Parton level Monte Carlo at NLO

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with thanks to John Campbell / University of Glasgow

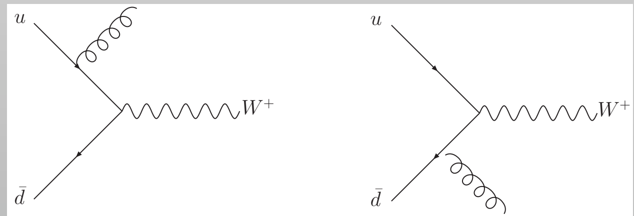
Outline

- Overview of next-to-leading order
- What NLO can do for you
- What not to expect from NLO
- Summary

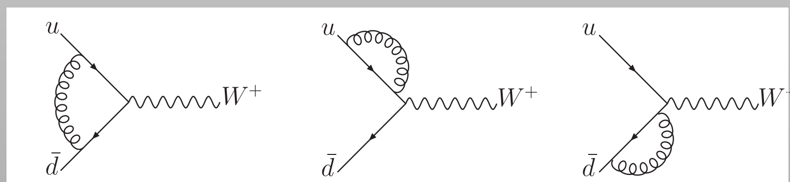
Anatomy of a NLO calculation

Next-to-leading order basics

- The perturbative expansion of an observable to one order higher in the coupling constant than the first approximation.
- Since $\alpha_{em}(M_Z) = 1/137$ and $\alpha_s(M_Z) \sim 0.12$, the corrections associated with the strong coupling of QCD are the most important ones.
- Typically the lowest order prediction is based on the calculation of tree graphs (although this is not always the case). Extra factors of the coupling are obtained by adding vertices representing the radiation of an additional gluon.
- The Feynman diagrams that must be calculated fall into two categories. For example, when calculating the cross section for the production of a W boson by the Drell-Yan mechanism at a hadron collider:



an additional gluon is radiated and is present in the final state (REAL diagrams)



a virtual gluon is emitted in one place and reabsorbed in another (VIRTUAL or ONE-LOOP diagrams)

Real diagrams

- The calculation of the real diagrams is straightforward (tree level). Applying the Feynman rules one finds the kinematic structure,

$$|\mathcal{M}|^2_{\rm real} \sim \left(\frac{s_{ug}}{s_{\bar{d}g}} + \frac{s_{\bar{d}g}}{s_{ug}} + \frac{2m_W^2\, s_{u\bar{d}}}{s_{ug}s_{\bar{d}g}} \right) .$$

- Since all particles are massless we can parametrize the final term by,

$$\frac{2m_W^2(1-\cos\theta_{u\bar{d}})}{E_g^2(1-\cos\theta_{ug})(1-\cos\theta_{\bar{d}g})}$$

  so that when combined with the phase space for the gluon emission, $\int d^4p_g \longrightarrow \int E_g dE_g\; d\cos\theta_{ug}$ we are left with expressions of the form,

$$\int \frac{dE_g\; d\cos\theta_{ug}}{E_g(1-\cos\theta_{ug})} .$$

- Thus there are logarithmic singularities when $\cos\theta_{ug} \longrightarrow 1$ (the gluon is COLLINEAR to the quark) and when $E_g \longrightarrow 0$ (the gluon is SOFT).
- This behaviour of the matrix elements is universal.

Subtraction

- In order to proceed with a NLO calculation, the infrared (collinear and soft) singularities must be isolated in some way.
- A common technique is called SUBTRACTION, with the basic idea that the singular behaviour is compensated for by a simple function that is easy to integrate analytically.
- In order to expose the singularities, we pass from four dimensions to $4 - 2\epsilon$ as an intermediate step. Schematically, this corresponds to:

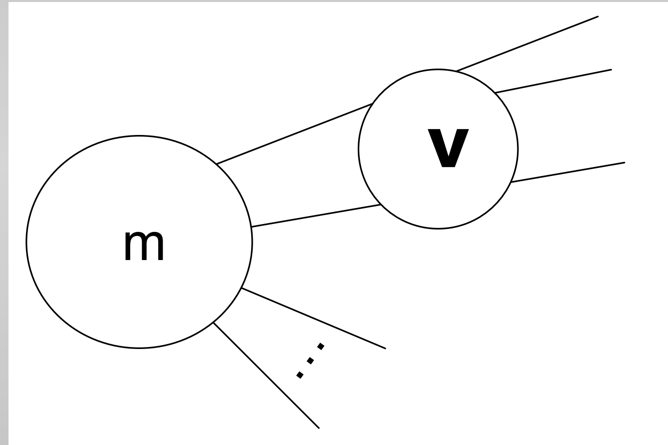
$$\mathcal{I} = \underbrace{\int_0^1 \frac{dx}{x^{1+\epsilon}} \left[\mathcal{M}(x)F(x) - \mathcal{M}(0)F(0)\right]}_{\text{finite as } x \to 0} + \underbrace{\mathcal{M}(0)F(0) \int_0^1 \frac{dx}{x^{1+\epsilon}}}_{\text{singular term}} ,$$

  where $\mathcal{M}$ represents the matrix elements and x corresponds to the energy of the gluon, for instance.
- A different subtraction term is required for each singular region of phase space. As the number of partons in the final state grows, the number of subtractions performed in the calculation increases.

