Machine Learning in HEP-TH

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Introduction

- What is ML in HEP-TH physics?
- The status of ML in HEP-TH.
- The most relevant applications.

What is ML in HEP-TH physics?

Today's landscape can be grouped into 2 levels:

Level-0: computational techniques and tools

- Advanced numerical methods and applications
- MC event generators
- Higher orders
- Computer algebra techniques

These are the most popular computational HEP-TH physics topics which may include modern ML techniques on top of advanced computational physics.

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Level-0 examples:

- MC output storage e.g. ntuples development (see Maitre's talk),
- Subtraction schemes (see Liu's talk),
- Numerical methods-techniques for N-loop integrals (Freitas et al.'s talks),
- ... and many other applications, see talks in Track 3

What is ML in HEP-TH physics?

However we talking about ML in *sensu stricto* we obtain a second group

Level-1: application of ML modern techniques (alla ICML)

- Regression and classification (supervised learning)
- Techniques for uncertainty propagation and combination
- Experimental mathematics using ML optimization

Usually Level-1 is closer to HEP-EXP applications ($\Rightarrow$ requires data input).

Easy to find hybrid projects covering experimental and theoretical physics.

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Some Level-1 examples:

- ***Regression, NN models, reweighting:*** Parton distribution functions, fragmentation functions, Monte Carlo tunes (NNPDF arXiv:1612.01551, arXiv:1706.07049, arXiv:1605.06515)
- ***Classification:*** Deep CNN jet discrimination (Komiske et al. arXiv:1612.01551)
- ***Uncertainty estimation-combination:*** PDF4LHC15 tools, higher-order uncertainty modeling (PDF4LHC et al. arXiv:1612.01551, SC arXiv:1704.00471)
- ***Experimental mathematics:*** Multivariate densities and integration (Bendavid arXiv:1707.00028, Likas CPC135, Garrido 9807018)

Case study: the proton structure determination

During the last months the parton distribution function (PDF) community have published innovative results in HEP-TH using ML methods:

- **NNPDF**: (arXiv:1612.01551, 1706.07049, 1605.06515)
  - determination of the internal structure of composite particles, e.g. polarized and unpolarized proton and fragmentation functions.
- **PDF4LHC recommendation**: (arXiv:1612.01551, 1504.06459, 1504.06736)
  - PDF combination
  - PDF information optimization/compression

In the next slides we show a quick overview of recent developments.

Outline

1. NNPDF methodology
2. PDF4LHC tools for LHC Run II

   (Butterworth et al., arXiv:1510.03865)
3. CMC-PDFs

   (S.C. et al., arXiv:1504.06459)
4. MC2H & Meta PDFs

   (S.C. et al., arXiv:1504.06736)
5. SMPDF

   (S.C., Forte, Kassabov, Rojo, arXiv:1601.00005)
6. Summary

NNPDF methodology

Why ML in PDFs determination?

- **PDFs** are **essential** for a **realistic computation** of hadronic particle physics **observable**, σ, thanks to the factorization theorem, e.g. in *pp* collider:

$$\underbrace{\sigma_X(s, M_X^2)}_{Y} = \sum_{a,b} \int_{x_{\min}}^{1} dx_1 dx_2 \; \underbrace{\hat{\sigma}_{a,b}(x_1, x_2, s, M_X^2)}_{X} \; f_a(x_1, M_X^2) f_b(x_2, M_X^2),$$

  where the elementary **hard cross-section** $\hat{\sigma}$ is convoluted with f the **PDF**.
- **PDFs** are **not calculable**: reflect non-perturbative physics of confinement
- **PDFs** are **extracted** by comparing theoretical predictions to real data
- $f_i(x_1, M_X^2)$ is the PDF of parton i carrying a fraction of momentum x at scale $M \Rightarrow$ needs to be learned from data.

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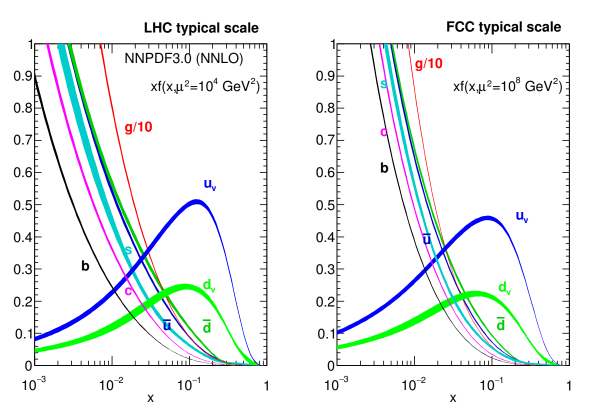
- $f_i(x_1, M_X^2)$ is the PDF of parton i carrying a fraction of momentum x at scale $M \Rightarrow$ needs to be learned from data.

- Constraints come in the form of convolutions:

$$X \otimes f \to Y$$

- Experimental data points is ~4000 → not a big data problem
- Data from several process and experiments over the past decades $\Rightarrow$ deal with data inconsistencies

Why ML in PDFs determination?



- PDF determination requires a sensible estimate of the **uncertainty**
- Not a well researched topic in ML

The NNPDF methodology

The NNPDF (Neural Networks PDF) implements the Monte Carlo approach to the determination of a global PDF fit. We propose to:

1. **reduce** all sources of **theoretical bias**:
   - no fixed functional form
   - possibility to reproduce non-Gaussian behavior

   ⇒ use Neural Networks instead of polynomials
2. provide a sensible estimate of the **uncertainty**:
   - uncertainties from input experimental data
   - minimization inefficiencies and degenerate minima
   - theoretical uncertainties

   ⇒ use MC artificial replicas from data, training with a GA minimizer
3. Test the setup through **closure tests**

The NNPDF methodology

Parametrization, minimization and stopping:

- **Neural Network** parametrization (MLP 2-5-3-1, sigmoids-linear)

  $$f_i(x, Q_0) = A \cdot x^{\alpha}(1-x)^{\beta} NN(x, \log x)$$

  x8 independent PDFs ⇒ 296 free parameters

- Minimization driven by a **genetic algorithm**

  $$\chi^2 = \sum_{ij} (D_i - O_i)\sigma^{-1}_{i,j}(D_j - O_j)$$

  where D_i is exp. measure, O_i the prediction, σ the covariance matrix

  - does not require the gradient evaluation
  - good performance with complex analytic behaviour

- Optimization controlled by **training/validation method**

  - long training of 30000 iterations
  - Select minimum of the validation set as the parameters for the replica

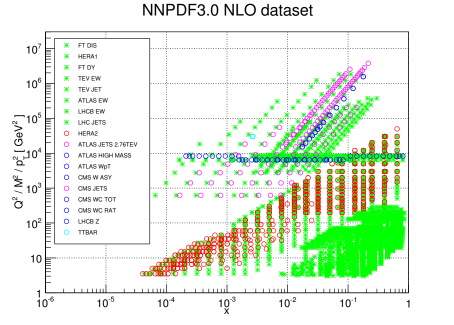
The NNPDF methodology

Uncertainty estimation, pseudodata replicas:

- Generate artificial Monte Carlo data replicas from experimental data:
- we perform O(1000) fits, sampling pseudodata replicas

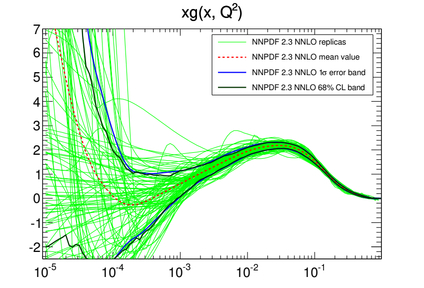
$$D_i^{(r)} \to D_i^{(r)} + \mathrm{chol}(\Sigma)_{i,j}\mathcal{N}(0,1), \quad i,j = 1..N_{\mathrm{dat}},\ r = 1...N_{\mathrm{rep}}$$

We obtain N_{rep} PDF replicas, no assumptions at all about the Gaussianity of the errors.



