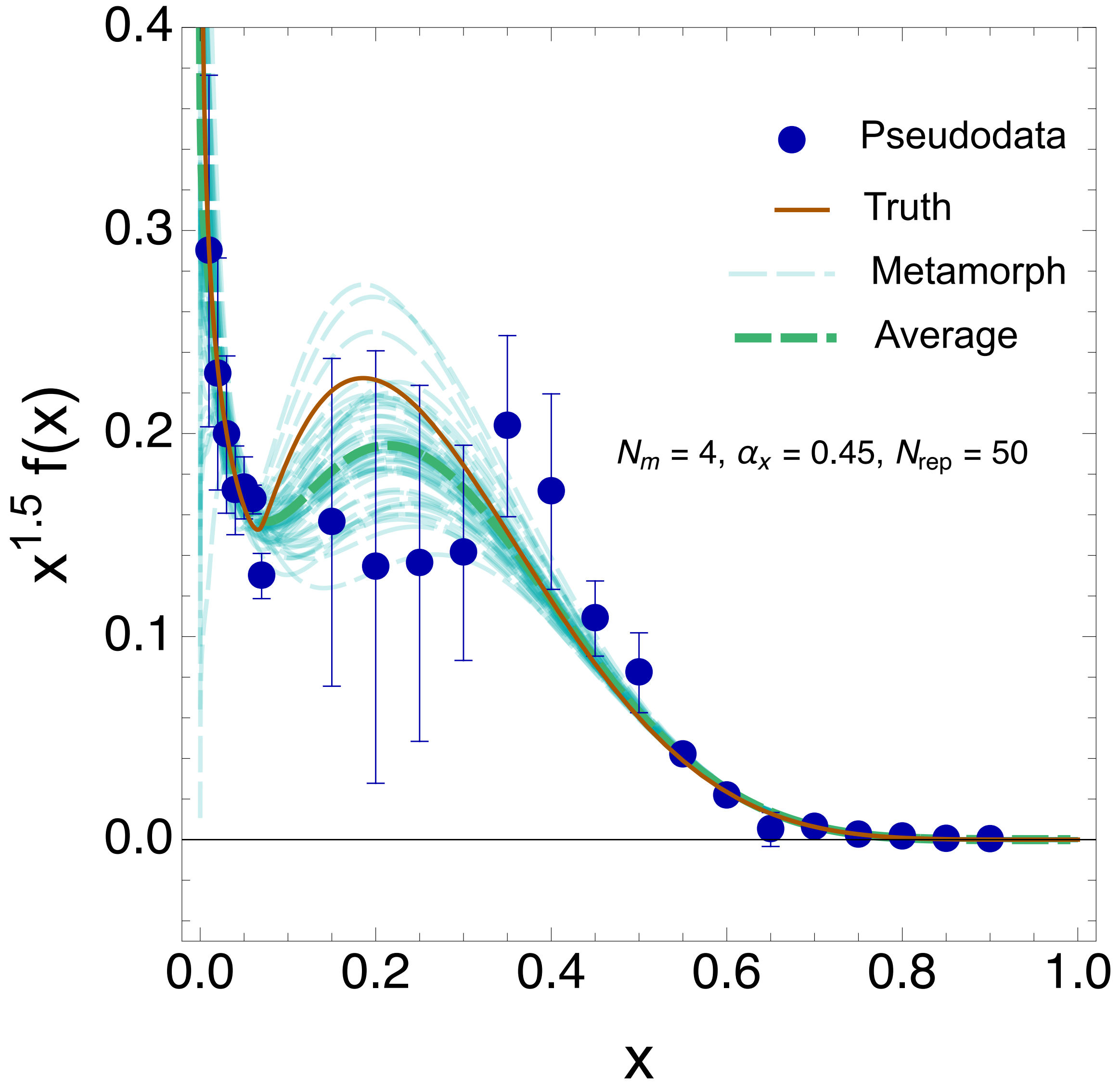
$$x\, q(x, Q_0^2) = A'_q\, x^{B_q} (1-x)^{C_q} \times \left(1 + \mathcal{B}^{(N_m)}(x^{\alpha_x}, Q_0^2; \underline{v})\right)$$

Bézier-curve methodology for global analyses — toy model



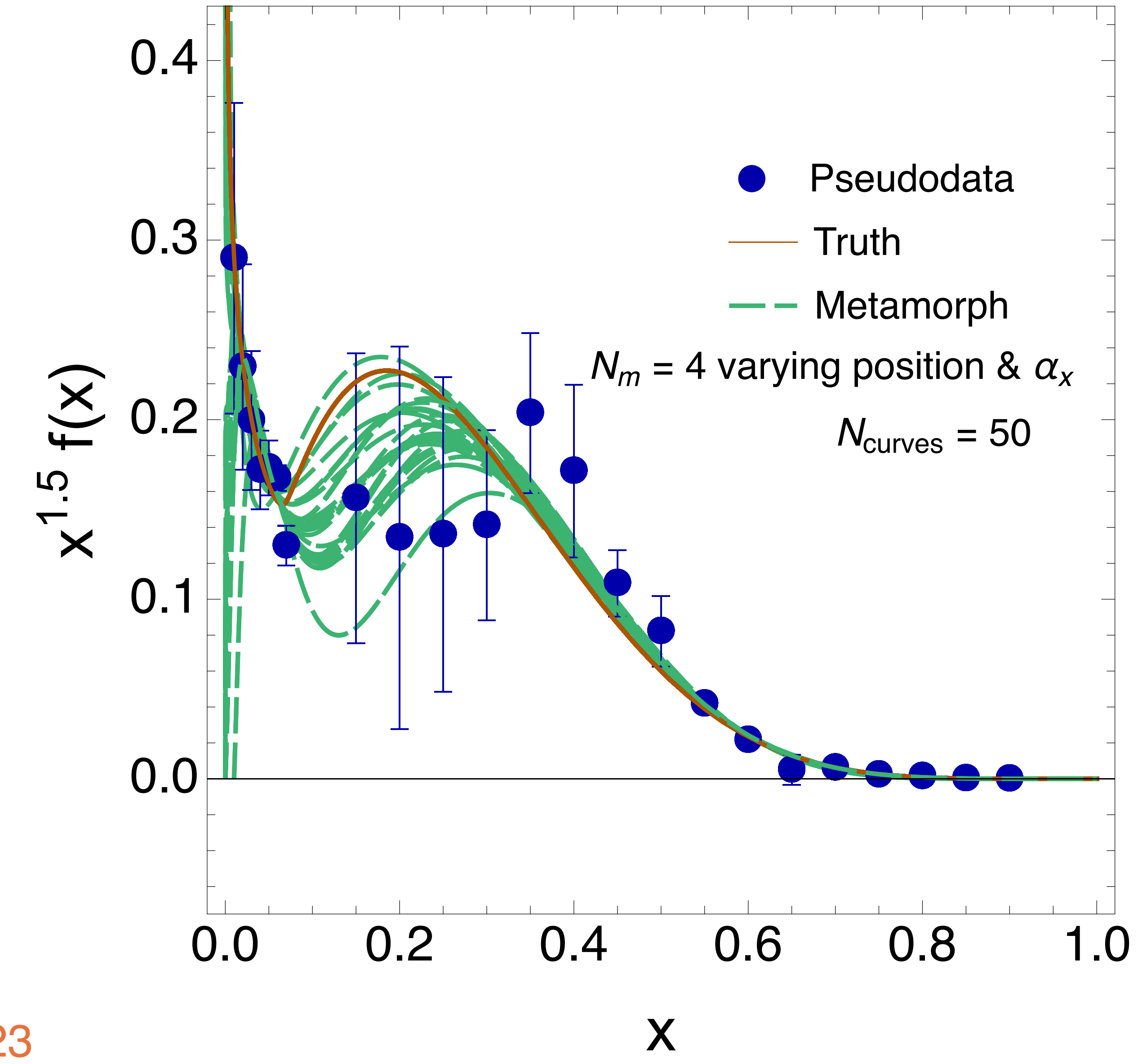
if bootstrapped

sampling on the distribution of data uncertainties



if sampled over `metamorph` settings

sampling over parametrizations



Both samplings can be done in the same analysis, they are not mutually exclusive.

metamorph routine in xFitter

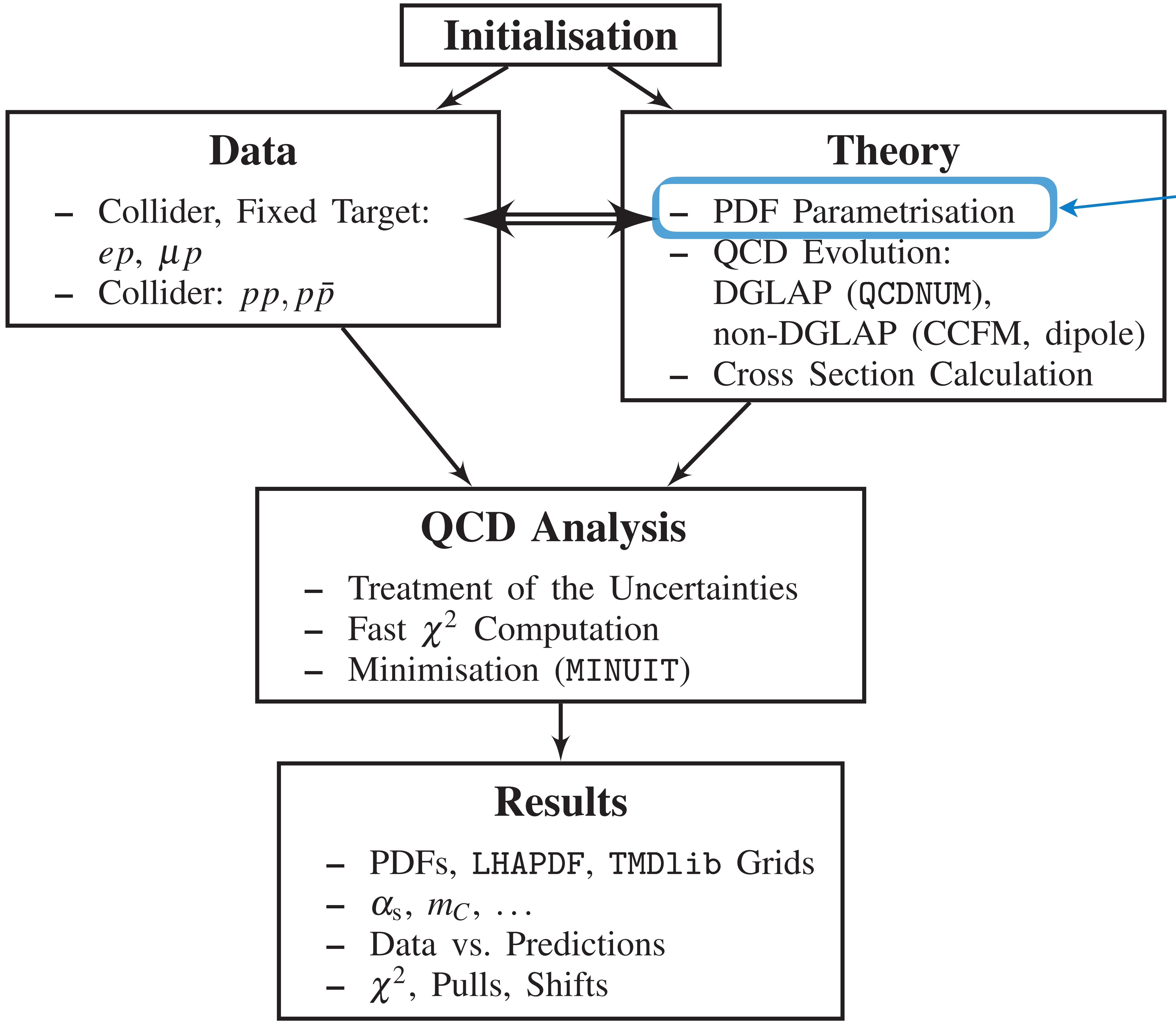


Figure 1: Schematic structure of the xFitter program.

metamorph requires inputs from the user:

- N_m — degree of polynomial
- $\{x, f_{\text{in}}(x)\}$ of control points
- fixed or free control points
- stretching parameter

First application of Fantômas: pion PDF

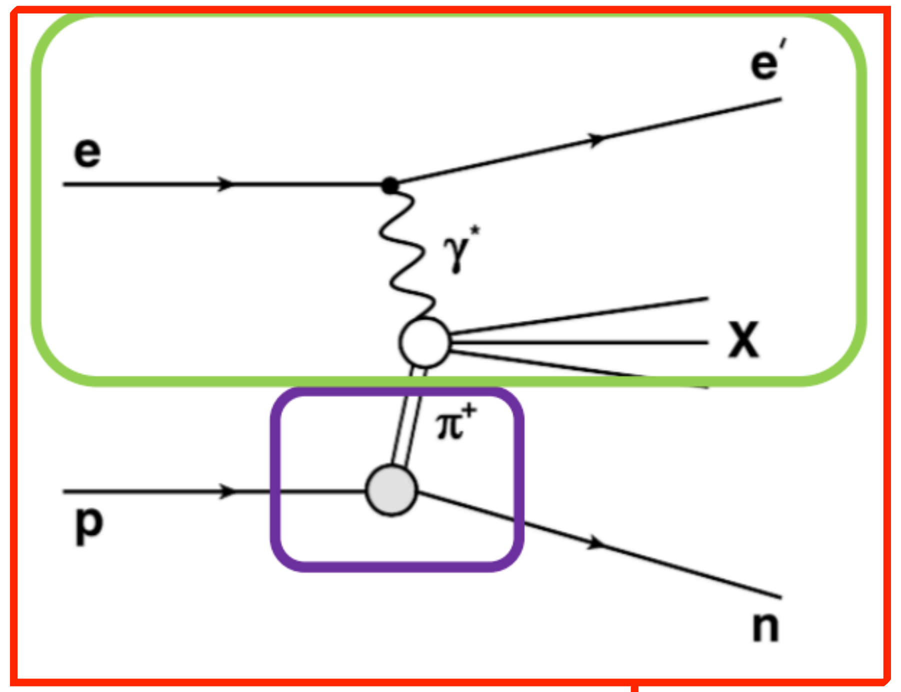
Previous pion analyses:

