mc²hessian

An unbiased Hessian representation for Monte Carlo PDFs

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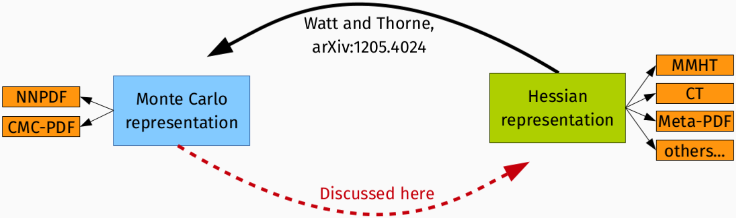
in collaboration with S. Forte, Z. Kassabov, J.I. Latorre and J. Rojo

PDF4LHC, April 13, 2015, CERN

Panorama of PDF representations:



Problem addressed here:

⇒ Determine an **unbiased Hessian representation** for **MC** PDFs.

- Some **advantages** of each approach:

Monte Carlo approach:

- unbiased PDF parametrization
- no linear approximation to propagate uncertainties

Hessian approach:

- PDF probability density is Gaussian
- the use of PDF profiling

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MC to Hessian conversion problem:

Avoid the definition of an **intermediate** functional form which introduces **bias** in the **PDF parametrization**

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Our Strategy:

use MC replicas ***themselves*** *as the* ***basis*** *of the linear representation*

- **Methodology**
  - Definition and implementation
- **Validation and Benchmarking**
  - Hessian representation of MC PDFs
  - Self-closure of the algorithm
  - LHC phenomenology
- **Delivery**

THE `mc2hessian` METHODOLOGY

Given a Monte Carlo prior set of PDFs

$$\{f_\alpha^{(k)}\}_{k=1,\ldots,N_{\rm rep}}\,, \quad \alpha = \{g, u, d, s, \ldots\}\,,$$

use a subset of replicas as parameters of linear expansion:

$$f_\alpha^{(k)} \approx f_{H,\alpha}^{(k)} \equiv f_\alpha^{(0)} + \sum_{i=1}^{N_{\rm eig}} a_i^{(k)} (\eta_\alpha^{(i)} - f_\alpha^{(0)})\,, \quad k = 1, \ldots, N_{\rm rep}$$

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The methodology in 4 steps:

(a) We define the **covariance matrix** for the prior set

$$\mathrm{cov}^{\mathrm{pdf}}_{ij,\alpha\beta} \equiv \frac{N_{\mathrm{rep}}}{N_{\mathrm{rep}}-1}\left(\left\langle f_\alpha^{(k)}(x_i,Q_0^2)\cdot f_\beta^{(k)}(x_j,Q_0^2)\right\rangle_{\mathrm{rep}} - \left\langle f_\alpha^{(k)}(x_i,Q_0^2)\right\rangle_{\mathrm{rep}}\left\langle f_\beta^{(k)}(x_j,Q_0^2)\right\rangle_{\mathrm{rep}}\right)$$

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(b) Then we minimize the **figure of merit**

$$\chi^{2(k)}_{\mathrm{pdf}} \equiv \sum_{i,j=1}^{N_x}\sum_{\alpha,\beta=1}^{N_f}\left(\left[f^{(k)}_{H,\alpha}(x_i,Q_0^2) - f^{(k)}_{\alpha}(x_i,Q_0^2)\right]\cdot\left(\mathrm{cov}^{\mathrm{pdf}}\right)^{-1}_{ij,\alpha\beta}\cdot\left[f^{(k)}_{H,\beta}(x_j,Q_0^2) - f^{(k)}_{\beta}(x_j,Q_0^2)\right]\right)$$

- in a suitable sampling in x and flavors $\rightarrow (N_x, N_f)$
- at fixed Q_0^2 $\rightarrow$ higher values by DGLAP evolution

DESCRIPTION OF THE METHOD

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Minimization strategy

- impose $\chi^{2(k)}_{\mathrm{pdf}} \rightarrow 0$ for each replica of the prior (e.g. SVD)
- determination of the coefficients $\{a_i^{(k)}\}$ for each original replica k

(c) We construct the covariance matrix of $\{a_i^{(k)}\}$ coefficients

$$\mathrm{cov}_{ij}^{(\mathrm{a})} \equiv \frac{N_{\mathrm{rep}}}{N_{\mathrm{rep}}-1}\left(\left\langle a_i \cdot a_j \right\rangle_{\mathrm{rep}} - \left\langle a_i \right\rangle_{\mathrm{rep}} \left\langle a_j \right\rangle_{\mathrm{rep}}\right), \quad i,j = 1,\ldots,N_{\mathrm{eig}}$$

