In the recent years enormous efforts have gone into higher order QCD calculations of physical quantities. Example: Moch, Vermaseren, Vogt


Motivation:

Search for signals of “New Physics” requires good knowledge of the conventional one.
The third-order QCD corrections to deep-inelastic scattering by photon exchange

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Received 2 May 2005; accepted 7 June 2005
Available online 14 July 2005
Observable: nucleon structure functions

\[ x^{-1} F_a = C_{a,ns} \otimes q_{ns} + \left\langle e^2 \right\rangle (C_{a,q} \otimes q_s + C_{a,g} \otimes g) \]

**hard scattering cross section**

**quark distribution functions**

**QED:**

\[ c^{(0)}_{2,ns}(x) = \delta(x_1), \quad c^{(0)}_{2,ps}(x) = c^{(0)}_{2,g}(x) = c^{(1)}_{2,ps}(x) = 0 \]

**LO:**

\[ c^{(1)}_{2,ns}(x) = C_F \left\{ 4D_1 - 3D_0 - (9 + 4\xi_2)\delta(x_1) - 2(1 + x)(L_1 - L_0) - 4x_1^{-1}L_0 + 6 + 4x \right\}, \]

\[ c^{(1)}_{2,g}(x) = n_f \left\{ (2 - 4xx_1)(L_1 - L_0) - 2 + 16xx_1 \right\} \]

with \( C_F = (N_c^2 - 1)/(2N_c) = 4/3 \) in QCD. Here and below we use the a

\[ x_1 = 1 - x, \quad L_0 = \ln x, \quad L_1 = \ln x_1, \quad D_k = \left[ x_1^{-1} L_1^k \right]_+ \]
in terms of polylogarithmic functions

\[ H(0; x) = \ln x, \]
\[ H(1; x) = \int_0^x \frac{dx'}{1 - x'} = -\ln(1 - x), \]
\[ H(-1; x) = \int_0^x \frac{dx'}{1 + x'} = \ln(1 + x). \]

\[ H(0, 0; x) = \frac{1}{2} \ln^2 x, \]
\[ H(0, 1; x) = \int_0^x \frac{dx'}{x'} H(1; x') = -\int_0^x \frac{dx'}{x'} \ln(1 - x'), \]
\[ H(0, -1; x) = \int_0^x \frac{dx'}{x'} H(-1; x') = \int_0^x \frac{dx'}{x'} \ln(1 + x'), \]
\[ H(1, 0; x) = \int_0^x \frac{dx'}{1 - x'} H(0; x') = \int_0^x \frac{dx'}{1 - x'} \ln x', \]
\[ H(1, 1; x) = \int_0^x \frac{dx'}{1 - x'} H(1; x') = -\int_0^x \frac{dx'}{1 - x'} \ln(1 - x'), \]
\[ H(1, -1; x) = \int_0^x \frac{dx'}{1 - x'} H(-1; x') = \int_0^x \frac{dx'}{1 - x'} \ln(1 + x'), \]
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\[ H(-1, -1; x) = \int_0^x \frac{dx'}{1 + x'} H(-1; x') = \int_0^x \frac{dx'}{1 + x'} \ln(1 + x'). \]
NNLO:

just one coefficient function takes 10 full pages like this one!
The questions I want to address:

- Do we understand theoretical ambiguities resulting from using finite order perturbative approximants?
- What is the theoretical uncertainty of these calculations?
- How it relates to the (enormously complicated) NNLO and higher order calculations?

There can be no definite answer to these questions but contrary to the situation two decades ago, when people like Stevenson, Grunberg and Brodsky developed different approaches to resolving the ambiguities of finite order QCD calculations, these questions are now largely ignored and common inertia has set in.
For a number of interesting physical quantities measured at HERA and TEVATRON the ambiguities resulting from the freedom in the choice of the renormalization and factorization scales prevent us from drawing conclusions on the presence of signals of new physics, like the BFKL dynamics.

