A Matrix Approach to Numerical Solution of the DGLAP Evolution Equations

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Abstract

A matrix-based approach to numerical integration of the DGLAP evolution equations is presented. The method arises naturally on discretisation of the Bjorken $x$ variable, a necessary procedure for numerical integration. Owing to peculiar properties of the matrices involved, the resulting equations take on a particularly simple form and may be solved in closed analytical form in the variable $t = \ln(\alpha_0/\alpha)$. Such an approach affords parametrisation via data $x$ bins, rather than fixed functional forms. Thus, with the aid of the full correlation matrix, appraisal of the behaviour in different $x$ regions is rendered more transparent and free of pollution from unphysical cross-correlations inherent to functional parametrisations. Computationally, the entire programme results in greater speed and stability; the matrix representation developed is extremely compact. Moreover, since the parameter dependence is linear, fitting is very stable and may be performed analytically in a single pass over the data values.

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1. INTRODUCTION

Since the pioneering work of Duke and Owens [1] in the early eighties there has been an enormous investment in the phenomenological study of parton densities. As is well-known, the quark and gluon distributions inside hadrons acquire a scale ($Q^2$) dependence via higher-order PQCD corrections. Account of such dependence is necessary, both for correct analysis of experimental data and for various questions of theoretical importance. The evolution of the parton densities with $Q^2$ is governed by the DGLAP equations [2, 3, 4], the integro-differential nature of which hampers their numerical solution. In the literature there exist numerous techniques: such as, the so-called brute-force method [5], the use of Laguerre polynomials [6, 7] and solution in Mellin moment space with subsequent inversion. Shortcomings common to almost all are the computer time required and decreasing accuracy for $x \to 0$.

The precise motivation for developing this approach was an attempt to avoid the strong interplay between parameters (and $x$ regions) to which standard approaches are prone. For example, typically, in any standard approach the overall normalisation is a function of all available parameters and thus, in particular, the low-$x$ asymptotic power is prisoner to any fluctuations that may occur in the high-$x$ region. As will emerge, the natural solution to this problem, i.e., to use function values themselves (binned in $x$ and $Q^2$) as the parameters, leads to a gross simplification of the integro-differential equations involved. Indeed, suitable discretisation of the $x$ variable immediately allows exact integration of the differential equations in $Q^2$ and, moreover, most calculations may be performed prior to actual evolution or data fitting. A further enormous simplification of the equations is obtained by a suitable choice of the $x$ bins—the matrices governing evolution are then “banded” lower triangular, with two crucial effects: they commute (and may be expressed in terms of sums of the unit matrix and nil-potent matrices); moreover, multiplication of such matrices is an order $n^2$ operation (as opposed to the usual $n^3$) and they may be stored in very compact form, i.e., storage requirements are order $n$ (as opposed to the usual $n^2$).

Before proceeding it should be pointed out that an approach related to that proposed here has been presented by Santorelli and Scrimieri [8]. Rather than comment immediately on the similarities and differences, it is probably more convenient to highlight such in the following, as and when appropriate.

This paper is structured as follows: the following section contains the basic derivation of the approach to evolution while the subsequent covers its extension to singlet densities and higher-orders; in section 4 numerical results are presented and section 5 describes the application to data fitting. Finally, some conclusions and prospects for the technique are presented. The appendices contain a brief demonstration of the special properties of the matrices involved and details of kernel integration.

2. OUTLINE OF THE METHOD

In the following the general form of the evolution equations is first presented and simplifying substitutions of variables are then applied. Finally, the matrix equation is derived and solved formally.
2.1. The Evolution Equations

In the simplest case, non-singlet (NS) to leading logarithmic approximation (LLA), the evolution equations for parton densities take on the form:

\[
\frac{df(x, Q^2)}{d \ln Q^2} = \frac{\alpha_s(Q^2)}{2\pi} \int_x^1 \frac{dy}{y} P\left(\frac{x}{y}\right) f(y, Q^2),
\]

(2.1)

where \(f(x, Q^2)\) represents some NS parton density and \(P\) the corresponding splitting function. The convolution form does allow exact \(\ln Q^2\) integration if transformed to Mellin moment space. However, this requires knowledge of the function over the *entire* \(x\) region. Thus, if data analysis is the main aim, it is desirable to remain in \(x\) space.

