KRAKOW SCHOOL
OF INTERDYSCIPLINARY
PHD STUDIES

Nuclear PDF Determination Using Markov Chain Monte Carlo Methods

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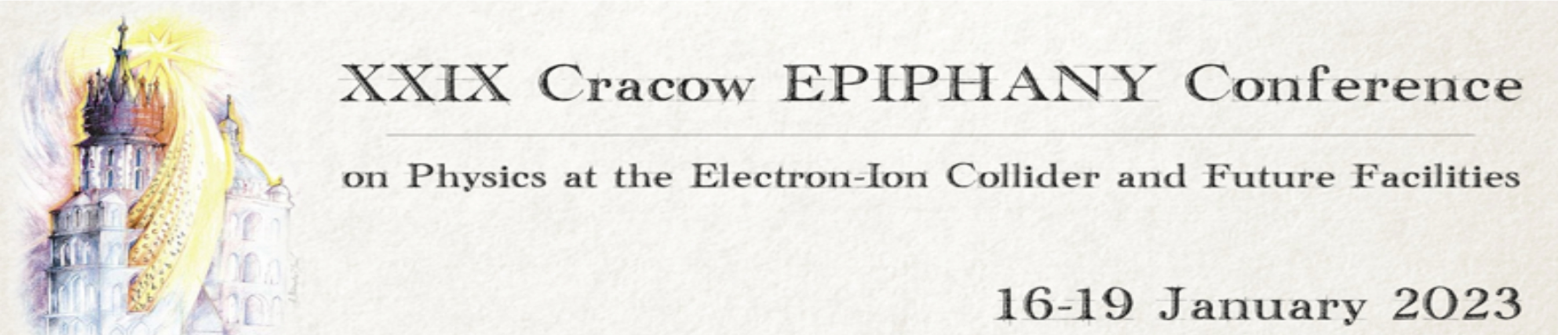

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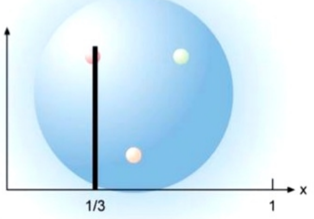
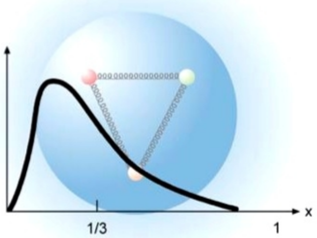
Outline:

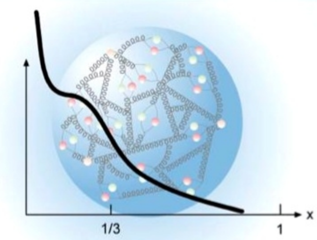
- Nuclear Parton Distribution Function (nPDF)
- nPDF extraction and the uncertainties
- Markov Chain Monte Carlo method
- Preliminary results (MCMC analysis)
- Conclusion



Free quarks



Bound quarks



Bound quarks
+ QCD effects

Parton Distribution Function (PDF):

The probability $f_{a/p}(x,\mu)$ that a parton a carries fraction x of the proton’s momentum is called parton distribution function (PDF).

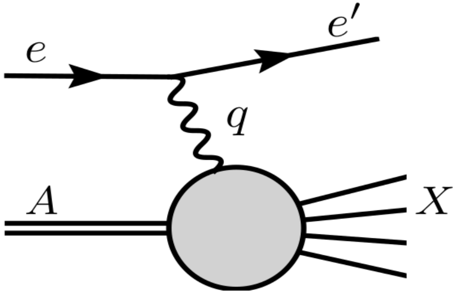
μ: Factorization scale
X: momentum fraction

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

Parton densities (PDFs)

PDFs are obtained from a **fit to experimental data**

Calculable Parton interaction (pQCD)



Nuclear Parton Distribution Function (nPDF):

What are nPDFs?

Parton Distribution of nucleons in a nucleus

Where are nPDFs useful?

