Response to “Parton distributions need representative sampling”

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Abstract

We respond to the criticism raised by Courtoy et al. [1], in which the faithfulness of the NNPDF4.0 sampling is questioned and an under-estimate of the NNPDF4.0 PDF uncertainties is implied. We list, correct, and clarify in detail a number of inaccurate or misleading claims that are made in Ref. [1]. Specifically, we explain and explicitly demonstrate why the central value of the PDF distribution does not generally coincide with the absolute minimum of the $\chi^2$ to the data. We examine some PDFs that have been constructed in the above study and claimed to be “good solutions”: we show that similar PDFs are found with the NNPDF methodology, but with very low probability.
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1 Introduction

Progress in the understanding and testing of the Standard Model is increasingly relying on precision measurements, which may reveal statistically significant discrepancies between theory and experiment. The increase in luminosity at the LHC, together with results from dedicated experiments, will drive a significant increase in the precision of experimental results. It has been emphasized multiple times that theory predictions need to match the forthcoming experimental precision. A robust framework to estimate the statistical and systematic errors in the determination of PDFs is one of the necessary ingredients in this program.

A recent publication [1] advocates a new technique for sampling in the space of PDFs, or possibly for constructing PDFs. Unfortunately, the statistical foundations of this recipe are unclear and may lead to incorrect conclusions. In what follows, we briefly summarize the challenges involved in the extraction of PDFs, focusing on the statistical formulation, and point out some of the problems with the claims in [1].

The plan of this note is the following: In Sect. 2, after reviewing the meaning of a PDF determination, we summarize how PDFs can be represented by Monte Carlo samples, the way in which the Monte Carlo sample must be constructed, and show that NNPDF4.0 replicas provide a representative sampling. A reader who is familiar with statistics and is mostly interested in the rebuttal can go directly to Sect. 3, where we list and correct a number of misleading or false statements that are made in Ref. [1]. In Sect. 4 we examine some PDFs constructed in [1], we show that PDF replicas having similar features can be obtained with the NNPDF4.0 methodology, but that these PDFs correspond to overlearning, thus have a low probability.

In Appendix A we summarize the closure and future test indicators that have been used in order to validate NNPDF4.0 PDFs, and a metric that can be used to measure overlearning.

2 Statement of the problem

The determination of PDFs from a (necessarily finite) set of data is a classical example of an inverse problem; the functions that we are trying to reconstruct are elements of infinite-dimensional spaces, and hence the problem is clearly under-determined and its solution will depend on the assumptions we make.

Prior and posterior. A Bayesian approach is well suited to tackle these problems: the assumptions we make about the solution are encoded in a prior probability measure in the space of functions. The probability measure is then updated, yielding a so-called posterior distribution, using the available data. Our knowledge about the solution of the inverse problem is encoded in the posterior [2].

In the particular case of PDFs, we are interested in functions $f_k(x)$ where the index $k$ spans the set of PDFs in some chosen basis. For instance in the evolution basis used for NNPDF fits:

$$f_k \in \{V, V_3, V_8, T_3, T_8, T_{15}, \Sigma, g\}$$

(2.1)

We refer to Ref. [3] for a detailed description of the flavor combinations that enter in the evolution basis.

The observables delivered by experiments can be expressed as convolutions of these PDFs with coefficient functions, as dictated by factorization theorems. A simple example of such a convolution is the factorization of the DIS non-singlet structure function, see e.g. Ref. [4]. In the case of a global fit, many observables corresponding to a large number of different processes are combined in order to determine all the PDFs in the basis in Eq. (2.1). Note that PDFs are defined, and can be extracted from data, only within a well-defined theoretical framework (e.g. using perturbative QCD in a given scheme and at a given order of perturbation theory). These choices, together with any of the theoretical assumptions such as integrability, positivity and sum rules, determine the prior for the probability measure.

Some parametrization for the functions $f_k$ needs to be chosen, so that the problem can be cast in terms of a finite number of parameters. This is broadly accepted by all collaborations that perform PDFs fits, albeit with different choices of the parametrization. Henceforth the finite-dimensional space of parametrized functions is denoted by $\mathcal{F}$. In the NNPDF approach, the parton distributions are parametrized using a single fully connected deep neural network, so that the set of parameters corresponds to the thresholds and weights of the network as explained in Ref. [3]. The set of parameters is traditionally denoted as $\theta$.

Bayes theorem allows us to write the posterior probability, given a dataset $D$:

$$p(\theta|D, \mathcal{H}) \propto p(D|\theta, \mathcal{H})p(\theta|\mathcal{H}),$$

(2.2)
where $p(\theta|\mathcal{H})$ is the prior probability distribution, i.e. the probability distribution in the space of parametrized functions before being given any experimental results. The prior probability encodes all the theoretical knowledge about the PDFs, as discussed above, and depends on the hyperparameters $\mathcal{H}$ of the neural networks.

**Monte Carlo representation of the posterior.** It is customary to approximate the posterior probability distribution by its mode

$$\theta^* = \arg \max_{\theta} p(\theta|D, \mathcal{H}), \quad (2.3)$$

called the MAP (Maximum A Posteriori) estimator, complemented with the fluctuations of the MAP estimator induced by the fluctuations in the data. As explained since the very early publications [5], the posterior distribution in the NNPDF approach is constructed by a Monte Carlo sampling procedure. An ensemble of artificial data $D^{(k)}$, called replicas, is generated, which reproduce the statistical distribution of the experimental data. For each replica, the MAP estimator is evaluated, which yields an ensemble of replicas of sets of parameters $\theta^{(k)}$. It is important to note that in Eq. (2.2), the first factor is the likelihood,

$$p(D^{(k)}|\theta, \mathcal{H}), \quad (2.4)$$

which is related as usual to the $\chi^2$ of the artificial data generated for that given replica – a quantity that we will consistently denote $\chi^2(k)$. This should not be confused with the $\chi^2$ of that replica to the central data, that we will consistently denote as $\chi^2(k,c)$.

