

# Bayesian PDF reweighting meets the Hessian methods

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## Abstract

New data coming from the LHC experiments have a potential to extend the current knowledge of parton distribution functions (PDFs). As a short cut to the cumbersome and time consuming task of performing a new PDF fit, reweighting methods have been proposed. In this talk, we introduce the so-called Hessian re-weighting, valid for PDF fits that carried out a Hessian error analysis, and compare it with the better-known Bayesian methods. We determine the existence of an agreement between the two approaches, and illustrate this using the inclusive jet production at the LHC.

## 1. Introduction

The interpretation of high-energy collider data relies strongly on the precise description of the parton distribution functions (PDFs). Usually they are obtained from global fits to data, the extraction being done nowadays up to NNLO accuracy [1, 2, 3, 4]. However, due to the complexity of PDF fits it has been impossible for those outside the groups dedicated to the PDF fitting (like experimentalists) to work out the implications that new measurements would have in a global PDF fit. The situation underwent an improvement when the NNPDF collaboration revived [5, 6] an old idea [7] of the Bayesian reweighting technique that tests the consistency between new data and data previously included in a PDF fit and also provides with a quantitative estimate on how the new data will affect the known PDFs. This method has become extremely popular [8, 9, 10, 11, 12, 13, 14]. Unfortunately, it has been unclear how to extend the reweighting outside the NNPDF fits. Indeed, while the NNPDF fits use Monte-Carlo methods for the uncertainty determination, most of the rival groups make use of the Hessian technique [15], and provide error sets that quantify the neighborhood of the central fit within a certain confidence level

$\Delta\chi^2$ . In order to use the Bayesian reweighting technique with these Hessian PDFs sets, an extension was proposed in Ref. [16], and has been employed to some extent [9, 17, 18]. However the accuracy of the proposed generalization has been put in the spotlight by a recent study [19] in which the results of reweighting were observed to deviate from the ones obtained by a direct fit.

In this contribution we review the results presented in Ref. [21] in which, building on the ideas introduced in Ref. [20], we put forward a different strategy to study the consistency and impact of a new data set within an existing set of PDFs that comes with Hessian error sets.

## 2. The Hessian re-weighting

The description of experimental data by a set of PDFs  $f \equiv f(x, Q^2)$  depending on fit parameters  $\{a\}$ , is done usually by finding the minimum of a  $\chi^2$ -function

$$\chi^2\{a\} = \sum_k \left[ \frac{X_k^{\text{theory}}[f] - X_k^{\text{data}}}{\delta_k^{\text{data}}} \right]^2, \quad (1)$$

where  $X_k^{\text{theory}}[f]$  are the theory predictions depending on the parameters  $\{a\}$ ,  $X_k^{\text{data}}$  the experimental values and

$\delta_k^{\text{data}}$  their uncertainties. The PDF errors are quantified in the Hessian approach [15] by assuming the behaviour of  $\chi^2$  function around the minimum to be sufficiently quadratic in the space of fit parameters  $\{a\}$

$$\chi^2\{a\} \approx \chi_0^2 + \sum_{ij} \delta a_i H_{ij} \delta a_j, \quad (2)$$

where  $\delta a_j \equiv a_j - a_j^0$  are departures from the best-fit values and  $\chi_0^2$  is the minimum value of  $\chi^2$ . The Hessian matrix  $H_{ij}$  has  $N_{\text{eig}}$  eigenvalues  $\epsilon_k$  and orthonormal eigenvectors  $\mathbf{v}^{(k)}$  that satisfy

$$H_{ij} v_j^{(k)} = \epsilon_k v_i^{(k)}, \quad (3)$$

$$\sum_j v_j^{(k)} v_j^{(\ell)} = \sum_j v_k^{(j)} v_\ell^{(j)} = \delta_{k\ell}. \quad (4)$$

