Estimation of uncertainties from missing higher orders in perturbative calculations

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Talk based on Bagnaschi et al JHEP **1502** (2015) 133 arXiv:1409.5036 [hep-ph]

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Talk structure

Goals of our study

Statistical survey of two models for MHOU

Scale variation

- Revisit the SV procedure and analyze statistically its performance on a wide set of observables to improve our knowledge/control on what is currently used in the experimental analysis

The Bayesian approach

- Improve the Bayesian approach first proposed by Cacciari and Houdeau[1] to work around some of its imperfections
- Analyze the performance of the newly improved model on a wide set of observables

[1] Cacciari-Houdeau JHEP **1109** (2011) 039 arXiv:1105.5152 [hep-ph]

Perturbative QCD and MHOUs

Baseline

- The perturbative expansion of an observable known up to order k is

$$O_k(Q,\mu) = \sum_{n=l}^{k} \alpha_s^n(\mu) c_n(Q,\mu) \quad \text{(known)}$$

- Q is the hard scale of the process, μ represents the unphysical scale(s) (e.g. the renormalization scale) from which the truncated perturbative expansion depends. We assume it set at the value Q
- The remainder of the series expansion is unknown and it is our MHOU

$$\Delta_k = \sum_{n=k+1}^{\infty} \alpha_s^n(Q) c_n(Q) \simeq \alpha_s^{k+1} c_{k+1} = ?$$

Scale variation

Procedure

- Vary the unphysical scale(s) μ around the central scale Q by an **arbitrary** factor r
- Different prescriptions used in the literature. We will use the following ones:
  1. **Scan**: vary μ between Q/r and $r \times Q$ and use the maximum/minimum value of the observable to define the uncertainty
  2. **Extrema**: Use the maximum/minimum of the value of the observable obtained for $\mu = r \times Q, Q/r$
- **Caveat**: the factor r is arbitrary and the interval obtained has **no** statistical meaning

The CH model

Bayesian framework

- Suppose there is an upper bound on the coefficients magnitude and call it $\bar{c}$
- The priors for the model are then given by

$$f_\epsilon(\ln \bar{c}) = \frac{1}{2|\ln \epsilon|} \chi_{|\ln \bar{c}| \leq |\ln \epsilon|}$$

$$f(c_n|\bar{c}) = \frac{1}{2\bar{c}} \begin{cases} 1 & \text{if } |c_n| \leq \bar{c} \\ 0 & \text{if } |c_n| > \bar{c} \end{cases}$$

$$f(\{c_i, i \in I\}|\bar{c}) = \prod_{i \in I} f(c_i|\bar{c})$$

- Bayesian inference gives then the uncertainty interval posterior

$$f(\Delta_k|c_l, \dots, c_k) \simeq \left(\frac{n_c}{n_c+1}\right) \frac{1}{2\alpha_s^{k+1}\bar{c}_k} \begin{cases} 1 & \text{if } |\Delta_k| \leq \alpha_s^{k+1}\bar{c}_k \\ \frac{1}{(|\Delta_k|/(\alpha_s^{k+1}\bar{c}_k)^{n_c+1}} & \text{if } |\Delta_k| > \alpha_s^{k+1}\bar{c}_k \end{cases}$$

  where $n_c = k - l + 1$ and $\bar{c}_k = \max(c_l, \dots, c_k)$
- Intervals have a statistical meaning in term of Degree of Belief (DoB)

The $\overline{\mathrm{CH}}$ model

Recent developments

- **Issue:** the uncertainty estimate **depends** on the expansion parameter of the series
- **Approach:** rewrite the observable as

$$O_k(Q) = \sum_{n=l}^{k} \left(\frac{\alpha_s(Q)}{\lambda} \right)^n (n-1)!\, b_n(Q)$$

- Apply the same prior to b_n
- The $(n-1)!$ factor is suggested by renormalon based analysis
- λ estimated empirically from the performance of the model

Methodology

To study the behavior of the models we define the following performance parameter

Success rate

- Call θ the external free parameter of the model (λ for the $\overline{\text{CH}}$ and r for SV)

1. Fix θ and the order n; for the Bayesian model, fix also the requested DoB of the interval
2. Compute the interval at the order n with the fixed θ for every observable in the set
3. Define the **success rate** of the model as the **ratio of the number of observables whose order $n+1$ is contained in the uncertainty interval of the order n over the total number of observables in the set**

Non-hadronic survey

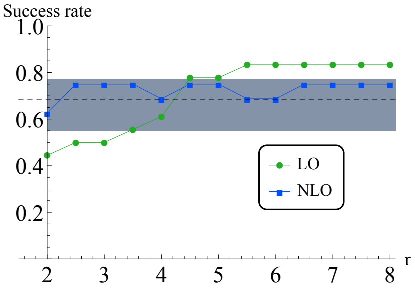
We first study observables without initial state hadrons.

