# Uncertainty of the Uncertainty of $\alpha_s$

Kirtimaan Mohan @Alphas-2025, Savoie, France Dec 2025

**CTEQ-TEA**
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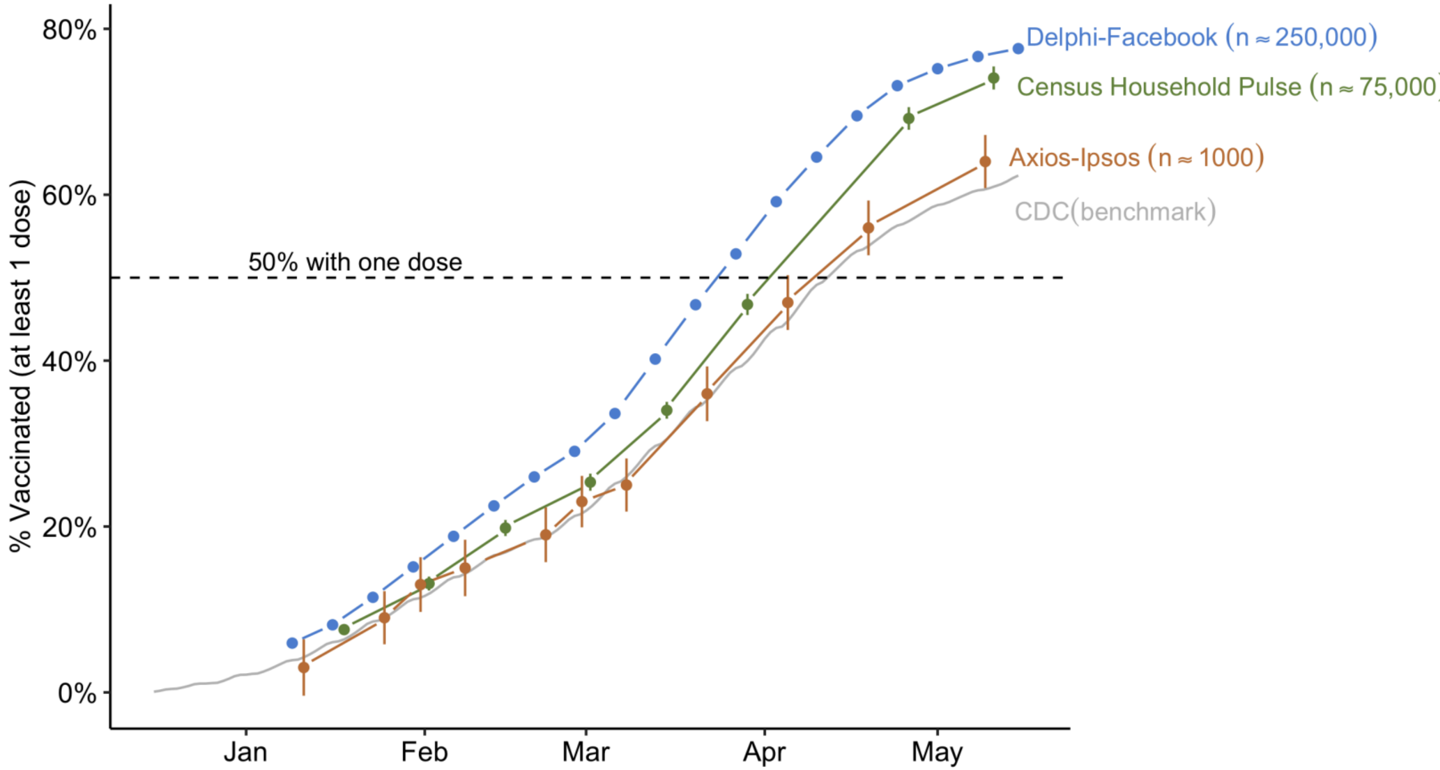
# Big Data Paradox: *The bigger the data, the surer we fool ourselves*, if we do pay attention to data quality




[Slide from Xiao Li Meng, PHYSTAT 2025]

# Uncertainty Quantification

- **Aleatoric** ("dicey") Uncertainty:
  - Statistical uncertainty in data that is reduced by improving data quantity and quality
- **Epistemic** ("knowledge") Uncertainty:
  - Due to lack of knowledge, which can introduce bias. Improved through better (or at least) representative modelling. Aka Systematic uncertainty.

Hullermeier & Waegeman (2021)

# This Talk

Present challenges of quantifying uncertainty preliminary results of the CTEQ-TEA's simultaneous determination of the strong coupling and PDFs using updated data sets.

# NNLO fits with new data (nD) from LHC at 8 and 13 TeV

$\chi^2/N_{pt}$ for CT18A + new data (*vs.* CT18A at right) NNLO fits; 68% CL

| ID | Experimental data set | $N_{pt}$ | CT25prel | CT18A |
|---|---|---|---|---|
| | **Drell-Yan pair production** | | | |
| 211 | ATLAS 8 TeV W | 22 | $2.37^{+1.30}_{-0.68}$ | $3.56^{+2.26}_{-1.65}$ |
| 212 | CMS 13 TeV Z | 12 | $2.10^{+2.20}_{-0.38}$ | $2.13^{+3.46}_{-0.30}$ |
| 214 | ATLAS 8 TeV Z 3D | 188 | $1.14^{+0.10}_{-0.04}$ | $1.21^{+0.32}_{-0.15}$ |
| 215 | ATLAS 5.02 TeV W,Z | 27 | $0.70^{+0.27}_{-0.06}$ | $0.74^{+0.31}_{-0.08}$ |
| 217 | LHCb 8 TeV W | 14 | $1.36^{+0.37}_{-0.34}$ | $1.47^{+0.43}_{-0.38}$ |
| 218 | LHCb 13 TeV Z | 16 | $1.06^{+0.76}_{-0.38}$ | $1.29^{+0.95}_{-0.44}$ |
| | **13 TeV $t\bar{t}$ production** | | | |
| 521 | ATLAS all-hadronic $y_{t\bar{t}}$ | 12 | $1.07^{+0.08}_{-0.05}$ | $1.07^{+0.12}_{-0.07}$ |
| 528 | CMS dilepton $y_{t\bar{t}}$ | 10 | $1.10^{+0.56}_{-0.40}$ | $1.13^{+0.85}_{-0.53}$ |
| 581 | CMS lepton+jet $m_{t\bar{t}}$ | 15 | $1.38^{+0.65}_{-0.40}$ | $1.44^{+0.89}_{-0.56}$ |
| 587 | ATLAS lepton+jet $m_{t\bar{t}} + y_{t\bar{t}} + y^B_{t\bar{t}} + H^{t\bar{t}}_T$ | 34 | $0.94^{+0.13}_{-0.11}$ | $0.94^{+0.28}_{-0.09}$ |
| | **Inclusive jet production** | | | |
| 553 | ATLAS 8 IncJet | 171 | $1.54^{+0.09}_{-0.06}$ | $1.57^{+0.12}_{-0.07}$ |
| 554 | ATLAS 13 IncJet | 177 | $1.25^{+0.07}_{-0.03}$ | $1.26^{+0.08}_{-0.04}$ |
| 555 | CMS 13 IncJet | 78 | $1.11^{+0.13}_{-0.09}$ | $1.10^{+0.21}_{-0.10}$ |

