Evolution of Parton Distributions

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Abstract
I present a highly efficient method for evolving parton distributions in perturbative QCD. The method allows evolving the parton distribution functions according to any of the commonly-used truncations of the evolution equations (which differ in their treatment of higher-order terms). I also give formulæ for computing crossing functions within the method.

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1. Introduction

The parton distribution functions of the nucleon are fundamental ingredients in the description of short-distance scattering experiments involving hadronic initial states, whether these be in hadron-hadron collisions, or in deeply inelastic scattering. Indeed, along with the running coupling $\alpha_s$, they are the only ingredients needed from outside perturbation theory for a complete description of such processes ignoring subleading power corrections.

Both the parton distributions and the running coupling depend on the momentum scale at which they are evaluated. As is well known, the variation in each of these quantities as one moves from one momentum scale to another is described by an evolution equation that can be computed perturbatively. It is only the values of the distributions and of the coupling at a fixed scale which are required inputs from outside perturbation theory.

Lattice gauge theorists may calculate these quantities someday, but for the moment they must be extracted from experiments. The modern approaches [1,2] involve global fits to all available experiments. The experiments in fact involve different scale arguments to the distribution functions, but as these are related by a perturbative evolution equation, we can regard the fits as determining the distributions at a certain fixed scale $Q_0$.

Present theoretical abilities allow extensive calculations at next-to-leading order (NLO), and there are growing indications that next-to-next-to-leading order (NNLO) calculations are required if we are to determine $\alpha_s$ to 1%. To the required precision, the evolution equation for the running coupling can be solved in closed form. This is not true, however, of the evolution equation for the parton distributions; these must be evolved numerically from the original fixed scale.

Workers have used two main approaches to evolve the distribution functions numerically: direct integration of the evolution equations, and an approach based on Mellin transformations. This paper presents an improvement to the techniques heretofore used, within the framework of the latter approach.

2. Evolution Equations

A parton distribution function $f(x, Q^2)$ obeys an evolution equation [3] in momentum,

$$Q^2 \frac{\partial f(x, Q^2)}{\partial Q^2} = P(x, Q^2) \otimes f(x, Q^2), \quad (2.1)$$

where $P(x, Q^2)$ is the Altarelli-Parisi kernel, and $\otimes$ denotes a convolution,

$$A(x) \otimes B(x) = \int_0^1 dy \int_0^1 dz \, \delta(x - yz) A(y) B(z), \quad (2.2)$$
(For a different early discussion, see ref. [4].) For the quark non-singlet distributions, each of the quantities in eqn. (2.1) is a scalar; in the singlet sector, \( f \) is a two-component vector containing the quark singlet distribution and the gluon distribution, and \( P(x, Q^2) \) is a \( 2 \times 2 \) matrix.

The kernel \( P(x, Q^2) \) has a perturbative expansion,

\[
P(x, Q^2) = a_s(Q^2)P_0(x) + a_s^2(Q^2)P_1(x) + \mathcal{O}(a_s^3),
\]

in which \( a_s(Q^2) = \alpha_s(Q^2)/(4\pi) \) is a rescaled version of the usual running coupling. As mentioned in the introduction, one approach to evolving the parton distribution functions \( f \), known as the \( x \)-space method, is to integrate the perturbative approximation to eqn. (2.1) directly. I will return to the issues surrounding the choice of method in section 8. For the moment, let us proceed by Mellin transforming the evolution equation; with Mellin moments \( h^z \) of a function \( h(x) \) defined via

\[
h^z = \int_0^1 dx \ x^{z-1}h(x),
\]

the evolution equation, truncated to next-to-leading order, becomes

\[
Q^2 \frac{\partial f^z(Q^2)}{\partial Q^2} = \left[ a_s(Q^2)P_0^z + a_s^2(Q^2)P_1^z \right] f^z(Q^2)
\]

since the Mellin transformation turns convolutions into products. (That is reason for using it.) It is convenient to change variables, and to use \( a_s \) as the evolution variable. We can do this using the beta function,

\[
\beta(a_s) \equiv \frac{\partial a_s}{\partial \ln Q^2} = -\beta_0 a_s^2 - \beta_1 a_s^3 + \mathcal{O}(a_s^4),
\]

obtaining

\[
\frac{\partial f^z}{\partial a_s} = \frac{[P_0^z + a_s P_1^z]}{a_s \left[ \beta_0 + \beta_1 a_s \right]} f^z.
\]

The usual approach [5] expands the right-hand side, in keeping with a perturbative treatment of the equation, upon which we obtain

\[
\frac{\partial f^z}{\partial a_s} = -\frac{1}{\beta_0 a_s} \left[ P_0^z + a_s \left( P_1^z - \frac{\beta_1}{\beta_0} P_0^z \right) \right] f^z.
\]

The boundary condition is \( f^z(Q_0^2) = f_0^z \). Conventionally one proceeds by introducing an evolution operator \( E \) such that

\[
f^z(Q^2) = E^z(a_s(Q^2), a_s(Q_0^2))f^z(Q_0^2).
\]

In the non-singlet case, \( E \) is just a scalar function of \( z \); in the singlet case, it is a \( 2 \times 2 \) matrix. The evolution operator satisfies the same equation (2.8) we have been considering above,

\[
\frac{\partial E^z}{\partial a_s} = -\frac{1}{\beta_0 a_s} \left[ P_0^z + a_s \left( P_1^z - \frac{\beta_1}{\beta_0} P_0^z \right) \right] E^z,
\]
but has a boundary condition, \(E^z(a_0, a_0) = 1\), that renders it an entirely perturbative object.

Solving the evolution equation is straightforward in the non-singlet case; expanding in \(a_s\) beyond the leading terms, we obtain \([6,7]\)

\[
E^z_\eta(a_s, a_0) = \left[ 1 - \frac{a_s - a_0}{\beta_0} \mathcal{P}_1^z(\eta) \right] \left( a_s/a_0 \right)^{-P^0_0/\beta_0}.
\] (2.11)

where \(\eta = \pm 1\) correspond respectively to the combinations \(q - \overline{q}\) and \((u + \overline{u}) - (d + \overline{d}),\ldots\), and where \(\mathcal{P}_1^z(\eta) \equiv P^z_1(\eta) - \frac{\beta_1}{\beta_0} P^z_0\). In the singlet case, we need first to define two matrices which project onto the eigenvectors of the leading-order AP coefficient matrix,

\[
P^z_\pm = \pm \frac{1}{(\lambda^z_+ - \lambda^z_-)} \left( P^z_0 - \lambda^z_\pm \right),
\]

in which

\[
\lambda^z_\pm = \frac{1}{2} \left[ P^z_{0,gg} + P^z_{0,qq} \pm \sqrt{(P^z_{0,gg} - P^z_{0,qq})^2 + 4P^z_{0,gg} P^z_{0,qq}} \right] \quad (2.12)
\]

are the eigenvalues of \(P^z_0\). With these definitions, we can write the evolution operator in the singlet sector as \([6,7]\),

\[
E^z(a_s, a_0) = \left[ P^z_\mp - \frac{a_s - a_0}{\beta_0} P^z_\mp \mathcal{P}_1^z P^z_\pm \right. \\
- \left. \frac{1}{\beta_0 - \lambda^z_+ + \lambda^z_-} \left( a_s \left( \frac{a_s}{a_0} \right) \frac{(\lambda^z_+ - \lambda^z_-)/\beta_0}{-a_0} \right) P^z_\mp \mathcal{P}_1^z P^z_\pm \right] \left( a_s/a_0 \right)^{-\lambda^z_\pm/\beta_0} \quad (2.13)
\]

\[+ (+ \leftrightarrow -) .
\]

With the normalizations used here and \(n_f\) the number of active flavors, the beta function \([8]\) coefficients are

\[
\beta_0 = 11 - \frac{2}{3} n_f, \quad \beta_1 = 102 - \frac{38}{3} n_f; \quad (2.14)
\]

the Mellin moments of the Altarelli-Parisi function may be found in ref. \([9]\), noting that \(P^z_i = -\gamma^{(i)z}/2\). The analytic continuations of these moments are given by Glück, Reya, and Vogt \([7]\); I discuss the analytic continuation of a certain term involving the dilogarithm in an appendix.

Of course, for use in perturbative cross section calculations, we want the evolved distributions as functions of the parton momentum fraction \(x\), not their Mellin transforms as functions of the conjugate variable \(z\). To obtain the evolved parton distribution in \(x\)-space, we must invert the Mellin transform,

\[
f(x, Q^2) = \frac{1}{2\pi i} \int_C dz \: x^{-z} f^z(Q^2), \quad (2.15)
\]

where the contour \(C\) runs parallel to the imaginary axis, to the right of the rightmost pole in the integrand.
Up to this point, everything I have written is completely standard. I now wish to investigate how one may deform the contour \( C \) in order to obtain an efficient method for evaluating the integral. Note that the integrand has poles only along the real axis; denote the rightmost pole by \( c_r \). (It is typically around 0.5 for the non-singlet case, and 1.3 for the singlet case.)

One can in principle perform the contour integral along the textbook contour \( z = c + iy \) \((-\infty < y < \infty \text{ and } c > c_r\) ), as was done in the original work of Glück and Reya [10]. One then obtains the expression

\[
\frac{x^{-c}}{2\pi} \int_0^\infty dy \left( x^{-iy} f^{c+iy}(Q^2) + x^{iy} f^{c-iy}(Q^2) \right)
= \frac{x^{-c}}{\pi} \int_0^\infty dy \ \text{Re} \left[ x^{-iy} f^{c+iy}(Q^2) + x^{iy} f^{c-iy}(Q^2) \right].
\] (2.16)

The large-\( y \) behavior of the integrand is determined by the behavior of the initial distribution as \( x \to 1 \). Initial distributions of the form \( x^a(1-x)^\beta \) give rise to a power decay, \( f \sim y^{-\beta-1} \) as \( y \to \infty \). Because the contour is parallel to the imaginary axis, the \( x^{-z} \) factor is a purely oscillating; it does not damp the integrand as \( y \to \infty \). On the other hand, because the integrand has no poles off the real axis, and because the integral along a half-circle at \( \infty \) in the left half-plane (or along part of this half-circle) vanishes, we can freely deform the contour into the left-half plane, so long as we stay away from the real axis. Were we to choose a contour such that \( z \) has an increasingly negative real part as it heads off to infinity, the \( x^{-z} \) factor would contribute an exponential suppression, improving the convergence of the integral. (Recall that the base point \( x \) lies between 0 and 1.)

