

xFitter 2.0.0: Heavy quark matching scales:

Unifying the FFNS and VFNS

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xFitter [1] is an open-source package that provides a framework for the determination of the parton distribution functions (PDFs) of the proton for many different kinds of analyses in Quantum Chromodynamics (QCD). It incorporates experimental data from a wide range of experiments including fixed-target, Tevatron, HERA, and LHC. xFitter version 2.0.0 has recently been released, and offers an expanded set of tools and options. The new xFitter 2.0.0 program links to the APFEL code [2] which has implemented generalized matching conditions that enable the switch from N_F to $N_F + 1$ active flavors at an arbitrary matching scale μ_m . This enables us to generalize the transition between a FFNS and a VFNS and essentially vary continuously between the two schemes; in this sense the matching scale μ_m allows us to unify the FFNS and VFNS in a common framework [3]. This paper provides a brief overview of xFitter with emphasis of these new features.

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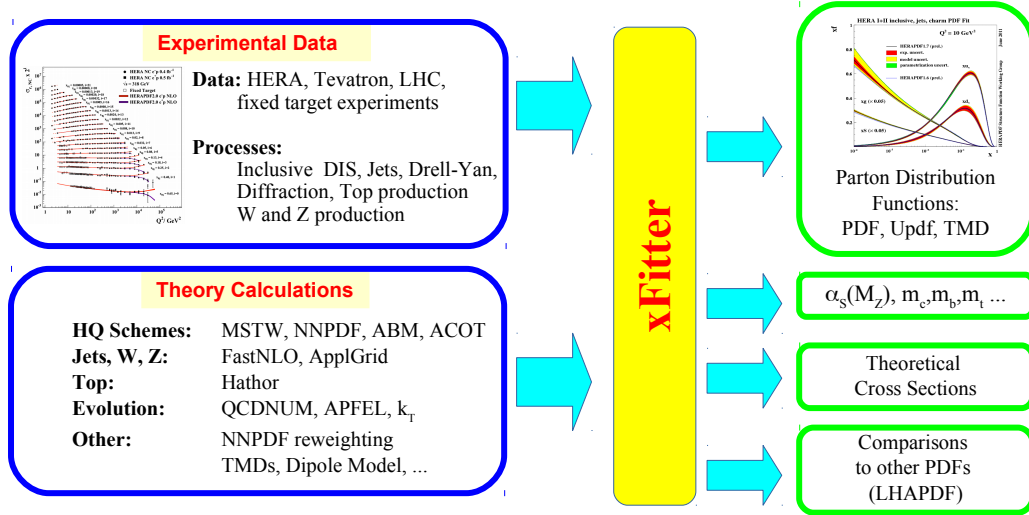


Figure 1: Schematic of the modular structure of xFitter illustrating the components and capabilities of the program.

1. Introduction

The Parton Distribution Functions (PDFs) are the essential components that allow us to make theoretical predictions for experimental measurements of protons and hadrons. The precision of the PDF analysis has advanced tremendously in recent years, and these studies are now performed with very high precision at NLO and NNLO in perturbation theory. The xFitter project¹ is an open source QCD fit framework that can perform PDF fits, assess the impact of new data, compare existing PDF sets, and perform a variety of other tasks [1]. The modular structure of xFitter allows for interfaces to a variety of external programs including: QCDNUM [4], APFEL [2], LHAPDF [5], APPLGRID [6], APFELGRID [7], FastNLO [8] and HATHOR [9]. A schematic of the modular structure is illustrated in Fig. 1.



xFitter 2.0.0
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An overview of the recent xFitter updates and available tutorials is available in Ref. [10]. In this short report we will focus on the implementation of a generalized heavy quark matching scale μ_m and the implications for PDF fits.²

2. The VFNS and FFNS

The inclusion of heavy quarks $Q = \{c, b, \dots\}$ into the PDF framework has been a formidable challenge. In the Fixed Flavor Number Scheme (FFNS), the heavy quark is excluded from the PDF parton-model framework; here, the heavy quark Q must be produced explicitly such as in the process $\gamma g \rightarrow Q\bar{Q}$. In contrast, in the Variable Flavor Number Scheme (VFNS), the heavy quark is included as a parton in the PDF at scales above the μ_m matching scale;³ thus, we have the option of exciting a heavy quark Q from within the proton, e.g. $\gamma Q \rightarrow Qg$.

¹xFitter can be downloaded from www.xFitter.org. An overview of the program can be found in Ref. [1].

²A more extensive report of these features can be found in Ref. [3].

