Investigation of the factorization scheme dependence of finite order perturbative QCD calculations: searching for approximately ZERO factorization scheme

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Abstract

The possibility of an improvement of current NLO Monte Carlo event generators by means of choosing a suitable factorization scheme is studied. The optimal factorization scheme for combining initial state parton showers and NLO hard scattering cross-sections is the ZERO factorization scheme, in which all NLO splitting functions vanish. However, it has turned out that the ZERO factorization scheme has a limited range of practical applicability. Hence, this paper is focused on searching for a factorization scheme which is applicable at the NLO in the full range of $x$ relevant for QCD phenomenology and simultaneously close to the ZERO factorization scheme (i.e. the corresponding NLO splitting functions are close to zero).

1 Introduction

At present time many QCD cross-sections at parton level are known at the NLO accuracy and necessary algorithms, e.g. [1, 2, 3, 4, 5], for their incorporation in Monte Carlo event generators have been developed. However, these algorithms attach initial state parton showers that are generated on the basis of the LO splitting functions to NLO hard scattering cross-sections obtained in the standard $\overline{\text{MS}}$ factorization scheme because no satisfactory algorithm for generating parton showers at the NLO accuracy has been found so far. The reasons why generating initial state parton showers at the NLO accuracy is difficult in the $\overline{\text{MS}}$ factorization scheme are following. The NLO splitting functions no longer correspond to basic QCD vertices, are expressed by much more complicated formulae than the LO ones and are negative for some $x$, which prevents us from using straightforward probabilistic interpretation, which is crucial for Monte Carlo simulations.

Initial state parton showers induce the scale dependence of parton distribution functions, which is described by the evolution equations. Monte Carlo simulations of initial state parton showers have some important advantages in comparison with the analytical calculations represented by the evolution equations — they take into account transverse momenta, include the color description and the partons radiated in initial state parton showers participate in hadronization.

Since current NLO Monte Carlo event generators attach LO initial state parton showers to NLO hard scattering cross-sections corresponding to the $\overline{\text{MS}}$ factorization scheme, they
cannot predict some quantities, e.g. spectra of transverse momenta, at the NLO accuracy.

The deficiency lying in the combination of LO initial state parton showers and NLO hard scattering cross-sections calculated in the $\overline{\text{MS}}$ factorization scheme could be removed by using the ZERO factorization scheme, in which all NLO splitting functions vanish, and therefore all NLO corrections are included in hard scattering cross-sections. Attaching formally LO initial state parton showers to NLO hard scattering cross-sections is thus consistent if we use the ZERO factorization scheme. The change of the factorization scheme employed in NLO Monte Carlo event generators requires only to transform hard scattering cross-sections from the standard $\overline{\text{MS}}$ factorization scheme to a new one and to determine parton distribution functions in the new factorization scheme. The existing algorithms for parton showering and for attaching parton showers to NLO cross-sections need not be changed.

The ZERO factorization scheme was studied in detail in [6]. Unfortunately, it has turned out that from the practical point of view, the ZERO factorization scheme cannot be applied at the NLO in the full range of $x$ needed for QCD phenomenology. Hence, it is worth trying to find some factorization scheme which is applicable without any restrictions and simultaneously sufficiently close to the ZERO factorization scheme (i.e. the corresponding NLO splitting functions are sufficiently close to zero). A factorization scheme satisfying these conditions will be called an approximately ZERO factorization scheme in the following. An approximately ZERO factorization scheme does not allow the construction of fully consistent NLO Monte Carlo event generators based on initial state parton showers that are taken formally at the LO. But its exploitation in NLO Monte Carlo event generators still makes sense because it can significantly reduce the deficiency caused by combining LO initial state parton showers with NLO hard scattering cross-sections calculated in the standard $\overline{\text{MS}}$ factorization scheme.

This paper is focused on searching for an approximately ZERO factorization scheme. This search is described in detail in the next section. The summary and conclusion are presented in section 3. The notation used in this text is the same as that in [6].

