4 Lectures on

QCD

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Lecture 4

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Contents

Lecture 4:

✓ Matching of LO calculations with Parton Showers

✓ MC@NLO: the basic idea

✓ Some more specific points

   ✓ pdf at various orders
   ✓ Effective number of flavors inside the proton

✓ LHC applications
Why we need LO+PS matching?

- Multijet events are omnipresent at the LHC. QCD produces many of those; bSM too. To find bSM we need good understanding of the genuine QCD backgrounds.

![Background simulations](Image)

<table>
<thead>
<tr>
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<th>$Z \to \nu\bar{\nu}$</th>
<th>$t\bar{t}/W \to e, \mu, X$</th>
<th>$t\bar{t}/W \to \tau, X$</th>
<th>QCD</th>
<th>Total background</th>
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<td>&gt;200</td>
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<td>0.0±4.2</td>
<td>2.4±1.4</td>
<td>0.9±1.3</td>
</tr>
</tbody>
</table>

- Notice the limit of the simulation
- Notice the large number of jets that are actually measured. And this is for 8 TeV. The LHC now operates at 13 TeV!
Why we need LO+PS matching?

• The genuine shower programs cannot predict such events with any reasonable accuracy.
  
  • Pythia, for example, has only $2 \rightarrow 1$ and $2 \rightarrow 2$ processes genuinely built in. To generate many hard jets with a shower, one has to use the soft and collinear radiation of the shower well outside its intended “comfort” zone.
  
  • A warning – this can be achieved by playing with the scales – but would this be correct? And a more general warning: programs can produce any number. It is up to the user to make sense of produced results. The logic of “an imperfect number is better than no number” could be very useful but also very dangerous. One has to be very careful there!

• Large number of hard emissions are naturally described in fixed order perturbation theory. But these are single, colorful (typically massless) on-shell partons that look nothing like the jets we measure.

• Clearly, we need a combination of:
  
  • hard emissions generated by a complete fixed order calculation (these will give the proto-jets)
  
  • parton shower (builds the highly complex internal structure of the jets).

• Combining fixed order calculations with parton showers is a non-trivial task which is by now solved in many ways at LO. Doing this at NLO is still a very advanced problem. At NNLO this hasn’t even been seriously contemplated (not yet – but may not be far into the future!)
Before we match LO with PS: what’s a merging scheme?

• First, recall the distinction between inclusive and exclusive observable
  • Example: inclusive jets: typically, within QCD, this means two or more jets.
  • At LO however, we only include 2-to-2 diagrams. This way no final states with 3 or more particles (jets). At the same time a state with, e.g. 8 jets, also belongs to this inclusive observable.
  • Question is: how to account for such multi-jet events?
  • Exclusive event: one with a fixed number of final state particles (jets). For example:
    • Exactly 2
    • Exactly 3
    • ...
  • Note: at LO (and only at LO) the various final states are mutually exclusive, i.e. an inclusive sample is just a sum of exclusive ones. This absolutely doesn’t work at NLO and beyond!

• Thus, we arrive at the basic idea of merging samples at LO:
  • Introduce a separation measure between final states with n and n+1 partons.
  • Generate samples for all process with n final states, n<N_{max}. N_{max} \sim O(10) – see previous slide.
  • Add the samples. They are non-overlapping by construction, i.e. any double counting is avoided.
  • A question: this seems an easy thing to do. But then why do we need NLO calculations?
The difference between a merged LO sample and an NLO (or N^kLO) calculation

• Lets take as an example Higgs production:
  • Inclusive Higgs at LO: pp → H
  • Inclusive Higgs at NLO: pp → h; h+j
  • Inclusive Higgs at NNLO: pp→h;h+j;h+jj

• A merged LO sample with N_{max} = 2 would cover all of the above final states.
• But not in the full kinematic range!

• For example, in the merged LO sample we are not allowed to make any two final state partons too close to each other. In fact, the result would diverge if we attempted to do that!

• Thus, the LO merged sample depends on the parameter that separates the different multiplicities.

• In contrast, in an NLO calculation one can take the extra emitted final state parton and make it as close as desired to any other parton. The divergence is compensated by the divergence in the loop virtual corrections that are absent in the merged sample!