2.2. Simplifying Substitution of Variables

Let us start by applying two simplifying variable transformations. It is convenient to substitute the scale variable \(Q^2\) with the variable \(t\):

\[
t = \ln \frac{\alpha(Q_0^2)}{\alpha(Q^2)},
\]

(2.2)

where \(Q_0^2\) is some starting scale for evolution (typically a very few GeV\(^2\)). The second substitution is for the Bjorken variables \(x\) and \(y\):

\[
u = \ln \frac{1}{x}, \quad v = \ln \frac{1}{y}.
\]

(2.3)

With these two substitutions, eq. (2.1) simplifies to

\[
\frac{df(u, t)}{dt} = \int_0^u dv P(u - v) f(v, t),
\]

(2.4)

where we have taken into account that to LLA \(\alpha_s\) is proportional to \(1/\ln Q^2\) and various coefficients have been absorbed into the definition of \(P\).

2.3. The Matrix Equation and a First Solution

To examine the numerical approach, consider performing the right-hand side integral via a naïve trapezoidal rule over subintervals of size \(h\):

\[
\frac{df_m(t)}{dt} = \sum_{k=1}^m P_{mk} f_k(t),
\]

(2.5)

where the following rather obvious definitions have been made:

\[
u_k = k h, \quad f_k(t) = f(u_k, t), \quad P_{mk} = h P(u_m - u_k),
\]

(2.6)

the typical vanishing of \(f(x)\) at \(x = 1\) has been exploited and a factor one half in the last term of the series has been omitted. By noting that the sum in eq. (2.5) runs only up to
m, one sees that the matrix $P_{mk}$ is lower triangular. Thus, finally, writing the equation in matrix form, one obtains

$$\dot{f}(t) = P f(t),$$

where the dot indicates a derivative w.r.t. $t$.

One would now, at least in principle, need only diagonalise $P$, via a matrix $D$ say: left multiplication by $D^{-1}$ would then result in

$$D^{-1} \dot{f}(t) = D^{-1} P D D^{-1} f(t).$$

Defining $\tilde{f} = D^{-1} f$ and the diagonalised matrix $P_D = D^{-1} P D$, the final simple form would therefore be

$$\dot{\tilde{f}}(t) = P_D \tilde{f}(t).$$

The exact solution could thus be written down directly:

$$\tilde{f}_m(t) = e^{\gamma_m t} \tilde{f}_m(0),$$

where the $\gamma_m$ would be just the eigenvalues of the matrix $P$. Transforming back to the original basis, one would then have

$$f_m(t) = \sum_k e^{\gamma_k t} d_{mk} \tilde{f}_k(0).$$

This would then be an exact solution in $t$ of the differential equation, i.e., only the $x$ variable having been discretised and treated numerically.

It turns out that the eigenvalues are very close to one another and so diagonalisation is very nearly singular. A possible approach might be to avoid degeneracy by suitable choice of binning and also to work in extended precision on the computer; however, as we shall now show, this apparent obstacle may be turned into a virtue owing to the nature of the matrices generated.

### 2.4. A Better Solution to the Matrix Equation

The choice of equally spaced bins in $u$ leads, in fact, to total degeneracy. This impedes matrix diagonalisation and thus the solution must be obtained differently. However, in compensation, a natural simplification occurs: the elements $P_{km}$ only depend on the differences $k - m$ (see appendix [B] for a proof). Thus, first of all, such matrices may be stored numerically as vectors, there being only $n$ independent elements. More specifically, we may define

$$P_{km} = p_k - m,$$

where $p_k$ is just a vector of length $n$. Moreover, matrix multiplication, inversion etc. only require $O(n^2)$ floating-point operations as compared with the $O(n^3)$ for general $n \times n$ matrix manipulation. The banded triangular nature of the matrix provides a further remarkable simplification: the set of all such matrices is abelian. This means that the NS equation may effectively be solved algebraically. Thus, $P$ may be treated as a $c$-number in eq. (2.7); the solution is then trivial:

$$f(t) = e^{P t} f(0).$$

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There is a further useful property of the matrices appearing here: if the diagonal elements of such a matrix are zero then the matrix is nilpotent; i.e., if $A_{ij} = a_{i-j}$ is such an $n \times n$ matrix with $a_0 = 0$ then $A^n = 0$. Separating $P$ according to $P = p_0 \mathbf{1} + \tilde{P}$, commutation of the two terms being trivial, we may then write

$$f(t) = e^{p_0 t} e^{\tilde{P} t} f(0),$$

(2.14)

where, owing to the nilpotency of $\tilde{P}$, the factor $\exp[\tilde{P} t]$ is now given by a finite sum of power terms. It is easy to see that its calculation indeed only requires $O(n^3)$ multiplications and is thus equivalent to a single normal matrix product. Moreover, any function admitting a power-series expansion (e.g., sin, cos, log, square-root, etc.) is evaluated similarly. The $n$ terms of any such sum, of course, need only be calculated once and then stored (as an $n \times n$ matrix), providing for very rapid evaluation for any $t$.

3. EXTENSION TO SINGLET AND HIGHER-ORDER

In all modern analyses the extension to both singlet and higher logarithmic accuracy is an absolute necessity. Thus, we now turn first to the extension to the singlet case and secondly to higher-order QCD corrections.

3.1. The Singlet Equations

In the singlet case the equations become a $2 \times 2$ system:

$$\dot{\Sigma}(t) = P_{\Sigma \Sigma} \Sigma(t) + P_{\Sigma g} g(t),$$
$$\dot{g}(t) = P_{g \Sigma} \Sigma(t) + P_{gg} g(t),$$

(3.1)

where the singlet-quark density is $\Sigma = \sum_i q_i(x)$ and the $P_{ab}$ are individually of banded triangular form. If we rewrite eq. (3.1) as the outer product of $2 \times 2$ matrices and the banded triangular kernels, $P_{ab}$,

$$\dot{F}(t) = \mathcal{P} F(t),$$

(3.2)

one immediately sees that the form of the original solution still holds: namely,

$$F(t) = \exp[\mathcal{P} t] F(0).$$

(3.3)

Of course, the matrix $\mathcal{P}$, not being of the banded triangular type, does not permit direct evaluation of the exponential via a finite polynomial. However, the $2 \times 2$ matrix elements are commuting matrices which may still then be treated as $c$-numbers; the solution is thus trivially obtained by diagonalisation of the $2 \times 2$ system:

$$F(t) = D \exp[\mathcal{P}_D t] D^{-1} F(0),$$

(3.4)

where $\mathcal{P}_D = D^{-1} \mathcal{P} D$ is diagonal in the $2 \times 2$ space. Note also that the transformation matrix, $D$, may be chosen such that $D^{-1} = D$ (and is real). The upper-left and lower-right diagonal blocks may now be treated separately along the lines of the NS case. Note that, for the DGLAP kernels calculated in QCD, the matrix $\mathcal{P}$ is not singular; in the case that it were, the solution would in fact be trivial.
Alternatively, we may exploit the simple nature of $2 \times 2$ matrices. Let us use a basis of Pauli matrices:

$$\tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \tau_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \tau_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \quad (3.5)$$

Writing $\mathcal{P} = P_0 \mathbb{1} + P_3 \tau_3 + P_+ \tau_+ + P_- \tau_- = P_0 \mathbb{1} + \mathcal{P}$, where the unit matrix and $\mathcal{P}$ now lie in the $2 \times 2$ space and the $P_a$ lie in $x$-bin space, we obtain

$$\mathcal{P}^2 = (P_3^2 + P_+ P_-) \mathbb{1} \equiv \tilde{P}^2 \mathbb{1}, \quad (3.6)$$

and thus

$$e^{\mathcal{P} t} = e^{P_0 t} \left[ \cosh(\tilde{P} t) \mathbb{1} + \sinh(\tilde{P} t) \mathcal{P} / \tilde{P} \right]. \quad (3.7)$$

Note that although $P_0$ and $\tilde{P}$ remain matrices in $x$-bin space they are also still banded lower triangular and thus the hyperbolic functions and square-root may again be evaluated as finite polynomials. We note in passing that, while both forms are stable, the evaluation of eq. (3.4) requires slightly less computing time than does (3.7).

