Improved Approximations for the Three-Loop Splitting Functions in QCD

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Abstract

We update our approximate parametrizations of the three-loop splitting functions for the evolution of unpolarized parton densities in perturbative QCD. The new information taken into account is given by the additional Mellin moments recently calculated by Retey and Vermaseren. The inclusion of these constraints reduces the uncertainties of our approximations considerably and extends their region of applicability by about one order of magnitude to lower momentum fractions $x$.

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In order to achieve a high accuracy of the predictions of perturbative QCD for hard processes, the calculations need to transcend the standard next-to-leading order (NLO) approximation. For processes with initial-state hadrons, the next-to-next-to-leading order (NNLO) expressions include the three-loop splitting functions. The computation of these functions is under way \cite{1}, but will not be completed in the near future \cite{2}.

Partial results have already been obtained \cite{3–9}, however, most notably the five lowest even-integer moments for the flavour non-singlet combination entering electromagnetic deep-inelastic scattering (DIS) \cite{3}, and four moments for the singlet splitting functions \cite{4}. In refs. \cite{10, 11} we have demonstrated that this information — due to the smoothening effect of the ubiquitous convolution with the initial parton densities and the small size of the corrections — is fully sufficient for momentum fractions $x \gtrsim 0.1$ and leaves only small uncertainties down to $x \simeq 10^{-3}$ at scales above about 10 GeV$^2$. We have provided approximate parametrizations for the three-loop splitting functions, including quantitative estimates of their residual uncertainties. These results have already been applied \cite{12} to structure functions in DIS and Drell-Yan cross sections at hadron colliders, for which the subprocess cross sections have been computed up to NNLO \cite{13, 14}.

Very recently the fixed-moment calculations of refs. \cite{3, 4} have been extended, using improved computing resources, up to the twelfth moment \cite{2}. For the first time also (odd) moments of the three-loop valence splitting functions have been obtained there. These results provide a severe check of our approximation procedure, as the latter led to rather tight predictions for the (tenth and) twelfth moments. This test is passed by the results of refs. \cite{10, 11}. In this letter we update these parametrizations by including the moments of ref. \cite{2} in the derivation. As a result the residual uncertainties are greatly reduced, and the region of safe applicability is extended by about one order of magnitude in $x$, an improvement most relevant for applications to structure functions at HERA \cite{12}.

Our notations for the parton densities and splitting functions are as follows: the non-singlet combinations of quark and antiquark densities, $q_i$ and $\bar{q}_i$, are given by

$$q_{\text{NS}}^\pm = q_i \pm \bar{q}_i - (q_k \pm \bar{q}_k), \quad q_{\text{NS}}^V = \sum_{r=1}^{N_f} (q_r - \bar{q}_r).$$ (1)

$N_f$ stands for the number of effectively massless flavours. The corresponding splitting functions are denoted by $P_{\text{NS}}^\pm$ and $P_{\text{NS}}^V \equiv P_{\text{NS}}^+ + P_{\text{NS}}^-$. The latter function, $P_{\text{NS}}^S$, occurs for the first time at $O(\alpha_s^3)$. Except for the vanishing of the first moment, it was unknown before the calculation of ref. \cite{2}. The evolution equations in the singlet sector are written as

$$\frac{d}{d \ln \mu_f^2} \left( \Sigma \ g \right) = \left( \begin{array}{cc} P_{\text{NS}}^+ + P_{\text{PS}} & P_{gg} \\ P_{gg} & P_{gg} \end{array} \right) \otimes \left( \Sigma \ g \right), \quad \Sigma = \sum_{r=1}^{N_f} (q_r + \bar{q}_r).$$ (2)

Here $g$ represents the gluon density, and $\otimes$ denotes the Mellin convolution. The expansion of all these splitting functions in powers of the running coupling constant $\alpha_s$ reads

$$P(x, \alpha_s) = a_s P^{(0)}(x) + a_s^2 P^{(1)}(x) + a_s^3 P^{(2)}(x) + \ldots \text{ with } a_s \equiv \alpha_s/4\pi.$$ (3)
if the renormalization and factorization scales are identified, \( \mu_r = \mu_f \). The additional terms for \( \mu_r \neq \mu_f \) are exactly known up to NNLO and need not to be considered here.

