# Pion structure in global analyses focus on uncertainty quantification

### **Aurore Courtoy**

Instituto de Física Universidad Nacional Autónoma de México (UNAM)





Dirección General de Asuntos del Personal Académico **Non-Perturbative Physics: Tools** 

and Applications

UMSNH, Morelia 08/09/23





"Fantômas For QCD: parton distributions in a pion with Bézier parametrizations"

DIS23 proceedings [2309.00152] Full manuscript to be released (very) soon

#### Fantômas team

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

A. Courtoy-IFUNAM\_\_\_\_\_Fantômas4QCD: the pion PDF\_

# Towards epistemic parton distributions

### Mainly based in the following publications

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

### **CTEQ-TEA** collaboration

China: S. Dulat, J. Gao, T.-J. Hou, I. Sitiwaldi, M. Yan, and collaborators Mexico: A. Courtoy T.J. Hobbs, M. Guzzi, J. Huston, P. Nadolsky, C. Schmidt, D. Stump, K. Xie, C.-P. Yuan USA:

and forthcoming studies.

"Fantômas: global analysis of the pion PDF with Bézier curves" [upcoming]

#### Fantômas team

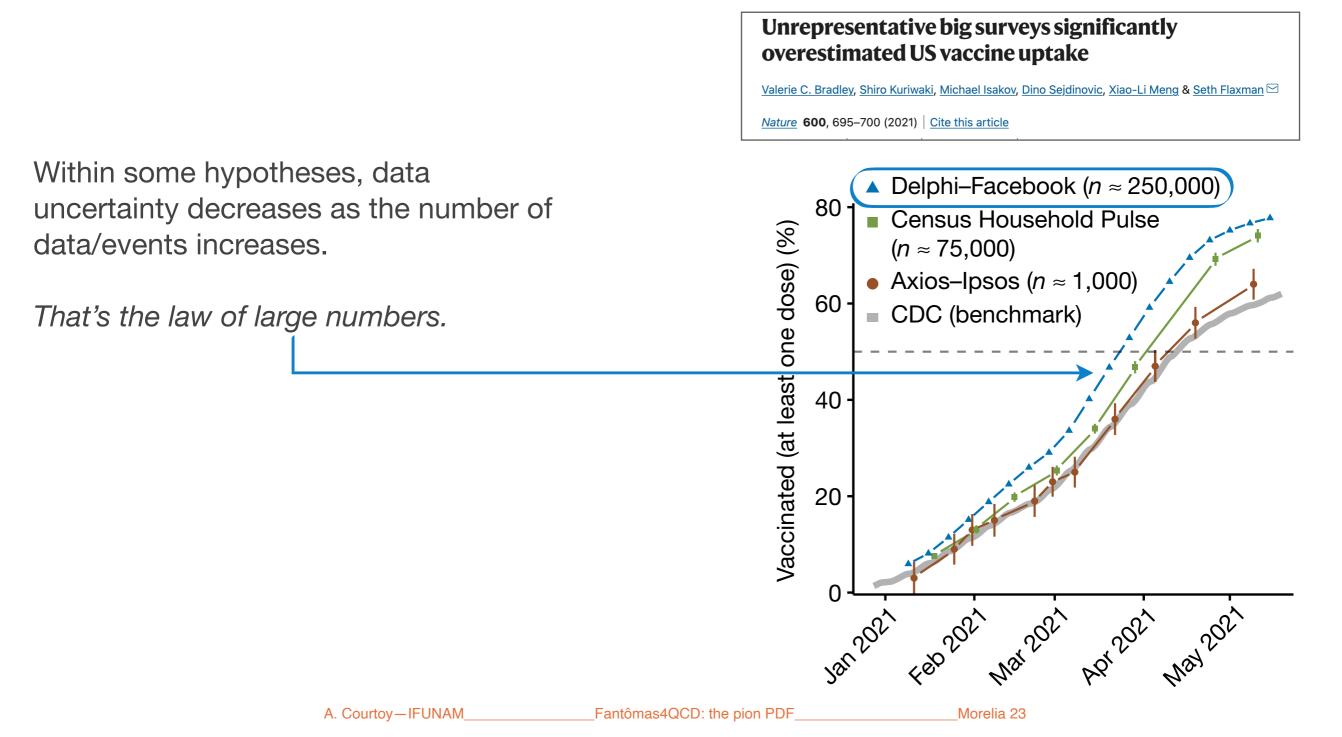
Mexico: A. Courtoy, D.M. Ponce-Chávez USA: L. Kotz, P. Nadolsky, F. Olness

based on [AC & Nadolsky, Phys.Rev.D 103].

# PDF phenomenology — a large population analysis

Precision and accuracy in PDF global analyses are possible thanks to a wealth of data, computer power and the correct statistical methods.

Multivariate problem that involves a high-dimensional space.



# PDF phenomenology — a large population analysis

Precision and accuracy in PDF global analyses are possible thanks to a wealth of data, computer power and the correct statistical methods.

Multivariate problem that involves a high-dimensional space.

Within some hypotheses, data uncertainty decreases as the number of data/events increases.

That's the law of large numbers.

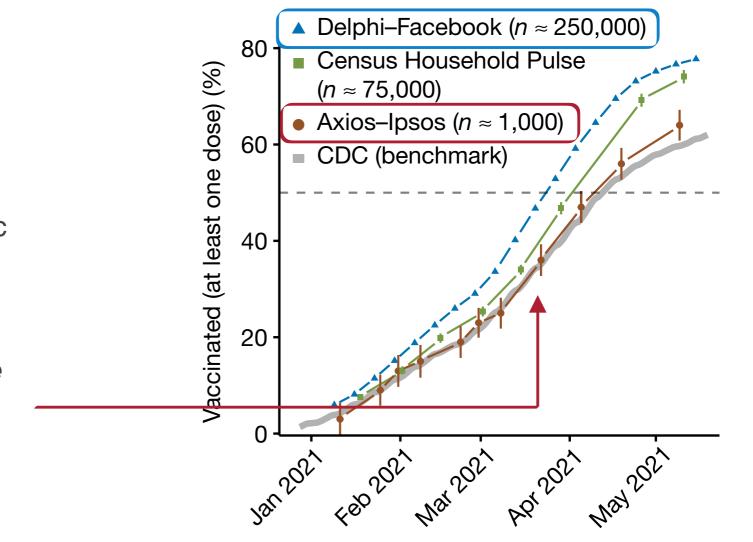
Smaller sample collected through specific methods display larger uncertainties but are closer to the benchmark.

There are other factors that determine the distance to the truth: big-data paradox.

### Unrepresentative big surveys significantly overestimated US vaccine uptake

Valerie C. Bradley, Shiro Kuriwaki, Michael Isakov, Dino Sejdinovic, Xiao-Li Meng & Seth Flaxman 🖂

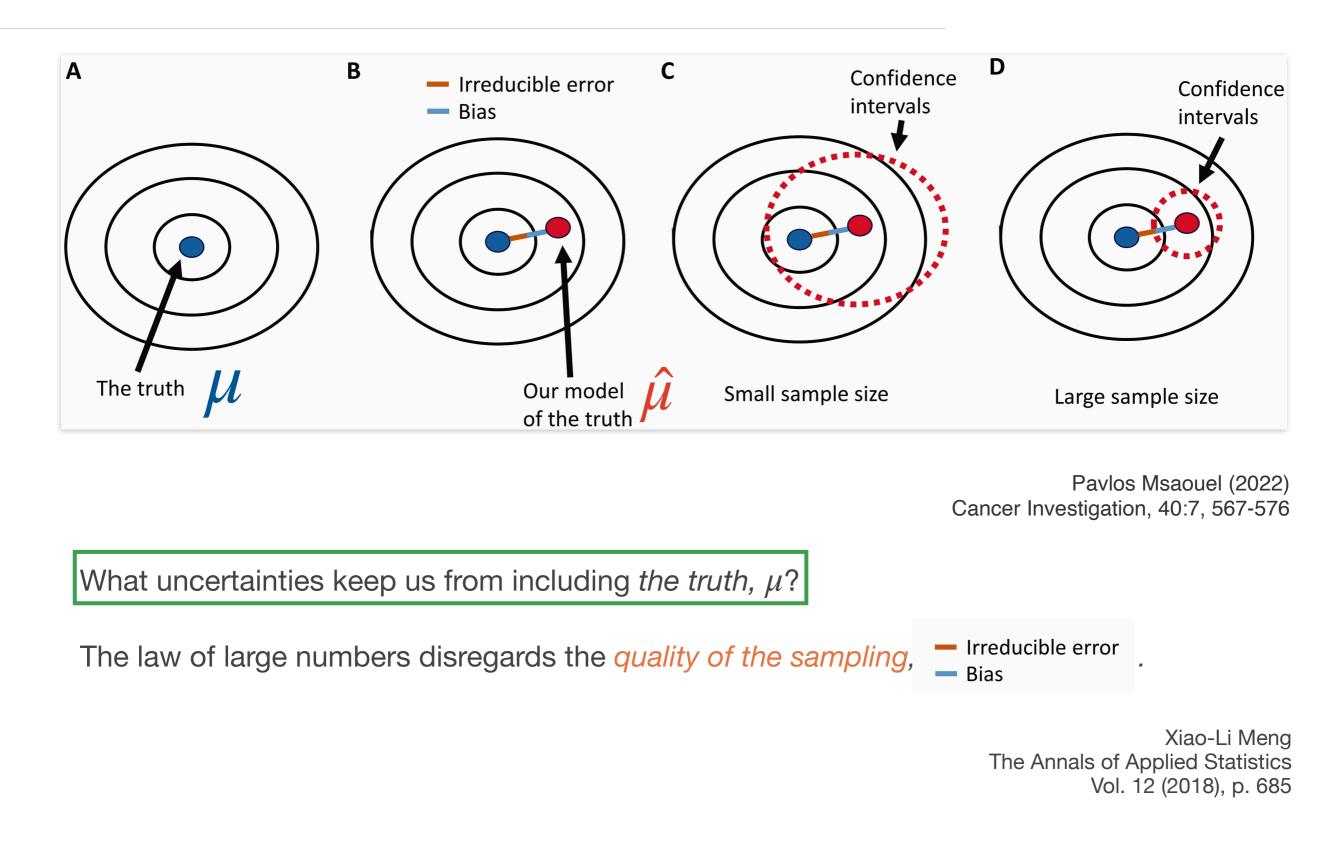
<u>Nature</u> 600, 695–700 (2021) Cite this article



Morelia 23

Fantômas4QCD: the pion PDF

# Sampling bias and big-data paradox

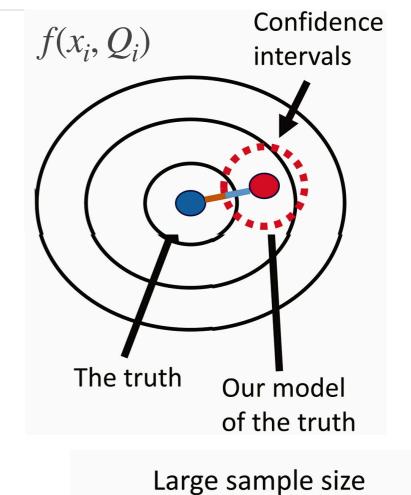


Towards epistemic Pion PDF

# Physics phenomenology and accuracy

Suppose we know the true parton distribution function at given  $(x_i, Q_i)$ .

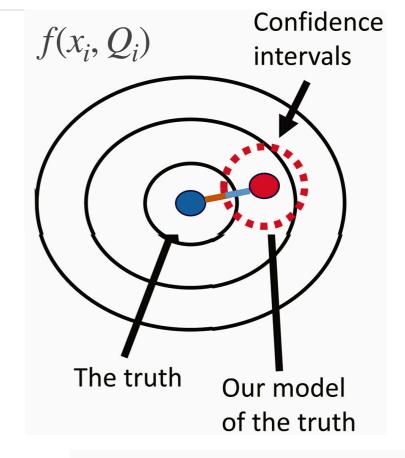
We want our determination from global analysis to encompass it.



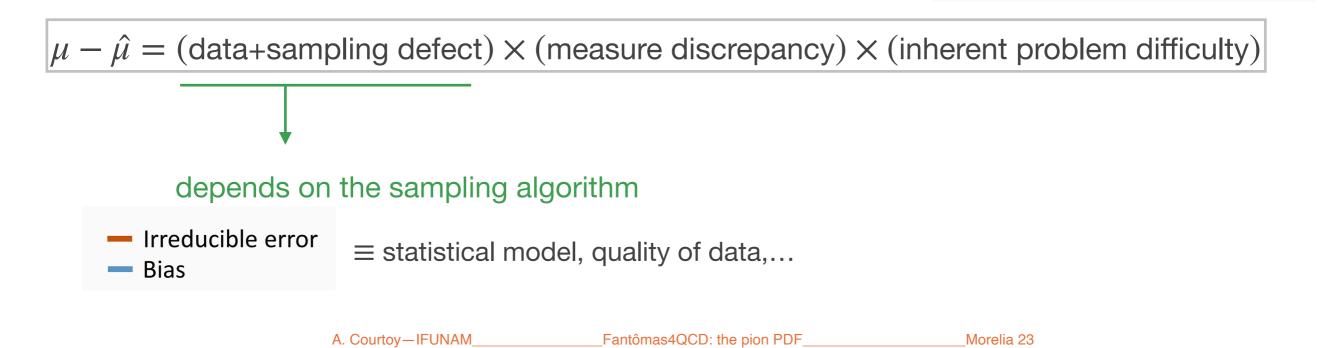
# Physics phenomenology and accuracy

Suppose we know the true parton distribution function at given  $(x_i, Q_i)$ .