The NNPDF methodology

The procedure delivers a **Monte Carlo** representation of results:



The central value of observables based on PDFs are obtained with:

$$\langle \mathcal{O}[f] \rangle = \frac{1}{N_{\mathrm{rep}}} \sum_{k=1}^{N_{\mathrm{rep}}} \mathcal{O}[f_k]$$

Phenomenological implications will be presented in the parallel section.

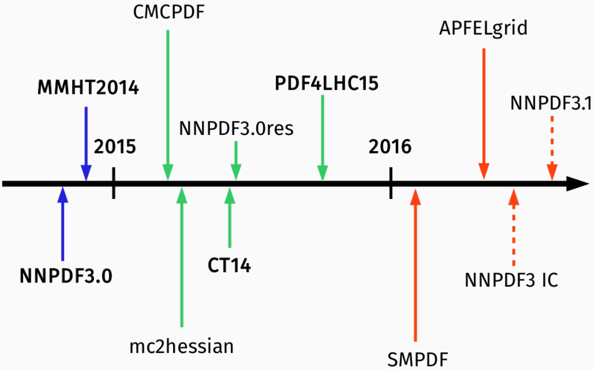
PDF4LHC tools for LHC Run II

(Butterworth et al., arXiv:1510.03865)

PDF releases and new tools

PDF tools for the PDF4LHC15:

- CMC-PDFs: compression algorithm for MC PDFs.
- mc2hessian: MC to hessian conversion tool for PDFs.
- SMPDF: Specialized Minimal PDFs.



Introduction

Challenge

Determine the **best combined PDF uncertainty** from **individual PDF sets**.

From 2010, the PDF4LHC WG released recommendations, updated several times to include newer versions and bug fixes.

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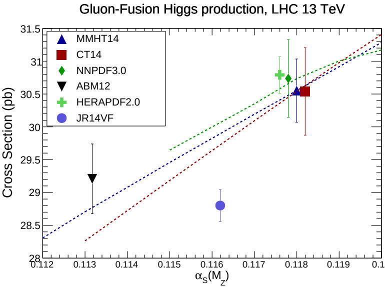
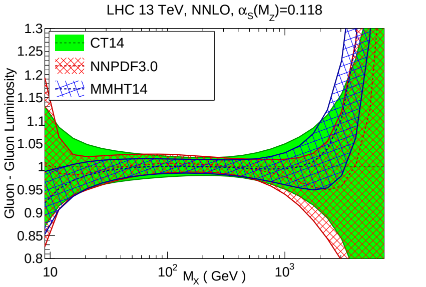
Towards the PDF4LHC15 recommendation

In 2014/2015 MMHT, CT and NNPDF **improve significantly agreement** due to new data, better theory treatment and better understanding of fitting issues.



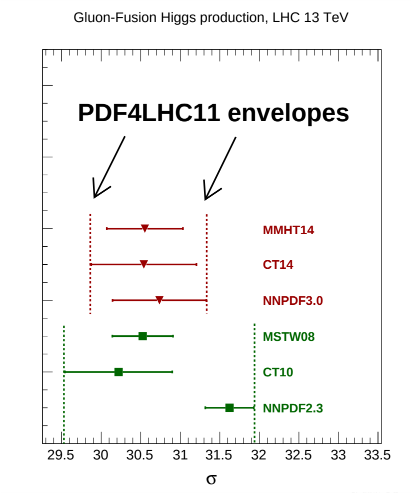


PDF4LHC recommendations

PDF4LHC11 recommendation

1. Use MSTW, CT and NNPDF PDFs
2. Take the **envelope** of uncertainties as uncertainty

- agreement was not so good, e.g. *ggH* cross section uncertainty was >2x the given by any individual set.
- over-conservative: **no proper statistical meaning**



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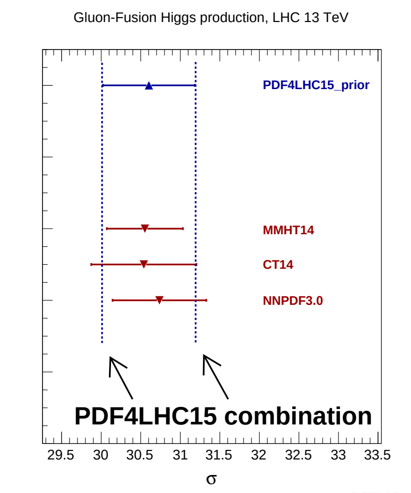
PDF4LHC15 possibility

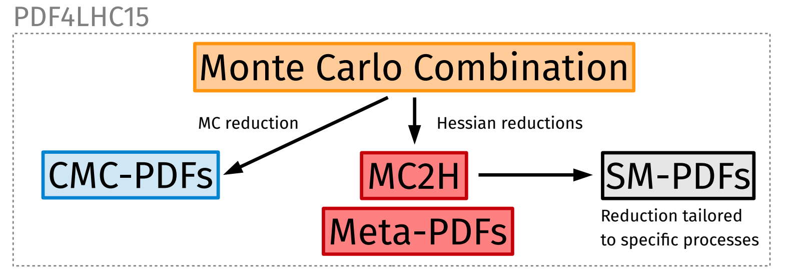
- Provide a clear **statistical interpretation**
- Deliver MC & Hessian **representations**



The PDF4LHC15 strategy

The new PDF4LHC15 prescription

1. Construct a **Monte Carlo combined** set from global PDF determinations
   - sets entering into the combination must satisfy requirements, e.g.: global datasets, use the GM-VFNS, α_s set to the PDG average.
2. Reduce **redundant information**
3. Deliver a single combined PDF set - either **Monte Carlo** or **Hessian** form.



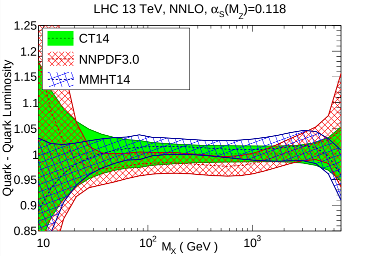
Monte Carlo combination

The combination strategy

We select the PDF sets that enter the combination

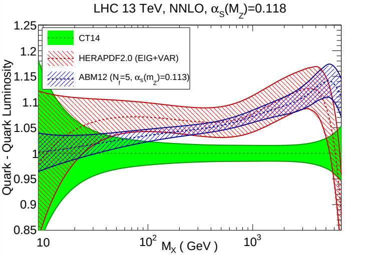
⇒ must be **reasonably consistent** among them.

Global sets:



- Sets are compatible.
- Good candidate for combination.

Non global + global sets:



- Clear incompatibility.
- Little data, different evolution, characterization of uncertainty.

The PDF4LHC15 implementation

The combined sets are based on a statistical combination of:

PDF4LHC15_prior: CT14, MMHT2014 and NNPDF3.0 (MC set, $N_{rep} = 900$)

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Reduced sets:

PDF4LHC15_*_mc: A compressed Monte Carlo set with $N_{rep} = 100$.
(*CMC-PDFs approach*, *arXiv:1504.06469*)

PDF4LHC15_*_100: A symmetric Hessian set with $N_{eig} = 100$.
(*MC2H approach*, *arXiv:1505.06736*)

PDF4LHC15_*_30: A symmetric Hessian set with $N_{eig} = 30$.
(*Meta-PDF approach*, *arXiv:1404.0013*)

Monte Carlo: contains **non-Gaussian** features important for **searches** at high masses (high x).

Hessian: useful for many experimental needs and when using **nuisance** parameters. 100 eigenvectors when **optimal precision** is needed.

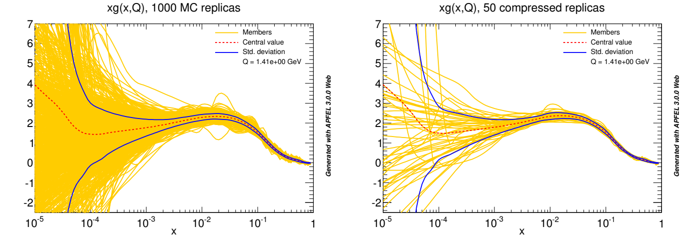
CMC-PDFs

(S.C. et al., arXiv:1504.06459)

The compression idea

Compression idea:

Reduce the size of a PDF set of Monte Carlo replicas with no/minimal **loss of information**, e.g.:



Problem: Preserve as much as possible *the underlying statistical distribution* of the prior MC PDF set.