Let us briefly illustrate our approximation procedure for the case of the \( N_f \) term, \( P_{qg,1}^{(2)}(x) \), of the gluon-quark splitting function \( P_{qg} \) which dominates the small-\( x \) evolution of the quark densities. Taking into account the small-\( x \) result of ref. \[5\], the expected form of this function in the \( \overline{\text{MS}} \) scheme employed throughout this paper is given by

\[
P_{qg,1}^{(2)}(x) = \sum_{m=1}^{4} A_m \ln^m (1-x) + f_{\text{smooth}}(x) + \sum_{n=1}^{4} B_n \ln^n x + \frac{C}{x} - \frac{896}{27} \ln x ,
\]

where \( f_{\text{smooth}} \) is finite for \( 0 \leq x \leq 1 \). We choose three or two of the large-\( x \) logarithms, one or two smooth functions (mainly low powers or simple polynomials of \( x \)) and two of the small-\( x \) terms \( (x^{-1} \text{ and } \ln x \text{ or } \ln^2 x) \). Their coefficients are then determined from the known six moments \[4, 5\]. Varying these choices we arrive at the about 50 approximations compared in Fig. 1. The two representatives spanning the error band for most of the \( x \)-range are finally selected as our estimates for \( P_{qg,1}^{(2)} \) and its residual uncertainty.

Analogous procedures are applied to the \( N_f^0 \) and \( N_f^1 \) terms of all other functions \( P^{(2)}(x) \). The non-singlet \( N_f^1 \) contribution is known \[6\]. The singlet \( N_f^2 \) pieces are smaller in absolute size and uncertainty than the \( N_f^0 \) and \( N_f^1 \) terms, hence for them it suffices to select just one central representative. Note that the previous information, four (five) moments in the singlet \( (P_{NS}^+) \) sector, respectively, was not sufficient to fix the coefficients of the subleading small-\( x \) terms \( \propto x^{-1} (\ln^3 x) \) from the moments. Thus we had to resort to conservatively varied, educated guesses inspired by the NLO results. Except for the case of \( P^{(2)+} \) (where the rightmost pole in Mellin space is not one, but two units away from the lowest calculated moment) we can now dispense with these ad hoc estimates.

We now write down our improved parametrizations, using the abbreviations

\[
L_0 \equiv \ln x , \quad L_1 \equiv \ln(1-x).
\]

Two approximations, denoted by \( P_{A}^{(2)} \) and \( P_{B}^{(2)} \), are provided for each function. Where both are present, the \( N_f^0 \) and \( N_f^1 \) terms have been combined such that the error bands are maximized at small \( x \). The averages \( 1/2 \ [A+B] \) represent the central results.

Our new expressions for the non-singlet splitting functions \( P_{NS}^{(2)+} \) read

\[
P_{NS,A}^{(2)}(x) = 1185.229 \ (1-x)^{-1}_+ + 1365.458 \delta(1-x) - 157.387 \ L_1^2 - 2741.42 \ x^2 \\
- 490.43 \ (1-x) + 67.00 \ L_2^3 + 10.005 \ L_0^4 + 1.432 \ L_0^4 \\
+ N_f \ \{ -184.765 \ (1-x)^{-1}_+ - 184.289 \delta(1-x) + 17.989 \ L_1^2 + 355.636 \ x^2 \\
- 73.407 \ (1-x)L_1 + 11.491 \ L_0^4 + 1.928 \ L_0^4 \} + P_{NS,2}^{(2)}(x)
\]

