Update of Parton Distributions at NNLO

A.D. Martin\textsuperscript{a}, W.J. Stirling\textsuperscript{a}, R.S. Thorne\textsuperscript{b,1} and G. Watt\textsuperscript{b}

\textsuperscript{a} Institute for Particle Physics Phenomenology, University of Durham, DH1 3LE, UK
\textsuperscript{b} Department of Physics and Astronomy, University College London, WC1E 6BT, UK

Abstract

We present a new set of parton distributions obtained at NNLO. These differ from the previous sets available at NNLO due to improvements in the theoretical treatment. In particular we include a full treatment of heavy flavours in the region near the quark mass. In this way, an essentially complete set of NNLO partons is presented for the first time. The improved treatment leads to a significant change in the gluon and heavy quark distributions, and a larger value of the QCD coupling at NNLO, $\alpha_S(M_Z^2) = 0.1191 \pm 0.002(\text{expt.}) \pm 0.003(\text{theory})$. Indirectly this also leads to a change in the light partons at small $x$ and modifications of our predictions for $W$ and $Z$ production at the LHC. As well as the best-fit set of partons, we also provide 30 additional sets representing the uncertainties of the partons obtained using the Hessian approach.

The highest level of precision so far achieved for cross sections calculated in fixed-order perturbative QCD is next-to-next-to-leading order (NNLO). The cross sections are known at NNLO for many processes involving incoming protons (or antiprotons), i.e. coefficient functions exist for deep-inelastic scattering [1], for hadro-production of electroweak particles such as $W$ and $Z$ bosons [2] (as a function of rapidity [3]), and even Higgs bosons [4, 5] (in both the standard and supersymmetric models). The appropriate parton distributions to use with these hard cross sections are those which have been evolved using NNLO evolution kernels. Approximations to these [6] based on exact moments [7] and small-$x$ limits [8] have been available for a number of years, and correspondingly approximate NNLO parton distributions have been extracted from global fits [9, 10], or fits to DIS data [11]. The complete calculation of the splitting functions was published in 2004 [12] (the results being numerically very similar to the previous estimates) and this allowed improved NNLO parton distributions to be obtained [13, 14]. Nevertheless, some additional, sometimes unmentioned, approximations still exist in the published sets of NNLO partons.

\textsuperscript{1}Royal Society University Research Fellow
Figure 1: Comparison of the NLO up distribution with the NNLO up distribution, concentrating on small $x$ (left) and high $x$ (right).

One of the most significant of these is the treatment of heavy flavour. At NNLO the partons become discontinuous at flavour transition points (conventionally chosen to be at $\mu^2 = m_H^2$, with $H = c, b$), due to the non-vanishing of transition matrix elements [15] if the flavour number is allowed to vary. There is no reason why any parton should be exactly zero at a particular scale, and it is an accident of the $\overline{\text{MS}}$ renormalisation and factorisation scheme that the structure of the perturbative heavy flavour is so simple that one can evolve from zero at a given scale even at NLO. This is not true, for example, in the MS renormalisation scheme or even in the DIS factorisation scheme (an all orders heavy flavour prescription in this scheme is presented in [16]) where an $x$-dependent input at $\mu^2 = m_H^2$ is required at NLO. These discontinuities in NNLO partons have so far been ignored, as explained in the appendices of [9]. In principle it is possible to avoid this problem of discontinuities at the transition points by simply remaining in a fixed flavour number scheme. However, in practice the heavy flavour coefficient functions appropriate for this choice are only known to NLO so this is not an option. A complete NNLO set of partons must have a properly defined treatment of heavy flavour. None of the previous sets satisfy this requirement. Also, the NNLO parton distributions should be obtained by a comparison to data using cross sections calculated at the same order.