- avoid bias in the extrapolation region.
- conserve physical requirements, e.g. positivity, correlations, etc.

The compression strategy

We define statistical estimator for the MC prior set:

1. **moments:** central value, variance, skewness and kurtosis
2. **statistical distance:** the Kolmogorov distance
3. **correlations:** between flavors at multiple x points

The compression strategy

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2. **statistical distance:** the Kolmogorov distance
3. **correlations:** between flavors at multiple *x* points

These estimators are them **compared** to subsets of replicas **interactively** driven by an *error function*, i.e.:

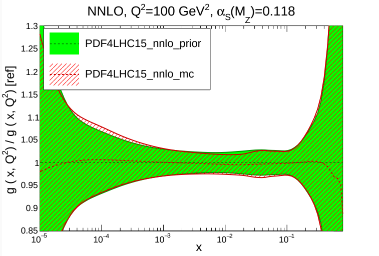
$$\mathrm{ERF} = \sum_k \frac{1}{N_k} \sum_i \left(\frac{C_i^{(k)} - O_i^{(k)}}{O_i^{(k)}} \right)^2$$

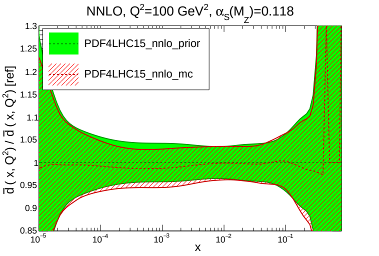
where k runs over the number of statistical estimators and

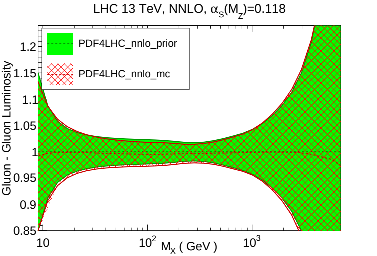
- N_k is a normalization factor extracted from random realizations
- $O_i^{(k)}$ is the value of the estimator for the prior
- $C_i^{(k)}$ is the corresponding value for the compressed set

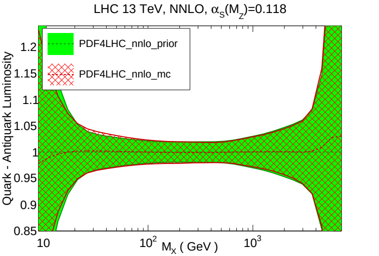
CMC-PDFs (aka PDF4LHC15_*_mc)

Good agreement between the **PDF4LHC15_prior** and **CMC-PDFs** from a number of compressed replicas $N_{rep} > 50$, e.g.:



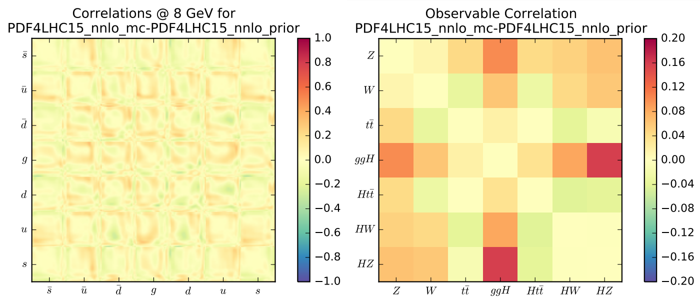






CMC-PDFs (aka PDF4LHC15_*_mc)

Reasonable agreement as well for the **correlations** between different PDF flavours and inclusive cross-sections.



A similar number of replicas from each of the three sets is automatically selected by the compression algorithm
⇒NNPDF3.0: 23 replicas; CT14: 36 replicas, MMHT14: 32 replicas

MC2H & Meta PDFs

(S.C. et al., arXiv:1504.06736)

Hessian representations

mc²hessian

Problem addressed here:

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

MC2H Strategy:

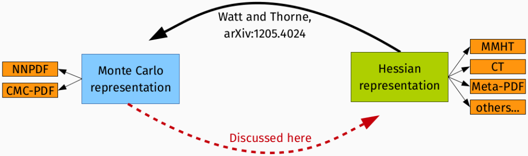
use MC replicas **themselves** as the **basis** of the linear representation.

use **Principal Component Analysis** (PCA) to reproduce PDF covariance matrix with arbitrary precision.

Meta-PDF Strategy:

each MC replica is **re-fitted** using a flexible “meta-parametrization”.

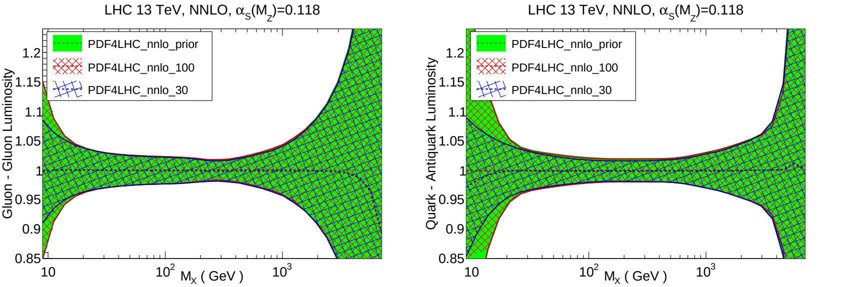
the best constrained combination are found by **diagonalization** of the covariance matrix on the PDF space



MC2H (aka PDF4LHC15_*_100)

A Hessian representation of the PDF4LHC15_prior has been constructed using

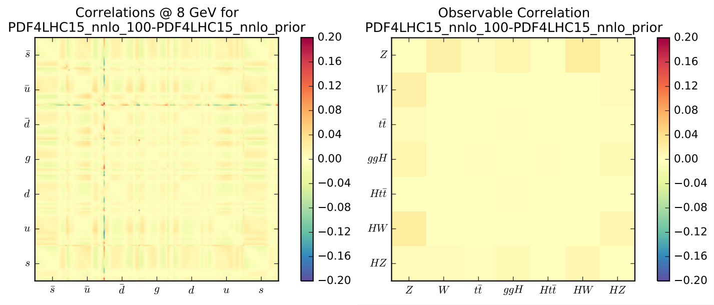
- MC2H ⇒ PDF4LHC15_*_100 with $N_{\mathrm{eig}} = 100$ (high accuracy)
- Meta-PDF ⇒ PDF4LHC15_*_30 with $N_{\mathrm{eig}} = 30$



Excellent level of agreement for PDFs and luminosities as compared with the prior.

MC2H (aka PDF4LHC15_*_100) correlations

Excellent agreement with the prior for PDF correlation and observable correlation.



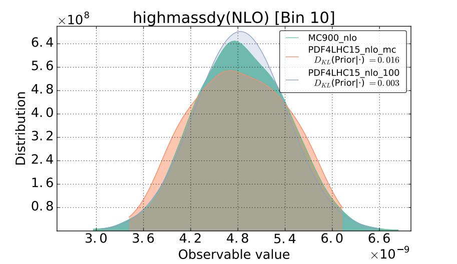
Correlations @ 8 GeV for PDF4LHC15_nnlo_100-PDF4LHC15_nnlo_prior

Observable Correlation PDF4LHC15_nnlo_100-PDF4LHC15_nnlo_prior

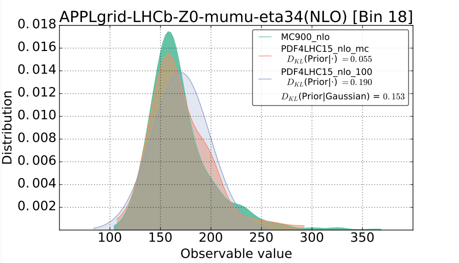
Tiny residual differences at the level of few percent, irrelevant for LHC phenomenology.

Gaussianity of the PDF4LHC15 combinations

MC2H works best for Gaussian bins and when using the results as Gaussian.



CMC works best for non-Gaussian bins, when treating the results as MC.



