



KRAKOW SCHOOL
OF INTERDISCIPLINARY
PHD STUDIES

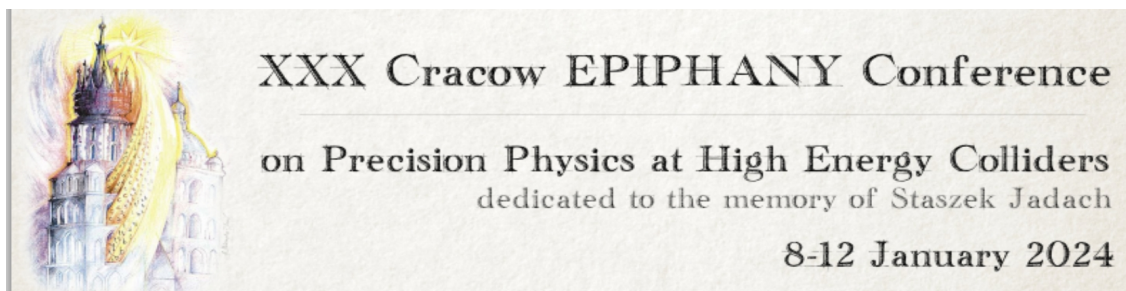
Markov Chain Monte Carlo Methods: An Alternative Approach for Nuclear PDF Determination

Nasim Derakhshanian

Dr. Aleksander Kusina

IFJ PAN

Department of Theoretical Particle Physics



nCTEQ
nuclear parton distribution functions

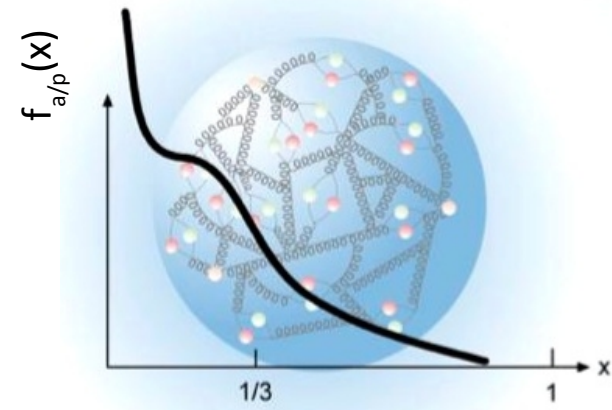


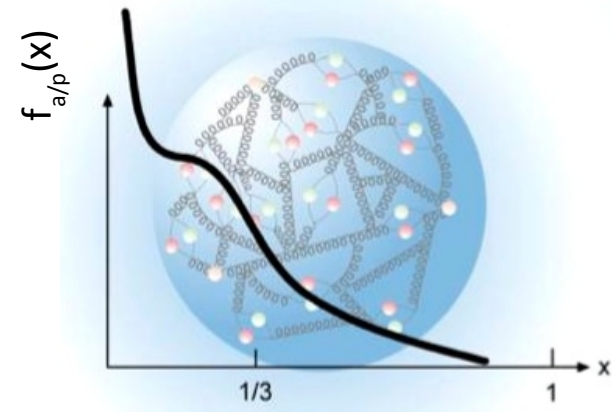
Parton Distribution Function (PDF):

The probability $f_{a/p}(x, \mu)$ that a parton **a** carries fraction **x** of the proton's momentum

μ : Factorization scale

x: momentum fraction





Parton Distribution Function (PDF):

The probability $f_{a/p}(\mathbf{x}, \mu)$ that a parton \mathbf{a} carries fraction \mathbf{x} of the proton's momentum

μ : Factorization scale

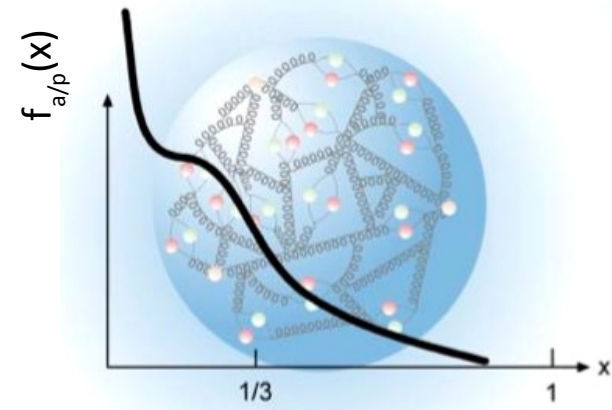
\mathbf{x} : momentum fraction

Factorization Theorem:

$$\sigma_{P\gamma\rightarrow c} = f_{P\rightarrow a} \otimes \hat{\sigma}_{a\gamma\rightarrow c}$$

Parton densities
(long-distance)

Parton interaction
(short-distance)



Parton Distribution Function (PDF):

The probability $f_{a/p}(\mathbf{x}, \mu)$ that a parton \mathbf{a} carries fraction \mathbf{x} of the proton's momentum

μ : Factorization scale

\mathbf{x} : momentum fraction

Factorization Theorem:

$$\sigma_{P \gamma \rightarrow c} = f_{P \rightarrow a} \otimes \hat{\sigma}_{a \gamma \rightarrow c}$$

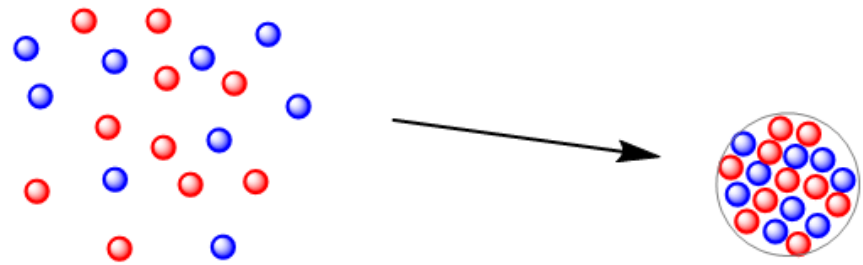
Parton densities
(long-distance)

Parton interaction
(short-distance)

PDF properties:

- Universal (independent of the process)
- Constrained through momentum and number sum rules
- μ^2 -dependence governed by DGLAP evolution equations
- **Non-perturbative:** x -dependence of PDF is NOT calculable in pQCD