This motivates the choice of contour in ref. [7], where it is taken to contain two line segments running diagonally into the left-half plane from a point \( c \) on the real axis to infinity.

However, we might ask: why this contour? Or, phrased differently: how should we choose a contour? I address this question in the next section.

3. Choosing a Contour

The most obvious answer is that we should choose the contour of steepest descent; this choice will yield an integral that converges most efficiently and (one therefore hopes) can be evaluated numerically with fewest function evaluations for a fixed desired accuracy. One might fear that finding the contour of steepest descent requires a complicated computation. For our problem, however, it will turn out that there is a simple but very good approximation to the desired contour.

Now, we don’t want to find a contour for each value of \( Q^2 \), especially if finding such a contour involves a significant number of function evaluations; this would defeat the whole purpose of the exercise! For use in a program evaluating a cross section, it is convenient to set up a grid of \( x \) and
points (à la MRS [1]), and interpolate between them. Instead of finding a contour for each \((x, Q^2)\) pair, use the following strategy: for each grid \(x\) value, find the contour of steepest descent for \(Q^2_0\), and then use it for evolution to all \(Q^2\) values. Since the evolution is relatively slow (it is only in \(\ln \ln Q^2\), after all), the contour at \(Q^2_0\) should be fairly close to the contour of steepest descent at \(Q^2\). From a programming point of view, this approach allows all the contours, points along them, and the associated anomalous dimensions to be computed as setup code; only the evolution operators at the given points will need to be evaluated anew for each \(Q^2\) to which we wish to evolve the distributions.

Let us then first consider the inverse Mellin transform of \(f^z(Q^2_0)\). (Yes, we already know the answer — it is just \(f(x, Q^2_0)\) — but that is not the point.) There are certain technical complications in the singlet sector, which I will discuss section 5, so let us restrict attention here to the non-singlet distributions.

The first step in determining the contour is to find the minimum of the integrand along the real axis. As the starting distribution is a positive function, its Mellin transform will be positive along the real axis to the right of its rightmost pole \(c_r\). Furthermore, the starting distribution is not infinitely concentrated at \(x = 1\), so its Mellin transform will decrease as \(z \to \infty\). On the other hand, since \(x < 1\), \(x^{-z}\) increases exponentially as \(z \to \infty\). The product of the two must therefore have a minimum somewhere, and the value of the product there will be positive. (If there happen to be multiple minima, pick the one closest to the rightmost pole.) Call this point \(c_0\).

The integrand is analytic as a function of \(z\). The minimum of the function along the real axis is therefore actually a saddle point of the function in the complex plane, and thus the place to start tracing out our desired contour. Furthermore (again because of analyticity), the desired contour is also a contour of stationary phase, so that the integrand will be real along it. (I will also assume that the rightmost singularity of the Mellin transform of the initial distribution is to the right of the rightmost pole in the anomalous dimensions; this assumption, which holds for realistic parton distributions, ensures that the minimum is only slightly different for \(f^z(Q^2)\) than for \(f^z(Q^2_0)\), and is in any event necessary if we are to use a contour as determined below for integrating \(f^z(Q^2)\).)

Define \(F(z) = x^{-z}f^z(Q^2_0)\); our inverse Mellin transform then has the form

\[
I = \frac{1}{2\pi i} \int_{C_s+(\overline{C}_s)} dz \ x^{-z}f^z(Q^2_0) = \frac{1}{2\pi i} \int_{C_s} [dz \ F(z) - d\bar{z} \ F(\bar{z})]
\]

\[
= \frac{1}{\pi} \int_{C_s} \text{Re} [-i \ dz \ F(z)]
\]

(3.1)

where \(C_s\) is the part of the contour of steepest descent running upwards from \(c_0\).

Let us examine the contour near the point \(c_0\). A generic saddle point will have a non-vanishing second derivative (and all the relevant minima for conventional choices of \(f(x, Q^2_0)\) are indeed
generic), so the contour will start out with a tangent parallel to the imaginary axis: that is the direction of steepest descent of

\[ F(z) \sim F(c_0) + \frac{F''(c_0)}{2} (z - c_0)^2 + \cdots, \]  

(3.2)

which is perhaps easiest to see if we parametrize \( z(t) = x(t) + iy(t) \), with

\[ x(t_0 = 0) = c_0, \quad y(0) = 0, \quad x, y \text{ real}. \]  

(3.3)

Note that the symmetry of the contour under reflection in the real axis forces \( x \) to be an even function of \( t \) (so that \( x'(0) = 0 \)), and \( y \) to be an odd function. We can rescale \( t \) to make \( y'(0) = 1 \).

The expansion in eqn. (3.2) is then

\[ F(z(t)) \sim F(c_0) + \frac{F''(c_0)}{2} (x'(0)^2 - y'(0)^2 + 2ix'(0)y'(0)) t^2 + \cdots \]  

(3.4)

Since all the derivatives of \( F(x) \) are real, the equation \( \text{Im} F(z(t)) = 0 \) is then satisfied to this order, and as \( F''(c_0) \) is positive, the function decreases with \( t \). However, for conventional choices of \( f(x, Q_0^2) \), the contour does not continue parallel to the imaginary axis; to see where it does go, we need to consider the expansion to one higher order,

\[ F(z(t)) \sim F(c_0) - \frac{F''(c_0)}{2} t^2 + \frac{1}{6} \left(-iF^{(3)}(c_0) + 3iF''(c_0)x''(0)\right) t^3 + \cdots \]  

(3.5)

To \( O(t^3) \), \( \text{Im} F(z(t)) = 0 \) then requires

\[ x''(0) = \frac{F^{(3)}(c_0)}{3F''(c_0)}. \]  

(3.6)

Thus in the neighborhood of \( c_0 \), the contour has the form

\[ z(t) = c_0 + it + \frac{F^{(3)}(c_0)}{6F''(c_0)} t^2. \]  

(3.7)

\( (F^{(3)}(c_0) \) is typically negative for the class of functions in which we are interested, as is necessary for this to be a useful truncation.) What is not so obvious — but turns out to be true — is that for our purposes, the contour \( C' \) described by this equation is essentially indistinguishable from the true contour of steepest descent. That is, in the region where the integrands of interest give the bulk of the contributions to the inverse Mellin transform, the two contours are extremely close, and so we incur almost no efficiency penalty in choosing the simplified contour given by eqn. (3.7).

With this choice, our inverse Mellin transform can now be written

\[ \frac{1}{\pi} \int_0^\infty dt \text{ Re} \left[ \left(1 - \frac{iF^{(3)}(c_0)}{3F''(c_0)}t\right) F(z(t)) \right]. \]  

(3.8)

As we shall see in later sections, this quadratic contour is a significant improvement over the linear contour chosen in ref. [7], not to mention the textbook contour.
4. Evaluating the Inverse Transform

The next point we must consider is the evaluation of the inverse Mellin transform using our new contour \((3.7)\). We want to choose a few points along the contour at which to evaluate the function in order to approximate the integral by a finite sum,

\[
\frac{1}{\pi} \int_{C'} \Re \left[ -i \zeta F(\zeta) \right] \simeq \sum_{\zeta_i \in C'} w_i F(\zeta_i)
\]  

(4.1)

In order to find a ‘good’ set of points, we should in principle first find a set of functions in which to expand \(f_x(Q^2)\). A possible (though not necessarily “optimal”) choice is a set of orthogonal polynomials with an astutely-chosen weight function. In fact, for integrating \(f_x(Q^2)\), such a choice is optimal if we pick the weight function to be \(F(z)\) itself! We might therefore be tempted to construct a set of orthogonal polynomials with respect to this weight function.

First, though, let us examine the behavior of the integrand along the contour near \(c_0\). Assume that \(f_x(Q^2)\) does not vary exponentially, so that it cannot eliminate the exponential fall-off expected from the \(e^{-z}\) factor. We then expect a behavior of the form \(F(c_0) e^{-g(t)}\), where the power series expansion of \(g(t)\) can be determined by matching coefficients with the power series expansion in the integrand of eqn. \((3.8)\). (Note that the imaginary part of \(z(t)\) in the prefactor does not contribute until order \(t^5\).) We then obtain

\[
g(t) \sim \frac{F''(c_0)}{2F(c_0)} t^2 + \ldots
\]  

(4.2)

(As discussed in the previous section, both \(F''(c_0)\) and \(F(c_0)\) will be positive.) This suggests that we perform a change of variables \(u = \frac{F''(c_0)}{2F(c_0)} t^2\), whereupon the integral of eqn. \((3.8)\) becomes

\[
\frac{1}{\pi} \sqrt{\frac{F(c_0)}{2F''(c_0)}} \int_0^\infty \frac{du}{\sqrt{u}} \Re \left[ \left( 1 - \frac{i}{3} \frac{F^{(3)}(c_0)}{F''(c_0)} \right) \frac{2F(c_0)}{\sqrt{u}} \right] F \left( \sqrt{u} \right)
\]  

(4.3)

\[
= \frac{c_2}{2\pi} \int_0^\infty \frac{du}{\sqrt{u}} e^{-u} \Re \left[ e^{u} \left( 1 - ic_2 c_3 \sqrt{u} \right) F \left( c_2 \sqrt{u} \right) \right]
\]

where \(c_2 = \sqrt{2F(c_0)/F''(c_0)}\) and \(c_3 = F^{(3)}(c_0)/(3F''(c_0))\). For small \(u\), we expect the factor inside the brackets on the second line to vary slowly. What is again not so obvious, but turns out to be true for initial parton distributions of interest, is that the factor in brackets varies very little, and smoothly at that, in the entire region where the integral receives noticeable contributions. It is thus an excellent candidate for approximation by polynomials. The same statements continue to hold for the inverse Mellin transform of \(f_x(Q^2)\), in which the factor inside the brackets in eqn. \((4.3)\) is now multiplied by the evolution operator \(E_x(a_x(Q^2), a_s(Q^2))\).