This expression can be simplified by a change of variables that brings the Hessian matrix to a diagonal form

$$z_k \equiv \sqrt{\epsilon_k} \sum_j v_j^{(k)} \delta a_j, \quad (5)$$

so that

$$\chi^2\{a\} \approx \chi_0^2 + \sum_i z_i^2. \quad (6)$$

Just how much  $\sum_i z_i^2$  can increase with the fit still being *acceptable* is a choice left to those performing the fit, though generally it is preferred to take  $\Delta\chi^2 > 1$  [2, 3]. The corresponding uncertainty for a PDF-dependent quantity  $O = O[f]$  can then be calculated as

$$(\Delta O)^2 = \Delta\chi^2 \sum_k \left( \frac{\partial O}{\partial z_k} \right)^2. \quad (7)$$

In addition to the best fit  $S_0$ , the Hessian approach introduces the PDF error sets  $S_k^\pm$ , defined in the  $z$ -space as

$$z(S_0) = (0, 0, \dots, 0),$$

$$\vdots$$

$$z(S_{N_{\text{eig}}}^\pm) = \pm \sqrt{\Delta\chi^2} (0, 0, \dots, 1).$$

Using these, the derivatives in Eq. (7) can be evaluated by a linear approximation

$$\left( \frac{\partial O}{\partial z_k} \right) \approx \frac{O[S_k^+] - O[S_k^-]}{2\sqrt{\Delta\chi^2}}, \quad (8)$$

so that

$$(\Delta O)^2 = \frac{1}{4} \sum_k (O[S_k^+] - O[S_k^-])^2. \quad (9)$$

In the recent years the fixed  $\Delta\chi^2$  tolerance has been left aside in favor of a *dynamic tolerance*

$$z_i(S_k^\pm) \equiv \pm t_k^\pm \delta_{ik}. \quad (10)$$

Consider now a new set of data  $\mathbf{y} = y_1, y_2, \dots, y_{N_{\text{data}}}$  with covariance matrix  $C$ . We want to know whether or not it is consistent with an original set of PDFs and, if so, how including the data would affect the PDFs. For this purpose we introduce a new function defined as

$$\chi_{\text{new}}^2 \equiv \chi_0^2 + \sum_k z_k^2 + \sum_{i,j=1}^{N_{\text{data}}} (y_i[f] - y_j) C_{ij}^{-1} (y_j[f] - y_i), \quad (11)$$

which is just Eq. (6) plus the contribution of the new data. Employing a linear approximation, the theoretical values  $y_i[f]$  in arbitrary  $z$ -space coordinates can be approximated by

$$y_i[f] \approx y_i[S_0] + \sum_{k=1}^{N_{\text{eig}}} D_{ik} w_k, \quad (12)$$

with

$$D_{ik} \equiv \frac{y_i[S_k^+] - y_i[S_k^-]}{2} \quad (13)$$

$$w_k \equiv \frac{z_k}{\frac{1}{2}(t_k^+ + t_k^-)}. \quad (14)$$

Then,  $\chi_{\text{new}}^2$  is a quadratic function of the new parameters  $w_k$ , with its minimum given by

$$\vec{w}^{\text{min}} = -\mathbf{B}^{-1} \vec{a}, \quad (15)$$

where the matrix  $\mathbf{B}$  and vector  $\vec{a}$  are

$$B_{kn} = \sum_{i,j} D_{ik} C_{ij}^{-1} D_{jn} + \left( \frac{t_k^+ + t_k^-}{2} \right)^2 \delta_{kn}, \quad (16)$$

$$a_k = \sum_{i,j} D_{ik} C_{ij}^{-1} (y_j[S_0] - y_j). \quad (17)$$

The solution presents a *penalty term*

$$P \equiv \sum_{k=1}^{N_{\text{eig}}} \left[ \left( \frac{t_k^+ + t_k^-}{2} \right) w_k^{\text{min}} \right]^2 \rightarrow \Delta\chi^2 \sum_{k=1}^{N_{\text{eig}}} (w_k^{\text{min}})^2, \quad (18)$$

which allows us to determine whether the new data is consistent or not with the original PDFs. If a  $\Delta\chi^2$  was taken in the original fit,  $P \ll \Delta\chi^2$  means that the new data could have been incorporated without a conflict. However, if  $P \gtrsim \Delta\chi^2$  the new data shows clear tension with the set of PDFs in question. This does not, however, always mean that the new data would be incompatible with the other data. For instance, it might

be the case that the new data probe unconstrained components of PDFs whose behaviour was initially fixed by hand. The set of PDFs  $f^{\text{new}}$  corresponding to the new global minimum is determined by the components of the weight vector  $\vec{w}^{\text{min}}$

$$f^{\text{new}} \approx f_{S_0} + \sum_{k=1}^{N_{\text{rep}}} \left( \frac{f_{S_k^+} - f_{S_k^-}}{2} \right) w_k^{\text{min}}. \quad (19)$$