### 3.2. Higher Logarithmic Accuracy

Extending to higher logarithmic accuracy presents no obstacle in the NS case, indeed, it is trivial to all orders in $\alpha_s$. The evolution equation now becomes

$$\dot{q}(t) = \sum_{n=0}^{N} (\alpha(Q^2))^n P^{(n)} q(t), \quad (3.8)$$

where the sum runs up to $N$, the order of the approximation. Since the matrices $P^{(n)}$ are still all of the banded triangular type (i.e., commuting), an exponential solution of the form of eq. (2.13) is still valid for any $N$:

$$q(t) = e^{P^{(0)} t} e^{P^{(1)} (1-e^{-t})} e^{P^{(2)} \frac{1}{2} (1-e^{-2t})} \cdots q(0). \quad (3.9)$$

From the above form, it is also clear that the corrections actually factorise order-by-order and thus it is even possible to examine their effects separately and in parallel in a single calculation.

Turning next to the singlet case, we encounter the first and only serious complication: in

$$\dot{F}(t) = \sum_{n=0}^{N} P^{(n)} e^{-nt} F(t), \quad (3.10)$$

the $2 \times 2$ matrices, $P^{(n)}$, do not commute and thus naïve exponentiation cannot furnish the required solution. Let us examine the system in the next-to-leading-logarithmic approximation (NLLA), which we rewrite as follows:

$$\dot{F}(t) = [\mathcal{A} + \mathcal{B} e^{-t}] F(t). \quad (3.11)$$

If $D$ is the matrix that diagonalises $\mathcal{A}$ at the $2 \times 2$ level, with the diagonal $\mathcal{A}'_D = D^{-1} \mathcal{A} D$ and $\mathcal{B}' = D^{-1} \mathcal{B} D$, then defining the vector $G(t)$ via

$$F(t) \equiv D \exp \left[ \mathcal{A}'_D t + \mathcal{B}'_D (1 - e^{-t}) \right] G(t) \quad (3.12)$$
where $B'_D$ is the diagonal part of $B'$ and transforming to the variable $s \equiv e^{-t}$ we obtain

$$\frac{dG(s)}{ds} = -\exp\{2 [A'_3 \ln s + B'_3 (s - 1)] \sigma_3\} [B'_+ \sigma_+ + B'_- \sigma_-] G(s).$$

(3.13)

Defining upper and lower elements of $G$ by $G_{\pm}$, the coupled first-order equations transform into a pair of decoupled second-order equations:

$$\frac{d^2 G_{\pm}(s)}{ds^2} = \pm 2 \left( \frac{A'_3}{s} + B'_3 \right) \frac{dG_{\pm}(s)}{ds} + B'_3 B'_{\pm} G_{\pm}(s).$$

(3.14)

The solution may then be obtained in a relatively straight-forward manner via power-series substitution. However, while the banded triangular nature of the matrices certainly facilitates evaluation, the series is infinite here and thus must be truncated. Fortunately, the compact form of the matrices permits cheap computer storage of a large number of terms.

We note here that the natural expansion is a power series in $s$ and not $t$. Indeed, while for small $t$ the two are essentially equivalent, for large values (where $s \to 0$) the expansion in $t$ contains only a part of the series expressed in terms of $s$. In the following section we shall comment further on this point with regard to the approach of [8].

4. NUMERICAL RESULTS ON EVOLUTION

We have thoroughly tested the approach to LLA for the both the NS and full singlet evolution equations: the performance is highly satisfactory both in terms of precision and computing time. For the purposes of testing we have used the following representative set of input distributions at $Q^2_0 = 4$ GeV$^2$:

$$q_{NS}(x, Q^2_0) = A_{NS} x^{-0.5} (1 - x)^3,$$

$$\Sigma(x, Q^2_0) = A_S x^{-1} (1 - x)^3,$$

$$g(x, Q^2_0) = A_g x^{-1} (1 - x)^{6.5}.$$  

(4.1)

The normalisations are fixed by various sum rules, which also provide means of cross-checking the accuracy of the method.