We want our determination from global analysis to encompass it.



Large sample size



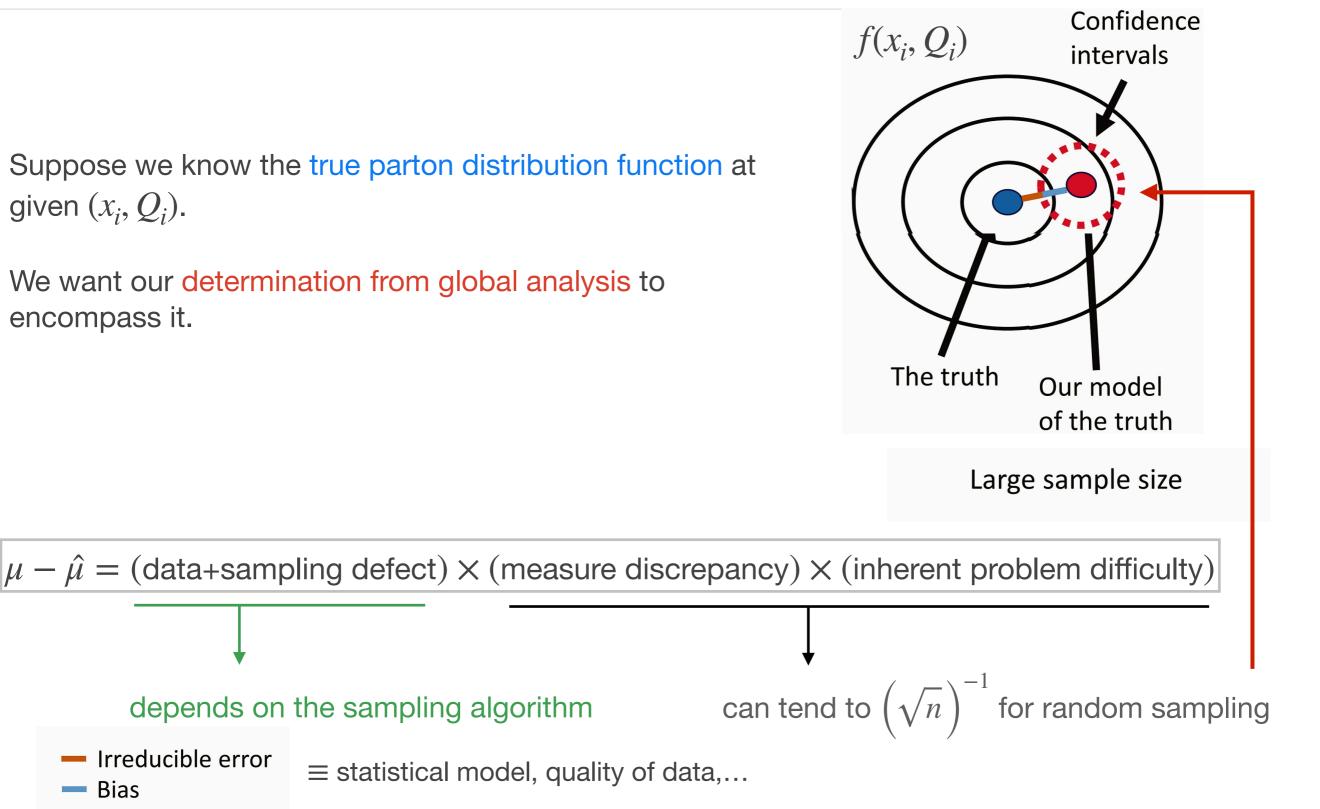
# Physics phenomenology and accuracy

Suppose we know the true parton distribution function at given  $(x_i, Q_i)$ .

We want our determination from global analysis to encompass it.

Irreducible error

Bias

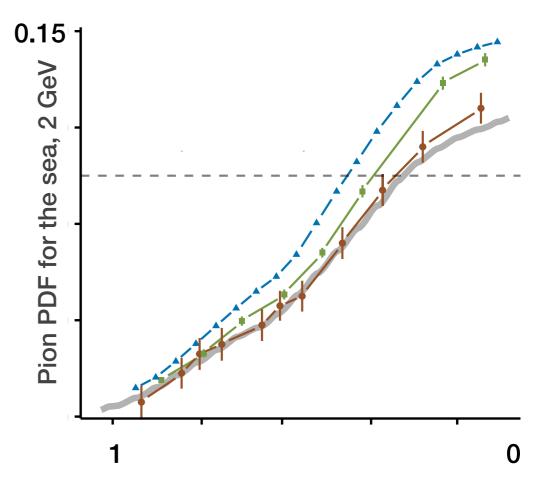


Morelia 23

#### very fanciful!!

If the light-gray curve is the truth, hence its shape would reveal information on the underlying non-perturbative mechanisms.

e.g., in our fairy-tale example, that the sea quarks freeze about x = 0.1 at Q = 2 GeV or the slope at which it falls down at  $x \rightarrow 1$ .



#### **Disclaimer:**

I purposedly adapted to vaccination plot for illustration. It's not a true PDF.

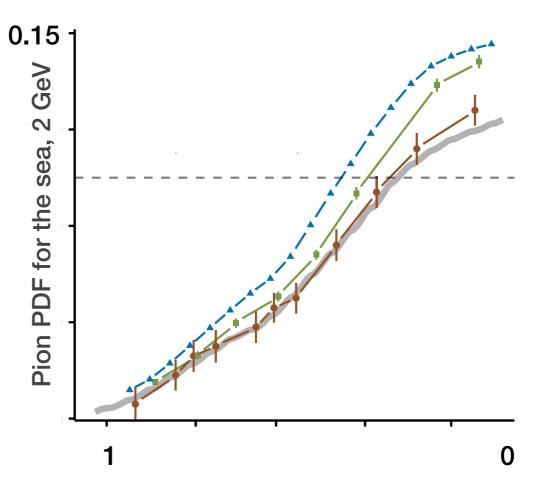
### very fanciful!!

If the light-gray curve is the truth, hence its shape would reveal information on the underlying non-perturbative mechanisms.

e.g., in our fairy-tale example, that the sea quarks freeze about x = 0.1 at Q = 2 GeV or the slope at which it falls down at  $x \rightarrow 1$ .

If sampling only focuses on the quantity of the data/replicas/parameters/..., we risk to reproduce the blue curve and its tiny uncertainty [that misses the truth].

and wrongly deduce that there are, e.g., more sea quarks at small *x* than there is.



#### **Disclaimer:**

I purposedly adapted to vaccination plot for illustration. It's not a true PDF.

### very fanciful!!

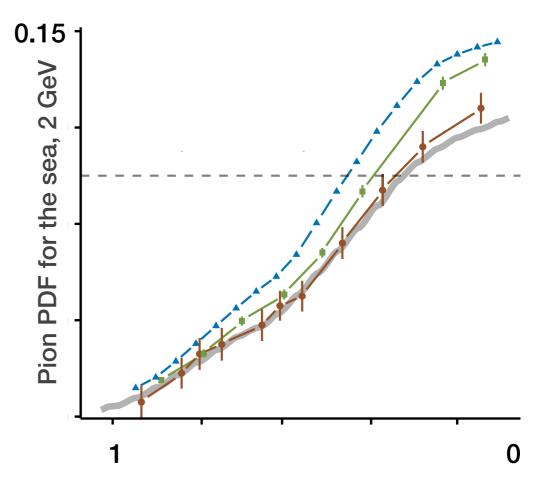
If the light-gray curve is the truth, hence its shape would reveal information on the underlying non-perturbative mechanisms.

e.g., in our fairy-tale example, that the sea quarks freeze about x = 0.1 at Q = 2 GeV or the slope at which it falls down at  $x \rightarrow 1$ .

If sampling only focuses on the quantity of the data/replicas/parameters/..., we risk to reproduce the blue curve and its tiny uncertainty [that misses the truth].

and wrongly deduce that there are, e.g., more sea quarks at small *x* than there is.

If sampling is inclusive of various factors [optimization of the space exploration], we might reproduce the maroon curve together with a larger uncertainty [and include the truth].



#### **Disclaimer:**

I purposedly adapted to vaccination plot for illustration. It's not a true PDF.

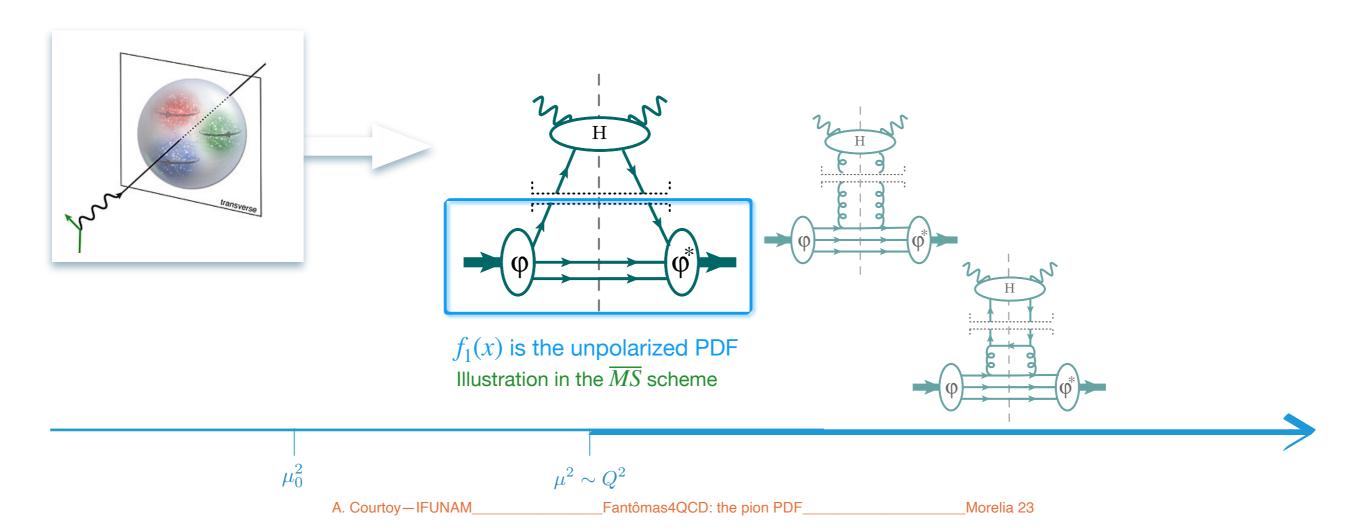
# PDFs in QCD phenomenology

### In the realm of QCD...

The two regimes of QCD demand that non-perturbative objects are accessed through *factorization theorems*,

*i.e.,* theory is expressed through a convolution of hard and soft part to which corrections are added.

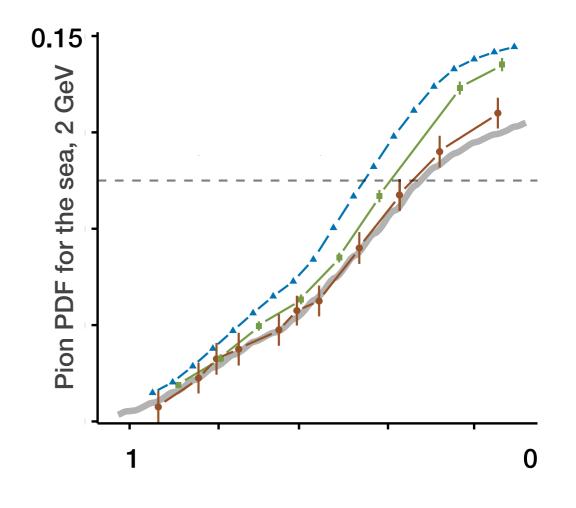
 $\Rightarrow$  the data is not reproduced by the PDF only



What are the conventions on "QCD phenoma"? [first principles may need adaptation to the present understanding of perturbative QCD].

> [AC & Nadolsky, PRD103] [Candido et al, *JHEP* 11& 2308.00025] [Collins et al, PRD105]

E.g., what is the smoking-gun sign for role of chiral symmetry in the emergence of hadronic mass? On how many and which parameters does that smoking gun depend?



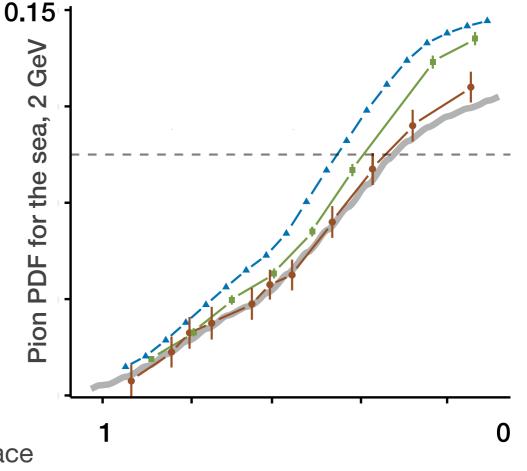
What are the conventions on "QCD phenoma"? [first principles may need adaptation to the present understanding of perturbative QCD].

> [AC & Nadolsky, PRD103] [Candido et al, *JHEP* 11& 2308.00025] [Collins et al, PRD105]

E.g., what is the smoking-gun sign for role of chiral symmetry in the emergence of hadronic mass? On how many and which parameters does that smoking gun depend?