Dipole Subtraction Method

$$\sigma_R = \int dPS_{m+1} \left\{ |\mathcal{M}_{m+1}|^2 F_{m+1}(\{p\}_{m+1}) - \sum_{\text{dipoles},i} \mathcal{D}_i F_m(\{p\}_{m,i}) \right\}$$

$$\begin{aligned} \mathcal{D}_i &= \langle \{p\}_{m,i} | \mathbf{V}_i | \{p\}_{m,i} \rangle \\ dPS_{m+1} &= dPS_m \, dPS_1 \\ \int dPS_1 \mathbf{V}_i &= \mathbf{I}_i \end{aligned}$$



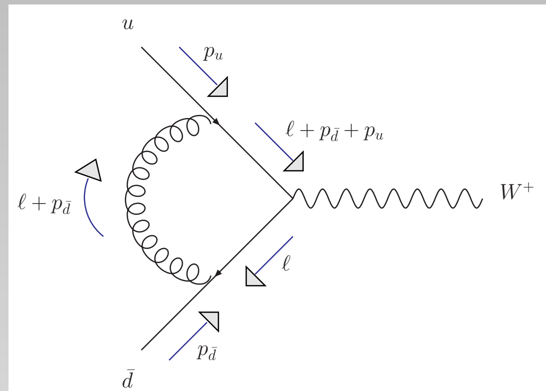
$$\int dPS_{m+1} \sum_i \mathcal{D}_i F_m(\{p\}_{m,i}) = \int dPS_m \left\langle \{p\}_m \left| \sum_i \mathbf{I}_i \right| \{p\}_m \right\rangle F_m(\{p\}_m)$$

- All analytical integrals done once and for all.

S. Catani & MHS Nucl.Phys.B485 (1997) 291

Virtual diagrams

- An arbitrary LOOP MOMENTUM ℓ is introduced, which must be integrated over to obtain a final result.
- The contribution from this diagram is,



$$\int \frac{d^4\ell \quad \mathcal{N}}{\ell^2(\ell + p_{\bar{d}})^2(\ell + p_{\bar{d}} + p_u)^2}$$

where $\mathcal{N} = \bar{u}(\bar{d})\gamma^\alpha \not{\ell} \not{\epsilon}(\not{\ell} + \not{p}_{\bar{d}} + \not{p}_u)\gamma_\alpha v(u)$.

- Evaluating these types of integrals – in particular as the number of propagators in the denominator grows and as the complexity of $\mathcal{N}$ increases – is the major challenge for NLO calculations.
- Inspecting the denominator of the integral, there is a singularity when $\ell \to -p_{\bar{d}}$, with two propagators vanishing. This occurs when the virtual gluon is SOFT.
- In fact, $\ell \propto p_{\bar{d}}$ has the same effect. In this general case, the singularity occurs when the virtual gluon is COLLINEAR to the external $\bar{d}$ quark.
- Just as when dealing with the singular configurations in the real diagrams, the singularities can be exposed by moving out of four dimensions, $d^4\ell \to d^{4-2\epsilon}\ell$.

Putting it all together

REAL	$\left\|\mathcal{M}_{u\bar{d}\to W+g}\right\|^2 - \sum(\text{singular})\left\|\mathcal{M}_{u\bar{d}\to W}\right\|^2$	FINITE
	$\left(\frac{2}{\epsilon^2}+\frac{3}{\epsilon}+\mathcal{O}(\epsilon^0)\right)\left\|\mathcal{M}_{u\bar{d}\to W}\right\|^2$	SINGULAR
VIRTUAL	$\mathcal{O}(\epsilon^0)$	FINITE
	$\left(-\frac{2}{\epsilon^2}-\frac{3}{\epsilon}\right)\left\|\mathcal{M}_{u\bar{d}\to W}\right\|^2$	SINGULAR

- The singularities from the REAL and VIRTUAL contributions are equal and opposite, so that they cancel in the sum. This is true for every properly-defined observable in any process (Bloch-Nordsieck and KLN theorems).

