Challenges and progress associated to PDF determinations

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A common trend in presentations

"The LHC has found no New Physics. Therefore further progress relies on precision studies."

Consequently we have to

- *Improve experimental data.*
- *Improve theory.*

- Any low hanging fruits?

Precision studies

Precision studies typically answer two kinds of question:

Parameter estimation What are the values and errors of the best fitting parameters given a model and a dataset?

Hypothesis testing Does a given dataset allow to reject a given model?

- Note that these two do not commute.
- Significative improvements can be made in the process of comparing data and theory, namely in the statistical treatment.
- Crucially related to PDF determinations.

Improvements in statistical treatment

- Maximize the sensitivity w.r.t. the things we want to understand.
- Minimize it w.r.t. the things we don't understand (*robustness*).
- Consider all relevant degrees of freedom.
- Understand the underlying optimization problem.
- Perform the optimization effectively.
- Consider all relevant sources of uncertainty.

This talk:

- Examples of how improvements in each of these can result in better precision studies.
- Related progress in PDF determination.

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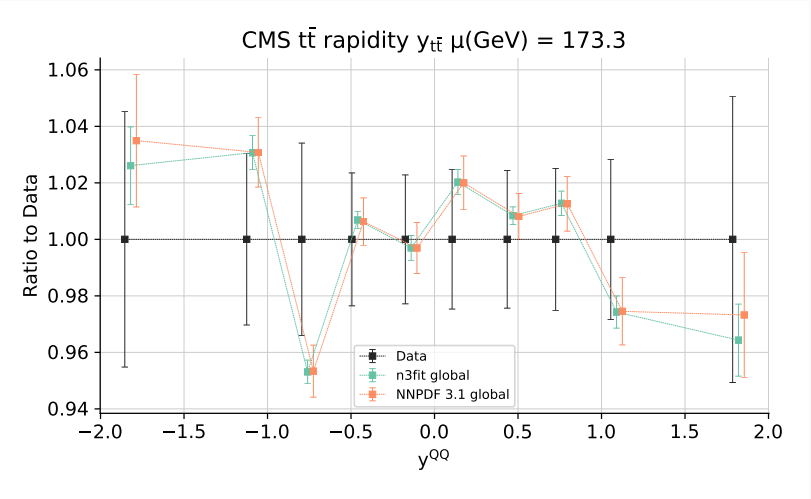
Overall effect is to improve consistency of parameter estimations and decrease sensitivity to new models. But can inform on the best way forward.

Unstable covariance matrices: Introduction

Can compare data and theory by looking at plots

But:

- Need a quantitative measure.
- Insensitive to correlations.



The χ^2 statistic is typically used

$$\chi^2 = \sum_i^N \sum_j^N (\text{data}_i - \text{prediction}_i)\Sigma_{ij}^{-1}(\text{data}_j - \text{prediction}_j) = \delta^T \Sigma^{-1} \delta$$

- Predictions supplied by the theoretical model.
- Central measurement of data and covariance matrix Σ supplied by experiments.
- Expected value (under suitable assumptions): $\langle \chi^2 \rangle = N$. Larger values indicate disagreement between data and theory.

Problems with covariance matrices

- Datasets with problematic correlation models have become common recently
  - ATLAS Jets at 7 TeV (arxiv: 1410.8857): Enormous sensitivity to correlations studied in detail in [Harland-Lang, Martin, Thorne arxiv:1711.05757].

	Full	21	62	21,62
$\chi^2/N_{\text{pts.}}$	2.85	1.58	2.36	1.27

Table 1: χ^2 per number of data points ($N_{\text{pts}} = 140$) for fit to ATLAS jets data [23], with the default systematic error treatment ('full') and with certain errors, defined in the text, decorrelated between jet rapidity bins.

  - CMS 8 TeV double-differential Drell-Yan data at 8 TeV (arXiv:1412.1115) had to be discarded from NNPDF 3.1 (arxiv:1706.00428).
  - Similar issues found in *"several"* newer datasets.
- We now study the issue within a toy model. Will showcase a request to experimentalists and a warning to theorists.

Systematics dominated covariance matrices

- Experiments have reached an impressive level of statistical precision.
  - Statistical component of the uncertainty (typically uncorrelated across bins) less important.
  - Systematic uncertainties (correlated across bins) tend to dominate.
- A somewhat realistic toy model for a covariance matrix from HepData:

$$\Sigma \propto \begin{bmatrix} \epsilon^2 + 1 & 1 & 1 & 1 \\ 1 & \epsilon^2 + 1 & 1 & 1 \\ 1 & 1 & \epsilon^2 + 1 & 1 \\ 1 & 1 & 1 & \epsilon^2 + 1 \end{bmatrix}$$

with $\epsilon^2 \ll 1$.

  - Assumes 4 data points, and uncorrelated error of size ϵ and one completely correlated systematic of size 1.

Allowed fluctuations

$$\Sigma \propto \begin{bmatrix} \epsilon^2+1 & 1 & 1 & 1 \\ 1 & \epsilon^2+1 & 1 & 1 \\ 1 & 1 & \epsilon^2+1 & 1 \\ 1 & 1 & 1 & \epsilon^2+1 \end{bmatrix}$$

The eigenvector decomposition is:

$$\left(\lambda_{1,2,3} = \epsilon^2,\ e_{1,2,3} = \begin{bmatrix} -1 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ -1 \end{bmatrix}, \begin{bmatrix} -1 \\ -1 \\ 1 \\ 1 \end{bmatrix} \right), \left(\lambda_4 = \epsilon^2 + 4,\ e_4 = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \right)$$

$$\chi^2 = \sum_\ell \langle \delta | e_\ell \rangle \frac{\lambda_\ell^{-1}}{\|e_\ell\|^2} \langle e_\ell | \delta \rangle$$

Fluctuations in $\delta = (\text{data} - \text{theory})$ larger than ϵ in the subspace spanned by $e_{1,2,3}$ lead to $\chi^2 \gg N$.

