Universität Münster

Graduiertenkolleg 2149 Research Training Group

nCTEQ nuclear parton distribution functions

Markov chain Monte Carlo determination of Proton PDF uncertainties at NNLO

DIS 2024 – Grenoble

Peter Risse (risse.p@uni-muenster.de)

living.knowledge

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Markov chain Monte Carlo

- sampling representation of the likelihood
- autocorrelation: a bridge to lattice QCD

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- fixing a flaw in the parametrization

Definition of Uncertainties

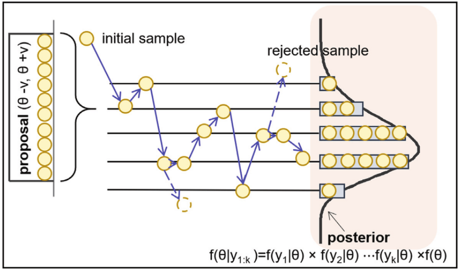
- From samples to PDF-Uncertainties
- Comparison with Hessian

Contents

Markov chain Monte Carlo representation of the likelihood

- **draw random samples** from the posterior function

$$\mathrm{post}(\mathbf{c}|D) = \frac{1}{\mathcal{Z}} \exp\left(-\frac{1}{2}\chi^2(\mathbf{c}, D)\right)$$
$$\rightarrow \{\mathbf{c_1}, \mathbf{c_2}, \ldots, \mathbf{c_n}\}$$



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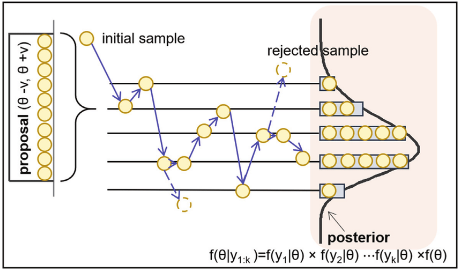
$$\rightarrow \{\mathbf{c_1}, \mathbf{c_2}, \ldots, \mathbf{c_n}\}$$

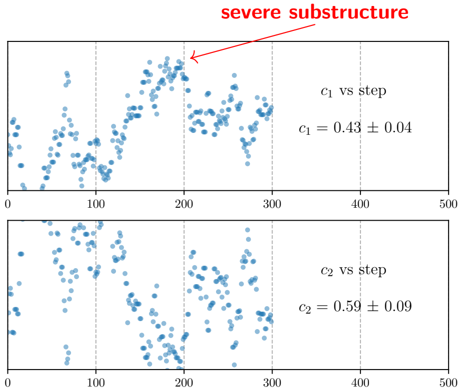
- samples have to **reproduce the expectation value and higher modes**

$$E\{\mathcal{O}(\mathbf{c})\} = \frac{1}{n}\sum_{i=1}^{n}\mathcal{O}(\mathbf{c}_i)$$



Autocorrelation

- we **cannot use the simple equations** to estimate variances and higher modes
  - these severely underestimate the true PDF-Uncertainties



autocorrelation at full force

Autocorrelation

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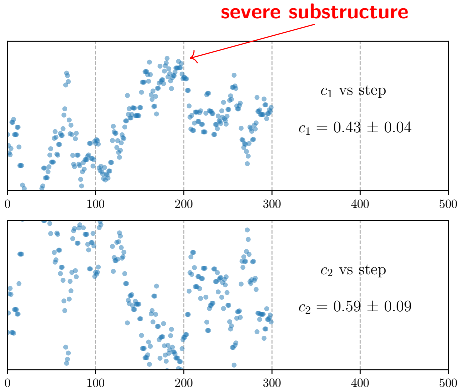
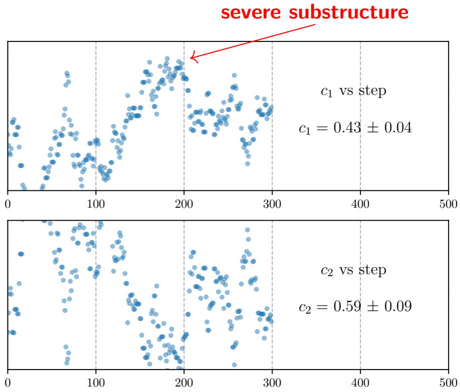
- since every new sample depends on the current **the gain in information is reduced**



