Perturbative QCD predictions in fixed order for cross section ratios

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ABSTRACT: In the standard approach, predictions of perturbative Quantum Chromodynamics for ratios of cross sections are computed as the ratio of fixed-order predictions for the numerator and the denominator. Beyond the lowest order in the perturbative expansion, the result does, however, not correspond to a fixed-order prediction for the ratio. This article describes how exact fixed-order results for ratios of arbitrary cross sections can be obtained. The general method for computations in any order of the perturbative expansion is derived, and results for next-to-leading order and next-to-next-to-leading order calculations are given. The approach is applied to theory predictions for various multi-jet cross section ratios measured at hadron colliders. The two methods are compared with each other and with the experimental data. Recommendations are made how to obtain improved theory predictions with more realistic uncertainty estimates.

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1 Introduction

Measurable quantities, defined as ratios of cross sections, R, are studied for a variety of reasons. Due to the cancellation of uncertainties which are correlated between numerator and denominator, such ratios can often be measured with higher experimental precision and also be more precisely predicted by theory. Among such quantities are normalized distributions where a differential cross section is divided by its integral, or ratios of production cross sections for different processes. Examples for the latter are ratios of multi-jet cross sections in hadron collisions with different jet multiplicities, which are frequently used for phenomenological tests of perturbative Quantum Chromodynamics, pQCD, for determinations of the strong coupling constant, α_s , and for tests of the renormalization group predictions for its running [1–5].

In most cases, phenomenological analyses of experimental data use pQCD predictions in fixed order in α_s . The pQCD predictions for a ratio R are then typically computed from the ratio of the corresponding fixed-order predictions for the cross sections in the numerator and the denominator. For consistency, both of these are computed at the same relative order in α_s , i.e. both at leading order, LO, next-to-leading order, NLO, or next-to-next-to-leading order, NNLO, in α_s . Beyond the LO, however, such computations do not provide exact fixed-order pQCD predictions for the ratio R.

In this article, we discuss how the cross section results for the numerator and denominator can be used to compute an exact fixed-order result for the ratio R of arbitrary cross sections. We present the general procedure for any order pQCD, and provide the solutions for predictions at NLO and NNLO. Specific results for both methods are computed for a set of multi-jet cross section ratios, measured at the CERN LHC and the Fermilab Tevatron Collider. From the comparison of both methods and their description of the experimental data, and based on general considerations, we derive recommendations for theoretical calculations of cross section ratios. We motivate how this can lead to improved predictions with more realistic uncertainty estimates in future phenomenological analyses of cross section ratios.

2 Calculation

Definitions

A measurable quantity $R = \frac{\sigma_n}{\sigma_d}$ is defined as the ratio of two cross sections σ_n and σ_d , where n and d denote the order of α_s of the LO contributions to the pQCD predictions $(\sigma_{n,LO} \propto \alpha_s^n \text{ and } \sigma_{d,LO} \propto \alpha_s^d)$ and it is assumed that $n \geq d$. It is also assumed that the quantity R is defined in bins of an energy or transverse momentum related variable p which is defined for both σ_n and σ_d . At a fixed value (or in a given bin) of p, the quantity R is given by $R(p) = \frac{\sigma_n(p)}{\sigma_d(p)}$, and it is assumed that in a pQCD calculation the renormalization scale μ_r can be related to p by the same simple function (like $\mu_r = p$ or $\mu_r = p/2$) for both, σ_n and σ_d . In other words, in a given bin of p, the ratio R is probing α_s and the pQCD matrix elements for σ_n and σ_d at the same μ_r . In the following, for the sake of brevity, the dependence on p is omitted The perturbative expansions of the two cross sections in orders of α_s are given by

$$\sigma_{\rm n} = \sum_{i=0}^{\infty} \sigma_{n,i}$$
 and $\sigma_{\rm d} = \sum_{i=0}^{\infty} \sigma_{d,i}$, (2.1)

where the pQCD contribution in LO corresponds to i = 0, NLO to i = 1, and NNLO to i = 2.