³Details on the distinction between the matching and transition scales can be found in Ref. [11]

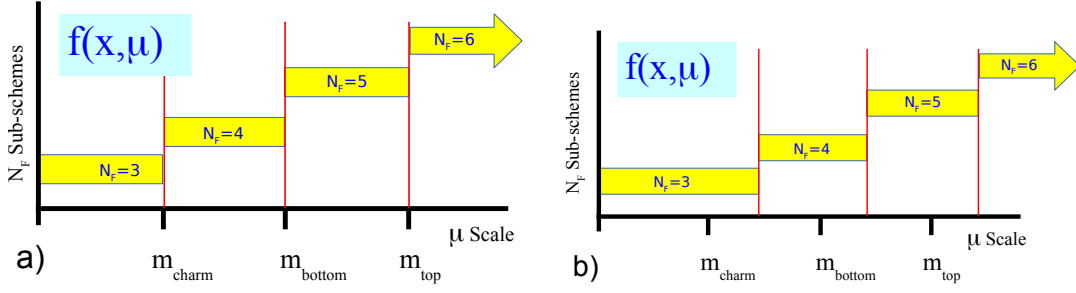


Figure 2: An illustration of the separate N_F renormalization sub-schemes which define a VFNS. Historically, the matching scales μ_m were chosen to be exactly the mass values $m_{c,b,t}$ as in Fig.-a. Fig.-b is a generalized case where the μ_m scales are chosen to be different from the mass values.

Both the FFNS and VFNS, as traditionally implemented, have advantages and disadvantages. The FFNS has the simplicity of avoiding an N_F flavor threshold in the PDFs, but at large energy scales (such as at the LHC) the heavy quarks $Q = \{c, b, \dots\}$ are treated differently from the light quarks.

Conversely, the VFNS has the advantage that it resums the heavy quark contributions using the DGLAP evolution and treats all the quarks on an equal footing at large energy scales; however, the VFNS can have some delicate cancellations when the heavy quark matching scale μ_m is similar to the heavy quark mass m_H . Traditionally in most implementations of the VFNS, the heavy quark matching scale was chosen equal to the heavy quark mass $\mu_m = m_H$ for a number of reasons as outlined in Ref. [3, 11]. The new xFitter 2.0.0 program does not impose $\mu_m = m_H$, and has the flexibility to choose any value for the matching scale μ_m ; thus, the difficulties of the traditional VFNS implementation with $\mu_m = m_H$ are avoided. In a general sense, the variable matching scale allows us to interpolate continuously between the traditional VFNS (with $\mu_m = m_H$) and the FFNS (with $\mu_m \rightarrow \infty$).

This situation is summarized diagrammatically in Fig. 2. In Fig. 2-a), we see the traditional choice where the matching scale μ_m is set equal to the heavy quark mass m_H . In Fig. 2-b), we remove the $\mu_m = m_H$ constraint and allow μ_m to take an arbitrary values. This is the new flexibility provided by xFitter 2.0.0.

3. Boundary Conditions

One of the key steps for implementing the variable heavy quark matching scales is the correct boundary conditions between the N_F and $N_F + 1$ active flavors. These boundary conditions are displayed in Fig. 3 for the case of the bottom quark PDF.

At NLO, if we match exactly at the bottom quark mass $\mu_b = m_b$, we find⁴ $f_b(x, \mu = m_b) = 0$. For values $\mu_b \neq m_b$, the boundary conditions are determined by the NLO contributions from the DGLAP evolution kernels, and this is displayed in Fig. 3-a). These contributions are driven by the $\ln(\mu/m_b)$ terms which are negative for $\mu < m_b$. At large μ scales, we observe the differences due to the choice of different boundary conditions; this is due to the (un-resummed) higher order $\mathcal{O}(\alpha_s^2)$ terms which are not included at NLO.

In Fig. 3-b) we display the NNLO matching conditions. In this case we find $x f_b(x, \mu) \neq 0$ for $\mu_b = m_b$. At this order, we have included terms of one higher order in α_s compared to the

⁴This accidental cancellation for \overline{MS} at NLO was, in part, the reason for the traditional VFNS choice $\mu_m = m_H$.

