EXACT SOLUTIONS OF THE QCD EVOLUTION EQUATIONS USING MONTE CARLO METHOD*

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We present the exact and precise ($\sim 0.1\%$) numerical solution of the QCD evolution equations for the parton distributions in a wide range of Q and x using Monte Carlo (MC) method, which relies on the so-called Markovian algorithm. We point out certain advantages of such a method with respect to the existing non-MC methods. We also formulate a challenge of constructing non-Markovian MC algorithm for the evolution equations for the initial state QCD radiation with tagging the type and x of the exiting parton. This seems to be within the reach of the presently available computer CPUs and the sophistication of the MC techniques.

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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. This process consists of the random steps forward in the logarithm of the energy scale, $t = \ln Q$, and the collinear decay of partons. Such a Markovian process can be readily used as a basis of the Monte Carlo (MC) algorithm producing events in the so called Parton Shower MC (PSMC), see for example Ref. [2]. The Markovian MC provides, in principle, an exact solution of the evolution equations. This possibility was not exploited in practice in the past, mainly because alternative non-MC numerical methods and programs solving the QCD evolution equations on

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the finite grid of points in the space of t and parton energy x are much faster than the MC method. Typical non-MC program of this type is QCDnum16 of Ref. [3]. For comparisons with other codes see Ref. [4].

In this work we test practical feasibility of applying the MC Markovian method to solve the QCD evolution equations exactly and precisely (per-mill level), exploiting computer CPU power available today, in a wide range of $\ln Q$ and x.

Apart from pure exploratory aspect, we believe that MC method has certain advantages over non-MC methods, see discussion below.

It is also commonly known that the basic Markovian algorithm cannot be used in the PSMC to model the initial state radiation (ISR), because of its extremely poor efficiency. In the latter part of this work we formulate a *challenge* of constructing non-Markovian type of MC algorithm for ISR PSMC, in which the exact evolution of the parton distributions is a builtin feature, like in the Markovian MC case¹. We claim that with present CPU power and sophistication of the MC techniques such a scenario may be feasible. With the advent of the future high quality and high statistics experimental data coming from LHC and HERA, such a solution is worth to consider.

The layout of the paper is the following: In Section 2 we summarize basic concepts on the Markovian process and its application to solution of the QCD evolution equations. In Section 3 we present exact high precision Markovian MC solution of the QCD evolution equations. Section 4 discusses the results and perspectives.

2. The formalism

Let us briefly review basic definitions and concepts concerning the *evolu*tion equations and the Markovian process. The generic evolution equations read

$$\partial_t D_I(t) = \sum_K \mathcal{P}_{IK}(t) D_K(t), \tag{1}$$

where $t = \ln Q$ and I and K are discrete indexes numbering states of a certain physical system. The extension to continuous sets of states is straightforward, see below. The necessary and sufficient condition for this equation to have its representation as a probabilistic Markovian process in the evolution time t, with a properly normalized probability of a forward step, is the following:

$$\mathcal{P}_{II}(t) = -\sum_{K \neq I} \mathcal{P}_{KI}(t) \equiv -R_I(t), \qquad \mathcal{P}_{IK}(t) \ge 0, \text{ for } I \neq K, \quad (2)$$

¹ This is contrary to most of the existing MC PSMCs, in which evolved parton distributions come from a table obtained using an independent non-MC program.

where $R_I(t) \ge 0$ is the *decay rate* of the *I*-th parton. The evolution equation

$$\partial_t D_I(t) + R_I(t) D_I(t) = \sum_{K \neq I} \mathcal{P}_{IK}(t) D_K(t)$$
(3)

can be easily brought to a homogeneous form

$$e^{-\Phi_I(t,t_0)}\partial_t \left(e^{\Phi_I(t,t_0)}D_I(t) \right) = \sum_{K \neq I} \mathcal{P}_{IK}(t)D_K(t),$$

$$\Phi_I(t,t_0) \equiv \int_{t_0}^t dt_1 R_I(t_1)$$
(4)

