

## Theoretical Procedures and the effect on PDFs and $\alpha_S(M_Z^2)$

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I consider the effect on partons distribution functions (PDFs) of changes in the theoretical procedure used in a PDF fit. I consider using the 3-flavour fixed flavour number scheme instead of the standard general mass variable flavour number scheme used in the MSTW analysis. This results in the light quarks increasing at most  $x$  values, the gluon distribution becoming softer at high values of  $x$  and larger at small  $x$ , and the coupling constant  $\alpha_S(M_Z^2)$  falling, particularly at NNLO. The fit quality also deteriorates. I also consider lowering the kinematic cut on  $W^2$  for DIS data and introducing higher twist terms which are fit to data. This results in much smaller effects on both PDFs and  $\alpha_S(M_Z^2)$ , with changes generally smaller than uncertainties, except for quarks at very high  $x$ . I show that the fixed flavour scheme and variable flavour scheme structure functions differ significantly for  $x \sim 0.01$  at high  $Q^2$ . I demonstrate that in the fixed flavour scheme there is a slow convergence of large logarithmic terms of the form  $(\alpha_S \ln(Q^2/m_c^2))^n$  in this regime. I conclude that some major differences in PDF sets are largely due to the choice of flavour scheme used.

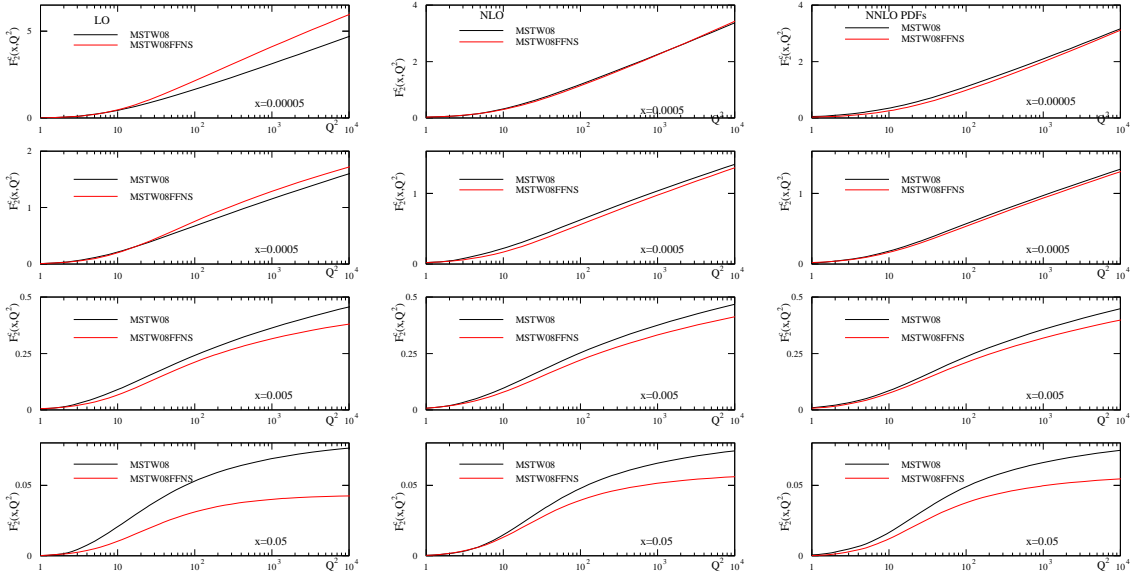
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There have recently been improvements in the PDF determinations by the various groups, generally making the predictions more consistent. However, there are still some large differences which are sometimes much bigger than the individual PDF uncertainties [1, 2, 3]. This is particularly the case for cross sections depending on the high- $x$  gluon. In this article I investigate potential reasons, based on different theoretical procedures that can be chosen for a PDF fit.

