Progress in NNLO calculations for scattering processes

E. W. N. Glover*

Institute for Particle Physics Phenomenology, University of Durham
South Road, Durham, DH1 3LE, U.K.
E-mail: E.W.N.Glover@durham.ac.uk

ABSTRACT: The various motivations for improving the perturbative prediction to next-to-next-to-leading order (NNLO) for basic scattering processes in proton-(anti)proton, electron-proton and electron-positron scattering are discussed in detail. Recent progress in the field of next-to-next-to-leading order calculations is reviewed.

KEYWORDS: QCD, Jets, LEP HERA and SLC Physics, NLO and NNLO Computations.

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1. Why NNLO calculations are important.

In the past decade, QCD has become a quantitative science and comparisons of experimental data with NLO QCD have become the standard. However, there are many reasons why extending perturbative calculations to NNLO is vital in reducing the theoretical uncertainty. In the following we list six of them.

1.1 Renormalisation scale uncertainty

In many cases, the uncertainty from the pdf’s and from the choice of the renormalisation scale $\mu_R$ give uncertainties that are as big as or bigger than the experimental errors. Of course, the theoretical prediction should be independent of $\mu_R$. However, a scale dependence is introduced by truncating the perturbative series. The change due to varying the scale is formally higher order. If an observable $O\!bs$ is known to order $\alpha_s^N$,  

$$O\!bs = \sum_0^N A_n(\mu_R) \alpha_s^n(\mu_R),$$

then,  

$$\frac{\partial}{\partial \ln(\mu_R^2)} O\!bs = \mathcal{O} \left( \alpha_s^{N+1} \right).$$

Often the uncertainty due to uncalculated higher orders is estimated by varying the renormalisation scale upwards and downwards by a factor of two around a typical hard scale in the process. However, the variation only produces copies of the lower order terms, e.g.

$$O\!bs = A_1 \alpha_s(\mu_R) + A_2 + b_0 A_1 \ln \left( \frac{\mu_R^2}{\mu_0^2} \right) \alpha_s^2(\mu_R).$$

$A_2$ will generally contain infrared logarithms and constants that are not present in $A_1$ and therefore cannot be predicted by varying $\mu_R$. For example, $A_1$ may contain infrared logarithms $L$ up to $L^2$, while $A_2$ would contain these logarithms up to $L^4$. $\mu_R$ variation is only an estimate of higher order terms and a large variation probably means that predictable higher order terms are large.

To illustrate the improvement in scale uncertainty that may occur at NNLO, let us consider the production of a central jet in $p\bar{p}$ collisions. The renormalisation scale dependence is entirely predictable, 

$$\frac{d\sigma}{dE_T} = \alpha_s^2(\mu_R) A_0 + \alpha_s^3(\mu_R) \left( A_1 + 2b_0 A_0 \right) + \alpha_s^4(\mu_R) \left( A_2 + 3b_0 L A_1 + (3b_0^2 L^2 + 2b_1 L) A_0 \right)$$
Figure 1: Single jet inclusive distribution at $E_T = 100$ GeV and $0.1 < |\eta| < 0.7$ at $\sqrt{s} = 1800$ GeV at LO (green), NLO (blue) and NNLO (red). The solid and dashed red lines show the NNLO prediction if $A_4 = 0$, $A_4 = \pm A_3^2/A_2$ respectively. The same pdf’s and $\alpha_s$ are used throughout.

with $L = \log(\mu_R/E_T)$. $A_2$ and $A_3$ are the known LO and NLO coefficients while $A_4$ is the presently unknown NNLO term. Inspection of Fig. 1 shows that the scale dependence is systematically reduced by increasing the number of terms in the perturbative expansion. At NLO, there is always a turning point where the prediction is insensitive to small changes in $\mu_R$. If this occurs at a scale far from the typically chosen values of $\mu_R$, the $K$-factor (defined as $K = 1 + \alpha_s(\mu_R)A_3/A_2$) will be large. At NNLO the scale dependence is clearly significantly reduced, although a more quantitative statement requires knowledge of $A_4$.

1.2 Factorisation scale dependence

Similar qualitative arguments can be applied to the factorisation scale inherent in perturbative predictions for quantities with initial state hadrons. Including the NNLO contribution reduces the uncertainty due to the truncation of the perturbative series.

1.3 Jet algorithms

There is also a mismatch between the number of hadrons and the number of partons in the event. At LO each parton has to model a jet and there is no sensitivity to the size of the jet cone. At NLO two partons can combine to make a jet giving sensitivity to the shape and size of the jet cone. Perturbation theory is starting to reconstruct the parton shower within the jet. This is further improved at NNLO where up to three partons can form a single jet, or alternatively two of the jets may be formed by two partons. This should lead to a better matching of the jet algorithm between theory and experiment.