SMPDF

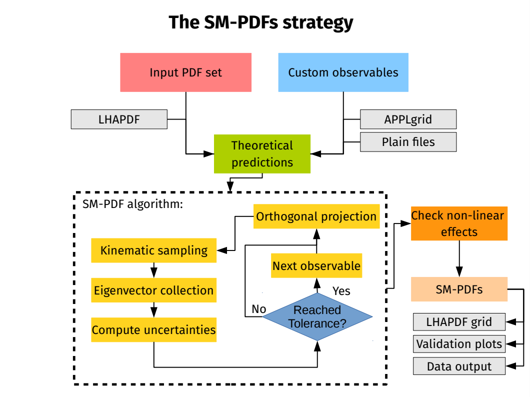
(S.C., Forte, Kassabov, Rojo, arXiv:1601.00005)

Specialized Minimal PDFs

Idea overview

Efficient and accurate PDF **process-specific** PCA Hessian reduction algorithm.

- Prior PDF, list of observables $\Longrightarrow$ Reduced representation (**SMPDF**)



Example cases

We have generated SMPDFs for the most important **Higgs prod. processes**:

Process	PDF4LHC15_prior		NNPDF3.0		MMHT14	
	$T_R = 5\%$	$T_R = 10\%$	$T_R = 5\%$	$T_R = 10\%$	$T_R = 5\%$	$T_R = 10\%$
$gg \to h$	4	5	4	4	3	3
VBF hjj	7	5	10	5	4	3
hW	6	5	6	4	6	3
hZ	11	7	6	4	8	5
$ht\bar{t}$	3	2	4	4	3	2
Total h	15	11	13	8	8	7

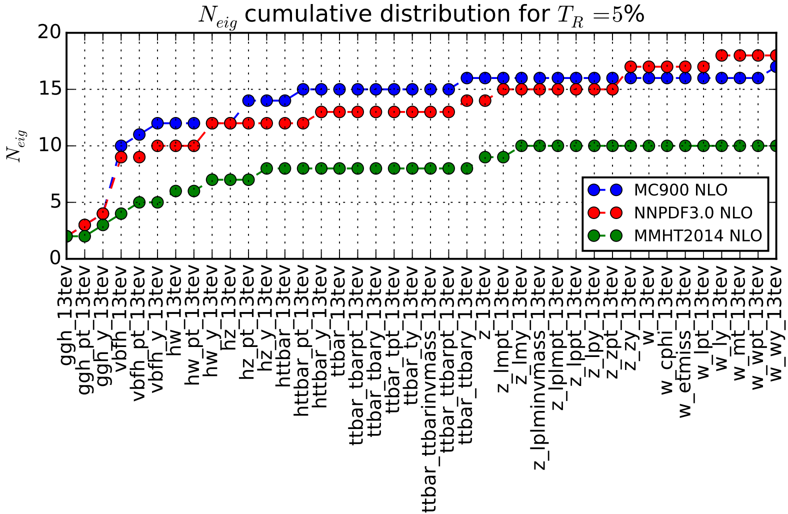
and the **main backgrounds**:

Process	PDF4LHC15_prior		NNPDF3.0		MMHT14	
	$T_R = 5\%$	$T_R = 10\%$	$T_R = 5\%$	$T_R = 10\%$	$T_R = 5\%$	$T_R = 10\%$
h	15	11	13	8	8	7
$t\bar{t}$	4	4	5	4	3	3
W, Z	14	11	13	8	10	9
Ladder	17	14	18	11	10	10

T_R (set by user) is the maximum allowed deviation from the prior for any bin.
⇒ Typical difference is **much smaller**.

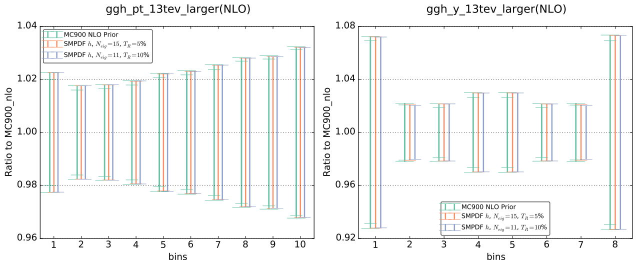
Ladder SMPDF

Multiple processes can be efficiently stacked together.

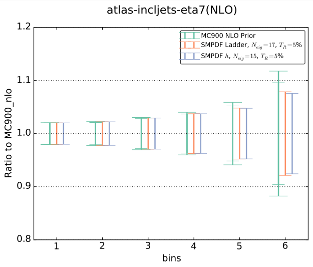


SMPDF stability

Kinematical ranges that double those used as input (p_T^h and y^h)



Breakdown only when going in extreme regions (large $|\eta|$):



Summary

Summary

- Recent ML applications to HEP-TH confirm success.
- Results from the PDF community are encouraging.
  - Unbiased parton structure determinations
  - New ways of combining PDFs.
  - New methods and tools for the reduction of PDF sets are available.
- ***Future developments:***
  - new cutting edge ML methodologies are under investigation, e.g.
    - Deep NN and RNN
    - Reinforcement learning
    - Gradient based methods

Thanks for your attention!

The PDF4LHC15 deliverables

LHAPDF6 grid	Pto.	ErrorType	N_{mem}	$\alpha_S(m_Z^2)$
`PDF4LHC15_(n)nlo_mc`	(N)NLO	`replicas`	100	0.118
`PDF4LHC15_(n)nlo_100`	(N)NLO	`symmhessian`	100	0.118
`PDF4LHC15_(n)nlo_30`	(N)NLO	`symmhessian`	30	0.118
`PDF4LHC15_(n)nlo_mc_pdfas`	(N)NLO	`replicas+as`	102	mem 0:100→0.118 mem 101→0.1165 mem 102→0.1195
`PDF4LHC15_(n)nlo_100_pdfas`	(N)NLO	`symmhessian+as`	102	mem 0:100→0.118 mem 101→0.1165 mem 102→0.1195
`PDF4LHC15_(n)nlo_30_pdfas`	(N)NLO	`symmhessian+as`	32	mem 0:30→0.118 mem 31→0.1165 mem 32→0.1195
`PDF4LHC15_(n)nlo_asvar`	(N)NLO	-	1	mem 0→0.1165 mem 1→0.1195

Table 1: Summary of the combined PDF4LHC15 sets with $n_f^{\max} = 5$.

The PDF4LHC15 deliverables

LHAPDF6 grid	Pto.	ErrorType	N_{mem}	$\alpha_S^{(n_f=5)}(m_Z^2)$
PDF4LHC15_nlo_nf4_100	NLO	symmhessian	100	0.118
PDF4LHC15_nlo_nf4_30	NLO	symmhessian	30	0.118
PDF4LHC15_nlo_nf4_100_pdfas	NLO	symmhessian+as	102	mem 0:100→0.118
				mem 101→0.1165
				mem 102→0.1195
PDF4LHC15_nlo_nf4_30_pdfas	NLO	symmhessian+as	32	mem 0:30→0.118
				mem 31→0.1165
				mem 32→0.1195
PDF4LHC15_nlo_nf4_asvar	NLO	-	1	mem 0→0.1165
				mem 1→0.1195

Table 2: Summary of the combined PDF4LHC15 in the $n_f = 4$.

Monte Carlo combination

The combination strategy

1. We select the PDF sets that enter the combination
   ⇒ must be **reasonably consistent** among them.
2. **Transform** the Hessian PDF sets into their **Monte Carlo representation** (Watt and Thorne '12):

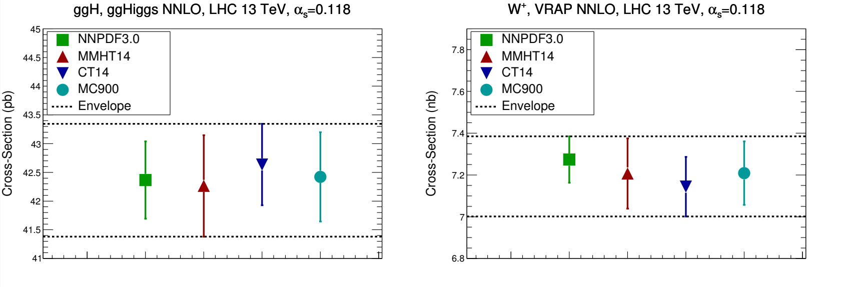
$$F^k = F(q_0) + \frac{1}{2}\sum_{j=1}^{N_{eig}} \left[F(q_j^+) - F(q_j^-)\right] R_j^k, \quad k = 1, \ldots, N_{\mathrm{rep}}$$

3. **Combine** the same number of replicas from each of the prior sets, assuming **equal weight** in the combination (i.e. an unweighted set).