2 Searching for approximately ZERO factorization scheme

The NLO splitting functions should be as small as possible in an approximately ZERO factorization scheme. If NLO splitting functions are small, then they should have little influence on the evolution of parton distribution functions. Hence, the evolution of parton distribution functions in any factorization scheme that can be considered as an approximately ZERO factorization scheme should be close to their evolution calculated with absolutely zero NLO splitting functions. This fact can be exploited in searching for an approximately ZERO factorization scheme. Since an approximately ZERO factorization scheme is aimed at using for the description of proton collisions, it is desirable to minimize the influence of NLO splitting functions on the evolution of parton distribution functions in the case of the proton.

To quantify the influence of NLO splitting functions on the evolution of parton distribution functions in a factorization scheme FS, let us introduce a set of auxiliary parton distribution functions $D_0(x, M, FS, M_S)$ that are defined as follows:

- their evolution in the factorization scale $M$ is formally LO (i.e. the evolution is calculated with vanishing NLO splitting functions), independently of the factorization scheme FS,

\footnote{However, the NLO accuracy of some predictions, like those for total cross-sections, is not disturbed by using LO parton showers if the NLO parton distribution functions are used in the simulation of the hard scattering cross-section.}
• the initial condition of the evolution is given as
  \[ D_0(x, M = M_S, FS, M_S) = D(x, M = M_S, FS) \]

where \( D(x, M, FS) \) represents the parton distribution functions of the proton. The auxiliary “zero” parton distribution functions \( D_0(x, M, FS, M_S) \) are fully calculable from the parton distribution functions \( D(x, M, FS) \). In any factorization scheme \( FS \) that is close to the ZERO factorization scheme, the “zero” parton distribution functions \( D_0(x, M, FS, M_S) \) should be close to the parton distribution functions \( D(x, M, FS) \) for all values of \( x \) and \( M \), independently of the “starting” factorization scale \( M_S \), which specifies the initial condition of the evolution of the “zero” parton distribution functions.

An approximately ZERO factorization scheme was searched by minimizing the difference between \( D_0(x, M, FS, M_S) \) and \( D(x, M, FS) \). A small difference between \( D_0(x, M, FS, M_S) \) and \( D(x, M, FS) \) is a necessary, but not sufficient, condition for the factorization scheme \( FS \) to be close to the ZERO factorization scheme. The reason why this condition was used for searching for an approximately ZERO factorization scheme is that it takes into account the fact that an approximately ZERO factorization scheme is aimed at using for the description of proton collisions.

In \[6\], it has been shown that factorization schemes specified via the corresponding NLO splitting functions, which can be chosen at will, may have unexpected restrictions of their practical applicability — NLO splitting functions appearing at first sight as reasonable may specify a factorization scheme that cannot be applied in the full range of \( x \) relevant for QCD phenomenology. Unexpected restrictions of practical applicability are ruled out if the Mellin moments of the appropriate NLO splitting functions satisfy (see subsection 4.4 in \[6\])

\[
P_{GG}^{(0)}(n) \left( P_{QQ}^{(0)}(n) - P_{GG}^{(0)}(n) - b \right) \left( P_{QQ}^{(1)}(n) - P_{GG}^{(1)}(n, \overline{MS}) \right) + \\
+ P_{QQ}^{(0)}(n) \left( P_{QQ}^{(0)}(n) - P_{GG}^{(0)}(n) + b \right) \left( P_{QQ}^{(1)}(n) - P_{GG}^{(1)}(n, \overline{MS}) \right) - \\
- 2 P_{QQ}^{(0)}(n) P_{GG}^{(0)}(n) \left( P_{QQ}^{(1)}(n) - P_{GG}^{(1)}(n) - P_{QQ}^{(1)}(n, \overline{MS}) + P_{GG}^{(1)}(n, \overline{MS}) \right) = 0 \quad (1)
\]

for \( n \) for which

\[
b^2 - \left( P_{QQ}^{(0)}(n) - P_{GG}^{(0)}(n) \right)^2 - 4 P_{QQ}^{(0)}(n) P_{GG}^{(0)}(n) = 0 \quad \text{and} \quad \text{Re} \, n > 1. \quad (2)
\]