Problem: Uncertainties in the correlations

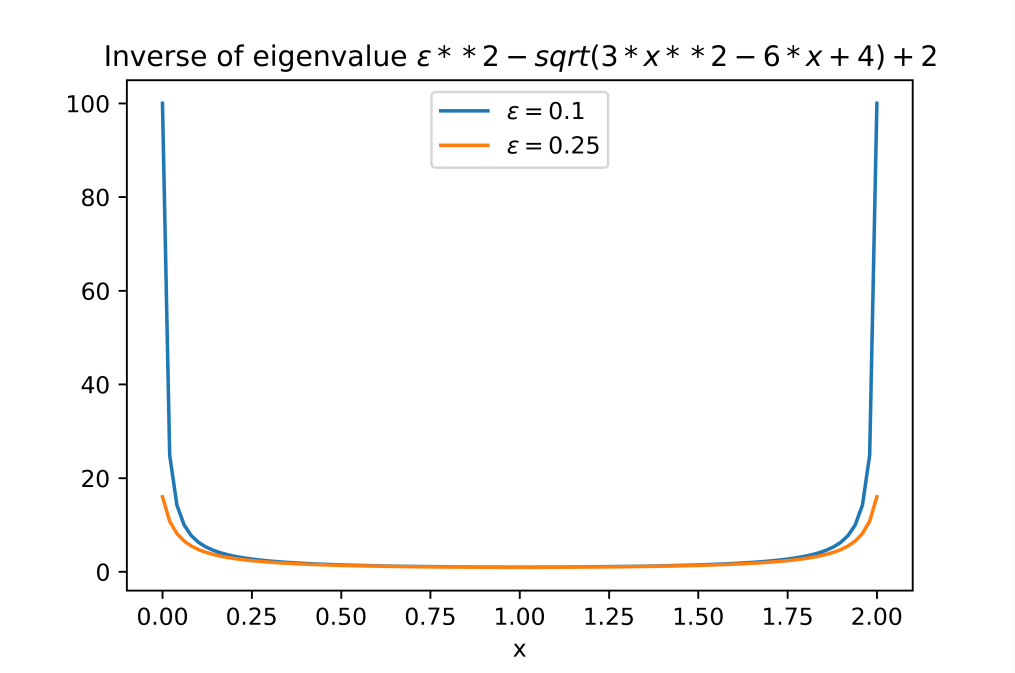
- Well known that exact experimental correlations are hard to determine precisely.
- Model the uncertainty in correlations with unknown parameter $x \in [0, 2]$ controlling the correlations of the last bin.

$$\begin{bmatrix} \epsilon^2 + 1 & 1 & 1 & 1 - x \\ 1 & \epsilon^2 + 1 & 1 & 1 - x \\ 1 & 1 & \epsilon^2 + 1 & 1 - x \\ 1 - x & 1 - x & 1 - x & \epsilon^2 + 1 \end{bmatrix}$$

  - We are keeping the total variance fixed. It is realistic to think that x could be anywhere in the range.
- Experimental results often presented by default with the highest correlation (i.e. $x = 0$).

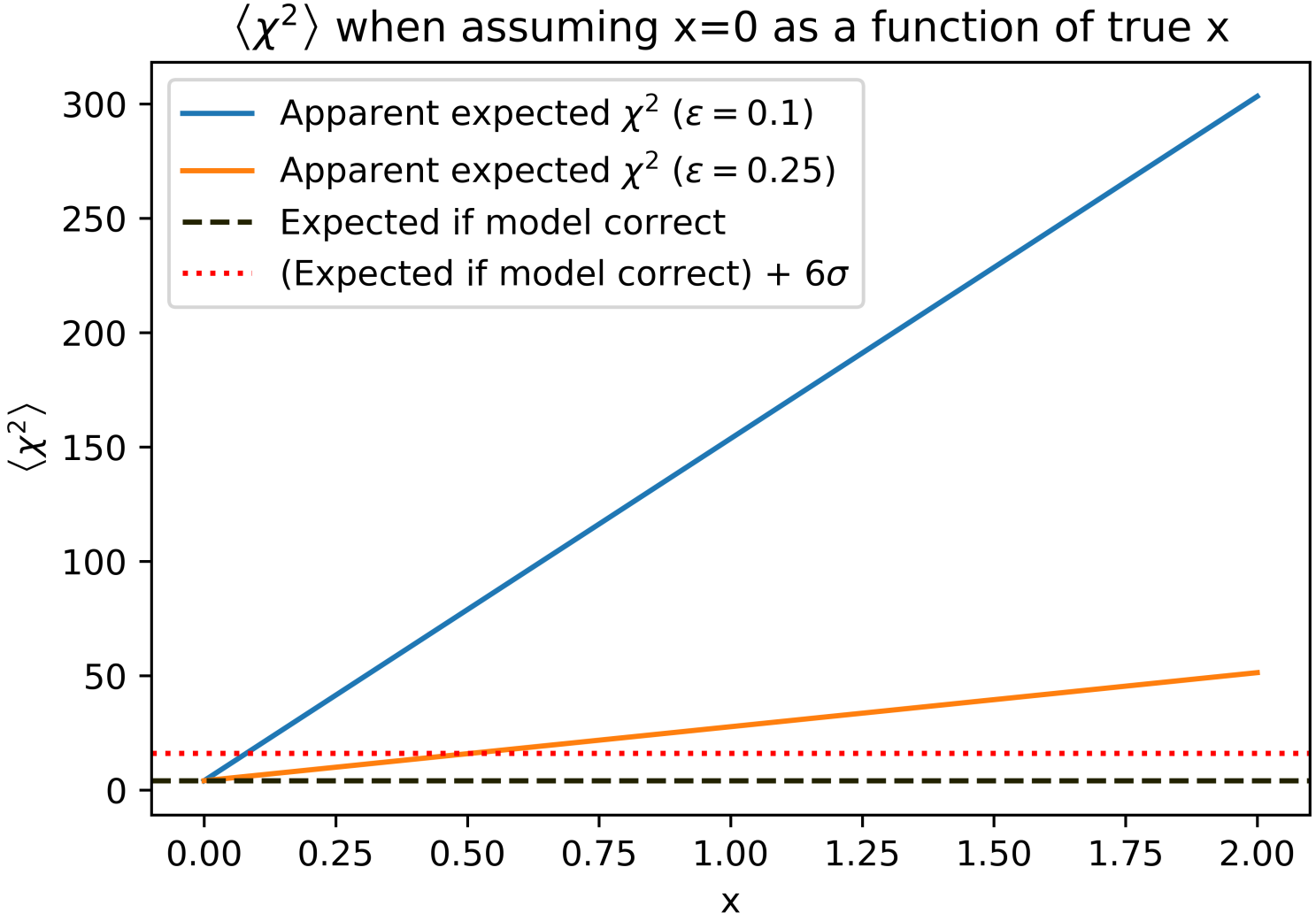
Modified eigenvalue

- Now one eigenvalue depends critically on x.



- The problematic situation is where:
  - Experimental analysis claims high correlations ($x = 0$).
  - Actual correlations are lower (e.g. $x = 0.3$).
- Instability translates directly to the χ^2.

χ^2 with incorrectly predicted correlations



Note: this is all assuming that there are no free parameters to fit.

Choices of correlation models

- A plethora of correlations models (up to 18) was proposed to address issues with ATLAS Jets at 7 TeV, (B. Malescu QCD@LHC'18).
- Also done in other datasets (e.g. ATLAS dijets offer three correlation models)
- This is a positive development but:
  - Pushes the work to test each correlation model downstream.
  - Causes fragmentation among different analyses.
  - Data should inform PDF (and other theory) models; not the other way around.