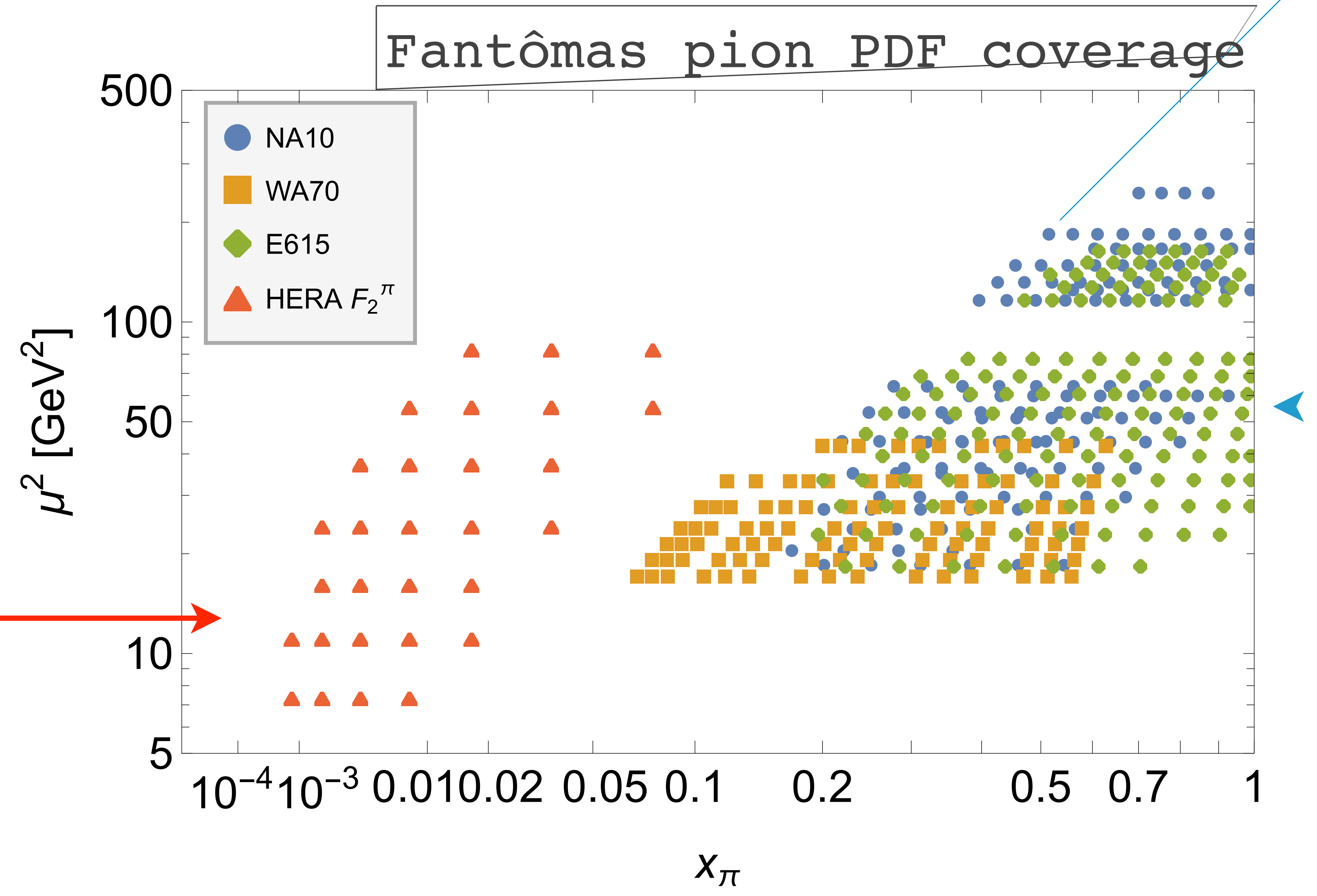
xFitter [*PRD* 102 (2020)]
JAM [PRL 121 (2018), *PRD* 103, *PRL* 127 (2021)]

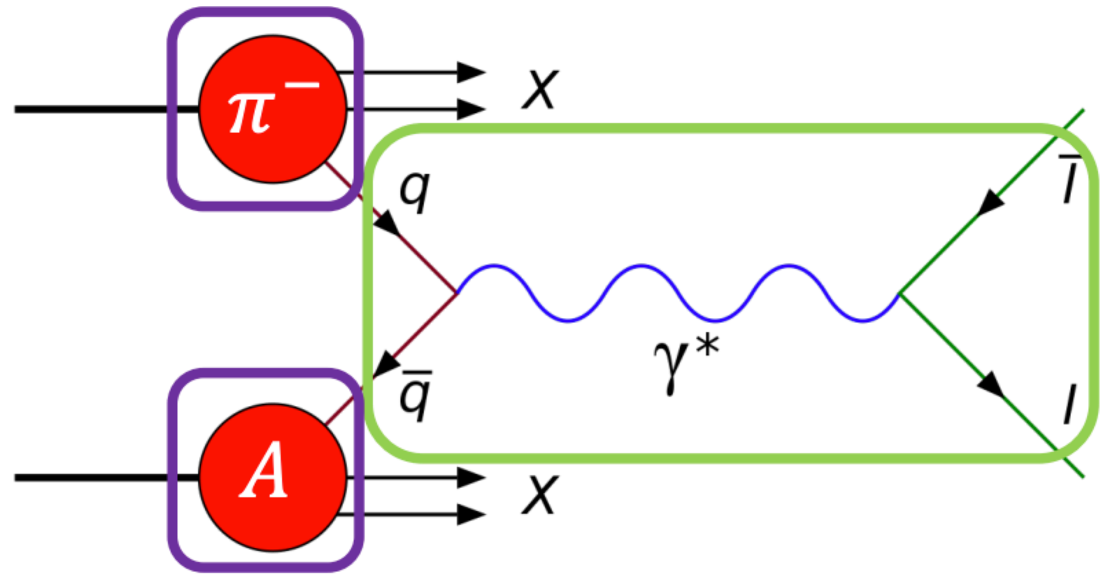
Pion PDF now accessible through more experiments as well as through lattice QCD studies — exciting playground!

We use the xFitter framework, in which `metamorph` was implemented as an independent parametrization.

We also extend the xFitter data by adding leading neutron (Sullivan process) data.







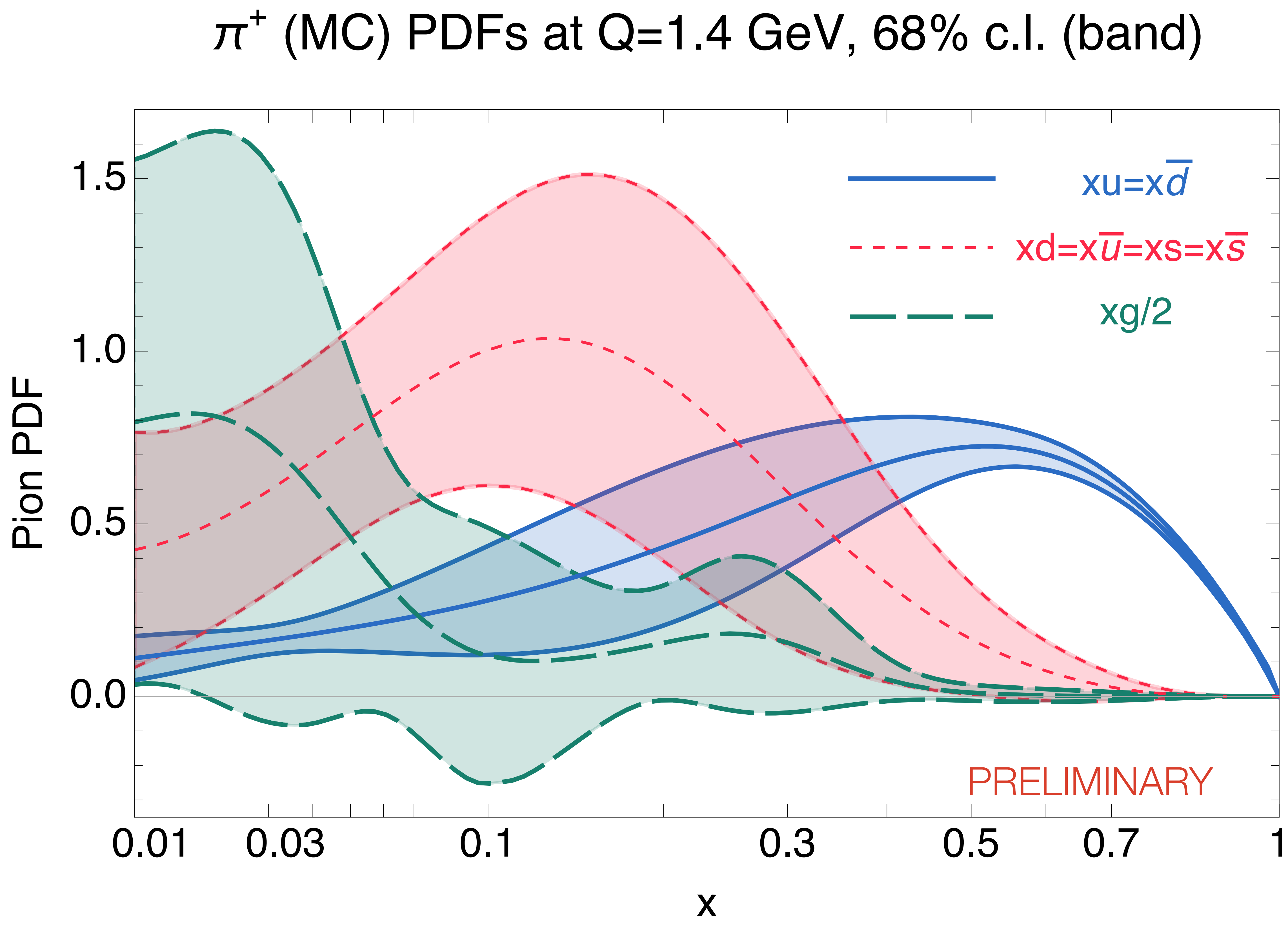
Diagrams from P. Barry

The Fantômas pion PDFs

[Kotz, Ponce-Chávez, AC, Nadolsky & Olness]
Proceedings in 2309.00152.

First physics use of the Fantômas framework:

- We generated $N \sim 100$ fits corresponding to N sets for $\{N_m, \underline{P}, \alpha_x\}$.
- Well-behaved (convergence + soft constraints) fits are kept.
- Fits within $\chi^2 + \delta\chi^2 = \chi^2 + \sqrt{2(N_{\mathrm{pts}} - N_{\mathrm{par}})}$ are kept.
- The final bundle is generated from the 5 most diverse shapes at Q_0.
- Bundled uncertainty with `mcgen` [Gao & Nadolsky, JHEP07]



The Fantômas pion PDFs

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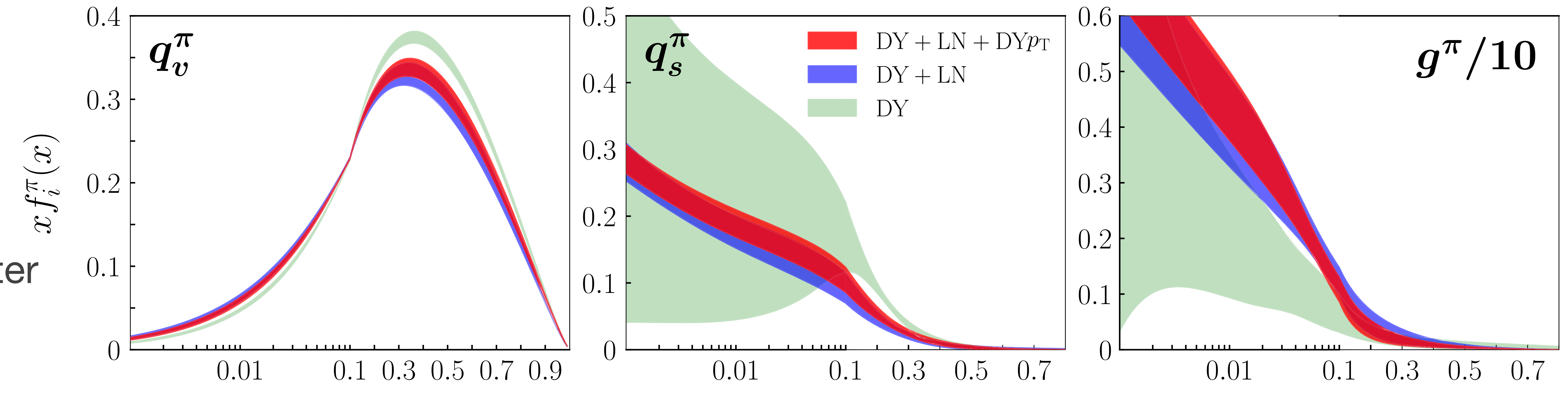
PRELIMINARY