As a first examination, let us consider NS evolution using just 20 points per decade (i.e., there are 20 bins between any $x$ and $x/10$) and a simple two-point interpolation to evolve over a range of $t = 0$ to 2; this corresponds to an astronomical final $Q^2 = 2.3 \times 10^{12}$ GeV$^2$ (taking $Q^2_0 = 4$ GeV$^2$ and $\lambda_{QCD} = 0.240$ GeV for three active flavours) but we feel that this is important to test stability of the algorithm (we shall make further comments later). Under these extreme conditions (using double-precision arithmetic) the first moment of the valence quark distribution remains constant to one part in $10^5$ while the second moments (the momentum sum rule) agree with the analytical evaluation to 1% (valence and singlet quark) and 2% (gluon). Note, however, that to obtain $10^{-5}$ precision in the first-moment integral it is necessary (for this number of bins) to cover the region $x \in (10^{-10}, 1)$ and to employ higher-order interpolation formulæ for the moment integral itself. The precision decreases rapidly with increasing moment (owing to heavier sampling of the large-$x$ region): it is down to the 10% level by the sixth (fourth) moment for the valence and singlet quark (gluon).

A significant improvement is obtained by also using higher-order interpolation formulæ to calculate the matrices. Note that, in order to maintain the matrix properties, it is necessary
to interpolate in each $x$ bin using only function values at the bin boundaries and higher values of $x$. This means that fake zero values must be introduced for a very few $x$ values larger than one (this essentially cancels the gain for the last bins). Eight-point interpolation leads to a gain in precision of around three orders of magnitude for the second moments of all the distributions.

Clearly, a substantial gain may also be made by increasing the density of the $x$ points, this also permits a check of precision as a function of $x$; moments are only sensitive to a very limited range of $x$, around the peak of $x^{n-1}q(x)$. Doubling the density of points to 40 per decade results in an improvement in precision of a factor 3 (50) for the two-point (8-point) interpolation. Doubling again to 80 points per decade (i.e., only 400 in the range $x \in (10^{-5}, 1)$, the precision for 8-point interpolation is better than one part in $10^4$ for all moments up to $n = 12$ and better than one in $10^6$ for the momentum sum rule, the gain for the higher-order interpolation is still overwhelming. As a final step we double once more to 160 points per decade, but find no further significant improvement.

Thus, we choose to compare results with a benchmark of 80 points per decade using 8-point interpolation. For evolution with 20 points per decade and 8-point interpolation, the precision from $x = 0.25$ down to $x = 10^{-10}$ is better than 5 parts in $10^6$, for the valence density, still 2% for the highest value available for this binning ($x = 0.8$) but already 2.4 in $10^4$ for $x = 0.5$. The singlet-quark (gluon) density has a roughly factor 20 (30) poorer accuracy except for the higher $x$ values where the singlet-quark precision is comparable to that of the valence. As a final test, we compare evolution with 10 points. Even here performance is excellent: the valence precision is better than 1 in $10^4$ for $x \leq 0.2$ while that of the singlet quark and gluon is better than one per mille over most of the range. Note that if better precision in the high $x$ region is necessary, then a separate (parallel) evaluation may be made with a greater concentration of points over a limited region ($x \geq 0.2$ say).

With regard to the large value of $t$ chosen for testing, we now comment on the method proposed in [8]: there the truncation of the power series in $t$ at no more than 12 terms is justified on the basis of rapid convergence. Direct examination of the full finite expansion calculated here suggests this might be illusory: some coefficients do not become truly small until much later in the series and thus it may be that convergence is only achieved in [8] thanks to the not large values of $t$ considered there. We have studied the problem only superficially, but find that truncation at small order of the series obtained here renders the procedure unstable and, moreover, the onset of instability is very sudden with increasing $t$. We should point out, however, the authors of [8] claim to see no evidence for such behaviour in their studies [9].

It might be held that the typical size of $t$ corresponding to physically accessible energy scales is not normally larger than about 0.3, as considered in [8]. On the other hand, if one wishes to study the dynamical generation of parton distributions starting at some very small scale (see, for example, [10]), then the range of $t$ may be considerably larger. Finally, as commented above, a more suitable variable would be $s$; in this case the starting point being $s = 1$ requires expansion in the variable $s - 1$, which is still always a small variable ($0 < s - 1 \leq 1$).

