



KRAKOW SCHOOL  
OF INTERDISCIPLINARY  
PHD STUDIES

# Nuclear PDF Determination Using Markov Chain Monte Carlo Methods

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*nCTEQ collaboration*

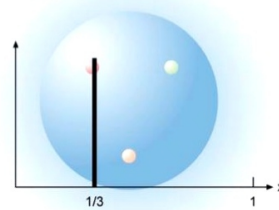
IFJ PAN

Department of Theoretical Particle Physics

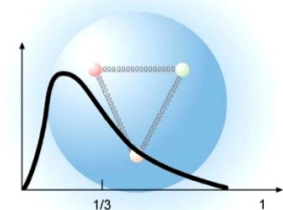


Polish Particle and Nuclear Theory Summit (2PiNTS)

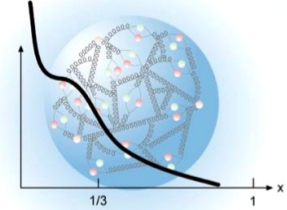
November 2023, Krakow



Free quarks



Bound quarks



Bound quarks + QCD effects

## 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

$\mu$ : Factorization scale

$X$ : 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)

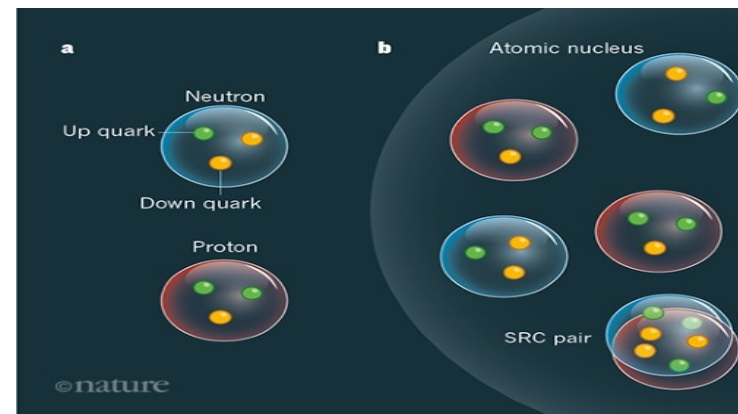
### PDF properties:

- Universal
- Constrained through momentum and number sum rules
- $\mu^2$ -dependence governed by DGLAP evolution equations
- Non-perturbative:  $x$ -dependence of PDF is NOT calculable in pQCD

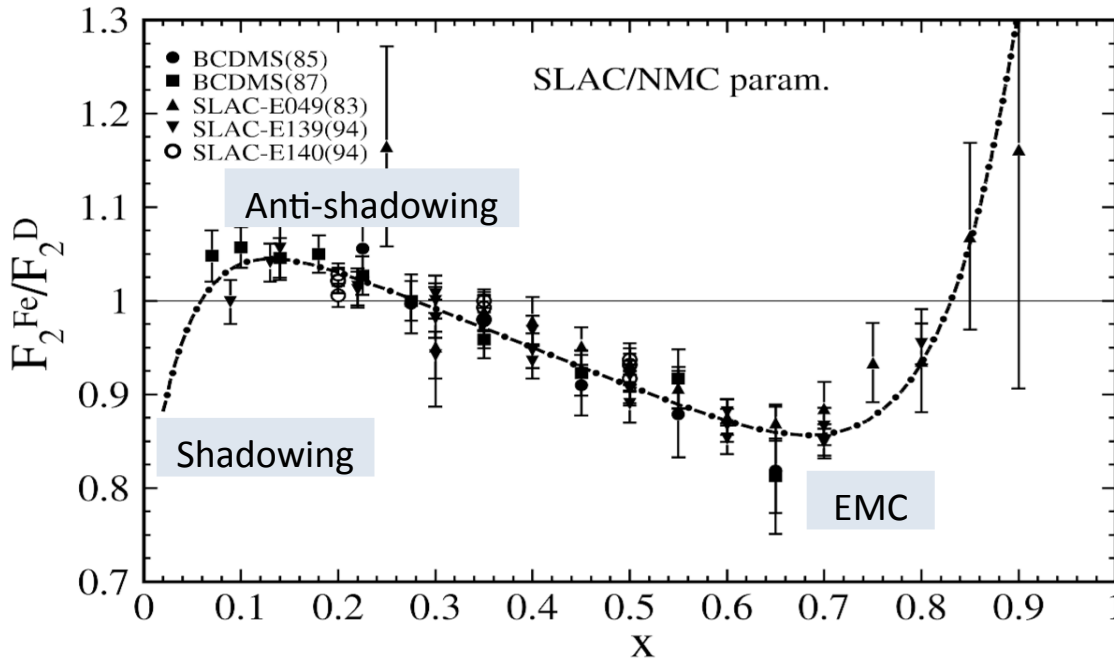
→ extracting from a fit to experimental data



