

Parton pseudo distribution functions from Lattice QCD

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Distribution functions: Lattice QCD meets phenomenology

Paphos, Cyprus

In collaboration with J. Karpie (Columbia), K. Orginos (College of William & Mary and JLAB), A. Radyushkin (ODU and JLAB)
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PDFs from the lattice: Pseudo-PDFs Formalism

Starting point: the equal time hadronic matrix element with the quark and anti-quark fields separated by a finite distance [Radyushkin \(2017\)](#)

$$\mathcal{M}^\alpha(z, p) \equiv \langle p | \bar{\psi}(0) \gamma^\alpha \hat{E}(0, z; A) \tau_3 \psi(z) | p \rangle$$

$z = (0, 0, 0, z_3)$
 $p = (p^0, 0, 0, p)$
 $\alpha = 0$

Lorentz inv. \rightarrow

$$\mathcal{M}^\alpha(z, p) = 2p^\alpha \underbrace{\mathcal{M}_p(-z p, -z^2)}_{\text{Leading twist}} + z^\alpha \underbrace{\mathcal{M}_z(-z p, -z^2)}_{\text{Higher twist}}$$


- The Lorentz invariant quantity $\nu = -(z p)$, is the "loffe time"
- loffe time PDFs $\mathcal{M}(\nu, z_3^2)$ defined at a scale $\mu^2 = 4e^{-2\gamma_E}/z_3^2$ (at leading log level) are the Fourier transform of regular PDFs $f(x, \mu^2)$ [Balitsky, Braun \(1988\)](#), [Braun et al. \(1995\)](#)

$$\mathcal{M}(\nu, z_3^2) = \int_{-1}^1 dx f(x, 1/z_3^2) e^{i x \nu}$$

Obtaining the Ioffe time PDF

$$z_3 \rightarrow 0 \Rightarrow \mathcal{M}_p(\nu, z_3^2) = \mathcal{M}(\nu, z_3^2) + \mathcal{O}(z_3^2)$$

But.... large $\mathcal{O}(z_3^2)$ corrections **prohibit** the extraction.

Conservation of the vector current implies $\mathcal{M}_p(0, z_3^2) = 1 + \mathcal{O}(z_3^2)$, but in a **ratio** z_3^2 corrections (related to the transverse structure of the hadron) might cancel  [Radyushkin \(2017\)](#)

$$\mathfrak{M}(\nu, z_3^2) \equiv \frac{\mathcal{M}_p(\nu, z_3^2)}{\mathcal{M}_p(0, z_3^2)}$$

- Much **smaller** $\mathcal{O}(z_3^2)$ corrections and therefore this ratio could be used to extract the Ioffe time PDFs
- All UV singularities are **exactly cancelled** and when computed in lattice QCD it can be extrapolated to the continuum limit at fixed ν and z^2 .

Numerical implementation

First case study in an unphysical setup [Karpie, Orginos, Radyushkin SZ, Phys.Rev. D96 \(2017\) no.9, 094503](#)

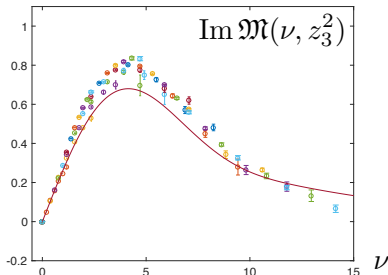
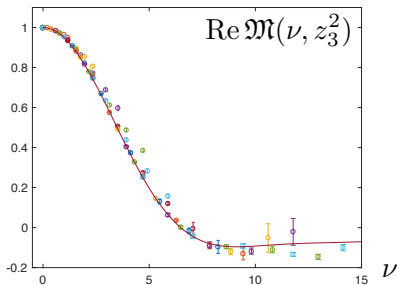
- Quenched approximation
- $32^3 \times 64$ lattices with $a = 0.093\text{fm}$.
- $m_\pi = 601\text{MeV}$ and $m_N = 1411\text{MeV}$

Now employing dynamical ensembles

$a(\text{fm})$	$M_\pi(\text{MeV})$	β	$L^3 \times T$
0.127(2)	415	6.1	$24^3 \times 64$
0.127(2)	415	6.1	$32^3 \times 96$
0.094(1)	390	6.3	$32^3 \times 64$
0.094(1)	280	6.3	$32^3 \times 64$
0.094(1)	172	6.3	$64^3 \times 128$

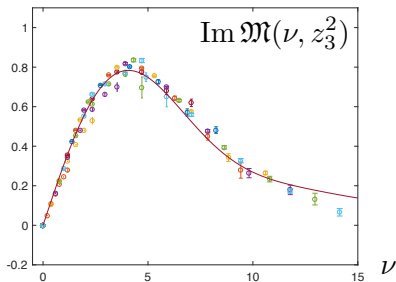
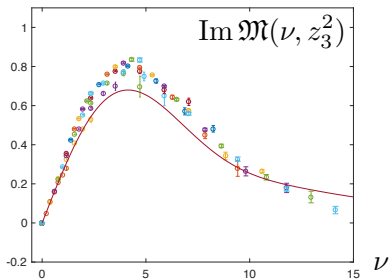
Table: Parameters for the lattices generated by the JLab/W&M collaboration using 2+1 flavors of clover Wilson fermions and a tree-level tadpole-improved Symanzik gauge action. The lattice spacings, a , are estimated using the Wilson flow scale w_0 . Stout smearing implemented in the fermion action makes the tadpole corrected tree-level clover coefficient c_{SW} used, to be very close to the value determined non-pertubatively with the Schrödinger functional method

Results for the Re and Im parts of $\mathfrak{M}(\nu, z_3^2)$



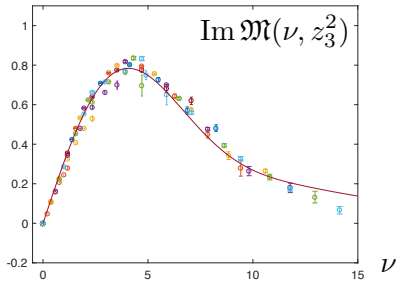
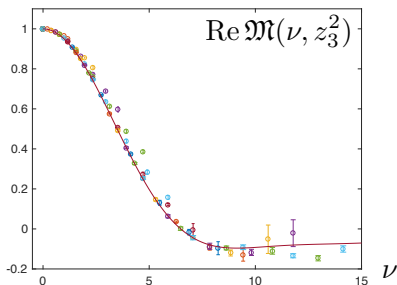
- Curves represent Re and Im Fourier transforms of $q_\nu(x) = \frac{315}{32} \sqrt{x}(1-x)^3$.
- Considering CP even and odd combinations
 - ▶ even: $q_-(x) = f(x) + f(-x) = q(x) - \bar{q}(x) = q_\nu(x)$
 - ▶ odd: $q_+(x) = f(x) - f(-x) = q(x) + \bar{q}(x) = q_\nu(x) + 2\bar{q}(x)$

Results for the Im part of $\mathfrak{M}(\nu, z_3^2)$



- Curves represent the Im Fourier transforms of $q_v(x) = q(x) - \bar{q}(x)$ and $q_+(x) = q(x) + \bar{q}(x) = q_v(x) + 2\bar{q}(x)$ respectively.
- The agreement with the data is strongly improved if we use a non-vanishing antiquark contribution, namely $\bar{q}(x) = \bar{u}(x) + \bar{d}(x) = 0.07[20x(1-x)^3]$.