Poor sampling can sometimes be due to over-constrained space where solutions are deemed acceptables — i.e., through priors or penalties.

For the Hessian-methodology based global analyses, a functional form is required. A parametrization is a prior-like penalty.



What are the conventions on "QCD phenoma"? [first principles may need adaptation to the present understanding of perturbative QCD].

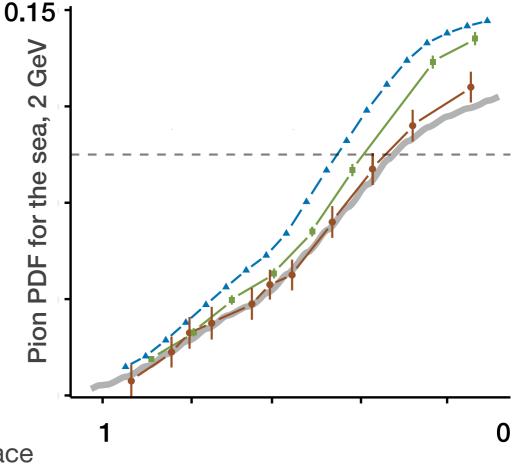
> [AC & Nadolsky, PRD103] [Candido et al, *JHEP* 11& 2308.00025] [Collins et al, PRD105]

E.g., what is the smoking-gun sign for role of chiral symmetry in the emergence of hadronic mass? On how many and which parameters does that smoking gun depend?

Poor sampling can sometimes be due to over-constrained space where solutions are deemed acceptables — i.e., through priors or penalties.

For the Hessian-methodology based global analyses, a functional form is required. A parametrization is a prior-like penalty.

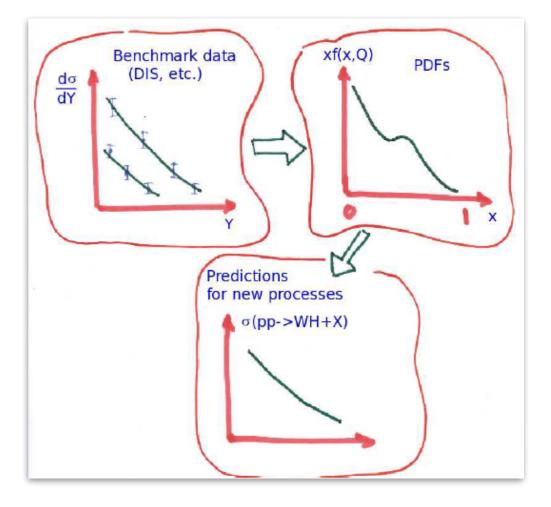




Low-energy QCD dynamics, encapsulated in PDFs, are learned from experimental data.

Shape in *x* extracted from data that are sensitive to specific PDF flavors, etc.

- I. hints of behavior of partons at low scales
- II. predictions for other (new) processes



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

Shape in *x* extracted from data that are sensitive to specific PDF flavors, etc.

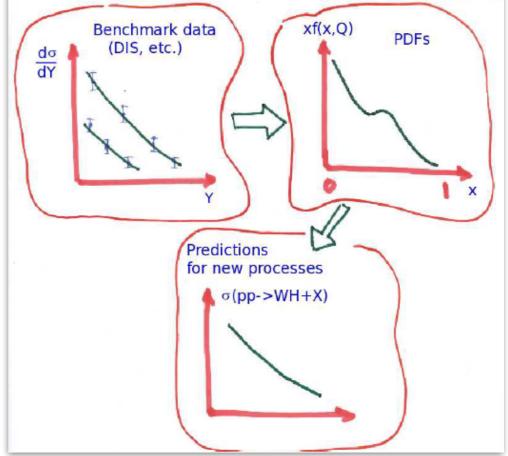
- I. hints of behavior of partons at low scales
- II. predictions for other (new) processes

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:  $\langle x \rangle_n = \int_0^1 dx \, x^{n-1} f(x)$

*Model* evaluation of *x*-dependence (in parallel to data learning)

- use QFT description of f(x) together with model description of hadron wave function (non trivial to define)
- ensure symmetries are fulfilled



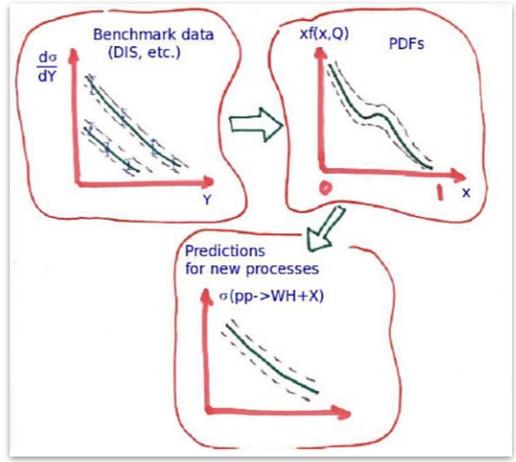
Morelia 23

A. Courtoy-IFUNAM\_\_\_\_\_Fantômas4QCD: the pion PDF\_\_\_\_\_

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

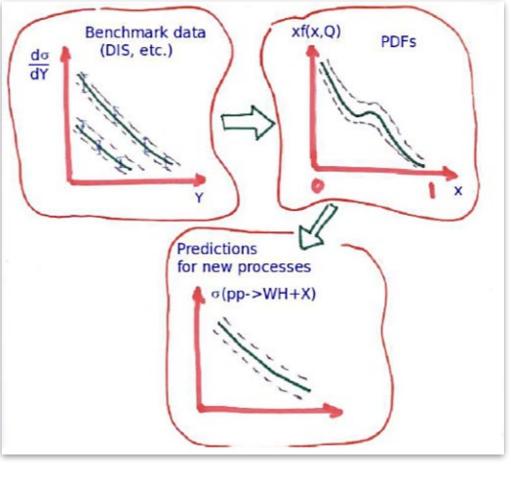


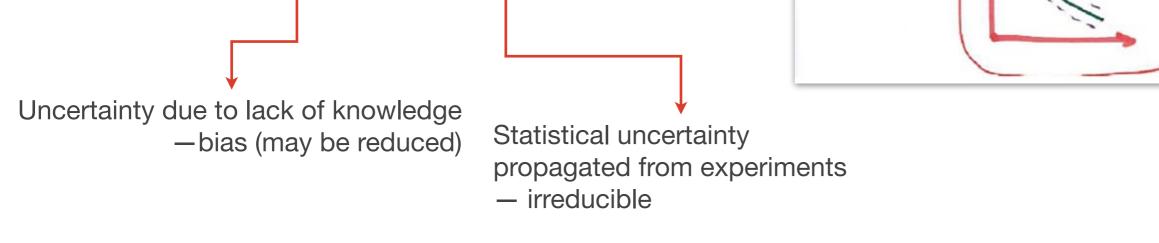
# The shape of parton distributions

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

#### Uncertainty propagates from data and methodology to the PDF determination

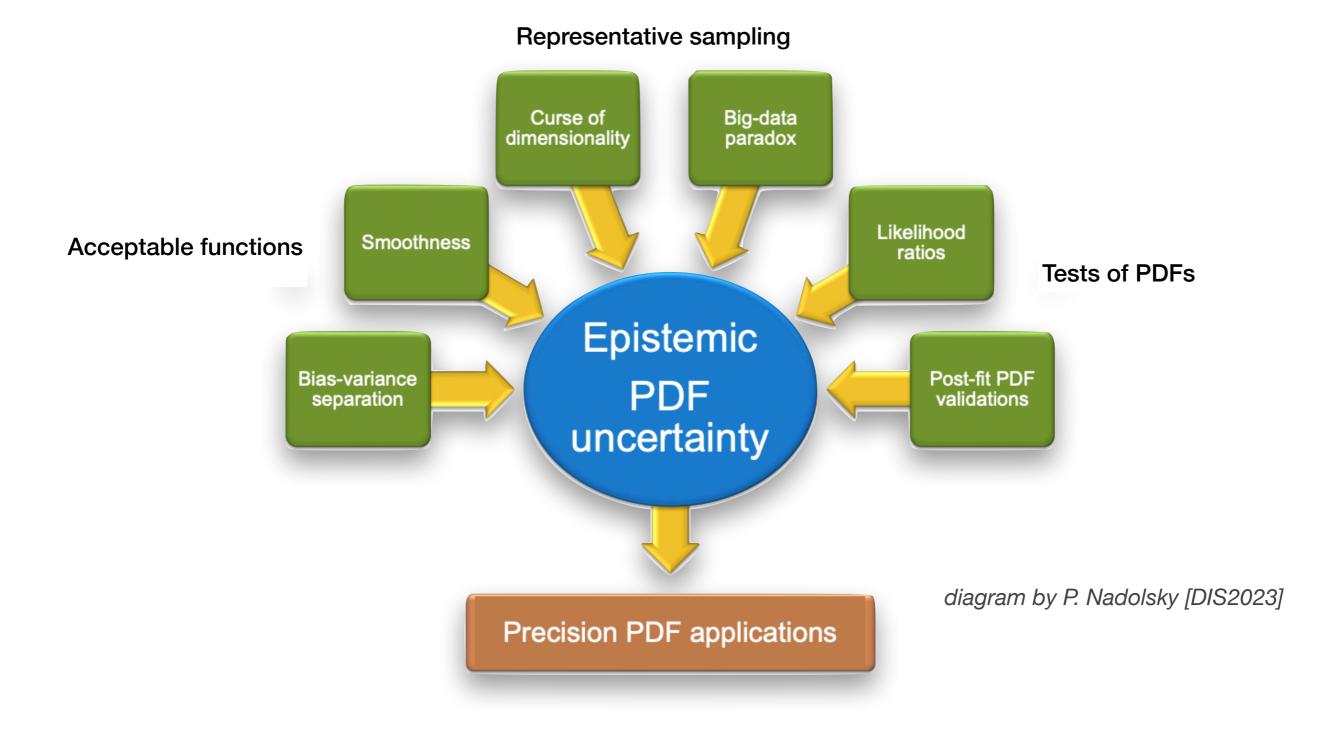
- I. assessment of uncertainty magnitude is key
- II. advanced statistical problem
- III. evolving topic in the era of AI/ML





**Epistemic vs. aleatory uncertainties** 

# Hypothesis testing and parton distributions



# Fantômas4QCD

*Fantômas4QCD*: systematize the role of functional form in global analyses, alternative to neural networks.



CTEQ-TEA and xFitter members + students

Collaboration between Southern Methodist University (SMU) and Institute of Physics at UNAM.

Supported by CONACyT (Mexico) and IANN-QCD.







\_Towards epistemic Pion PDF\_

### **Testing specific** *x***-shapes:**

Polynomial mimicry=Mathematical equivalence of polynomials of different orders.

<u>Bézier curves</u> give an example of mathematical equivalence of polynomials of different orders

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.

$$B_{n,l}(x) \equiv \binom{l}{n} x^l (1-x)^{n-l}$$

### **Testing specific** *x***-shapes:**

Polynomial mimicry=Mathematical equivalence of polynomials of different orders.

<u>Bézier curves</u> give an example of mathematical equivalence of polynomials of different orders

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:

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

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

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

• <u>*T*</u> is now a matrix of  $x^l$  expressed at the control points.

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

Such that the coefficients can be expressed in terms of known matrices

$$\underline{C} = \underline{\underline{M}}^{-1} \cdot \underline{\underline{T}}^{-1} \cdot \underline{\underline{P}}$$

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

• <u>*T*</u> is now a matrix of  $x^l$  expressed at the control points.

A. Courtoy—IFUNAM

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

LFTC workshop 23

Such that the coefficients can be expressed in terms of known matrices

$$\underline{C} = \underline{\underline{M}}^{-1} \cdot \underline{\underline{T}}^{-1} \cdot \underline{\underline{P}}$$

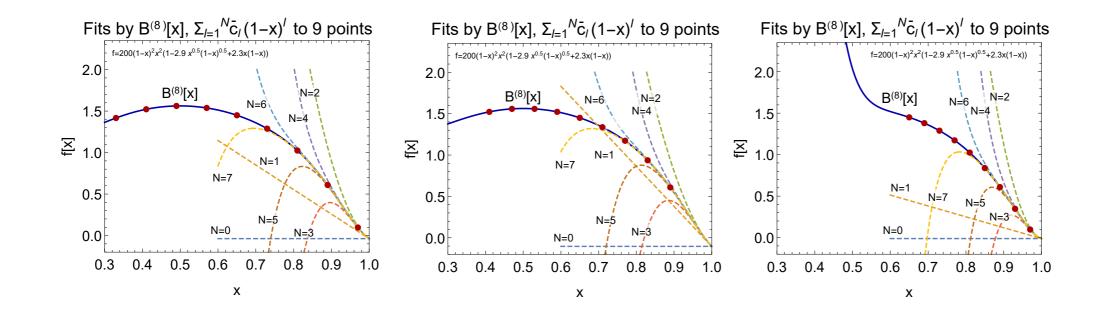
To test a (1 - x) behavior, we expand the interpolation through Fits by  $B^{(4)}[x]$ ,  $\Sigma_{l=1}^{N} \bar{c_l} (1-x)^l$  to 9 points Bézier curves about x = 1:  $u_{\pi}(x \to 1) = \sum_{i=0}^{n} \bar{c}_i (1-x)^i$ 3.0  $f=30x^2(1-x)^2$ 2.5  $B^{(4)}[x]$ 2.0 The red points represent the control points, the number of which  $\ge 1.5$ is related to the degree of the polynomial. 1.0 N=3 0.5 N=0 and <sup>2</sup> 0.0 0.3 0.4 0.5 0.6 0.8 0.9 1.0 0.7 Х

Towards epistemic Pion PDF

# Bézier-curve methodology for global analyses

<u>Reconstruction of a parametrization</u>  $f=200(1-x)^2 x^2 (1-2.9 x^{0.5}(1-x)^{0.5}+2.3x(1-x))$ 

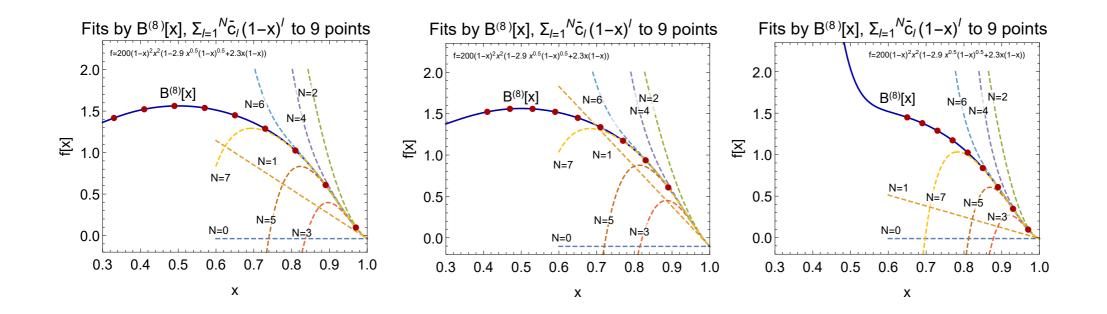
⇒ The lowest powers of the expansion cannot be meaningfully reconstructed.