We have not yet implemented higher-order corrections; however, in the NS case the algorithm will suffer no change, indeed, examination of eqs. (3.12, 3.13) reveals that higher-order corrections are implemented as further multiplicative (smaller) corrections. A possible strategy in the singlet case might be to exponentiate the leading corrections (possibly together with all diagonal pieces) and then apply the approach of [8] to the residual equations. Al-
ternatively, as shown in Section 3.2, after all possible simple factorisation the remaining differential equation is amenable to power-series solution.

5. DATA FITTING

It is now relatively straight-forward to perform data fitting. The \( f_m(0) \) in eq. (2.14) may be taken as the input parameters to fit, directly providing the parton density at some starting \( Q_0^2 \). The exact nature of the solution in \( t \) means that to fit a data point at some given \( t \) it is possible to obtain the necessary \( f_m \) at precisely that value and then interpolate in \( x \) to the required \( x \) value. Thus, since the matrix \( P \) is calculated once-and-for-all at the start of the fit (and only once even for many fits), the number of operations necessary to evaluate the fit function for a given set of values of \( x \) and \( Q^2 \) is drastically reduced with respect to all standard approaches. The number of floating-point operations may be reduced further by pre-calculating the evolution operator, \( e^{P t} e^{P t} \), for a set of \( t \) values and then interpolating both in \( x \) and \( t \). Note that the compact matrix storage requires just a single vector of length \( n \) for each value of \( t \). Note too that evolution may be performed using a larger number of \( x \) bins than are used for parametrisation.

In a fit, since each evolved value, \( f(x, t) \), depends only linearly on the input starting values, \( f_m(0) = f(x_m, 0) \), \( \chi^2 \) is quadratic in the parameters, precisely the \( f_m(0) \). Thus, minimisation and calculation of the full error matrix can, in principle, be performed with a single pass over the data points; this affords considerable saving in computer time and storage space. Indeed, data values need never be stored, the only memory requirements being for the evolution matrices (in vector form) and parameter vectors, together with the resulting covariance matrix.

Moreover, fixing the overall normalisation (i.e., imposing sum rules) at this stage is entirely superfluous and so has no influence, while the fit will naturally return a full covariance matrix for the parameters \( f_m(0) \), from which it is then possible to deduce whatever is of interest as to asymptotic behaviour, satisfaction of sum rules, etc., in an entirely independent manner.

So far we have only tested a NS code by generating fake data (with nominal but realistic errors) at some fixed large \( Q^2 \). The data generated were not smeared statistically so that any resulting non-zero \( \chi^2 \) would be due purely to inaccuracy in the evolution (based on a limited number of parameters). As an example we have used 200 data points generated over the interval \( x \in [10^{-5}, 1] \) and for the same extreme \( Q^2 \) as above, with 5 equally spaced parameter values per decade (note, however, that there is no restriction on the parameter spacing) and evolution using 20 points per decade. We find a total resulting \( \chi^2 = 0.6 \) (i.e., 0.004/DoF), the highest \( x \) parameter (corresponding to \( x = 0.63 \)) is returned to within \( 8\% \) of its true value while for all \( x < 0.1 \) the precision is better than 2 parts per mille. The entire fitting procedure (including data reading) takes around one second on a Pentium-driven laptop. As a final test, we generate an accurate set of 400 data points over four \( Q^2 \) slices (equally spaced in \( t \)) in the same \( x \) range and fit using the same number of parameters and evolution points as above. The results are very similar to the previous.
6. FINAL COMMENTS

There remain certain technical issues to address, in particular, the matrix manipulations involved: at any point instabilities may, in principle, arise. However, this is unlikely; for $h$ small the matrix solution will always be equivalent to other methods (and, in particular, it must be precisely equivalent to the so-called brute-force method) and will therefore have a well-defined and unique solution. Moreover, much of the procedure may be performed to essentially arbitrary precision beforehand, the resulting matrices then being used as fixed input to the evolution/fitting procedure.

A further technical issue concerns the discretisation in $x$: the number of points will always be small, compared with what might normally be adopted for accurate numerical integration. However, the real data do actually lie in a finite number of finite-size bins and thus discretisation is in any case effectively forced even in methods where some functional form is fit to the binned data.

