Markov Chain Monte Carlo technics applied to Parton Distribution Functions determination: proof of concept

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Outline

1 Introduction

2 From minimization to Bayesian inference
   - Formulation of PDFs determination in terms of Bayesian inference
   - Markov chains
   - Metropolis algorithm
   - Hybrid (or Hamiltonian) Monte Carlo

3 Markov chain analysis
   - Thermalisation, autocorrelation and all that....

4 First results
   - PDFs Parameters
   - PDFs probability distribution functions

5 Conclusions
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Precise assessment of PDFs uncertainties has become crucial.

PDFs subject both to theoretical (input parametrization, neglected higher order corrections, heavy flavors treatment, ... ) and experimental uncertainties.

To deal with experimental errors:

- Hessian method: based on linear error propagation
- Lagrange multiplier method
- ...

Assumption on the permissible range of "acceptable" $\Delta \chi^2$ for the fit and choice of a tolerance parameter $T$ $^1$.

$^1$ This excepts Neural Networks technics
Traditional propagation of experimental uncertainties

- $\Delta \chi^2 = 1$ for 68% C.L. IF fitting consistent data sets with ideal gaussian errors
- In practice: inconsistencies between fitted data sets and unknown exp. and theoretical uncertainties, so not appropriate for global PDFs analysis $\Rightarrow$ choice of tolerance criteria $\Delta \chi^2 \neq 1$.

Ex.: MRST\[hep-ph/0211080]\ 

"We estimate $\Delta \chi^2 = 50$ to be a conservative uncertainty (perhaps of the order of a 90% confidence level or a little less than 2$\sigma$) due to the observation that an increase of 50 in the global $\chi^2$ [...] usually signifies that the fit to one or more data sets is becoming unacceptably poor. We find that an increase $\Delta \chi^2$ of 100 normally means that some data sets are very badly described by the theory."

What can MCMC methods tell us about PDFs uncertainties?
Traditional propagation of experimental uncertainties

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What can MCMC methods tell us about PDFs uncertainties?
Very general flow diagram of PDFs extraction

1. Choice of PDFs parametrization at a starting scale $Q_0 \rightarrow f_i(Q_0, x)$ (typically ~ 20-30 parameters)

2. Evolution at $Q_{\text{data}}$ by DGLAP equations $\rightarrow f_i(Q_{\text{data}}, x)$

3. $\chi^2$ construction from $\sigma_{\text{data}}(Q)$ and $\sigma_{\text{theo}}(Q)$ (computed from $f_i(Q_{\text{data}}, x)$)

4. Minimisation

5. MCMC technics

6. Extraction of Probability Density Functions of PDFs

7. Extraction of parameters and PDFs
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PDFs determination in terms of Bayesian inference

- $\vec{q}$: vector of PDFs parameters to be determined:
  
  $\vec{q} = (q^{(1)}, q^{(2)}, \ldots, q^{(m)})^T$

- $xFitter$ functional form at $Q^2_0 \sim 2$ GeV$^2$:

  $xf_a(x) = A_a \ x^B_a \ (1 - x)^C_a \ (1 + D_a x + E_a x^2)$. \hspace{1cm} \text{where } a \text{ labels a parton } (g, u_{val}, d_{val}, \ldots).

- $D$: data

**Bayesian inference:**

Both model parameters and observables considered random quantities. Aims at determining a joint probability distribution $P(D, \vec{q})$ over all random quantities:

$$P(D, \vec{q}) = P(D|\vec{q})P(\vec{q})$$

- $P(\vec{q})$ prior distribution
- $P(D|\vec{q})$: likelihood of the data $\mathcal{L}(\vec{q})$
Bayes theorem

Express $P(\vec{q}|D)$ in terms of the likelihood $P(D|\vec{q})$:

$$P(\vec{q}|D) = \frac{P(D|\vec{q})P(\vec{q})}{\int d\vec{q}P(D|\vec{q})P(\vec{q})}$$  \hspace{1cm} (1)

- $P(\vec{q}|D)$: *posterior* probability density
- Can be sampled using a Monte Carlo algorithm
PDFs determination in terms of Bayesian inference

**Likelihood**

Let’s note

- \(D_i\) and \(T_i\): respectively the \(i^{th}\) experimental point and the corresponding theoretical calculation
- \(\sigma_i^2\): the uncertainty associated with the measured data \(i\).

If \(\frac{(D_i - T_i)}{\sigma_i}\) independent and normally distributed:

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

(2)

Possibility to construct more involved likelihood with correlated data

**Prior distribution**

We choose \(P(\vec{q})\) uniform

Remark: If \(D_i\) distributed according to a Gaussian law, MLE and LSM equivalent
In summary...