Other solutions and take away

- Experimental uncertainties should be **robust** w.r.t. unknown parameters, particularly correlations.
- Possible improvements:

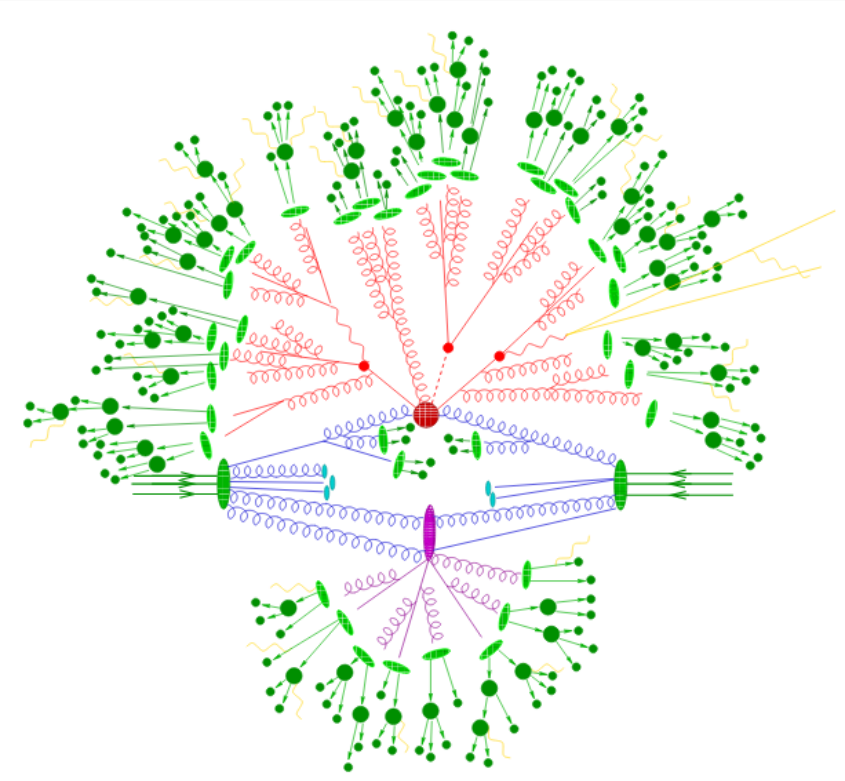
  Decorrelation Assume lower correlations unless proven otherwise. Note that even a small decorrelation (e.g. make $x = 0.3$) makes a big difference.

  Regularization Add a term to Σ that makes Σ^{-1} more stable. E.g. Tikhonov regularization: Add a diagonal term making $\Sigma \to \Sigma + \rho I$

    - Advatage: Best fit theory could be the same.

- Both experimentalist and theorists should be aware of these issues when comparing results.
- Improvements here crucial. Can't do precision physics with unstable precision tests.

On partial fits to partial data



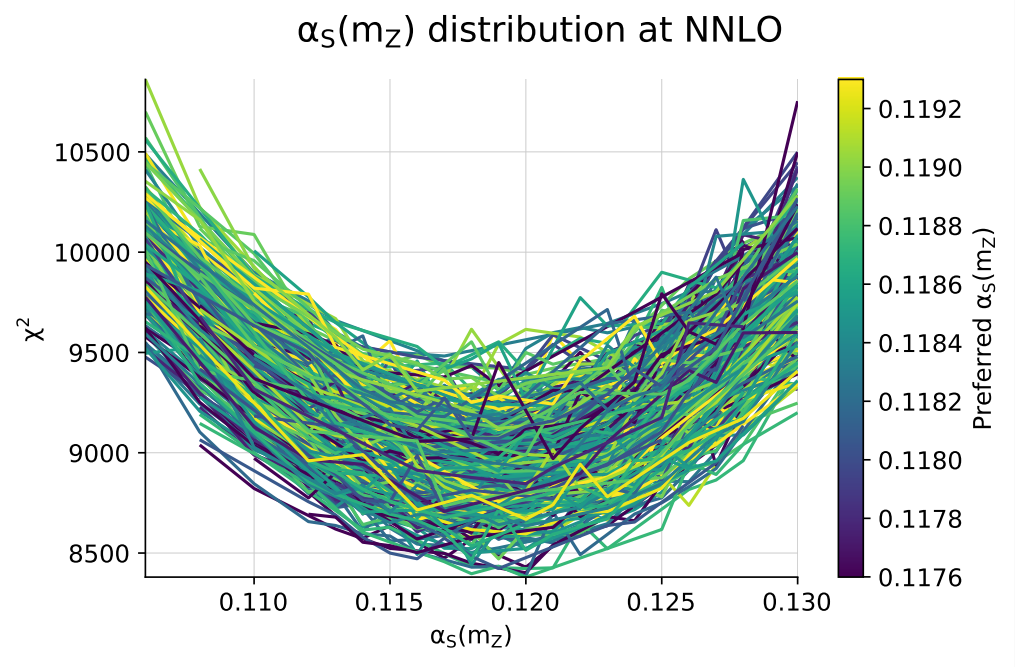
From SHERPA, arxiv:0811.4622

If a given parameter is to be fitted from hadronic data, its best fit value depends on its effect on the full *picture.*

Example: Interaction of α_s and PDF fits.

α_S from PDFs

- α_S Can be determined from global PDF fits. Most recently [NNPDF, arxiv:1802.03398].
- Methodology: Determine simultaneously (α_s, PDF), by minimizing the global χ^2 of the full (NN)PDF dataset (see Z.K., QCD@LHC'18).



- Best attainable total χ^2 changes **strongly** with α_s (leading to a very precise prediction, if theory uncertainties are ignored).

α_S from hadronic data

- Many determinations of α_S based on hadronic data exist. For example CMS $t\bar{t}$ determination at 7 TeV (arXiv:1307.1907), included as "independent" category in the PDF average.
- Methodology:
  - Compute the χ^2 of the particular dataset in a range of α_S and determine the minimum.
  - Use external PDFs scanned fitted at each scanned value of α_S. Value of PDF χ^2 ignored.
- Some also provide simultaneous PDF determinations although with limitations in dataset and parametrization (e.g. H1 jets, arXiv:1709.07251; see talk by K. Rabbertz).

Interplay between partial and global χ^2

(See Z.K., arxiv:1802.05236)

- Hadronic predictions (and thus the partial χ^2) depend on PDFs.
- The PDFs are themselves the result of a global χ^2 optimization.
- Suddenly there are *two* χ^2s in the problem as well as *two* datasets: Partial and global.
    - Certainly PDF and hadronic based determinations cannot be considered independent.
- The methodology, i.e.
    1. Restricting to the best fit PDF and
    2. then minimizing the partial χ^2 along α_S

  minimizes neither the partial or the total χ^2 nor a combination of them.

Erroneous minimization in a real example

- Can perform an "hadronic" determination with any subset of data used in the global NNPDF α_s fit.
- Choose Z p_T data and find that *"best fit"* is $\alpha_S = 0.124$.
- Could find a *"better best fit"* at $\alpha_S = 0.120$. Both Z p_T and the rest of the data agree better.

χ^2/d.o.f..	$\alpha_S = 0.120$ weighted Zp_T	$\alpha_S = 0.124$ default
Total	1.226	1.281
Zp_T	0.94	1.11

- Found it by minimizing $(\text{global } \chi^2) + 31(Zp_T\ \chi^2)$, but that's a detail.