\[
P_{NS,B}^{(2)-}(x) = 1174.348 \ (1-x)^{-1}_+ + 1286.799 \delta(1-x) + 115.099 \ L_1^2 + 1581.05 \ L_1 \\
+ 267.33 \ (1-x) - 127.65 \ L_2^3 - 25.22 \ L_0^4 + 1.432 \ L_0^4 \\
+ N_f \ \{ -183.718 \ (1-x)^{-1}_+ - 177.762 \delta(1-x) + 11.999 \ L_1^2 + 397.546 \ x^2 \\
+ 41.949 \ (1-x) - 1.477 \ L_0^4 - 0.538 \ L_0^4 \} + P_{NS,2}^{(2)}(x)
\]

(6)
and

\[ P_{NS,A}^{(2)+}(x) = 1183.762 (1 - x)^{-1} + 1347.032 \delta(1 - x) + 1047.590 L_1 - 843.884 x^2 - 98.65 (1 - x) - 33.71 L_0^2 + 1.580 (L_0^4 + 4L_0^2) \\
+ N_f \left\{ -183.148 (1 - x)^{-1} - 174.402 \delta(1 - x) + 9.649 L_1^2 + 406.171 x^2 \\
+ 32.218 (1 - x) + 5.976 L_0^2 + 1.60 L_0^3 \right\} + P_{NS,2}^{(2)}(x) \]

\[ P_{NS,B}^{(2)+}(x) = 1182.774 (1 - x)^{-1} + 1351.088 \delta(1 - x) - 147.692 L_1 - 2602.738 x^2 - 170.11 + 148.47 L_0 + 1.580 (L_0^4 - 4L_0^3) \\
+ N_f \left\{ -183.931 (1 - x)^{-1} - 178.208 \delta(1 - x) - 89.941 L_1 + 218.482 x^2 \\
+ 9.623 + 0.910 L_0^2 - 1.60 L_0^3 \right\} + P_{NS,2}^{(2)}(x). \]  

The \( \ln^4 x \) terms in Eqs. (6) and (7) stem from ref. [7]. The exactly known \( N_f^2 \) contribution \( P_{NS,2}^{(2)}(x) \) for both cases [3] is given in Eq. (4.13) of ref. [10]. \( P_{NS}^{(2)+}(x) \) and \( P_{NS}^{(2)-}(x) \) are compared at \( x < 1 \) in Fig. 2, for \( N_f = 4 \), to our previous approximations based on one moment less for \( P_{NS}^{(2)+} \) and mostly indirect information on \( P_{NS}^{(2)-}(x) \). Our present results are consistent with, but considerably more accurate than those of ref. [10].

In contrast to \( P_{qg} \) and \( P_{q\bar{q}} \), the transition from one to two loops leads only to \( \ln^1(1-x) \) terms in \( P_{NS} \) and \( P_{qg} \). Assuming correspondingly that no large-\( x \) logarithms beyond \( \ln^2(1-x) \) occur in \( P_{NS}^{(2)+} \), the coefficients of the \( 1/(1-x)_+ \) term of the (also about 50) test functions considered for \( P_{NS}^{(2)-}(x) \) cover the range 1167.3 \ldots 1190.3 for the \( N_f^0 \) part, and \(-184.8 \ldots -183.1\) for the \( N_f^1 \) contribution. The findings for \( P_{NS}^{(2)+} \), where one moment less is known, are consistent with these results. Note that terms \( [\ln^k(1-x)/(1-x)]_+ \) with \( k \geq 1 \) do not occur in the \( MS \) splitting functions, as proven in ref. [13].

