Scale Dependence and Uncertainties of Fixed Order pQCD Cross sections: How precise is the Higgs cross section?

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• This discussion is really about the questions you should ask your theory colleagues when they give you a pQCD result.

• I am not currently in the business of doing the hard pQCD work, but I do remember the history.

• We’ll start with inclusive jets and move on to inclusive Higgs.

• You know all this stuff – but do you talk about it enough?
Recall the basic structure of pQCD calculations: Factorized so that

A) Important UV/short-distance physics at momentum scales larger than $\mu_R$ are summed to all orders (in $\alpha_s$) and some fixed order in logarithms (of $\mu_R/\Lambda_{QCD}$) into the running coupling $\alpha_s(\mu_R)$, which is the solution of the appropriate renormalization group equation;

B) Important IR/long distance physics at momentum scales smaller than $\mu_F$ are summed to all orders (in $\alpha_s$) and some fixed order in logarithms (of $\mu_F/\Lambda_{QCD}$) into the running parton distributions functions, which are solutions of DGLAP equations;

C) The fixed order pQCD cross section describes the “hard” physics between these two scales, typically characterized by a “physics” scale, e.g., a jet pT or Higgs mass.

D) The final expression is a convolution of all of these components

$$d\sigma \left( p_T, \sqrt{s}, y; R; \mu_F, \mu_R \right) \sim \int \int \int \sum_{a,b,c,x} f_{a/p} \left( x_a, \mu_F \right) \otimes f_{b/p} \left( x_b, \mu_F \right)$$

$$\otimes d\hat{\sigma}_{ab\rightarrow cX} \left( p_T, \sqrt{x_a x_b s}, y; R; \alpha_s(\mu_R), \mu_F, \mu_R \right)$$
But..

A) The data do NOT depend on the scales $\mu_R$ and $\mu_F$.

B) We expect a “complete” (all orders) pQCD result to also have vanishing dependence on the scales $\mu_R$ and $\mu_F$. 
While at fixed, low order expect -

• Past lowest order the integrated parton cross section will exhibit explicit logarithms of the scales $\mu_R$ and $\mu_F$ that partially cancel the dependence in the running coupling and PDFs.

• But this cancellation is always incomplete and the pQCD theoretical results do depend on this scales.

• To obtain a numerical pQCD result we must choose explicit numerical values for the scales $\mu_R$ and $\mu_F$!

  How do we make that choice?

  How much does it matter?

• We can use the residual scale dependence to estimate the residual theoretical uncertainty!

  WARNING: this last technique is necessarily ad hoc, i.e., it is difficult to estimate the uncertainty in the estimated uncertainty!
Important lesson – can use the pQCD calculation itself to choose scales and estimate uncertainties!

This is what you want to ask of your theory colleagues!

• Choosing a scale - since the goal is independence of both $\mu$’s and the perturbative order, two possibilities immediately suggest themselves:

a) choose a scale where the residual $\mu$ dependence is minimal in the current fixed order result, or

b) choose a scale where the cross section does not change as the order of the calculation changes (i.e., the higher correction vanishes), or

c) both.
EXAMPLE - consider first the inclusive (EKS = Ellis, Kunszt, Soper) jet cross section, where we take central (small rapidity) jets as a function of $p_J \approx p_T$, set $\mu_R = \mu_F = \mu$ and vary $\mu$ with fixed $p_J$. The jet cross section in the figure is for jets defined by the Anti-kT algorithm with $R = 0.6$, $p_J = 200$ GeV and $\sqrt{s} = 7$ TeV.

The blue, LO curve exhibits the expected monotonic decrease with $\mu$ (both the PDFs and the coupling decrease with $\mu$). Any value for the cross section can be obtained by an appropriate scale choice and so the uncertainty is very large.

At NLO (the red curve) there is a local maxima, which is near where the two curves intersect.

By both criteria the appropriate NLO scale choice is $\mu = p_J/2$, and this is the typical choice. But it is important to recall that there is a reason for this choice.

