

MARKOVIAN MONTE CARLO SOLUTIONS OF THE NLO QCD EVOLUTION EQUATIONS*

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We present precision Monte Carlo calculations solving the QCD evolution equations up to the next-to-leading-order (NLO) level. They employ forward Markovian Monte Carlo (FMC) algorithms, which provide the rigorous solutions of the QCD evolution equations. Appropriate Monte Carlo algorithms are described in detail. They are implemented in the form of the Monte Carlo program `Evo1FMC`, which features the NLO kernels for the QCD evolution. The presented numerical results agree with those from independent, non-MC, programs (`QCDNum16`, `APCheb33`) at the level of 0.1%. In this way we have demonstrated the feasibility of the precision MC calculations for the QCD evolution and provided very useful numerical tests (benchmarks) for other, non-Markovian, MC algorithms developed recently.

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1. Introduction

It is commonly known that the so-called evolution equations of the quark and gluon distributions in the hadron, derived in QED and QCD using the renormalization group or diagrammatic techniques [1], can be interpreted probabilistically as a Markovian process, see *e.g.* Ref. [2]. Such a process can be modeled using Monte Carlo (MC) methods. The corresponding MC algorithm, called in the following the Markovian MC, provides, in principle,

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an exact solution of the evolution equations for parton distribution functions (PDFs). In practice, the main limitation of a such solution is the size of a generated MC sample, *i.e.* corresponding statistical errors of numerical results. This is probably the main reason why this possibility has not been exploited until recently. Instead, alternative numerical methods and programs solving the QCD evolution equations much faster than the Markovian MC have been used. Typical examples of such non-MC programs are QCDNum16 [3] and APCheb33 [4], see also Ref. [5].

Feasibility of solving efficiently the DGLAP equations [1] at the leading-order (LO) approximation with the Markovian MC was demonstrated for the first time by two of us (S.J. and M.S.) in Ref. [6]. There, the basic formalism was briefly sketched and the first numerical results were presented. Good agreement between the constructed Markovian MC program and QCDNum16 for gluon and quark singlet distribution functions was achieved. However, some small residual differences, at the level of 0.2%, between the two programs were found. Their origin was not understood at that time. Here we repeat the above comparisons, explain the source of these discrepancies and show the corrected results which agree at the level of 0.1%. The main conclusion of Ref. [6] was that the currently available computer CPU power allows to solve efficiently and precisely (at the per-mill level) the QCD evolution equations with the use of the Markovian MC algorithm. Of course, this method will always be slower in CPU time than non-MC techniques. However, it has several advantages, such as: no biases and/or numerical instabilities related to finite grids of points, use of quadratures, decomposition into finite series of polynomials, accumulation of rounding errors, *etc.* It is also more flexible in treatment of PDFs (*e.g.* no need to split them into singlet and non-singlet components) and easier to extend into higher orders, new contributions, *etc.*

The above Markovian algorithm can be a basis for the final-state radiation (FSR) parton shower MC program that not only solves numerically the evolution equations but also generates events in terms of parton flavours and four-momenta. Moreover, this algorithm can be a starting point and a testing tool for various kinds of constrained MC algorithms [7–10] being developed for the initial-state radiation (ISR).

This paper is devoted to the Markovian MC solution of the DGLAP evolution equations up to the next-to-leading order (NLO) in the perturbative QCD. It is organized as follows: In Sec. 2 we present a general structure of the DGLAP equations and discuss their basic features up to the next-to-next-to-leading order (NNLO). In Sec. 3 we describe in detail the Markovian MC algorithm for parton density distributions. We start from a classic iterative solution of the DGLAP equations and show how it can be expressed in terms of Markovian transition probabilities. Then we provide a method

for generation of a single Markovian step according to these probabilities. Subsec. 3.4 is devoted to construction of a weighted Markovian MC algorithm, where some importance sampling is used to generate evolution variables. In the last subsection we show how the above algorithm can be modified in order to account for the running QCD coupling constant. In Sec. 4 we present the Markovian MC algorithm for parton-momentum distributions. It has certain advantages over the previous algorithm due to momentum sum rules that can be applied to evolution kernels. Both the above algorithms have been implemented in the MC program called `Evo1FMC` [11]. Numerical results from `Evo1FMC` at the LO and the NLO are presented in Sec. 5. They are compared with the results of non-MC programs `QCDNum16` and `APCh33`. Sec. 6 summarizes the paper and gives some outlook for the future. In Appendix A we collect formulae for the QCD kernels (splitting functions) up to the NLO as well as explicit expressions for the NLO Sudakov form-factor. Appendices B and C contain formulae for simplified evolution kernels that are used for importance sampling in the weighted Markovian algorithm. Finally, in Appendix D we discuss a generic discrete Markovian process. It can be seen as an illustration of basic features of the DGLAP-like evolution equations and their solution in terms of the Markovian MC algorithm.

2. QCD evolution equations

2.1. General structure of DGLAP equations

The DGLAP evolution equations for quark, antiquark and gluon distributions,

$$\{q_1, \dots, q_{n_f}, \bar{q}_1, \dots, \bar{q}_{n_f}, G\}(\mu, x), \quad (1)$$

take the following general form [1, 12]

$$\begin{aligned} \frac{\partial}{\partial \ln \mu^2} q_i &= \sum_j \left(P_{q_i q_j} \otimes q_j + P_{q_i \bar{q}_j} \otimes \bar{q}_j \right) + P_{q_i G} \otimes G, \\ \frac{\partial}{\partial \ln \mu^2} \bar{q}_i &= \sum_j \left(P_{\bar{q}_i q_j} \otimes q_j + P_{\bar{q}_i \bar{q}_j} \otimes \bar{q}_j \right) + P_{\bar{q}_i G} \otimes G, \\ \frac{\partial}{\partial \ln \mu^2} G &= \sum_j \left(P_{G q_j} \otimes q_j + P_{G \bar{q}_j} \otimes \bar{q}_j \right) + P_{GG} \otimes G, \end{aligned} \quad (2)$$

where the summation is performed over quark flavours, $j = 1, \dots, n_f$. The parton distributions are functions of the Bjorken variable x and the factorization scale μ , identified with a hard scale in a given process (*e.g.* $\mu = \sqrt{Q^2}$ in deep inelastic scattering). The functions $P = P(\mu, x)$ are splitting functions to be discussed below. The integral convolution denoted by \otimes involves only *longitudinal* momentum fractions

$$\begin{aligned}
(P \otimes q)(\mu, x) &= \int_0^1 dy \int_0^1 dz \delta(x - zy) P(\alpha_s, z) q(\mu, y) \\
&= \int_x^1 \frac{dz}{z} P(\alpha_s, z) q\left(\mu, \frac{x}{z}\right) = \int_x^1 \frac{dz}{z} P\left(\alpha_s, \frac{x}{z}\right) q(\mu, z). \quad (3)
\end{aligned}$$

The splitting functions $P(\alpha_s, z)$ depend on μ through the strong coupling constant $\alpha_s = \alpha_s(\mu)$:

$$P(\alpha_s, z) = \frac{\alpha_s}{2\pi} P^{(0)}(z) + \left(\frac{\alpha_s}{2\pi}\right)^2 P^{(1)}(z) + \left(\frac{\alpha_s}{2\pi}\right)^3 P^{(2)}(z) + \dots \quad (4)$$

The superscripts (0), (1), (2) refer, respectively, to the leading (LO), next-to-leading (NLO) and next-to-next-to-leading order (NNLO) approximations in which the splitting functions are computed¹.

From charge conjugation and $SU(n_f)$ symmetry the splitting functions P have the following general structure which is independent of the approximation in which they have been computed

$$\begin{aligned}
P_{q_i q_j} &= P_{\bar{q}_i \bar{q}_j} = \delta_{ij} P_{qq}^V + P_{qq}^S, \\
P_{q_i \bar{q}_j} &= P_{\bar{q}_i q_j} = \delta_{ij} P_{q\bar{q}}^V + P_{q\bar{q}}^S, \\
P_{q_i G} &= P_{\bar{q}_i G} = P_{FG}, \\
P_{G q_i} &= P_{G \bar{q}_i} = P_{GF}. \quad (5)
\end{aligned}$$

Substituting these relations to (2), we find

$$\begin{aligned}
\frac{\partial}{\partial \ln \mu^2} q_i &= P_{qq}^V \otimes q_i + P_{q\bar{q}}^V \otimes \bar{q}_i + P_{qq}^S \otimes \sum_j q_j + P_{q\bar{q}}^S \otimes \sum_j \bar{q}_j + P_{FG} \otimes G, \\
\frac{\partial}{\partial \ln \mu^2} \bar{q}_i &= P_{q\bar{q}}^V \otimes q_i + P_{q\bar{q}}^V \otimes \bar{q}_i + P_{q\bar{q}}^S \otimes \sum_j q_j + P_{qq}^S \otimes \sum_j \bar{q}_j + P_{FG} \otimes G, \\
\frac{\partial}{\partial \ln \mu^2} G &= P_{GF} \otimes \sum_j (q_j + \bar{q}_j) + P_{GG} \otimes G. \quad (6)
\end{aligned}$$

¹ We adopt the convention of Curci, Furmanski and Petronzio [13, 14] in which the expansion parameter equals $\alpha_s/(2\pi)$. The NNLO analysis of Moch and Vogt [15, 16] uses $\alpha_s/(4\pi)$.

This is the basic form of the DGLAP evolution equations.

Within a given approximation some splitting functions may vanish or be equal. In particular,

- in the LO [1]

$$P_{q\bar{q}}^{V(0)} = P_{q\bar{q}}^{S(0)} = P_{qq}^{S(0)} = 0, \quad (7)$$

- in the NLO [13,14]

$$P_{qq}^{S(1)} = P_{q\bar{q}}^{S(1)}, \quad (8)$$

- but in the NNLO [15,16]

$$P_{qq}^{S(2)} \neq P_{q\bar{q}}^{S(2)}. \quad (9)$$

Eqs. (6) can be rewritten in an alternative form which involves quark singlet and non-singlet distributions. We will present this form below.

2.1.1. Singlet case

The quark singlet distribution is defined as

$$\Sigma(\mu, x) = \sum_{j=1}^{n_f} (q_j(\mu, x) + \bar{q}_j(\mu, x)). \quad (10)$$

Performing summation over quark flavours in the first two equations (6), we find

$$\frac{\partial}{\partial \ln \mu^2} \Sigma = \{P_{qq}^V + P_{q\bar{q}}^V + n_f(P_{qq}^S + P_{q\bar{q}}^S)\} \otimes \Sigma + (2n_f P_{FG}) \otimes G. \quad (11)$$

Introducing the notation

$$P_{FF} = P_+^V + n_f P_+^S, \quad (12)$$

$$P_+^{V,S} = P_{qq}^{V,S} + P_{q\bar{q}}^{V,S}, \quad (13)$$

the following closed set of equations is obtained for the quark singlet and gluon distributions

$$\frac{\partial}{\partial \ln \mu^2} \Sigma = P_{FF} \otimes \Sigma + (2n_f P_{FG}) \otimes G, \quad (14)$$

$$\frac{\partial}{\partial \ln \mu^2} G = P_{GF} \otimes \Sigma + P_{GG} \otimes G. \quad (15)$$

The splitting functions in these equations obey the general relations

$$\begin{aligned} & \int_0^1 dz \{ zP_{FF}(\mu, z) + zP_{GF}(\mu, z) \} \\ &= \int_0^1 dz \{ 2n_f zP_{FG}(\mu, z) + zP_{GG}(\mu, z) \} = 0. \end{aligned} \quad (16)$$

They immediately leads to the momentum sum rule

$$\int_0^1 dx \{ x\Sigma(\mu, x) + xG(\mu, x) \} = \text{const} \quad (17)$$

which is conserved during the evolution. In the parton model interpretation the constant is set to one by normalizing the initial conditions for Eqs. (14), (15): $\Sigma(\mu_0, x)$ and $G(\mu_0, x)$.

2.1.2. Non-singlet case

Introducing the quark non-singlet distribution

$$V(\mu, x) = \sum_{j=1}^{n_f} (q_j(\mu, x) - \bar{q}_j(\mu, x)), \quad (18)$$

the following evolution equation is obtained from Eqs. (6)

$$\frac{\partial}{\partial \ln \mu^2} V = P_{NS}^V \otimes V, \quad (19)$$

where the new splitting function reads

$$P_{NS}^V = P_-^V + n_f P_-^S, \quad (20)$$

$$P_-^{V,S} = P_{qq}^{V,S} - P_{q\bar{q}}^{V,S}. \quad (21)$$

Similarly, for the non-singlet quark distributions

$$q_i^-(\mu, x) = q_i(\mu, x) - \bar{q}_i(\mu, x) - \frac{1}{n_f} V(\mu, x), \quad (22)$$

$$q_i^+(\mu, x) = q_i(\mu, x) + \bar{q}_i(\mu, x) - \frac{1}{n_f} \Sigma(\mu, x), \quad (23)$$

we find from Eqs. (6), (14) and (19) the following equations

$$\frac{\partial}{\partial \ln \mu^2} q_i^- = P_-^V \otimes q_i^-, \quad (24)$$

$$\frac{\partial}{\partial \ln \mu^2} q_i^+ = P_+^V \otimes q_i^+. \quad (25)$$

Notice that there is no gluon distribution in the derived equations.

2.2. Summary of the forms

With the splitting functions usually presented in the literature

$$\{P_{\pm}^V, P_{\pm}^S, P_{FG}, P_{GF}, P_{GG}\}, \quad (26)$$

the evolution equations for the parton distributions $\{q_i^-, q_i^+, V, \Sigma, G\}$ are given by Eqs. (24), (25), (19), (14) and (15), respectively.

According to relations (7)–(9), the perturbative expansions for the kernels P_{\pm}^V and P_{\pm}^S take the following form

$$\begin{aligned} P_{\pm}^V(\alpha_s, z) &= \frac{\alpha_s}{2\pi} P_{qq}^{V(0)}(z) + \left(\frac{\alpha_s}{2\pi}\right)^2 P_{\pm}^{V(1)}(z) + \left(\frac{\alpha_s}{2\pi}\right)^3 P_{\pm}^{V(2)}(z) + \dots, \\ P_+^S(\alpha_s, z) &= \left(\frac{\alpha_s}{2\pi}\right)^2 P_{qq}^{S(1)}(z) + \left(\frac{\alpha_s}{2\pi}\right)^3 P_+^{S(2)}(z) + \dots, \\ P_-^S(\alpha_s, z) &= \left(\frac{\alpha_s}{2\pi}\right)^3 P_-^{S(2)}(z) + \dots. \end{aligned} \quad (27)$$

The remaining kernels $\{P_{FG}, P_{GF}, P_{GG}\}$ have the nonzero splitting functions in each approximation.

Alternatively, the parton distributions $\{q_i, \bar{q}_i, G\}$ could be evolved with the help of Eqs. (6) with the kernels

$$\{P_{qq}^{V,S}, P_{q\bar{q}}^{V,S}, P_{FG}, P_{GF}, P_{GG}\}, \quad (28)$$

where $P_{qq}^{V,S}$ and $P_{q\bar{q}}^{V,S}$ are computed by inverting relations (13) and (21):

$$P_{qq}^{V,S} = \frac{1}{2} \left(P_+^{V,S} + P_-^{V,S} \right), \quad (29)$$

$$P_{q\bar{q}}^{V,S} = \frac{1}{2} \left(P_+^{V,S} - P_-^{V,S} \right). \quad (30)$$

2.3. Behaviour at $z \rightarrow 1$

Let us consider the splitting functions (26). All the kernels, except the P_+^S , are divergent for $z = 1$.