# Nuclear PDFs(nPDFs):



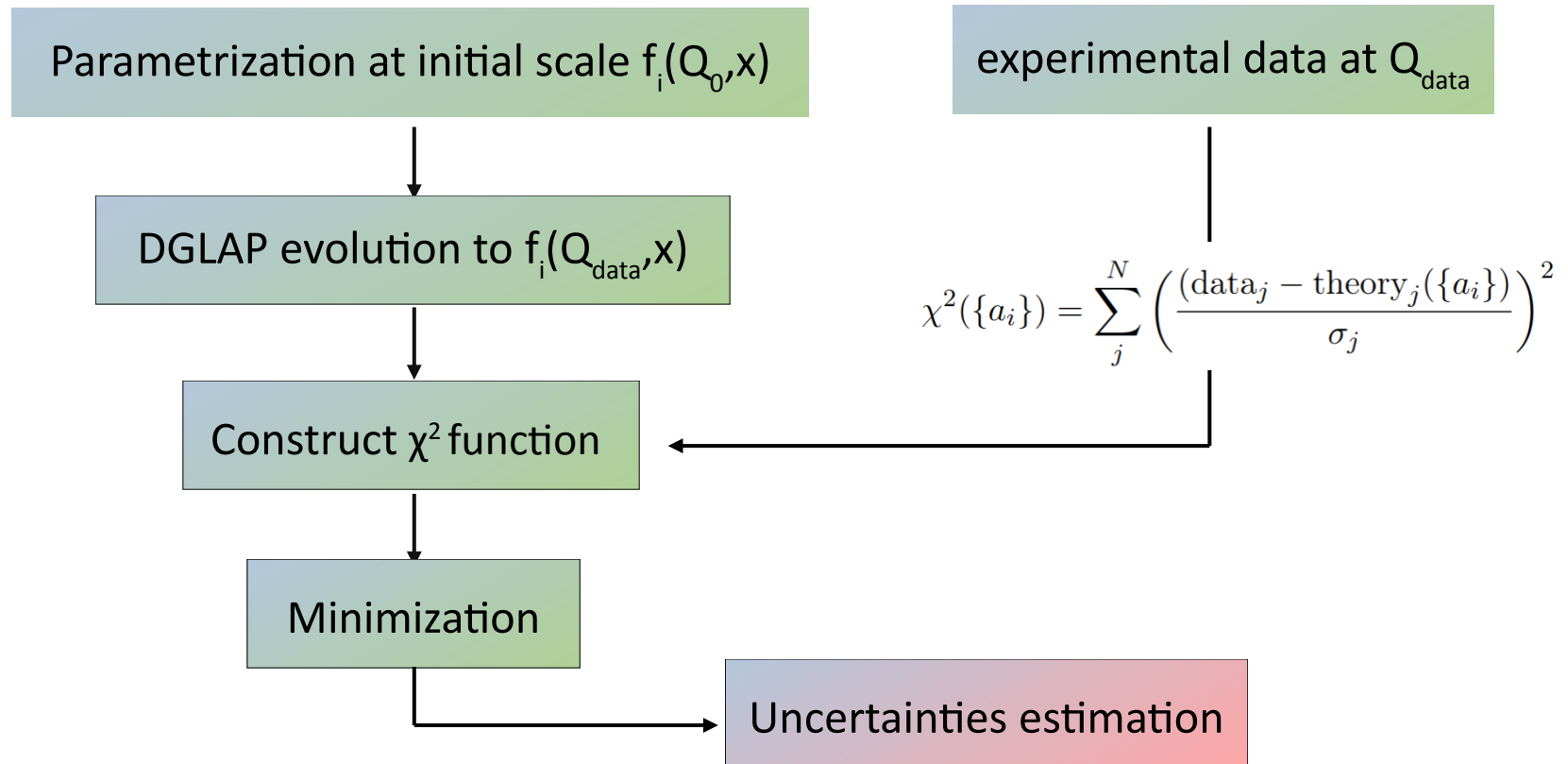
$$F_2^A(x) \neq ZF_2^p(x) + NF_2^n(x)$$



## Motivations:

- Interpreting heavy-ion collision data
- Understanding Nuclear Structure

## 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):

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



## new nCTEQ global nPDF release: CJ15

Accardi et al., arXiv:1602.03154

Functional form for bound protons at  $Q_0$ :