I first examine the number of active quark flavour used in the calculation of structure functions, where there are two choices for how one treats the charm and bottom quark contributions. In the  $n_f = 3$  Fixed Flavour Number Scheme (FFNS)  $F(x, Q^2) = C_k^{FF, n_f}(Q^2/m_H^2) \otimes f_k^{n_f}(Q^2)$ , i.e. for  $Q^2 \sim m_c^2$  massive quarks are only created in the final state. This is exact but does not sum all  $\alpha_S^n \ln^n Q^2/m_c^2$  terms in the perturbative expansion. The FFNS is known at NLO [4] but not fully at NNLO ( $\mathcal{O}(\alpha_S^3 C^{FF,3})$ ). Approximate results can be derived e.g. [5], (and are sometimes used in fits, e.g. [6]) but these NNLO corrections are not large except near threshold and very low  $x$ . In a variable flavour scheme one uses the fact that at  $Q^2 \gg m_c^2$  the heavy quarks behave like massless partons and the  $\ln(Q^2/m_c^2)$  terms are summed via evolution. PDFs in different number regions are related perturbatively,  $f_j^{n_f+1}(Q^2) = A_{jk}(Q^2/m_H^2) \otimes f_k^{n_f}(Q^2)$  where the perturbative matrix elements  $A_{jk}(Q^2/m_H^2)$  are known exactly to NLO [7]. The original Zero Mass Variable Flavour Number Scheme (ZM-VFNS) ignores  $\mathcal{O}(m_c^2/Q^2)$  corrections in cross sections, i.e.  $F(x, Q^2) = C_j^{ZM, n_f} \otimes f_j^{n_f}(Q^2)$ , but this is an approximation at low  $Q^2$  and PDF groups use a General-Mass Variable Flavour Number Scheme (GM-VFNS) taking one from the two well-defined limits of  $Q^2 \leq m_c^2$  and  $Q^2 \gg m_c^2$  instead. Some variants are reviewed in [8].

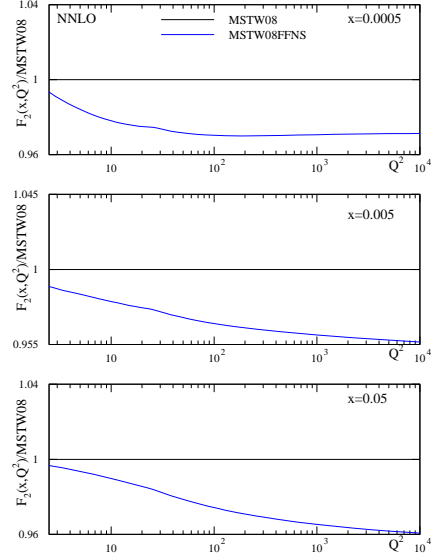


**Figure 1:**  $F_2^c(x, Q^2)$  using the FFNS and GM-VFNS at LO, NLO and NNLO.

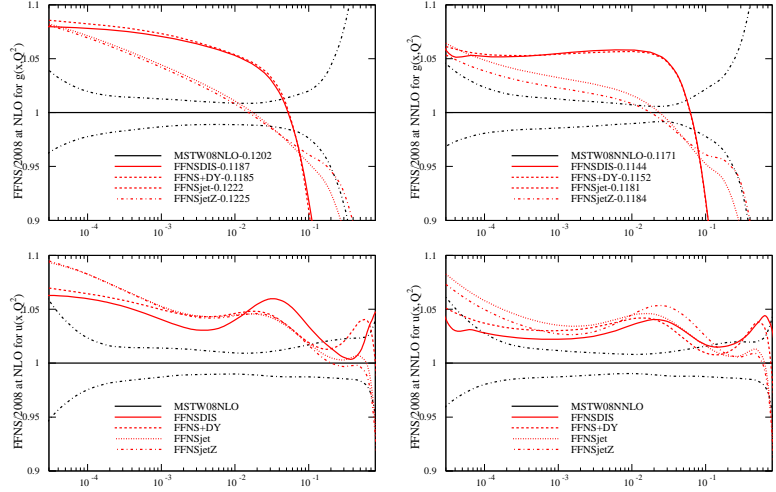
The predictions using FFNS and the TR' GM-VFNS [9] for  $F_2^c(x, Q^2)$  using the MSTW2008 input distributions [10] are shown in Fig. 1. At LO there is a big difference between the two. At NLO  $F_2^c(x, Q^2)$  at high  $Q^2$  for the FFNS is nearly always lower than for the GM-VFNS, significantly so at higher  $x \sim 0.01$ . For FFNS at NNLO only NLO coefficient functions are used, but (various choices of) approximate  $\mathcal{O}(\alpha_S^3)$  corrections give only minor increases. There is no dramatic improvement in the agreement between FFNS and GM-VFNS at NNLO compared to NLO, contrary to what one might expect.

