Perturbative QCD 3

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3rd Lecture



Nordita Winter School 2024 in Particle Physics and Cosmology January 2024

DGLAP Evolution

The DGLAP evolution is a key to precision LHC phenomenology: it allows to measure PDFs at some scale (say in DIS) and evolve upwards to make LHC (7, 8, 13, 14, 33, 100....TeV) predictions



Typical features of PDFs

- vanish at $x \rightarrow I$
- valence quarks peak at $x \approx 1/3$
- gluon and sea distribution rise for $x \rightarrow 0$ (region dominated by gluons)



Progress in PDFs

PDFs are an essential ingredient for the LHC program.

Recent progress includes

- better assessment of uncertainties (e.g. different groups now agree at the $I \sigma$ level where data is available)
- exploit wealth of new information from LHC Run I, II and III measurements
- progress in tools and methods (e.g. Neural Network PDFs) to include these data in the fits
- inclusion of PDFs for photons, leptons

Progress in PDFs

Issues under discussion

- which data to include in the fits (and how to deal with incompatible data)
- enhance relevance of some data (reduce effect of inconsistent data sets)
- heavy-quark treatment and masses
- parametrization for PDFs (theoretical bias, reduced in Neural Network PDFs)
- include theoretical improvement (e.g. resummation) for some observables
- unphysical behaviour close to x=0 and x=1
- meaning of uncertainties
- α_s as external input or fitted with PDFs
- how not to "fit away" New Physics effects in PDFs

Summary

- In the QCD parton model, hadrons are treated as bound states of quasifee point-like quarks is very successful to explain DIS measurements
- In this model, the probability to find a parton with a given momentum fraction is given by the (scale independent) parton distribution function
- The model breaks down once one includes initial state radiation since collinear divergences do not cancel
- This leads to scale dependent parton distribution functions
- The dependence is governed by the DGLAP evolution equations
- QCD factorisation means that PDFs are universal and processindependent quantities: they can be measured in some process, at some scale, and use in a different process at a different scale
- PDFs are today determined by global fits to data

Perturbative calculations

Perturbative calculations rely on the idea of an order-by-order expansion in the small coupling

$$\sigma \sim A + B\alpha_s + C\alpha_s^2 + D\alpha_s^3 + \dots$$

lo nlo nnlo nnnlo

- Perturbative calculations are possible because the coupling is small at high energy
- In QCD (or in a generic QFT) the coupling depends on the energy (renormalization scale)
- So changing scale the result changes. By how much? What does this dependence mean?
- In the following will discuss these issues through examples

Hard cross section

Born level cross section straightforward in principle



Leading order with Feynman diagrams

Get any LO cross-section from the Lagrangian

- I. draw all Feynman diagrams
- 2. put in the explicit Feynman rules and get the amplitude
- 3. do some algebra, simplifications
- 4. square the amplitude
- 5. integrate over phase space + flux factor + sum/average over outgoing/ incoming states

Automated tools for (1-3): FeynArts/Qgraf, Mathematica/Form etc.

Bottlenecks

- a) number of Feynman diagrams diverges factorially
- b) algebra becomes more cumbersome with more particles

But given enough computer power everything can be computed at LO

Diagrams for gluon amplitudes

Number of diagrams for gg \rightarrow n gluons

n	2	3	4	5	6	7	8
diag.	4	25	220	2485	34300	559405	10525900

•number of diagrams grows very fast

• complexity of each diagrams grows with n

Alternative methods?

Techniques beyond Feynman diagrams



Is it necessary to go beyond LO?