(fits with 1 new process, 'nProcces')

nDY

nTT

nIncJet

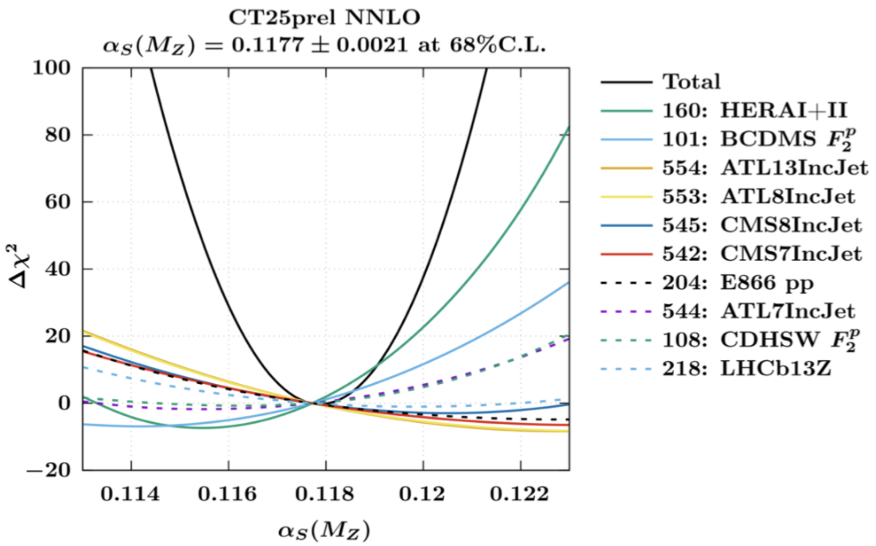
nD

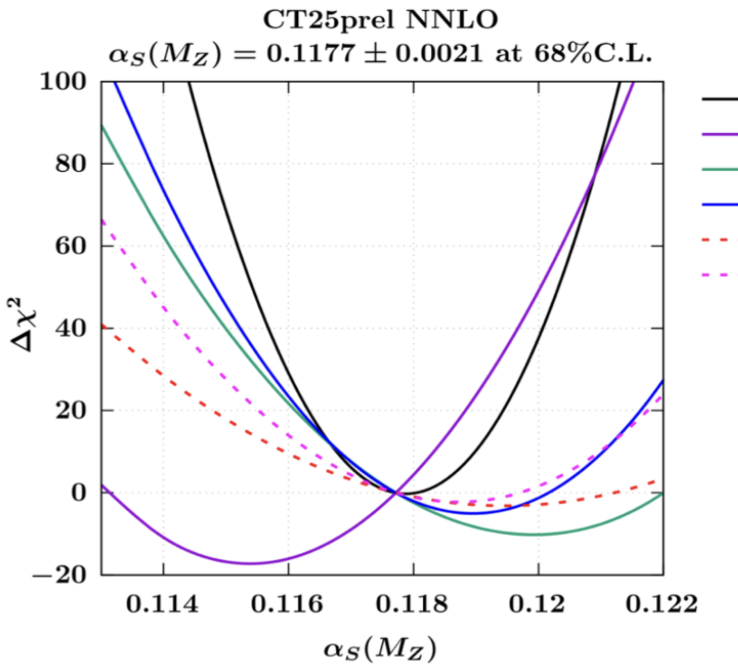
(combined fit)

# Impact of new data on fits

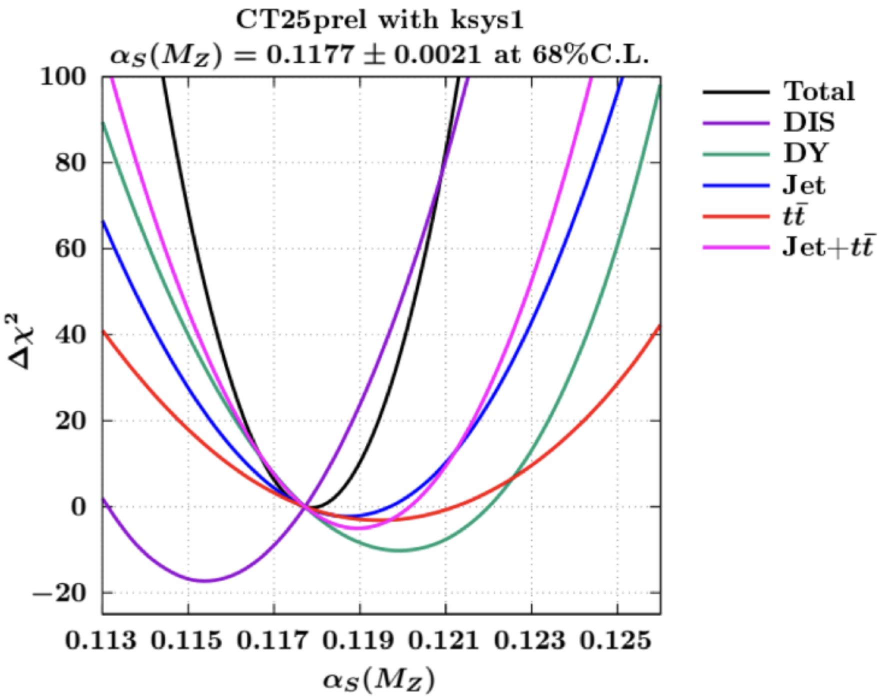
Updates from the upcoming CT25 NNLO fits

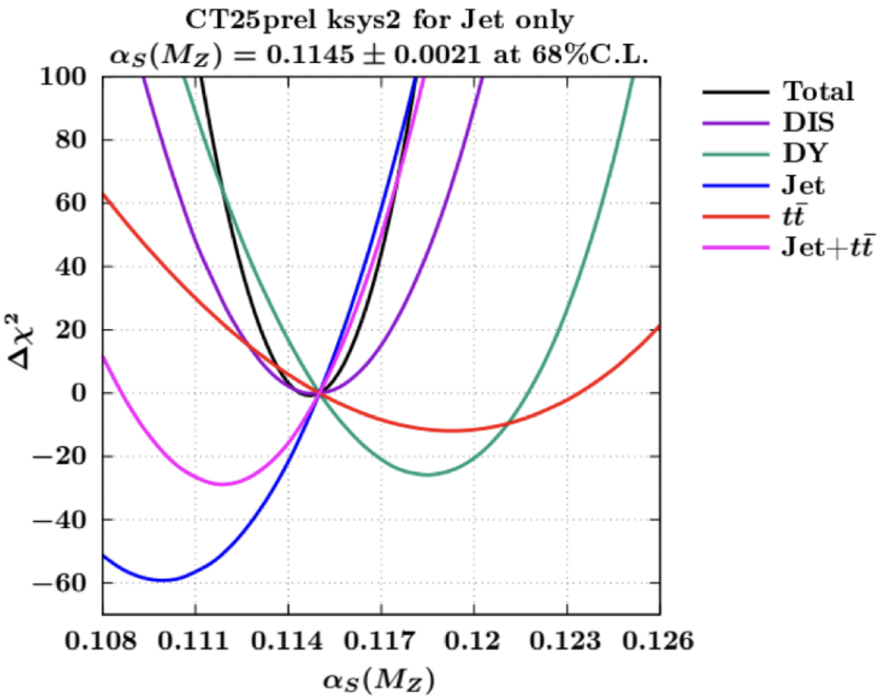
- Significant pulls on $\alpha_s$ from ATLAS Incl. Jets [553, 554] and 13 TeV LHCb Z data [218] and $t\bar{t}$ production data
- Large tension between DIS, DY and Jet+ $t\bar{t}$



