Uncertainty quantification in lattice determinations of unpolarised PDFs

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PDFLattice 2024 Workshop

QUARK-GLUON TOMOGRAPHY COLLABORATION

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The ‘spirit’ of this talk

My charge:

“provide an overview on the uncertainty quantification in lattice-QCD unpolarized-PDF--related calculations. Emphasizing broader aspects of the topic and highlighting unresolved issues and future challenges would be appreciated…”

I proceed under the assumptions that:

1. a) Quantification of “standard” lattice uncertainties (discretisation, finite volume, excited state contamination) is an internal matter for lattice theorists
   b) New technical developments thoroughly reviewed by M. Constantinou

   See, M. Constantinou’s talk

   c) These uncertainties will reach the few percent level in the next five years (at least, pointwise in the relevant distribution space)
2. Uncertainties related to the Fourier transform inverse problem, finite momentum and factorisation are of primary interest to this audience

Outline

Numerics

Fourier transforms

Factorisation

Distributions from the lattice perspective

$$\langle H(P)|\overline{\psi}(n^{\alpha})W^{(f)}(n,0)\psi(0)|H(P)\rangle$$

Distributions from the lattice perspective

$$f^{(0)}_{q/H}(x) = \int_{-1}^{1} \frac{\mathrm{d}\xi^-}{4\pi} e^{-i\xi^- x P^+} \langle H(P)|\overline{\psi}(n^\alpha) W^{(f)}(n,0)\psi(0)|H(P)\rangle$$

PDFs

$n^2 = 0$ ξ^-

$$\langle H(P)|\overline{\psi}(n^\alpha) W^{(f)}(n,0)\psi(0)|H(P)\rangle$$

Distributions from the lattice perspective

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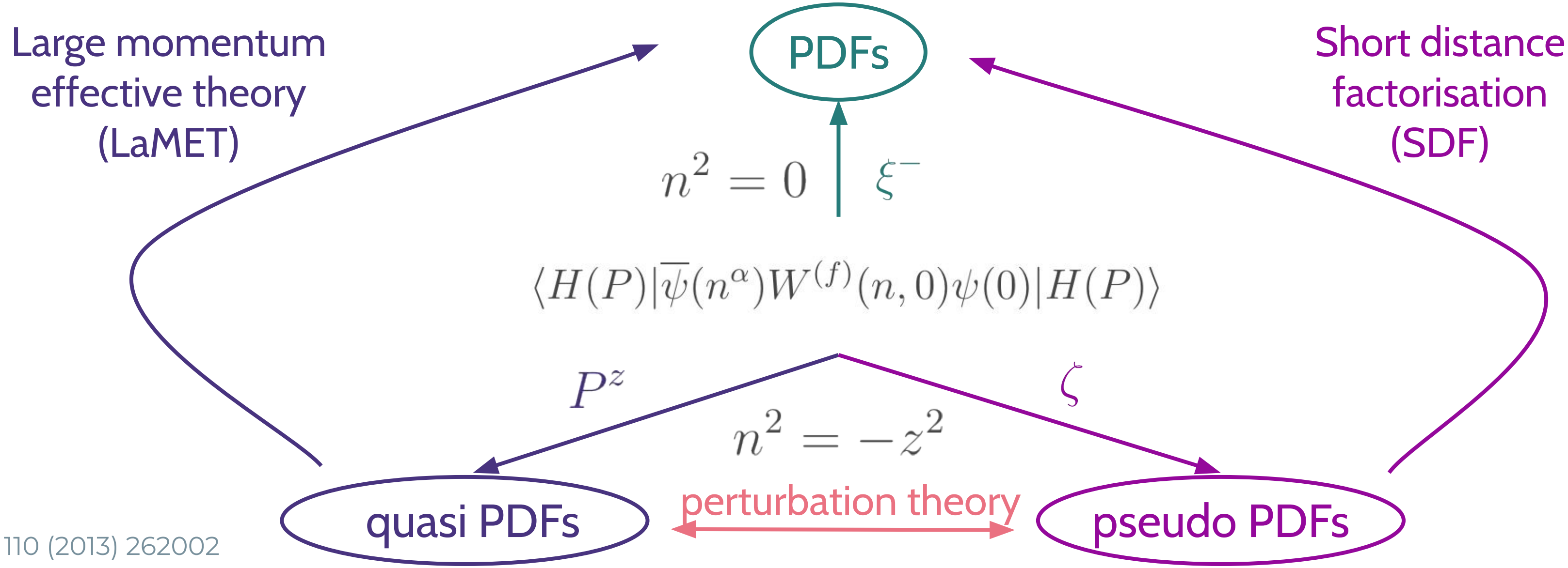

Ji, PRL 110 (2013) 262002

$$\widetilde{f}^{(0)}_{j/H}(\xi, P^z) = \int_{-\infty}^{\infty} \frac{\mathrm{d}z}{4\pi} e^{i\xi P_z z} \langle H(P)\left|\overline{\psi}(0,z,\mathbf{0}_\mathrm{T}) W(z,0)\Gamma_j \psi(0)\right| H(P)\rangle$$

$$\widetilde{p}^{(0)}_{j/H}(\xi, z^2) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\zeta}{4\pi} e^{i\xi\zeta} \langle H(P)\left|\overline{\psi}(0,z,\mathbf{0}_\mathrm{T}) W(z,0)\Gamma_j \psi(0)\right| H(P)\rangle$$

Radyushkin, PRD 96 (2017) 034025

Distributions from the lattice perspective

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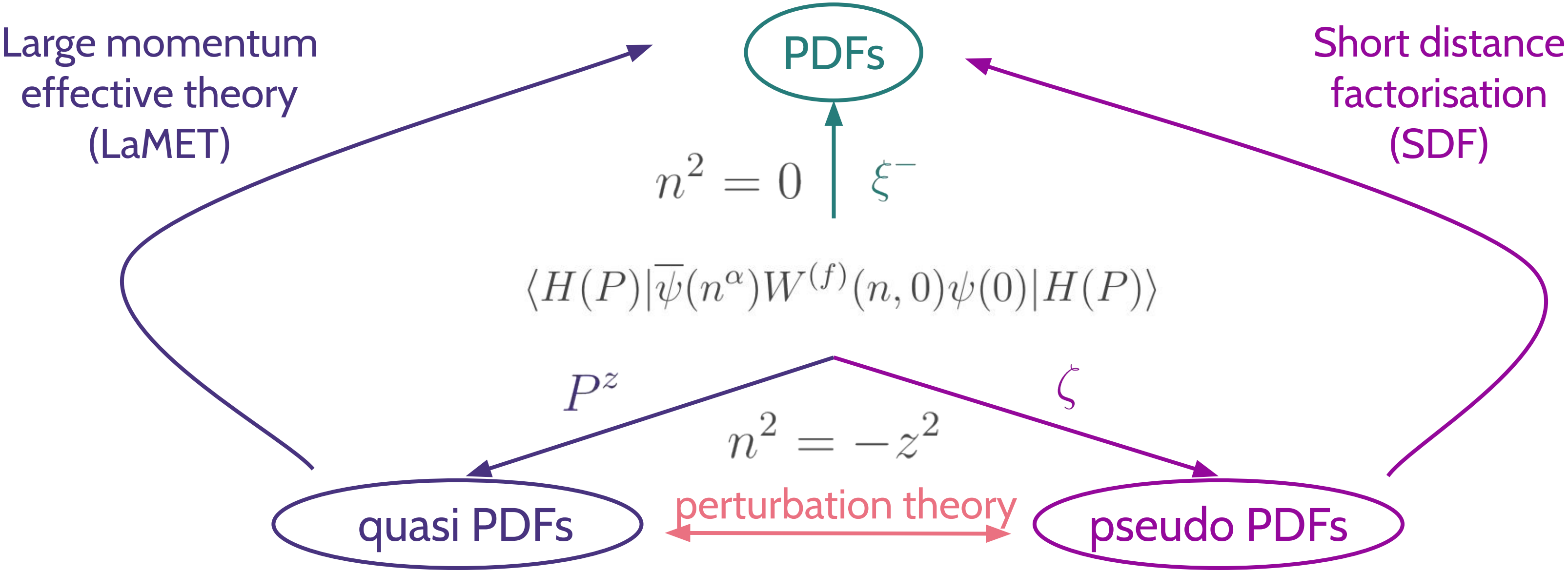


"How do we define the regimes of validity and equivalence between zP^z and $\xi^- P^+$?"

