

BAYESIAN ESTIMATES FOR TH UNCERTAINTIES

Discussion of theoretical systematics in LHC precision measurements — February 26th 2024 — CERN

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WHAT IS THE UNCERTAINTY Δ_{TH} of MY RESULT?

- increasingly urgent to address with $\Delta_{\rm EXP} \searrow (\leftrightarrow\to \rm HL\text{-}LHC)$
	- \triangleright what does 5σ mean if Δ_{TH} non-negligible?
	- interpretation of data in need for robust Δ_{TH} : PDF fits, χ^2 in ATLAS jets, ... Δ_{TH} : PDF fits, χ^2
- \bullet various sources that contribute to Δ_{TH} :
	- **↓** Δ_{α_s} , Δ_{param} : parametric uncertainties ↔ exp. extraction
	- \rightarrow Δ_{PDF} : parton distribution functions (PDFs) \leftrightarrow fits
	- Δ _{non pert.}: hadronisation, UE, ... \leftrightarrow parton showers [e.g. HERWIG vs. PYTHIA]
	- Δ_{MHO}: *missing higher-order (MHO)* corrections

Focus here

CONVENTIONAL APPROACH FOR Δ_{MHO} – SCALE VARIATION

• approximation for an observable ω (next-to-)^{*n*} leading order: *n* $\propto \alpha_s^{n_0+k}$

- \blacktriangleright NⁿLO: n $\Sigma \simeq \Sigma_n(\mu) =$ ∑ $k=0$ $\Sigma^{(k)}(\mu)$
- ๏ truncation of series induces a sensitivity to terms of the next order Cremienten variation.

$$
\mu \frac{\mathrm{d}}{\mathrm{d}\mu} \Sigma_n(\mu) = \mathcal{O}(\alpha_s^{n_0+n+1}) = \mathcal{O}(\math>
$$

electroweak (EW): ↪ scheme dependence $\hookrightarrow \alpha \ll \alpha_s$

ISSUES WITH STANDARD SCALE VARIATIONS

- ๏ known to be insufficient:
	- exclusive jet(s) (veto)
	- ratios (correlation?)
	- ‣ cancellations (e.g. *qq*¯ vs. *qg* in DY)

- fastest apparent convergence (FAC) $\hookrightarrow \sum(n)$ $(\mu_{\text{FAC}}) = 0$
- ‣ principle of minimal sensitivity (PMS) $\leftrightarrow \frac{\partial}{\partial u}$ ∂*μ* $\Sigma^{(n)}(\mu)$ *μ*PMS $= 0$
- ‣ BLM/PMC

๏ choice of the central scale

‣

๏ crucially: *no probabilistic interpretation!* can we do better? ⇝

… [Brodsky, Lepage, Mackenzie '83]; [Brodsky, Di Giustino '12]

PROBABILITY DISTRIBUTIONS FOR
$$
\Delta_{MHO}
$$
 [Cacciari, Houdeau '11]
\n• Sequence of perturbative corrections δ_k normalised w.r.t. LO (dimensionless)
\n
$$
\Sigma_n = \Sigma^{(0)} (1 + \delta_1 + ... + \delta_n) \qquad \leadsto \delta_k = \mathcal{O}(\alpha_s^k)
$$
\nProbability distribution for δ_{n+1} , given $\delta_n = (\delta_0, \delta_1, ..., \delta_n)$
\n
$$
P(\delta_{n+1} | \delta_n) = \frac{P(\delta_{n+1})}{P(\delta_n)} = \frac{\int d^m p \ P(\delta_{n+1} | p) P_0(p)}{\int d^m p \ P(\delta_n | p) P_0(p)}
$$

 $P(A, B) = P(A | B) P(B)$ $P(A) = \text{d}B P(A, B)$

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 $\mathsf{Model}: P(\mathcal{S}_n | p)$ Priors: $P_0(p)$ ⊕

 δ_{n+1} , given $\delta_n = (\delta_0, \delta_1, ..., \delta_n)$ $p(p) P_0(p)$ $p P_0(p)$ \rightarrow $\delta_k = O(\alpha_s^k)$

THE CH MODEL

• perturbative expansion $\delta_k = c_k \alpha_s^k$ bounded by a geometric series: $|c_k| \leq \bar{c}$ $\forall k$

- ▸ one hidden parameter: *c*
- \triangleright constrain upper bound \bar{c} from known orders \rightarrow constraint on unknown coefficients c_{n+1}
- ๏ limitations:

*a*_{*s*} at what scale? why not: $\frac{d^2y}{dx^2}$, $\frac{d^2y}{dx^2}$, α_s $\ln^2(v)$, α_s $\ln(v)$, ...? *αs π αs* 2*π*

why not let the model figure out the expansion parameter itself?