• Similarly at NNLO: there one or two partons can become very close to any other parton. The divergences are much worse than at NLO but this is again compensated by the (now even more complicated) loop corrections.
A note of caution: the terms merging and matching are not always assigned the same meaning in the literature. Keep an open mind and all should eventually be clear from the context.

- There is no one “best” or unique way of doing this: the final result always contains ambiguities and dependence on unphysical scales as long as we work to finite orders in perturbation theory
- The main requirements for a good matching scheme are:
  - Avoid double counting (all emissions look the same: be they hard, or from the shower)
  - Avoid dead regions (i.e. kinematical regions unpopulated by radiation while they should be)
  - One scheme is better than another one if it is a better approximation (in the sense that both LO and NLO are imperfect, but NLO is clearly better than LO).
Common strategies for PS matching procedures

Follow the comparative study http://arxiv.org/pdf/0706.2569v2.pdf

1. A jet measure is defined and all relevant cross sections including jets are calculated for the process under consideration. I.e. for the production of a final state X in pp-collisions, the cross sections for the processes pp → X + n jets with n = 0, 1, ..., N = N_{max} are evaluated.

2. Hard parton samples are produced with a probability proportional to the respective total cross section, in a corresponding kinematic configuration following the matrix element.

3. The individual configurations are accepted or rejected with a dynamical, kinematics-dependent probability that includes both effects of running coupling constants and of Sudakov form factors. In case the event is rejected, step 2 is repeated, i.e. a new parton sample is selected, possibly with a new number of jets.

4. The parton shower is invoked with suitable initial conditions for each of the legs. In some cases, like, e.g. in the MLM procedure, this step is performed together with the step before, i.e. the acceptance/rejection of the jet configuration. In all cases the parton shower is constrained not to produce any extra jet; stated in other words: configurations that would fall into the realm of matrix elements with a higher jet multiplicity are vetoed in the parton shower step.

The matching procedures discussed below differ mainly in:

- the jet definition used in the matrix elements;
- how acceptance/rejection of jet configurations from the matrix element is performed;
- Details of, and the jet vetoing inside, the parton showering.
Restate the problem

- Let’s make it even more evident where’s the problem
  
  - We need a separation parameter at parton level \( R_{\text{part}} \), i.e. any two partons must have \( R > R_{\text{part}} \). It is needed, because if \( R_{\text{part}} \to 0 \) then the partonic x-section is IR divergent.
  
  - We also need a jet-level separation parameter (connected to jet definition, etc) \( R_{\text{jet}} \) which separates jets from each other.

- Clearly, only \( R_{\text{jet}} \) is physical because it is related to the measurement; not \( R_{\text{part}} \).

- Yet, it is easy to see that an unmatched sample has strong dependence on the value of \( R_{\text{part}} \): by taking smaller and smaller values for \( R_{\text{part}} \) the x-section grows unbounded.

- Basically our prediction strongly depends on an unphysical parameter. This is a problem.

- \( R_{\text{part}} \) should be smaller than \( R_{\text{jet}} \) (because otherwise we will have unpopulated regions – or dead zones) which is undesirable.

- The goal of the FO+PS matching procedure is to minimize the dependence on this parton level cut

  Ideally it should be independent of it, but this is never the case.

- How to achieve this is not obvious. There are 3 main proposals.
Main LO + PS matching procedures

• Main algorithms:
  • MLM (Mangano ’02)
  • CKKW (Catani, Kraus, Kuhn, Webber ‘01)
  • Dipole (Lonnblad’02)

• Their approaches are: if two partons are very close (can happen when $R_{\text{part}}$ is small) we somehow suppress or outright veto such event (a veto is a form of suppression).

• In MLM the parton level generation and shower are done without any intermediate checks. Only the final jets are checked for:
  • mutual separation
  • If each jet can be associated with one hard parton
  • all jets and partons can be paired
  • Any event where the above are not satisfied is vetoed.
  • The $R_{\text{part}}$ sensitivity is reduced because if two partons are very close they will produce jets that are close to each other and this is vetoed.