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

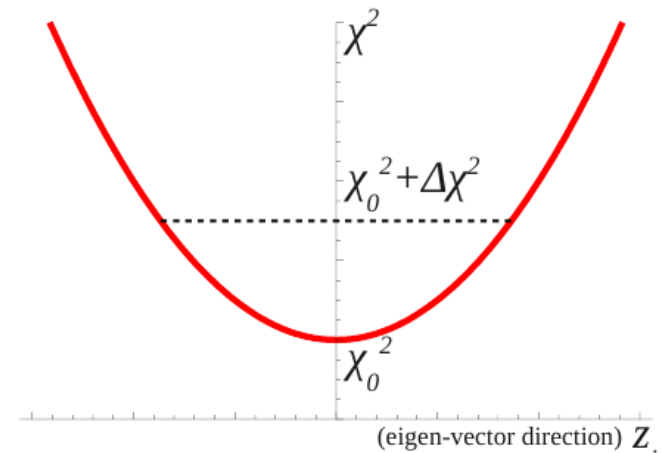
$$i = u_v, d_v, g, \bar{u} + \bar{d}, s, \bar{s}$$

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):

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



## 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

nPDF difficulties

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



deeper insight

**Markov Chain Monte Carlo method**



## 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 and arrows:

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

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.

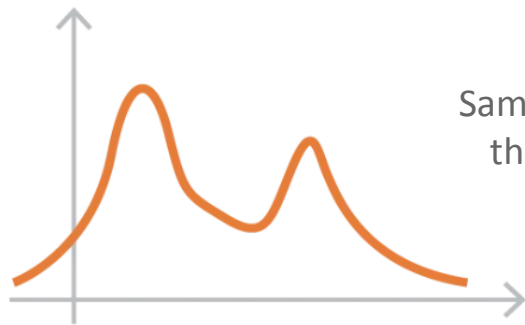


We aim to find the set of nPDF parameters that maximizes the posterior probability distribution given the experimental data.

Bayesian inference

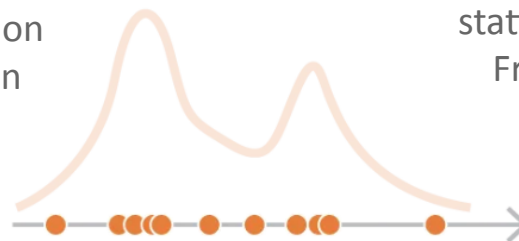


MCMC algorithms



Posterior distribution

Sampling based on the distribution



samples

statistics/estimations From the sample



$\mu, \sigma, \dots$



## Metropolis algorithm:

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

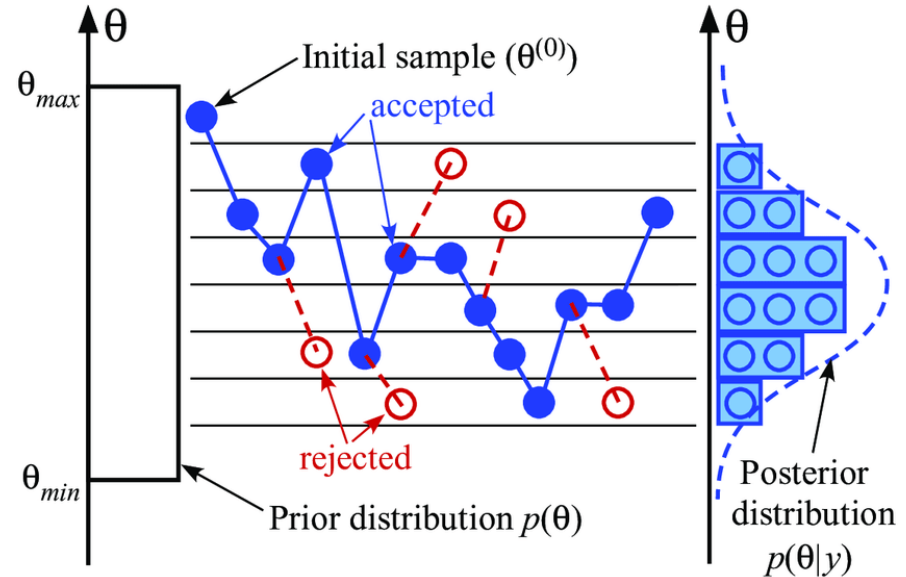
Generate proposed parameters via proposition function:  $\theta^* \sim q(\theta^* | \theta_i)$