The quark–quark and gluon–gluon splitting functions $\{P_{\pm}^V, P_{\pm}^S, P_{GG}\}$ have the following form

$$P(\alpha_s, z) = \frac{A(\alpha_s)}{(1-z)_+} + B(\alpha_s) \delta(1-z) + \bar{P}(\alpha_s, z), \quad (31)$$

where the “+” prescription regularizes the $1/(1-z)$ singularity

$$[f(z)]_+ = f(z) - \delta(1-z) \int_0^1 dz' f(z'), \quad (32)$$

and the functions $A(\alpha_s)$, $B(\alpha_s)$ and $\bar{P}(\alpha_s, z)$ are computed in powers of α_s , see Eq. (4). In particular

$$\bar{P}(\alpha_s, z) = \sum_{k=0} \alpha_s^{k+1} D^{(k)}(z). \quad (33)$$

In the LO approximation ($k = 0$) $D^{(0)}(z = 1)$ is finite [1] while in the NLO ($k = 1$) and NNLO ($k = 2$) approximations, the coefficients are logarithmically divergent [13–16]:

$$D^{(k)}(z) = D_k \ln(1-z) + \mathcal{O}(1). \quad (34)$$

Similarly, the quark–gluon and gluon–quark splitting functions $\{P_{FG}, P_{GF}\}$ contain logarithmically divergent terms for $z = 1$ [14, 16]:

$$P(\alpha_s, z) = \sum_{k=0} \alpha_s^{k+1} \left\{ \sum_{i=1}^{2k} D_i^{(k)} \ln^i(1-z) + \mathcal{O}(1) \right\}. \quad (35)$$

Thus in the limit $z \rightarrow 1$, we have for P_{FG} and P_{GF} :

$$P(\alpha_s, z) = \begin{cases} \mathcal{O}(\alpha_s) & \text{in LO (k = 0),} \\ \mathcal{O}(\alpha_s^2 \ln^2(1-z)) & \text{in NLO (k = 1),} \\ \mathcal{O}(\alpha_s^3 \ln^4(1-z)) & \text{in NNLO (k = 2).} \end{cases} \quad (36)$$

2.4. Behaviour at $z \rightarrow 0$

As in the previous section, let us consider the splitting functions (26).

The splitting functions $\{P_{\pm}^V, P_{\pm}^S\}$ are logarithmically divergent at $z = 0$ starting from the NLO approximation: [13–16]:

$$P(\alpha_s, z) = \sum_{k=0} \alpha_s^{k+1} \left\{ \sum_{i=1}^{2k} \overline{D}_i^{(k)} \ln^i z + \mathcal{O}(1) \right\}. \quad (37)$$

Thus for $z \rightarrow 0$, we find for P_{\pm}^V and P_{\pm}^S :

$$P(\alpha_s, z) = \begin{cases} \mathcal{O}(\alpha_s) & \text{in LO } (k = 0), \\ \mathcal{O}(\alpha_s^2 \ln^2 z) & \text{in NLO } (k = 1), \\ \mathcal{O}(\alpha_s^3 \ln^4 z) & \text{in NNLO } (k = 2). \end{cases} \quad (38)$$

The remaining splitting functions $\{P_+^S, P_{FG}, P_{GF}, P_{GG}\}$ have the following behaviour for $z \rightarrow 0$ [14, 16]:

$$P(\alpha_s, z) = E_1(\alpha_s) \frac{\ln z}{z} + E_2(\alpha_s) \frac{1}{z} + \mathcal{O}(\ln^{2k} z). \quad (39)$$

The logarithmic term is present starting from the NLO ($k = 1$) approximation:

$$E_1(\alpha_s) = \alpha_s^2 E_1^{(1)} + \alpha_s^3 E_1^{(2)} + \dots, \quad (40)$$

while the $1/z$ term is present from the LO ($k = 0$) approximation:

$$E_2(\alpha_s) = \alpha_s E_2^{(0)} + \alpha_s^2 E_2^{(1)} + \alpha_s^3 E_2^{(2)} \dots \quad (41)$$

2.5. Monte Carlo form of DGLAP equations

The $z = 1$ singularity in Eq. (31) needs special treatment in the Monte Carlo formulation of the DGLAP equations. Rewriting Eqs. (6) for the parton distributions multiplied by x , denoted in the matrix form as

$$\{xq_1, \dots, xq_{n_f}, x\bar{q}_1, \dots, x\bar{q}_{n_f}, xG\}(\mu, x) \equiv x\mathbf{D}(\mu, x) \equiv \mathbf{Q}(\mu, x),$$

we have

$$\frac{\partial}{\partial \ln \mu^2} \mathbf{Q}(\mu, x) = \int_x^1 dz \mathbf{P}(\alpha_s, z) \mathbf{Q}(\mu, (x/z)), \quad (42)$$

where \mathbf{P} is the matrix of the splitting functions, which can be easily read off from Eqs. (6).

Based on the results of Sec. 2.3, we can write the general structure of the splitting functions in the following form

$$\mathbf{P}(\alpha_s, z) = \frac{\mathbf{A}(\alpha_s)}{(1-z)_+} + \mathbf{B}(\alpha_s) \delta(1-z) + \overline{\mathbf{P}}(\alpha_s, z), \quad (43)$$

where A , B , $\overline{\mathbf{P}}$ are computed in powers of α_s . The function $\overline{\mathbf{P}}(\alpha_s, z)$ may contain singular terms in the limit $z \rightarrow 1$, proportional to powers of $\ln(1-z)$.

For simplicity of the notation we suppress the μ -dependence of the parton distribution and the splitting functions in the following. Substituting (43) to Eq. (42) and using definition (32), we find

$$\begin{aligned} \frac{\partial}{\partial \ln \mu^2} \mathbf{Q}(x) &= \int_x^1 dz \left\{ \mathbf{A} \frac{\mathbf{Q}(x/z) - \mathbf{Q}(x)}{1-z} + \overline{\mathbf{P}}(z) \mathbf{Q}(x/z) \right\} \\ &+ \{ \mathbf{A} \ln(1-x) + \mathbf{B} \} \mathbf{Q}(x). \end{aligned} \quad (44)$$

Now, we introduce a small cutoff in the upper limit of the integration, $1 \rightarrow (1-\varepsilon)$, which isolates the $z=1$ singularity. Performing the integration,

$$\int_x^{1-\varepsilon} dz \mathbf{A} \frac{-\mathbf{Q}(x)}{1-z} = \{ \mathbf{A} \ln \varepsilon - \mathbf{A} \ln(1-x) \} \mathbf{Q}(x),$$

we find for Eq. (44)

$$\begin{aligned} \frac{\partial}{\partial \ln \mu^2} \mathbf{Q}(x) &= \int_x^{1-\varepsilon} dz \mathbf{A} \frac{\mathbf{Q}(x/z)}{1-z} + \int_x^1 dz \overline{\mathbf{P}}(z) \mathbf{Q}(x/z) \\ &+ \{ \mathbf{A} \ln \varepsilon + \mathbf{B} \} \mathbf{Q}(x). \end{aligned} \quad (45)$$

Inserting back the μ -dependence, the equation above can be written as

$$\frac{\partial}{\partial \ln \mu^2} \mathbf{Q}(\mu, x) = \int_x^1 dz \mathbf{P}(\alpha_s, z, \varepsilon) \mathbf{Q}(\mu, x/z) \quad (46)$$

with the kernel

$$\mathbf{P}(\alpha_s, z, \varepsilon) = \frac{\mathbf{A}(\alpha_s)}{1-z} \Theta(1-z-\varepsilon) + \{ \mathbf{A}(\alpha_s) \ln \varepsilon + \mathbf{B}(\alpha_s) \} \delta(1-z) + \overline{\mathbf{P}}(\alpha_s, z). \quad (47)$$

This form of the DGLAP equations is a starting point for the Monte Carlo generation. Let us notice that the presented formulae are valid for both representations of the parton distributions and splitting functions discussed in Sec. 2.2. Explicit expressions for the splitting functions up to the NLO are given in Appendix A.

3. Markovian algorithm for parton distributions

In the following we show how to transform the QCD evolution equation (DGLAP type) into an integral homogeneous equation and solve it by means of iteration. The general properties of the evolution equations and the related diffusion equations are discussed in Appendix D using simple environment of the discrete space. Below we discuss a more complicated case of the mixed, discrete-continuous, space of the QCD evolution equations.

3.1. Classic iterative solution

Introducing the variable

$$t = \ln \mu \equiv \ln Q, \quad (48)$$

the evolution equations (42) in the component form read

$$\begin{aligned} \frac{\partial}{\partial t} D_K(t, x) &= \sum_J (\mathcal{P}_{KJ} \otimes D_J)(t, x) \\ &= \sum_J \int_x^1 \frac{dz}{z} \mathcal{P}_{KJ}(t, z) D_J\left(t, \left(\frac{x}{z}\right)\right). \end{aligned} \quad (49)$$

Notice that due to the definition of the evolution variable t , the splitting functions \mathcal{P}_{KJ} are related to those from Sec. 1, Eqs. (4), by

$$\mathcal{P}_{KJ}(t, z) = 2P_{KJ}(\alpha_s(t), z) \quad (50)$$

with a possible dependence of $\alpha_s(t)$ also on z in order to accommodate coherence effects.

The next important step is to introduce the infra-red (IR) cut ε and to isolate a part of the kernel \mathcal{P} diagonal both in the parton (flavour) index and in the z -variable²

$$\begin{aligned} \mathcal{P}_{KJ}(t, z) &= -\mathcal{P}_{KK}^\delta(t, \varepsilon(t)) \delta_{KJ} \delta(1-z) + \mathcal{P}_{KJ}^\theta(t, z), \\ \mathcal{P}_{KJ}^\theta(t, z) &= \mathcal{P}_{KJ}(t, z) \Theta(1-z-\varepsilon(t)) \Theta(z-\varepsilon'), \end{aligned} \quad (51)$$

² All components proportional to $\delta(1-z)$ reside in the diagonal part of the matrix \mathcal{P}_{KJ} anyway.

where we also introduced a facultative lower limit ε' on z -variable, equivalent to the minimal global x of the evolution. Note that in the DGLAP case there is no reason for the IR regulator ε to be t -dependent. However, for applications in the context of parton-shower algorithms and of the CCFM equations [17] it is worthwhile to keep this option open. In any case we always assume that ε and $\varepsilon(t)$ are small. A more detailed discussion of the LO kernels is given in Appendix B. After the above splitting of the kernels the evolution equation becomes inhomogeneous

$$\frac{\partial}{\partial t} D_K(t, x) + \mathcal{P}_{KK}^\delta(t) D_K(t, x) = \sum_J (\mathcal{P}_{KJ}^\ominus \otimes D_J)(t, x). \quad (52)$$

It is easily made again homogeneous

$$e^{-\Phi_K(t, t_0)} \frac{\partial}{\partial t} \left(e^{\Phi_K(t, t_0)} D_K(t, x) \right) = \sum_J (\mathcal{P}_{KJ}^\ominus \otimes D_J)(t, x),$$

$$\Phi_K(t, t_0) = \int_{t_0}^t dt' \mathcal{P}_{KK}^\delta(t', \varepsilon(t')), \quad (53)$$

and turned into an integral equation

$$e^{\Phi_K(t, t_0)} D_K(t, x) = D_K(t_0, x) + \int_{t_0}^t dt_1 e^{\Phi_K(t_1, t_0)} \sum_J (\mathcal{P}_{KJ}^\ominus \otimes D_J)(t_1, x). \quad (54)$$

Its another equivalent form, which is more convenient for iteration, reads

$$D_K(t, x) = e^{-\Phi_K(t, t_0)} D_K(t_0, x) + \int_{t_0}^t dt_1 e^{-\Phi_K(t, t_1)} \sum_J (\mathcal{P}_{KJ}^\ominus \otimes D_J)(t_1, x). \quad (55)$$

The iteration of the above equation provides a solution in terms of a series of integrals

$$D_K(t, x) = e^{-\Phi_K(t, t_0)} D_K(t_0, x) \quad (56)$$

$$+ \sum_{n=1}^{\infty} \sum_{K_0, \dots, K_{n-1}} \prod_{i=1}^n \left[\int_{t_0}^t dt_i \Theta(t_i - t_{i-1}) \int_0^1 dz_i \right] e^{-\Phi_K(t, t_n)}$$

$$\times \int_0^1 dx_0 \prod_{i=1}^n \left[\mathcal{P}_{K_i K_{i-1}}^\ominus(t_i, z_i) e^{-\Phi_{K_{i-1}}(t_i, t_{i-1})} \right] D_{K_0}(t_0, x_0) \delta \left(x - x_0 \prod_{i=1}^n z_i \right),$$

where $k_n \equiv k$. At this point we have many options for the MC implementation of the multidimensional integrals given by the above expression. Quite generally, they can be divided into Markovian and non-Markovian groups of the MC implementations. In the following we shall describe solutions of the Markovian type. However, it will be done such that the mechanism to switch to a non-Markovian method will be as easy as possible.

3.2. Markovianization

Contrary to the evolution of the non-singlet PDF or of the singlet one-component PDF, in the most general case represented by the Eq. (56) one cannot express its integrand as an exact product of the Markovian single-step probabilities, each normalized to 1. However, the general iterative solution of the evolution equation in Eq. (56) can be expressed in terms of the (unnormalized) transition density

$$\begin{aligned} \Omega(t_i, x_i, K_i | t_{i-1}, x_{i-1}, K_{i-1}) &\equiv \Theta(t_i - t_{i-1}) \mathcal{P}_{K_i K_{i-1}}^\Theta(t_i, x_i / x_{i-1}) \\ &\times e^{-\Phi_{K_{i-1}}(t_i, t_{i-1})}, \end{aligned} \quad (57)$$

as follows

$$\begin{aligned} D_K(t, x) &= e^{-\Phi_K(t, t_0)} D_K(t_0, x) \\ &+ \sum_{n=1}^{\infty} \sum_{K_0, \dots, K_{n-1}} \int_0^1 dx_0 \prod_{i=1}^n \left[\int_{t_0}^t dt_i \int_0^1 dz_i \right] e^{-\Phi_K(t, t_n)} \\ &\times \prod_{i=1}^n \Omega(t_i, x_i, K_i | t_{i-1}, x_{i-1}, K_{i-1}) \delta \left(x - x_0 \prod_{i=1}^n z_i \right) D_{K_0}(t_0, x_0). \end{aligned} \quad (58)$$

The above expression looks almost as a product of Markovian transition probabilities, except that Ω lacks a proper normalization

$$\begin{aligned} &\int_{t_{i-1}}^{\infty} dt_i \int_0^1 dz_i \sum_{K_i} \Omega(t_i, x_i, K_i | t_{i-1}, x_{i-1}, K_{i-1}) \\ &= \int_0^{\infty} d(T_{K_{i-1}}(t_i, t_{i-1})) e^{-\Phi_{K_{i-1}}(t_i, t_{i-1})} \neq 1, \end{aligned} \quad (59)$$

where

$$T_K(t, t_0) = \int_{t_0}^t dt' \int_0^1 dz \sum_J \mathcal{P}_{JK}^\Theta(t', z). \quad (60)$$

The above problem cannot be cured by changing integration variables or normalization of the PDFs. On the other hand, one can define a properly normalized transition probability

$$\begin{aligned} \omega(t_i, x_i, K_i | t_{i-1}, x_{i-1}, K_{i-1}) &\equiv \Theta(t_i - t_{i-1}) \mathcal{P}_{K_i K_{i-1}}^\Theta(t_i, x_i/x_{i-1}) \\ &\quad \times e^{-T_{K_{i-1}}(t_i, t_{i-1})}, \\ \int_{t_{i-1}}^{\infty} dt_i \int_0^1 dz_i \sum_{K_i} \omega(t_i, x_i, K_i | t_{i-1}, x_{i-1}, K_{i-1}) &\equiv 1, \end{aligned} \quad (61)$$

and express

$$\begin{aligned} \Omega(t_i, x_i, K_i | t_{i-1}, x_{i-1}, K_{i-1}) &= e^{\Delta_{K_{i-1}}(t_i, t_{i-1})} \\ &\quad \times \omega(t_i, x_i, K_i | t_{i-1}, x_{i-1}, K_{i-1}), \end{aligned} \quad (62)$$

where

$$\Delta_K(t, t_0) = T_K(t, t_0) - \Phi_K(t, t_0) = \int_{t_0}^t dt' \int_0^1 dz \sum_J \mathcal{P}_{JK}(t', z), \quad (63)$$

which is independent of the IR regulator $\varepsilon(t)$. This opens a way to the Monte Carlo algorithm with weighted events, in which the Markovian algorithm is based on the ω distributions and the correcting weight $w = \prod(\Omega/\omega)$ brings back the MC distributions to the original ones.