Observable	Available accuracy	Reference
$R(e^+e^- \to \text{hadr})$	NNLO-QCD	Baikov et al., 2008
Bjorken sum rule GLS sum rule	NNLO-QCD NNLO-QCD	Larin et al, 1991 Larin et al, 1991
$\Gamma(b \to ce\bar{\nu}_e)$	NLO-QCD	Biswas & Melnikov, 2010
$\Gamma(Z \to \text{hadr})$ $\Gamma(Z \to b\bar{b})$	N3LO-QCD NNLO-QCD	Baikov et al., 2012 Chetyrkin et al., 1994
Event shape variables (6) e.g. thrust, heavy jet mass	NNLO-QCD	Weinzierl, 2009
Splitting kernels $\gamma_{ns}^{(+)}, \gamma_{qq}, \gamma_{qg}$	NNLO-QCD	Larin et al., 1996
$H \to b\bar{b}\|_{m_b=0}$ $H \to gg$ $H \to \gamma\gamma$	N3LO-QCD N3LO-QCD NNLO-QCD	Baikov et al., 2005 Baikov et al., 2006 Maierhöefer et al, 2013

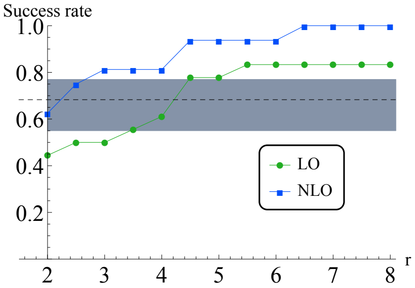
List of all the non-hadronic observables used in the survey

Scale variation performance

Success rate for SV for different values of r



SV with just the three finite choices $\{Q/r, Q, r \times Q\}$



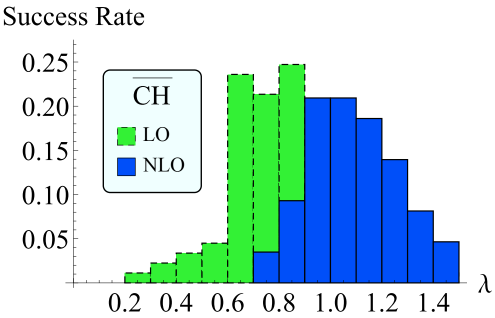
SV with the full scan in the interval $[Q/r, r \times Q]$

We can assign a heuristic a posteriori 68% Confidence Level (CL) for $r = 2 \sim 3$

$\overline{\text{CH}}$ performance and tuning

Procedure

- Vary λ between 0.1 and 2 for a given DoB
- Find the *optimal* value for which **success rate = input DoB**
- Repeat for all DoBs between 0.05 and 0.95 in steps of 0.01 and histogram the results

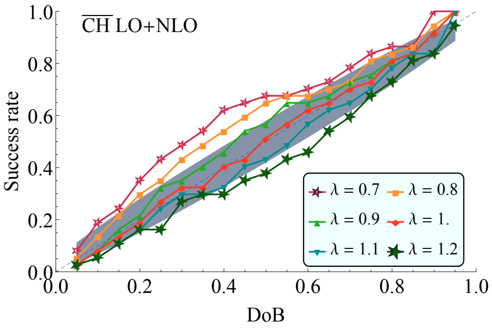


- **LO**: optimal value $\lambda \sim 0.7 - 1.0$
- **NLO**: optimal value $\lambda \sim 0.9 - 1.1$