As the new PDFs  $f^{\text{new}}$  are a linear combination of the primary central and error sets, we may say that the original ones have just been *reweighted*. The new distributions  $f^{\text{new}}$  obey the same evolution equations and satisfy the same sum rules as the individual members  $f_{S_k^\pm}$  and can thereby be consistently utilized in perturbative QCD calculations.

### 3. Bayesian re-weighting

Given a Monte-Carlo ensemble of PDFs  $f_k$ ,  $k = 1 \dots N_{\text{rep}}$  (like those of the NNPDF collaboration [4]), that represent the probability density  $\mathcal{P}_{\text{old}}(f)$  of the PDFs, the expectation value  $\langle O \rangle$  and variance  $\delta\langle O \rangle$  for a PDF-dependent observable  $O$  can be computed as

$$\langle O \rangle = \frac{1}{N_{\text{rep}}} \sum_{k=1}^{N_{\text{rep}}} O[f_k], \quad (20)$$

$$\delta\langle O \rangle = \sqrt{\frac{1}{N_{\text{rep}}} \sum_{k=1}^{N_{\text{rep}}} (O[f_k] - \langle O \rangle)^2}. \quad (21)$$

The initial probability distribution  $\mathcal{P}_{\text{old}}(f)$  can be updated to include information from a new set of data  $\vec{y}$ , since

$$\mathcal{P}_{\text{new}}(f) \propto \mathcal{P}(\vec{y}|f) \mathcal{P}_{\text{old}}(f), \quad (22)$$

where  $\mathcal{P}(\vec{y}|f)$  is the likelihood function for the new data, given a set of PDFs. Consequently, for the observable  $O$  above, the expectation value becomes a weighted average

$$\langle O \rangle_{\text{new}} = \frac{1}{N_{\text{rep}}} \sum_{k=1}^{N_{\text{rep}}} \omega_k O[f_k], \quad (23)$$

$$\delta\langle O \rangle_{\text{new}} = \sqrt{\frac{1}{N_{\text{rep}}} \sum_{k=1}^{N_{\text{rep}}} \omega_k (O[f_k] - \langle O \rangle_{\text{new}})^2}, \quad (24)$$

where the weights  $\omega_k$  are proportional to  $\mathcal{P}(\vec{y}|f)$ . How to choose the likelihood appropriately has been a somewhat controversial issue and two options have been put forward so far. The original proposal by Giele and

Keller [7] (abbreviated by GK from now on) is to take  $\mathcal{P}(\vec{y}|f)d^n y$  as the probability to find the new data to be confined in an element  $d^n y$  centered around  $\vec{y}$  leading to

$$\omega_k^{\text{GK}} = \frac{\exp[-\chi_k^2/2]}{(1/N_{\text{rep}}) \sum_{k=1}^{N_{\text{rep}}} \exp[-\chi_k^2/2]}, \quad (25)$$

with

$$\chi_k^2 = \sum_{i,j=1}^{N_{\text{data}}} (y_i[f_k] - y_i) C_{ij}^{-1} (y_j[f_k] - y_j). \quad (26)$$

The other option, cherished by the NNPDF collaboration, considers  $\mathcal{P}(\vec{y}|f)d\chi$  as the probability for  $\chi \equiv \sqrt{\chi^2}$  to be confined in a volume element  $d\chi$  around  $\chi$ , resulting in

$$\omega_k^{\text{chi-squared}} = \frac{(\chi_k^2)^{(N_{\text{data}}-1)/2} \exp[-\chi_k^2/2]}{(1/N_{\text{rep}}) \sum_{k=1}^{N_{\text{rep}}} (\chi_k^2)^{(N_{\text{data}}-1)/2} \exp[-\chi_k^2/2]}. \quad (27)$$

We label these weights  $\omega_k^{\text{chi-squared}}$  as their behaviour is similar to the usual  $\chi^2$  distribution. The latter choice has been proven consistent with a direct fit in the NNPDF framework [5, 6]. However it was pointed out in Ref. [22] that  $\omega_k^{\text{GK}}$  contain more information on the new data, as a fixed  $\chi^2$  may correspond to different data sets.