which can be turned into an integral equation

$$D_{I}(t) = e^{-\Phi_{I}(t,t_{0})} D_{I}(t_{0}) + \int_{t_{0}}^{t} dt_{1} e^{-\Phi_{I}(t,t_{1})} \sum_{K} \mathcal{P}'_{IK}(t_{1}) D_{K}(t_{1}),$$

$$\mathcal{P}'_{KJ} \equiv \begin{cases} \mathcal{P}_{KJ}, & \text{for } K \neq J, \\ 0, & \text{for } K = J, \end{cases}$$
(5)

and finally can be solved by means of multiple iteration:

$$D_{K}(t) = e^{-\Phi_{K}(t,t_{0})} D_{K}(t_{0}) + \sum_{n=1}^{\infty} \sum_{K_{0}...K_{n-1}} \prod_{i=1}^{n} \left[\int_{t_{0}}^{t} dt_{i} \ \Theta(t_{i} - t_{i-1}) \right] \\ \times e^{-\Phi_{K}(t,t_{n})} \prod_{i=1}^{n} \left[\mathcal{P}'_{K_{i}K_{i-1}}(t_{i}) e^{-\Phi_{K_{i-1}}(t_{i},t_{i-1})} \right] D_{K_{0}}(t_{0}), \qquad (6)$$

where $K \equiv K_n$ is understood, for the brevity of the notation. The above series of integrals with positively defined integrands can be interpreted in terms of a random Markovian process starting at t_0 and continuing until twith the following, properly normalized, transition probability of a single Markovian random step forward, $(t_{i-1}, K_{i-1}) \rightarrow (t_i, K_i), t_i > t_{i-1}, K_i \neq K_{i-1}$:

$$\omega(t_i, K_i | t_{i-1}, K_{i-1}) \equiv \Theta(t_i - t_{i-1}) \mathcal{P}'_{K_i K_{i-1}}(t_i) e^{-\Phi_{K_{i-1}}(t_i, t_{i-1})},$$

$$\int_{t_{i-1}}^{\infty} dt_i \sum_{K_i} \omega(t_i, K_i | t_{i-1}, K_{i-1}) = 1.$$
(7)

Each term in the sum in Eq. (6) can be expressed as a product of the single step probabilities of Eq. (7) as follows:

$$D_{K}(t) = e^{-\Phi_{K}(t,t_{0})} D_{K}(t_{0}) + \sum_{n=1}^{\infty} \sum_{K_{0}...K_{n-1}} \prod_{j=1}^{n} \int_{t_{0}}^{t} dt_{j}$$
$$\times e^{-\Phi_{K}(t,t_{n})} \prod_{i=1}^{n} \omega(t_{i}, K_{i}|t_{i-1}, K_{i-1}) D_{K_{0}}(t_{0}).$$
(8)

The Markovian process does not run forever — it is stopped by the so called *stopping rule*, which in our case is $t_{n+1} > t$. The variable t_{n+1} is added in Eq. (8) by means of inserting an extra integration with the help of an identity

$$e^{-\Phi_{K_n}(t,t_n)} = \int_{t}^{\infty} dt_{n+1} \sum_{K_{n+1}} \omega(t_{n+1}, K_{n+1}|t_n, K_n) \,. \tag{9}$$

The resulting solution

$$D_{K}(t) = \int_{t_{1}>t} dt_{1} \sum_{K_{1}} \omega(t_{1}, K_{1}|t_{0}, K_{0}) D_{K}(t_{0}) + \sum_{n=1}^{\infty} \sum_{K_{0}...K_{n-1}} \int_{t_{n+1}>t} dt_{n+1} \sum_{K_{n+1}} \omega(t_{n+1}, K_{n+1}|t_{n}, K_{n}) \prod_{j=1}^{n} \int_{t_{j}(10)$$

represents clearly a Markovian process, in which, starting from a point (t_0, K_0) distributed according to $D_{K_0}(t_0)$, we generate step by step the points $(t_i, K_i), i = 1, 2, \ldots, n+1$, using transition probability ω , until the stopping rule $t_{n+1} > t$ acts. In such a case the point (t_{n+1}, K_{n+1}) is trashed and the previous point (t_n, K_n) is kept as the last one. Eq. (10) tells us that the points (t_n, K_n) obtained in the above Markovian process are distributed exactly according to the solution of the original evolution equations² of Eq. (1).

