Simultaneous QCD analysis of quantum probability distributions

Wally Melnitchouk
— Jefferson Lab —
Overview

- JAM (Jefferson Lab Angular Momentum) collaboration studies the parton structure of hadrons through extraction of “quantum probability distributions” (PDFs, FFs, TMDs) via global QCD analysis using Monte Carlo-based methods.

- Methodology is based on Bayesian statistics and Monte Carlo sampling of the parameter space.

- Inter-dependence of observables on distributions requires simultaneous extraction of unpolarized and polarized PDFs & fragmentation functions.
Strange quark suppression from a simultaneous Monte Carlo analysis of PDFs and fragmentation functions

First Monte Carlo global QCD analysis of pion parton distributions

First Monte Carlo global analysis of nucleon transversity with lattice QCD constraints

First simultaneous extraction of spin-dependent PDFs and fragmentation functions from a global QCD analysis

First Monte Carlo analysis of fragmentation functions from e^+e^- annihilation

Iterative Monte Carlo analysis of spin-dependent parton distributions

Constraints on spin-dependent parton distributions at large x from global QCD analysis

Impact of hadronic and nuclear corrections on global analysis of spin-dependent PDFs
Parton distributions in hadrons

- Parton distribution functions (PDFs) are light-cone correlation functions

\[ q(x) = \int_{-\infty}^{\infty} d\xi^- e^{-ixP^+\xi^-} \langle P \mid \bar{\psi}(\xi^-) \gamma^+ \mathcal{W}(\xi^-, 0) \psi(0) \mid P \rangle \]

\[ \rightarrow \text{light cone momentum fraction} \quad x = \frac{k^+_c}{P^+} \]

\[ \rightarrow \text{Wilson line (gauge invariance)} \quad \mathcal{W}(\xi^-, 0) = \exp \left\{ -ig \int_0^{\xi^-} d\eta^- A^+(\eta^-) \right\} \]

- In \( A^+ = 0 \) gauge, in fast-moving frame PDF has a probabilistic interpretation as a particle density

\[ \int_{-1}^{1} dx \ q(x) = \langle P \mid \bar{\psi}(0) \gamma^+ \psi(0) \mid P \rangle \approx \langle P \mid \psi^\dagger(0) \psi(0) \mid P \rangle \]

\[ \bar{\psi} \gamma^0 \psi \approx \bar{\psi} \gamma^z \psi \]
Parton distributions in hadrons

- Inclusive high-energy particle production $AB \rightarrow CX$

\[ \sigma_{AB \rightarrow CX}(p_A, p_B) = \sum_{a,b} \int d x_a \, d x_b \, f_{a/A}(x_a, \mu) \, f_{b/B}(x_b, \mu) \times \sum_n \alpha_s^n(\mu) \, \hat{\sigma}_{ab \rightarrow CX}^{(n)}(x_a p_A, x_b p_B, Q/\mu) \]

- QCD factorization: separation of hard (perturbative, calculable) from soft (nonperturbative, parametrized) physics

- Process-independent parton distribution functions $f_{a/A}$ characterizing structure of bound state $A$

Collins, Soper, Sterman (1980s)
Parton distributions in hadrons

- Most information on PDFs obtained from lepton-hadron deep-inelastic scattering (DIS)

\[
\frac{d^2 \sigma}{d\Omega dE'} = \frac{4\alpha^2 E'^2 \cos^2 \frac{\theta}{2}}{Q^4} \left( 2 \tan^2 \frac{\theta}{2} \frac{F_1}{2M} + \frac{F_2}{\nu} \right)
\]

\[
x_B = \frac{Q^2}{2M\nu} \quad Q^2 = q^2 - \nu^2 \quad \nu = E - E'
\]

\[\rightarrow\] structure function given as convolution of hard Wilson coefficient with PDF

\[
F_2(x_B, Q^2) = x_B \sum_q e_q^2 \int_{x_B}^{1} \frac{dx}{x} C_q \left( \frac{x_B}{x}, \alpha_s \right) q(x, Q^2)
\]

\[\rightarrow x_B \sum_q e_q^2 q(x_B, Q^2)\]

for leading order approximation

\[
C_q \rightarrow \delta \left( 1 - \frac{x_B}{x} \right)
\]
Parton distributions in hadrons