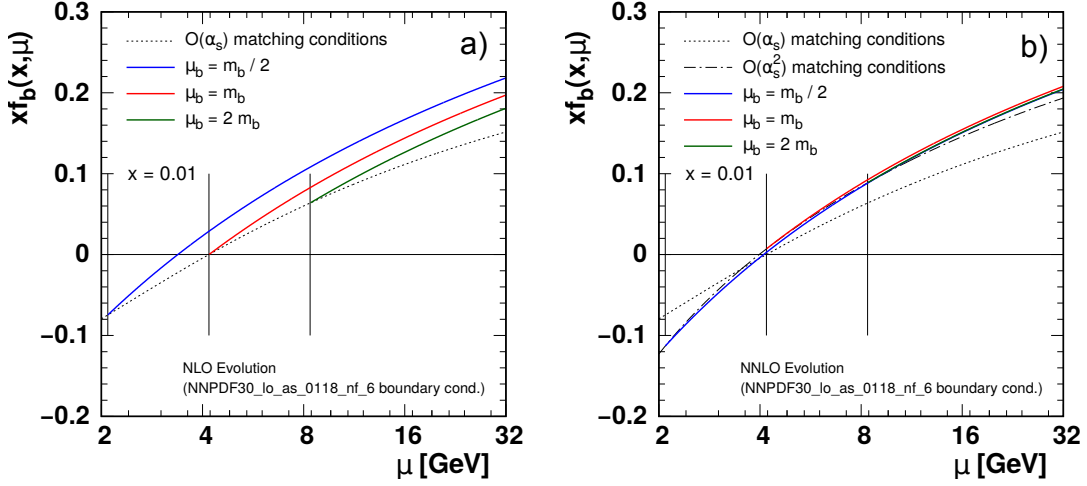


Figure 3: We display the b-quark PDF $x f_b^{(5)}(x, \mu)$ for different choices of the matching scales $\mu_m = \{m_b/2, m_b, 2m_b\}$ (indicated by the vertical lines) computed at NLO (Fig.-a) and NNLO (Fig.-b).

previous case, and we see this tremendously reduces the variation of $x f_b(x, \mu)$ for different choices of the matching scale μ_m . This behavior is crucial as the choice of the heavy quark matching scale amounts to a scheme choice, and the resulting physics observables should be insensitive up to the corresponding order of perturbation theory.

4. Scheme Independence

We can further illustrate the insensitivity of the physical observables to the choice of the heavy quark matching scale μ_m by examining the structure function $F_2^b(x, Q)$ displayed in Fig. 4. In Fig. 4-a) we compute $F_2^b(x, Q)$ at NLO for a choice of μ_m values; at large energy scales $Q \sim 32$ GeV we observe a large dependence on the choice of μ_m . In contrast, at NNLO in Fig. 4-b) the variation of $F_2^b(x, Q)$ is significantly reduced. Thus, the inclusion of the $\mathcal{O}(\alpha_s^2)$ NNLO contributions yields a result for the physical $F_2^b(x, Q)$ which is very stable w.r.t. μ_m .

Therefore, the NNLO implementation of the heavy quark matching scale in xFitter 2.0.0 has eliminated many of the difficulties previously encountered with the NLO VFNS with the traditional choice of $\mu_m = m_H$.

5. Impact on Fits

To facilitate comparisons of the NLO and NNLO results, Fig. 5 displays the ratio χ^2/χ_0^2 for charm (on the left) and bottom (on the right) where χ_0^2 is the value of the χ^2 at $\mu_m = m_H$. By plotting χ^2/χ_0^2 , we can better compare the fractional variation of χ^2 across the matching scale values.⁵ At NLO for the case of charm, the optimal heavy quark matching scale for μ_c is in the general range $\mu_c \sim m_c$. For lower scales ($\mu_c \ll m_c$), $\alpha_s(\mu)$ is large and the charm PDFs are negative. For higher scales ($\mu_c \gg m_c$), χ^2/χ_0^2 increases. At NNLO for the case of charm, the χ^2/χ_0^2 variation is greatly reduced ($\sim 2\%$), and there is minimal sensitivity to the μ_c scale in this range. For the case of bottom, the χ^2/χ_0^2 variation is very mild ($\sim 1\%$) for both NLO and NNLO; hence, the physics results are relatively insensitive to the particular choice of the heavy quark matching scale μ_b .

⁵See Ref. [3] for the full details of the fit.

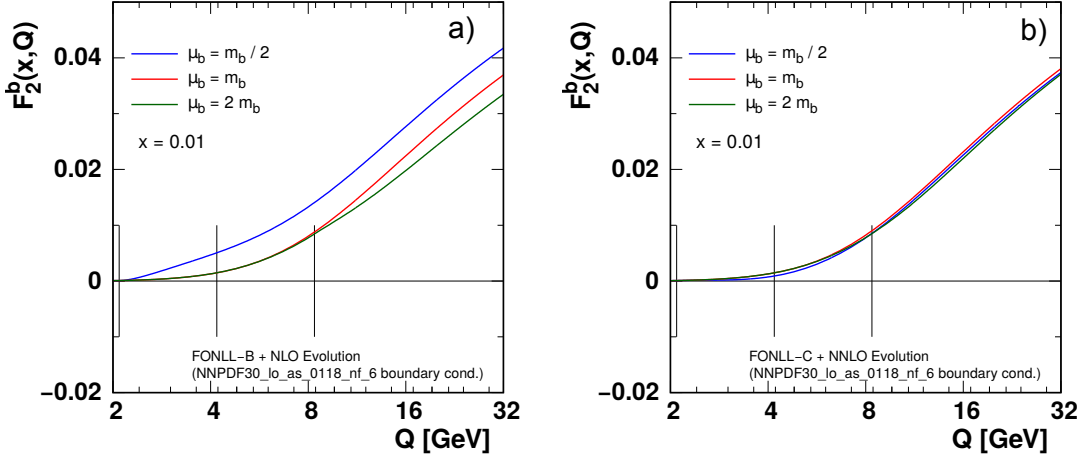


Figure 4: We display $F_2^b(x, Q)$ for different choices of the matching scales $\mu_m = \{m_b/2, m_b, 2m_b\}$ (indicated by the vertical lines) computed at NLO (Fig.-a) and NNLO (Fig.-b). Here, we have chosen $\mu = Q$. For details on the FONLL calculation see Ref. [12].