² The above MC solution is exact and unbiased contrary to other non-MC methods which have inherent biases due to choice of finite grid decomposition into polynomials and other technical artifacts present there. The main disadvantage of the MC method is its slowness.

Two technical point have to be clarified before we apply the above solution to the QCD parton distribution evolution equations: one concerns the t dependence of the \mathcal{P} matrix and another one concerns extension of the above formalism to continuous indexes in the \mathcal{P} matrix.

The transition matrix \mathcal{P} , in the case of the QCD parton distributions, includes the running coupling constant $\alpha(t)$

$$\mathcal{P}(t)_{KL} = \alpha(t) \ P_{KL},\tag{11}$$

which depends rather strongly on t at low $t = \ln Q$. In the above we have explicitly assumed that the kernel P_{KL} is independent of t, which is true in the leading-logarithmic (LL) case and is not true in the next-to-leadinglogarithmic (NLL) case. However, even in the NLL case this is a very good approximation, which can be easily corrected in the MC calculation using an extra weight (and event rejection). So, we can safely assume the validity of Eq. (11) without any loss of generality, even beyond the LL level. If the above factorization (11) is true, then we may employ the standard trick which eliminates t-dependence from \mathcal{P} completely. This is realized by introducing a new evolution time variable

$$\tau \equiv \frac{1}{\alpha(t_0)} \int_{t_0}^t dt_1 \ \alpha(t_1), \quad \frac{\partial t}{\partial \tau} = \frac{\alpha(t_0)}{\alpha(t)}.$$
(12)

With this choice we have

$$\partial_{\tau} D_{I}(\tau) = \sum_{K} \bar{\mathcal{P}}_{IK} D_{K}(\tau), \quad \bar{\mathcal{P}}_{IK} = \frac{\alpha(t_{0})}{\alpha(t)} \mathcal{P}_{IK}(t) = \alpha(t_{0}) P_{KL}, \quad (13)$$

where $\overline{\mathcal{P}}$ does not depend on the new evolution time variable τ anymore, because $\alpha(t)$ in $\overline{\mathcal{P}}$ is effectively replaced by $\alpha(t_0)$. The rest of the formalism following Eq. (1) is the same, provided we substitute $t \to \tau$ and $\mathcal{P} \to \overline{\mathcal{P}}$ everywhere.

Concerning the continuous indexes, indeed in the QCD case we deal with the composite index $K = \{k, x\}$, where k is the parton type; let it be $k = G, q, \bar{q}$ in the simple case of gluon and one type of quark, and x, which is a fraction of the energy of the primary (proton) beam particle carried by the parton – the usual definition. The standard parton distribution evolution equations read

$$\partial_{\tau} x_1 D_{k_1}(\tau, x_1) = \sum_{k_0} \int_{x_1}^1 dx_0 \ \frac{\alpha_{\rm S}(t_0)}{\pi} \ \frac{x_1}{x_0^2} P_{k_1 k_0}\left(\frac{x_1}{x_0}\right) x_0 D_{k_0}(\tau, x_0) \tag{14}$$

from which we deduce the following substitution rule

$$\sum_{K_i} \to \sum_{k_i} \int dx_i, \tag{15}$$

while for the matrix elements, excluding IR region $x_i = x_{i-1}$ from the consideration, we have the explicit expression

$$\bar{\mathcal{P}}_{K_i K_{i-1}} = \frac{\alpha_{\rm S}(t_0)}{\pi} \, \frac{x_i}{x_{i-1}^2} P_{k_i k_{i-1}} \left(\frac{x_i}{x_{i-1}}\right) \, \Theta\left(1 - \frac{x_i}{x_{i-1}}\right),\tag{16}$$

where $K_i = \{k_i, x_i\}.$

Another two points require now clarification: the meaning of the *diagonal* part K = J in the $\bar{\mathcal{P}}_{K,J}$, the *off-diagonal* part $\bar{\mathcal{P}}'_{KJ}$ and the validity of the condition of Eq. (2) necessary for the feasibility of the Markovianization.

