Bayesian Reweighting for Global Fits

Nobuo Sato, J. F. Owens, and Harrison Prosper

Department of Physics, Florida State University, Tallahassee, Florida 32306-4350

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Abstract

Two different techniques for adding additional data sets to existing global fits using Bayesian reweighting have been proposed in the literature. The derivation of each reweighting formalism is critically reviewed. A simple example is constructed that conclusively favors one of the two formalisms. The effects of this choice for global fits is discussed.
I. INTRODUCTION

In general, the understanding of a given phenomenon relies on our ability to construct a model that describes the relevant data and their corresponding uncertainties. One way to summarize what the data tell us about a model is to find a probability density function for its parameters. For such a task, standard fitting techniques such as $\chi^2$ minimization are commonly used to determine this probability density. Typically, this process is iterative: once new data are available, a new fit is performed combining the old and new data. We shall refer to this procedure as a global fit. In some cases, the complexity of the model is such that its numerical evaluation makes the fitting procedure time consuming. For practical reasons, it would be desirable to update the probability density by incorporating the information from new data without having to perform a full global fit. Such updating can be achieved by a statistical inference procedure, based on Bayes theorem, known as the reweighting technique.

A particular example, where the reweighting technique is useful, is in the context of global fits for the determination of parton distribution functions (PDFs). Modeling and fitting these functions has been the central task of several collaborations, e.g., CTEQ, CJ, MSTW, and NNPDF, among others. But still, there are kinematic regions where the PDFs are relatively unconstrained. Given the complexity of the calculations, it is desirable to use the reweighting technique to update our knowledge of the PDFs or to quantify the potential impact of anticipated data sets on the PDFs.

The idea of reweighting PDFs was originally proposed in [1] and later discussed by the NNPDF collaboration in [2, 3]. However, there is disagreement about the reweighting procedure, which has led to methods that differ mathematically. The purpose of this paper is to discuss the differences between the reweighting methods. In particular, we investigate the degree to which the reweighting procedures yield results that are consistent with those from global fits. We shall argue that this is the case for the method proposed in [1].

The paper is organized as follows. In Sec. II we describe the basics of the reweighting technique. In Sec. III we will discuss subtleties in the NNPDF arguments. In Sec. IV we will present a simple numerical example to display the differences between the reweighting methods. Our conclusions are given in Sec. V.
II. THE REWEIGHTING METHOD

The reweighting of probability densities in order to incorporate the information from new data is merely the recursive application of Bayes theorem. Suppose a probability density function (pdf) \( P(\vec{\alpha}) \) of the parameters \( \vec{\alpha} \) in a model is known. (To avoid confusion, we shall take “PDF” to mean parton distribution function, and “pdf” to mean probability density function.) Given new data \( D \), Bayes theorem states that

\[
P(\vec{\alpha}|D) = \frac{P(D|\vec{\alpha})}{P(D)} P(\vec{\alpha}),
\]

where \( P(\vec{\alpha}|D) \), known as posterior density, is the updated pdf from the prior density (or prior for short) \( P(\vec{\alpha}) \), which can serve as the prior in a subsequent analysis. The quantity \( P(D|\vec{\alpha}) \) called the likelihood function, represents the conditional probability for a data set \( D \) given the parameters \( \vec{\alpha} \) of the model. The quantity \( P(D) \) ensures the normalization of the posterior density. With the new data, the expectation value of an observable \( O \) can be written as,

\[
E[O] = \int d^n \alpha P(\vec{\alpha}|D) O(\vec{\alpha})
\]

\[
= \int d^n \alpha \frac{P(D|\vec{\alpha})}{P(D)} P(\vec{\alpha}) O(\vec{\alpha})
\]

\[
= \frac{1}{N} \sum_k w_k O(\vec{\alpha}_k).
\]

In the last line, we have used a Monte Carlo approximation of the integral in which the parameters \( \{\vec{\alpha}_k\} \) are distributed according to the prior \( P(\vec{\alpha}_k) \). Similarly, the variance is given by

\[
\text{Var}[O] = \frac{1}{N} \sum_k w_k (O(\vec{\alpha}_k) - E[O])^2.
\]

The quantities \( \{w_k\} \) are weights that are proportional to \( P(D|\vec{\alpha}_k) \). Their normalization is fixed by demanding \( E[1] = 1 \), that is, \( \sum_k w_k = N \).