Putting it all together

REAL	$\left\lvert\mathcal{M}_{u\bar{d}\to W+g}\right\rvert^2 - \sum(\text{singular})\,\lvert\mathcal{M}_{u\bar{d}\to W}\rvert^2$	FINITE
	$\left(\frac{2}{\epsilon^2}+\frac{3}{\epsilon}+\mathcal{O}(\epsilon^0)\right)\,\lvert\mathcal{M}_{u\bar{d}\to W}\rvert^2$	SINGULAR
VIRTUAL	$\mathcal{O}(\epsilon^0)$	FINITE
	$\left(-\frac{2}{\epsilon^2}-\frac{3}{\epsilon}\right)\lvert\mathcal{M}_{u\bar{d}\to W}\rvert^2$	SINGULAR

- The implementation of NLO matrix elements within a Monte Carlo phase space integration program is thus divided into two contributions. For an obervable calculated from an n particle final state:
  - ⋆ Contributions containing $(n+1)$ particles, with n-particle singular configurations subtracted. As a result, this piece may be negative at any given point and its overall integral may be negative too (REAL).
  - ⋆ Contributions with exactly n particles in the final state (VIRTUAL).
- Although each contribution is separately finite, only the sum is meaningful.

Features of NLO

Normalization

- The overall cross section for each process changes at NLO. It is not guaranteed to increase, but for usual choices of scales this is indeed the case.
- The information provided by a NLO calculation is often encapsulated in the form of a $K-$factor that is the ratio of the NLO cross section to the LO one.

hadron-collider process	scale	Tevatron	LHC
W production	m_W	1.33	1.15
top pairs	m_t	1.08	1.40
$W + 1$ jet ($p_T^{\text{jet}} > 20$ GeV, $\lvert\eta^{\text{jet}}\rvert < 2.5$)	m_W	1.24	1.31
weak boson fusion (m_H=120 GeV)	m_H	1.07	1.23

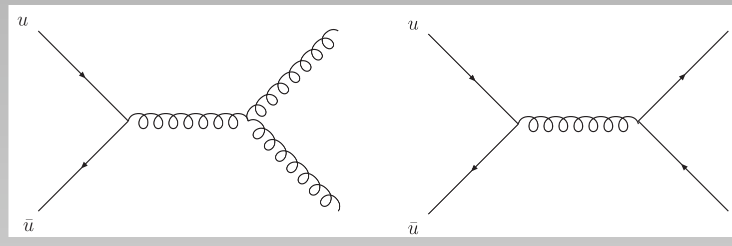
- The K-factor depends upon the process and the collider. For more complicated processes it also depends upon the cuts used to define the lowest order cross section.
- The value also depends upon input parameters such as masses and parton distribution functions. In particular, it is common practice to use leading order PDF's (α_s and evolution) in the denominator and NLO PDF's in the numerator (as in the table above).
- USE WITH CARE!

Renormalization and factorization scales

- Both of these scales (μ_R, μ_F) are introduced in order to calculate predictions in QCD perturbatively. The full result to all orders (if it could be calculated) does not depend on the values that they take.
- The renormalization scale is needed to redefine “bare” fields in terms of physical ones.
- In hadronic collisions, the factorization scale appears when absorbing collinear divergences into the parton densities. One can think of this scale as separating the soft physics inside the protons from the hard process represented by the partonic matrix elements.
- Usually both scales are chosen based on a hard scale present in the process - for example m_W, $p_T^{\rm min}$, or some factor thereof. Any reasonable value is allowed though and other strategies for choosing the scale are sometimes favoured.
- By truncating the perturbative expansion at a given order, residual dependence upon the values of μ_R, μ_F remains.

Scale example

- The single jet inclusive distribution at the Tevatron. The dominant lowest order diagrams at high E_T are shown here.



- The NLO prediction can be written schematically as,

$$\frac{d\sigma}{dE_T} = \left[\alpha_s^2(\mu_R)\,\mathcal{A} + \alpha_s^3(\mu_R)\Big(\mathcal{B} + 2b_0\log(\mu_R/E_T)\,\mathcal{A} - 2P_{qq}\log(\mu_F/E_T)\,\mathcal{A}\Big)\right]$$
$$\otimes f_q(\mu_F) \otimes f_{\bar{q}}(\mu_F).$$