The problem of defining off-diagonal elements in $\bar{\mathcal{P}}'_{K,J}$ coincides with the problem of defining an infrared (IR) cut-off and is dealt with in a standard way by introducing a dimensionless small parameter $\varepsilon \to 0$, which defines/separates real gluon emission by requiring $x_i/x_{i-1} < 1 - \varepsilon$. The off-diagonal (real emission) part is defined in the usual way³

$$\bar{\mathcal{P}}'_{K_jK_i} = \Theta\left(1 - \varepsilon - \frac{x_j}{x_i}\right) \frac{\alpha_{\rm S}(t_0)}{\pi} \frac{x_j}{x_i^2} P_{k_jk_i}\left(\frac{x_j}{x_i}\right) + \mathcal{O}(\varepsilon)(1 - \delta_{k_ik_j}).$$
(17)

The condition of Eq. (2), $\sum_{K_j} \bar{\mathcal{P}}_{K_j K_i} = 0$, coincides in fact with the energy conservation sum rule, which reads as follows

$$\bar{R}_{K_i} = \sum_{K_j} \bar{\mathcal{P}}'_{K_j K_i} = \frac{\alpha_{\rm S}(t_0)}{\pi} \sum_{k_j} \int dz_{ji} \, z_{ji} P_{k_j k_i}(z_{ji}) \, \Theta(1 - \varepsilon - z_{ji}) \,, \quad (18)$$

where $z_{ji} = x_j/x_i$, and the nice feature is that \bar{R}_{K_i} depends only on the parton type k_i and not on x_i (unless we introduce more complicated IR cut). At this point it is understandable why Eq. (14) was written for the energy distributions xD(x) and not for the parton distributions $D_K(x)$ themselves. In the latter case the condition of Eq. (2) is not generally valid⁴ and the Markovian MC calculation is not possible. The significance of the energy sum rules in the evolution equations was underlined in many works, see for instance Refs. [5, 6].

³ The $\mathcal{O}(\varepsilon)$ term is related to the fact that for the sake of simplicity we apply the $\Theta(x_j/x_i - 1 + \varepsilon)$ factor also to the $k_i \neq k_j$ part, which is not IR singular.

⁴ It is, however, valid for the non-singlet component.

Collecting all the above material we can write the normalized transition probability for the actual MC Markovian calculation as follows

$$\omega(\tau_i, k_i, x_i | \tau_{i-1}, k_{i-1}, x_{i-1}) = \Theta(\tau_i - \tau_{i-1}) e^{-(\tau_i - \tau_{i-1})R_{i-1}} \bar{\mathcal{P}}'_{K_i K_{i-1}}, \quad (19)$$

where the necessary ingredients are provided by Eqs. (17) and (18). The LL QCD evolution kernels can be found in any QCD textbook and we skip details of the actual formulas entering the above equation.

3. Numerical results

In the following we present numerical results obtained for the distributions of three light quarks and gluons evolved from Q = 1 GeV up to 1 TeV in the range $x \in (10^{-4}, 1)$. The starting parton distribution at $Q_0 = 1$ GeV is the proton distribution defined in a conventional way:

$$xD_{G}(x) = 1.9083594473 x^{-0.2} (1-x)^{5.0},$$

$$xD_{q}(x) = 0.5 xD_{sea}(x) + xD_{2u}(x),$$

$$xD_{\bar{q}}(x) = 0.5 xD_{sea}(x) + xD_{d}(x),$$

$$xD_{sea}(x) = 0.6733449216 x^{-0.2} (1-x)^{7.0},$$

$$xD_{2u}(x) = 2.187500000 x^{0.5} (1-x)^{3.0},$$

$$xD_{d}(x) = 1.2304687500 x^{0.5} (1-x)^{4.0}.$$
(20)

We use in this exercise the LL version of the evolution kernels [1,7]. Extension to the NLL level requires to use the NLL kernels [8]. The rest of the MC algorithm/program is the same as in the LL case. Such an extension will be presented elsewhere.