Very early observation:

at least NLO corrections are needed to describe data



Drell Yan production is one of the first processes for which NLO corrections have been computed

Leading order n-jet cross-section

• Consider the cross-section to produce n jets. The leading order result at scale μ result will be

$$\sigma_{\rm njets}^{\rm LO}(\mu) = \alpha_s(\mu)^n A(p_i, \epsilon_i, \ldots)$$

- Instead, choosing a scale μ ' one gets

$$\sigma_{\rm njets}^{\rm LO}(\mu') = \alpha_s(\mu')^n A(p_i, \epsilon_i, \ldots) = \alpha_s(\mu)^n \left(1 + n \, b_0 \, \alpha_s(\mu) \ln \frac{\mu^2}{\mu'^2} + \ldots\right) A(p_i, \epsilon_i, \ldots)$$

So the change of scale is an NLO effect ($\propto \alpha_s$), but this becomes more important when the number of jets increases ($\propto n$)

• Notice that at Leading Order the normalization is not under control:

$$\frac{\sigma_{\rm njets}^{\rm LO}(\mu)}{\sigma_{\rm njets}^{\rm LO}(\mu')} = \left(\frac{\alpha_s(\mu)}{\alpha_s(\mu')}\right)^n$$

NLO n-jet cross-section

Now consider n-jet cross-section at NLO. At scale μ the result reads

$$\sigma_{\rm njets}^{\rm NLO}(\mu) = \alpha_s(\mu)^n A(p_i, \epsilon_i, \dots) + \alpha_s(\mu)^{n+1} \left(B(p_i, \epsilon_i, \dots) - nb_0 \ln \frac{\mu^2}{Q_0^2} \right) + \dots$$

- So the NLO result compensates the LO scale dependence. The residual dependence is NNLO.
- Scale dependence and normalization start being under control only at NLO, since compensation mechanism kicks in
- Notice also that a good scale choice automatically resums large logarithms to all orders, while a bad one spuriously introduces large logs and ruins the PT expansion
- Scale variation is conventionally used to estimate theory uncertainty, but the validity of this procedure should not be overrated (see later)

NLO calculations

NLO accuracy requires to dress a process with one real or one virtual parton



Sample diagrams shown. All diagrams must be included.

We won't have time to do detailed NLO calculations, but let's look a bit more in detail at the issue of divergences/subtraction

Regularization procedures in QCD

<u>Regularization</u>: a way to make intermediate divergent quantities meaningful

 In QCD dimensional regularization is today the standard procedure, based on the fact that d-dimensional integrals are more convergent if one reduces the number of dimensions.

$$\int \frac{d^4 l}{(2\pi)^4} \to \mu^{2\epsilon} \int \frac{d^d l}{(2\pi)^d} \,, \ d = 4 - 2\epsilon < 4$$

- N.B. to preserve the correct dimensions a mass scale μ is needed
- Divergences show up as intermediate poles $1/\epsilon$

$$\int_0^1 \frac{dx}{x} \to \int_0^1 \frac{dx}{x^{1-\epsilon}} = \frac{1}{\epsilon}$$

• This procedure works both for UV divergences and IR divergences

Alternative regularization schemes: photon mass (EW), cut-offs, Pauli-Villard ... Compared to those methods, dimensional regularizatiom has the big virtue that it leaves the regularized theory Lorentz invariant, gauge invariant, unitary etc.

Subtraction and slicing methods

• Consider e.g. an n-jet cross-section with some arbitrary infrared safe jet definition. At NLO, two divergent integrals, but the sum is finite

$$\sigma_{\rm NLO}^J = \int_{n+1} d\sigma_{\rm R}^J + \int_n d\sigma_{\rm V}^J$$

- Since one integrates over a different number of particles in the final state, real and virtual need to be evaluated first, and combined then
- This means that one needs to find a way of removing divergences before evaluating the phase space integrals
- Two main techniques to do this
 - phase space slicing \Rightarrow used mostly at NNLO (not NLO)
 - subtraction method \Rightarrow most used in NLO applications

Subtraction method

• The real cross-section can be written schematically as

$$d\sigma_R^J = d\phi_{n+1} |\mathcal{M}_{n+1}|^2 F_{n+1}^J(p_1, \dots, p_{n+1})$$

where F^J is the arbitrary infrared-safe jet-definition

• The matrix element has a non-integrable divergence

$$|\mathcal{M}_{n+1}|^2 = \frac{1}{x}\mathcal{M}(x)$$

where x vanishes in the soft/collinear divergent region

• IR divergences in the loop integration regularized by taking D=4-2 ϵ

$$2\operatorname{Re}\{\mathcal{M}_V\cdot\mathcal{M}_0^*\}=\frac{1}{\epsilon}\mathcal{V}$$