Erroneous minimization in a toy model

- Imagine PDF characterized by a single parameter b. (α, PDF) parameter space simply a plane.
- Assume both partial and total χ^2 are paraboloids

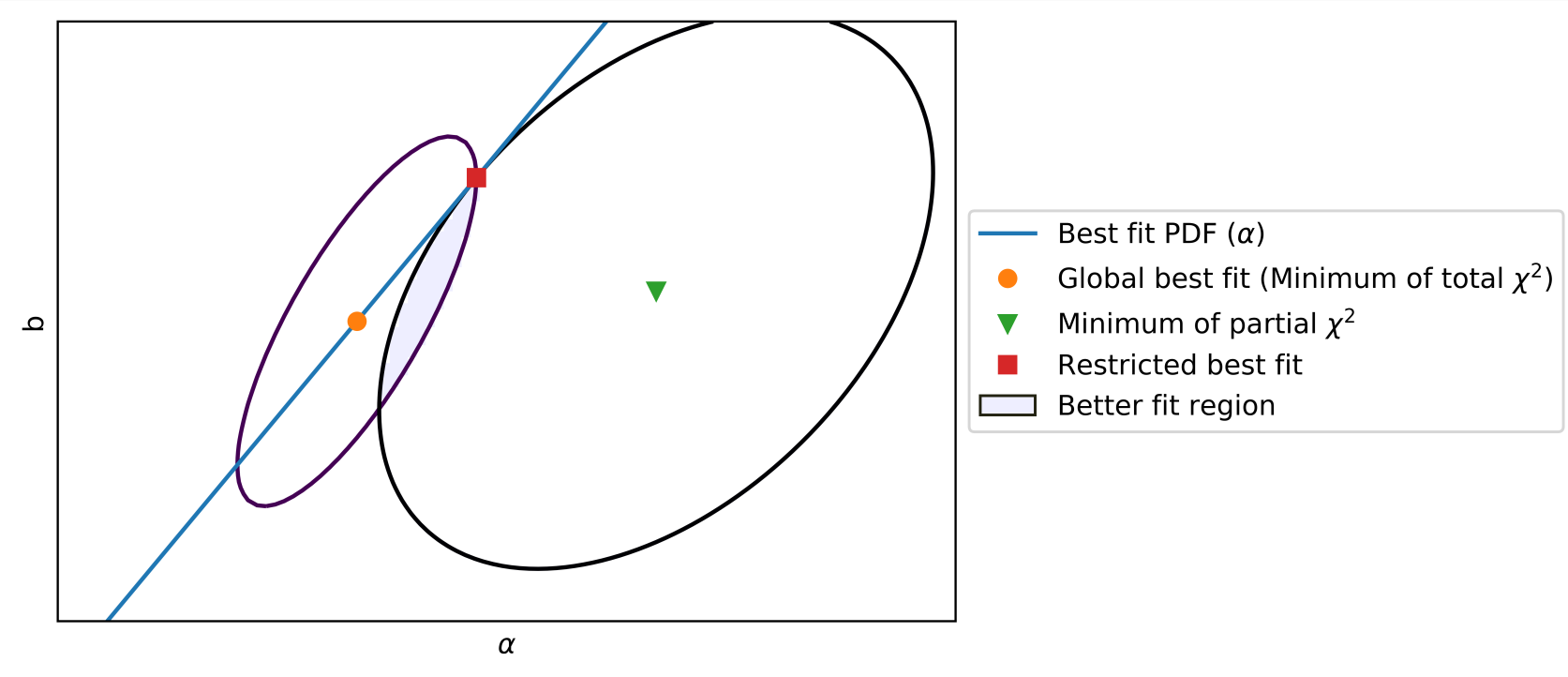
$$\chi^2_{\text{total}}(\alpha, b) = t_1 \left(\alpha \cos\theta + b \sin\theta\right)^2 + t_2 \left(-\alpha \sin\theta + b \cos\theta\right)^2$$

$$\chi^2_{\text{partial}}(\alpha, b) = p_1 \left((\alpha - \delta_\alpha)\cos\phi + (b - \delta_b)\sin\phi\right)^2$$
$$+ p_2 \left(-(\alpha - \delta_\alpha)\sin\phi + (b - \delta_b)\cos\phi\right)^2$$

The best PDF for a given α is

$$b_{\text{best}}(\alpha) = \arg\min_b \chi^2_{\text{total}}(\alpha, b)$$

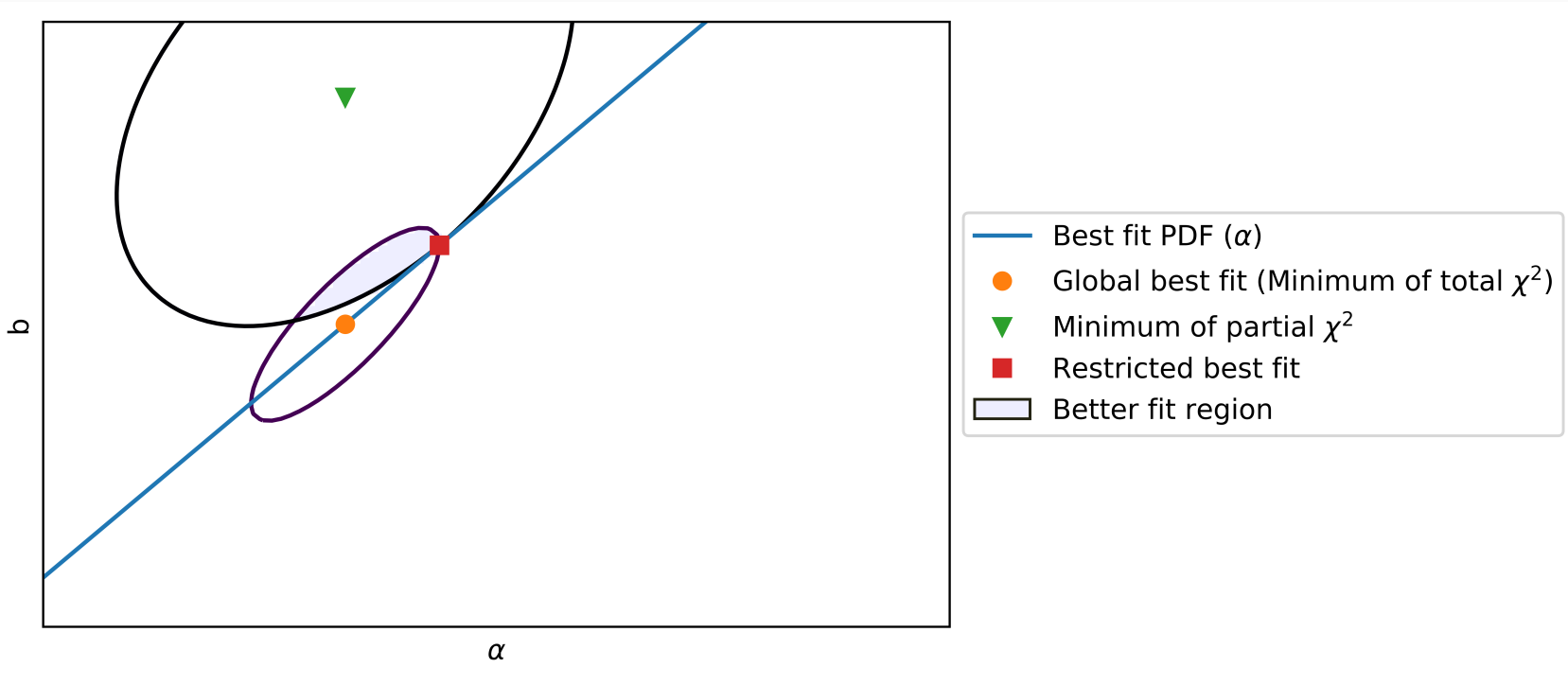
Better fit regions



- The procedure using best fit PDFs would yield the minimum of the partial χ^2 along the best fit PDF (red square)
- In fact the overlapping region describes better both datasets.