As usual, Markovianization cannot be accomplished without adding one extra integration variable. We do this starting from the identity

$$\int_t^{\infty} dt_i \int_0^1 dz_i \sum_{K_i} \omega(t_i, x_i, K_i | t_{i-1}, x_{i-1}, K_{i-1}) = e^{-T_{K_{i-1}}(t, t_{i-1})}, \quad (64)$$

and then we add the $(n+1)$ -th “spill-over” variables in the integrals using

$$e^{\Delta_{K_n}(t, t_n)} \int_t^{\infty} dt_{n+1} \int_0^1 dz_{n+1} \sum_{K_{n+1}} \omega(t_{n+1}, x_{n+1}, K_{n+1} | t_n, x_n, K_n) = e^{-\Phi_{K_n}(t, t_n)}. \quad (65)$$

Summarizing all the above discussion, we transform Eq. (56) into a new equivalent form

$$\begin{aligned}
 D_K(t, x) = & e^{\Delta_K(t, t_0)} \int_{t_1 > t} dt_1 dz_1 \sum_{K_1} \omega(t_1, x_1, K_1 | t_0, x, K) D_K(t_0, x) \\
 & + \sum_{n=1}^{\infty} \int_0^1 dx_0 \int_{t_{n+1} > t} dt_{n+1} dz_{n+1} \sum_{K_{n+1}} \sum_{K_0, \dots, K_{n-1}} \prod_{i=1}^n \int_{t_i < t} dt_i dz_i \\
 & \times e^{\Delta_{K_n}(t, t_n)} \omega(t_{n+1}, x_{n+1}, K_{n+1} | t_n, x_n, K_n) \\
 & \times \prod_{i=1}^n e^{\Delta_{K_{i-1}}(t_i, t_{i-1})} \omega(t_i, x_i, K_i | t_{i-1}, x_{i-1}, K_{i-1}) \\
 & \times \delta \left(x - x_0 \prod_{i=1}^n z_i \right) D_{K_0}(t_0, x_0). \tag{66}
 \end{aligned}$$

In the Markovian Monte Carlo algorithm implementing exactly the above series of the integrals we neglect primarily the factor

$$w = e^{\Delta_{K_n}(t, t_n)} \prod_{i=1}^n e^{\Delta_{K_{i-1}}(t_i, t_{i-1})}, \tag{67}$$

such that the whole series of integrals can be implemented readily as a Markovian chain of steps with the normalized transition probability $\omega(t_i, x_i, K_i | t_{i-1}, x_{i-1}, K_{i-1})$ for each single step. The original integrals and distributions can be recovered by means of applying the MC correcting weight w defined above. The only technical problem is that $w \geq 1$ and one may struggle to find the maximum weight, in order to turn weighted events into unweighted ones. It is an unavoidable price to pay in this method.

In the case of the single-component evolution (singlet or non-singlet) we recover automatically the constant-weight algorithm

$$w = e^{\Delta(t, t_n)} \prod_{i=1}^n e^{\Delta(t_i, t_{i-1})} = e^{\Delta(t, t_0)}. \tag{68}$$

In the case of the non-singlet evolution we even have $w = 1$.

3.3. Generation of a single Markovian step

The description of the Markovian algorithm of the previous section is incomplete without providing at least one method to generate *exactly* the

distribution of a single step forward, $(t_0, x_0, K_0) \rightarrow (t_1, z_1 x_0, K_1)$, in the primary Markovian algorithm

$$d\omega(t_1, z_1 x_0, K_1 | t_0, x_0, K_0) = \Theta(t_1 - t_0) \mathcal{P}_{K_1 K_0}^\Theta(t_1, z_1) e^{-T_{K_0}(t_1, t_0)} dt_1 dz_1. \quad (69)$$

The natural method of generating the above 3-dimensional distribution (including one discrete variable) can be read from the reorganized normalization integral

$$\begin{aligned} 1 &\equiv \int_{t_0}^{\infty} dt_1 \sum_{K_1} \int_0^1 dz_1 \omega(t_1, z_1 x_0, K_1 | t_0, x_0, K_0) \\ &= \int_0^1 d(e^{-T_{K_0}(t_1, t_0)}) \sum_{K_1} \frac{\int dz' \mathcal{P}_{K_1 K_0}^\Theta(t_1, z')}{\sum_{X=q,g} \int dz' \mathcal{P}_{X K_0}^\Theta(t_1, z')} \int_0^1 dz_1 \frac{\mathcal{P}_{K_1 K_0}^\Theta(t_1, z_1)}{\int dz' \mathcal{P}_{K_1 K_0}^\Theta(t_1, z')} \\ &= \int_0^1 dr(t_1) \sum_{K_1} p(K_1 | t_1) \int_0^1 dz_1 p(z_1 | K_1, t_1), \end{aligned} \quad (70)$$

where the two final integrals and the parton sum are each equal to 1 separately.

One may generate the first variable t_1 by inverting the cumulative distribution $r(t_1)$. Because of the possible t -dependence of the coupling constant and the cut-off parameters, this requires inverting the distribution $r(t_1)$ numerically or preparing look-up tables for $T_K(t_1, t_0)$ form factors and their inverse, for each parton type K separately.

Knowing t_1 , one can generate the parton type K_1 according to the probability $\pi_{K_1 K_0}$ proportional to $\int dz \mathcal{P}_{K_1 K_0}^\Theta(t_1, z)$. Look-up tables of the t_1 dependent $\pi_{K_1 K_0}$ branching ratios are needed for better efficiency.

Finally, knowing t_1 and K_1 one can generate the variable z_1 according to the probability distribution proportional to $\mathcal{P}_{K_1 K_0}^\Theta(t_1, z_1)$. Here one can generate z_1 starting from some approximate distribution and execute an internal rejection loop with the correcting weight, about which the external part of the MC algorithm knows nothing.

As one can see, $\omega(t_1, z_1 x_0, K_1 | t_0, x_0, K_0)$ can be generated exactly. However, because of the need to pretabulate the form factors and the branching probabilities there will always be some irreducible numerical bias in the MC results. This requires some extra effort to control quantitatively and reduce, if necessary.

3.4. Weighted Markovian algorithm

The above Markovian scenario is close to what is used in the standard parton-shower MCs. Here we shall describe another class of MC solutions for Eq. (56). We shall stay within the class of the Markovian algorithms, but our aim will be to use a MC implementation which allows for easy and quick transition to constrained Markovian algorithms. Quite generally, in the MC algorithm described above, there is a tendency of “micromanaging” the generation of the component sub-distributions (*i.e.* ω distributions) such that they are generated exactly and there is only one extra global MC weight of Eq. (67). This is an efficient method but the efficiency comes at a price of using look-up tables for generation of the ω distributions.

The alternative (implemented in the MC program `Evo1FMC` [11]) is to simplify intelligently the kernels, phase space boundaries, coupling constant, *etc.*, such that all component distributions in the MC algorithm are easily generated. The compensating weight is applied at a later stage to exactly retrieve the original distributions and integrals. This also comes at a price because an extra weight will lead to a wider weight distribution and a less efficient algorithm, especially if one wants to turn weighted events into unweighted ones at the end of the MC generation. These negative aspects can be minimized by a better choice of approximations and the use of internal rejection loops, wherever possible. On the positive side, there is no need to deal with annoying procedures of controlling quantitatively the numerical bias due to the use of the look-up tables. Moreover, since the approximate distributions reflect well the singularity structure of the integrand, we have better insight into the physics and a better chance to move away from the Markovian algorithm (if we find it profitable for some other reasons).

Looking into the LO and NLO evolution kernels in QCD, one can see that they all have the following structure

$$\begin{aligned}
 P_{IK}(t, z) = & \frac{1}{(1-z)_+} \delta_{IK} A_{KK}(t) + \delta(1-z) \delta_{IK} B_{KK}(t) \\
 & + \frac{1}{z} C_{IK}(t) + D_{IK}(t, z), \tag{71}
 \end{aligned}$$

where $D_{IK}(z)$ is completely regular. The coefficient constants A_{KK}, B_{KK}, C_{IK} and the coefficient functions $D_{IK}(z)$ can be decomposed into the LO and NLO parts:

$$\begin{aligned}
A_{KK}(t) &= \frac{\alpha_s(t)}{2\pi} A_{KK}^{(0)} + \left(\frac{\alpha_s(t)}{2\pi}\right)^2 A_{KK}^{(1)}, \\
B_{KK}(t) &= \frac{\alpha_s(t)}{2\pi} B_{KK}^{(0)} + \left(\frac{\alpha_s(t)}{2\pi}\right)^2 B_{KK}^{(1)}, \\
C_{IK}(t) &= \frac{\alpha_s(t)}{2\pi} C_{IK}^{(0)} + \left(\frac{\alpha_s(t)}{2\pi}\right)^2 C_{IK}^{(1)}, \\
D_{IK}(t, z) &= \frac{\alpha_s(t)}{2\pi} D_{IK}^{(0)}(z) + \left(\frac{\alpha_s(t)}{2\pi}\right)^2 D_{IK}^{(1)}(z). \tag{72}
\end{aligned}$$

Once we have made the above decomposition, we may readily express all the form factors and constants entering into our integrals of Eqs. (56) and (58).

The virtual diagonal IR-divergent elements in the kernel matrix and the corresponding form factor read as follows

$$\begin{aligned}
\mathcal{P}_{KK}^\delta(t) &= 2 \left(A_{KK}(t) \ln \frac{1}{\varepsilon(t)} - B_{KK}(t) \right), \\
\Phi_K(t, t_0) &= \int_{t_0}^t dt' \mathcal{P}_{KK}^\delta(t') = \int_{t_0}^t dt' 2 \left(A_{KK}(t') \ln \frac{1}{\varepsilon(t')} - B_{KK}(t') \right), \tag{73}
\end{aligned}$$

The integrated real-emission off-diagonal elements needed to generate the parton type in the Markovian MC is now

$$\begin{aligned}
\pi_{IK}(t) &= \int_0^1 dz \mathcal{P}_{IK}^\Theta(t, z) \\
&= 2 \left[\delta_{IK} A_{KK}(t) \ln \frac{1}{\varepsilon(t)} + C_{IK}(t) \ln \frac{1}{\varepsilon'} + \int_0^1 dz D_{IK}(t, z) \right]. \tag{74}
\end{aligned}$$

The real-emission form factors T_K , $K = q, g$, are given by

$$\begin{aligned}
T_K(t, t_0) &= \int_{t_0}^t dt' \sum_X \pi_{XK}(t') \\
&= \int_{t_0}^t dt' 2 \left[A_{KK}(t') \ln \frac{1}{\varepsilon(t')} + \sum_X C_{XK}(t') \ln \frac{1}{\varepsilon'} + \sum_X \int_0^1 dz D_{XK}(t', z) \right]. \tag{75}
\end{aligned}$$

Finally, the form factors Δ_K , needed in the final MC weight for the correct overall normalization, read

$$\begin{aligned} \Delta_K(t, t_0) &= \int_{t_0}^t dt' \sum_X \int dz \mathcal{P}_{XK}(t') = \int_{t_0}^t dt' \left\{ -\mathcal{P}_{KK}^\delta(t') + \sum_X \pi_{XK}(t') \right\} \\ &= \int_{t_0}^t dt' 2 \left[B_{KK}(t') + \sum_X C_{XK}(t') \ln \frac{1}{\varepsilon'} + \sum_X \int_0^1 dz D_{XK}(t', z) \right]. \end{aligned} \quad (76)$$

Having expressed all the elements in Eq. (66) of the standard Markovian algorithm, let us construct an alternative MC Markovian scenario starting from Eq. (56) (before Markovianization). First, we simplify the kernel matrix elements

$$\begin{aligned} \mathcal{P}_{IK}^\Theta(t, z) \rightarrow \hat{\mathcal{P}}_{IK}^\Theta(t_0, z) &= \Theta(z - \varepsilon') \Theta(1 - z - \hat{\varepsilon}) \frac{\alpha_s(t_0)}{\pi} \\ &\times \left\{ \frac{1}{1-z} \delta_{IK} A_{KK}^{(0)} + \frac{1}{z} C_{IK}^{(0)} + \hat{D}_{IK} \right\}, \end{aligned} \quad (77)$$

where D is replaced by the constant \hat{D} , which is chosen to be zero when $A^{(0)}, B^{(0)}$ are nonzero or equal the maximum (positive) value of $D_{IK}^{(0)}(z)$; see Appendix B. The above simplification is of course compensated by the MC weight

$$w_P = \prod_{i=1}^n \frac{\mathcal{P}_{K_i K_{i-1}}^\Theta(t_i, z_i)}{\hat{\mathcal{P}}_{K_i K_{i-1}}^\Theta(t_0, z_i)}. \quad (78)$$

Let us remark that the replacement $\alpha_s(t_i) \rightarrow \alpha_s(t_0)$ of the running coupling which stands in front of the LO kernel might cause poor overall MC efficiency. This problem is addressed separately in the next section.