# Bézier-curve methodology for global analyses

<u>Reconstruction of a parametrization</u>  $f=200(1-x)^2 x^2 (1-2.9 x^{0.5}(1-x)^{0.5}+2.3x(1-x))$ 

⇒ The lowest powers of the expansion cannot be meaningfully reconstructed.

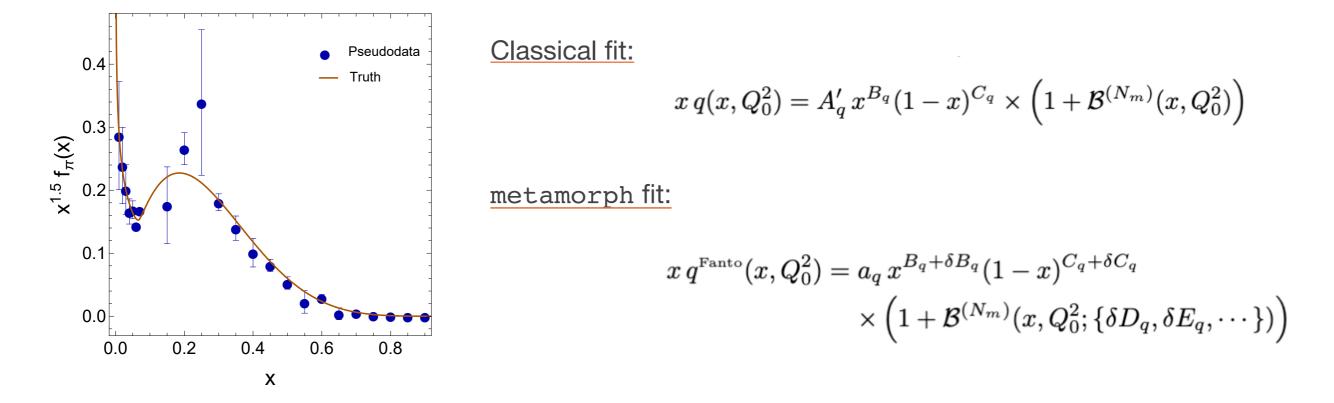


⇒ The reconstructed function depends on the position and number of control points.

This property can be exploited in favor of global analyses: by varying settings of the Bézier curves, we generate a variety of curves, beyond reconstruction.

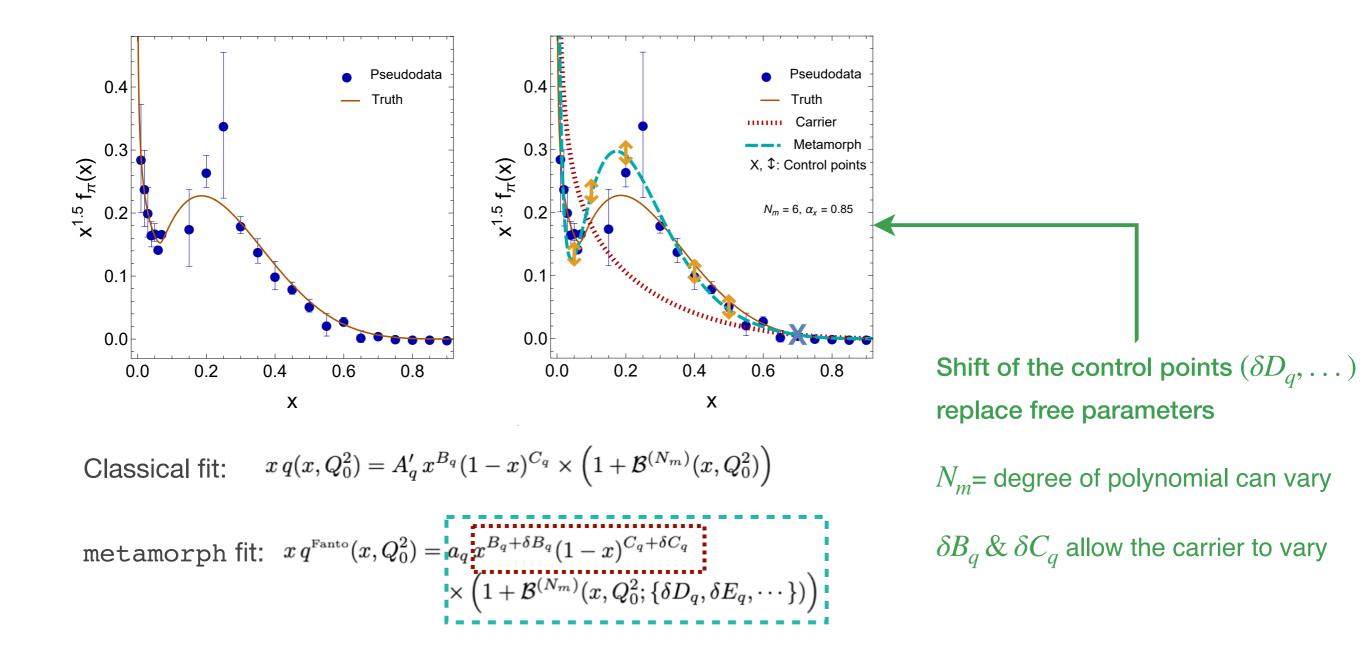
### Fantômas4QCD program

- $\Rightarrow$  From interpolation to minimization over parameters through  $\mathscr{B}$
- ⇒ Exploit polynomial mimicry to systematically improve and flexibilize parametrization of PDFs.



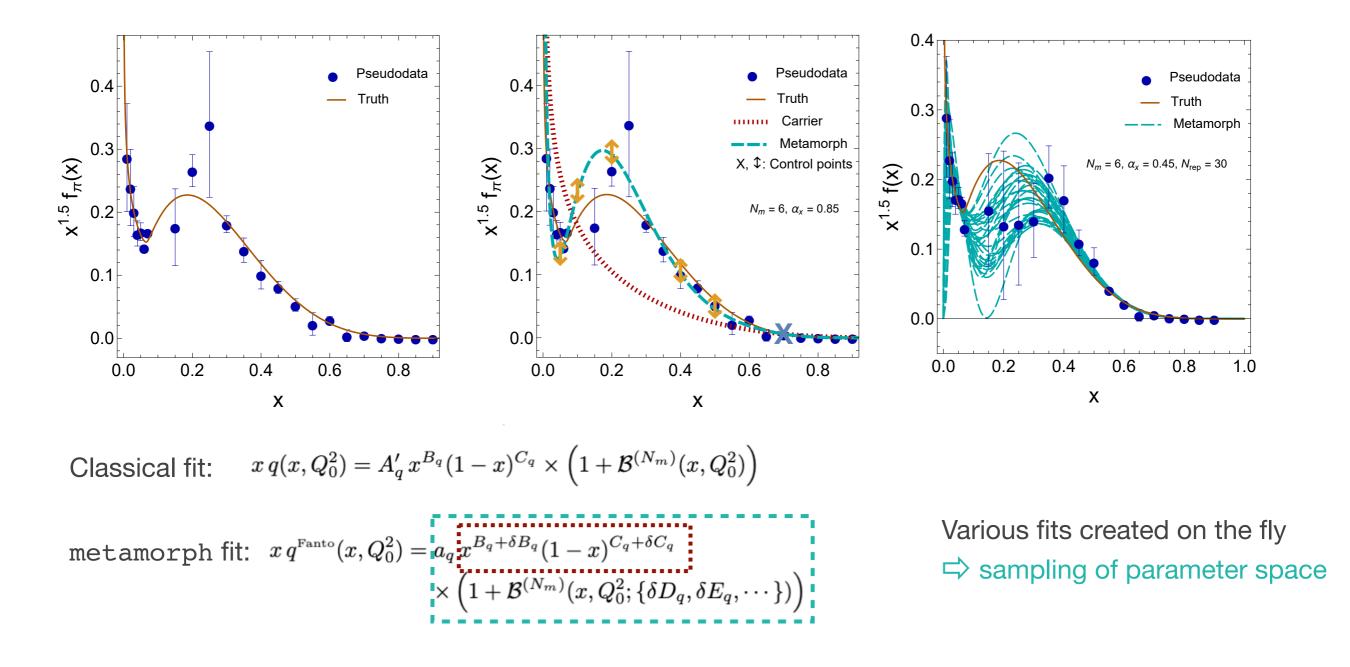
We parametrize the Bézier coefficients as the shifts of the position of the control points:

$$P_i = \mathcal{B}(x_i) \to P'_i = \mathcal{B}(x_i) + \delta \mathcal{B}(x_i)$$
  
$$\to \underline{P}' = (\mathcal{B}_0(x_1) + \delta D, \mathcal{B}_0(x_2) + \delta E, \cdots)$$



Exploit polynomial mimicry to systematically improve and flexibilize parametrization of PDFs.

→ Fantômas4QCD program



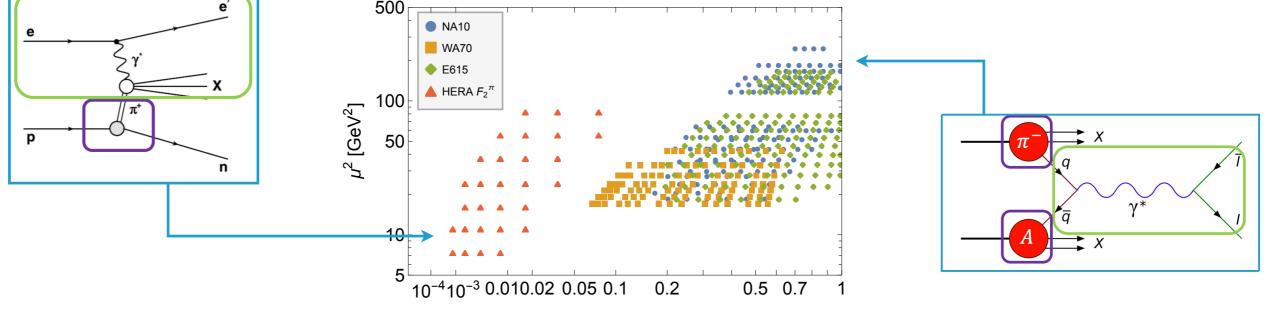
We use the xFitter framework, in which metamorph was implemented as an independent parametrization.

We also extend the xFitter data:

pion-induced Drell-Yan 0

 $\rightarrow$  constraints valence PDF at large x

- prompt photons  $\overline{\mathbf{O}}$
- 0
- $\rightarrow$  may constrain gluon PDF at largish x
- <u>leading neutron (Sullivan process</u>)  $\rightarrow$  only constraints on sea and gluon at  $x \leq 0.1$

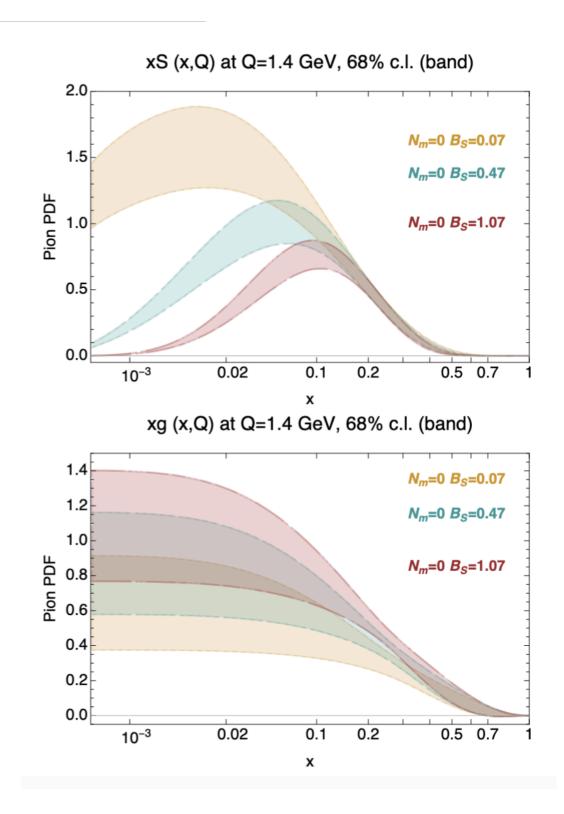


# Drell-Yan only analysis

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 within xFitter uncertainty.