- **Spin-dependent PDFs are defined similarly**

  \[ \Delta q(x) = q^\uparrow(x) - q^\downarrow(x) \]

  \[ = \int_{-\infty}^{\infty} d\xi^- e^{-ixP^+\xi^-} \langle P | \bar{\psi}(\xi^-) \gamma^+ \gamma_5 \mathcal{W}(\xi^-, 0) \psi(0) | P \rangle \]

  measured in polarized lepton-nucleon DIS

\[ A_\parallel = \frac{\sigma^{\uparrow\downarrow} - \sigma^{\uparrow\uparrow}}{\sigma^{\uparrow\downarrow} + \sigma^{\uparrow\uparrow}} = D (A_1 + \eta A_2) \]

\[ A_1 \approx \frac{2x_B g_1(x_B, Q^2)}{F_2(x_B, Q^2)} \]

- **Polarized structure function in terms of spin-dependent PDFs**

  \[ g_1(x_B, Q^2) = \frac{1}{2} \sum_q e_q^2 \int_{x_B}^1 \frac{dx}{x} \Delta C_q \left( \frac{x_B}{x}, \alpha_s \right) \Delta q(x, Q^2) \]

  \[ \rightarrow \frac{1}{2} \sum_q e_q^2 \Delta q(x_B, Q^2) \text{ at leading order} \]
Global PDF analysis

Universality of PDFs allows data from many different processes (DIS, SIDIS, weak boson/jet production in $pp$, Drell-Yan …) to be analyzed simultaneously

→ distributions parametrized using a specific functional form, with parameters fitted to data

Extraction of PDFs is challenging because usually there exist multiple solutions — “inverse problem”

→ PDFs are not directly measured, but inferred from observables involving convolutions with other functions
Bayesian approach to global analysis

Analysis of data requires estimating expectation values $E$ and variances $V$ of “observables” $\mathcal{O}$ (functions of PDFs) which are functions of parameters

$$
E[\mathcal{O}] = \int d^m a \, \mathcal{P}(\tilde{a}|\text{data}) \, \mathcal{O}(\tilde{a})
$$

$$
V[\mathcal{O}] = \int d^m a \, \mathcal{P}(\tilde{a}|\text{data}) \left[ \mathcal{O}(\tilde{a}) - E[\mathcal{O}] \right]^2
$$

“Bayesian master formulas"

Using Bayes’ theorem, probability distribution $\mathcal{P}$ given by

$$
\mathcal{P}(\tilde{a}|\text{data}) = \frac{1}{Z} \, \mathcal{L}(\text{data}|\tilde{a}) \, \pi(\tilde{a})
$$

in terms of the likelihood function $\mathcal{L}$ and priors $\pi$
Bayesian approach to global analysis

**Likelihood function**

\[
\mathcal{L}(\text{data}|\vec{a}) = \exp\left(-\frac{1}{2}\chi^2(\vec{a})\right)
\]

is a Gaussian form in the data, with \(\chi^2\) function

\[
\chi^2(\vec{a}) = \sum_i \left(\frac{\text{data}_i - \text{theory}_i(\vec{a})}{\delta(\text{data})}\right)^2
\]

with priors \(\pi(\vec{a})\) and evidence \(Z\)

\[
Z = \int d^n a \, \mathcal{L}(\text{data}|\vec{a}) \, \pi(\vec{a})
\]

→ \(Z\) tests if e.g. an \(n\)-parameter fit is statistically different from \((n+1)\)-parameter fit
Bayesian approach to global analysis

- **Standard method for evaluating** $E$, $V$ via maximum likelihood
  
  $\Rightarrow$ maximize probability distribution
  
  $P(\tilde{a}|\text{data}) \rightarrow \tilde{a}_0$

  $\Rightarrow$ if $\mathcal{O}$ is linear in parameters, and if probability is symmetric in all parameters
  