In analogy to Eq. (19), the ensemble of PDFs required by the Bayesian approach can be constructed by

$$f_k \equiv f_{S_0} + \sum_i^{N_{\text{eig}}} \left( \frac{f_{S_i^+} - f_{S_i^-}}{2} \right) R_{ik}. \quad (28)$$

The coefficients  $R_{ik}$  are Gaussian random numbers with mean zero and 1-sigma variance. After computing the weights  $\omega_k$ , the reweighted PDFs can be written as

$$f^{\text{new}} = f_{S_0} + \sum_i^{N_{\text{eig}}} \left( \frac{f_{S_i^+} - f_{S_i^-}}{2} \right) \left( \frac{1}{N_{\text{rep}}} \sum_k \omega_k R_{ik} \right), \quad (29)$$

and the penalty induced becomes

$$P = \Delta\chi^2 \sum_i^{N_{\text{eig}}} \left( \frac{1}{N_{\text{rep}}} \sum_k \omega_k R_{ik} \right)^2. \quad (30)$$

The Bayesian methods have also another estimator for the new data compatibility: the effective number of replicas  $N_{\text{eff}}$  which is defined as

$$N_{\text{eff}} \equiv \exp \left\{ \frac{1}{N_{\text{rep}}} \sum_{k=1}^{N_{\text{rep}}} \omega_k \log(N_{\text{rep}}/\omega_k) \right\}. \quad (31)$$

If  $N_{\text{eff}} \ll N_{\text{rep}}$ , the method becomes inefficient and indicates that either the new data contains too much new information or that it is incompatible with the previous data.

#### 4. A pedagogical example

Let us consider a function

$$g(x) = a_0 x^{a_1} (1-x)^{a_2} e^{x a_3} (1+x e^{a_4})^{a_5}, \quad (32)$$

a typical fit function used in PDF fits. First, we construct a set of pseudodata (data set 1) for  $g(x)$ , the value of each data point  $y_k$  and its uncertainty  $\delta y_k$  obtained by

$$y_k = (1 + \alpha r_k) y_k^0, \quad \delta y_k = \alpha y_k^0$$

where  $y_k^0 = g(x)$  evaluated with fixed parameters. We make a  $\chi^2$  fit with free parameters  $a_0, a_1, a_2, a_3$  and construct the corresponding Hessian error sets with a certain  $\Delta\chi^2$  criteria. After that, we construct a second set of pseudodata (data set 2) and reweight the original fit by these data with all the introduced reweighting techniques in turn. Finally, we perform a direct fit considering both data sets and compare it with the predictions given by the reweighting methods. As the global fits of PDFs usually use  $\Delta\chi^2 > 1$ , we choose (arbitrarily) in our example  $\Delta\chi^2 = 10$ . The results are shown in Figs. 1 and 2. While all the reweighting methods yield

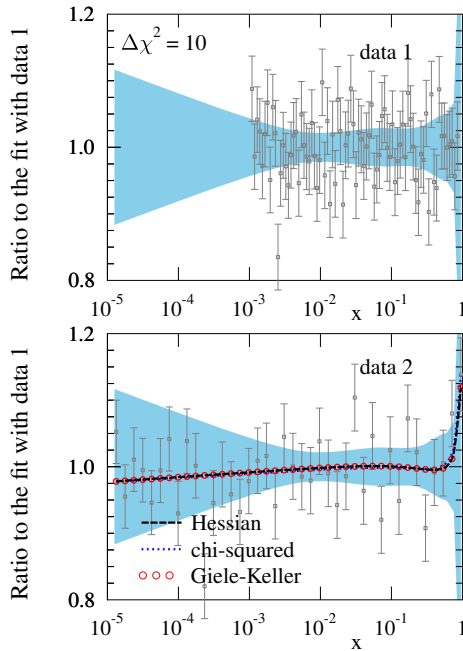


Figure 1: Upper panel: Data set 1 normalized by the fit to these data. Lower panel: Data set 2 normalized by the fit to the data set 1. In both panels the light blue band is the fit uncertainty for  $\Delta\chi^2 = 10$ , and in the lower panels we also show the results using the Hessian (black dashed), Bayesian with  $\omega_k^{\text{chi-squared}}$  (blue dotted) and Bayesian with  $\omega_k^{\text{GK}}$  (red circles) reweighting.