$\overline{\text{CH}}$ performance and tuning

Complementary Procedure

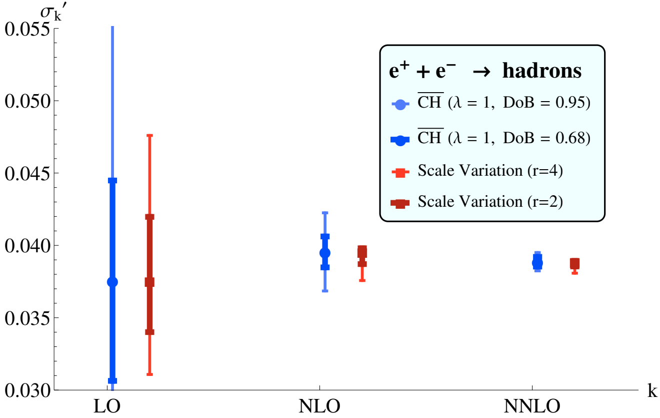
- Consider a fixed list of values for $\lambda = 0.7 \ldots 1.2$
- Plot the **success rate vs the requested DoB**
- The optimal value of λ should produce a curve close to the straight line defined by success rate $=$ DoB



- **All orders:** optimal value $\lambda \sim 0.9 - 1.1$

Benchmarks

$e^+e^- \to$ hadrons: $\overline{\text{CH}}$ vs scale variation



Where we have defined $\sigma_k' \equiv \frac{\sigma_k}{\sigma_0} - 1$.

Application to hadronic observables

Issues

- The model was formulated originally for observables without initial state hadrons
- A hadronic observable can be written as

$$O_k(\tau, Q) = \mathscr{L}(Q) \otimes \sum_{n=l}^{k} \alpha_s^n C_n(Q)$$

- **To what should we apply the $\overline{\text{CH}}$ Bayesian model?** Short-scale "coefficients" C_n are distributions
- **How to account for the convolution of the partonic cross-section with the PDFs?** Non-perturbative physics is involved

Plan A: convolution

Algorithm

- After the PDFs integration we can write the observable in the same form as in the non-hadronic case

$$O_k(\tau, Q) = \sum_{n=l}^{k} \left(\frac{\alpha_s(Q)}{\lambda_h} \right)^n (n-1)!\, H_n(Q, \tau)$$

The coefficients H_n will include a non-perturbative content from the convolution with the PDFs. In first approximation we assume that this content is equal at all orders and that therefore is just a global rescaling factor

The λ value is retuned using the same procedure as in the non-hadronic case.

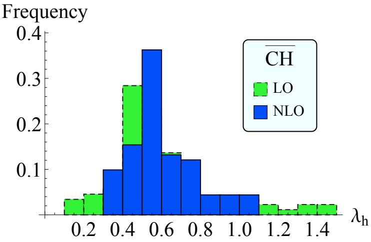
Plan A: convolution

Observables used for the estimation of λ_h

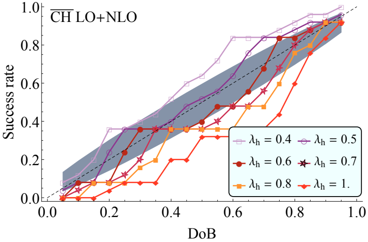
Observable	Available accuracy	Reference
$gg \to H$ at $\sqrt{s} = 8$ TeV	NNLO	HIGLU, Spira et al, 1995
$b\bar{b} \to H$ associated production at $\sqrt{s} = 8$ TeV	NNLO	bbh@nnlo, Harlander et al, 2003
$gg \to t\bar{t}$ at $\sqrt{s} = 8$ TeV	NNLO	Czakon et al, 2013
on-shell $pp \to Z + X \to e^+e^- + X$ at $\sqrt{s} = 8$ TeV	NNLO	DYNNLO, Catani et al, 2009
on-shell $p\bar{p} \to W^\pm + X \to l^\pm \nu_l + X$ at $\sqrt{s} = 8$ TeV (2×3)	NNLO	DYNNLO, Catani et al, 2009
Higgs strahlung production at $\sqrt{s} = 8$ TeV	NNLO	Brein et al, 2003
$b\bar{b}$ at $\sqrt{s} = 8$ TeV	NLO	MCFM, Campbell et al
$Z + \mathrm{j}$ at $\sqrt{s} = 8$ TeV	NLO	MCFM, Campbell et al
$Z + 2\mathrm{j}$ at $\sqrt{s} = 8$ TeV	NLO	MCFM, Campbell et al
$W^\pm + \mathrm{j}$ at $\sqrt{s} = 8$ TeV	NLO	MCFM, Campbell et al
$W^\pm + 2\mathrm{j}$ at $\sqrt{s} = 8$ TeV	NLO	MCFM, Campbell et al
ZZ at $\sqrt{s} = 8$ TeV	NLO	MCFM, Campbell et al
WW at $\sqrt{s} = 8$ TeV	NLO	MCFM, Campbell et al