autocorrelation at full force

Autocorrelation

- we **cannot use the simple equations** to estimate variances and higher modes
  - these severely underestimate the true PDF-Uncertainties
- since every new sample depends on the current **the gain in information is reduced**
- this is what is called **autocorrelation**
  - twice the **autocorrelation-time τ** estimates the number of links in the chain **until the next independent sample is drawn**



autocorrelation at full force

Bridge to Lattice QCD

- lattice QCD has several methods dealing with this problem

Bridge to Lattice QCD

- lattice QCD has several methods dealing with this problem
- one example is the **Γ-method**
  - this method estimates the autocorrelation time directly from the chain
  - used to **enlarge error estimates** as to eliminate bias
  - **or filter** the time series to get uncorrelated samples

Monte Carlo errors with less errors.

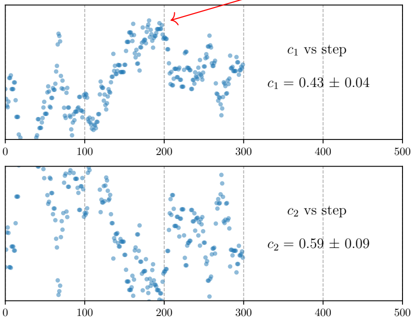
Ulli Wolff*
Institut für Physik, Humboldt Universität
Newtonstr. 15
12489 Berlin, Germany

Abstract
We explain in detail how to estimate mean values and assess statistical errors for arbitrary functions of elementary observables in Monte Carlo simulations. The method is to estimate and sum the relevant autocorrelation functions, which is argued to produce more certain error estimates than binning techniques and hence to help toward a