In Figs. 1, 2 we show numerical results for the gluon and quark distributions evolved from Q = 1 GeV to higher scales Q = 10,100,1000 GeV, obtained from our Markovian Monte Carlo EvolMC1⁵. In the plots we also show the results from the standard program QCDnum16 evolving parton distributions using a finite grid of points in the x and Q space. As we see, these two calculations agree within 0.2% for gluons and even better for the quark singlet. This is clearly seen from the plotted ratio of the MC result and the result of QCDnum16. The biggest discrepancy is in the region close to x = 1, where all parton distributions are extremely small. The origin of 0.2% discrepancy for gluons is not identified unambiguously. Variation of the grid parameters change the results of QCDnum16 quite substantially, while the variation of the IR cut ε and of the minimum x parameters in the

 $^{^5}$ The actual MC program is rather compact, it consists of about 3k lines of the C++ code.

MC run has no visible influence on the MC results. We tend to conclude that the difference between the MC and QCDnum16 is due to a numerical bias in the QCDnum16 program, although more work is required to reach a firm conclusion. In the MC we generated 1.2×10^9 events (96nh CERN units). It would be possible to increase MC statistics by a factor of 10, obtaining a sub per-mill statistical errors in the MC results, if necessary.



Fig. 1. The upper plot shows gluon distribution $xD_G(x, Q_i)$ evolved from $Q_0 = 1$ GeV to $Q_i = 10,100,1000$ GeV obtained from QCDnum16 and EvolMC1, while the lower plot shows their ratio. The horizontal axis is $\log_{10}(x)$. See the text for details.



Fig. 2. The upper plot shows the singlet quark distribution $D_{\bar{q}+q}(x)$ evolved from $Q_0 = 1$ GeV to $Q_i = 10,100,1000$ GeV obtained from QCDnum16 and EvolMC1, while the lower plot shows their ratio. The horizontal axis is $\log_{10}(x)$. See the text for details.

4. Discussion

The main lesson from the above numerical exercises is that with the modern computing power the precision of 10^{-4} in the solutions of the QCD evolution equations is within the reach of the MC method for most of the *x*-range. MC will always be slower than the non-MC methods, however, it has no biases related to the finite grid, the use of quadratures, decomposition into finite series of polynomials, accumulation of the rounding errors, *etc.* MC method can therefore be used to test any other non-MC tool for the QCD evolution. Let us stress that in the MC method there is also no need to split PDFs into a singlet component and several types of non-singlet

components, each of them evolved separately and combined in the very end of the calculation. This simplifies the calculation, and the MC Markovian method is clearly well suited for the evolution of PDFs with many components, for example QCD+QED, SUSY theory or QCD+electroweak theory at very large energies, modeling showers of extremely high energetic cosmic rays in the intergalactic space (see Ref. [9]), *etc.*