Comparison of methodologies:

bootstrap+ IMC vs. `metamorph` parametrization in xFitter

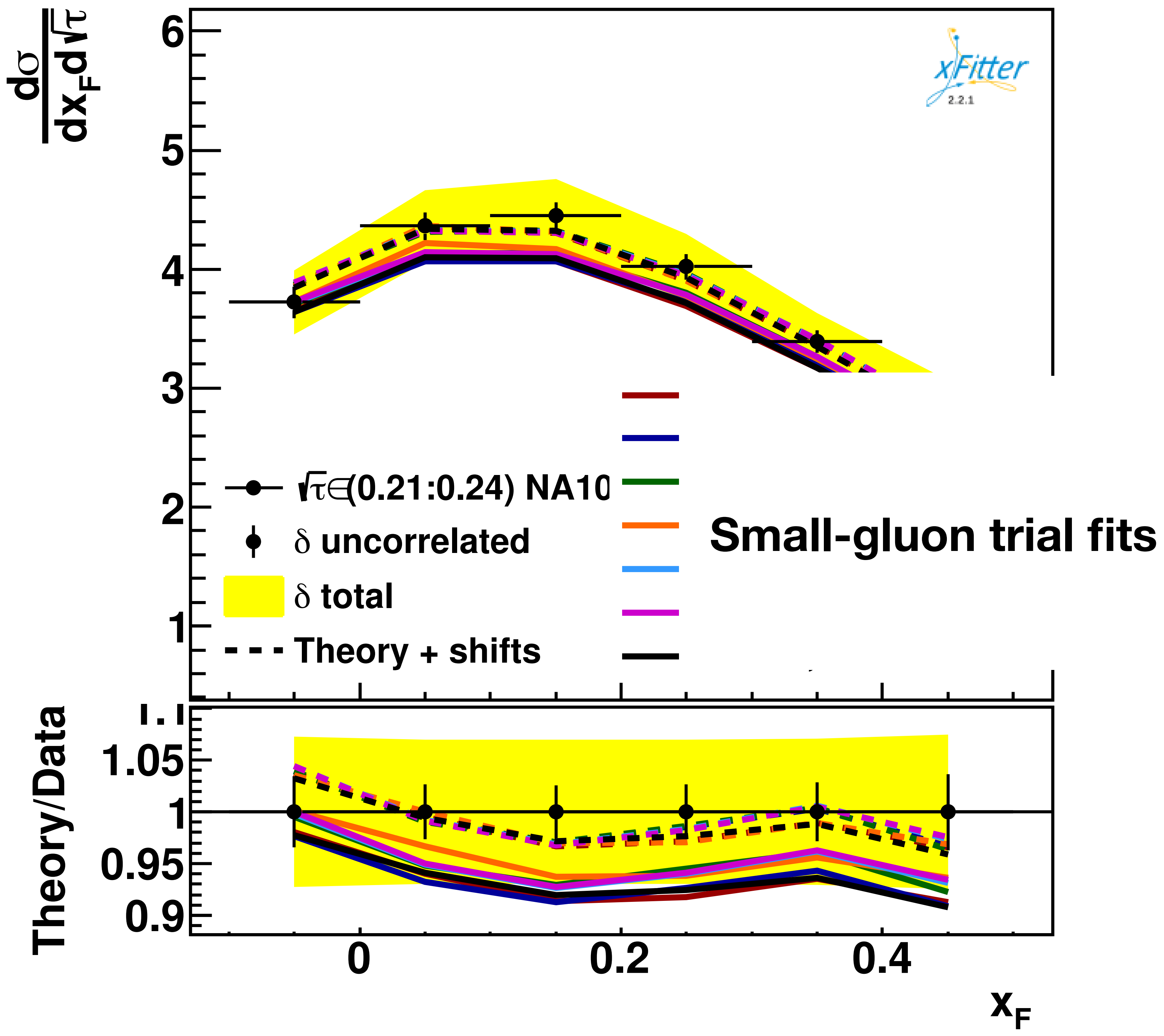


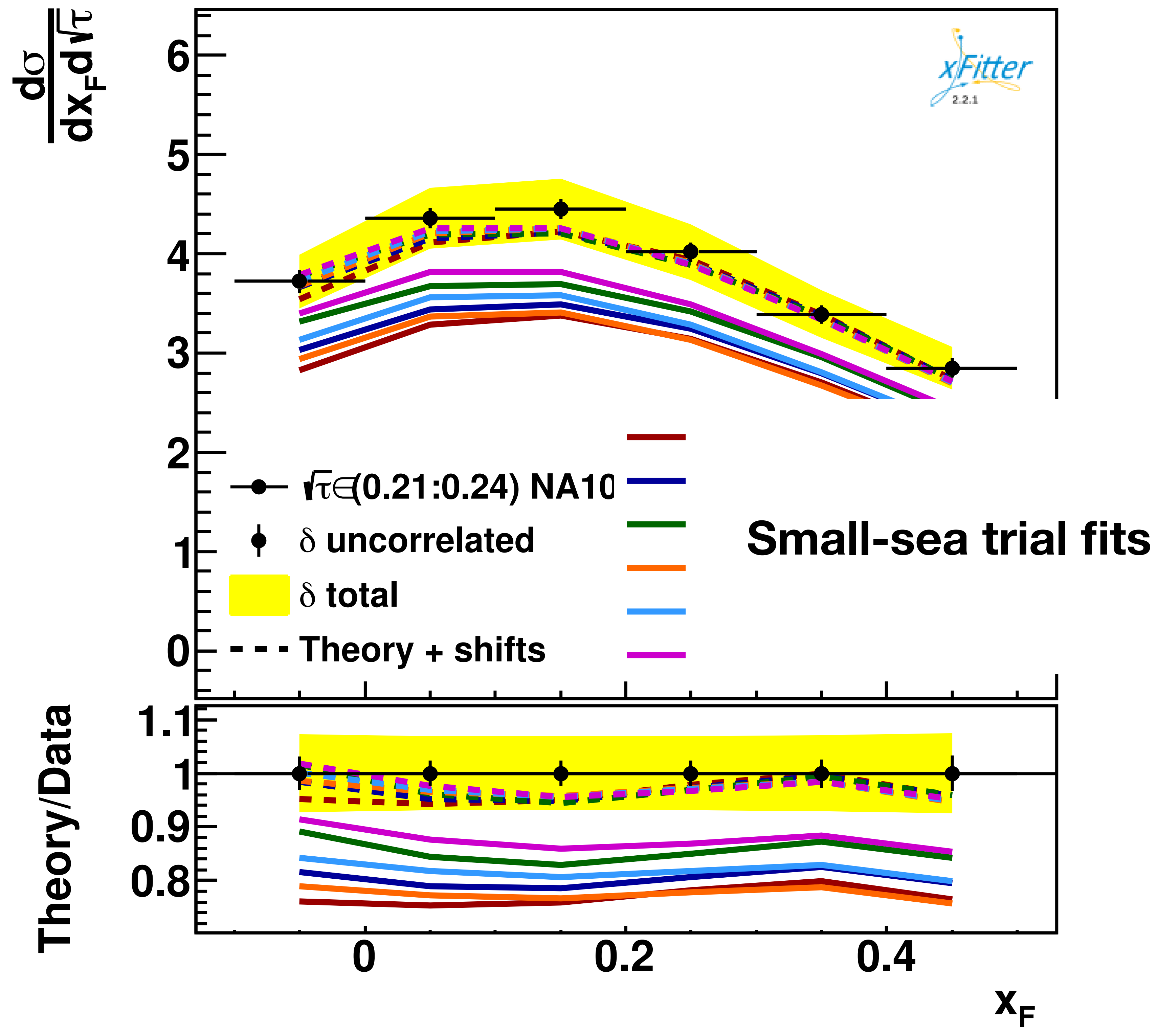
JAM [Phys.Rev.D103]

Sea and gluon behavior

Data sets vary between JAM and Fantômas: higher number of NA10 data points for us.

We explored small gluon and small sea scenarios: at small $\sqrt{\tau}$, zero-gluon solutions are allowed; zero-sea are unfavored.

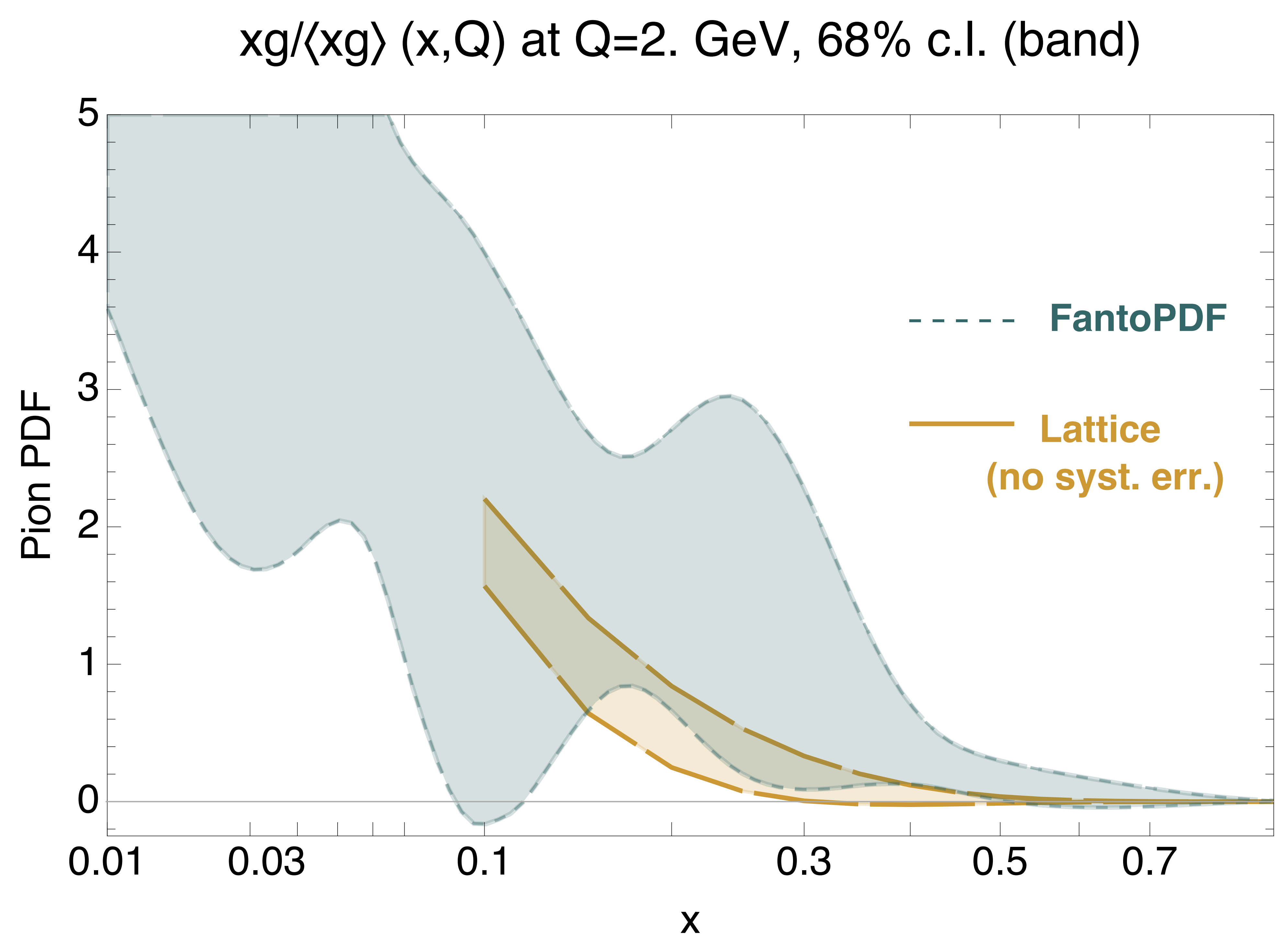


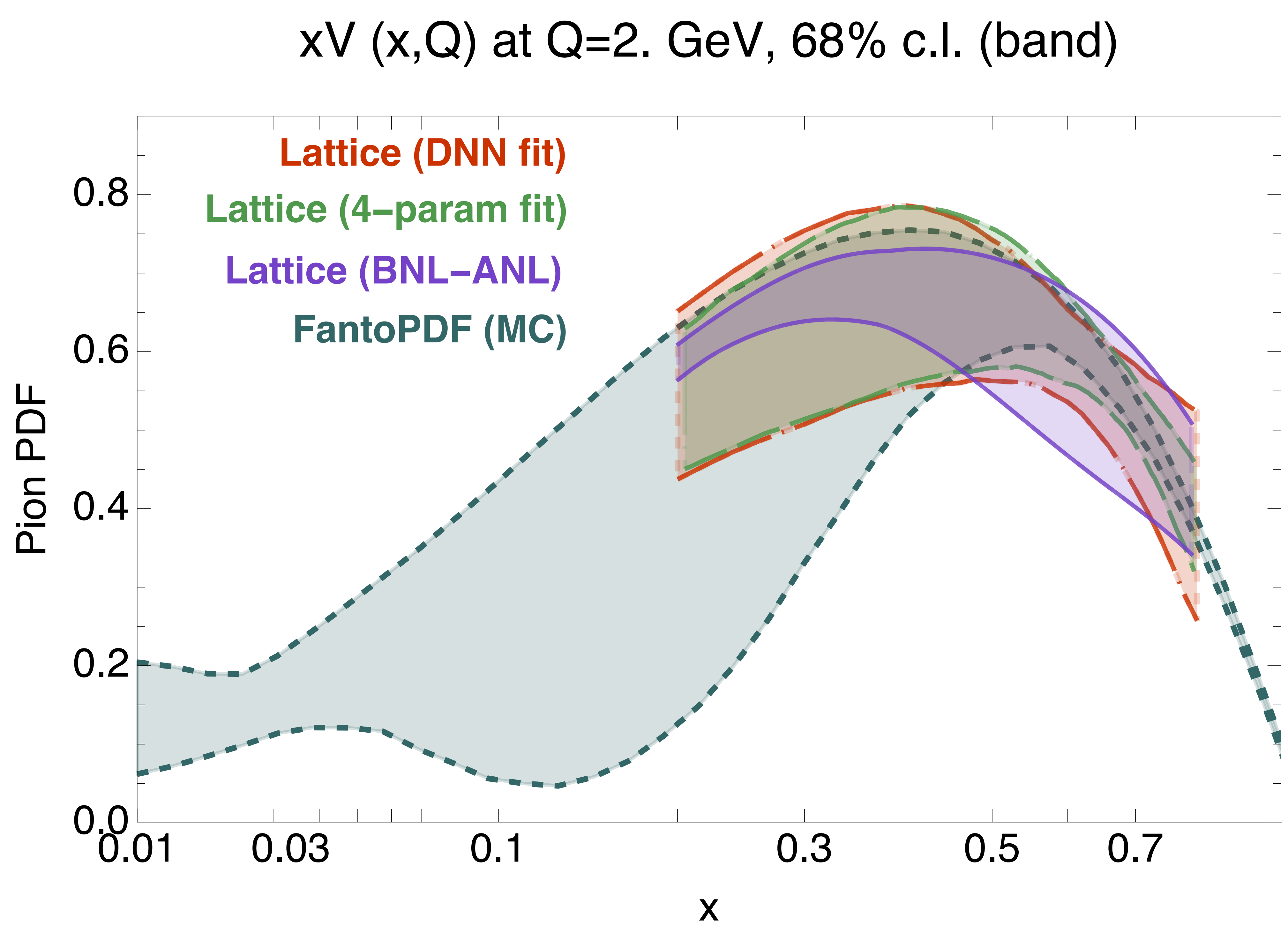


Pion PDF compared with lattice QCD results

Gluon shape averaged to momentum fraction given by
[Fan & Lin, PLB 823 (2021)]