(d) We diagonalize the inverse of $\mathrm{cov}_{ij}^{(\mathrm{a})}$, the one-sigma uncertainty is

$$\sigma_{H,\alpha}^{\mathrm{PDF}}(x,Q^2) = \sqrt{\sum_{i=1}^{N_{\mathrm{eig}}}\left[\sum_{j=1}^{N_{\mathrm{eig}}} \frac{v_{ij}}{\sqrt{\lambda_i}}\left(\eta_{\alpha}^{(j)}(x,Q^2) - f_{\alpha}^{(0)}(x,Q^2)\right)\right]^2}$$

where v_{ij} is rotation matrix, and λ_i the set of eigenvalues.

The final symmetric Hessian eigenvectors

$$\widetilde{f}_{\alpha}^{(i)}(x, Q^2) = f_{\alpha}^{(0)}(x, Q^2) + \sum_{j=1}^{N_{\mathrm{eig}}} \frac{v_{ij}}{\sqrt{\lambda_i}} \left(\eta_{\alpha}^{(j)}(x, Q^2) - f_{\alpha}^{(0)}(x, Q^2) \right)$$

The one-sigma uncertainty band is then

$$\sigma_{H,\alpha}^{\mathrm{PDF}}(x, Q^2) = \sqrt{\sum_{i=1}^{N_{eig}} \left(\widetilde{f}_{\alpha}^{(i)}(x, Q^2) - f_{\alpha}^{(0)}(x, Q^2) \right)^2}$$

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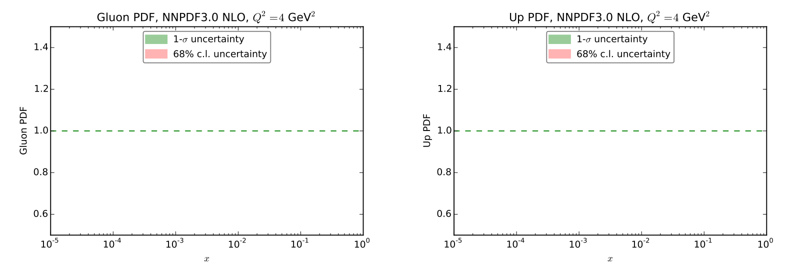
To be compared to the standard deviation of the prior MC set:

$$\sigma_{\alpha}^{\rm PDF}(x, Q^2) = \sqrt{\left\langle \left(f_{\alpha}^{(k)}(x, Q^2) \right)^2 \right\rangle_{\rm rep} - \left\langle f_{\alpha}^{(k)}(x, Q^2) \right\rangle_{\rm rep}^2}$$

THE `mc2hessian` NUMERICS

Practical implementation issues

1. the **grid of points in** x: 1-σ and the 68% confidence level intervals

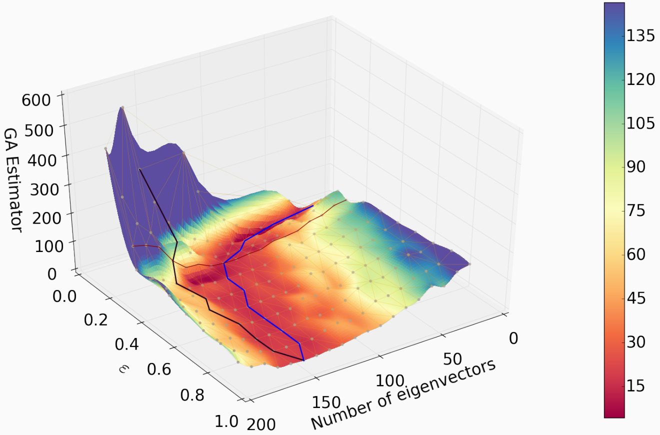


2. the **optimal basis** of replicas, the **optimal number** of symmetric eigenvectors for the Hessian representation

We define an **estimator** which measures the distance between the prior MC and its Hessian representation:

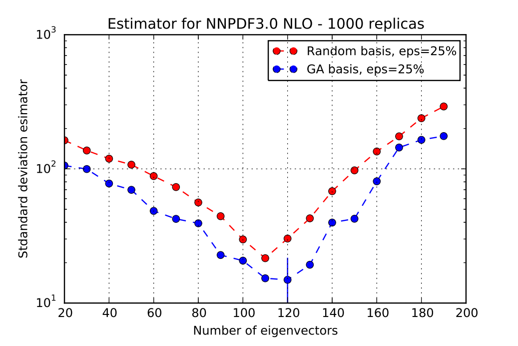
$$\mathrm{ERF}_\sigma = \sum_{i=1}^{N_x} \sum_{\alpha=1}^{N_f} \left| \frac{\sigma_{H,\alpha}^{\mathrm{PDF}}(x_i, Q_0^2) - \sigma_{\alpha}^{\mathrm{PDF}}(x_i, Q_0^2)}{\sigma_{\alpha}^{\mathrm{PDF}}(x_i, Q_0^2)} \right|$$

- We **introduce** an ϵ threshold for the **exclusion** of regions in x where the Gaussian approximation is no reliable.
- We **implement** a Genetic Algorithm in function of ϵ and N_{eig} which **minimizes** the **estimator**.



- **Surface:** GA minimum for estimator in function of ϵ and N_{eig}.
- **Blue curve:** surface minimum; **black curve:** estimator with large ϵ.

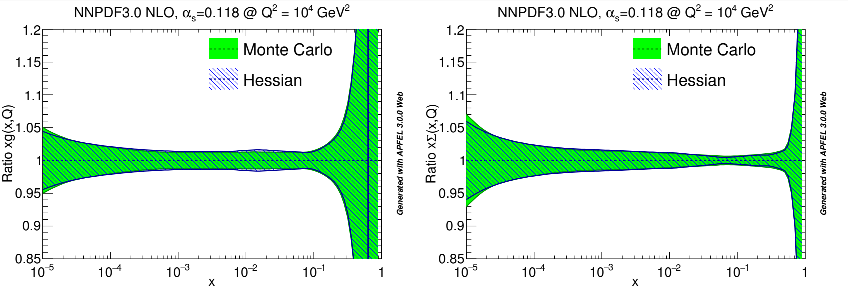
Estimator: Random vs. GA basis



- **NNPDF3.0 NLO** $\longrightarrow$ Hessian representation with $N_{\rm eig} = 120$
- We use $\epsilon = 25\%$ motivated by the previous slide.

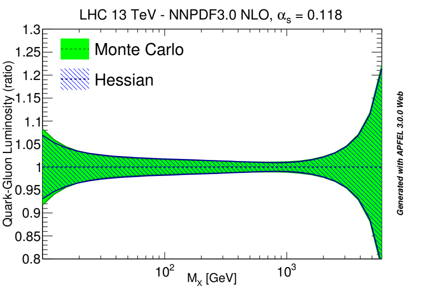
VALIDATION AND BENCHMARKING

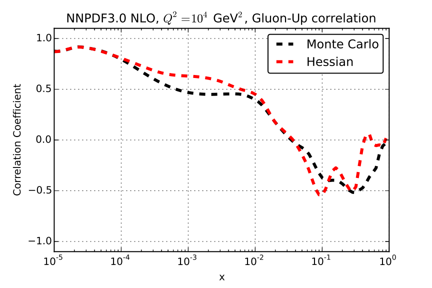
PDF comparison: MC vs. Hessian representations



- **Good agreement:** differences in the one-sigma PDF uncertainty bands of the order 5% at most between the two representations.

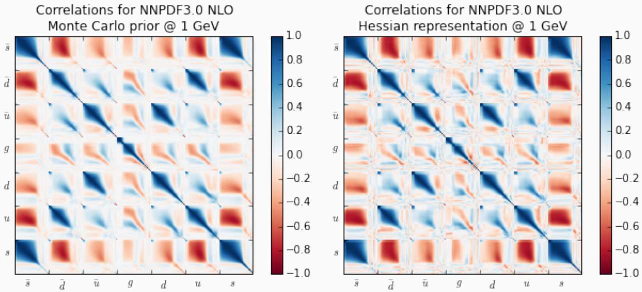
Luminosities and Correlations:





- **Reasonable agreement:** small differences due to the information loss when moving from the MC to the Hessian representation.