Results for the Re and Im parts of $\mathfrak{M}(\nu, z_3^2)$



- Data as function of the loffe time. A **residual** z_3 -dependence can be seen.
- This is more visible when, for a **particular** ν we have several data points corresponding to **different values of** z_3 .
- Different values of z_3^2 for the same ν correspond to the loffe time distribution at different scales.

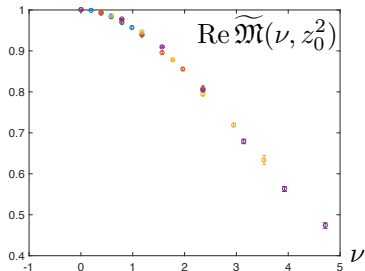
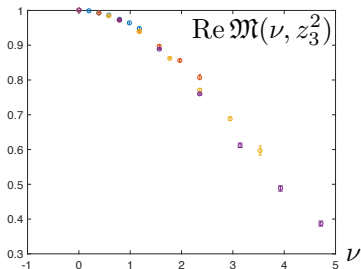
Residual z_3 -dependence

- Is the residual scatter in the data points **consistent with evolution**? By solving the evolution equation at LO, the loffe time PDF at z'_3 is related to the one at z_3 by

$$\mathfrak{M}(\nu, z'_3{}^2) = \mathfrak{M}(\nu, z_3^2) - \frac{2}{3} \frac{\alpha_s}{\pi} \ln(z'_3{}^2/z_3^2) \int_0^1 du B(u) \mathfrak{M}(u\nu, z_3^2)$$

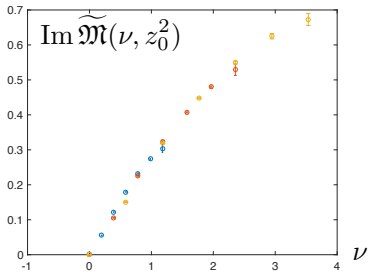
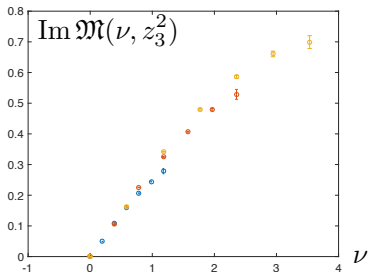
- Only applicable at small z_3

Before and after evolution



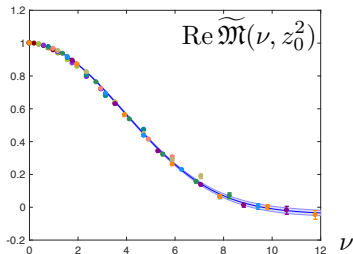
The ratio $\mathfrak{M}(\nu, z_3^2)$ for $z_3/a = 1, 2, 3,$ and 4 . **LHS:** Data before evolution. **RHS:** Data after evolution. The reduction in scatter indicates that evolution collapses all data to the same universal curve.

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Comparison to global fits



- Evolved points fitted with cosine FT of

$$q_v(x) = N(a, b) x^a (1 - x)^b$$

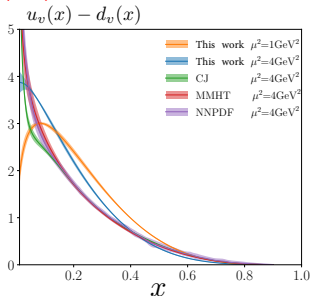
$$a = 0.36(6), \quad b = 3.95(22)$$

 Karpie, Orginos, Radyushkin, S.Z. (2017)

- Evolved data can be exploited to build

$$u_v(x) - d_v(x)$$

- Results compared with predictions from global fits

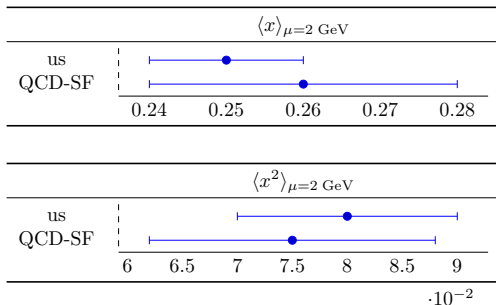


Sanity checks vs other lattice results

- Extract lowest PDF moments from our data [Karpie, Orginos, S.Z., JHEP 1811 \(2018\)](#) and compare with the lattice literature [QCD-SF collaboration \(1996\)](#)
- \overline{MS} moments up to $\mathcal{O}(\alpha_s^2, z^2)$ directly from the reduced function $\mathfrak{M}(\nu, z^2)$

$$a_{n+1}(\mu) = (-i)^n \frac{1}{c_n(z^2 \mu^2)} \left. \frac{\partial^n \mathfrak{M}(\nu, z^2)}{\partial \nu^n} \right|_{\nu=0} + \mathcal{O}(z^2, \alpha_s^2)$$

- Our method avoids mixing and allows the extraction of any moment



The pertinent systematics in PDF extraction


- Parton distribution functions or distribution amplitudes may be defined in lattice QCD by inverting the quasi-Fourier transform of a certain class of hadronic position-space matrix elements
- One example are the Ioffe-time PDFs, \mathfrak{M}_R , related to the physical PDF $q_v(x, \mu^2)$ via the integral relation

$$\mathfrak{M}_R(\nu, \mu^2) \equiv \int_0^1 dx \cos(\nu x) q_v(x, \mu^2)$$

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Cosine not orthogonal in $[0, 1]$

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Cosine not orthogonal in $[0, 1]$

- The task at hand is then to **reconstruct the PDF $q_v(x, \mu^2)$ given a limited set of simulated data** for $\mathfrak{M}_R(\nu, \mu^2)$.
- The extraction is highly ill-posed, so one has to resort to regularization strategies in order to find a way to reliably estimate the PDF from the data at hand