PDF reconstruction

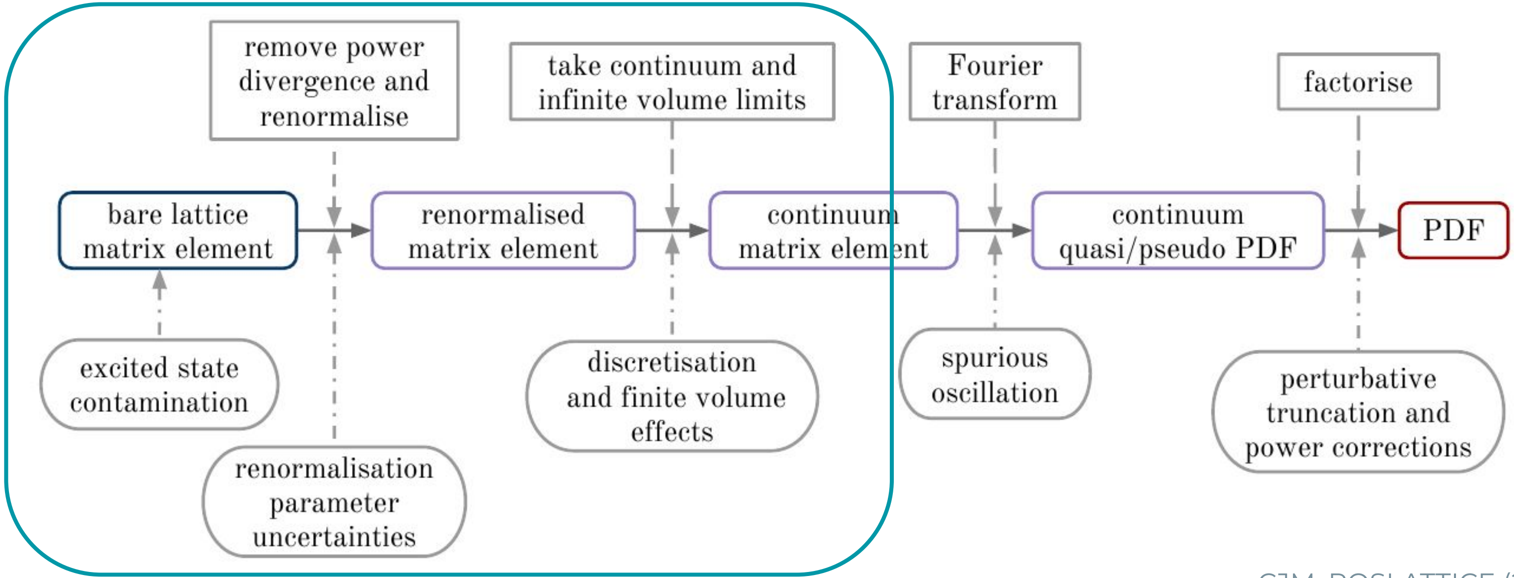
Extraction of light-cone PDFs from lattice QCD is a three-step process

1. Numerical determination of relevant matrix elements
2. Determination of quasi- and pseudo-PDFs via Fourier transform
3. Factorisation of light-cone PDF through LaMET or SDF

Numerical methods

Extraction of light-cone PDFs from lattice QCD is a “three-step” process

1. Numerical determination of relevant matrix elements



CJM, POSLATTICE (2018) 018

Fourier transforms and inverse problems

Extraction of light-cone PDFs from lattice QCD is a three-step process

1. Numerical determination of relevant matrix elements
2. Determination of quasi- and pseudo-PDFs via Fourier transform

an ill-posed inverse problem

Inverse problems:

"Starting with the effects to discover the causes"

Given a (forward) map *M(p)*, we want model parameters {*p*} that match observed data

$$d_{\text{obs.}} = M(p) \qquad \Rightarrow \qquad p = M^{-1}(d_{\text{obs.}})$$

Fourier transforms and ill-posed inverse problems

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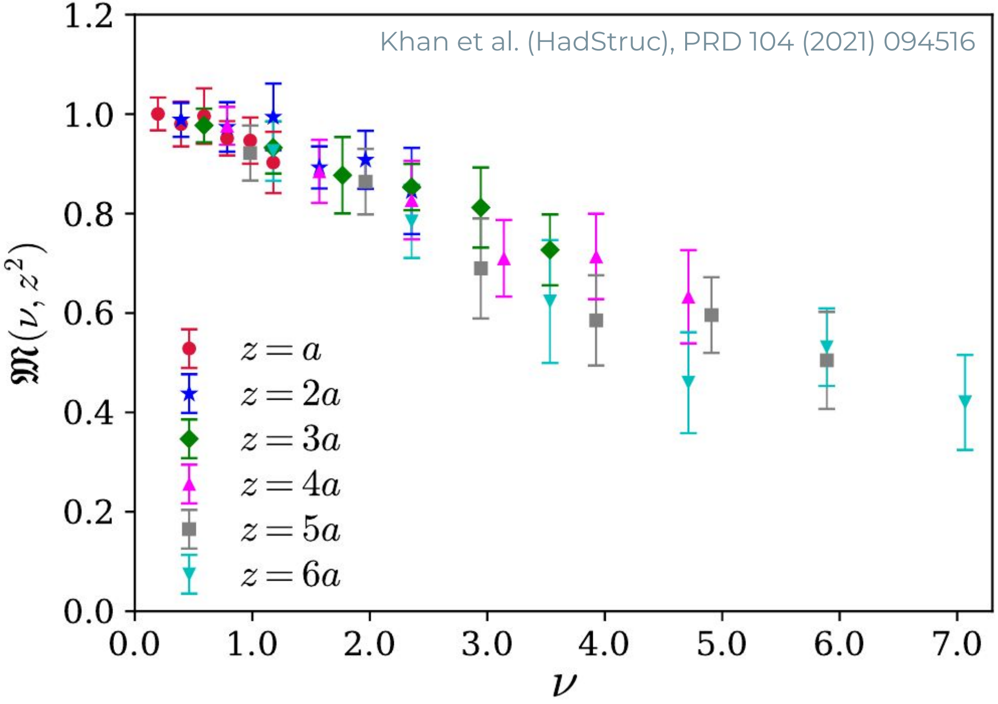
Ill-posed (according to Hadamard):