- Structure of nucleus
- Heavy-ion collisions

x-dependence of PDF is NOT calculable in pQCD

μ^2-dependence of PDF is calculable in pQCD by **DGLAP** eqs

Number of free parameters ????

nCTEQ framework for nuclear PDF:

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

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

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

Functional form for bound protons:

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

Atomic number dependence is characterized in the c_k coefficients as

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

PDF Uncertainties:

Hessian method: Common method to propagating the experimental errors to PDFs

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

- Non-gaussian errors
- Global minima judgment
- Tolerance definition

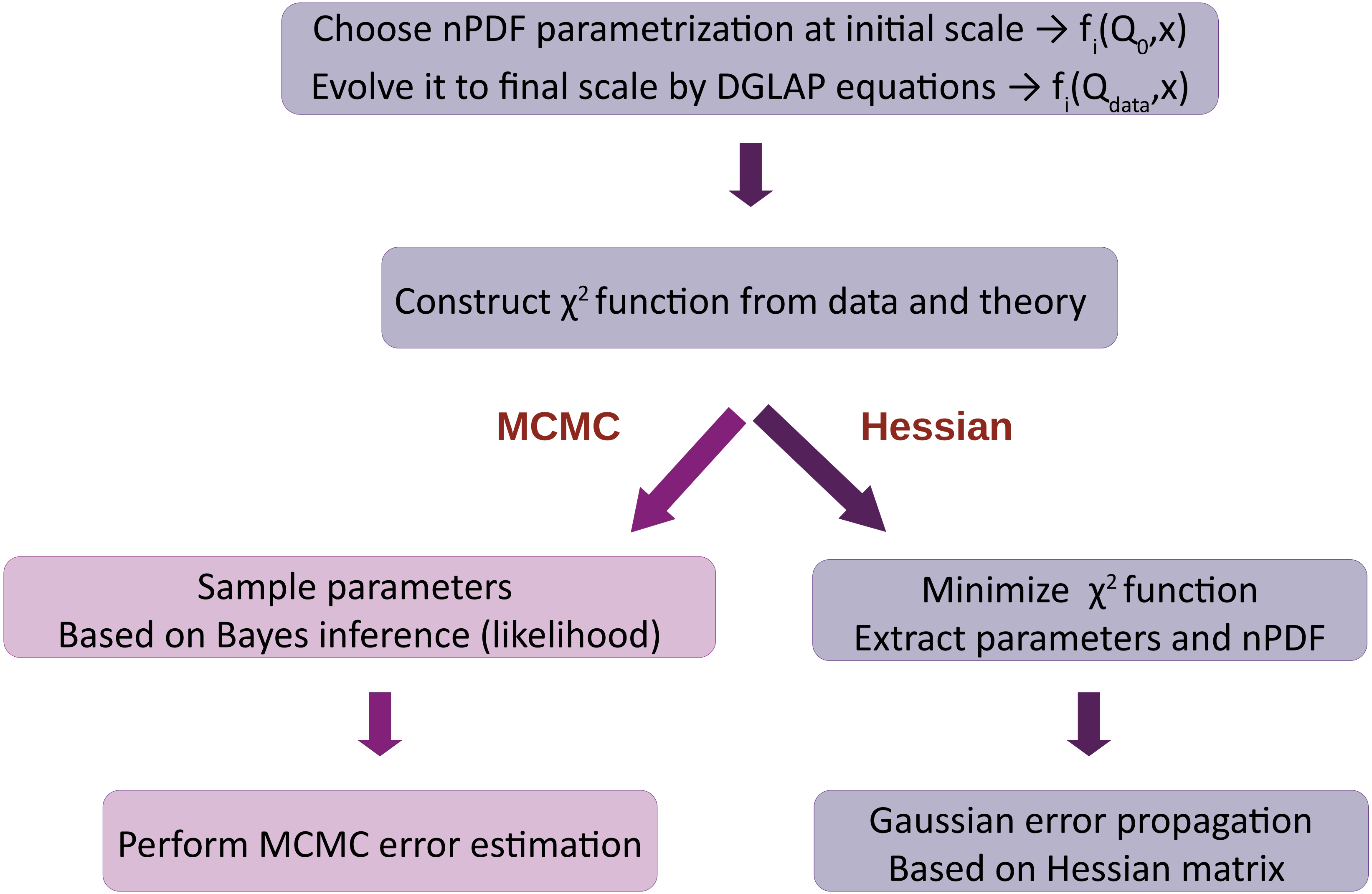
nPDF difficulties

- lacking data (need low-x & precise data, for several nuclei)
- largely unconstrained nuclear gluon PDF

deeper insight

Markov Chain Monte Carlo method

nPDF extraction, Hessian VS MCMC:



Choose nPDF parametrization at initial scale → $f_i(Q_0,x)$

Evolve it to final scale by DGLAP equations → $f_i(Q_{data},x)$

Construct χ^2 function from data and theory

MCMC

Hessian

Sample parameters
Based on Bayes inference (likelihood)

Minimize χ^2 function
Extract parameters and nPDF

Perform MCMC error estimation

Gaussian error propagation
Based on Hessian matrix

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.

likelihood

Prior probability

Bayes theorem:

$$P(\hat{q}|D) = \frac{P(D|\hat{q})P(\hat{q})}{\int d\hat{q}P(D|\hat{q})P(\hat{q})}$$

Posterior probability

$$\log \mathcal{L}(\hat{q}) = -\frac{1}{2}\sum_{i=1}^{n}\frac{(D_i - T_i)^2}{\sigma_i^2} = -\frac{1}{2}\chi^2$$

We sample the likelihood function of each parameter via MCMC method

Generating the Markov Chain of nPDF parameters:

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

$$\Downarrow$$

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

$$\downarrow$$

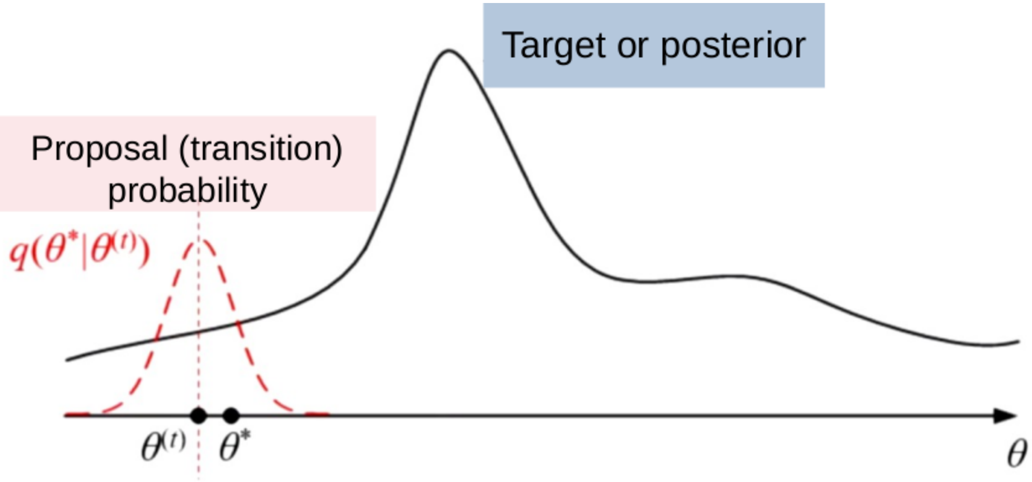
Sampling by adaptive MH algorithm

Each unit of the chain is representing a set of nPDF parameters

Markov Chain: $\mathbf{X}^0, \mathbf{X}^1, \mathbf{X}^2, \ldots$

$$\downarrow$$

{uv-a1, uv-a2, uv-a5, dv-a1, dv-a2, dv-a5, ūd̄-a1, ūd̄-a2}



Metropolis algorithm:

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

Propose a new sample

Generate proposed parameters via proposition function: θ * ~ q(θ * | θ i)

Sample from uniform distribution: u ~ U(0,1)

Compute acceptance ratio: α = p(θ * | D) / p(θ i | D)

If u < min(1, α) then x_{i+1} =x *

Judgment of proposed sample

- Else x_{i+1} =x i

Metropolis-Hasting:

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

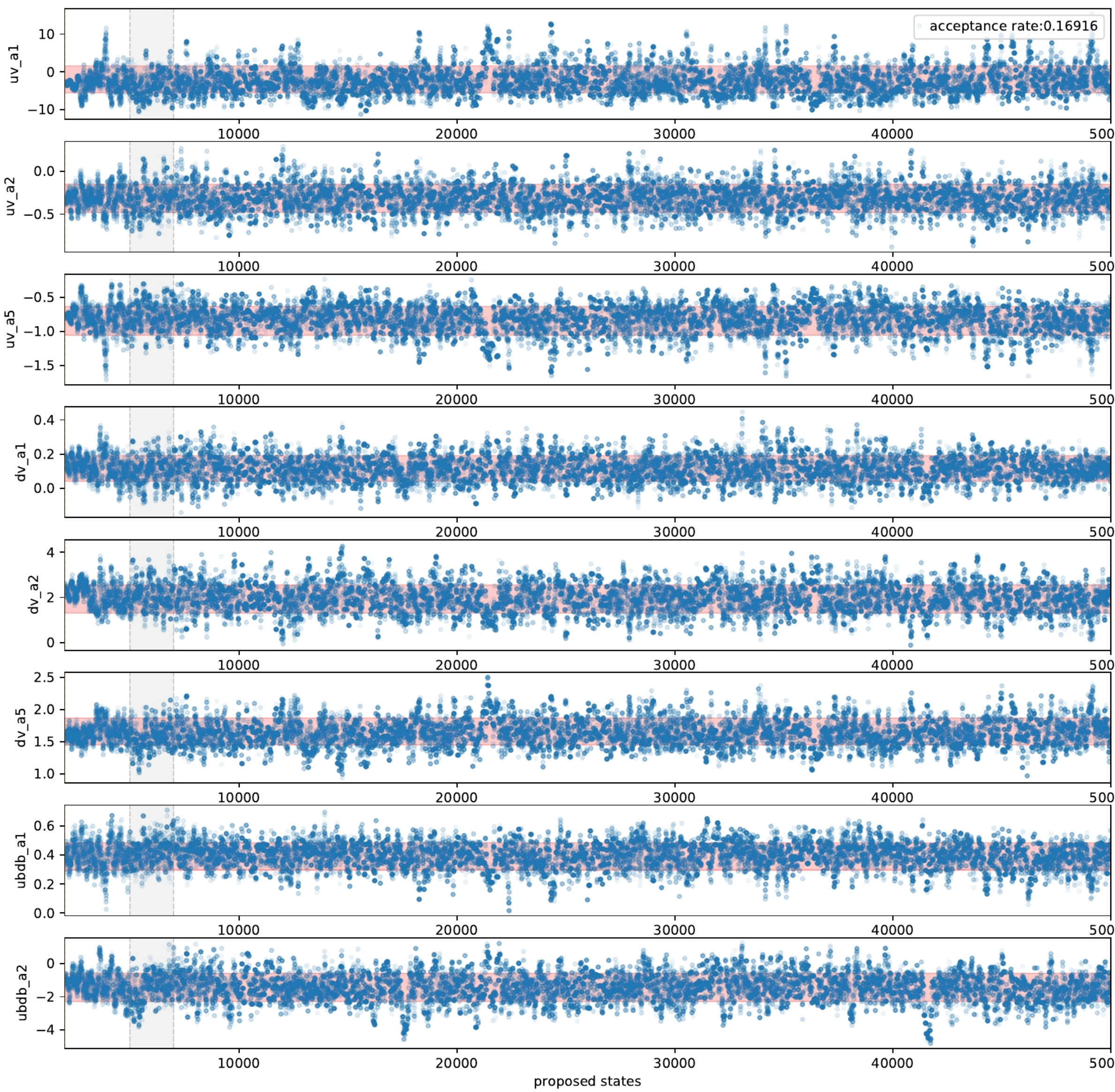
Adaptive Metropolis-Hasting:

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

Markov chain of 8 fitting parameters:

- 3 parameters for u-valence
- 3 parameters for v-valence
- 2 parameters for $\bar{u}\bar{d}$

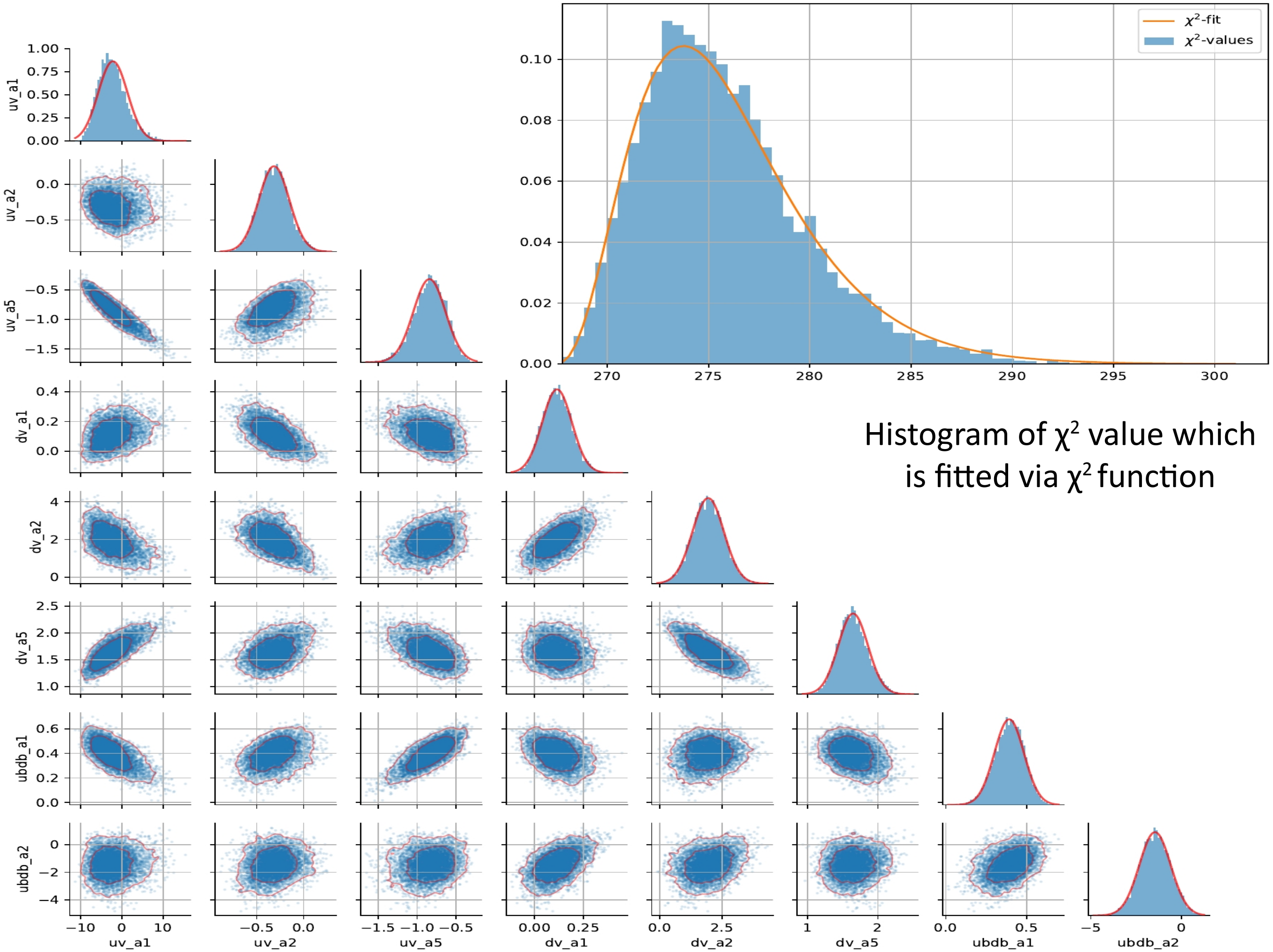
chains representing time series of parameter's value



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

The inner and outer contours are regions containing respectively 68% and 95% of the probability density

Pairwise plot for 8 fitting parameters:



Histogram of χ^2 value which is fitted via χ^2 function

Autocorrelation and statistical errors:

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

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

Lag k is the number of interval between two unit of the chain

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

MC error (uncorrelated)

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

MCMC error (correlated)

$$\sigma^2_{MCMC} = 2\,\tau_{int}\,\sigma^2_{MC}$$

Thinning method:

In order to reduce the correlation of samples I perform the **Thinning** method

↓

discard all except every k-th steps

Why Thinning?