  $E[\mathcal{O}(\tilde{a})] = \mathcal{O}(\tilde{a}_0), \quad V[\mathcal{O}(\tilde{a})] \rightarrow \text{Hessian} \quad H_{ij} = \frac{1}{2} \frac{\partial^2 \chi^2(\tilde{a})}{\partial a_i \partial a_j} \bigg|_{\tilde{a} = \tilde{a}_0}$

- In practice, since in general $E[f(\tilde{a})] \neq f(E[\tilde{a}])$, maximum likelihood method sometimes fails

  $\Rightarrow$ need more robust (Monte Carlo) approach

  $E[\mathcal{O}] \approx \frac{1}{N} \sum_k \mathcal{O}(\tilde{a}_k), \quad V[\mathcal{O}] \approx \frac{1}{N} \sum_k [\mathcal{O}(\tilde{a}_k) - E[\mathcal{O}]]^2$
Bayesian approach to global analysis

- First group to use MC for global PDF analysis was NNPDF, using neural network to parametrize $P(x)$ in

$$f(x) = N x^\alpha (1 - x)^\beta P(x)$$

→ “unbiased”? not really… “pre-processing” coefficients… there is no such thing as an unbiased PDF fit!

Ball, Forte et al. (2002)

- JAM — iterative, multi-step Monte Carlo

→ traditional functional form for distributions, but sample much larger parameter space

→ no assumptions for exponents

→ iterate until convergence (posteriors = priors)

→ robust determination of PDF uncertainties

Accardi, WM, Nocera, Sato et al. (2019)
First application of IMC — spin structure

First JAM MC analysis studied impact of JLab data on spin structure of the nucleon

\[ x \Delta u^+ \]

\[ x \Delta d^+ \]

\[ x \Delta s^+ \]

\[ x \Delta g \]

\( Sato, WM, Kuhn, Ethier, Accardi (2016) \)

\( Q^2 \) evolution

- inclusion of JLab data increases # data points by factor \( \sim 2 \)
- reduced uncertainty in \( \Delta s^+, \Delta g \)
- \( s \)-quark polarization negative from inclusive DIS data (assuming SU(3) symmetry)
First application of IMC — spin structure

First JAM MC analysis studied impact of JLab data on spin structure of the nucleon

- inclusion of JLab data increases # data points by factor ~ 2
- reduced uncertainty in $\Delta s^+$, $\Delta g$ through $Q^2$ evolution
- $s$-quark polarization negative from Inclusive DIS data (assuming SU(3) symmetry)
First application of IMC — spin structure

- Inclusive DIS data cannot distinguish between \( q \) and \( \bar{q} \)
  - 2 observables \( (g_1^p, g_1^n) \) can determine up to 2 unknowns, e.g. \( \Delta u + \Delta \bar{u}, \Delta d + \Delta \bar{d} \) — sea quarks from \( Q^2 \) dependence

- Semi-inclusive DIS sensitive to \( \Delta q \) & \( \Delta \bar{q} \)
  \[
  \sim \sum_q e_q^2 \left[ \Delta q(x) D_q^h(z) + \Delta \bar{q}(x) D_{\bar{q}}^h(z) \right]
  \]
  fragmentation functions

- Global analysis of DIS + SIDIS data gives different sign for strange quark polarization for different fragmentation functions!
  - \( \Delta s > 0 \) for “DSS” FFs, but \( \Delta s < 0 \) for “HKNS” FFs

- Need to understand origin of differences in fragmentation functions
IMC analysis of fragmentation functions

Analysis of single-inclusive $e^+ e^-$ annihilation data for $\pi$, $K$
production (from DESY, CERN, SLAC & KEK) from $Q \sim 10$ GeV to $M_Z$

$e^+ e^- \rightarrow h X$
single-inclusive
annihilation (SIA)

Sato, Ethier, WM, Hirai, Kumano, Accardi (2016)

→ convergence after $\sim 20$ iterations
**Analysis of single-inclusive $e^+e^-$ annihilation data for $\pi$, $K$ production (from DESY, CERN, SLAC & KEK) from $Q \sim 10$ GeV to $M_Z$**