Typically, the "NLO k-factor", k_{NLO} , for a given quantity is defined as the ratio of its NLO and LO pQCD predictions. For σ_n it is therefore

$$k_{\text{NLO}} = \frac{\sigma_{n,\text{NLO}}}{\sigma_{n,\text{LO}}} = \frac{\sigma_{n,0} + \sigma_{n,1}}{\sigma_{n,0}} = 1 + \frac{\sigma_{n,1}}{\sigma_{n,0}}.$$
 (2.2)

We name the last piece $k_{n,1} \equiv \frac{\sigma_{n,1}}{\sigma_{n,0}}$ a "reduced NLO k-factor", since $k_{n,1} = (k_{\text{NLO}} - 1)$. This definition is then extended to all orders, such that for each order i, a reduced k-factor is defined as

$$k_{n,i} = \frac{\sigma_{n,i}}{\sigma_{n,0}}$$
 for $i = 1, 2, 3, \cdots$. (2.3)

With this definition, the perturbative expansions of σ_n and σ_d can be written in terms of their LO contributions and their reduced k-factors as

$$\sigma_{\rm n} = \sigma_{n,0} \cdot (1 + k_{n,1} + k_{n,2} + ...)$$
 and $\sigma_{\rm d} = \sigma_{d,0} \cdot (1 + k_{d,1} + k_{d,2} + ...)$. (2.4)

The standard approach for computing the ratio

The LO pQCD prediction for the ratio $R = \frac{\sigma_n}{\sigma_d}$ is uniquely given by the ratio of the LO pQCD results for the numerator and denominator

$$R_{\rm LO} = \frac{\sigma_{n,\rm LO}}{\sigma_{d,\rm LO}} = \frac{\sigma_{n,0}}{\sigma_{d,0}}.$$
 (2.5)

Beyond LO, however, the pQCD prediction for R can be obtained in different ways. In phenomenological analyses of experimental data, the NLO (NNLO) pQCD prediction for R is usually computed from the ratio of the NLO (NNLO) predictions for σ_n and σ_d as

$$R_{\text{NLO}} = \frac{\sigma_{n,\text{NLO}}}{\sigma_{d,\text{NLO}}}$$
 and $R_{\text{NNLO}} = \frac{\sigma_{n,\text{NNLO}}}{\sigma_{d,\text{NNLO}}}$. (2.6)

With (2.4) and (2.5), the NLO result can be written as

$$R_{\text{NLO}} = \frac{\sigma_{n,0} \cdot (1 + k_{n,1})}{\sigma_{d,0} \cdot (1 + k_{d,1})} = R_{\text{LO}} \cdot \frac{1 + k_{n,1}}{1 + k_{d,1}},$$
(2.7)

the NNLO result as

$$R_{\text{NNLO}} = \frac{\sigma_{n,0} \cdot (1 + k_{n,1} + k_{n,2})}{\sigma_{d,0} \cdot (1 + k_{d,1} + k_{d,2})} = R_{\text{LO}} \cdot \frac{1 + k_{n,1} + k_{n,2}}{1 + k_{d,1} + k_{d,2}}, \tag{2.8}$$

and the general expression as

$$R_{\text{fixed-order}} = \frac{\sigma_{n,0} \cdot (1 + \sum_{i=1}^{i_{\text{max}}} k_{n,i})}{\sigma_{d,0} \cdot (1 + \sum_{i=1}^{i_{\text{max}}} k_{d,i})} = R_{\text{LO}} \cdot \frac{1 + \sum_{i=1}^{i_{\text{max}}} k_{n,i}}{1 + \sum_{i=1}^{i_{\text{max}}} k_{d,i}},$$
(2.9)

where i_{max} specifies the highest order in the pQCD calculations (1: NLO, 2: NNLO, ...). In the following, we refer to the results (2.6)–(2.9), as the "standard" approach. Note that, beyond LO, these ratios do not directly correspond to fixed-order pQCD results for the quantity R.

