METHOD OF FITTING PDFs FOR THE MONTE CARLO SOLUTIONS OF THE EVOLUTION EQUATIONS IN QCD*

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We present a framework for fitting the parton density functions obtained from the Monte Carlo solutions of the QCD evolution equations of various types to the F_2 data. To speed up the fitting it is enough to perform the Monte Carlo simulation only once. The actual parton density functions as functions of the fitting parameters are then reconstructed by fast one-dimensional numerical integration. Such a tool is necessary in order to determine initial values for parton density functions in case of non-DGLAP Monte Carlo evolutions.

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1. Introduction

In a series of recent papers [1–7], co-authored by one of us (M.S.), it has been demonstrated that the Monte Carlo (MC) simulations can be used to obtain precise solutions of the evolution equations in QCD [8]. MC is a mathematically rigorous method, and with the help of todays computers it is feasible to reach the precision of the order of 10^{-4} within a reasonable computing time. Such MC algorithms not only provide the evolution of the inclusive parton density functions (PDFs), but also emulate the whole exclusive process of multiple emission of partons described by the evolution equations. The evolution starts from a certain initial value Q_0 of the evolution variable Q and then develops up to the scale of the hard process. Such a cascade of emissions, described originally by two-dimensional evolution in x and Q space, can be extended into the full-scale parton shower

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MC program in which all four-momenta of the emitted partons are reconstructed. This in turn allows for inclusion of the complicated detector effects. In order to do that one has to specify the type of evolution, the meaning of evolution variables and the initial values of PDFs at Q_0 for that particular evolution setup. The shape of the PDFs at Q_0 cannot be obtained by means of perturbative calculations due to collinear singularities arising from non-perturbative, long-distance sector of QCD, *cf. e.g.* [9, 10]. On the other hand the non-perturbative methods, like lattice gauge theory, are still not precise enough as compared with the typical accuracy required by the experiments. Therefore the common way of proceeding is to determine the shape of PDFs at Q_0 by fitting structure functions F_i calculated from these PDFs to the experimental data. Such a fitting procedures have been extensively studied by various groups [11–18] and others; for a recent overview see [19]. Numerous effects and approximation levels have been included in these analyzes: perturbative higher orders (LO/NLO/NNLO), heavy quark effects (zero-mass/general-mass variable-flavor-number; fixed-flavor-number) or non-perturbative higher twist effects. Also the treatment of experimental errors varies in the level of sophistication from simple Gaussian errors to complicated correlated ones.

In the earlier mentioned series of papers a family of new MC algorithms has been presented. Initially these algorithms [1–4] solved DGLAP-type equations, including some of the listed above effects (NLO for example) [7]. Later on the non-DGLAP evolutions have also been simulated. Namely, by means of clever choice of argument of the running coupling one can resum some of the logarithmically enhanced higher order terms or include some of the low-x effects [20–24]. In practical terms the modified argument is of the form $Q(1-z)$, $Q(1-z)^{1/2}/z$, or in general $Qf(z)$. In the above mentioned series of MC algorithms the scheme with $\alpha(Q(1-z))$ has been chosen and implemented [25]. In the next step the CCFM-like evolution [26] with α being the function of the true transverse momentum k_{T} of emitted gluons, with non-Sudakov form-factor and with ordering in rapidity has also been implemented in these MC algorithms [27].

The PDF fits to such non-DGLAP schemes are difficult to find in the literature [28]. For that reason it is important for us that in parallel with the MC parton shower algorithms we develop a framework that would enable us to perform fits of PDFs to experimental data.

In this paper we present such a framework, suitable for fitting PDFs calculated by MC codes with any general form of α that depends on Q and z variables. The requirement that the fitting procedure uses MC code to solve evolution equations is a nontrivial one because MC codes are much slower than the codes based on other numerical methods. In consequence it is very difficult to repeat the evolution many times for various input pa-

rameters during fitting. To overcome this problem, we based our method on the factorizability of the evolution equations which allows us to write their solutions in a form of a convolution of a boundary condition which depends on the fitting parameters and the universal Green-function-type solution of the evolution equations independent of the fitting parameters.

It should be mentioned here that the use of MC simulation as the basis of fitting is not restricted to structure functions but can be used for other observables as well. In such a general case MC has the unique feature of allowing for inclusion of the detector effects into the fitting procedures. How much of these effects can be included in an efficient way (without excessive number of long generations) depends on the observable.

This paper is organized as follows. In the next section we show how the construction of PDFs is done, based on the numerical convolution of results of MC simulation. In Section 3 we discuss the actual fitting procedure for F_2 at LO and NLO levels. Section 4 contains concluding remarks.

2. Construction of PDFs

We begin by showing how the solution of evolution equations can be decomposed into two parts: the universal one, of the Green-function type, describing evolution and the actual initial condition.