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

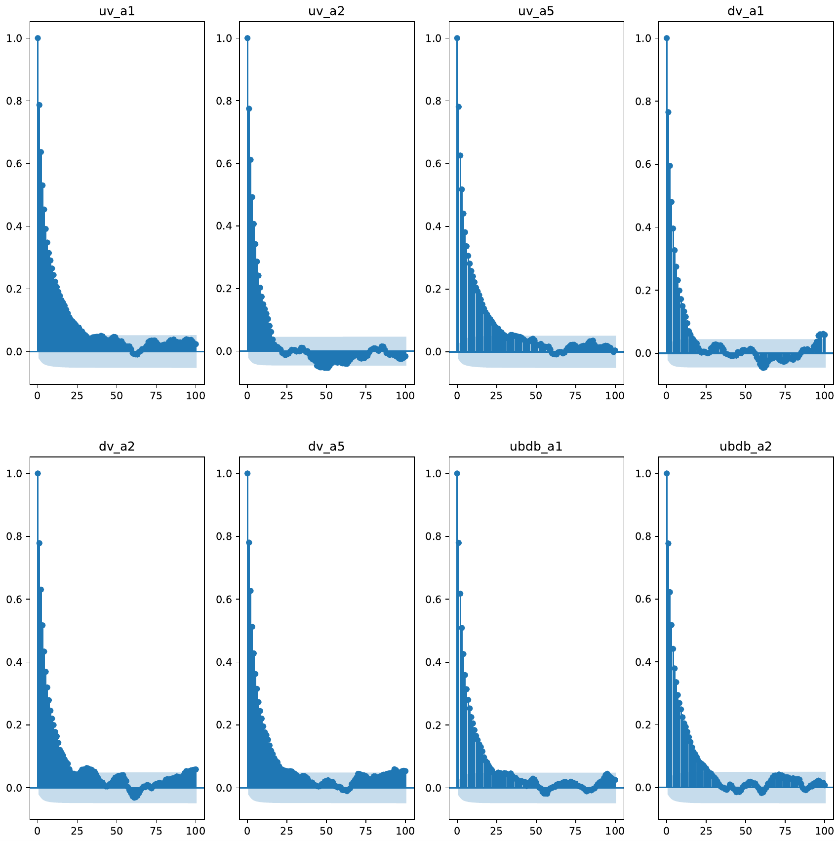
$$\sigma^2_{MCMC} = 2\,\tau_{int}\,\sigma^2_{MC} \quad \Longrightarrow \quad \sigma^2_{MC} = \frac{1}{n-1}\sum_{t=1}^{n}(X_t - \hat{\mu})^2$$