Making it worse

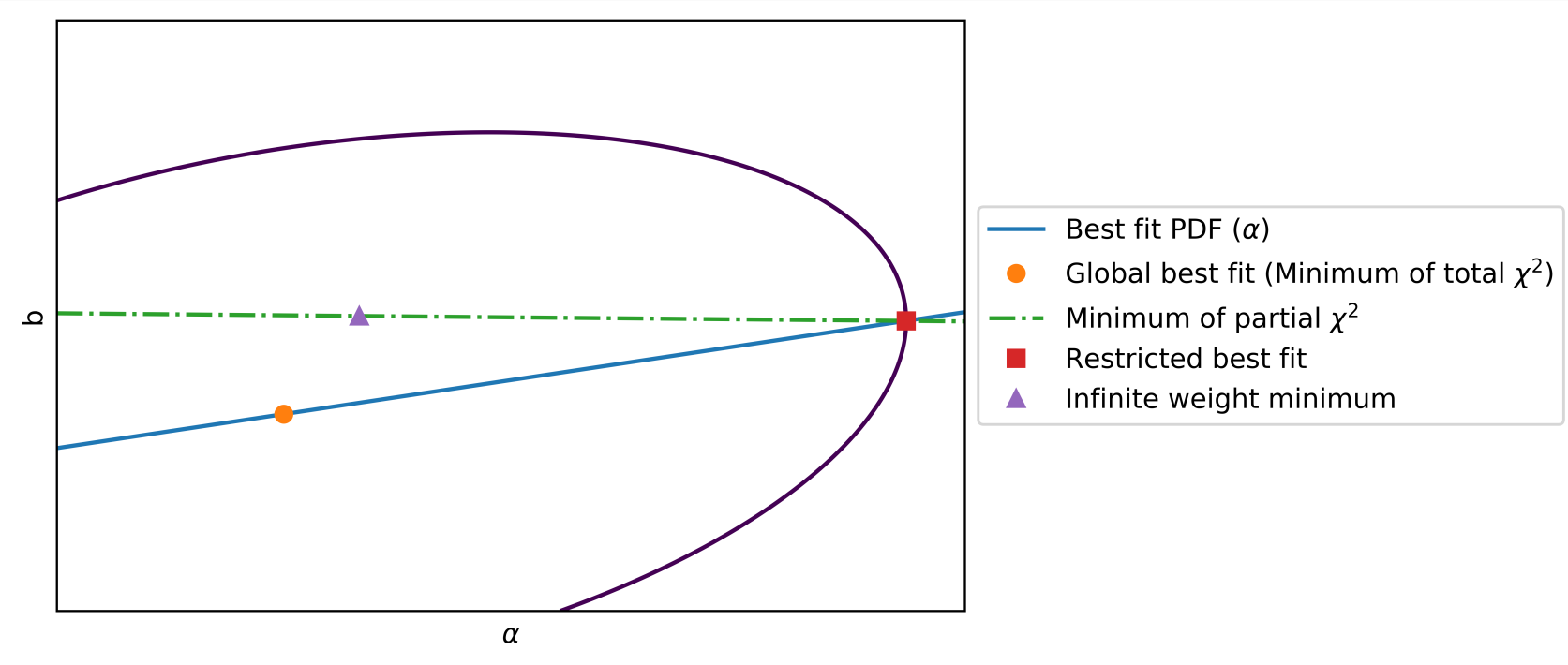
- Parameters can be tweaked so that the restricted minimum is far away from a desirable value.



A slightly more realistic model

- A more realistic situation is where the partial set doesn't determine both α_s and the PDF on its own, but only a combination of them.

$$\chi^2_{\text{partial}}(\alpha, b) = p_1 \left((\alpha - \delta_\alpha) \cos\phi + (b - \delta_b) \sin\phi \right)^2$$



- Similar situation: Now there is a better fit segment.
- Datasets with little handle on α can look artificially inconsistent.
- Can consider the $\lim_{w\to\infty} \chi^2_{\text{total}} + w\chi^2_{\text{partial}}$