This 20-40% difference in  $F_2^c(x, Q^2)$  can lead to over 4% changes in the total  $F_2(x, Q^2)$ , see Fig 2. At  $x \sim 0.01$  this is mainly due to  $F_2^c(x, Q^2)$ . At lower  $x$  there is a contribution to the difference from light quarks evolving slightly more slowly in FFNS. For  $x > 0.1$  the FFNS and GM-VFNS are very similar. In order to test the importance of this difference I have extended an investigation in [12] and performed fits using the FFNS scheme. At NNLO  $\mathcal{O}(\alpha_S^2)$  heavy flavour coefficient functions are used as default (which has been done in other fits, e.g. [11]). Approximate  $\mathcal{O}(\alpha_S^3)$  expressions change the results very little. Fits are primarily to only DIS and Drell-Yan data, but are also extended to Tevatron jet and Drell-Yan data using the 5-flavour scheme in these cases. The data chosen are as in [10]. The fit quality for DIS and Drell-Yan data are at least a few tens of units higher in  $\chi^2$  in the FFNS fit than in the MSTW2008 fit. FFNS is often slightly better for  $F_2^c(x, Q^2)$ , but is flatter in  $Q^2$  for  $x \sim 0.01$  for the total  $F_2(x, Q^2)$ . When using the FFNS the fit quality for DIS and Drell Yan deteriorates by  $\sim 50$  units when Tevatron jet and  $W, Z$  data are included, as opposed to 10 units or less when using a GM-VFNS. The resulting PDFs evolved up to  $Q^2 = 10,000\text{GeV}^2$  (using variable flavour evolution for consistent comparison) are shown in Fig. 3. The PDFs and  $\alpha_S(M_Z^2)$  are different in form to the MSTW2008 PDFs, with larger light quarks, a gluon which is bigger at low  $x$  and much smaller at high  $x$  and a smaller  $\alpha_S(M_Z^2)$ . Some similar differences have been noted in [13, 14]. Using FFNS rather than GM-VFNS leads to much larger changes than any variation in choice of GM-VFNS [12].

I have also investigated the effect of lowering the  $W^2$  cut to  $5\text{ GeV}^2$  and parameterising higher twist corrections in the form  $(D_i/Q^2)F_2(x, Q^2)$  in 13 bins of  $x$ , and fitting the  $D_i$  and PDFs simultaneous, as in [15]. The  $D_i$  are similar to this older study, though larger at the smallest  $x$ . The effect on the PDFs and  $\alpha_S(M_Z^2)$  is small, using either FFNS or GM-VFNS, except for very high- $x$  quarks, as shown in Fig. 4. I also perform FFNS fits restricting higher twist from the lowest  $x$  values and omitting the less theoretically clean nuclear target data (except dimuon cross sections, which constrain the strange quark). This results in values of  $\alpha_S$  of  $\alpha_S(M_Z^2) = 0.1179$  at NLO and  $\alpha_S(M_Z^2) = 0.1136$  at NNLO, very close to those in [11], where the scheme choice, data types, and form of higher twist (and the resulting PDFs) are similar.



**Figure 2:** The ratio of  $F(x, Q^2)$  using the FFNS to that using the GM-VFNS.



**Figure 3:** Ratios of PDFs in various FFNS fits to the MSTW2008 PDFs.

I also perform fits where  $\alpha_S(M_Z^2)$  is fixed to the higher value obtained in the GM-VFNS. This results in the FFNS gluon being a little closer to that using GM-VFNS, as shown in the left of Fig. 5 and very similar to [14], where studies are performed with fixed  $\alpha_S(M_Z^2)$ . The fit quality to DIS and low-energy DY data in the FFNS fit is 8 units worse when  $\alpha_S(M_Z^2) = 0.1171$  than for 0.1136. The fit to HERA data is better, but worse for fixed target data. One can understand the need for  $\alpha_S$  to be smaller in FFNS. To compensate for smaller  $F_2^c(x, Q^2)$  at  $x \sim 0.05$  the FFNS gluon must be bigger in this region, and from the momentum sum rule, is smaller at high  $x$ . The correlation between the high- $x$  gluon and  $\alpha_S$  when fitting high- $x$  DIS data drives  $\alpha_S$  down (for reduced gluon the quarks fall with  $Q^2$  too quickly, hence the need to lower  $\alpha_S$ ), requiring the small  $x$  gluon to even bigger, until stability is reached.