PDF4LHC15: we combine $N_{rep} = 300$ replicas from NNPDF3.0, CT14 and MMHT2014, however any **other choice is possible**.

Monte Carlo combination

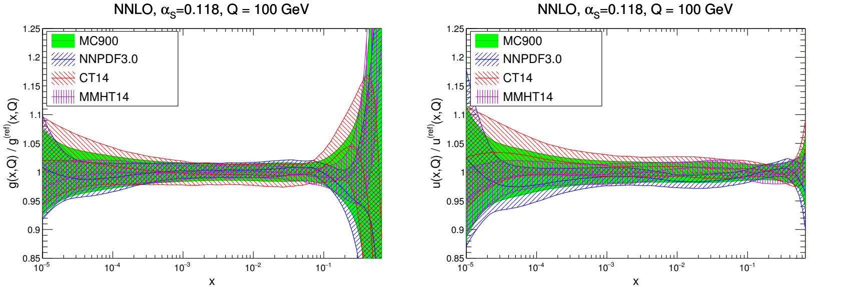
The resulting combined Monte Carlo set has **statistical properties** which lead to **smaller uncertainties** than the PDF4LHC11 envelope.



Proper treatment of **outliers** ⇒ the envelope gives more weight to **outliers**.

Monte Carlo combination

PDF4LHC15_prior 900 MC replicas required to **stabilize** the combination.



Issues before the development of reduction strategies:

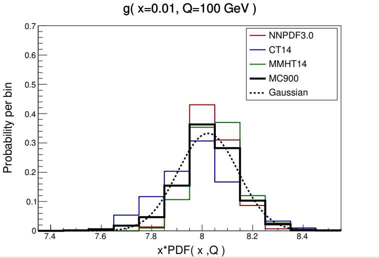
- too many replicas for practical applications ($N_{rep} = 900$)
- no possible Hessian representation
- no reduced way to preserve non-Gaussian features

Monte Carlo combination

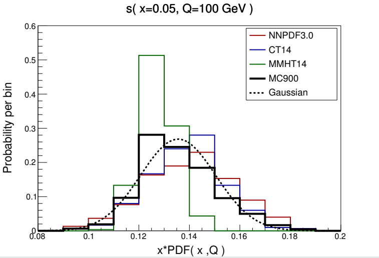
The MC combination is usually **Gaussian** but in many cases **non-Gaussian features** are observed.

Particular important for **BSM searches**, which rely on PDFs in regions where PDF errors are large.

Gaussian



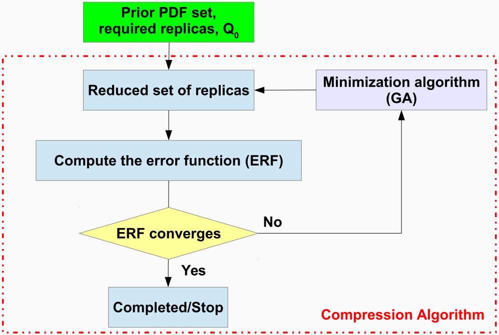
Non-Gaussian



The compression strategy

The algorithm **selects replicas** from the prior that minimize the **error function**. The minimization is driven by a **genetic algorithm**.

Validation: estimators, PDF plots, theoretical predictions, distances, χ^2 to experimental data, etc.

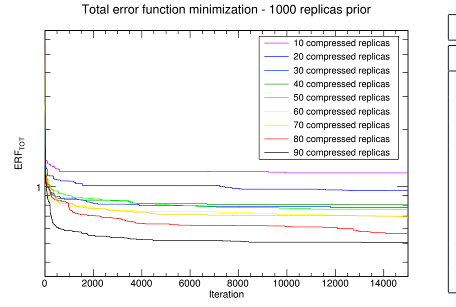


Prior PDF set, required replicas, Q_0
Reduced set of replicas
Minimization algorithm (GA)
Compute the error function (ERF)
ERF converges
No
Yes
Completed/Stop
Compression Algorithm

The compression strategy

Test case:

Example of ERF minimization for $N_{rep} = 1000$ from NNPDF3.0 NLO.



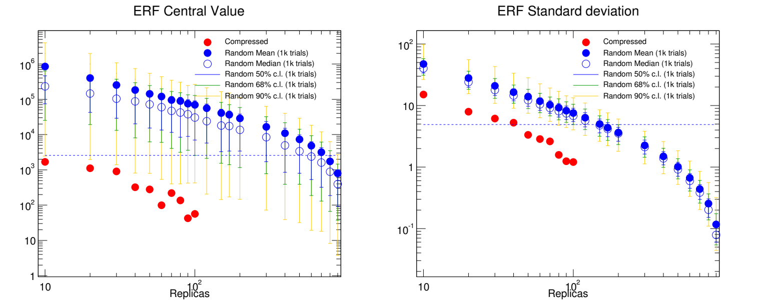
compressor v1.0.0	
GA Parameters	
$N_{\rm gen}^{\rm max}$	15000
$N_{\rm mut}$	5
$N_{\rm x}$	70
$x_{\rm min}$	10^{-5}
$x_{\rm max}$	0.9
n_f	7
Q_0	user-defined
$N_{\rm x}^{\rm corr}$	5
$N_{\rm rand}$	1000

- The algorithm reaches the stability plateau after 2k iterations.
- Large prior of MC replicas ⇒ increases possible combinations.

The compression strategy

Moment estimators for the **compression** and **random selections**.

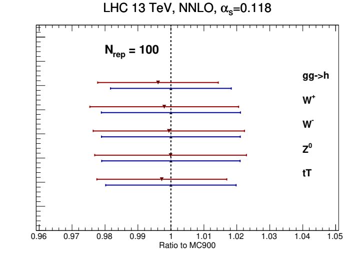
- horizontal lines ⇒ lower 68% c.l. for random selection with $N_{rep} = 100$

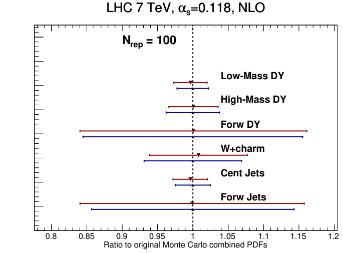


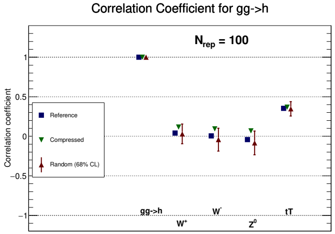
- Substantial **improvements** as compared to random selections.
- Compression is able to successfully reproduce **higher moments** and **correlations**.
- In this test case $N_{rep} = 50$ are equivalent to MC fits with 100 replicas.

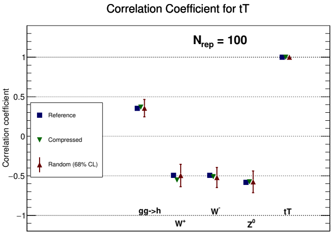
LHC Phenomenology

CMC-PDFs also validated for LHC inclusive cross-sections and differential distributions, including correlations.