In the case of five massless quark flavours, the approximate values of \( n \) satisfying the preceding condition \[2\] are 1.9001 and 3.1798. The condition \[1\] depends only on singlet splitting functions, and therefore it does not put any constraints on the choice of non-singlet NLO splitting functions. Hence, the choice of non-singlet NLO splitting functions cannot cause any unexpected restrictions of practical applicability. Since an approximately ZERO factorization scheme is required to be applicable in the full range needed for QCD phenomenology, the influence of NLO splitting functions on the evolution of parton distribution functions should be minimized on a set of NLO splitting functions that satisfy the condition of practical applicability \[1\].

The difference between \( D_0(x, M, FS, M_S) \) and \( D(x, M, FS) \) was minimized on the set of factorization schemes in which the non-singlet NLO splitting functions vanish and the matrix of the singlet NLO splitting functions \( P^{(1)}(x) \) is expressed as

\[
P^{(1)}(x) = P_{0}^{(1)}(x) + \sum_{k=1}^{N} \lambda_k P_k^{(1)}(x) \quad (3)
\]
where the real parameters $\lambda_k$ are completely arbitrary. All matrices in the preceding relation are square matrices of dimension 2. The set in which an approximately ZERO factorization scheme is sought is characterized by the functions $D^{(1)}_k(x), \ k \geq 0$ which have to be chosen such that the singlet NLO splitting functions $P^{(1)}_k(x)$ satisfy:

- the condition of practical applicability (1),
- $\int_0^1 x \left( P^{(1)}_{qQ}(x) + P^{(1)}_{GQ}(x) \right) \, dx = 0, \quad \int_0^1 x \left( P^{(1)}_{qQ}(x) + P^{(1)}_{GQ}(x) \right) \, dx = 0.$

Both conditions must be satisfied independently of the values of the parameters $\lambda_k$. The second condition, which is satisfied trivially in the ZERO factorization scheme, ensures that the sum of momentum fractions of all partons is independent of the factorization scale. The difference between $D_0(x, M, FS, M_S)$ and $D(x, M, FS)$ was minimized for several different choices of the functions $P^{(1)}_k(x)$.

The factorization scheme that has been found on the basis of the minimization of the difference between $D_0(x, M, FS, M_S)$ and $D(x, M, FS)$ for five massless quark flavours will be denoted as EP0 in the following. The comparison of the parton distribution functions $D(x, M, EP0)$ to the “zero” parton distribution functions $D_0(x, M, EP0, M_S)$ is displayed in figures 1 and 2. The non-singlet parton distribution functions are not displayed because any “zero” non-singlet parton distribution function $q^{NS}_0(x, M, EP0, M_S)$ is identical to the appropriate non-singlet parton distribution function $q^{NS}_0(x, M, EP0)$, which follows from the fact that the non-singlet NLO splitting functions vanish in the EP0 factorization scheme. The parton distribution functions are compared at small factorization scales $M$ because the differences between $D(x, M, EP0)$ and $D_0(x, M, EP0, M_S)$ increase with increasing distance from the initial condition at the factorization scale $M_S$.

The parton distribution functions in the EP0 factorization scheme were calculated as follows. Using formula (4.5) in 6, the parton distribution functions were calculated at the factorization scale $M_T = 10^7$ GeV from the $\overline{\text{MS}}$ ones that corresponded to the MSTW 2008 set 7. The parton distribution functions at a general factorization scale $M$ were then obtained by the evolution from $M_T$ to $M$ in the EP0 factorization scheme (the EP0 factorization scheme is defined only for five massless quark flavours, and therefore the evolution corresponded to this number of massless quark flavours even for factorization scales smaller than the mass of the $b$ quark). Figures 1 and 2 show that the influence of the NLO splitting functions on the evolution of the parton distribution functions corresponding to the MSTW 2008 set 7 is almost negligible in the EP0 factorization scheme. From the point of view of the evolution of the parton distribution functions of the proton, the EP0 factorization scheme is thus very close to the ZERO factorization scheme.