Eqs. (2.2,2.3) show that the quantity that is maximized when computing the MAP estimator is the posterior probability, which also includes the prior distribution for the PDFs. Each fitted replica is the mode of the posterior distribution for an instance of the data that is generated with the probability distribution dictated by the experimental uncertainties. In this way, the probability distribution of the data induces the probability distribution of the parameters $\theta$ and through the Monte Carlo sampling procedure, it generates a sample of the posterior distribution. In order to propagate the distribution correctly, each replica in the ensemble must have the same statistical weight. Indeed, it has been shown analytically that this procedure yields the correct posterior distribution in the case of linear fits to Gaussian data [6], so that the expectation value of a generic function $O(\theta)$ of the parameters $\theta$ can be computed as

$$\int d\theta p(\theta|F, \mathcal{H}) O(\theta) = \frac{1}{n_{\text{rep}}} \sum_{k=1}^{n_{\text{rep}}} O(\theta^{(k)}), \quad \text{for} \quad n_{\text{rep}} \to \infty. \quad (2.5)$$

The important points to keep in mind are:

1. each PDF replica is obtained as the mode of the posterior distribution given one sample of the distribution of data;
2. the posterior distribution is the product of the likelihood times the prior – not just the likelihood;
3. each replica has the same statistical weight;
4. the $\chi^2$ of a replica to the central value of the experimental data is not a measure of the posterior probability of that replica, since the contribution of the prior is missing;
5. outliers in the distribution of fitted replicas are typically good fits to some unlikely fluctuation of the data.

**Regularization.** It is important to understand that even though each replica is obtained by optimizing $\chi^2(k)$, it does not correspond to the absolute minimum of this quantity. Indeed, this absolute minimum generally corresponds to an overfitted or overlearned solution. An overfitted solution is a solution that does not generalize correctly the information contained in the specific instance of the data. This means that, rather than fitting the true underlying law, it fits particular features of the input data set or of the specific data instance (such as a random statistical fluctuation). In the NNPDF methodology, such overfitting is avoided through carefully constructed regularization methods.

First, before performing the final fit, the methodology is hyperoptimized [7] through a K-folding algorithm [8], that guarantees that choices related to the minimization algorithm are not tuned to the specific
Figure 2.1. The NNPDF4.0 PDF replicas (1000 replica sample) in the $\sigma_Z - \sigma_H$ plane (referred to as ZH in the main text). The two, three and four $\sigma$ contours are shown.

datasets, thereby guaranteeing that the specific datasets are not overfitted. Then, during the fitting itself, by using a cross-validation algorithm, in which the minimization process is stopped before reaching the absolute minimum using a training/validation split of the data. Specifically, the minimization algorithm only receives as input the training part of the data, while the validation part of the data is used as a control set. The final result of a fit corresponds to the instance with lowest $\chi^2$ as defined with respect to the validation part of the data. This ensure that any noise present in the data is not inferred by the neural network. The training set (which in NNPDF4.0 [3] is taken to be a random set of 75% of the points per dataset) is used to build the likelihood function. The hyperoptimized methodology then employs a gradient-descent-based algorithm to take (for each replica) the path that maximizes the posterior probability. Note that the settings of this algorithm are determined through the hyperoptimization itself. Note also that the algorithm partly depends on a random state that changes on a replica-by-replica basis. The fit is stopped when the validation $\chi^2$ stops improving, regardless of the value of the training $\chi^2$.

A number of tests of the robustness of the procedure have been performed extensively by NNPDF: namely closure tests [6, 9] that check sampling in the data region and future tests [10] that check sampling in the extrapolation region. These tests are briefly reviewed in Appendix A.

We illustrate the outcome of this procedure when correctly implemented by showing probability contours for the final replica distribution from the NNPDF4.0 [11] PDF determination. Of course, a PDF set is a set of functions, so confidence levels for it should be shown in a space of functions [2], which is difficult to visualize. We can instead consider a projection of the PDF on a finite dimensional space. In order to make contact with the discussion in the following Sections, we choose a two-dimensional space of LHC cross sections, that of the Z and Higgs total production cross section (ZH plane, henceforth), a choice that is also made in Ref. [1]. This is a useful choice in that the Higgs cross section is gluon driven and the Z cross section is quark-driven: so points in the ZH plane can be interpreted in terms of the size of the quark and gluon luminosities. Cross sections are computed as in [3]. In particular, partonic cross sections accurate to next-to-leading order (NLO) in the strong coupling are convoluted with PDFs accurate to next-to-next-to-leading order (NNLO). A center-of-mass energy of 14 TeV is assumed, and cross sections are integrated in the fiducial phase space specified in Sect. 9.2 of [3]. Contours in this plane provide a test of the fact that the PDFs are correctly sampled, given that the cross sections depend on several different combinations of PDFs, evolved to the appropriate scale and convoluted over $x$ with hard cross sections.