One might hope that at much higher energies available at the LHC, perturbative QCD predictions will be much more stable. In this talk

I will argue that this is not always the case and that the problem of scale/scheme setting may hinder even such important and seemingly clean observables like the ttbar production cross section.
Perturbative calculations involve a number of variables that emerge in the process of renormalization and factorization procedures due to ambiguities in the definition of the renormalized couplant and dressed PDF and FF. Physics is independent of these ambiguities provided perturbative expansions are taken to all orders, but they matter if these expansions are truncated.

At any finite order perturbative QCD yields a function of the associated free parameters. Their choice is an integral part of any application of PQCD.

The calculations themselves can be carried out for any set of these parameters as transforming the results from one set to another is simple and straightforward.
Renormalized couplant \( a \equiv \alpha_s / \pi \)

\[ \frac{da(\mu, c_i)}{d \ln \mu} = -ba^2(\mu, c_i) \left[ 1 + ca(\mu, c_i) + c_2a^2(\mu, c_i) + \cdots \right] \]

\[ b = \frac{11N_c - 2n_f}{6} \quad ; \quad c = \frac{51N_c - 19n_f}{22N_c - 4n_f} \]

\text{arbitrary!}

But even for a given r.h.s. there is an infinite number of solutions differing by the choice of initial condition.

renormalization scheme (RS): choice of \( c_k, k > 1 \) and the initial condition specified, for instance, by \( \Lambda_{RS} \), where

\[ a(\mu = \Lambda_{RS}) = \infty \quad \Rightarrow \quad a = a(\mu / \Lambda_{RS}) \]
Observable

Example:

\[ R(Q) \equiv \frac{\sigma(Q, e^+e^- \rightarrow \text{hadrons})}{\sigma(Q, e^+e^- \rightarrow \mu^+\mu^-)} = \left(3 \sum_i e_i^2\right) (1 + r(Q)) \]

\[ r(Q) = a(\mu / \Lambda, c_i) \left( r_0 + r_1(\mu / Q)a(\mu / \Lambda, c_i) + r_2(\mu / Q, c_2)a^2(\mu / \Lambda, c_i) + \cdots \right) \]

the internal consistency requires

\[ \frac{dr(Q)}{d \ln \mu} = \frac{dr(Q)}{dc_i} = 0; \quad i \geq 2 \]

which in turn implies

\[ r_1(Q / \mu, RS) = b \ln \frac{\mu}{\Lambda_{RS}} - \rho(Q) \]

\[ r_2(Q / \mu, RS) = \rho_2 - c_2 + (r_1 + c / 2)^2 \]

renormalization group invariants
instead of $\mu$ and $c_2$ we can use $a$ and $c_2$

$$\rho(Q) = b \ln(Q/\Lambda) - r_1(1)$$

Which point to choose?

For $c=0$

$$\rho(Q) = \frac{1}{\rho(Q)}$$

invariant arbitray
Parton distribution functions

\[ \frac{d \Sigma(M)}{d \ln M^2} = P_{qq}(M) \otimes \Sigma(M) + P_{qG}(M) \otimes G(M), \]
\[ \frac{d G(M)}{d \ln M^2} = P_{Gq}(M) \otimes \Sigma(M) + P_{GG}(M) \otimes G(M), \]
\[ \frac{d q_{NS}(M)}{d \ln M^2} = P_{NS}(M) \otimes q_{NS}(M). \]

Splitting functions

\[ P_{ij}(x, M) = \frac{\alpha_s(M)}{2\pi} P_{ij}^{(0)}(x) + \left( \frac{\alpha_s(M)}{2\pi} \right)^2 P_{ij}^{(1)}(x) + \cdots \]

Similarly for fragmentation functions.

arbitrary!
**Observables**

**Factorization procedure:** cross sections of physical processes can be written as convolutions of PDF, FF and partonic hard cross sections.

