

THEORY UNCERTAINTIES

Zurich Phenomenology Workshop — January 8th 2025 — Zurich

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THEORY UNCERTAINTIES IN HIGH-ENERGY PRECISION MEASUREMENTS AT THE LHC

* I will focus on select <u>recent developments & trends</u> which I find interesting/important/concerning/...

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LHC – FROM A DISCOVERY TO A PRECISION MACHINE



[CMS-PAS-SMP-22-010]LEP + SLD: $A_{FB}^{0,b}$ 0.23221 ± 0.00029 SM 0.23098 ± 0.00026 SLD: A, CDF 2 TeV 0.23221 ± 0.00046 D0 2 TeV 0.23095 ± 0.00040 ATLAS 7 TeV 0.23080 ± 0.00120 LHCb 7+8 TeV 0.23142 ± 0.00106 CMS 8 TeV 0.23101 ± 0.00053 ATLAS 8 TeV Preliminary 0.23140 ± 0.00036 CMS 13 TeV 0.23157 ± 0.00031 Preliminary 0.229 0.231 0.233 0.23 0.232 0.234 $\sin^2 \theta_{eff}^l$







What is the Uncertainty Δ_{TH} of my Result?

- increasingly urgent to address with $\Delta_{\text{EXP}} \searrow (\leftrightarrow \text{HL-LHC})$
 - what does 5σ mean if Δ_{TH} non-negligible?
 - interpretation of data in need for robust Δ_{TH} : precision measurements, PDF fits, ...
- various sources that contribute to Δ_{TH} :
 - $\Delta_{\alpha_{s'}} \Delta_{\text{param}}$: parametric uncertainties $\leftrightarrow \Rightarrow$ exp. extraction
 - Δ_{PDF} : parton distribution functions (PDFs) $\leftrightarrow \beta$ fits to data, lattice, ...
 - $\Delta_{\text{non pert.}}$: intrinsic k_T , hadronisation, UE, ... \leftrightarrow TMD, parton showers, ...
 - $\Delta_{\text{pert.}}$: missing higher-order corrections $\leftrightarrow \rightarrow$ conceptually tricky



- MOTIVATION
- 1. Scale Variations
- "QCD modelling" **2**. Bayesian Estimates
 - 3. Theory Nuisance Parameters
 - **4.** Parton Distribution Functions
 - CONCLUSIONS



GENERAL IDEA & CONVENTIONS

approximation for an observable (next-to-)ⁿ leading order:

truncation of series induces a sensitivity to terms of the next order $\mu \frac{\mathrm{d}}{\mathrm{d}\mu} \sigma^{\mathrm{N^{n}LO}}(\mu) = \mathcal{O}(\alpha_{s}^{n_{0}+n+1}) = \mathcal{O}(\Delta_{\mathrm{pert.}})$



$$d\sigma^{\text{N}^{n}\text{LO}} = d\sigma^{(0)} + \alpha_{s} d\sigma^{(1)} + \dots + \alpha_{s}^{n} d\sigma^{(n)}$$



CREDIT WHERE CREDIT IS DUE

- quite neat & simple
- can work very well... ... lot of experience if it doesn't ← new channels, jet bins, "giant *K* factors", ratios, ... \hookrightarrow strategies to mitigate





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- quite neat & simple
- can work very well... ... lot of experience if it doesn't \hookrightarrow new channels, jet bins, "giant *K* factors", ratios, ... \hookrightarrow strategies to mitigate
- failure of Δ_{scl} beyond repair(?) ↔ difficult for any method

13

 $\frac{27}{\sqrt{s} \,[\text{TeV}]}$

50

100

 10^{-}

-1 [%]

 σ NNLO/ σ NLO



MAIN ISSUES WITH SCALES

- choice of the central scale μ_0
- 2 no probabilistic interpretation
- no correlation model 3

fastest apparent convergence (FAC) $\hookrightarrow \sigma^{(n)}(\mu_{\text{FAC}}) = 0$

principle of minimal sensitivity (PMS)

$$\hookrightarrow \left. \frac{\partial}{\partial \mu} \sigma^{(n)}(\mu) \right|_{\mu_{\text{PMS}}} = 0$$

incl. jets @ NNLO w.r.t. $\mu_0 = 2p_T$

or combination:

- convergence
- band overlap
- stability

• • •







MAIN ISSUES WITH SCALES

- choice of the central scale μ_0
- no probabilistic interpretation 2
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MAIN ISSUES WITH SCALES