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  $x_{i+1} = x^*$

**Propose a new sample**



**Judgment of proposed sample**

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

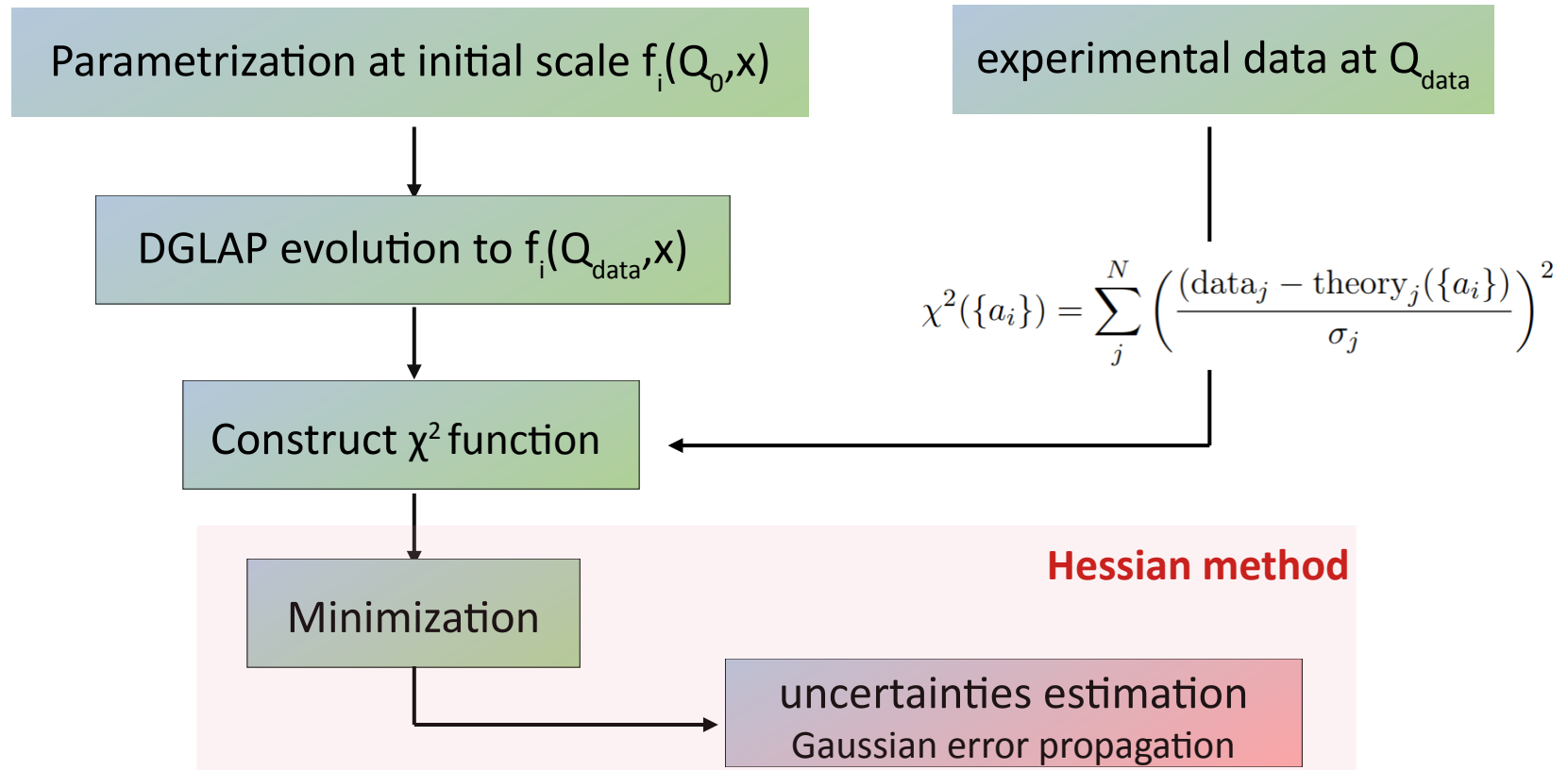
**Metropolis-Hasting:**

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