The evolution equations are of the standard form

$$\partial_t D_A(x,t) = P_{AB}(x,t) \otimes^x D_B(x,t)\,, \tag{1}$$

$$D_A(x,t=0) = D_A^0\left(x,\alpha_1^A,\ldots,\alpha_k^A\right)\,. \tag{2}$$

$D_A(x,t)$ denotes PDF of the type A with $A = q_i, \bar{q}_i, g;\ i = 1.\ldots, n_f.$ and t is the evolution time. The splitting kernels $P_{AB}(x,t)$ include also coupling constants and the convolution symbol $\otimes^x$ stands for

$$\big(f(x,\alpha) \otimes^x g(x,\beta)\big)(x) = \int\limits_0^1 dydz\delta(x-yz) f(y,\alpha) g(z,\beta)\,. \tag{3}$$

The actual decomposition of the solution $D_A(x,t)$ of Eq. (1) can be written as follows

$$D_A(x,t) = D_{AB}^{\delta}(x,t) \otimes^x D_B^0\left(x,\alpha_1^B,\ldots,\alpha_k^B\right)\,, \tag{4}$$

where

$$\partial_t D_{AB}^{\delta}(x,t) = P_{AC}(x,t) \otimes^x D_{CB}^{\delta}(x,t)\,, \tag{5}$$

$$D_{AB}^{\delta}(x,0) = \delta_{AB}\delta(1-x)\,. \tag{6}$$

It is easy to verify that, by virtue of Eq. (5), the D_A of Eq. (4) fulfills Eq. (1) and, due to (6), it fulfills condition (2).

The decomposition (4) allows us now to perform the time-consuming MC evolution only *once* for each of $2n_f + 1$ columns of D^{δ}_{AB} matrix, *i.e.* for $B = q_i, \bar{q}_i, g$, starting in each case from the appropriate "unit" initial condition (6). The entire dependence on the initial parameters is hidden in the functions $D^0_B(x, \alpha^B_1, \ldots, \alpha^B_k)$. In order to obtain the actual value of $D_A(x,t)$, needed for the fitting procedure, it is enough to perform only fast one-dimensional numerical integration[1]. To achieve high precision (10^{-3}) of this integration we employed a few technical tricks. First, the results of MC calculation, which have a form of a histogram of a finite binning (typically 100 bins), have been parameterized by a series of second order polynomial functions. Secondly, because in the MC run we use logarithmic scale for x-variable, the value of D^{δ} at x close to 1 is not known exactly and we extrapolate it from the neighboring bins. We could in principle use linear scale in that region in MC and generate the missing points. However, it turns out that extrapolation is sufficient for the precision of 10^{-3} within the range of $x < 0.5$ and for the precision of 10^{-2} for $x > 0.5$.

Let us now present technical tests of this integration procedure. For this purpose we use gluon (G) and singlet (Σ) PDFs

$$D_{\Sigma} = \sum_i \Big(D_{q_i} + D_{\bar{q}_i} \Big) \tag{7}$$

which can be regarded as a two-dimensional system

$$\begin{aligned} D_G(x,t) &= D^{\delta}_{GG}(x,t) \otimes D^0_G(x) + D^{\delta}_{G\Sigma}(x,t) \otimes D^0_{\Sigma}(x)\,, \\ D_{\Sigma}(x,t) &= D^{\delta}_{\Sigma G}(x,t) \otimes D^0_G(x) + D^{\delta}_{\Sigma\Sigma}(x,t) \otimes D^0_{\Sigma}(x)\,. \end{aligned} \tag{8}$$

We took the following initial distributions for the evolution

$$\begin{aligned} D^0_G(x) &= 1.908 x^{-1.2}(1-x)^{5.0}\,, \\ D^0_{\rm sea}(x) &= 0.6733 x^{-1.2}(1-x)^{7.0}\,, \\ D^0_{u_{\rm val}}(x) &= 2.187 x^{-0.5}(1-x)^{3.0}\,, \\ D^0_{d_{\rm val}}(x) &= 1.230 x^{-0.5}(1-x)^{4.0}\,. \end{aligned} \tag{9}$$

[1] It should be noted here, however, that such a scheme does not allow fitting $\Lambda_{\rm QCD}$ because in general case $\Lambda_{\rm QCD}$ enters into D^{δ}_{AB} function. That would violate the universality of D^{δ}_{AB}. This problem will be addressed elsewhere [29].