Plan A: convolution

Global tuning of the λ value



Best λ value for $0.05 < \text{DoB} < 0.95$



Fraction vs requested DoB for $\lambda = 0.4 \ldots 1$

The estimated value of λ is 0.6 ± 0.2

Plan B: Mellin moment

Algorithm

- In Mellin space we can rewrite the convolution as a simple product

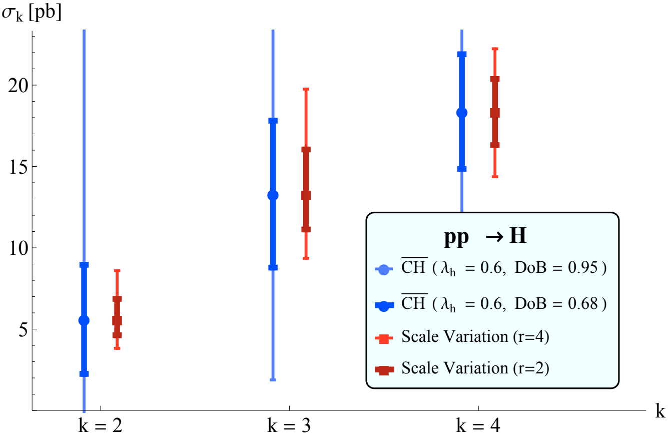
$$O_k(N,Q) = \mathscr{L}(N+1,Q) \sum_{n=l}^{k} \frac{\alpha_s^n}{\lambda_h^n} (n-1)!\, B_n(N,Q)$$

- Find the dominant Mellin moment N^*
- Apply the $\overline{\text{CH}}$ method to $B_n(N^*)$ to get an uncertainty band for the coefficient function
- Calculate the uncertainty band on the full cross-section by proportionally rescaling the value obtained in Mellin space

Uncertainty on the total cross section in the SM

$pp(gg) \to H$ at the LHC 8 TeV (coefficient)

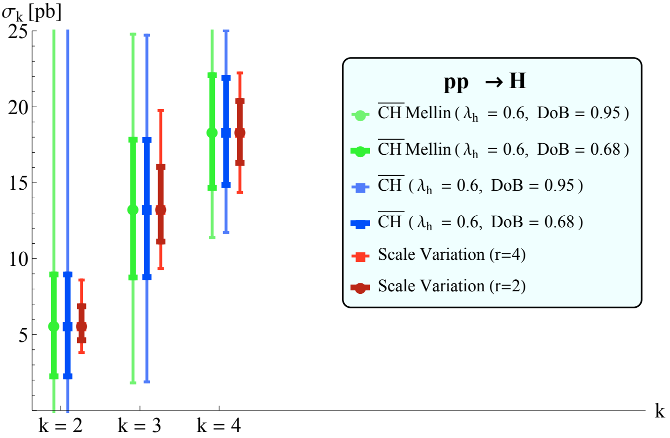
Error bars: $\overline{\text{CH}}$ vs scale variation



Uncertainty on the total cross section in the SM

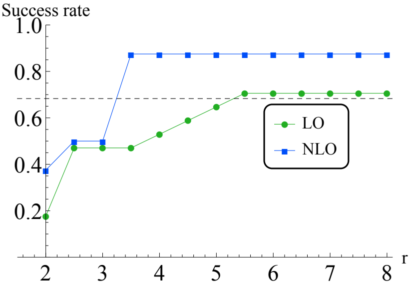
$pp(gg) \to H$ at the LHC 8 TeV (Mellin)