1. Existence - for any data, there exist parameters that fit the data
2. Uniqueness - *M* is injective (parameters are mapped uniquely to data)
3. Stability - M^{-1} is continuous (data are mapped smoothly to parameters)

Unfortunately…

Lattice data are:

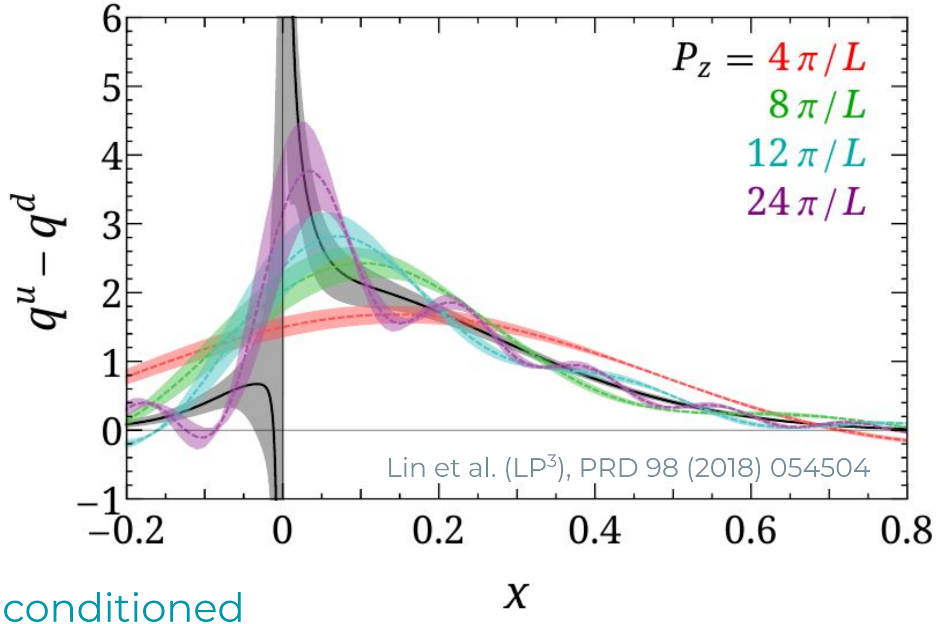
1. Statistically noisy
2. Subject to systematic biases
3. Limited in kinematic range



PDF reconstruction

Carrying out the Fourier transform is certainly an ill-posed problem

- fails criterion 2 (uniqueness)
- fails criterion 3 (stability)



And even the direct Fourier inversion is ill-conditioned

Karpie et al., JHEP 04 (2019) 057

Noise and ill-posed inverse problems

In the presence of noisy data, we can capture stability through stability estimates

$$|p_1 - p_2| \leq f(|M(p_1) - M(p_2)|)$$

Provides a numerical, but subjective, approach to ill-posedness:

- when noise is significantly amplified, the problem is ill-posed
- noise can also lead to data falling outside the range of *M(p)*

Natural to introduce noise through a modified forward map

$$d_{\text{obs.}} = M(p) + \eta$$

- statistical properties of noise become important
- Monte Carlo statistical uncertainty well-modelled by Gaussian noise
- less clear how to analytically model lattice systematic uncertainties

Overcoming noise

Three obvious strategies to overcome noise in inverse problems

1. Acquire more accurate data to reduce $|p_1 - p_2|$ arising from $|\eta|$
2. Change the map $M(p)$ and acquire different data
3. Restrict the space in which parameters are sought

In other words, introduce a prior model:

1. Penalisation procedure (e.g. a regularisation)
2. Bayesian framework

Note that some authors consider the first option a subset of the latter, with Bayesian methods having the advantage of making the impact of prior information explicit.

Some historical strategies

Three obvious strategies to overcome noise in inverse problems

1. Acquire more accurate data to reduce $|p_1 - p_2|$ arising from $|\eta|$
2. Change the map $M(p)$ and acquire different data
3. Restrict the space in which parameters are sought

Direct Fourier transform — Lin et al. (LP^3), PRD 91 (2014) 054510

Low-pass filtering — Lin et al. (LP^3), PRD 98 (2018) 054504

"Derivative method" — Ishikawa et al., SCPMA 62 (2019) 991021

Gaussian weighting

Backus-Gilbert — Karpie et al., JHEP 04 (2019) 057

Maximum entropy method

Bayesian reconstruction

Neural nets — Izubuchi et al., PRD 100 (2019) 034516; Cichy, Del Debbio & Giani, JHEP 2019 (2019) 137

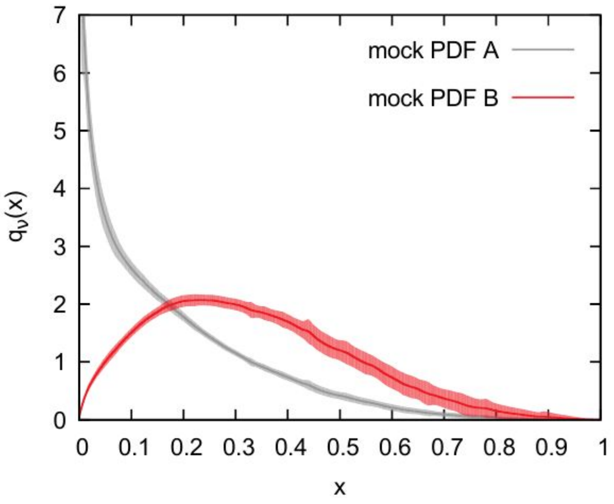
Global fits

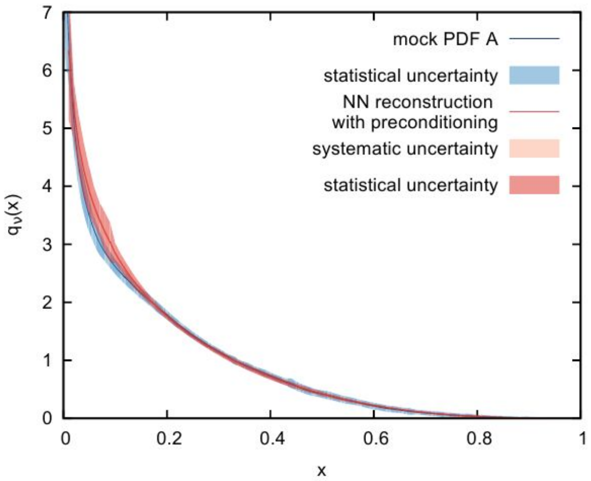
Model data and closure tests

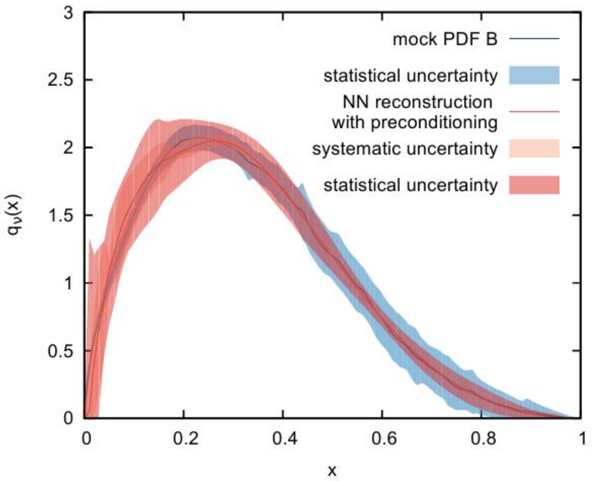
Reconstruction methods first systematically studied in Karpie et al., JHEP 04 (2019) 057

