Soft gluons and gauge-invariant subtractions in NLO parton-shower Monte Carlo event generators

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Abstract: We address the problem of decomposing graphs in perturbative QCD into terms associated with particular regions. Motivated by asking how to incorporate next-to-leading order (NLO) QCD corrections in parton-shower algorithms, we require that: (a) The integrand for the hard part is to be integrable even if the corrections are applied to a process that is not infrared and collinear safe. (b) The splitting between the terms should be defined gauge-invariantly. (c) The dependence on cut-offs should obey homogeneous evolution equations. In the context of one-gluon-emission graphs for deep inelastic scattering, we explain a subtractive technique that is based on gauge-invariant Wilson-line operators. Appropriate organization of subtractions involving the soft region allows a connection to previous work where evolution equations with respect to the directions of the Wilson lines have been derived.

Keywords: QCD, NLO Computations.
1. Introduction

Current parton-shower Monte Carlo event generators are essentially leading-order (LO) QCD tools. For precision phenomenology at present and future high-energy colliders, it is valuable to be able to go beyond this level of approximation [1]. Although there are a number of treatments of various next-to-leading-order (NLO) effects in event generators (see [2, 3, 4, 5] and references in [1]), there is as yet no method for going beyond the leading approximation systematically. This implies that event generators are not able to incorporate fully the known NLO (and NNLO) calculations of hard scattering cross sections.

Recently, systematic subtractive procedures have been proposed [6, 7, 8] to correct this situation. An important step in the implementation of this program is to show how to decompose Feynman graphs into sums of terms over different regions; the terms are to be arranged to correspond to factors in a factorization theorem that is in a form suitable for the Monte Carlo application. In Ref. [7] an implementation was presented for a simple, but phenomenologically important case: the photon-gluon fusion process in leptoproduction. This case was simple because soft gluons do not enter at the leading power, so that leading regions do not overlap. The purpose of the present work is to show how to extend the method to decompose graphs with soft gluons and hence with overlapping leading regions. We will treat the simplest such case in leptoproduction, i.e., the photon-quark process to NLO.

A Monte Carlo event generator treats observables that are not infrared and collinear safe. So the kind of subtraction method used in Refs. [9] and [10] is not directly applicable, since it relies on the calculated observable being infrared and collinear safe. In particular we cannot use a cancellation of soft gluon contributions
between real and virtual graphs. More general factorization theorems are to be used in which the soft contributions factor instead of canceling [11], and all the factors are defined gauge-invariantly in terms of Wilson-line operators [12]. We will require that the following properties be satisfied:

(a) The integrand for the hard scattering coefficient is to be an integrable function, and not merely a distribution. Thus the hard scattering coefficient is usable even when one is calculating an infrared and collinear unsafe observable. See Eq. (3.9) for an example.

(b) The terms in the expansion of each Feynman graph should arise from matrix elements of gauge-invariant operators.

(c) In particular, the necessary cut-offs on rapidity integrations are to be defined gauge-invariantly. This involves the use of Wilson-line operators along non-lightlike directions.

(d) The evolution equations [12, 13] with respect to these cut-offs should be simple, in the sense that there should be no power-law remainder terms. That is, the equations are homogeneous, like the renormalization-group equations, rather than the Callan-Symanzik equations. This is achieved by the technique proposed in Ref. [14].

In Sec. 2 we briefly describe the framework provided by the subtraction method for Monte Carlo event generators. In Sec. 3 we treat gauge-invariant subtractions and construct the decomposition of the partonic cross section. In Sec. 4 we comment on graph-by-graph subtractions. In Sec. 5 we give conclusions.

2. Subtraction scheme

To put our result in the Monte Carlo context, we schematically represent the cross section in an event generator as

$$\sigma[W] = \sum_{\text{final states } X} W(X) \, \text{PS} \otimes \hat{H}. \quad (2.1)$$