The above reorganization leads us to the following new formula

$$\begin{aligned} D_K(t, x) &= e^{-\Phi_K(t, t_0)} D_K(t_0, x) \\ &+ \sum_{n=1}^{\infty} \sum_{K_0, \dots, K_{n-1}} \int_0^1 dx_0 \prod_{i=1}^n \left[\int_{t_0}^t dt_i \Theta(t_i - t_{i-1}) \int_0^1 dz_i \right] \\ &\times e^{-\Phi_K(t, t_n)} \prod_{i=1}^n \left[\hat{\mathcal{P}}_{K_i K_{i-1}}^\Theta(t_0, z_i) e^{-\Phi_{K_{i-1}}(t_i, t_{i-1})} \right] \\ &\times D_{K_0}(t_0, x_0) \delta \left(x - x_0 \prod_{i=1}^n z_i \right) w_P, \end{aligned} \quad (79)$$

completely equivalent to Eq. (56). Markovianization is now done for the variant of the above formula in which w_P is neglected. We define a new transition probability as follows

$$\begin{aligned} \hat{\omega}(t_i, x_i, K_i | t_{i-1}, x_{i-1}, K_{i-1}) &\equiv \Theta(t_i - t_{i-1}) \hat{\mathcal{P}}_{K_i K_{i-1}}^\Theta(t_0, x_i/x_{i-1}) \\ &\quad \times e^{-\hat{T}_{K_{i-1}}(t_i, t_{i-1})}, \\ \int_{t_{i-1}}^{\infty} dt_i \int_0^1 dz_i \sum_{K_i} \hat{\omega}(t_i, x_i, K_i | t_{i-1}, x_{i-1}, K_{i-1}) &\equiv 1, \end{aligned} \quad (80)$$

where

$$\begin{aligned} \hat{T}_K(t_i, t_{i-1}) &= \int_{t_{i-1}}^{t_i} dt' \int_0^1 dz \sum_J \hat{\mathcal{P}}_{JK}^\Theta(t', z) \\ &= (t_i - t_{i-1}) \frac{\alpha_s(t_0)}{\pi} \left[A_{KK}^{(0)} \ln \frac{1}{\hat{\varepsilon}} + \sum_X C_{XK}^{(0)} \ln \frac{1}{\varepsilon'} + \sum_X \hat{D}_{XK}^{(0)} \right] \\ &= \int_{t_{i-1}}^{t_i} dt' \sum_X \hat{\pi}_{XK} = (t_i - t_{i-1}) \sum_X \hat{\pi}_{XK} = (t_i - t_{i-1}) R_K, \end{aligned} \quad (81)$$

and the probability rate of the parton transition $K \rightarrow I$ is now constant

$$\begin{aligned} \hat{\pi}_{IK} &= \int_0^1 dz \hat{\mathcal{P}}_{IK}^\Theta(t_0, z) \\ &= \frac{\alpha_s(t_0)}{\pi} \left[\delta_{IK} A_{KK}^{(0)} \ln \frac{1}{\hat{\varepsilon}} + C_{IK}^{(0)} \ln \frac{1}{\varepsilon'} + \hat{D}_{IK} \right], \end{aligned} \quad (82)$$

independent of t ; see Appendix B for explicit formulae. Summarizing, the transition probability

$$\begin{aligned} \hat{\omega}(t_i, x_i, K_i | t_{i-1}, x_{i-1}, K_{i-1}) &\equiv \Theta(t_i - t_{i-1}) \hat{\mathcal{P}}_{K_i K_{i-1}}^\Theta(t_0, x_i/x_{i-1}) \\ &\quad \times e^{-(t_i - t_{i-1}) R_{K_{i-1}}} \end{aligned} \quad (83)$$

is now such a simple function that can be generated using elementary MC methods, without any pretabulation. The last thing necessary, as usual, for the Markovianization is introduction of the ‘‘spill-over’’ variable. This is done with the help of the identity

$$\begin{aligned}
 e^{-\Phi_{K_n}(t,t_n)} &= e^{\hat{\Delta}_{K_n}(t,t_n)} \int_t^\infty dt_{n+1} \int_0^1 dz_{n+1} \\
 &\times \sum_{K_{n+1}} \hat{\omega}(t_{n+1}, x_{n+1}, K_{n+1} | t_n, x_n, K_n), \quad (84)
 \end{aligned}$$

where

$$\hat{\Delta}_K(t_i, t_{i-1}) = \hat{T}_K(t_i, t_{i-1}) - \Phi_K(t_i, t_{i-1}) = (t_i - t_{i-1}) R_K - \Phi_K(t_i, t_{i-1}). \quad (85)$$

Let us stress that now, contrary to the previous standard Markovian scenario, $\hat{\Delta}$ has an explicit residual dependence on the IR cut $\hat{\varepsilon}$ which is necessary to cancel *exactly* the analogous dependence of the average weight w_P (similarly as in a typical MC algorithm for QED exponentiation).

Summarizing all the above discussion, we transform Eq. (79) in a new equivalent form

$$\begin{aligned}
 D_K(t, x) &= e^{\hat{\Delta}_K(t,t_0)} \int_{t_1 > t} dt_1 dz_1 \sum_{K_1} \hat{\omega}(t_1, x_1, K_1 | t_0, x, K) D_K(t_0, x) \\
 &+ \sum_{n=1}^\infty \int_0^1 dx_0 \int_{t_{n+1} > t} dt_{n+1} dz_{n+1} \sum_{K_{n+1}} \sum_{K_0, \dots, K_{n-1}} \prod_{i=1}^n \int dt_i dz_i \\
 &\times \hat{\omega}(t_{n+1}, x_{n+1}, K_{n+1} | t_n, x_n, K_n) \prod_{i=1}^n \hat{\omega}(t_i, x_i, K_i | t_{i-1}, x_{i-1}, K_{i-1}) \\
 &\times \delta \left(x - x_0 \prod_{i=1}^n z_i \right) D_{K_0}(t_0, x_0) w_P w_\Delta, \quad (86)
 \end{aligned}$$

where

$$w_\Delta = e^{\hat{\Delta}_{K_n}(t,t_n)} \prod_{i=1}^n e^{\hat{\Delta}_{K_{i-1}}(t_i, t_{i-1})}. \quad (87)$$

In the MC generation we proceed as before. Neglecting the weight $w = w_P w_\Delta$, we generate primary MC events using the Markovian algorithm with the simplified transition probability $\hat{\omega}$. The original distributions and integrals are recovered by applying the correction weight w . As already stressed, the MC efficiency will be worse than in the previous case, but the whole MC program is now much simpler and most likely provides better control of the technical precision.

Let us note that we shall still need a precise 1-dimensional pretabulation of all the form factors $\Phi_K(t, t_0)$, entering into w_Δ through $\hat{\Delta}_K$.

3.5. Importance sampling for running $\alpha_s(t)$

In the above we took into account the t -dependence ($t = \ln Q$), that is running, of the strong coupling constant $\alpha_s(t)$ by reweighting MC events. This is very inefficient and it is rather easy to introduce the relevant t -dependence of $\alpha_s(t)$ at least at the one-loop level

$$\alpha_s^{(0)}(t) = \frac{4\pi}{\beta_0(2t - 2 \ln \Lambda_0)} \quad (88)$$

already in the underlying MC distributions.

One can see that in the t -integration in Eq. (79) we have effectively

$$\int dt_i \alpha_s^{(0)}(t_i) = \int dt_i \frac{2\pi}{\beta_0(t_i - \ln \Lambda_0)} = \frac{2\pi}{\beta_0} \int d \ln(t_i - \ln \Lambda_0). \quad (89)$$

It is, therefore, natural to introduce the variable τ_i ,

$$\begin{aligned} \tau_i &= \ln(t_i - \ln \Lambda_0), & t_i &= \ln \Lambda_0 + \exp(\tau_i), \\ dt_i &= (t_i - \ln \Lambda_0) d\tau_i = e^{\tau_i} d\tau_i, \end{aligned} \quad (90)$$

instead of³ t_i . This change of variables will lead to the Jacobian factor $e^{\tau_i} = t_i - \ln \Lambda_0$ in the integrand, which will cancel the unwanted factor $e^{-\tau_i} = (t_i - \ln \Lambda_0)^{-1}$ present in $\alpha_s(t)$ in the MC weight. The two-loop and more complicated contributions to $\alpha_s(t)$ may still be added by reweighting events, without spoiling much the efficiency.

We start again from Eq. (56) (before Markovianization). The kernel matrix elements are now simplified more “gently” with respect to Eq. (77)

$$\begin{aligned} \mathcal{P}_{IK}^\Theta(t, z) \rightarrow \bar{\mathcal{P}}_{IK}^\Theta(t, z) &= \Theta(z - \varepsilon') \Theta(1 - z - \bar{\varepsilon}) \frac{\alpha_s^{(0)}(t)}{\pi} \\ &\times \left\{ \frac{1}{(1-z)_+} \delta_{IK} A_{KK}^{(0)} + \frac{1}{z} C_{IK}^{(0)} + \bar{D}_{IK} \right\}, \end{aligned} \quad (91)$$

where $\bar{D}_{IK} = \hat{D}_{IK}$ and $\varepsilon(t) \rightarrow \bar{\varepsilon}$. The new compensating MC weight is

$$\bar{w}_P = \prod_{i=1}^n \frac{\mathcal{P}_{K_i K_{i-1}}^\Theta(t_i, z_i)}{\bar{\mathcal{P}}_{K_i K_{i-1}}^\Theta(t_i, z_i)}. \quad (92)$$

³ Of course, we are aware of a possibility of introducing τ as an evolution “time” in the original differential equation from the very beginning. We proceed this way in order to get more insight into various versions of the MC algorithm.

The above reorganization leads us to the following new formula, completely equivalent to Eq. (56),

$$\begin{aligned}
 D_K(\tau, x) &= e^{-\Phi_K(\tau, \tau_0)} D_K(\tau_0, x) \\
 &+ \sum_{n=1}^{\infty} \sum_{K_0, \dots, K_{n-1}} \prod_{i=1}^n \left[\int_{\tau_0}^{\tau} d\tau_i \Theta(\tau_i - \tau_{i-1}) \int_0^1 dz_i \right] \\
 &\times e^{-\Phi_K(\tau, \tau_n)} \int_0^1 dx_0 \prod_{i=1}^n \left[e^{\tau_i} \bar{\mathcal{P}}_{K_i K_{i-1}}^{\Theta}(\tau_i, z_i) e^{-\Phi_{K_{i-1}}(\tau_i, \tau_{i-1})} \right] \\
 &\times D_{K_0}(\tau_0, x_0) \delta \left(x - x_0 \prod_{i=1}^n z_i \right) \bar{w}_P. \tag{93}
 \end{aligned}$$

In the following we shall use a new function

$$\bar{\mathcal{P}}_{K_i K_{i-1}}^{\Theta}(z_i) = e^{\tau_i} \bar{\mathcal{P}}_{K_i K_{i-1}}^{\Theta}(\tau_i, z_i), \tag{94}$$

because it *does not depend* on τ_i anymore. This is the whole point of the $t_i \rightarrow \tau_i$ change of variables.

Omitting \bar{w}_P , we proceed to Markovianization following the example of the previous section

$$\begin{aligned}
 \bar{\omega}(\tau_i, x_i, K_i | \tau_{i-1}, x_{i-1}, K_{i-1}) &\equiv \Theta(\tau_i - \tau_{i-1}) \bar{\mathcal{P}}_{K_i K_{i-1}}^{\Theta}(x_i/x_{i-1}) \\
 &\times e^{-\bar{T}_{K_{i-1}}(\tau_i, \tau_{i-1})}, \\
 \int_{\tau_{i-1}}^{\infty} d\tau_i \int_0^1 dz_i \sum_{K_i} \bar{\omega}(\tau_i, x_i, K_i | \tau_{i-1}, x_{i-1}, K_{i-1}) &\equiv 1, \tag{95}
 \end{aligned}$$

where

$$\begin{aligned}
 \bar{T}_K(\tau_i, \tau_{i-1}) &= \int_{\tau_{i-1}}^{\tau_i} d\tau' \int_0^1 dz \sum_J \bar{\mathcal{P}}_{JK}^{\Theta}(z) \\
 &= (\tau_i - \tau_{i-1}) \frac{2}{\beta_0} \left[A_{KK}^{(0)} \ln \frac{1}{\bar{\epsilon}} + \sum_X C_{XK}^{(0)} \ln \frac{1}{\bar{\epsilon}'} + \sum_X \bar{D}_{XK}^{(0)} \right] \\
 &= (\tau_i - \tau_{i-1}) \bar{R}_K, \\
 \bar{R}_K &= \sum_X \bar{\pi}_{XK},
 \end{aligned} \tag{96}$$

and the probability rate of the parton transition $K \rightarrow I$ is now a constant

$$\bar{\pi}_{IK} = \int_0^1 dz \bar{\mathcal{P}}_{IK}^{\Theta}(z) = \frac{2}{\beta_0} \left[\delta_{IK} A_{KK}^{(0)} \ln \frac{1}{\varepsilon} + C_{IK}^{(0)} \ln \frac{1}{\varepsilon'} + \bar{D}_{IK} \right], \quad (97)$$

again independent of t . The final transition probability to be generated in each step of the Markovian algorithm reads

$$\begin{aligned} \bar{\omega}(\tau_i, x_i, K_i | \tau_{i-1}, x_{i-1}, K_{i-1}) &\equiv \Theta(\tau_i - \tau_{i-1}) \bar{\mathcal{P}}_{K_i K_{i-1}}^{\Theta}(x_i/x_{i-1}) \\ &\times e^{-(\tau_i - \tau_{i-1}) \bar{R}_{K_{i-1}}}, \end{aligned} \quad (98)$$

where

$$\bar{\mathcal{P}}_{IK}^{\Theta}(z) = \Theta(z - \varepsilon') \Theta(1 - z - \bar{\varepsilon}) \frac{2}{\beta_0} \left\{ \frac{1}{1-z} \delta_{IK} A_{KK}^{(0)} + \frac{1}{z} C_{IK}^{(0)} + \bar{D}_{IK} \right\} \quad (99)$$

is again a simple function which can be generated, without any pretabulation, using elementary MC methods. The overall recipe, as compared with the previous MC algorithm, is to replace: $t_i \rightarrow \tau_i$ and $\alpha_s(t_0)/\pi \rightarrow 2/\beta_0$ in the generation of the primary MC distribution $\bar{\omega}$, before applying $\bar{\omega}_P$.

Inevitably, to complete the Markovianization, the integral over a “spillover” variable τ_{n+1} is added with the usual identity

$$\begin{aligned} e^{-\Phi_{K_n}(\tau, \tau_n)} &= e^{\bar{\Delta}_{K_n}(\tau, \tau_n)} \int_{\tau}^{\infty} d\tau_{n+1} \int_0^1 dz_{n+1} \\ &\times \sum_{K_{n+1}} \bar{\omega}(\tau_{n+1}, x_{n+1}, K_{n+1} | \tau_n, x_n, K_n), \end{aligned} \quad (100)$$

where

$$\begin{aligned} \bar{\Delta}_K(\tau_i, \tau_{i-1}) &= \bar{T}_K(t_i, \tau_{i-1}) - \Phi_K(\tau_i, \tau_{i-1}) \\ &= (\tau_i - \tau_{i-1}) \bar{R}_K - \Phi_K(\tau_i, \tau_{i-1}). \end{aligned} \quad (101)$$

The final formula, equivalent to original Eq. (79), for this MC scenario with the importance sampling for the running α_s reads as follows

$$\begin{aligned}
 D_K(\tau, x) &= e^{\bar{\Delta}_K(\tau, \tau_0)} \int_{\tau_1 > \tau} d\tau_1 dz_1 \sum_{K_1} \bar{\omega}(\tau_1, x_1, K_1 | \tau_0, x, K) D_K(\tau_0, x) \\
 &+ \sum_{n=1}^{\infty} \int_0^1 dx_0 \int_{\tau_{n+1} > \tau} d\tau_{n+1} dz_{n+1} \sum_{K_{n+1}} \sum_{K_0, \dots, K_{n-1}} \prod_{i=1}^n \int d\tau_i dz_i \\
 &\times \bar{\omega}(\tau_{n+1}, x_{n+1}, K_{n+1} | \tau_n, x_n, K_n) \prod_{i=1}^n \bar{\omega}(\tau_i, x_i, K_i | \tau_{i-1}, x_{i-1}, K_{i-1}) \\
 &\times \delta \left(x - x_0 \prod_{i=1}^n z_i \right) D_{K_0}(\tau_0, x_0) \bar{w}_P \bar{w}_\Delta, \tag{102}
 \end{aligned}$$

where

$$\bar{w}_\Delta = e^{\bar{\Delta}_{K_n}(\tau, \tau_n)} \prod_{i=1}^n e^{\bar{\Delta}_{K_{i-1}}(\tau_i, \tau_{i-1})}. \tag{103}$$

The above formula looks almost identical to Eq. (86).