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$$
\left|\sum_{k} \delta_{k}\right| \leq \sum_{k} |c_{k}| \alpha_{s}^{k} \leq \sum_{k} \bar{c} \alpha_{s}^{k}
$$

THE GEOMETRIC MODEL **•** bounded by a geometric series with expansion parameter *a*: ๏ model: *P*(*k*) $P_0(a, c) = P_0(a) P_0(c)$ $|\delta_k| \leq c \ a^k \quad \forall k \qquad \leftrightarrow \text{two model parameters: } a, c$ $\int_{\text{geo}}^{(k)}(\delta_k | a, c)$ = $\frac{1}{2c \ a^k} \ \Theta\left(c - \frac{|\delta_k|}{a^k}\right)$ $P_0(a) = (1 + \omega) (1 - a)^{\omega} \Theta(a) \Theta(1 - a)$ $P_0(c) =$ *ε c*1+*^ε* $\Theta(c-1)$

[Bonvini '20]

↭ d*c*/*c* ∼ d ln(*c*) (*ε*: regulator)

The Inference Step $-$ Geometric series: $\delta_k = (0.7)^k$

 \circ LO $\delta_0 \equiv 1$

 $P_0(a, c) = \Theta(a) \Theta(1 - a) P_0(c)$

 $\mathbf{choose} \ \omega = 0$ for flat prior in *a*

 $P(\delta_1) = \int da \int dc \ P_{\text{gec}}^{(1)}$ $P_0(1)(\delta_1 | a, c) P_0(a, c)$

no inference yet! $P(\delta_1)$ entirely determined by the *model & priors*

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The Inference Step $-$ Geometric series: $\delta_k = (0.7)^k$

 \circ LO $\delta_0 \equiv 1$ $\delta_1 = 0.7$ $\delta_2 = 0.7^2$ $P(a, c | \delta_1) \propto P_{\text{geo}}^{(1)}(\delta_1 | a, c) P_0(a, c)$ $P(a, c | \delta_1, \delta_2) \propto P(\delta_2 | \delta_1, a, c) P(a, c | \delta_1)$ $\propto P_{\text{geo}}^{(2)}(\delta_2 | a, c) P_{\text{geo}}^{(1)}(\delta_1 | a, c) P_0(a, c)$ 1 1 2 3 4 $P_0(a, c) = \Theta(a) \Theta(1 - a) P_0(c)$ *P*(*a*) 1 Bayes' theorem

& independence *also:*

 $a \sim 0.7$ also: $c \sim 1$

The Inference Step $-$ Geometric series: $\delta_k = (0.7)^k$

 \circ LO $\delta_0 \equiv 1$ $\delta_1 = 0.7$ $\delta_2 = 0.7^2$ \bullet $P(a, c | \delta_1) \propto P_{\text{geo}}^{(1)}(\delta_1 | a, c) P_0(a, c)$ $P(a, c | \delta_1, \delta_2) \propto P(\delta_2 | \delta_1, a, c) P(a, c | \delta_1)$ $\propto P_{\text{geo}}^{(2)}(\delta_2 | a, c) P_{\text{geo}}^{(1)}(\delta_1 | a, c) P_0(a, c)$ $P_0(a, c) = \Theta(a) \Theta(1 - a) P_0(c)$

$$
P(\delta_{n+1} | \delta_n) \propto \int da \int dc \prod_{k=1}^n \left[P_{\text{geo}}^{(k)}(\delta_k | a, c) \right] P_0(a, c)
$$

can be solved analytically

THE *abc* MODEL — ASYMMETRIC GEOMETRIC MODEL

-
- ๏ allow for different lower & upper bound: $b - c \leq$ δ_k

• **priors:**
$$
P_0(a, b, c) = P_0(a) P_0(b, c)
$$

\n
$$
P_0(a) = \frac{1}{2} (1 + \omega) (1 - |a|)^{\omega}
$$
\n
$$
P_0(b, c) = \frac{\varepsilon \eta^{\varepsilon}}{c^{1 + \varepsilon}} \Theta(c - \eta) \frac{1}{2\xi c}
$$