# Sensitivity to treatment of systematics




Left: **multiplicative errors** for all data sets

$\alpha_s(M_Z) \approx 0.118$

… but possible theory bias in syst. effects

Right: **additive errors** for jet data sets

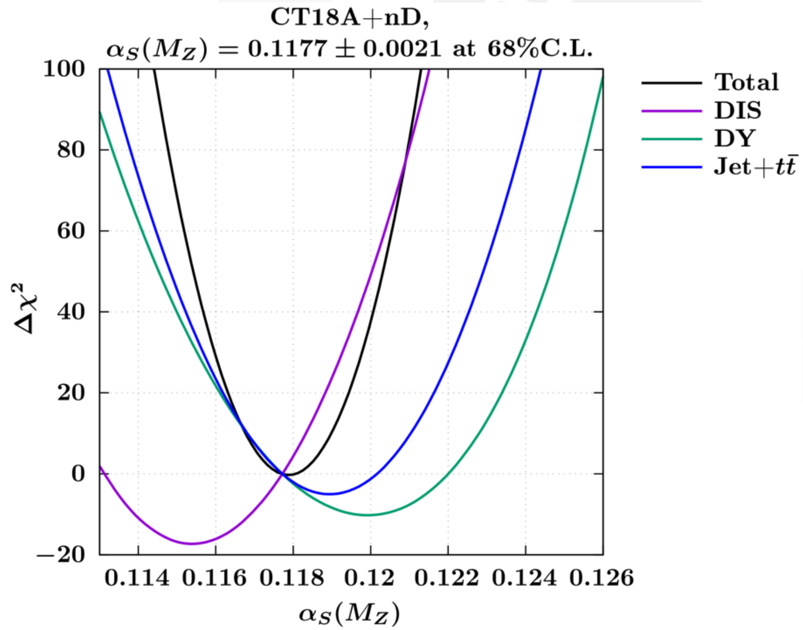
$\alpha_s(M_Z) \approx 0.115$

… likely reflects D'Agostini's bias – cf. also a similar shift in the 2025 NNPDF4.0 $\alpha_s$ study

The truth is within a range between the extremes

# Tolerance for Tolerating Tension

- It is easy to see that there is a large tension between DIS and other data sets.
- Treat each of the sets (DIS, DY, Jet $+t\bar{t}$) as independent and identically distributed measurements of $\alpha_s$
- $\chi^2_{tot} = \sum_i \chi^2_i$
- Mean and Error given by minimizing
- $\tilde{\chi}^2 = \sum_i \frac{(\alpha_{s_i} - \bar{\alpha}_s)}{\sigma_i^2}$
- $\bar{\alpha}_s = \sigma^2_{tot} \sum_i \frac{\alpha_{s_i}}{\sigma_i^2}$ , $\frac{1}{\sigma^2_{tot}} = \sum_i \frac{1}{\sigma_i^2}$
- Large Tension: $\frac{\tilde{\chi}^2}{dof} \simeq 17$
- Yet small uncertainty:
  - $\alpha_s = 0.1179 \pm 0.000329$
  - (Profile Likelihood)



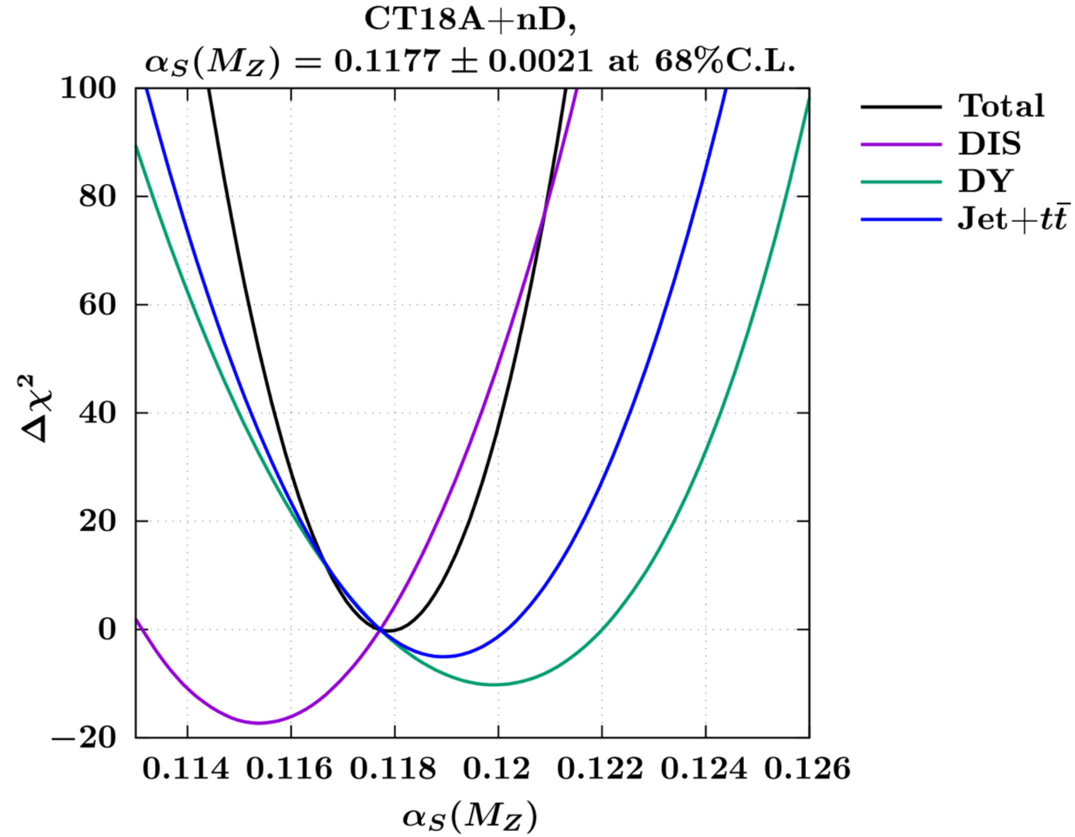

| | DIS | DY | Jet $+t\bar{t}$ | $\chi^2_{tot}$ |
|---|---|---|---|---|
| $\alpha_s \times 10^3$ $at\ \min of\ \chi^2_i$ | 115.88 | 119.91 | 118.94 | **117.88** |
| Error $(\sigma_i \times 10^3)$ $(\Delta\chi^2_i = 1)$ | 0.553 | 0.655 | 0.539 | **0.329** |

# How to proceed?

What should we do when we don’t know how to proceed?

Form committees!

# Committee #1: Global Tolerance




Use global Tolerance:

$$\Delta\chi^2 = T^2$$

$$\alpha_s(M_Z) = 0.1177 \pm 0.0021 \; at \; 68\% \; CL$$

How should we justify the choice of Tolerance here?