arXiv:hep-lat/0306017

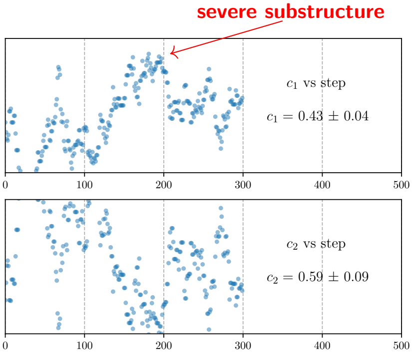
Filtering based on the Γ-method

severe substructure



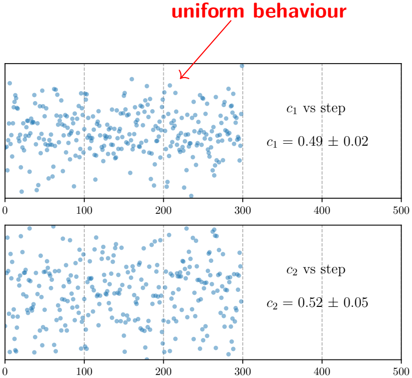
using 300 samples directly

Filtering based on the Γ-method



using 300 samples directly

$\Longrightarrow$

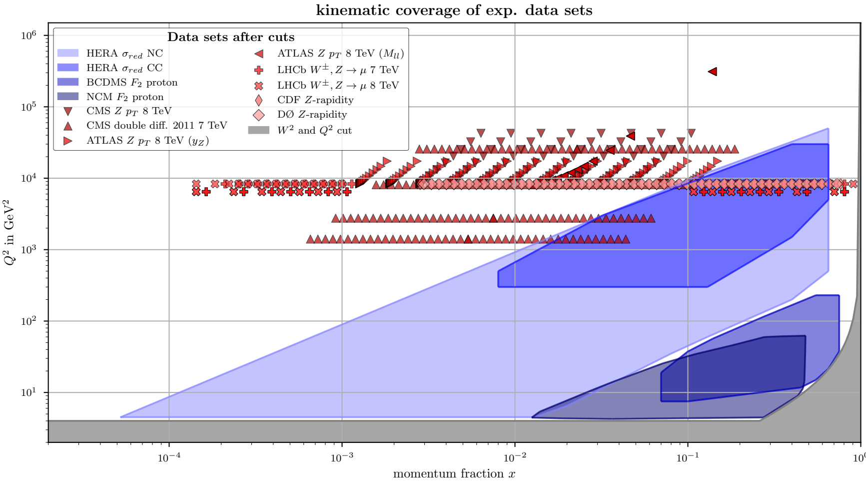


thinning 10^4 samples to a total of 300

Contents

Experimental data

- DIS: 1660 points
  - HERA NC/CC
  - NMC F_2
  - BCDMS F_2
- DY: 324 points
  - CDF & DØ
  - CMS
  - ATLAS
  - LHCb
- Total: 1984 points



Fitting setup

PDF parameters

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

$\mathbf{u_v}$	$\rightarrow$	c_1	c_2	c_4		
$\mathbf{d_v}$	$\rightarrow$	c_1	c_2	c_4		
$\mathbf{\bar{u} + \bar{d}}$	$\rightarrow$	c_1	c_2	c_4		
$\mathbf{s + \bar{s}}$	$\rightarrow$	c_0				
$\mathbf{g}$	$\rightarrow$	c_0	c_1	c_2	c_3	c_4

Total: 15 parameters

Hyperparameters

A flaw in the Parametrization

Down-valence Distribution

$$xd_v(x,Q_0) = c_0 x^{\mathbf{c_1}} (1-x)^{\mathbf{c_2}} \left(1 + c_3\sqrt{x} + \mathbf{c_4} x\right)$$

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becomes independent of $\mathbf{c_4}$

$$\lim_{\mathbf{c_4}\to\infty} xd_v(x, Q_0) = \lim_{\mathbf{c_4}\to\infty} c_0 x^{\mathbf{c_1}} (1-x)^{\mathbf{c_2}} \left[\mathbf{c_4} x\right]$$
$$= \tilde{\mathbf{c}}_{\mathbf{0}} x^{\mathbf{c_1}+1} (1-x)^{\mathbf{c_2}}$$

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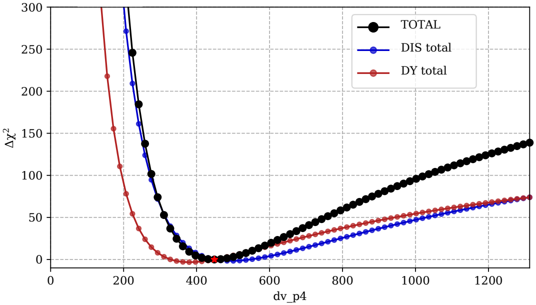
1D parameter scan



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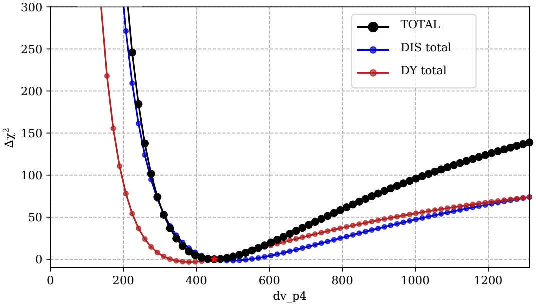
$$= \tilde{\mathbf{c}}_0 x^{\mathbf{c_1}+1}(1-x)^{\mathbf{c_2}}$$