The reader may also recognize the prefactor in front of the brackets as the weight function for the generalized Laguerre polynomials \(L_n^{-1/2}(u)\), and it is a generalized Gauss-Laguerre quadrature.
formula employing these polynomials which we should use for evaluating the integral in eqn. (4.3). This formula approximates an integral

\[ \int_0^\infty \frac{du}{\sqrt{u}} e^{-u} h(u) \simeq \sum_{j=1}^n w_j h(u_j), \]  

where the \( u_j \) are the zeros of \( L_n^{-1/2}(u) \), and the weights are given by standard formulæ \[11\],

\[ w_j = \frac{\Gamma(n+1/2)}{n!(n+1)^2} \frac{u_j}{\left[ L_{n+1}^{-1/2}(u_j) \right]^2}. \]  

5. Singlet Evolution

The same considerations discussed in the previous two sections apply to singlet evolution, with some important differences. In the non-singlet case, the integrand in the inverse Mellin transform of \( f^z(Q_0^2) \) is modified by a simple (and modest) multiplicative factor to obtain the integrand for \( f(x,Q^2) \). In contrast, in the singlet case, the evolution operator has non-trivial matrix structure, and is not close to the identity matrix even for \( Q^2 \) near \( Q_0^2 \). This happens because the \( (\Sigma, g) \) basis is not an eigenbasis even for the lowest-order Altarelli-Parisi function. Accordingly, contours chosen according to either \( \Sigma \) or \( g \) will not be particularly good ones. What we want is a basis in which the evolution operator does not twist one direction into another as we move around in the complex plane. Such a basis is given by the eigenvectors of the lowest-order Altarelli-Parisi matrix, that is by \( P_{\pm}^{z}(\Sigma) \). Thus in the singlet sector, we could rewrite our Mellin integral as

\[ \int_C \text{Re} \left[ -idz \ x^{-z} E^z(a_s,a_0)s^z(Q_0^2) \right] = \int_C \text{Re} \left[ -idz \ x^{-z} E^z(a_s,a_0)P_{-} s^z(Q_0^2) \right] + \int_C \text{Re} \left[ -idz \ x^{-z} E^z(a_s,a_0)P_{+} s^z(Q_0^2) \right], \]  

where

\[ s^z(Q^2) = \left( \Sigma^z(Q^2) \ g^z(Q^2) \right). \]  

In each of these integrals, each of the components is now modified multiplicatively (up to \( \mathcal{O}(a_s) \) corrections), like the non-singlet Mellin integrals I analyzed in previous sections. We might expect them to be treatable in the same fashion — contours chosen according to the components of \( P_\pm s^z(Q_0^2) \). Indeed, following this approach we would choose four different contours for the different integrations above. There are, however, two complications we would confront.

Analyticity assures us that it is legitimate to choose different contours for the \( P_- \) and \( P_+ \) integrals, but there is a subtlety: the integrands have branch cuts in the complex plane, and the
contours chosen according to section 3 may cross these branch cuts. So long as we use the same contour for both integrals, this is completely harmless, because all that happens upon crossing a branch cut is that $\lambda_{\pm}$ interchange roles. This merely interchanges the two integrands, and the sum is unaffected. If we want to choose different contours, however, we should either shift the branch cuts so that neither integral crosses them (which is possible only some of the time), or else we must compute the integral around the branch cut. While the latter is possible, it will not allow an efficient evaluation of the integral.

The other complication is that the components of $P_{\pm}^z s^z(Q_0^2)$ are no longer necessarily positive functions. As a result, they no longer necessarily have a minimum to the right of the rightmost pole. (Typically $\Sigma^z$ and $g^z$ will have nearly the same rightmost pole, as it controls the $x \rightarrow 0$ behavior; the gluon distribution will be slightly steeper [1].) Indeed, in practice one combination — $P^z s^z(Q_0^2)$ — is roughly a sum of the two components, and hence is positive, and can be handled according to the prescriptions of the previous section; while the other combination $(P_+ s^z(Q^2))$ is not, and in fact has no minimum to the right of the rightmost pole for certain choices of $f^z(Q_0^2)$. (The contour of steepest descent heads straight into the pole.)

Thus instead it is better to pick a slightly different approach to choosing the contour-determining function in this case. Instead of the parton distributions at the original scale $Q_0^2$, take the distributions evolved (using leading-order evolution) to another fixed scale $Q_1^2$ as the contour-determining function $F(z)$. The latter is of course just given by the evolution operator $E_{\text{LO}}^z(Q_1^2, Q_0^2)$ multiplied by the starting distributions $s^z(Q_0^2)$. While in principle we might choose different contours for the two different components in the singlet sector, in practice it is more efficient overall to choose a single contour using the gluon component in the role of $F(z)$. That is, for the purposes of determining the contour of integration, and the integration points along it, take

$$
\left[ \left( a_s(Q_1^2/a_0) \right)^{-\lambda^z_+/\beta_0} + a_s(Q_1^2/a_0)^{-\lambda^z_-/\beta_0} \right] s^z(Q_0^2) \right]_2
$$

for $F(z)$ in the singlet sector. In this expression, $Q_1$ would be a scale intermediate between $Q_0^2$ and the highest scale to which we wish to evolve the parton distributions.

6. Numerical Performance

At how many points do we need to evaluate the integrands constructed according to the prescriptions in previous sections, in order to obtain an evolved parton distribution function to a given accuracy? While the answer will depend on the precise form of the initial distribution functions, and on the desired accuracy, we can obtain a very good idea by studying the numerics of
the evolution of the toy parton distribution set considered by Blümlein et al. [12]. Those authors consider the \( \overline{\text{MS}} \) massless four-flavor evolution from a reference scale \( Q_0 = 2 \text{ GeV} \), with \( \Lambda_{\text{MS}}^{(4)} = 250 \text{ MeV} \). The initial distributions are taken to have the following form,

\[
\begin{align*}
    u_v(x, Q_0^2) &= A_u x^{-0.5}(1 - x)^3, \\
    d_v(x, Q_0^2) &= A_d x^{-0.5}(1 - x)^4, \\
    S(x, Q_0^2) &= A_S x^{-1.2}(1 - x)^7, \\
    c(x, Q_0^2) &= 0, \\
    g(x, Q_0^2) &= A_g x^{-1.2}(1 - x)^5.
\end{align*}
\]

(6.1)

The sea \( S(x, Q^2) = [\Sigma - u_v - d_v](x, Q^2) \) includes the charm content, and is taken to carry 15\% of the nucleon momentum at the input scale. This fixes \( A_S \); the remaining \( A_i \) are fixed by the flavor and momentum sum rules.

Take the desired accuracy to be the same 2 parts in \( 10^4 \) sought by the above authors. For the non-singlet evolution (for example, the valence up or down densities) to \( Q = 10 \text{ GeV} \) requires around 30 points at small \( x \), rising to around 80 points for \( x = 0.7 \), using Gauss-Legendre quadrature on the contour of ref. [7]. (Evolution to \( Q = 10 \text{ TeV} \) requires about 10\% more points at larger \( x \).) In constrast, using contour derived in the present work requires only three or four points for all \( 10^{-5} < x < 0.9 \). In the singlet sector, the new contour typically requires four points, while the contour of ref. [7] requires roughly the same number of points as the non-singlet sector at small \( x \), and somewhat more at larger \( x \). Obtaining the toy parton set to the stated accuracy typically requires more points, because the charm distribution is a small difference of two larger numbers. The quadratic contour derived in this paper requires a lone additional point for most \( x \) values, and a total of seven points at the largest \( x \) value. (For the contour of ref. [7], the toy parton set typically requires 30 points at small \( x \) to over 120 at the largest \( x \) value.)

The answers obtained using this new approach should be compared with those of the ‘truncated analytic solution,’ that is the lower half, of the table of ref. [12]. The following table illustrates the convergence of sample values using the new contour, with one, two, or four Gauss-Laguerre
crossing functions arise naturally in a crossing-symmetric formalism [13] for evaluating general next-to-leading order distributions in a collider environment. They give the change in the differential cross section as a colored final-state particle is crossed from the final state into the initial state. The crossing functions $C_{a\to p}(x, Q^2)$ are factorization-scheme dependent. They can be expressed in terms of scheme-independent functions $A_{a\to p}$ and scheme-dependent functions $B_{a\to p}$ as follows,

$$C_{a\to p}(x, Q^2) = \left( \frac{N}{2\pi} \right) \left[ A_{a\to p}(x, Q^2) \ln \left( \frac{s_{\text{min}}}{Q^2} \right) + B_{a\to p}(x, Q^2) \right],$$