Computing the ratio at fixed order

The goal is to obtain an exact fixed-order result for R, in the form

$$R = R_{\text{LO}} \cdot \left(1 + \sum_{i=1}^{i_{\text{max}}} \alpha_s^i c_i \right) . \tag{2.10}$$

To find the terms of the sum, we rewrite (2.9) as

$$R_{\text{fixed-order}} = R_{\text{LO}} \cdot \left(1 + \sum_{i=1}^{i_{\text{max}}} k_{n,i} \right) \cdot \frac{1}{1 + \sum_{i=1}^{i_{\text{max}}} k_{d,i}},$$
 (2.11)

and expand the right term in a Taylor series

$$\frac{1}{1+x} = 1 - x + x^2 - x^3 + x^4 - \dots \quad \text{with} \quad x = \sum_{i=1}^{i_{\text{max}}} k_{d,i} . \tag{2.12}$$

The terms of this series are multiplied with the terms in parenthesis in (2.11), and the resulting products are sorted in their powers of α_s . The infinite series is then truncated at the corresponding order at which σ_n and σ_d were computed.¹ This can be done at any order pQCD. To compute a corresponding fixed-order pQCD result for R requires, of course, to compute both σ_n and σ_d at the same corresponding relative order in α_s (e.g. NLO, NNLO, ...).

¹The sorting is facilitated by the fact that the $k_{n,i}$ and $k_{d,i}$ are both proportional to α_s^i , which follows directly from their definition in (2.3).

Results for NLO and NNLO

At NLO, with $x = k_{d,1}$ in the Taylor series, one obtains

$$R_{\text{NLO}} = R_{\text{LO}} \cdot (1 + k_{n,1} - k_{d,1}), \qquad (2.13)$$

and at NNLO, with $x = (k_{d,1} + k_{d,2})$ in the Taylor series,

$$R_{\text{NNLO}} = R_{\text{LO}} \cdot \left[1 + (k_{n,1} - k_{d,1}) + (k_{n,2} - k_{d,2}) - k_{d,1}(k_{n,1} - k_{d,1}) \right]. \tag{2.14}$$

The individual pieces in (2.13) and (2.14) can simply be computed from the LO and (N)NLO pQCD results from the cross section calculations for σ_n and σ_d . The calculation of $R_{\rm NLO}$ requires

$$R_{\rm LO} = \frac{\sigma_{n,\rm LO}}{\sigma_{d,\rm LO}} , \qquad k_{n,1} = \frac{\sigma_{n,\rm NLO} - \sigma_{n,\rm LO}}{\sigma_{n,\rm LO}} , \qquad k_{d,1} = \frac{\sigma_{d,\rm NLO} - \sigma_{d,\rm LO}}{\sigma_{n,\rm LO}} , \qquad (2.15)$$

and the calculation of $R_{
m NNLO}$ requires in addition

$$k_{n,2} = \frac{\sigma_{n,\text{NNLO}} - \sigma_{n,\text{NLO}}}{\sigma_{n,\text{LO}}}, \qquad k_{d,2} = \frac{\sigma_{d,\text{NNLO}} - \sigma_{d,\text{NLO}}}{\sigma_{n,\text{LO}}}.$$
 (2.16)

The difference of the two results at NLO

The fixed-order result (2.13) differs from the "standard" result (2.7) due to the truncation of the series of the products of the terms in parenthesis in (2.11) and the terms from the Taylor series. An estimate of this difference can be obtained from the leading term of the truncated piece. At NLO, this is the term proportional to α_s^2 . The difference of the results from the two methods is

$$R_{\text{NLO,fixed-order}} - R_{\text{NLO,standard}} = R_{\text{LO}} \cdot [k_{d,1} \cdot (k_{n,1} - k_{d,1})] + \text{higher orders}.$$
 (2.17)