Here $W$ is a weight function that specifies the definition of the particular cross section under consideration. The symbol PS denotes the parton shower and the symbol $\otimes$ denotes its action on the initial and final partons in the hard scattering, whose cross section is denoted by $\hat{H}$. In a standard Monte Carlo, the hard scattering is taken to the leading order, $H^{(LO)}$, and PS denotes showering from the partons in $H^{(LO)}$. In an NLO Monte Carlo, the cross section involves a structure of the form

$$\text{PS} \otimes \left[ H^{(LO)} + \alpha_s \left( H^{(NLO)} - \text{PS}_I(1) \otimes H^{(LO)} - \text{PS}_F(1) \otimes H^{(LO)} \right) \right]. \quad (2.2)$$
Here the first term in the square brackets is the LO hard-scattering function, and the second term is the subtracted NLO hard-scattering function. \( H^{(\text{NLO})} \) is the result of computing the partonic cross section from the NLO graphs, while \( \text{PS}_I(1) \) and \( \text{PS}_F(1) \) are the order \( \alpha_s \) approximations to the initial-state and final-state showering. The subtraction terms avoid double counting of events already included by showering from \( H^{(\text{LO})} \).

We will construct a decomposition of \( H^{(\text{NLO})} \) into a sum of pieces, one for each of the leading regions \( R \),

\[
H^{(\text{NLO})} = \sum_{\text{regions } R} A_H(R) + \text{nonleading power}, \tag{2.3}
\]

that holds uniformly over the whole of the phase space. Each of the pieces in (2.3) will contain counterterms that prevent double counting and provide the suppression for going outside the region in which that particular piece was originally supposed to give a good approximation to the matrix element. This is to be contrasted with approaches based on splitting the phase space in different domains and using different approximations to the matrix element in these different domains (see, e.g., Refs. [2, 3]).

Once we have established a result of the type (2.3), the term corresponding to the ultraviolet region will give precisely the subtracted hard-scattering function to be used in Eq. (2.2). The collinear terms will correspond to factors in the cross section that are associated with showering; they therefore imply the evolution kernels to be used in the showering. The soft term would correspond to a new element in the Monte Carlo, but, at the order to which we work, we will show that the soft term can be eliminated by a suitable choice of the cut-offs. This is a result analogous to one in [9]. However the results of [11] indicate that this is unlikely to be an all-order result.

Our decomposition of graphs of order \( \alpha_s \) entails a specific definition of the collinear factors, which will not necessarily coincide with the definitions used in any current event generator. However, we will not address in this paper the issue of how to obtain a showering algorithm that corresponds to our collinear terms. A correct solution of this problem will encompass known results about coherent emission of gluons and angular ordering of gluon emission [15].

3. Decomposition of partonic cross section

Let us consider deep inelastic scattering \( \gamma^* + P \rightarrow X \), in which we consider a generic cross section or observable associated with the reaction \( \gamma^*(q) + q(p) \rightarrow g(k) + q(k') \) — see Fig. 1. We denote this by \( \Sigma[\varphi] \), where \( \varphi \) is a weight function that is the product of the weight function \( W(X) \) concerned with the final state \( X \) in Eq. (2.1) and the factors in the cross section associated with the showering, including the
parton density. Thus $\phi$ contains all the infrared sensitive and nonperturbative parts of the observable.

Figure 1: DIS with quark-induced hard scattering.

We work in the $\gamma^* + \text{hadron}$ reference frame, and we use light-front coordinates $v^\mu = (v^+, v^-, v_T)$ with $v^\pm = (v^0 \pm v^3)/\sqrt{2}$. The hadron and photon momenta are $P^\mu = (P^+, m^2/2P^+, 0_T)$ and $q^\mu = (-xP^+, Q^2/2xP^+, 0_T)$. Then we parameterize the gluon momentum $k$ as

$$k^\mu = \left( \alpha xP^+, \beta \frac{Q^2}{2xP^+}, |k_T| \hat{\phi} \right),$$

where $\hat{\phi}$ is a unit transverse vector at azimuthal angle $\phi$.