(7.1)

where $s_{\text{min}}$ is the boundary between the real contributions integrated analytically and those integrated numerically. A physical quantity will be independent of $s_{\text{min}}$, in the limit that $s_{\text{min}} \to 0$. The $A$ and $B$ functions are convolutions of universal kernels with the parton distribution functions,

$$A_{a\to p}(x, Q^2) = K_{a\to b}^A(x) \otimes f_{b\to p}(x, Q^2),$$

$$B_{a\to p}(x, Q^2) = K_{a\to b}^B(x) \otimes f_{b\to p}(x, Q^2),$$

(7.2)

| $x$ | $f$ | $xf(x)$ | $n=1$ | 2 | 4 | exact |
|-----|-----|---------|--------|---|---|-------|
| $10^{-5}$ | $u_v$ | frac. error | 0.0096683 | $2.7 \cdot 10^{-2}$ | $3.4 \cdot 10^{-3}$ | $2.7 \cdot 10^{-5}$ | 0.0094114 |
| $10^{-3}$ | $u_v$ | frac. error | 0.089636 | $1.8 \cdot 10^{-2}$ | $1.0 \cdot 10^{-3}$ | $1.0 \cdot 10^{-4}$ | 0.088086 |
| 0.1 | $u_v$ | frac. error | 0.47445 | $3.8 \cdot 10^{-3}$ | $5.2 \cdot 10^{-4}$ | $7.4 \cdot 10^{-7}$ | 0.47267 |
| 0.3 | $u_v$ | frac. error | 0.31061 | $8.6 \cdot 10^{-3}$ | $1.0 \cdot 10^{-4}$ | $2.1 \cdot 10^{-6}$ | 0.30797 |
| $10^{-5}$ | $g$ | frac. error | 102.92 | $4.9 \cdot 10^{-2}$ | $97.879$ | $98.080$ | 0.088086 |
| $10^{-3}$ | $g$ | frac. error | 22.052 | $4.5 \cdot 10^{-2}$ | $21.106$ | $21.112$ | 21.112 |
| 0.1 | $g$ | frac. error | 1.4168 | $1.2 \cdot 10^{-3}$ | $1.4152$ | $1.4151$ | 1.4151 |
| 0.3 | $g$ | frac. error | 0.18849 | $5.0 \cdot 10^{-3}$ | $0.18754$ | $0.18755$ | 0.18755 |

7. Crossing Functions

Crossing functions arise naturally in a crossing-symmetric formalism [13] for evaluating general next-to-leading order distributions in a collider environment. They give the change in the differential cross section as a colored final-state particle is crossed from the final state into the initial state. The crossing functions $C_{a\to p}(x, Q^2)$ are factorization-scheme dependent. They can be expressed in terms of scheme-independent functions $A_{a\to p}$ and scheme-dependent functions $B_{a\to p}$ as follows,
(again with implicit summation over $b$). Explicit expressions for the kernels $K^{A,B}$ may be extracted from ref. [13],

\[
K_{g_{\rightarrow}g}^{A}(x) = \frac{(11N - 2n_f)}{6N} \delta(1 - x) + 2 \left( \frac{x}{(1-x)_+} + \frac{(1-x)}{x} + x(1-x) \right),
\]

\[
K_{g_{\rightarrow}q}^{A}(x) = \delta_{qq'} \left( 1 - \frac{1}{N^2} \right) \left[ \frac{3}{4} \delta(1 - x) + \frac{1}{2} \left( \frac{1 + x^2}{(1-x)_+} \right) \right],
\]

\[
K_{q_{\rightarrow}g}^{A}(x) = \frac{1}{2N} \left( z^2 + (1-z)^2 \right),
\]

\[
K_{g_{\rightarrow}q}^{A}(x) = \frac{1}{2} \left( 1 - \frac{1}{N^2} \right) \frac{1 + (1-z)^2}{z},
\]

\[
K_{g_{\rightarrow}g}^{B, MS}(x) = \left( \frac{\pi^2}{3} - \frac{67}{18} + \frac{5n_f}{9N} \right) \delta(1 - x) + 2x \left( \frac{\ln(1-x)}{1-x} \right) + \]
\[
+ 2 \left( \frac{(1-x)}{x} + x(1-x) \right) \ln(1-x),
\]

\[
K_{g_{\rightarrow}q}^{B, MS}(x) = \delta_{qq'} \left( 1 - \frac{1}{N^2} \right) \left[ \frac{\pi^2}{6} - \frac{7}{4} \delta(1 - x) - \frac{1}{2} (1-x) + \frac{1}{2} (1 + x^2) \left( \frac{\ln(1-x)}{1-x} \right) \right],
\]

\[
K_{q_{\rightarrow}g}^{B, MS}(x) = \frac{1}{2N} \left[ (x^2 + (1-x)^2) \ln(1-x) + 1 - x^2 - (1-x)^2 \right],
\]

\[
K_{g_{\rightarrow}q}^{B, MS}(x) = \frac{1}{2} \left( 1 - \frac{1}{N^2} \right) \left[ \frac{1 + (1-x)^2}{x} \ln(1-x) + x \right].
\]

(Note that $K_{g_{\rightarrow}q}^{A,B} = K_{q_{\rightarrow}g}^{A,B}$, etc.) In this equation the $(.)_+$ prescription is defined by

\[
(F(z))_+ = \lim_{\beta \to 0} \left( \theta(1 - z - \beta) F(z) - \delta(1-z-\beta) \int_0^{1-\beta} F(y) dy \right),
\]

such that,

\[
\int_x^1 dz \left( \frac{g(z)}{(1-z)_+} \right) = \int_x^1 dz \frac{g(z) - g(1)}{1-z} + g(1) \log(1-x),
\]

\[
\int_x^1 dz g(z) \left( \frac{\log(1-z)}{1-z} \right)_+ = \int_x^1 dz \frac{g(z) - g(1)}{1-z} \log(1-z) + \frac{g(1)}{2} \log^2(1-x),
\]

provided that $g(z)$ is a function well behaved at $z = 1$. 

13
The Mellin moments of the kernels are

\[
K_{q\rightarrow q}^{A,z} = \frac{11}{6} - \frac{n_f}{3N} + 2 \left( \psi(1) - \psi(z+1) + \frac{1}{z(z-1)} + \frac{1}{(z+1)(z+2)} \right),
\]

\[
K_{q\rightarrow q'}^{A,z} = \delta_{qq'} \left( \frac{1}{1 - \frac{1}{N^2}} \right) \left[ \frac{3}{4} + \psi(1) - \psi(z+1) + \frac{1}{2z(z+1)} \right],
\]

\[
K_{A,z}^{g\rightarrow q} = \frac{1}{2N} \left( \frac{1}{z+2} + \frac{2}{z(z+1)(z+2)} \right),
\]

\[
K_{A,z}^{g\rightarrow q} = \frac{1}{2} \left( \frac{1}{z-1} + \frac{2}{z(z-1)(z+1)} \right),
\]

\[
K_{B,MS,z}^{g\rightarrow g} = \frac{\pi^2}{3} - \frac{67}{18} + \frac{5n_f}{9N} + (\psi(z+1) - \psi(1))^2 + \psi'(1) - \psi'(z+1)
\]

\[
+ \left( \frac{2}{z(z-1)} + \frac{2}{z(z+1)(z+2)} \right) (1 + \psi(1) - \psi(z+1) - \frac{2}{z+1} + \frac{2}{z+2}),
\]

\[
K_{B,MS,z}^{g\rightarrow g'} = \delta_{qq'} \left( \frac{1}{1 - \frac{1}{N^2}} \right) \left[ \frac{\pi^2}{6} - \frac{7}{4} + \frac{1}{2z^2} - \frac{1}{2z(z+1)^2} + \frac{1}{2}(\psi(z+1) - \psi(1))^2
\]

\[
+ \frac{1}{2z(z+1)}(\psi(1) - \psi(z+1)) + \frac{1}{2}(\psi'(1) - \psi'(z)) \right],
\]

\[
K_{B,MS,z}^{g\rightarrow g} = \frac{1}{2N} \left[ \left( \frac{1}{z+2} + \frac{2}{z(z+1)(z+2)} \right) (\psi(1) - \psi(z+3))
\]

\[
+ \frac{2}{z(z+1)} + \frac{1}{z(z+1)(z+2)} \right],
\]

\[
K_{B,MS,z}^{g\rightarrow q} = \frac{1}{2} \left( \frac{1}{z-1} + \frac{2}{z(z-1)(z+1)} \right) (\psi(1) - \psi(z+1) + \frac{z}{z+1} + \frac{2}{z(z-1)} \right].
\]

(7.6)

These moments allow us to write

\[
A_{a\rightarrow p}^{z}(Q^2) = K_{a\rightarrow b}^{A,z} f_{b\rightarrow p}^{z}(Q^2)
\]

\[
B_{a\rightarrow p}^{z}(Q^2) = K_{a\rightarrow b}^{B,z} f_{b\rightarrow p}^{z}(Q^2)
\]

and then using eqn. (2.9),

\[
A_{a\rightarrow p}^{z}(Q^2) = K_{a\rightarrow b}^{A,z} E_{bc}^{z}(\alpha_s(Q^2), \alpha_0) f_{c\rightarrow p}^{z}(Q_0^2)
\]

\[
B_{a\rightarrow p}^{z}(Q^2) = K_{a\rightarrow b}^{B,z} E_{bc}^{z}(\alpha_s(Q^2), \alpha_0) f_{c\rightarrow p}^{z}(Q_0^2)
\]

(7.8)

We can evaluate the crossing function, given by the inverse Mellin transform of this moment, using the same approach described in previous sections, but with \( f^{z}(Q_0^2) \) replaced by \( K^{X,z} f^{z}(Q_0^2) \) \( (X = A, B) \).

The conjugation identities mentioned above, along with the fact that \( K_{q\rightarrow q}^{X,z} = 0 \), imply that the non-singlet and singlet sectors do not mix in eqn. (7.8), and that the kernel in the non-singlet sector is simply \( K_{q\rightarrow q}^{X,z} \), while the \( 2 \times 2 \) matrix in the singlet sector is

\[
\begin{pmatrix}
K_{q\rightarrow q}^{X,z} & K_{q\rightarrow q}^{X,z} \\
K_{q\rightarrow q}^{X,z} & K_{q\rightarrow q}^{X,z}
\end{pmatrix}
\]

(7.9)
8. Comparison with $x$-Space Codes

As mentioned in the introduction, the two main methods now commonly used to evolve parton distribution functions are the Mellin transform method [7,14] pursued in previous sections, or direct integration [15] of the differential equations for $f(x,Q^2)$. While formally equivalent to NLO, these techniques differ in the higher-order terms implicitly retained. As noted by Blümlein et al. [5], these differences can have a substantial effect on the parton distributions, as much as several percent even at moderate $x$. One lesson from this comparison is that a determination of $\alpha_s(M_Z^2)$ to 1% will require NNLO calculations; in the meantime, however, it is useful to be able to reproduce answers obtained through the $x$-space method as well. The purpose of this section is to show that solutions identical to those obtained by direct integration can be obtained using the Mellin transform technique, taking advantage of the same enhancements considered in previous sections.

