Hyperoptimization - detecting overfitting

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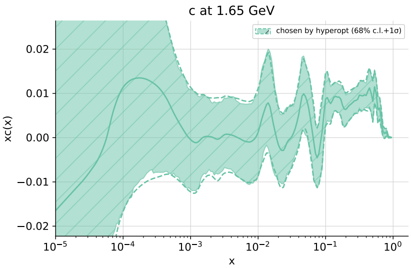
Hyperparameter selection

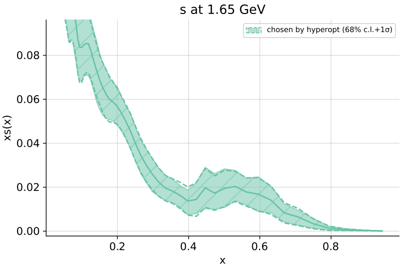
Currently: k-folds Hyperoptimization

This results in the possiblity of overfitted or underfitted setups, in part due to fluctuations (think preprocessing exponents)

To get a “nice” PDF we do a manual selection after the automated hyperoptimization, re-introducing human bias

To reduce bias we would like a numerical objective metric for overfitting or underfitting





The idea

Ideally, we have an objective metric that is not relative (such as arc-length), but absolute

Correlation between PDFs and validation data suggests overfitting

How can we detect when this happens?

The idea

Realization: for any PDF the validation loss χ^r_{val} should be equal to the "validation loss" calculated for any other pseudodata set $\chi^{\hat{r}}_{\mathsf{val}}$ (with the same tr/vl mask)

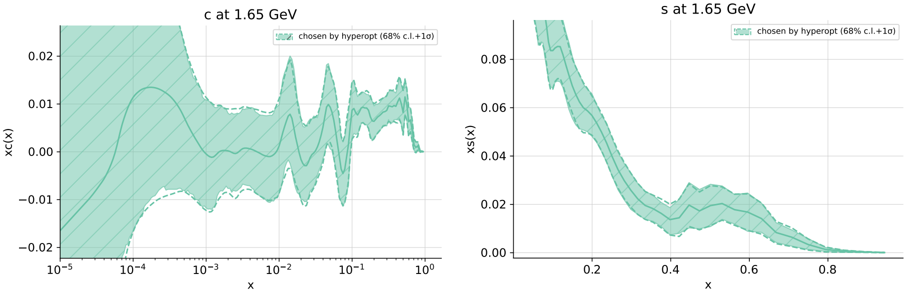
Thus as a metric for overfitting we might consider

$$\Delta\chi^2_{\mathsf{overfit}} = \langle \chi^2_{\mathsf{val},\hat{r}} - \chi^2_{\mathsf{val,r}} \rangle \quad (< 0 \text{ if overfitted})$$

While **underfitted** setups will be filtered due to their higher χ^2 values

(How) does this work?

Let's have a look at a clearly overfitted PDF (preferred by hyperopt):

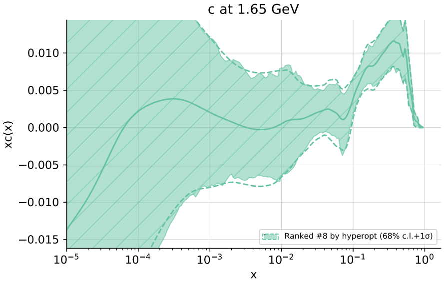


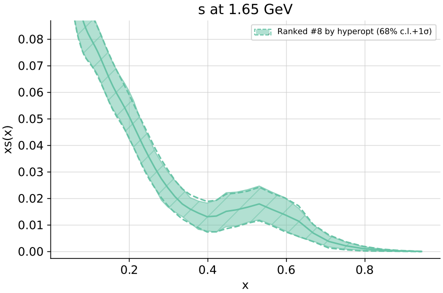
$$\Delta\chi^2_{\text{overfit}} = -0.0459 \pm 0.0078 \qquad 5.9\sigma \text{ from } 0$$

The $\Delta\chi^2_{overfit}$ values and bootstrap errors in these slides are determined using PDFs with $N_{rep} = 100$

(How) does this work?

And now for a PDF that is a bit smoother (ranked #8 by hyperopt):



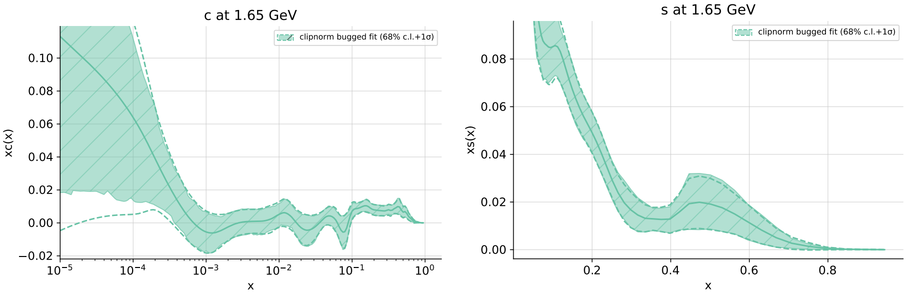


$$\Delta\chi^2_{\text{overfit}} = -0.0168 \pm 0.0105 \qquad 1.6\sigma \text{ from } 0$$

The distance from 0 decreases as expected

(How) does this work?

In the past we have had a scenario where this metric would have helped a lot:

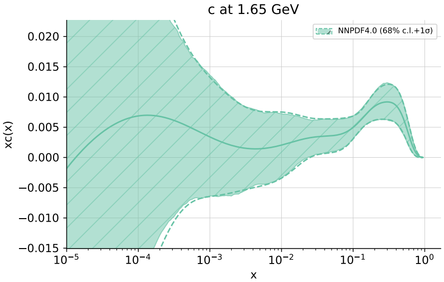


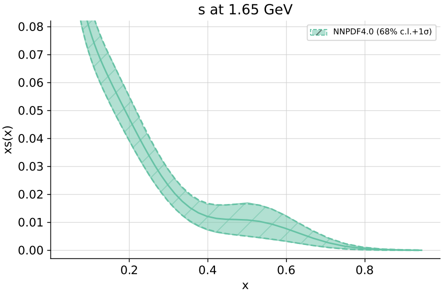
$$\Delta\chi^2_{\text{overfit}} = -0.0236 \pm 0.0126 \qquad 1.9\sigma \text{ from } 0$$

A clear indicator that the clipnorm bugged fit is overfitted!

(How) does this work?

And what about NNPDF4.0?





$$\Delta\chi^2_{\text{overfit}} = -0.0012 \pm 0.0130 \qquad 0.1\sigma \text{ from } 0$$

How can this be used in NNPDF?

As an a-posteriory check similar to (but cheaper than) the closure test

1. Run hyperoptimization
2. Select N best setups and do full 100 replica fits for each
3. Calculate the estimators for all
4. Discard setups with e.g. $R_{\text{overfit}} < -1$
5. 5.1 Increase number of replicas and repeat...
   5.2 or select the best of the remaining fit

5.1: If the bootstrap error becomes small enough we will likely always get a negative $\Delta\chi^2_{\text{overfit}}$
5.2: What is an acceptable $\Delta\chi^2_{\text{overfit}}$?
How do we define the best fit (χ^2_{val}, χ^2_{tr}, χ^2_{exp}, $\ldots$)?

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Conclusion: The $\Delta\chi^2_{\text{overfit}}$ provides a metric for overfitting that can be used to flag overfitted hyperparameter setups and thereby reduce human bias

Backup

Hyperopt demonstration

Demonstration file