This difference is proportional to the LO result, $R_{\rm LO}$, and it depends on the NLO k-factors for the numerator and denominator. It becomes small if either the NLO k-factor for the denominator is close to unity (corresponding to a reduced k-factor of $|k_{d,1}| \ll 1$) and/or if the NLO k-factors for the numerator and denominator become equal $(k_{n,1} \simeq k_{d,1})$. It is interesting to note the asymmetry: For the difference to become small, it is sufficient that the k-factor for the denominator is small while it is not affected by the k-factor for the numerator alone. Based on (2.17), the two k-factors can be used to obtain a quick estimate of the difference between the "standard" method and the fixed-order result at NLO.

3 Comparison with data

In the following, we use the formulae obtained in the previous section to compute NLO pQCD predictions for selected quantities which are then compared to the results from experimental measurements. For this purpose, we focus on five measurements of different multi-jet cross section ratios at the CERN LHC (in pp collisions at $\sqrt{s} = 7 \,\text{TeV}$ and $8 \,\text{TeV}$) and the Fermilab Tevatron Collider (in $p\bar{p}$ collisions at $\sqrt{s} = 1.96 \,\text{TeV}$). These include

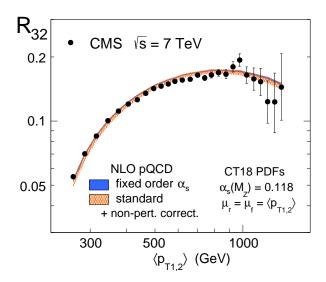


Figure 1. The multi-jet cross section ratio $R_{3/2}$, measured in pp collisions at $\sqrt{s} = 7 \text{ TeV}$ as a function of $\langle p_{T1,2} \rangle$ in the CMS experiment [4]. Two sets of pQCD predictions, corrected for non-perturbative contributions, are compared to the data: the fixed-order results for $R_{3/2}$, and the results from the "standard" approach, computed from the ratio of the fixed-order results for the two cross sections. The shaded areas represent the ranges of the scale dependences of the calculations.

measurements of the quantities $R_{3/2}$, $R_{\Delta\phi}$, and $R_{\Delta R}$, which are different ratios of three-jet and two-jet production processes.

The theoretical predictions for the ratios at NLO are obtained from the LO and NLO pQCD results for the two-jet and three-jet cross section calculations which are computed using NLOJET++ [6, 7] with fastNLO [8, 9]. Parametrizations of the parton distribution functions, PDFs, of the proton are taken from the results of the global analysis CT18 [10]. The renormalization, μ_r , and factorization scales, μ_f , are set to the same values as used in the experimental publications of the measurement results, either to one of the relevant jet p_T variables, or to half of the total jet p_T sum, $H_T/2$. The uncertainty of the pQCD results due to the $\mu_{r,f}$ dependence is computed from independent variations of μ_r and μ_f by factors of 0.5–2 around the nominal choices. The corresponding range of variations is referred to as "scale dependence". Correction factors, to account for non-perturbative contributions are taken from the estimates that were obtained in the experimental analyses. PDF uncertainties are not relevant for the following discussions and have not been evaluated. Computations according to (2.13) are referred to as "fixed-order" results, and those, based on the left equation in (2.6) as the "standard" method.

The CMS Collaboration has measured the ratio of the inclusive three-jet cross section and the inclusive two-jet cross section, $R_{3/2}$, for jets with $p_T > 150\,\text{GeV}$ and rapidities of |y| < 2.5 [4]. The results are published as a function of the average transverse momentum of the two leading jets in the event, $\langle p_{T1,2} \rangle$, over the range $0.42 < \langle p_{T1,2} \rangle < 1.39\,\text{TeV}$, as displayed in Figure 1. The results of the fixed-order and "standard" calculations for $R_{3/2}$ are compared to the data, with their error bands representing the range of their respective scale dependences. Both results are in agreement, and both describe the data equally well.

