

# **BAYESIAN ESTIMATES FOR TH UNCERTAINTIES**

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## What is the Uncertainty $\Delta_{TH}$ of my Result?

- increasingly urgent to address with  $\Delta_{\text{EXP}} \searrow ( \leftrightarrow \text{HL-LHC} )$ 
  - what does  $5\sigma$  mean if  $\Delta_{TH}$  non-negligible?
  - interpretation of data in need for robust  $\Delta_{TH}$ : PDF fits,  $\chi^2$  in ATLAS jets, ...
- various sources that contribute to  $\Delta_{TH}$ :
  - $\Delta_{\alpha_{s'}} \Delta_{\text{param}}$ : parametric uncertainties  $\leftrightarrow \Rightarrow$  exp. extraction
  - $\Delta_{\text{PDF}}$ : parton distribution functions (PDFs)  $\leftrightarrow \rightarrow$  fits
  - ▶  $\Delta_{\text{non pert.}}$ : hadronisation, UE, ...  $\leftrightarrow$  parton showers [e.g. HERWIG vs. PYTHIA]
  - $\Delta_{\text{MHO}}$ : missing higher-order (MHO) corrections

Focus here



#### Conventional Approach for $\Delta_{\rm MHO}$ – Scale Variation

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

- N<sup>n</sup>LO:  $\Sigma \simeq \Sigma_n(\mu) = \sum_{k=1}^{n} \Sigma^{(k)}(\mu)$ k=0
- truncation of series induces a sensitivity to terms of the next order

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



electroweak (EW):  $\hookrightarrow$  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.  $q\bar{q}$  vs. qg in DY)



#### choice of the central scale

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

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

**crucially:** *no probabilistic interpretation!*  $\rightarrow$  can we do better?







PROBABILITY DISTRIBUTIONS FOR 
$$\Delta_{\text{MHO}}$$
  
• Sequence of perturbative corrections  $\delta_{k}$   
 $\Sigma_{n} = \Sigma^{(0)} (1 + \delta_{1} + ... + \delta_{n}) \quad \Rightarrow \delta_{n}$   
• Probability distribution for  $\delta_{n+1}$ , give  
 $P(\delta_{n+1} | \delta_{n}) = \frac{P(\delta_{n+1})}{P(\delta_{n})} = \frac{\int d^{m}p \ P(\delta_{n+1})}{\int d^{m}p \ P(\delta_{n})}$ 

P(A, B) = P(A | B) P(B) $P(A) = \left| \mathrm{d}B \ P(A, B) \right|$ 

Model:  $P(\boldsymbol{\delta}_n | \boldsymbol{p})$  $\bigcirc$ Priors:  $P_0(\mathbf{p})$ 

[Cacciari, Houdeau '11]

 $_{k}$  normalised w.r.t. LO (dimensionless)

 $\delta_k = \mathcal{O}(\alpha_s^k)$ en  $\boldsymbol{\delta}_n = (\delta_0, \delta_1, \dots, \delta_n)$  $(p) P_0(p)$  $(p) P_0(p)$ 



# THE CH MODEL

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

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

- one hidden parameter:  $\bar{c}$
- constrain upper bound  $\bar{c}$  from known orders  $\rightarrow$  constraint on unknown coefficients  $C_{n+1}$
- limitations:

 $\alpha_s$  at what scale? why not:  $\frac{\alpha_s}{\pi}$ ,  $\frac{\alpha_s}{2\pi}$ ,  $\alpha_s \ln^2(v)$ ,  $\alpha_s \ln(v)$ , ...? why not let the model figure out the expansion parameter itself?

| [Cacciari, | Houdeau '                     |
|------------|-------------------------------|
| <br>       | • • • • • • • • • • • • • • • |

#### $\forall k$

 $c_k \sim \eta^k$  $\hookrightarrow$  survey of observables [Bagnaschi, Cacciari, Guffanti, Jenniches '14]  $\hookrightarrow$  fitting [Forte, Isgro, Vita '13]

#### 11]

# THE GEOMETRIC MODEL bounded by a geometric series with expansion parameter *a*: $|\delta_k| \leq c a^k \quad \forall k \quad \iff \text{two model parameters: } a, c$ **model:** $P_{\text{geo}}^{(k)}(\delta_k | a, c) = \frac{1}{2c a^k} \Theta\left(c - \frac{|\delta_k|}{a^k}\right)$ **priors:** $P_0(a, c) = P_0(a) P_0(c)$ $P_0(a) = (1 + \omega) (1 - a)^{\omega} \Theta(a) \Theta(1 - a)$ $P_0(c) = \frac{\varepsilon}{c^{1+\varepsilon}} \Theta(c-1)$