<u>Need for complementary processes</u> <u>universality and flavor separation – EIC</u> <u>and JLab22(?)</u>



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

We also extend the xFitter data:

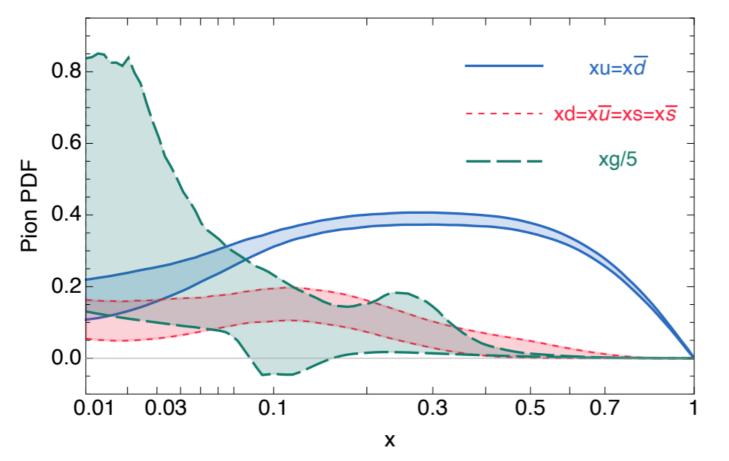
pion-induced Drell-Yan

 $\rightarrow$  constraints valence PDF at large *x* 

prompt photons

- $\rightarrow$  may constrain gluon PDF at largish *x*
- <u>leading neutron (Sullivan process</u>)  $\rightarrow$  only constraints on sea and gluon at  $x \leq 0.1$

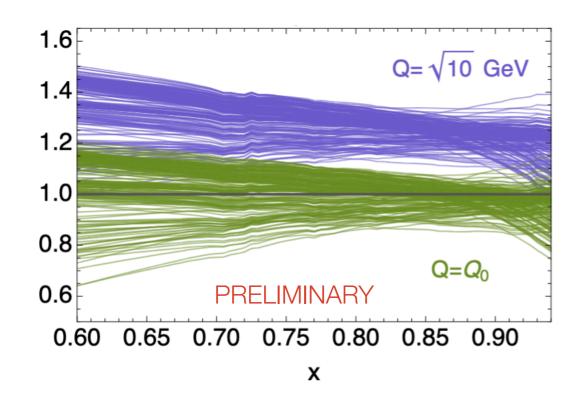
### $\pi^+$ PDFs at Q=2. GeV, 68% c.l. (band)



For a selection of  $\{N_m, CP\}$  sets. Bundled uncertainty with mcgen [Gao & Nadolsky, JHEP07]

[Kotz, Ponce-Chávez, **AC**, Nadolsky & Olness, <u>soon</u>] Proceedings in 2309.00152.

\_\_\_\_LFTC workshop 23



At NLO (MSbar), the valence PDF is well determined at large x $\Rightarrow$  doesn't fall very much like  $(1 - x)^2$  $\Rightarrow$  very similar to JAM and xFitter at large x

Corrective terms might need to be taken into account [large-x resummation]. JAM did and found an exponent between 1 to ~2.5, depending on the prescription [JAM, PRL127].

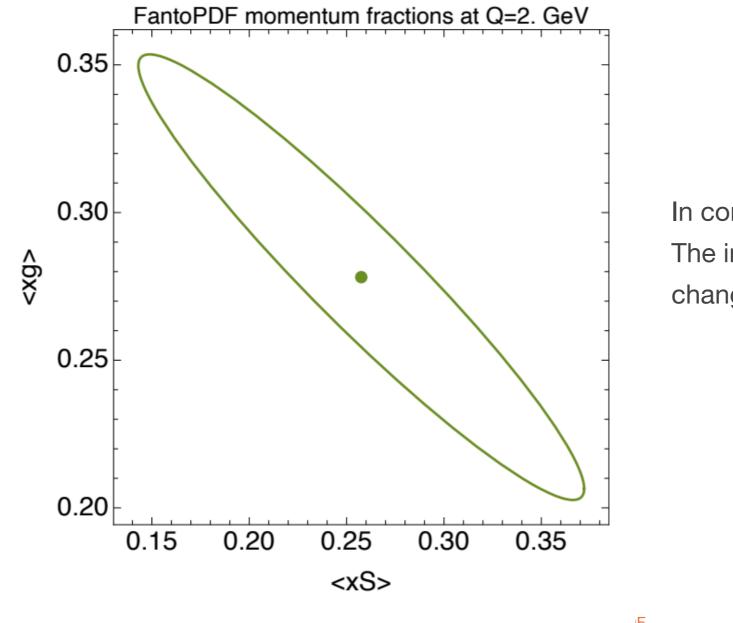
Lattice studies contribute to the information on hadron structure. Mindful analysis of the determination of the effective exponent of the PDF fall-off on the lattice [Gao et al., PRD102].

➡ inverse problem

# The Fantômas pion PDF

Towards epistemic uncertainty: sampling over parameter space more representative

Momentum-fraction distributions for gluon and sea are largely (anti)-correlated.



In contrast with the findings of JAM: The inclusion of LN data does not drastically change the momentum fractions.

\_LFTC workshop 23

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



➡ End-point behavior of pion distributions seems to follow the trend given by mass generation vs. quark-counting rules.

Uncertainty quantification in non-perturbative calculations? At what Q will pQCD (constraints) take over?

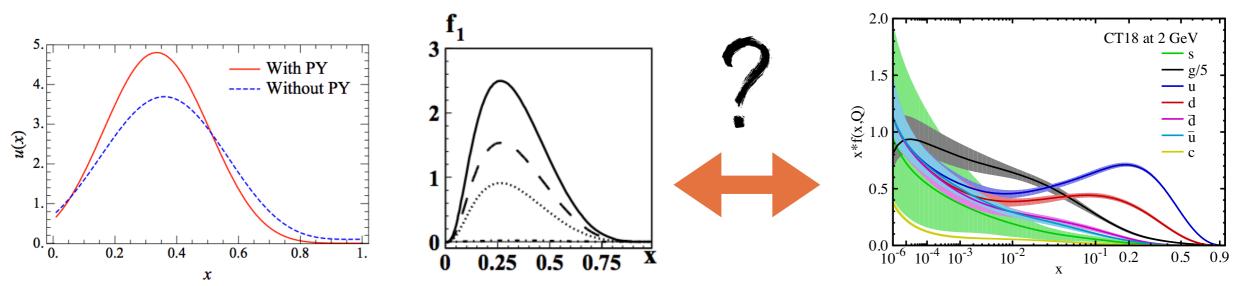


\_Morelia 23



How to compare phenomenological distribution functions to nonperturbative manifestations or behaviors that are characteristic of models for hadron structure?

#### But pheno PDFs cannot validate those specifics so easily



Behaviors in e.g. MIT bag model, light-cone constituent quark model, ...

Global analysis groups: CT (illustrated), MSHT, NNPDF, JAM,...

#### Hypothesis testing from phenomenological PDF:

- $\Rightarrow$  for local true or false statements
- ⇒ for functional behavior constraints

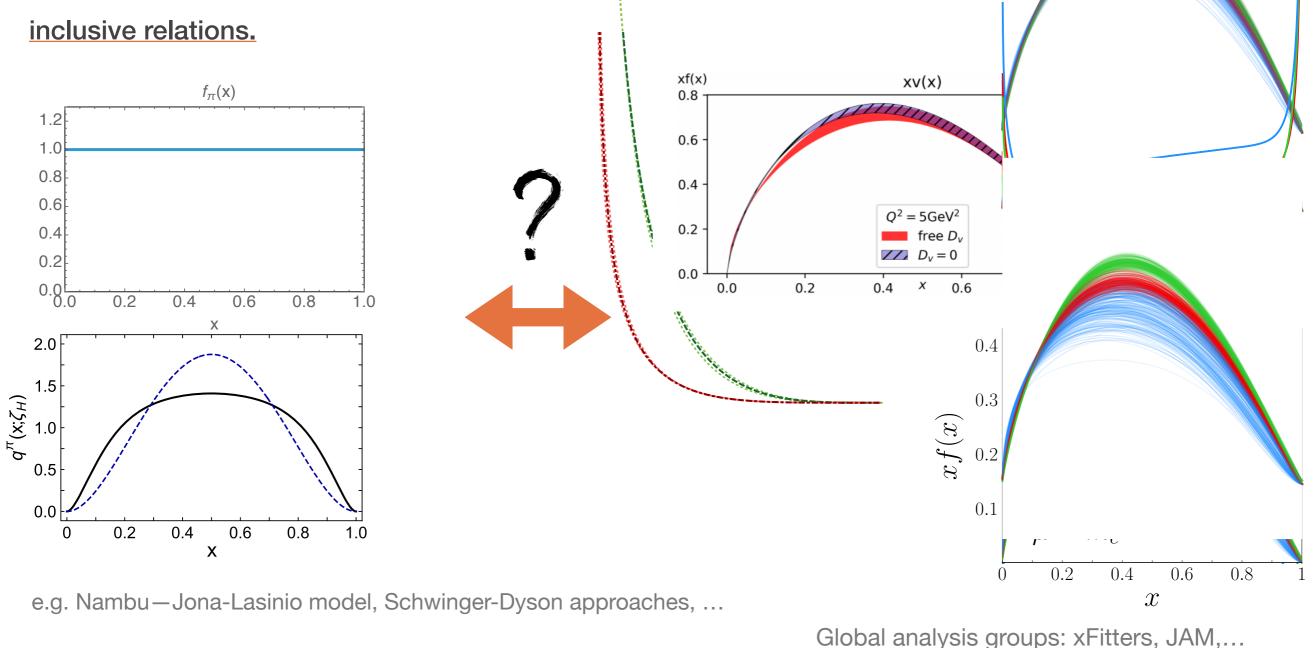
[AC & P. Nadolsky, Phys.Rev.D 103 (2021)]

\_Morelia 23

# Model inputs and connection to phenomenology: the pion

Pion PDFs are closely related to the dynamics of QCD in non-perturbative

Trickier interpretation due to its pseudo-Goldstone nature and ansatze for exclu

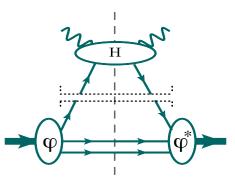


A. Courtoy-IFUNAM\_\_\_\_\_Fantômas4QCD: the pion PDF\_\_\_\_\_Morelia 23

# Can we test quark counting rules with pheno PDFs?

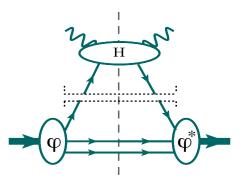
Early-QCD predicted behavior for structure functions when one quark carries almost all the momentum fraction:

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



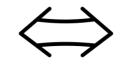
Can we test quark counting rules with pheno PDFs?

Early-QCD predicted behavior for structure functions when one quark carries almost all the momentum fraction:  $f_{q_v/P}(x) \xrightarrow[x \to 1]{} (1-x)^3, \qquad f_{q_v/\pi}(x) \xrightarrow[x \to 1]{} (1-x)^2$ 



## **Evidence of polynomial form**

There is more than one possible solution to the choice of functional form.



## Agreement of model with data

Uncertainties needed for a faithful conclusion.

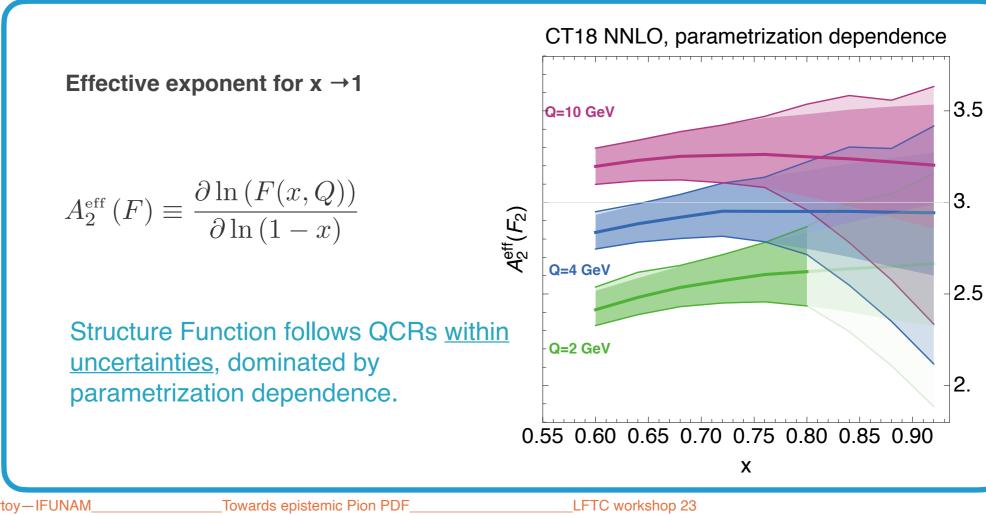
Can we test quark counting rules with pheno PDFs?

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

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



Uncertainties needed for a faithful conclusion.



## **Evidence of polynomial form**

There is more than one possible solution to the choice of functional form.