in present case a good approximation of the direct fit, only the Hessian reweighting can accurately reproduce the direct fit. This could have been expected as the replicas were generated using  $\Delta\chi^2 = 10$  but the likelihood function  $\mathcal{P}(\vec{y}|f)$  does not compensate for this in either case of the two Bayesian weights. However, as taking  $\Delta\chi^2 > 1$  is equivalent to increasing all the data errors correspondingly by  $\sqrt{\Delta\chi^2}$ , it should be the case that by rescaling  $\chi_k^2 \rightarrow \chi_k^2/\Delta\chi^2$  in Eqs. (25) and (27) when computing the weight for each replica, compensates for the tolerance  $\Delta\chi^2 > 1$ . The results are shown in Fig. 3.

It is clear that an agreement is reached between the

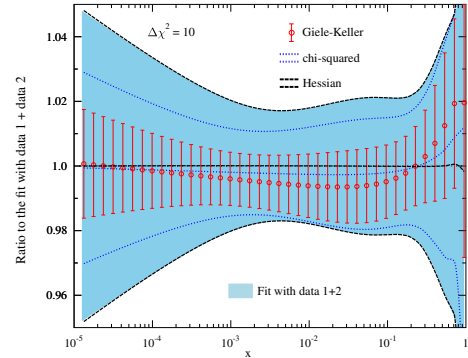


Figure 2: The results of reweighting for the function  $g(x)$  normalized to the fit using data sets 1 and 2. Black dashed: Hessian reweighting. Blue dotted: Bayesian reweighting with  $\omega_k^{\text{chi-squared}}$ . Red circles: Bayesian reweighting with  $\omega_k^{\text{GK}}$ .

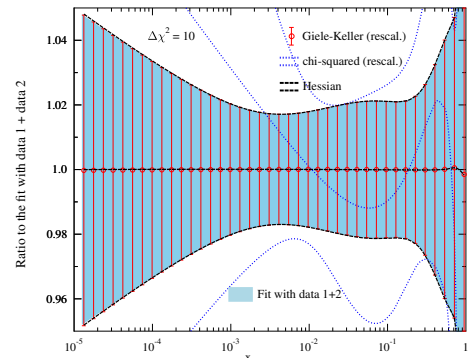


Figure 3: As Figure 1, but rescaling the values of  $\chi^2$  by  $(\Delta\chi^2)^{-1}$  in the case of Bayesian reweighting.

Bayesian method with rescaled GK weights, the Hessian reweighting, and the re-fit (a detailed mathematical proof for this correspondence is given in Ref.[21]). The Bayesian reweighting with chi-squared weights, on the

other hand, does not behave correctly and the rescaling  $\chi_k^2 \rightarrow \chi_k^2 / \Delta\chi^2$  makes the chi-squared weights to go haywire.

## 5. Inclusive jet production at the LHC

Now we apply the reweighting methods to the production of inclusive jets in proton+proton collisions at the LHC. The quadratic PDF dependence of the proton+proton cross sections

$$\sigma^{\text{PP}}[S] = f[S] \otimes \hat{\sigma} \otimes f[S], \quad (33)$$

could potentially decrease the accuracy of the linear approximation

$$\sigma^{\text{PP}}[S] \approx \sigma^{\text{PP}}[S_0] + \frac{\sum_k (\sigma^{\text{PP}}[S_k^+] - \sigma^{\text{PP}}[S_k^-]) w_k}{2}, \quad (34)$$

which one effectively makes when using Eq. (12). However, if the result of reweighting does not end up being very far from the original central fit, the nonlinear corrections should remain subdominant [21].

