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TOWARDS THE COMPRESSION OF PARTON DENSITIES THROUGH MACHINE LEARNING ALGORITHMS

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One of the most fascinating challenges in the context of parton density function (PDF) is the determination of the best combined PDF uncertainty from individual PDF sets. Since 2014 multiple methodologies have been developed to achieve this goal. In this proceedings we first summarize the strategy adopted by the PDF4LHC15 recommendation and then, we discuss about a new approach to Monte Carlo PDF compression based on clustering through machine learning algorithms.

The PDF4LHC15 recommendation and tools for LHC Run II In October 2015 the PDF4LHC Working Group released a new set of guidelines for the combination of PDF sets, known as the "PDF4LHC15 recommendation" published in Ref. [1]. This updated recommendation proposes the construction of a combined prior PDF set of Monte Carlo (MC) replicas, where each replica comes from global PDF determinations. The prior set is then compressed to a minimal number of PDF members through reduction algorithms specialized in the removal of information redundancy.

The PDF4LHC15 prior consists in $N_{\rm rep} = 900$ MC replicas from NNPDF3.0 [2], CT14 [3] and MMHT2014 [4]. Eigenvectors from CT14 and MMHT2014 are transformed into MC replicas through the method developed by Watt and Thorne in Ref. [6] and implemented in the `LHAPDF6` [5] library. The PDF sets entering in the current combination satisfy requirements which guarantee the consistency of results: use global datasets, compute theoretical predictions and DGLAP in the GM-VFNS, set α_s to the PDG average [7].

The subsequent step consists in removing the redundant information from the prior set through reduction algorithms. For the PDF4LHC15 recommendation we have used 3 different strategies: CMC-PDF [8], MC2H [9] and Meta-PDF [10]. The CMC-PDF approach outputs a subset of MC replicas which preserves the statistical properties of the prior set. The MC2H strategy provides a symmetric Hessian PDF set obtained by using the MC replicas themselves as the basis of the linear representation in combination with principal component analysis (PCA) to reproduce the PDF covariance matrix with arbitrary precision. The Meta-PDF approach refit each MC replica with a flexible meta-parametrization, from which the best constrained combination are found by diagonalization of the covariance matrix on the PDF space.

The delivery of results in the MC representation is useful when considering regions where predictions are non-Gaussian, such as searches at high-masses and generally wherever the PDF is probed at large x. On the other hand, Hessian sets are useful for many experimental needs, *e.g.* when using nuisance parameters, or when high accuracy is required. The PDF4LHC15 recommendation delivers sets at NLO and NNLO with $n_f = 4, 5$, noted as: `PDF4LHC15_mc`, the compressed Monte Carlo set with $N_{\rm rep} = 100$ obtained with CMC-PDF; `PDF4LHC15_100`, the symmetric Hessian set with $N_{\rm eig} = 100$ obtained with MC2H; `PDF4LHC15_30`, the symmetric Hessian set with $N_{\rm eig} = 30$ obtained with Meta-PDF.

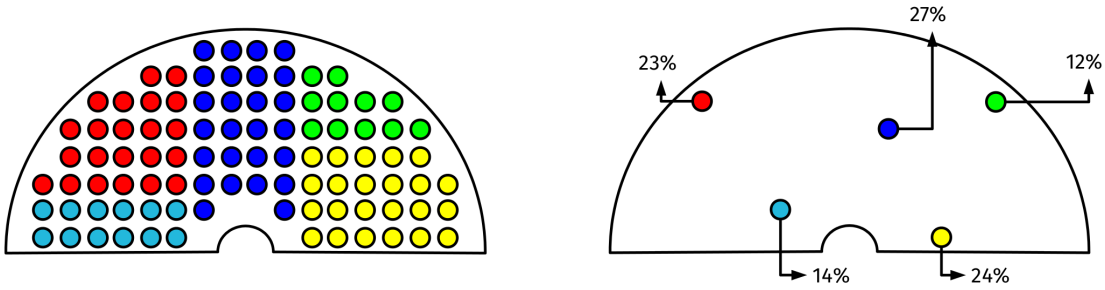

Figure 1 – Illustrative example of the clustering idea. A parliament is composed by several elements (left), for each of them it is possible to determine the most representative exemplars and the fraction of elements similar to them (right).

Finally, thanks to developments for the PDF4LHC15 recommendation, a recent Hessian reduction algorithm called Specialized Minimal PDF (SMPDF) was published in Ref. [11]. The SMPDF methodology constructs PDFs designed to provide an accurate representation of PDF uncertainties for specific processes or classes of processes with a minimal number of PDF error sets.