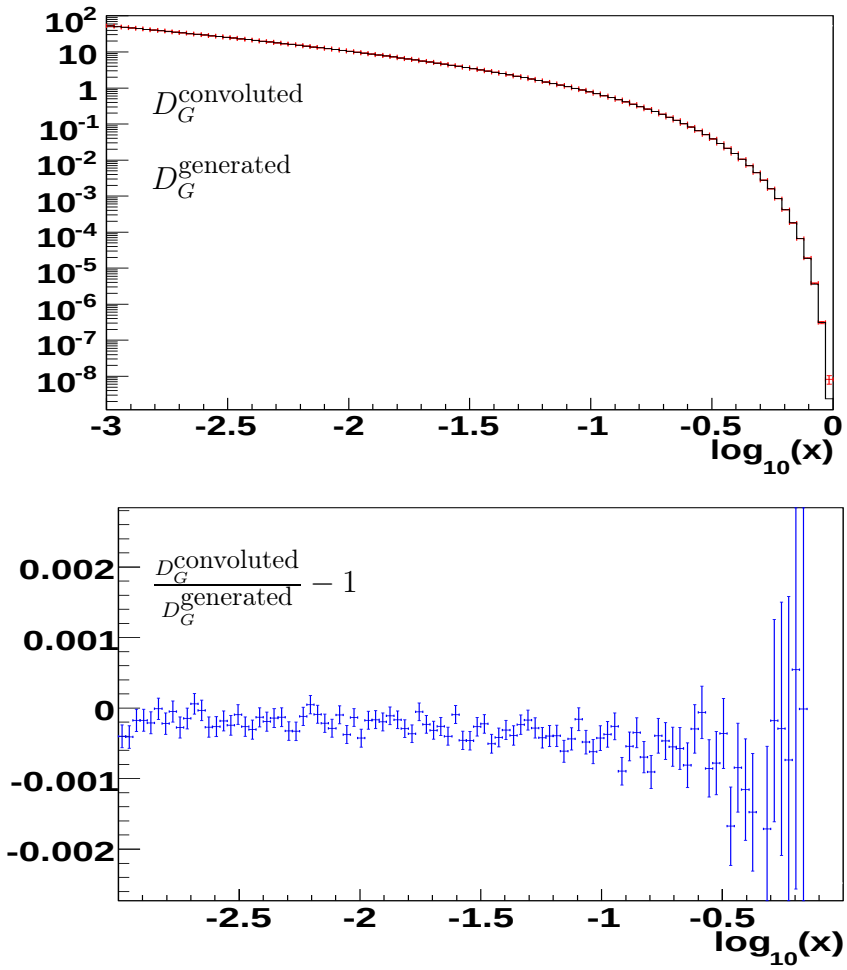

Fig. 1. Top frame: gluon PDF generated directly from the initial distributions (9) — dotted red line and from the convolution (8) — solid black line. Bottom frame: their ratio minus 1. Evolution from $Q = 1$ GeV to $Q = 100$ GeV, LO type. Statistical errors correspond to direct evolution (9).

and

$$\begin{aligned} D_u^0(x) &= D_{u_{\text{val}}}^0(x) + \frac{1}{6} D_{\text{sea}}^0(x)\,, \\ D_d^0(x) &= D_{d_{\text{val}}}^0(x) + \frac{1}{6} D_{\text{sea}}^0(x)\,, \\ D_s^0(x) &= D_{\bar{u}}^0(x) = D_{\bar{d}}^0(x) = D_{\bar{s}}^0(x) = \frac{1}{6} D_{\text{sea}}^0(x)\,, \\ D_\Sigma^0(x) &= D_{\text{sea}}^0(x) + D_{u_{\text{val}}}^0(x) + D_{d_{\text{val}}}^0(x)\,. \end{aligned} \tag{10}$$