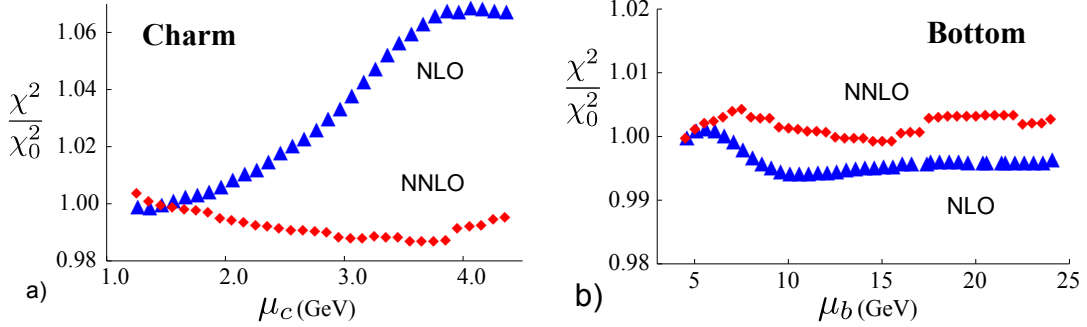


Figure 5: The ratio (χ^2/χ_0^2) of total χ^2 values (all data sets combined) as a function of the a) charm and b) bottom matching scale $\mu_{c,b}$ in GeV. χ_0^2 is the χ^2 value for μ_m equal to the quark mass. The triangles (blue \blacktriangle) are NLO and the diamonds (red \blacklozenge) are NNLO. The fits are from Ref. [3].

While the detailed characteristics of the above fits will depend on specifics of the analysis, there are two general patterns which emerge: i) the χ^2 variation of the NNLO results are generally reduced compared to the NLO results, and ii) the relative χ^2 variation across the bottom transition is reduced compared to the charm transition. For example, although the global χ^2 can be modified by different choices of data sets and weight factors, these general properties persist across separate data sets.[3] Additionally, there are a variety of prescriptions for computing the heavy flavor contributions; these primarily differ in how the higher order contributions are organized. As a cross check, we performed a NLO fit using the FONLL-A scheme; while the absolute value of χ^2 differed, the above general properties persisted.

The net result is that we can now quantify the theoretical uncertainty associated with the transition between different N_F sub-schemes. In practical applications, if we choose $\mu_c \sim m_c$, the impact of the $N_F = 3$ to $N_F = 4$ transition is reduced as this is often below the minimum kinematic cuts of the analysis (e.g. Q_{min}^2 and W_{min}^2). Conversely, the $N_F = 4$ to $N_F = 5$ transition is more likely to fall in the region of fitted data; hence, it is useful to quantify the uncertainty associated with the μ_b choice.

6. Conclusion

The xFitter 2.0.0 program is a versatile, flexible, modular, and comprehensive tool that can facilitate analyses of the experimental data and theoretical calculations. In this study we have examined the impact of the heavy flavor matching scales μ_m on a PDF fit to the combined HERA data set. These observations can be useful when performing fits. While charm has a larger χ^2 variation (especially at NLO), the charm quark mass $m_c \sim 1.45$ GeV lies in a region which is generally excluded by cuts in Q^2 and/or W^2 . On the contrary, the χ^2 variation for the bottom quark is relatively small at both NLO and NNLO. Since the bottom quark mass $m_b \sim 4.5$ GeV is in a region where there is abundance of precision HERA data, this flexibility allows us to shift the heavy flavor threshold (and the requisite discontinuities) away from any particular data set. Functionally, this means that we can analyze the HERA data using an $N_F = 4$ flavor scheme up to relatively large μ scales, and then perform the appropriate NNLO matching (with the associated constants and log terms) so that we can analyze the high-scale LHC data in the $N_F = 5$ or even $N_F = 6$ scheme.

These variable heavy flavor matching scales μ_m allow us to generalize the transition between a FFNS and a VFNS, and provides a theoretical “laboratory” which can quantitatively test proposed implementations. In conclusion, we find that the ability to vary the heavy flavor matching scales μ_m , not only provides new insights into the intricacies of QCD, but also has practical advantages for PDF fits.

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