A given fixed order pQCD calculation can (itself) provide information about what scale choice to make by exploring the calculated $\mu$ dependence. Any pQCD analysis claiming precision should perform such a study.
NOTE: there is another scale in the jet problem (i.e., $\sqrt{s}$) and the calculated $\mu$ dependence can depend on it, e.g., through the variable $x_T = 2 \ p_T/\sqrt{s}$ as exhibited in the 3D plot below. Like the previous plot this is for NLO (EKS), Anti-$k_T$, $R = 0.6$, $\mu_R = \mu_F = \mu$, scaled to the cross section at $\mu = p_J/2$ for each $x_T$ ($p_J$) value.

For $x_T > 0.05$ (the blue region) we see essentially the same $\mu$ dependence as on the previous slide (a local maximum).

HOWEVER, we see that the NLO result becomes monotonic (like LO) at small $p_J$, $x_T < 0.03$ ($p_J < 100$ GeV at 7 TeV), i.e., NLO becomes “unreliable” (much larger uncertainty) at small $p_J$, $x_T$ values.
We should think about this behavior in terms of $x_T$ because it is (presumably) really a small $x$ (of the partons) scaling behavior when $p_J \ll \sqrt{s}$.

Note that $x_T$ is the geometric mean of the $x$‘s of the 2 incoming partons. When $x_T$ is $\ll 1$, at least one of the parton $x$‘s is also small. Also true at large $y$.

Generically at small $x$ the scaling of the PDFs (especially the gluons) changes from decreasing with $\mu_F$ (as is true at larger $x$) to increasing with $\mu_F$, and we should not be surprised by this change of behavior at small $x_T$. 

![Graph showing $d\sigma(pJ,\mu)/dpJ$ for $p_J = 30$ GeV and $p_J = 200$ GeV]
I believe that we should think about this behavior in terms of $x_T$ because it is (presumably) really a small $x$ (of the partons) scaling behavior when $p_J << \sqrt{s}$. Note that $x_T$ is the geometric mean of the $x$'s of the 2 incoming partons. When $x_T$ is << 1, at least one of the parton $x$'s is also small. Generically at small $x$ the scaling of the PDFs changes from decreasing with $\mu$ (as is true at larger $x$) to increasing with $\mu$ at small $x$, and we should not be surprised by this change of behavior at small $x_T$.

To further suggest this scaling behavior, the plot below exhibits very similar behavior and is a plot that I made for Run I at the Tevatron (for the different value $\sqrt{s} = 1.8$ TeV) in 1993. In this plot the transition to monotonic behavior occurs at about the same $x_T$, but smaller $p_J (=ET)$.

(Note also that this plot is for the old seedless iterative cone jet algorithm with $R = 0.7$.)
Next Consider the full 2 D structure in $\mu_F$ and $\mu_R$

We start with the inclusive single jet cross section, which is a function of jet $p_T$, jet rapidity $y$, jet parameter $R$, $\sqrt{s}$, and the scales $\mu_R$ and $\mu_F$. Next we introduce reference scales ($\mu_{0,F}$, $\mu_{0,R}$) and expand around them, i.e., substitute $\ln \mu_F = \ln \mu_{0,F} + \ln(\mu_F/\mu_{0,F})$ and $\ln \mu_R = \ln \mu_{0,R} + \ln(\mu_R/\mu_{0,R})$ in the original result and keep up to quadratic terms in $\ln(\mu_F/\mu_{0,F})$ and $\ln(\mu_R/\mu_{0,R})$ (we are assuming $\mu \approx \mu_0$). Near the reference point the resulting (approximate) expression will look like

$$\sigma(\mu_F, \mu_R) \approx \sigma(\mu_{0,F}, \mu_{0,R}) \left[ 1 + b_R \ln(\mu_R/\mu_{0,R}) + b_F \ln(\mu_F/\mu_{0,F}) + c_R \ln^2(\mu_R/\mu_{0,R}) + c_F \ln^2(\mu_F/\mu_{0,F}) + c_{RF} \ln(\mu_R/\mu_{0,R}) \ln(\mu_F/\mu_{0,F}) \right].$$

All of the quantities in this expression (except the explicit logs), i.e., the coefficients, will, in general, depend on all of the possible variables, typically logarithmically, i.e., $\ln (p_T/\mu_{0,F})$, $\ln (p_T/\mu_{0,R})$, $\ln(R)$, $\ln(p_T/\sqrt{s})$, $y$. 
The underlying suggestion is that the best estimate of the “full” is where the derivatives wrt both scales vanish, typically a SADDLE POINT.