# State-of-the-art of the pion at large *x*

### Polynomial mimicry prevents functional behaviors from being validated as if and only if conditions.

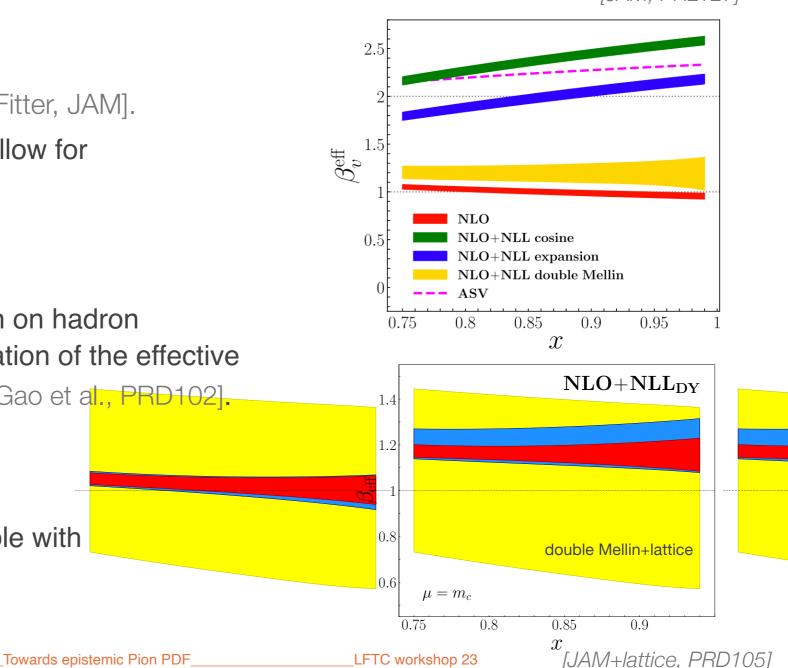
Mathematical equivalence of polynomials of different orders can be illustrated with Bézier curves. QCD corrections, at low and large  $Q^2$ , also inhibit the  $(1 - x)^{\beta}$  power to be tested.

Most global analyses find A<sub>2,eff</sub> ( $\beta_{eff}$ ) ~1 [xFitter, JAM]. Corrections from threshold resummation allow for A<sub>2,eff</sub> ( $\beta_{eff}$ ) from 1 to ~2.5.

Lattice studies contribute to the information on hadron structure. Mindful analysis of the determination of the effective exponent of the PDF fall-off on the lattice [Gao et al., PRD102]. ⇒ inverse problem

Pheno and lattice PDF of the pion compatible with within uncertainties.

A. Courtoy—IFUNAM



## ${\ensuremath{^{\circ}}}$ at hadronic scale $\mu_0^2 < 1 \, {\rm GeV}^2$

⇒ prefactorization picture

⇒ nonperturbative dynamics

 $\Rightarrow$  model's degrees of freedom

**at factorization scale**  $\mu^2 > 1 \, \text{GeV}^2$ 

⇒ quasi-free partonic degrees of freedom

⇒ defined in the MSbar scheme

 $\Rightarrow$  leading-power approximation to full dynamics

## • at hadronic scale $\mu_0^2 < 1 \, {\rm GeV}^2$

⇒ prefactorization picture

- ⇒ nonperturbative dynamics
- ⇒ model's degrees of freedom

(a) at factorization scale  $\mu^2 > 1 \, {\rm GeV}^2$ 

⇒ quasi-free partonic degrees of freedom

 $\Rightarrow$  defined in the MSbar scheme

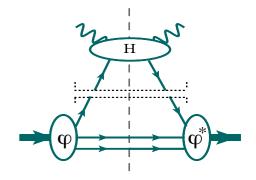
⇒ leading-power approximation to full dynamics

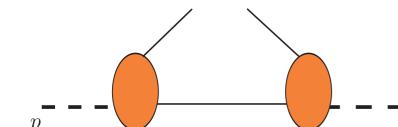
#### How to relate the x dependence of the perturbative and nonperturbative pictures?

Fantômas4QCD: the pion PDF

$$\int \frac{dz^{-}}{2\pi} e^{i(x-\frac{1}{2})z^{-}p^{+}} \langle \pi^{+}(p) | \bar{q} \left(-\frac{z}{2}\right) \not n \frac{1}{2} (1+\tau^{3}) q \left(\frac{z}{2}\right) | \pi^{+}(p) \rangle = \frac{1}{p^{+}} q(x)$$

A. Courtoy-IFUNAM



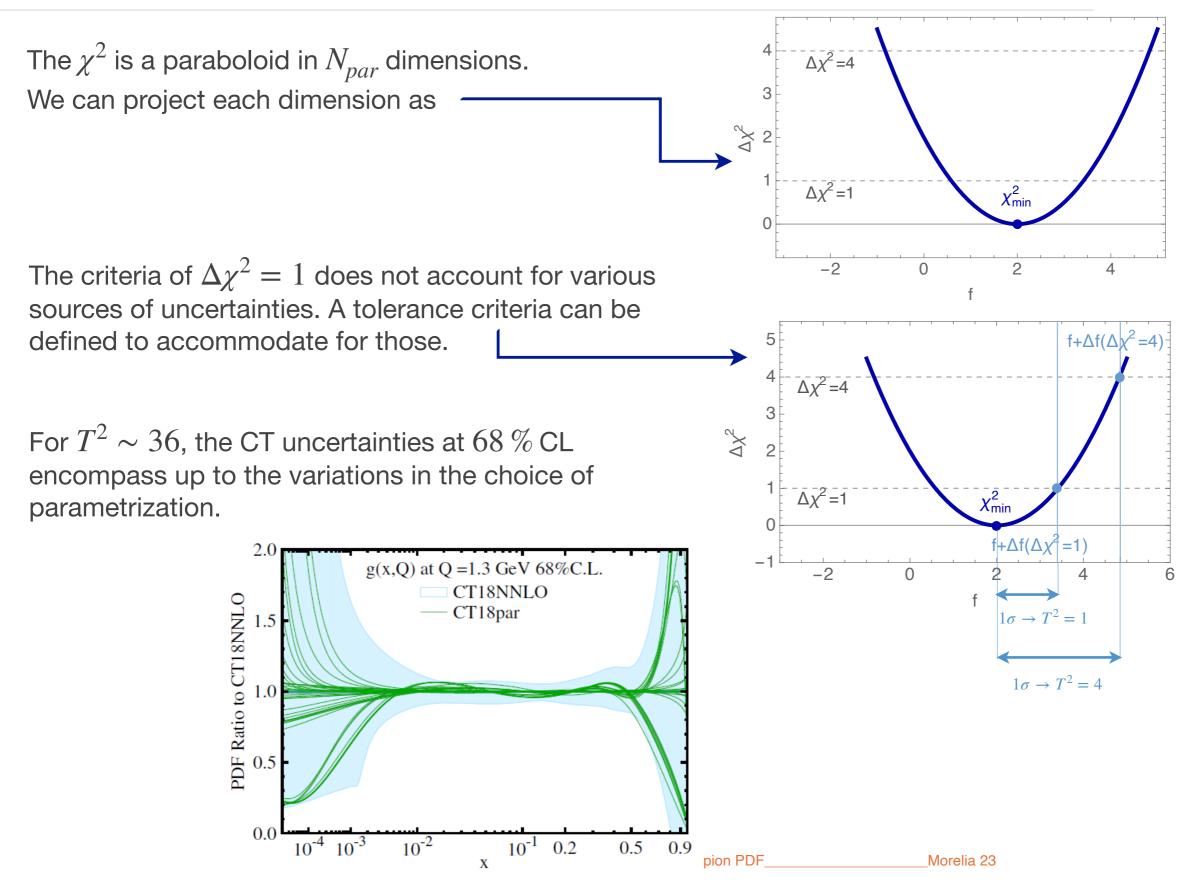


$$F(x_{\rm B}, Q^2) = \sum_a \int_{x_{\rm B}}^1 \frac{dx}{x} f_{a/p}(x, \mu^2) H_a\left(\frac{x_{\rm B}}{x}, \frac{\mu^2}{Q^2}\right) + \mathcal{O}(M/Q),$$

$$\sigma = \sum_{a,b} \int dx_a \int dx_b f_{a/A}(x_a, \mu_{\rm F}^2) f_{b/B}(x_b, \mu_{\rm F}^2) H_{a,b,x_a,x_b,\mu_{\rm F}^2}$$

Morelia 23

 $+ \mathcal{O}(M/Q)$ 

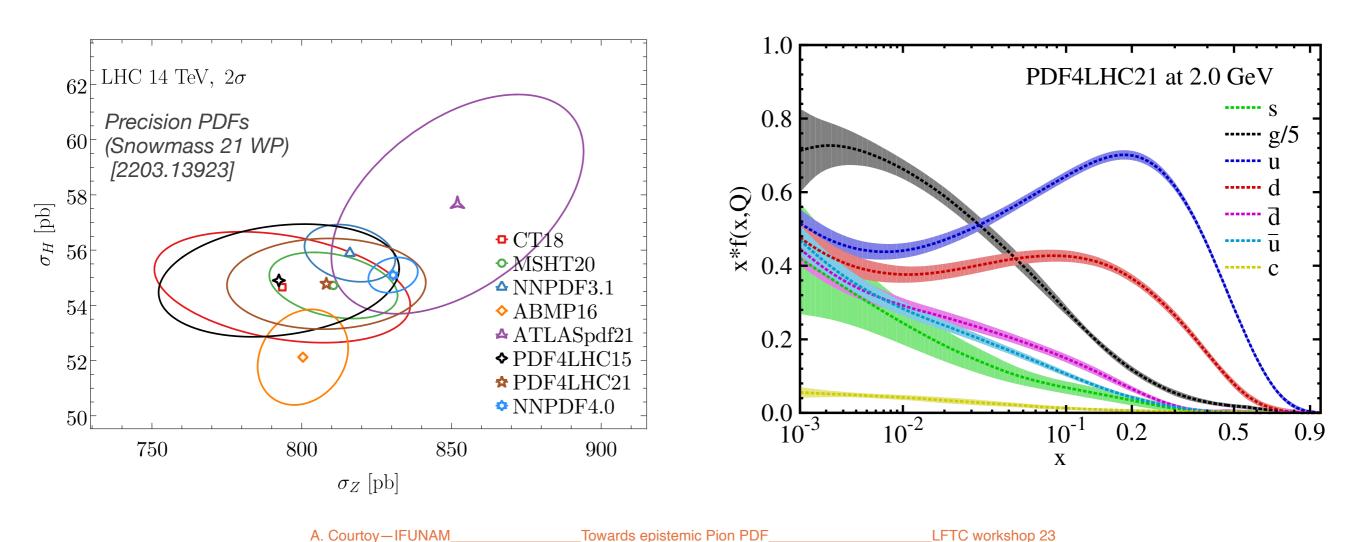


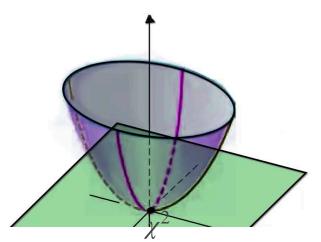
Recent advancements in the determination of unpolarized PDFs: CT18, MSHT20, NNPDF4.0, ATLASpdf21 as well as PDF4LHC21.

#### PDF4LHC21:

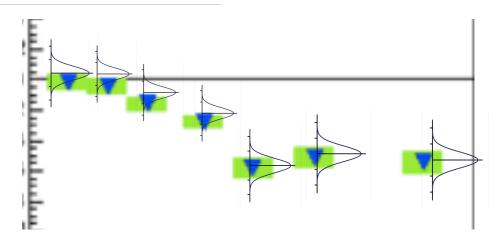
benchmarking and combination of the leader PDF sets, CT, MSHT & NNPDF, for the run III of the LHC.

[Ball, [...], AC, et al, J.Phys.G 49 (2022)]



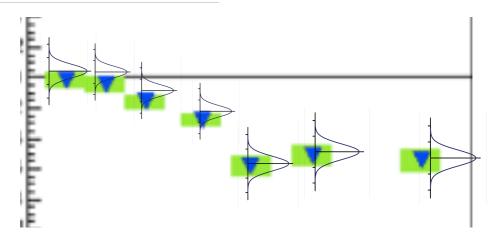


Hessian methodology finds the global minimum and explores the parameter space.

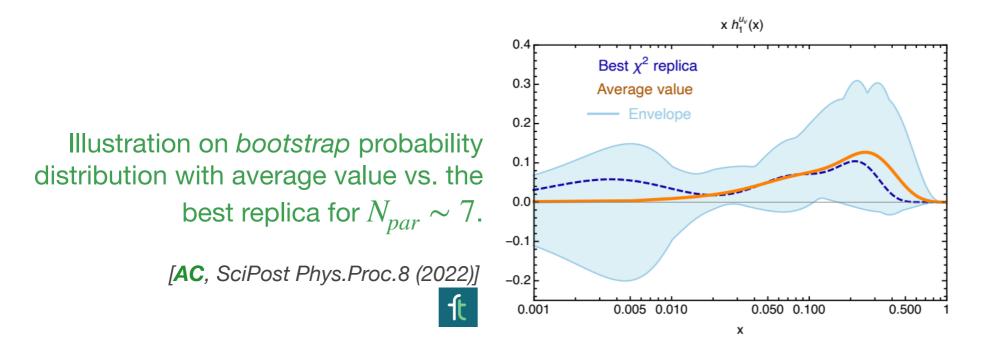


Monte-Carlo methodology (neural network, AI/ML) replicates fluctuated data, then optimizes each replica (up to training).