$$
\text{ \textcolor{red}{\bullet} \text{ model:} \quad P_{abc}^{(k)}(\delta_k | a, b, c) = \frac{1}{2c|a|^k} \Theta\bigg(c - \Big|\frac{\delta_k}{a^k} - b\Big|\bigg) \qquad \qquad \overbrace{\big|_{(b-c)a^k}^{(b-c)a^k} \quad (b+c)a^k}}
$$

Θ(*ξc* − *b*)

^ω Θ(1 − |*a*|) ↭ support: [−1,+1] (alternating ✔)

WHAT TO DO WITH THE THE SCALE μ ?

 Θ $\forall \mu \rightsquigarrow P(\delta_3 | \delta_0, \delta_1, \delta_2; \mu)$ • $CI_{68/95}$ \parallel (geo) \parallel (abc)

๏ geo

- ‣ always entered around NNLO
- ‣ very narrow peak

- $\mu/\mu_0 \gtrsim 1 \rightsquigarrow$ anticipate pos. N3LO
- ‣ bias slowly disappears *μ*/*μ*⁰ ≲ 1 ⇝

๏ *abc*

WHAT TO DO WITH THE THE SCALE *μ*?

 Θ $\forall \mu \rightsquigarrow P(\delta_3 | \delta_0, \delta_1, \delta_2; \mu)$ • $CI_{68/95}$ \parallel (geo) \parallel (abc)

> **F**astest **A**pparent **C**onvergence $\Sigma_n(\mu_{\text{FAC}}) = \Sigma_{n-1}(\mu_{\text{FAC}})$

> > *15*

- ๏ two options:
	- 1. invoke some *principle* to pick the *"optimal"* scale
		- FAC, PMS, PMC, ...

depends on order might not be unique

WHAT TO DO WITH THE THE SCALE *μ*?

 Θ $\forall \mu \rightsquigarrow P(\delta_3 | \delta_0, \delta_1, \delta_2; \mu)$ • $CI_{68/95}$ \parallel (geo) \parallel (abc)

> **P**rinciple of **M**inimal **S**ensitivity $\sum_{n}(\mu)\big|_{\mu_{\rm PMS}}$ $= 0$

> > *15*

- ๏ two options:
	- 1. invoke some *principle* to pick the *"optimal"* scale
		- FAC, PMS, PMC, ...

depends on order might not be unique

WHAT TO DO WITH THE THE SCALE μ ?

 Θ $\forall \mu \rightsquigarrow P(\delta_3 | \delta_0, \delta_1, \delta_2; \mu)$

- ๏ two options:
	- 1. invoke some *principle* to pick the *"optimal"* scale
		- FAC, PMS, PMC, ...
	- 2. combine different $P(\delta_{n+1} | \delta_n; \mu)$

pursued in the following

PRESCRIPTIONS FOR SCALES

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Scale Marginalisation (sm):

 o treat *μ* as a hidden model parameter & *marginalise* over it:

Scale Average (sa):

 $P(\mu | \delta_n) \propto P(\delta_n; \mu) P_0(\mu)$ with prior: $P_0(\mu) =$ 1 $\frac{1}{2\mu \ln F} \Theta(\ln F - |\ln (\ln$ *μ μ*0

๏ has no probabilistic interpretation *μ average* over it: ⇝

$$
P_{\rm sm}(\delta_{n+1} | \delta_n) = \int d\mu \ P(\delta_{n+1}, \mu | \delta_n)
$$

=
$$
\int d\mu \ P(\delta_{n+1} | \delta_n; \mu) \ P(\mu | \delta_n)
$$

with prior:
\n
$$
w(\mu) = \frac{1}{2\mu \ln F} \Theta\left(\ln F - \left|\ln\left(\frac{\mu}{\mu_0}\right)\right|\right)
$$
\n
$$
\lim_{\mu = \mu_0/F} \mu_0 \qquad F \mu_0
$$

$$
P_{\rm sa}(\delta_{n+1} | \delta_n) = \int d\mu \ w(\mu) P(\delta_{n+1} | \delta_n; \mu)
$$