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

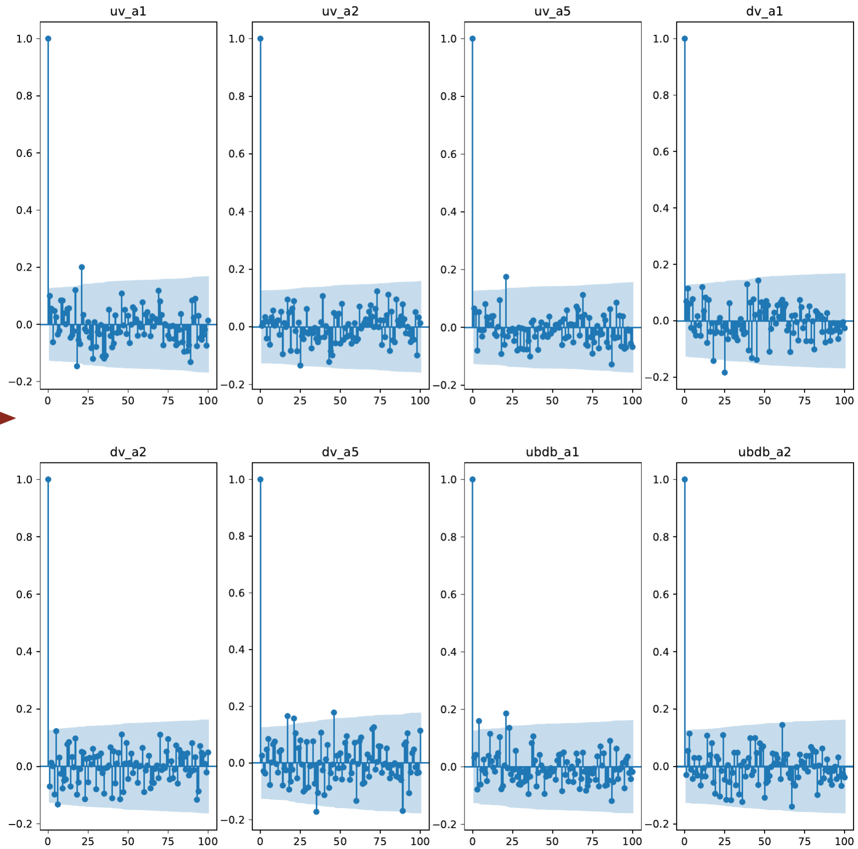
Thinning reduces the autocorrelation of the chain

$$\mathrm{Cov}(k) = \frac{1}{n}\sum_{t=1}^{n-k}(x_{t+k} - \bar{x})(x_t - \bar{x}), \quad \rho(k) = \frac{\mathrm{Cov}(k)}{\mathrm{Cov}(0)}$$

