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The Effect of Variable Flavour Number Scheme Variations on PDFs and Cross Sections

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I consider variations in the definition of a general-mass variable flavour number scheme (GM-VFNS) for heavy flavour structure functions, both at next-to-leading order (NLO) and at next-to-next-to leading order (NNLO).I also define a new "optimal" scheme choice improving the smoothness of the transition from one flavour number to the next. At both NLO and NNLO I investigate the variation of the structure function for a fixed set of parton distribution functions (PDFs) and also the change in the distributions when a new MSTW-type global fit to data is performed for each GM-VFNS. At NLO the parton distributions, and predictions using them at hadron colliders, can vary by $\sim 2\%$ from the mean value. Use of the the zero-mass variable flavour number scheme, which is simpler but only an approximation, leads to results a further couple of percent or more outside this range. At NNLO there is far more stability with varying GM-VFNS definition. Typical changes in PDFs and predictions are less than 1%, with most variation at very small x values. This demonstrates that mass-scheme variation is an additional and significant source of uncertainty when considering parton distributions, but like other theoretical uncertainties, it diminishes quickly as higher orders are included.

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The treatment of heavy flavours, charm and bottom, in structure functions has an important impact on the PDFs extracted in fits, due to direct data on $F_2^h(x,Q^2)$ and also the contribution the total structure function at small x. There are two distinct regimes with different descriptions. For $Q^2 \sim m_h^2$ massive quarks are created in the final state, and described using the Fixed Flavour Number Scheme (FFNS) (see [1] for NLO results), $F(x,Q^2) = C_k^{FF,n_f}(Q^2/m_h^2) \otimes f_k^{n_f}(Q^2)$, where n_f is the number of light quarks. This does not sum $\alpha_S^n \ln^n Q^2/m_h^2$ terms in the perturbative expansion which may be important. At high scales, $Q^2 \gg m_h^2$, heavy quarks behave like massless partons and the logs are summed via evolution equations. The distributions for different light quark number are related to each other perturbatively $f_j^{n_f+1}(Q^2) = A_{jk}(Q^2/m_H^2) \otimes f_k^{n_f}(Q^2)$, where the matrix elements $A_{jk}(Q^2/m_H^2)$, calculated at $\mathcal{O}(\alpha_S^2)$ in [2], contain the fixed-order $\ln(Q^2/m_h^2)$ contributions. In the $Q^2/m_h^2 \to \infty$ limit the description is the Zero-Mass Variable Flavour Number Scheme (ZM-VFNS), $F(x,Q^2) = C_j^{ZMVF,n_f} \otimes f_j^{n_f}(Q^2)$. This is approximate, ignoring all $\mathcal{O}(m_h^2/Q^2)$ corrections. To correct this shortcoming and obtain a correct description between the two limits of $Q^2 \leq m_H^2$ and $Q^2 \gg m_H^2$, one can use a General-Mass Variable Flavour Number Scheme (GM-VFNS).

The GM-VFNS can be defined from equivalence of the n_f flavour and n_f+1 flavour descriptions at all orders, resulting in $C_k^{FF,n_f}(Q^2/m_h^2) = C_j^{GMVF,n_f+1}(Q^2/m_h^2) \otimes A_{jk}(Q^2/m_h^2)$, e.g. at $\mathcal{O}(\alpha_S)$

$$C_{2,hg}^{FF,n_f,(1)}(Q^2/m_h^2) = C_{2,h\bar{h}}^{GMVF,n_f+1,(0)}(Q^2/m_h^2) \otimes P_{qg}^0 \ln(Q^2/m_h^2) + C_{2,hg}^{GMVF,n_f+1,(1)}(Q^2/m_h^2), \quad (1)$$