Let us now elaborate more on the issues related to the construction of the efficient PSMC for the QCD initial state radiation. As it is well known, the cross section of the hard scattering, especially in the presence of narrow resonances, discriminates very strongly on the parton type and x of the parton exiting PSMC and entering the hard scattering. The Markovian PSMC does not provide for any control (tagging) of the flavor and x of the exiting parton, consequently, the overall efficiency of such a MC for the initial state would be drastically bad. The solution adopted in the most of the existing ISR QCD PSMCs is the so-called backward parton shower of Ref. [10], in which one starts with the parton next to the hard process, defining its type and energy x, and then the Markovian random walk continues toward the lower Q and higher x, until the hadron mass scale is reached. This beautiful algorithm requires, however, the *a priori* knowledge of the parton distribution functions (PDF) at all intermediate Q scales. These PDFs are, therefore, tabulated using results of the non-MC evolution programs, and are also fitted to the deep inelastic scattering (DIS) data. In other words, the evolution of PDFs is not a built-in feature of the standard ISR PSMC. The two most important reasons for that are the following: (i) one is purely technical — the low efficiency of the standard Markovian ISR PSMC and another one is (ii) the convenience in porting PDFs from DIS data to hadron-hadron scattering. We notice that both of these reasons seem nowadays to fade away. For (i), the CPU power of the present computer systems is bigger by the factor $\sim 10^4$ than 15 years ago, when the problem of the efficiency of the PSMC for ISR was considered for the first time. That widens considerably the range of the practically realizable MC algorithms. In addition, there exist now working examples of the efficient non-Markovian algorithms with built-in evolution (albeit in the soft approximation) for the pure multi-bremsstrahlung process in the Abelian case (QED), see Refs. [11, 12], which can be treated as a partial solution of the problem of tagging x. For *(ii)*, PDFs in the future LHC experiments will be constrained not only by DIS but also by the LHC data (W and Z production) themselves. One should, therefore, consider the genuine MC solution for the QCD evolution as an integral part of the PSMC, with the aim of fitting the LHC and DIS data simultaneously. The obvious advantage of such a scenario is that the detector effects can be removed from the data more efficiently. No doubt, to realize it in practice will be

technically rather challenging. Nevertheless, we claim that it is feasible and at present it makes sense to consider it seriously.

In view of the above discussion let us formulate the challenge in the construction of the MC event generators: It would be desirable to construct a MC program/algorithm, which evolves the parton distribution functions using the QCD NLL \overline{MS} kernels from the PDFs at low Q_{\min} to higher Q_{\max} , in which we are able to fix beforehand the type (flavor) and the energy fraction x of the parton at the scale Q_{\max} . The *a priori* knowledge of the PDFs at all intermediate Qs should not be required/used; the input from the perturbative QCD would be the expressions for the kernels. The PDFs at all intermediate Qs would be the result from the MC.

Additional remarks:

- (i) We do not assume that the solution is based on the Markovian process. Any, even brute force solution, but feasible with the present CPU power, is worth consideration.
- (ii) The above challenge concerns primarily the (Q, x) space. The construction of a full scale parton shower MC on top of the above twodimensional MC we treat as a separate (important) issue.
- (*iii*) In our opinion, solving the above technical challenge would open new interesting avenues in the realm of the MC event generators for DIS and hadron-hadron scattering.

For the moment we do not offer any solution of our own. We can see one hint, which comes from the exercises we have done using the presented MC of the Markovian type. In the left hand side plot in Fig. 3 we show the average number of all "emissions" in the Markovian process on the way from Q = 1 GeV to Q = 1 TeV, for the proton case, as a function of the final x at Q = 1 TeV. The IR cut-off $\varepsilon = 10^{-4}$ is used. Due to a sizable value of $\alpha_{\rm S}$ and large phase space the average number of emissions is about 20 (for a single proton beam). However, the average number of the transitions $q, \bar{q} \to G$ and $G \to q, \bar{q}$, shown in the right hand side plot in the same figure, is much smaller — it is in the range from 0.5 to 1. This feature suggests the brute force solutions in which $q, \bar{q} \to G$ and $G \to q, \bar{q}$ transition are pretabulated (solving the problem of tagging the parton type), while the pure bremsstrahlung transition $G \to G$ and $q \to q$ are treated using the algorithm of the QED (with the constrained final x). However, we hope that more elegant and efficient solution can be found. Finally, we would like to refer the reader to extensive literature on the subject of the QCD evolution and parton shower MC algorithms, which can be found for instance in Refs. [7, 13].



Fig. 3. Average multiplicities of all emissions (left plot) and of the transitions $G \to q$ and $q \to G$ only (right plot) as a function of $\log_{10}(x)$. Results are for the proton "showering" up to 1 TeV scale according to Markovian MC with the IR cut $\varepsilon = 10^{-4}$.

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