Finally, as discussed, while the extension to NLLA in the NS case proves entirely trivial and to singlet in LLA is relatively straight-forward (it becomes a $2 \times 2$ system of equations), a full extension to the singlet case in NLLA proves less direct as the $2 \times 2$ system is non-commuting. However, the expansion that is to be truncated should be well-behaved insofar as the parameter is $\alpha_s$ itself.

7. NOTE ADDED TO COMPLETED MANUSCRIPT

On completion of this manuscript the author became aware of unpublished work by Pascaud and Zomer [11, 12], which contains many of the basic ideas presented here. There are however certain comments we should like to make. Firstly, the discussion of the treatment of the high-$x$ region is unnecessarily complicated; it is sufficient to simply choose a second $x$ grid starting at $x \sim 0.2$ with $n \gtrsim 100$ and not 1000 via the complicated formula suggested in [12]. Moreover, the interpolation adopted there is linear and no comment is made on the possibility of choosing higher-order polynomials, which, as noted here, do improve the precision considerably. Finally, and this is the most serious criticism: as discussed in the present work, a solution of the form of eq. (9) in [12] cannot be trivially extended to the $2 \times 2$ set of singlet equations; the LLA and NLLA matrices do not commute, thus direct exponentiation is not possible. In other words, the expression for $e^{A_k}$, despite having the simplified form given in the cited papers, does not correspond to the correct evolution operator for the singlet densities. Indeed, the authors present only limited cross-checking of their results using the analytically calculable moments of the parton distributions, relying purely on the assumed accuracy of the largest-$n$ calculation.

APPENDIX A: THE DGLAP KERNELS IN NUMERICAL FORM

The kernel matrices may be calculated by hand with no great difficulty. For simplicity, only the NS case will be treated here (the singlet case is more involved numerically but not conceptually). Thus, the equation to solve implies a convolution integral of some NS parton distribution, which is taken to be of the form[13] \( f(x) = xq(x) \), with the following kernel:

\[
P(x) \propto x \left[ \frac{(1+x^2)}{(1-x)^+} + \frac{3}{2} \delta(x-1) \right],
\]  

(A1)
where the ‘+’ regularisation is defined by

\[ \int_0^1 dx \frac{f(x)}{(1-x)_+} \equiv \int_0^1 dx \frac{f(x) - f(1)}{(1-x)}. \]  

(A2)

A simplification is obtained by observing that, under the integral, the plus regularisation obeys the following identity:

\[ \int_x^1 dy \left( \frac{y^n}{1-y} \right)_+ f(y) \equiv \int_x^1 dy \frac{y^n}{(1-y)_+} f(y) + \sum_{m=1}^n \frac{1}{m} f(1). \]  

(A3)

The integral to evaluate may therefore be cast into the form

\[ \int_x^1 \frac{dy}{y} \left[ \frac{1+y^2}{1-y} \right] f\left( \frac{x}{y} \right) \equiv \int_x^1 dy \left( \frac{1+y^2}{1-y} \right) f\left( \frac{x}{y} \right) - \int_0^1 dy \left( \frac{1+y^2}{1-y} \right) f(x) \]

\[ = \int_x^1 dy \left( \frac{1+y^2}{1-y} \right) \left[ f\left( \frac{x}{y} \right) - f(x) \right] - \int_0^x dy \left( \frac{1+y^2}{1-y} \right) f(x). \]  

(A4)

We choose to compute the integrals using the x variable rather than the transformed variable u introduced in the main text for simplicity of calculation; note that since the x-step ratio is always rather close to unity, there is negligible numerical difference between the two approaches.

The integrals may be simplified via integration by parts to obtain

\[ - \left[ \left( 2 \ln(1-y) + y + \frac{1}{2} y^2 \right) \left( \frac{x}{y} \right) - f(x) \right]_x^1 + \int_x^1 dy \left( 2 \ln(1-y) + y + \frac{1}{2} y^2 \right) \frac{d}{dy} f\left( \frac{x}{y} \right) + \left[ 2 \ln(1-y) + y + \frac{1}{2} y^2 \right]_0^x f(x), \]  

(A5)

in which careful examination reveals that the first and third terms completely cancel. Upon substitution of \( y \to x/y \) we finally obtain

\[ - \int_x^1 \frac{dy}{y} \frac{x}{y} \left[ \ln\left( \frac{1-x}{y} \right) + \frac{x}{y} + \frac{1}{2} y^2 \right] \frac{d}{dy} f(y). \]  