- need constrain $\mathbf{c_4}$ by Uniform Prior:

$$-1000 \leq \mathbf{c_4} \leq 10.000$$

1D parameter scan



Fitting setup

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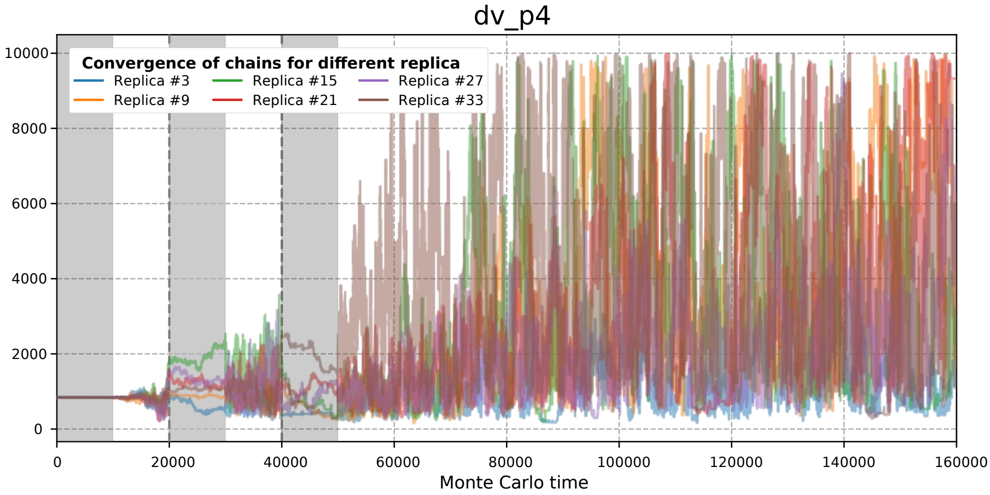
Hyperparameters

- Proposals: Adaptive Metropolis Hastings
- 36 independent chains with 479.000 samples each

Thermalization



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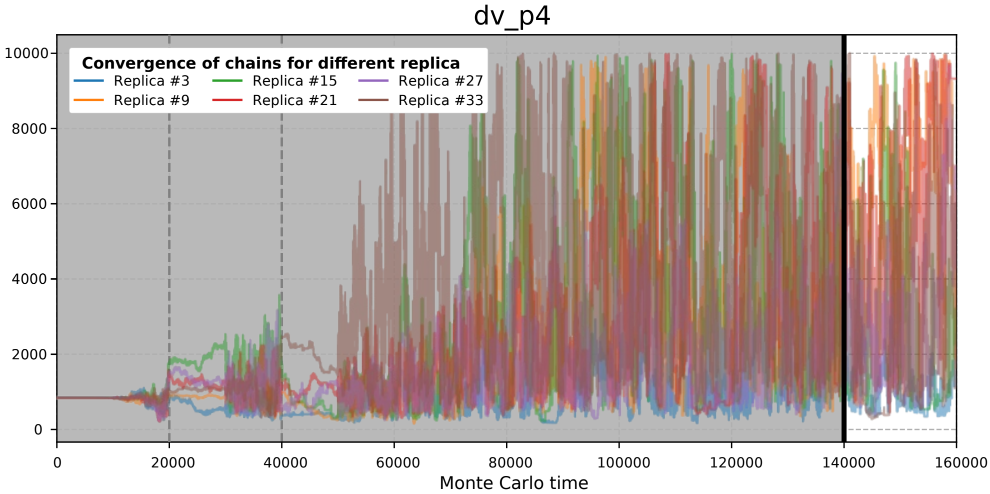

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Hyperparameters

- Proposals: Adaptive Metropolis Hastings
- 36 independent chains with 479.000 samples each
  - burn-in phase: 140.000 samples
  - **Total:** 17 million samples
- removing autocorrelation and burn-in:

Total: 4068 uncorrelated samples

Fitting setup

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$$\chi^2/\text{d.o.f.} = 2380.25/1969 = 1.20$$

Contents

From Samples to PDF-Uncertainties

Confidence interval for observable $\mathcal{O}(c)$

$$\mathcal{O}_- \leq \mathcal{O} \leq \mathcal{O}_+$$

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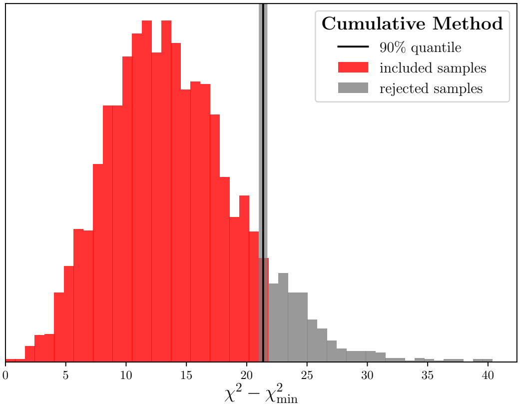
Cumulative χ^2-Method