4. Markovian MC for parton-momentum distributions

The factor $1/z$ in the bremsstrahlung kernels causes a significant loss of MC efficiency due to $\exp(\Delta_K)$ which contains uncompensated $\ln(\varepsilon')$. We can get rid of this annoying phenomenon by switching to the $xD(x)$ which evolve with the kernels $zP(z)$. The reason for improvement is that kernels $zP(z)$ fulfill the momentum-conservation sum rules. The evolution equations for $xD(x)$ read

$$\partial_t xD_K(t, x) = \sum_J \int_x^1 \frac{dz}{z} z\mathcal{P}_{KJ}(t, z) \frac{x}{z} D_J(t, (x/z)). \tag{104}$$

The iterative solution can be obtained from the above formulae, or equivalently by multiplying both sides of Eq. (56) by x ,

$$\begin{aligned}
xD_K(t, x) &= e^{-\Phi_K(t, t_0)} x D_K(t_0, x) \\
&+ \sum_{n=1}^{\infty} \int_0^1 dx_0 \sum_{K_0, \dots, K_{n-1}} \prod_{i=1}^n \left[\int_{t_0}^t dt_i \Theta(t_i - t_{i-1}) \int_0^1 dz_i \right] \\
&\times e^{-\Phi_K(t, t_n)} \prod_{i=1}^n \left[z_i \mathcal{P}_{K_i K_{i-1}}^{\Theta}(t_i, z_i) e^{-\Phi_{K_{i-1}}(t_i, t_{i-1})} \right] \\
&\times x_0 D_{K_0}(t_0, x_0) \delta \left(x - x_0 \prod_{i=1}^n z_i \right), \tag{105}
\end{aligned}$$

where $K \equiv K_n$. It was essential to exploit the condition $x = x_0 \prod_{i=1}^n z_i$ imposed by the overall δ -functions⁴. We also feel free to introduce such an overall factor x in the $x D(x)$, because our ultimate aim is to use a constrained Markovian algorithm, hence such a factor will be dealt in the MC separately and independently with other dedicated MC methods. At the technical level, we may multiply both sides of the above equation by $1/x$ and absorb $1/x$ in the MC weight, pretending that we generate $D(x)$ distribution as before; in such a case the fluctuations of the weight in the histograms of x will change but the distribution of x will be the same. The main change will be in the probability distribution ω for the forward leap in the Markovian random walk.

Before we enter into details of the Markovian MC, let us introduce the evolution variable τ , similarly as in the previous section

$$\tau \equiv \frac{1}{\alpha_s(t_A)} \int_{t_A}^t dt_1 \alpha_s(t_1), \quad \frac{\partial t}{\partial \tau} = \frac{\alpha_s(t_A)}{\alpha_s(t)}. \tag{106}$$

In the above transformation we may use various choices of t_A and of $\alpha_s(t)$. For instance, we may employ the same $\alpha_s(t)$ as in the evolution equations (LO or NLO) or we may stay with the one-loop LO: $\alpha_s^{(0)}(t) = 2\pi/(\beta_0(t - \ln \Lambda_0))$. In the latter case, with t_A chosen such that $\alpha_s^{(0)}(t_A) = 2\pi/\beta_0$ (e.g. $t_A - \ln \Lambda_0 = 1$, $t_A = \ln(e\Lambda_0)$), we recover the definition $\tau = \ln(t - \ln \Lambda_0)$ of the previous section. Let us adjust $t_A = t_0$ to the starting point of the evolution and use $\alpha_s^{(0)}(t)$ in the definition of τ . With such a choice we have:

⁴ This way we could introduce any power of x , say x^α , in front of $D(x)$ and z^α in the kernels.

$$\begin{aligned}
 xD_K(\tau, x) &= e^{-\Phi_K(\tau, \tau_0)} xD_K(\tau_0, x) \\
 &+ \sum_{n=1}^{\infty} \int_0^1 dx_0 \sum_{K_0, \dots, K_{n-1}} \prod_{i=1}^n \left[\int_{\tau_0}^{\tau} d\tau_i \Theta(\tau_i - \tau_{i-1}) \int_0^1 dz_i \right] \\
 &\times e^{-\Phi_K(\tau, \tau_n)} \prod_{i=1}^n \left[\mathcal{P}_{K_i K_{i-1}}^{\Theta}(\tau_i, z_i) e^{-\Phi_{K_{i-1}}(\tau_i, \tau_{i-1})} \right] \\
 &\times x_0 D_{K_0}(\tau_0, x_0) \delta \left(x - x_0 \prod_{i=1}^n z_i \right), \tag{107}
 \end{aligned}$$

where $K \equiv K_n$, and

$$\mathcal{P}_{K_i K_{i-1}}^{\Theta}(\tau_i, z_i) = \frac{\alpha_s^{(0)}(t_0)}{\alpha_s^{(0)}(t_i)} z_i \mathcal{P}_{K_i K_{i-1}}^{\Theta}(\tau_i, z_i), \tag{108}$$

which depends on τ_i very weakly. In the LO case it is completely independent of τ_i .

In the general (NLO) case we may decompose the evolution kernels multiplied by z as follows

$$\begin{aligned}
 \frac{1}{2} z \mathcal{P}_{IK}(t, z) &\equiv z P_{IK}(t, z) \\
 &= \frac{1}{(1-z)_+} \delta_{IK} A_{KK}(t) + \delta(1-z) \delta_{IK} B_{KK}(t) + F_{IK}(t, z), \tag{109}
 \end{aligned}$$

where the finite part F can be expressed in terms of the previously defined functions A , C and D as follows

$$F_{IK}(t, z) = z D_{IK}(t, z) + C_{IK}(t) - \delta_{IK} A_{KK}(t). \tag{110}$$

In the MC we replace, as before, the full kernels for the real emission with the LO approximation with the constant IR regulator $\bar{\varepsilon} \leq \varepsilon(t)$:

$$\begin{aligned}
 \mathcal{P}_{IK}^{\Theta}(\tau, z) &\rightarrow \bar{\mathcal{P}}_{IK}^{\Theta}(\tau_0, z) = \Theta(1-z-\bar{\varepsilon}) \frac{\alpha_s^{(0)}(t_0)}{\pi} z P_{IK}^{(0)}(z), \\
 z P_{IK}^{(0)}(z) &= \frac{1}{(1-z)_+} \delta_{IK} A_{KK}^{(0)} + \delta(1-z) \delta_{IK} B_{KK}^{(0)} + F_{IK}^{(0)}(z). \tag{111}
 \end{aligned}$$

The approximate kernels do not depend on τ . The corresponding compensating weight is now

$$\bar{w}_P = \prod_{i=1}^n \frac{\mathcal{P}_{K_i K_{i-1}}^{\Theta}(\tau_i, z_i)}{\bar{\mathcal{P}}_{K_i K_{i-1}}^{\Theta}(\tau_0, z_i)}. \tag{112}$$

The probability of the forward Markovian leap reads now as follows

$$\begin{aligned} \bar{\omega}(\tau_i, x_i, K_i | \tau_{i-1}, x_{i-1}, K_{i-1}) &\equiv \Theta(\tau_i - \tau_{i-1}) \\ &\quad \times \bar{\mathcal{P}}_{K_i K_{i-1}}^\Theta(\tau_0, x_i/x_{i-1}) e^{-\bar{T}_{K_{i-1}}(\tau_i, \tau_{i-1})}, \\ \int_{\tau_{i-1}}^{\infty} d\tau_i \int_0^1 dz_i \sum_{K_i} \bar{\omega}(\tau_i, x_i, K_i | \tau_{i-1}, x_{i-1}, K_{i-1}) &\equiv 1, \\ z_i &= x_i/x_{i-1}, \end{aligned} \quad (113)$$

where the new real-emission form factor is defined as follows

$$\begin{aligned} \bar{T}_K(\tau_i, \tau_{i-1}) &= \int_{\tau_{i-1}}^{\tau_i} d\tau' \int_0^1 dz \sum_J \bar{\mathcal{P}}_{JK}^\Theta(\tau_0, z) \\ &= (\tau_i - \tau_{i-1}) \frac{\alpha_s^{(0)}(t_0)}{\pi} \left[A_{KK}^{(0)} \ln \frac{1}{\varepsilon} + \sum_J \int_0^1 F_{JK}^{(0)}(z) dz \right] \\ &= (\tau_i - \tau_{i-1}) \sum_J \bar{\pi}_{JK} = (\tau_i - \tau_{i-1}) \bar{R}_K. \end{aligned} \quad (114)$$

The rate of the parton transition $K \rightarrow I$ is now

$$\bar{\pi}_{IK} = \int_0^1 dz \bar{\mathcal{P}}_{IK}^\Theta(\tau_0, z) = \frac{\alpha_s^{(0)}(t_0)}{\pi} \left[\delta_{IK} A_{KK}^{(0)} \ln \frac{1}{\varepsilon} + \int_0^1 F_{IK}^{(0)}(z) dz \right]. \quad (115)$$

On the other hand, the exact virtual form factor is

$$\Phi_K(\tau, \tau_0) = \int_{\tau_0}^{\tau} d\tau' \frac{\alpha_s^{(0)}(t_0)}{\alpha_s^{(0)}(t')} 2 \left[A_{KK}(\tau') \ln \frac{1}{\varepsilon(\tau')} - B_{KK}(\tau') \right]. \quad (116)$$

In the LO, for the one-loop $\alpha_s^{(0)}$ and if, in addition, we choose $\varepsilon(\tau) = \varepsilon = \text{const}$, then the virtual form factor becomes simply

$$\Phi_K(\tau, \tau_0) = (\tau - \tau_0) \frac{\alpha_s^{(0)}(t_0)}{\pi} \left(A_{KK}^{(0)} \ln \frac{1}{\varepsilon} - B_{KK}^{(0)} \right). \quad (117)$$

Summarizing, the final transition probability to be generated in each step of the Markovian algorithm reads

$$\begin{aligned} \bar{\omega}(\tau_i, x_i, K_i | \tau_{i-1}, x_{i-1}, K_{i-1}) &\equiv \Theta(\tau_i - \tau_{i-1}) \\ &\quad \times \bar{\mathcal{P}}_{K_i K_{i-1}}^\Theta(\tau_0, x_i/x_{i-1}) e^{-(\tau_i - \tau_{i-1}) \bar{R}_{K_{i-1}}}, \end{aligned} \quad (118)$$

where

$$\bar{\mathcal{P}}_{IK}^{\Theta}(\tau_0, z) = \Theta(1 - z - \bar{\varepsilon}) \frac{\alpha_s^{(0)}(t_0)}{\pi} \left\{ \frac{1}{1-z} \delta_{IK} A_{KK}^{(0)} + F_{IK}^{(0)}(z) \right\}. \quad (119)$$

To complete the Markovianization, the integral over the “spill-over” variable τ_{n+1} is added with the help of the usual identity

$$e^{-\Phi_{K_n}(\tau, \tau_n)} = e^{\bar{\Delta}_{K_n}(\tau, \tau_n)} \quad (120)$$

$$\times \int_{\tau}^{\infty} d\tau_{n+1} \int_0^1 dz_{n+1} \sum_{K_{n+1}} \bar{\omega}(\tau_{n+1}, x_{n+1}, K_{n+1} | \tau_n, x_n, K_n),$$

where $z_{n+1} = x_{n+1}/x_n$, and

$$\begin{aligned} \bar{\Delta}_K(\tau_i, \tau_{i-1}) &= \bar{T}_K(\tau_i, \tau_{i-1}) - \Phi_K(\tau_i, \tau_{i-1}) \\ &= (\tau_i - \tau_{i-1}) \bar{R}_K - \Phi_K(\tau_i, \tau_{i-1}). \end{aligned} \quad (121)$$

The advantage of the method outlined in this section is that at the LO level we obtain for $\varepsilon = \bar{\varepsilon}$

$$\bar{\Delta}_K = 0 \quad (122)$$

due to the fact that the kernels obey the momentum sum rules. In most renormalization schemes (*e.g.* \overline{MS}) this will be also valid at the NLO level⁵.

The final formula for this MC scenario with the importance sampling for the running α_s reads:

$$\begin{aligned} xD_K(\tau, x) &= e^{\bar{\Delta}_K(\tau, \tau_0)} \int_{\tau_1 > \tau} d\tau_1 dz_1 \sum_{K_1} \bar{\omega}(\tau_1, z_1 x, K_1 | \tau_0, x, K) xD_K(\tau_0, x) \\ &+ \sum_{n=1}^{\infty} \int_0^1 dx_0 \int_{\tau_{n+1} > \tau} d\tau_{n+1} dz_{n+1} \sum_{K_{n+1}} \sum_{K_0, \dots, K_{n-1}} \prod_{i=1}^n \int_{\tau_i < \tau} d\tau_i dz_i \\ &\times \bar{\omega}(\tau_{n+1}, x_{n+1}, K_{n+1} | \tau_n, x_n, K_n) \prod_{i=1}^n \bar{\omega}(\tau_i, x_i, K_i | \tau_{i-1}, x_{i-1}, K_{i-1}) \\ &\times \delta \left(x - x_0 \prod_{i=1}^n z_i \right) x_0 D_{K_0}(\tau_0, x_0) \bar{w}_P \bar{w}_{\Delta}, \end{aligned} \quad (123)$$

where $z_i = x_i/x_{i-1}$, $K \equiv K_n$ and

$$\bar{w}_{\Delta} = e^{\bar{\Delta}_{K_n}(\tau, \tau_n)} \prod_{i=1}^n e^{\bar{\Delta}_{K_{i-1}}(\tau_i, \tau_{i-1})}. \quad (124)$$

⁵ A small non-zero value of $\bar{\Delta}_K$ may be present for technical reasons, that is, if we use slightly simplified kernels at the low MC generation level.

5. Numerical tests

We have performed comparisons of the MC solution of the DGLAP evolution equations implemented in the program `Evo1FMC` [11] with another solution provided by the non-MC program `QCDnum16` [3]. In both cases we have evolved singlet PDF for gluons and three doublets of massless quarks from $Q_0 = 1$ GeV to $Q = 10, 100, 1000$ GeV. The comparisons have been done both for the LO and the NLO evolution, including the running α_s in the corresponding approximation.

In our test, we have used the following parameterization of the starting parton distributions in the proton at $Q_0 = 1$ GeV:

$$\begin{aligned}
 xD_G(x) &= 1.9083594473 x^{-0.2}(1-x)^{5.0}, \\
 xD_q(x) &= 0.5 xD_{\text{sea}}(x) + xD_{2u}(x), \\
 xD_{\bar{q}}(x) &= 0.5 xD_{\text{sea}}(x) + xD_d(x), \\
 xD_{\text{sea}}(x) &= 0.6733449216 x^{-0.2}(1-x)^{7.0}, \\
 xD_{2u}(x) &= 2.1875000000 x^{0.5}(1-x)^{3.0}, \\
 xD_d(x) &= 1.2304687500 x^{0.5}(1-x)^{4.0}.
 \end{aligned} \tag{125}$$

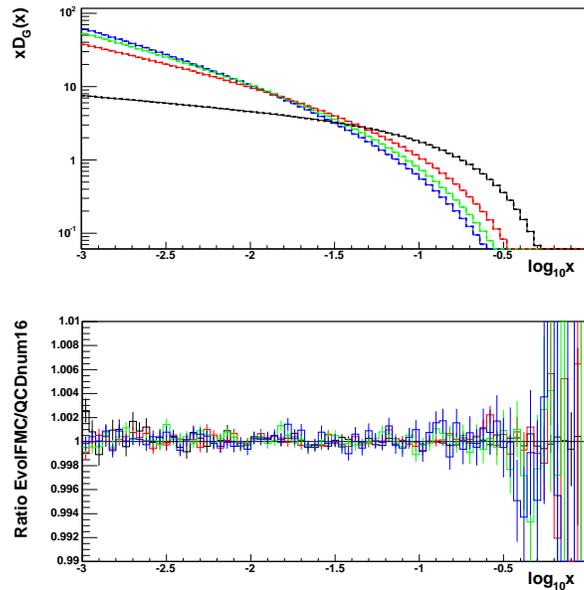


Fig.1. The upper plot shows the gluon distribution $x D_G(x, Q_i)$ evolved from $Q_0 = 1$ GeV (black) to $Q_i = 10$ (red), 100 (green) and 1000 (blue) GeV, obtained in the LO approximation from `Evo1FMC` (solid lines) and `QCDnum16` (dashed lines), while the lower plot shows their ratio.

