

Robust estimates of theoretical uncertainties at fixed-order in perturbation theory

Matthew A. Lim^{1,*} and Rene Poncelet^{2,†}

¹*Department of Physics and Astronomy, University of Sussex,
Sussex House, Brighton, BN1 9RH, United Kingdom*

²*Institute of Nuclear Physics, Ulica Radzikowskiego 152, 31–342 Krakow, Poland*



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Calculations truncated at a fixed order in perturbation theory are accompanied by an associated theoretical uncertainty, which encodes the missing higher orders (MHOU). This is typically estimated by a scale variation procedure, which has well-known shortcomings. In this work, we propose a simple prescription to directly encode the missing higher order terms using theory nuisance parameters (TNPs) and estimate the uncertainty by their variation. We study multiple processes relevant for Large Hadron Collider physics at next-to-leading and next-to-next-to-leading order in perturbation theory, obtaining MHOU estimates for differential observables in each case. In cases where scale variations are well-behaved we are able to replicate their effects using TNPs, while we find significant improvement in cases where scale variation typically underestimates the uncertainty.

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Introduction. A longstanding problem in using quantum field theories for phenomenological predictions in perturbation theory is how one reliably estimates missing higher-order uncertainties (MHOU). The conventional method to gauge the size of these terms relies on the fact that, for a prediction truncated at a given order, the difference between predictions computed at different values of the unphysical renormalization scale μ is of genuinely higher order. Typically, practitioners choose a “good” value of the central scale and take an envelope of scale variations as a measure of the uncertainty. The size of this uncertainty is expected to reduce with successive orders. There remains, however, an arbitrariness in the choice of the central scale and in the size of the variations. In practice, scale variations often underestimate the theoretical uncertainty, due to, e.g., emergence of new partonic channels at higher orders, cancellations rendering corrections artificially small, etc. In addition, scale variations do not correlate uncertainties between bins of a differential distribution (or between multiple differential distributions) correctly; moreover, μ itself does not represent an actual parameter with a true value which the prediction depends upon, and thus cannot be relied upon to determine a true uncertainty.

Various attempts have been made to place the MHOU estimation problem on a more stable footing. Reference [1] aimed to associate the MHOU with a Bayesian degree of confidence, based on the perturbative expansion of an observable. This was further refined in Ref. [2], which aimed to better treat cases with large higher-order corrections. Both methods were scrutinized in Ref. [3], which incorporated the dependence on the renormalization and factorization scales μ_R , μ_F into Bayesian inference. Reference [4] took a different approach, proposing an uncertainty estimate for an arbitrary process based on the scale variations of a set of QCD reference processes.

Theory nuisance parameters (TNPs) were introduced in Ref. [5] as a way to directly parametrize unknown higher-order terms. Recent applications have used TNPs with scale variations to estimate the uncertainty from unknown higher-loop ingredients at a given order in resummed perturbation theory [6,7]. This is convenient, since factorization in soft-collinear effective theory dictates the structure of the resummed calculation to all orders. This information allows direct identification of TNPs with unknown terms in the resummation, e.g. anomalous dimensions. Similarly, TNPs have been employed to obtain approximate N^3 LO parton distribution functions by the MSHT Collaboration [8], where they parameterize both partially known PDF ingredients at N^3 LO and completely unknown cross sections. TNPs thus serve as an appealing alternative to the scale variation procedure, even for calculations at fixed order [5].

Here, we apply TNPs to estimate missing higher-order uncertainties for fixed-order differential distributions.

*Contact author: m.a.lim@sussex.ac.uk

†Contact author: rene.poncelet@ifj.edu.pl

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Unlike the resummed case, the all-order structure of a fixed-order calculation is *a priori* unknown, introducing a greater arbitrariness in accomplishing the parameterization. We shall show that our relatively simple TNP *Ansätze* produce uncertainty bands which show a good convergence between orders, replicate the effects of scale variation procedures in cases where these work well, and greatly improve on scale variation in cases where it fails.

Implementation. In contrast to resummed perturbation theory, given a computation at a certain fixed order we can infer very little about the structure of higher-order corrections *a priori*. We must therefore introduce some parametrization of the missing higher orders. We begin by expanding a differential cross section in the strong coupling α_s as

$$d\sigma = \alpha_s^n N_c^m d\bar{\sigma}^{(0)} \left[1 + \alpha_s N_c \left(\frac{d\bar{\sigma}^{(1)}}{d\bar{\sigma}^{(0)}} \right) + \dots \right] \quad (1)$$

where we abbreviate the differential cross section as $d\sigma$ and factored out the leading power of the number of colors N_c .