Valence pion PDF compared to lattice results from
[X. Gao, PRL128 & PRD106]





Further motivation for pion PDFs in phenomenology

⇨ Hypothesis testing for functional behavior constraints — *do PDFs fall off like* $(1-x)^\beta$*?*

Quark-counting rules:

Early-QCD predicted behavior for structure functions when one quark carries almost all the momentum fraction

$$f_{q_v/P}(x) \xrightarrow[x\to 1]{} (1-x)^3, \qquad f_{q_v/\pi}(x) \xrightarrow[x\to 1]{} (1-x)^2$$

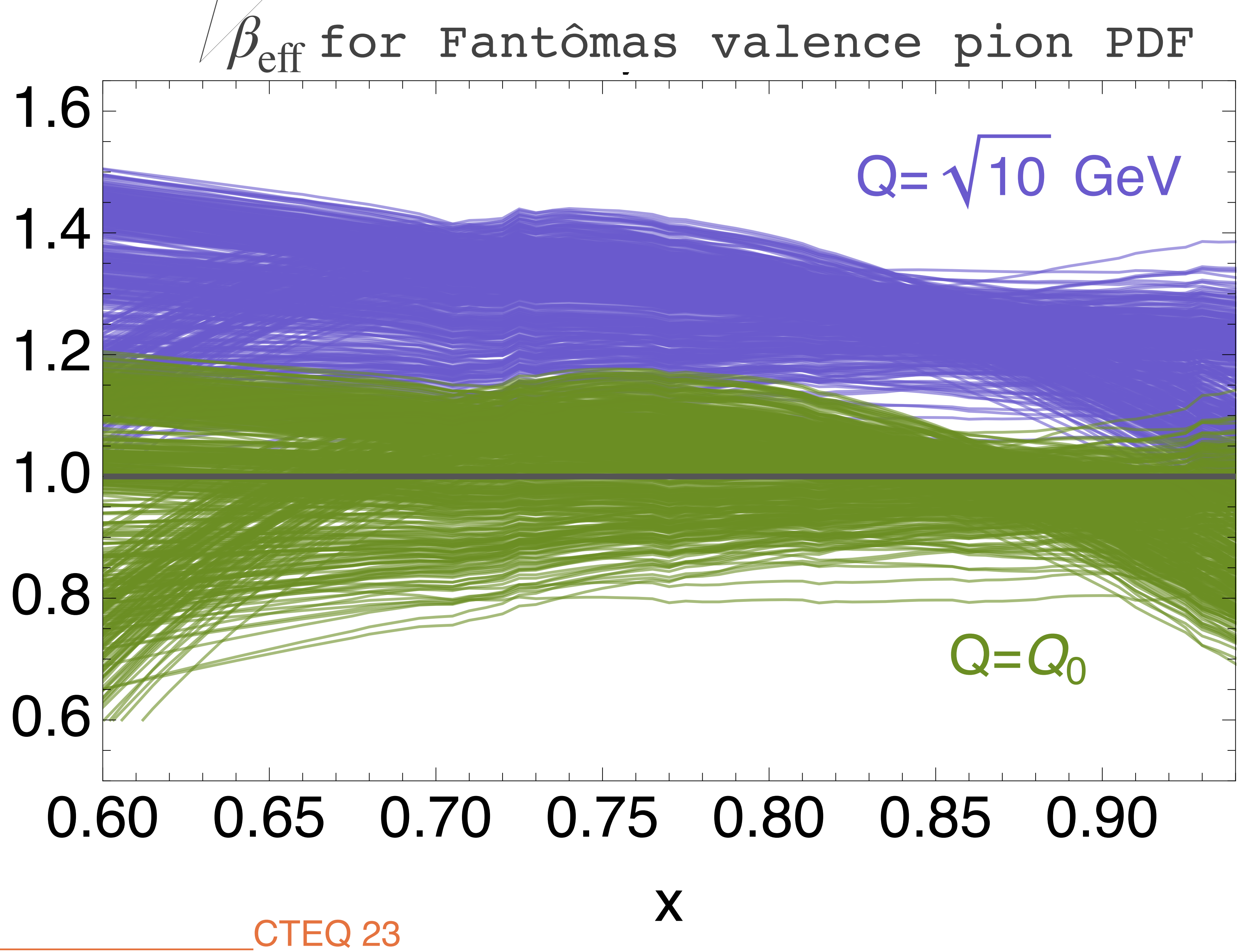
At NLO (MSbar), the valence PDF is well determined at large x

⇨ doesn't fall very much like $(1-x)^2$

⇨ very similar to JAM and xFitter at large x

This result can be understood through non-perturbative QCD corrections as well aspolynomial mimicry.

[2011.10078]



Momentum fractions

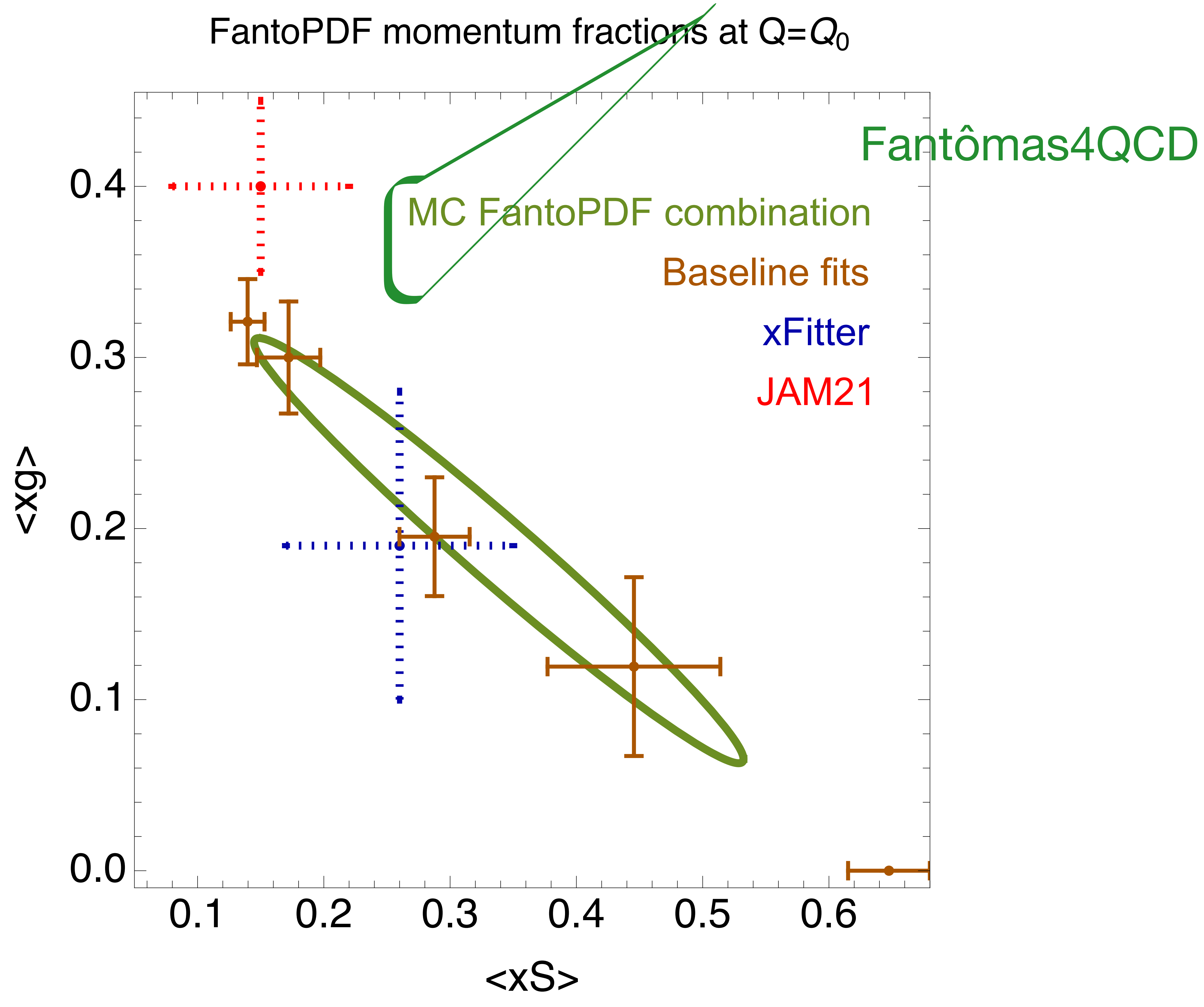
As it turns out, the valence sector was not as exciting as expected — sea and gluon separation got most of our attention!

The addition of leading-neutron data does not dramatically change the momentum fractions once the uncertainty appropriately include representative sampling.

Increased uncertainty on all three $\langle xf_q \rangle$.

Lattice estimates for $\langle xf_g \rangle$ vary in a non-negligible way!

Valence fraction $\langle xf_v \rangle (Q = \sqrt{1.9}\ \mathrm{GeV}) = 0.48(8)$
—compatible with theoretically calculated momentum fractions.



The Fantômas pion PDF

First analysis within the Fantômas framework!

Pion PDFs with representative sampling over the space of solutions — here, parametrization is extended.

Not included (for now): uncertainties from scale dependence, nuclear PDF set, threshold resummation.

Towards epistemic uncertainty: sampling over parameter space more representative

Fantômas to be used for proton PDFs in the future, extending CT's use of Bernstein basis.

A variety of applications of our routine are possible — some settings are still being studied by the FantoTeam

Fantômas will be included in the original xFitter framework

xFitter

Once the code will be released, everyone will be vert welcome to use it and/or collaborate on it.

Conclusions

- Uncertainties come from various sources in global analyses.
  Extension to sampling accuracy, here sampling occurs over parametrization forms.

- Rôle of the parametrization in the sampling accuracy: we make use of Bézier-curve methodology

  Fantômas4QCD framework *[to appear very soon]*
  metamorph can be used to study many functions

  Reliable uncertainty on the pion PDF analysis (to NLO)
  re: larger where no data constrains $q^{\pi}(x, Q^2)$

  - Sea-gluon separation requires more data — a very interesting sector!
  - End-point behavior of valence pion distributions seems to follow a $(1-x)$ fall-off.

- Fantômas code can be used in inverse problems for other correlation functions — transversity, nuclear PDFs,…
- positivity constraints can be implemented, too

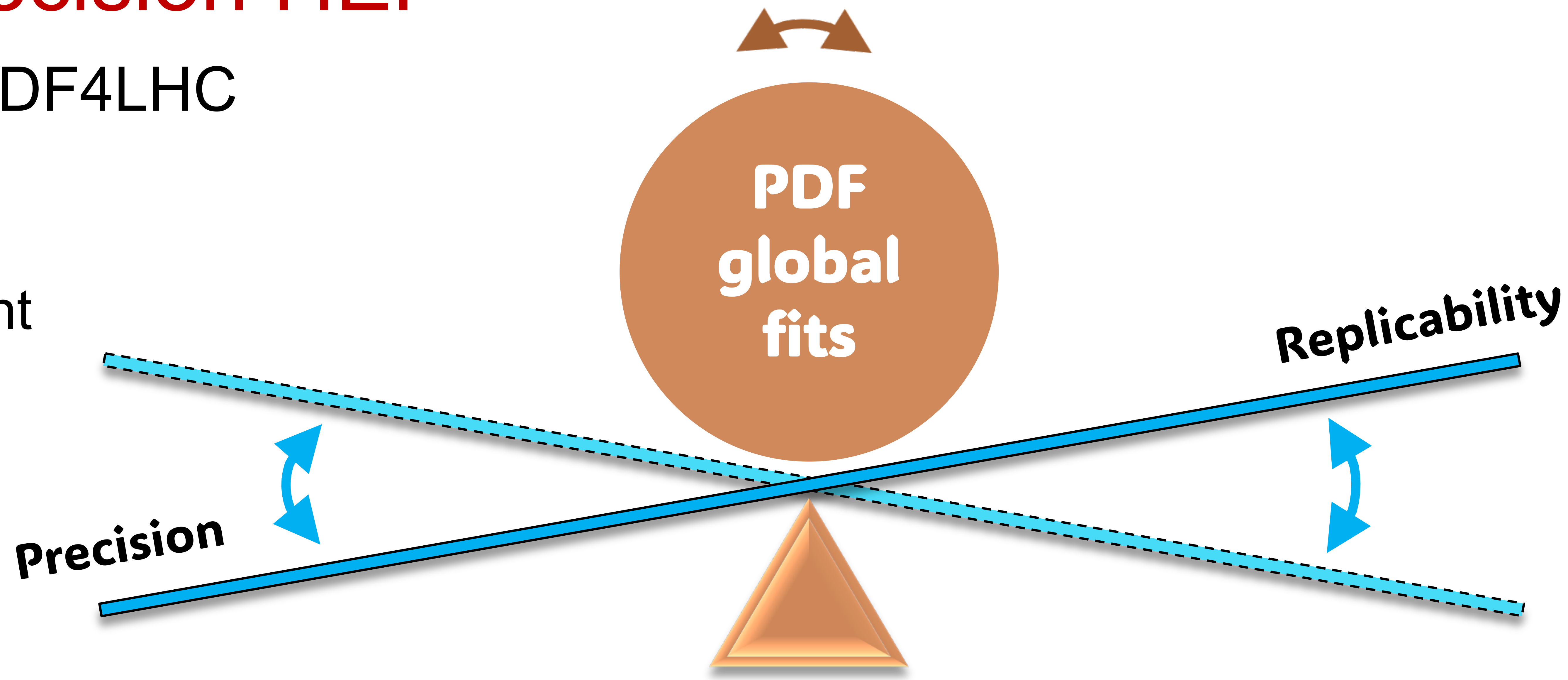
Fantômas was born in the context of Uncertainty Quantifications for CT global analyses.