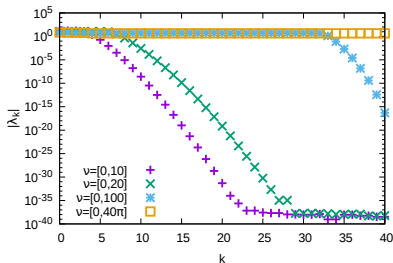
 Karpie, Orginos, Rothkopf, S.Z. JHEP 1904 (2019) 057

Naive Reconstruction

- Discretize the integral, employing the trapezoid rule

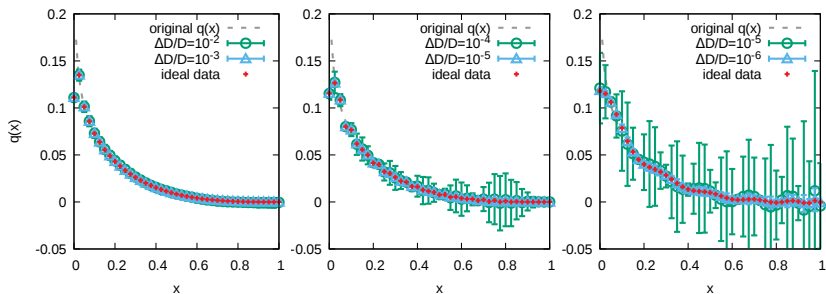
$$\mathfrak{M}_R(\nu) = \frac{1}{2} \cos(\nu x_0) q_v(x_0) + \sum_{k=1}^{N_x-1} \delta x \cos(\nu x_k) q_v(x_k) + \frac{1}{2} \cos(\nu x_{N_x}) q_v(x_{N_x})$$

- Casting our problem in a matrix equation $\mathfrak{m} = \mathfrak{C} \cdot \mathfrak{q}$,
- The conditioning of the problem is easily elucidated by considering the eigenvalues of the matrix \mathfrak{C} .



 Karpie, Orginos, Rothkopf, S.Z. - arXiv:1901.05408 - JHEP 1904 (2019) 057

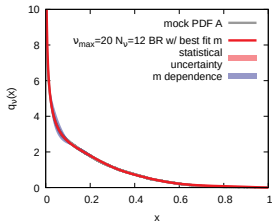
Naive Reconstruction



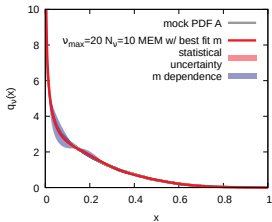
Results for the direct inversion for different discretization intervals
(left $\nu = [0, 40\pi]$, center $\nu = [0, 100]$, right $\nu = [0, 20]$).

Advanced PDF Reconstructions

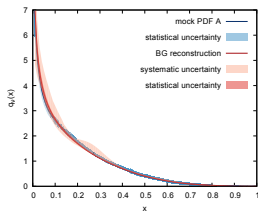
Bayesian Reconstruction



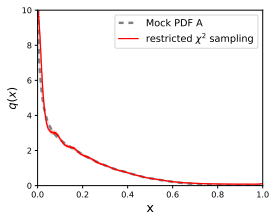
Max. Entropy Method



Backus-Gilbert algorithm

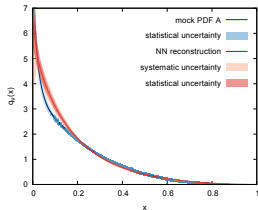


HMC χ^2 evaluation



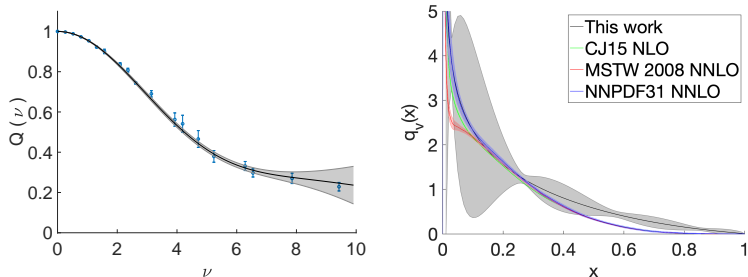
Capitalize of the good scanning in loffe time and use advanced reconstruction methods to extract the maximum amount of information also for the small- x region.

Neural Network



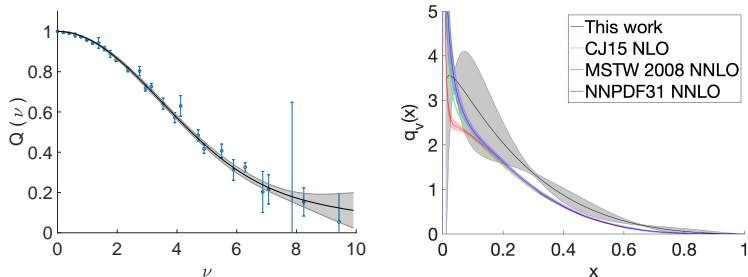
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New results with $N_f = 2 + 1$ fermions for the nucleon



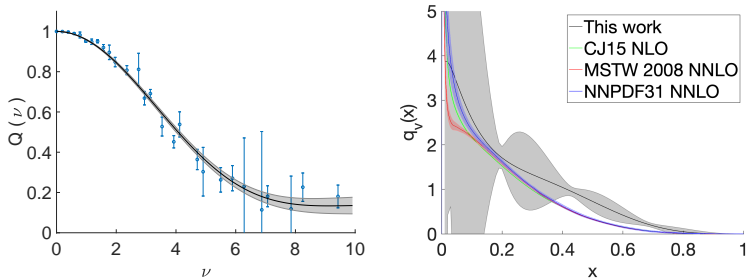
The nucleon valence distribution obtained from the ensemble $a_{127}m_{415}$ fit to the form used by the JAM collaboration. The $\chi^2/\text{d.o.f.}$ for the fit with all the data is 2.5(1.5). The uncertainty band is obtained from the fits to the Jackknife samples of the data.