The difference \( P_{NS}^S = P_{NS}^V - P_{NS}^P \) and the pure-singlet splitting function \( P_{PS} \) in Eq. (2) result as \( N_f(P_{q\bar{q}_k}^S - P_{q\bar{q}_k}^S) \) and \( N_f(P_{q\bar{q}_k}^S + P_{q\bar{q}_k}^S), \) respectively, from the flavour independent ('sea') parts of the quark-quark and quark-antiquark splitting functions. The former combination carries the colour factor \( d^{abc}d^{abc} \) which does not occur in \( P_{NS}^-; \) this fact facilitates the separations of the two terms in the results of ref. [2]. Both \( P_{NS}^S(x) \) and \( P_{PS}(x) \) vanish at \( x = 1 \), but are large at small \( x \). The parametrizations selected for the \( a_s \) contributions to these two functions are given by

\[ P_{NS,A}^{(2)S}(x) = N_f \left\{ (1-x)(-1441.57 x^2 + 12603.59 x - 15450.01) + 7876.93 xL_0^2 \\
- 4260.29 L_0 - 229.27 L_0^2 + 4.4075 L_0^3 \right\} \]

\[ P_{NS,B}^{(2)S}(x) = N_f \left\{ (1-x)(-704.67 x^3 + 3310.32 x^2 + 2144.81 x - 244.68) \\
+ 4490.81 x^2L_0 - 4127.85 L_0 - 11.0165 L_0^3 \right\} \]

and

\[ P_{PS,A}^{(2)} = N_f \left\{ (1-x)(-229.497 L_1 - 722.99 x^2 + 2678.77 - 560.20 x^{-1}) \\
+ 2008.61 L_0 + 998.15 L_0^2 - 3584/27 x^{-1}L_0 \right\} + P_{PS,2}^{(2)}(x) \]

\[ P_{PS,B}^{(2)} = N_f \left\{ (1-x)(73.845 L_1^2 + 305.988 L_1 + 2063.19 x - 387.95 x^{-1}) \\
+ 1999.35 xL_0 - 732.68 L_0 - 3584/27 x^{-1}L_0 \right\} + P_{PS,2}^{(2)}(x) \]
with

\[ P_{\text{PS,2}}^{(2)}(x) = N_f^2 \left\{ (1-x)(-7.282 L_1 - 38.779 x^2 + 32.022 x - 6.252 + 1.767 x^{-1}) + 7.453 L_0^2 \right\}. \]  

(10)

The \((\ln x)/x\) term in Eq. (3) has been derived in ref. [1].

Our new approximations for the off-diagonal singlet splitting functions \(P_{qq}^{(2)}\) and \(P_{gg}^{(2)}\) are given by

\[ P_{qq,A}^{(2)}(x) = N_f \left\{ -31.830 \, L_1^3 + 1252.267 \, L_1 + 1999.89 \, x + 1722.47 + 1223.43 \, L_0^2 - 1334.61 \, x^{-1} - 896/3 \, x^{-1} \, L_0 \right\} + P_{qq,2}^{(2)}(x) \]

\[ P_{qq,B}^{(2)}(x) = N_f \left\{ 19.428 \, L_1^4 + 159.833 \, L_1^3 + 309.384 \, L_1^2 + 2631.00 \, (1-x) - 67.25 \, L_0^2 - 776.793 \, x^{-1} - 896/3 \, x^{-1} \, L_0 \right\} + P_{qq,2}^{(2)}(x) \]  

(11)

with

\[ P_{gg,2}^{(2)}(x) = N_f^2 \left\{ -0.9085 \, L_1^2 - 35.803 \, L_1 - 128.023 + 200.929 \, (1-x) + 40.542 \, L_0 + 3.284 \, x^{-1} \right\}. \]  