The VFNS coefficient functions tend to the massless limits as $Q^2/m_h^2 \to \infty$, but $C_j^{GMVF}(Q^2/m_h^2)$ is only uniquely defined in this limit. One can swap $\mathcal{O}(m_h^2/Q^2)$ terms between $C_{2,h\bar{h}}^{GMVF,(0)}(Q^2/m_h^2)$ and $C_{2,g}^{GMVF,(1)}(Q^2/m_h^2)$ in Eq. (1), and at higher orders, leading to various prescriptions [3, 4, 5, 6, 7]. The TR GM-VFNS [4] highlighted the freedom in choice, and enforced correct kinematics via a quite complicated definition. The (S)ACOT(χ) prescription [6] applied the simple choice $C_{2,h\bar{h}}^{GMVF,(0)}(Q^2/m_h^2,z) \propto \delta(z-x_{\max})$, which gives $F_2^{h,(0)}(x,Q^2) \propto e_h^2(h+\bar{h})(x/x_{\max},Q^2)$, where $x_{\max} = Q^2/(Q^2+4m_h^2)$, and imposes the threshold $W^2 = Q^2(1-x)/x \geq 4m_h^2$. This gives the usual limit $C_{2,h\bar{h}}^{ZMVF,(0)}(z) = \delta(1-z)$ for $Q^2/m_h^2 \to \infty$. The TR' scheme [7] adopted this and extensions to higher orders (though uses a different multiplicative factor of $Q^2/(Q^2+4m_h^2)$ [8]). However, ACOT-type schemes have used the same order of α_S above and below $Q^2 = m_h^2$, despite the fact that FFNS is LO at $\mathcal{O}(\alpha_S)$ while ZM-VFNS starts at zeroth order. Instead the TR' definition uses, for example, at LO the $\mathcal{O}(\alpha_S)$ FFNS result for $Q^2 < m_h^2$, and for $Q^2 > m_h^2$

$$F_2^h(x,Q^2) = \alpha_S(m_h^2) C_{2,hg}^{FF,n_f,(1)}(1) \otimes g^{n_f}(m_h^2) + C_{2,h\bar{h}}^{GMVF,n_f+1,(0)}(Q^2/m_h^2) \otimes (h+\bar{h})(Q^2), \quad (2)$$

i.e. it freezes the higher order α_S term when going upwards through $Q^2 = m_h^2$. This difference in choice can be phenomenologically important. As an alternative, but ultimately equivalent, formulation of a GM-VFNS, BMSN [2] and FONLL [8] define a scheme in general terms as

$$F^{\rm GMVF}(x,Q^2) = F_2^{\rm FF}(x,Q^2) - F_2^{\rm asymp}(x,Q^2) + F_2^{\rm ZMVF}(x,Q^2) \quad (3)$$

where the second (subtraction) term is the asymptotic version of the first, i.e., all terms $\mathcal{O}(m_h^2/Q^2)$ are omitted. There are differences in exactly how the second and third terms are defined in detail in different schemes. In the simplest applications the α_S order of $F^{\rm FF}(x,Q^2)$ at low Q^2 is the same as that of $F^{\rm ZMVF}(x,Q^2)$ as $Q^2 \to \infty$. There is a version of FONLL which uses one power higher in the FFNS term, but it leads to part of the higher order contribution persisting as $Q^2 \to \infty$.

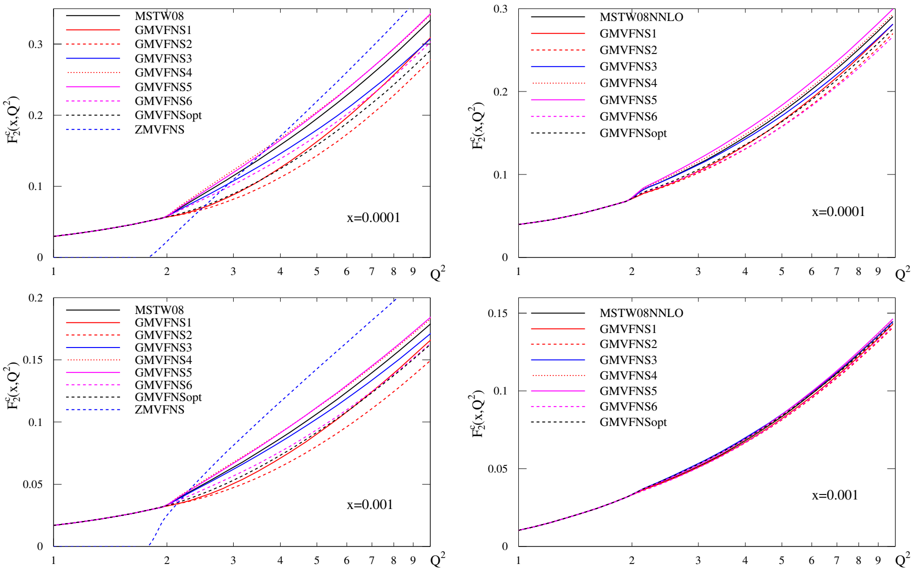

Figure 1: The variation in $F_2^c(x,Q^2)$ generated from a variety of choices of GM-VFNS at NLO (left) and NNLO (right) using the MSTW2008 pdfs in each case.