- choice of the central scale μ_0
- no probabilistic interpretation 2
- no correlation model

new approaches try to mainly address 2 & 3 I remains a challenge ∀













GENERAL IDEA

consider the perturbative series as a sequence of dimensionless numbers $d\sigma = d\sigma^{(0)} \left[1 + \delta_1 + \delta_2 + \dots \right] \qquad \rightsquigarrow \quad \delta_k = \mathcal{O}(\alpha_s^k)$ Q: after observing $\delta_n \equiv (\delta_0, \delta_1, \dots, \delta_n)$, prob. to observe δ_{n+1} ? $P(\boldsymbol{\delta}_{n+1} | \boldsymbol{\delta}_n) = \frac{P(\boldsymbol{\delta}_{n+1}, \boldsymbol{\delta}_n)}{P(\boldsymbol{\delta}_n)} = \frac{\int d^m \boldsymbol{p} \ P(\boldsymbol{\delta}_{n+1}, \boldsymbol{\delta}_n | \boldsymbol{p}) \ P_0(\boldsymbol{p})}{\int d^m \boldsymbol{p} \ P(\boldsymbol{\delta}_n | \boldsymbol{p}) \ P_0(\boldsymbol{p})}$ P(A, B) = P(A | B) P(B) $P(A) = \left| \mathrm{d}B \ P(A, B) \right|$

[Cacciari, Houdeau '11], [Bonvini '20] [Duhr, Huss, Mazeliauskas, Szafron '21]





THE CH MODEL [Cacciari, Houdeau '11]

THE GEOMETRIC MODEL [Bonvini '20]

model:

$$P_{\text{geo}}^{(k)}(\delta_k | \boldsymbol{a}, \boldsymbol{c}) = \frac{1}{2\boldsymbol{c} \ \boldsymbol{a}^k} \Theta\left(\boldsymbol{c} - \frac{|\delta_k|}{\boldsymbol{a}^k}\right) \qquad P_0(\boldsymbol{a})$$

$$P_0(\boldsymbol{a}) = \frac{1}{2\boldsymbol{c} \ \boldsymbol{a}^k} \Theta\left(\boldsymbol{c} - \frac{|\delta_k|}{\boldsymbol{a}^k}\right) \qquad P_0(\boldsymbol{a})$$

pert. exp. $\delta_k = c_k \alpha_s^k$ bounded by geometric series: $|c_k| \leq \overline{c} \quad \forall k \quad \nleftrightarrow 1$ param: \overline{c} $\sim \alpha_s$ at what scale? why not: α_s/π , $\alpha_s/(4\pi)$, $\alpha_s \ln^2(v)$, $\alpha_s \ln(v)$, ... ?

let the model learn the expansion parameter: $|\delta_k| \leq c a^k \quad \forall k \quad \nleftrightarrow 2 \text{ parameter: } a, c$ priors:

 $(\mathbf{a}) = (1 + \omega) \ (1 - \mathbf{a})^{\omega} \ \Theta(|\mathbf{a}| < 1)$

 $P_0(\mathbf{c}) = \frac{\varepsilon}{\mathbf{c}^{1+\varepsilon}} \Theta(\mathbf{c}-1)$

 $dc/c \sim d \ln(c)$ (*ɛ*: regulator)









Higgs production in gluon fusion at LHC 13 TeV, $m_H = 125$ GeV



 $\mu_{\rm F} = m_{\rm H}/2$ $\mu_{\rm R} = m_{\rm H}/2$ 60 50 70

THE GEOMETRIC MODEL

- full prob. dist. $P(\sigma)$
- broad lower orders: \hookrightarrow stronger dependence on priors P_0
- narrow higher orders: \hookrightarrow inference of hidden parameters





THE ABC MODEL

allow for a bias & alt. series: $b - c \le \frac{\delta_k}{a^k} \le b + c \quad \forall k$

INCORPORATION OF SCALES

scale marginalisation (sm)

$$\int \mathrm{d}\mu \ P(\delta_n$$











THE ABC MODEL

allow for a bias & alt. series: $b - c \le \frac{\delta_k}{c^k} \le b + c \quad \forall k$

INCORPORATION OF SCALES

 $\leftrightarrow P_{\rm sm}(\delta_{n+1} | \boldsymbol{\delta}_n)$ peaks at μ_{FAC}

scale average (sa) 2 $\leftrightarrow P_{sa}(\delta_{n+1} | \boldsymbol{\delta}_n)$

peaks at μ_{PMS}



 \leftrightarrow prescription



scale interpretation











overall: not radically different estimates for $\Delta_{\text{pert.}}$ $(n \ge 2)$

- δ_3 is large and outside of 9pt!
- similar unc.: sa \simeq 9pt
- n = 2: sm \ll others (μ_{FAC})
- n = 3: all prescriptions similar