Generated two PDF models and analysed advanced reconstruction methods

See, e.g., L. Harland-Lang's talk







Model data and closure tests

Reconstruction methods first systematically studied in Karpie et al., JHEP 04 (2019) 057

Conclusions:

1. Advanced reconstruction methods "leads to satisfactory reconstruction results" for $x > 0.1$ with approximately ten points up to Ioffe times of 10
2. Goal of doubling available range of Ioffe time is "reasonable and achievable in the near future" and would "significantly reduce the uncertainty of the reconstruction for all three tested methods"
3. "However, tripling or quadrupling the maximum Ioffe time accessible would require concerted by the lattice community working on PDFs"

Real data and multiple analysis approaches

High precision pion data systematically studied in Gao et al., PRD 106 (2022) 114510

Analysed high statistics chiral-continuum extrapolated isovector quark PDF of the pion

1. Data constrain only the first few Mellin moments
2. Fit pseudo-distribution data (using ratio method) to two models
3. Deep neural network reconstruction of Ioffe time distribution
4. Direct Fourier transform of the quasi-distribution (using hybrid renormalisation), with explicit model of large distance behaviour

Gao et al., PRL 128 (2022) 142003

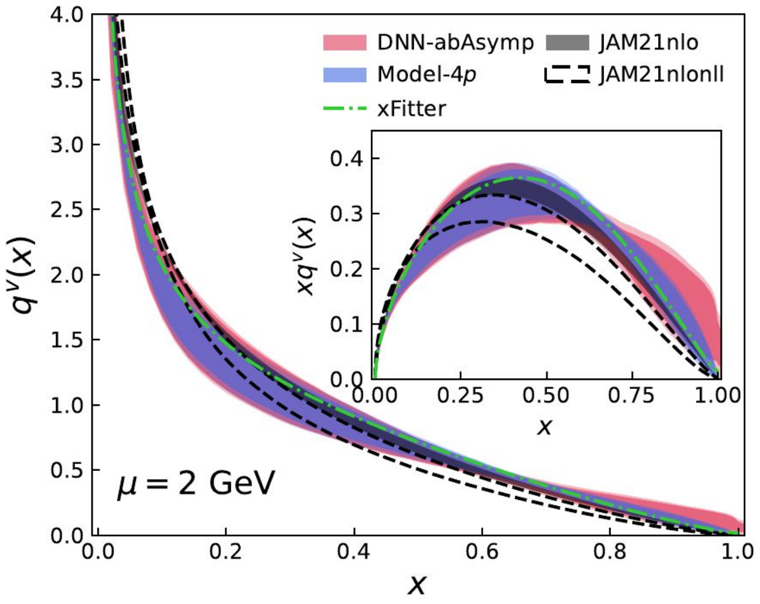
Real data and multiple analysis approaches

High precision pion data systematically studied in Gao et al., PRD 106 (2022) 114510

Comments:

1. Reconstruction systematic qualitatively under control for moderate to large x
2. Thorough analysis of reconstruction methods
3. Future community refinements require quantitative analysis of e.g. model dependence or systematic uncertainties associated with reconstruction method - natural to implement model averaging

See E. Neil's talk



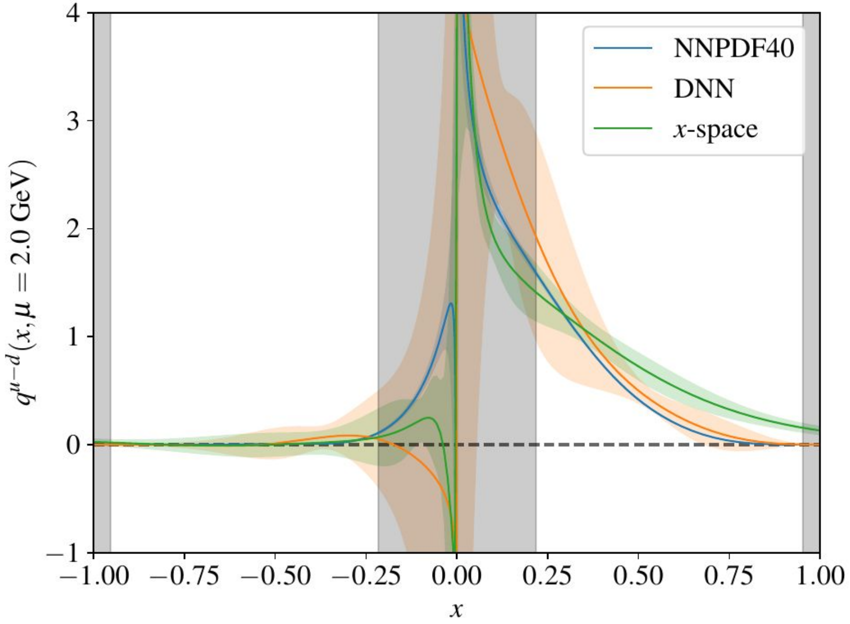
Real data and multiple analysis approaches

High precision proton data systematically studied in Gao et al., PRD 107 (2023) 074509

Note: analysis uses a single lattice spacing

Conclusions:

1. Difference between NLO and NNLO matching is “small but non-negligible”
2. Excited state contamination “significant”
3. “statistical errors dominate” in PDF reconstruction
4. “some tension” between LaMET and DNN and NNPDF results and “a need for larger P_z”



Real data and model averaging

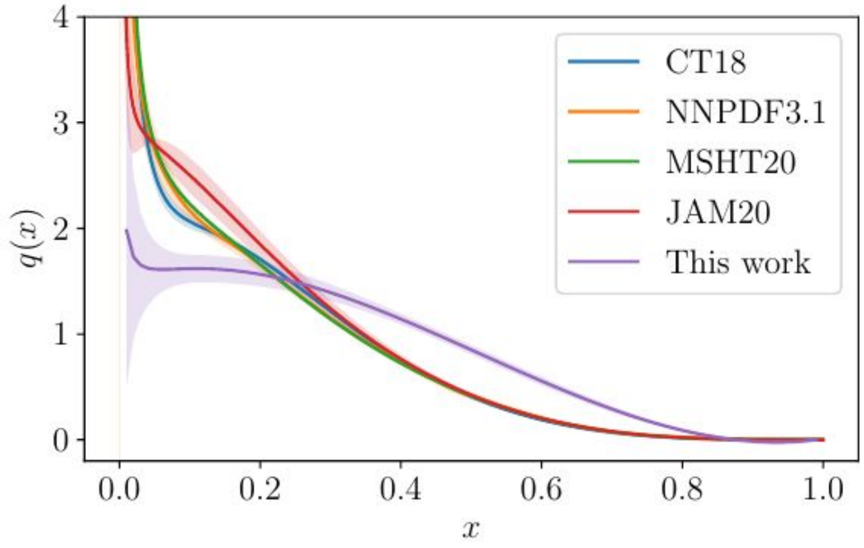
High precision proton data systematically studied in Karpie et al., JHEP 11 (2021) 024

Parameterised PDF through Jacobi polynomials, which provide flexible parameterisation of functions in [0,1]

“Nuisance” terms included to account for discretisation and higher-twist effects

Bayesian model averaging via the Akaike Information Criterion (AIC)