(A6)

The integral to be performed requires the division of the interval \([x_{\text{min}},1]\) into n sub-intervals of equal size in the variable u, introduced earlier. While one might directly apply a trapezoidal (or better) rule, since the integrand is a product of the unknown distribution function and a known splitting function (with singularities), it is clearly better to use the latter as a weight function. Thus, if we define the k-th interval as \([x_k, x_{k-1}]\), with \( x_k \equiv \lambda^k \) (and \( x_{\text{min}} = \lambda^n \)), then from eq. (2.4) we have

\[ - \sum_{k=1}^m \int_{x_k}^{x_{k-1}} \frac{dy}{y} \frac{x_m}{y} \left[ \ln\left( \frac{1-x_m}{y} \right) + \frac{x_m}{y} + \frac{1}{2} y^2 \right] \left( \frac{f_k - f_{k-1}}{(x_k - x_{k-1})} \right). \]  

(A7)
where we have identified $x$ with $x_m$ and assumed for simplicity a two-point interpolation formula for $f(y)$. The coefficients of $f_k$ for each $x_m$ are then just the elements $P_{mk}$ of the DGLAP kernel matrix required.

It is immediately clear that precision will be poorer in the region $x \to 1$. However, two points should be borne in mind: firstly, the data are sparse in this region and thus high precision is superfluous, and secondly, the absolute value of $q(x)$ there is so small as to be negligible. Moreover, as and when greater precision for $x \to 1$ might be necessary, at no more than the cost of doubling computer time, evolution could be performed in parallel for the entire region of interest and for just the region $x \in [0.2, 1]$, say.

In concluding this appendix let us remark that the form in which the elements are calculated numerically is crucial for the avoidance of large round-off errors due to repeated division and multiplication by $1 - \lambda$, where $\lambda$ is defined just after eq. (2.10). We note also in passing that as the interval size tends to zero, the coefficients diverge only logarithmically, as all pole terms explicitly cancel. We further note that the use of higher-order interpolation formulae leads to significantly greater precision: we have tested Lagrange polynomials up to order seven and found improvements in precision of rather more than two orders of magnitude.

**APPENDIX B: PROOF OF BANDED FORM OF THE DGLAP MATRICES**

Here we prove the statement that the matrix elements $P_{km}$ only depends on $k - m$. First of all we note that the plus regularisation involves the subtraction of an integral over the entire interval $[0, 1]$, which therefore depends neither on $m$ nor $k$, indeed, it contains no $x$ dependence, except in the factor $f(x)$ itself. Thus, for the proof we may ignore the subtleties of the plus regularisation, then the typical integral to evaluate takes the form

$$
\sum_{k=1}^{m} \int_{x_k}^{x_{k-1}} \frac{dy}{y} P\left(\frac{x_m}{y}\right) f(y).
$$

(B1)

The two-point interpolating (Lagrange) function for $f(y)$ between the points $x = x_k$ and $x_{k-1}$ is just

$$
f(y) \approx \frac{y - x_k}{x_{k-1} - x_k} f_{k-1} + \frac{y - x_{k-1}}{x_k - x_{k-1}} f_k
$$

(B2)

Making the substitution $y = x_{k-1} \xi$ and using $x_k = \lambda^k$ we obtain

$$
\sum_{k=1}^{m} \int_{1}^{\lambda^m} \frac{d\xi}{\xi} P\left(\frac{\xi^{m-k+1}}{\lambda}\right) f(\lambda^{k-1} \xi),
$$

(B3)

where the interpolation formula now becomes

$$
f(\lambda^{k-1} \xi) \approx \frac{\xi - \lambda}{1 - \lambda} f_{k-1} + \frac{\xi - 1}{\lambda - 1} f_k.
$$

(B4)

Thus the final result for the coefficients of the $f_k$, in the integral governing the evolution at $x_m$, clearly only depend on the difference $m - k$, which in turn only appears in the numerator of the argument of $P$ in eq. (B3). Clearly, increasing the number of interpolation points
does not affect the argument, provided the set of points used for any given bin terminates at the lower \( x \) boundary of that bin.

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