The location of the saddle point \((\mu_{S,F}, \mu_{S,R})\) is determined by solving the (implicit) equations (substitute \((\mu_{0,F}, \mu_{0,R}) \Rightarrow (\mu_{S,F}, \mu_{S,R})\) in the b’s and solve)

\[
\begin{align*}
  b_R \left( \ln \left( \frac{p_T}{\mu_{S,R}} \right), \ln \left( \frac{p_T}{\mu_{S,F}} \right), \ln \left( \frac{p_T}{\sqrt{s}} \right), \ln R, y \right) &= 0, \\
  b_F \left( \ln \left( \frac{p_T}{\mu_{S,R}} \right), \ln \left( \frac{p_T}{\mu_{S,F}} \right), \ln \left( \frac{p_T}{\sqrt{s}} \right), \ln R, y \right) &= 0.
\end{align*}
\]

Of course, these equations may have no real solutions near \(p_T\), in which case we see no saddle point. These equations are expected to largely factorize, i.e., \(b_F\) depends primarily on \(\mu_{S,F}\) (not \(\mu_{S,R}\)) and \(b_R\) depends on \(\mu_{S,R}\) (not \(\mu_{S,F}\)). In any case, it is not surprising that the resulting saddle point moves around as the kinematic variables change, as we will see in detail. To see the saddle point in the formalism we set \(\mu_0 = \mu_S\) (where the b’s vanish) and write

\[
\sigma \left( \mu_F, \mu_R \right) \approx \sigma \left( \mu_{S,F}, \mu_{S,R} \right) \left[ 1 + c_R \ln^2 \left( \frac{\mu_R}{\mu_{S,R}} \right) + c_F \ln^2 \left( \frac{\mu_F}{\mu_{S,F}} \right) \\
+ c_{RF} \ln \left( \frac{\mu_R}{\mu_{S,R}} \right) \ln \left( \frac{\mu_F}{\mu_{S,F}} \right) \right],
\]

where the \(c\) coefficients still depend on the variables \(x_T, y\) and \(R\).
The “orientation” of the saddle point (the orientation of its axes) can be characterized in terms of the relative size and signs of the $c$ coefficients (at the saddle point). For the case $c_F > 0$, $c_R < 0$ and $c_F$, $|c_R| >> |c_{RF}|$, the saddle point axes are aligned with the plot axes, which we will see is the “low pT” behavior and is indicated in the upper figure to the right.

If instead $c_{RF} < 0$ and $c_F, |c_R| << |c_{RF}|$ (still $c_F > 0$, $c_R < 0$), we obtain the “rotated” saddle point ($\sim 45^\circ$) indicated in the lower figure to the right, which we will associate with large pT behavior.

Different relative sizes (and signs) of the $c$’s leads to other rotations of the saddle point.

As we will see, the $\mu$ behavior along the diagonal ($\mu_R = \mu_F$) can dramatically change with the orientation.
So one way to proceed is to try to understand the behavior of the $b$’s (i.e., the location of the saddle point) and the $c$’s (i.e., the character of the saddle point) as functions of the kinematic and experimental parameters. Since the explicit logarithms must act to cancel the running behavior of the couplings and the PDFs, one can hope to proceed analytically. This is not a solved problem but see the recent SCET analysis by Matt Schwartz and collaborators – 1206.6115, which studies the logarithms directly (but with 4 scales).

QUALITATIVELY the perturbative functions $\rightarrow 0$ as $\mu$’s $\rightarrow \infty$ and become large in magnitude for small $\mu$ values. But the sign of this divergence depends on the higher order explicit logarithms ($\ln (\mu_R/p_T) \& \ln(p_T/\mu_F)$) and on the $x$ value in the splitting vertex (running PDFs).

⇒ SADDLE POINTS

⇒ But numbers depend on details (of convolutions)
Here we will proceed “experimentally” results and look at some plots. The first introductory plots are EKS results and the detailed jet results are from Joey Huston.

Our goal is to understand how/why the saddle point moves, especially with respect to the diagonal, and rotates when we vary one of the parameters (pT, $\sqrt{s}$, R, y) with the others held fixed. Here we briefly note the movement

The following plots all have (ln) $\mu_R/pT$ along the x-axis and (ln) $\mu_F/pT$ along the y-axis. Where appropriate, the diagonal, the saddle point and other commonly used scale choices are indicated.