Subtraction method

• The n-jet cross-section becomes

$$\sigma_{\rm NLO}^J = \int_0^1 \frac{dx}{x^{1+\epsilon}} \mathcal{M}(x) F_{n+1}^J(x) + \frac{1}{\epsilon} \mathcal{V} F_n^J$$

• Infrared safety of the jet definition implies

$$\lim_{x \to 0} F_{n+1}^J(x) = F_n^J$$

• KLN cancelation guarantees that

$$\lim_{x \to 0} \mathcal{M}(x) = \mathcal{V}$$

• One can then add and subtract the analytically computed divergent part

$$\sigma_{\rm NLO}^J = \int_0^1 \frac{dx}{x^{1+\epsilon}} \mathcal{M}(x) F_{n+1}^J(x) - \int_0^1 \frac{dx}{x^{1+\epsilon}} \mathcal{V}F_n^J + \int_0^1 \frac{dx}{x^{1+\epsilon}} \mathcal{V}F_n^J + \frac{1}{\epsilon} \mathcal{V}F_n^J$$

Subtraction method

• This can be rewritten exactly as

$$\sigma_{\rm NLO}^J = \int_0^1 \frac{dx}{x^{1+\epsilon}} \left(\mathcal{M}(x) F_{n+1}^J - \mathcal{V} F_n^J \right) + \mathcal{O}(1) \mathcal{V} F_n^J$$

 \Rightarrow Now both terms are finite and can be evaluated numerically

- Subtracted cross-section must be calculated separately for each process (but mostly automated now). It must be valid everywhere in phase space
- Systematised in the seminal papers of Catani-Seymour (dipole subtraction, '96) and Frixione-Kunszt-Signer (FKS method, '96)
- Subtraction used in all recent NLO applications and public codes

Ingredients at NLO

A full N-particle NLO calculation requires:

- ✓ tree graph rates with N+I partons
 → soft/collinear divergences
- virtual correction to N-leg process
 divergence from loop integration, use e.g. dimensional regularization
- set of subtraction terms





bottleneck for a very long time

Virtual one-loop: two breakthrough ideas

Aim: NLO loop integral without doing the integration

1) "... we show how to use generalized unitarity to read off the (box) coefficients. The generalized cuts we use are quadrupole cuts ..."



Britto, Cachazo, Feng '04

Quadrupole cuts: 4 on-shell conditions on 4 dimensional loop momentum) freezes the integration. But rational part of the amplitude, coming from $D=4-2\varepsilon$ not 4, computed separately

One-loop: two breakthrough ideas

Aim: NLO loop integral without doing the integration

2) The OPP method: "We show how to extract the coefficients of 4-, 3-, 2- and I-point one-loop scalar integrals...."



Ossola, Pittau, Papadopolous '06

Coefficients can be determined by solving a system of equations!

Virtual (one-loop) amplitude

Bottleneck for a long time... but thanks to these and other theoretical breakthrough ideas



the problem of computing NLO QCD corrections is now solved

Automated NLO (aka NLO revolution)

Example: single Higgs production processes (similar results available for all SM processes of similar complexity, backgrounds to Higgs studies)