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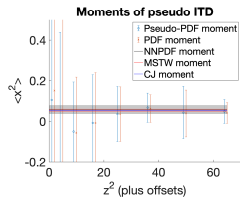
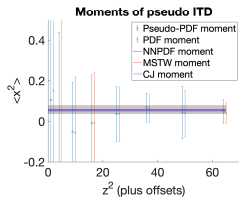
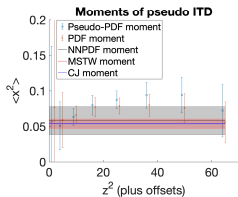
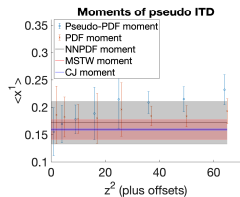
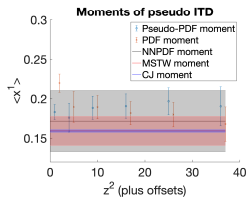
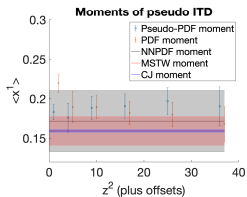
The nucleon valence distribution obtained from the ensemble $a_{127m415L}$ fit to the form used by the JAM collaboration. The $\chi^2/\text{d.o.f.}$ for the fit with all the data is 2.1(6). The uncertainty band is obtained from the fits to the Jackknife samples of the data.

New results with $N_f = 2 + 1$ dynamical fermions

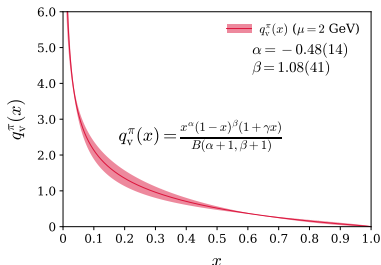
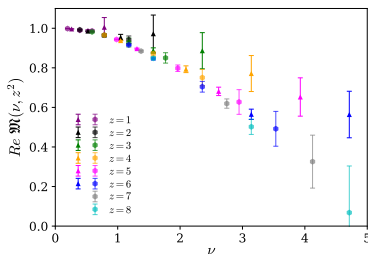


The nucleon valence distribution obtained from the ensemble $a094m390$ fit to the form used by the JAM collaboration. The $\chi^2/\text{d.o.f.}$ for the fit with all the data is 2.0(5). The uncertainty band is obtained from the fits to the Jackknife samples of the data.

New results with $N_f = 2 + 1$ fermions for the nucleon

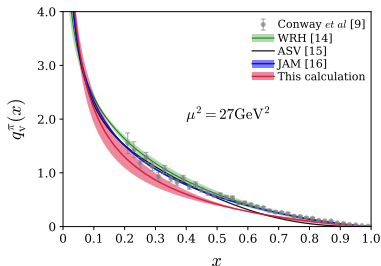
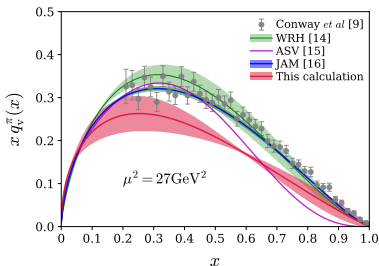


Results with $N_f = 2 + 1$ fermions for the pion



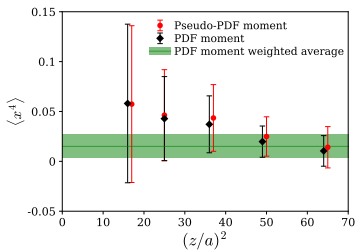
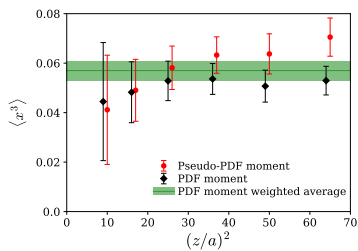
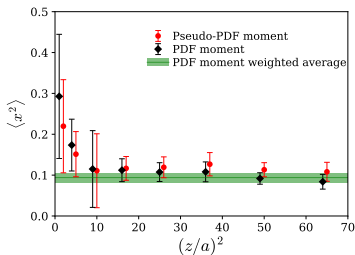
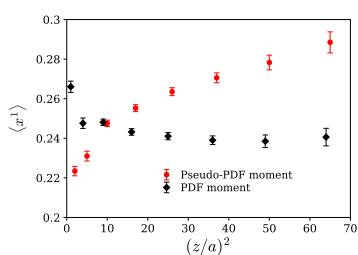
ITD obtained from ensembles $a_{127m415}$ and $a_{127m415L}$ after 1-loop perturbative matching at $\mu = 2$ GeV. The circle (\circ) symbols indicate the reduced pseudo-ITD matrix elements M^0 extracted from the $a_{127m415}$ ensemble and the diamond (\diamond) symbols denote those for the $a_{127m415L}$ ensemble. The red band is obtained from a simultaneous fit to the matched ITDs on these two ensembles in the limit of infinite volume (LHS). The pion valence distribution (RHS).

Results with $N_f = 2 + 1$ flavors for the pion



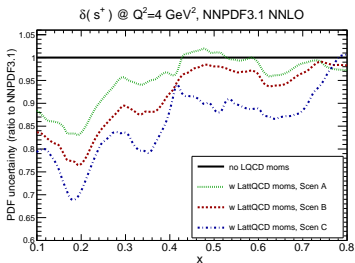
(LHS) Comparison of the pion $xq_V^\pi(x)$ -distribution with the LO extraction from DY data (gray data points), NLO fits (green, maroon, and blue). This lattice QCD calculation of $q_V^\pi(x)$ is evolved from an initial scale $\mu_0^2 = 4\text{GeV}^2$ at NLO. All the results are evolved to an evolution scale of $\mu^2 = 27\text{GeV}^2$. Similar comparison of the pion $q_V^\pi(x)$ -distribution (RHS).

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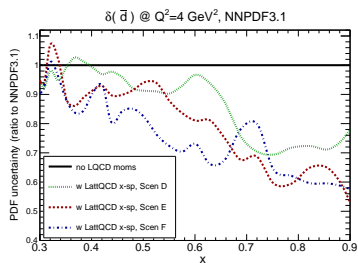


Lattice impact in the precision of global fits

s^+ quark PDFs, percentage PDF uncertainty



\bar{d} quark PDFs, percentage PDF uncertainty



- The comparison is with the results of including lattice-QCD pseudo-data for moments of PDFs (left) and info from lattice-QCD pseudo-data on x-space PDFs (right). [Lin et al. \(2018\)](#), [Cichy, Del Debbio and Giani JHEP 1910 \(2019\) 137](#)

Take home messages

- Realization that $\mathcal{M}(\nu, z_3^2)$ should be treated as a function of Lorentz invariants ν and z^2 .
- Only the ν -dependence is responsible for the x -dependence of the PDFs.
- μ^2 serves the same role as z^2 in the pseudo-PDF
- Don't mix z^2 and ν .
- The ITpD $\mathcal{M}(\nu, z_3^2)$ can be directly matched to the light cone ITD $\mathcal{I}(\nu, \mu^2)$ with no intermediaries needed.
- Knowing $\mathcal{I}(\nu, \mu^2)$ means that we know $f(x, \mu^2)$.
- Small difference between the pseudo-ITD and the light cone ITD

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Take home messages

- Issues with the Fourier transform
- In the pseudo-approach the Fourier transform is in the end over ν
- However a FT over z could be a source of systematics.
- Extrapolating from z_{max} to ∞ and then carry out the integral?
- The renormalized m.e. have growing and growing errors at z_{max} saying that this is equal to zero is not a precision statement.
- pPDFs allow for a good control of higher twist effects
- We study the residual z^2 effects for the moments as well as the matched ITD and have a concrete idea of the size of these effects.
- If one carries the FT over z instead you can not clearly control the higher twist effects because the integral over z mixes the leading and higher twist regions.