(12)

and

\[ P_{qq,A}^{(2)}(x) = 13.1212 \, L_1^4 + 126.665 \, L_1^3 + 308.536 \, L_1^2 + 361.21 - 2113.45 \, L_0 \]

\[ - 17.965 \, x^{-1} L_0 + N_f \left\{ 2.4427 \, L_1^4 + 27.763 \, L_1^3 + 80.548 \, L_1^2 - 227.135 - 151.04 \, L_0^2 + 65.91 \, x^{-1} \, L_0 \right\} + P_{qq,2}^{(2)}(x) \]

\[ P_{qq,B}^{(2)}(x) = -4.5108 \, L_1^4 - 66.618 \, L_1^3 - 231.535 \, L_1^2 - 1224.22 \, (1-x) + 240.08 \, L_0^2 + 379.60 \, x^{-1} (L_0 + 4) + N_f \left\{ -1.4028 \, L_1^4 - 11.638 \, L_1^3 + 164.963 \, L_1 \right\}
\]

\[- 1066.78 \, (1-x) - 182.08 \, L_0^2 + 138.54 \, x^{-1} (L_0 + 2) \right\} + P_{gg,2}^{(2)}(x) \]  

(13)

with

\[ P_{gg,2}^{(2)}(x) = N_f^2 \left\{ 1.9361 \, L_1^2 + 11.178 \, L_1 + 11.632 - 15.145 \, (1-x) + 3.354 \, L_0 - 2.133 \, x^{-1} \right\}. \]  

(14)

Unlike the case of \(P_{gg}^{(2)}\) discussed above, the coefficients of the leading small-\(x\) terms \((\ln x)/x\) have not been derived for \(P_{gg}^{(2)}\) up to now. Thus these coefficients in Eq. (13) have been determined, as before [1], from the available moments.

The \(1/[1-x]_+\) soft-gluon contributions to the one- and two-loop gluon-gluon splitting functions, \(P_{gg}^{(0)}\) and \(P_{gg}^{(1)}\), are related to their quark-quark (non-singlet) counterparts by a factor \(C_A/C_F\). The same holds for the \(N_f^2\) terms at third order [3, 8]. Assuming that this relation holds generally for \(P_{gg}^{(3)}\), the results given below Eq. (7) can be employed. In this way we arrive at the approximate expressions
\[ P_{gg,A}^{(2)}(x) = 2626.38 \,(1-x)^{-1} + 4424.168 \,\delta(1-x) - 732.715 \,L_1^2 - 20640.069 \,x \]
\[ - 15428.58 \,(1-x^2) - 15213.60 \,L_0^2 + 16700.88 \,x^{-1} + 2675.85 \,x^{-1} L_0 \]
\[ + N_f \,\{-415.71 \,(1-x)^{-1} - 548.569 \,\delta(1-x) - 425.708 \,L_1 + 914.548 \,x^2 \}
\[ - 1122.86 - 444.21 \,L_0^2 + 376.98 \,x^{-1} + 157.18 \,x^{-1} L_0 \} + P_{gg,A}^{(2)}(x) \]
\[ P_{gg,B}^{(2)}(x) = 2678.22 \,(1-x)^{-1} + 4590.570 \,\delta(1-x) + 3748.934 \,L_1 + 60879.62 \,x \]
\[ - 35974.45 \,(1+x^2) + 2002.96 \,L_0^2 + 9762.09 \,x^{-1} + 2675.85 \,x^{-1} L_0 \]
\[ + N_f \,\{-412.00 \,(1-x)^{-1} - 534.951 \,\delta(1-x) + 62.630 \,L_1^2 + 801.90 \}
\[ + 1891.40 \,L_0 + 813.78 \,L_0^2 + 1.360 \,x^{-1} + 157.18 \,x^{-1} L_0 \} + P_{gg,B}^{(2)}(x) \] (15)

with
\[ P_{gg,2}^{(2)}(x) = N_f^2 \,\{ -16/9 \,(1-x)^{-1} + 6.4882 \,\delta(1-x) + 37.6417 \,x^2 - 72.926 \,x \]
\[ + 32.349 - 0.991 \,L_0^2 + 2.818 \,x^{-1} \} \] . (16)

The \((\ln x)/x\) terms in Eq. (15) have been determined in ref. [5] in a scheme equivalent to the DIS scheme up to NNLO. The transformation to \(\overline{\text{MS}}\) can be found in ref. [11].