Monte Carlo PDF compression through machine learning In the next paragraphs we present a new concept of compression approach for MC PDFs based on clustering through machine learning algorithms.

Let us consider a generic PDF set composed by a large number of MC replicas. Starting from a simple visual inspection we observe that groups of replicas have similar shapes, positions and lengths. This observation suggests that in the PDF space there is a limited number of shapes and directions privileged by replicas and so, if we want to reduce the number of members contained in a PDF set we should extract the most important replicas and their respective weights. This observation is illustrated in Figure 1 by the analogy of the politicians and their parties in a parliament which in our case study are identified to PDF replicas. The left plot shows the initial distribution of elements. In this example similar objects are identified by a color, and we have 5 groups. The right plot shows the most representative exemplars of each group and their weight. The next step is to setup a clustering algorithm able to identify the number of groups, the most representative exemplars and their weights.

Here we use Affinity Propagation (AP), by messaging passing algorithm presented in Ref. [12] where the authors show its impressive capability of grouping data with complex structure. The choice of this particular algorithm is motivated by its capability of determining automatically the number of final clusters and its members without requiring as input an *a prior* knowledge or guess of the number of clusters. The only requirement of AP is to set a distance definition to quantify the similarity between elements of a given ensemble of PDF replicas. In the AP approach, we construct a similarity matrix, defined as:

$$S_{i,j} = -d(\ell_i, \ell_j), \tag{1}$$

where $d(\ell_i, \ell_j)$ is the distance estimator defined by the user. We performed the current analysis with the squared euclidean distance between the arc-length of replicas defined as:

$$\ell_k = \sum_{\alpha=-n_f}^{n_f} \int_0^1 \sqrt{1 + \left(\frac{df_\alpha^{(k)}(x,Q)}{dx} \right)^2} dx, \tag{2}$$

where k is the replica index and α runs over the n_f independent PDF flavors at the factorization scale Q. We observed that similar results are also obtained when using just the spatial euclidean distance between replicas.

In Figure 2 we show the results of this clustering procedure for the NNPDF3.0 NLO set with $N_{\rm rep} = 1000$ replicas. The AP algorithm identifies 14 clusters which are represented by different colors for the down (left plot) and strange (right plot) PDFs. The final step consists in computing the weight associated to each cluster center exemplar. For each cluster i we define its associated weight, w_i, as:

$$w_i = N_i/N_{\rm rep}, \quad \sum_i w_i = 1, \tag{3}$$

where N_i is the number of elements contained in the cluster i. The output of this procedure is a MC set of PDFs with $N_{\rm rep} = 14$ MC replicas and a list of $N_{\rm rep}$ weights.

In Figure 3 we compare the central value and its uncertainty for the down and strange PDFs for the NNPDF prior and the compressed set obtained with AP. For the AP PDF set we plot the weighted mean and standard deviation. In general, we observe that a good level of agreement is obtained. Furthermore, in Figure 4 we compare theoretical predictions of both sets for the ATLAS inclusive jets setup with $|\eta| < 0.3$ from Ref. [14] (left plot) and a $t\bar{t}$ rapidity distribution at LHC with $\sqrt{s} = 13$ TeV (right plot). Also in this case, the level of agreement is satisfactory.

Similar results are obtained when using the PDF4LHC prior set. This approach has two advantages in comparison to the CMC-PDF method: the instantaneous computation time, and the possibility to compress to a very lower number of replicas due to the flexibility of weights. We are confident that this or similar approaches based on the idea of weighting MC replicas are the right future direction to obtain fast and outstanding compression performance of MC PDF sets.

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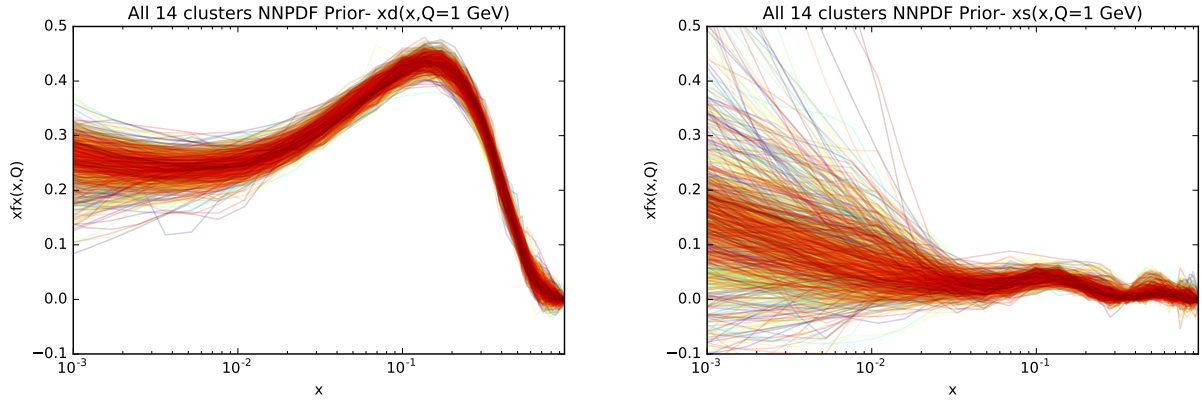