- Iarge cancellations in the ratio
- n < 2: 9pt performs poorly
- $(A_W)_n \nearrow$ (anticipated by *abc*)
- size: $abc \leq others$

c)



DIFFERENTAIL DISTRIBUTIONS



• *n* < 2:

- CI₆₈ bigger than 9pt
- *abc* captures pos. shift

•
$$n = 2$$
:

- almost identical bands
- $\Delta_{\rm MHO}$ very robust
- sm vs. sa
 - almost identical CI



GENERAL IDEA & STEPS

- parametrise the unknown order using nuisance parameters $\vec{\theta}$ (TNP) $d\sigma = d\sigma^{(0)} + \alpha_s d\sigma^{(1)} + \alpha_s^2 d\sigma^{(2)}_{TNP}(\theta)$
- assign a probability distribution $P(\theta)$ 2 \hookrightarrow stat. interpretation & correlation model
- possibility to constrain $\hat{\theta}$ using data 3

[McGowan, Cridge, Harland-Lang, Thorne '23] [Tackmann '24], [Lim, Poncelet '24]

$\rightarrow \mathcal{N}\theta \quad (simplest case)$



most interesting when we have information on the functional dependence of an observable ↔ <u>correlations</u>





RESUMMED PREDICTION

factorization in limit $p_T \rightarrow 0 \iff$ functional dependence known

$$\frac{\mathrm{d}\sigma}{\mathrm{d}p_{\mathrm{T}}} = \begin{bmatrix} H \otimes B_{a} \otimes B_{b} \otimes S \end{bmatrix} (\alpha_{s}; L) + \mathcal{O}(p_{T}/Q) \qquad L \equiv \ln(p_{T}/Q)$$

$$RGE$$

$$\mathcal{X} \in \{H, B_{a}, B_{b}, S\} \longrightarrow \mathcal{X}(\alpha_{s}; L) = \mathcal{X}(\alpha_{s}) \exp \int_{0}^{L} \mathrm{d}L' \left\{ \Gamma(\alpha_{s}(L')) L' + \gamma_{\mathcal{X}}(\alpha_{s}(L')) \right\}$$

boundary conditions: $\mathscr{X}(\alpha_{s}) = \mathscr{X}_{0} + \alpha_{s} \mathscr{X}_{1} + \alpha_{s}^{2} \mathscr{X}_{2} + \dots$ anomalous dimensions: $\Gamma(\alpha_s) = \alpha_s \left[\Gamma_0 + \alpha_s \Gamma_1 + \alpha_s^2 \Gamma_2 + \dots \right]$ Yx(

$$(\alpha_s) = \alpha_s \left[\gamma_0 + \alpha_s \gamma_1 + \alpha_s^2 \gamma_2 + \dots \right]$$







RESUMMED PREDICTION

- 1'
 - boundary conditions: $\mathcal{X} \in \{H, B_a, B_b, S\}$

$$\mathcal{X}_n = \mathcal{N}_{\mathcal{X}}^{(n)} \, \boldsymbol{\theta}_{\mathcal{X}}$$

anomalous dimensions: (+ beta function β & splitting functions $P_{a \rightarrow b}$)

$$\Gamma_n = \mathcal{N}_{\Gamma}^{(n)} \,\boldsymbol{\theta}_{\Gamma} \qquad \boldsymbol{\gamma}_{\mathcal{X},n} = \mathcal{N}_{\boldsymbol{\gamma}_{\mathcal{X}}}^{(n)} \,\boldsymbol{\theta}_{\boldsymbol{\gamma}_{\mathcal{X}}}$$

implements a correlation model for the (low-ish) p_T spectrum

Tackmann '24

parametrise unknown resummation ingredients using nuisance parameters $\hat{\theta}$ \rightarrow actually functions: $B_i(x_i)$





RESUMMED PREDICTION

assign a probability distribution (statistics over \exists calculations) 2 ↔ assume universality in order *n* as well as processes/ingredients valid?



selection bias?