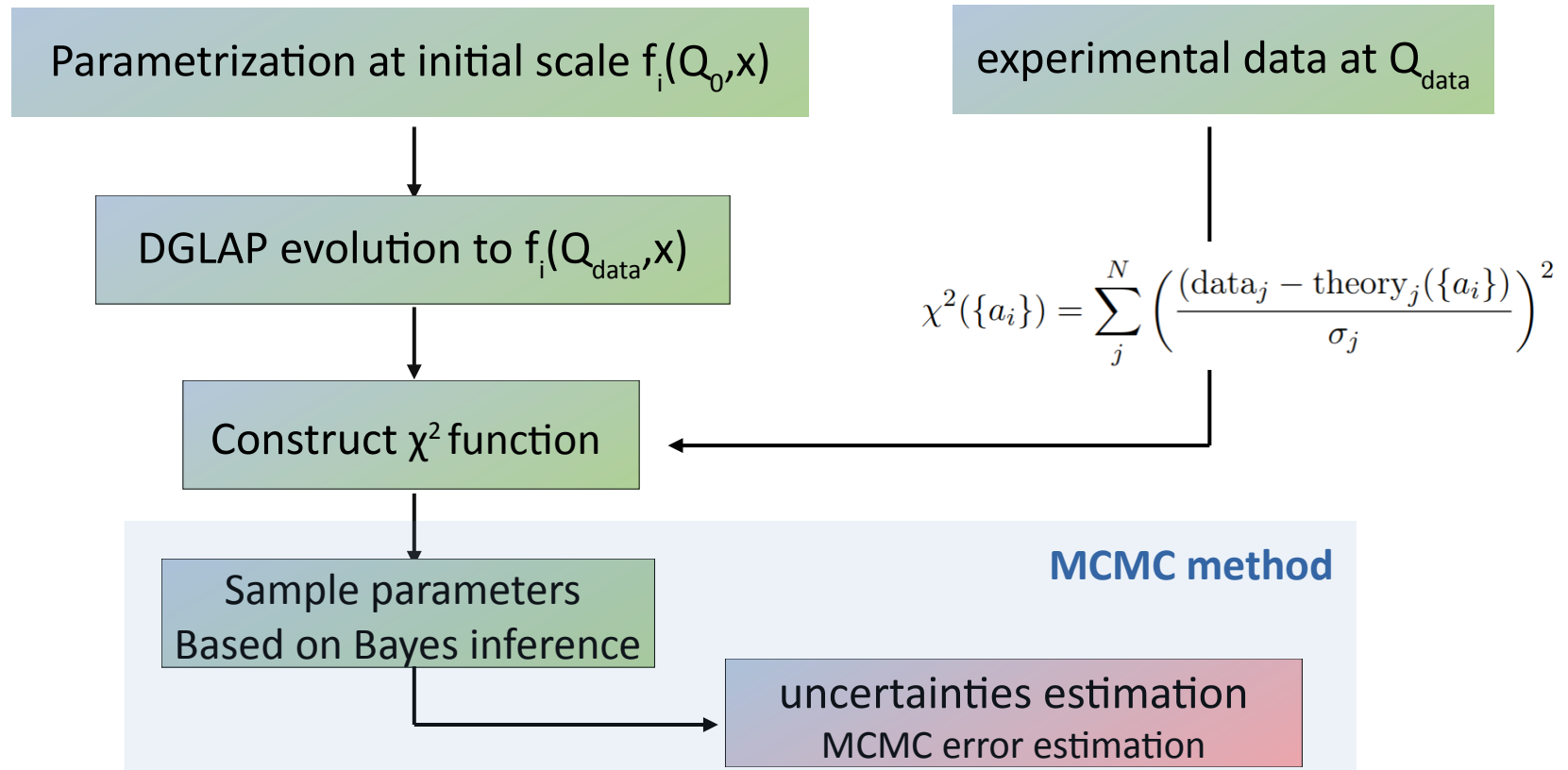
**Adaptive Metropolis-Hasting:**

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

## PDF Global analysis:



## PDF Global analysis:





CJ15 nPDF  
parametrization

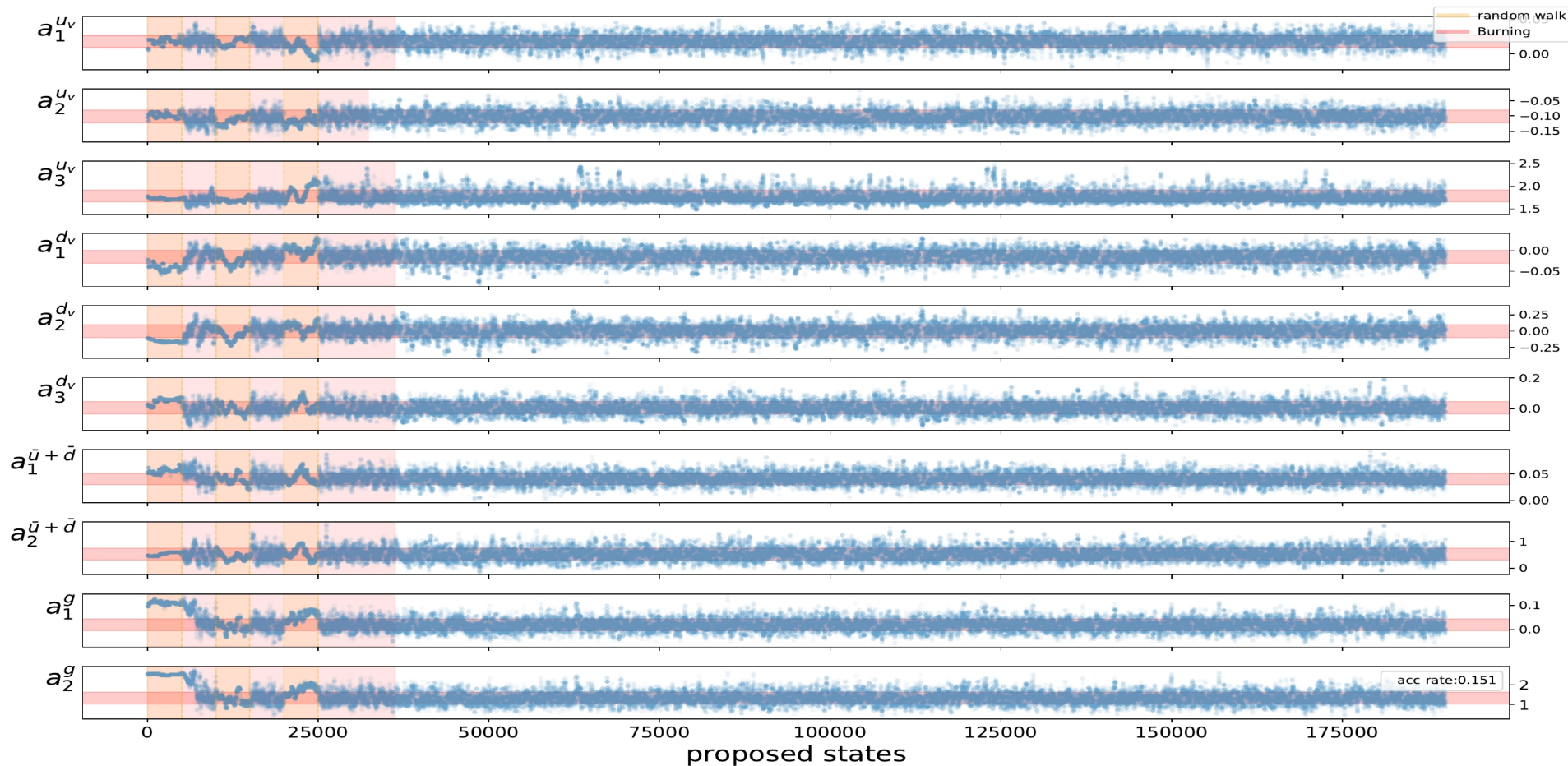
$$x f_i^{p/A}(x, Q_0) = c_0 x^{c_1} (1-x)^{c_2} (1 + c_3 \sqrt{x} + c_4 x)$$

$$c_k \rightarrow p_k + a_k \ln(A) + b_k \ln^2(A).$$

## Generating the Markov Chain of nPDF parameters:

Each point of the chain is representing a set of nPDF parameters  
(6 valance, 2 sea quarks and 2 gloun)