LHC 13 TeV, NNLO, α_s=0.118

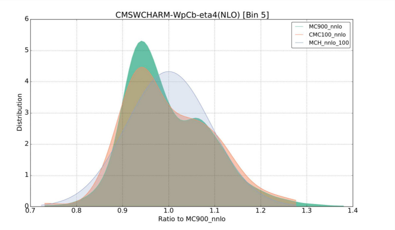

LHC 7 TeV, α_s=0.118, NLO

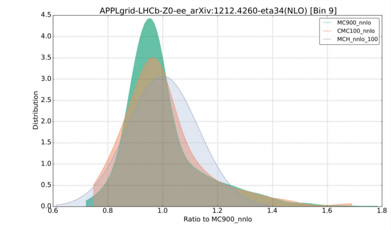

Correlation Coefficient for gg->h


Correlation Coefficient for tT

Non-Gaussian features in LHC cross-sections

Non-Gaussian features are also clearly observed at the level of LHC processes, e.g. most forward bin of the CMS W+charm differential cross-section measurement and DY measurement from LHCb.





Hessian reduction fails by construction when reproducing such features.

However, in regions where the **Gaussian approximation** is reasonable, one should use a Hessian representation.

General strategy

1. Given a Monte Carlo prior set of PDFs

$$\{f^{(k)}_{\alpha,\mathrm{mc}}\}_{k=1,\dots,N_{\mathrm{rep}}}\,, \quad \alpha = \{g,u,d,s,\dots\}\,,$$

2. Fix the central value to be the same as the prior:

$$f^{(0)}_{\alpha,\mathrm{hessian}} = f^{(0)}_{\alpha,\mathrm{mc}}$$

3. We define the matrix for the deviations wrt central value:

$$X_{lk}(Q) \equiv f^{(k)}_{\alpha,\mathrm{mc}}(x_i,Q) - f^{(0)}_{\alpha}(x_i,Q), \quad l \equiv N_x(\alpha-1)+i$$

4. The covariance matrix is given in terms of X:

$$\mathrm{cov}^{\mathrm{pdf}}_{\mathrm{ij},\alpha\beta}(Q) \equiv \frac{1}{N_{\mathrm{rep}}-1}XX^t$$

General strategy

SVD

A diagonal representation of the covariance matrix in terms of replicas is found by SVD of the matrix X:

$$X = USV^t,$$

V is an orthogonal $N_{\mathrm{rep}} \times N_{\mathrm{rep}}$ matrix of coefficients, and

$$XV,$$

provides a representation of the multigaussian covariance matrix in terms of the original replicas.

PCA Reduction

Many eigenvectors lead to a very small contribution to the covariance matrix $\Rightarrow$ we can select a smaller set of N_{eig}, with largest eigenvalues, which still provides a good approximation to the covariance matrix.

General strategy

The PCA optimization retains the principal components, i.e. the largest singular values.

- U, S are replaced by their submatrices u, s respectively.
    - $\dim u = N_x N_f \times N_{\rm eig}$ and $\dim s = N_{\rm eig} \times N_{\rm rep}$
- Only the $N_{\rm rep} \times N_{\rm eig}$ orthogonal upper left submatrix of V contributes
- This is the principal submatrix P of V:

$$P_{ki} = V_{ki}, \quad k = 1, \ldots N_{\rm rep}; i = 1, \ldots, N_{\rm eig}$$

General strategy

The PCA optimization retains the principal components, i.e. the largest singular values.

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    - $\dim u = N_x N_f \times N_{\mathrm{eig}}$ and $\dim s = N_{\mathrm{eig}} \times N_{\mathrm{rep}}$
- Only the $N_{\mathrm{rep}} \times N_{\mathrm{eig}}$ orthogonal upper left submatrix of V contributes
- This is the principal submatrix P of V:

$$P_{ki} = V_{ki}, \quad k = 1, \ldots N_{\mathrm{rep}}; i = 1, \ldots, N_{\mathrm{eig}}$$

Thus we write the Hessian eigenvectors as a linear combination of replicas:

$$\begin{aligned} f^{(i)}_{\alpha,\mathrm{hessian}}(x_j, Q) &= f^{(0)}_{\alpha}(x_j, Q) + X_{lk} P_{ki}, \qquad l \equiv N_x(\alpha - 1) + j \\ &= f^{(0)}_{\alpha}(x_j, Q) + \sum_{k=1}^{N_{\mathrm{rep}}} a^{(i)}_k \left(f^{(k)}_{\alpha,mc}(x_j, Q) - f^{(0)}_{\alpha}(x_j, Q) \right) \end{aligned}$$

Note the $a^{(i)}_k$ independence in (x, Q). It takes care of evolution automatically.

Robustness and gaussianity of the PDF4LHC15 combinations

Idea

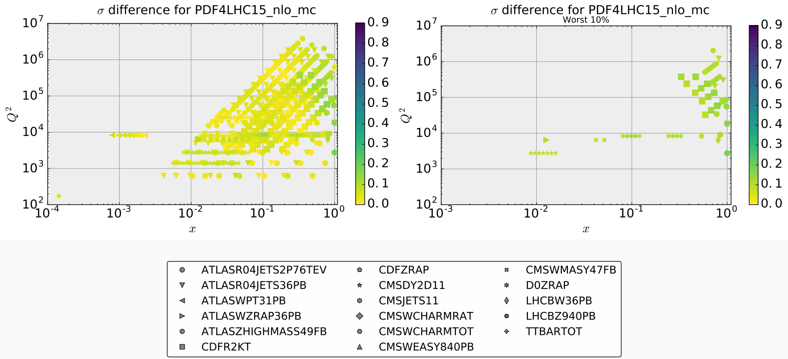
Test the **accuracy** and **Gaussianity** of the PDF4LHC15 sets.

- Verify the range of validity of prediction using data included in PDF fits.
- Discriminate Gaussianity of predictions ⇒ verify MC vs Hessian representations.

Results elaborated for the Les Houches 2015 proceedings.

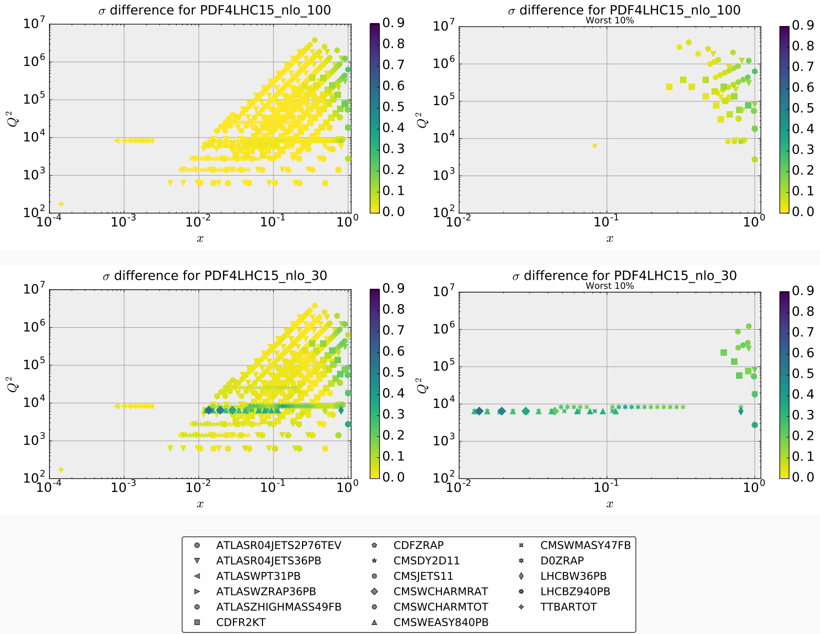
Robustness of the PDF4LHC15 combinations

We have computed predictions with **PDF4LHC15_prior** and the three reduced sets, for all data hadronic data included in the NNPDF3.0 dataset.



Deviations are generally small, and concentrated in regions in which experimental information is scarce and PDF uncertainties are largest ⇒ large x and large Q.