Central: sample with minimal $\chi^2 \rightarrow \mathcal{O}_{\chi^2_{min}}$

Lower bound: $\min(\{\mathcal{O}\}_{90\%})$

Upper bound: $\max(\{\mathcal{O}\}_{90\%})$

A. Putze et al., arXiv: 0808.2437



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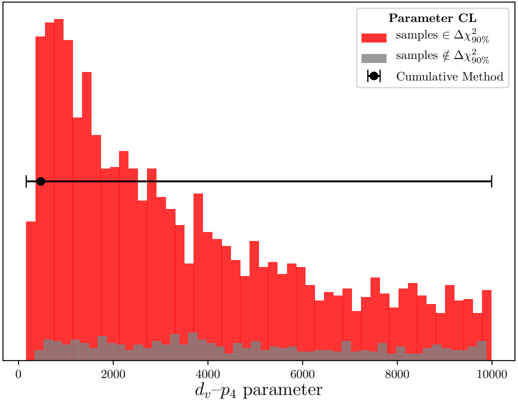


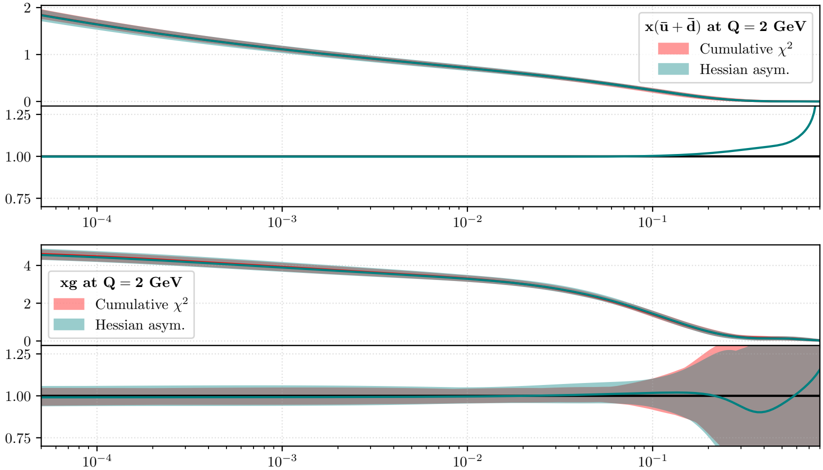
Comparison with Hessian – Gaussian parameters

Cumulative χ^2

$$\Delta\chi^2_{90\%} = 22$$

Hessian Method

$$\Delta\chi^2 = 22$$



Comparison with Hessian – non-Gaussian parameters

Cumulative χ^2

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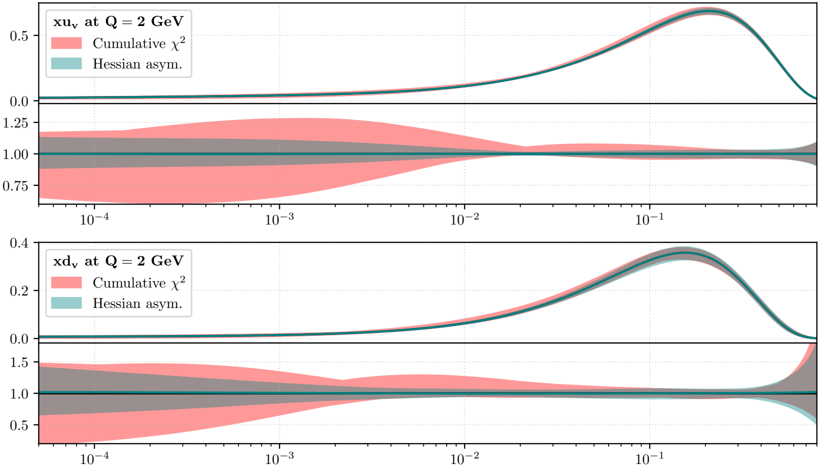
Hessian Method

$$\Delta\chi^2 = 22$$



Conclusion

Markov chain Monte Carlo

- access uncertainties without approximations
- Γ-method to deal with autocorrelation