Process	Syntax	Cross section (pb)			
Single Higgs production		LO 13 TeV	NLO 13 TeV		
$ \begin{array}{ll} {\rm g.1} & pp \rightarrow H \ ({\rm HEFT}) \\ {\rm g.2} & pp \rightarrow Hj \ ({\rm HEFT}) \\ {\rm g.3} & pp \rightarrow Hjj \ ({\rm HEFT}) \end{array} $	p p > h p p > h j p p > h j j	$\begin{array}{rrrr} 1.593 \pm 0.003 \cdot 10^1 & +34.8\% & +1.2\% \\ -26.0\% & -1.7\% \\ 8.367 \pm 0.003 \cdot 10^0 & +39.4\% & +1.2\% \\ -26.4\% & -1.4\% \\ 3.020 \pm 0.002 \cdot 10^0 & +59.1\% & +1.4\% \\ -34.7\% & -1.7\% \end{array}$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$		
$ \begin{array}{ll} {\rm g.4} & pp \mathop{\rightarrow} Hjj \ {\rm (VBF)} \\ {\rm g.5} & pp \mathop{\rightarrow} Hjjj \ {\rm (VBF)} \end{array} $	p p > h j j \$\$ w+ w- z p p > h j j j \$\$ w+ w- z	$\begin{array}{cccc} 1.987 \pm 0.002 \cdot 10^{0} & {}^{+1.7\%}_{-2.0\%} {}^{+1.9\%}_{-1.4\%} \\ 2.824 \pm 0.005 \cdot 10^{-1} & {}^{+15.7\%}_{-12.7\%} {}^{+1.5\%}_{-10.0\%} \end{array}$	$\begin{array}{cccc} 1.900 \pm 0.006 \cdot 10^{0} & {}^{+0.8\%}_{-0.9\%} {}^{+2.0\%}_{-1.5\%} \\ 3.085 \pm 0.010 \cdot 10^{-1} & {}^{+2.0\%}_{-3.0\%} {}^{+1.5\%}_{-1.1\%} \end{array}$		
g.6 $pp \rightarrow HW^{\pm}$ g.7 $pp \rightarrow$ g.8* $pp \rightarrow$	рр>h wpm	$1.195 \pm 0.002 \cdot 10^{0}$ $^{+3.5\%}_{4.5\%}$ $^{+1.9\%}_{1.5\%}$	$\begin{array}{cccc} 1.419 \pm 0.005 \cdot 10^0 & {}^{+2.1\%}_{-2.6\%} & {}^{+1.9\%}_{-1.4\%} \\ {}^{+1.2\%}_{-1.0\%}_{-0.6\%} \end{array}$		
$\begin{array}{ccc} g.9 & pp \rightarrow \\ g.10 & pp \rightarrow \\ g.11^* & pp \rightarrow \end{array}$	solve	d probl	E -1.4% +1.1% -0.9% +0.7% -0.6%		
$ \begin{array}{ll} {\rm g.12^*} & pp \mathop{\rightarrow} HW^+W^- \ (\rm 4f) \\ {\rm g.13^*} & pp \mathop{\rightarrow} HW^\pm \gamma \\ {\rm g.14^*} & pp \mathop{\rightarrow} HZW^\pm \\ {\rm g.15^*} & pp \mathop{\rightarrow} HZZ \end{array} $	p p > h w+ w- p p > h wpm a p p > h z wpm p p > h z z	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	$\begin{array}{cccccc} 1.065 \pm 0.003 \cdot 10^{-2} & +2.3\% & +2.0\% \\ -1.9\% & -1.5\% \\ 3.309 \pm 0.011 \cdot 10^{-3} & +2.7\% & +1.7\% \\ -2.0\% & -1.4\% \\ 5.292 \pm 0.015 \cdot 10^{-3} & +3.9\% & +1.8\% \\ -3.1\% & -1.4\% \\ 2.538 \pm 0.007 \cdot 10^{-3} & +1.9\% & +2.0\% \\ -1.4\% & -1.5\% \end{array}$		
$ \begin{array}{ll} {\rm g.16} & pp \rightarrow Ht\bar{t} \\ {\rm g.17} & pp \rightarrow Htj \\ {\rm g.18} & pp \rightarrow Hb\bar{b} \ (\rm 4f) \end{array} $	p p > h t t~ p p > h tt j p p > h b b~	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$		
$ \begin{array}{ll} {\rm g.19} & pp \mathop{\rightarrow} Ht\bar{t}j \\ {\rm g.20^*} & pp \mathop{\rightarrow} Hb\bar{b}j \ ({\rm 4f}) \end{array} \end{array} $	p p > h t t~ j p p > h b b~ j	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$		

NLO revolution?