Error bars: $\overline{\text{CH}}$ vs scale variation

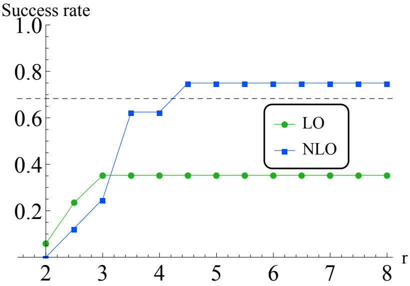


Scales variation for hadronic observables

Frequentist evaluation of the scales variation procedure in the hadronic case



Hadronic scale variation, NNLO PDF



Hadronic scale variation, order matched PDF

Conclusions

Final thoughts and comments

- The study of the SV performances seems to imply that a slightly bigger r than 2 correspond to an heuristic 68% CL
- The extension of the $\overline{\text{CH}}$ model to hadronic observables has been accomplished in two ways.
- We have parameterized the dependence of the $\overline{\text{CH}}$ model on the expansion parameter with the use of a specific parameter λ.

Potential future developments

- Replace the λ value estimation procedure by introducing another prior in the Bayesian model.
- Analyze different classes of observables and possibly define more refined models for each of them.
- Investigate how the $\overline{\text{CH}}$ model depend on the chosen central value for the unphysical scales.

Backup slides

Characterization of MHOUs

Experimental

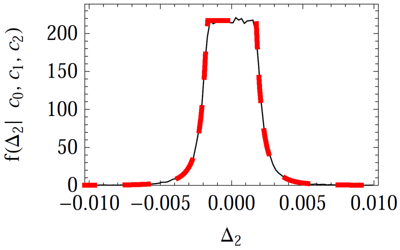
- Lack of of clear signals from LHC data. New physics, if it exists at the EW scale, will appear as a deviation in precision measurements
- In some cases, experimental uncertainties start to be comparable to theoretical ones

Theoretical

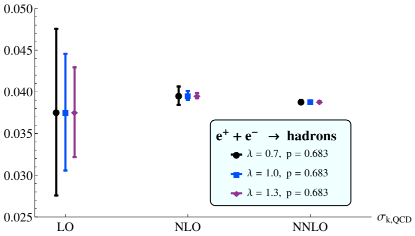
- One of the most important source of theoretical uncertainties are Missing Higher Order Uncertainties (MHOU)
- The standard method used to account for this, Scale Variation (SV), does **not** provide a full statistical framework to treat the problem

How can we improve our handling of MHOUs?

Features and issues



Posterior distribution for Δ_k. In red-dashed the analytic approximation, in black the numerical result

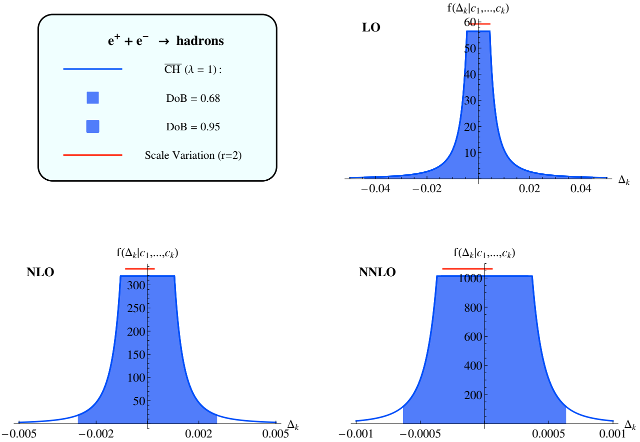


Effect of the rescaling of the expansion parameter $\alpha_s \to \frac{\alpha_s}{\lambda}$ for various values of λ

Benchmarks

$e^+e^- \to$ hadrons

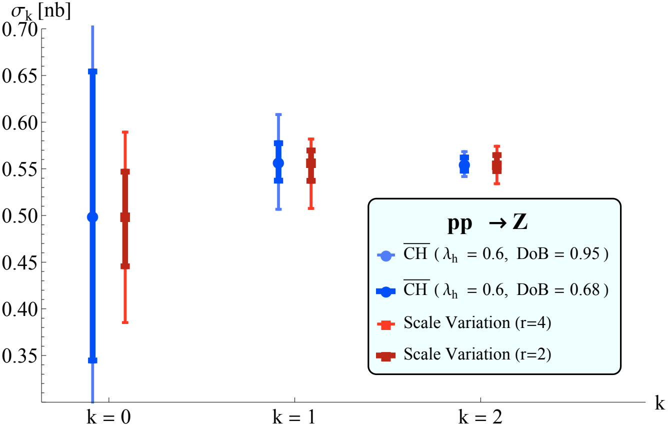
Density profile for the posterior distribution