The comparison of the parton distribution functions $D(x, M, \overline{\text{MS}})$ to the “zero” parton distribution functions $D_0(x, M, \overline{\text{MS}}, M_S)$ is displayed in figures 3 and 4. The $\overline{\text{MS}}$ parton distribution functions that were used for the construction of these graphs corresponded to the MSTW 2008 set 7 for factorization scales greater than the mass of the $b$ quark. The parton

- Since the evolution of initial state parton showers is backward in Monte Carlo event generators, the parton distribution functions are compared at factorization scales $M$ smaller than $M_S$.
- Similarly as in the case of the EP0 factorization scheme, only the quark singlet and gluon distribution functions are displayed. However, contrary to the EP0 factorization scheme, displaying the non-singlet parton distribution functions would make sense in the case of the $\overline{\text{MS}}$ factorization scheme because non-singlet parton distribution functions $q^{NS}(x, M, \overline{\text{MS}})$ differ from the appropriate “zero” non-singlet parton distribution functions $q^{NS}_0(x, M, \overline{\text{MS}}, M_S)$. 

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Figure 1: Comparison of the quark singlet distribution functions in the EP0 factorization scheme. The differences between the curves are so small that the curves overlap. Note that the ranges of the axes of the left graphs differ from those of the right graphs.
Figure 2: Comparison of the gluon distribution functions in the EP0 factorization scheme. Note that the ranges of the axes of the left graphs differ from those of the right graphs.
distribution functions at factorization scales less than the mass of the $b$ quark were then obtained by the evolution from greater factorization scales in the $\overline{\text{MS}}$ factorization scheme for five massless quark flavours (and therefore the $\overline{\text{MS}}$ parton distribution functions differ from those of the MSTW 2008 set \cite{7} for factorization scales smaller than the mass of the $b$ quark). Figures 3 and 4 show that the effect of the NLO splitting functions on the evolution of the parton distribution functions cannot be neglected in the $\overline{\text{MS}}$ factorization scheme, especially in the low $x$ region. The influence of the NLO splitting functions on the evolution of the parton distribution functions also manifests itself by the dependence of the “zero” parton distribution functions $D_0(x, M, FS, M_S)$ on the “starting” factorization scale $M_S$. Comparing figures 1-4, one sees that the “zero” parton distribution functions $D_0(x, M, FS, M_S)$ depend on $M_S$ significantly more in the case of the $\overline{\text{MS}}$ factorization scheme than in the case of the EP0 factorization scheme, for which the dependence is almost negligible. From the point of view of the evolution of the parton distribution functions of the proton, the EP0 factorization scheme is significantly closer to the ZERO factorization scheme than the $\overline{\text{MS}}$ one.

The singlet NLO splitting functions in the EP0 factorization scheme are plotted in figures 5 and 6. The figures show that the singlet NLO splitting functions in the EP0 factorization scheme are not small in comparison with those in the $\overline{\text{MS}}$ factorization scheme \cite{8} and the singlet LO splitting functions. In the low $x$ region, the singlet NLO splitting functions in the EP0 factorization scheme even strongly dominate over the $\overline{\text{MS}}$ and LO ones. Hence, the EP0 factorization scheme cannot be regarded as a factorization scheme close to the ZERO factorization scheme. The little influence of the singlet NLO splitting functions on the evolution of the parton distribution functions of the proton in the EP0 factorization scheme is thus not a consequence of the closeness of the singlet NLO splitting functions to zero, but it is a consequence of their suitable shape.