**Least square method**
- $\chi^2$ construction
- Minimization

- $\chi^2_{min}$ and neighborhood

**MCMC method**
- Choice of prior
- Likelihood construction
- Monte Carlo sampling of posterior probability

- Probability distributions, confidence intervals...
Metropolis [Metropolis et al., J. Chem Phys. 21 (1953)]

- one of the simplest Monte Carlo algorithm
- standard computational workhorse of MCMC methods
- in principle applicable to any system
- extremely straightforward to implement and to sample a target density $P(\vec{q}|D)$
- at each Monte Carlo time $t$, the next state $\vec{q}_{t+1}$ is chosen by sampling a candidate point $\vec{q}'$ from a proposal distribution ($\ast$). The candidate point is then accepted with the probability

$$\alpha(\vec{q}_t, \vec{q}') = \min \left(1, \frac{P(\vec{q}'|D)}{P(\vec{q}_t|D)} \right)$$

i.e. in our case

$$\alpha(\vec{q}_t, \vec{q}') = \min \left(1, e^{-\frac{1}{2}\Delta\chi^2} \right)$$

($\ast$) Proposal distribution assumed symmetric here
and why we do not use it.....

Metropolis algorithms (even flavored with multivariate Gaussian distributions or binary space partitioning) are NOT suited for realistic PDFs determination ($m \sim 25$).

**Acceptance test**
- typically for 1 parameter: 30-50%
- decreases as $\sim 0.5^m$
  $\rightarrow$ For $m=10$ parameters, unacceptable acceptance...

**Initialize** $\vec{q}_0$; set $t = 0$
Repeat {
  Sample a point $\vec{y}$ from a proposal distribution
  Sample a Uniform[0,1] random variable $u$
  If $u \leq \alpha(\vec{q}_t, \vec{y})$ set $\vec{q}_{t+1} = \vec{y}$
  otherwise set $\vec{q}_{t+1} = \vec{q}_t$
  Increment $t$
}

trial point far from the initial one $\rightarrow$ large change in the distribution to sample
point close to the initial one $\rightarrow$ inefficient exploration of the parameter space
HMC

- Developed originally for lattice field theory [Duane et al, 1987]
- Combines molecular dynamics evolution with a Metropolis accept/reject step

Introduce for each set of parameters $\vec{q}$ a set of conjugate momenta $\vec{p}$

Associates an Hamiltonian $H(\vec{q},\vec{p}) = \vec{p}^T M^{-1} \vec{p}/2 + U(q)$, where $M$ is a mass matrix, and $U(q)$ an arbitrary potential energy.

This allows to define a joint distribution as

$$P(q,p) = \frac{1}{Z} e^{-H(q,p)} = \frac{1}{Z} e^{-K(p)} e^{-U(q)}$$

$Z$ normalizing constant

We use for the potential energy $U(q) = -\log[P(D|\vec{q})P(\vec{q})]$. 
From minimization to Bayesian inference

Hybrid (or Hamiltonian) Monte Carlo

- choose $\vec{p}_0$ normally distributed
- let the system evolve deterministically
- candidate point $\vec{q}_1$ accepted with probability $\min(1, e^{-\Delta H})$ i.e. 100% !!!

In practice: acceptance degraded because of numerical resolution of Hamilton equations, but still very high (typically $\sim 80 - 90\%$, independently of the dimension of the chain).

Sampling of a 100D gaussian. Values of the variable with largest standard deviation.

[R. M. Neal, arXiv:1206.1901]
Implementation of HMC in xFitter package

- parametrized HERA PDFs: $xu_v, xd_v, xg, x\overline{U} = xu, x\overline{D} = xd + x\overline{s}$

- functional form at $Q_0^2 \sim 2 \text{ GeV}^2$:

  \[
  x f_a(x) = A_a \, x^{B_a} \, (1 - x)^{C_a} \, (1 + D_a \, x + E_a \, x^2) \tag{3}
  \]

  where $a$ labels a parton ($g$, $u_{val}$, $d_{val}$, ...).

- we consider 10 free parameters: $B_g$, $C_g$, $B_{u_{val}}$, $C_{u_{val}}$, $E_{u_{val}}$, $C_{d_{val}}$, $C_{\overline{U}}$, $A_{\overline{D}}$, $B_{\overline{D}}$ and $C_{\overline{D}}$

- validation study, with combined inclusive $e^\pm p$ scattering cross-sections from H1 and ZEUS ($\sim 600$ data points), and ZMVFN scheme.

- comparison with HERAPDF1.0 with ZMVFNs.
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Extracting observables and their statistical errors from Monte Carlo simulations: subtle task, requiring careful treatment of the Markov chain.