The reweighting procedure depends on the form assumed for the likelihood function. The form of the likelihood function is not unique since it depends on the amount of information we want to extract from the new data. To clarify, suppose the new data consist of \( n \) data points \( \{(x_i, y_i)\} \) with uncertainties in \( \{y_i\} \) given by a covariance matrix \( \Sigma \). Let us call \( \{t_i = f(x_i, \vec{\alpha})\} \) the \( n \) predictions from the model \( f \) with parameters \( \vec{\alpha} \). Assuming a Gaussian
model, the conditional probability for new data to be confined in a differential volume \( d^n y \) around \( \vec{y} \) for a given configuration of parameters \( \vec{\alpha} \) is

\[
\mathcal{P}(\vec{y}|\vec{\alpha}) d^n y = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} e^{-\frac{1}{2} \chi^2(\vec{y},\vec{t})} d^n y,
\]

(4)

where the \( \chi^2(\vec{y},\vec{t}) \) is defined in the standard way

\[
\chi^2(\vec{y},\vec{t}) = (\vec{y} - \vec{t})^T \Sigma^{-1} (\vec{y} - \vec{t}).
\]

(5)

On the other hand, we might be interested in the probability for the new data to be confined only in a differential shell \( \chi \) to \( \chi + d\chi \). This probability density can be obtained by integrating \( \mathcal{P}(\vec{y}|\vec{\alpha}) \) inside the shell (see Appendix A). The result,

\[
\mathcal{P}(\chi|\vec{\alpha}) d\chi = \frac{1}{2^{n/2-1} \Gamma(n/2)} \chi^{n-1} e^{-\frac{1}{2} \chi^2} d\chi,
\]

(6)

is the well-known \( \chi^2 \) distribution. Using the functions from Eqs. (4) and (6) as likelihoods in Eq. (1), we obtain the corresponding posterior densities and weights,

\[
\mathcal{P}(\vec{\alpha}|\vec{y}) = \frac{\mathcal{P}(\vec{y}|\vec{\alpha})}{\mathcal{P}(\vec{y})} \mathcal{P}(\vec{\alpha}) \rightarrow w_k \propto \exp \left( \frac{1}{2} \chi^2(\vec{y},\vec{t}_k) \right),
\]

(7)

\[
\mathcal{P}(\vec{\alpha}|\chi) = \frac{\mathcal{P}(\chi|\vec{\alpha})}{\mathcal{P}(\chi)} \mathcal{P}(\vec{\alpha}) \rightarrow w_k \propto (\chi^2(\vec{y},\vec{t}_k))^{\frac{1}{2}(n-1)} \exp \left( \frac{1}{2} \chi^2(\vec{y},\vec{t}_k) \right).
\]

(8)

Note that \( \mathcal{P}(\chi|\vec{\alpha}) \) has less information than \( \mathcal{P}(\vec{y}|\vec{\alpha}) \): a given data set \( y \) uniquely determines \( \chi \), but a given \( \chi \) is consistent with infinitely many data sets \( y \). Therefore, the posterior density \( \mathcal{P}(\vec{\alpha}|\chi) \) has less information than \( \mathcal{P}(\vec{\alpha}|\vec{y}) \), a mathematical fact that we shall quantify using a standard information-theoretic measure.