DIS and W/Z boson data:  
436 data points

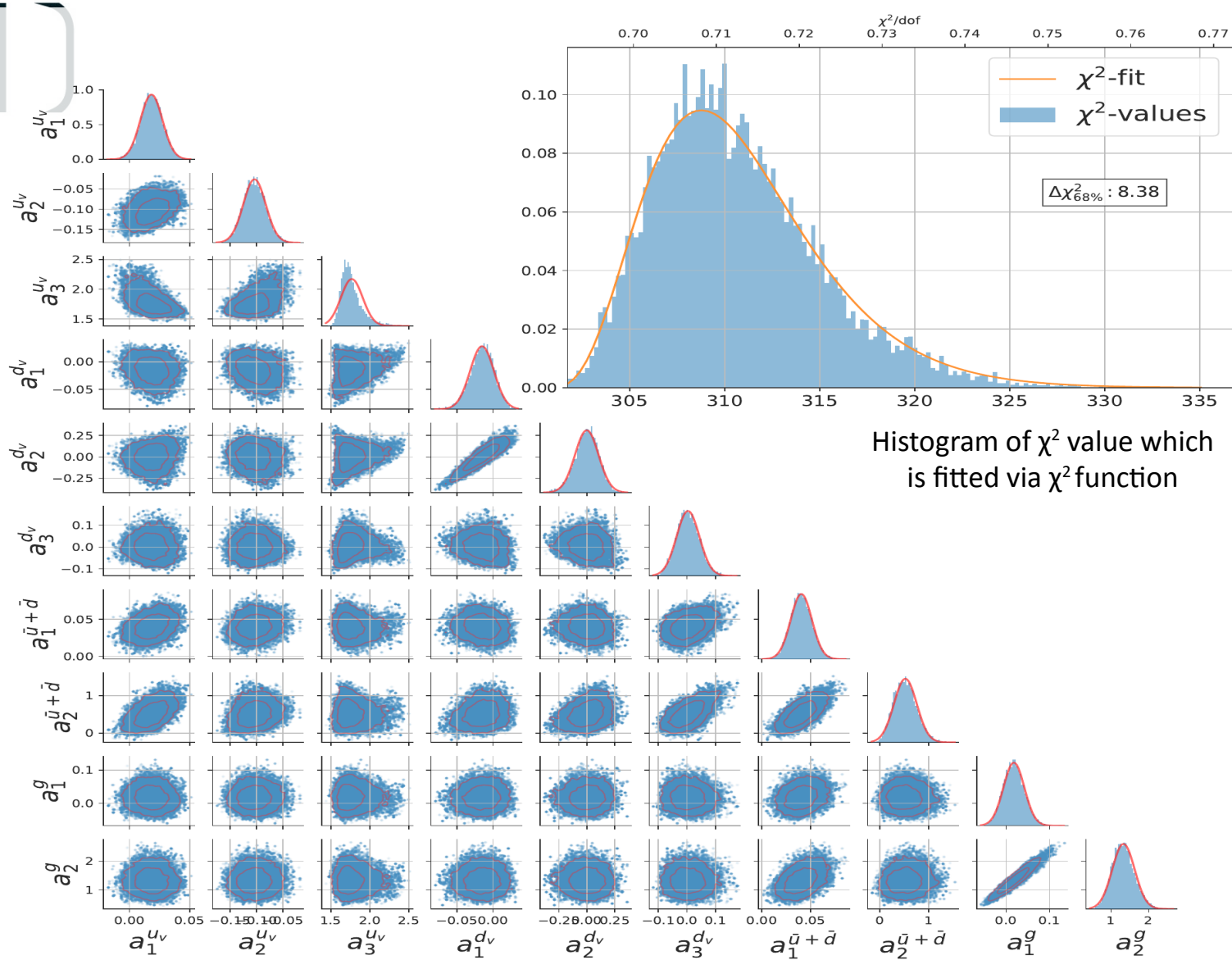


# MCMC can reveal non-Gaussian features of the underlying distribution



## Pairwise plot

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





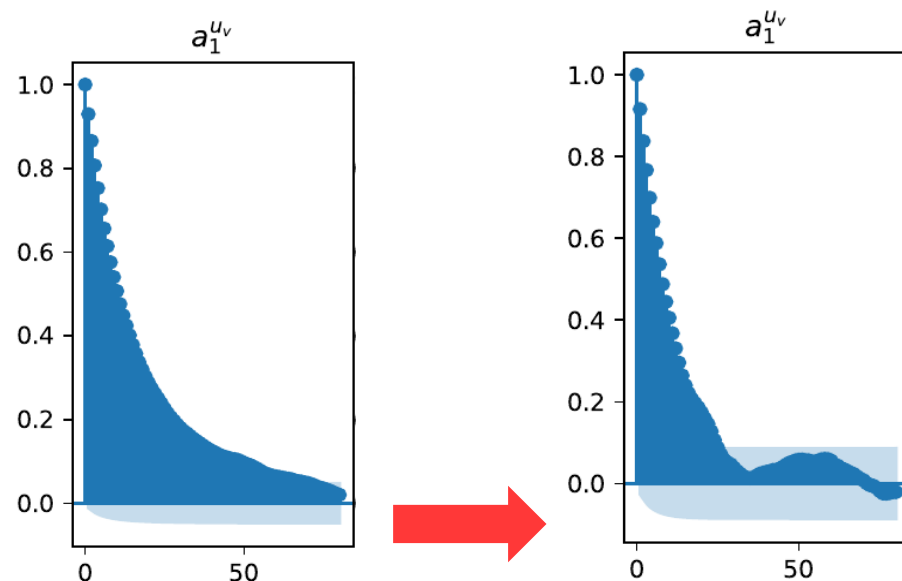
## Error estimation:

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

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

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

Autocorrelation function versus time interval



**Thinning** by rate 40

discard all except every k-th point of the chain

**MCMC error (correlated)**

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

**MC error (uncorrelated)**

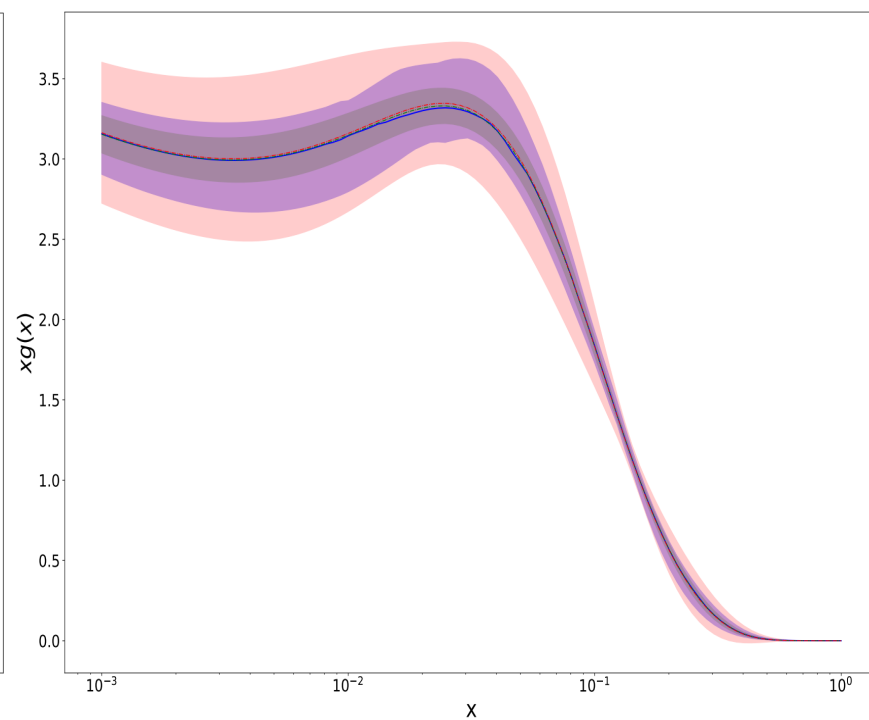
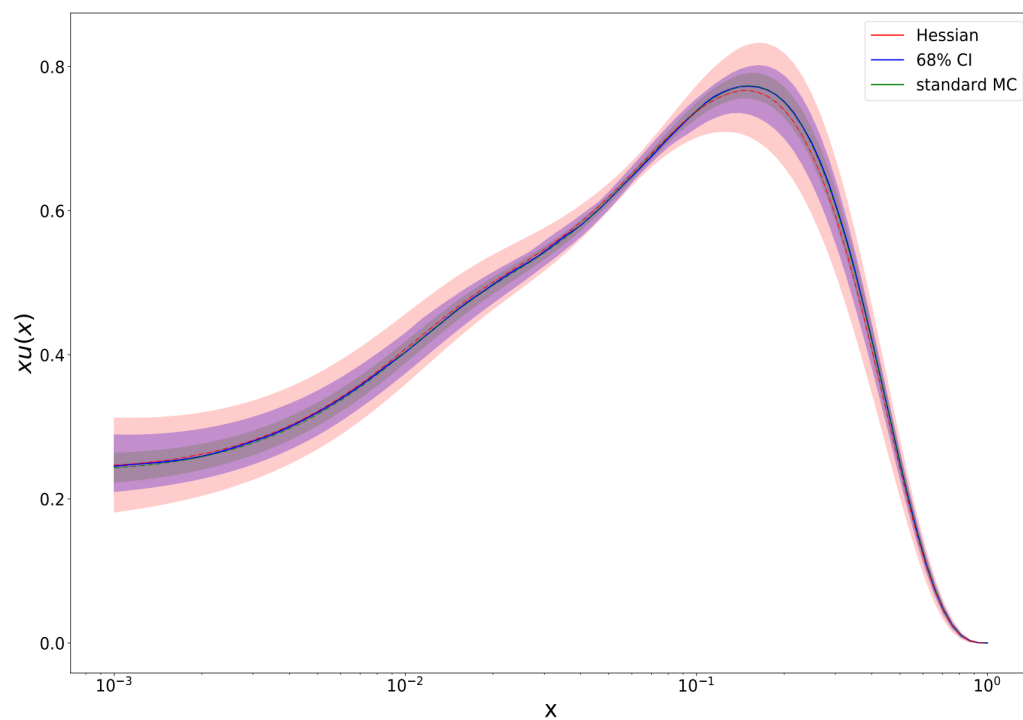
$$\sigma_{MC}^2 = \frac{1}{n-1} \sum_{t=1}^n (X_t - \hat{\mu})^2$$



MCMC approach:

- Generating the Markov Chain
- Thinning the chain
- Dumping PDF corresponding to each unit of the thinned chain
- Evaluating the error band determined from Monte Carlo error

LHAPDF (set of nPDF grids):







Thank you for your attention

**Acknowledgment:**

This work was supported by Narodowe Centrum Nauki under grant no. \ 2019/34/E/ST2/00186.