For our calculation, the external partons are on-shell, and the incoming quark $p$ has zero transverse momentum, so that $\Sigma$ can be written as follows:

$$\Sigma[\phi] = \int_0^\infty d\alpha \int_0^\infty d\beta \int_0^{2\pi} \frac{d\phi}{2\pi} \varphi(x, Q^2, \alpha, \beta, \phi) J(x, \alpha, \beta) M(\alpha, \beta).$$

Here, $J$ is the Jacobian factor

$$J(x, \alpha, \beta) = \frac{1}{16\pi^2} \frac{1}{1 + \alpha - \beta} \Theta \left( \frac{1-x}{x} - \alpha \right) \Theta \left( 1 - \frac{x}{1-x} \alpha - \beta \right),$$

and $M$ is the next-to-leading-order matrix element for $\gamma^* q$ obtained by contracting the photon Lorentz indices with the projector corresponding to the structure function $F_2$ [16]

$$M = 4 e_q^2 g_s^2 C_F M(\alpha, \beta), \quad M(\alpha, \beta) = (1 - \beta)^2 \frac{1 + (1 + \alpha - \beta)^2}{\alpha \beta (1 + \alpha - \beta)} + 2 + 6 \frac{(1 - \beta)^2}{1 + \alpha - \beta}. $$

The physical region for $\alpha, \beta$ is the interior of the triangle in Fig. 2.

Standard arguments [17] determine the infrared sensitive regions contributing to the leading power behavior of $\Sigma[\phi]$, which are located on Fig. 2 as follows: The region in which the gluon is collinear to the initial state is a neighborhood of the axis
\( \beta = 0 \), the region in which the gluon is collinear to the final state is a neighborhood of the axis \( \alpha = 0 \), and the soft region is a neighborhood of the origin \( \alpha = 0, \beta = 0 \). The truly hard region lies away from the \( \alpha = 0 \) and \( \beta = 0 \) axes.

To obtain a decomposition for \( \Sigma \) of the type of Eq. (2.3), we now employ the technique of Ref. [14]. This generalizes the R-operation techniques of renormalization. (See Ref. [18] for a related approach.) To ensure that the procedure is gauge-invariant, each of the terms in the right hand side of Eq. (2.3) is constructed from matrix elements involving Wilson line operators,

\[
V_I(n) = \mathcal{P} \exp \left( ig \int_{-\infty}^{0} dy \, n \cdot A(y) \right), \quad V_F(n) = \mathcal{P} \exp \left( ig \int_{0}^{+\infty} dy \, n \cdot A(y) \right),
\]

(3.5)

with suitable directions \( n \) for the lines. Evolution equations in \( n \) enable one to connect the results corresponding to different directions [12, 13, 14]. We define lightlike vectors \( \hat{p} = (1, 0, \mathbf{0}_T) \), \( \hat{p}' = (0, 1, \mathbf{0}_T) \). We will also use non-lightlike vectors \( u = (u^+, u^-, \mathbf{0}_T) \), \( u' = (u'^+, u'^-, \mathbf{0}_T) \), all of whose components are positive. It is convenient to define \( \eta = (2x^2P^2/Q^2)u^-/u^+ \), and \( \eta' = (Q^2/2x^2P^2)u'^+/u'^- \).

As in [14], we start with the smallest region, the soft region \( \alpha, \beta \to 0 \), and determine the corresponding contribution to the matrix element (3.4):

\[
M_S(\alpha, \beta) = \frac{2}{\alpha \beta} - \frac{2}{(\alpha + \eta' \beta) \beta} - \frac{2}{\alpha (\beta + \eta \alpha)}. \quad (3.6)
\]

Observe that the first term in the right hand side of this formula is just obtained by taking the soft approximation to Eq. (3.4). It can be thought of as the one-loop contribution to the square of a vacuum–to–gluon matrix element of a product of eikonal Wilson lines taken along lightlike directions \( \hat{p}, \hat{p}' \) [14]. This first term reproduces the behavior of the matrix element \( M \) when \( \alpha \) and \( \beta \) simultaneously approach zero. But there are also logarithms in its integral associated with the collinear regions where \( \alpha/\beta \) or \( \beta/\alpha \) go to zero. The subtractions provided by the other two terms conveniently cancel these regions. They can be derived from operators analogous to those for the first term, except for replacing one of the lightlike eikonal lines by a line along a non-lightlike direction. In particular, the second term subtracts
the divergence from a region collinear to the initial state, i.e., from the region \( \beta/\alpha \to 0 \). At the same time, the non-lightlike vector \( u' \) in this term provides a cut-off on the region of small \( \alpha \). Similarly, the third term in Eq. (3.6) subtracts the divergence from the region collinear to the final state, i.e., from the region \( \alpha/\beta \to 0 \).