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Take home messages

- No need for infinite p for the pseudo-PDFs.
- Large p is useful for good scanning in ν but no $p \rightarrow \infty$ is required.
- The ratio is an RGI quantity agnostic to the regulator
- Finite moments which make our goal twofold (extraction of moments beyond the x -dependence).

Conclusions and outlook

- PDFs are needed as theoretical inputs to all hadron scattering experiments and in some cases are the largest theory uncertainty.
- The lattice community is by now able to provide ab-initio determinations of PDFs without theoretical obstructions.
- The interplay between lattice QCD and global fits is very important
- Also important in the search of New Physics [Gao, Harland-Lang, Rojo \(2018\)](#)
- What next? Polarized, Transversity, gluon PDFs and GPDs eventually
- **Many thanks for your attention!!!**

Formalism

- The quasi-PDF $Q(x, p^2)$ is related to $\mathcal{M}_p(\nu, z_3^2)$ by

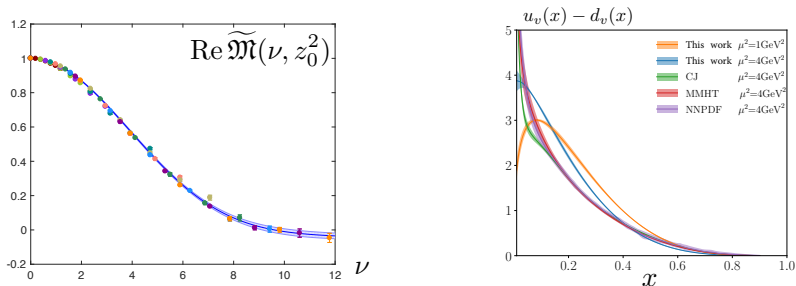
$$Q(x, p^2) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\nu e^{-ix\nu} \mathcal{M}_p(\nu, [\nu/p]^2)$$

Quasi PDF mixes invariant scales until p_z is effectively large enough

- While the pseudo-PDF has fixed invariant scale dependence

$$P(x, z_0^2) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\nu e^{-ix\nu} \mathcal{M}_p(\nu, z_0^2)$$

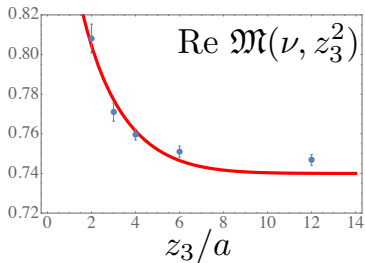
Comparison to global fits



LHS: Data points for $\text{Re } \widetilde{\mathcal{M}}(\nu, z_3^2)$ with $z_3 \leq 10a$ evolved to $z_3 = 2a$. By fitting these evolved points with a cosine FT of $q_v(x) = N(a, b)x^a(1-x)^b$ we obtain $a = 0.36(6)$ and $b = 3.95(22)$ (statistical errors). RHS: Curve for $u_v(x) - d_v(x)$ built from the evolved data shown in the left panel and treated as corresponding to the $\mu^2 = 1 \text{ GeV}^2$ scale; then evolved to the reference point $\mu^2 = 4 \text{ GeV}^2$ of the global fits. 1-loop matching to $\overline{\text{MS}}$ still to be done on our data

A. Radyushkin 1710.08813, Zhang et al 1801.03023, Izubuchi et al 1801.03917

More on evolution



- LO evolution cannot be extended to very low scales.
- It is known that evolution stops below a certain scale (by observing our data we infer that this is the case for $z_3 \geq 6a$.)
- Adopt an evolution that leaves the PDF unchanged for length scales above $z_3 = 6a$ and use the leading perturbative evolution formula to evolve to smaller z_3 scales.

Numerical implementation

Following [C. Bouchard et.al Phys. Rev. D 96, no. 1, 014504 \(2017\)](#) , we compute a regular nucleon two point function

$$C_p(t) = \langle \mathcal{N}_p(t) \overline{\mathcal{N}}_p(0) \rangle ,$$

$$C_p^{\mathcal{O}^0(z)}(t) = \sum_{\tau} \langle \mathcal{N}_p(t) \mathcal{O}^0(z, \tau) \overline{\mathcal{N}}_p(0) \rangle$$

with $\mathcal{O}^0(z, t) = \overline{\psi}(0, t) \gamma^0 \tau_3 \hat{E}(0, z; A) \psi(z, t)$

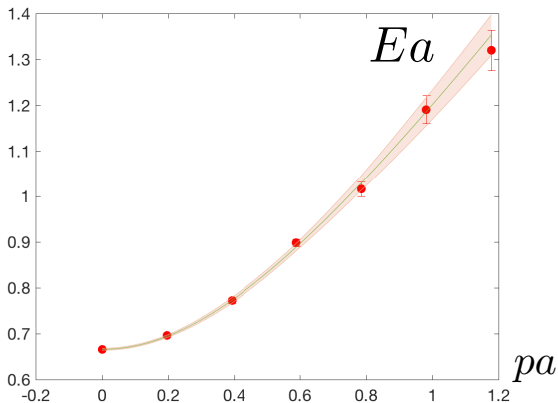
Proton momentum and displacement of the quark fields along the \hat{z} axis

$$\mathcal{M}_{\text{eff}}(z_3 p, z_3^2; t) = \frac{C_p^{\mathcal{O}^0(z)}(t+1)}{C_p(t+1)} - \frac{C_p^{\mathcal{O}^0(z)}(t)}{C_p(t)}$$