See E. Neil’s talk

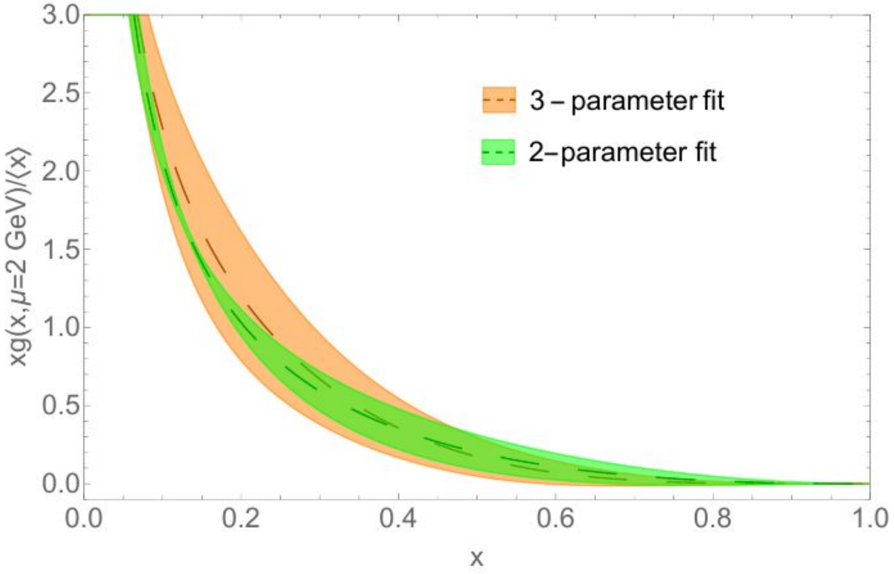


Gluon PDF of the nucleon

High statistics chiral-continuum gluon data studied in Fan et al., PRD 108 (2023) 014508

Fits to two choices of model

- Model dependency clearly smaller than statistical uncertainties



A less historical approach

Dutrieux et al. (HadStruc), JHEP 04 (2024) 061

Three obvious strategies to overcome noise in inverse problems

1. Acquire more accurate data to reduce $|p_1 - p_2|$ arising from $|\eta|$
2. Change the map $M(p)$ and acquire different data

Constrain PDF properties through real-space evolution

Leverage small-volume simulations

Typical lattice simulations have a "window problem"

$$a \ll P^{-1}, z \ll \Lambda_{\rm QCD}^{-1} \ll L \qquad x \sim (zP_z)^{-1}$$

Mitigated by working in small volumes and applying step-scaling

Enables access to large Ioffe-times and evolution to perturbative scales

Back to our outline of PDF reconstruction

Extraction of light-cone PDFs from lattice QCD is a three-step process

1. Numerical determination of relevant matrix elements
2. Determination of quasi- and pseudo-PDFs via Fourier transform
3. Factorisation of light-cone PDF through LaMET or SDF

Here we confront (at least) one of the central questions posed by organisers:
"What role do large-momentum corrections play?"
should be augmented with the analogous question
"What role do large-distance corrections play?"

Large momenta?

Some recent typical lattice parameters

Reference	Parton/hadron	Max momentum (GeV)	Lattice spacing (fm)
2208.02297	Pion quark PDF	1.78	0.04, 0.06, 0.076
2105.13313	Nucleon quark PDF	4.8	0.048, 0.065, 0.075
2212.12569	Nucleon quark PDF	1.53	0.076
2210.09985	Nucleon gluon PDF	3.05	0.09, 0.12, 0.15

Note that generative machine learning has been proposed as a tool for surpassing current computational limits - Chowdhury et al., 2409.17234

Role of higher twist contributions?

Short-distance factorisation relies on short distances to control higher-twist effects

- Large momentum still required to access a wide range Ioffe times

LaMET relies on large momenta to control higher-twist effects

Estimating these can be carried out in three primary ways

1. Perturbative analysis
2. Renormalon analysis
3. Numerical analysis

Braun et al., PRD 99 (2019) 014013

Renormalon analysis

Provides
"a minimal model for the higher-twist corrections that captures effects that are necessary for the selfconsistency of the theory, but possibly misses other nonperturbative corrections"

Power corrections to quasi-PDFs (i.e. LaMET framework) take the form

$$\mathcal{Q}(x,p) = q(x)\left\{1 + \mathcal{O}\left(\frac{\Lambda^2}{p^2}\cdot\frac{1}{x^2(1-x)}\right)\right\}$$

and for pseudo-PDFs (i.e. SDF framework)

$$\mathcal{P}(x,z) = q(x)\left\{1 + \mathcal{O}\left(z^2\Lambda^2(1-x)\right)\right\}$$

Results depend on choice of renormalisation procedure

For a recent review, see Zhang PoSLATTICE2023 (2024) 117

Numerical evidence?

Ratio method: renormalisation procedure for Wilson-line operators, via RGI ratios of matrix elements

Numerical evidence suggests that the ratio method works well to distances ~ 1 fm

> "the predicted bands from short distances are consistent with the matrix elements at relatively large distances, suggesting that the matching kernel works well up to … z ~ 1 fm … within our current statistics. This observation … seems to support the argument that the ratio-scheme indeed reduces the higher-twist effect $O(z^2\Lambda^2_{QCD})$ by the cancellation between the numerator and denominator, even though it is naively not expected that the leading-twist OPE can approximately work up to 1 fm."

Gao et al., PRD 106 (2022) 114510

And that, in the LaMET framework, momenta of 2-3 GeV are insufficient

In the SDF framework, synthetic data indicate that Ioffe times ~ 20 significantly improve control over inverse problem

Summary - broad brush

Lattice calculations have matured:

- sophisticated analyses of systematic uncertainties now possible
- multiple advanced methods for regulating the inverse problem
- unlikely to provide new information on quark isovector PDFs, which may be better suited as benchmark quantities for lattice calculations
- lattice will contribute meaningfully where experimental data are lacking
- inclusion in global fitting paradigm has been demonstrated to be a productive approach to pursue

Summary - in slightly more detail

State-of-the-art calculations feature:

- chiral-continuum limit, with evidence of mild pion mass dependence
- NNLO factorisation, with evidence of reasonable convergence behaviour
- hadron momentum of 2-3 GeV, with evidence that this is too small
    - clear quantitative evidence of “required” momentum not available
    - question off what is “large enough” is only well-defined at a specified precision
- typical Ioffe times of 8-10
    - closure tests suggest Ioffe times ~ 20 will significantly improve reconstruction
- dominant “lattice” uncertainties
    - discretisation effects
    - excited state contamination
- generally qualitative inverse problem regularisation
    - typically use multiple model parameterisations to observe model dependence
    - evidence that neural nets provide appropriate nonparametric reconstruction

Summary - a personal take on uncertainty quantification

Ultimately, community needs to move beyond current “kitchen sink” approach

- assessment of inverse problem regularisation currently generally qualitative
- plotting multiple fits in the same figure is great, but not uncertainty quantification

I expect that we will move towards situation similar to global fitting community
(or heavy quark flavour physics or muon g-2 ...)

Our aim (should be):

1. to provide complete pointwise error budgets
2. for multiple groups, using different frameworks, to agree within quantified errors

One of the central challenges: Quantifying inverse problem regularisation uncertainty

- synthetic data and closure tests will be important tool
- unpolarised isovector quark PDFs of the nucleon provide benchmarks
- Bayesian methods have the advantage of making prior assumptions explicit
- model averaging should be used as part of uncertainty quantification

Treating lattice data in a comprehensive global fit seems (to me) like a natural way forward

Thank you!