Hessian methodology finds the global minimum and explores the parameter space.



Monte-Carlo methodology (neural network, AI/ML) replicates fluctuated data, then optimizes each replica (up to training).



In multivariate analyses, sampling occurs at various levels — parameter space, bootstrap but also priors, ... In large-dimensional problems, sampling is complex.

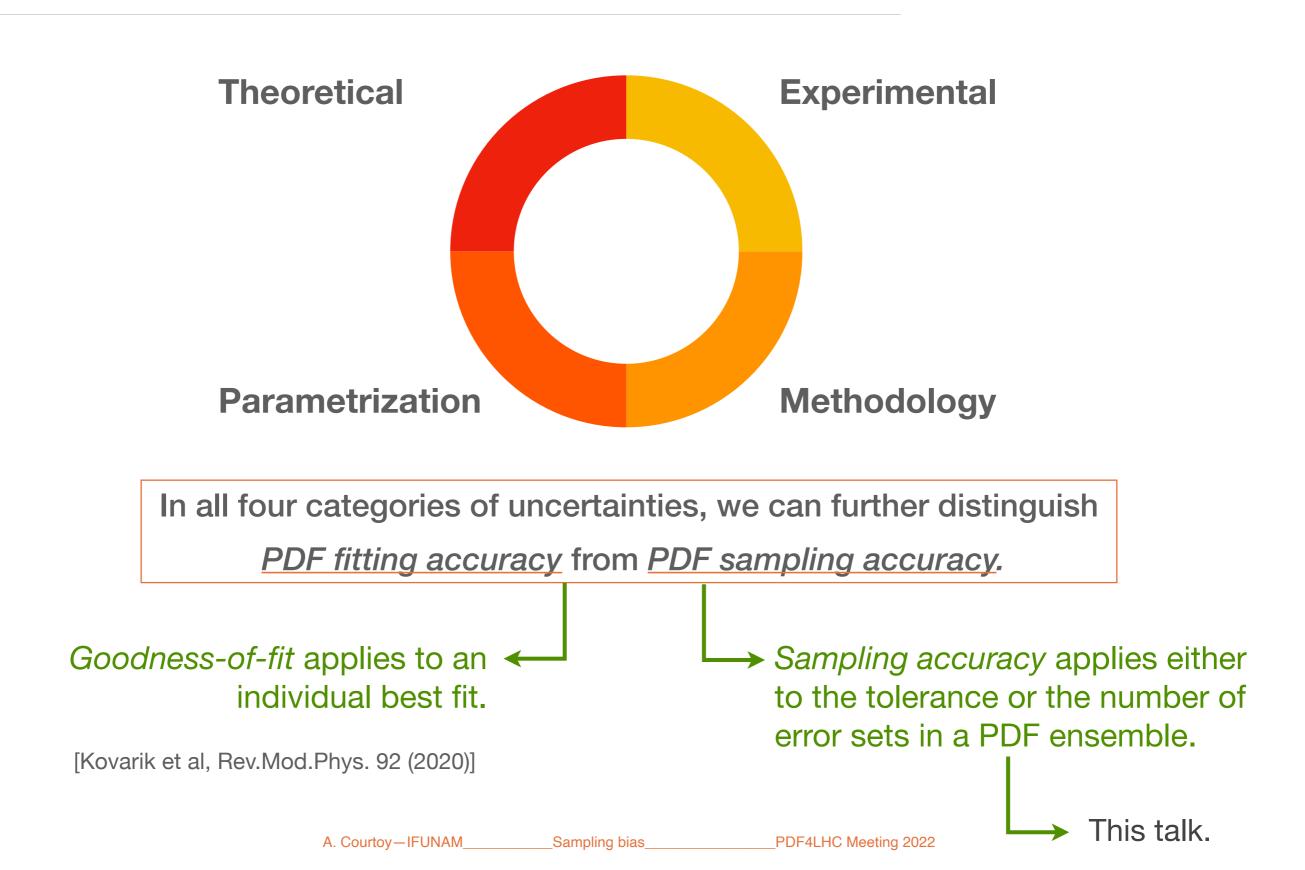
Towards epistemic Pion PDF

# The tolerance puzzle and the big-data paradox

Outside of HEP, there is significant interest in statistical problems that are similar to the PDF tolerance problem. These studies introduce a fundamental distinction between the <u>fitting uncertainty</u> and <u>sampling uncertainty</u>, often overlooked in the PDF fits.

Article Unrepresentative big surveys significantly overestimated US vaccine uptake <u>Nature</u> v. 600 (2021) 695	
https://doi.org/10.1038/s4158 Received: 18 June 2021	Valerie C. Bradley <sup>1,6</sup> , Shiro Kuriwaki <sup>2,6</sup> , Michael Isakov <sup>3</sup> , Dino Sejdinovio <sup>1</sup> , Xiao-Li Meng <sup>4</sup> & Seth Flaxman <sup>511</sup>
	SCIENCE ADVANCES   RESEARCH ARTICLE
	MATHEMATICS
	Models with higher effective dimensions tend to produce more uncertain estimates
	Arnald Puy <sup>1,2,3</sup> *, Pierfrancesco Beneventano <sup>4</sup> , Simon A. Levin <sup>2</sup> , Samuele Lo Piano <sup>5</sup> , Tommaso Portaluri <sup>6</sup> , Andrea Saltelli <sup>3,7</sup>
The Big Data Paradox in Clinical Practice Pavlos Msaouel To cite this article: Pavlos Msaouel (2022) The Big Data Paradox in Clinical Practice, Cancer Investigation, 40:7, 567-576, DOI: <u>10.1080/07357907.2022.2084621</u>	
Investigation, 40	7, 567-576, DOI: <u>10.1080/07357907.2022.2084621</u>

A new avenue to understand PDF tolerance



# Sampling bias in PDF global analyses—I

How do we know the "data+sampling defect=confounding correlation" of our analysis?

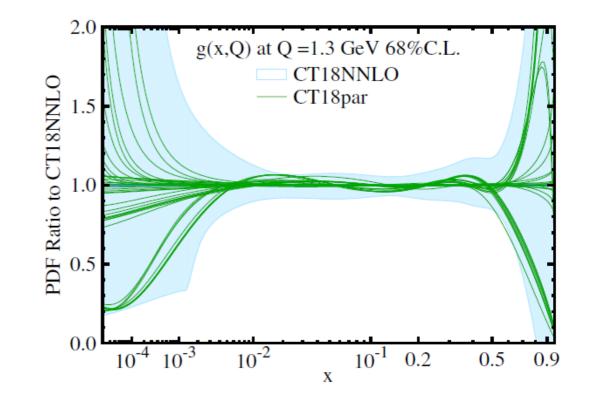
#### Hessian-based analysis:

objective function includes penalties, establishing the tolerance criteria.

Size of uncertainties reflect a series of confounding sources —selection of fitted experiments, treatment of correlated systematic errors, functional forms of PDFs, ...

<u>Verification</u> that proper spanning of parameter space is compatible with total uncertainties (*a posteriori*). >300 functional forms are tested in CT18.

**Dimensions** of the problem given by the number of parameters=eigenvector (EV) directions.



Sampling bias\_\_\_\_\_

# Sampling bias in PDF global analyses—II

## How do we know the "data+sampling defect=confounding correlation" of our analysis?

### Monte Carlo-based analysis:

### optimization implies selection of hyperparameters

The usage of Neural Networks had as primary goal eliminating the biases associated with the choice of a specific functional form.

However, there are still many choices associated with the optimization:

- Number and with of the layers
- Activation functions and initialization
- Optimization algorithm (and associated parameters)
- Training length, stopping patience, etc.
- Strength of lagrange multipliers (positivity, integrability)

Collectively called "hyperparameters", usually selected manually.



Sampling bias



## Do we understand sampling for QCD global analyses?

Sampling of multidimensional spaces ( $d \gg 20$ ) is exponentially inefficient and may require  $n > 2^d$ replicas to obtain a convergent expectation value.

In general, an intractable problem.

[Hickernell, MCQMC 2016, 1702.01487] [Sloan, Wo'zniakowski, 1997]

# Do we understand sampling for QCD global analyses?

Sampling of multidimensional spaces ( $d \gg 20$ ) is exponentially inefficient and may require  $n > 2^d$  replicas to obtain a convergent expectation value.

In general, an intractable problem.

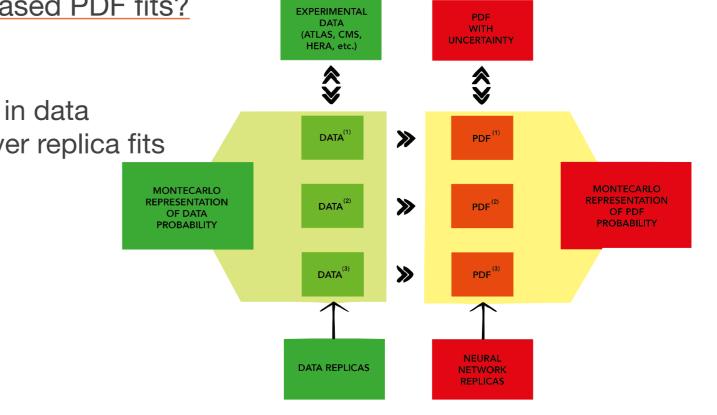
[Hickernell, MCQMC 2016, 1702.01487] [Sloan, Wo´zniakowski, 1997]

- 1. Justification for tolerance criteria for Hessian-based PDF fits
- 2. How is sampling achieved in Monte Carlo-based PDF fits?

Importance sampling, as defined by NNPDF

- =bootstrap/resampling of random fluctuations in data
- expectations are then unweighted averages over replica fits

Such sampling does not include sampling over hyperparameters and priors.



# Do we understand sampling for QCD global analyses?

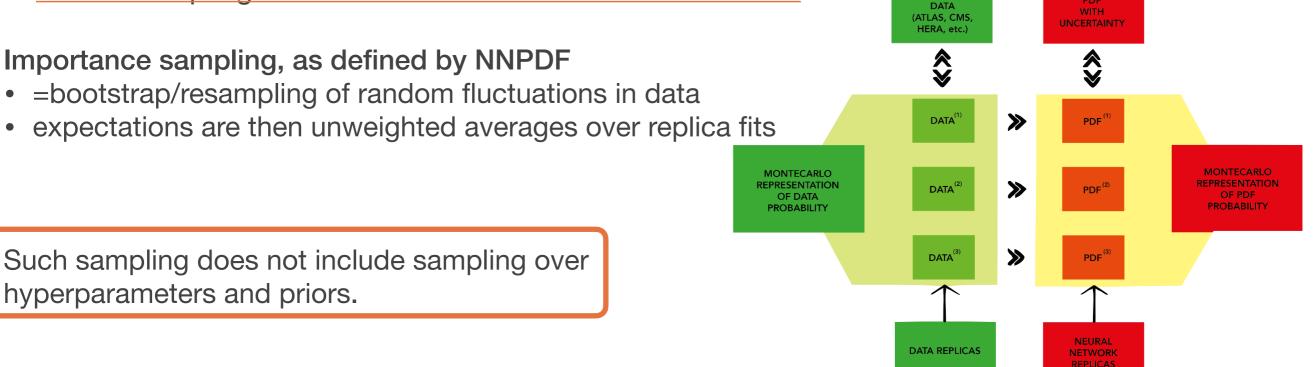
Sampling of multidimensional spaces ( $d \gg 20$ ) is exponentially inefficient and may require  $n > 2^d$  replicas to obtain a convergent expectation value.

In general, an intractable problem.

[Hickernell, MCQMC 2016, 1702.01487] [Sloan, Wo´zniakowski, 1997]

PDF

- 1. Justification for tolerance criteria for Hessian-based PDF fits
- 2. How is sampling achieved in Monte Carlo-based PDF fits?



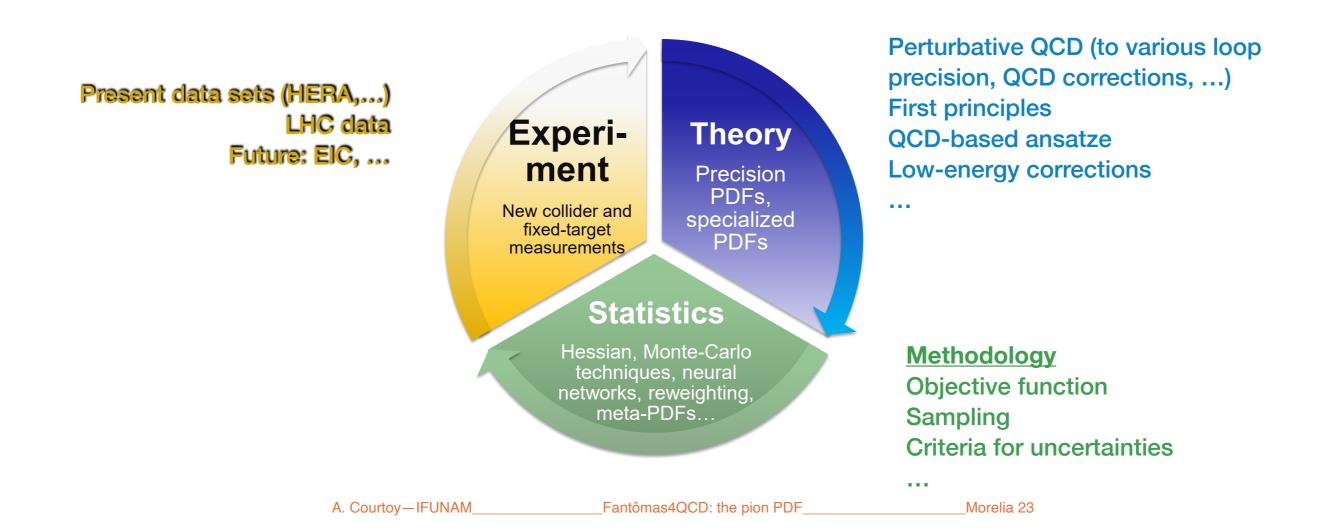
**EXPERIMENTAL** 

# Global analyses of unpolarized PDF — CT

The **C**oordinated **T**heoretical-**E**xperimental project on **Q**CD (CTEQ) is a high-energy physics collaboration whose efforts include *fits* of unpolarized PDFs. This is done in the **C**TEQ-**T**ung et al (CT) group.