• In CKKW there are both parton-level and jet-level checks:
  • Associate a Sudakov factor at each vertex. This is an exponential which dampens parton-level events with small separation.
  • PS emissions which are hard (off-jet) are vetoed.
  • Important: this gives a prescription for how to choose the value of the renormalization scale at each vertex (i.e. for each emission)!
CKKW merging procedure

- The separation of the matrix-element and parton-shower domains for different multi-jet processes is achieved through a $k_\perp$ measure which controls the internal separation cut, also called the merging scale;

- The acceptance/rejection of jet configurations proceeds through a reweighting of the matrix elements with analytical Sudakov form factors and factors due to different scales in $\alpha_s$;

- A vetoed parton-shower algorithm is used to guarantee that no unwanted hard jets are produced during jet evolution.

- The starting scale for the parton shower evolution of each parton is given by the scale where it appeared first:

\begin{center}
\begin{tikzpicture}
\node[inner sep=0pt] (Q) at (0,0) {\small $Q$};
\node[inner sep=0pt] (q) at (0,-2) {\small $q$};
\node[inner sep=0pt] (Q1) at (0,-4) {\small $Q_1$};
\draw[->] (Q) -- (q) node [midway, above] {shower from $Q$};
\draw[->] (q) -- (Q1) node [midway, below] {shower from $q$};
\draw[->] (Q1) -- (Q) node [midway, below] {shower from $Q$, not $q$};
\end{tikzpicture}
\end{center}

Fig. courtesy of B. Webber
The Sudakov Formfactor

• In our discussion of soft-gluon resummation (lecture 2) we encountered the Sudakov formfactor
• It was resumming soft emission from an independently evolving hard parton
• It included both virtual (loop) and real emission corrections.
• Separately, Real and Virtual corrections were divergent, but together they were finite.
• We interpreted it as a probability for no resolved emission.

• In the context of parton showers it reads:

\[
\Delta_{i\rightarrow j}(q_1, q_2) = \exp \left[ - \int_{q_2^2}^{q_1^2} \frac{dq^2}{q^2} \frac{\alpha_S(q^2)}{2\pi} \int_{Q_0^2/q^2}^{1-Q_0^2/q^2} dz \int_0^{2\pi} d\phi P_{ij}(z, \phi) \right]
\]

  • Evolution of parton i from scale \( q_1 \) down to scale \( q_2 \) without resolved radiation
  • \( Q_0 \) is a scale 1GeV, at which the shower terminates.

• How does the shower work?
  • Start with a hard parton i;
  • It is on-shell; we shift it off-shell and assign some virtuality \( Q \) (the initial scale) to the parton (all momenta need to be reshuffled for this!).
  • Solve the equation \( \Delta(Q, q_1) = R \) for \( q_1 \), where R is a uniform random number.
    • If \( q_1 < Q_0 \): terminate the shower (no resolved emission was made)
    • If \( q_1 > Q_0 \): then splitting \( i\rightarrow j \) occurred.
  • Repeat the above for the secondary parton j starting from a scale \( q_1 \).
The MC@NLO approach

- Combine NLO matrix element with a shower
  - The NLO matrix element is formulated within the subtractions method we discussed yesterday. The matrix elements either have an emission or not (virtual)
  - The shower is based upon the Sudakov formfactor and describes emissions (0,1,2...) that are independent of the matrix element emissions

- The goal is to ensure:
  - No double counting (after all, emissions from matrix elements and Shower look the same...)
  - Simple interpretation: the definition of the observable enters through the shower; the matrix elements only modify the weight of the shower (compared to the LO case).
  - Improved numerical convergence compared to a fixed order calculation
The MC@NLO approach

- Assume the following form:

\[ d\sigma_{\text{MC@NLO}}(O) = W_0S(O, x_M) + \int_{x_0}^{x_M} dyW(y)S(O, y) + \ldots \]

- A combination of sets of (0,1,...)-emission events with:

  - Weight \( W_0, W_1 \), to be determined by matching to a fixed order calculation
  - Each emission is interfaced to a shower \( S() \). The kinematics of the shower is dependent on the real emission (i.e. the shower can emit only the energy left after the hard emission is made)
  - \( x_0 \) and \( x_M \) are the minimum/maximum energies available to radiate.
  - Denote the energy of the real emission, if any, as \( y: x_0 < y < x_M \).