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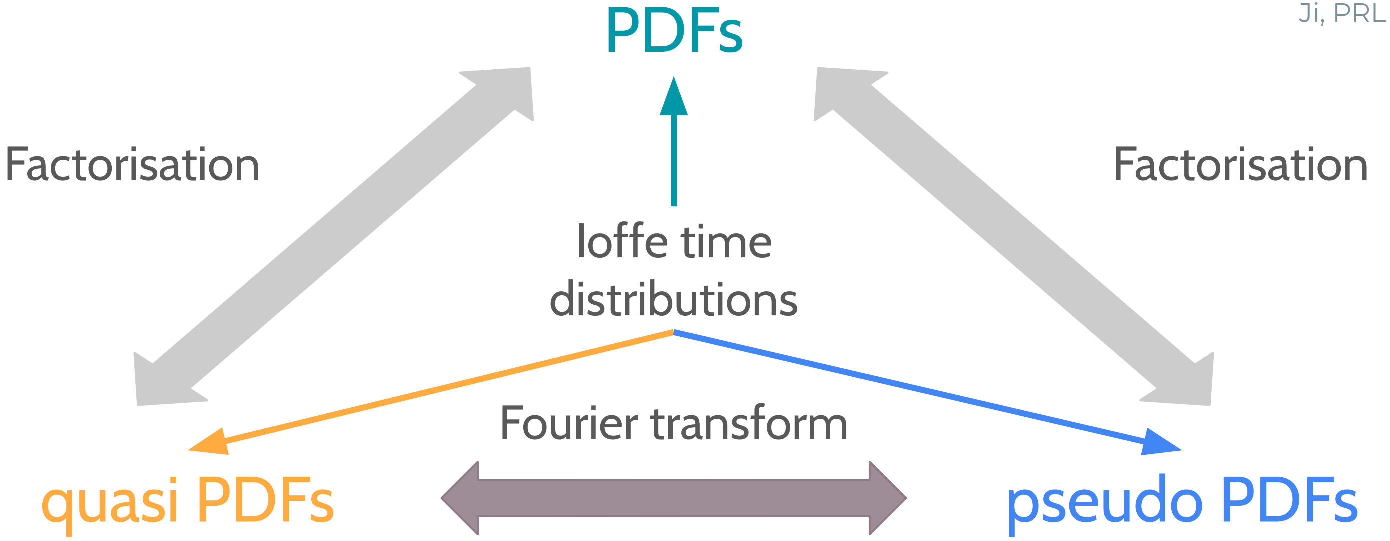
Distributions from the lattice perspective

Izubuchi et al., PRD 98 (2018) 03917
Zhang, Chen & CJM, PRD 97 (2018) 074508
Radyushkin, PLB 781 (2018) 433
Ji et al., NPB 924 (2017) 326
Ji, PRL 110 (2013) 262002

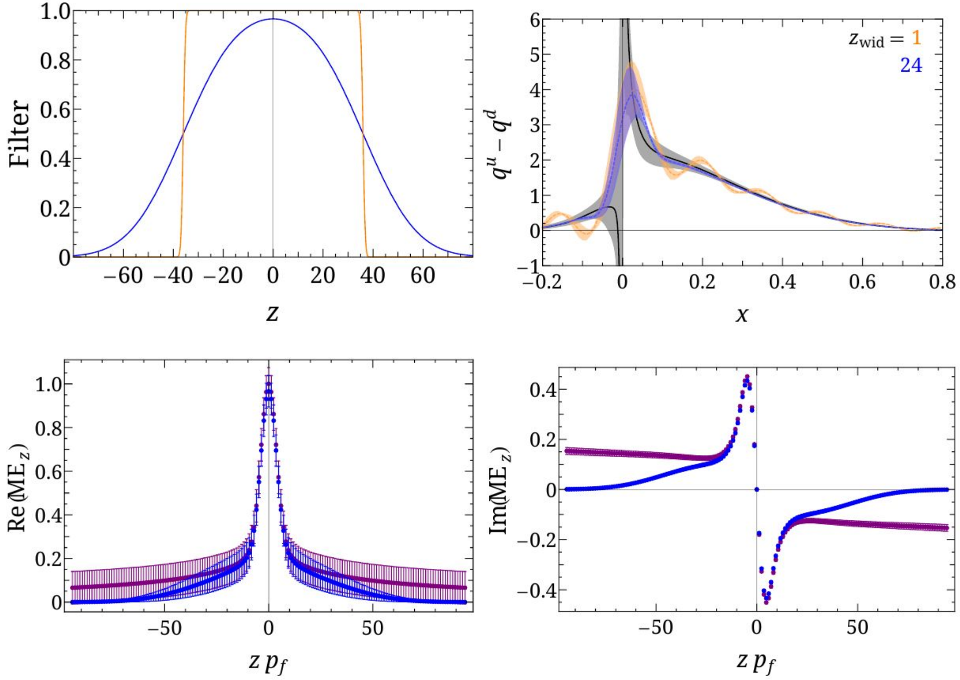


Low-pass filter

Lin et al. (LP[3]), PRD 98 (2018) 054504

Apply the filter

$$F(z_{\rm lim}, z_{\rm wid}) = \frac{1+\mathrm{erf}\left(\frac{z+z_{\rm lim}}{z_{\rm wid}}\right)}{2}\,\frac{1-\mathrm{erf}\left(\frac{z-z_{\rm lim}}{z_{\rm wid}}\right)}{2}$$



Derivative method

Lin et al. (LP3), PRD 98 (2018) 054504

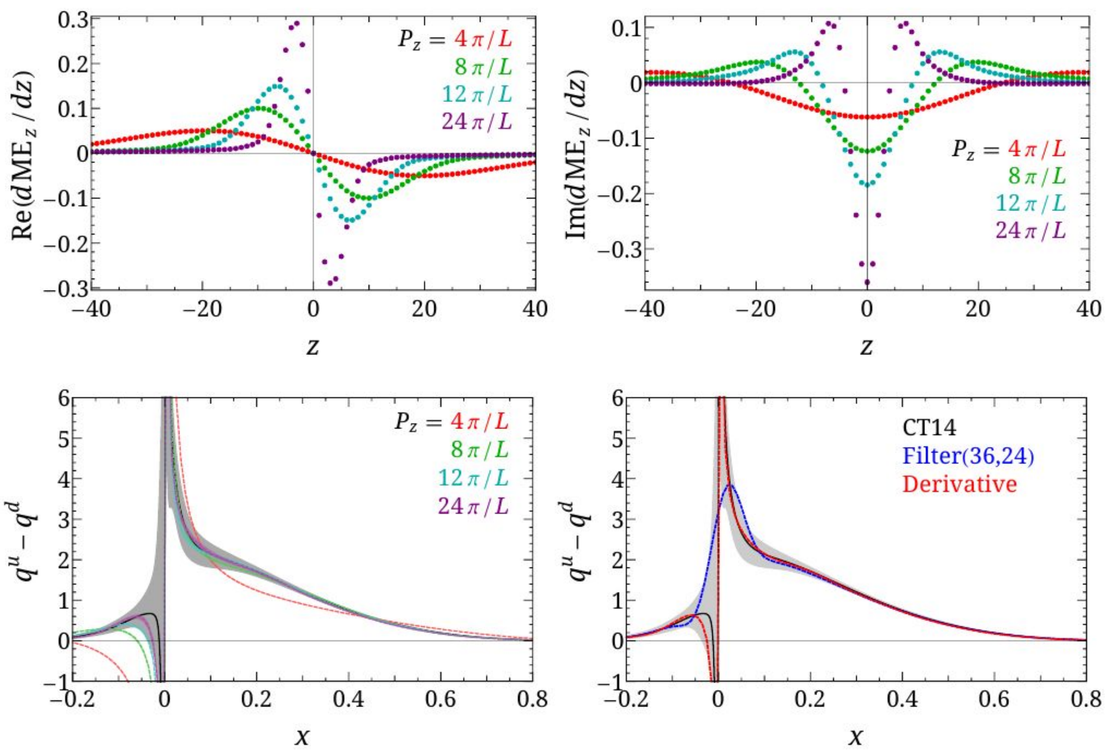
Apply the derivative

$$q(x) = \int_{-z_{\max}}^{+z_{\max}} dz \frac{-1}{2\pi} \frac{e^{ixP_z z}}{iP_z x} h'(z)$$