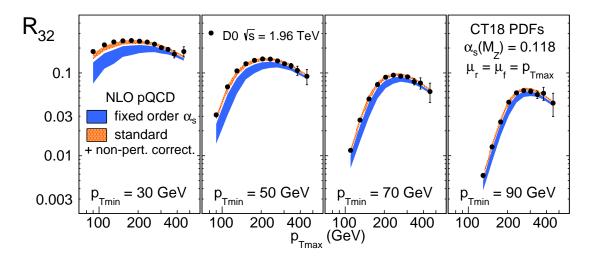


Figure 2. The multi-jet cross section ratio $R_{3/2}$, measured in $p\bar{p}$ collisions at $\sqrt{s}=1.96\,\mathrm{TeV}$ as a function of p_T^{max} in the D0 experiment [2]. Two sets of pQCD predictions, corrected for non-perturbative contributions, are compared to the data: the fixed-order results for $R_{3/2}$, and the results from the "standard" approach, computed from the ratio of the fixed-order results for the two cross sections. The shaded areas represent the ranges of the scale dependences of the calculations.

Another measurement of the ratio $R_{3/2}$ was made by the D0 Collaboration for jets with rapidities |y| < 2.4 and for various lower jet p_T requirements, $p_{T\min}$. The results are published as a function of the leading jet p_T , p_T^{\max} , over the range $80 < p_T^{\max} < 500 \,\text{GeV}$ and for four $p_{T\min}$ choices from 30 to 90 GeV, as displayed in Figure 2. The pQCD prediction from the "standard" method gives a reasonable description of the data over the whole p_T^{\max} range for all $p_{T\min}$ requirements, except for the lowest p_T^{\max} bins for $p_{T\min} = 30 \,\text{GeV}$. The fixed-order calculation predicts lower values everywhere and the scale uncertainty bands of the two calculations do either not, or hardly, overlap. Only towards larger $p_{T\min}$ and larger p_T^{\max} , the uncertainty bands get closer.

The D0 Collaboration also published measurement results of a new quantity, $R_{\Delta R}$ [1]. This quantity, while defined in a more inclusive way, also probes the ratio of three-jet and two-jet production. Starting point is an inclusive jet sample (which probes the two-jet production process). The presence of a neighboring jet with $\Delta R < \pi$ is a sign of an event topology with three or more jets. The fraction of all inclusive jets with a neighboring jet, $R_{\Delta R}$, is therefore also a three- over two-jet ratio. The quantity $R_{\Delta R}$ was measured for different p_T requirements, $p_{T\min}^{\text{nbr}}$, and different angular separations, ΔR , for the neighboring jets, as a function of inclusive jet p_T from 50 to 450 GeV. The results of the fixed-order and the "standard" calculations for $R_{\Delta R}$ are compared to the data in Figure 3. In almost all of the phase space the conclusions mirror those for the theoretical description of the CMS $R_{3/2}$ data in Figure 1: The fixed-order pQCD predictions agree with those from the "standard" method, and both give a good description of all data with $p_{T\min}^{\text{nbr}} \geq 50 \text{ GeV}$. Only in the softer regime, for $p_{T\min}^{\text{nbr}} = 30 \text{ GeV}$ at smaller p_T , they slightly underestimate the experimental measurement results.