Robustness of the PDF4LHC15 combinations



σ difference for PDF4LHC15_nlo_100

σ difference for PDF4LHC15_nlo_100
Worst 10%

σ difference for PDF4LHC15_nlo_30

σ difference for PDF4LHC15_nlo_30
Worst 10%

Gaussianity of the PDF4LHC15 combinations

In order to estimate the gaussianity of predictions we construct a continuous probability density from a Monte Carlo sample (Kernel Density Estimate):

$$P(\sigma_i) = \frac{1}{N_{\mathrm{rep}}} \sum_{k=1}^{N_{\mathrm{rep}}} K(\sigma_i - \sigma_i^{(k)}), \quad i = 1, \ldots, N_{\mathrm{dat}}$$

We use the Kullback-Leibler divergence to measure how much information we are loosing by approximating the prior $P(\sigma)$ with the distribution spanned form each of the optimized representations $Q(\sigma)$.

$$D_{KL}^{(i)}(P|Q) = \int_{-\infty}^{\infty} \left(P(\sigma_i) \cdot \frac{\log P(\sigma_i)}{\log Q(\sigma_i)} \right) d\sigma_i$$

Gaussianity of the PDF4LHC15 combinations

We use the Kullback-Leibler divergence to measure how much information we are loosing by approximating the prior $P(\sigma)$ with the distribution spanned form each of the optimized representations $Q(\sigma)$.

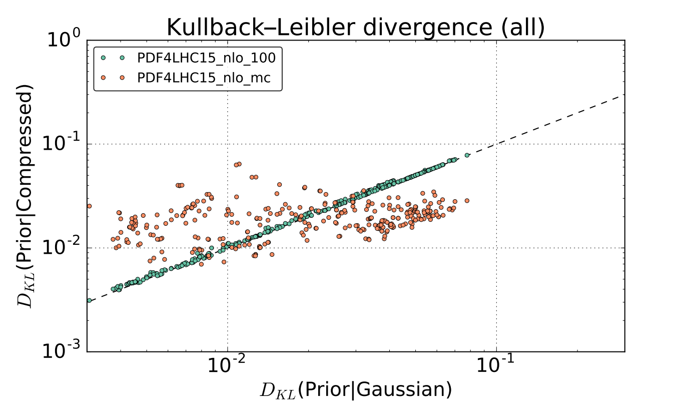
$$D_{KL}^{(i)}(P|Q) = \int_{-\infty}^{\infty} \left(P(\sigma_i) \cdot \frac{\log P(\sigma_i)}{\log Q(\sigma_i)} \right) d\sigma_i$$

We compare the KDE of the prior with

- A Gaussian given by $\mu = \langle \sigma_i \rangle_i$, $\sigma = \frac{1}{N-1}\sqrt{\sum(\sigma_i - \mu)^2}$.
- The MC2H Gaussian.
- The CMC KDE.

Here we have used the SMPDF dataset.

Gaussianity of the PDF4LHC15 combinations

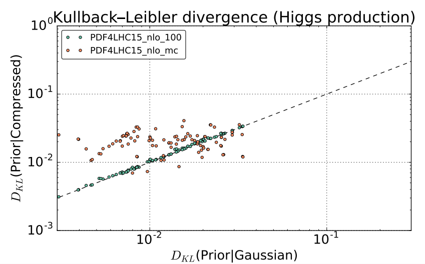


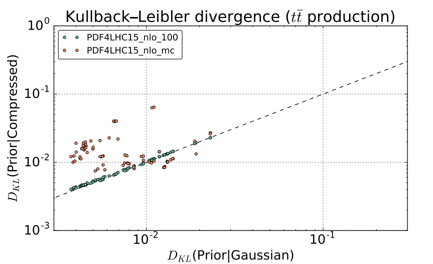
Points in the diagonal ⇒ agrees exactly with the purely Gaussian approx.

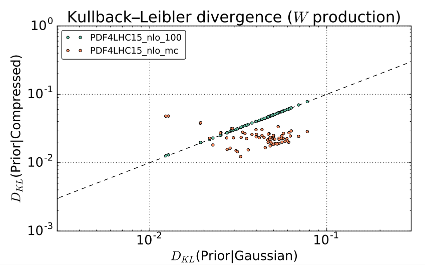
Orange points below diagonal ⇒ CMC better than MC2H

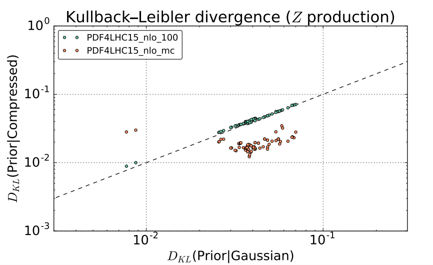
Gaussianity of the PDF4LHC15 combinations

KL divergence process by process:



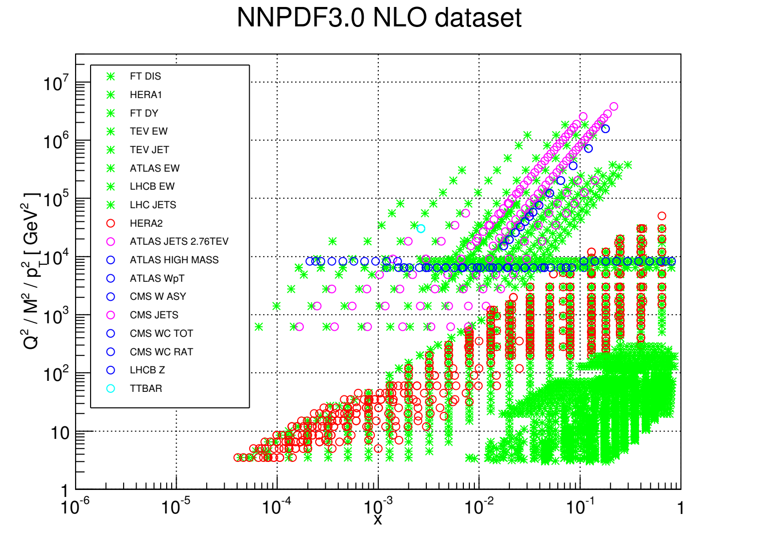






Robustness of the PDF4LHC15 combinations

We have computed predictions with **PDF4LHC15_prior** and the three reduced sets, for all data in the NNPDF3.0 dataset.



SMPDF backup - algorithm strategy

Following the MC2H PCA methodology we can find a subspace with a smaller number of parameters which optimizes the agreement for some quantities.

$$\tilde{X} = XP \in \mathbb{R}^{N_x N_{\mathrm{pdf}}} \times \mathbb{R}^{N_{\mathrm{eig}} \ll N_{\mathrm{rep}}}$$

We can greatly improve the reduction by targeting specific processes:

$$\{\sigma_i\}, \quad i = 1, \ldots, N_\sigma$$

$$s_{\sigma_i} = \left(\frac{1}{N_{\mathrm{rep}} - 1} \sum_{k=1}^{N_{\mathrm{rep}}} \left(\sigma_i^{(k)} - \sigma_i^{(0)} \right)^2 \right)^{\frac{1}{2}}$$

The worst-case accuracy target can be tuned by user:

$$T_R < \max_{i \in (1, N_\sigma)} \left| 1 - \frac{\tilde{s}_{\sigma_i}}{s_{\sigma_i}} \right|$$

This is implemented in an interactive procedure.

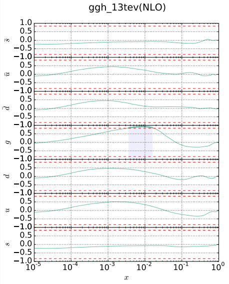
SMPDF backup - selection algorithm

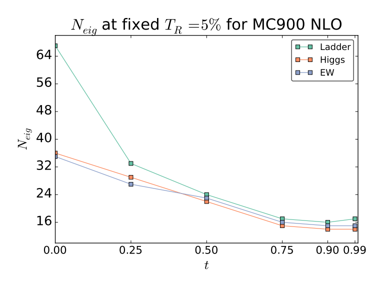
For each iteration, select points in (x, α, Q) correlated with variations in σ

$$\rho(x_i, Q, \alpha, \sigma) = \frac{N_{\mathrm{rep}}}{N_{\mathrm{rep}} - 1} \frac{\langle X(Q_\alpha)_{lk} \cdot (\sigma^{(k)} - \sigma^{(0)}) \rangle_{\mathrm{rep}} - \langle X(Q_\sigma)_{lk} \rangle_{\mathrm{rep}} \cdot \langle \sigma^{(k)} - \sigma^{(0)} \rangle_{\mathrm{rep}}}{s_\alpha^{\mathrm{PDF}} \cdot s_\sigma}$$

$$\Xi = \{(X_i, \alpha) : \rho(X_i, Q_\alpha, \alpha, \sigma) \geq t \cdot \rho_{\max}\}, \quad X \to X_\Xi(Q_\sigma)$$

The correlation threshold t is the only free parameter of the algorithm $\Rightarrow$ $t = 0.9$ optimal choice.