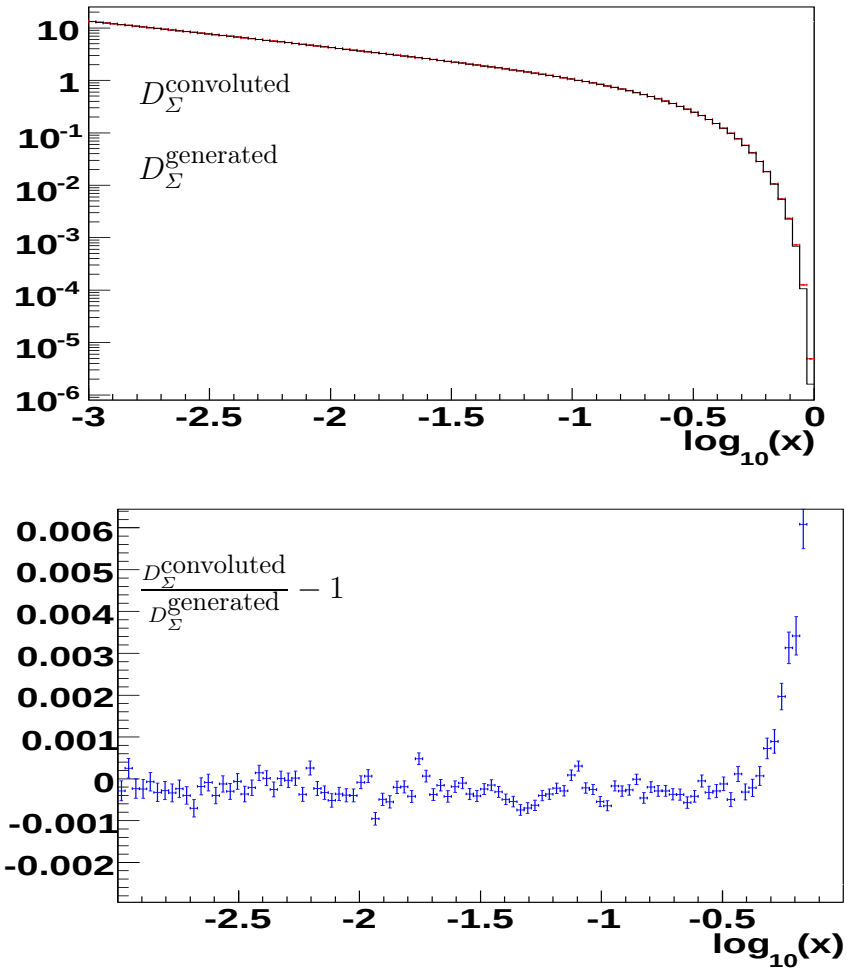

Fig. 2. Top frame: singlet PDF generated directly from the initial distributions (9) — dotted red line and from the convolution (8) — solid black line. Bottom frame: their ratio minus 1. Evolution from $Q = 1$ GeV to $Q = 100$ GeV, LO type. Statistical errors correspond to direct evolution (9).

In the upper frames of figures 1 and 2 we show respectively the G and Σ PDFs, generated by MC code EvolFMC [30], directly from the initial distributions (9) and from the convolutions (8). The curves are almost indistinguishable. In the lower frames we plot their ratio (minus 1). The D^δ functions are also generated by EvolFMC. The evolution is of the LO type and carried from $Q = 1$ GeV to $Q = 100$ GeV. The errors shown are purely statistical and correspond only to the direct MC generation from the initial

distributions (9). From the figures we see that the agreement is well within the 10^{-3}, except for the very high values of $\log_{10} x > -0.25$ in the Σ case, where it drops to 10^{-2}, as discussed earlier. Increase of errors for high x is statistical: PDFs decrease sharply and number of generated MC events is much lower in that region. Similar plots for the case of NLO evolution are shown in figures 3 and 4. As in the LO case the agreement is well within the 10^{-3}, except for the very high values of $\log_{10} x > -0.25$ in the Σ case.

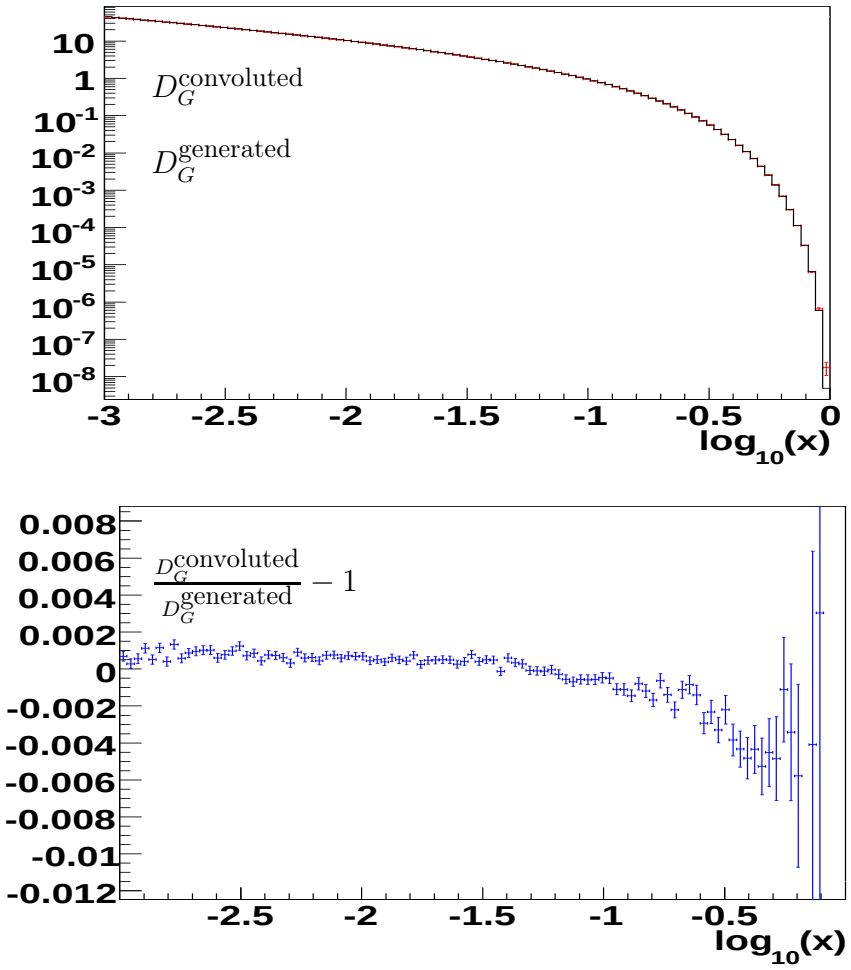

Fig. 3. Top frame: gluon PDF generated directly from the initial distributions (9) — dotted red line and from the convolution (8) — solid black line. Bottom frame: their ratio minus 1. Evolution from $Q = 1$ GeV to $Q = 100$ GeV, NLO type. Statistical errors correspond to direct evolution (9).