# Committee #2: Global Tolerance through Effective Gaussian variable

$$S_n = \sqrt{2\chi^2(N_n)} - \sqrt{N_n - 1}$$

Criteria determined by values of $S_n \approx 0.468$
for 68% CL for the total $\chi^2$
Note: Related to Quantile of $\chi^2$

$$\alpha_s(M_Z) = 0.1179 + 0.0024 - 0.0025$$

# Committee #3: Dynamical Tolerance

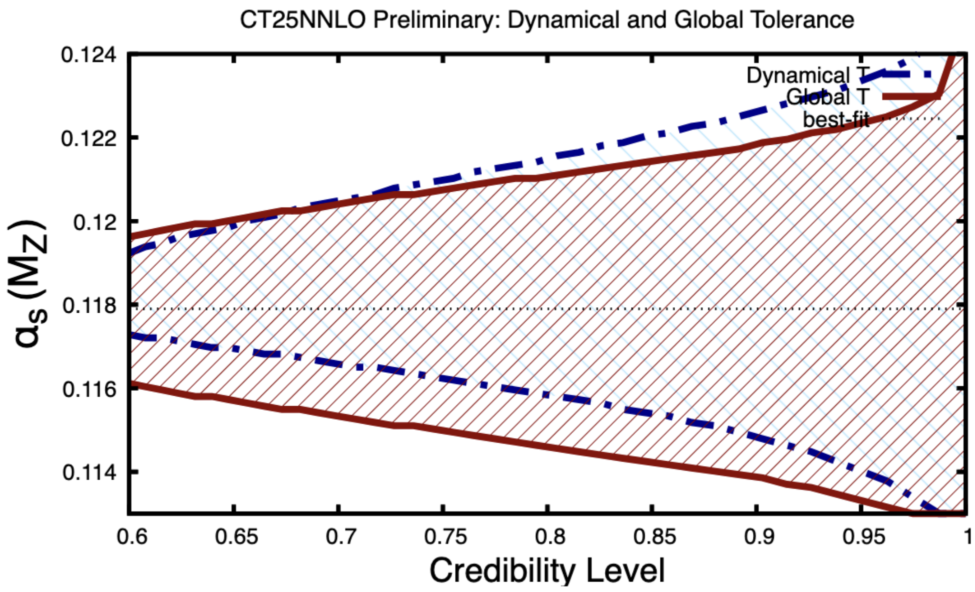
$$\chi_E^2(a,\lambda) = \sum_{k=1}^{N_{pt}} \frac{1}{s_k^2}\left(D_k - T_k(a) - \sum_{\alpha=1}^{N_\lambda} \beta_{k\alpha}\lambda_\alpha\right)^2 - \sum_{\alpha=1}^{N_\lambda} \lambda_\alpha^2\,,$$

Dynamic Tolerance determine by using Lewis formula for 52 individual experiments

$$\alpha_s(M_Z) = 0.1179 + 0.0024 - 0.0012$$

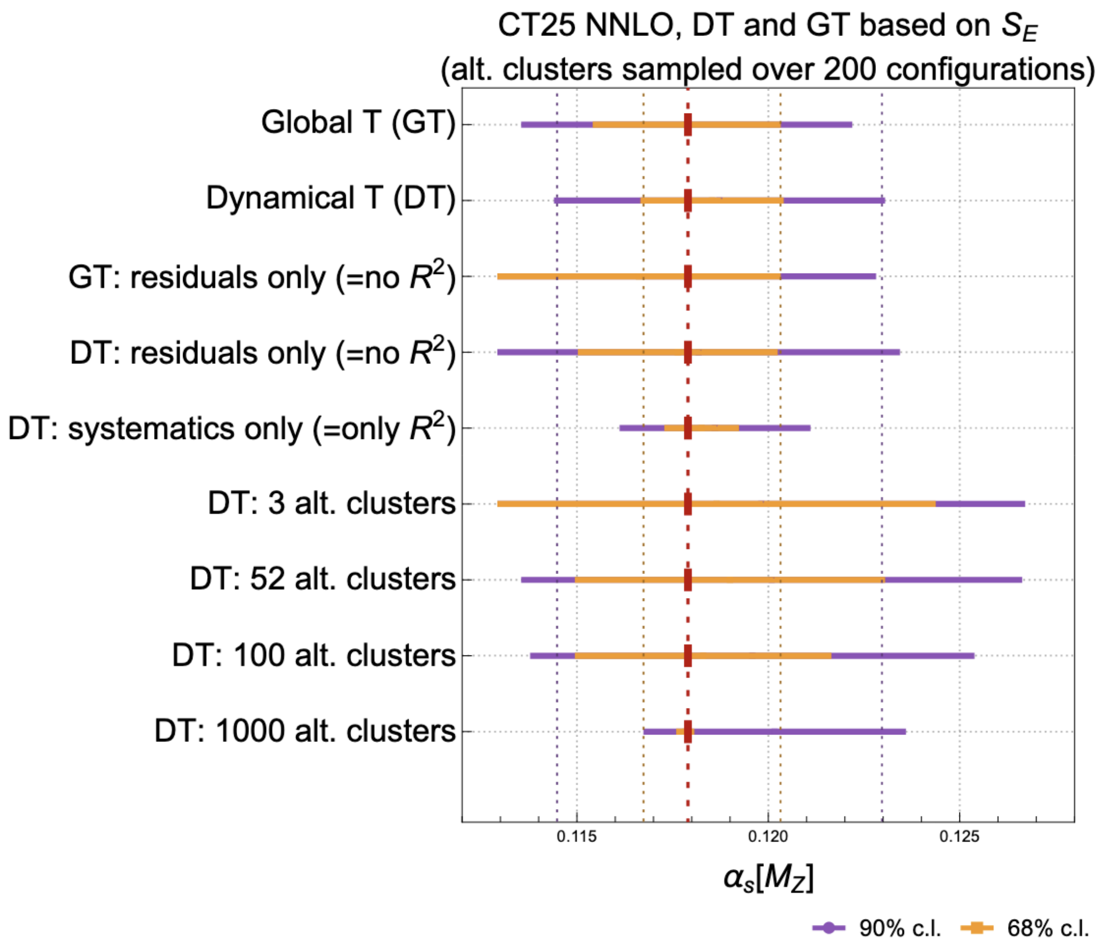
Comparison of Credibility level for Global Tolerance and Dynamic Tolerance

Dynamic Tolerance shows dependence one how data is partitioned



# Sensitivity to partitioning of data sets

In an ideal scenario, in which all residuals are normally distributed according to $N(0,1)$, alternative clusters would produce approximately the same estimate for the uncertainty.