PDF4LHC and replicability in precision HEP

An upcoming talk by Pavel Nadolsky at the PDF4LHC meeting, November 17, 2023

PDF parametrization dependence is an important **epistemic uncertainty.** It affects precision measurements when other experimental and theoretical uncertainties are small

Adequate estimation of such uncertainties is important for **replicability** of precision analyses.



Achieving replicability requires community-wide strategies to mitigate complexity of analyses with rigor.

Two immediate steps to improve replicability in PDF applications:

1. Avoid naïve application of the $\Delta\chi^2 = 1$ criterion for PDF uncertainties [cf. T.J. Hou et al., 1912.10053, App. F].
2. Thoroughly sample dependence on the PDF parametrizations or NN architecture when other errors are small.

Fantômas team:

L. Kotz
A. Courtoy
P. Nadolsky
F. Olness
D.M. Ponce-Chávez


LA AMENAZA ELEGANTE

Why study the pion?

- ➡ xFitter's framework set up the pion PDF analysis— https://www.xfitter.org/xFitter/
- ➡ less data *wrt* proton, still at NLO accuracy
- ➡ recent "come back" thanks to increased fitting activity in the nuclear community —theory and experiment-wise

⇨ Pion PDFs are closely related to the dynamics of QCD in non-perturbative regime— trickier interpretation due to its pseudo-Goldstone nature and ansatze for exclusive-to-inclusive relations.

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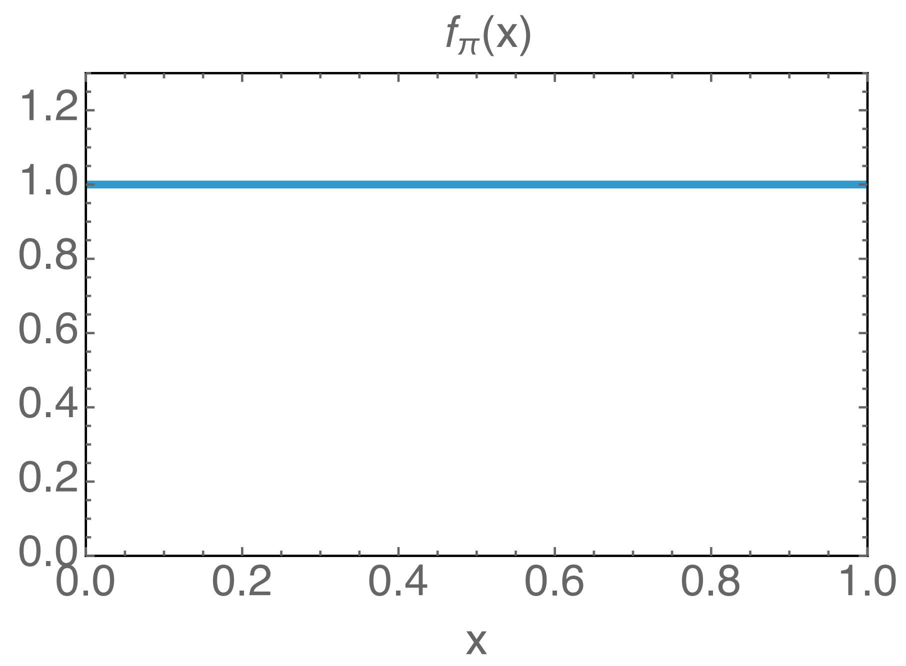
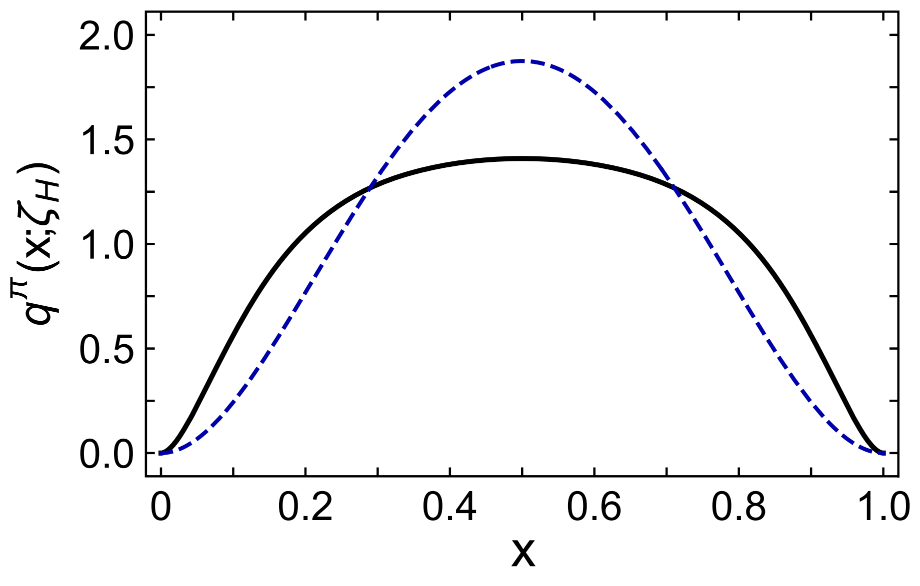
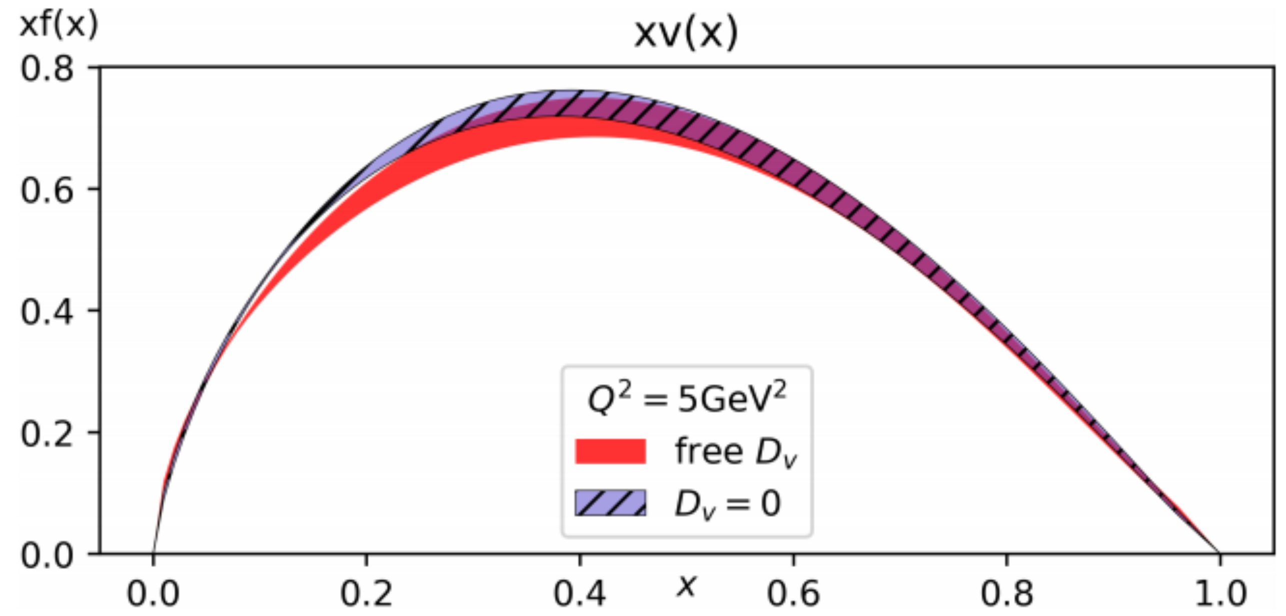
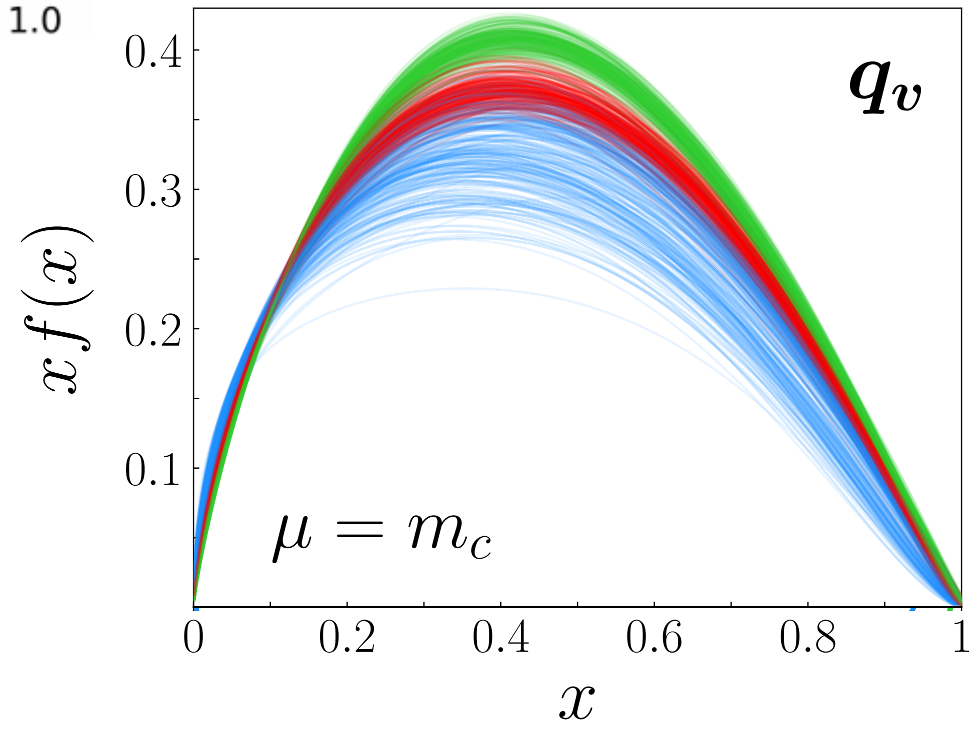


e.g. Nambu—Jona-Lasinio model, Schwinger-Dyson approaches, …



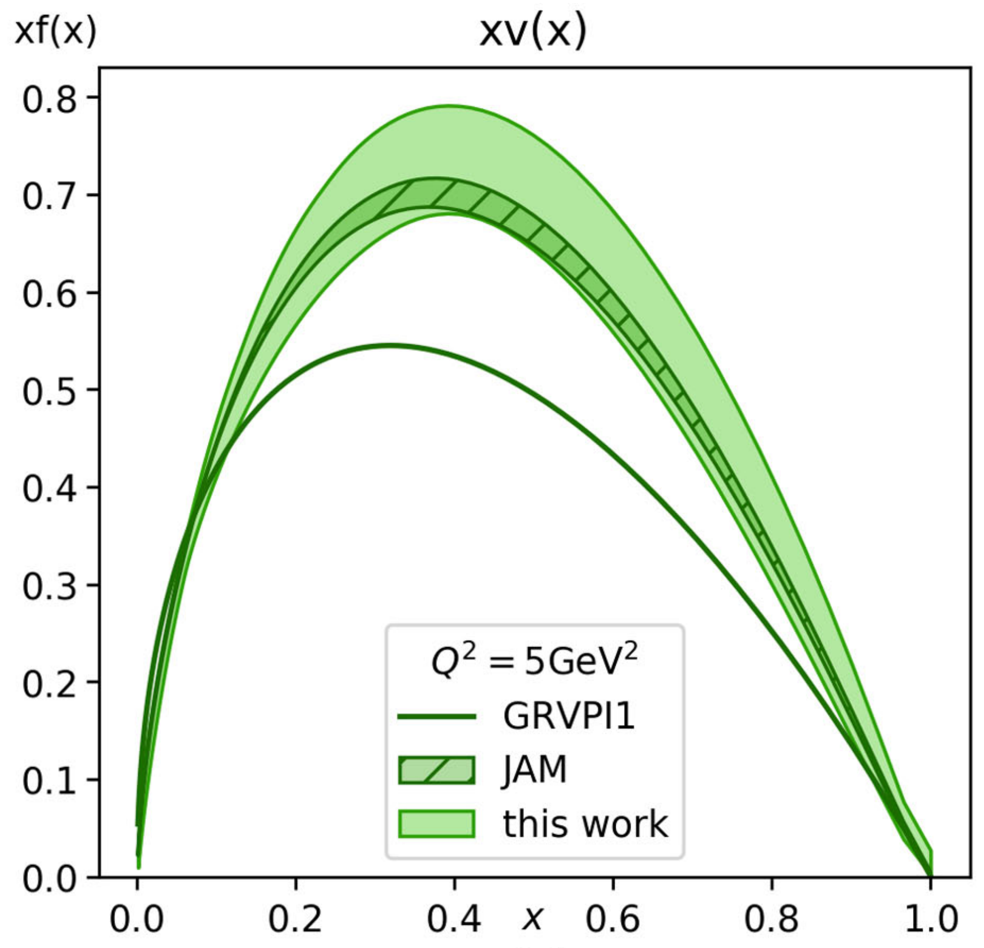


Global analysis groups:
xFitter [*PRD* 102 (2020)]
JAM [PRL 121 (2018), *PRD* 103, *PRL* 127 (2021)]
…