In Fig. 2.1 we show the results for 1000 NNPDF4.0 PDF replicas in the ZH plane, along with two, three and four $\sigma$ contours.

The replicas are distributed as expected given that the underlying distribution of the experimental uncertainties is Gaussian and it is expected (and has explicitly shown [12]) to lead to a Gaussian distribution of physical predictions. Indeed, more replicas are concentrated at the center and less in the tails, with no local distortions or clusters. For example, the two dimensional three $\sigma$ contour corresponds to a 98.9% confidence level, so one would expect 11 NNPDF4.0 replicas outside the three $\sigma$ contour, to be compared to 14 found in Fig. 2.1 in good agreement with the expected value. This result displays no evidence for
sampling bias in the NNPDF4.0 replica sample and instead confirms that the replica sample is representative of the probability distribution in the ZH plane.

3 Inaccurate or misleading claims

In this section we discuss a number of misleading, inaccurate or false claims that are made in Ref. [1]. These claims may suggest that the PDF uncertainty on key LHC cross sections obtained with the NNPDF4.0 PDF sets is underestimated.

First, we list individual claims and comment on them one by one. Then, we discuss and correct a misconception on the meaning of the $\chi^2$ figure of merit that appears to underlie much of the discussion in Ref. [1].

• In Section II it is stated that “analyses that fit a large number of flexible functions using a modest number of fitted replicas might fail at finding all possible solutions due to a sampling bias”. It is then stated that “dense sampling of a high-dimensional volume requires an exponentially growing number $N_p$ of replicas, such as $2^{N_{par}} \sim 10^{30}$ for $N_{par} = 100$”.

This is misleading, as it suggests that a similar number of replicas is needed for sets of PDFs. As discussed in Sect. 2, PDF fitting is an example of an inverse problem: the aim is to find a posterior probability of $f$ given the data $D$. In the NNPDF approach, the MC ensemble is not a random sampling, but rather an importance sampling of the PDF space $F$. As a result the number of replicas needed to obtain a faithful representation in the PDF space does not require an exponentially growing number of replicas. A replica sample with $n_{\text{rep}} \sim 1000$ is sufficiently large to reproduce the correlations of the experimental data to per-cent accuracy and to determine the the same accuracy. Note that this well-known fact is at the basis of the PDF4LHC15 [13] and PDF4LHC21 [14] combinations, and its correctness has been verified a posteriori several times in the construction of these sets, e.g. by checking that samples of replicas of this size accurately represent prior underlying sets of Hessian PDFs [15, 16]. For example, even with PDF sets with a relatively small number of parameters such as CT18 or MSHT20, if the number of replicas required in order to obtain a faithful representation did scale as $2^{N_{par}}$, then a number of replicas of order $10^9 - 10^{10}$ would be required for a faithful representation, instead of the 300 used and shown to be adequate for the PDF4LHC combinations. Conversely, most information contained in a replica sample can be represented with a small number of Hessian parameters regardless of the size of the sample [17] suggesting a larger sample does not add significantly more information.

• In Section III it is stated that the NNPDF4.0 publication [3] “interchangeably uses two forms of $\chi^2$ as the figure-of-merit, called “$t_0$” and “exp”, which differ in implementation of experimental systematic uncertainties.”

This statement is false. The only figure of merit used by NNPDF for minimization is the $\chi^2_{t_0}$. This figure of merit, used for minimization since the first NNPDF global set [18] is designed to avoid significant multiplicative uncertainties.

The $t_0$ covariance matrix is then defined as

$$
(cov_{t_0})_{ij} = \delta_{ij} \sigma_i^{(\text{uncorr})} \sigma_j^{(\text{uncorr})} + \sum_{m=1}^{N_{\text{norm}}} \sigma_{i,m}^{(\text{norm})} \sigma_{j,m}^{(\text{norm})} + \sum_{l=1}^{N_{\text{corr}}} \sigma_{i,l}^{(\text{corr})} \sigma_{j,l}^{(\text{corr})} \delta_{ij} D_i D_j,
$$

(3.1)

where the indices $i,j$ label the datapoints, $\sigma_i^{(\text{uncorr})}$ are the uncorrelated uncertainties obtained by adding the uncorrelated systematic uncertainties and statistical uncertainties in quadrature, $m$ runs over the $N_{\text{norm}}$ multiplicative normalization uncertainties, $\sigma_{i,m}^{(\text{norm})}$, and $l$ runs over the $N_{\text{corr}}$ other correlated systematic uncertainties, $\sigma_{i,l}^{(\text{corr})}$. Finally, $D_i$ are the measured central values.
where $T_i^{(0)}$ is a theoretical prediction for the $i$-th data point evaluated using a $t_0$ input PDF.

In the $t_0$ method [18], PDFs are determined by optimizing

$$
\chi^2_{t_0} = \sum_{i,j} N_{\text{dat}} (T_i - D_i) (\text{cov}_{t_0}^{-1})_{ij} (T_j - D_j).
$$

(3.3)

This leads to a set of PDFs that is then used to iteratively compute the theoretical predictions $T_i^{(0)}$ that are needed for the construction of a new $t_0$ covariance matrix, which is then used for a new PDF determination. This procedure is iterated until convergence.

Note that all PDF determinations use similar procedures for the treatment of multiplicative uncertainties, since, as mentioned, if the experimental $\chi^2$ were used for minimization, biased results would be obtained. The $\chi^2$ definitions used by different groups in order to avoid the D’Agostini bias were benchmarked in Ref. [20], where in particular it was shown that the $t_0$ definition is entirely equivalent to that used by the CT and MSTW groups.