# Committee #4: PDG Prescription: Scaling Errors

- **PDG proposal:** scale errors by a factor $e_s$ to make fits more consistent, i.e. each $\sigma_i \rightarrow e_s\, \sigma_i$
- $e_{s_{PDG}} = \sqrt{\frac{\tilde{\chi}^2}{dof}} \simeq 4.1$ so that each $\sigma_i \rightarrow 4.1 \times \sigma_i$ and $\frac{\tilde{\chi}^2}{dof} \rightarrow 1$
- **Caveat:** For very large $\sqrt{\frac{\tilde{\chi}^2}{dof}}$, PDG recommends making an educated guess of the uncertainty rather than scaling the errors.
- $\bar{\alpha}_s = 0.11795 \pm 0.00135$

# Sensitivity to partitioning of data sets

- $N = 3$
- $\alpha_s = 0.1179 \pm 0.000329.$
- $\frac{\tilde{\chi}^2}{dof} \simeq 17$
- $\bar{\alpha}_s = 0.11795 \pm 0.00135$

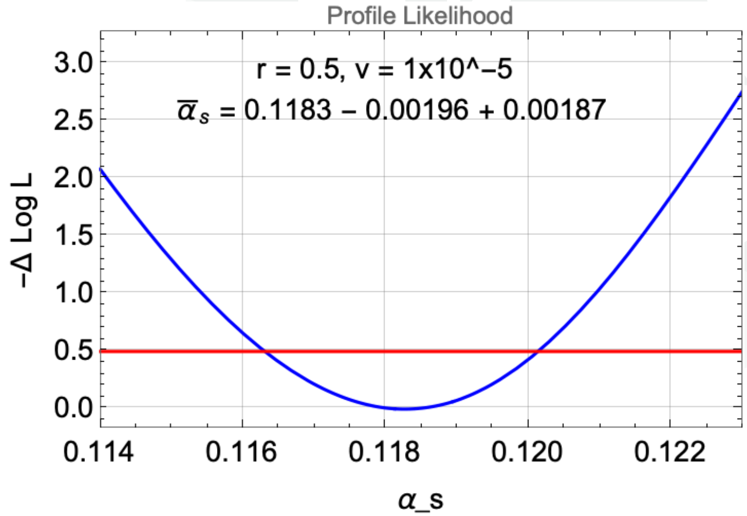
- $N = 52$
- $\alpha_s = 0.1181 \pm 0.000334.$
- $\frac{\tilde{\chi}^2}{dof} \simeq 3.1$
- $\bar{\alpha}_s = 0.1181 \pm 0.0006$

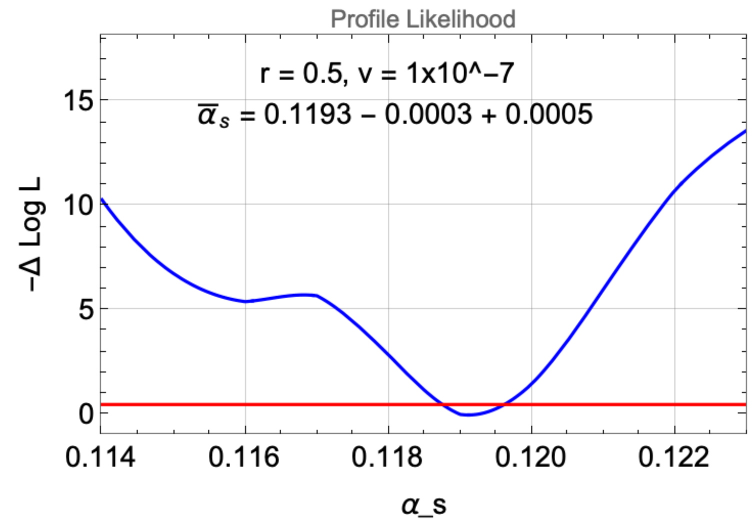
# Committee #5: The "Error on the error"

$$\ln L(\boldsymbol{\mu}, \boldsymbol{\theta}, \boldsymbol{\sigma}_{\mathbf{u}}^2) = \ln P(\mathbf{y}|\boldsymbol{\mu}, \boldsymbol{\theta})$$

$$-\frac{1}{2}\sum_{i=1}^{N}\left[\frac{(u_i-\theta_i)^2}{\sigma_{u_i}^2} + \left(1+\frac{1}{2r_i^2}\right)\ln\sigma_{u_i}^2 + \frac{v_i}{2r_i^2\sigma_{u_i}^2}\right]$$

$$P(\mathbf{y}|\boldsymbol{\mu}, \boldsymbol{\theta}) = \prod_{i=1}^{N}\frac{1}{\sqrt{2\pi}\sigma_{y_i}}e^{-(y_i-\varphi(x_i;\boldsymbol{\mu})-\theta_i)^2/2\sigma_{y_i}^2}$$




Needs as input an estimate of the uncertainty on the systematic uncertainty characterized by r.

Sensible values of r need to be chosen by analyst, making and educated guess.

G. Cowan arXiv:1809.05778, see also
M. Reader arxiv.org:2408.12922

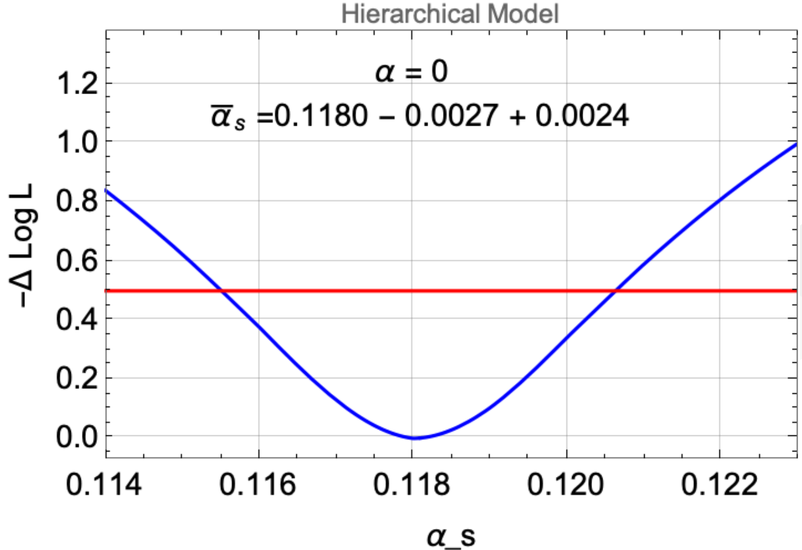
# Committee #6: Bayesian Hierarchical Model

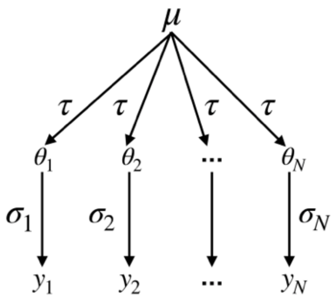
$$p(\mu|y_i) \propto \int_0^\infty \prod_{i=1}^{N} (\sigma_i^2+\tau^2)^{-\frac{1}{2}(1+\frac{\alpha}{N})} e^{-\frac{(\mu-y_i)^2}{2(\sigma_i^2+\tau^2)}} d\tau^2.$$

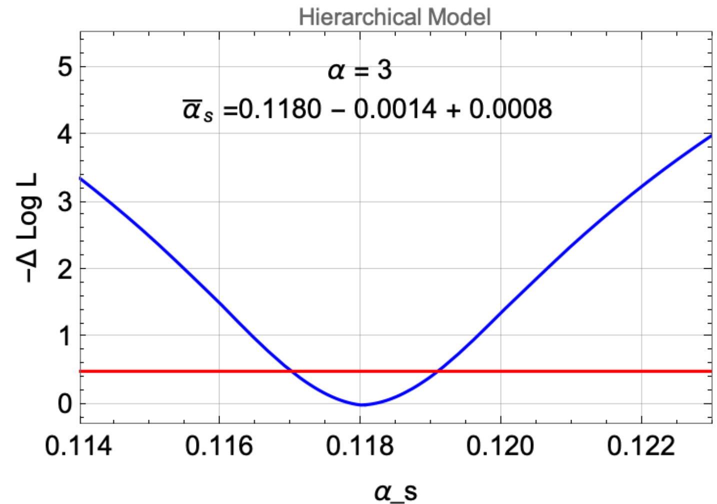
Depends on choice of $\alpha$:

$0 \leq \alpha \leq 3$ for large unknown systematics.