To explain the differences between FFNS and GM-VFNS evolution, shown for  $Q^2 = 500\text{GeV}^2$  in the right of Fig. 5, I consider high  $Q^2$ . At LO in the FFNS (setting all scales as  $Q^2$ )

$$\begin{aligned} F_2^{c,1,FF} &= \alpha_S \ln(Q^2/m_c^2) p_{qg}^0 \otimes g + \mathcal{O}(\alpha_S \cdot g) \equiv \alpha_S A_{Hg}^{1,1} \otimes g + \mathcal{O}(\alpha_S \cdot g), \\ \rightarrow dF_2^{c,1,FF}/d\ln Q^2 &= \alpha_S p_{qg}^0 \otimes g + \ln(Q^2/m_c^2) d(\alpha_S p_{qg}^0 \otimes g)/d\ln Q^2 + \dots \end{aligned} \quad (1)$$

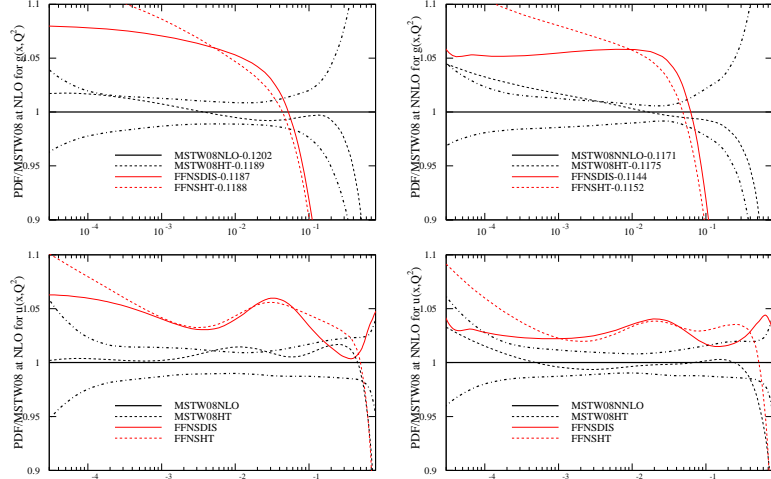
At LO in the GM-VFNS, where  $F_2^{c,1,VF} = (c + \bar{c}) = c^+$  we have

$$dc^+/d\ln Q^2 = \alpha_S p_{qg}^0 \otimes g + \alpha_S p_{qq}^0 \otimes c^+, \quad c^+ \equiv \alpha_S \ln(Q^2/m_c^2) p_{qg}^0 \otimes g + \dots \equiv \alpha_S A_{Hg}^{1,1} \otimes g + \dots \quad (2)$$

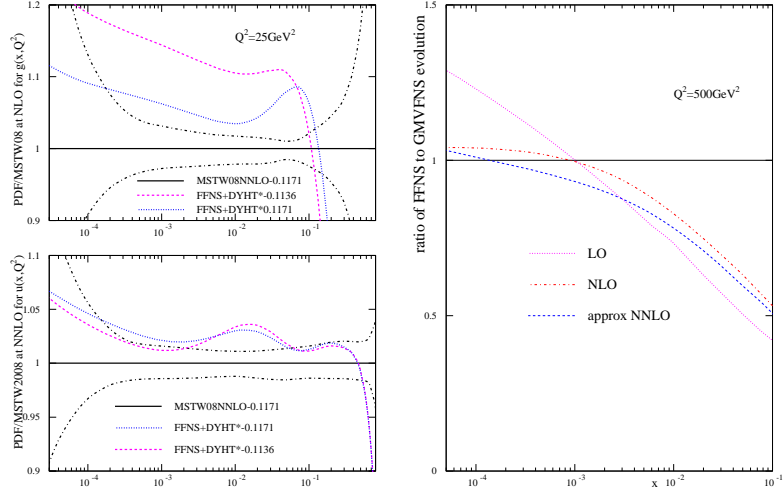
The first terms in each expression are equivalent. The difference between the LO expressions is

$$d(F_2^{c,1,VF} - F_2^{c,1,FF})/d\ln Q^2 = \alpha_S^2 \ln(Q^2/m_c^2) p_{qg}^0 \otimes (p_{qq}^0 + \beta_0 - p_{gg}^0) \otimes g + \dots \equiv P_{VF-FF}^{\text{LO}} \otimes g + \dots \quad (3)$$

where  $\beta_0 = 9/(4\pi)$ . The effect of  $p_{gg}^0$  is negative at high  $x$  and positive at small  $x$ . That of  $p_{qq}^0$  is negative at high  $x$ , but smaller than  $p_{gg}^0$ . Hence, the difference is large and positive at high  $x$  and



**Figure 4:** Ratios of PDFs with higher twist corrections to PDFs without. The fit to HERA data is better, but worse for fixed target data. One can understand the need for  $\alpha_S$  to be smaller in FFNS. To compensate for smaller  $F_2^c(x, Q^2)$  at  $x \sim 0.05$  the FFNS gluon must be bigger in this region, and from the momentum sum rule, is smaller at high  $x$ . The correlation between the high- $x$  gluon and  $\alpha_S$  when fitting high- $x$  DIS data drives  $\alpha_S$  down (for reduced gluon the quarks fall with  $Q^2$  too quickly, hence the need to lower  $\alpha_S$ ), requiring the small  $x$  gluon to even bigger, until stability is reached.