At a given order N in fixed-order perturbation theory, the term of order $N + 1$ in Eq. (1) estimates the theoretical uncertainty associated with truncating the series. We wish to model this term using TNPs. To do this, we use information from available lower orders of the calculation. Specifically, we assume the coefficients of $\alpha_s N_c$ in the square brackets of Eq. (1) are simple functions of the kinematics and can be modeled by a polynomial with coefficients of order 1 multiplying a lower-order term. We find this empirically to be true for a range of processes and distributions. We thus write the order $N + 1$ estimate as

$$\frac{d\bar{\sigma}_{\text{TNP}}^{(N+1)}}{d\bar{\sigma}^{(0)}} = \sum_{j=1}^N f_k^{(j)}(\vec{\theta}, x) \left(\frac{d\bar{\sigma}^{(j)}}{d\bar{\sigma}^{(0)}} \right) \quad (2)$$

where f_k is a polynomial of degree k in a (suitably rescaled) kinematic variable x and the θ_i are the TNPs.¹ We have experimented with different choices of polynomial basis, and present results using Bernstein polynomials

$$f_k^B(\vec{\theta}, x) = \sum_{i=0}^k \theta_i \binom{k}{i} x^{k-i} (1-x)^i \quad (3)$$

defined in the range $x \in [0, 1]$ as well as for Chebyshev polynomials of the first kind,

$$f_k^C(\vec{\theta}, x) = \frac{1}{2} \sum_{i=0}^k \theta_i T_i(x), \quad (4)$$

¹In the notation of Ref. [5], this is then an N^{m+1} LO model for a fixed value of the scale μ .

defined in the range $x \in [-1, 1]$. The choice of the integer k modulates the amount of shape variation permitted. In this work we always use $k = 2$.²

While the parametrization in Eq. (2) is arbitrary, all choices should be equivalent in the limit $k \rightarrow \infty$. The arbitrariness enters as soon as we truncate the polynomial expansion, inducing dependence on the exact parametrization and the truncation order. Parameterization sensitivity is discussed in Ref. [5]. Empirically, we find that employing our procedure at NLO gives a good approximation to the known NNLO term for $\theta_i \sim \mathcal{O}(1)$, which we use as justification to extend this one order higher to gauge the size of missing N^3 LO terms. We believe this still represents an improvement on the scale variation procedure, despite any residual ambiguities. For some choice of the θ_i in Eq. (2) and $k = 2$, we find that it is always possible to construct at least a fair approximation to the next unknown order. In contrast, frequently no choice of μ at a given order will reproduce the next order. We do not attempt to construct a TNP model for the LO uncertainty. In this case, there is no lower-order information upon which to base our ansatz. Given that NLO is now the de facto minimum standard for most processes, this is not a major shortcoming.

We note that strict adherence to the philosophy espoused in Ref. [5] would dictate that our model be independent of the size (if not the shape) of lower-order corrections. The motivation for this is to avoid significant underestimation of the MHOU when the lower-order terms happen by chance to be smaller than might be naively expected. While this is certainly a desirable property in principle, in practice we have found it difficult to achieve, even after factoring in known structures (flavor decomposition of partonic channels, etc.). Since our aim is to provide a prescription which can be applied generally and to a range of processes, we have conceded on this particular tenet.³ We observe no instances where we believe the MHOU has been significantly underestimated (in contrast to results obtained using scale variations). While we do not exclude the possibility of achieving a parametrization which does not utilise this information, its form is likely to be specific to a given interest case, given that it depends on an interplay of factors.

Another criticism is that we are still required to make a choice for the central value of our scales, which remains arbitrary. Examining different central choices, our uncertainty estimates remain consistent—our construction

²In principle, in cases where one has additional information about the process it would be possible to refine Eq. (2) further. For example, for processes where new channels appear at higher orders, one could decompose each $d\bar{\sigma}^{(i)}$ according to the partonic initial states $d\bar{\sigma}_{gg}^{(i)}$, $d\bar{\sigma}_{q\bar{q}}^{(i)}$, etc. and treat each separately.