These considerations make it necessary to update the NNLO parton distributions. Compared to the previous version, MRST2004 [13], there are two main changes in the theory: an implementation of a new variable flavour number scheme (VFNS) for the heavy quark ($c, b$)
flavours [17] (based on the NLO schemes in [18] and [19]) which maintains the continuity (up to N^3LO corrections which are very small) of both neutral and charged current structure functions by introducing discontinuities in coefficient functions which counter those in the parton distributions; and the inclusion of NNLO corrections [3] to the Drell–Yan cross sections. The most important change compared to the previous NNLO partons, which already used the exact splitting functions [12], is the new VFNS which leads to a significant change in the gluon and heavy quark distributions. Moreover, because we knew that the previous NNLO treatments were approximate, we did not provide uncertainties along with the central values. Now that the NNLO procedure is essentially complete we rectify this. The size of the uncertainties due to the experimental errors on the data fitted, which is obtained using the Hessian approach [21], is similar to that at NLO [22]. There is more work to do in order to estimate the theoretical uncertainty, which is certainly important in some regions [10].

The procedure that we use to obtain the partons, and their uncertainties, is very similar to previous analyses, with the data used in the fit being essentially the same as in the MRST2004 analysis. We provide 15 different eigenvector sets of partons, with an “up” and “down” set for each. Each of the 30 parton sets corresponds to a $\Delta \chi^2$ of 50 compared to the best fit, this corresponding to an approximate 90% confidence-level for the uncertainty of the partons.\footnote{Some of the most important features of these new distributions have been highlighted in [20].}

\footnote{Note that it does not always correspond precisely to a rescaling of the uncertainty for $\Delta \chi^2 = 1$ by a factor}
Figure 3: The charm distribution, $x_c(x, \mu^2)$, at the transition point $\mu^2 = m_c^2 = 2.045 \text{GeV}^2$. The distribution, which is zero for $\mu^2 < m_c^2$, turns on, at NNLO in the $\overline{\text{MS}}$ scheme, with a non-zero value at $\mu^2 = m_c^2$ given by the curve above. (The discontinuity in the charm distribution, and other parton densities, at $\mu^2 = m_c^2$ is compensated by discontinuities in the coefficient functions such that structure functions are continuous up to tiny $N^3\text{LO}$ contributions [17].)

These partons can be used to estimate the uncertainty of physical quantities in exactly the manner explained for the NLO partons in [22].

The central values for the light quarks are similar to the previous NNLO analysis, though the evolution with $Q^2$ is a little different in order to obtain the best fit with the different heavy flavour procedure. This leads to the most marked change being at small $x$ and high $Q^2$, and we will return to this. At lower $Q^2$ it is most illuminating to instead examine the difference between the NNLO quarks and the quarks at NLO [22]. The change in the up quark distribution when going from NLO to NNLO is shown in Fig. 1. At small $x$ the effect of the coefficient functions, particularly $C_{2,g}^{(2)}(x)$, is important and the difference between the NLO and the NNLO distribution is greater than the uncertainty in each. At large $x$ the coefficient functions are again important, i.e.

$$C_{2,q}^{(2)}(x) \sim \left( \frac{\ln^3(1-x)}{(1-x)} \right)_+$$

and the difference between NLO and NNLO is again larger than the uncertainty in each as of $\sqrt{50}$, because the increase in $\chi^2$ about the minimum is not completely quadratic for every eigenvector.
Figure 4: The charm contribution to $F_2(x,Q^2)$ at NLO and NNLO as a function of $Q^2$. 

seen in Fig. 1. At small $x$ the effect of the splitting functions is also important, particularly due to $P_{qg}^{(2)}(x)$, which has a positive $\ln(1/x)/x$ contribution. This affects the gluon distribution via the fit to $dF_2(x,Q^2)/d\ln Q^2$, and the NNLO gluon is smaller at very low $x$ than the NLO gluon, as shown in Fig. 2.

The major change in the partons comes about due to the improved treatment of the heavy quarks, $H = c, b$. As before, we assume that the heavy quark distributions are generated by perturbative evolution, i.e. by $g, \Sigma \rightarrow H\bar{H}$ transitions, where $\Sigma$ is the singlet light quark distribution. At NNLO, heavy flavour no longer evolves from zero at $\mu^2 = m_H^2$. Rather the distributions, $H = c, b$, have an input value given by the convolution

$$(H + \bar{H})(x, m_H^2) = A_{Hg}^{(2)}(m_H^2) \otimes g(m_H^2) + A_{Hq}^{(2)}(m_H^2) \otimes \Sigma(m_H^2),$$

where, in practice, the heavy flavour distribution starts from a negative value at low $x$, since the main contribution is from the matrix element at small $x$ which is