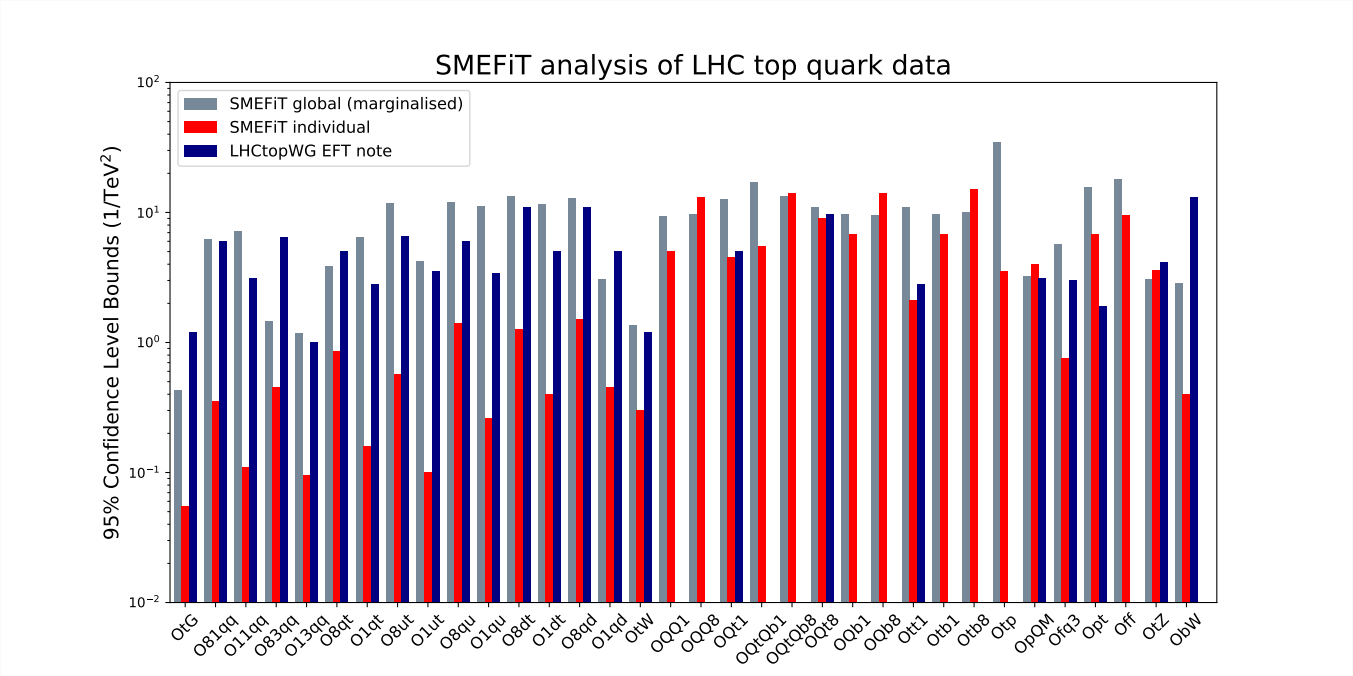
Dangers of partial fits

- Inconsistent minimization puts into question several determinations of α_S, as well as the QCD average.
- PDFs generally cannot be considered external to fitting problems.
- Problems not limited to α_S, but affect any parameter that changes PDFs.

Fits of EFT coefficients

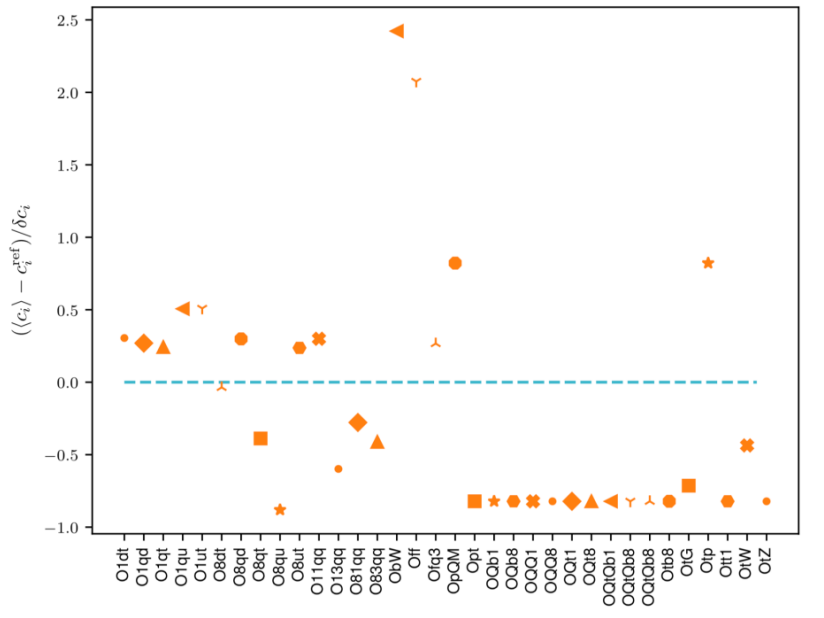
(See talk by Emma Slade and Hartland et al, arxiv:1901.05965)

- Used fitting methodology and validation inspired by NNPDF to constrain EFT coefficients in the top sector.
- Some results:
  - Bounds derived from fitting only one operator at a time (and fixing the rest to zero) much tighter than in a full fit.
  - Including more operators results in looser bounds.

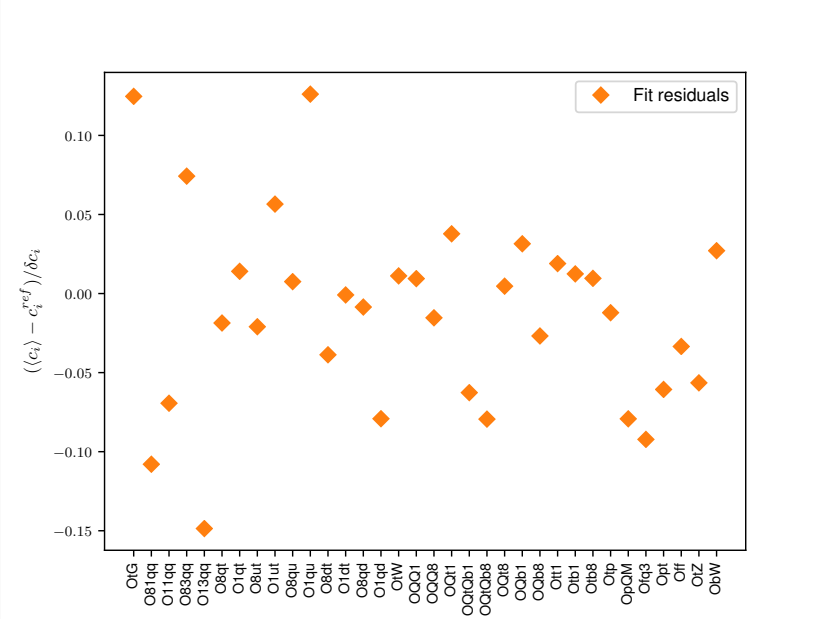


Residuals on a closure test

- Methodology tested on simulated data assuming SM only.



(a) Individual fit. Note: Marker shapes not meaningful



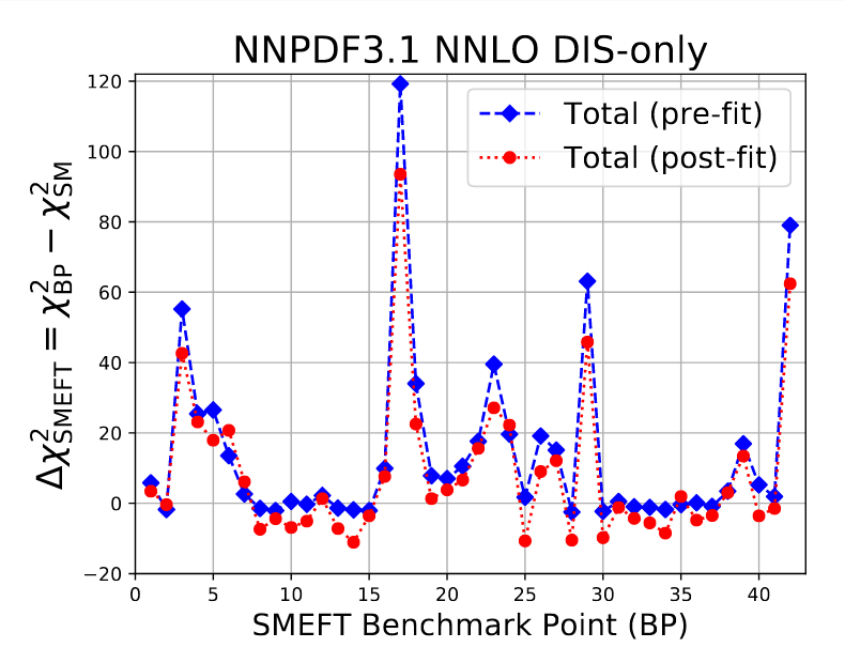
(b) Simultaneos fit

- Suggests EFT bounds only reliable when constrained globally.