³The closest analog in Ref. [5] would be strategy 3 of Sec. IV.3. In that case, however, the author is explicit about the normalization required to make the estimate independent of the size of lower order terms. In using this information, our approach is instead closer to that adopted in Ref. [8] with $k = 0$.

TABLE I. Processes and NNLO distributions included in meta-analysis.

Process	$\sqrt{s}/\text{TeV}$	Scale	PDF	Distributions	References
$pp \rightarrow H$ (full theory)	13	$m_H/2$	NNPDF3.1	y_H	[17,18]
$pp \rightarrow ZZ^* \rightarrow e^+e^-\mu^+\mu^-$	13	M_T	NNPDF3.1	$M_{e^+\mu^+}, p_T^{e^+e^-}, y_{e^+}$	[19]
$pp \rightarrow WW^* \rightarrow e\nu_e\mu\nu_\mu$	13	m_W	NNPDF3.1	M_{WW}, p_T^μ, y_{W^-}	[20]
$pp \rightarrow (W \rightarrow \ell\nu) + c$	13	$E_T + p_T^c$	NNPDF3.1	$p_T^\ell, y_\ell $	[21,22]
$pp \rightarrow t\bar{t}$	13	$H_T/4$	NNPDF3.1	$M_{t\bar{t}}, p_T^t, y_t$	[23,24]
$pp \rightarrow t\bar{t} \rightarrow b\bar{b}\ell\bar{\ell}$	13	$H_T/4$	NNPDF3.1	$M_{\ell\bar{\ell}}, p_T^{b_1}, p_{T,\ell_1}/p_{T,\ell_2}$	[23,24]
$pp \rightarrow \gamma\gamma$	8	$M_{\gamma\gamma}$	NNPDF3.1	$M_{\gamma\gamma}, p_T^{\gamma_1}, y_{\gamma\gamma}$	[25]
$pp \rightarrow \gamma\gamma j$	13	$H_T/2$	NNPDF3.1	$M_{\gamma\gamma}, p_T^{\gamma\gamma}, \cos\phi_{CS}, y_{\gamma_1} , \Delta\phi_{\gamma\gamma}$	[26]
$pp \rightarrow jjj$	13	$\hat{H}_T$	MMHT2014	TEEC with $H_{T,2} \in [1000, 1500), [1500, 2000), [3500, \infty)$ GeV	[27,28]
$pp \rightarrow \gamma jj$	13	H_T	NNPDF3.1	$M_{\gamma jj}, p_T^j, y_{\gamma-jet} , E_{T,\gamma}$	[29]

naturally overcomes “poor” scale choices, in the sense that these result in large K -factors which inflate the TNP uncertainty. This issue is also discussed in detail in Ref. [5].

Results. We obtain our (N)NLO cross sections from published results obtained within the STRIPPER framework [9–12]: a full list of included processes can be found in Table I. We study both NLO uncertainties (where NNLO corrections are known) and NNLO uncertainties (where N³LO corrections are at present unknown). We explicitly present results for two processes, namely $pp \rightarrow t\bar{t} \rightarrow b\bar{b}\ell\bar{\ell}$ and $pp \rightarrow W^+W^- \rightarrow \ell\bar{\ell}\nu\bar{\nu}$, defined in appropriate fiducial regions. More processes are available using a Jupyter notebook interface to HighTEA at Ref. [13]. Each case has a distinct behavior with respect to scale variations. The first process features colored final states and large higher-order corrections, where the leading-order scale band does not contain the NLO result. The second example is pathological with respect to scale variations, and the NNLO uncertainty band lies completely outside that of the NLO. This allows us to test our procedure in different scenarios. For the original NNLO computations of each process, see Refs. [14–16].

For each process and distribution we consider, we compute the central curve using a fixed scale choice. We compute uncertainty estimates by summing in quadrature variations by ± 1 of each TNP separately. This is appropriate if the parameters are independently and normally distributed, a matter which we shall address. We have verified that results using Bernstein and Chebyshev polynomials are very similar.

We begin with the $t\bar{t}$ process with a central scale choice. In Fig. 1 we show the invariant mass of the lepton pair, the transverse momentum of the hardest b -jet and the ratio of lepton transverse momenta. The scale variation plots show that the LO uncertainty is generally underestimated but that scale variations estimate the MHO well beyond this order. The TNP approach reproduces this behavior, with marginally smaller estimates of the NLO uncertainty.