→ extracting from a fit to experimental data

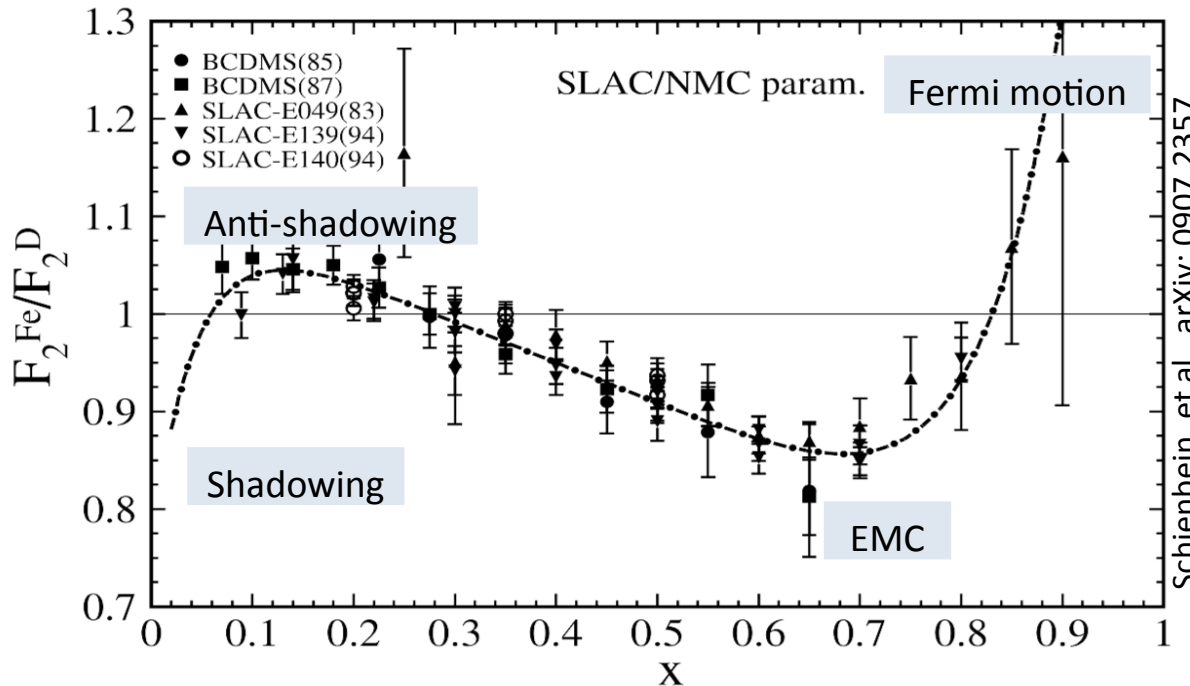


Nuclear PDFs(nPDFs):

Free nucleons

Bound nucleons within a nucleus

$$F_2^A(x) \neq ZF_2^p(x) + NF_2^n(x)$$





Nuclear PDFs(nPDFs):

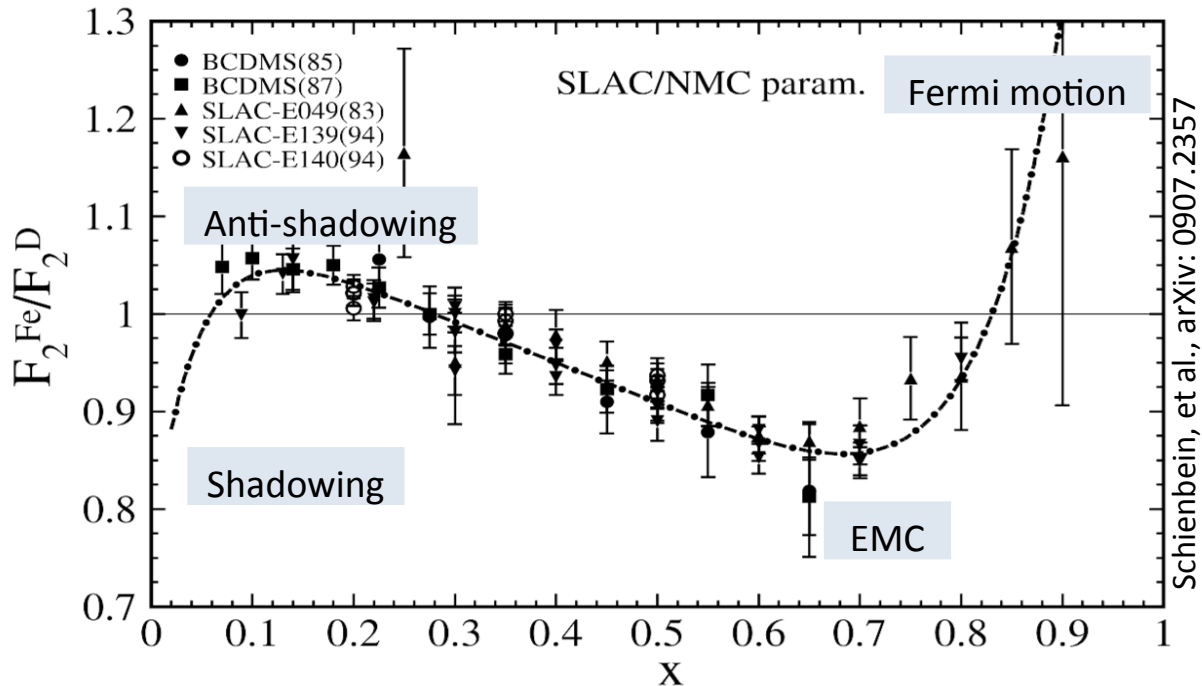
Motivations:

- Interpreting heavy-ion collision data
- Understanding Nuclear Structure

The accuracy of PDF(nPDF) determination plays an important role in high-energy physics