What lead to this remarkable progress?

The fact that

 l.leading order can be computed automatically and efficiently (e.g. via recursion relations)
 one can reduce the one-loop to product of tree-level amplitudes
 it was well understood how to subtract singularities
 the basis of master integrals was known

But for item 2. everything was there since the time of Passarino-Veltman (even item 2. was understood, but no efficient/practical method exited). We will later on compare this to the current status of NNLO

NLO status

Various public tools developed: Blackhat+Sherpa, GoSam+Sherpa, Helac-NLO, Madgraph5_aMC@NLO, NJet+Sherpa, OpenLoops+Sherpa, Samurai, Recola ...

- Practical limitation: high-multiplicity processes still difficult because of numerical instabilities, need long run-time on clusters to obtain stable results (edge: around 6 particles in the final state, depending on the process)
- Today focus on
 - automation of NLO for BSM signals
 - Ioop-induced processes: formally higher-order, but enhanced by gluon PDF
 - automation of NLO electroweak corrections (necessary to match accuracy of NNLO)
 - automation of NLO in SMEFT

Comparison to NLO is the standard now in most LHC analyses

Uncertainties

The "unpleasant" feature that cross-sections depend on the choice of renormalization and factorization scale can be turned into something useful, i.e. a way to quantify the theoretical error

Example: R-ratio

Fix both scales to the scale at which the hard process occurs (Q) and vary them up and down by a factor 2 1.1

<u>NB:</u>

- the factor 2 is conventional
- it is a procedure that seemed to work well in practice
- in complicated processes large degree of freedom in the choice of the scale



I. LHC example of NLO: tt+ljet



- Scale variation is not a perfect procedure to assess the theory uncertainty
- Ambiguities in the central scale choice (more so for more complicated processes)
- Scale variation for ratios (asymmetries etc.) underestimates the uncertainty

2. LHC example of NLO:W+3jets

<u>Scale choice:</u> example of W+3 jets (problem more severe with more jets)



... large logarithms can appear in some distributions, invalidating even an NLO prediction. Bern et al. '09

Is NNLO needed?



LHC data clearly already requires NNLO Same conclusion in all measurements examined so far With more data NLO likely to be insufficient

Why is NNLO difficult



Cancelation manifest after phase space integration, but to have fully differential results must achieve cancelation before integration

Ingredients for NNLO

At NNLO the situation is very different from NLO

- I. leading order of very limited importance
- 2. no procedure to reduce two-loop to tree-level (unitarity approaches still face many outstanding issues)
- 3. subtraction of singularities far from trivial
- 4. basis set of master integrals not known, integrals not all/always known analytically

What changed in the last years (and keeps changing rapidly)

- I. technology to compute integrals
- 2. extension of systematic subtraction to NNLO

NNLO: status



NNLO uncertainty?

NNLO *scale* uncertainty bands of 1-2%. Is the *theory* uncertainty indeed 1-2%?

N3LO: only 3 LHC process known so far

Gluon fusion Higgs production (in the large m_t effective theory)

Vector boson fusion Higgs production (in the structure function approximation, i.e. double DIS process)

Drell Yan (W and Z bosons to leptons)

Higgs production at N3LO

- O(100000) interference diagrams (1000 at NNLO)
- 68273802 loop and phase space integrals (47000 at NNLO)
- about 1000 master integrals (26 at NNLO)

Higgs production at N3LO

- N³LO finally stabilizes the perturbative expansion
- also matched to resummed calculation (essentially no impact on central value at preferred scale $m_H/2$)

Error budget: one example

Gluon-fusion Higgs productions (known to N³LO fully differential)

Summary of perturbative calculations

- LO: fully automated. Edge: 10-12 particles in the final state
- NLO: also automated. Edge: 4-6 particles in the final state
- NNLO: the new frontier. Lots of new 2 → 2 processes in recent years.
 First 2 → 3 calculations for the LHC
- NNNLO: fully inclusive Higgs production via gluon fusion (large mt effective theory), vector boson fusion (factorised approximation) and Drell Yan production