Ideally one would like any GM-VFNS to reduce to exactly the correct order FFNS at low Q^2 and exactly the correct order (one power of α_S lower) ZM-VFNS as $Q^2 \to \infty$. At present none do, but this can easily be rectified. Let us return to the TR' version of the GM-VFNS. The obstacle is the presence of the frozen term as $Q^2 \to \infty$ (which depends on the PDFs only at low scales, so is a small effect at large Q^2). In fact, this is not strictly necessary and one can have instead

scheme	a	b	c	d
GM-VFNS1	0	-1	1	0
GM-VFNS2	0	-1	0.5	0
GM-VFNS3	1	0	0	0
GM-VFNS4	0	0.3	1	0
GM-VFNS5	0	0	0	0.1
GM-VFNS6	0	0	0	-0.2
optimal	1	-2/3	1	0

Table 1: Parameter values for different extreme GM-VFNS definitions.

$$(m_h^2/Q^2)^a \alpha_S^n(m_h^2) \sum C_{2,i}^{\rm FF}(m_h^2) \otimes f_i(m_h^2) \qquad \text{or} \qquad (m_h^2/Q^2)^a \alpha_S^n(Q^2) \sum C_{2,i}^{\rm FF}(Q^2) \otimes f_i(Q^2). \tag{4}$$

Any $a > 0$ provides the correct limit, though strictly from factorization one should have (m_H^2/Q^2) times $\ln(Q^2/m_H^2)$ terms. There is also more freedom. One can modify the heavy quark coefficient function as long as the $Q^2/m_h^2 \to \infty$ limit is maintained. However, since this appears in convolutions for higher order subtraction terms, we do not want a complicated x dependence. A simple choice is

$$C_{2,h\bar{h}}^{GMVF,(0)}(Q^2/m_h^2, z) \to (1 + b(m_h^2/Q^2)^c)\delta(z - x_{\rm max}), \tag{5}$$

where again variation in c really mimics (m_h^2/Q^2) with logarithmic corrections. One can also modify the argument of the δ-function, similar to the Intermediate-Mass IM scheme [9],

$$\xi = x/x_{\rm max} \to x\big(1 + (x(1 + 4m_h^2/Q^2))^d 4m_h^2/Q^2\big), \tag{6}$$

so the kinematic limit stays the same, but if $d > 0 (< 0)$ small x is less (more) suppressed. The default a, b, c, d are all zero, but can vary, being limited by fit quality or *sensible* choices.

A variety of different choices defined in Table 1 has been tried at NLO and at NNLO along with the ZM-VFNS (at NLO). The resulting variations in $F_2^c(x,Q^2)$ near the transition point due to different choices of GM-VFNS at NLO are shown in the left of Fig. 1. I also define an “optimal”

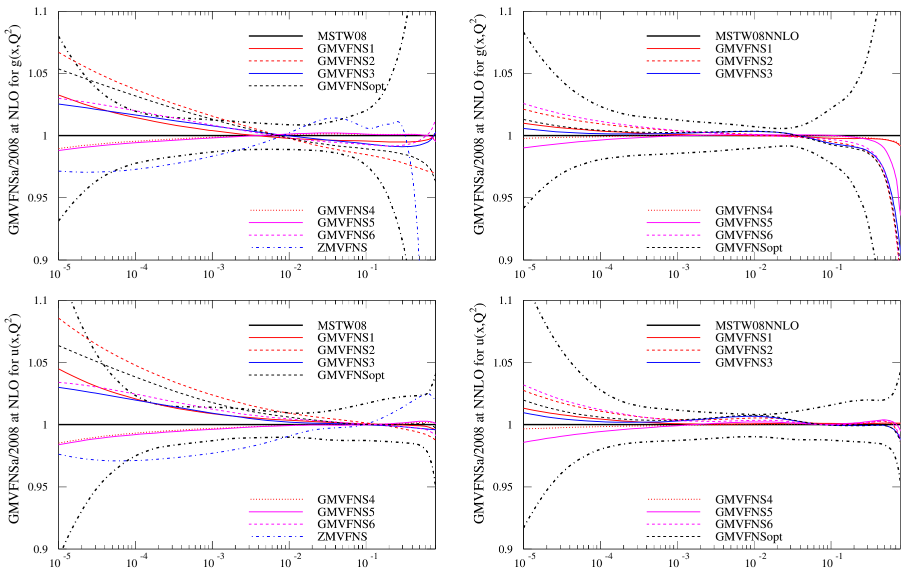

Figure 2: The variation of PDFs obtained from the best fit from a variety of choices of GM-VFNS and the ZM-VFNS at NLO (left) and NNLO (right) as a ratio to the MSTW2008 PDFs.

scheme which is smooth at threshold and reduces to exactly the right limits at high and low Q^2. There is quite a spread at NLO, though the ZM-VFNS is far steeper at low Q^2 than any GM-VFNS. This spread is very much reduced at NNLO, the right of Fig. 1, with almost zero variation until very small x, showing that NNLO evolution effects are most important in this regime.