We consider  $\sqrt{s} = 7 \text{ TeV}$  jet measurements by the CMS collaboration [23], and take the CTEQ6.6 PDFs [24] as a baseline. For CTEQ6.6 we have  $\Delta\chi_{\text{CTEQ6.6}}^2 = 100$  ( $t_k^\pm = 10$ ) and  $N_{\text{eig}} = 22$ . We have employed the FASTNLO program [25, 26, 27] to compute the cross sections. In line with the CTEQ6.6 analysis, the factorization ( $\mu_f$ ) and renormalization ( $\mu_r$ ) scales were fixed to the transverse momentum of the jets ( $\mu_r = \mu_f = p_T/2$ ), and the QCD coupling was set by taking  $\alpha_s(M_Z) = 0.118$  at the Z boson mass pole. To evaluate the  $\chi^2$  values, we construct a covariance matrix  $C$  from the uncorrelated errors  $\sigma_i^{\text{uncorr}}$  and the systematic shifts  $\beta_i^k$  (1-sigma variation of the  $k$ th systematic parameter) by

$$C_{ij} = \delta_{ij} (\sigma_i^{\text{uncorr}})^2 + \sum_k \beta_i^k \beta_j^k, \quad (35)$$

The uncorrelated errors  $\sigma_i^{\text{uncorr}}$  include a 1% uncorrelated systematic uncertainty and the statistical error added in quadrature. Computing the  $\chi^2$  using Eq. (26) corresponds to [28, 29, 30] directly minimizing

$$\chi^2 = \sum_i \left[ \frac{y_i^{\text{theory}} - y_i^{\text{data}} - \sum_k s_k \beta_i^k}{\sigma_i^{\text{uncorr}}} \right]^2 + \sum_k s_k^2, \quad (36)$$

with respect to the  $s_k$  parameters resulting in

$$s_k^{\text{min}} = \sum_j \left[ \beta_j^k - \sum_{i,\ell,s} \beta_i^k C_{i\ell}^{-1} \beta_\ell^s \beta_j^s \right] \frac{y_j^{\text{theory}} - y_j^{\text{data}}}{(\sigma_j^{\text{uncorr}})^2}. \quad (37)$$

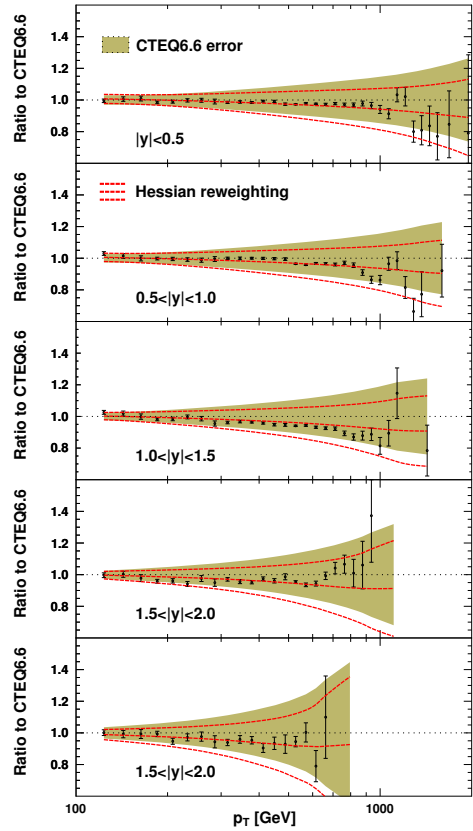


Figure 4: The CMS inclusive jet cross sections compared to the predictions after the Hessian reweighting and applying the systematic shifts. All values have been normalized to the central prediction of CTEQ6.6 and only the statistical data errors are shown.

From this we can compute the aggregate  $-\sum_k s_k^{\text{min}} \beta_i^k$  of the systematic shifts for a given data point  $y_i^{\text{data}}$ .