Use large values of $\alpha$ if quoted uncertainties are trusted.



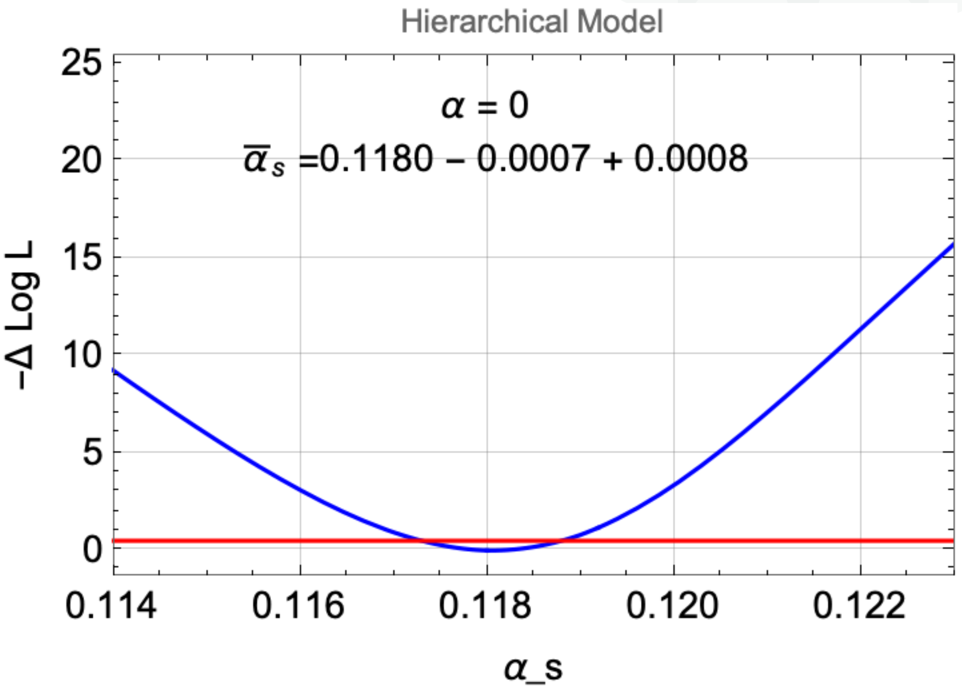

J. Erler & R. Ferro-Hernandez, arXiv:2004.01219

# Impact of Clustering

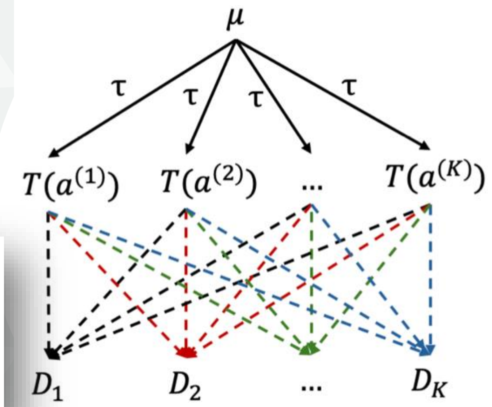
N=52 , $e_{S_{PDG}} \approx 1.8$

More consistent fit?

Tracks PDG error scaling factor



# Gaussian Mixture Model




1. Modified Posterior

$$\prod_{i=1}^{N_D}\left(\sum_{k=1}^{K} P(T(a^{(k)})|D_i)\right) \propto \prod_{i=1}^{N_D}\left(\sum_{k=1}^{K} w_k \mathcal{N}(D_i|T(a^{(k)}),\sigma_i)\right)$$

2. Implementation via MLE of Mixture of Gaussians

$$\pi(Y|\vec{\theta}) = \prod_{j=1}^{N_{\mathrm{pt}}} \pi(y_j,\Delta y_j|\vec{\theta}) = \prod_{j=1}^{N_{\mathrm{pt}}}\sum_{i=1}^{K} \omega_i \mathcal{N}(y_j,\Delta y_j|\theta_i),$$
$$0 \le \omega_k \le 1 \quad \text{and} \quad \sum_k \omega_k = 1,$$

3. Calculate Mean

$$\mathbb{E}[\theta] = \sum_{i=1}^{K} \omega_i \hat{\theta}_i.$$

4. Estimate uncertainty via observed Fisher Information Matrix

$$\begin{aligned}\mathrm{cov}_{\mathrm{GMM}} &= \sum_{i=1}^{K}\omega_i\, \mathrm{cov}_{\mathrm{GMM},i} + \sum_{i=1}^{K}\omega_i(\mathbb{E}[\theta]-\hat{\theta}_i)^2 \\ &= \sum_{i=1}^{K}\omega_i\left(\sum_{j=1}^{N_{\mathrm{pt}}}\frac{1}{\Delta y_j^2}\left(\frac{\partial y_j(\theta_i)}{\partial\theta_i}\right)^2\frac{\mathcal{N}(y_j,\Delta y_j|\theta_i)}{\pi(y_j,\Delta y_j|\vec{\theta})}\right)^{-1} + \sum_{i=1}^{K}\omega_i(\mathbb{E}[\theta]-\hat{\theta}_i)^2.\end{aligned}$$

5. Use Information Criteria (AIC/BIC) to determine the number of Gaussians

$$\begin{aligned}\mathrm{AIC} &= N_{\mathrm{parm}}\,\log N_{\mathrm{pt}} - 2\log L\big|_{\theta=\hat{\theta}}, \\ \mathrm{BIC} &= 2N_{\mathrm{parm}} - 2\log L\big|_{\theta=\hat{\theta}}.\end{aligned}$$

$$N_{\mathrm{parm}} = 2K + (K-1).$$

M.Yan, T.-J. Hou, Z. Li, KM, C.-P. Yuan, arxiv: 2406.01664

# Committee #7: $\alpha_s$ Uncertainty with GMM

GMM (K=2) (Yellow shaded)

$$\bar{\alpha}_s = 0.11801 \pm 0.00192$$

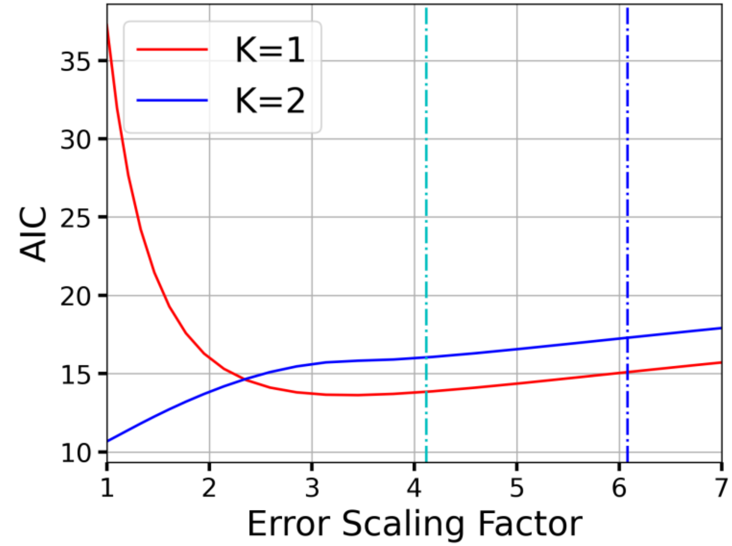
$e_{s_{PDG}} \sim 4.1$ *(Green shaded, Cyan line)*