The experimental $\chi^2$, which is obtained using the experimental covariance matrix $\text{cov}_{\text{exp}}$ of Eq. (3.1) instead of $\text{cov}_{t_0}$ of Eq. (3.2) in the definition of Eq. (3.3) is never used by NNPDF for fitting. It is only quoted for the sake of comparison to $\chi^2$ values computed and quoted by experimental collaborations.

Hence, any value of the experimental $\chi^2$, such as those displayed in Figs. 2, 5 and 6 of Ref. [1], is meaningless if the purpose is to discuss fit quality, given that this is not the figure of merit that is used for PDF determination. Specifically, it is meaningless if the goal is to show that there exists PDF combinations that display a better $\chi^2$ than the one obtained in the NNPDF4.0 fit. In the sequel, when referring to $\chi^2$ values we will always mean the $t_0 \chi^2$.

- In Section III it is stated that “Each replica fit achieves a good $\chi^2$ with respect to its fluctuated data set, while practically all MC replicas have a very high $\chi^2$ (by hundreds of units) with respect to the published (unfluctuated) data values. The individual MC PDFs are thus poor fits to the published (unfluctuated) data set – but their average (called the ”central replica”, or ”replica 0”) agrees with the unfluctuated data much better.”

This statement is misleading, in that it suggests that the quality of the fit of PDF replicas to the central unfluctuated data is a relevant measure of their fit quality. This is incorrect. Each PDF replica is determined through a fit to its data replica and therefore the fluctuations of the fits truly reflect the fluctuations in the PDFs induced by the fluctuations in the data.

- In Section III.D it is stated that “in the current NNPDF procedure, small data sets may acquire a larger effective $\chi^2$ weight, because during the cross validation the small data sets may be included in their entirety in the fitted sample and not divided between the fitted and control samples. The resulting PDFs are then biased toward the smaller data sets.”

The statement is false. As clearly stated in Ref. [3] (see Section 3.2.4) for all datasets (regardless of whether large or small) 75% of data enters the training set. In NNPDF4.0, the training fraction was increased from the value 50% used in previous NNPDF determinations based on the observation that the dataset analyzed in the NNPDF4.0 fit is so wide that, even with just 25% validation, overlearning does not occur. This observation was backed up by the closure test studies performed in Ref. [6] and an explicit check using the $R_O$ metric of Eq. (B.2).

Finally, a clear misconception emerges in [1], which leads to various confusing or wrong statements. Recall that in the NNPDF approach, the central PDF is obtained as the expected value, i.e. as the average over the replica sample. It is sometimes also referred to as replica 0 (because this is how it is delivered through the LHAPDF6 interface [21]). We denote the $\chi^2$ of this mean, replica 0 PDF to the central data as $\chi^2_{0,c}$. The misconception is that $\chi^2_{0,c}$ should be the absolute minimum of $\chi^2$. This is incorrect for several reasons that we recall here:

- As already mentioned, in order to avoid overfitting each PDF replica, $f^{(k)}$, to the corresponding data replica, $D^{(k)}$, an early stopping procedure is implemented. Hence a PDF replica does not correspond to the absolute minimum of $\chi^2^{(k)}$. Likewise, it is easy to construct PDFs that provide an overfit to central data, such as the PDF shown in Fig. 3.7 of Ref. [3]. These correspond to a lower value of $\chi^2$ than the average of the replica sample.
Whatever the value of the average obtained from a given sample, there always exists any number of PDFs with lower values, trivially because the average of any given replica sample is just an instance of a probability distribution. There will be an instance of the distribution that corresponds to the minimum of the $\chi^2$ for the given distribution, but the probability of sampling exactly this instance is of course zero. These PDFs will be indistinguishable from the ones that are provided within PDF uncertainties.

As already explained, NNPDF replicas are constructed as fits to data replicas, i.e. by minimizing $\chi^2(k)$, which is clearly not the same as $\chi^2(k, c)$, where the latter measures the agreement to central data. This means that $\chi^2(k, c)$ should have a probability distribution, that depends on the likelihood of individual data replicas. Hence, in particular, for a large enough replica sample there will always exist increasingly unlikely data replicas, leading to correspondingly unlikely PDF replicas, with arbitrarily high $\chi^2(k, c)$. Conversely, some of them will be in the opposite tail of the distribution, such that their $\chi^2(k, c)$ is lower than $\chi^2(0, c)$. This is illustrated in Fig. 3.1, where we show the values of $\chi^2(k, c)$ of each replica $k$ plotted in a frequency histograms with the $\chi^2$ of the central PDF marked as a vertical line. Results are shown for a sample of 1000 (red) and 3000 (blue) replicas. It is clear that for a large enough number of replicas there are some that have a value of $\chi^2$ smaller than that of the average.

4 The hopscotch PDFs

The main result presented in Ref. [1] is the construction of a set of PDFs by the so-called hopscotch (HS) method. We first summarize the construction of these PDFs, then their possible interpretation, and finally state some questions that they may raise. We then present the answer to these questions.