Benchmarks

Z production at the LHC 8 TeV

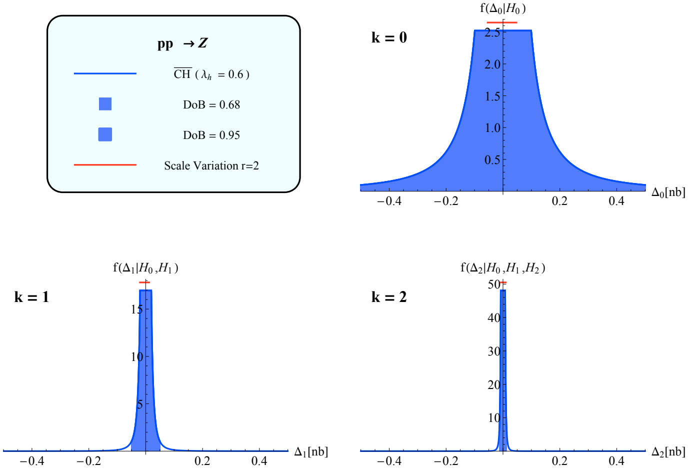
Error bars: $\overline{\text{CH}}$ vs scale variation



Benchmarks

Z production at the LHC 8 TeV

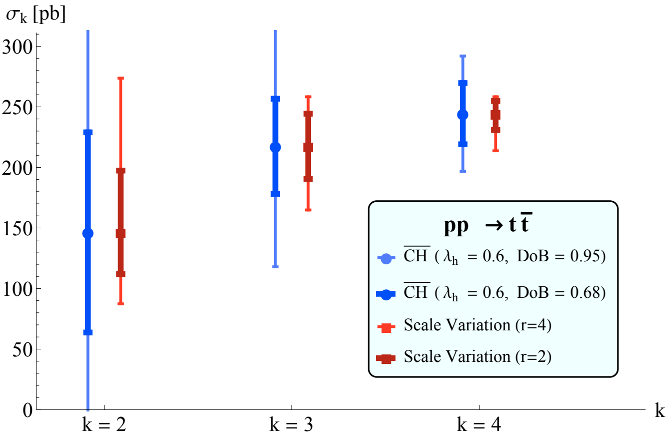
Density profile for the posterior distribution at NNLO



Benchmarks

$t\bar{t}$ production at the LHC 8 TeV

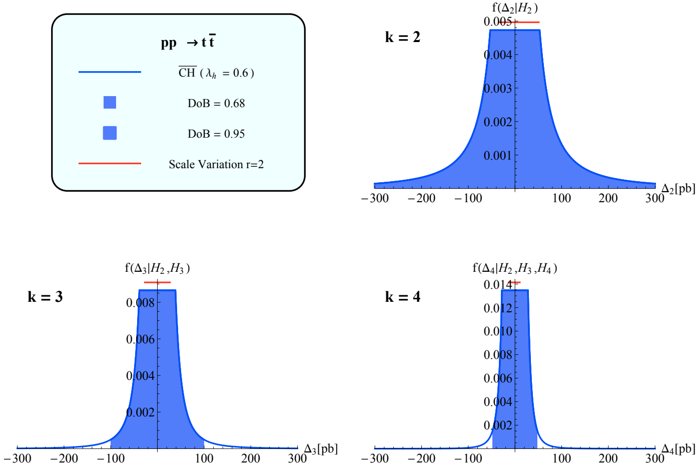
Error bars: $\overline{\text{CH}}$ vs scale variation



Benchmarks

$t\bar{t}$ production at the LHC 8 TeV

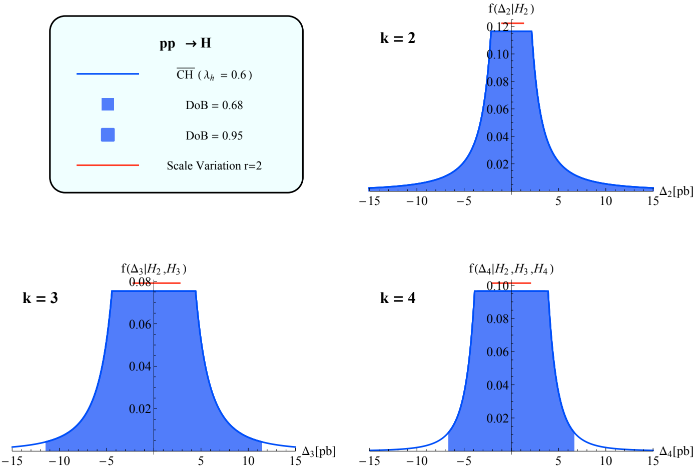
Density profile for the posterior distribution at NNLO