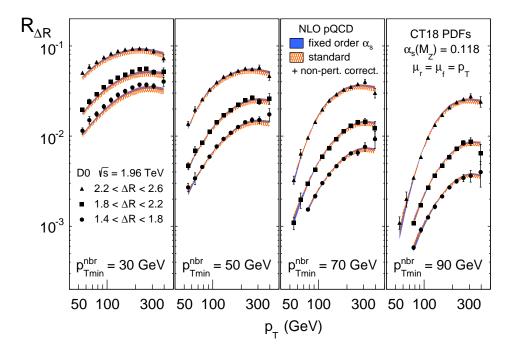


Figure 3. The multi-jet cross section ratio $R_{\Delta R}$, measured in $p\bar{p}$ collisions at $\sqrt{s}=1.96\,\mathrm{TeV}$ in the D0 experiment [1], as a function of p_T , in four values of $p_{T\mathrm{min}}^{\mathrm{nbr}}$ and in three regions of ΔR . Two sets of pQCD predictions, corrected for non-perturbative contributions, are compared to the data: the fixed-order results for $R_{\Delta R}$, and the results from the "standard" approach, computed from the ratio of the fixed-order results for the two cross sections. The shaded areas represent the ranges of the scale dependences of the calculations.

The multi-jet ratio $R_{\Delta\phi}$ was proposed [11] as another ratio of three- and two-jet production processes that probes the azimuthal decorrelations of the two leading p_T jets in an event. The $R_{\Delta\phi}$ measurements by the D0 and ATLAS Collaborations [3, 5] both follow the recommendations from the original proposal, and the two results are shown in Figure 4. Both measurements are performed in the same three rapidity regions, y^* , and for the same azimuthal decorrelation requirements, $\Delta \phi_{\rm max}$. The ATLAS (D0) data are presented as a function of the scalar p_T sum of all jets in an event, H_T , over the range 0.46–4 TeV (180– 900 GeV). Since both data sets are measured at different center-of-mass energies, \sqrt{s} , their results should be compared to each other at the same H_T/\sqrt{s} . The degree of agreement between the NLO pQCD predictions from the fixed-order and the "standard" calculations and how they describe the data is pretty much the same for the ATLAS and D0 data sets. In different y^* and $\Delta\phi_{\rm max}$ regions, however, the two calculations exhibit a rather different behavior. At $y^* < 1.0$, for $\Delta \phi_{\rm max} = 7\pi/8$ and $5\pi/6$, both calculations agree very well, exhibit a relatively small scale dependence, and both describe the data. At $\Delta \phi_{\rm max} = 3\pi/4$, the two predictions start to deviate from each other, and in some cases their larger scale uncertainty bands have only a small overlap. The data are described by both predictions. At $1 < y^* < 2$, for $\Delta \phi_{\rm max} = 7\pi/8$ and $5\pi/6$, the two predictions have a different H_T dependence and disagree at high H_T . In these regions, the fixed-order calculation gives a better description of the overall H_T shape for both data sets.