Let us first consider $a_s$ itself; in terms of the QCD scale parameter $\Lambda$, it can be written [6] at NLO as

$$a_s(Q^2) = \frac{1}{\beta_0 \ln Q^2/\Lambda^2} \left[ 1 - \frac{\beta_1}{\beta_0^2} \ln \ln Q^2/\Lambda^2 + O (\ln^{-3} Q^2/\Lambda^2) \right] ;$$

(8.1)

let us replace it with an approximation (to NLO) for $a_s$ in terms of $a_s$ at a different scale, instead of one in terms of $\Lambda_{QCD}$,

$$a_s(Q^2,Q_0^2,a_0) = \frac{a_0(1 + a_0 \beta_0 \ln Q^2/Q_0^2)}{(1 + a_0 \beta_0 \ln Q^2/Q_0^2)^2 + a_0 \beta_r (1 + a_0 \beta_r + a_0 \beta_0 \ln Q^2/Q_0^2) \ln \left( 1 + \frac{a_0 \beta_0 \ln Q^2/Q_0^2}{1 + a_0 \beta_r} \right) } ,$$

(8.2)

where $\beta_r = \beta_1/\beta_0$, and the number of flavors is taken to be constant throughout the interval $[Q_0, Q]$. This particular form of $a_s$ emerges by performing one Newton-Raphson improvement to the 1-loop solution. We could recover the solution of the implicit (beta function) equation for $a_s$,

$$\frac{1}{a_s(Q^2)} = \frac{1}{a_s(Q_0^2)} + \beta_0 \ln \left( Q^2/Q_0^2 \right) - \frac{\beta_1}{\beta_0} \ln \left[ \frac{a_s(Q^2)(\beta_0 + \beta_1 a_s(Q_0^2))}{a_s(Q_0^2)(\beta_0 + \beta_1 a_s(Q_0^2))} \right]$$

(8.3)

if we iterate the evolution$^\dagger$,

$$a_s^{[n]}(Q^2,Q_0^2,a_0) = a_s^{[n-1]}(Q^2,Q_0^2,a_s^{[n-1]}(Q_1^2,Q_0^2,a_0)) ,$$

$$a_s^{[0]}(Q^2,Q_0^2,a_0) = a_s(Q^2,Q_0^2,a_0) .$$

(8.4)

where $Q_1$ lies in the interval $[Q_0,Q]$; since the evolution is logarithmic, we would presumably choose $Q_1 = \sqrt{Q Q_0}$. Formally, we want to take the limit $n \to \infty$, so that

$$a_s(Q^2,Q_0^2,a_0) = \lim_{n \to \infty} a_s^{[n]}(Q^2,Q_0^2,a_0) .$$

(8.5)

$^\dagger$ Iteration will result in convergence to the numerical solution of eqn. (2.6) only if the form of the approximation is suitable; for a slowly varying function whose true zero is near the initial approximation, a Newton-Raphson approximation is indeed suitable.
In practice, however, this is a completely pointless exercise, because the form (8.2) is already within one part in $10^4$ of the ‘exact’ answer for $Q > Q_0$, so long as $Q_0 \geq 1.5$ GeV; in the other direction, for $Q_0 = M_Z$, the fractional error is less than $2 \cdot 10^{-4}$ for $Q > 4$ GeV. (The ‘exact’ answer refers to the numerical solution of the implicit NLO equation (8.3).) As $Q$ grows for fixed $Q_0$, the fractional error reaches a maximum for some $Q^2_m$, and then falls off; for $Q_0 = 2$ GeV, it is as noted less than 1 part in $10^4$, around $Q_m = 27$ GeV.

With a formula for $a_s$ that reproduces a direct integration of the $\beta$ function in hand, we can turn to the evolution equations for the parton distributions. Equation (2.7), for the Mellin transform of the evolved parton distribution, is identical to the original $x$-space equation. In the usual Mellin space approach, one performs the further truncations discussed in section 2, effectively dropping terms which are $O(a_s^3)$, to obtain the usual solution (2.11,2.13). I should stress that from a physical point of view, to next-to-leading order the truncated equations are no less valid than the original, and the solutions qualify no less as NLO solutions. What is of interest is the discrepancy between the two solutions: one or both has higher-order corrections at least as large as half the difference between them. In order to study this difference, we must solve the untruncated equation (2.7).

Introduce an evolution operator just as in equation (2.9). In the non-singlet case, we can integrate the equation directly, obtaining

$$E^z(a_s, a_0) = \exp \left( \int_{a_0}^{a_s} \frac{P^z(a)}{\beta(a)} \, da \right). \quad (8.6)$$

In the case at hand,

$$\int_{a_0}^{a_s} \frac{P^z(a)}{\beta(a)} \, da = - \int_{a_0}^{a_s} \frac{P_0^z + aP_1^z}{a(\beta_0 + \beta_1 a)} \, da$$

$$= - \frac{P_0^z}{\beta_0} \ln \left( \frac{a_s}{a_0} \right) - \frac{P_1^z}{\beta_1} \ln \left( \frac{\beta_0 + \beta_1 a_s}{\beta_0 + \beta_1 a_0} \right), \quad (8.7)$$

so that

$$E^z(a_s, a_0) = \left( \frac{a_s}{a_0} \right)^{-P_0^z/\beta_0} \left( \frac{\beta_0 + \beta_1 a_s}{\beta_0 + \beta_1 a_0} \right)^{-P_1^z/\beta_1}. \quad (8.8)$$

It is worth noting that this evolution operator is not much more expensive to evaluate on a computer than the conventional one, eqn. (2.11).

Now, although we can solve the equation in closed form in the non-singlet case, we will not be able to do so in the singlet case, so it is useful to understand what alternative means we have of computing the operator in eqn. (8.8). Since it is an evolution operator, we can write it in the form

$$E^z(a_s, a_0) = \Pi_{j=1}^{a_n} E^z(a_j, a_{j-1}), \quad (8.9)$$

with $a_n = a_s$, where (for example),

$$a_j = a_0 + (a_s - a_0)j/n. \quad (8.10)$$
Equation (8.9) is, of course, exact; but can we take advantage of it to approximate \( E^z(a_j, a_{j-1}) \)? We would then hope to recover the full evolution operator by taking the \( n \to \infty \) limit,

\[
E^z(a_s, a_0) = \lim_{n \to \infty} \Pi_{j=1}^n E^z(a_j, a_{j-1}).
\] (8.11)

In fact, we can, but there is a subtlety concerning the expansion parameter. Define \( \delta a = (a_s - a_0)/n \), the total evolution length for each step in eqn. (8.9), and expand \( E^z(a_j, a_{j-1}) \) in \( \delta a \),

\[
E^z(a_j, a_{j-1}) = 1 + e_1(a_j)\delta a + e_2(a_j)(\delta a)^2 + \cdots
\] (8.12)

We then find

\[
E^z(a_s, a_0) = 1 + \delta a \sum_{j=1}^n e_1(a_j) + (\delta a)^2 \sum_{j_1, j_2=1 \atop j_1 \neq j_2}^n e_1(a_{j_1})e_1(a_{j_2}) + \cdots + (\delta a)^n e_1(a_1) \cdots e_1(a_n)
\]

\[
+ (\delta a)^2 \sum_{j=1}^n e_2(a_j) + (\delta a)^4 \sum_{j_1, j_2=1 \atop j_1 \neq j_2}^n e_2(a_{j_1})e_2(a_{j_2}) + \cdots + (\delta a)^2e_2(a_1) \cdots e_2(a_n) + \cdots
\]

\[
= \left( 1 + \delta a \sum_{j=1}^n e_1(a_j) \right)^n + \text{terms with fewer sums than powers of } \delta a.
\] (8.13)

If the \( e_i \) are well-behaved functions (as they are in our case), roughly speaking each complete sum over an index produces a factor of \( n \) compensating the \( 1/n \) implicit in \( \delta a \), so that when we take the limit the terms with fewer sums than powers will vanish because they are suppressed by powers of \( n \). Thus in the limit we obtain

\[
E^z(a_s, a_0) = \lim_{n \to \infty} \left( 1 + \delta a \sum_{j=1}^n e_1(a_j) \right)^n
\]

\[
= \exp \left[ \int_{a_0}^{a_s} da \frac{d \ln E^z(a, a_0)}{da} \right]
\] (8.14)

which using (2.7) is of course equivalent to eqn. (8.6). So we learn that expansion in \( \delta a \) is legitimate, and that the higher-order terms don’t matter in the limit (they would of course accelerate convergence if they were present). This is neither surprising nor subtle; the subtlety comes when we consider in addition expanding in \( a_j \), which is also a small parameter,

\[
e_i(a) = e_{i,0} + e_{i,1}a + e_{i,2}a^2 + \cdots
\] (8.15)

and truncating at order \( m \), to obtain \( \tilde{e}_i(a) \). Running through the above argument, we find that no matter how large the number of segments \( n \) gets, there is always an error of \( \mathcal{O}(a^{m+1}) \) in the
estimate of \( E^z(a_s, a_0) \),

\[
\tilde{E}^z(a_s, a_0) = \lim_{n \to \infty} \left( 1 + \delta a \sum_{j=1}^{n} \tilde{c}_1(a_j) \right)^n
\]

\[= \exp \left[ \int_{a_0}^{a_s} \frac{d \ln E^z(a, a_0)}{da} \right] + O(a^{m+1}) \tag{8.16}\]

Unfortunately, the standard evolution operator (2.11) does involve precisely these sorts of truncations, so we can’t use it to recover the missing higher-order terms. We can obtain a kernel that will work by exponentiating only the leading-order term of the integral (8.7), and leaving the rest expanded,

\[
E^z(a_s, a_0) = \left( \frac{a_s}{a_0} \right)^{-P_z^0/\beta_0} \left[ 1 - \frac{P_z^1}{\beta_1} \ln \left( \frac{\beta_0 + \beta_1 a_s}{\beta_0 + \beta_1 a_0} \right) \right]. \tag{8.17}\]

This is equivalent to (formally) expanding in \( P_z^1 \), which is in general not a small parameter; the expansion only works because the accompanying logarithm is small. We may thus expect that the speed of convergence varies as we move around the complex plane, and the question then arises of how large \( n \) has to be in equation (8.9) before we converge to the ‘exact’ answer given by eqn. (8.8).