Proton PDF extraction

- 15 parameter fit to DIS & DY data
- $\chi^2/\text{d.o.f.} = 2380.25/1969 = 1.20$
- Full MCMC chain: 17 million samples
- Result: 4068 uncorrelated samples

Definition of Uncertainties

- Confidence limits using χ^2-values
- Estimation of Tolerance from χ^2-samples
- good agreement for Gaussian parameters
- differences for non-Gaussian parameters

backup

Markov chain Monte Carlo representation of the likelihood

- posterior distribution too complicated to sample directly
  - need clever way to choose Monte Carlo samples
- construct the Monte Carlo samples via a Markov chain

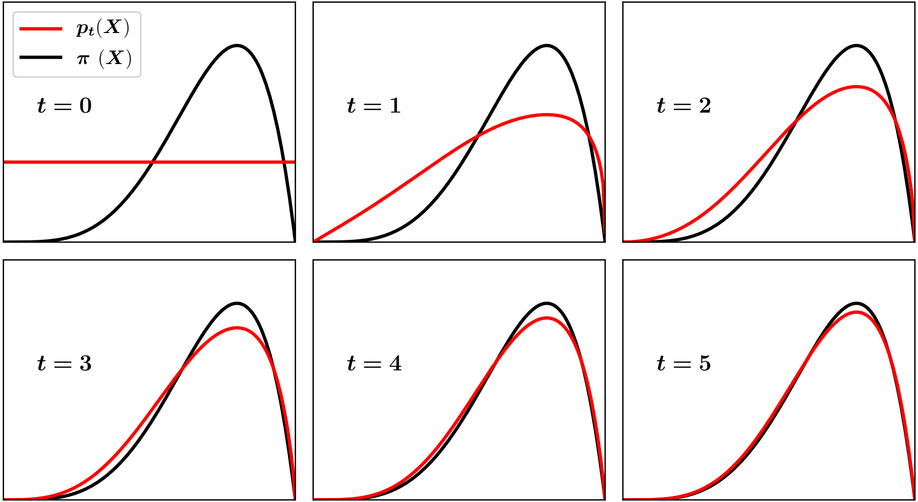
$$\{\mathbf{c}_1 \to \mathbf{c}_2 \to \cdots \to \mathbf{c}_{n-1} \to \mathbf{c}_n\}$$

$$\text{with} \quad p_i(\mathbf{c}) = \int \mathrm{d}\mathbf{c}'\, p_{i-1}(\mathbf{c}') T(\mathbf{c}', \mathbf{c})$$

- with the **transition kernel** $T(\mathbf{c}, \mathbf{c}')$

$$\underbrace{p_t(\mathbf{c}) \quad \xrightarrow{t\to\infty} \quad \mathrm{post}(\mathbf{c}|D)}_{\text{proper MCMC algorithm: } T(\mathbf{c}, \mathbf{c}')}$$

Markov chain Monte Carlo representation of the likelihood



Choosing the proposal distribution – Adaptive Metropolis-Hastings

1. Use **normal random walk Metropolis-Hastings** until N_0 samples have been obtained
   - proposal distribution: multivariate Gaussian

$$\tilde{\mathbf{c}}_{i+1} \quad \text{proposed from} \quad q(\tilde{\mathbf{c}}_{i+1}, \mathbf{c}_i) = \mathcal{N}(\mathbf{c}_i, C_0) \quad \text{with} \quad C_0: \ \text{covariance matrix from user input}$$