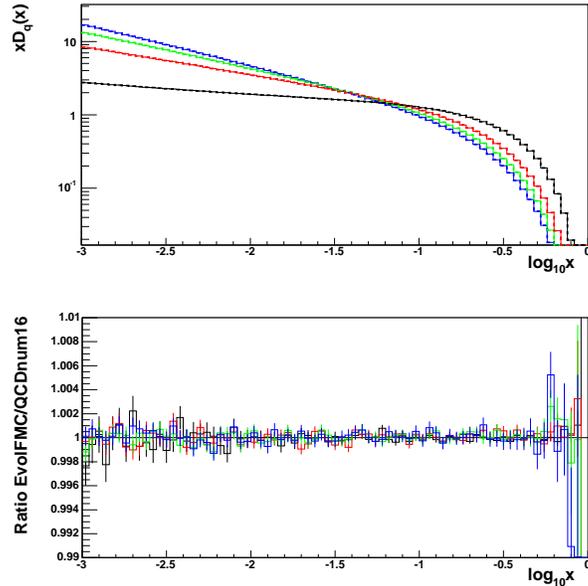


Fig. 2. The upper plot shows the singlet quark distribution $x D_{\bar{q}}(x, Q_i)$ evolved from $Q_0 = 1$ GeV (black) to $Q_i = 10$ (red), 100 (green) and 1000 (blue) GeV, obtained in the LO approximation from *EvolFMC* (solid lines) and *QCDnum16* (dashed lines), while the lower plot shows their ratio.

The first results of these comparisons for the LO evolution were presented in Ref. [6]. They showed a 0.2% discrepancy for the gluon distributions between *EvolFMC* and *QCDnum16*. This numerical bias is eliminated in this paper. In Figs. 1 and 2 we show the resulting gluon and quark distributions evolved to $Q = 10, 100, 1000$ GeV in the LO approximation. As one can see, these two calculations agree to within 0.1% for the gluon as well as for the quark singlet distributions. The origin of the previous 0.2% discrepancy for gluon was identified as a result of too high values of the dummy IR cut-offs: $\varepsilon = \bar{\varepsilon} = 10^{-3}$. The new results have been obtained for $\varepsilon = \bar{\varepsilon} = 10^{-4}$. In the small- x region ($x < 0.1$), we have found a similar agreement with the program *APCheb33* [4], which uses the Chebyshev-polynomial technique to solve the DGLAP equations.

In Figs. 3 and 4 we present the results of similar comparisons for the NLO evolution. In the NLO, there is some ambiguity in calculation of the running α_s . In *EvolFMC* we use a definition of α_s given in Appendix A. However, in the original version of *QCDnum16* a different definition of α_s at the NLO was employed. For the sake of our comparisons, we have replaced in the *QCDnum16* code the routine for α_s evaluation with the appropriate routine from *EvolFMC*. We have checked for several values of Q^2 , that after replacement the two programs give numerically the same values of $\alpha_s(Q^2)$.

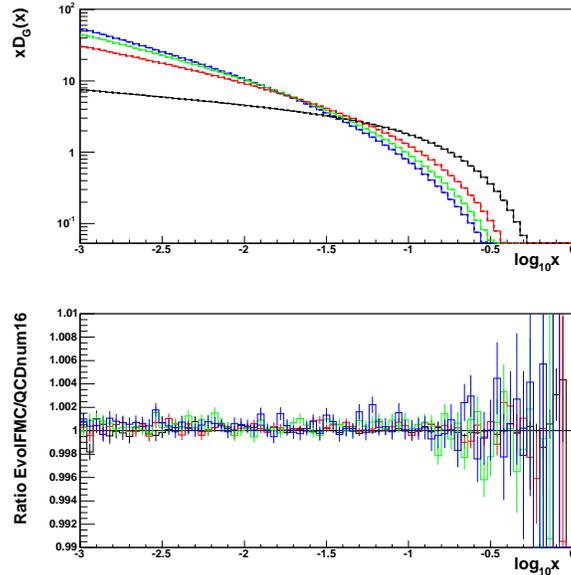


Fig. 3. The upper plot shows the gluon distribution $x D_G(x, Q_i)$ evolved from $Q_0 = 1$ GeV (black) to $Q_i = 10$ (red), 100 (green) and 1000 (blue) GeV, obtained in the NLO approximation from Evo1FMC (solid lines) and QCDnum16 (dashed lines), while the lower plot shows their ratio.

The NLO results for the gluon and quark singlet distributions from Evo1FMC and QCDnum16 agree within $\sim 0.1\%$, as in the LO case. Again, for $x < 0.1$ we have found a similar agreement with APCh33.

The MC calculation for the NLO evolution is, of course, slower and less efficient than for the LO one but not very much. In comparison with the LO results given above, the NLO results were obtained for the statistics about 2 times higher and their computation required about 3 times more CPU time.

All the above results were obtained in the weighted-event mode of Evo1FMC. In the LO case the weighted events can be turned into the unweighted (weight = 1) ones without difficulty — the event weight is well-behaved, non-negative and bounded from above. At the NLO, however, the situation is problematic. As was described in Sec. 2.3, the P_{FG} and P_{GF} splitting functions at the NLO acquire logarithmic singularities at $z = 1$. In our MC algorithm this leads to large positive weights for the $F \rightarrow G$ transitions and to negative weights for the $G \rightarrow F$ transitions in the region of $z \gtrsim 0.95$. While the problem of large positive weights can be cured with appropriate importance sampling, there is no technical method to turn negative-weight events into unweighted events. The current version of Evo1FMC implements only the weighted-event solution for the NLO DGLAP evolution. These problems will be addressed in our future works.

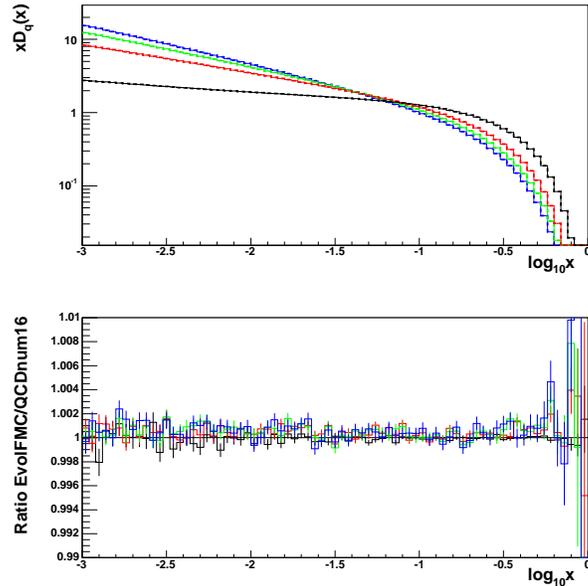


Fig. 4. The upper plot shows the singlet quark distribution $x D_{\bar{q}}(x, Q_i)$ evolved from $Q_0 = 1$ GeV (black) to $Q_i = 10$ (red), 100 (green) and 1000 (blue) GeV, obtained in the NLO approximation from Evo1FMC (solid lines) and QCDnum16 (dashed lines), while the lower plot shows their ratio.

6. Summary and outlook

In this paper we have presented in detail two Markovian MC algorithms for solving the DGLAP equations up to the NLO accuracy. The one of them is based directly on the evolution of the PDFs and the other one instead of pure PDFs uses the parton-momentum distributions. The latter algorithm is more efficient due to the momentum-conservation sum rules. The evolution is done in parton flavour space, in the current version for gluons and three light quarks but it can be easily extended to include more flavours. Both the above algorithms have been implemented in the MC generator Evo1FMC (written in C++). This program has been cross-checked against two independent non-MC programs: QCDnum16 and APCh33. The numerical tests show that with today computer CPU power the Markovian MC is able to solve efficiently and precisely (to the per-mil level) the QCD evolution equation up to the NLO. Therefore, it can be used to cross-check other, non-MC methods or even as an alternative to them. As was pointed out in Introduction, the MC method is not competitive with other techniques in terms of the CPU time but it has certain advantages that may be important in some cases – it is usually less biased and more stable numerically as well as more flexible for possible extensions.

So far we have included only light (massless) quarks in our MC algorithm, however, extending it to heavy quarks does not pose any problem. It can be realized either by simple rejection of extra massless quarks below mass thresholds or by some importance sampling that accounts for these thresholds. Also extension to the NNLO seems straightforward — one only needs to implement the NNLO evolution kernels [15,16]. A more serious problem concerns the divergences of the NLO kernels at $z \rightarrow 1$ which for some transitions lead to negative weights. This indicates that some resummation in this region might be necessary.

As was mentioned in Introduction, we do not consider the Markovian MC algorithm described in this paper to be only a tool for solving numerically the evolution equations for parton densities. It can be also used as the basis for constructing the FSR parton shower MC event generator which would generate physical events in terms of particle flavours and four-momenta. This algorithm cannot be directly used for the ISR evolution (parton shower), since in that case one needs to impose some energy-momentum constraints on the partons entering the hard process. However, it can be used as a starting point for developing any kind of constraint MC algorithms as well as it can play a role of a testing tool for corresponding MC programs, see Refs. [7–10].

Yet another way of development of the above Markovian MC algorithm can go into the direction of solving the CCFM equations [17]. In this case one deals with the so-called unintegrated parton distribution functions, which in addition to x and Q^2 depend on the partonic transverse momenta k_T . This may be important for better modeling physical events in deep inelastic scattering as well as hadron–hadron collisions, see *e.g.* Ref. [18]. We have already implemented the so-called one-loop approximation of the CCFM equation [19–21] which will be reported in our forthcoming paper [22].

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Appendix A

QCD kernels at NLO

A general parton-parton transition matrix for a gluon and three quark flavours (d, u, s) can be written as

$$\mathbf{P}(\alpha_s, z) = \begin{bmatrix} P_{G \leftarrow G}, & P_{G \leftarrow d}, & P_{G \leftarrow u}, & P_{G \leftarrow s}, & P_{G \leftarrow \bar{d}}, & P_{G \leftarrow \bar{u}}, & P_{G \leftarrow \bar{s}} \\ P_{d \leftarrow G}, & P_{d \leftarrow d}, & P_{d \leftarrow u}, & P_{d \leftarrow s}, & P_{d \leftarrow \bar{d}}, & P_{d \leftarrow \bar{u}}, & P_{d \leftarrow \bar{s}} \\ P_{u \leftarrow G}, & P_{u \leftarrow d}, & P_{u \leftarrow u}, & P_{u \leftarrow s}, & P_{u \leftarrow \bar{d}}, & P_{u \leftarrow \bar{u}}, & P_{u \leftarrow \bar{s}} \\ P_{s \leftarrow G}, & P_{s \leftarrow d}, & P_{s \leftarrow u}, & P_{s \leftarrow s}, & P_{s \leftarrow \bar{d}}, & P_{s \leftarrow \bar{u}}, & P_{s \leftarrow \bar{s}} \\ \hline P_{\bar{d} \leftarrow G}, & P_{\bar{d} \leftarrow d}, & P_{\bar{d} \leftarrow u}, & P_{\bar{d} \leftarrow s}, & P_{\bar{d} \leftarrow \bar{d}}, & P_{\bar{d} \leftarrow \bar{u}}, & P_{\bar{d} \leftarrow \bar{s}} \\ P_{\bar{u} \leftarrow G}, & P_{\bar{u} \leftarrow d}, & P_{\bar{u} \leftarrow u}, & P_{\bar{u} \leftarrow s}, & P_{\bar{u} \leftarrow \bar{d}}, & P_{\bar{u} \leftarrow \bar{u}}, & P_{\bar{u} \leftarrow \bar{s}} \\ P_{\bar{s} \leftarrow G}, & P_{\bar{s} \leftarrow d}, & P_{\bar{s} \leftarrow u}, & P_{\bar{s} \leftarrow s}, & P_{\bar{s} \leftarrow \bar{d}}, & P_{\bar{s} \leftarrow \bar{u}}, & P_{\bar{s} \leftarrow \bar{s}} \end{bmatrix}, \quad (\text{A.1})$$

where $P_{J \leftarrow I} \equiv P_{J \leftarrow I}(\alpha_s, z)$. At the NLO, the kernels can be decomposed as follows

$$\mathbf{P}(\alpha_s, z) = \frac{\alpha_s(t)}{2\pi} \mathbf{P}^{(0)}(z) + \left(\frac{\alpha_s(t)}{2\pi} \right)^2 \mathbf{P}^{(1)}(z), \quad (\text{A.2})$$

where the NLO QCD coupling in the \overline{MS} -scheme is

$$\begin{aligned} \alpha_s(t) &= \alpha_s^{(0)}(t) \left\{ 1 - \alpha_s^{(0)}(t) \frac{b_1}{b_0} \ln(2[t - \ln A_{\overline{MS}}]) \right\}, \\ b_0 &= \frac{\beta_0}{4\pi}, \quad b_1 = \frac{\beta_1}{(4\pi)^2}, \\ \beta_0 &= 11 - \frac{2}{3} n_f, \quad \beta_1 = 102 - \frac{38}{3} n_f, \end{aligned} \quad (\text{A.3})$$

and $t = \ln Q$ (n_f is the number of active flavours).

The LO kernel matrix takes a simple form

$$\mathbf{P}^{(0)}(z) = \begin{bmatrix} P_{GG}^{(0)}, & P_{GF}^{(0)}, & P_{GF}^{(0)}, & P_{GF}^{(0)}, & P_{GF}^{(0)}, & P_{GF}^{(0)}, & P_{GF}^{(0)} \\ P_{FG}^{(0)}, & P_{FF}^{(0)}, & 0, & 0, & 0, & 0, & 0 \\ P_{FG}^{(0)}, & 0, & P_{FF}^{(0)}, & 0, & 0, & 0, & 0 \\ P_{FG}^{(0)}, & 0, & 0, & P_{FF}^{(0)}, & 0, & 0, & 0 \\ \hline P_{FG}^{(0)}, & 0, & 0, & 0, & P_{FF}^{(0)}, & 0, & 0 \\ P_{FG}^{(0)}, & 0, & 0, & 0, & 0, & P_{FF}^{(0)}, & 0 \\ P_{FG}^{(0)}, & 0, & 0, & 0, & 0, & 0, & P_{FF}^{(0)} \end{bmatrix}, \quad (\text{A.4})$$

where

$$\begin{aligned}
P_{GG}^{(0)}(z) &= 2C_A \left[\frac{1}{(1-z)_+} - 2 + z(1-z) + \frac{1}{z} \right] + \frac{11C_A - 4T_f}{6} \delta(1-z), \\
P_{FG}^{(0)}(z) &= T_R [z^2 + (1-z)^2], \\
P_{GF}^{(0)}(z) &= C_F \frac{1 + (1-z)^2}{z}, \\
P_{FF}^{(0)}(z) &= C_F \left[\frac{1+z^2}{(1-z)_+} + \frac{3}{2} \delta(1-z) \right],
\end{aligned} \tag{A.5}$$

and the colour-group factors are: $C_A = N_c = 3$, $C_F = (N_c^2 - 1)/2N_c = 4/3$, $T_R = 1/2$.