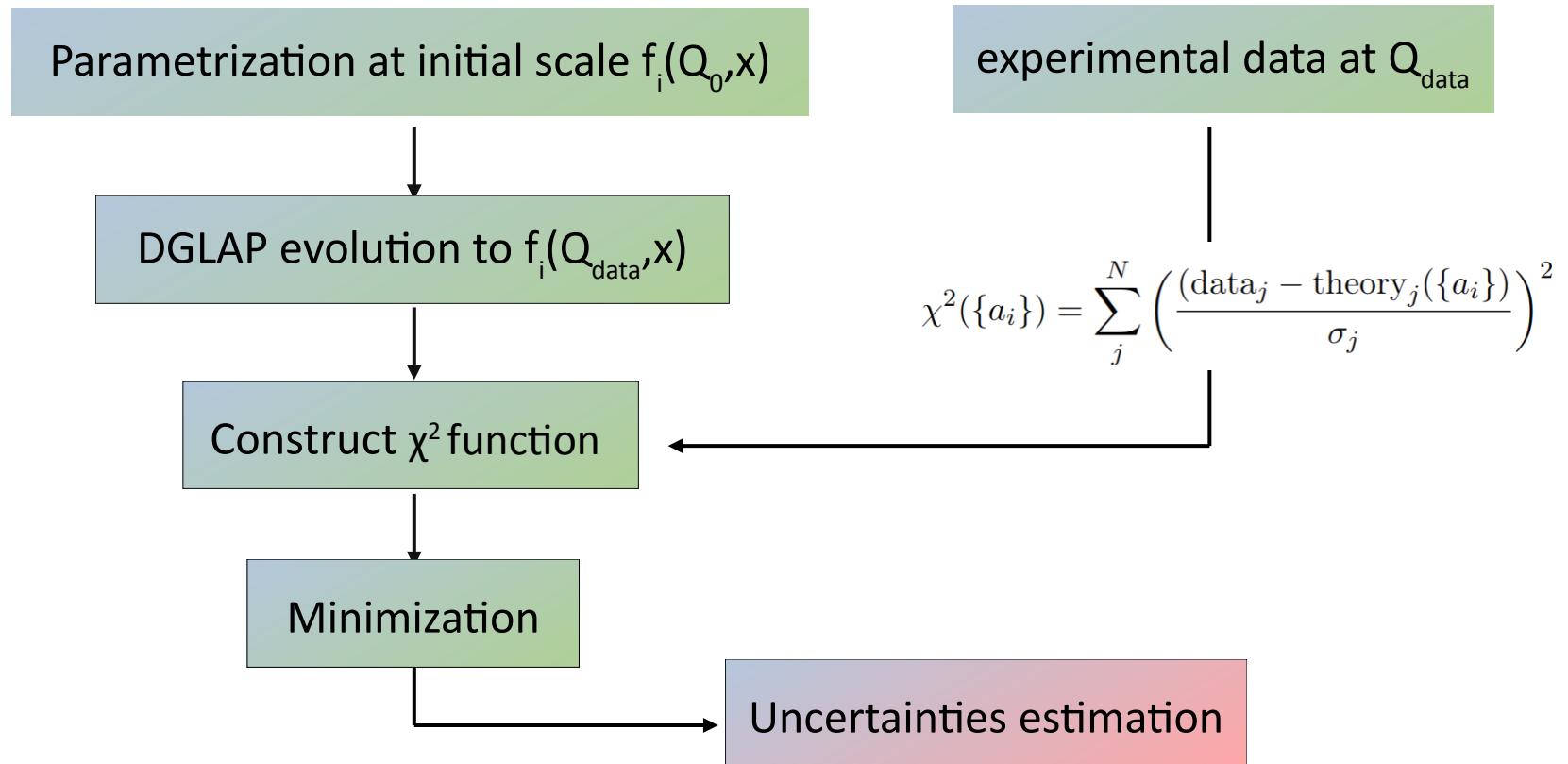
$$F_2^A(x) \neq ZF_2^p(x) + NF_2^n(x)$$

Nuclear correction ratio:



Schienbein, et al., arXiv: 0907.2357

QCD Global analysis:





nCTEQ15 framework for nuclear PDF:

Kovarik et al., arXiv:1509.00792

Functional form for bound proton at Q_0 :

$$x f_i^{p/A}(x, Q_0) = c_0 x^{c_1} (1-x)^{c_2} e^{c_3 x} (1 + e^{c_4 x})^{c_5}$$

$$i = u_v, d_v, g, \bar{u} + \bar{d}, s, \bar{s}$$

Atomic number dependence is characterized in the c_k coefficients as

$$c_k \rightarrow c_k(A) \equiv p_k + a_k(1 - A^{-b_k}), \quad k = \{1, \dots, 5\}.$$

PDF of a nucleus (A – mass, Z – charge):

$$f_i^{(A,Z)}(x, Q) = \frac{Z}{A} f_i^{p/A}(x, Q) + \frac{A-Z}{A} f_i^{n/A}(x, Q)$$

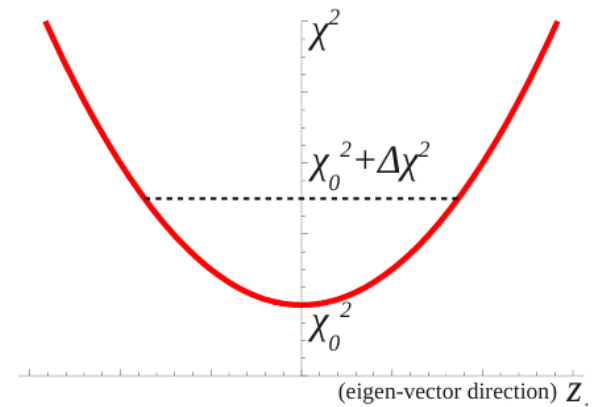


PDF uncertainties estimation:

Hessian method: Common method for estimating uncertainties in PDFs.



relying on the Gaussian approximation of $\Delta\chi^2$



Shortcomings:

- Non-gaussian errors
- Global minima judgment
- Choice of $\Delta\chi^2$

PDF uncertainties estimation:

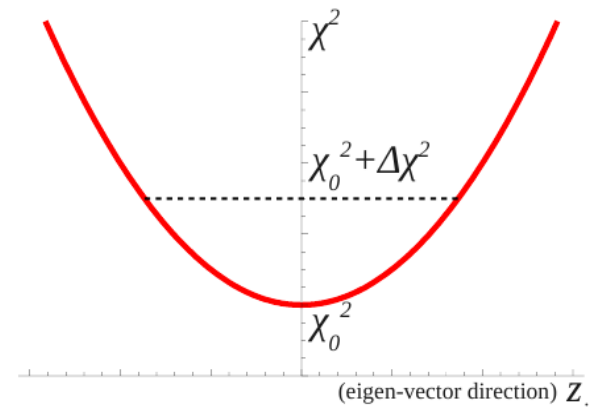
Hessian method: Common method for estimating uncertainties in PDFs.