[Bonvini '20] [Duhr, AH, Mazeliauskas, Szafron '21]

PEAK OF THE DISTRIBUTIONS*

Scale Marginalisation (sm):

- ω if $\mu_{\text{FAC}} \in [\mu_0/F, F\mu_0]$ then $P_{\rm sm}(\delta_{n+1} | \delta_n)$ peaks at $\Sigma_n(\mu_{\rm FAC})$
	- $P(\delta_n | \mu)$ dominated by $(k = n)$ term
	- ‣ symmetric model \rightarrow $\delta_n(\mu) = 0$ enhanced

Scale Average (sa):

- ω if $\mu_{\text{PMS}} \in [\mu_0/F, F\mu_0]$ then $P_{sa}(\delta_{n+1} | \delta_n)$ peaks at $\Sigma_n(\mu_{PMS})$
	- **•** overlap between $P(\delta_{n+1} | \delta_n; \mu)$ enhanced at stationary point \rightarrow $\Sigma'_n(\mu_{\rm PMS}) \approx 0$

* for symmetric models, a convergent series, and reasonable assumptions

Choice of how to interpret the scale has consequences for predictions!

INCLUSIVE CROSS SECTIONS UP TO N3LO

-
- \bullet similar unc.: sa \simeq 9pt
- $n = 2$: sm \ll others (μ_{FAC})
- renormalisation scales. Computations were performed with the proVBFH code [124].

In the left panel of figure 16 we display the CIs for different models and prescriptions for

 \smile *A*

 $\cancel{\approx}$

 \int_{n+1}^{n} *n*+1

- **•** δ_3 is large and outside of 9pt!
•• large cancellations in the ratio • δ_3 is large and outside of 9pt! • • large cancellations in the ratio
- **o** similar unc.: sa \simeq 9pt **o** $n < 2$: 9pt performs poorly
	- $O (A_W)_n \nearrow$ (anticipated by abc)
	- ๏ size: others *abc* ≲

0 1
0 (
0 S single Higgs VBF production. For *n <* 2 the Bayesian approach gives a larger uncertainty m different estimates for Λ_{max} (n > 2) abc_a **abc** sa **19.6, 46.6, 46.6, 46.6, 46.6, 46.6, 46.6, 46.6, 46.6, 46.6, 47.4, 4** abc_a **abc** sa **14.6, 46.6, 46.6, 46.6, 46.6, 46.6, 46.6, 46.6, 46.6, 46.6, 47.4, 4** *overall:* not radically different estimates for $\Delta_{\rm MHO}$ $(n \ge 2)$

DIFFERENTIAL DISTRIBUTIONS

- ๏ Bayesian approach also applicable to distributions \rightarrow treat each bin individually \leftrightarrow will not include correlations!
- ๏ new challenges
	- **no longer "easy" to identify an appropriate hard scale** μ_0 **(up to rescaling)** \rightarrow inclusive ggH: M_H vs. $\frac{1}{2}M_H$? Just let the model figure it out. 1 $\frac{1}{2} M_{\text{H}}$
	- ‣ differential distributions can probe different kinematic regimes **→ dynamical scale choice <→ many choices!** 1

▸ re-cycling via quadrature limited $→$ ideally interpolation grids

$$
\rightarrow
$$
 e.g. in jet production: p_T^j , $p_T^{j_1}$, $\langle p_T^j \rangle_{avg}$, $H_T \equiv \sum_{i \in jets} p_T^i$, $\hat{H}_T \equiv \sum_{i \in parts} p_T^i$, ...

W-BOSON + JET PRODUCTION

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 \bullet $n < 2$:

- ‣ almost identical bands
- ‣ very robust ΔMHO
- ๏ sm vs. sa
	- almost identical CI

- \cdot CI₆₈ bigger than 9pt *n* < 2:
 a CI₆₈ bigger than
 a *abc* captures po
 n = 2:
 almost identical
 A A_{MHO} very robus
 sm vs. sa
 almost identical
- ‣ captures pos. shift *abc*

$$
n=2:
$$

D I-PHOTON PRODUCTION

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- ๏ example where 9pt fails
	- large corrections

- ‣ marginal overlap for geo
- ‣ differences in *size* & *position*
- \rightarrow ideally N3LO for robust Δ_{MHO}