Figure 2 – Examples of clustering of MC replicas using affinity propagation and arc-length distance metrics.

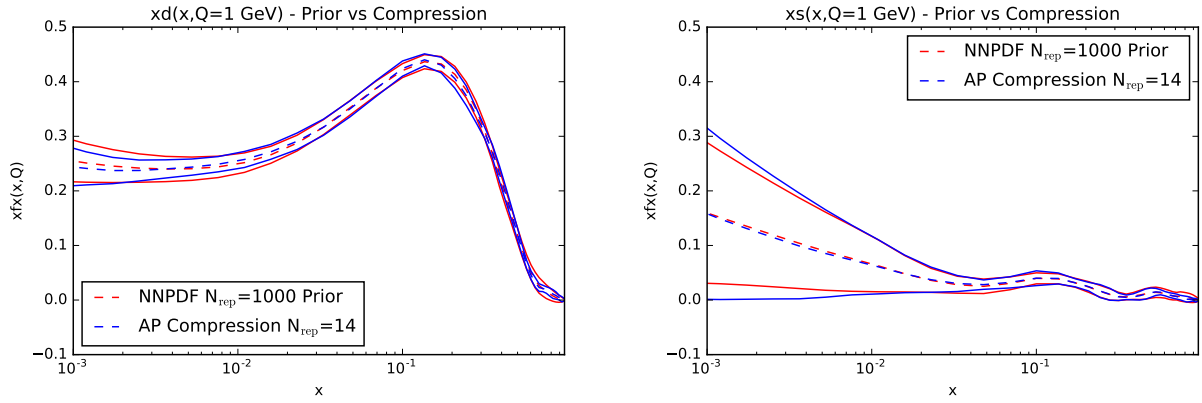

Figure 3 – Comparisons for central values and uncertainties between the prior PDF set and the affinity propagation clustering compression.

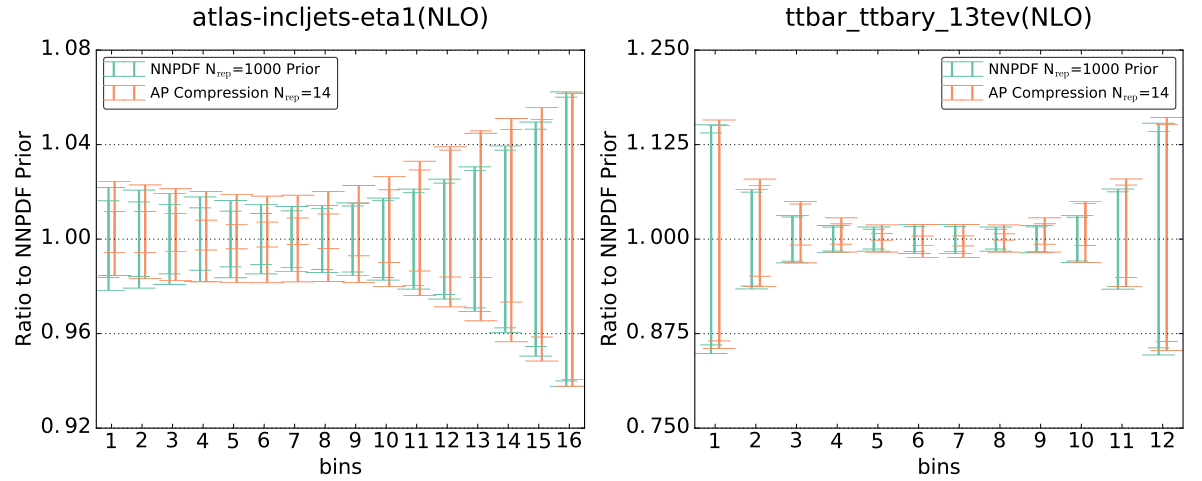

Figure 4 – Comparisons of theoretical predictions for the prior PDF set and the affinity propagation clustering compression sets. Plots obtained with SMPDF.