III. THE NNPDF PARADOX

The NNPDF collaboration argues in Ref. [2, 3] that we should avoid the use of the likelihood \( \mathcal{P}(y|\vec{\alpha}) \) because of the Borel-Kolmogorov paradox, the observation that conditional probabilities, such as \( \Pr(\vec{\alpha}, y = D)/\Pr(y = D) \), for continuous variables \( y \) are ambiguous because they condition on a set of measure zero for which the probability is strictly zero. In the present context, the probability that \( y \) is exactly equal to \( D \) is zero. In order to give meaning to \( \Pr(f, y = D)/\Pr(y = D) \), the latter must be defined by a limit. The paradox
arises because different ways of taking the limit can yield different results. However, no issue arises in Bayes theorem, Eq. (1), even when $y = D$ is multidimensional. Indeed, statisticians (and some physicists) routinely use multivariate densities in Bayes theorem. Our intuitive understanding of why Eq. (1) is mathematically sound is that, first, the probabilities are defined by integrals about the point $y$ and second that the shapes of the sequence of nested sets about the limit point $y$ is the same in both the numerator and the denominator. When the sets become sufficiently small, the integrals can be approximated by the probability density times a small, but finite, volume element which cancels in Bayes theorem. Crucially, this is true for all shapes of the $n$-dimensional, small but finite, volume element and therefore for all sequences of (measurable) sets. Therefore, the suggestion by the NNPDF authors that, in effect, Bayes theorem, Eq. (1), is problematic when $y = D$ is multidimensional is not convincing. Indeed, Eq. (1) is the bedrock of state-of-the-art Bayesian analyses (see for example, Ref. [4].)

IV. A SIMPLE NUMERICAL EXAMPLE

This section aims to study the differences between the reweighting results from the likelihoods $P(y|\vec{\alpha})$ and $P(x|\vec{\alpha})$ by a numerical example. Simulated data from the function

$$f(x, \vec{\alpha}) = x^{\alpha_0}(1 - x)^{\alpha_1},$$

are generated by adding gaussian noise with independent random variances for each value of $x$. The parameters of the function has been arbitrary set to $\vec{\alpha} = (-2, 2)$ and a sample 100 points equally spaced in the range $0 < x < 1$ is taken. This particular functional form is inspired by a typical parton distribution function parametrization used in global fits.

For the analysis, the data are divided into 11 equally spaced regions in $x$ and labeled as \{d_0, d_1, ..., d_{10}\} from the lowest $x$ region ($d_0$) to the highest $x$ region ($d_{10}$). Then, the data sets are organized as described in table I. Using $\chi^2$ minimization, we perform global fits to each data set $A_i$. The uncertainties in the fitted parameters are obtained using the Hessian method (see Appendix B). As a result we obtain four parameter vectors $\vec{\alpha}_j^{\pm} = \vec{\alpha}_0 \pm \delta \vec{\alpha}_j$ with $j = 1, 2$ for each data set $A_i$. These vectors encode the 1$\sigma$ confidence interval of the fitted parameters. For the reweighting, is necessary to construct a Monte Carlo representation of
the fitted results. This is done by sampling the parameters as

\[ \vec{\alpha}_k = \vec{\alpha}_0 + \sum_j \delta\vec{\alpha}_j R_{kj} \]  

(10)

where \( R_{kj} \) are normally distributed random numbers with variance 1 and mean 0. \( k \) is the number of samples. Evaluating Eq. (9) with parameters \( \vec{\alpha}_k \) from the fit \( A_i \) yields the desired Monte Carlo sample \( \{f_k|A_i\} \). We compute the latter and its corresponding expectation value \( E[f|A_i] \) and variance \( \text{Var}[f|A_i] \) for each set \( A_i \). In order to perform the reweighting, we select the Monte Carlo sample \( \{f_k|A_0\} \) as the prior to be reweighted. Using the data sets \( \{B_i\} \) as new evidence, we compute the expectation value \( E[f|A_0, B_i] \) and variance \( \text{Var}[f|A_0, B_i] \) using Eqs. (2) and (3) with the weights from Eq. (7) or Eq. (8) for each set \( B_i \).