relying on the Gaussian approximation of $\Delta\chi^2$

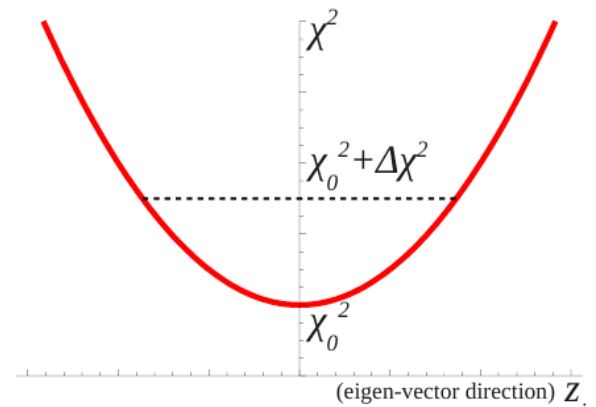
nPDF difficulties

- Lacking data (need low-x & precise data, for several nuclei)
- Complexity and nature of nuclear effects



Shortcomings:

- Non-gaussian errors
- Global minima judgment
- Choice of $\Delta\chi^2$



PDF uncertainties estimation:

Hessian method: Common method for estimating uncertainties in PDFs.



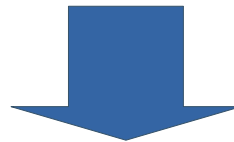
relying on the Gaussian approximation of $\Delta\chi^2$

Shortcomings:

- Non-gaussian errors
- Global minima judgment
- Choice of $\Delta\chi^2$

nPDF difficulties

- Lacking data (need low-x & precise data, for several nuclei)
- Complexity and nature of nuclear effects



Markov Chain Monte Carlo method

advanced statistical method as an alternative for Hessian



Markov Chain Monte Carlo (MCMC)

A sequence of random variables where the current value is dependent on the value of the prior variable (Memory-less property)

A technique for randomly sampling a probability distribution and approximating a desired quantity.

Bayes theorem:

$$p(\theta \mid \text{data}) = \frac{p(\text{data} \mid \theta) \cdot p(\theta)}{p(\text{data})}$$

Diagram illustrating Bayes' theorem with labels:

- Posterior: $p(\theta \mid \text{data})$
- Likelihood: $p(\text{data} \mid \theta)$
- Prior: $p(\theta)$
- Normalization: $p(\text{data})$

Prior: initial belief about the parameter before considering the data.

Likelihood: probability of observing the data given a specific value of the parameter.

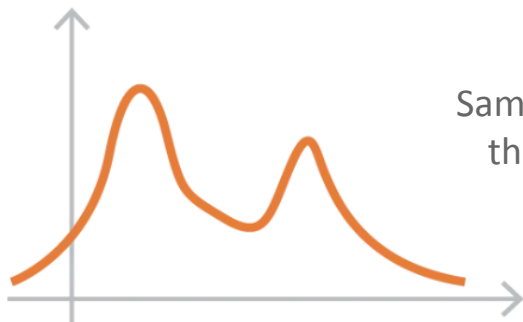
Posterior: updated belief about the parameter given the data.

We aim to find the set of nPDF parameters that maximizes the posterior probability distribution given the experimental data.

Bayesian inference

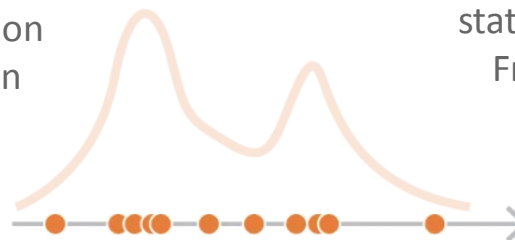


MCMC algorithms



Posterior distribution

Sampling based on the distribution



samples

statistics/estimations From the sample



μ, σ, \dots



Metropolis algorithm:

- Initialize parameters
- for $i=1$ to $i=N$:

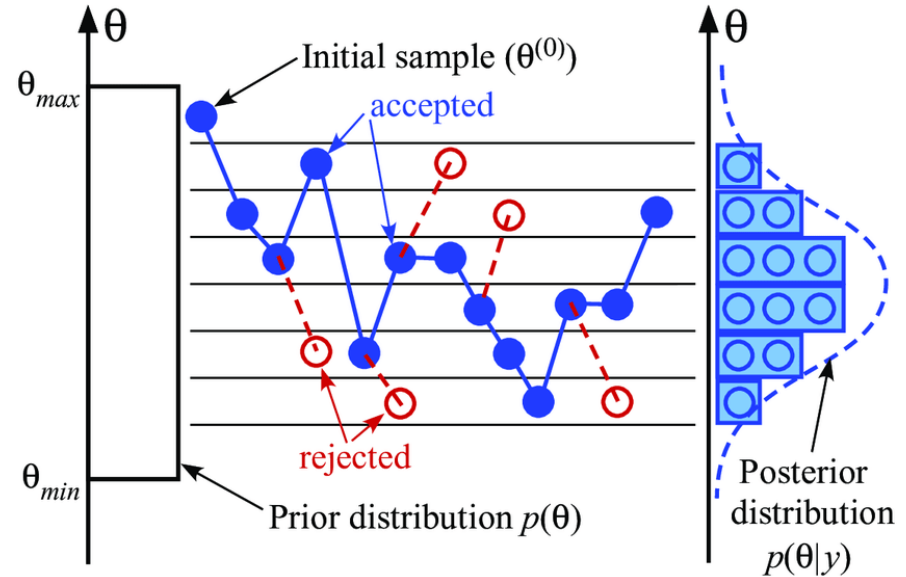
Generate proposed parameters via proposition function: $\theta^* \sim q(\theta^* | \theta_i)$