**generic expression for hard collision of particles A, B**

$$\sum_{a,b} D_{a/A}(M_a) \otimes D_{b/B}(M_b) \otimes \sigma_{a+b\to f}^{\text{hard}}(M_a, M_b, \mu) \otimes \sigma_f(\text{final state})$$

(usually $M_a=M_b$)

**cancellation of factorization scale dependence**

Renormalization scale $\mu$ enters only when partonic hard scattering cross section is expanded in PQCD.

$$\sigma_{a+b\to f}^{\text{hard}} = \alpha_s^k(\mu, c_i)C^{LO} + \alpha_s^{k+1}(\mu, c_i)C^{NLO}(M_a, M_b, \mu) + \cdots$$

**cancellation of renormalization scale dependence**
Scales and schemes appear due to ambiguities in the treatment of singularities at

short distances: renormalization scale and scheme
long distances: factorization scale and scheme

Dependence on scales has intuitively clear physical interpretation but their choice is insufficient to unambiguously specify perturbative calculations, as the schemes are as important as the scales!!

In other words, the existence of “natural physical scale” of a given hard process does not help in resolving the scale/scheme setting problem.
The common practice of identifying $\mu=M$ and setting it equal to some “natural scale” $Q$ has no justification apart from simplicity (Politzer, 1987).

Moreover, the conventional way of estimating theoretical uncertainty due to scale choice, i.e. plotting the band of results corresponding to

$$Q/2 \leq \mu \leq 2Q$$

makes little sense because it
- depends on selected scheme
- is actually misleading: at LO

$$\frac{\alpha_s(\mu/2) - \alpha_s(2\mu)}{\alpha_s(\mu)} \approx \beta_0 \alpha_s(\mu) \ln 4 \to 0 \text{ as } \mu \to \infty$$

i.e. LO predictions would appear to have very small “uncertainty” at short distances, which is nonsense.
So how should we proceed?

Make a choice of scales and schemes, based on some general idea, and look whether it leads to meaningful phenomenology for wide range of processes.

Keep the renormalization and factorization scales $\mu$ and $M$ as independent parameters and investigate the dependence of perturbative results on these parameters in the whole $(\mu, M)$ plane, looking for regions of local stability.

Such investigation makes sense even if one does not subscribe to PMS!
Factorization scale

\[ \mu_{\text{factorization}} \neq \mu_{\text{renormalization}} \]

- Arbitrary separation of soft and hard physics

- Dependence on factorization scale not associated with beta function - present even in conformal theory

- Keep factorization scale separate from renormalization scale

\[ \frac{d\mathcal{O}}{d\mu_{\text{factorization}}} = 0 \]

- Residual dependence when one works in fixed order in perturbation theory.
Principle of Minimal Sensitivity (PMS, Stevenson): scales and schemes chosen at points of local stability

\[ \frac{dF(\mu, M, c_i)}{d\mu} = \frac{dF(\mu, M, c_i)}{dM} = \frac{dF(\mu, M, c_i)}{dc_i} = 0 \]

Effective Charges (EC, Grunberg): earlier also called “Fastest apparent convergence” scales and schemes chosen at points where all higher order contributions vanish

\[ r_1 = b \ln(\mu / \Lambda) - \rho(Q) = 0, \quad r_2 = \rho_2 - c_2 + (r_1 + c / 2)^2 = 0 \]

Brodsky-Lepage-McKenzie (BLM): mimics QED, applicable to renormalization scale only
Inclusive particle production in $\gamma^*p$ collisions

an example how the scale dependence can mar the searches for signals of “new physics”

Forward pions in $ep$ collisions has been suggested by A. Mueller as a process where the BFKL effects, characteristic for low $x$ region, should be manifest.

But due to large scale dependence, we cannot distinguish BFKL or merely direct $\gamma$ or resolved $\gamma$ needed?

Conventional choice identifies four different scales!!

$$\mu^2 = M_p^2 = M_\gamma^2 = M_h^2 = \kappa^2 (Q^2 + E_T^2)$$

renormalization $\gamma$-factorization photon virtuality pion $E_T$

p-factorization fragmentation
The optimists: Kniehl, Kramer and Maniatis 05

\( \pi^0 \) and charged hadrons spectra compared to H1(99) data.