$$A_{Hg}^{(2)}(x, \mu^2 = m_H^2) \to \left(\frac{\alpha_s(m_H^2)}{4\pi}\right)^2 \left(\frac{40}{3} - \frac{8\pi^2}{3}\right) \frac{1}{x},$$

plus less singular contributions, and the singlet matrix element has the same small-$x$ behaviour up to a colour factor of $4/9$. These negative small-$x$ matrix elements are combined with the positive high- and moderate-$x$ parton distributions in the convolution to give negative heavy flavour contributions. The resulting discontinuity at $\mu^2 = m_H^2$ in the heavy flavour
distributions is by no means insignificant, see Fig. 3. The discontinuities make the use of a general-mass variable-flavour scheme essential, otherwise the structure functions would have sizable discontinuities at NNLO [17].\footnote{One could choose the transition point away from $\mu^2 = m_H^2$, but there is little sensitivity to this choice since the $\ln(\mu^2/m_H^2)$-dependent terms in the matrix elements account for evolution (without a complete resummation, of course). If one made the transition at $\mu^2 \sim 2m_H^2$ the input for the heavy partons would be smaller, although it would not be exactly zero anywhere. This would be more complicated to implement and the discontinuities in the other partons would change as well.} Alternatively, ignoring the discontinuities leads to large errors in the heavy flavour partons. The discontinuities in the light partons are much less significant, being at most a few percent for the gluon, the change quickly being overshadowed by evolution, and are very small indeed for light quarks. The increased evolution from the NNLO splitting function allows the NNLO charm distribution to catch up partially with respect to that at NLO, which starts from zero at $m_c^2$, but it always lags a little behind at higher $Q^2$.

(2.27) The increase at low $Q^2$ and the decrease which persists to high $Q^2$, means unambiguously

Figure 5: Comparison of the NNLO gluon distribution (together with its uncertainty) with the previous approximate NNLO distribution at $Q^2 = 5$ GeV$^2$ (left), and the ratio at $Q^2 = 10^4$ GeV$^2$ for both the gluon and the up quark (right).
that $F_2^c(x,Q^2)$ tends to be flatter in $Q^2$ at NNLO than NLO. Note that this comparison is made after a refit to data so that the corresponding evolution for light quarks must be such as to fit the HERA inclusive data on $F_2(x,Q^2)$. In detail this means that the light quarks at NNLO now actually need to evolve slightly more quickly than at NLO (or than in the previous approximate NNLO treatment) to make up for the decrease in the evolution for the heavy flavour. This correction in the charm procedure then automatically affects the gluon, since it has to compensate for the change in evolution of $F_2^c(x,Q^2)$. The comparison with the low $Q^2$ MRST2004 NNLO gluon is shown in the left of Fig. 5, while the right of Fig. 5 shows the ratio after a long evolution length for both the gluon and the up quark (the effect on the down quark being much the same). We see that the change in the gluon, and on the light quarks at very high $Q^2$, is greater than the uncertainty in some places. The correct heavy flavour treatment is vital.

Our other theoretical improvement at NNLO is also non-trivial. The NNLO corrections to the Drell–Yan cross section are significant [3]. There is an enhancement at high $x_F = x_1 - x_2$ due to large logarithms, which is similar to the $\ln(1 - x)$ enhancement in structure functions. The NLO correction is large and the NNLO corrections are 10% or more, as seen in Fig. 6. The quality of the fit to E866 Drell–Yan production [23] in proton–proton collisions\(^5\) is $\chi^2 = 223/174$ at NLO and $\chi^2 = 240/174$ at NNLO. The scatter of points is large and a $\chi^2 \sim 220$ is approaching

\(^5\)We use the data corrected for radiative corrections [24].
Figure 7: Comparison of the NLO and NNLO Drell–Yan cross sections with the data.

the best possible with a smooth distribution. The quality of the fit is good, as seen in Fig. 7. It is worse for proton–deuterium data. The positive correction at NNLO requires the data normalisation to be 106% (99% at NLO), there being little freedom since both the sea quarks for $x \leq 0.1$ and the valence quarks are already well determined by structure function data. The normalisation uncertainty on the data is 6.5%, and a change of 6% is large but acceptable.\(^6\)