The answer, somewhat amusingly, is that for the non-singlet parton distribution functions one encounters in practice, a real-world value of \( a_s \), and evolution over the range from \( Q_0 = 2 \text{ GeV} \) to \( Q = 15 \text{ GeV} \), \( n = 1 \) suffices (except at the smallest values of \( x \), for which we need \( n = 3 \)). That is, using eqn. (8.17) already gives the limiting answer, to within 2 parts in \( 10^4 \). More generally, \( n = 2 \) limits the error to 6 parts in \( 10^4 \) for \( Q \leq 10 \text{ TeV} \).

In the singlet sector, equation (2.7) has the solution

\[
E^z(a_s, a_0) = T_a \exp \left[ \int_{a_0}^{a_s} \frac{P_z^z(a)}{\beta(a)} \, da \right]. \tag{8.18}\]

where the \( a \)-ordering operator \( T_a \), the analog of the usual path-ordering operator, orders matrices \( P_z^z(a) \) according to their distance from \( a_0 \), putting matrices of arguments further away from \( a_0 \) further to the left. It appears because in general \( P_z^z \) matrices at different points \( a, a' \) do not commute.

Equation (8.18) is still a formal expression, and one must make further approximations to obtain an explicit expression. We can make use of eqn. (8.9), in which for singlet evolution we must also order the matrices,

\[
E^z(a_s, a_0) = E^z(a_n, a_{n-1}) \cdots E^z(a_1, a_0). \tag{8.19}\]

Let us take a \( \delta a \) sufficiently small that we can formally expand NLO terms in the \( a \)-ordered exponential (8.18) to first order, without assuming that the same is true of LO terms; we can then
write
\[ E^z(a_s, a_0) = T_a \left\{ \exp \left[ \frac{P_0}{\beta_0} \int_{a_0}^{a_s} da \right] \exp \left[ \int_{a_0}^{a_s} \frac{P^z(a)}{\beta(a)} - \left( \frac{P^z}{-\beta_0 a} \right) da \right] \right\} \]
\[ = T_a \left\{ \exp \left[ \frac{P_0}{\beta_0} \int_{a_0}^{a_s} da \right] \left( 1 + \int_{a_0}^{a_s} \frac{P^z(a)}{\beta(a)} - \left( \frac{P^z}{-\beta_0 a} \right) da \right) \right\} \]  (8.20)

Evaluating the time-ordered product gives us our final expression for the singlet evolution operator,
\[ E^z(a_s, a_0) = \]
\[ \left( \frac{a_s}{a_0} \right)^{-\lambda_{\perp}^z/\beta_0} \left\{ P_- - \frac{1}{\beta_1} P_- P^z_1 P_- \ln \left[ \frac{\beta_0 + \beta_1 a_s}{\beta_0 + \beta_1 a_0} \right] \right\} \]
\[ - P_- P^z_1 P_+ \frac{1}{\beta_0 - \lambda_{\perp}^z + \lambda_{\parallel}^z} \]
\[ \times \left[ a_0 \left( \frac{a_s}{a_0} \right)^{(\lambda_{\perp}^z - \lambda_{\parallel}^z)/\beta_0} 2 F_1 \left( 1, 1 - \frac{\lambda_{\perp}^z - \lambda_{\parallel}^z}{\beta_0}; 2 - \frac{\lambda_{\perp}^z - \lambda_{\parallel}^z}{\beta_0}; -\frac{\beta_1}{\beta_0} a_s \right) \right. \]
\[ - a_0 \left. 2 F_1 \left( 1, 1 - \frac{\lambda_{\perp}^z - \lambda_{\parallel}^z}{\beta_0}; 2 - \frac{\lambda_{\perp}^z - \lambda_{\parallel}^z}{\beta_0}; -\frac{\beta_1}{\beta_0} a_0 \right) \right\} \]  (8.21)

In this equation, \( 2 F_1 \) is the hypergeometric function; while \( \beta_1 \) is substantially larger than \( \beta_0 \), the argument of the hypergeometric function will still be much smaller (in absolute magnitude) than one, so that we can evaluate it using its series expansion,
\[ 2 F_1 (a, b; c; z) = \frac{\Gamma(c)}{\Gamma(a) \Gamma(b)} \sum_{n=0}^{\infty} \frac{\Gamma(n+a) \Gamma(n+b)}{\Gamma(n+c) n!} z^n \]  (8.22)

To reproduce the toy parton as discussed in section 6, we would need a rather large number of subintervals \( n \) in eqn. (8.19) for evolution at small and large \( x \). It is possible to reduce this number by resumming the terms in \( P_1 \) that are proportional to \( P_0 \). To do so, define
\[ \mu_{-}^z = \text{Tr} \left( P_- P^z_1 \right), \quad \mu_{+}^z = \text{Tr} \left( P_+ P^z_1 \right). \]  (8.23)

Then
\[ \overline{P}^z = \mu_{-}^z P_- + P_- P^z_1 P_+ + \mu_{+}^z P_+ + P_+ P^z_1 P_-, \]  (8.24)

and
\[ E^z(a_s, a_0) = \]
\[ \left( \frac{a_s}{a_0} \right)^{-\lambda_{\perp}^z/\beta_0} \left( \frac{\beta_0 + \beta_1 a_s}{\beta_0 + \beta_1 a_0} \right)^{-\mu_{-}^z/\beta_1} \left\{ P_- - P_- P^z_1 P_+ \frac{1}{\beta_0 - \lambda_{\perp}^z + \lambda_{\parallel}^z} \left( 1 + \frac{\beta_1}{\beta_0} a_0 \right) \right\} \]
\[ \times \left[ a_0 \left( \frac{a_s}{a_0} \right)^{(\lambda_{\perp}^z - \lambda_{\parallel}^z)/\beta_0} 2 F_1 \left( 1 + \mu_{+}^z - \mu_{-}^z, 1 - \frac{\lambda_{\perp}^z - \lambda_{\parallel}^z}{\beta_0}; 2 - \frac{\lambda_{\perp}^z - \lambda_{\parallel}^z}{\beta_0}; -\frac{\beta_1}{\beta_0} a_s \right) \right. \]
\[ - a_0 \left. 2 F_1 \left( 1 + \mu_{+}^z - \mu_{-}^z, 1 - \frac{\lambda_{\perp}^z - \lambda_{\parallel}^z}{\beta_0}; 2 - \frac{\lambda_{\perp}^z - \lambda_{\parallel}^z}{\beta_0}; -\frac{\beta_1}{\beta_0} a_0 \right) \right\} \]
\[ + (+ \leftrightarrow -) \]  (8.25)
With this form, 20 subintervals suffice at \( x \sim 10^{-5} \), 10 or fewer at intermediate \( x \), and only at the largest \( x \sim 0.7 \) do we still require a large number (> 100) of subintervals.

Using equations (8.2,8.8,8.25,8.19) yields the evolution as would be given by a direct integration of the untruncated evolution equation (2.1) along with a direct integration of the beta function (2.6). One might have thought that this would be the evolution as computed by various \( x \)-space programs; but it isn’t. The reason is that these programs do not appear to integrate the beta function numerically, but rather use the approximate solution (8.1). This provides yet a third inequivalent version of NLO evolution. It isn’t difficult to reproduce it in the Mellin approach, however; avoid changing variables to \( a_s \), and instead integrate eqn. (2.5) with respect to \( Q^2 \). In the non-singlet sector, we obtain

\[
\hat{E}^z(Q^2, Q_0^2) = \left( \frac{L_0}{L} \right)^{-P_0^z/\beta_0} \exp \left[ \beta_1 \frac{1}{\beta_0^2} \frac{P^z_1}{P_0^z} \left( \frac{1}{L_0} - \frac{1}{L} \right) - \beta_1 \frac{1}{\beta_0} \frac{P^z_0}{P_0^z} \left( \frac{\ln L_0}{L_0} - \frac{\ln L}{L} \right) - \beta_1 \frac{1}{\beta_0} \frac{P^z_1}{P_0^z} \left( \frac{1 + 2 \ln L_0}{L_0^2} - \frac{1 + 2 \ln L}{L^2} \right) + \frac{\beta_1^2}{27 \beta_0^2} \frac{P^z_1}{P_0^z} \left( \frac{2 + 6 \ln L_0 + 9 \ln^2 L_0}{L_0^3} - \frac{2 + 6 \ln L + 9 \ln^2 L}{L^3} \right) \right] \tag{8.26}
\]

where the hat on \( E \) indicates that its arguments are momentum scales instead of running couplings, and where \( L_i = \ln Q_i^2 / \Lambda^2 \). We can obtain the analog to equation (8.17) by formally expanding the exponential in the \( P_i^z \), but leaving the power prefactor unexpanded. In the singlet sector, the first-order expansion in eqn. (8.20) yields