Extract the desired ME \mathcal{J} at large Euclidean time separation as

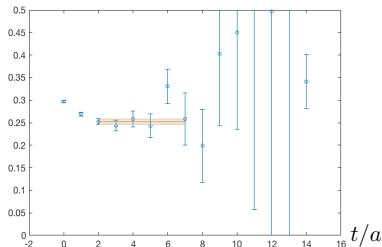
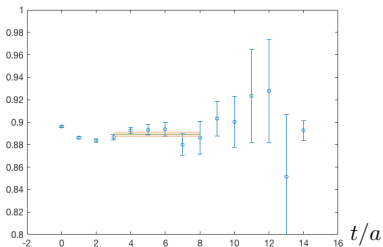
$$\frac{\mathcal{J}(z_3 p, z_3^2)}{2p^0} = \lim_{t \rightarrow \infty} \mathcal{M}_{\text{eff}}(z_3 p, z_3^2; t) , \text{ where } p^0 \text{ is the energy of the nucleon.}$$

Results for the nucleon dispersion relation



Energies and momenta are in lattice units. The solid line is the continuum dispersion relation (not a fit) while the errorband is an indication of the statistical error of the lattice nucleon energies

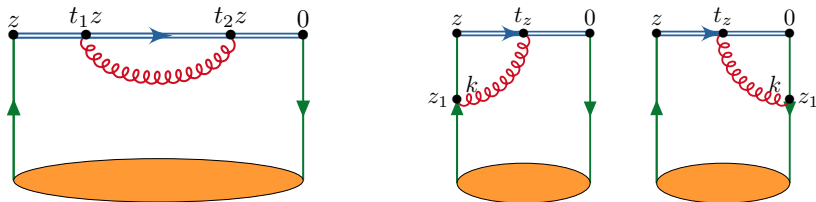
Results



Typical fits used to extract the reduced matrix element (here $p = 2\pi/L \cdot 2$ and $z = 4$ (LHS) and $p = 2\pi/L \cdot 3$ and $z = 8$ (RHS)). The average χ^2 per degree of freedom was $\mathcal{O}(1)$. All fits are performed with the full covariance matrix and the error bars are determined with the jackknife method.

Renormalization

- In a series of articles [Dotsenko Nucl.Phys. B169 \(1980\) 527](#), [Ishikawa et al. Phys. Rev. D 96, 094019 \(2017\)](#), [Chen et al. Nucl.Phys. B915 \(2017\)](#) and [A. V. Radyushkin Phys.Lett. B781 \(2018\) 433-442](#) the one loop renormalizability of $\mathcal{M}^\alpha(z, p, a)$ has been discussed
- by analyzing the pertinent diagrams one can see that there is a linear divergence from the link self-energy contribution and a logarithmic divergence associated to the anomalous dimension $2\gamma_{\text{end}}$ due to two end-points of the link.



Renormalization

- \mathcal{M} has been shown to renormalize multiplicatively as $\mathcal{M}_R(\nu, z^2, \mu) = Z_j^{-1} Z_{\bar{j}}^{-1} e^{-\delta m |z|} \mathcal{M}_B(\nu, z^2, a)$, where $\delta m = C_F \frac{\alpha_s}{2\pi} \frac{\pi}{a}$, is an effective mass counterterm removing power divergences in the Wilson line and $Z_j^{-1}, Z_{\bar{j}}^{-1}$ are renormalization constants (RCs) associated with the endpoints of the Wilson line independent of z, p .
- The entire renormalization is independent of the external momentum
- Forming the ratio, the RCs cancel and thus the reduced Ioffe time distribution has a great potential to reduce systematic effects related to renormalization. The UV divergences generated by the link-related and quark-self-energy diagrams cancel in the ratio.

Numerical implementation

- Renormalization of the ME?
- For $z_3 = 0$ $\mathcal{M}(z_3 p, z_3^2) \rightarrow$ the local iso-vector current, should be = 1 (but ...) lattice artifacts...
- Introduce an RC $Z_p = \frac{1}{\mathcal{J}(z_3 p, z_3^2)|_{z_3=0}}$
- Z_p has to be independent from p . But lattice artifacts or potential fitting systematics ...
- renormalize the ME for each momentum with its own $Z_p \rightarrow$ maximal statistical correlations to reduce statistical errors, and cancellation of lattice artifacts in the ratio

Numerical implementation

- in practise use the double ratio

$$\mathfrak{M}(\nu, z_3^2) = \lim_{t \rightarrow \infty} \frac{\mathcal{M}_{\text{eff}}(z_3 p, z_3^2; t)}{\mathcal{M}_{\text{eff}}(z_3 p, z_3^2; t)|_{z_3=0}} \times \frac{\mathcal{M}_{\text{eff}}(z_3 p, z_3^2; t)|_{p=0, z_3=0}}{\mathcal{M}_{\text{eff}}(z_3 p, z_3^2; t)|_{p=0}},$$

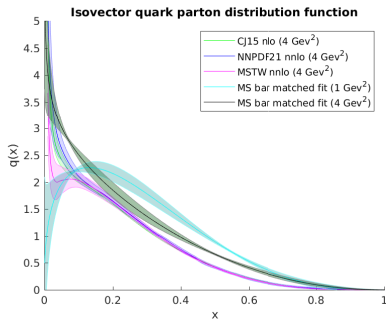
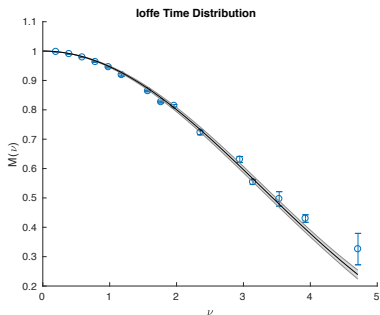
- infinite t limit is obtained with a fit to a constant for a suitable choice of a fitting range.

Matching to \overline{MS}

- In 1801.02427 it was shown by Radyushkin that at 1-loop evolution and matching to \overline{MS} can be done simultaneously.
- This establishes a direct relation between the Ioffe time distribution function (ITDF) and pseudo-ITDF.
- Scales are needed as such that we are in a regime dominated by perturbative effects

$$\begin{aligned} \mathcal{I}(\nu, \mu^2) = & \mathfrak{M}(\nu, z_3^2) + \frac{\alpha_s}{\pi} C_F \int_0^1 dw \mathfrak{M}(w\nu, z_3^2) \\ & \times \left\{ B(w) \ln \left[(1-w) z_3 \mu \frac{e^{\gamma_E + 1/2}}{2} \right] \right. \\ & \left. + [(w+1) \ln(1-w) - (1-w)]_+ \right\} \end{aligned}$$

Comparison to global fits after converting to the \overline{MS} scheme



Bayesian Reconstruction

$$P[q|\mathfrak{M}, I] = \frac{P[\mathfrak{M}|q, I]P[q|I]}{P[\mathfrak{M}|I]}.$$

- The likelihood probability $P[\mathfrak{M}|q, I]$ denotes how probable it is to find the data \mathfrak{M} if q were the correct PDF.
- Finding the most probable q by maximizing the likelihood is nothing but a χ^2 fit to the \mathfrak{M} data, which as we saw from the direct inversion is by itself ill-defined.
- The prior probability $P[q|I]$, which quantifies, how compatible our test function q is with respect to any prior information we have (e.g. appearance of non-analytic behavior of $q(x)$ at the boundaries of the x interval).
- $P[\mathfrak{M}|I]$, the so called evidence is a q independent normalization.