- The Sudakov formfactor is:

\[ \Delta(x_M, x_0) = \exp \left[ -a \int_{x_0}^{x_M} \frac{dz}{z} P(z) \right] = 1 - a \int_{x_0}^{x_M} \frac{dz}{z} P(z) + \mathcal{O}(a^2) \]

- It drives the shower (i.e. shower contains all possible emissions with probability derived from the Sudakov):

\[
S(O, x(y)) = \left[ 1 - a \int_{x_0}^{x} \frac{dz}{z} P(z) + \mathcal{O}(a^2) \right] \delta(O - O(y)) + \left[ a \int_{x_0}^{x} \frac{dx_1}{x_1} P(x_1) + \mathcal{O}(a^2) \right] \delta(O - O(y; x_1)) + \mathcal{O}(a^2)
\]

- No emission from shower
- 1 emission from shower
- 2 emissions from shower
The MC@NLO approach

\[ d\sigma_{\text{MC@NLO}}(O) = W_0 S(O, x_M) + \int_{x_0}^{x_M} dy W_i(y) S(O, y) + \ldots \]

- To determine the weights \( W_0, W_1 \) one expands MC@NLO and requires that to NLO it agrees with the NLO result (derived within the subtraction method)

\[
d\sigma_{\text{NLO}} = B + a \left( \frac{V_{\text{pole}}}{\varepsilon} + V_{\text{fin}} \right) + \mathcal{O}(a^2)
\]

\[
+ a \int_0^1 \frac{dx}{x^{1+\varepsilon}} R(x) + \mathcal{O}(a^2)
\]

\[
= B + a \left( V_{\text{fin}} + \int_0^1 \frac{dx}{x} (R(x) - R(0)) \right) + \mathcal{O}(a^2)
\]

- The MC@NLO weights read:

\[
W_0 = B + a \left[ V_{\text{fin}} + \int_0^1 \frac{dx}{x} (BP(x) - R(0)) \right]
\]

\[
W_1 = a \frac{R(x) - BP(x)}{x}
\]

- Notice the “miracle”:
  - Weights are similar to the NLO ones but the real emission counterterm got replaced by the shower: \( R(0) = \text{B} \rightarrow BP(x) \)

  - This implies that the subtraction kinematics is the same as the one for the event. Improved convergence; less negative weight events compared to fixed order calculation
PDF evolution and number of active flavors in the proton

• How to treat the heavy flavors (c, b, t) in the proton?

• It depends on the scale at which we measure the pdfs:

\[
f_i(x, \mu) \begin{cases} 
  i = u, d, s & \text{if } \mu < m_c \\
  i = u, d, s, c & \text{if } m_c < \mu < m_b \\
  i = u, d, s, c, b & \text{if } m_b < \mu < m_t \\
  i = u, d, s, c, b, t & \text{if } \mu > m_t 
\end{cases}
\]

• Unlikely to need top quark pdf’s at the LHC but should be absolutely essential at a future 100 TeV hadron collider
PDF (and fragmentation functions) at different orders (LO NLO,...)

\[ O = \sum_{ij} f_i f_j \left( d\sigma_{ij}^{(0)} \right) \]

\[ O = \sum_{ij} f_i f_j \left( d\sigma_{ij}^{(0)} + d\sigma_{ij}^{(1)} \right) \]

\[ O = \sum_{ij} f_i f_j \left( d\sigma_{ij}^{(0)} + d\sigma_{ij}^{(1)} + d\sigma_{ij}^{(2)} \right) \]

- Using the same data, we can extract pdf’s at LO, NLO NNLO,...
- Clearly, the change in perturbative cross-section gets “absorbed” by a change in the pdf.
- Therefore, pdf’s at LO, NLO,... are different.
- They should be used consistently in subsequent computations.
LHC applications
The most basic hadron collider process:

\[ pp \rightarrow \gamma^* \rightarrow \mu^+ \mu^- \]

- NLO corrections shown above
- Now know through NNLO
- It is the “inverted” version of \( e^+ e^- \rightarrow \) hadrons
Vector boson rapidity distribution

Notice the scale variation.