[Bonvini '20]



 $\leftrightarrow dc/c \sim d\ln(c)$  ( $\varepsilon$ : regulator)



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

• LO  $> \delta_0 \equiv 1$ 

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

chose  $\omega = 0$  for flat prior in a

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



$$P(\delta_{1}) = \int da \int dc \ P_{geo}^{(1)}(\delta_{1} | a, c) \ P_{0}(a, c)$$





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

 $> \delta_0 \equiv 1$  $P_0(a,c) = \Theta(a) \ \Theta(1-a) \ P_0(c)$ **NLO** >  $\delta_1 = 0.7$  $P(a, c | \delta_1) \propto P_{geo}^{(1)}(\delta_1 | a, c) P_0(a, c)$ • N<sup>2</sup>LO >  $\delta_2 = 0.7^2$  $P(a, c \mid \delta_1, \delta_2) \propto P(\delta_2 \mid \delta_1, a, c) P(a, c \mid \delta_1)$  $\propto P_{geo}^{(2)}(\delta_2 | a, c) P_{geo}^{(1)}(\delta_1 | a, c) P_0(a, c)$ 

Bayes' theorem & independence

*a* ~ 0.7 <u>also:</u> *c* ~ 1





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

 $> \delta_0 \equiv 1$ LO  $P_0(a,c) = \Theta(a) \ \Theta(1-a) \ P_0(c)$ • NLO >  $\delta_1 = 0.7$  $P(a, c | \delta_1) \propto P_{geo}^{(1)}(\delta_1 | a, c) P_0(a, c)$ • N<sup>2</sup>LO >  $\delta_2 = 0.7^2$  $P(a, c \mid \delta_1, \delta_2) \propto P(\delta_2 \mid \delta_1, a, c) P(a, c \mid \delta_1)$  $\propto P_{\text{geo}}^{(2)}(\delta_2 | a, c) P_{\text{geo}}^{(1)}(\delta_1 | a, c) P_0(a, c)$ 

can be solved analytically



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





### THE *abc* MODEL – ASYMMETRIC GEOMETRIC MODEL

- allow for different lower & upper bound:  $b - c \leq \frac{\delta_k}{a^k} \leq b + c \quad \forall k \quad \iff \text{ three model parameters: } a, b, c$

• model: 
$$P_{abc}^{(k)}(\delta_k | a, b, c) = \frac{1}{2c |a|^k} \Theta\left(c - \left|\frac{o_k}{a^k} - b\right|\right)$$
  
 $(b - c)a^k$   $(b + c)a^k$ 

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



 $\Theta(1 - |a|) \iff \text{support: } [-1, +1] \text{ (alternating })$ 

 $\Theta(\xi c - b)$ 







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

#### • geo

- always entered around NNLO
- very narrow peak
- abc
  - ▶  $\mu/\mu_0 \gtrsim 1 \implies$  anticipate pos. N3LO
  - $\mu/\mu_0 \lesssim 1 \Rightarrow$  bias slowly disappears





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

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



Fastest Apparent Convergence  $\Sigma_n(\mu_{\text{FAC}}) = \Sigma_{n-1}(\mu_{\text{FAC}})$ 

depends on order might not be unique



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

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





Principle of Minimal Sensitivity  $\frac{\partial}{\partial \mu} \Sigma_n(\mu) \big|_{\mu_{\rm PMS}} = 0$ 

depends on order might not be unique



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

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

pursued in the following





### PRESCRIPTIONS FOR SCALES

#### Scale Marginalisation (sm):

[Bonvini '20]

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

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

•  $P(\mu | \boldsymbol{\delta}_n) \propto P(\boldsymbol{\delta}_n; \mu) P_0(\mu)$  with prior:  $P_0(\mu) = \frac{1}{2\mu \ln F} \Theta\left(\ln F - \left|\ln\left(\frac{\mu}{\mu_0}\right)\right|\right)$ 

 $\mu = \mu_0 / F \quad \mu_0 \quad F \, \mu_0$ 

#### Scale Average (sa):

[Duhr, AH, Mazeliauskas, Szafron '21]

μ has no probabilistic interpretation
 → average over it:

$$P_{\text{sa}}(\delta_{n+1} | \boldsymbol{\delta}_n) = \int d\mu \ w(\mu) \ P(\delta_{n+1} | \boldsymbol{\delta}_n; \mu)$$