Besides the EP0 factorization scheme, other factorization schemes in which the influence of the NLO splitting functions on the evolution of the parton distribution functions of the proton is almost negligible have been found. However, in all these factorization schemes the behaviour of NLO splitting functions and parton distribution functions is similar to that in the EP0 factorization scheme. If the functions $P^{(1)}_k(x)$ in formula (3) were chosen in such a way that they did not allow the singlet NLO splitting functions $P^{(1)}(x)$ to be large in absolute value in the low $x$ region, then no NLO splitting functions with sufficiently small influence on the evolution of the parton distribution functions of the proton in the corresponding factorization scheme were found. It thus seems that in order that NLO splitting functions have little influence on the evolution of the parton distribution functions of the proton, which is a necessary condition that the factorization scheme specified by them be close to the ZERO factorization scheme, they have to be large in the low $x$ region (provided that they satisfy the condition of practical applicability \cite{1}). But large values of NLO splitting functions are in contradiction with the closeness to the ZERO factorization scheme. The results of searching for an approximately ZERO factorization scheme based on the minimization of the difference between $D_0(x, M, FS, M_S)$ and $D(x, M, FS)$ thus indicate that there is no factorization scheme which has no restrictions of its practical applicability at the NLO and simultaneously is sufficiently close to the ZERO factorization scheme. This conclusion is also confirmed by the results of a direct minimization of the singlet NLO splitting functions $P^{(1)}(x)$ given by formula (3) because the NLO splitting functions that have been obtained by the direct minimization do not have a negligible influence on the evolution of the parton distribution functions of the proton, and therefore the corresponding factorization schemes cannot be considered as close.
Figure 3: Comparison of the quark singlet and gluon distribution functions in the $\overline{\text{MS}}$ factorization scheme for large $x$. 
Figure 4: Comparison of the quark singlet and gluon distribution functions in the $\overline{\text{MS}}$ factorization scheme.
Figure 5: Comparison of singlet LO and NLO splitting functions for five massless quark flavours. The singlet NLO splitting functions are plotted for the \( \overline{\text{MS}} \) and EP0 factorization scheme.
Figure 6: Comparison of singlet LO and NLO splitting functions at low $x$ for five massless quark flavours. The singlet NLO splitting functions are plotted for the $\overline{\text{MS}}$ and EP0 factorization scheme. Note that the singlet LO splitting functions and the singlet NLO splitting functions in the $\overline{\text{MS}}$ factorization scheme are multiplied by 100.
to the ZERO factorization scheme.

3 Summary and conclusion

A factorization scheme suitable for current NLO Monte Carlo event generators is the ZERO factorization scheme because its employment makes the combination of formally LO initial state parton showers and NLO hard scattering cross-sections consistent. But it has turned out [6] that the ZERO factorization scheme is not applicable in the full range of $x$ needed for QCD phenomenology. The deficiency of current NLO Monte Carlo event generators lying in combining formally LO initial state parton showers and NLO hard scattering cross-sections can thus be removed by means of choosing a suitable factorization scheme only in a certain kinematic region in which the ZERO factorization scheme is applicable. Since this region covers, for instance, the production of heavy objects, which is important in searches for new physics, the use of the ZERO factorization scheme makes sense despite its limited range of practical applicability. However, if we require applicability in the full range relevant for QCD phenomenology, then the freedom in the choice of the factorization scheme does not allow us to remove the mentioned deficiency of current NLO Monte Carlo event generators because of the limited practical applicability of the ZERO factorization scheme. Hence, we have tried to find some factorization scheme which is applicable at the NLO in the full range needed for QCD phenomenology and simultaneously sufficiently close to the ZERO factorization scheme. Such a factorization scheme could at least significantly reduce the mentioned deficiency of current NLO Monte Carlo event generators.

We have found NLO splitting functions which satisfy the condition of practical applicability [1] and the influence of which on the evolution of the parton distribution functions of the proton is almost negligible. However, these NLO splitting functions are not small in comparison with those in the $\overline{\text{MS}}$ factorization scheme, and therefore the corresponding factorization scheme cannot be regarded as a factorization scheme close to the ZERO factorization scheme. Moreover, it has turned out that the condition of practical applicability [1] does not allow NLO splitting functions to be significantly smaller (in the absolute value) than those in the $\overline{\text{MS}}$ factorization scheme. The deficiency of current NLO Monte Carlo event generators lying in combining formally LO initial state parton showers and NLO hard scattering cross-sections can thus not be significantly reduced by means of choosing a suitable factorization scheme if we require applicability in the full range relevant for QCD phenomenology.

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