Where

$$\tilde{q}(x, P_z, \tilde{\mu}) = \int_{-\infty}^{\infty} \frac{dz}{2\pi} \; e^{ixP_z z} h(z, P_z, \tilde{\mu})$$

$$\tilde{q}(x, P_z, \tilde{\mu}) = \int_{-1}^{+1} \frac{dy}{|y|} \; C\left(\frac{x}{y}, \frac{\tilde{\mu}}{P_z}, \frac{\mu}{P_z}\right) q(y, \mu)$$

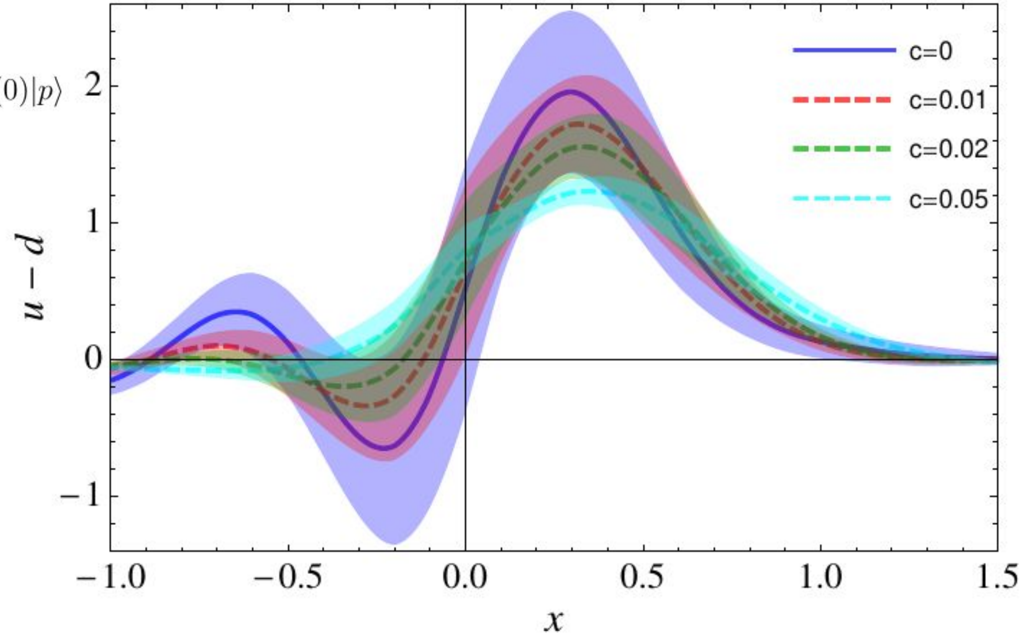


Gaussian weighting

Ishikawa et al., SCPMA 62 (2019) 991021

Apply weighting factor

$$\tilde{q}_{\rm GW}(x,\Lambda,p_z)=\int\frac{dz}{4\pi}e^{ixp_zz-z^2/l^2}\langle p|\overline{\psi}(0,0_\perp,z)\gamma^zL(z,0)\psi(0)|p\rangle$$



Backus-Gilbert

Karpie et al., JHEP 04 (2019) 057
Llang, Liu, Yang, EPJ Conf. 175 (2018) 14014

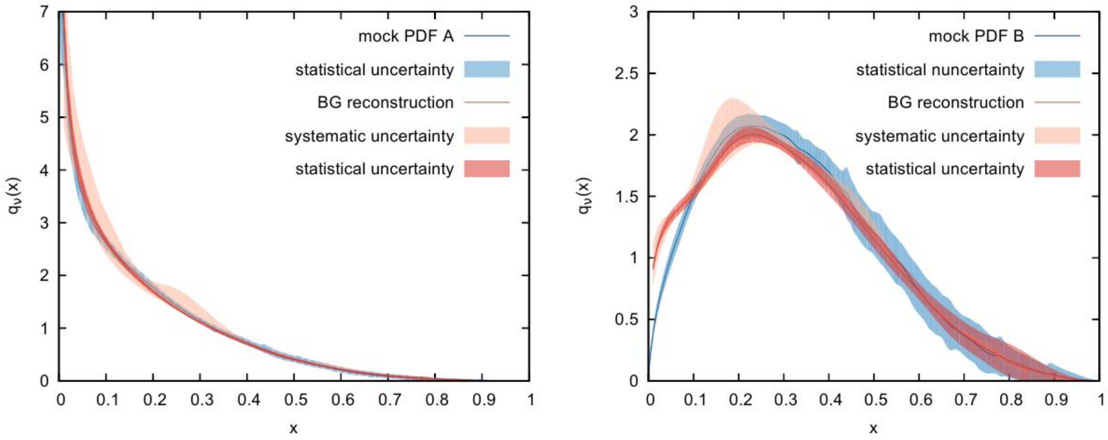
Define

$$d_j \equiv \mathcal{Q}_R(\nu_j) = \int_0^1 dx K_j(x) h(x)$$

$$\Delta(x - \bar{x}) = \sum_j a_j(\bar{x}) K_j(x)$$

and then estimate

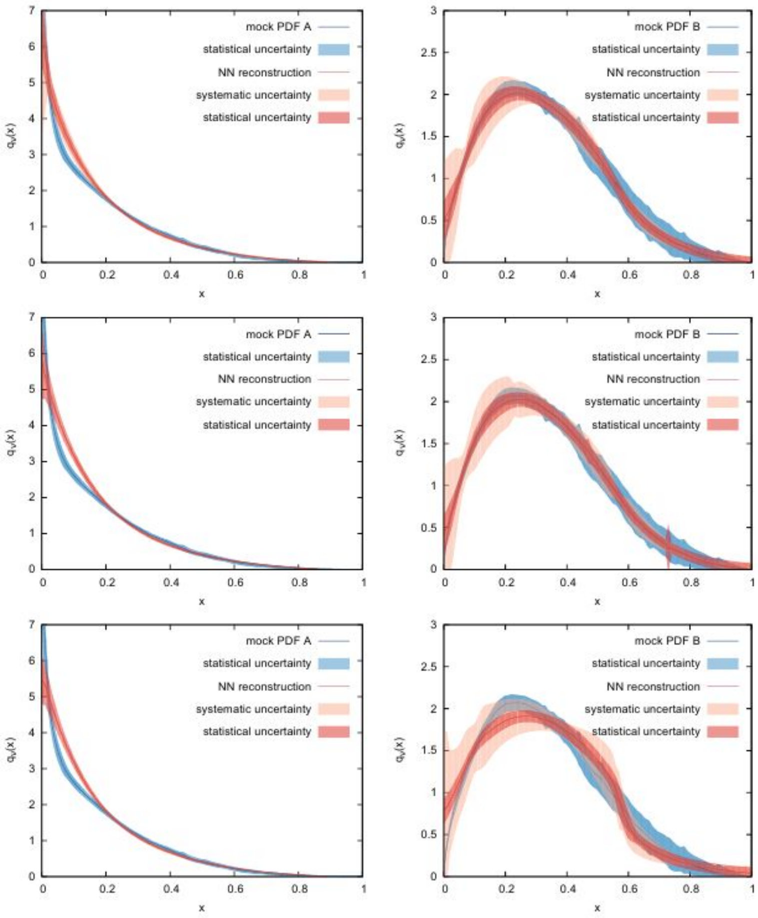
$$\hat{h}(\bar{x}) = \sum_j a_j(\bar{x}) d_j$$