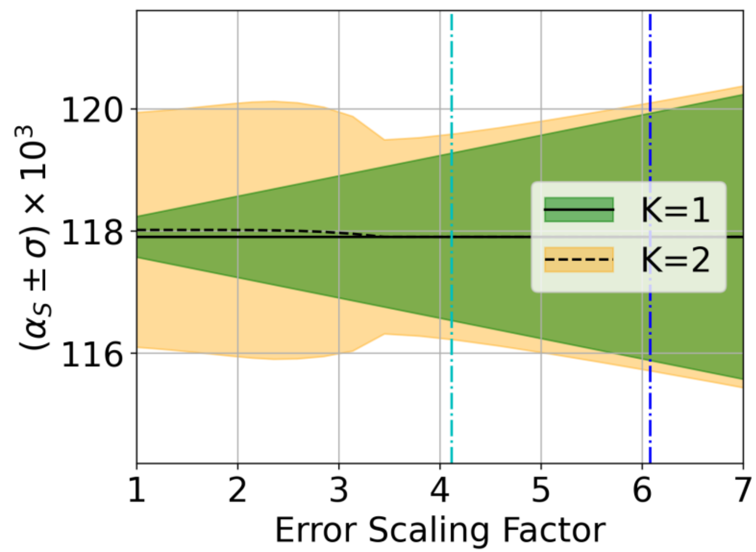
$$\bar{\alpha}_s = 0.11795 \pm 0.00135$$

$e_s \sim 6.1$ (Green shaded, Blue line)

$$\bar{\alpha}_s = 0.11795 \pm 0.0020$$

Caveat: How we partition the data sets does have an impact on uncertainty determination. More complete study is underway



# Impact of clustering

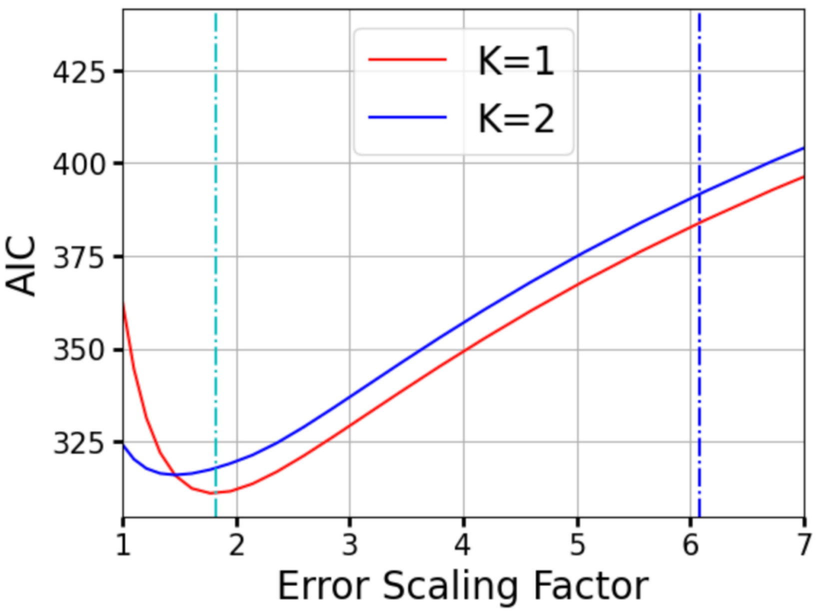
Using 52 data sets.
Caveat: This is a simplified application of the GMM on the profile likelihood of the strong coupling.
Full application needs fits over GMM likelihood

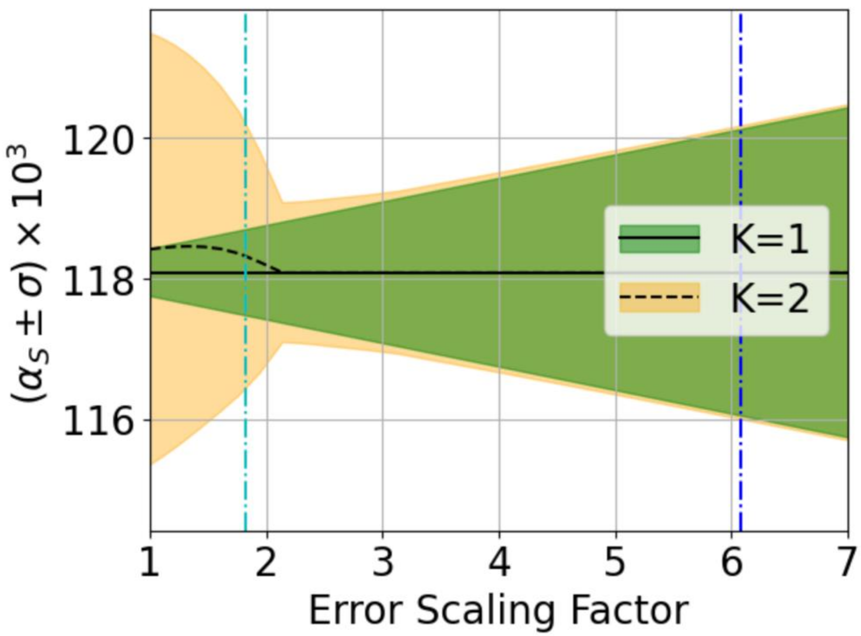
GMM (K=2, N=3)

$$\bar{\alpha}_s = 0.11801 \pm 0.00192$$

GMM (K=2,N=52) (Yellow shaded)

$$\bar{\alpha}_s = 0.1184 \pm 0.003$$

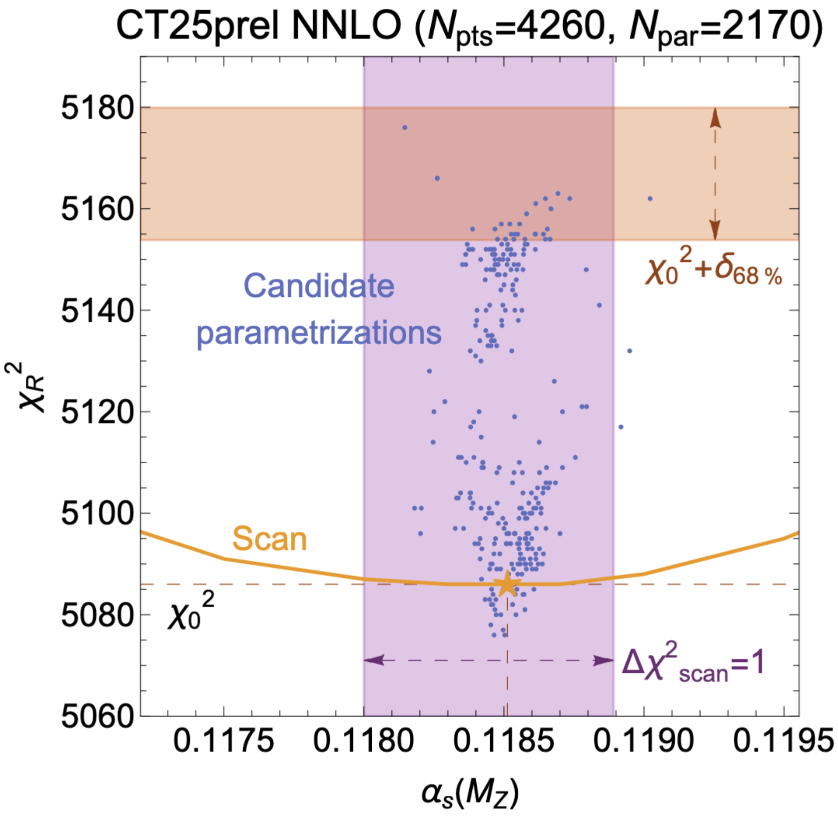


# Committee #8: PDF Parametrization Uncertainty for $\alpha_s$

$\alpha_s$ has low correlation with PDF parametrizations.