• weight function:  

$$w(\mu) = \frac{1}{2\mu \ln F} \Theta\left(\ln F - \left|\ln\left(\frac{\mu}{\mu_0}\right)\right|\right)$$

$$\ln \mu$$

$$F \mu_0$$



### **PEAK OF THE DISTRIBUTIONS\***

#### Scale Marginalisation (sm):

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

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

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

#### Scale Average (sa):

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





# INCLUSIVE CROSS SECTIONS UP TO N<sup>3</sup>LO



• n < 2: CI<sub>68</sub> bigger than 9pt •  $\delta_1 < 0 \Rightarrow abc$  alternating n > 2: all prescriptions similar



- $\delta_3$  is large and outside of 9pt!
  - similar unc.: sa  $\simeq$  9pt
- n = 2: sm  $\ll$  others ( $\mu_{\text{FAC}}$ )
  - n = 3: all prescriptions similar

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

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



### **DIFFERENTIAL DISTRIBUTIONS**

- Bayesian approach also applicable to distributions → treat each bin individually ↔ will not include correlations!
- new challenges
  - → inclusive ggH:  $M_{\rm H}$  vs.  $\frac{1}{2}M_{\rm H}$ ? Just let the model figure it out.
  - differential distributions can probe different kinematic regimes → dynamical scale choice ↔ *many choices!*  $\rightarrow$  e.g. in jet production:  $p_{T}^{j}$ ,  $p_{T}^{j_{1}}$ ,  $\langle p_{T}^{j} \rangle$

re-cycling via quadrature limited  $\rightsquigarrow$  ideally interpolation grids

no longer "easy" to identify an appropriate hard scale  $\mu_0$  (up to rescaling)

 $II - \nabla - i \hat{II}$ 

$$\langle p_{\rm T}' \rangle_{\rm avg}$$
,  $H_{\rm T} \equiv \sum_{i \in jets} p_{\rm T}'$ ,  $H_{\rm T} \equiv \sum_{i \in partons} p_{\rm T}'$ , ...



### W-BOSON + JET PRODUCTION



● *n* < 2:

- CI<sub>68</sub> bigger than 9pt
- *abc* captures pos. shift

• 
$$n = 2$$
:

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



### **DI-PHOTON PRODUCTION**



- example where 9pt fails
  - large corrections
  - $\Delta_{\rm MHO}^{\rm NNLO}\gtrsim\Delta_{\rm MHO}^{\rm NLO}$
  - no sign of convergence

$$\sim$$
 CI<sub>68</sub> ~ 2-3 × 9pt

• *n* = 2:

- marginal overlap for geo
- differences in *size* & *position*
- ideally N3LO for robust  $\Delta_{MHO}$

• sm  $\simeq$  sa

large correctionsprohibit FAC points







#### THE PROBLEM WITH JETS...











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









### 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 IN miho

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

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

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

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

[AH, Mazeliauskas w.i.p]

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







use inference to constrain c



# CONCLUSIONS & OUTLOOK

- Bayesian inference is a powerful framework to estimate  $\Delta_{MHO}$ probabilistic interpretation  $\leftrightarrow P(\delta_{n+1} | \delta_n)$
- - exposes our *assumptions* & *biases* clearly  $\leftrightarrow \rightarrow$  model & priors
  - *but*: it is not more reliable than scale variation  $\rightarrow$  <u>careful analysis required</u>
- typically for n < 2:  $CI_{68} > 9pt$ ;  $n \ge 2$ :  $CI_{68} \simeq 9pt$
- public code: ミホ (miho) ---> https://github.com/aykhuss/miho
- future directions
  - 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 <u>single</u> prescription for TH unc. in precision measurements that does not admit a probabilistic interpretation is potentially dangerous!

[AH, Mazeliauskas w.i.p]





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[AH, Mazeliauskas w.i.p] Thank you!









### TOY EXAMPLE – $\delta_k = (0.7)^k$



• Confidence Intervals  $\operatorname{CI}_{x} = [\Sigma_{x}^{\operatorname{low}}, \Sigma_{x}^{\operatorname{upp}}]$ containing x % of the probability

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

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

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



 $S_{n+1}^{\text{est}}$ 

 $S_{n+1}^{\text{est}}$ 





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

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

n



#### Sensitivity on the Range F

#### Scale Marginalisation (sm):



#### Scale Average (sa):



- the integration over  $\mu$  is in general very costly (numerical)  $\rightarrow$  approximate it using quadrature rule (works well for CI<sub>68/95</sub>)  $\rightarrow$  recycle existing calculations done for  $\{\mu_0/2, 2\mu_0\}$
- Gauss-Legendre  $(w_0 = \frac{8}{18}; w_{\pm 1} = \frac{5}{18}) \rightarrow \text{corresponds to } F \simeq 2.45$  $d\mu w(\mu) f(\mu) \simeq w_{-1} f(\mu_0/2) + w_0 f(\mu_0) + w_{+1} f(2\mu_0)$