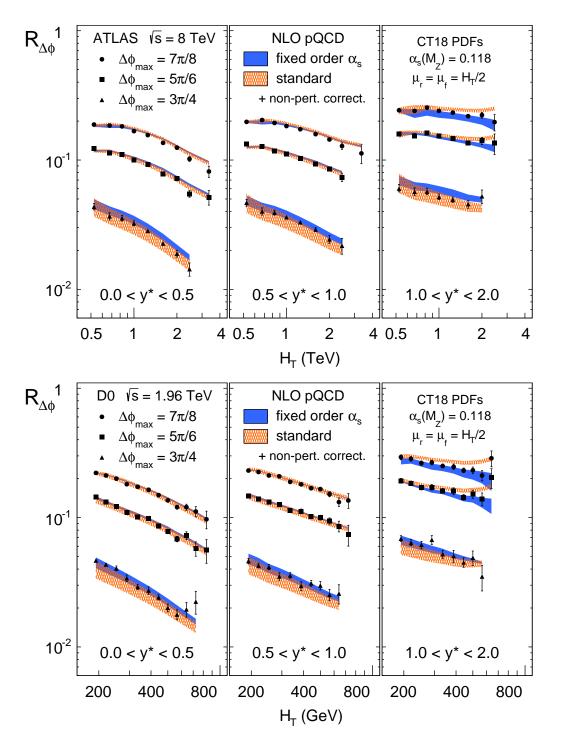


Figure 4. The multi-jet cross section ratio $R_{\Delta\phi}$, measured in pp collisions at $\sqrt{s}=8\,\mathrm{TeV}$ in the ATLAS experiment [5] (top) and in $p\bar{p}$ collisions at $\sqrt{s}=1.96\,\mathrm{TeV}$ in the D0 experiment [3] (bottom), as a function of H_T , in three regions of y^* and for three values of $\Delta\phi_{\mathrm{max}}$. Two sets of pQCD predictions, corrected for non-perturbative contributions, are compared to the data: the fixed-order results for $R_{\Delta\phi}$, and the results from the "standard" approach, computed from the ratio of the fixed-order results for the two cross sections. The shaded areas represent the ranges of the scale dependences of the calculations.

4 Summary and recommendations

In the "standard" approach, pQCD predictions for cross section ratios are computed as the ratio of the fixed-order results of the numerator and the denominator. Such a calculation does, however, not represent an exact fixed-order result for the ratio. A method, how to obtain exact fixed-order results for ratios of cross sections is presented in this article. NLO pQCD predictions according to the new fixed-order method and the "standard" method were calculated for five different experimental measurements of multi-jet cross section ratios. For these measured quantities the two predictions were compared to each other and to the experimental data. It was found that in all cases where the results from the two methods agree with each other (as seen for the CMS $R_{3/2}$, the D0 $R_{\Delta R}$, and some regions of the ATLAS and D0 $R_{\Delta\phi}$ measurements in Figures 1, 3, and 4), they also both describe the data. In all cases where the two methods disagree (meaning that their scale uncertainty bands do not overlap, as seen for the D0 $R_{3/2}$ data and the high H_T tails in some of the ATLAS and D0 $R_{\Delta\phi}$ data at $y^* > 1$ in Figures 3 and 4), one of them (but not always the same) is describing the data. In some intermediate cases, where the scale uncertainty bands from the two methods have little overlap (as for the ATLAS and D0 $R_{\Delta\phi}$ data with $\Delta \phi_{\rm max} = 3\pi/4$ in Figure 4), both predictions are somehow consistent with the data.

It is important here to note, that neither of the two methods is fundamentally preferable over the other and both stand exactly on the same footing. In any given order pQCD, the results from both methods are equally valid representation of the perturbative expansion, and they only differ in higher-order terms, just like for the scale dependence of the calculation.² Consequently, both results should be taken into account, and their discrepancy should be regarded as a genuine uncertainty, which is not always covered by the range of the scale uncertainties of the individual methods (for example in Figure 4).

For future phenomenological studies of cross section ratios, we make the following recommendations:

1. For the central pQCD prediction

Typically, the goal of phenomenological studies is to find if a theory can describe the data. Therefore we recommend to consider both methods, and use the one that gives a better description of the data. In general, this can be decided by a χ^2 calculation (especially in the case of parameter determinations) or sometimes simply by eye (as in Figure 2).

2. For the uncertainty of the prediction

Based on the arguments given above, we recommend to use the full envelope of the scale uncertainty bands from both methods as an estimate of the pQCD uncertainty related to uncalculated terms of higher order in α_s .

While sometimes the two methods differ only in their normalization (as in Figure 2), in other cases they can also feature very different shapes (as in Figure 4). The first recom-

The results of fixed-order pQCD calculations obtained at different scales $\mu_{r,f}$ differ only due to terms which are of higher orders of α_s . Since the scale dependence is a reflection of some higher-order terms, it is typically used as an estimate of the potential size of the uncalculated higher order contributions.

mendation ensures that one does not rule out a theory which, in an equally valid alternative form, would actually be able to describe a given data set. The second recommendation acknowledges the additional uncertainty contribution related to the difference of two equally valid representations of the pQCD calculation which may exceed the uncertainty estimate based on simple scale variations (as seen in Figure 4). This will provide more realistic estimates of theoretical uncertainties and will be helpful in future phenomenological studies when identifying robust measurable quantities for which the theoretical approximations are more reliable.

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