The results are shown in Fig. 1 where a clear disagreement between the two reweighting methods is exhibited. The variances obtained by using the likelihood \( P(\chi|\vec{\alpha}) \) are greater than the variances obtained from the likelihood \( P(\vec{y}|\vec{\alpha}) \) and the convergence of the expectation values is much faster for the latter case. This is consistent with the discussion in section 11 where we argued that the posterior \( P(\vec{\alpha}|\chi) \) contains less information than \( P(\vec{\alpha}|\vec{y}) \). More importantly, reweighting with the likelihood \( P(\vec{y}|\vec{\alpha}) \) yields a result that is more compatible with that obtained from the global fits than is that obtained using the likelihood \( P(\chi|\vec{\alpha}) \). This is illustrated by the dotted and dashed curves being nearly identical while the solid and dashed curves show significant differences.

In the light of above, it is important to discuss why the NNPDF collaboration has obtained reweighting results compatible with global fits in [2, 3] even when they have used the likelihood \( P(\chi|\vec{\alpha}) \) instead of \( P(\vec{y}|\vec{\alpha}) \). In their case, their prior corresponds to PDFs fitted using deep inelastic scattering data (DIS) and Lepton Pair Production data (LPP). By performing the reweighting and comparing it with a new global fit using the W-lepton asymmetry data, they have proven the consistency of their reweighting method. However, it is also known that PDFs are already reasonably well constrained by the DIS and LPP data. This means that the information provided by the W-lepton data is sub-dominant with respect to the DIS and LPP data.

We have performed a similar exercise as before but this time using the Monte Carlo sample \( \{f_k|A_4\} \) as the prior and the data set \( C_5 \) as the new evidence. This setup aims to mimic the conditions at which NNPDF had studied the reweighting technique: the data set \( A_4 \) contains more data than \( C_5 \) and therefore the effects of including the later must be
| SET  | data       | SET  | data       | SET  | data       |
|------|------------|------|------------|------|------------|
| A0   | d5         | B1   | d4, d6     | B2   | d3, d4, d5, d6, d7 |
| A1   | d4, d5, d6 | B3   | d2, d3, d4, d5, d6, d7, d8 | B4   | d1, d2, d3, d4, d5, d6, d7, d8, d9 |
| A2   | d3, d4, d5, d6, d7 |      |            |      |             |
| A3   | d2, d3, d4, d5, d6, d7, d8 | B5   | d0, d1, d2, d3, d4, d5, d6, d7, d8, d9, d10 | C5   | d0, d10 |
| A4   |           |      |            |      |             |
| A5   | d0, d1, d2, d3, d4, d5, d6, d7, d8, d9, d10 |      |            |      |             |

TABLE I: Data sets.

| prior data | new evidence | \mathcal{D}(\mathcal{P}(\vec{\alpha}|\vec{y})||\mathcal{P}(\vec{\alpha})) | \mathcal{D}(\mathcal{P}(\vec{\alpha}|\chi)||\mathcal{P}(\vec{\alpha})) |
|------------|--------------|-------------------------------------------------|-------------------------------------------------|
| A0         | B1           | 2.94                                            | 1.86                                            |
| A0         | B2           | 3.96                                            | 2.62                                            |
| A0         | B3           | 4.77                                            | 3.13                                            |
| A0         | B4           | 5.32                                            | 3.51                                            |
| A0         | B5           | 5.84                                            | 3.94                                            |
| A4         | C5           | 0.83                                            | 0.08                                            |

TABLE II: KL divergences.

sub-dominant for a global fit as well as the reweighting. The results are shown in Fig. 2. It is clear that in this situation the reweighting of both methods yield similar results compatible with global fits.