EFT effects inside the PDF

(See Carrazza et al, arxiv:1905.05215)

- PDF fits sensible to inclusion of EFT effects in the determination itself.
- Added EFT corrections to DIS structure functions and used the result to determine PDFs .



- Results might vary more with an increased dataset.
- Putting it all together should be interesting: Global dataset + “complete” set of operators + PDFs + other parameters.

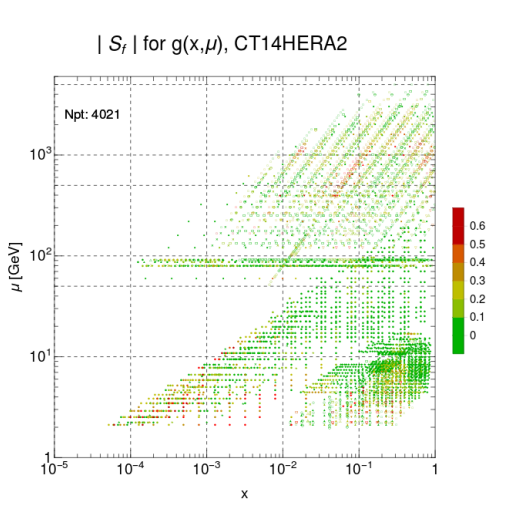
Visualization and analysis tools

(See talks by Carl Schmidt and Timothy Hobbs)

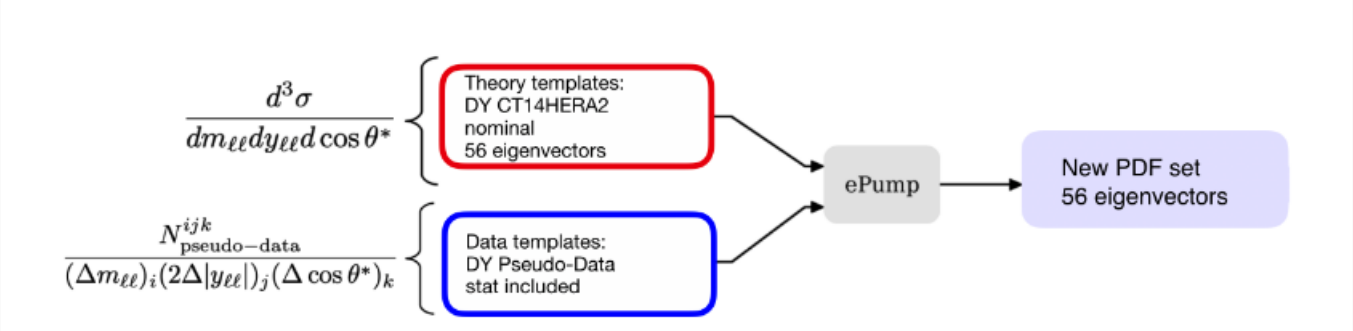
- Existing ways to understand how PDFs change upon inclusion of new data and which datasets cause discrepancies are ad hoc and manual.
- It would be good to be able to *visualize* data dependency.
- Lots of work on open source tools done by CTEQ lately.

Examples of tools

PDFSense (Wang et al, arxiv:1808.07470) code to study various data dependency, such as cluster data points by their effect on PDFs.



ePump (Willis et al, arxiv:1809.09481) Can estimate the effect of new data in PDFs.



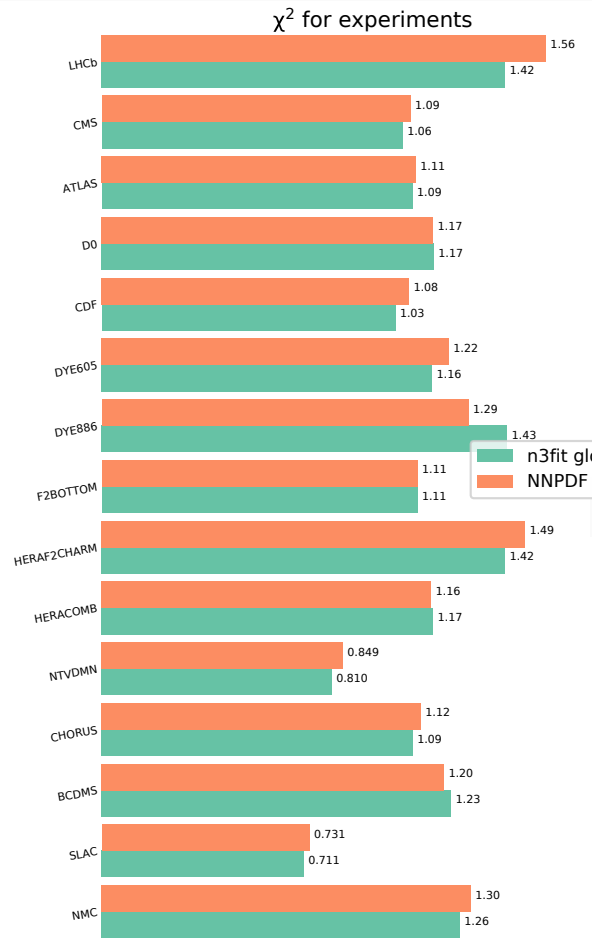
Improvements in the NNPDF fitting methodology

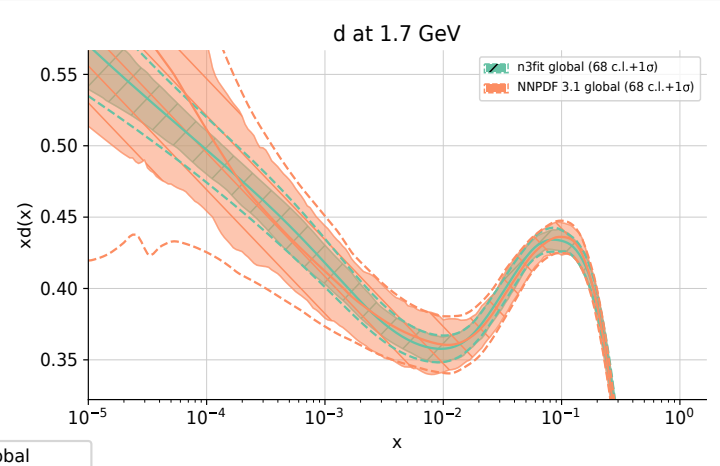
(See talk by Juan Cruz, and Carrazza, Cruz-Martinez arxiv:1907.05075)