You are encouraged to think that you should always be shown such plots to understand the pQCD results and uncertainties.
Consider the full behavior in \( \mu_R \) and \( \mu_F \) in terms of 2D contour plots for jets at the LHC.

The left panel is a “large pT” saddle point (red dot, \( \mu_R = 0.65 \, p_T \), \( \mu_F = 0.70 \, p_T \)) with approximately symmetric \( \mu \) dependence along the two axes, except for the sign, and with shallow behavior in both directions.

The right panel is a low pT saddle point (blue dot, \( \mu_R = 0.55 \, p_T \), \( \mu_F = 0.82 \, p_T \)), which is shifted up and to the left (although still within the factor of 2 uncertainty circle about the previous – red - location), and “rotated” (to align with the axes) with steep behavior in \( \mu_R \) and more shallow behavior in \( \mu_F \).
Now with the diagonal line, $\mu_F = \mu_R$, explicit

- The left panel explains why we see an extremum versus $\mu = \mu_F = \mu_R$, the diagonal passes right through the saddle point in the direction to see a local maximum (at the saddle point).

- The right panel explains what happens as we decrease $p_T$. As the saddle point drifts away from the diagonal (up and left), the maximum along the diagonal moves towards the origin and eventually we see only the low $x_T$ monotonic behavior of slides 3 and 4.
To illustrate what I think happens at low pT, here is a contour plot from fake data (the previous 70 GeV data shifted further to the left and up, and multiplied by 3).

Now the diagonal misses the saddle point completely and the behavior along the diagonal ($\mu_R = \mu_F = \mu$) is monotonic. I believe this explains the structure seen in the plots on slides 3 and 4 at small xT (pT).

Next we study a variety of plots from Joey indicating how the saddle point varies with the kinematic variables and R.
As pT increases, the saddle point structure rotates CCW and the saddle point itself shifts along the diagonal to smaller $\mu/pT$. At the smallest pT the variation along the diagonal is monotonic.

In the language of the $c$’s, $|c_{RF}|$ apparently grows with respect to $|c_R|$ and $|c_F|$, with $c_{RF}$ small and positive at low pT and then becoming large and negative (passing thru 0 around pT = 80 GeV).

For this value of R, the 2 $b$’s are very similar leading to a saddle point on the diagonal with $\mu$ values that grow slightly less rapidly than pT ($\mu/pT$ decreases with increasing pT).
$R = 0.6$, small $y$, versus $p_T$

For this value of $R$, as $p_T$ increases, the $c$’s behave similarly to the $R = 0.4$ case and the saddle point structure rotates CCW.

However, the $2b$’s are different and the saddle point at low $p_T$ has $\mu_{S,R} < \mu_{S,F}$ (above the diagonal). As $p_T$ increases it shifts asymmetrically to smaller $\mu/p_T$ with $|\Delta \mu_{S,R}| < |\Delta \mu_{S,F}|$ so that it passes through the diagonal around $p_T \sim 200$ GeV.

Note that, for larger $R$, there is less “splash-out” meaning smaller parton $x$’s for the same jet $p_T$, and conversely.
The orientation of the saddle point structure seems to be essentially R independent (i.e., the c’s are largely R independent).

The location of the saddle point shifts with R at most pT values, but in different directions at large and small pT (i.e., the b’s have correlated R and pT dependence – for R = 0.4 the pT dependences of $\mu_{S,R}$ and $\mu_{S,F}$ are about equal, while for R = 0.6 $\mu_{S,R}/pT$ decreases less rapidly with increasing pT than $\mu_{S,F}/pT$.

The R dependence is also smaller at large pT where the QCD showers are presumably intrinsically more narrow.
The orientation of the saddle point structure seems to be largely \( y \) independent (maybe some CCW rotation at the largest \( y \)), i.e., the \( c \)'s are approximately \( y \) independent.

The location of the saddle point (the \( b \)'s) moves slowly to larger \( \mu \) (along the diagonal) as \( y \) increases, with a rate that seems to increase slightly with \( pT \), i.e., the \( y \) dependence of the \( b \)'s is approximately the same for \( R = 0.4 \).
y dependence at R=0.6

Again the orientation of the saddle point structure seems to be largely $y$ independent, i.e., the $c$’s are largely independent of both $y$ and $R$.