Benchmarks

$pp(gg) \to h$ at the LHC 8 TeV (coefficient)

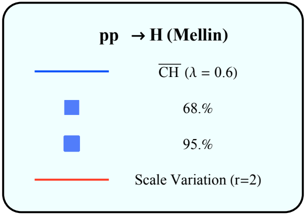
Density profile for the posterior distribution at NNLO

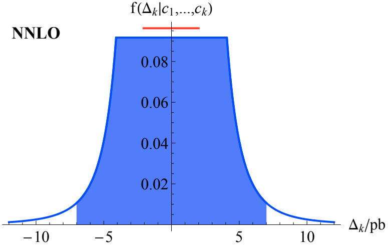


Benchmarks

$pp(gg) \rightarrow h$ at the LHC 8 TeV (Mellin)

Density profile for the posterior distribution at NNLO





Benchmarks

Comments

- The uncertainty intervals given by $\overline{\text{CH}}$ for a 68% DoB tend to be larger than the intervals obtained with scales variation with $r = 2$
- A separate study of the scale variation intervals shows that an heuristic 68% CL is obtained by taking a range of scales in the interval $3 \ldots 4$

Saddle point approximation[1] for $pp(gg) \to H$ (1)

We can write in x-space

$$\sigma(\tau, m_h^2) = \int_\tau^1 dz\, \mathscr{L}\left(\frac{\tau}{z}, m_H^2\right) \hat{\sigma}(z, \alpha_s(m_H^2))$$

with

$$\hat{\sigma}(z, \alpha_s) = \sigma_0\, z\, C(z, \alpha_s)$$
$$C(z, \alpha_s) = \delta(1-z) + \alpha_s C^{(1)}(z) + \alpha_s^2 C^{(2)}(z) + \mathcal{O}(\alpha_s^3)$$

[1] Bonvini,Forte,Ridolfi Phys. Rev. Lett. **109**, 102002 (2012) arXiv:1204.5473v2 [hep-ph]

Saddle point approximation for $pp(gg) \to H$ (2)

After a Mellin transform we have

$$\sigma(N, m_H^2) = \int_0^1 d\tau\ \tau^{N-1} \sigma(\tau, m_H^2)$$

$$C(N, \alpha_s) = \int_0^1 dz\, z^{N-1} C(z, \alpha_s)$$

$$\mathcal{L}(N) = \int_0^1 dz\, z^{N-1} \mathcal{L}(z)$$

We have then

$$\sigma(N, m_H^2) = \sigma_0 \mathcal{L}(N, m_H^2) C(N, \alpha_s)$$

Saddle point approximation for $pp(gg) \to H$ (3)

The Mellin inversion integral is given by

$$\sigma(\tau, m_H^2) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dN\, \tau^{-N} \sigma(N, m_H^2)$$

With the definition of

$$E(N, \tau, m_H^2) \equiv N \ln \frac{1}{\tau} + \ln \sigma(N, m_H^2)$$

We can rewrite the integral as

$$\sigma(\tau, m_H^2) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dN\, e^{E(N, \tau, m_H^2)}$$

Saddle point approximation for $pp(gg) \to h$ (4)

The inversion integral is then

$$\sigma(\tau, m_H^2) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dN\, e^{E(N,\tau,m_H^2)}$$

This integral can be computed with the saddle-point approximation, where it is assumed to be dominated by the value of the exponent E for the dominant moment N_0 which satisfy

$$\left. \frac{\partial E(N, \tau, m_H^2)}{\partial N} \right|_{N=N_0} = 0$$

David-Passarino prescription[1]

An alternative approach

- Direct estimation of the theoretical uncertainty by using sequence transformation on the known perturbative expansion
- The uncertainty does not depend on the expansion parameter of the series

[1] David,Passarino Phys. Lett. B **726** (2013) 266 arXiv:1307.1843 [hep-ph]