The single-inclusive annihilation process

<table>
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<th>Experiment</th>
<th>Ref.</th>
<th>Observable</th>
<th>$Q$ (GeV)</th>
<th>$N_{dat}$</th>
<th>norm.</th>
<th>$\chi^2$</th>
<th>$N_{dat}$</th>
<th>norm.</th>
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<td>(*)</td>
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<td>0.998 (1.001)</td>
<td>30.2 (40.4)</td>
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<td>Total:</td>
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<td>599.3 (671.2)</td>
<td>391</td>
<td>395.0</td>
<td>1.31 (1.46)</td>
<td>1.01</td>
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$\chi^2/N_{dat} = 1.31 (1.46)$  \hspace{1cm} $\chi^2/N_{dat} = 1.01$
IMC analysis of fragmentation functions

- Analysis of single-inclusive $e^+ e^-$ annihilation data for $\pi$, $K$ production (from DESY, CERN, SLAC & KEK) from $Q \sim 10$ GeV to $M_Z$

$u^+ = u + \bar{u}$ & $s^+ = s + \bar{s}$ FFs well constrained

$\rightarrow$ larger $s \rightarrow K$ fragmentation $cf.$ HKNS suggests less negative $\Delta s$
Simultaneous spin PDF + FF analysis

- First simultaneous extraction of spin PDFs and FFs, fitting polarized DIS + SIDIS (HERMES, COMPASS) and SIA data

- No assumption of SU(3) symmetry
  \( \Delta u^+ - \Delta d^+ = g_A \equiv F + D \)
  \( \Delta u^+ + \Delta d^+ - 2\Delta s^+ = a_8 \equiv 3F - D \)

- \( \Delta s \) slightly > 0 at high \( x \), consistent with zero

- \( \Delta s - \Delta \bar{s} \) & \( \Delta \bar{u} - \Delta \bar{d} \) consistent with zero

**Ethier, Sato, WM (2017)**
Simultaneous spin PDF + FF analysis

Polarized strangeness in previous, DIS-only analyses was negative at $x \sim 0.1$, induced by SU(3) and parametrization bias.

![Graph showing $x\Delta s^+$](image)

- weak sensitivity to $\Delta s^+$ from DIS data & evolution
  - SU(3) pulls $\Delta s^+$ to generate moment $\sim -0.1$
  - negative peak at $x \sim 0.1$ induced by fixing $b \sim 6 - 8$

Ethier, Sato, WM (2017)
Simultaneous spin PDF + FF analysis

SIDIS data, especially for $K$ production, clearly prefer a less negative $\Delta s$

Ethier, Sato, WM (2017)
Simultaneous spin PDF + FF analysis

Statistical distribution of lowest moments (axial charges)

- triplet charge $g_A$ consistent with $SU(2)$ value
- hint of $SU(3)$ breaking in octet charge $a_8$  
  \[ a_8 = 0.46(21) \]
- less negative $\Delta s = -0.03(10)$ gives larger total helicity $\Delta \Sigma = 0.36(9)$

Ethier, Sato, WM (2017)
Simultaneous spin PDF + FF analysis

- What impact does unpolarized strange PDF have on the extraction of polarized strange?
  
  → only systematic way is to fit unpolarized PDFs, polarized PDFs and fragmentation functions simultaneously…

- Shape of unpolarized strange PDF is interesting (and controversial) in its own right!
  
  → historically, strange to nonstrange ratio $R_s = \frac{s + \bar{s}}{u + \bar{d}} \sim 0.4$

\begin{itemize}
  \item $Q^2 = 1.9$ GeV$^2$, $x=0.023$
  \item $pp \to W(Z) + X$
  \item $r_s = \frac{(s + \bar{s})/2\bar{d}}{\bar{d}} = 1.00^{+0.25}_{-0.28}$
\end{itemize}
Study the impact of SIDIS data on unpolarized PDFs

- unpolarized fixed-target DIS on $p, d$ (SLAC, BCDMS, NMC), HERA collider data (runs I & II)
- Drell-Yan (Fermilab E866), jet production (CDF, D0)
- SIDIS pion & kaon multiplicities for deuteron (COMPASS)
- $e^+e^-$ annihilation (DESY, LEP/CERN, SLAC, KEK)