Full correlations matrix:



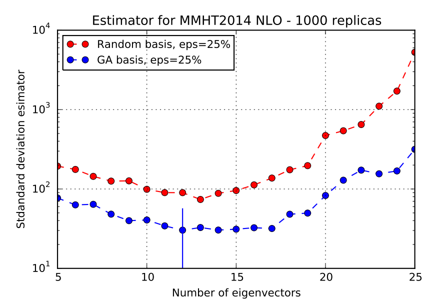
- **Good agreement:** small differences due to the information loss when moving from the MC to the Hessian representation.

SELF-CLOSURE TEST

Starting from the original Hessian MMHT14 NLO set:

1. Construct its **MC representation** (Watt & Thorne '12)
2. Run the `mc2hessian` algorithm

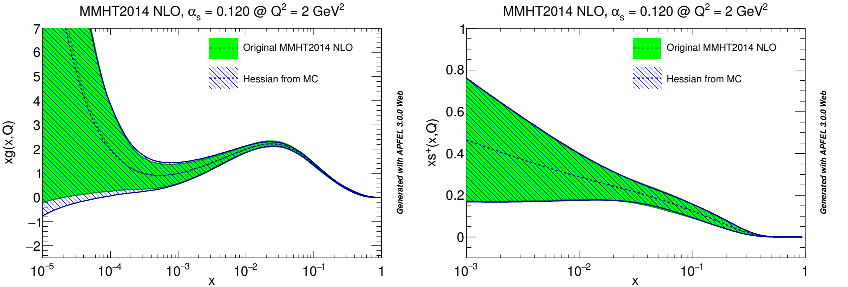
In this case, the estimator minimum is obtained with **12 symmetric eigenvectors**.



Self-closure Test Output:

`mc2hessian` successful ⇒ **original** and the **new** Hessian representations are **close to each other**

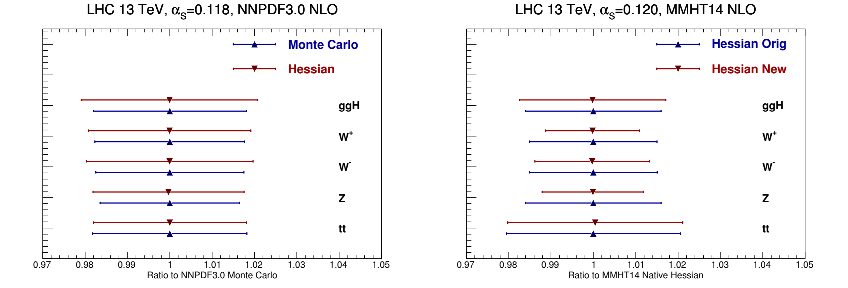
PDF comparison: Original MMHT2014 vs. Hessian from MC



- Agreements **better than 5%** of the uncertainty between the two Hessian representations.
- The `mc2hessian` is able to **compress information** of the native Hessian representations, **reducing the total number of eigenvectors**.

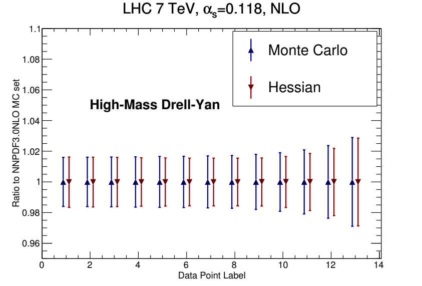
PHENOMENOLOGY

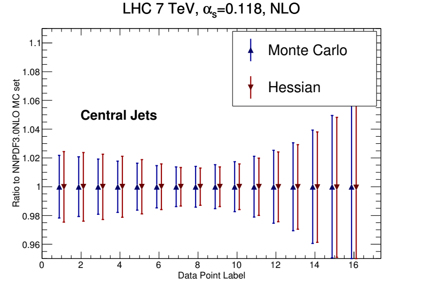
LHC inclusive cross-sections @ 13 TeV



- **Good agreement** for LHC inclusive cross-sections, discrepancies below 10%.

LHC differential distributions @ 7 TeV for NNPDF3.0 NLO





- **Very good agreement** for a large number of differential distributions at the LHC 7 TeV, differences always below 10%.

DELIVERY

- The `mc2hessian` program is public available at

  `github.com/scarrazza/mc2hessian`

- Further **optimizations** in progress before final release.
- NNPDF3.0 Hessian version available in `LHAPDF6` soon:
  - `NNPDF30_nlo_as_0118_hessian`
  - `NNPDF30_nnlo_as_0118_hessian`
- Any other MC set can be converted using directly the public code.

Questions?