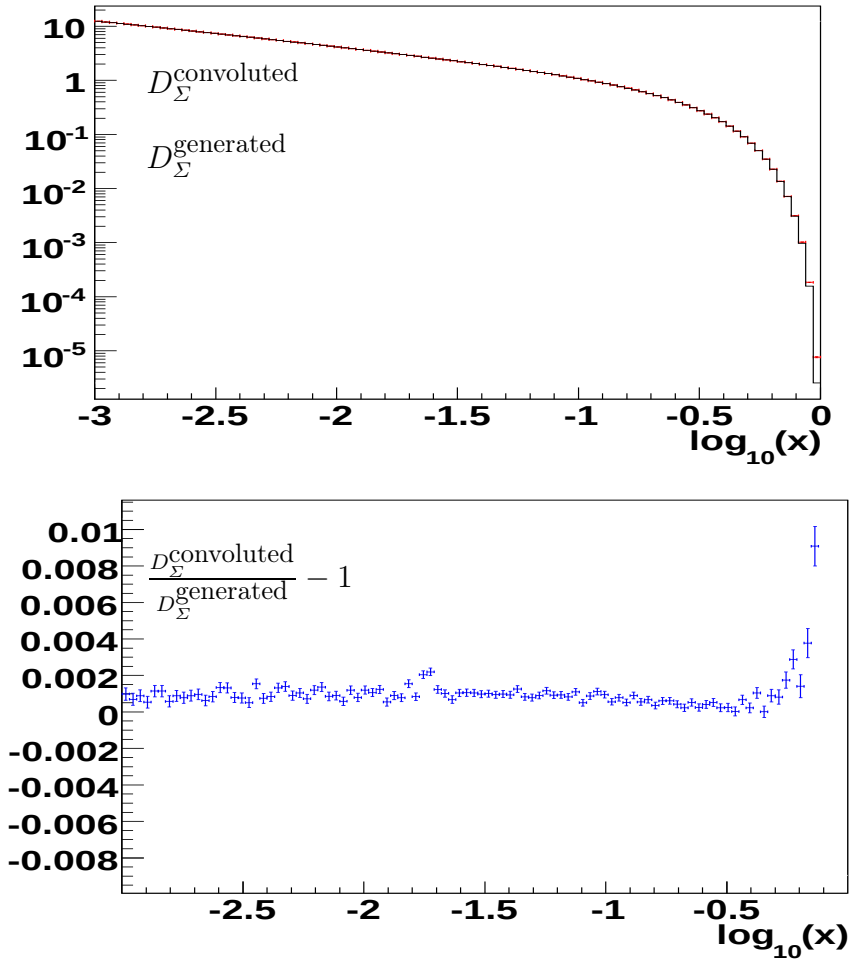

Fig. 4. Top frame: singlet PDF generated directly from the initial distributions (9) — dotted red line and from the convolution (8) — solid black line. Bottom frame: their ratio minus 1. Evolution from $Q = 1$ GeV to $Q = 100$ GeV, NLO type. Statistical errors correspond to direct evolution (9).

3. Fitting procedure

Having prepared the efficient method of calculating PDFs as functions of initial parameters we proceed to the fitting. To this end we use the program MINUIT [31] and perform the least-squares fit by minimizing the chi-square function. As a first step we will do fits at the level of PDFs themselves. This exercise will mainly check correctness of the procedure but it will also

provide some interesting comparisons of different evolution types. As before, let us consider two-dimensional system of PDFs of Eq. (8) for G and Σ and define the chi-square function as

$$\chi^2(\alpha_1^G,\ldots,\alpha_k^G;\alpha_1^\Sigma,\ldots,\alpha_k^\Sigma) = \sum_{A=G,\Sigma}\sum_i \frac{(D_A^X(x_i,t,\alpha_1^A,\ldots,\alpha_k^A) - D_A^Y(x_i,t))^2}{e_A^Y(x_i,t)^2}, \tag{11}$$

where the time t is fixed. The "data points" are generated by EvolFMC according to some evolution type Y. The fitted functions D_A^X are calculated according to Eq. (8) with D^δ generated also by EvolFMC. If both evolutions X and Y are the same (*i.e.* $X = Y$) we plainly test the fitting procedure. We show such tests for the LO and NLO evolutions. The initial densities are parameterized as

$$\alpha_1^A x^{-\alpha_2^A}(1-x)^{\alpha_3^A}; \qquad A = G, u, d, \text{sea}. \tag{12}$$

In Tables I and II we compare the values of α_i^A used for generation (I) with the ones obtained from fits (F) for the cases of LO and NLO evolutions respectively. As we can see, the agreement is very good in both cases.