52 shape parameters + 41 “nuisance” parameters for systematic uncertainties (data normalizations)

953 fits to 4366 data points (2680 DIS, 992 SIDIS, 250 DY, 444 SIA)

such an analysis has never been attempted before…
JAM 2019 analysis

mean reduced $\chi^2 = 1.3$ for all data

→ valence & light sea quark broadly in agreement with other groups
→ striking suppression of strange PDF compared to ATLAS extraction
→ SIDIS + SIA data force strange to kaon FF to be larger
JAM 2019 analysis

--- solutions with large $s(x)$

fully constrained solutions
JAM 2019 analysis

- - - - solutions with large \( s(x) \)

--- fully constrained solutions

SIA data at large \( z \) strongly disfavor small strange \( \rightarrow K_{\text{FF}} \)
vital role played by SIDIS + SIA data in constraining strange PDF
Recent progress in extracting $x$ dependence of PDFs in lattice QCD from matrix element of nonlocal operator

$$h(z, P_z) = \langle P | \bar{\psi}(0, z) \gamma_z \mathcal{W}(z, 0) \psi(0, 0) | P \rangle$$

$$= \int_{-\infty}^{\infty} dy \ e^{i y P_z z} \bar{q}(y, P_z)$$

→ quasi-PDF $\tilde{q}$ related to light-cone PDF via matching kernel $\tilde{C}$

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

Conflicting results on sign of $\bar{d} - \bar{u}$ asymmetry

$d > u$

$d < u$
PDFs in lattice QCD

Fit lattice observable directly within JAM framework

→ cannot determine \( \bar{d} - \bar{u} \) from present lattice data
PDFs in lattice QCD

- Fit lattice observable directly within JAM framework

better agreement between lattice and experiment for polarized PDFs (within larger uncertainties)

Bringewatt, Sato, WM (2019)
PDFs in the pion

- MC analysis combining pQCD with chiral EFT to fit $\pi N$ Drell-Yan + leading neutron electroproduction data from HERA

$\text{DY} = \pi N$ Drell-Yan data (medium/high $x$)

$\text{LN} =$ leading neutron electroproduction (low $x$)

- Larger gluon fraction in the pion than without LN constraint

$\langle x_\pi \rangle$ vs. $Q^2$ (GeV$^2$)
PDFs in the pion

- MC analysis combining pQCD with chiral EFT to fit $\pi N$ Drell-Yan + leading neutron electroproduction data from HERA

- Provides new insights into the origin of the $\bar{d} - \bar{u}$ asymmetry in the proton

  → chiral effective theory relates asymmetry to structure of pion

$$ (\bar{d} - \bar{u})(x) = \int \frac{dy}{y} f_{\pi + n}(y) \bar{q}^\pi(x/y) $$

DY = $\pi N$ Drell-Yan data (medium/high $x$)

LN = leading neutron electroproduction (low $x$)
PDFs in the pion

- $x \to 1$ behavior of pion PDF is controversial: $\sim (1 - x)$ or $(1 - x)^2$?

- Hard scattering coefficient function kinematically enhanced when $z \to 1$ because of gluon emissions

- Effect of resummation on phenomenology?
PDFs in the pion

- New analysis examines whether large-$q_T$ DY data can be simultaneously described with $q_T$-integrated DY + HERA LN data

  $$\rightarrow$$ large-$q_T$ photon requires hard gluon to recoil against — sensitivity to gluon PDF in pion at large $x$!

- Generalization of chiral model to SU(3) octet & decuplet baryons

  * Nina Cao et al. (2019)

  Marston Copeland et al. (2019)

  * expected Oct. 2019
Outlook

- New paradigm in global analysis — simultaneous determination of collinear distributions using MC sampling of parameter space

- Next steps: simultaneous analysis of all collinear distributions — unpolarized & polarized PDFs and FFs (including jet, $W$ production, … data)

- Longer-term: technology developed here will be applied to global QCD analysis of transverse momentum dependent (TMD) distributions — map out full 3-d image of hadrons