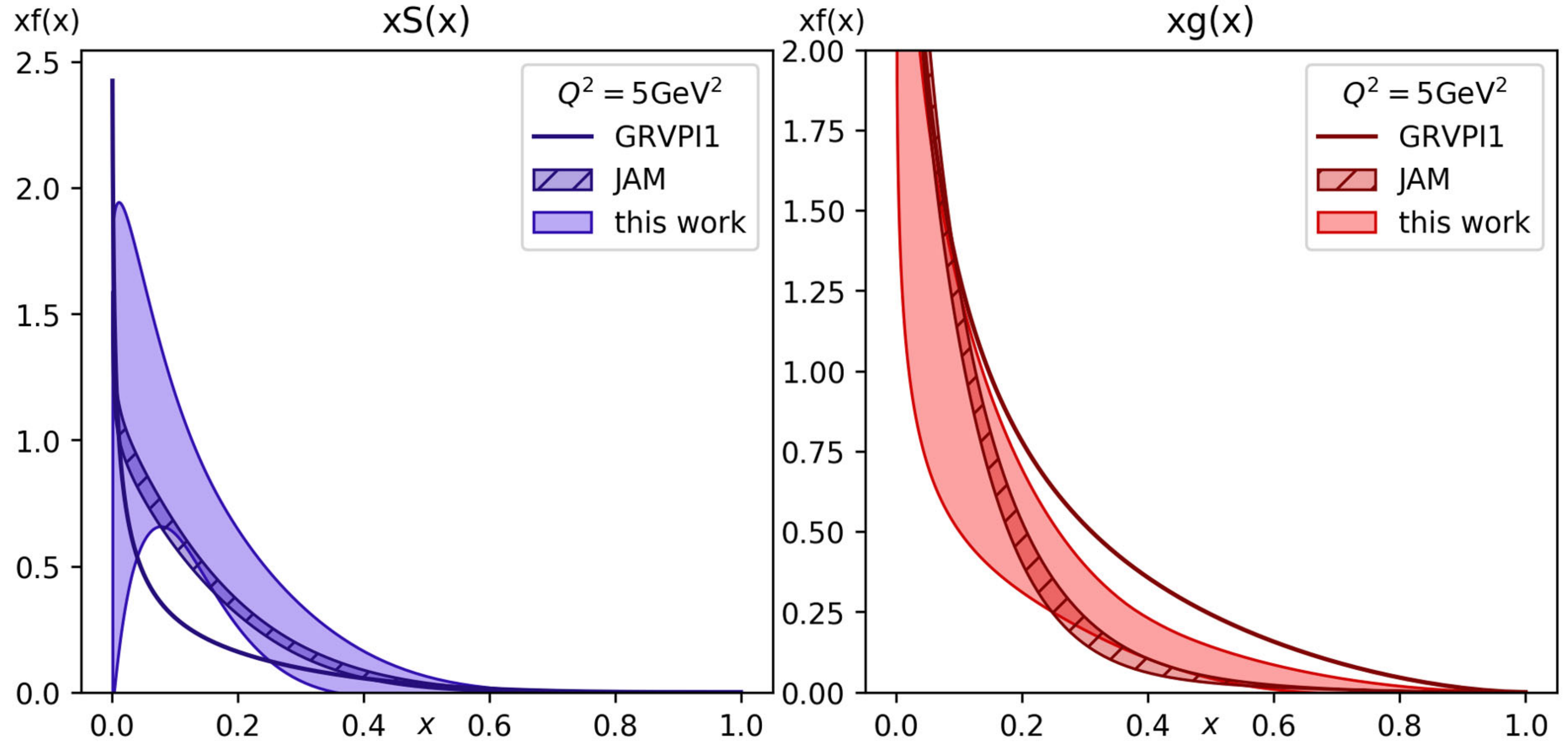
State-of-the-art of pion PDF in global analyses

Pioneer pion-induced Drell-Yan analyses (GRV, SMRS….) replaced by modern analyses



by **xFitter** [from which I took the plot]

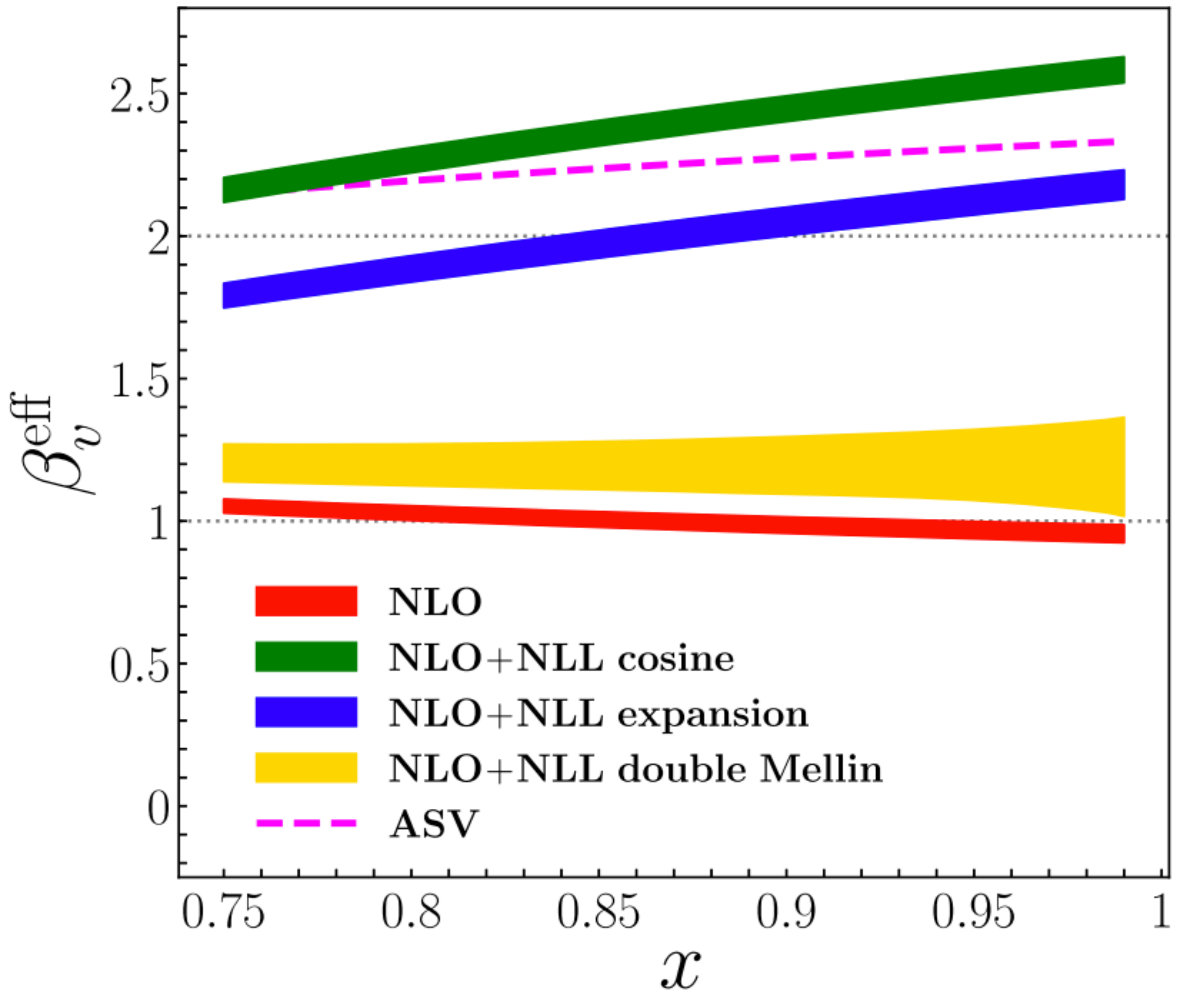
complemented by [model-dependent] leading-neutron data [**JAM**]



include large-x resummation

➡ ASV [Aicher etal., PRL105]

➡ **JAM21** [Barry et al., PRL127]



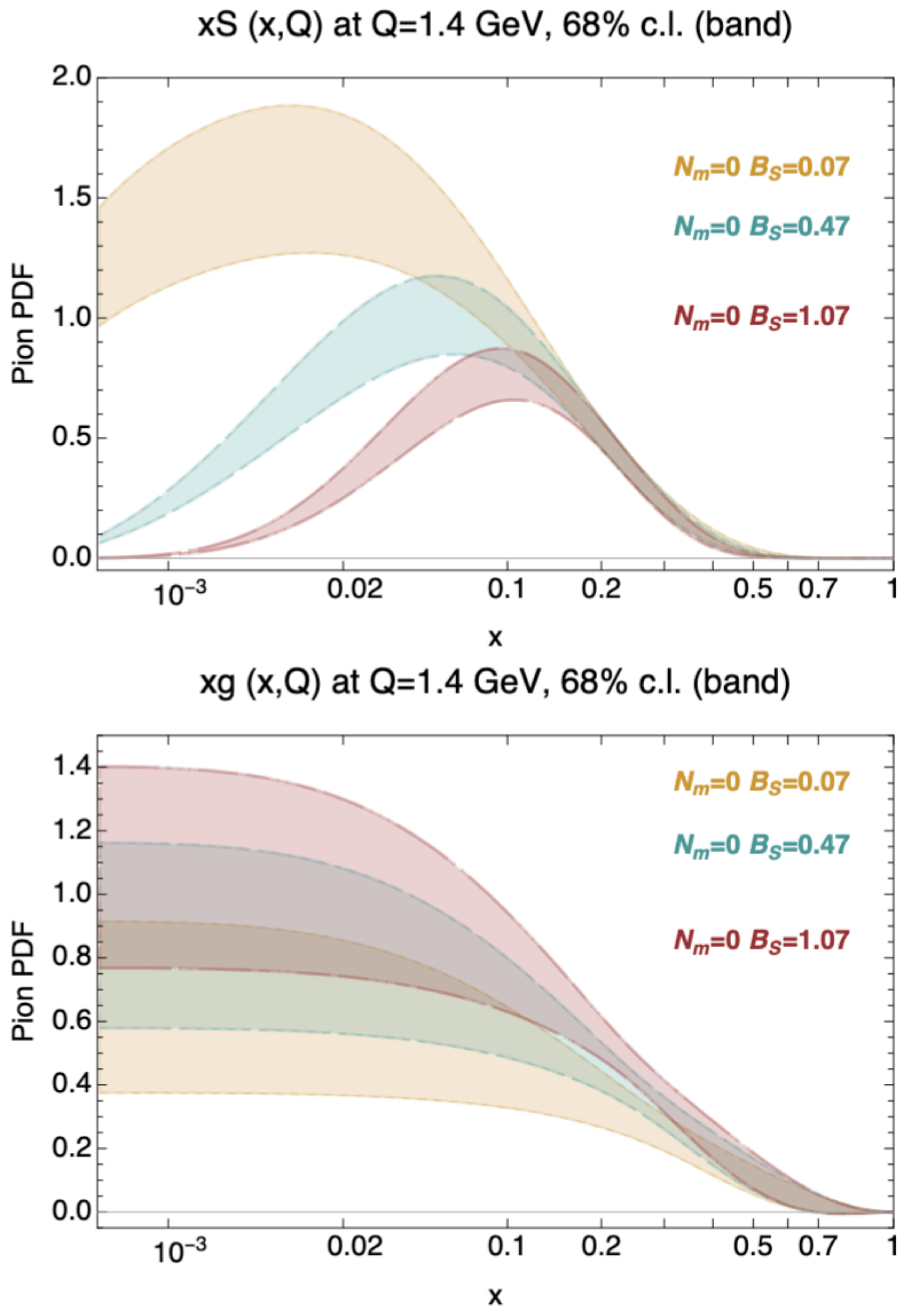
Drell-Yan only analysis

Previous analyses used a fairly basic parametrization

$$xf_{q/\pi}(x, Q_0) = Nx^{\alpha}(1-x)^{\beta} \times \left(1 + \gamma\sqrt{x} + \cdots\right)$$

With a rigid parametrization, in Drell-Yan only analysis, the sea and gluon pion distributions are not well determined.

We can achieve equally good or better fits by varying the small-x behaviour of the sea PDF [B_S] within xFitter uncertainty.



Drell-Yan only analysis

Previous analyses used a fairly basic parametrization

$$xf_{q/\pi}(x, Q_0) = Nx^{\alpha}(1-x)^{\beta} \times \left(1 + \gamma\sqrt{x} + \cdots\right)$$

With a rigid parametrization, in Drell-Yan only analysis, the sea and gluon pion distributions are not well determined.