1.4 Transverse momentum of the incoming partons

At LO, the incoming particles have no transverse momentum with respect to the beam so that the final state is produced at rest in the transverse plane. At NLO,
Figure 2: The average value of $\langle 1 - T \rangle$ given by Eq. 1.1 showing the NLO prediction (dashed red), the NLO prediction with power correction of $\lambda = 1$ GeV (solid blue) and an NNLO estimate with $A_3 = 3$ and a power correction of $\lambda = 0.5$ GeV (green dots).

single hard radiation off one of the incoming particles gives the final state a transverse momentum kick even if no additional jet is observed. In some cases, this is insufficient to describe the transverse momentum distribution observed in the data and one appeals to the intrinsic transverse motion of the partons confined in the proton to provide an enhancement. However, at NNLO, double radiation from one particle or single radiation off each incoming particle gives more complicated transverse momentum to the final state and should provide a better, and more theoretically motivated, description of the data.

1.5 Power corrections

Current comparisons of NLO predictions with experimental data generally reveal the need for power corrections. For example, in electron-positron annihilation, the experimentally measured average value of 1-Thrust lies well above the NLO predictions. The difference can be accounted for by a $1/Q$ power correction. While the form of the power correction can be theoretically motivated, the magnitude is generally extracted from data and, to some extent, can be attributed to uncalculated higher orders. Including the NNLO may therefore reduce the size of the phenomenological power correction needed to fit the data.

Before the calculation of the NNLO contribution it is not possible to make a more quantitative statement. However to illustrate the qualitative point, let us take the simple example of an observable like $\langle 1 - T \rangle$ which can be modelled by the simplified series,

$$\langle 1 - T \rangle = 0.33\alpha_s(Q) + 1.0\alpha_s(Q)^2 + A_3\alpha_s(Q)^3 + \frac{\lambda}{Q},$$

with $\alpha_s(Q) \sim 6\pi/23/\log(Q/\Lambda)$ and $\Lambda = 200$ MeV. Fig 2 shows the NLO perturbative prediction $A_3 = 0, \lambda = 0$ as well as the NLO prediction combined with a power correction, $A_3 = 0, \lambda = 1$ GeV which can be taken to model the data. If the
Kinematic scales | Tree | One-loop | Two-loop
---|---|---|---
\frac{(u^2 + t^2)}{s^2} & √ & √ & √
\frac{(u^2 - t^2)}{s^2}, 1 & √ & √
\frac{u^3}{s^2 t}, \frac{t^3}{s^2 u} & & √

Table 1: Ratios of kinematic scales for the scattering of unlike massless quarks, \( q\bar{q} \rightarrow q'\bar{q}' \)

NNLO coefficient turns out to be positive (which is by no means guaranteed), then the size of the power correction needed to describe the data will be reduced. For example, if we estimate the NNLO coefficient as \( A_3 = 3 \), which is large but perhaps not unreasonably, then the NLO prediction plus power correction can almost exactly be reproduced with a power correction of the same form, but \( \lambda = 0.6 \) GeV. We are effectively trading a contribution of \( \mathcal{O}(1/Q) \) for a contribution of \( 1/\log^3(Q/\Lambda) \). At present the data is insufficient to distinguish between these two functional forms.

1.6 The shape of the prediction

It is an oft repeated statement that NLO predictions affect the normalisation of the leading order prediction but not the shape of the distribution. This is wrong for two reasons. First, as indicated in Table 1, the loop contribution gets new kinematic contributions. Of course, each ratio of kinematic scales is further multiplied by logarithms and polylogarithms of ratios of scales. Second, as the number of final state particles increases, the allowed phase space is enlarged - leading, for example, to lower values of thrust in electron-positron annihilation and jet production at higher rapidities in hadron-hadron collisions. These effects simply cannot be modelled by scaling the lowest order cross section.

1.7 Parton densities at NNLO

Consistent NNLO predictions for processes involving hadrons in the initial state require not only the NNLO hard scattering cross sections, but also parton distribution functions which are accurate to this order.

The evolution of parton distributions is governed at NNLO by the three-loop splitting functions, which are not fully known at present, although the expectation is that they will be determined shortly, see Ref. [1] and references therein.

The determination of NNLO parton distributions requires a global fit to the available data on a number of hard scattering observables, with all observables computed consistently at NNLO. At present, the NNLO coefficient functions are available for
the inclusive Drell-Yan process \cite{2, 3} and for deep inelastic structure functions \cite{4}. These two observables are by themselves insufficient to fully constrain all parton species. In particular large transverse energy jet production in hadron-hadron collisions provides a vital constraint on the gluon at large $x$ and therefore requires the determination of the single jet inclusive cross section at NNLO.

2. Recent progress in the field

There has been enormous progress in calculating two-loop matrix elements since the previous “Loops and Legs” workshop in April 2000. To a large extent this has been due to breakthroughs in the calculation of two-loop master integrals with massless propagators. In tour de force calculations through the summer of 1999, Smirnov \cite{5} and Tausk \cite{6} computed the planar and non-planar double box master integrals with four on-shell legs using Mellin Barnes integrals. The other four four-point master integrals needed for the on-shell case were much easier to calculate \cite{7, 8, 9, 10, 11}.