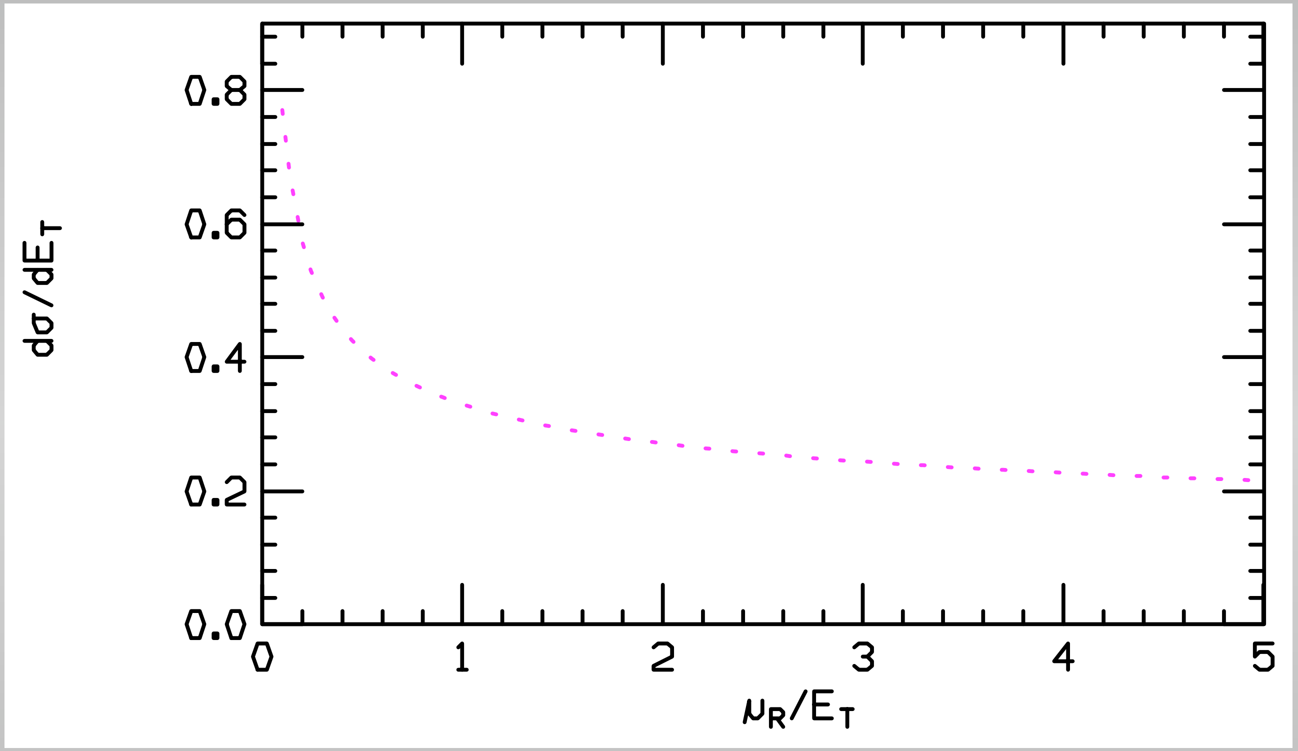
where $b_0 = (33 - 2n_f)/6\pi$ and P_{qq} is the Altarelli-Parisi splitting function.

- In this expression, the explicit logarithms involving the renormalization and factorization scales have been exposed. The remainder of the $\mathcal{O}(\alpha_s^3)$ corrections lie in the function $\mathcal{B}$.
- Using the running of the coupling α_s and the DGLAP equation describing the evolution of the splitting functions,

$$\frac{\partial\alpha_s(\mu_R)}{\partial\log\mu_R} = -b_0\alpha_s^2(\mu_R) + \mathcal{O}(\alpha_s^3)\ , \qquad \frac{\partial f_i(\mu_F)}{\partial\log\mu_F} = \alpha_s(\mu_R)P_{qq}\otimes f_i(\mu_F) + \mathcal{O}(\alpha_s^2).$$