Sample from uniform distribution: $u \sim U(0,1)$

Compute acceptance ratio: $\alpha = p(\theta^* | D) / p(\theta_i | D)$

If $u < \min(1, \alpha)$ then $x_{i+1} = x^*$

- Else $x_{i+1} = x_i$



Propose a new sample

Judgment of proposed sample

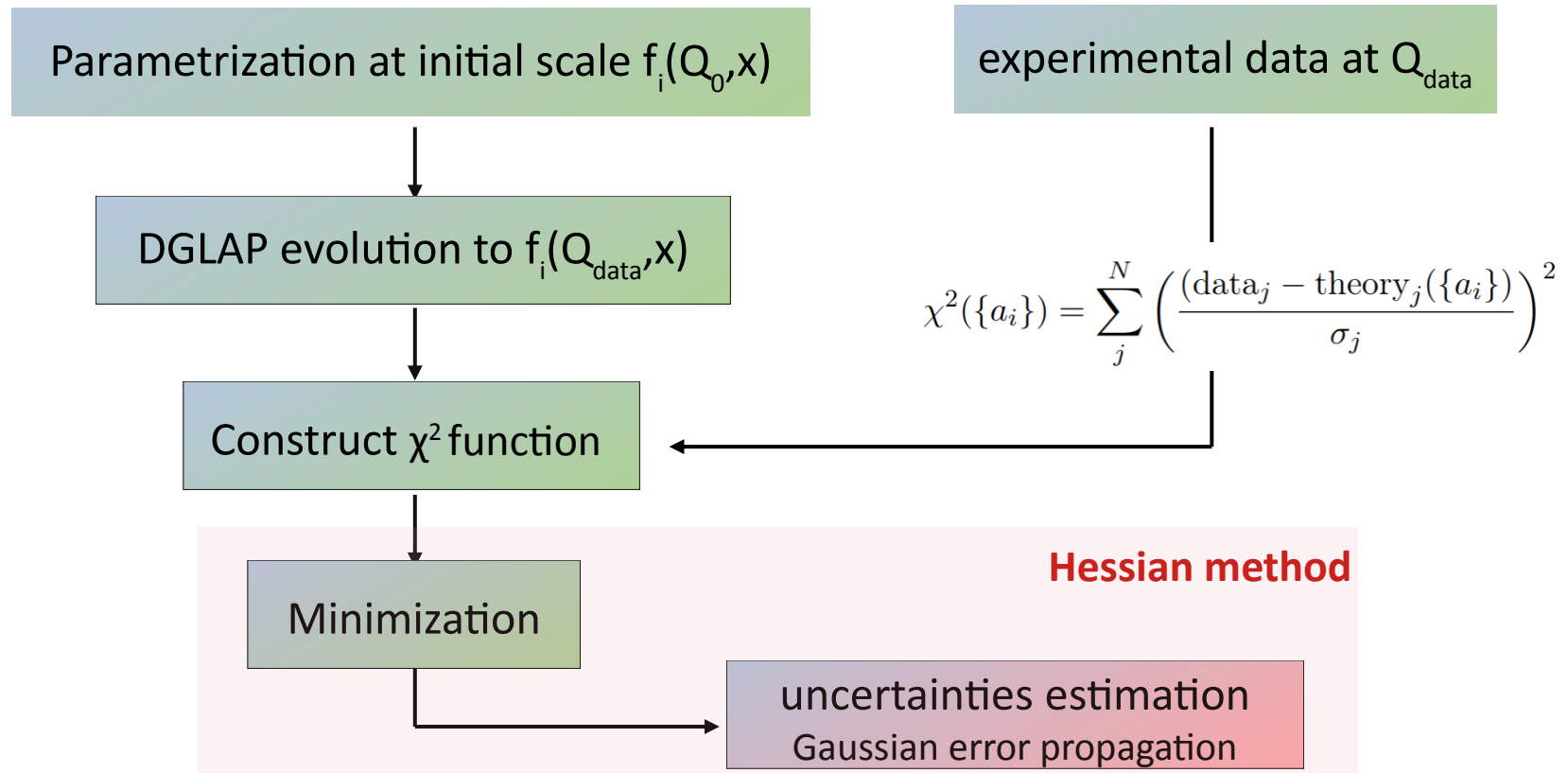
Metropolis-Hasting:

$$x_{t+1} = \mathcal{N}(x_t, C_0)$$

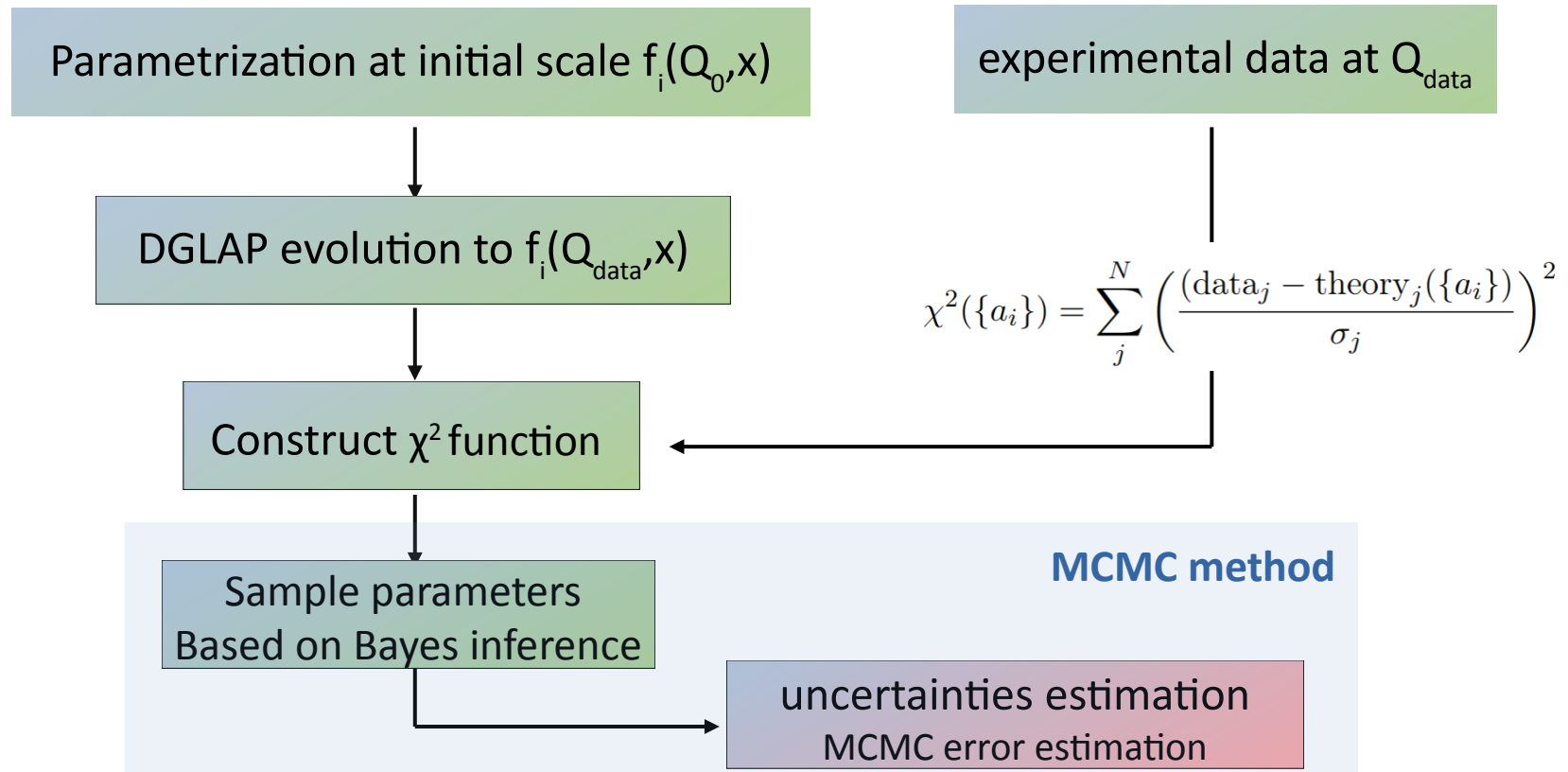
Adaptive Metropolis-Hasting:

$$x_{t+1} = \beta \mathcal{N}(x_t, C_0) + (1 - \beta) \mathcal{N}(x_t, \hat{C}_n)$$

PDF Global analysis:



PDF Global analysis:





$$\text{Parametrization: } x f_i^{p/A}(x, Q_0) = c_0 x^{c_1} (1-x)^{c_2} e^{c_3 x} (1 + e^{c_4 x})^{c_5}$$

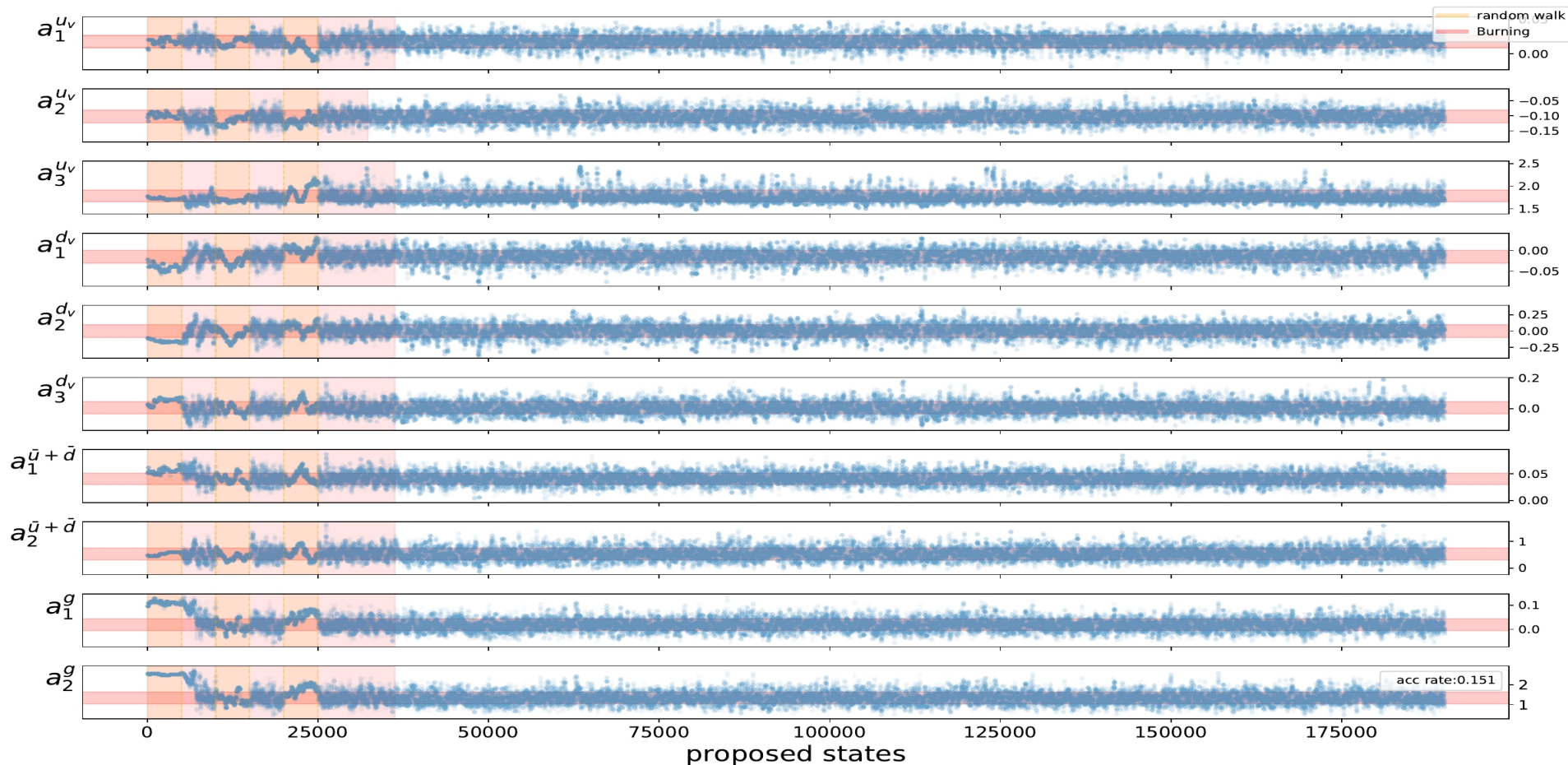


$$c_k \rightarrow c_k(A) \equiv p_k + a_k(1 - A^{-b_k}),$$

Generating the Markov Chain of nPDF parameters:

Each point of the chain is representing a set of nPDF parameters
(parameter a_k for 6 valances, 2 sea quarks and 2 gluon)

DIS and W/Z boson data:
436 data points

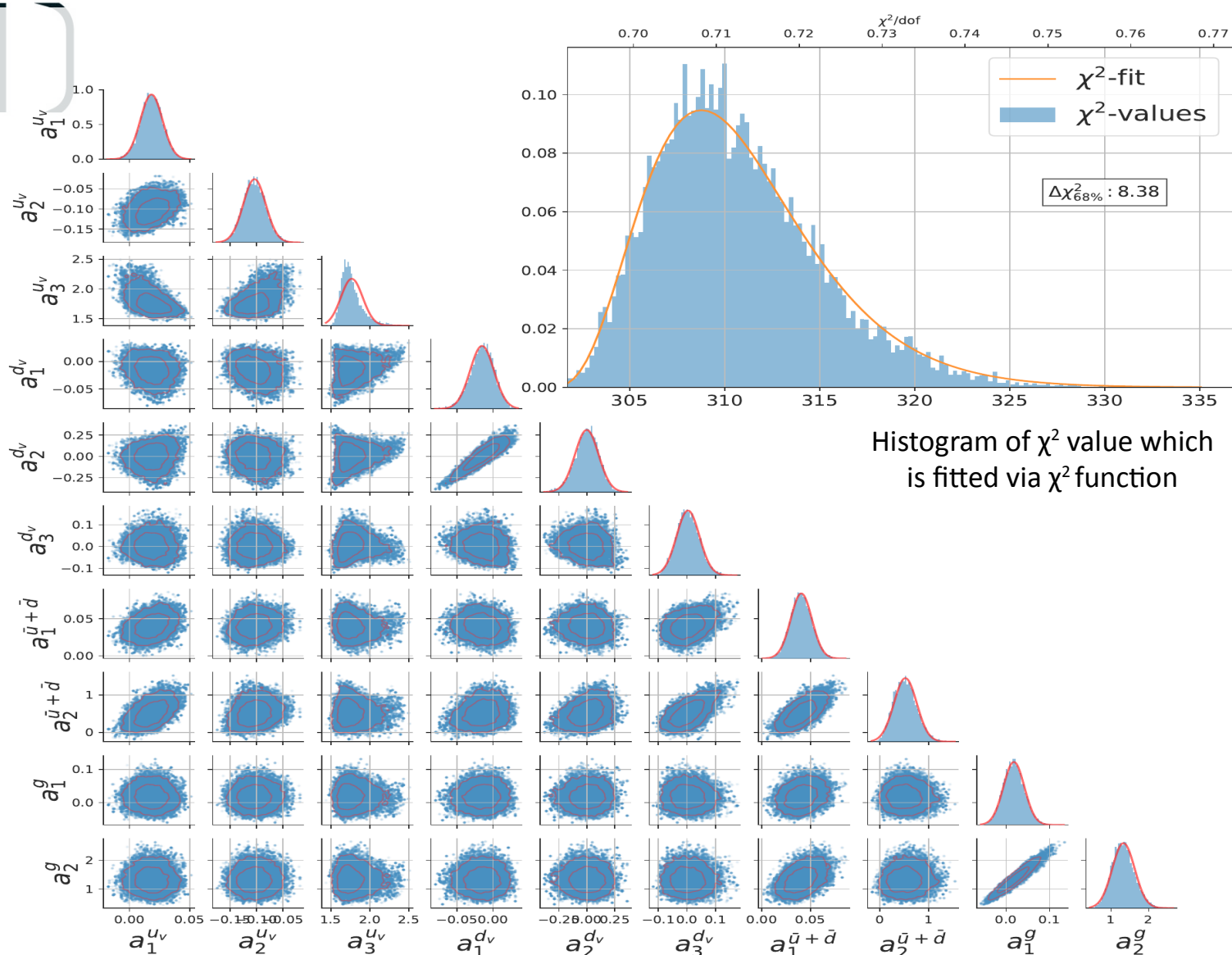


MCMC can reveal non-Gaussian features of the underlying distribution



Pairwise plot

diagonal: histogram of each parameter
off-diagonal: 2D correlation plots between parameters





Error estimation:

Monte Carlo error estimation
(uncorrelated)

$$\sigma_{MC}^2 = \frac{1}{n-1} \sum_{t=1}^n (X_t - \hat{\mu})^2$$

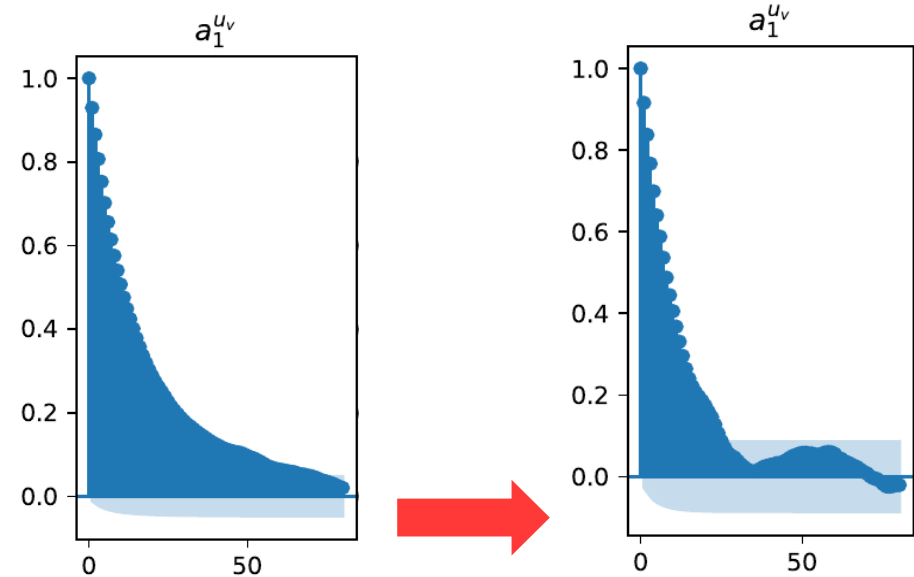
MCMC error estimation
(correlated)

$$\sigma_{MCMC}^2 = 2 \tau_{int} \sigma_{MC}^2$$

Autocorrelation function (ACF) $\rho(k) = \frac{\text{Cov}(k)}{\text{Cov}(0)}$

$$\text{Cov}(k) = \frac{1}{n} \sum_{t=1}^{n-k} (x_{t+k} - \bar{x})(x_t - \bar{x}),$$

Autocorrelation time $\tau_{int} = \frac{1}{2} \sum_{-\infty}^{+\infty} \rho(k)$



Thinning by rate 40

Thinning method:

keep only every k-th sample in the Markov chain and discard the rest

Why Thinning?