Global fits are also performed using the same procedure as the MSTW08 fit [10] for all schemes. At NLO the initial χ^2 for a new scheme can change by 250, but converges to within 20 of the original. There are improved fits for options 1, 3 and 6 and the fit is best for the for optimal scheme. The variations in the partons extracted at NLO are shown in the left of Fig. 2. The default TR' scheme sits near the low end. Some changes in PDFs exceed the one σ *uncertainty*. $\alpha_S(M_Z^2)$ changes by < 0.0007 except for the ZM-VFNS where it falls by 0.0015. The ZM-VFNS PDF is clearly outside than the GM-VFNS band. For fits at NNLO the initial changes in χ^2 are < 20 and they converge to within 10 of the original. The variations in PDFs extracted at NNLO are shown in the right of Fig. 2. At worst the changes approach the *uncertainty*, but are usually far less. Variations in $\alpha_S(M_Z^2)$ are ~ 0.0003. However, at NNLO the TR' scheme models the $\mathcal{O}(\alpha_S^3)$ FFNS terms at low Q^2 using leading threshold logarithms [11] and $\ln(1/x)$ terms [12]. The latter take the form $\propto (1-z/x_{\max})^{\tilde{a}}(\ln(1/z)-\tilde{b})/z$, where the default is $\tilde{a}=20, \tilde{b}=4$, so $\tilde{a}$ and $\tilde{b}$ can be varied. Changes in $\tilde{a}$ make little difference. The maximum *sensible* variation to $\tilde{b}=2$ leads to an effect of order the uncertainty at $x \leq 0.001$. However, this is largely eliminated if the $\mathcal{O}(\alpha_S^3)$ contribution dies away, rather than being frozen.

PDF set	Tev		LHC	(14 TeV)
	σ_Z (nb)	σ_H(pb)	σ_Z (nb)	σ_H(pb)
MSTW08	7.207	0.7462	59.25	40.69
GMvar1	+0.3%	−0.5%	+1.1%	+0.2%
GMvar2	+0.7%	−1.1%	+3.0%	+1.5%
GMvar3	+0.1%	−0.3%	+1.1%	+0.8%
GMvar4	+0.0%	−0.1%	−0.4%	−0.2%
GMvar5	−0.1%	−0.1%	−0.5%	−0.3%
GMvar6	+0.3%	−0.4%	+1.6%	+0.8%
GMvaropt	+0.3%	−1.5%	+2.0%	+0.4%
ZM-VFNS	−0.7%	−1.2%	−3.0%	−3.1%
GMvarcc	+0.0%	−0.1%	+0.0%	−0.1%

Table 2: Predicted cross-sections at NLO for Z and a 120 GeV Higgs boson at the Tevatron and LHC.

PDF set	Tev		LHC	(14 TeV)
	σ_Z (nb)	σ_H(pb)	σ_Z (nb)	σ_H(pb)
MSTW08	7.448	0.9550	60.93	50.51
GMvar1	+0.1%	−0.5%	+0.1%	−0.2%
GMvar2	+0.3%	−0.8%	+0.5%	+0.1%
GMvar3	+0.4%	−0.1%	+0.5%	+0.7%
GMvar4	+0.0%	−0.2%	+0.1%	−0.1%
GMvar5	+0.1%	−0.3%	−0.2%	−0.2%
GMvar6	+0.1%	−0.9%	+0.3%	−0.2%
GMvaropt	+0.4%	−0.2%	+0.6%	+0.8%
GMvarmod	−0.2%	−0.4%	−1.4%	−1.0%
GMvarmod′	+0.0%	−0.7%	+0.0%	+0.1%

Table 3: Predicted cross-sections at NNLO for Z and a 120 GeV Higgs boson at the Tevatron and LHC.

The predictions for cross-sections are shown at NLO in Table. 2. There is at most a 1.5% variation at the Tevatron. There is a +3% down to −0.5% variation in σ_Z at the LHC. The spread in σ_H is about halved due to the higher average x sampled. The ZM-VFNS is the clear outlier in the low direction at the LHC. GMvarcc denotes variation in the GM-VFNS for charged current processes, and clearly the effect is very small indeed. The predictions at NNLO are seen in Table. 3. Other than model dependence – GMvarmod denotes the variation to $\tilde{b} = 2$ in the $\mathscr{O}(\alpha_S^3)$ term – the maximum variations are of order 0.5% at LHC. GMvarmod' is when the $\mathscr{O}(\alpha_S^3)$ falls with Q^2, and also exhibits a very small deviation.

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