One way to quantify the information about the parameters $\vec{\alpha}$ provided by the likelihood $p(x|\vec{\alpha})$, where $x$ is either $\vec{y}$ or $\chi$ is to calculate the Kullback-Leibler (KL) divergence (see Appendix C. Table II shows the KL divergences for the reweighting results performed above. The values in the table confirms the loss of information when using $\mathcal{P}(\vec{\alpha}|\chi)$ as the likelihood instead of $\mathcal{P}(\vec{\alpha}|\vec{y})$ in the reweighting procedure.
FIG. 1: Column 1 shows the data $A_0$ (black) from which the prior distribution is obtained and the new evidence $B_i$ (colored) that is used for reweighting or appended to $A_0$ to perform a global fit. The data is normalized respect to the “true” model. Columns 2,3,4 shows expectation values and variances from global fits and reweighting. Dashed lines are the results from global fits. Black dashed uses only the data $A_0$ while the colored dashed line includes the new evidences. Solid and dotted lines are reweighting results of data set $A_0$ using the evidences of data $B_i$. Dotted uses $w_k \propto \exp \left(-\frac{1}{2} \chi_k^2 \right)$ while solid uses $w_k \propto \chi_k^{n-1} \exp \left(-\frac{1}{2} \chi_k^2 \right)$.

FIG. 2: Similar to Fig. 2. In this case, set $A_4$ is used to obtain the prior distribution and set $C_5$ is used for reweighting or appended to $A_4$ for a global fit.
V. CONCLUSIONS

The technique of statistical inference is a useful tool to constrain probability density functions in the presence of new evidence. It is an alternative method to obtain updated distributions without having to perform a global fit by appending the old data and the new data. The NNPDF collaboration has argued that the method proposed in [2, 3] is not adequate and they proposed their own method. In the light of the results presented in this paper, we conclude that both methods are statistically equivalent in the limit when the prior densities are well constrained by the data and the new evidence do not provide significant information. We have shown using a numerical example that, if the uncertainties in the prior distribution are larger compared to the uncertainties obtained by the inclusion of new data, the method proposed by NNPDF collaboration is less efficient than the method proposed by [1] and the latter yields results that are significantly closer to those obtained from global fits.

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Appendix A: proof of Eq. (6)

The distribution \( P(\chi^2 | \vec{\alpha}) \) can be obtained by integrating \( P(\vec{y} | \vec{\alpha}) \) subjected to \( \chi^2 = \chi^2(\vec{y}, \vec{t}) \). Mathematically this is simply

\[
P(\chi^2 | \vec{\alpha}) = \int \delta[\chi^2 - \chi^2(\vec{y}, \vec{t})] p(y|\vec{\alpha}) \, d^n y
\]

\[
= \frac{1}{2\pi i} \int_{-\infty}^{\infty} d(i\omega) \int e^{i\omega\chi^2} \frac{1}{(2\pi)^{n/2}\Sigma^{1/2}} e^{-\frac{1}{2}(2i\omega+1)\chi^2} \, d^n y,
\]

\[
= \frac{1}{2^{n/2} 2\pi i} \int_{-\infty}^{\infty} d(i\omega) \frac{1}{(i\omega + 1/2)^{n/2}}
\]

\[
= \frac{1}{2^{n/2} \Gamma(n/2)} \left(\chi^2\right)^{\frac{1}{2}(n-2)} e^{-\frac{1}{2} \chi^2}.
\]

(A1)
Then we obtain

\[
\mathcal{P}(\chi|\vec{\alpha}) = \int d\bar{\chi}^2 \delta[\chi - \bar{\chi}] \mathcal{P}(\bar{\chi}^2|\vec{\alpha})
\]

\[
= \frac{1}{2^{n/2-1} \Gamma(n/2)} (\chi^2)^{\frac{1}{2}(n-1)} e^{-\frac{1}{2}\chi^2}.
\]  

(A2)