The one remaining set of data for which we cannot use NNLO coefficient functions is the Tevatron high-$E_T$ inclusive jet data \cite{25}, since the calculation is not complete.\(^7\) However, the systematic uncertainties on these data are of order 10%, which is representative of the size of the NLO corrections, and indications \cite{27} are that the NNLO corrections are somewhat less than this (the coupling being rather small at these very high scales, of course). Whether one includes these data or not can lead to changes in the high-$x$ gluon of over 100%, so a potential error of probably less than 10% from using only the NLO coefficient functions seems trivial in comparison, and we keep these data in the fit.

The quality of the full fit for the set of data used is $\chi^2 = 2406/2287$ at NLO and $\chi^2 = 2366/2287$ at NNLO. The NNLO fit is consistently better than the NLO fit. There is most improvement in the description of the high-$x$ structure function data, where the NNLO coefficient function leads to a quicker evolution at low $Q^2$. Most DIS data sets, and the Tevatron jet

\(^6\)The NNLO Drell–Yan cross section is also used in the latter reference of \cite{14}.

\(^7\)Progress is continually being made in evaluating NNLO cross sections of this type \cite{26}.
Figure 8: Comparison of the NNLO gluon distribution with that of Alekhin.

data, have a slightly better fit quality at NNLO. The exception is the E866 Drell–Yan data, as already noted. There is a tendency for the NNLO $\alpha_S(M_Z^2)$ to increase with the improved theoretical treatment. An exactly analogous NLO fit yields $\alpha_S(M_Z^2) = 0.1212$, i.e. much the same as in [13] since the analysis is extremely similar. In comparison, at NNLO $\alpha_S(M_Z^2) = 0.1191 \pm 0.002(\text{expt.}) \pm 0.003(\text{theory})$, whereas in [13] $\alpha_S(M_Z^2) = 0.1167 \pm 0.002(\text{expt.}) \pm 0.003(\text{theory})$. The difference can be traced mainly to the slowing of the heavy flavour evolution using the full treatment, leading to an increased coupling as well as a modified gluon distribution to compensate. Overall, although the fit is generally good, particularly at NNLO, there is some room for improvement, and the data would prefer a little more gluon at both high and moderate $x$.

We examine the effect of the change in the NNLO partons on the predictions for $W$ and $Z$ production at the LHC and the Tevatron. The results, compared to those using the NNLO partons of MRST2004, are shown in Table 1, where we use $B_{l\nu} = 0.1068$ and $B_{l^+l^-} = 0.033658$. The uncertainties on these cross sections are roughly $\pm 2\% (\text{expt.})$. The results are largely unchanged for the Tevatron cross sections, but there is an increase of 6% in the LHC cross sections using the updated partons. This is not difficult to understand. We have already seen the difference in the gluon distribution in Fig. 5. The larger gluon in the region $0.001 \lesssim x \lesssim 0.1$, and the larger coupling, are required to drive the evolution of the light quarks more quickly to match the small-$x$ HERA data when the new procedure produces a flatter $F_2^c(x, Q^2)$. This results in the larger light quark distributions at high $Q^2$ for $x \lesssim 0.01$, as seen in the right of Fig. 5, and a 6% increase in the LHC cross sections, which are dominated by light quark–antiquark annihilation.
Table 1: Total $W$ and $Z$ cross sections multiplied by leptonic branching ratios at the Tevatron and the LHC, calculated at NNLO using the updated NNLO parton distributions. The predictions using the 2004 NNLO sets are shown in brackets.

|        | $B_{W} \cdot \sigma_{W}$ (nb) | $B_{t+1-} \cdot \sigma_{Z}$ (nb) |
|--------|--------------------------------|----------------------------------|
| Tevatron | 2.727 (2.693) | 0.2534 (0.2518) |
| LHC     | 21.42 (20.15) | 2.044 (1.918) |

with $x \sim 0.006$. The Tevatron probes the distributions at $x \sim 0.05$ resulting in little change in the predictions. Ratios of heavy boson cross sections are also essentially unchanged. The 6% change in the predictions of the $W, Z$ rates at the LHC should not be regarded as an uncertainty — it is a consequence of correcting an over-simplified treatment of heavy flavours in previous NNLO analyses. We also note that this change is for different reasons than the recent change in predictions for vector boson cross sections at the LHC observed in going from the CTEQ6.1 to CTEQ6.5 parton distributions [28]. The latter was for NLO partons and came about due to the implementation of a general-mass VFNS instead of a zero-mass VFNS. Our change is due to an improvement in the general-mass VFNS, the most important modification being the treatment of parton discontinuities, which is a feature which only appears at NNLO.