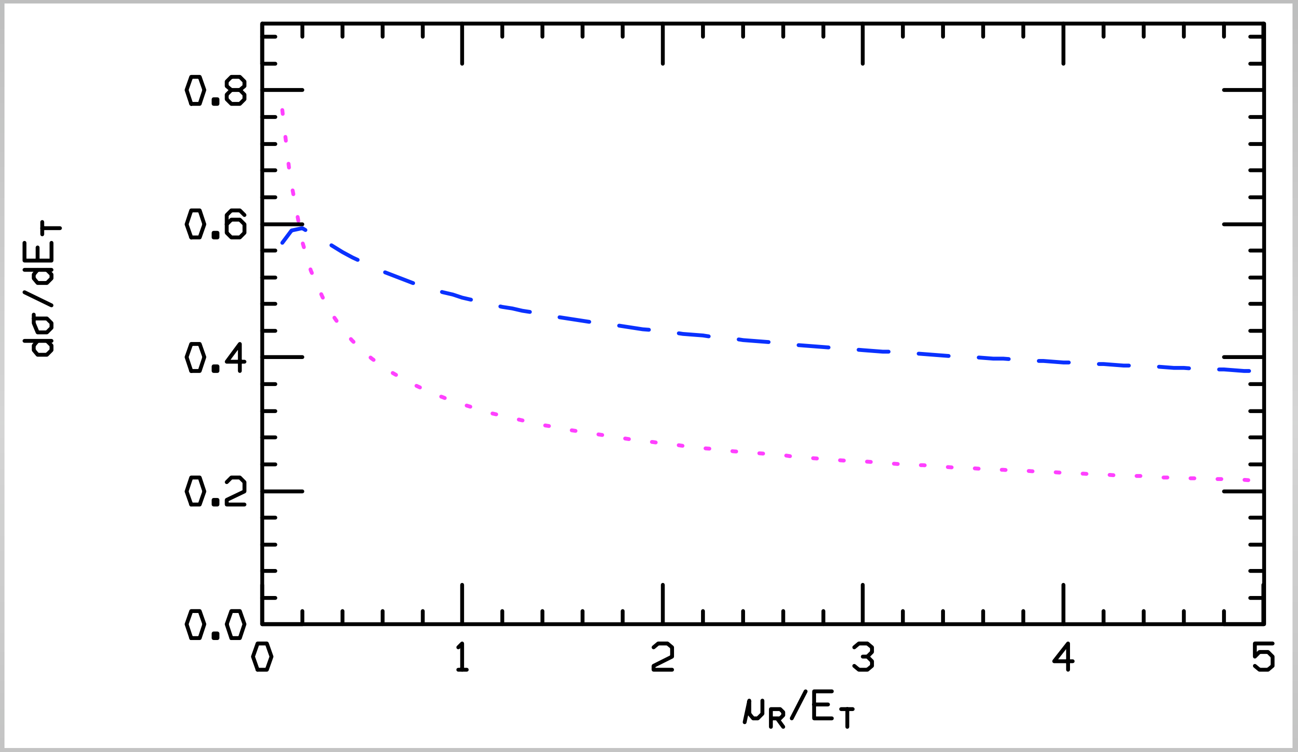
the NLO result is independent of μ_R, μ_F up to (unspecified) higher order terms.

LO scale dependence



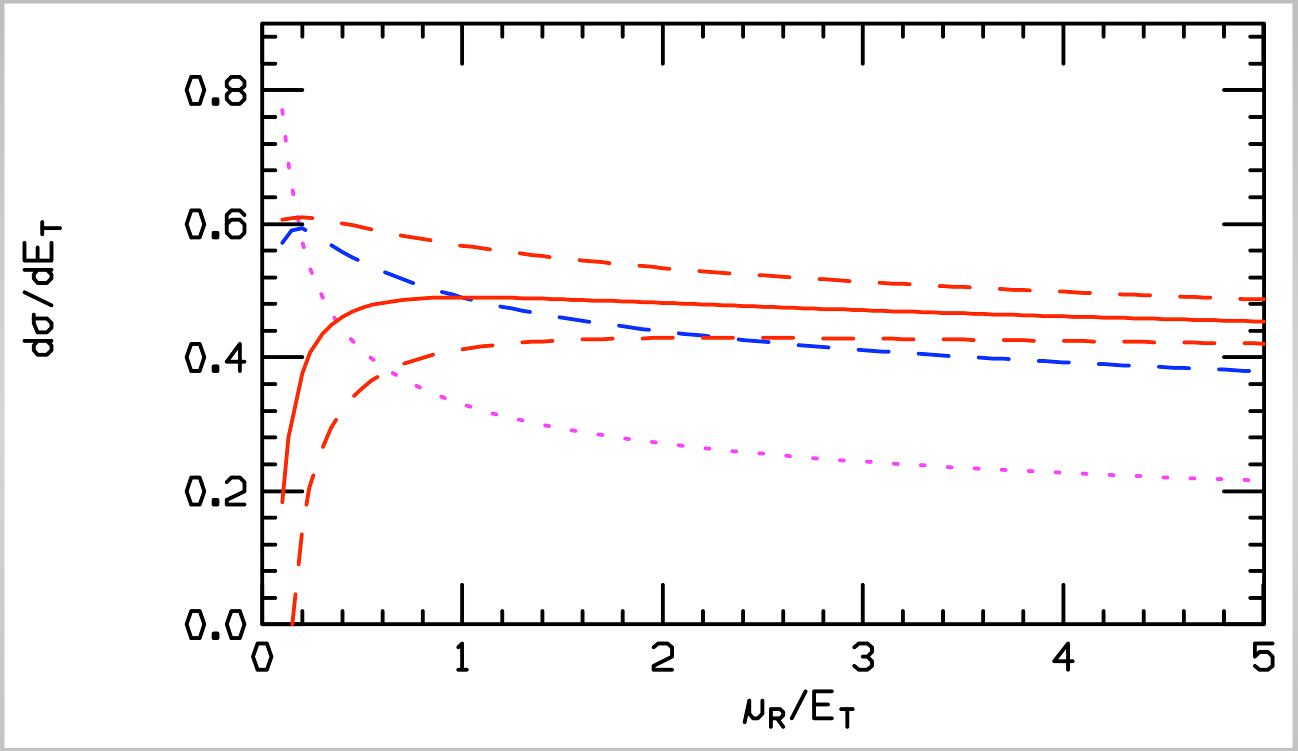
- The distribution at the Tevatron, for $E_T = 100$ GeV. The factorization scale is kept fixed at $\mu_F = E_T$ and the ratio μ_R/E_T varied about a central value of 1.
- At lowest order, the behaviour is dominated by the running of α_s. The prediction varies considerably as μ_R is changed so that the normalization of the cross section is unreliable.