The HS PDFs are constructed as follows: first, the Hessian version of the NNPDF4.0 is used. This Hessian version has been constructed [3] using the mc2hessian [22] code, which determines a multigaussian projection of the probability distribution obtained from a given replica sample with a desired number of Hessian eigenvectors by sampling the replica probability distribution, performing a singular value decomposition of the result, and retaining the eigenvectors with largest eigenvalues. The set delivered in Ref. [3] contains 50 eigenvectors, which is sufficient to guarantee percent-level accuracy on the PDFs. Then, new PDFs are sought for by moving along each Hessian eigenvector direction, monitoring the $\chi^2$ value, and specifically looking for the lowest $\chi^2$ configurations. These HS PDFs thus correspond to first, taking PDFs that correspond to one-σ deviations from the center of the given NNPDF4.0 replica sample, and then performing linear combinations of them. Hence, they can be thought of as linear combinations of NNPDF4.0 replicas — though strictly speaking the PDFs of which they are linear combinations are not NNPDF4.0 replicas, but rather Hessian PDFs constructed out of the replica distribution. Note that these HS PDFs are not a part of an ensemble of replicas and must therefore considered as isolated PDF instances. Indeed, as correctly stated in Ref. [16], replicas are only useful as an ensemble.

Several of these HS PDFs are constructed by looking at and minimizing the experimental $\chi^2_{exp}$. As discussed in Sect 3, $\chi^2_{exp}$ is never used as a figure of merit for PDF minimization, by either NNPDF or other fitting group, since its minimization would lead to PDFs affected by d’Agostini bias. Hence the HS PDFs
constructed by looking at this figure of merit are devoid of interest or significance and we will ignore them: they only confuse the relevant issues.

Further HS PDFs are instead constructed looking at and minimizing the $t_0$ $\chi^2$ (that we are consistently denoting as $\chi^2$ for short) and we discuss them now. Specifically, these PDFs are constructed by minimizing $\chi^2(k,c)$, namely the $\chi^2$ to central data — unlike NNPDF4.0 replicas that are determined minimizing $\chi^2(k)$, the $\chi^2$ to a data replica. Note that here the index $k$ merely numbers the HS PDFs, which as already stated are not an ensemble of replicas, but rather isolated PDF instances. Fig. 4.1 show the 300 HS PDFs that have values of $\chi^2(k,c)$ comparable or lower than $\chi^2(0,c)$, the value of the central NNPDF4.0 PDF: $\chi^2(k,c) \lesssim \chi^2(0,c)$. They are shown in the ZH plane, superposed to the set of 1000 NNPDF4.0 replicas of Fig. 2.1.

It is manifest that whereas the NNPDF4.0 replicas provide a representative sampling of the underlying probability distribution, the HS PDFs instead are mostly cluster along one line in the ZH plane. These HS PDFs generally have large values of the Higgs cross section, and a large number of them, denoted by red points in Fig. 4.1, fall outside the three $\sigma$ interval for $\sigma_H$ is denoted by two vertical bands, and the HS PDFs that falls outside it are shown in red.

Figure 4.1. Same ad Fig. 2.1, but now also including a set of 300 HS PDFs with $\chi^2$ values similar to that of the NNPDF4.0 central value, $\chi^2(k,c) \lesssim \chi^2(0,c)$ (orange and red points). The three $\sigma$ interval for $\sigma_H$ is denoted by two vertical bands, and the HS PDFs that falls outside it are shown in red.
clarify this point we study the following two questions:

1. Does the NNPDF4.0 methodology have difficulties in producing PDF replicas that look like the HS PDFs, and specifically that have large values of the Higgs cross-section, specifically outside the three $\sigma$ interval and with $\sigma_H$ bigger or much bigger than the mean? Or is there perhaps some reason (such as, for instance, an excessive stiffness for some reason built in the NNPDF4.0 methodology) that prevents such PDFs being obtained, so that e.g. there is a “hard wall” along the $\sigma_H$ axis, so that the NNPDF4.0 methodology cannot produce replicas with sufficiently large Higgs cross-section?

2. If instead the NNPDF4.0 methodology can produce replicas with large $\sigma_H$, and/or replicas that look like the HS PDFs, why are these replicas so unlikely, despite having $\chi^2(k, c) \sim \chi^2(0, c)$? As discussed in Sect. 2, there is nothing wrong with a PDF being unlikely despite having a low $\chi^2(k, c)$, because the posterior distribution is the product of the likelihood times the prior, so a PDF could have high likelihood yet low prior probability. However, this then begs the question, why is the prior probability for these replicas so low?

We now address these two questions in turn, in two dedicated subsections. Specifically we show that

1. the NNPDF4.0 fitting methodology has no difficulty in producing replicas that look like the HS PDFs and/or PDFs leading to the largest values of $\sigma_H$ of the HS PDFs;

2. the HS PDFs have low likelihood because they correspond to overfitted solutions.

### 4.1 NNPDF4.0 replicas reproducing the HS PDFs

Fig. 4.1 shows that NNPDF4.0 predicts a multigaussian distribution in the ZH plane. Therefore, one expects that in order to get an arbitrarily large number of PDF replicas in any given region (specifically with large $\sigma_H$) it is sufficient to increase the number of replicas by a sufficiently large amount. Yet it could be that this is not the case and that something makes it more difficult for the NNPDF4.0 methodology to produce PDFs with large values of the Higgs cross-section. We can test whether this is the case in various ways.

As a first test, we recall that NNPDF4.0 replicas are fitted to data replicas by minimizing $\chi^2(k)$. If for the NNPDF4.0 methodology it is more difficult to fit replicas in the rightmost region of the ZH plane, then we should see a correlation between the value of $\chi^2(k)$ and the position of the replica in the ZH plane.