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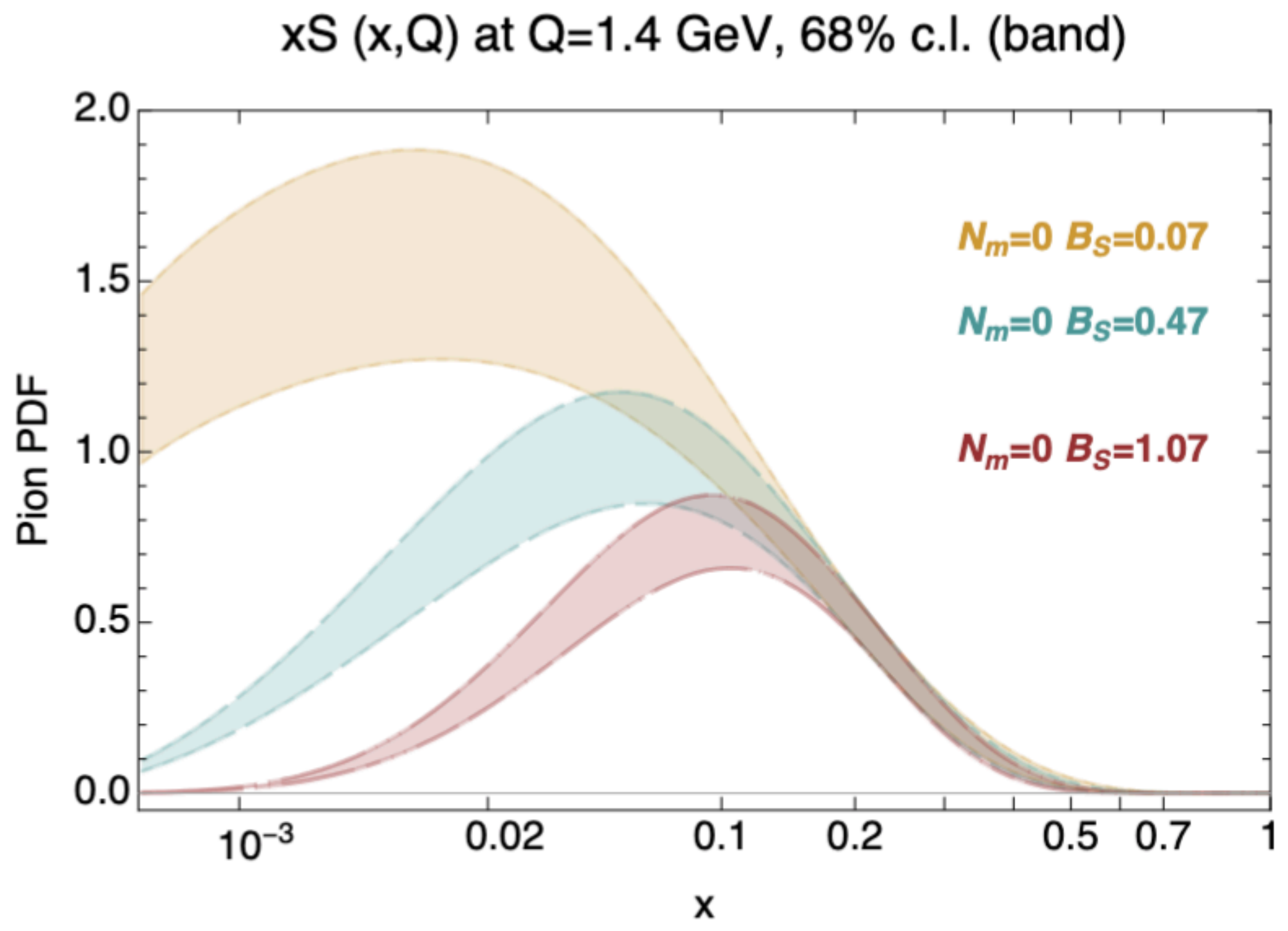
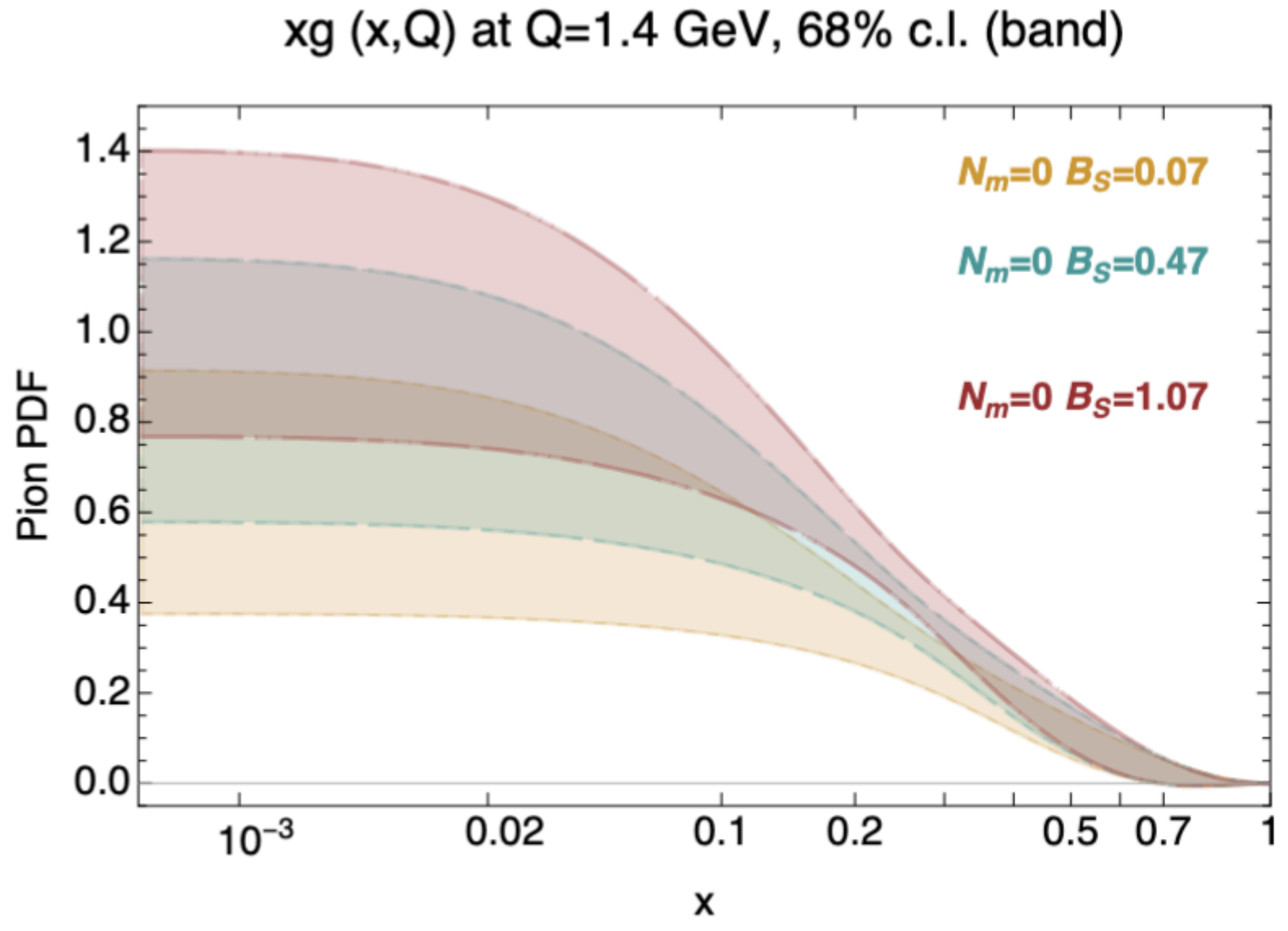


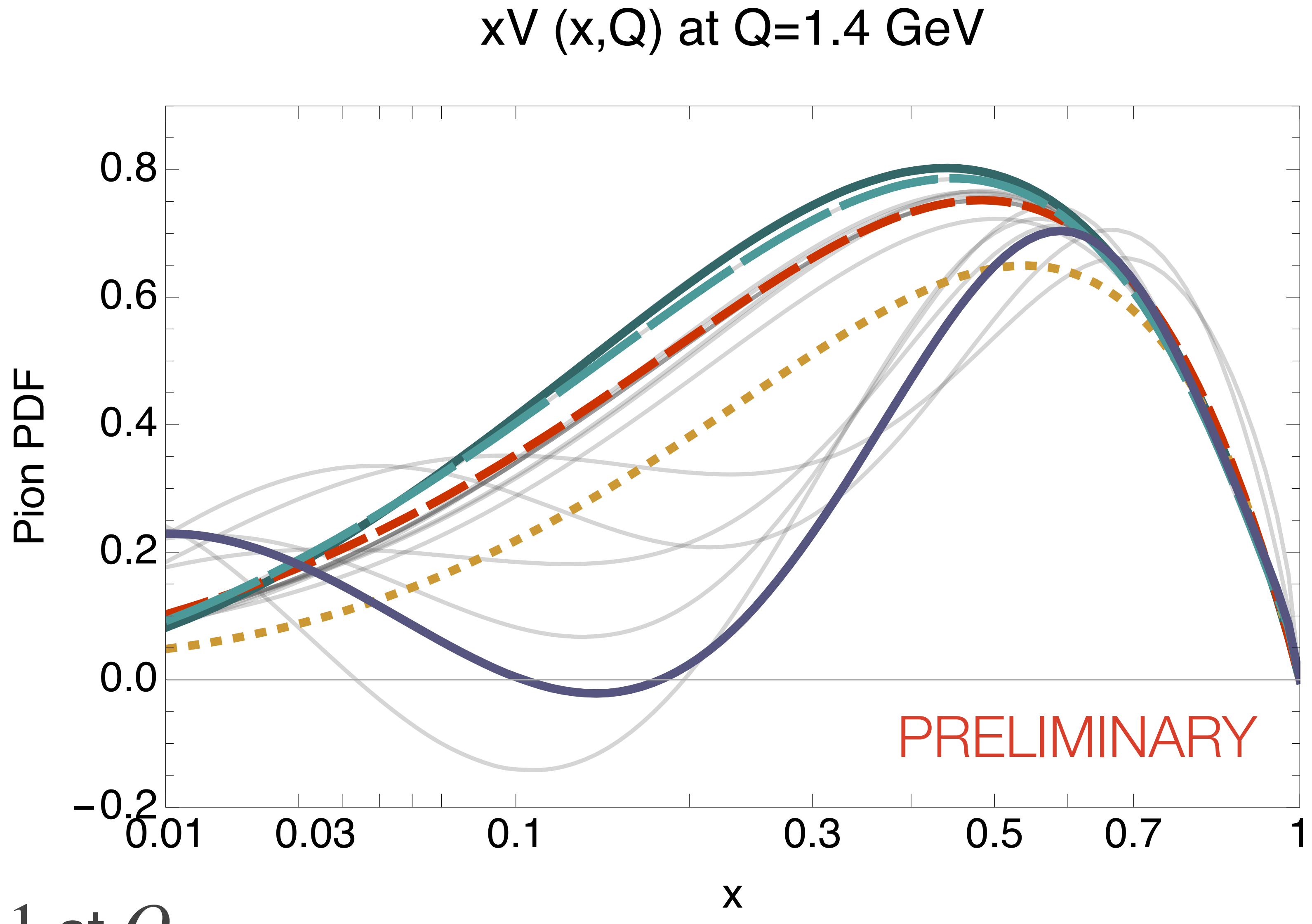


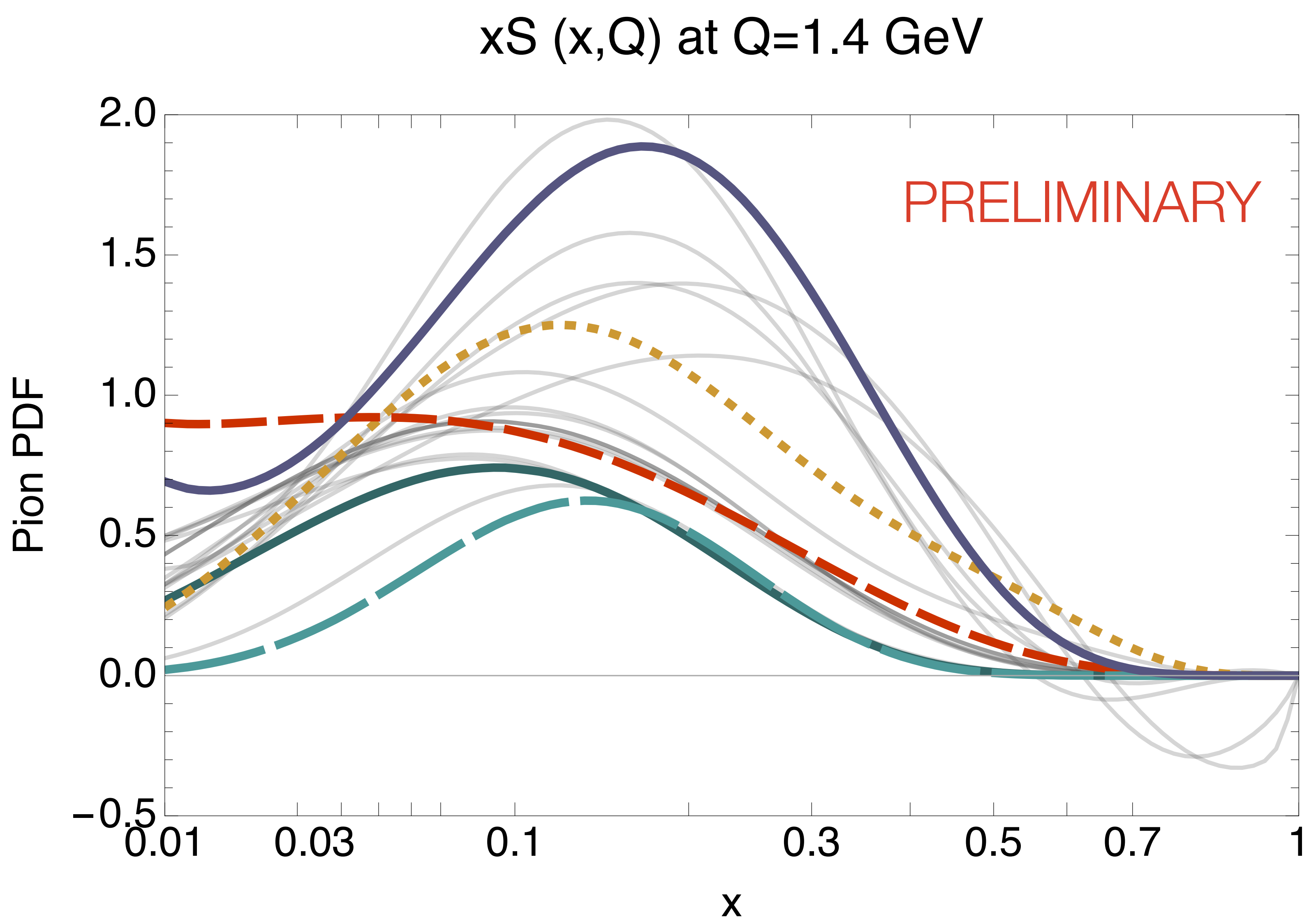
Need for complementary processes— universality and flavor separation

⇨ JAM (and HERA before them) proposed to use leading-neutron data

⇨ future experiments at EIC and JLab22(?)