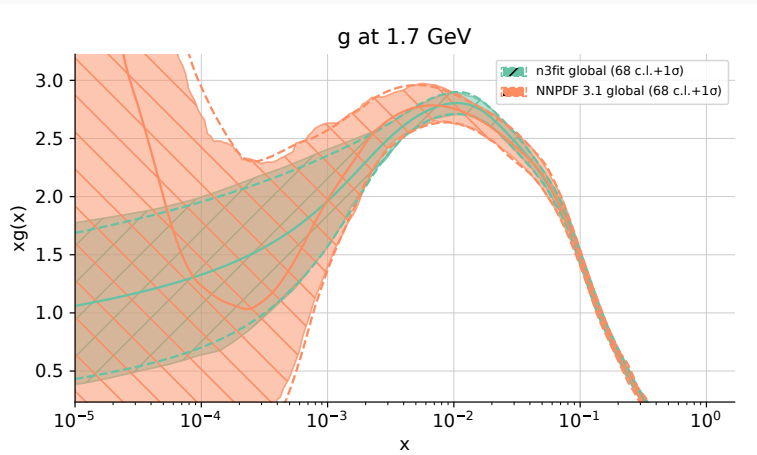
- Current NNPDF methodology was state of art Machine Leaning some 10 years ago. But the field has moved:
  - Gradient based optimization of large networks and complicated function.
  - Quality industry backed library present.
- The NNPDF methodology has been implemented with Keras + Tensorflow using gradient techniques.
  - Performance increased by a factor 20.
  - Allows to remove a lot of legacy code.
  - Still have to patch Tensorflow a bit to get good memory usage with convolutions.
- Increased speed will open the door to new classes of studies!

Results (so far)

- Central values and fit quality remarkably stable.
- PDF uncertainties significatively reduced.
  - Not so much at the level of predictions: High frequency component removed.





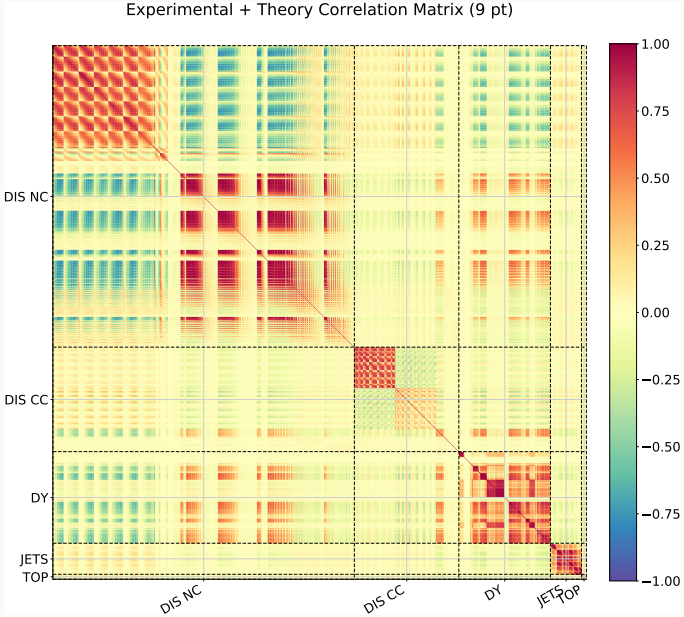


Theory uncertainties in PDFs

- Most important issue in current PDF sets is that they do not account for any uncertainty in the underlying theory, and specifically Missing Higher Order Uncertainties.
- Scale variations typically used as a proxy. Only method known to generalize to multiscale problems like PDF fits.
- Much work towards improving on it lately. E.g. (Harland-Lang, Thorne, arxiv:1811.08434)
- A First Determination of Parton Distributions with Theoretical Uncertainties (NNPDF, arxiv:1905.04311)
    - NLO PDFs with a model for MHOUs available for first time.
    - General formalism: NNPDF, arxiv:1906.10698.

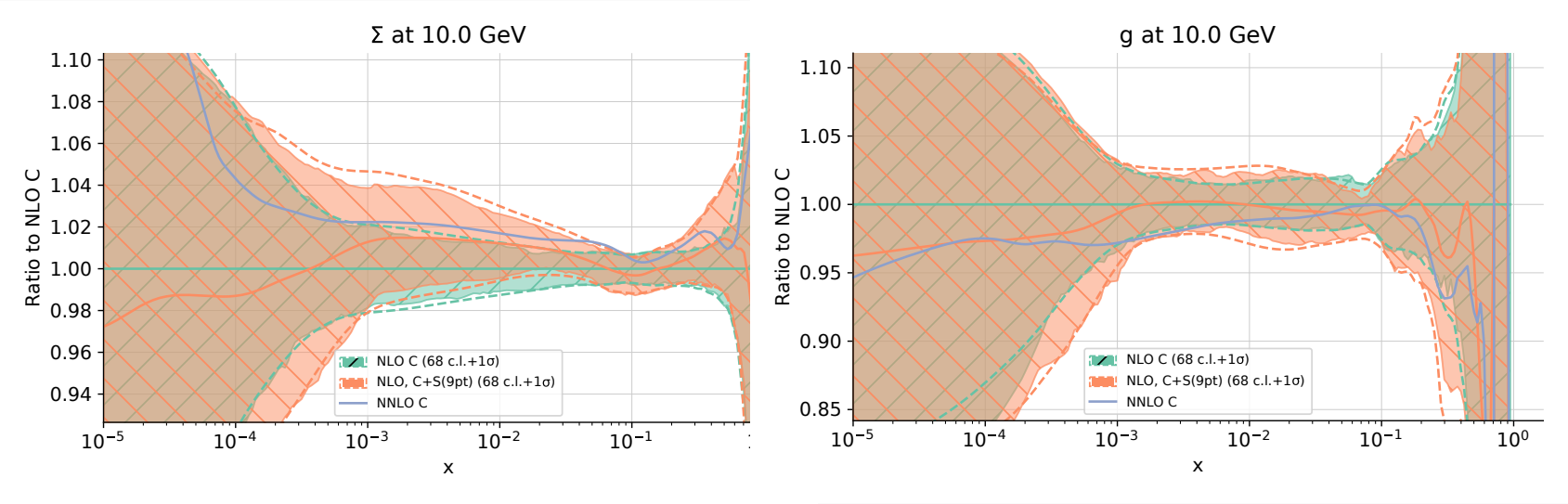
Theory covariance fit in NNPDF

- Idea: Include the integrated effect of scale variations in each PDF replica.
- In that case “scale variation systematics” can simply be added in quadrature to the experimental uncertainties. Define by:
  1. Labelling each dataset with a *process*: DIS CC, DIS NC, DY, Top, Jets
  2. Defining a covariance model for points belonging to the same or a different process.
     - Note that both the size of the uncertainties and the correlation model are heuristic. Choose to generalize envelopes with plausible correlations (“9 point prescription”).



Effects of the theory covariance matrix

- Data with large scale scale uncertainties weighted down in favour of more perturbatively stable data.
- Central value shift towards NNLO.



Concluding remarks

- PDF fits might be obsolete for precision physics. Need global fits including PDF parameters.
- Frameworks (both the theoretical and software ones) need to become more open and integrated.
- Independent cross checks very valuable
  - E.g. photon PDF in (Harland–Lang, Martin, Nathvani, Thorne, arxiv: 1907.02750, talk by Thomas Cridge) re-derives a LUXQED-like framework in an elegant way and finds consistent results.

Thank you!