- It provides an **uncorrelated** chain so we can use Monte-Carlo error estimation:

$$\sigma_{MCMC}^2 = 2 \tau_{int} \sigma_{MC}^2 \quad \longrightarrow \quad \sigma_{MC}^2 = \frac{1}{n-1} \sum_{t=1}^n (X_t - \hat{\mu})^2$$

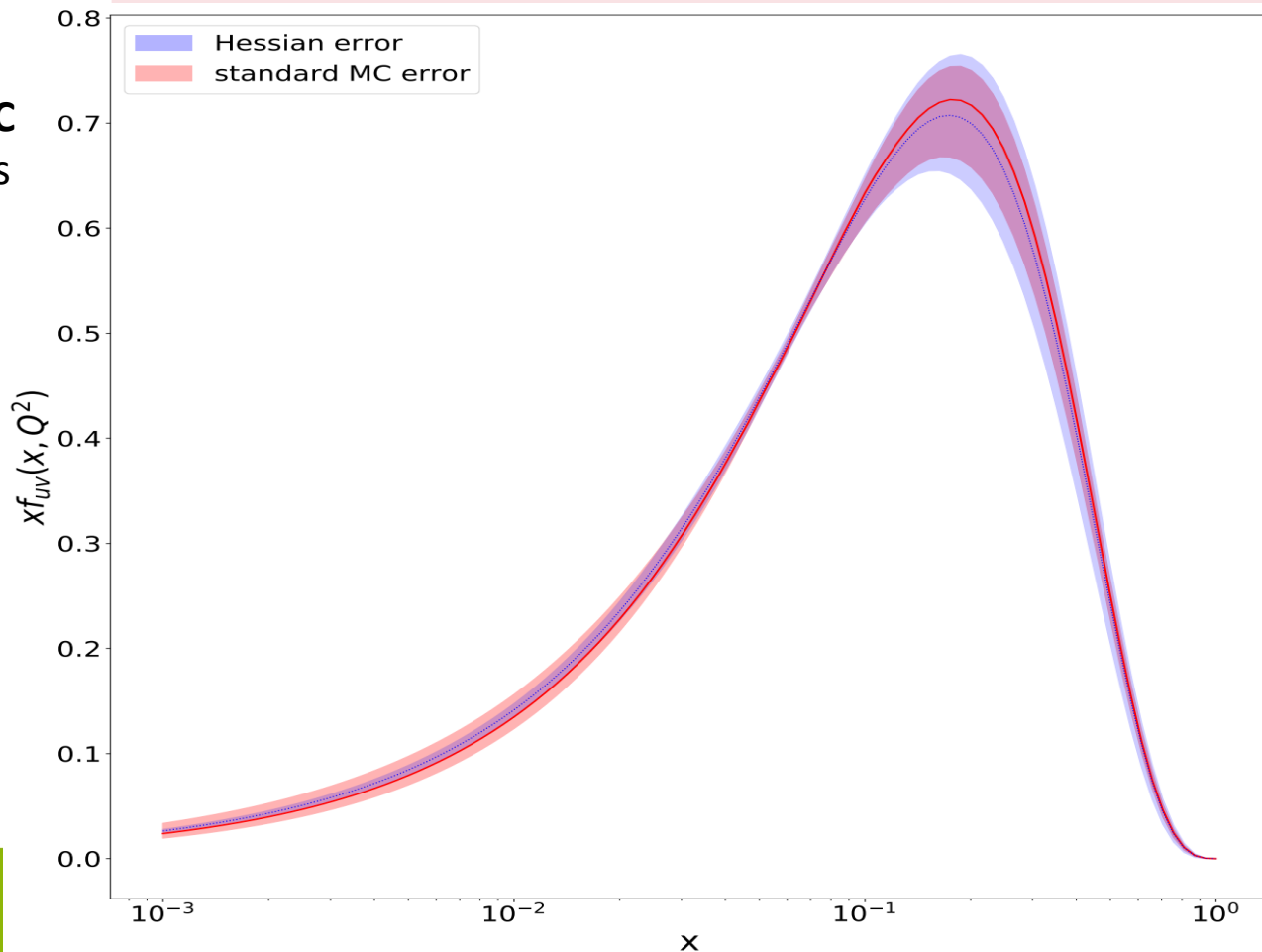
- We aim to generate a set of PDF grids corresponding chain's units. Thinning the chain makes it more applicable.



MCMC approach:

- Generating the Markov Chain
- Thinning the chain
- Construct nPDF corresponding to each unit of the thinned chain and perform standard MC error estimation (Saving them in the standard LHAPDF format so that anyone can use such nPDFs)

Pb²⁰⁸ PDF(u-valence)
resulting from **MCMC**
and **Hessian** methods





Conclusion:

- ◆ Despite the MCMC challenges (mainly computational cost), this method has become a powerful tool for determining nPDFs.
- ◆ The implementation of this alternative method hasn't finished yet, but so far we have obtained promising results (comparing with Hessian).

new nCTEQ global nPDF release: CJ15

Accardi et al., arXiv:1602.03154

Functional form for bound protons at Q_0 :

$$x f_i^{p/A}(x, Q_0) = c_0 x^{c_1} (1-x)^{c_2} (1 + c_3 \sqrt{x} + c_4 x)$$

$$i = u_v, d_v, g, \bar{u} + \bar{d}, s, \bar{s}$$

Atomic number dependence is characterized in the c_k coefficients as

$$c_k \rightarrow p_k + a_k \ln(A) + b_k \ln^2(A). \quad k = \{1, \dots, 5\}.$$

PDF of a nucleus (A – mass, Z – charge):

$$f_i^{(A,Z)}(x, Q) = \frac{Z}{A} f_i^{p/A}(x, Q) + \frac{A-Z}{A} f_i^{n/A}(x, Q)$$