TABLE I

Comparison of fitted values of coefficients with the original ones used for generation for the LO evolution at $Q = 100$ GeV. I: values used for generation, F: fitted values. The initial distributions are $\alpha_1^A x^{-\alpha_2^A}(1-x)^{\alpha_3^A}$.

	α_1^G	α_2^G	α_3^G	α_1^u	α_2^u	α_3^u	α_1^d	α_2^d	α_3^d	α_1^{sea}	α_2^{sea}	α_3^{sea}
I	1.908	1.200	5.000	2.187	0.500	3.000	1.230	0.500	4.000	0.67	1.200	7.00
F	1.907	1.199	4.994	2.186	0.501	3.008	1.229	0.505	3.991	0.68	1.199	7.06

TABLE II

Comparison of fitted values of coefficients with the original ones used for generation for the NLO evolution at $Q = 100$ GeV. I: values used for generation, F: fitted values. The initial distributions are $\alpha_1^A x^{-\alpha_2^A}(1-x)^{\alpha_3^A}$.

	α_1^G	α_2^G	α_3^G	α_1^u	α_2^u	α_3^u	α_1^d	α_2^d	α_3^d	α_1^{sea}	α_2^{sea}	α_3^{sea}
I	1.908	1.200	5.000	2.187	0.500	3.000	1.230	0.500	4.000	0.67	1.200	7.00
F	1.905	1.200	5.002	2.187	0.503	3.013	1.230	0.513	3.997	0.67	1.198	7.09

As a next step we fit a different type of evolution than the one used to prepare "data points". More specifically, we use again the same setup of PDFs for G and Σ, Eq. (8), and the same initial condition (9). We evolve PDFs with the z-dependent coupling constant of the form $\alpha_S = \alpha_S(Q(1-z))$. For the fit however we use the coupling independent of z: $\alpha_S = \alpha_S(Q)$. This way we can asses how big the change of initial conditions must be in order to compensate for different evolution scheme at a given value of Q. In the Table III we show results for the case of LO evolution with $\alpha_S(Q(1-z))$ used for generation, which is then fitted with NLO evolution with $\alpha_S(Q)$. The evolution runs from $Q = 1$ GeV up to $Q = 100$ GeV. We see from the table that the changes in some of the parameters are quite big. Therefore even such a very simple exercise suggests that the NLO effects not included through modified argument of α_S significantly change the evolution and one should be careful with choosing proper initial distributions for a given evolution type.

TABLE III

Fitting different evolutions: Generated LO DGLAP with $\alpha(Q(1-z))$, fitted NLO DGLAP with $\alpha(Q)$. Evolution from $Q = 1$ GeV to $Q = 100$ GeV. I — values used for generation, F — fitted values. The initial distributions are $\alpha_1^A x^{-\alpha_2^A}(1-x)^{\alpha_3^A}$.

	α_1^G	α_2^G	α_3^G	α_1^u	α_2^u	α_3^u	α_1^d	α_2^d	α_3^d	$\alpha_1^{\rm sea}$	$\alpha_2^{\rm sea}$	$\alpha_3^{\rm sea}$
I	1.908	1.200	5.000	2.187	0.500	3.000	1.230	0.500	4.000	0.67	1.200	7.00
F	1.775	1.197	4.657	1.974	0.341	2.736	0.437	0.142	2.523	0.601	1.471	7.232

Finally, we turn to the F_2. In the LO approximation F_2 is a linear combination of PDFs

$$F_2^{\rm LO}(x,t) = \sum_{A=q,\bar{q}} \int_0^1 d\xi D_A(\xi,t) x e_A^2 \delta(x-\xi) = \sum_{A=q,\bar{q}} D_A(x,t) x e_A^2 \,. \tag{13}$$

Apart from computing PDFs from Eq. (4) and constructing F_2 directly from Eq. (13) we have also used rearranged form of Eq. (13). Inserting representation (4) of D_A into Eq. (13) we obtain

$$F_2^{\rm LO}(x,t,\vec{\alpha}_1,\ldots,\vec{\alpha}_k) = x \sum_B \left(\sum_{A=q,\bar{q}} e_A^2 D_{AB}^{\delta}(x,t) \right) \otimes^x D_B^0\left(x,\alpha_1^B,\ldots,\alpha_k^B\right) . \tag{14}$$

Eq. (14) is faster to compute numerically due to smaller number of convolutions, especially if one takes into account further symmetries of D_{AB}^{δ} for various combinations of indices A and B.