The NLO contribution to the kernel matrix can be expressed in the following form

$$\mathbf{P}^{(1)}(z) = \begin{bmatrix} P_{GG}^{(1)} & P_{GF}^{(1)} & P_{GF}^{(1)} & P_{GF}^{(1)} & P_{GF}^{(1)} & P_{GF}^{(1)} & P_{GF}^{(1)} \\ P_{FG}^{(1)} & P_{qq}^{V+S(1)} & P_{qq}^S(1) & P_{qq}^S(1) & P_{q\bar{q}}^{V+S(1)} & P_{q\bar{q}}^S(1) & P_{q\bar{q}}^S(1) \\ P_{FG}^{(1)} & P_{qq}^S(1) & P_{qq}^{V+S(1)} & P_{qq}^S(1) & P_{q\bar{q}}^S(1) & P_{q\bar{q}}^{V+S(1)} & P_{q\bar{q}}^S(1) \\ P_{FG}^{(1)} & P_{qq}^S(1) & P_{qq}^S(1) & P_{qq}^{V+S(1)} & P_{q\bar{q}}^S(1) & P_{q\bar{q}}^S(1) & P_{q\bar{q}}^{V+S(1)} \\ P_{FG}^{(1)} & P_{q\bar{q}}^{V+S(1)} & P_{q\bar{q}}^S(1) & P_{q\bar{q}}^S(1) & P_{qq}^{V+S(1)} & P_{qq}^S(1) & P_{qq}^S(1) \\ P_{FG}^{(1)} & P_{q\bar{q}}^S(1) & P_{q\bar{q}}^{V+S(1)} & P_{q\bar{q}}^S(1) & P_{qq}^S(1) & P_{qq}^{V+S(1)} & P_{qq}^S(1) \\ P_{FG}^{(1)} & P_{q\bar{q}}^S(1) & P_{q\bar{q}}^S(1) & P_{q\bar{q}}^{V+S(1)} & P_{qq}^S(1) & P_{qq}^S(1) & P_{qq}^{V+S(1)} \end{bmatrix}, \tag{A.6}$$

where $P_{IJ}^{(1)} \equiv P_{IJ}^{(1)}(z)$ and we have used a short-hand notation $P_{IJ}^{V+S(1)} \equiv P_{IJ}^{V(1)} + P_{IJ}^{S(1)}$. The above matrix can be simplified by exploiting the identity (8)

$$P_{qq}^S(1) = P_{q\bar{q}}^S(1), \tag{A.7}$$

which is true up to the NLO. However, we prefer to keep a more general form of the kernel matrix which can be useful for some tests and possible future extensions. The above kernel matrices can be easily extended to include more quark flavours.

The non-singlet and singlet-quark kernels can be expressed in terms of the basic NLO splitting functions P_+ , P_- and P_{FF} , defined in Refs. [13,14], as follows:

$$\begin{aligned}
P_{qq}^V(1) &= \frac{1}{2} [P_+^{(1)} + P_-^{(1)}], \\
P_{q\bar{q}}^V(1) &= \frac{1}{2} [P_+^{(1)} - P_-^{(1)}], \\
P_{qq}^S(1) &= \frac{1}{2n_f} [P_{FF}^{(1)} - P_+^{(1)}].
\end{aligned} \tag{A.8}$$

Finally, all the elements of the above kernel matrix can be calculated (*e.g.* numerically) from the six basic NLO splitting functions of Refs. [13,14]

$$[P_+^{(1)}, P_-^{(1)}, P_{FF}^{(1)}, P_{FG}^{(1)}, P_{GF}^{(1)}, P_{GG}^{(1)}]. \tag{A.9}$$

These basic splitting functions are given at the NLO by the following expressions:

$$P_{\pm}^{(1)}(z, \varepsilon) = \frac{A_{\pm}^{(1)}(z)}{1-z} \Theta(1-z-\varepsilon) + B_{\pm}^{(1)}(z) + [C_S^{(1)} + A_S^{(1)} \ln \varepsilon] \delta(1-z), \tag{A.10}$$

$$P_{FF}^{(1)}(z, \varepsilon) = \frac{A_S^{(1)}}{1-z} \Theta(1-z-\varepsilon) + B_S^{(1)}(z) + [C_S^{(1)} + A_S^{(1)} \ln \varepsilon] \delta(1-z), \tag{A.11}$$

$$P_{GG}^{(1)}(z, \varepsilon) = \frac{A_G^{(1)}}{1-z} \Theta(1-z-\varepsilon) + B_G^{(1)}(z) + [C_G^{(1)} + A_G^{(1)} \ln \varepsilon] \delta(1-z), \tag{A.12}$$

$$\begin{aligned}
P_{FG}^{(1)}(z) &= \frac{1}{2} C_F T_R \left\{ 4 - 9z + (4z - 1) \ln z + (2z - 1) \ln^2 z + 4 \ln(1 - z) \right. \\
&\quad \left. + \left[10 - \frac{2}{3} \pi^2 + 2 \ln^2 \left(\frac{1-z}{z} \right) - 4 \ln \left(\frac{1-z}{z} \right) \right] [z^2 + (1-z)^2] \right\} \\
&\quad + \frac{1}{2} C_A T_R \left\{ \frac{182}{9} + \frac{14}{9} z + \frac{40}{9z} + \left(\frac{136}{3} z - \frac{38}{3} \right) \ln z - 4 \ln(1 - z) \right. \\
&\quad - (2 + 8z) \ln^2 z + 2 [z^2 + (1+z)^2] S_2(z) + \left[\frac{\pi^2}{3} - \frac{218}{9} + \frac{44}{3} \ln z \right. \\
&\quad \left. \left. - \ln^2 z + 4 \ln(1 - z) - 2 \ln^2(1 - z) \right] [z^2 + (1 - z)^2] \right\},
\end{aligned} \tag{A.13}$$

$$\begin{aligned}
P_{GF}^{(1)}(z) = & C_F^2 \left\{ -\frac{5}{2} - \frac{7}{2}z - 2z \ln(1-z) - \frac{1+(1-z)^2}{z} \ln(1-z) [3 + \ln(1-z)] \right. \\
& + \left(2 + \frac{7}{2}z \right) \ln z - \left(1 - \frac{1}{2}z \right) \ln^2 z \left. \right\} \\
& + C_F C_A \left\{ \frac{28}{9} + \frac{65}{18}z + \frac{44}{9}z^2 - \left(12 + 5z + \frac{8}{3}z^2 \right) \ln z + (4+z) \ln^2 z \right. \\
& + 2z \ln(1-z) + \frac{1+(1-z)^2}{z} \left[\frac{1}{2} - \frac{\pi^2}{6} + \frac{11}{3} \ln(1-z) \right. \\
& + \left. \left. \ln^2(1-z) - 2 \ln z \ln(1-z) + \frac{1}{2} \ln^2 z \right] - \frac{1+(1+z)^2}{z} S_2(z) \left. \right\} \\
& - C_F T_f \left\{ \frac{4}{3}z + \frac{1+(1-z)^2}{z} \left[\frac{20}{9} + \frac{4}{3} \ln(1-z) \right] \right\}, \tag{A.14}
\end{aligned}$$

where

$$\begin{aligned}
C_S^{(1)} &= C_F^2 \left(\frac{3}{8} - \frac{\pi^2}{2} + 6\zeta_3 \right) + \frac{1}{2} C_F C_A \left(\frac{17}{12} + \frac{11\pi^2}{9} - 6\zeta_3 \right) - C_F T_f \left(\frac{1}{6} + \frac{2\pi^2}{9} \right), \\
A_S^{(1)} &= C_F \left\{ C_A \left(\frac{67}{9} - \frac{\pi^2}{3} \right) - \frac{20}{9} T_f \right\}, \\
C_G^{(1)} &= C_A^2 \left(\frac{8}{3} + 3\zeta_3 \right) - \left(\frac{4}{3} C_A + C_F \right) T_f, \\
A_G^{(1)} &= C_A \left\{ C_A \left(\frac{67}{9} - \frac{\pi^2}{3} \right) - \frac{20}{9} T_f \right\}, \tag{A.15}
\end{aligned}$$

with $\zeta_3 \equiv \zeta(3) \approx 1.2020569$.

The non-singlet coefficients take the form

$$\begin{aligned}
A_{\pm}^{(1)}(z) = & C_F^2 [-2(1+z^2) \ln z \ln(1-z) - 3 \ln z] \\
& + \frac{1}{2} C_F C_A \left[\ln^2 z + \frac{11}{3} \ln z + \frac{67}{9} - \frac{\pi^2}{3} \right] (1+z^2) \\
& - C_F T_f \frac{2}{3} \left[\ln z + \frac{5}{3} \right] (1+z^2), \tag{A.16}
\end{aligned}$$

$$\begin{aligned}
 B_{\pm}^{(1)}(z) = & C_F^2 \left[-2z \ln z - \frac{1}{2}(1+z) \ln^2 z - 5(1-z) \pm P_A(z) \right] \\
 & + \frac{1}{2} C_F C_A \left[2(1+z) \ln z + \frac{40}{3}(1-z) \mp P_A(z) \right] - C_F T_f \frac{4}{3}(1-z),
 \end{aligned} \tag{A.17}$$

where

$$P_A(z) = 2 \frac{1+z^2}{1+z} S_2(z) + 2(1+z) \ln z + 4(1-z). \tag{A.18}$$

Notice that, as it should be, $A_{\pm}^{(1)}(1) = A_S^{(1)}$. The function S_2 is defined in the interval $(0, 1]$

$$S_2(z) = \int_{z/(1+z)}^{1/(1+z)} \frac{dy}{y} \ln \frac{1-y}{y} = -2 \text{Li}_2(-z) + \frac{1}{2} \ln^2 z - 2 \ln z \ln(1+z) - \frac{\pi^2}{6}, \tag{A.19}$$

where the dilogarithm function Li_2 is given by

$$\text{Li}_2(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^2} = \int_z^0 \frac{dt}{t} \ln(1-t), \tag{A.20}$$

with a branch point discontinuity on a complex plane along $[1, +\infty]$.

For the singlet and gluon coefficients we have

$$\begin{aligned}
 B_S^{(1)}(z) = & C_F^2 \left\{ -1+z + \frac{1}{2} [1-3z - (1+z) \ln z] \ln z \right. \\
 & \left. - 2 \left(\frac{1+z^2}{1-z} \right) \left[\frac{3}{4} + \ln(1-z) \right] \ln z + 2 \frac{1+z^2}{1+z} S_2(z) \right\} \\
 & + C_F C_A \left\{ - \left(\frac{67}{18} - \frac{\pi^2}{6} \right) (1+z) + \frac{14}{3} (1-z) \right. \\
 & \left. + \frac{1}{2} \left(\frac{1+z^2}{1-z} \right) \left(\frac{11}{3} + \ln z \right) \ln z - \frac{1+z^2}{1+z} S_2(z) \right\} \\
 & + C_F T_f \left\{ - \frac{16}{3} + \frac{10}{9} (1+z) + \frac{40}{9z} + \frac{40z}{3} - \frac{112z^2}{9} \right. \\
 & \left. - \frac{2}{3} \left(\frac{1+z^2}{1-z} \right) \ln z + \left(2+10z + \frac{16}{3} z^2 \right) \ln z - 2(1+z) \ln^2 z \right\},
 \end{aligned} \tag{A.21}$$

$$\begin{aligned}
B_G^{(1)}(z) = & C_A^2 \left\{ \frac{27}{2}(1-z) + \frac{67}{9}(z^2 - z^{-1}) - \frac{1}{3}(25 - 11z + 44z^2) \ln z \right. \\
& + 4(1+z) \ln^2 z + [\ln^2 z - 4 \ln z \ln(1-z)] \frac{1}{1-z} \\
& + \left[\ln^2 z - 4 \ln z \ln(1-z) + \frac{67}{9} - \frac{\pi^2}{3} \right] \left[\frac{1}{z} - 2 + z(1-z) \right] \\
& \left. + 2 \left(\frac{1}{1+z} - \frac{1}{z} - 2 - z - z^2 \right) S_2(z) \right\} \\
& + C_A T_f \left\{ 2(1-z) + \frac{26}{9}(z^2 - z^{-1}) - \frac{4}{3}(1+z) \ln z - \frac{20}{9} \left[\frac{1}{z} - 2 + z(1-z) \right] \right\} \\
& + C_F T_f \left\{ 8(z-2) + \frac{20}{3}z^2 + \frac{4}{3z} - (6+10z) \ln z - 2(1+z) \ln^2 z \right\}. \quad (\text{A.22})
\end{aligned}$$

It is easy to check that the above functions have no singularity at $z = 1$.

It is worth noticing that the non-singlet quark kernels have particularly simple analytical representations

$$\begin{aligned}
P_{qq}^{V(1)}(z, \varepsilon) = & \left[C_S^{(1)} + A_S^{(1)} \ln \varepsilon \right] \delta(1-z) + \frac{A_+^{(1)}(z)}{1-z} \Theta(1-z-\varepsilon) \\
& + C_F^2 \left[-2z \ln z - \frac{1}{2}(1+z) \ln^2 z - 5(1-z) \right] \\
& + \frac{1}{2} C_F C_A \left[2(1+z) \ln z + \frac{40}{3}(1-z) \right] - C_F T_f \frac{4}{3}(1-z), \\
P_{q\bar{q}}^{V(1)}(z) = & C_F \left(C_F - \frac{1}{2} C_A \right) P_A(z). \quad (\text{A.23})
\end{aligned}$$

Using these analytical formulae in numerical evaluations of the kernels $P_{qq}^{V(1)}$ and $P_{q\bar{q}}^{V(1)}$ can be faster and more stable numerically than computing them indirectly from the splitting functions $P_{\pm}^{(1)}$.

In the Monte Carlo implementation, the above kernel matrices are used for generation of real-parton radiation, *i.e.* for $z < 1 - \varepsilon$. This has to be compensated by the appropriate Sudakov form factor summing up virtual and soft-parton corrections, *i.e.* terms proportional to $\delta(1-z)$. At the NLO, the Sudakov exponent Φ_K takes the form

$$\Phi_K(t_2, t_1) = 2 \int_{t_1}^{t_2} dt \left\{ \frac{\alpha_s(t)}{2\pi} P_{KK}^{\delta(0)}(z) + \left(\frac{\alpha_s(t)}{2\pi} \right)^2 P_{KK}^{\delta(1)}(z) \right\}, \quad (\text{A.24})$$

where the NLO $\alpha_s(t)$ has to be taken for both terms. The factor of 2 in front of the integral is due to the fact that our evolution “time” is $t = \ln Q$. Integrating over $\tau = \ln(t - \ln A)$, we obtain for gluons

$$\begin{aligned} \Phi_G(\tau_2, \tau_1) = & \frac{2}{\beta_0} \left\{ [\chi_0(\tau_2) - \chi_0(\tau_1)] \left[2C_A \ln \frac{1}{\varepsilon} - \frac{11}{6}C_A + \frac{2}{3}T_f \right] \right. \\ & \left. + [\chi_1(\tau_2) - \chi_1(\tau_1)] \left[A_G^{(1)} \ln \frac{1}{\varepsilon} - C_G^{(1)} \right] \right\} \end{aligned} \quad (\text{A.25})$$

and for fermions (both quarks and anti-quarks)

$$\begin{aligned} \Phi_F(\tau_2, \tau_1) = & \frac{2}{\beta_0} \left\{ [\chi_0(\tau_2) - \chi_0(\tau_1)] \left[2C_F \ln \frac{1}{\varepsilon} - \frac{3}{2}C_F \right] \right. \\ & \left. + [\chi_1(\tau_2) - \chi_1(\tau_1)] \left[A_S^{(1)} \ln \frac{1}{\varepsilon} - C_S^{(1)} \right] \right\}, \end{aligned} \quad (\text{A.26})$$

where

$$\chi_0(\tau) = \tau + \frac{\beta_1}{2\beta_0^2}(\tau + \ln 2 + 1)e^{-\tau}, \quad (\text{A.27})$$

and

$$\begin{aligned} \chi_1(\tau) = & -\frac{1}{\beta_0} \left\{ \frac{\beta_1}{2\beta_0^2} \left(\frac{\beta_1}{6\beta_0^2} \left[\tau^2 + 2 \left(\ln 2 + \frac{1}{3} \right) \left(\tau + \frac{1}{3} \right) + \ln^2 2 \right] e^{-\tau} \right. \right. \\ & \left. \left. - \tau - \ln 2 - \frac{1}{2} \right) e^{-\tau} + 1 \right\} e^{-\tau}. \end{aligned} \quad (\text{A.28})$$

Appendix B

Gluon and quark singlet kernels at LO

As already advocated, we isolate all singular parts from the kernels (*cf.* Eq. (71))

$$P_{IK}(t, z) = \frac{1}{(1-z)_+} \delta_{IK} A_{KK}(t) + \delta(1-z) \delta_{IK} B_{KK}(t) + \frac{1}{z} C_{IK}(t) + D_{IK}(t, z). \quad (\text{B.1})$$

After expanding to LO (see Eq. (72)) the resulting components $A^{(0)}, B^{(0)}, C^{(0)}, D^{(0)}$ are listed in Table I.