Autocorrelation function versus time interval



thinning

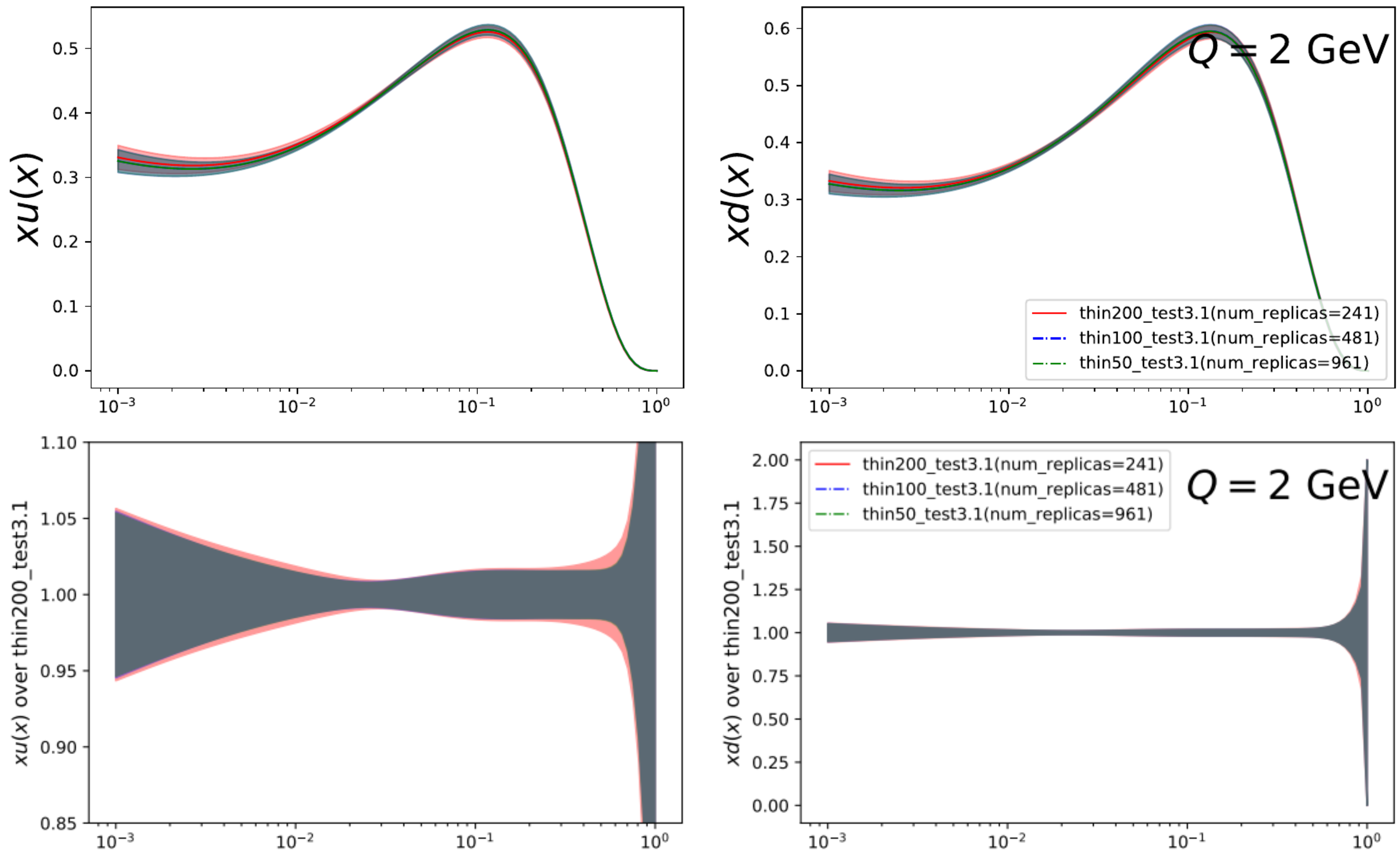


MCMC approach:

- 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 PDF grids):

Full-PDF and ratio-PDF for thinned chain of 8 parameters



Thank you for your attention

Acknowledgment:
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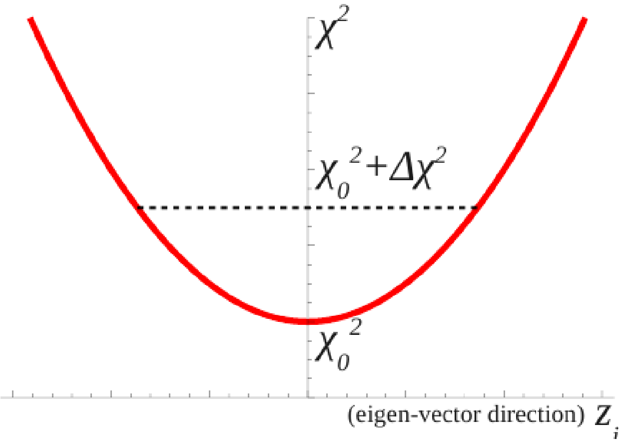

Hessian method:

Expand χ² function around minimum and diagonalize it:

$$\chi^2 = \chi_0^2 + \sum_{i,j} H_{ij}\, y_i\, y_j \qquad y_i = a_i - a_i^0$$

Fitting parameters

Minimum value

Hessian matrix

$$H_{ij} = \frac{1}{2}\left(\frac{\partial^2\chi^2}{\partial y_i \partial y_j}\right)_{a_i = a_i^0}$$

diagonalization

$$\chi^2 = \chi_0^2 + \sum_i \lambda_i z_i^2$$

$$f_i^{\pm} = f(\{z_i\}) = f(0, \ldots, z_i = \pm\sqrt{\Delta\chi^2}, \ldots, 0)$$

$$z_i = \pm\sqrt{\Delta\chi^2}$$

$$\Delta X = \sqrt{\sum_i \left(\frac{\partial X}{\partial z_i} \times \delta z_i\right)^2} \simeq \frac{1}{2}\sqrt{\sum_i \left[X(f_i^+) - X(f_i^-)\right]^2}$$

LHAPDF (set of PDF grids):

Full-PDF and ratio-PDF for thinned chain of 10 parameters