The NLO case is more complicated because coefficient functions become nontrivial. In the $\overline{\rm MS}$ scheme one finds

$$F_2^{\rm NLO}(x,t) \;=\; x\sum_{A=q,\bar{q}} e_A^2 D_A(x,t) + \Delta F_2\,, \tag{15}$$

$$\begin{aligned}\Delta F_2 \;=\; & x\sum_{A=q,\bar{q}} e_A^2 D_A(x,t)\otimes^x \frac{\alpha_s}{2\pi} C_A^{\overline{\rm MS}}(x) \\ & + x\sum_{A=q,\bar{q}} e_A^2 D_g(x,t)\otimes^x \frac{\alpha_S}{2\pi} C_g^{\overline{\rm MS}}(x)\;,\end{aligned} \tag{16}$$

where [32]

$$\begin{aligned} C_q^{\overline{\rm MS}} \;=\; & C_{\rm F}\left(2\left(\frac{\ln(1-z)}{1-z}\right)_+ - \frac{3}{2}\left(\frac{1}{1-z}\right)_+ - (1+z)\ln(1-z) - \frac{1+z^2}{1-z}\ln(z)\right. \\ & \left. + 3 + 2z - \left(\frac{\pi^2}{3}+\frac{9}{2}\right)\delta(1-z)\right) \end{aligned} \tag{17}$$

$$= C_{\rm F}\left(\frac{1+z^2}{1-z}\left(\ln\frac{1-z}{z} - \frac{3}{4}\right) + \frac{1}{4}(9+5z)\right)_+\,, \tag{18}$$

$$C_g^{\overline{\rm MS}} \;=\; T_{\rm R}\left(\left((1-z)^2+z^2\right)\right)\ln\left(\frac{1-z}{z}\right) - 8z^2 + 8z - 1\Big)\;. \tag{19}$$

The plus distribution is defined in a usual way

$$[f(z)]_+ = f(z) - \delta(1-z)\int\limits_0^1 f(x)dx\,. \tag{20}$$

The only new components, as compared to the LO case, are the convolutions of the PDFs D_A (stored in the form of histograms) with the coefficient functions $C^{\overline{\rm MS}}(x)$. The convolutions have been done numerically. In the quark case we used representation (18) and we applied directly the definition (20) of the plus distribution.

The test of the convolution is presented in Fig. 5 where we show the correction ΔF_2 obtained by means of double convolutions (8) and (15) from D^δ functions generated by EvolFMC. As a reference we used the numerical results obtained from the `QCDNum16` code [33]. The two curves are indistinguishable (upper frame) and their difference is shown in the lower frame. Note that the difference is not normalized due to the presence of zeroes of ΔF_2 at high x. As one can see the agreement is excellent — at the level of 10^{-5} in absolute units.