Drell-Yan

Anastasiou, Dixon, Melnikov, Petriello ‘03
Drell-Yan, W and Z

• These processes are the best known ones at hadron colliders


• Known fully differentially through NNLO in QCD for all processes

• For Drell-Yan also NLO EW included.

• Relevance of these processes:
  
  • Standard calibration tool for detectors.
  • Were proposed for LHC luminosity measurement due to the very good theory control.
  • Searches for Z’ and related bSM processes
  • The W+ and W- asymmetries allow direct access to the flavor asymmetries of the proton pdf’s.
  • Uncertainties at percent level.
Higgs production

LO Feynman diagrams:

- Higgs–strahlung
- Vector boson fusion
- gluon–gluon fusion
- in associated with $Q\bar{Q}$

Note the top loop in $Hgg$

Production at Tevatron and LHC7:
Higgs production

Higgs decay channels:
Higgs production

Theoretical uncertainties in Differential Higgs production:

And for the total cross-section:
Higgs production

- The slow convergence of the perturbative expansion in Higgs production prompted work beyond NNLO QCD.

\[
\sigma = \tau \sum_{ij} \left( f_i \otimes f_j \otimes \frac{\hat{\sigma}_{ij}(z)}{z} \right)(\tau)
\]

\[
\tau = \frac{m_H^2}{S} \quad \text{and} \quad z = \frac{m_H^2}{s} \quad \frac{\hat{\sigma}_{ij}(z)}{z} = \frac{\pi C^2}{8V} \sum_{k=0}^{\infty} \left( \frac{\alpha_s}{\pi} \right)^k \eta_{ij}^{(k)}(z)
\]

- Expansion around the soft limit (normally \(n=1\)):

\[
\frac{\hat{\sigma}_{ij}(z)}{z^{1+n}} \approx \hat{\sigma}_{ij}(z)_{(1-z)^{-1}} + \hat{\sigma}_{ij}(z)_{(1-z)^0} + n(1-z) \hat{\sigma}_{ij}(z)_{(1-z)^{-1}} + \mathcal{O}(1-z)^1
\]

- The soft and next to soft expansion at N\(^3\)LO is now known

Higgs production

- The (essentially) full N³LO result is now also known

![Graph showing scale variation of the gluon fusion cross-section at different perturbative orders through N³LO.](image)

**FIG. 2:** Scale variation of the gluon fusion cross-section at all perturbative orders through N³LO.

<table>
<thead>
<tr>
<th>(\mu = \frac{m_H}{2})</th>
<th>2 TeV</th>
<th>7 TeV</th>
<th>8 TeV</th>
<th>13 TeV</th>
<th>14 TeV</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m_H)</td>
<td>0.99+0.43%−4.65%</td>
<td>15.31+0.31%−3.08%</td>
<td>19.47+0.32%−2.99%</td>
<td>44.31+0.31%−2.64%</td>
<td>49.87+0.32%−2.61%</td>
</tr>
</tbody>
</table>

- So far the choice of central scale was always tenuous.

- It seems at N³LO it doesn’t really matter any more (which is a very good news)

Top-pair production

Scale error at 3%; similar to parametric errors due to $\alpha_s$, $m_{\text{top}}$, pdf

Impressive convergence of perturbation theory in this process. Much faster than Higgs!

For more details see arXiv:1305.3892
Top-pair production

• The scale variation in top production is small. Indicates good perturbative convergence.

Fig. 1. – Scale dependence of the total cross-section at LO (blue), NLO (red) and NNLO (black) as a function of $m_{\text{top}}$ at the Tevatron (left) and the LHC 8 TeV (right). No soft gluon resummation is included. For reference the most precise experimental measurements are also shown.