The location of the saddle point shifts slowly to larger $\mu$ as $y$ increases in a symmetric ($\Delta\mu_{S,R} \approx \Delta\mu_{S,F}$) fashion, with a rate that seems to increase slightly with $p_T$, i.e., the $b$’s have some $y$ dependence that is essentially the same for $b_F$ and $b_R$ and largely independent of the $R$ parameter.
Summary for inclusive jets -

c's: the general behavior is $c_F > 0$, $c_R < 0$ with $c_R$ somewhat larger in magnitude;

the primary variation is in $c_{RF}$ which, at low $pT$ is positive and substantially smaller in magnitude
than $c_F$ and $c_R$ but, as $pT$ increases, $c_{RF}$ goes thru 0 and becomes more negative until it is larger in
magnitude than $c_F$ and $c_R$ at large $pT$, leading to a systematic CCW rotation of the saddle point;

the c's exhibit essentially no y or R dependence.

⇒ The saddle point rotates CCW with increasing $pT$ in a fashion that is largely y and R independent.

b's: exhibit dependence on R, y and pT such that –

for $R = 0.4$ and low $pT$, $\mu_{S,R} \approx \mu_{S,F}$ and both increase more slowly than $pT$ as $pT$ increases
($\mu_{S,R}/pT \approx \mu_{S,F}/pT$ decreases with $pT$) with $\Delta \mu_{S,R} \approx \Delta \mu_{S,F}$ (along the diagonal);

for $R = 0.6$ and low $pT$, $\mu_{S,R} < \mu_{S,F}$ (above the diagonal) and both increase more slowly than $pT$ as $pT$
increases (i.e., $\mu_{S,R}/pT$ and $\mu_{S,F}/pT$ decrease with $pT$) but with $|\Delta \mu_{S,R}| < |\Delta \mu_{S,F}|$ so that the saddle
point crosses the diagonal near $pT = 200$ GeV;

both $\mu_{S,R}/pT$ and $\mu_{S,F}/pT$ increase slowly with increasing y with $\Delta \mu_{S,R} \approx \Delta \mu_{S,F}$ (parallel to the
diagonal) in a fashion that is essentially independent of R and $pT$.

⇒ The y dependence is largely decoupled from the R and $pT$ dependences, while the R and $pT$
dependences are coupled.

For jets it is the R dependence that breaks the $\mu_{S,R} \approx \mu_{S,F}$ approximate symmetry.
Now consider inclusive Higgs production. The specific fixed order results presented here are from C. Anastasiou, S. Buehler, F. Herzog, and A. Lazopoulos of ETH (1202.3638). They generate their inclusive fixed order numbers with the public program \textit{ihixs} (the pT cut numbers come from the non-public program “Fehipro”). I believe this to be a complete fixed order pQCD calculation at NLO plus NNLO corrections in the HQET (top quark) approximation and some EW corrections. I also believe there are small differences from the two pQCD results used by the LHC Higgs XC Working group. One of those (dFG) sums $\mu R$ logs which matter numerically for $\mu > m_H/2$, but not for smaller $\mu$.

First consider the 1-D behavior along $\mu_R = \mu_F = \mu$ for both inclusive Higgs production (upper plot $m_H = 125$ GeV, middle plot $m_H = 450$ GeV) and with a cut on the pT of the Higgs (> 100 GeV, lower plot, $m_H = 125$ GeV). In these plots $\sqrt{s} = 8$ TeV. (Note that, with the pT cut, the result labeled NLO is actually the LO result for the process with a recoiling jet.)

Note how similar the NLO and NNLO curves in these plots are to the LO and NLO curves for inclusive jets on slide 2. In the plots here the suggested “best” $\mu$ value (where NNLO is flat and NLO $\approx$ NNLO) is about $\mu \approx m_H/5$, $\ln(\mu/m_H) \approx -1.6$ for $m_H = 125$ GeV and more like $\mu \approx m_H/2.7$, $\ln(\mu/m_H) \approx -1.0$ for $m_H = 450$ GeV.