Epistemic uncertainty from PDF parametrization is small



# No unique solution to PDF’s inverse problem

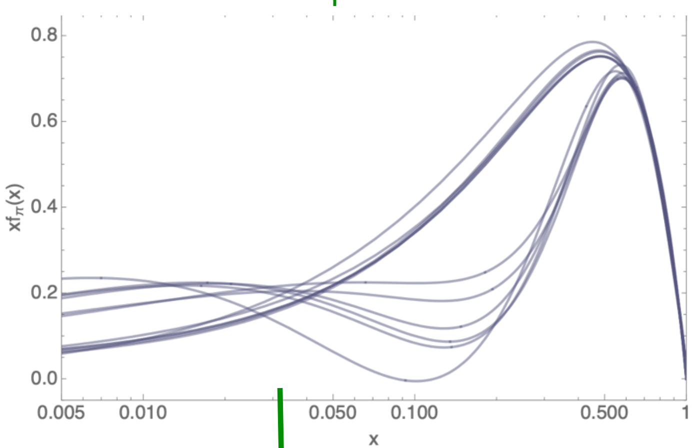
CT error bands quantify parametrization choice as a crucial source of epistemic uncertainty

— representative sampling over PDF models=study of parameter dependence

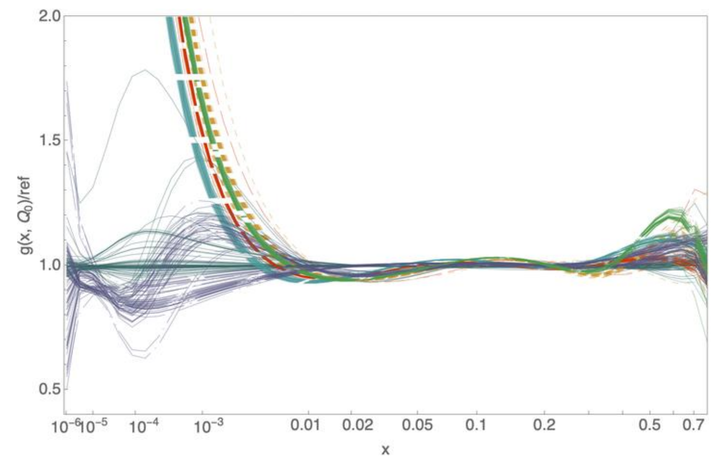
(Bernstein basis ad-hoc forms or adaptable Bernstein basis—Fantômas )

— fitting methodologies also contribute to epistemic uncertainties

Pion PDF with adaptable Bernstein basis —a sandbox




Proton PDF with Bernstein basis ad-hoc forms




*Fantômas*:

*flexible basis with hyperparameters on top of trainable parameters,* $c_i$

$$xf^{q}(x,Q_0^2) = A_q x^{\alpha_q}(1-x)^{\beta_q} \times \sum_i^N c_i \phi_i(g(x))$$

[Kotz et al, Phys.Rev.D109, 2507.22969]

To be applied to proton PDF soon!

# Combination of solutions for epistemic PDF uncertainty

CT error bands quantify parametrization choice as a crucial source of epistemic uncertainty

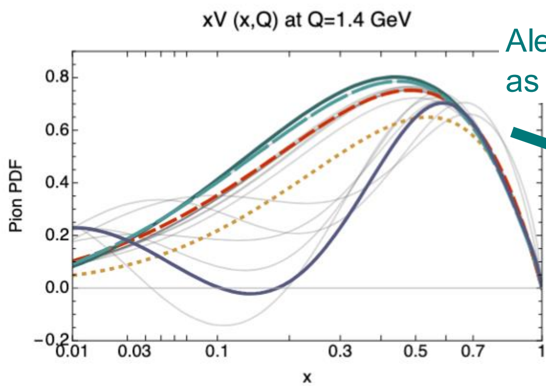
Statistical meaning of the sampling over parametrization:

*Unknown truth: all acceptable solutions stem from an unknown latent distribution of shapes*

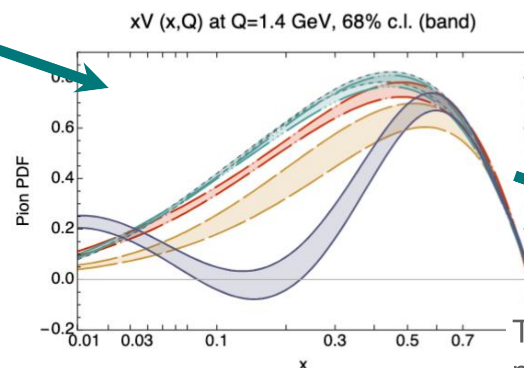
— no probability density interpretation in the space of data (aleatoric uncertainty accounted for the Hessian way)

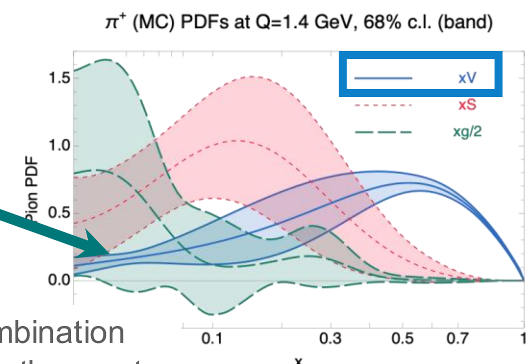
— sufficient to select a few solutions with most diverse shapes in $N_{\text{flavor}}$-dimensional space for $x \in [0,1]$

A convex log-likelihood justifies the combination à la METAPDF




Aleatoric uncertainties as single error band




[Gao & Nadolsky, JHEP07], updated for [Kotz et al, PRDXXX, 2505.13594]

The combination provides the most comprehensive UQ

Next:

— information criteria to systematize the selection of solutions

# Central Committee (Preliminary)

| Statistical Method | Eq. | $\alpha_s(M_Z)$ |
|---|---|---|
| Global Tolerance | 4.8 | $0.1179 + 0.0024 - 0.0025$ |
| Dynamical Tolerance | 4.10 | $0.1179 + 0.0024 - 0.0012$ |
| BHM | 4.13 | $0.118 + 0.0024 - 0.0027$ |
| GMM | 4.15 | $0.11801 \pm 0.00192$ |
| Average | | $0.11795 + 0.00225 - 0.00182$ |

# Outlook

- Presented (Preliminary) updated CTEQ-TEA fits to $\alpha_s$
- Significant upward pulls from Jet and ttbar data from LHC
- Statistical Modeling is challenging!
- Set up committees to determine the uncertainty on the strong coupling.
- Each committee has its own estimate on the uncertainty – represents uncertainty on the uncertainty
- Central committee to build consensus between committees.