**Appendix B: the Hessian method**

For completeness in this appendix we present the standard Hessian method for error propagation. Suppose the model parameters \(\vec{\alpha_0}\) that minimizes the \(\chi^2\) is found. The method consists of expanding the \(\chi^2\) around the minima as a function of the parameters:

\[
\chi^2(\vec{y}, \vec{\alpha}) \equiv \sum_{ij} (y_i - t_i(\vec{\alpha})) \Sigma^{-1}_{ij} (y_j - t_j(\vec{\alpha}))
\]

\[
\approx \chi_0^2 + \sum_{ij} (\alpha_i - \alpha_0^i) C^{-1}_{ij} (\alpha_j - \alpha_0^j),
\]  

(B1)

where \(C^{-1}_{ij}\) is the Hessian matrix given by

\[
H_{ij} = \frac{1}{2} \frac{\partial^2 \chi^2}{\partial a_i \partial a_j}
\]  

(B2)

that is evaluated at \(\vec{\alpha} = \vec{\alpha}_0\). Next we diagonalize the matrix \(C\) which gives eigenvectors \(\vec{v}_j\) with eigenvalues \(\lambda_j\). The displacements \((\vec{\alpha} - \vec{\alpha}_0)\) in Eq. (B1) can be written in terms of rescaled vectors \(e_k = \sqrt{\lambda_k} \vec{e}_k\)

\[
\delta \vec{\alpha} \equiv \vec{\alpha} - \vec{\alpha}_0 = \sum_k z_k \vec{e}_k
\]  

(B3)

Replacing Eq. (B3) in Eq. (B1) gives

\[
\chi^2(\vec{y}, \vec{\alpha}) \approx \chi_0^2 + \sum_{kq} z_k z_q (\vec{e}_k)^t C^{-1}_{ij} \vec{e}_q
\]

\[
= \chi_0^2 + \sum_k z_k^2
\]  

(B4)

Notice that each displacements \(\pm \delta \alpha_k = \pm \vec{e}_k\) \((z_k = 1)\) corresponds in Eq. (B4) a \(\chi^2\) change of 1 unit. The interval defined by these displacements is known as the one-sigma confidence interval.
Appendix C: Kullback-Leibler divergence

The Kullback-Leibler (KL) divergence \cite{6} of the posterior density \( P(\vec{\alpha}|x) \) from the prior \( P(\vec{\alpha}) \) is given by

\[
D(P(\vec{\alpha}|x)||P(\vec{\alpha})) = \int P(\vec{\alpha}|x) \ln \frac{P(\vec{\alpha}|x)}{P(\vec{\alpha})} \, d^n\alpha,
\]

\[
= \int \frac{P(x|\vec{\alpha})}{P(x)} P(\vec{\alpha}) \ln \frac{P(x|\vec{\alpha})}{P(x)} \, d^n\alpha,
\]

\[
\approx \frac{1}{N} \sum_{k=1}^{N} w_k \ln w_k,
\]

(C1)

where the weights are defined as in Sec. \[11\]. The larger the KL divergence, the greater the difference between \( P(\vec{\alpha}|x) \) and \( P(\vec{\alpha}) \) and, therefore, the more informative are the data \( x \) about the PDF parameters, relative to what was known about them prior to inclusion of these data. A similar quantity called effective number of replicas \( N_{\text{eff}} \) was defined in the references \[2, 3\]:

\[
N_{\text{eff}} = \exp \left( \frac{1}{N} \sum_k w_k \ln \left( \frac{N}{w_k} \right) \right)
\]

(C2)

Here \( N \) is the number of Monte Carlo sample (replicas) taken from the prior distribution. Clearly the KL divergence is related to \( N_{\text{eff}} \) via

\[
D(P(\vec{\alpha}|x)||P(\vec{\alpha})) \approx \ln \left( \frac{N_{\text{eff}}}{N} \right)
\]

(C3)

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