![Figure 4.2. Scatter plot of the training (left) and validation (right) values of $\chi^2(k)$ for NNPDF4.0 replicas in the $\sigma_H - \sigma_Z$ plane. The value of $\chi^2(k)$ is shown as a color code.](image)

The values of $\chi^2(k)$ for both the training and validation data for the NNPDF4.0 replicas are shown in Fig. 4.2. It is clear that there is no visible correlation between the position in the ZH plane, specifically the position along the $\sigma_H$ axis, and the value of the $\chi^2(k)$. In fact, the fit quality of each PDF replica to its data replica is similar, and essentially independent of the position in the ZH plane. This means that outlier replicas are fitted equally well as replicas close to the center of the distribution. Outlier replicas simply correspond to unlikely data fluctuations. The NNPDF4.0 methodology has no difficulties in fitting PDFs that correspond to large (or small) values of the Higgs (or Z) cross-section.
As a second test, we check explicitly that we can fit the HS PDFs if we assume them to be the underlying truth. To this purpose, we have performed a level-0 closure test [9]. The closure test procedure is summarized in Appendix A. Level-0 means that we have generated data with zero uncertainty, assuming a given underlying true PDF, and then fitted these data. Because the data are fitted at zero uncertainty, the fit can obtain vanishing $\chi^2$. We have picked as an underlying true PDF the HS PDF that gives the largest Higgs cross-section. We have then fitted 100 PDF replicas to it, with standard methodology (including training-validation split). We find $\langle \chi^2(k) \rangle_{\text{tr}} = 0.03 \pm 0.01$, $\langle \chi^2(k) \rangle_{\text{val}} = 0.04 \pm 0.02$, so indeed we reach a near-perfect fit. A scatter plot of results in the ZH plane is shown in Fig. 4.3. It is clear that even though all the fits are equally good and fit the data perfectly (with zero uncertainty) there is still a distribution of results, due to the fact that of course the data do not determine the PDF completely. Each replica can be thought of as a different equally good interpolation of the given data, distributed in the ZH plane. Several of these results have values of $\sigma_H$ that are in fact larger than the input underlying truth. So there is surely no “hard wall”, and we must conclude that the NNPDF4.0 methodology has no difficulty in producing replicas with large Higgs cross section and/or of fitting the HS PDF exactly.
4.2 The HS PDFs and overfitting

Having shown that the NNPDF4.0 methodology has no particular difficulty in fitting the HS PDF, we now address the question of why these PDFs are unlikely in the NNPDF methodology.

As a preliminary observation, we note that, given the extremely flexible NNPDF parametrization (with about 800 free parameters), it is very easy to obtain fits with a value of $\chi^2(0,c)$ that is much lower than that of the reference NNPDF4.0 determination, and that provide an overfit to the data, i.e. fit features of the specific datasets or processes that do not generalize to other cases. The NNPDF4.0 methodology is carefully tuned in order to avoid such overfits, by a K-folding procedure [3] that checks the power of the PDFs to correctly generalize, and, as already mentioned, tested a posteriori through closure tests [6, 9] (that check generalizing power in the data region) and future tests [10] (that check generalizing power in the extrapolation region) — see Appendix A for a brief review.

As an example of such overfits, in Fig. 4.4 we show the gluon distribution obtained in a fit in which we have artificially modified the minimization procedure in order to obtain a very low value of $\chi^2(0,c)$. Indeed, in this overfit the final value of $\chi^2(0,c)$ is by about $\delta = 0.08$ smaller than that of the default NNPDF4.0, i.e. $\delta \times N_{\text{dat}} \approx 300$, a difference that is about one order of magnitude bigger than that of the HS PDFs. The unphysical behavior of the PDFs thus obtained is manifest and representative of overfitting.

In light of this observation, in Fig. 4.5 we compare the NNPDF4.0 PDF gluon PDF to the HS PDFs: for NNPDF we show both the central value and one-σ uncertainty (left plot) and the corresponding replica set (right), while for HS we can only show the set of individual PDFs since their ensemble has no statistical meaning. It is apparent that the HS PDFs are characterized by a kink in the region $10^{-5} \lesssim x \lesssim 10^{-3}$. This kink is absent both in the central NNPDF4.0 gluon, and also in individual replicas.

In Fig. 4.6 we show a detail of the small $x$ region, in which the kink is clearly visible. For comparison, in Fig. 4.6 we also show a similar comparison for the octet valence combination ($V_8 = u^− + d^− - 2s^-$, with
Figure 4.7. The gluon PDF obtained from the level-0 PDF replicas of Fig. 4.3 (green), compared to the underlying assumed truth, namely the HS PDF with largest Higgs cross-section taken as underlying truth (orange).

Figure 4.8. The kinetic energy Eq. (4.1) for the gluon (left) and down PDFs (right), for NNPDF4.0 (green) and for the HS PDFs (red).

$q_i^-=q_i-\bar{q}_i$ in which even more pronounced kinks are seen in the HS PDFs.

It is important to observe that there are essentially no data constraining the gluon in the region of $x \lesssim 10^{-4}$, so the kink displayed by the HS PDFs is likely not data-driven. We can actually prove this explicitly by looking at the PDFs obtained in the level-0 closure determination of Fig. 4.3. Recall that this PDF produces a perfect fit to the data, i.e. it has vanishing $\chi^2$. In Fig. 4.7 the gluon PDF from this set is shown and compared to the underlying assumed truth HS PDF. Even though the assumed truth has the kink that characterizes the HS PDFs, a perfect fit to data as predicted by a HS PDF has no kink. This indicates that the HS kink is not data driven, but rather an overfitted feature.