Smirnov has applied the same Mellin Barnes technique to the case where one leg is off-shell \cite{12, 13}, however, the main breakthrough here is due to Gehrmann and Remiddi \cite{14, 15} who have provided expansions for all of the relevant master integrals by making use of differential equations for two-loop four point functions \cite{16}. For integrals with singularities through to $1/\epsilon^4$ it proved necessary to introduce two-dimensional harmonic polylogarithms in addition to the standard Nielsen polylogarithms. Numerical evaluations of the master integrals \cite{17, 18} and analytic continuations have been provided in Ref. \cite{19}.

The next major step is to reduce the tensor integrals appearing in Feynman diagram calculations to the few master integrals for which series expansions are known. The main tool here is integration-by-parts (IBP) \cite{20, 21} which, for two-loop four point integrals, generates 10 equations relating integrals with different powers of propagators. To this can be added the three Lorentz Invariance (LI) identities \cite{16}. Together, these equations represent the fact that loop integrals exhibit Poincare invariance. Together, the IBP and LI equations form a linear system that can be automatically solved with algebraic methods to relate all tensor integrals to the master integrals \cite{16, 22}.

These technological tools have allowed the computation of a whole raft of two-loop matrix elements for scattering processes with up to one off-shell leg as detailed in Table 2.

A vital check on the infrared structure of these two-loop matrix elements is given by Catani \cite{37}. In Catani’s formalism, the singular $\mathcal{O}(1/\epsilon^4)$, $\mathcal{O}(1/\epsilon^3)$, $\mathcal{O}(1/\epsilon^2)$ structure can be straightforwardly be determined while the non-logarithmic coefficient $H_2$ multiplying the $\mathcal{O}(1/\epsilon)$ can also be extracted. For some time, the origins of this formula were lost in transit, however Sterman and Tejeda-Yeomans \cite{38} have now
On-shell Process Tree Helicity
\[ e^+e^- \rightarrow \mu^+\mu^-(e^+e^-) \] \[ q\bar{q} \rightarrow q\bar{q}(q'\bar{q}') \] \[ q\bar{q} \rightarrow gg \] \[ gg \rightarrow gg \] \[ gg \rightarrow \gamma\gamma \] \[ \gamma\gamma \rightarrow \gamma\gamma \] \[ q\bar{q} \rightarrow g\gamma(\gamma\gamma) \]

Off-shell Process
\[ e^+e^- \rightarrow q\bar{q}g \]

| On-shell Process | Tree | Helicity |
|------------------|------|----------|
| \[ e^+e^- \rightarrow \mu^+\mu^-(e^+e^-) \] | [23] | \[ q\bar{q} \rightarrow q\bar{q}(q'\bar{q}') \] | [24, 25] |
| \[ q\bar{q} \rightarrow gg \] | [26] | \[ gg \rightarrow gg \] | [27] \[ 28, 29 \] |
| \[ gg \rightarrow \gamma\gamma \] | – | \[ \gamma\gamma \rightarrow \gamma\gamma \] | – \[ 30 \] |
| \[ q\bar{q} \rightarrow g\gamma(\gamma\gamma) \] | [33] |

Table 2: Current status of available two-loop amplitudes for scattering processes with all legs on-shell and with one leg off-shell

rederived it from the basis of factorisation of inter-jet and intra-jet radiation and given a more concrete explanation of how \( H_2 \) is produced.

3. What remains to be done

Of course knowledge of the two-loop amplitudes is only one of the ingredients needed in the construction of a NNLO parton level Monte Carlo. In addition we also need:

- square of the one-loop \( 2 \rightarrow 2 \) amplitudes,
- interference of tree and one-loop \( 2 \rightarrow 3 \) amplitudes,
- square of the tree-level \( 2 \rightarrow 4 \) amplitudes.

The tree level \( 2 \rightarrow 4 \) amplitudes have been known for some time, while the five point amplitudes with zero [39, 40, 41] and one [42, 43, 44, 45] off-shell legs have also been worked out.

These latter two processes contribute when either one or two of the partons are unresolved and there is a much more sophisticated infrared cancellation between

- \( n \) and \( n + 1 \) particle contributions when one particle is unresolved,
- \( n \) and \( n + 2 \) particle contributions when two particles are unresolved.

At present, a detailed method for subtracting the singularities and numerically evaluating the finite remainders has not been worked out.

Nevertheless, the prognosis is favourable. If the rate of technical development maintains its current pace, it is extremely likely that by the time of the next workshop, NNLO Monte Carlo’s will be available for some of the most basic scattering
processes, leading to a more complete and quantitative understanding of hard inter-

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