Let us consider evolution of the simple two-component state consisting of the gluon and the (singlet) quark with the LO evolution kernel

$$\mathbf{P}^{(0)}(z) = \begin{bmatrix} P_{GG}^{(0)}(z), & P_{Gq}^{(0)}(z) \\ P_{qG}^{(0)}(z), & P_{qq}^{(0)}(z) \end{bmatrix}, \quad (\text{B.2})$$

TABLE I

The elements of the singlet LO kernels ($T_f = n_f T_R$).

IK	$A_{KK}^{(0)}$	$B_{KK}^{(0)}$	$C_{IK}^{(0)}$	$D_{IK}^{(0)}(z)$	$\hat{D}_{IK}(z)$	$\int dz D_{IK}^{(0)}(z)$
GG	$2C_A$	$\frac{11}{6}C_A - \frac{2}{3}T_f$	$2C_A$	$2C_A(-2+z-z^2)$	0	$-\frac{11}{3}C_A$
qG	—	—	0	$2T_f(z^2 + (1-z)^2)$	$2T_f$	$\frac{4}{3}T_f$
qq	$2C_F$	$\frac{3}{2}C_F$	0	$C_F(-1-z)$	0	$-\frac{3}{2}C_F$
Gq	—	—	$2C_F$	$C_F(-2+z)$	0	$-\frac{3}{2}C_F$

where

$$\begin{aligned}
P_{qG}^{(0)}(z) &= n_f P_{FG}^{(0)}(z), \\
P_{qq}^{(0)}(z) &= P_{FF}^{(0)}, \\
P_{Gq}^{(0)}(z) &= P_{GF}^{(0)},
\end{aligned}
\tag{B.3}$$

and $P_{GG}^{(0)}$, $P_{FG}^{(0)}$, $P_{FF}^{(0)}$, $P_{GF}^{(0)}$ are given explicitly in Appendix A.

Let us concentrate now on the second (less standard) Markovian algorithm described in Sec. 3.4. The definition of the simplified kernel matrix elements, Eq. (77)

$$\hat{\mathcal{P}}_{IK}^{\mathcal{O}}(t_0, z) = \Theta(z - \varepsilon') \Theta(1 - z - \hat{\varepsilon}) \frac{\alpha_s(t_0)}{\pi} \left\{ \frac{1}{1-z} \delta_{IK} A_{KK}^{(0)} + \frac{1}{z} C_{IK}^{(0)} + \hat{D}_{IK} \right\}
\tag{B.4}$$

needs \hat{D}_{IK} , which are also provided in Table I.In this simple case we may explicitly list the parton $K \rightarrow I$ transition rates

$$\hat{\pi}_{IK} = \frac{\alpha_s(t_0)}{\pi} \left[\delta_{IK} A_{KK}^{(0)} \ln \frac{1}{\hat{\varepsilon}} + C_{IK}^{(0)} \ln \frac{1}{\varepsilon'} + \hat{D}_{IK} \right]
\tag{B.5}$$

as follows

$$\begin{bmatrix} \hat{\pi}_{GG}, & \hat{\pi}_{Gq} \\ \hat{\pi}_{qG}, & \hat{\pi}_{qq} \end{bmatrix} = \frac{\alpha_s(t_0)}{\pi} \begin{bmatrix} 2C_A \left(\ln \frac{1}{\hat{\varepsilon}} + \ln \frac{1}{\varepsilon'} \right), & 2C_F \ln \frac{1}{\varepsilon'} \\ 2T_f, & 2C_F \ln \frac{1}{\hat{\varepsilon}} \end{bmatrix},
\tag{B.6}$$

and also the characteristic decay rates $R_K = \sum_X \hat{\pi}_{XK}$, $K = g, q$ (in a primary MC)

$$\begin{aligned}
R_G &= \frac{\alpha_s(t_0)}{\pi} \left\{ 2C_A \left(\ln \frac{1}{\hat{\varepsilon}} + \ln \frac{1}{\varepsilon'} \right) + 2T_f \right\}, \\
R_q &= \frac{\alpha_s(t_0)}{\pi} \left\{ 2C_F \ln \frac{1}{\varepsilon'} + 2C_F \ln \frac{1}{\hat{\varepsilon}} \right\}.
\end{aligned}
\tag{B.7}$$

Appendix C

LO kernels for parton-momentum distributions

We may decompose the evolution kernels for parton-momentum distributions in the LO and NLO as follows, see Eq. (109)

$$zP_{IK}(t, z) = \frac{1}{(1-z)_+} \delta_{IK} A_{KK}(t) + \delta(1-z) \delta_{IK} B_{KK}(t) + F_{IK}(t, z), \quad (\text{C.1})$$

where q represents one quark flavour and the corresponding LO components are listed in Table II. Comparing to the previous appendix, we have

$$F_{IK}(t, z) = zD_{IK}(t, z) + C_{IK}(t) - \delta_{IK} A_{KK}(t). \quad (\text{C.2})$$

In the MC we use the simplified kernels (Eq. (111))

$$\bar{\mathcal{P}}_{IK}^{\Theta}(\tau_0, z) = \theta(1-z-\bar{\varepsilon}) \frac{\alpha_s^{(0)}(t_0)}{\pi} \left\{ \frac{1}{1-z} \delta_{IK} A_{KK}^{(0)} + F_{IK}^{(0)}(z) \right\}. \quad (\text{C.3})$$

In this simple case we may explicitly list the parton transition $K \rightarrow I$ rates (Eq. (115))

$$\bar{\pi}_{IK}(\tau_0) = \int_0^1 dz \bar{\mathcal{P}}_{IK}^{\Theta}(\tau_0, z) = \frac{\alpha_s^{(0)}(t_0)}{\pi} \left[\delta_{IK} A_{KK}^{(0)} \ln \frac{1}{\bar{\varepsilon}} + f_{IK}^{(0)} \right], \quad (\text{C.4})$$

TABLE II

The elements of the LO kernels for parton-momentum distributions ($T_f = n_f T_R$).

IK	$A_{KK}^{(0)}$	$B_{KK}^{(0)}$	$F_{IK}^{(0)}(z)$	$\max F_{IK}^{(0)}(z)$	$\int F_{IK}^{(0)}(z) dz$
$G \leftarrow G$	$2C_A$	$\frac{11}{6}C_A - \frac{2}{3}T_f$	$2C_A z(-2+z-z^2)$	0	$-\frac{11}{6}C_A$
$q \leftarrow G$	0	0	$T_R z(z^2 + (1-z)^2)$	T_R	$\frac{1}{3}T_R$
$\bar{q} \leftarrow G$	0	0	$T_R z(z^2 + (1-z)^2)$	T_R	$\frac{1}{3}T_R$
$G \leftarrow q$	0	0	$C_F(2-2z+z^2)$	$2C_F$	$\frac{4}{3}C_F$
$q \leftarrow q$	$2C_F$	$\frac{3}{2}C_F$	$C_F(-2-z-z^2)$	0	$-\frac{17}{6}C_F$
$\bar{q} \leftarrow q$	0	0	0	0	0
$G \leftarrow \bar{q}$	0	0	$C_F(2-2z+z^2)$	$2C_F$	$\frac{4}{3}C_F$
$q \leftarrow \bar{q}$	0	0	0	0	0
$\bar{q} \leftarrow \bar{q}$	$2C_F$	$\frac{3}{2}C_F$	$C_F(-2-z-z^2)$	0	$-\frac{17}{6}C_F$

where

$$f_{IK}^{(0)} \equiv \int_0^1 dz F_{IK}^{(0)}(z) \quad (\text{C.5})$$

are listed in the Table II.

The momentum-conservation sum rule reads

$$\sum_X \int_0^1 dz z P_{XK}(t, z) = B_{KK}(t) + \sum_X \int_0^1 dz F_{XK}(t, z) = 0, \quad (\text{C.6})$$

which is manifest in Table II for the LO case but it also holds for the \overline{MS} NLO kernels. Note that the above sum rule determines unambiguously the virtual part of the kernels

$$B_{KK} = - \sum_X f_{XK} = - \sum_X \int_0^1 dz F_{XK}(z), \quad (\text{C.7})$$

both in the case of the LO and the NLO.

Appendix D

Generic discrete Markovian process

Diffusion and evolution equations

Let us consider a general “evolution equation” for the multistate *discrete* system

$$\partial_t N_I(t) = \sum_L P_{IL}(t) N_L(t). \quad (\text{D.1})$$

Let us ask whether the time dependence of the above system can *always* be interpreted (implemented) as a probabilistic stochastic Markovian process, *i.e.* in terms of MC events with weight equal to 1. We shall see that this is not true in the general case and we shall show under which restriction on the transition matrix P_{IL} the above conjecture on Markovianization is true. Weighted MC events are excluded from the consideration, *i.e.* by the Markovian process we understand the probabilistic process with weight=1 events. Without any loss of generality, in our starting Eq. (D.1) we have chosen a discrete system in order to simplify the reasoning.

An answer is found by examining a general “diffusion” process in the discrete space. We shall derive the evolution equation (D.1) finding restriction on the transition matrix P_{IL} . Following this path of reasoning we first define a general transition probability of an object which is exactly in the state I

at the initial time t_0 . The explicit *transition probability* $(t_0, I) \rightarrow (t_1, K)$ at the later time $t_1 > t_0$ into another state $K \neq I$ is defined as follows

$$dp(K, t_1 | I, t_0) \Big|_{K \neq I} = \theta(t_1 - t_0) P_{KI}(t_1) dt_1 e^{-\int_{t_0}^{t_1} dt' \sum_{J \neq I} P_{JI}(t')}. \quad (\text{D.2})$$

It is properly normalized by the construction, *i.e.* it must fulfill

$$\int_{t_1 > t_0} \sum_{K \neq I} dp(k, t_1 | I, t_0) \equiv 1, \quad (\text{D.3})$$

for an *arbitrary* starting point (t_0, I) . The probability that the transition to any other state occurs *before* some time t is obtained as

$$\int_{t_0 < t_1 < t} \sum_{K \neq I} dp(K, t_1 | I, t_0) = 1 - e^{-\Phi_I(t, t_0)}, \quad (\text{D.4})$$

where we have denoted

$$\Phi_I(t, t_0) = \int_{t_0}^t dt' \sum_{J \neq I} P_{JI}(t'). \quad (\text{D.5})$$

The probability that such a transition occurs *after* the time $t_1 = t$ is just equal to

$$\int_{t_1 > t} \sum_{K \neq I} dp(k, t_1 | I, t_0) = e^{-\Phi_I(t, t_0)}. \quad (\text{D.6})$$

All the above is a repetition of the very standard description of the Poissonian “decay mechanism” with the “time-dependent” transition (decay) constants $P_{JI}(t) > 0$; it describes precisely what we basically do understand as a Markovian process⁶.

Let us now imagine a very large ensemble of identical objects, each of them at a given time t in one well defined state k , and evolving statistically *independently* according to the transition probability distribution defined above. Let us introduce the population $N_I(t)$ of the objects which are at a given time t in the state I . Given the above probabilistic transition rule, we may easily calculate the change of the population $\Delta N_I(t)$ from the time t to the time $t + \Delta t$. The *original* population $N_I(t)$ is diminished to $N_I(t)e^{-\Phi_I(t+\Delta t, t)}$. At the same time interval Δt the population of the state I

⁶ In the literature one may find many different definitions of the Markovian process, see *e.g.* [23–25].

is also increased by the influx from all other states $L \neq I$ by $\sum_{L \neq I} P_{IL} N_L \Delta t$. Altogether we get

$$N_I(t + \Delta t) = N_I(t) e^{-\Phi_I(t+\Delta t, t)} + \sum_{L \neq I} P_{IL}(t) N_L(t) \Delta t, \quad (\text{D.7})$$

and

$$\Delta N_I(t) = N_I(t + \Delta t) - N_I(t) = -N_I(t) \sum_{J \neq I} P_{JI}(t) \Delta t + \sum_{I \neq L} P_{IL}(t) N_L(t) \Delta t, \quad (\text{D.8})$$

or equivalently

$$\partial_t N_I(t) = - \left(\sum_{J \neq I} P_{JI}(t) \right) N_I(t) + \sum_{I \neq L} P_{IL}(t) N_L(t). \quad (\text{D.9})$$

We, therefore, conclude that the differential evolution equation (D.1) can only be compatible with the probabilistic Markovian process if the following property of the transition matrix is true

$$P_{II}(t) \equiv - \sum_{J \neq I} P_{JI}(t). \quad (\text{D.10})$$

This is what we shall always assume to be true in the standard Markovian process.

The QCD singlet evolution kernels do not fulfill the above condition. Hence, perfect Markovianization (with weight = 1 events) is not possible in this context and the use of the weighted events is mandatory, at least at the internal level of the parton-shower MC. MC events can always be turned into weight = 1 events with the usual rejection methods, but at some price. The remedy is to use $z P_{IK}(z)$, which fulfill the above condition, instead of $P_{IK}(z)$.

Iterative solution

For completeness let us write down the iterative solution of the evolution equation

$$\partial_t N_I(t) = -R_I N_I(t) + \sum_{K \neq I} P_{IK}(t) N_K(t), \quad R_I \equiv -P_{II}, \quad (\text{D.11})$$

in the discrete space. The above equation can be easily brought to a homogeneous form

$$e^{-\Phi_I(t,t_0)} \partial_t \left(e^{\Phi_I(t,t_0)} N_I(t) \right) = \sum_{K \neq I} P_{IK}(t) N_K(t),$$

$$\Phi_I(t, t_0) \equiv \int_{t_0}^t dt_1 R_I(t_1), \quad (\text{D.12})$$

which then can be turned into an integral equation

$$N_I(t) = e^{-\Phi_I(t,t_0)} N_I(t_0) + \int_{t_0}^t dt_1 e^{-\Phi_I(t,t_1)} \sum_K P'_{IK}(t_1) N_K(t_1),$$

$$P'_{KJ} \equiv \begin{cases} P_{KJ}, & \text{for } K \neq J, \\ 0, & \text{for } K = J, \end{cases} \quad (\text{D.13})$$

and finally can be solved by means of multiple iteration

$$N_K(t) = e^{-\Phi_K(t,t_0)} N_K(t_0) + \sum_{n=1}^{\infty} \sum_{K_0, \dots, K_{n-1}} \prod_{i=1}^n \left[\int_{t_0}^t dt_i \Theta(t_i - t_{i-1}) \right]$$

$$\times e^{-\Phi_K(t,t_n)} \prod_{i=1}^n \left[P'_{K_i K_{i-1}}(t_i) e^{-\Phi_{K_{i-1}}(t_i, t_{i-1})} \right] N_{K_0}(t_0), \quad (\text{D.14})$$

where $K \equiv K_n$, for the brevity of the notation. The above series of integrals with positively defined integrands (assuming $P_{IK} \geq 0$) can be interpreted in terms of a random Markovian process starting at t_0 and continuing until t .

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