The uncertainty bands for the three-loop singlet splitting functions resulting from Eqs. (9)–(13) are displayed in Fig. 3 for \(N_f = 4\). As in the non-singlet cases considered above, our new parametrizations considerably improve on the previous uncertainties. While the small-\(x\) behaviour of our approximations obviously depends on the results of refs. [3, 4], it is worthwhile to note that reducing the \(N_f^0\) coefficient of \((\ln x)/x\) in \(P_{gg}^{(2)}\) by a factor of two does not lead to approximations outside the error band in Fig. 3.

In Fig. 4 we finally illustrate the impact of the NNLO terms on the scale derivatives (2) of the singlet quark and gluon densities. As in ref. [11] the initial conditions are chosen as
\[ x \Sigma(x, \mu_f^2) = 0.6 \,x^{-0.3} \,(1-x)^{3.5} \,(1+5 \,x^{0.8}) \]
\[ x \,g(x, \mu_f^2) = 1.0 \,x^{-0.37} \,(1-x)^5 \] (17)
and
\[ \alpha_s(\mu_r^2 = \mu_f^2) = 0.2 \] , (18)
corresponding to \(\mu_f^2 \simeq 30\,\text{GeV}^2\). Under these conditions the residual uncertainties of the three-loop contributions amount to about \(\pm 2\%\) or less down to \(x \simeq 10^{-4}\), even if the bands in Fig. 4 were increased by 50\% in order to account for any possible underestimate of the errors. At lower scales the flatter small-\(x\) shapes of the quark and gluon densities, together with the larger \(\alpha_s\), lead to larger uncertainties at small \(x\). At \(x = 10^{-4}\) and \(\mu_f^2 \simeq 3\,\text{GeV}^2\), for example, they reach about \(\pm 4\%\) and \(\pm 3\%\) for the singlet quark and gluon derivatives, respectively, for standard NLO distributions like CTEQ4M [13]. These numbers represent improvements by about a factor of three on our previous results [11]. Thus our present approximations, based on the results of ref. [2], facilitate a reliable NNLO evolution of unpolarized parton densities down to, at least, \(\mu_f^2 \gtrsim 10\,\text{GeV}^2\) and \(x \gtrsim 10^{-4}\).

FORTRAN subroutines of the above approximations of the three-loop splitting functions can be obtained via email to neerven@lorentz.leidenuniv.nl or avogt@lorentz.leidenuniv.nl.
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Figure 1: Approximations of the $N_f^1$ part $P_{qg,1}^{(2)}$ of the three-loop splitting function $P_{qg}^{(2)}(x)$, as obtained from the six lowest even-integer moments [2, 4] together with the leading small-$x$ term of ref. [5]. The full curves represent those functions selected for Eq. (11).
Figure 2: Top: Our new approximations of $P_{NS}^{(2)+}(x)$ for $N_f = 4$, as obtained from Eq. (7) together with Eq. (4.13) of ref. [10]. The dotted curves represent our previous parametrizations [10]. Bottom: The same for $P_{NS}^{(2)-}(x)$ using Eq. (8).
Figure 3: Our new approximations of the singlet splitting functions $P_{ij}^{(2)}(x)$ for $N_f = 4$. $P_{qq}^{(2)}$ is obtained by adding $P_{NS}^{(2)}(x)$ of Fig. 2 (separately shown by the dash-dotted curve) and $P_{PS}^{(2)}(x)$ of Eqs. (9) and (10). Our previous parametrizations [11] are also shown.
Figure 4: The size and remaining uncertainties of the NNLO corrections for the scale derivatives, $\dot{\Sigma} \equiv \frac{d\Sigma}{d\ln \mu_f^2}$ and $\dot{g} \equiv \frac{dg}{d\ln \mu_f^2}$, of the singlet quark and gluon densities at $\mu_f^2 = \mu_r^2 \simeq 30 \text{ GeV}^2$ ($\alpha_s = 0.2$). The input densities are specified in Eq. (17).