We compare with the only other publicised NNLO partons available, those of Alekhin [14]. We have a much larger $\alpha_{S}(M_{Z}^{2})$, i.e. $\alpha_{S}(M_{Z}^{2}) = 0.1191 \pm 0.002$ (expt.) $\pm 0.003$ (theory), as compared to $0.1143 \pm 0.0014$ (expt.) and $0.1128 \pm 0.0015$ (expt.) of Refs. [14][8]. There is not much difference in the high-$x$ valence quarks, except that explained by the difference in $\alpha_{S}(M_{Z}^{2})$. There are differences in the low-$x$ sea quarks but these are dominated by differences in the flavour treatments of $\bar{u} - \bar{d}$ and $s(x, Q^{2})$. The difference between our and Alekhin’s gluon distribution at small $x$ is seen in Fig. 8, and is much bigger than the uncertainties. This is due to the different heavy flavour treatments, which we do not believe to be consistent in [14][9], and which we have already shown to be important, as well as to differences in the data fitted and in the value of $\alpha_{S}(M_{Z}^{2})$. The gluons also differ a great deal at high $x$, where, in our analysis, they are determined by the Tevatron jet data [25] (the comparison now being excellent [13]). In [14] the gluon is unconstrained here, and should presumably have a large uncertainty. In the $\overline{\text{MS}}$ scheme the gluon is more important for Tevatron jets at high $x$ at NNLO than at NLO because the high-$x$ quarks are automatically significantly smaller, as seen in Fig. 1.

In summary, we have new theoretical corrections in our global analysis, and have obtained NNLO partons with uncertainties for the first time. These NNLO partons (denoted MRST2006)

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8It should be remembered that there are choices in the definition of $\alpha_{S}$ at a given order, even for a given renormalisation scheme. The differences are formally of higher order, but may be significant at the level of 1% or so for an extraction of $\alpha_{S}(M_{Z}^{2})$ [29]. Different parton analyses tend to use different definitions. The details of our procedure can be found in [30] with extension to NNLO.

9The fit in [14] is performed in the fixed flavour number scheme using heavy flavour coefficient functions only up to NLO, and the variable flavour scheme partons are generated by evolution of these input partons without the inclusion of the discontinuities at heavy flavour transition points.
can be found at http://durpdg.dur.ac.uk/hepdata/mrs, where, in order to have a precise

treatment in the heavy quark transition region, there has been a major upgrade of the inter-

polation code, which now also allows a reliable extrapolation outside of the grid (now defined

for $10^{-6} \leq x \leq 1$ and $1 \text{ GeV}^2 \leq Q^2 \leq 10^9 \text{ GeV}^2$) for high $Q^2$ and/or low $x$. The NNLO fit

improves on that at NLO, as well as correcting our previous NNLO analysis. With respect to

the latter, the value of $\alpha_s(M_Z^2)$ at NNLO moves upwards significantly, and all partons change

by a significant amount, particularly at small $x$. As we have seen, this has implications for

predictions for processes at the LHC.

For the future, there are more new data to be included: neutrino deep-inelastic scattering
data from NuTeV [31] and CHORUS [32], HERA jets [33], updated Tevatron high-$E_T$ jets
[34], new CDF lepton-asymmetry data in different $E_T$ bins [35], new heavy flavour data from
HERA [36], and a full treatment of NuTeV dimuon data [37]. There will also soon be averaged
HERA structure function data [38]. This will lead us to produce fully updated NLO and NNLO
partons for the LHC complete with uncertainties — both experimental and theoretical — in
a relatively short timescale. However, until this major update can be finalised, the NNLO
partons outlined in this note will serve as by far the most theoretically self-consistent, and most
stringently constrained set currently available at NNLO.

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