A factor of 2 difference

\[ M^2 = \frac{\xi (Q^2 + E_T^2)}{2} \]

Agreement for \( \frac{\xi}{1/2} \leq \xi \leq 2 \)

"moderate unphysical scale variations lead to a satisfactory description of the HERA data"
The realists: **Aurenche, Basu, Fontannaz, Godbole 05**

analyzed the same data on forward $\pi^0$ taking into account the resolved virtual photon as well and setting as default

$$\mu^2 = M^2 = Q^2 + E_T^2$$

A factor of 2 difference from Kniehl et al.

Large instability is observed when varying independently the renormalization and fragmentation scales.

This prevents a really quantitative prediction for the single pion inclusive distribution in the forward region.
But this was at relatively low (transverse) energy, perhaps at much larger transverse energies available at the LHC the situation will be better.

It may, but not always!

In the following I will discuss the $t\bar{t}$bar production at LHC using the NLO code of

Frixione&Mangano:

What is wrong with the conventional assumption $\mu=M$?

LO prediction for $\sigma_{\text{tot}}(pp \rightarrow bb, \mu, M, s)$ at $\sqrt{s} = 64$ GeV

- It fakes stability where there is none!
- It leads away from regions of genuine stability

Sometimes

- It fakes stability where there is none!
- It leads away from regions of genuine stability
$b\bar{b}$ at $\sqrt{s} = 64$ GeV

conventional

$\mu = M = \sqrt{E_T^2 + m_b^2}$

saddle
$b\bar{b}$ at $\sqrt{s} = 1.8$ TeV
$\bar{t}\bar{t}$ at $\sqrt{s} = 1.8\text{TeV}$

10-15% difference
$t\bar{t}$ at $\sqrt{s} = 14$ TeV

30-40% difference phenomenologically significant
Backup
Do ambiguities decrease at higher orders?

The usual claim that at higher orders the ambiguities of finite order perturbative approximations decrease is not true, because at each order of perturbation theory additional new free parameters, namely $\beta$-function coefficients and splitting functions do appear. We can ignore them and continue to work in the conventional (renormalization and factorization) schemes, which reflect our preference for dimensional regularization, but this does not make the mentioned claim true.

Note, that it makes no sense to compare functions of different number of variables.
The Renormalization Scale Problem

- No renormalization scale ambiguity in QED
- Running Gell Mann-Low QED Coupling sums all Vacuum Polarization Contributions
- QED Scale Identical to Photon Virtuality
- Examples: Lamb Shift, muonic atoms, $g-2$
- No renormalization scale ambiguity in EW theory
Scales and schemes appear due to ambiguities in the treatment of singularities at

**short distances:** \( \mu \) and renormalization scheme

**long distances:** \( M_p, M_\gamma, M_F \) and factorization schemes

Freedom in the choice of renormalization and factorization schemes **almost unexploited** and phenomenological applications calculations done **mostly** in MS RS and FS.

Dependence on scales has a **clear interpretation**, but their choice is **insufficient** to specify perturbative calculations.

Common practice \( \mu = M_p = M_\gamma = M_F \) = "natural scale"

**has no justification apart from simplicity (Politzer 87)."
Chyla (Photon 2005)

The same choice of the renormalization scale gives different results in different RS! In fact the schemes are as important as scales, but there is no “natural” RS or FS!

The conventional procedure which assumes working in MS is thus based on entirely ad hoc choice of RS.

Choice of scales and schemes should be done in more sophisticated way. This means keeping

\[ \mu \quad \text{and} \quad M_p, M_\gamma, M_F \quad \text{independent} \]

and investigating the dependence of perturbative results on these free parameters, looking for regions of local stability.

Such investigation makes sense even if one does not subscribe to PMS!

PHOTON#05 9-3-05

BLM Scale Setting

Stan Brodsky, SLAC
very different dependences
From A. Vogt's talk at PHOTON05:

NLO predictions not accurate enough for many important processes

NNLO: Harlander, Kilgore (02), . . . ;  \( N^3\text{LO}_{SV} \): Moch, A.V. (05)