Note, in particular, that this “best” value for the scale is quite different from the values of $m_H$ or $m_H/2$ used by the LHC Higgs Working group (although it would presumably approach $m_H/2$ for a much larger mass than 125 GeV).
The left panel (NNLO) is most similar to the low pT, inclusive jet case, steep behavior in $\mu_R$, shallow in $\mu_F$. While the 2 default $\mu$ values (red = $m_H$, green = $m_H/2$) are consistent within the factor-2 circles (by construction), they are not consistent with the cross section value at the saddle point. The position of the saddle point is $(\mu_R, \mu_F) \approx (0.15,0.24) m_H$.

The right panel (NLO) shows that there is no saddle point at NLO (in the indicated ranges of $\mu$'s), as we would expect from the 1-D $\mu$ plots on the previous slide.
Here we display the same NNLO inclusive Higgs contour plot with the $\mu_R = \mu_F = \mu$ diagonal indicated. The actual (NNLO) cross section values suggested are ($\sqrt{s} = 8$ TeV)

\[ \mu = m_H \text{ (red), } \sigma \approx 18.8 \text{ pb } \pm 8\% \text{ (scale)} \]

\[ \mu = m_H/2 \text{ (green), } \sigma \approx 20.7 \text{ pb } \pm 8.5\% \text{ (scale)} \pm 7.5\% \text{ (PDF)} \]

\[ \mu = \text{Saddle Pt } ((\mu_{R,t}) \approx (0.15,0.24) m_H, \text{ blue}), \]

\[ \sigma \approx 23.1 \text{ pb } ^{-10}_1 \% \]

The LHC Higgs Cross Section Working Group, see 1101.0593 and their web page, for $\sqrt{s} = 8$ TeV, provide the value below for $m_H = 125$ GeV, based on the dFG calculation with $\mu = m_H$ (the resumed logs matter here)

\[ \sigma \approx 19.5 \text{ pb } ^{+7.2}_{-7.8} \% \text{ (scale) } ^{+7.5}_{-6.9} \% \text{ (PDF+}\alpha_s) \]

Because the correlations are ill-defined, the Working Group recommends linear addition of the uncertainties to yield $\pm 14.7\%$ or $\pm 2.8$ pb. Thus the upper limit (22.3 pb) is nearly consistent with the saddle point value (and certainly consistent with $\mu = m_H$ number for the NNLO results here).
Next compare the results at $m_H = 125$ GeV and $m_H = 450$ GeV

The saddle point has rotated CCW (as you might expect from the jet analysis), but the large jump below the diagonal (as $m_H$ increases) is not so clearly explained or expected!?
Finally compare the inclusive results (left) to the results with a Higgs pT cut of 100 GeV (right). Note that the axes are slightly different (with a smaller range of $\mu$ values on the right and so the plot is scaled to match). As I expected, with a pT cut and larger total parton scattering energy $\sqrt{s}$ (with larger parton x values), the saddle point has rotated a bit (CCW) and moved to slightly larger $\mu/pT$ (essentially parallel to the diagonal, like jets at larger $y$).
Summary I:

• The NNLO Higgs results described here need further verification and understanding, while the inclusive jet results tell a fairly straightforward story.

• I believe that the qualitative behavior of the NNLO pQCD results for Higgs production discussed here is correct and leads to the following conclusions.

• NLO in pQCD is not sufficient to obtain a reliable estimate of the inclusive Higgs cross section, but the current NNLO calculations are probably yielding reasonable results.

• Linearly adding the theory uncertainties from the experimental determination of the PDFs and $\alpha_s$ (correlated) to those from varying the scale (the uncorrelated truncation uncertainty) is probably an appropriately conservative approach. But this does not address the question of what scale should define the center of this window.
Summary II:

• The NNLO pQCD results given here suggest that the best estimate of the true inclusive Higgs production cross section is somewhat above the estimated uncertainty window in the 8 TeV LHC Higgs Working Group numbers, suggesting a larger window is appropriate, or a shift of the window to larger cross section values!

• It would be very useful to have an analysis of the $\mu_F$ and $\mu_R$ dependence of the cross sections quoted in the LHC study (and for any other interesting pQCD calculation) – ask your theory friends!.

• The suggestion here is to estimate the central cross section value by the value at the saddle point.

• Estimate the residual uncertainty by the variation on the circle around the saddle point.