Fantômas parametrizations for the pion PDF



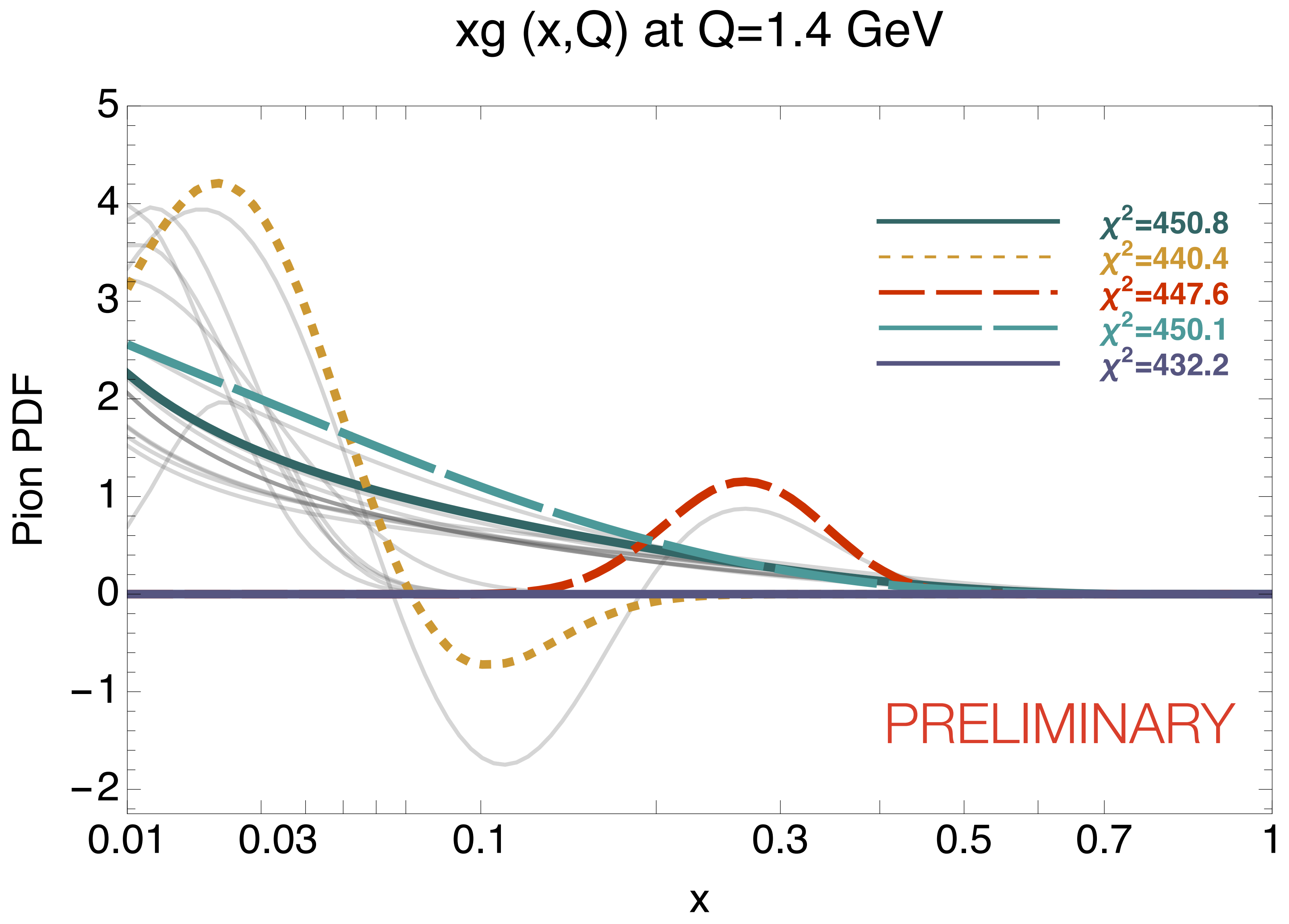


Fantômas analysis uses varying sets of

- degree of polynomial (0,1,2,3),
- position of fixed/free control points,
- stretching parameter of the argument

Extrapolation region for pion PDF is around $x = 0.1$ at Q_0.

Negative gluon are found to be possible at such a low scale [confirming JAM's findings].



Bold curves correspond to our selection for the final Fantômas set.

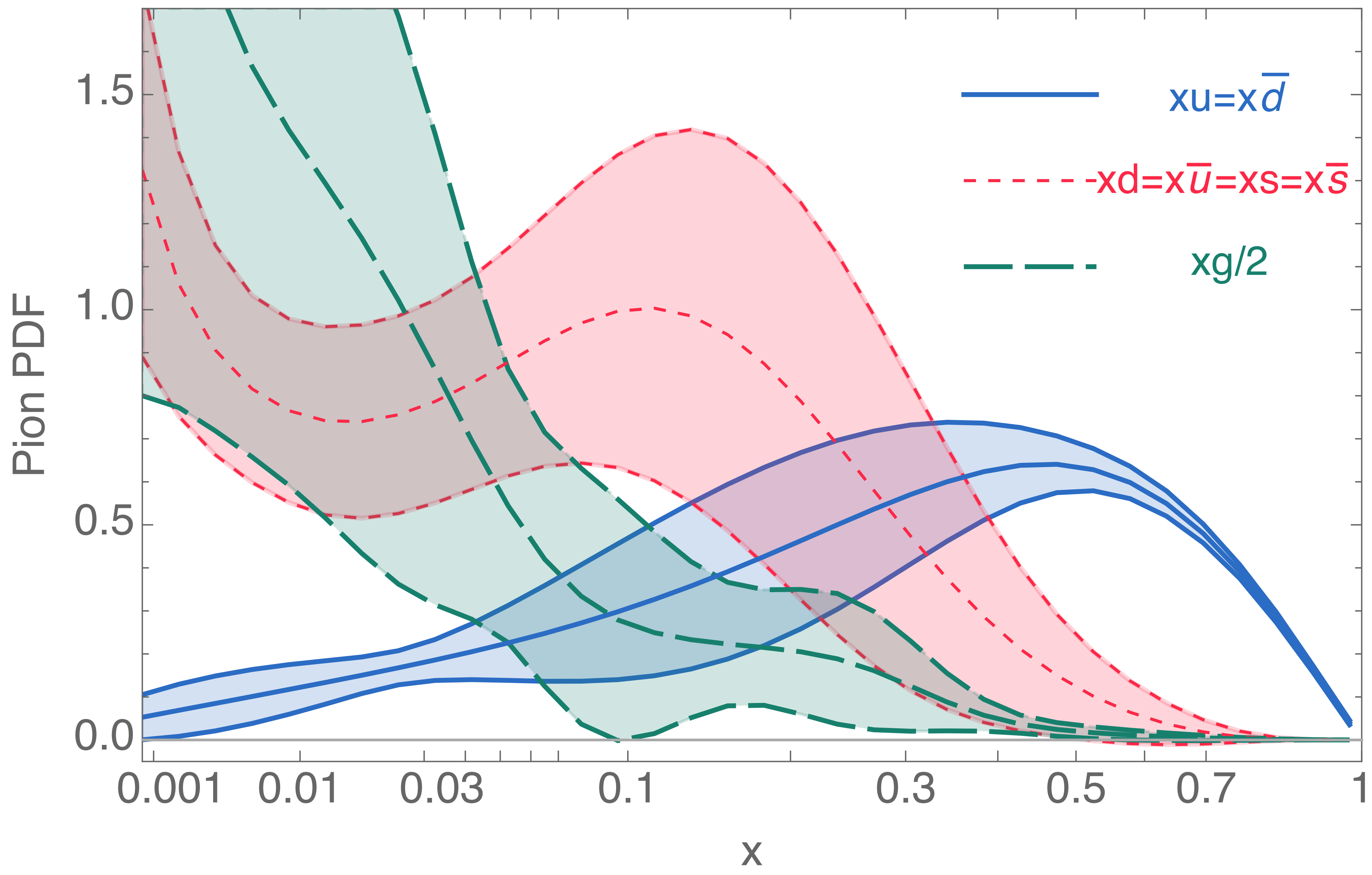
Representative curves within χ^2 range: $450 < \chi^2 + \delta\chi^2 = \chi^2 + \sqrt{2(N_{\rm pts} - N_{\rm par})} \simeq 430 + 30$

for 408 points and 7-13 parameters.

The Fantômas pion PDFs

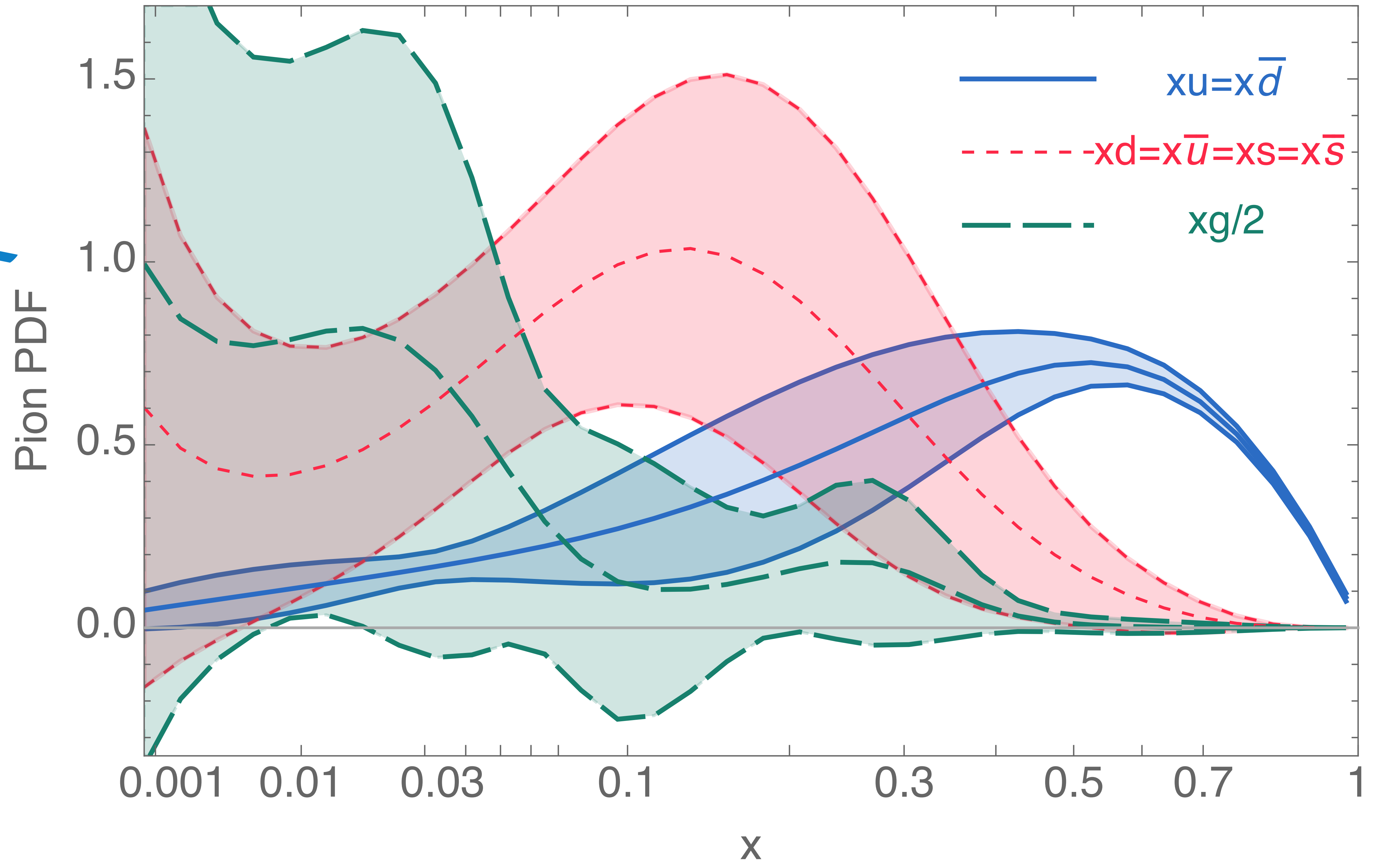
[Kotz, Ponce-Chávez, AC, Nadolsky & Olness]
Proceedings in 2309.00152.

π^+ (MC) PDFs at Q=2.5 GeV, 68% c.l. (band)



PRELIMINARY

π^+ (MC) PDFs at Q=1.4 GeV, 68% c.l. (band)



Sea and gluon behavior —prompt photon

Data sets vary between JAM and Fantômas: WA70 data points not included in JAM analysis.

We explored small gluon and small sea scenarios: they both undershoot the WA70 data for most bins.