The new cross sections after the Hessian reweighting are shown in Fig. 4 and, for curiosity, in Fig. 5 for the Bayesian chi-squared reweighting. For the Bayesian techniques we generated  $10^4$  PDF replicas using Eq. (28) and the chi-squared weights are computed as they are (without rescaling the  $\chi^2$  values). Given that jet production is mostly sensitive to the gluon distribution, in Fig. 6 we present the resulting modifications on the gluon PDFs. As expected from our earlier example, the Hessian technique and the Bayesian method with rescaled GK weights are in good agreement. The reweighting penalty  $P \approx 21$  is clearly lower than  $\Delta\chi_{\text{CTEQ6.6}}^2$  and only a small amount of replicas are “lost” ( $N_{\text{eff}}$  is large). Thus, had these data been incorporated into the CTEQ6.6 fit, they would have not caused a significant disagreement with the original data. In this

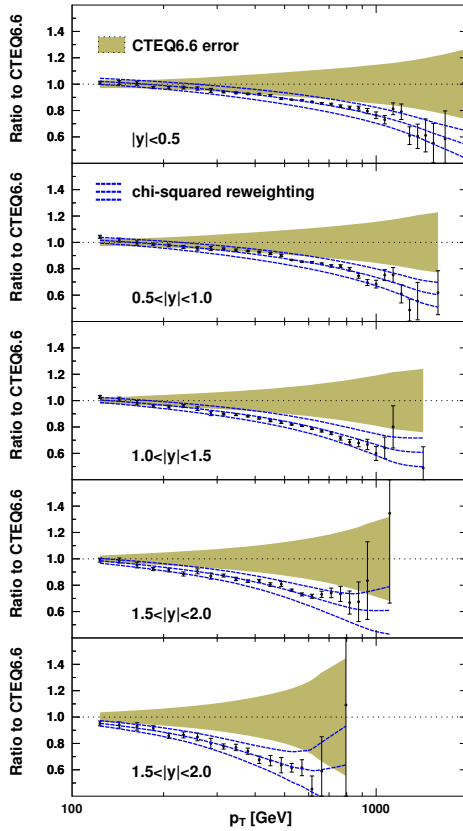


Figure 5: As Fig. 4 but with the Bayesian reweighting with chi-squared weights.

sense the data are compatible with the CTEQ6.6 PDFs in spite of the rather large  $\chi^2/N_{\text{data}} \approx 1.75$ . What comes to the chi-squared weights, they give rise to qualitatively similar but much larger effects. The value of  $\chi^2$  is almost ideal,  $\chi^2/N_{\text{data}} \approx 1$ , but the price to pay is increasing the original  $\chi^2$  of CTEQ6.6 clearly more than the tolerance,  $P \approx 480$ . As  $N_{\text{eff}}$  is also very low, one could think that these jet data completely disagree with CTEQ6.6. However, as our example of Section 4 demonstrated, the chi-squared weights do not properly account for the data in the original fit and such a conclusion would be flawed.

## 6. Summary

In summary, we have discussed different methods of PDF reweighting with an emphasis on a new technique, the Hessian reweighting. All the methods intend to “simulate” the full global fit and estimate the effects

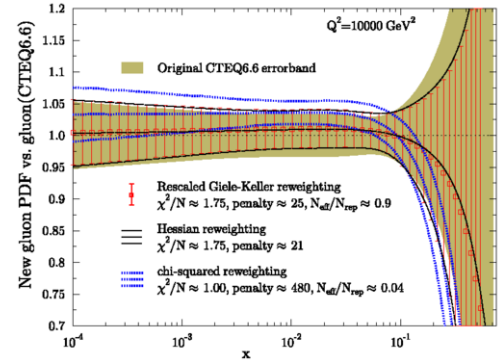


Figure 6: The gluon PDFs at  $Q^2 = 10000 \text{ GeV}^2$  after reweighting. Red points: Bayesian reweighting with rescaled GK weights. Blue dotted lines: Bayesian reweighting with chi-squared weights. Black dashed lines: Hessian reweighting. The colored band is the original CTEQ6.6 uncertainty. All results are normalized to the central set of CTEQ6.6.

that new experimental data would have on a set of PDFs. After outlining the underlying ideas, we compared the different approaches through a simple example identifying the correct ways to perform the reweighting in the case of Hessian PDF fits. Finally, we considered the inclusive jet production as an additional example. Our findings indicate that the correct way to reweight Hessian PDFs is different than what has been found to work for the PDF fits of NNPDF collaboration.

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