\[
\hat{E}^z(Q^2, Q_0^2) = r_L^{-\lambda^z / \beta_0} \times \left\{ P_+ + P_- \left[ \beta_1 \frac{1}{L_0^2 \beta_0^2} \frac{P^z_1}{P_0^z} \left( \frac{1}{L_0} - \frac{1}{L} \right) - 2 \frac{\beta_1^2}{\beta_0^2} \frac{P^z_0}{P_0^z} \left( \frac{\ln L_0}{L_0^2} - \frac{\ln L}{L^2} \right) \right] + P_+ \left[ \beta_1 \frac{1}{L_0^2 \beta_0^2} \frac{P^z_1}{P_0^z} \left( \frac{1}{L_0} - \frac{1}{L} \right) - 2 \frac{\beta_1^2}{\beta_0^2} \frac{P^z_0}{P_0^z} \left( \frac{\ln L_0}{L_0^2} - \frac{\ln L}{L^2} \right) \right] \right. \\
- 2 \frac{\beta_1}{\beta_0^2} \frac{P^z_1}{P_0^z} \left( \frac{1}{L_0^2 \beta_0^2} \frac{P^z_0}{P_0^z} \left( \frac{\ln L_0}{L_0^2} - \frac{\ln L}{L^2} \right) \right) + \frac{\beta_1^2}{\beta_0^2} \frac{P^z_0}{P_0^z} \left( \frac{\ln^2 L_0}{L_0^3} - \frac{\ln^2 L}{L^3} \right) \frac{1}{L_0^2 \beta_0^2} \frac{P^z_1}{P_0^z} \left( \frac{\ln L_0}{L_0^2} - \frac{\ln L}{L^2} \right) + \frac{\beta_1^2}{\beta_0^2} \frac{P^z_0}{P_0^z} \left( \frac{\ln^2 L_0}{L_0^3} - \frac{\ln^2 L}{L^3} \right) \frac{1}{L_0^2 \beta_0^2} \frac{P^z_1}{P_0^z} \left( \frac{\ln L_0}{L_0^2} - \frac{\ln L}{L^2} \right) \right\} \left[ P_+ + (\leftrightarrow -) \right] \tag{8.27}
\]

where \( r_L = L / L_0 \) and \( \delta^z \equiv (\lambda^z_+ - \lambda^z_-) / \beta_0 \). This form of the evolution operator should again be used in combination with eqn. (8.19); it does require a rather large number of subintervals \( n \) if we
want an answer accurate to 2 parts in $10^4$. It is thus better to add in the terms arising from an expansion of the time-ordered exponential to second order,

$$\delta E_z^z(Q^2, Q_0^2) = \sum_{\sigma_1, \sigma_2, \sigma_3 = \pm} P_{\sigma_1} z T_{\sigma_1} \delta E_z^z(\lambda_{\sigma_1}, \lambda_{\sigma_2}, \lambda_{\sigma_3}, P_{\sigma_2}) P_{\sigma_3}.$$ \hspace{1cm} (8.28)

The (somewhat lengthy) formula for $T_2$ is given in appendix II; it should be kept in mind that most of the computation need only be done once, not anew for each value of $Q^2$.

With the addition of the terms in $T_2$, most values of $x$ require $n = 3$ or 4 in eqn. (8.19), though at $x = 0.7$, 30 subintervals are required to provide an accuracy of $2 \cdot 10^{-4}$ for the toy parton set of ref. [12].

Using these evolution operators, along with eqn. (8.1), I find that I indeed reproduce the results of the ‘direct solution,’ that is the upper half of table 1 in ref. [12], mostly within their quoted errors. Curiously enough, the values of the evolved parton densities are quite close to what would be obtained from the ‘exact’ evolution described earlier in this section, typically within a few parts in $10^3$. Note, however, that the running coupling values are somewhat different: with $Q_0 = 2$ GeV, the two values for the running coupling differ by about 1% at $Q = 10$ GeV.

9. Conclusions

In this paper, I have derived a quadratic contour for calculating the evolution of parton distribution functions within the Mellin transform method, and demonstrated its superiority over other techniques in the literature. I have also shown how to reproduce the results obtained within the ‘$x$-space’ method using a modified evolution operator. In addition to the application discussed here, the method may also be used within a general framework for extracting parton distribution functions from collider data [16].

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Appendix I. Analytic Continuation of a Dilogarithm Integral

In order to evaluate the evolution operators along our chosen contours in the complex plane, we must be able to evaluate the moments of the leading- and next-to-leading order anomalous dimensions at essentially arbitrary points in the complex plane. As discussed in ref. [7], all functions appearing in the Mellin moments of these anomalous dimensions, save one, have expressions in terms of elementary functions or derivatives of the $\Gamma$ function. The latter can be calculated everywhere
in the complex plane via well-known techniques. The one exception is \( \tilde{S}(z) \), for which GRV give
the following expression,
\[
\tilde{S}(z) = -\frac{5}{8} \zeta(3) + \eta \left[ \frac{(\psi(z + 1) - \psi(1))}{z^2} - \frac{\zeta(2)}{2} (\psi((z + 1)/2) - \psi(z/2)) + \int_0^1 dx x^{z-1} \frac{\text{Li}_2(x)}{1 + x} \right]
\]
(I.1)
where \( \eta = \pm 1 \), \( \psi \) is the usual logarithmic derivative of the gamma function, and \( \text{Li}_2 \) is the dilogarithm. As it is not completely clear that the expansion given by the authors of ref. [7] for the last
term is valid for our purposes, I give an alternate one here.

Define
\[
M_1(z + 1) = \int_0^1 dx x^{z-1} \frac{\text{Li}_2(x)}{1 + x}.
\]
(I.2)
Using \( x^{z-1} = (1 + x)x^{z-2} - x^{z-2} \), we find the following recurrence relation for \( M_1 \),
\[
M_1(z + 1) = -M_1(z) + \int_0^1 dx x^{z-2} \text{Li}_2(x)
\]
(I.3)
\[
= M_1(z - 1) - \int_0^1 dx x^{z-3}(1 - x)\text{Li}_2(x).
\]
The other integrals in this equation may be performed by integration by parts. Let
\[
M_2(z) \equiv \int_0^1 dx x^{z-2} \text{Li}_2(x) = \frac{\zeta(2)}{z - 1} + \frac{1}{z - 1} \int_0^1 dx x^{z-2} \ln(1 - x)
\]
\[
= \frac{\zeta(2)}{z - 1} + \frac{1}{z - 1} d \left| \frac{d}{da} \int_0^1 dx x^{z-2}(1 - x)^a \right|_{a=0}
\]
(I.4)
\[
= \frac{\zeta(2)}{z - 1} + \frac{1}{(z - 1)^2} (\psi(1) - \psi(z))
\]
then
\[
M_2(z) - M_2(z - 1) = -\int_0^1 dx x^{z-3}(1 - x)\text{Li}_2(x)
\]
\[
= -\frac{\zeta(2)}{(z - 1)(z - 2)} - \frac{1}{(z - 2)^2} - \frac{1}{(z - 1)^2} \left( \psi(z - 1) - \psi(1) \right) + \frac{1}{(z - 1)^3}.
\]
(I.5)
On the other hand, we can also write down an ‘asymptotic’ expansion for \( M_1 \); to do so,
repeatedly rewrite
\[
\frac{1}{1 + x} = \frac{1 - x}{2(1 + x)} + \frac{1}{2},
\]
(I.6)
to obtain
\[
M_1(z) = \frac{1}{2} \int_0^1 dx x^{z-2} \text{Li}_2(x) + \frac{1}{2} \int_0^1 dx x^{z-2}(1 - x) \frac{\text{Li}_2(x)}{1 + x}
\]
\[
= \frac{1}{2} \sum_{j=0}^N 2^{-j} \int_0^1 dx x^{z-2}(1 - x)^j \text{Li}_2(x) + 2^{-N-1} \int_0^1 dx x^{z-2}(1 - x)^{N+1} \frac{\text{Li}_2(x)}{1 + x}
\]
(I.7)
\[
= \frac{1}{2} \sum_{j=0}^N 2^{-j} \sum_{l=0}^j (-1)^l \left( \begin{array}{c} j \\ l \end{array} \right) M_2(z + l) + 2^{-N-1} \int_0^1 dx x^{z-2}(1 - x)^{N+1} \frac{\text{Li}_2(x)}{1 + x}
\]
Since in the $z \rightarrow \infty$ limit, the integral is dominated by the region $x \sim 1$, the last term goes as $1/z^{N+2}$, and we can drop it if we are interested in the asymptotic expansion only through order $N + 1$. In fact, because of the factor of $2^{-N}$ in front, dropping this term is a reasonable approximation even for modest $z$. We can re-expand the resulting expression in terms of $1/z$, but this yields a rather poor representation. Instead we can rewrite the remainder term

$$2^{-N-1} \int_0^1 dx \, x^{z-2} (1 - x)^{N+1} \frac{\text{Li}_2(x)}{1 + x} =$$

$$2^{-N-2} \text{Li}_2(1) \int_0^1 dx \, x^{z-1} (1 - x)^{N+1} + 2^{-N-1} \int_0^1 dx \, x^{z-2} (1 - x)^{N+1} \left( \frac{\text{Li}_2(x)}{1 + x} - \frac{x \text{Li}_2(1)}{2} \right)$$

$$= 2^{-N-2} \zeta(2) \frac{\Gamma(z)\Gamma(N + 2)}{\Gamma(z + N + 2)} + 2^{-N-1} \int_0^1 dx \, x^{z-2} (1 - x)^{N+1} \left( \frac{\text{Li}_2(x)}{1 + x} - \frac{x \text{Li}_2(1)}{2} \right)$$

(I.8)

The second integral goes as $\ln z/z^{N+3}$. For Re $z$ sufficiently large, we simply drop the second term; for other $z$, we can use the recurrence relation (I.3) [backwards] to shift $z$ into this range. It’s worth using the recurrence relation (I.3) a few times explicitly, since we will certainly be interested in values near $z \sim 1$ or $2$ for which the approximation with reasonable $N$ won’t be enough; we can then simplify the transcendental functions to minimize the number of such function evaluations we need to perform.