NLO scale dependence



- At NLO, the growth as μ_R is decreased is softened by the logarithm that appears with coefficient α_s^3. The resulting turn-over is typical of a NLO calculation.
- As a result, the range of predicted values at NLO is much reduced and the first reliable normalization is obtained.

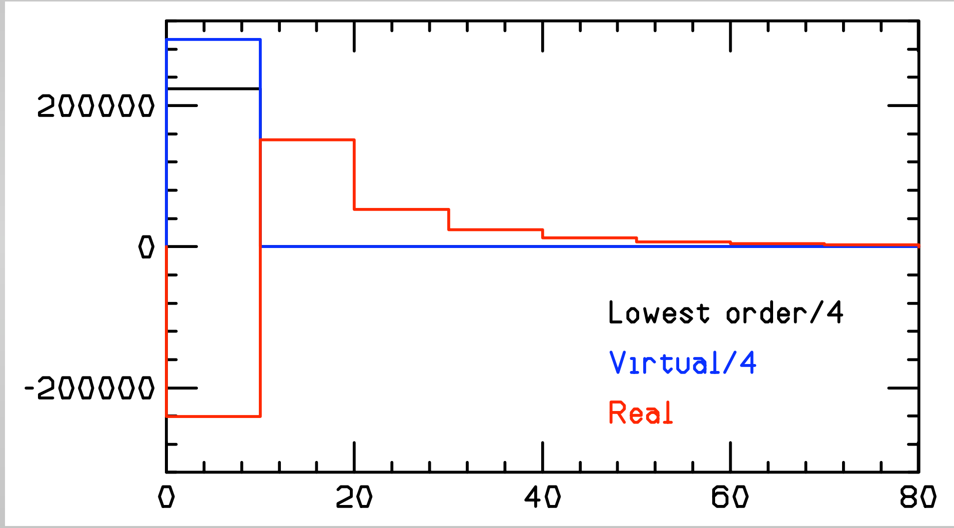
NNLO scale dependence



- The NNLO calculation for this process is not yet complete, but one can see the effect of reasonable guesses for the single unknown coefficient.
- Typical theoretical error estimate of a few percent, which is the level required for many LHC analyses.

Kinematic features

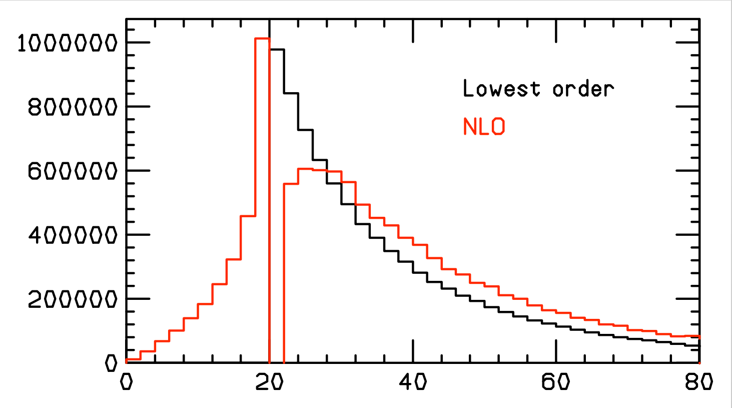
- The use of a K-factor completely washes out the important kinematic effects that the inclusion of NLO corrections introduces.
- For instance, consider the p_T of a W produced at the Tevatron.

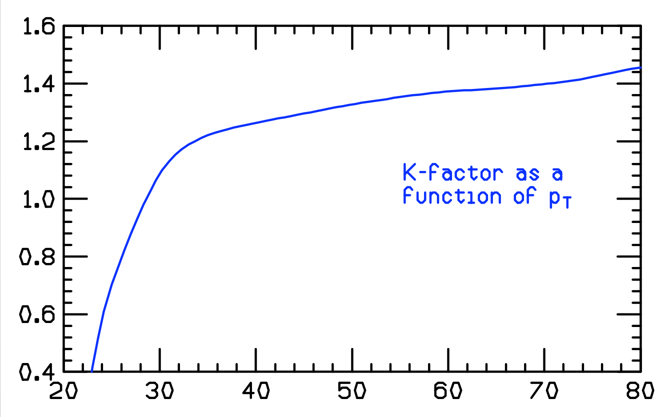


- Both the LO and VIRTUAL contributions have $2 \to 1$ kinematics. The W boson does not acquire any transverse momentum because the initial state has none.
- In the REAL calculation, some of the contributions are $2 \to 2$ processes in which the W boson transverse momentum balances against a hard parton.
- This is a trivial example, but clearly no K-factor can account for the richer kinematic structure encountered at NLO.