SMPDF backup - orthogonal projection algorithm

This approach allows to efficiently generalize to processes with similar PDF dependence, making the algorithm stable.

We compute the SVD of X_{Ξ} and select **one** eigenvector:

$$X_{\Xi}(Q_{\alpha}) = USV^{t}$$

$$(P \cdot R) = V \in \mathbb{R}^{N_{\mathrm{rep}}} \times \left(\mathbb{R}^{1}\mathbb{R}^{N_{\mathrm{rep}}-1}\right)$$

We project out the selected eigenvector for the next iteration

$$X \to XR$$

We iterate (select more eigenvectors) until we meet the tolerance criteria for the current observable, and move to the next observable, until we reproduce all.

SMPDF backup - APPLgrids

Input cross-sections for SM-PDFs for Higgs physics

process	distribution	grid name	$N_{\rm bins}$	range	kin. cuts
$gg \to h$	incl xsec	`ggh_13tev`	1	-	-
	$d\sigma/dp_t^h$	`ggh_pt_13tev`	10	[0,200] GeV	-
	$d\sigma/dy^h$	`ggh_y_13tev`	10	[-2.5,2.5]	-
VBF hjj	incl xsec	`vbfh_13tev`	1	-	-
	$d\sigma/dp_t^h$	`vbfh_pt_13tev`	5	[0,200] GeV	-
	$d\sigma/dy^h$	`vbfh_y_13tev`	5	[-2.5,2.5]	-
hW	incl xsec	`hw_13tev`	1	-	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma/dp_t^h$	`hw_pt_13tev`	10	[0,200] GeV	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma/dy^h$	`hw_y_13tev`	10	[-2.5,2.5]	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
hZ	incl xsec	`hz_13tev`	1	-	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma/dp_t^h$	`hz_pt_13tev`	10	[0,200] GeV	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma/dy^h$	`hz_y_13tev`	10	[-2.5,2.5]	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
$ht\bar{t}$	incl xsec	`httbar_13tev`	1	-	-
	$d\sigma/dp_t^h$	`httbar_pt_13tev`	10	[0,200] GeV	-
	$d\sigma/dy^h$	`httbar_y_13tev`	10	[-2.5,2.5]	-

SMPDF backup - APPLgrids

Input cross-sections for SM-PDFs for $t\bar{t}$ physics

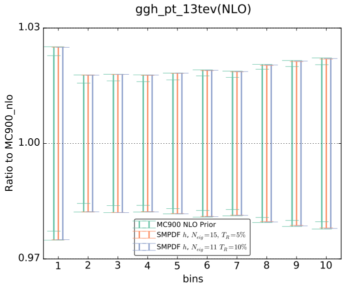
process	distribution	grid name	$N_{\rm bins}$	range	kin. cuts
$t\bar{t}$	incl xsec	`ttbar_13tev`	1	-	-
	$d\sigma/dp_t^{\bar{t}}$	`ttbar_tbarpt_13tev`	10	[40,400] GeV	-
	$d\sigma/dy^{\bar{t}}$	`ttbar_tbary_13tev`	10	[-2.5,2.5]	-
	$d\sigma/dp_t^{t}$	`ttbar_tpt_13tev`	10	[40,400] GeV	-
	$d\sigma/dy^{t}$	`ttbar_ty_13tev`	10	[-2.5,2.5]	-
	$d\sigma/dm^{t\bar{t}}$	`ttbar_ttbarinvmass_13tev`	10	[300,1000]	-
	$d\sigma/dp_t^{t\bar{t}}$	`ttbar_ttbarpt_13tev`	10	[20,200]	-
	$d\sigma/dy^{t\bar{t}}$	`ttbar_ttbary_13tev`	12	[-3,3]	-

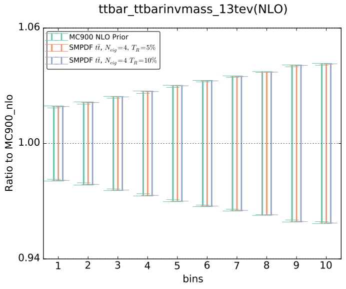
SMPDF backup - APPLgrids

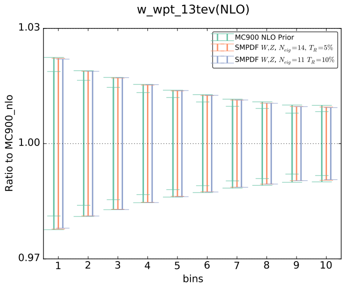
Input cross-sections for SM-PDFs for electroweak boson production physics

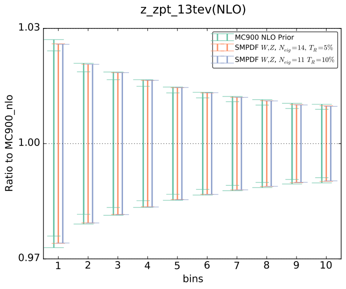
process	distribution	grid name	N_{bins}	range	kin. cuts
Z	incl xsec	`z_13tev`	1	-	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma\,/\,dp_t^{l^-}$	`z_lmpt_13tev`	10	[0,200] GeV	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma\,/\,dy^{l^-}$	`z_lmy_13tev`	10	[-2.5,2.5]	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma\,/\,dp_t^{l^+}$	`z_lppt_13tev`	10	[0,200] GeV	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma\,/\,dy^{l^-}$	`z_lpy_13tev`	10	[-2.5,2.5]	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma\,/\,dp_t^Z$	`z_zpt_13tev`	10	[0,200] GeV	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma\,/\,dy^Z$	`z_zy_13tev`	5	[-4,4]	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma\,/\,dm^{ll}$	`z_lplminvmass_13tev`	10	[50,130] GeV	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma\,/\,dp_t^{ll}$	`z_lplmpt_13tev`	10	[0,200] GeV	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
W	incl xsec	`w_13tev`	1	-	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma\,/\,d\phi$	`w_cphi_13tev`	10	[-1,1]	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma\,/\,dE_t^{\mathrm{miss}}$	`w_etmiss_13tev`	10	[0,200] GeV	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma\,/\,dp_t^l$	`w_lpt_13tev`	10	[0,200] GeV	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma\,/\,dy^l$	`w_ly_13tev`	10	[-2.5,2.5]	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma\,/\,dm_t$	`w_mt_13tev`	10	[0,200] GeV	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma\,/\,dp_t^W$	`w_wpt_13tev`	10	[0,200] GeV	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$
	$d\sigma\,/\,dy^W$	`w_wy_13tev`	10	[-4,4]	$p_T(l) \geq 10$ GeV, $\lvert\eta^l\rvert \leq 2.5$

SMPDF results


ggh_pt_13tev(NLO)
Ratio to MC900_nlo
bins
MC900 NLO Prior
SMPDF h, N_{eig}=15, T_R=5%
SMPDF h, N_{eig}=11 T_R=10%


ttbar_ttbarinvmass_13tev(NLO)
Ratio to MC900_nlo
bins
MC900 NLO Prior
SMPDF $t\bar{t}$, N_{eig}=4, T_R=5%
SMPDF $t\bar{t}$, N_{eig}=4 T_R=10%


w_wpt_13tev(NLO)
Ratio to MC900_nlo
bins
MC900 NLO Prior
SMPDF W,Z, N_{eig}=14, T_R=5%
SMPDF W,Z, N_{eig}=11 T_R=10%


z_zpt_13tev(NLO)
Ratio to MC900_nlo
bins
MC900 NLO Prior
SMPDF W,Z, N_{eig}=14, T_R=5%
SMPDF W,Z, N_{eig}=11 T_R=10%