Appendix II. Second-Order Terms for the $x$-Space Singlet Evolution Operator

To present the (somewhat lengthy) formula for $T_2$, used in equation (8.28), define the following
functions,

d_{c;ij} = c + \frac{\lambda^z_i - \lambda^z_j}{\beta_0},

P_{11} = \frac{1}{\beta_0} P_1 PP_1,

P_{10} = \frac{\beta_1}{\beta_0} P_1 PP_0,

P_{01} = \frac{\beta_1}{\beta_0} P_0 PP_1,

P_{00} = \frac{\beta_2}{\beta_0} P_0 PP_0, \quad (\text{II.1})

P'^{(a)}_{11} = P_{11} - d_{1;23} P_{10},

P'^{(b)}_{11} = P_{11} - d_{1;12} P_{01},

P'^{(a)}_{01} = P_{01} - d_{1;23} P_{00},

P'^{(a)}_{10} = P_{10} - d_{1;12} P_{00},

\delta_i^z = \frac{\lambda^z_i}{\beta_0}. 

As in section 8, r_L = L/L_0.
Then
\[ T_2^2(\lambda_1, \lambda_2, \lambda_3, P) = -\frac{d_{12}}{\beta_0^4 L_0} \left( P_{11}(a) d_{112} + P_{10}(a) d_{112} - P_{01} d_{112} + P_{00} d_{112}^2 + 2P_{00} d_{112}^3 \right) \]
\[ + \frac{d_{12}}{\beta_0^4 L_0^2} \left( P_{11}(a) d_{112} - P_{10}(a) d_{112} + P_{01} d_{112} + P_{00} d_{112}^2 - 2P_{00} d_{112}^3 \right) \]
\[ - \frac{2\beta_1 \ln L_0 r_{L_0}^\delta}{\beta_0^3 L_0^3} \left( P_{11}(a) d_{123} d_{212} + P_{11}(a) d_{123} d_{212} - P_{11}(a) d_{123} d_{212} - P_{11} d_{23} d_{312} - P_{01} d_{123} d_{212} \right) \]
\[ + \frac{2\beta_1 r_{L_0}^\delta}{\beta_0^3 L_0^4} \left( P_{11}(a) d_{123} d_{212} + P_{11}(a) d_{123} d_{212} - P_{11}(a) d_{123} d_{212} - P_{11} d_{23} d_{312} - P_{01} d_{123} d_{212} \right) \]
\[ + \frac{2\beta_1 r_{L_0}^\delta}{\beta_0^3 L_0^4} \left( 2P_{11} d_{222} d_{222} + 2P_{11} d_{222} d_{222} - 2P_{11} d_{222} d_{222} - P_{11} d_{222} d_{222} - P_{01} d_{222} d_{222} \right) \]
\[ - \frac{4P_{11} \ln L_{0} \beta_0^4 r_{L_0}^\delta}{\beta_0^8 L_0^5} \left( d_{222} d_{222} + d_{222} d_{222} - d_{222} d_{222} - d_{222} d_{222} - d_{222} d_{222} \right) \]
\[ - \frac{4P_{11} \ln L_{0} \beta_0^4 r_{L_0}^\delta}{\beta_0^8 L_0^5} \left( d_{222} d_{222} + d_{222} d_{222} - d_{222} d_{222} - d_{222} d_{222} - d_{222} d_{222} \right) \]
\[ - \frac{d_{12}}{\beta_0^4 L_0^2} \left( P_{11}(a) - P_{10}(a) d_{112} + P_{01} d_{112} + P_{00} d_{112}^2 + 2P_{00} d_{112}^3 \right) \]
\[ - \frac{d_{12}}{\beta_0^4 L_0^2} \left( P_{11}(a) - P_{10}(a) d_{112} + P_{01} d_{112} + P_{00} d_{112}^2 + 2P_{00} d_{112}^3 \right) \]
\[ - \frac{2\beta_1 P_{11}(a) d_{123} d_{212} \ln L_{0} r_{L_0}^\delta}{\beta_0^3 L_0^3} \left( d_{123} d_{212} + d_{123} d_{212} - d_{123} d_{212} - d_{123} d_{212} - d_{123} d_{212} \right) \]
\[ - \frac{2\beta_1 P_{11}(a) d_{123} d_{212} \ln L_{0} r_{L_0}^\delta}{\beta_0^3 L_0^3} \left( d_{123} d_{212} + d_{123} d_{212} - d_{123} d_{212} - d_{123} d_{212} - d_{123} d_{212} \right) \]
\[
+ \frac{2d_{4:13} \ln L \beta_{31}^4 r_{L}^{\delta_1} \delta_5}{L^4 \beta_0^8} \left(P_{1(a)} d_{1:23} d_{4:13} + 4P_{11} d_{1:23} d_{4:13} + P_{11} d_{3:23} d_{4:13} + 2P_{11} d_{2:23}^2 + P_{11} d_{3:23}^2 - 2P_{01} d_{4:13} d_{5:23}^2 - 3P_{10} d_{1:23} d_{4:13} - 3P_{01} d_{3:23} d_{4:13}^2 \right) \\
+ \frac{2d_{4:13} \beta r_{L}^{\delta_1} \delta_5}{L^4 \beta_0^8} \left(2P_{11} d_{1:23} d_{2:23}^2 + P_{11} d_{4:13} d_{3:23} + P_{11} d_{3:23}^3 - P_{01} d_{4:13} d_{3:23}^3 + P_{11}^{(a)} d_{1:23} d_{4:13} + 4P_{11} d_{2:23} d_{4:13} + P_{11} d_{3:23} d_{4:13}^2 + 2P_{01} d_{2:23} d_{4:13}^2 - 3P_{10} d_{1:23} d_{4:13}^3 - 3P_{01} d_{3:23} d_{4:13}^3 \right) \\
- \frac{4P_{11} d_{5:13} \ln L \beta_{31}^4 r_{L}^{\delta_1} \delta_5}{L^5 \beta_0^8} (d_{5:13} d_{2:23} + 2d_{5:13} d_{3:23} + d_{3:23}^3 + 3d_{2:23} d_{5:13}^2 + 3d_{3:23} d_{5:13}^2) \\
- \frac{4P_{11} d_{5:13} \beta_{31}^4 r_{L}^{\delta_1} \delta_5}{L^5 \beta_0^8} (d_{5:13} d_{2:23} + 2d_{5:13} d_{3:23} + d_{3:23}^3 + 3d_{2:23} d_{5:13}^2 + 3d_{3:23} d_{5:13}^2) \\
+ \frac{4P_{11} d_{2:23} \ln L d_{6:13} \beta_{31}^3 r_{L}^{\delta_1} \delta_5}{L^6 \beta_0^8} (3d_{3:23} d_{6:13} + d_{3:23}^2 + 6d_{6:13}^2) + \frac{2 \beta \beta_{1:23} \ln^2 L}{L^3 \beta_0^4} (P_{10} d_{1:23} + P_{10} d_{2:23}) \\
+ \frac{P_{00} d_{1:23} d_{1:23} \ln^2 L}{L^2 \beta_0^6} (3d_{3:23} d_{6:13} + d_{3:23}^2 + 6d_{6:13}^2) \\
+ \frac{d_{4:13} \beta_{31}^4 r_{L}^{\delta_1} \delta_5}{L^4 \beta_0^8} (P_{1(a)} d_{1:23} + 4P_{11} d_{2:23} + P_{11} d_{3:23} - 3P_{10} d_{1:23} d_{4:13} - 3P_{01} d_{3:23} d_{4:13} - 2P_{01} d_{3:23}^2) \\
- \frac{2 \beta r_{L}^{\delta_1} \ln^2 L}{\beta_0^6} (P_{10} d_{1:23} d_{2:12} + P_{01} d_{1:23} d_{2:12} - P_{10} d_{1:23} d_{3:13} - P_{01} d_{2:23} d_{3:13}) \\
+ \frac{\beta_{1:23}^2 \ln^2 L}{\beta_0^6} (4P_{11} d_{1:23} d_{2:23} + P_{11} d_{1:23} d_{3:12} + P_{11} d_{1:23} d_{3:12} - P_{11} d_{1:23} d_{3:13} - 4P_{11} d_{2:23} d_{3:13} + P_{11} d_{3:23} d_{4:13} - 2P_{10} d_{1:23} d_{3:12}^2 - 2P_{01} d_{1:23} d_{3:12}^2 + 2P_{01} d_{4:13} d_{3:23}^2 + 3P_{10} d_{1:23} d_{3:13} + 3P_{01} d_{3:23}^2) \\
- \frac{2 \beta r_{L}^{\delta_1} \ln^2 L}{\beta_0^6} \left(d_{3:23} d_{2:12} + d_{3:12} d_{2:23} + d_{1:23} d_{3:23}^2 + 2d_{2:23} d_{3:23} + d_{3:12}^2 - 2d_{5:13} d_{3:23}^2 - 3d_{2:23} d_{5:13}^2 - 3d_{3:23} d_{5:13}^2 \right) + \frac{P_{11} d_{3:23} \beta_{1:23}^4 r_{L}^{\delta_1} \ln^4 L}{\beta_0^{10} L_0^4} (d_{3:12} - d_{6:13}) \\
+ \frac{2 \beta r_{L}^{\delta_1} \ln^2 L}{\beta_0^6} \left(d_{3:23} d_{1:23} + d_{3:12} d_{2:23} - d_{6:13} d_{3:23} - 3d_{3:23} d_{6:13}^2 + 6d_{6:13}^3 \right) + \frac{2 \beta r_{L}^{\delta_1} \ln^3 L}{\beta_0^{10} L_0^6} (d_{3:12} d_{3:23} - d_{3:23} d_{6:13} + d_{3:12}^2 - 2d_{6:13}^2) .
\]

(II.2)
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