CT is a renown fitting group, whose PDF sets are widely used in colliders, ...

Leading the characterization of uncertainties in PDF analyses and on the connection to nuclear physics (relevant for EIC and JLab physics).



# Global analyses of unpolarized PDF — CT

## The CTEQ-Tung et al (CT) group.

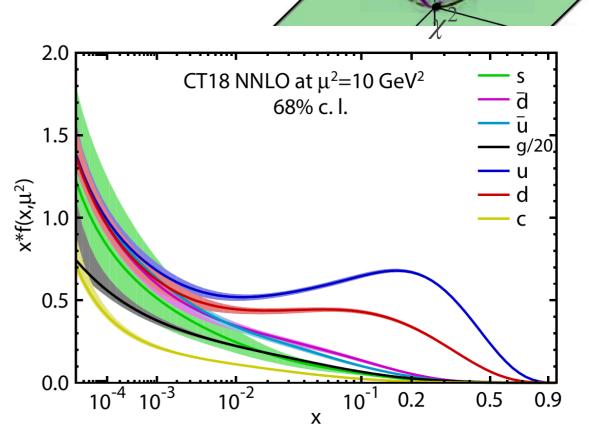
CTEQ-TEA members (as of 2023)

China: S. Dulat, J. Gao, T.-J. Hou, I. Sitiwaldi, M. Yan, and collaboratorsMexico: A. CourtoyUSA: T.J. Hobbs, M. Guzzi, J. Huston, P. Nadolsky, C. Schmidt, D. Stump, K. Xie,

### The CTEQ-Tung et al (CT) PDF set.

CT18 is the latest released PDF set.

CT methodology is based on minimizing a  $\chi^2$  expressed in terms of *parametrizations* for the PDFs, finding the global minimum and propagating the uncertainty through the Hessian formalism.



[Hou et al, Phys.Rev.D 103 (2021)]

# Hypothesis testing: role of uncertainties

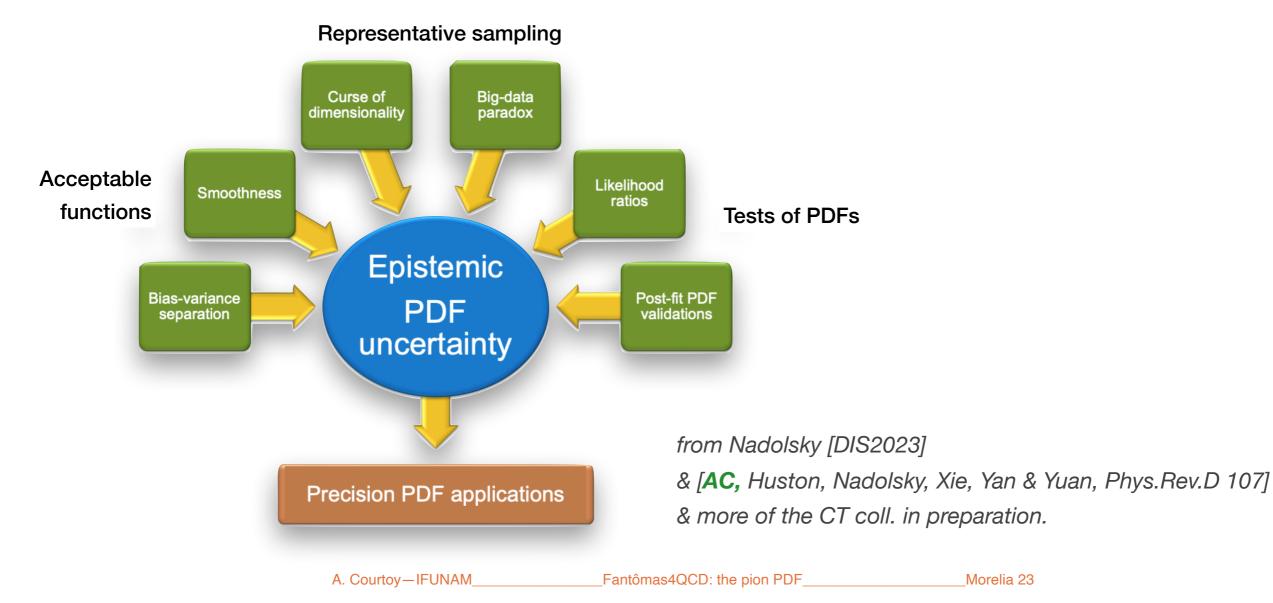
### Hypothesis testing of theoretical predictions relies on

- available data in x range, as well as value of Q, 1.
- sensitivity of data to the hypothesis, 2.
- quality of the data, 3.
- uncertainties found in the fits. 4.

# Hypothesis testing: role of uncertainties

Hypothesis testing of theoretical predictions relies on

- 1. available data in x range, as well as value of Q,
- 2. sensitivity of data to the hypothesis,
- 3. quality of the data,
- **4.** uncertainties found in the fits.

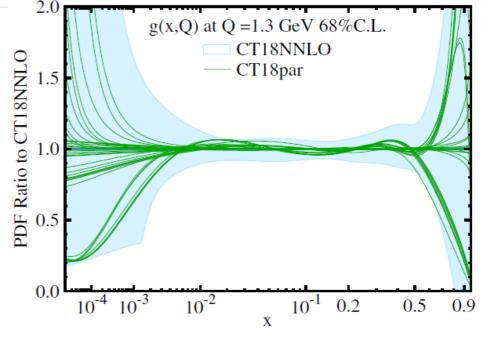


# Hypothesis testing: role of uncertainties

Representative sampling

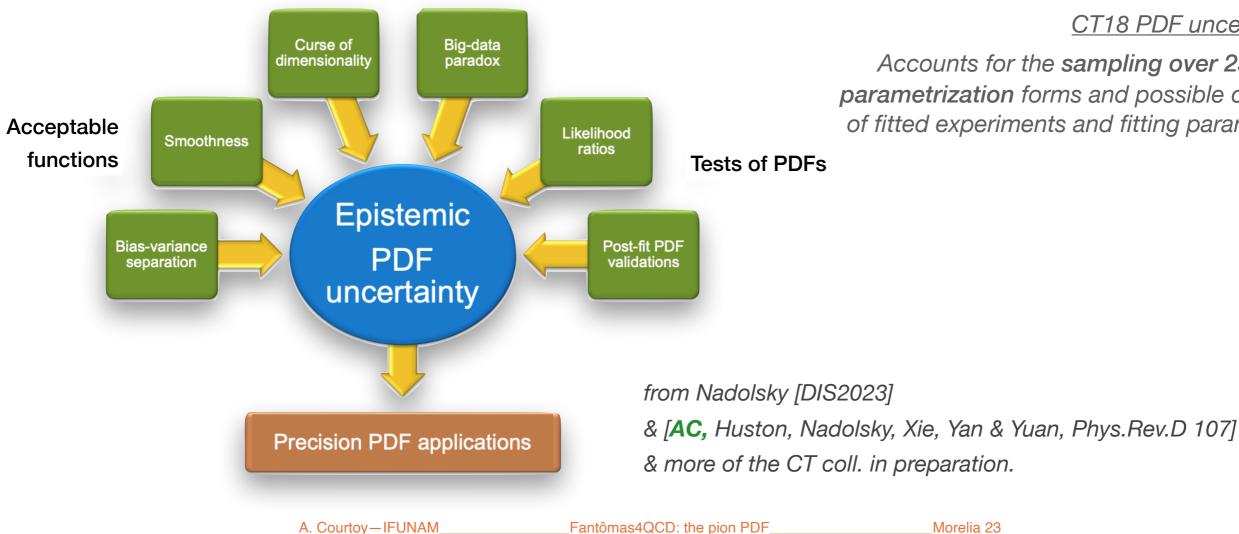
Hypothesis testing of theoretical predictions relies on

- available data in x range, as well as value of Q, 1.
- sensitivity of data to the hypothesis, 2.
- quality of the data, 3.
- uncertainties found in the fits. 4.

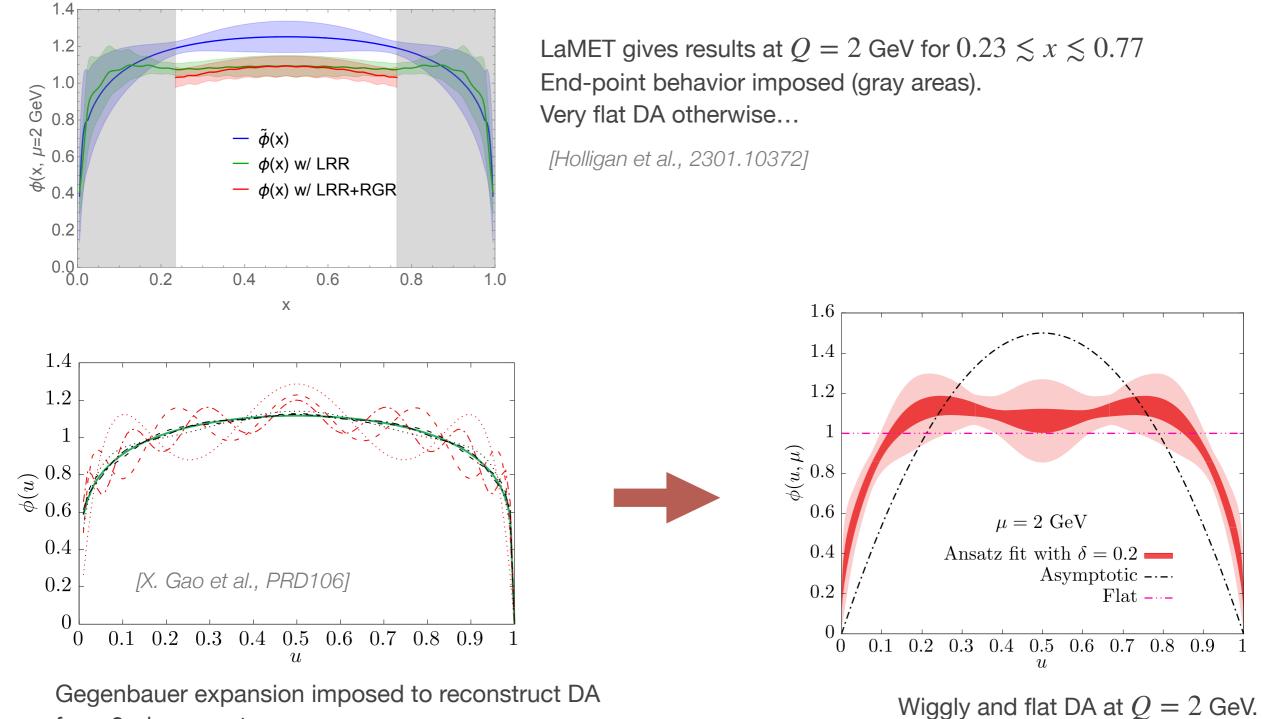


### CT18 PDF uncertainty:

Accounts for the sampling over 250-350 parametrization forms and possible choices of fitted experiments and fitting parameters.



## Pion objects and the inverse problem

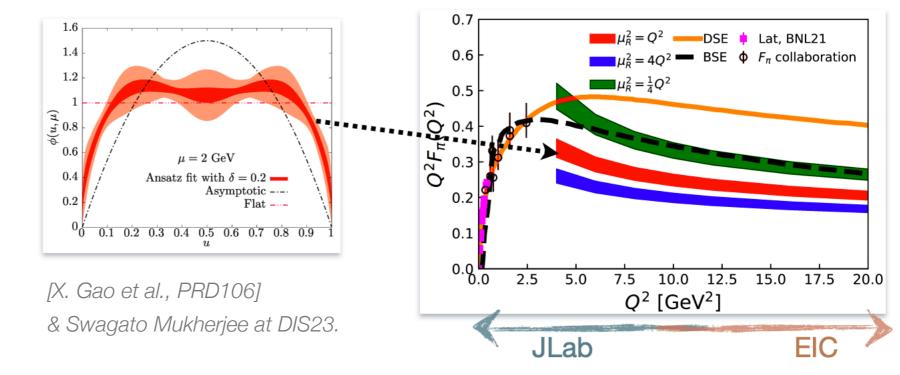


from 2nd moment

Second moment at Q = 2 GeV similar to NJL at  $Q_0$  !

## Pion objects and the inverse problem: convergence at end point.

Chiral symmetry seems to control the pion DA well over the Q spectrum.



#### Large-*x* convergence of the evolved pion DA seems to be key to problem.