Top-pair production

- Top is good for bSM searches (dominant background in high-PT searches)
- PDF determination: first fully known NNLO LHC process that is directly sensitive to the gluon
  - Implications for Higgs (which is also driven by gg)

- Top pair production has peculiar dependence on pdfs; changes drastically from Tevatron to LHC

<table>
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<tr>
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<th>TeVatron</th>
<th>LHC 7 TeV</th>
<th>LHC 8 TeV</th>
<th>LHC 14 TeV</th>
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<tr>
<td>$gg$</td>
<td>15.4%</td>
<td>84.8%</td>
<td>86.2%</td>
<td>90.2%</td>
</tr>
<tr>
<td>$qg + \bar{q}g$</td>
<td>-1.7%</td>
<td>-1.6%</td>
<td>-1.1%</td>
<td>0.5%</td>
</tr>
<tr>
<td>$qq$</td>
<td>86.3%</td>
<td>16.8%</td>
<td>14.9%</td>
<td>9.3%</td>
</tr>
</tbody>
</table>
Top-pair production: top-mass measurement

The fate of the Universe might depend on 1 GeV in $M_{\text{top}}$!

Cosmological implications:

- Higgs Inflation: Higgs = inflaton

\[
\mathcal{L}_h = -|\partial H|^2 + \mu^2 H^\dagger H - \lambda (H^\dagger H)^2 + \xi H^\dagger H \mathcal{R}.
\]

\[
m_h > 125.7 \text{ GeV} + 3.8 \text{ GeV} \left( \frac{m_t - 171 \text{ GeV}}{2 \text{ GeV}} \right) - 1.4 \text{ GeV} \left( \frac{\alpha_s(m_Z) - 0.1176}{0.0020} \right) \pm \delta.
\]

- Higgs mass and vacuum stability in the Standard Model at NNLO.

For more details see arXiv:1310.0799

Bezrukov, Shaposhnikov ‘07–’08
De Simone, Hertzberg, Wilczek’08

Strong dependence on the top mass!

Degrassi, Di Vita, Elias-Miro, Espinosa, Giudice, Isidori, Strumia ‘12

Instability scale $\Lambda$ [GeV]
$\delta M_{\text{top}}$ is the dominant uncertainty!
Cut diagrams

When we compute x-sections we need squared matrix elements.

Natural notation: cut diagrams (they put real and virtual loops on more equal footing):

\[
\begin{array}{cccc}
  u_i & u_f \\
  v_i & v_f \\
\end{array}
\times
\begin{bmatrix}
  u_i & u_f \\
  v_i & v_f \\
\end{bmatrix}
= \star
\]

\[
\begin{array}{cccc}
  u_i & u_i \\
  v_i & v_i \\
\end{array}
\star
\]

\[
2\pi\delta_+(p^2) \psi
\]

The “cut”, i.e. the physical final state
Modern computational methods: computing observables
Download/Install/Use Approach

✓ LO calculations are now completely automated and can be easily performed with a number of readily available software programs.
  • ALPGEN (http://mlm.web.cern.ch/mlm/alpgen/)

✓ NLO calculations can also be performed with automated software
  • aMC@NLO (uses MC@NLO + Madgraph) : a completely general program for performing (in principle) any NLO calculations,
    [http://amcatnlo.web.cern.ch/amcatnlo/ ]
  • Powheg Box: same as above, but for precomputed processes (a very large number of processes available) [http://powhegbox.mib.infn.it ]
  • MCFM: parton level NLO library. A classics. [http://mcfm.fnal.gov ]

✓ Parton showers / Monte Carlo event generators:
  • Pythia [http://home.thep.lu.se/~torbjorn/Pythia.html ]
  • Herwig [http://www.hep.phy.cam.ac.uk/theory/webber/Herwig/ ]
  • Herwig++ [http://herwig.hepforge.org ]
  • Sherpa [https://sherpa.hepforge.org/trac/wiki ]

These are programs that simulate the low-energy branching and subsequent fragmentation. They are very versatile and produce fully exclusive events (just the way they are measured by experiments)
  • NOTE: despite their very appealing features, their accuracy could be limited!
Some references:

[Shifman 2011], M. Shifman, “Historical curiosity: How asymptotic freedom of the Yang-Mills theory could have been discovered three times before Gross, Wilczek, and Politzer, but was not” in “At the frontier of particle physics”, vol. 1* 126-130


Lectures from Bryan Webber [see his website], especially what concerns parton showers and related subjects

R.K. Ellis: 5 lectures in QCD (online)