We can actually construct a quantitative overfitting estimator by defining the PDF kinetic energy

$$KE = \sqrt{1 + \left(\frac{d}{d\ln x} x f(x, Q^2)\right)^2}.$$  \hspace{1cm} (4.1)

This quantity, integrated between any two values of $x$ gives the arclength of the curve that $x f(x)$ traverses, viewed as a function of $\ln x$. The kinetic energy is thus a local measure of “wiggliness”: given a pair of curves with fixed extremes, the one with greater kinetic energy joins the two extremes with a longer curve. It coincides of course with the Lagrangian of a relativistic free particle (with $x f$ interpreted as space and $\ln x$ as time), hence its name, with its integral being equal to the action.

In Fig. 4.8 we compare the kinetic energy of the HS PDFs to that of NNPDF4.0: we show the gluon and also, for reference, the down quark. It is clear that the HS PDFs are characterized by higher kinetic energy, specifically for the gluon, but in fact for all HS PDFs. Furthermore, the kinetic energy itself displays greater
fluctuations for the HS PDFs. We conclude that the HS PDFs are characterized by having a feature which is not data driven and that corresponds to the given curve being further away from a least-action geodesic, which is disfavoured by the NNPDF methodology.

The fact that the HS PDFs display signs of overfitting should not come as a surprise, given that they have been constructed by starting from NNPDF4.0 replicas, which have been constructed in such a way as to avoid overfitting, and trying to further minimize the figure of merit. This suggests that PDF replicas with features similar to the HS PDFs could be obtained by forcing overfitting in the NNPDF4.0 methodology.

In order to check this explicitly, we have introduced overfitting in the NNPDF4.0 methodology by changing by hand the fit settings (which are set by the hyperoptimization procedure). In particular, we doubled the training length, which in turn implies increasing some parameters (such as the stopping patience) that are determined as functions of the training length. This leads to a decrease of \( \chi^2(0, c) \) by about 0.01, i.e. similar to the greatest reduction observed in the HS PDFs. We can explicitly check that these PDFs are overfitted by using an overfitting metric suggested in Ref. [24], and reviewed in Appendix B. This metric vanishes for a proper fit, and it is negative for an overfit. Results are shown in Fig. 4.9, where we compare this metric for the default NNPDF4.0 PDFs and for this overfitted variant. We see that while for the default \( R_O = -0.001 \pm 0.013 \), for the overfitted variant \( R_O = -0.027 \pm 0.001 \), which indicates an overfit at the three \( \sigma \) level.

A comparison of the gluon PDF in this overfitted variant to the default NNPDF4.0 gluon in Fig. 4.10 shows that it starts developing features that are similar to that of the HS PDFs, specifically a kink in the small \( x \) region and a somewhat higher peak. This provides further evidence that the HS PDFs are overfitted.

Summarizing, we have shown that the HS gluon is characterized by a feature that is not data-driven and that corresponds to being further away from a least-action curve, and that similar features can be
obtained in NNPDF4.0 replicas by forcing overfitting. We conclude that NNPDF4.0 replicas that look like
the HS PDFs are disfavored by the NNPDF methodology because they correspond to overfitting solutions.
Nevertheless, PDF replicas leading to results similar to the HS PDFs in the ZH plane (i.e. leading to similar
values of the Higgs and Z cross section) can be obtained as proper fits to unlikely data fluctuations, given
a large enough replica sample.

5 Conclusion

The main purpose of this note was to show that the NNPDF4.0 PDFs are constructed to give a representative
sampling of the probability distribution of PDFs, constrained by the experimental dataset that enter the
fit and the well-known theoretical constraints given by QCD, such as momentum and valence sum rules,
as well as integrability and positivity. We have explicitly examined the distribution of the NNPDF4.0
replicas and the fit quality of each replica. The faithfulness of the NNPDF sampling is confirmed by several
tests, for example the closure tests and future tests, which guarantee that the accuracy of the sampling is
consistent with its stated precision. We have considered an alternative sampling proposed in Ref. [1]. We
have explained that the features of these PDFs can be reproduced by NNPDF4.0 replicas, but with low
posterior probability. We show that such a low probability is related with the fact that hopscotch PDFs
are overfitted, namely they achieve a low $\chi^2$ to experimental data by fitting the random fluctuations in
the data. The extra wiggliness in the hopscotch PDFs is displayed explicitly, and explains why they are
relatively improbable.

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A Validation in NNPDF

To validate the resulting PDF distributions, several tests of the NNPDF methodology have been developed.
Specifically, the validity of the PDFs in the data region is validated using closure tests [6,9] and the validity
of the PDFs in the extrapolation region is validated using futures tests [10]. We briefly review these tests
here, while referring to the original publications for a more detailed treatment.

Closure test. In a closure test, instead of fitting to experimental data, a fit to pseudodata constructed
from predictions using a known input PDF is performed. Closure tests allow us to validate our methodology
by testing if it is able to faithfully reproduce the underlying input PDF and have been a characteristic of
NNPDF fits since they were first introduced in Ref. [9]. In order to quantify the accuracy of the posterior
distribution, a number of statistical estimators are considered that we will discuss here. These statistical
estimators have been evaluated for the NNPDF4.0 determination, and found to be within $1\sigma$ of the value
corresponding to a faithful representation of the input PDF. For a detailed motivation of these estimators
we refer the reader to Ref. [3].