Bayesian Reconstruction

- For sampled data, due to the central limit theorem, the likelihood probability may be written as the quadratic distance functional $P[\mathfrak{M}|q, I] = \exp[-L]$ with $L = \frac{1}{2} \sum_{k,l} (\mathfrak{M}_k - \mathfrak{M}_k^q) C_{kl}^{-1} (\mathfrak{M}_l - \mathfrak{M}_l^q)$.
- \mathfrak{M}_k^q are the loffe-time data arising from inserting the test function q into the cosine Fourier trafo and C_{kl} denotes the covariance matrix of the N_m measurements of simulation data \mathfrak{M}_k^h .
- We then specify an appropriate prior probability $P[q|I] = \exp[\alpha S[I]]$.
- Prior information enters in two ways here. On the one hand we deploy a particular functional form of the regularization functional

$$S_{BR}[q, m] = \sum_n \Delta x_n \left(1 - \frac{q_n}{m_n} + \log\left(\frac{q_n}{m_n}\right) \right)$$

which may be obtained by requiring positive definiteness of the resulting q , smoothness of q .

Bayesian Reconstruction

- The functional S depends on the function m , the default model.
- By construction constitutes its unique extremum.
- In the Bayesian logic m is the correct result for q in the absence of any data.
- We select m by a best fit of the Ioffe-PDF data and we will vary it to get a handle on systematics.

Bayesian Reconstruction

- What happens in the case of non-guaranteed positive definiteness?
- We need to change the regulator!
- Often the quadratic regulator is used

$$S_{QDR}[q, m] = \sum_n \Delta x_n (q_n - m_n)^2$$

- It is a comparatively strong regulator and usually imprints the form of the default model significantly onto the end result.
- Trying to keep the influence of the default model to a minimum, we extend the BR prior to non-positive functions.

$$S_{BRg}[q, m] = \sum_n \Delta x_n \left(-\frac{|q_n - m_n|}{h_n} + \log\left(\frac{|q_n - m_n|}{h_n} - 1\right) \right)$$

keeping the advantageous properties of the original BR prior at the price of having to introduce another default model related function h .

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Bayesian Reconstruction

- once L , S and m have been provided, the most probable PDF q , given simulation data and prior information is obtained by numerically finding the extremum of the posterior

$$\left. \frac{\delta P[q|\mathfrak{M}, I]}{\delta q} \right|_{q=q_{\text{Bayes}}} = 0.$$

- It has been proven that if the regulator is strictly concave, as is the case for all the regulators discussed above, there only exists a single unique extremum in the space of functions q on a discrete ν interval.
- With positive definiteness imposed on the end result, the space of admissible solutions is significantly reduced. Regulators admitting also q functions with negative contributions have to distinguish between a multitude of oscillatory functions, which if integrated over, resemble a monotonous function to high precision. We will observe the emergence of ringing artefacts for the quadratic and generalized BR prior.

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- We select m by a best fit of the Ioffe-PDF data and we will vary it to get a handle on systematics.
- In the definition of $P[q|I]$ we introduced a further parameter α , a so called hyperparameter
- Weighs the influence of simulation data and prior information. It has to be taken care of self-consistently.
- In the Maximum Entropy Method α is selected, such that the evidence has an extremum. In the BR method we deploy here, we marginalize the parameter α a priori, i.e. we integrate the posterior w.r.t the hyperparameter, assuming complete ignorance of its values $P[\alpha] = 1$.

Advanced PDF Reconstructions

- A versatile approach is Bayesian inference Y. Burnier and A. Rothkopf Phys.Rev.Lett. 111 (2013)
- It acknowledges the fact that the inverse problem is ill-defined and a unique answer may only be provided, once further information about the system has been made available.
- Formulated in terms of probabilities, one finds in the form of Bayes theorem that

$$P[q|\mathfrak{M}, I] = \frac{P[\mathfrak{M}|q, I]P[q|I]}{P[\mathfrak{M}|I]}.$$

It states that the so called **posterior probability** $P[q|\mathfrak{M}, I]$ for a test function q to be the correct x -space PDF, given our simulated loffe-time PDF \mathfrak{M} and additional prior information may be expressed in terms of three quantities.

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Bayesian Reconstruction

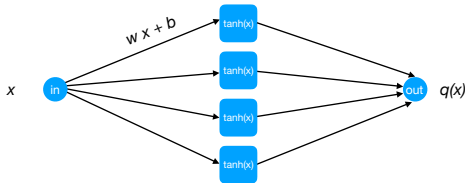
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Neural Network Reconstruction

- The ensemble average of data is obtained in two steps
 - ▶ Starting from random $[w, b]$, minimize χ^2 to find $[w, b]$.
 - ▶ Repeat 10 times to find 10 different Neural Nets (replicas).
- For each Neural Net, the minimizer is re-run for each jackknife sample to obtain a jackknife estimate $q(x)$ for each replica.
- Central value of $q(x)$ is the average over jackknife samples and replicas.
- Error by combining the fluctuations over the jackknife sample and replicas.



$$[\theta] = \{w, b\}$$

$$\min_{[\theta]} [\chi^2] \rightarrow [w, b]$$

$$\chi^2 = \sum_k \left(M(\nu_k) - \int_0^1 dx q_{[\theta]}(x) \cos(\nu_k x) \right) \sigma_k^2 \left(M(\nu_k) - \int_0^1 dx q_{[\theta]}(x) \cos(\nu_k x) \right)$$