- **CHOICES** (*« » ambiguities*)
- scheme dependence (scale, ren. scheme, IR subtr., ...)
 - parametrisation freedom $(\theta \rightarrow \theta')$: changes what is uncorrelated / independent)

"massaging"







RESUMMED PREDICTION

- 2' 100% correlation of $\vec{\theta}$
 - large cancellation in W⁺/Z
 - dominant residual
 uncertainties from *B*_{ab}
- similar absolute errors to Δ_{scl}
- valid at low p_T • requires matching @ high $p_T (\mu_R, \mu_F)$
- missing: non-pert. modelling



[Tackmann '24]











$\mathsf{CMS}\,M_{\mathrm{W}}\,\mathsf{MEASUREMENT}$

3 constrain $\vec{\theta}$ using data





Ц.,



BEYOND RESUMMED SPECTRA

$$\frac{\mathrm{d}\sigma}{\mathrm{d}x} = \frac{\mathrm{d}\sigma^{(0)}}{\mathrm{d}x} \left[1 + \alpha_s N_c \,\overline{K}^{(1)}(x) + \alpha_s^2 N_c^2 \,\overline{K}^{(2)}(x) + \dots\right] \qquad \overline{K}^{(n)}(x) \equiv \frac{1}{N_c^n} \,\frac{\mathrm{d}\sigma^{(n)}/\mathrm{d}x}{\mathrm{d}\sigma^{(0)}/\mathrm{d}x}$$

parametrise first unknown order as superposition of lower-order $\overline{K}^{(n)}$ $\overline{K}_{\text{TNP}}^{(n+1)}(\vec{\theta}; x) = \sum_{k=1}^{n} f_{k}^{(j)}(\vec{\theta}; x) \overline{K}^{(j)}(x)$ i = 1

polyn. modulation

•
$$k = 0 \Rightarrow f_0^{(j)}(\vec{\theta}; x) \to \theta_0^{(j)} \iff \text{approa}$$

pull out the Born prediction and split off leading-colour factor at each order *n*

$$\begin{cases} f_k^{(j)}(\vec{\theta}; x) = \sum_{i=0}^k \theta_i^{(j)} \begin{pmatrix} k \\ i \end{pmatrix} x^{k-i} (1-x)^i & \text{(Bernstein)} \\ f_k^{(j)}(\vec{\theta}; x) = \frac{1}{2} \sum_{i=0}^k \theta_i^{(j)} T_i(x) & \text{(Chebyshev)} \end{cases} \end{cases}$$

 $P(\theta_{i}^{(j)})$: uniform in [-1, +1], normal with $\sigma = 1$ ich to approx. N³LO in MSHT PDF fit



3 THEORY NUISANCE PARAMETERS $pp \to t\bar{t} \to \ell\bar{\ell} \ 2b - \text{jets}, \text{LHC} @ 13 \text{ TeV}$ central scale: $\mu = H_T/4^-$ Bernstein parameterisation (k=2)Errorbands: TNP (quad.) TNP's: symmetric by construction 0.6 -0.4 -Errorbands: 3-Point scale var. scale variation: 0.8 3-point, not 7-point 0.6 can be asymmetric 0.4 - 4500100 200300 400 $m(\vec{r})$ [GeV]





3 THEORY NUISANCE PARAMETERS $pp \to t\bar{t} \to \ell\bar{\ell} \ 2b - \text{jets}, \text{LHC} @ 13 \text{ TeV}$ central scale: $\mu = H_T/4^{-1}$ Bernstein parameterisation (k=2)Errorbands: TNP (quad.) TNP's: symmetric by construction 0.8 how to map x? 0.6multi-dim? 0.4 -Errorbands: 3-Point scale var. scale variation: 0.8 3-point, not 7-point 0.6 can be asymmetric 0.4500100 200300 400 $m(\vec{x})$ [GeV]





3 THEORY NUISANCE PARAMETERS $pp \ pp \rightarrow e^+ \bar{v_e} \mu^- \bar{v}_\mu \ LHC @ 13 \ TeV eV$ central scale: $\mu = H_T/2 \equiv$ Bernstein parameterisation (k=2)Errorbands: TNP (quad.) TND's: symmetric by constru 1.00 ·P 0.75 how to map x? 0.50multi-dim? NLO O Errorbands: 3-Point scale var. die voriation. 3-point, not 7-point 0.750.50 can be asymmetric 350 200250300 400 $m(W^+)V^-)$ [GV]



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DATASET & TOLERANCES

- $\mathcal{O}(4000)$ datapoints in a global fits \hookrightarrow inconsistencies between data, unknown/underestimated EXP/TH uncertainties, model, ...
- $\Delta \chi^2 = 1$ for 68% C.L. not suited \rightarrow "tolerance" $T^2 = 10-30$

THEORY UNCERTAINTIES IN PDFs

- NNPDF4+ (scale variation) MSHT aN³LO (nuisance parameter)
- mandatory in aN³LO as (almost) no predictions available at this order

more stable χ^2 in the progression of the orders







ggH @ N³LO

estimate ~ 1 % error $\left(\Delta_{\text{NNLO}}^{\text{app}} \equiv \frac{1}{2} \left| \frac{\sigma_{\text{NNLO-PDF}}^{\text{NNLO}} - \sigma_{\text{NLO-PDF}}^{\text{NNLO}}}{\sigma_{\text{NNLO-PDF}}^{\text{NNLO}}} \right|$ \hookrightarrow actual shift much larger:









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did we just see some artefacts from the mismatch between $\hat{\sigma}$ & PDFs? (uncompensated logs, ...)