2. switch to a **self learning proposal distribution**

$$\tilde{\mathbf{c}}_{i+1} \quad \text{proposed from} \quad q(\tilde{\mathbf{c}}_{i+1}, \mathbf{c}_i) = (1-\beta)\mathcal{N}\left(\mathbf{c}_i, \text{scale} \cdot \overline{C}_i\right) + \beta\mathcal{N}(\mathbf{c}_i, C_0)$$

with self learned $\overline{\mathbf{C}}_\mathbf{i}$

   - $0 \leq \beta \leq 1$ controls the impact of the 'learned' proposal

3. reset self learned proposal distribution **to boost convergence**
   - this reduces the impact of the starting point

H. Haario et al.: “An adaptive Metropolis algorithm”, *Bernoulli* 7.2 (Apr. 2001)

APFEL++ – A PDF evolution library in c++

Bertone, arXiv:1708.00911

- main author: **V. Bertone**
- rewrite of the Fortran APFEL code
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Precompute observables

$$F_\lambda(x, Q^2) = \sum_k \int_\chi^1 \frac{\mathrm{d}\xi}{\xi} C_k^\lambda\left(\frac{\chi}{\xi}, \frac{Q}{\mu}, \frac{M_i}{\mu}, \alpha_s(\mu)\right) f_k(\xi, \mu)$$

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Replace with interpolating functions: $\Uparrow$

$$\sum_\alpha^{N_\xi} w_\alpha(\xi) f_k(\xi_\alpha, \mu)$$

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Bertone, arXiv:1708.00911

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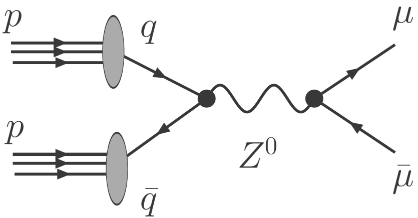
Precompute observables

$$F_\lambda(x, Q^2) = \sum_k \sum_\alpha \underbrace{\int_\chi^1 \frac{\mathrm{d}\xi}{\xi} C_k^\lambda\left(\frac{\chi}{\xi}, \frac{Q}{mu}, \frac{M_i}{\mu}, \alpha_s(\mu)\right) w_\alpha(\xi)}_{\textbf{Precompute}} f_k(\xi_\alpha, \mu)$$

Speed-up of theoretical predictions – Hadron collider

$$\sigma_{pp\to X} = \sum_s^{partons} \sum_p \int \mathrm{d}x_1 \mathrm{d}x_2\, \hat{\sigma}^{(s)(p)} \alpha_s^p(Q^2) F^{(s)}(x_1, x_2, Q^2)\ ,\ F^{(s)} = \sum_{ij} f_i(x_1, Q^2) f_j(x_2, Q^2)$$

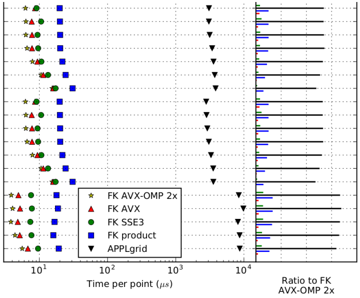


- computationally **expensive double integrals**
- increasing amount of experimental observables
- solution `APPLgrid`
  - interpolate the PDFs
  - precompute the integrals by including the interpolating functions as grids
  - now convolute grids with any pdf to get prediction