More complex processes

- For more complicated processes and observables, the phase space is extended but in less drastic ways.
- Consider a final state consisting of a W boson and one hard jet with a p_T above 20 GeV. At the LHC, the W boson p_T in these events is shown below.

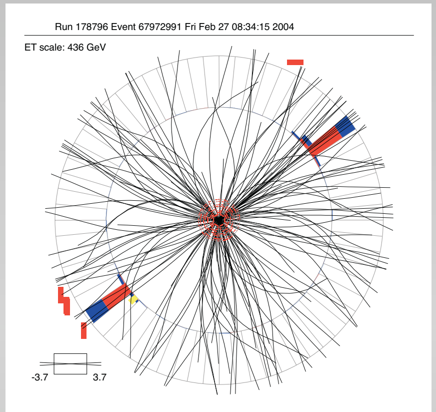




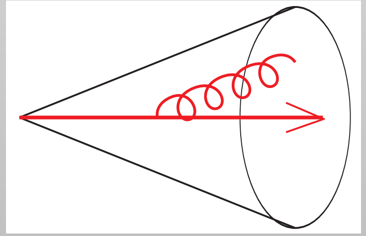
- Just as before, the W boson acquires a p_T by balancing the hard jet; clearly this precludes the region below 20 GeV at LO. At NLO, the real contribution contains configurations where the W boson balances against the vector sum of two partons, with $|\vec{p}_T^{\,1} + \vec{p}_T^{\,2}| < 20$ GeV, but $p_T^1, p_T^2 > 20$ GeV.
- The alarming behaviour which occurs as the LO phase space boundary is approached indicates the existence of a large logarithm which should be resummed. Away from this region, the NLO enhancement depends upon the p_T.

Jet structure

- At lowest order, each jet in the final state is modelled by a single parton.



- In the detector, a jet is the result of the combination of many tracks and has a definite size, for instance the radius of a cone in (η, ϕ) space.

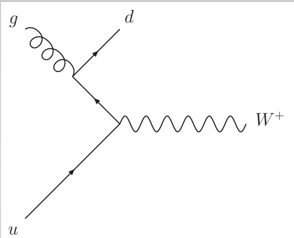


- At next-to-leading order, a similar procedure is used to combine the partons. The additional parton present in the real corrections can lie outside the original cone, or inside it.

- Thus, successive orders in α_s begin to build up the picture that we observe in the detectors, with multiple partons inside the jets. As a result, they become much more sensitive to the details of the jet-clustering algorithm, in particular the way the partons are combined and the size of the cone.

Additional initial states

- As well as the "obvious" extensions of the leading order diagrams, at a hadron collider the NLO real corrections also contain crossed diagrams. Returning to the Drell-Yan process, an example of such a diagram is:

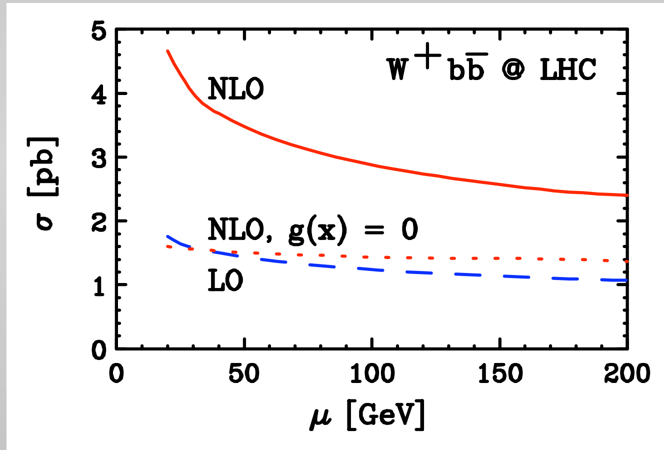


$$g + u \to W + d$$

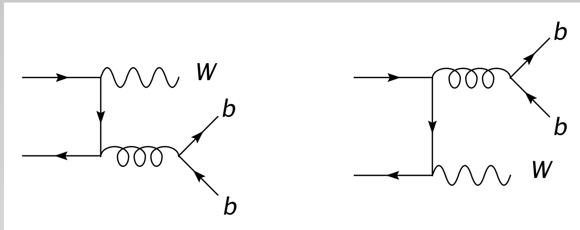
- The process now depends upon the gluon distribution at NLO, while it was completely insensitive to it at leading order.
- One can view this diagram as a gluon splitting into a $d\bar{d}$ pair and then the $\bar{d}$ participating in the reaction $\bar{d}u \to W$. This "factorized" approach is most accurate when the splitting is a collinear one; this is the basis of parton shower approaches to initial-state radiation.
- However, the full matrix elements included at NLO can describe the more general case when this is not true.