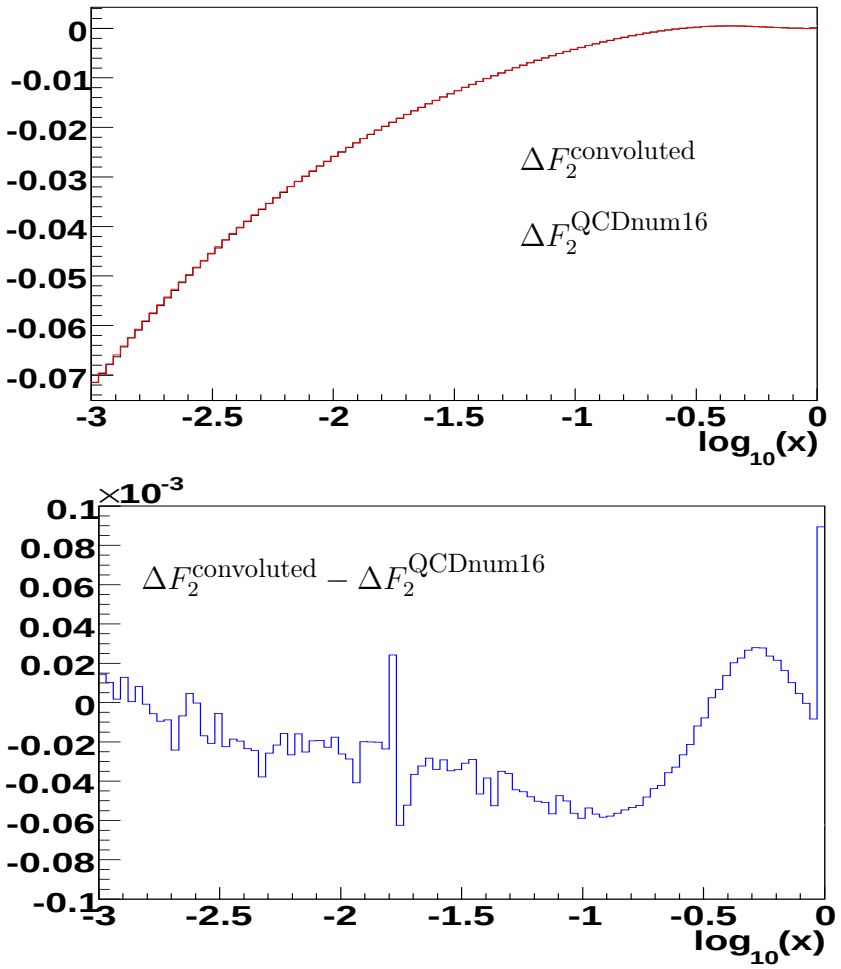

Fig. 5. Top frame: ΔF_2 from numerical convolution of EvolFMC results (red) and from `QCDNum16` (black). Bottom frame: their difference (note factor 10^{-3}); $Q = 100$ GeV.

To proceed with the fitting of F_2 we define chi-square function to be minimized by MINUIT:

$$\chi^2(\vec{\alpha}_1, \ldots, \vec{\alpha}_k) = \sum_n \sum_i \frac{\left(F_2(x_i, t_n, \vec{\alpha}_1, \ldots, \vec{\alpha}_k) - F_{2\text{exp}}(x_i, t_n)\right)^2}{e_{F_{2\text{exp}}}(x_i, t_n)^2}. \quad (21)$$

In order to test the whole procedure of constructing and fitting F_2 we generated a sample of "data points" of F_2 with the help of `QCDNum16` code. As

starting distributions we used again the same set of Eqs. (9)–(10). Then we performed fits to these F_2 "data points". The results of this comparison are shown in Tables IV and V for the case of LO and NLO evolutions respectively. As one can see the agreement is excellent in both cases. This is an important test of the procedure. It shows in particular, that the small inaccuracy in reconstruction of the PDFs for very high values of x discussed earlier in this section indeed has no influence on the accuracy of the whole procedure.

TABLE IV

Fitting two structure functions: F2 obtained from EvolFMC to F2 from `QCDNum16`. I — values used for generation in `QCDNum16`, F — fitted values. LO-type evolution. The initial distributions are of the form $\alpha_1^A x^{-\alpha_2^A}(1-x)^{\alpha_3^A}$.

	α_1^G	α_2^G	α_3^G	α_1^u	α_2^u	α_3^u	α_1^d	α_2^d	α_3^d	$\alpha_1^{\rm sea}$	$\alpha_2^{\rm sea}$	$\alpha_3^{\rm sea}$
I	1.908	1.200	5.000	2.187	0.500	3.000	1.230	0.500	4.000	0.67	1.200	7.00
F	1.908	1.199	4.988	2.187	0.502	3.07	1.241	0.507	4.08	0.674	1.200	6.944

TABLE V

Fitting two structure functions: F2 obtained from EvolFMC to F2 from `QCDNum16`. I — values used for generation in `QCDNum16`, F — fitted values. NLO-type evolution. The initial distributions are of the form $\alpha_1^A x^{-\alpha_2^A}(1-x)^{\alpha_3^A}$.

	α_1^G	α_2^G	α_3^G	α_1^u	α_2^u	α_3^u	α_1^d	α_2^d	α_3^d	$\alpha_1^{\rm sea}$	$\alpha_2^{\rm sea}$	$\alpha_3^{\rm sea}$
I	1.908	1.200	5.000	2.187	0.500	3.000	1.230	0.500	4.000	0.67	1.200	7.00
F	1.908	1.199	4.979	2.196	0.503	3.06	1.25	0.51	4.04	0.675	1.200	6.86

4. Summary and outlook

In this paper we presented a scheme of fitting the PDFs generated by the MC to the F_2 experimental data. The main technical difficulty in using the MC techniques to solve evolution equations is the slowness of the simulation. To overcome this problem we based the fitting procedure on the factorizability of the evolution equations. This way the MC is used only once to generate a universal evolution operator. The initial conditions are then taken into account by means of single numerical integration. We have shown in a series of numerical tests, both at the level of PDFs as well as F_2, in LO and NLO approximation, that such a procedure is indeed very fast and numerically precise.

The main limitation of this procedure is the inability of fitting the value of $\Lambda_{\rm QCD}$. Contrary to the other parameters the dependence on $\Lambda_{\rm QCD}$, which enters through the coupling constant, cannot be in the general case factored out in a form of a one-dimensional convolution of initial conditions with parameter-free evolution operator. Extension of the proposed procedure that would allow for this case is an important development to be done [29]. Another interesting line of development would be to construct a procedure for a more general evolution scheme which uses the actual $k_{\rm T}$ of emitted particles (CCFM-like). Such a scheme would in particular allow for performing fits of quantities other than F_2 with the inclusion of the detector effects.

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