PROFILING / REWEIGHTING

PDF uncert. often among dominant sources A exploit correlations to reduce impact \Rightarrow often a huge reduction (~ 2 ×) in $\Delta_{PDF}!$





PROFILING / REWEIGHTING FOR α_{c}

- situation is even more delicate for α_{s}
- quoted $\Delta_{PDF} = \pm 0.00051$





CONCLUSIONS & OUTLOOK

- Covered two dominant TH systematics in precision measurements → QCD modelling & PDF uncertainties.
 - <u>no time to cover</u>: EW corrections, PS, non-pert. uncertainties, ...
- Situation: $\Delta_{\text{EXP}} \ll \Delta_{\text{TH}}$ puts analyses in the position to constrain Δ_{TH} from data \rightarrow prob. interpretation & correlation model crucial in this endeavour
 - **Bayesian estimates:** prob. interpretation (can also implement correlations)
 - **Theory nuisance parameters:** "physical" correlation model $\bigoplus P(\theta)$
- \exists a "correct" $\Delta_{\text{pert.}}$ model (each approach relies on set of assumptions)
- PDF reweighting / profiling by now standard practice
 - can reduce nominal Δ_{PDF} by factors of 2–4
 - impact on global PDF fit picture needs to be better understood & potential missing model/methodology uncertainties?

relying on a <u>single</u> prescription is potentially dangerous!



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Thank you!







X PARTON SHOWERS

PERTURBATIVE **AND NON-PERTURBATIVE**

- Parton showers (PS) model all-order QCD emissions through the evolution from hard to soft scales
- no systematic approach (afaik) to assess *perturbative* uncertainties in PS
- tuning of PS further entangles the pert. part with the non-pert. (NP) model \hookrightarrow latter very sizeable
 - \hookrightarrow difficult to assess due to the notorious "Herwig vs. Pythia" effective two-point systematics





X PARTON SHOWERS

FORMAL ACCURACY

- tremendous progress in improving the formal accuracy of PS to
 → NLL [Alaric, Deductor, Herwig, Apollo, FHP, Panscales]
 → NNLL [PanScales 2406.02661]
- addresses long-standing issue with dipole showers that required an anomalously large $\alpha_s(M_Z) \gtrsim 0.130$
- NP effectively absorbing pert. effects?
 ⇒ can formally accurate PS lead to better alignment in NP modelling?







WORK IN PROGRESS - CORRELATIONS

- idea: if two bins show similar (opposite) perturbative behaviour \hookrightarrow two bins should be partially (anti-)correlated.
- we want: joint probability distribution P(x, y) for two bins x & y \rightarrow preserve projections for compatibility:

$$P(x) = \int dy \ P(x, y) = \int dz \ P(x, z)$$

possibilities: algorithmic "earth movers distance"; map P(x) onto P(y), ... \hookrightarrow can be done much simpler

[AH, Mazeliauskas w.i.p]

 \rightarrow hidden parameter -1 < c < +1 to smoothly implement the correlation





WORK IN PROGRESS - CORRELATION MODEL

projections of multi-dim. Gaussians (+ correlation matrix) are again Gaussian \rightarrow map P_i onto Gaussians, implement correlations, map back

$$P(x,y) = P_1(x)P_2(y)$$

$$\times \frac{d\Phi^{-1}(\alpha)}{d\alpha}\Big|_{\alpha=\Sigma_1(x)} \frac{d\Phi^{-1}(\beta)}{d\beta}\Big|_{\beta=\Sigma_2(y)}$$

$$\times \frac{1}{2\pi\sqrt{1-c^2}} \exp\left(-\frac{1}{2(1-c^2)}\left[\xi(x)^2 + \eta(y)^2 - c2\xi(x)\eta(y)\right]\right)$$



.

[AH, Mazeliauskas w.i.p]

 $\Sigma_i(x) = \int_{-\infty}^x dx' P_i(x')$ $\Phi^{-1}(p) = \sqrt{2} \mathrm{Erf}^{-1}(-1+2p)$ $\xi(x) = \Phi^{-1}\left(\Sigma_1(x)\right)$ $\eta(y) = \Phi^{-1}(\Sigma_2(y))$





use inference to constrain c





Kenneth Long