T. Carli, D. Clements et al., arXiv:0911.2985

Speed-up of theoretical predictions – Hadron collider

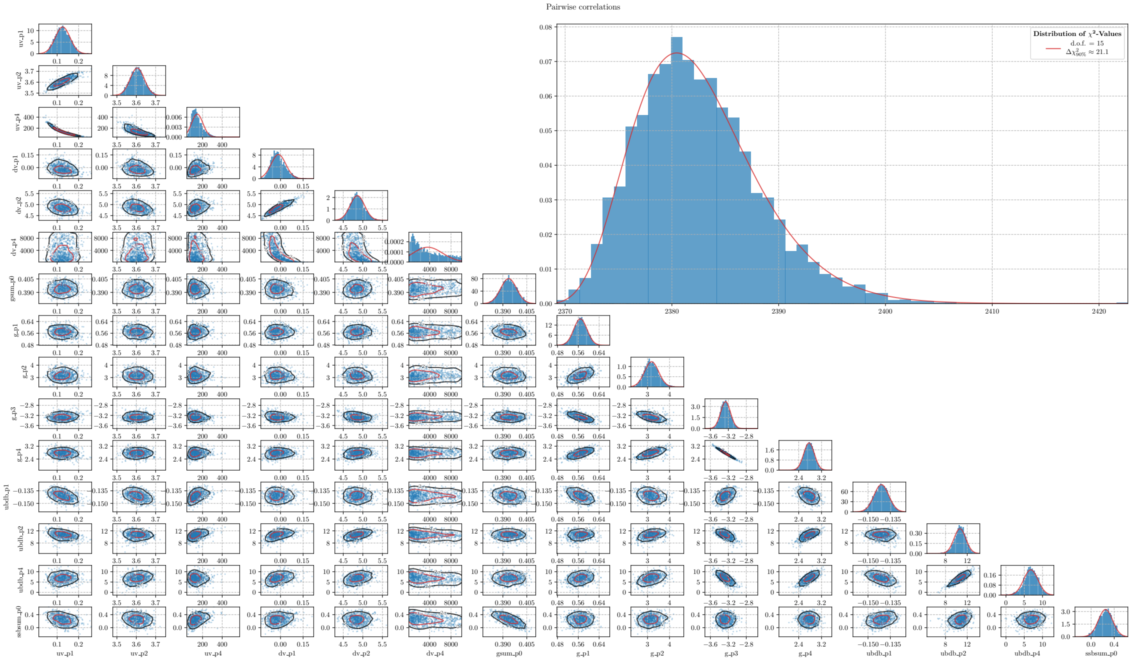
- APPLgrid is still too slow for several reasons
  - convolution of the grid with the PDFs is **not well optimized**
  - before one can convolute one has to compute the DGLAP evolution to get the PDFs at every Q
- solution **fast convolution tables** (FK-tables) by APFELgrid
  - combines APPLgrid tables with DGLAP-evolution tables
    - only need the PDFs at Q_0
  - well optimized by making use of vectorisation and multiprocessing
  - **possible speed-up** compared to APPLgrid: $\mathcal{O}(2) - \mathcal{O}(10^3)$



V. Bertone et al., arXiv:1605.02070

Description of Experimental Data

Data Set	Ref.	Data Points	χ^2/data
DIS			
HERA σ_{red} neutral current	[54]	1039	1.26
HERA σ_{red} charged current	[54]	81	1.08
BCDMS F_2 proton	[135]	339	1.09
NCM F_2 proton	[136]	201	1.54
DIS total		1660	1.25
DY			
CDF Z-rapidity	[137]	28	1.10
DØ Z-rapidity	[138]	28	0.60
ATLAS Z p_T 8 TeV (M_{ll})	[139]	44	1.06
ATLAS Z p_T 8 TeV (y_Z)	[139]	48	0.65
CMS Z p_T 8 TeV	[140]	28	0.46
CMS double diff. 2011 7 TeV	[141]	88	1.02
LHCb $W^{\pm}, Z \rightarrow \mu$ 7 TeV	[142]	29	1.07
LHCb $W^{\pm}, Z \rightarrow \mu$ 8 TeV	[143]	31	1.18
DY total		324	0.91
Total		1984	**1.20** (per dof)


Pairwise correlations
Distribution of χ^2-Values
d.o.f. = 15
$\Delta\chi^2_{90\%} \approx 21.1$
uv_p1
uv_p2
uv_p4
dv_p1
dv_p2
dv_p4
gsum_p0
g_p1
g_p2
g_p3
g_p4
ubdb_p1
ubdb_p2
ubdb_p4
ssbsum_p0