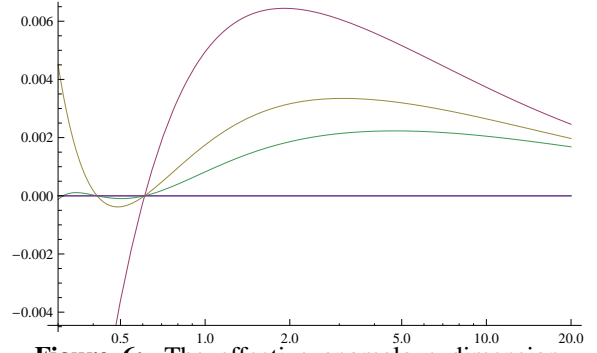
**Figure 5:** The ratio of FFNS fits with both free (red) and fixed  $\alpha_S(M_Z^2)$  (blue) to the MSTW2008 PDFs (left) and the ratio of  $dF_2^c/d\ln Q^2$  using the FFNS to that using the GM-VFNS (right).

large and negative at small  $x$ , as observed in Fig 5. Moreover, this difference must be eliminated at NLO by defining the leading-log term in the FFNS expression to provide cancellation, i.e.

$$F_2^{c,2,FF} = \alpha_S^2 A_{Hg}^{2,2} \otimes g + \dots = 1/2 \alpha_S^2 \ln^2(Q^2/m_c^2) p_{qg}^0 \otimes (p_{qq}^0 + \beta_0 - p_{gg}^0) \otimes g + \mathcal{O}(\alpha_S^2 \ln(Q^2/m_c^2)). \quad (4)$$

up to quark mixing corrections and sub-dominant terms. In the NLO evolution all  $\mathcal{O}(\alpha_S^2 \ln(Q^2/m_c^2))$  terms cancel in the difference. However, the derivative of  $F_2^{c,2,FF}$  contains  $1/2 \ln^2(Q^2/m_c^2) d(\alpha_S^2 p_{qg}^0 \otimes (p_{qq}^0 + \beta_0 - p_{gg}^0) \otimes g) / d \ln Q^2$  which does not cancel. This leads to  $P_{VF-FF}^{\text{NLO}} = 1/2 \alpha_S \ln(Q^2/m_c^2) (p_{qq}^0 + 2\beta_0 - p_{gg}^0) \otimes P_{VF-FF}^{\text{LO}}$ . The factor of  $(p_{qq}^0 + 2\beta_0 - p_{gg}^0)$  is large, positive at high  $x$  and negative at small  $x$ , but not until smaller  $x$  than at LO. Therefore,  $P_{VF-FF}^{\text{NLO}}$  is large and positive at high  $x$ , negative for smaller  $x$  and positive for extremely small  $x$ . This explains the behaviour correctly. Repeating the argument at NNLO  $P_{VF-FF}^{\text{NNLO}} = 1/3 \alpha_S \ln(Q^2/m_c^2) (p_{qq}^0 + 3\beta_0 - p_{gg}^0) \otimes P_{VF-FF}^{\text{LO}}$  This is large and positive at high  $x$  then changes sign twice but stays small until becoming negative at tiny  $x$ . Again this explains the behaviour correctly.

To look at the effect of this dominant high- $Q^2$  difference between GM-VFNS and FFNS evolution, it is useful to define the moment space anomalous dimension  $\mathcal{W}_{VF-FF}$  obtained from  $P_{VF-FF}$ . This is shown at LO, NLO and NNLO for  $Q^2 = 500\text{GeV}^2$  in Fig. 6. At high  $Q^2$ , values of  $x \sim 0.05$  correspond to  $N \sim 2$ , where  $\mathcal{W}_{VF-FF}$  only tends to zero slowly as the perturbative order increases. This explains why FFNS evolution for  $x \sim 0.05$  only slowly converges to the GM-VFNS result with increasing order.



**Figure 6:** The effective anomalous dimension  $\mathcal{W}_{VF-FF}(N)$  at LO (purple), NLO (brown) and NNLO (green).

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