Figure 2 shows off-shell WW production, a process notorious for the poor behavior of traditional methods in

estimating MHO terms. In this preliminary study, we do not include the effect of the loop-induced gg channel at NNLO. From the lower scale variation plots we see that the uncertainty at each order is completely underestimated. This is a result of so-called “giant” K -factors, which arise from NLO corrections in which a vector boson is emitted off a final-state parton [30,31]. The size of these corrections is exacerbated by fiducial cuts. In the case of the invariant mass distribution, the LO band is in fact smaller than the NLO which is of a similar size to the NNLO scale variation. In none of the distributions do the scale bands even overlap. In contrast, while the process is clearly challenging even for the TNP approach, a much more sensible behavior is observed. The TNP estimates decrease in size as one moves from NLO to NNLO, and the NLO error in particular is much better estimated.

Finally, we discuss neutral and charged current Drell-Yan production. This is a rare case where fully differential corrections in QCD are currently known through N³LO [32,33]—indeed, in Refs. [34,35] the first predictions at this order for the invariant mass distribution of the dilepton pair were presented. It was observed that, beginning at N³LO, the convergence of the perturbative series as measured by scale variation begins to deteriorate. While this is partly due to the effect of using NNLO PDFs (as opposed to aN³LO [36]), it is interesting to examine whether TNPs provide an uncertainty estimate which suggests greater consistency between perturbative orders. In Fig. 3 we show predictions for the invariant mass distribution at various orders in perturbation theory, for both charged and neutral current Drell-Yan production, and compare scale variations with (Chebyshev) TNP uncertainty estimates at the 95% confidence level.⁴ Results have been obtained using the public code N3LOXS [37]. A clear improvement of the description of the NNLO

⁴This corresponds to varying the TNPs by 2, rather than 1 as done elsewhere. We wish to stress that, given the statistical interpretation of the TNPs which we will demonstrate in the next section, this genuinely corresponds to a 2σ uncertainty—it is thus *not* analogous to a variation of μ by a factor of 4.

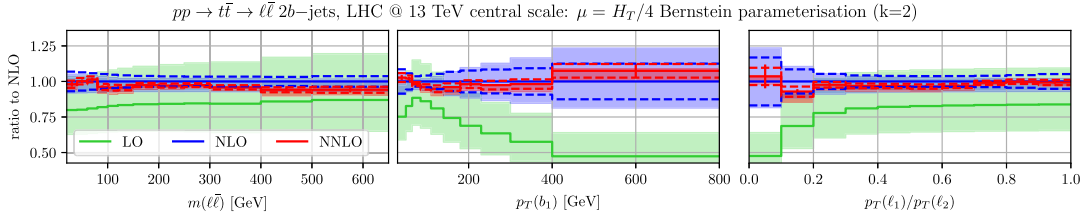


FIG. 1. Comparison between MHOUs estimates from TNP and scale variation for differential distributions in $t\bar{t}$ production, with QCD corrections treated in the narrow width approximation. From left to right, we show the lepton pair invariant mass $m(\ell\bar{\ell})$, the transverse momentum of the hardest b -jet $p_T(b_1)$ and the ratio of the lepton transverse momenta $p_T(\ell_1)/p_T(\ell_2)$. We take $\mu = H_T/4$ as our central scale and use a Bernstein parametrization. The solid lines represent the LO (green), NLO (blue), and NNLO (red) central predictions and the corresponding bands of the estimated MHOUs from scale variations, the dashed bands those from TNPs. The vertical lines indicate statistical uncertainties. We do not associate a TNP uncertainty with the LO prediction—see text for details.

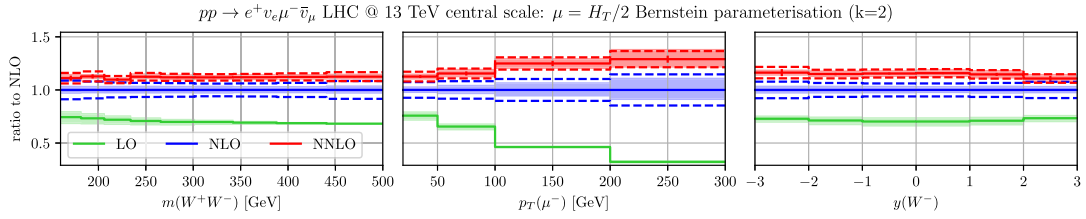


FIG. 2. As in Fig. 1, but for off-shell, fully decayed WW production. We take $\mu = H_T/2$ as our central scale choice and use a Bernstein parametrization. We show the pair invariant mass $m(W^+W^-)$, the transverse momentum of the muon $p_T(\mu^-)$ and the rapidity of one boson $y(W^-)$.