Lattice QCD requirements

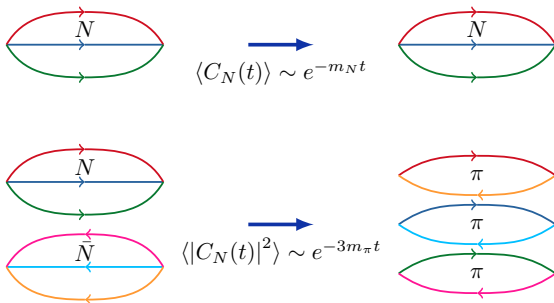
- Largest momentum on the lattice $aP_{max} = \pi/2 \propto \mathcal{O}(1)$
- $a = 0.1\text{fm} \rightarrow P_{max} = 10\Lambda$ where $\Lambda = 300 \text{ MeV}$
- $a = 0.05\text{fm} \rightarrow P_{max} = 20\Lambda$

Large momentum is required to suppress high twist effects (quasi-PDFs) and to provide a wide coverage of the loffe time ν

$P_{max} = 3 \text{ GeV}$ easily achievable with moderate values of the lattice spacing but still demanding due to statistical noise

$P_{max} = 6 \text{ GeV}$ exponentially harder requiring very fine values of the lattice spacing

Signal to Noise

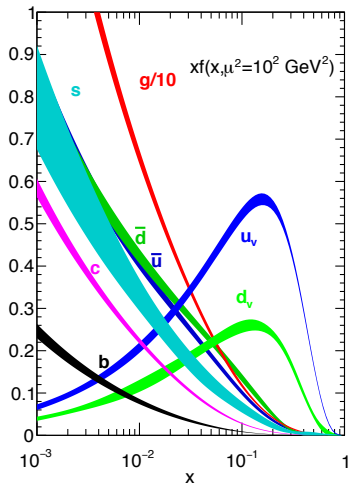
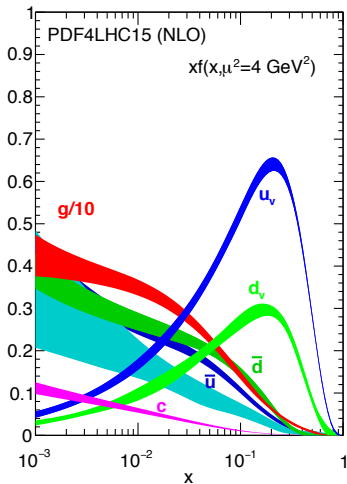


Statistical accuracy drops exponentially with increasing momentum P

$$\text{StN}(O) = \frac{\langle O \rangle}{\sqrt{\text{var}(O)}} \propto e^{-[E_N(P) - 3/2m_\pi]t}$$

G. Parisi (1984) P. Lepage (1989)

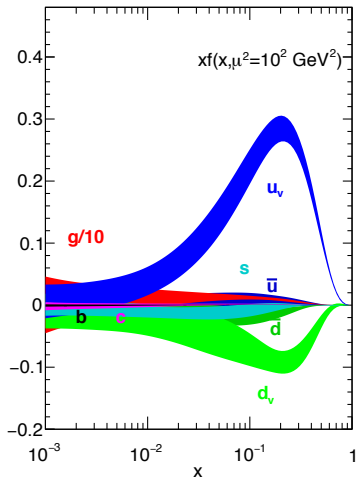
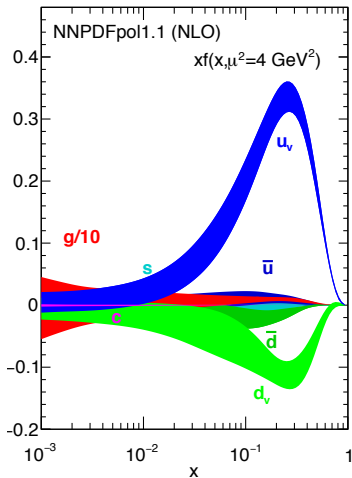
Determination of PDFs from Experiment



Global fits to experimental data [Parton distributions and lattice QCD calculations: a community white paper arXiv:](#)

1711.07916

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1711.07916

Backus-Gilbert Reconstruction

- The Backus-Gilbert (BG) method instead of imposing a smoothing condition on the resulting PDF $q(x)$ it imposes a minimization condition on the variance of the resulting function. G. Backus and F. Gilbert. *Geophysical Journal of the Royal*

Astronomical Society, 16:169205, (1968)

- Let us define a rescaled kernel and rescaled PDF $h(x)$

$$K_j(x) \equiv \cos(\nu_j x) p(x) \quad \text{and} \quad h(x) \equiv \frac{q_v(x)}{p(x)}$$

- where $p(x)$ corresponds to an appropriately chosen function that makes the problem easier to solve.
- We wish to incorporate into $p(x)$ most of the non-trivial structure of $q(x)$ apriorily, such that $h(x)$ is a slowly varying function of x and contains only the deviation of $q(x)$ from $p(x)$.

Backus-Gilbert Reconstruction

- Starting from the preconditioned expression with a rescaled PDF $h(x)$ that is only a slowly varying function of x our inverse problem becomes

$$d_j \equiv \mathfrak{M}_R(\nu_j) = \int_0^1 dx K_j(x) h(x).$$

- BG introduces a function $\Delta(x - \bar{x}) = \sum_j q_j(\bar{x}) K_j(x)$, where $q_j(\bar{x})$ are unknown functions to be determined.
- It then estimates the unknown function as a linear combination of the data

$$\hat{h}(\bar{x}) = \sum_j q_j(\bar{x}) d_j, \text{ or } \hat{q}_v(\bar{x}) = \sum_j q_j(\bar{x}) d_j p(\bar{x})$$

- If $\Delta(x - \bar{x})$ were to be a δ -function then $\hat{h}(\bar{x}) = h(\bar{x})$. If $\Delta(x - \bar{x})$ approximates a δ -function with a width σ , then the smaller σ is the better the approximation of $\hat{h}(x)$ to $h(x)$.

Backus-Gilbert Reconstruction

- In other words if $\hat{h}_\sigma(x)$ is the approximation resulting from $\Delta(x)$ with a width σ then $\lim_{\sigma \rightarrow 0} \hat{h}_\sigma(x) = h(x)$.
- With this in mind BG minimizes the width σ given by

$$\sigma = \int_0^1 dx (x - \bar{x})^2 \Delta(x - \bar{x})^2.$$

- Furthermore, if $\Delta(x)$ approximates a δ -function then one has to impose the constraint $\int_0^1 dx \Delta(x - \bar{x}) = 1$. Using a Lagrange multiplier λ one can minimize the width and impose the constraint by minimizing

$$\chi[q] = \int_0^1 dx (x - \bar{x})^2 \sum_{j,k} q_j(\bar{x}) K_j(x) K_k(x) q_k(\bar{x}) + \lambda \int_0^1 dx \sum_j K_j(x) q_j(\bar{x}).$$

- But let's see all this in practise ...