Next we construct terms for the collinear regions. By applying a treatment analogous to that for the soft region, we arrive at

\[
M_I(\alpha, \beta) = \frac{1}{\beta} \left( 1 + \frac{(1 + \alpha)^2}{\alpha (1 + \alpha)} \right) - \frac{2}{\alpha \beta} + \frac{2}{(\alpha + \eta' \beta)} = \frac{1}{\beta} \left( \frac{\alpha}{1 + \alpha} + \frac{2}{\alpha + \eta' \beta} \right)
\]

(3.7)

for the region collinear to the initial state, and

\[
M_F(\alpha, \beta) = \frac{1}{\alpha} \left( \frac{1 - \beta}{\beta} + (1 - \beta)^3 \right) - \frac{2}{\alpha \beta} + \frac{2}{\alpha (\beta + \eta \alpha)}
\]

\[
= \frac{1}{\alpha} \left( -4 + 3 \beta - \beta^2 + \frac{2}{\beta + \eta \alpha} \right)
\]

(3.8)

for the region collinear to the final state. The first term of the expression in the middle in each of these equations is the unsubtracted collinear approximation to the original matrix element (i.e., the \( \beta \to 0 \) or \( \alpha \to 0 \) limit of \( M \)). We will comment below on the subtraction terms.

The fully subtracted matrix element, associated with the hard region, is then given by

\[
M_H(\alpha, \beta) = M - M_S - M_I - M_F
\]

\[
= (1 - \beta)^2 \frac{1 + (1 + \alpha - \beta)^2}{\alpha \beta (1 + \alpha - \beta)} + 2 \frac{(1 - \beta)^2}{1 + \alpha - \beta} - \frac{1}{\beta} \frac{1 + (1 + \alpha)^2}{\alpha (1 + \alpha)} - \frac{1}{\alpha} \frac{1 + (1 - \beta)^2}{\beta (1 - \beta)} + \frac{2}{\alpha \beta}
\]

\[
= \beta + \frac{\alpha}{(1 + \alpha)(1 + \alpha - \beta)} + \frac{6(1 - \beta)^2}{(1 + \alpha - \beta)}
\]

(3.9)

This matrix element is finite in all of the infrared regions. It can be safely integrated down to \( \alpha = 0 \) or \( \beta = 0 \). Moreover, it is independent of the choice of the non-lightlike directions \( u, u' \): the dependence on \( \eta, \eta' \) has canceled in Eq. (3.9).

Eqs. (3.6)–(3.9) achieve a decomposition of the type (2.3) for the original matrix element. There is one term for each of the leading regions — in particular, a soft term. We now ask: can we reorganize it in a way that is suited for a parton-shower algorithm, such as, e.g., the algorithm [19] used in the event generators [20]?

The soft term can be eliminated by choosing the vectors \( u \) and \( u' \) so that \( \eta \eta' = 1 \); then there are only collinear terms, as is appropriate to match the structure of the parton-shower Monte Carlo algorithm, which has only initial-state or final-state branchings. The symmetric choice \( \eta = \eta' = 1 \) gives

\[
M_I^{(\text{MC})}(\alpha, \beta) = \frac{1}{\beta} \frac{1 + (1 + \alpha)^2}{\alpha (1 + \alpha)} - \frac{1}{\alpha} \frac{2}{\alpha + \beta}
\]

(3.10)
\[ M_F^{(MC)}(\alpha, \beta) = \frac{1}{\alpha} \frac{1 + (1 - \beta)^2}{\beta} (1 - \beta) - \frac{1}{\beta} \frac{2}{\alpha + \beta}. \]  

(3.11)

All of the infrared contributions are now associated with configurations that are either collinear to the initial state or collinear to the final state. We have inserted superscripts in the left hand sides of Eqs. (3.10) and (3.11) to indicate that this particular choice of the non-lightlike directions gives rise to a structure that corresponds to that of Monte Carlo algorithms.