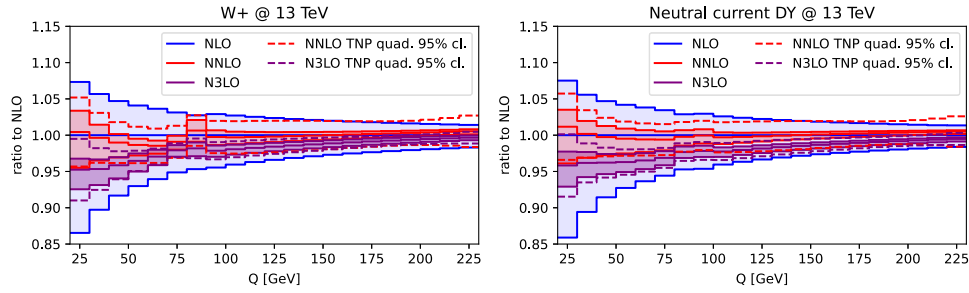


FIG. 3. Comparison between scale and TNP uncertainties for charged-current (W^+) and neutral-current Drell-Yan (Z/γ) through next-to-next-to-next-to-leading order. The colored bands indicate the uncertainties from 7-point scale variations, and dotted lines the quadrature combination of the TNP uncertainties at a 95% CL.

uncertainty in the TNP case with respect to the scale variation case is visible, particularly for $Q > 100$ GeV where the uncertainties now enclose the $N^3\text{LO}$ result. We can thus employ our method, without modification and in a simple and straightforward manner, to resolve an important discrepancy at the highest available order in perturbation theory.

As an *a posteriori* check on our procedure, we fitted our NLO uncertainty estimate in cases where the NNLO distribution is known. An example for the process $pp \rightarrow ZZ^*$ is shown in Fig. 4. This confirms that our parametrization is able to fit the NNLO data with values of $\theta_i \sim \mathcal{O}(1)$.

It is not possible to capture the correct bin-to-bin correlations of the uncertainties in a given differential distribution without knowledge of the functional form of the higher-order corrections (which one possesses, for example, in a resummed calculation). This is only possible to

the extent that the parametrization in Eq. (2) provides a good approximation of the true higher-order behavior. Given that this “true” behavior is always accompanied by a finite Monte Carlo error, the quality of the fits in Fig. 4 demonstrate that this is indeed the case: the parametrization describes correlations as well as the integration error allows. It is possible that by increasing statistics, one might find that a polynomial with $k = 2$ in fact underfits. In this case, one could always extend the parametrization by choosing $k > 2$. Alternatively, by including too many TNPs one overfits. The treatment here depends on the exact parametrization chosen. In the Chebyshev case, the orthogonality of the polynomial basis results in higher order coefficients naturally becoming smaller. In the Bernstein case, correlations between the TNPs are introduced which effectively set the coefficients of higher order

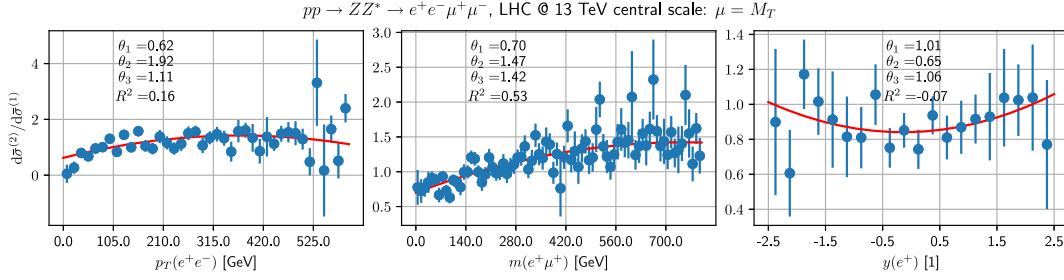


FIG. 4. Fit of the NLO uncertainty estimate using Bernstein polynomials (red) to the true NNLO result (blue) for the process $pp \rightarrow ZZ^* \rightarrow e^+e^-\mu^+\mu^-$. For each kinematic distribution the corresponding fit values of the nuisance parameters are shown.