Backus-Gilbert method minimises

$$\sigma = \int_0^1 dx (x - \bar{x})^2 \Delta(x - \bar{x})^2 \quad \text{so} \quad \lim_{\sigma \to 0} \hat{h}_\sigma(x) = h(x)$$

Neural net



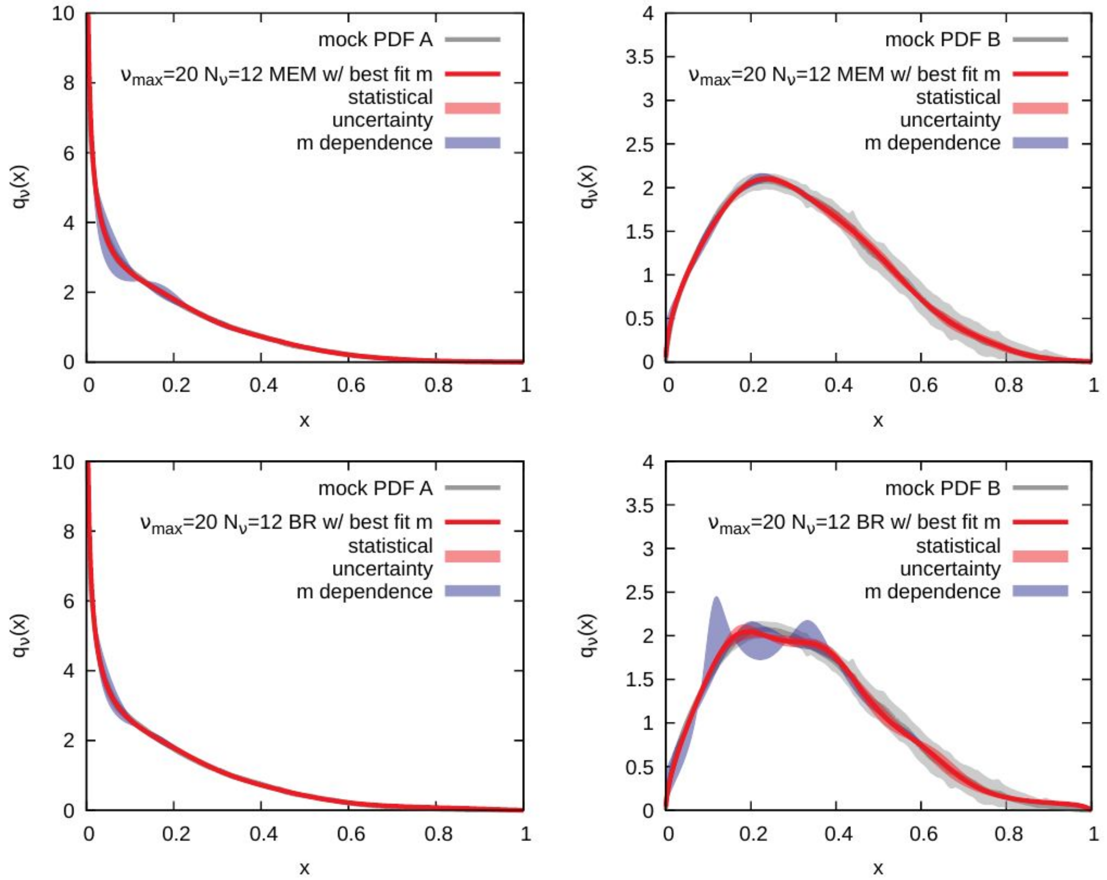
mock PDF A
statistical uncertainty
NN reconstruction
systematic uncertainty
statistical uncertainty
mock PDF B
$q_v(x)$
x

Karpie et al., JHEP 04 (2019) 057

Bayesian methods

Maximum entropy method

Bayesian reconstruction



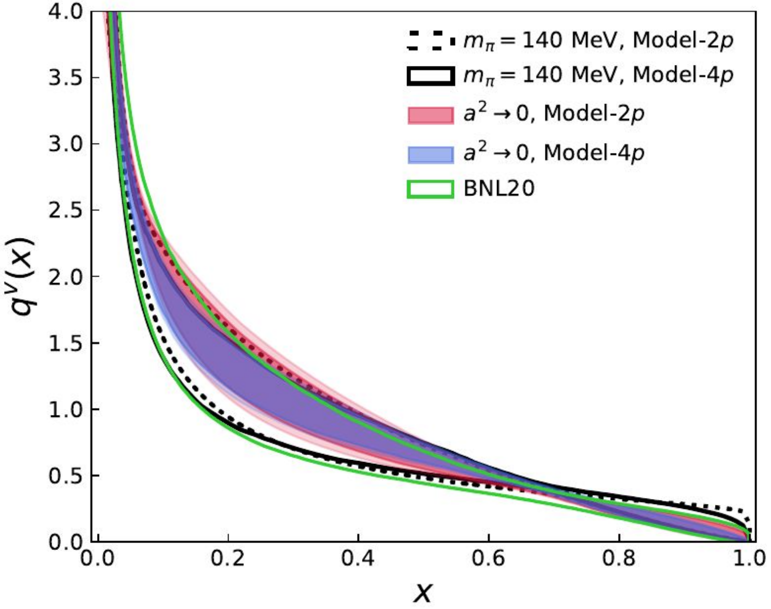
PDF reconstruction in selected recent results

Gao et al., PRD 106 (2022) 114510

Unpolarised isovector quark PDF of the pion in the chiral-continuum limit

1. Data constrain only the first few Mellin moments
2. Fit data to two models

$$q(x;\alpha,\beta) = \mathcal{N} x^{\alpha}(1-x)^{\beta}$$
$$q(x;\alpha,\beta,s,t) = \mathcal{N} x^{\alpha}(1-x)^{\beta}(1+s\sqrt{x}+tx)$$



Model uncertainty not explicitly quantified:

- qualitatively smaller than other systematics at moderate to large x
- natural to imagine using (Bayesian) model averaging to reduce model dependence

See E. Neil’s talk

PDF reconstruction in selected recent results

Gao et al., PRD 106 (2022) 114510

Unpolarised isovector quark PDF of the pion in the chiral-continuum limit

1. Data constrain only the first few Mellin moments
2. Fit data to two models
3. Deep neural network reconstruction of Ioffe time distribution