Eq. (3.9) determines the form of the counterterms to be used in the matrix element; Eqs. (3.10) and (3.11) determine the form of the counterterms to be used in the showering. The subtracted NLO matrix element (3.9) only receives contributions from the truly ultraviolet region. As for the modification to the showering, consider Eq. (3.10). \( M_I^{(MC)} \) is associated with the first branching from the initial state. As noted below Eq. (3.8), the first term in the right hand side is obtained from taking the collinear approximation \( \beta \to 0 \) to the original matrix element. The coefficient of \( 1/\beta \) is the standard quark \( \to \) quark splitting kernel:

\[ \frac{1 + (1 + \alpha)^2}{\alpha (1 + \alpha)} = P_{qq} \left( \frac{1}{1 + \alpha} \right). \]  

(3.12)

This first term corresponds to the standard form of the showering. It gives a good approximation in the initial-state collinear region, i.e., \( \beta \sim 0 \). The second term in the right hand side of Eq. (3.10), on the other hand, is non-standard. It effectively provides a cut-off when \( \alpha \to 0 \). Note that the second term is suppressed in the collinear region \( \beta \to 0 \) at fixed \( \alpha \). That is, the modified showering coincides with the usual one in the collinear limit and differs from it away from the collinear limit. Analogous remarks can be made based on the formula (3.11) associated with the final state.

Observe that if one regulated the \( \alpha \to 0 \) behavior of the first term in Eq. (3.10) by subtracting its \( \alpha \to 0 \) limit, given by \( 2/(\alpha \beta) \), this would bring about an extra \( \beta \to 0 \) singularity. This would not be suited for our application in a Monte Carlo algorithm. In contrast, the second term in Eq. (3.10) represents precisely what is, from our point of view, a better choice of a counterterm: it subtracts the \( \alpha \to 0 \) singularity without introducing any extra singular behavior at \( \beta \to 0 \).

Note also that this counterterm cuts off the integration over the region of small \( \alpha \) at a value of order \( \beta \): the leading behavior of \( M_I^{(MC)} \) for small \( \alpha \) is of the type

\[ \frac{2}{\beta (\alpha + \beta)} + \text{regular terms in } \alpha. \]  

(3.13)

Then we see that the procedure based on gauge-invariant subtractions that we have just applied, compared to the cut-off method, tells us precisely where the cut-off is to be placed. The position of the cut-off on \( \alpha \) turns out to be \( \beta \)-dependent. In more physical terms, this indicates that the cut-off to be applied in the initial-state shower
and the cut-off to be applied in the final-state shower are not to be set independently, but they are related.

4. Graph-by-graph subtractions

In our calculational example, the form of the four terms was determined by requiring them to be obtainable from matrix elements of gauge-invariant operators. However, the procedure can be applied graph-by-graph, as we will now explain. The basis of this procedure is the derivation of factorization for soft factors given in Refs. [11, 12].

Consider the connection of a gluon to a subgraph that consists of lines that are all collinear in the + direction. This factor we denote by $J^\mu(k)$, where $\mu$ is the Lorentz index that couples to the gluon. In a region where the gluon is either soft or collinear in the opposite direction, it is a good approximation to replace $J^\mu$ by its + component, and to replace the momentum $k$ in $J$ by its − component. Multiplying and dividing by $k^-$ gives

$$J^\mu(k) \mapsto g_+^\mu J^+(0, k^-, 0_T) = g_+^\mu \frac{1}{k^-} [k^- J^+(0, k^-, 0_T)].$$

Since the last factor is of the form of a gluon Green function contracted with the gluon’s momentum, a Ward identity can be applied. Then after a sum over all relevant graphs we obtain factors corresponding to matrix elements of operators that include path-ordered exponentials [12].

When this replacement is made, together with the corresponding replacement for gluonic connections to the opposite “jet” factor, some of the terms have new divergences when the gluon’s rapidity goes to $+\infty$ or $-\infty$, as explained earlier and in Ref. [14]. These divergences are cancelled by further subtractions that are constructed by manipulations on the $1/k^-$ and $1/k^+$ factors, to give a result like Eq. (3.6).

5. Conclusions

In conclusion, the above calculation tells us how to organize the subtractions in situations in which soft gluons are present and both initial-state and final-state branchings contribute. This is one of the issues that have to be dealt with to construct NLO Monte Carlo event generators. The subtractive technique [14] used for this calculation is based on graph-by-graph R-operation methods and enforces gauge invariance by relating the counterterms to matrix elements of Wilson-line operators. The calculations of this paper do not address the issue of how to generate the whole shower corresponding to the subtracted collinear terms. The investigation of this is left to future work.
Acknowledgments

This research is supported in part by the US Department of Energy under grant No. DE-FG02-90ER-40577.

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