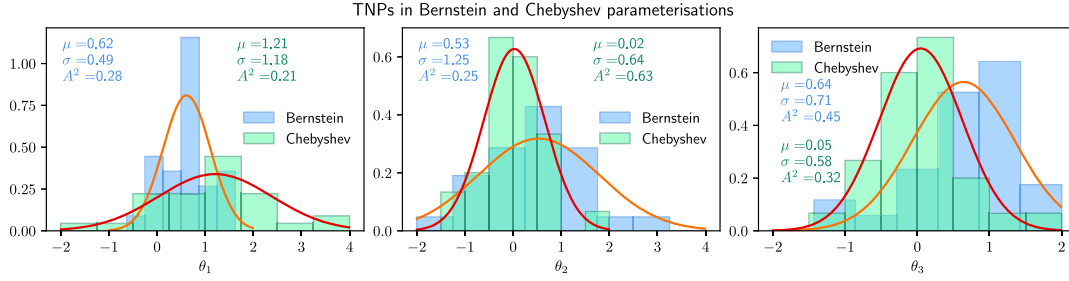


FIG. 5. Distribution of the values of the nuisance parameters θ_i in Bernstein and Chebyshev parametrizations at NNLO. For details of the data points included, see text. The mean and standard deviation of a fit Gaussian distribution are indicated on the plot, as is the Anderson-Darling test statistic (critical value 0.712 for $p = 0.05$). Binning is purely illustrative.

monomials to zero. Care must therefore be taken when combining uncertainties.

We have repeated the fit for a range of processes and distributions Table I. In selecting kinematic distributions for inclusion, we have endeavored to make quasi-independent choices—for example, choosing a rapidity distribution, an invariant mass and a transverse momentum rather than two invariant masses. In this way, we have tried to avoid double-counting information arising from strongly correlated distributions. This also restricts the amount of information we can include from each process—for $2 \rightarrow 2$ processes we limit ourselves to three distributions, while more can be included in the $2 \rightarrow 3$ cases due to the greater kinematic freedom they afford. In total, we include 30 data points. Results for the fit values of the TNPs are shown in Fig. 5, for both parametrizations. The resulting distributions are Gaussian, with values of the mean and standard deviation of order 1. Test statistics obtained using the Shapiro-Wilk and Anderson-Darling methods show no significant deviation from normality at the $p = 0.05$ level. This is a strong justification for our procedure, at least at NLO—a similar validation at NNLO is dependent on a greater availability of N^3 LO calculations.

Conclusions. In this work we have proposed a simple prescription to estimate missing higher-order uncertainties for fixed-order differential distributions using TNPs, which provides an appealing alternative to the scale variation paradigm. Our prescription is easily implemented at any

order in perturbation theory and can be applied to any process and any inclusive observable.

We have made a Jupyter notebook which implements the procedure discussed here publicly available [13], making use of the HighTEA interface to NNLO calculations [25]. HighTEA acts as a user-friendly repository for NNLO events, allowing the user to request desired kinematic distributions, PDF sets and binnings. At present, a number of processes have been implemented, including cases where the TNP approach provides a dramatic improvement on scale variations (e.g., $\gamma\gamma$ production).

Our method could also be used in the context of electroweak corrections. These present a problem to scale variation procedures due to the weak dependence on μ of the electroweak coupling. A TNP approach, would not suffer from this problem and could thus improve uncertainty estimates in a consistent fashion.

In practical applications, one is often interested in capturing not only the correlations in uncertainties between bins of a given kinematic distribution as is done here, but also between different distributions for a given process. Combining information in this way can be used to extract Standard Model parameters precisely, see, e.g., Refs. [38,39]. Such a combination would require a multidimensional TNP treatment, which parametrizes the joint dependence in multiple variables x_i . A simple attempt at this could for example use products of single-differential parametrizations. We leave a more detailed investigation of this topic to future work. Achieving the correct correlation model for differential distributions between processes would require substantially new ideas.

We would encourage practitioners of higher-order calculations to investigate our method, alongside normal scale variations. This would test how generalizable our method is, and potentially result in better convergence. Crucially, our simple proposal provides these estimates at no additional cost—the uncertainty can be calculated using results one would have already obtained.

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Data availability. Some of the data that support the findings of this article are openly available [13]. NNLO data extracted from other publications are not publicly available because they are owned by a third party and the terms of use prevent public distribution. The data are available from the authors upon reasonable request.

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