- The thermalization time (or burn-in length $b$): number of states \{\hat{q}_t\}_{t=1,...,b} to be discarded from the beginning so that the chain forgets its starting point.

\[ \chi^2/\text{d.o.f.} = 81.6 \]
\[ \chi^2/\text{d.o.f.} = 0.87 \]
\[ \chi^2/\text{d.o.f.} = 67.4 \]

We have taken $P(\hat{q}_b|D) > P_{1/2}$
Analysis (2/3)

- **Autocorrelation**: inherent correlations from one point to the next. Usual estimate of root-mean-square deviation of an observable $O$:

  $$\sigma^2_{naive} = \frac{N}{N-1} \left( \langle O^2 \rangle - \langle O \rangle^2 \right)$$

- Relies on the assumption that measurements performed on the Markov chain are NOT correlated
- Several methods to account for the correlations: jackknife binning (pre-averaging over blocks of data), $\Gamma$–method (explicit determination of autocorrelation functions and times), . . .
- In practice for this work: $\tau_{corr} \sim 2$. 

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Analysis (3/3)

- **Convergence**: start from different points, and check we reach the same distribution
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Ready to compare standard minimization and Monte Carlo method....

Comparison of results obtained for 2 parameters of the gluon PDF using Markov Chain procedure or $\chi^2$ (MINUIT) minimisation:

| parameter | values               | MCMC              | MINUIT minimization |
|-----------|----------------------|-------------------|---------------------|
| $B_g$     | mean $-0.0537 \pm 0.0002$ | $-0.0537 \pm 0.0002$ | $-0.0559$           |
|           | most probable $-0.0632 \pm 0.0168$ | $-0.0632 \pm 0.0168$ | $0.0288$           |
|           | standard deviation $0.0299 \pm 0.0001$ | $0.0299 \pm 0.0001$ |                     |
| $C_g$     | mean $5.9483 \pm 0.0025$ | $5.9483 \pm 0.0025$ |                     |
|           | most probable $5.8952 \pm 0.0615$ | $5.8952 \pm 0.0615$ |                     |
|           | standard deviation $0.5037 \pm 0.0019$ | $0.5037 \pm 0.0019$ |                     |

Much more information with MCMC
PDF Parameters: Marginal probability distribution and correlations

Marginal posterior parameter distributions

2D correlations

Inner and outer contours: 68% and 95% of the probability density resp.
PDF Parameters: Marginal probability distribution and correlations

Parameter marginal distributions not necessarily gaussian
PDF Parameters: $\chi^2$ distribution

$\chi^2$ distribution for a 10D MCMC. The solid line is an adjustment with a $\chi^2$ distribution law.

![Chi-squared distribution graph]

$\chi^2_{\text{min}} / \text{d. o. f.} = 0.89$

$\chi^2_{\text{min}} / \text{d. o. f.} + 0.02 \Rightarrow 68\% \text{ C.L.}$

$\chi^2_{\text{min}} / \text{d. o. f.} + 0.03 \Rightarrow 95\% \text{ C.L.}$
Probability distribution functions of PDFs (PDFs of PDFs...)

For each MC parameter set \( \vec{q}_t \), compute the corresponding PDFs

probability distribution of PDFs at fixed \((x, Q^2)\)

\[
\begin{align*}
  x &\approx 10^{-4} \quad \text{and} \quad Q^2 = 10 \text{ GeV}^2 \\
  x &\approx 0.83 \quad \text{and} \quad Q^2 = 10 \text{ GeV}^2
\end{align*}
\]

Gluon PDF probability distribution function for \( x \approx 10^{-4} \) (l.h.s.) and \( x \approx 0.83 \) at fixed \( Q^2 = 10 \text{ GeV}^2 \).

The 68% confidence interval is obtained considering the region of the distribution containing 68% of the data remaining on each side of the most probable value.
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Gluon PDF probability distribution function for $x \approx 10^{-4}$ (l.h.s.) and $x \approx 0.83$ at fixed $Q^2 = 10$ GeV$^2$.

The 68% confidence interval is obtained considering the region of the distribution containing 68% of the data remaining on each side of the most probable value.
The parton distribution functions obtained using MCMC (right) compared to HERAPDF1.0 (ZMVFN scheme) from xFitter output (left) for $xu_{val}$ and $xg$, at $Q^2 = 10$ GeV$^2$. The bands show the 68% confidence interval around the most probable value for the MCMC PDFs, and the standard $\Delta \chi^2 = 1$ deviation for HERAPDF.
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What we have done....

- MCMC, well-suited to multi-parameter determination, applicable to PDFs extraction
- Overcome the technical difficulties by a nice recycling of a lattice algorithm (HMC)
- Obtained probability densities of PDFs and as by-product, confidence intervals

What we would like to do....

- Consider more complex $\chi^2$ functions including correlations and study prior influence
- Extend this work to a competitive PDF ensemble with more parameters and data
- Extract $\alpha_s$ and possibly $m_c, m_b$ from data using MCMC

What we have NOT done....

- Tackled the problem of potentially incompatible data, but....

Bayesian approach applied to global analyses can lead to a deeper insight into PDFs uncertainties determination
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THANK YOU