 \bullet sm \simeq sa

large corrections $\Delta_{\rm MHO}^{\rm NNLO} \gtrsim \Delta_{\rm MHO}^{\rm NLO}$
no sign of converger
2:
CI₆₈ ~ 2-3 × 9pt
2:
marginal overlap fo:
differences in *size &*
ideally N3LO for rol
 \simeq sa
large corrections
prohibit FAC points

$$
n < 2
$$

$$
\cdot \quad \text{CI}_{68} \sim 2-3 \times 9 \text{pt}
$$

 \bullet $n = 2$:

$$
\Delta_{\rm MHO}^{\rm NNLO} \gtrsim \Delta_{\rm MHO}^{\rm NLO}
$$

no sign of convergence

THE PROBLEM WITH JETS…

non-trivial change of dynamical scales cannot be captured by a simple re-scaling

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

WORK IN PROGRESS — CORRELATIONS

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

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

[AH, Mazeliauskas w.i.p]

⇔ hidden parameter $-1 < c < +1$ to smoothly implement the correlation

WORK IN PROGRESS — CORRELATION MODEL IN miho

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

26

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

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

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

\n
$$
\times \bigg|_{\alpha = \beta}
$$

\n
$$
\times \bigg|_{\alpha = \beta}
$$

use inference to constrain *c*

[AH, Mazeliauskas w.i.p]

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

CONCLUSIONS & OUTLOOK

- Bayesian inference is a powerful framework to estimate $\Delta_{\rm MHO}$ **•** probabilistic interpretation \leftrightarrow $P(\delta_{n+1} | \delta_n)$
- - ▶ exposes our *assumptions & biases* clearly < **w>** model & priors
	- ◆ *but:* it is not more reliable than scale variation \rightarrow careful analysis required
- **Ⅰ** typically for $n < 2$: $CI_{68} > 9pt$; $n \ge 2$: $CI_{68} \approx 9pt$
- o public code: ミホ (miho) → https://github.com/aykhuss/miho
- ๏ future directions
	- *P* correlations $(p_T^W/p_T^Z, p_T^Z \text{ vs. } p_T^{\ell}, \text{ PDF fits & data interpretation, ...}$
	- ‣ marginalisation over models, …

relying on a single prescription for TH unc. in *precision measurements* that does not admit a probabilistic interpretation is potentially dangerous!

[AH, Mazeliauskas w.i.p]

CONCLUSIONS & OUTLOOK

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	-

๏ Confidence Intervals 3 containing x % of the probability $CI_{\mathcal{X}}$ *S*est

29 n

$\textsf{TOY EXAMPLE} \; - \; \delta_k = (0.7)^k$

$$
P_0(a) = \frac{1}{2} (1 + \omega) (1 - |a|)^{\omega} \Theta(1 - |a|)
$$

 S_{n+1}^{est}

 S_{n+1}^{est}

- ๏ dependence on priors decreases as *n* increases
- o less for $ξ$ as it controls the asymmetry of the distribution
- ๏ for geometric series:

$$
\begin{array}{c}\n\eta \to 0 \\
\xi \to \infty\n\end{array}\n\right\} \rightsquigarrow \quad S_{n+1}^{\text{est}} \to S_{n+1}
$$

• estimate for
$$
\Gamma_{\text{cusp}}^{\text{QCD}} - (\Gamma_{\text{cusp}}^{\text{QCD}})_4
$$
 $n = \frac{1}{2}$
\n
$$
\text{CI}_{68} = C_F \left(\frac{\alpha_s}{\pi}\right)^5 [2.1, 9.5]
$$

$$
\mathbf{CI}_{95} = C_F \left(\frac{a_s}{\pi}\right)^5 [-0.38, 21]
$$

SENSITIVITY ON THE RANGE *F*

Scale Marginalisation (sm): Scale Average (sa):

- \bullet the integration over μ is in general very costly (numerical) → approximate it using *quadrature rule* (works well for CI_{68/95}) \rightarrow recycle existing calculations done for $\{\mu_0/2, 2\mu_0\}$
- Gauss-Legendre $(w_0 = \frac{6}{18}; w_{\pm 1} = \frac{3}{18}) \rightsquigarrow$ corresponds to 8 $\frac{6}{18}$; $W_{\pm 1} =$ 5 18

 \rightarrow corresponds to $F \simeq 2.45$