Warning signs

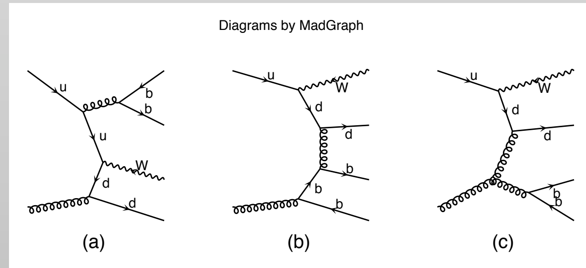
- Sometimes the inclusion of these NLO terms can drastically change the behaviour of the cross section.
- An example of this is provided by the production of a W boson and two b-quarks at the LHC.



LO



NLO



- It is a warning sign that the LO cross section may not be the basic process of interest.
- Naively one would expect that $\sigma(Wb\bar{b} + \text{jet}) < \sigma(Wb\bar{b})$, but this is not the case (for this definition of a jet, $p_T > 20$ GeV) because of the high gluon flux at the LHC. The $Wb\bar{b}$ final state is very likely to be accompanied by additional hadronic activity at the 20 GeV level.

Summary of NLO advantages

- More accurate normalization of the cross section, which is in general larger than the LO result.
  - ⋆ This is not always true – especially in restricted kinematic regions.
  - ⋆ Sometimes the scale dependence increases, so that either we change our view of the process, or must move to NNLO.
- Begin to model initial-state radiation and the effects of a jet-finding algorithm in the final state.
- The phase space available to observables is often extended at NLO, enabling comparison with a wider range of experimental data.
- Large corrections can help to identify regions in which a large logarithm exists and can be resummed. By matching with a NLO calculation, this gives an even more powerful prediction.

NLO MC Programs

MCFM

- http://mcfm.fnal.gov/ John Campbell & Keith Ellis
- Huge library of processes, implemented in a uniform way. . .
  - ⋆ $W^{\pm}/Z^0$
  - ⋆ $W^{\pm}/Z\ +\ j, + b, + \gamma$
  - ⋆ $W^{\pm}/Z\ +\ jj, + b\bar{b}$
  - ⋆ $W^{\pm}W^{\mp}$, $W^{\pm}Z^0$, Z^0Z^0
  - ⋆ $W^{\pm}H$, Z^0H
  - ⋆ H
  - ⋆ $H + j$, $H + b$, $H + b\bar{b}$
  - ⋆ $WW/ZZ \longrightarrow H$
  - ⋆ $t\bar{t}$
  - ⋆ t
- Each new process results in (requires to justify the effort. . . ?) a new publication. . .

NLOJET++

- http://www.ippp.dur.ac.uk/ nagyz/nlo++.html Zoltán Nagy
- Library of QCD processes, implemented in a uniform way. . .
  - ⋆ $e^+e^- \longrightarrow jj,\, jjj,\, jjjj$
  - ⋆ $ep \longrightarrow j + X,\, jj + X,\, jjj + X$ (DIS)
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papers/comment	C++ modules	F77 modules	Author(s)
hep-ph/0110315	hep-ph0110315-c++.tar.gz	N/A	Zoltán Nagy
hep-ph/0104315	hep-ph0104315-c++.tar.gz	N/A	Zoltán Nagy
one-jet inclusive kT alg. with CTEQ4	kT-1jet.tar.gz	N/A	Zoltán Nagy
hep-ph/9806317	hep-ph9806317-c++.tar.gz	N/A	Zoltán Nagy
hep-ph/9707309	hep-ph9707309-c++.tar.gz	N/A	Zoltán Nagy

Summary

- NLO Monte Carlo programs are more complicated than their LO counterparts but can provide vital additional information.
- This information is not limited to an overall normalization of a total cross section. Often kinematic distributions are extended and their shapes changed at NLO.
- Further benefits are (usually) reduced scale dependence and the first modelling of jet structure in the final state.
- NLO predictions are a vital counterpart to parton shower studies, but unfortunately are limited to $2 \to 3$ processes at present. The predictions are available in a number of different codes.
- Ripe for automation. . . several approaches in progress.
- Bottleneck: loop calculations for $2 \to 4$ (and beyond), much recent progress, from twistor-inspired to numerical and semi-numerical approaches.
- NNLO calculations are already available for some of the simplest processes and more will surely be available by the time the LHC turns on.

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