To estimate the faithfulness of the PDF uncertainty at the level of observables, the bias over variance ratio
as defined in Eq. (6.15) of Ref. [3] is used. Here “bias” can be understood as a measure of the fluctuations
of the observable values with respect to the central value prediction of the fitted PDF, while “variance” can
be understood as the fluctuations of the fitted PDF with respect to its central value prediction. Thus if
the methodology has faithfully reproduced the uncertainties in the underlying data (bias), this uncertainty
should be equal to the uncertainty in the predictions of the PDFs (variance), and hence the bias to variance ratio $R_{bv}$ is expected to be one.

To estimate the faithfulness of the PDF uncertainty at the level of the PDF we calculate a quantile estimator in PDF space $\xi^{(pdf)}_{1\sigma}$. This quantity corresponds to the number of fits for which the $1\sigma$ uncertainty band covers the PDF used as underlying law. The expected value is 0.68 for $\xi^{(pdf)}_{1\sigma}$, 0.95 for $\xi^{(pdf)}_{2\sigma}$, etc.

An analogous estimator can be calculated for the theory predictions in data space as opposed to PDF space, providing a generalization to quantile statics of the bias of variance ratio $R_{bv}$. The expected value of this quantile estimator depends on the bias over variance ratio and is $\text{erf}(R_{bv}/\sqrt{2})$, which is checked to be in agreement with the calculated value of $\xi^{(exp)}_{1\sigma}$.

Finally it should be noted that for each of these estimators the corresponding standard error on the calculated value is determined through a bootstrapping procedure [25, 26].

**Future test.** By definition, testing the accuracy in a region where there is no data to test against is impossible. Thus to test the accuracy of the predictions in the extrapolation region, a fit is performed using a “historic” dataset representing the knowledge available at an earlier point in time and its predictions compared to the more recent measurements. This is the basic premise of the the “future test” technique introduced in Ref. [10]. Specifically, the historic datasets for the validation performed for the NNPDF4.0 determination correspond to a pre-HERA and pre-LHC period where. For a detailed overview of exactly which datasets are included in each of the historic datasets we refer to Tab. 6.5 of Ref. [3].

Since the aim of doing a future test is to determine the ability of a methodology for PDF determination to provide a generalized fit, we need to take into account not only the uncertainty of the experimental data but also the uncertainty of the PDF itself. This is done by adding to the experimental covariance matrix (as will be defined in Sect. 3) also the covariance matrix of the observables calculated from PDF predictions:

$$
\text{cov}_{\text{future test}} = \text{cov}_{\text{exp}} + \text{cov}_{\text{pdf}},
$$

where $\text{cov}_{\text{pdf}}$ is defined as

$$
\text{cov}_{\text{pdf}} = \langle T_i T_j \rangle_{\text{rep}} - \langle T_i \rangle_{\text{rep}} \langle T_j \rangle_{\text{rep}},
$$

with $T_i^{(k)}$ the prediction of the $i$-th datapoint using the $k$-th PDF replica with the average defined over replicas.

While in general the expected disagreement between the predication of the unseen (or future) data and the actual data will be significant, the future test allows us to test whether methodology properly accounts for this by correspondingly increasing the PDF uncertainties. The $\chi^2$ as defined using the future test covariance matrix constructed by combining the PDF and experimental covariance matrices per Eq. (A.1) should reduce to the usual value of order one.

**B An overfitting metric**

If the optimal fit is determined through a cross-validation stopping criterion, based on splicing the data in training and validation sets, it is possible to construct a metric that explicitly detects the presence of overfitting in the final result [24]. We review here the way this metric is constructed.

Recall that the training-validation split is done randomly on a replica-by-replica basis. This means that for each replica, different data go into the training and validation sets. We call the way the data are split into training and validation sets a “validation mask”. So each data replica is characterized by the fact that (a) data are fluctuated differently and (b) a different mask is adopted. Based on this observation, define

$$
\chi^2_{\text{val}} \left[ T^{(k)}, F^{(k)} \right] = \frac{1}{N} \sum_{k' = 1}^{N} \chi^2 \left[ T^{(k)}, F^{(k')} \right]_{\text{fixed mask}}.
$$

The sum here is performed over different data replicas, but with a fixed validation mask: i.e. the data are fluctuated differently, but the same validation mask is adopted. Based on this observation, define

$$
\mathcal{R}_O = \chi^2_{\text{val}} \left[ T^{(k)}, F^{(k)} \right] - \frac{1}{\chi^2_{\text{val}} \left[ T^{(k)}, F^{(k)} \right]}.
$$

Now define

$$
\mathcal{R}_O = \frac{1}{\chi^2_{\text{val}}} \left[ T^{(k)}, F^{(k)} \right] - \frac{1}{\chi^2_{\text{val}}} \left[ T^{(k)}, F^{(k)} \right],
$$

16
where $\chi^2_{\text{val}}[T^{(k)}, F^{(k)}]$ is the usual validation $\chi^2$ for the fitting of the $k$-th replica, and $\chi^2_{\text{val}}[T^{(k)}, F^{(k)}]$ is computed using (for all replicas) the same validation mask that was used for this $k$-th replica.

If a PDF replica $f^{(k)}$ is overfitted, i.e. it does contain some information specific of the underlying data replica $F^{(k)}$, then the quantity $R_O$ is negative, meaning that its $\chi^2$ is lower than that which is obtained on average when comparing to a random fluctuation of the same validation data. If instead it is correctly fitted, then $R_O$ should be compatible with zero.

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