Parton densities with deep learning models

based on arXiv:1907.05075

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PDF challenges

The PDF priorities

Parton distribution functions have been developed in a systematic way from the 2000s. Since that time, the PDF community gave priority to:

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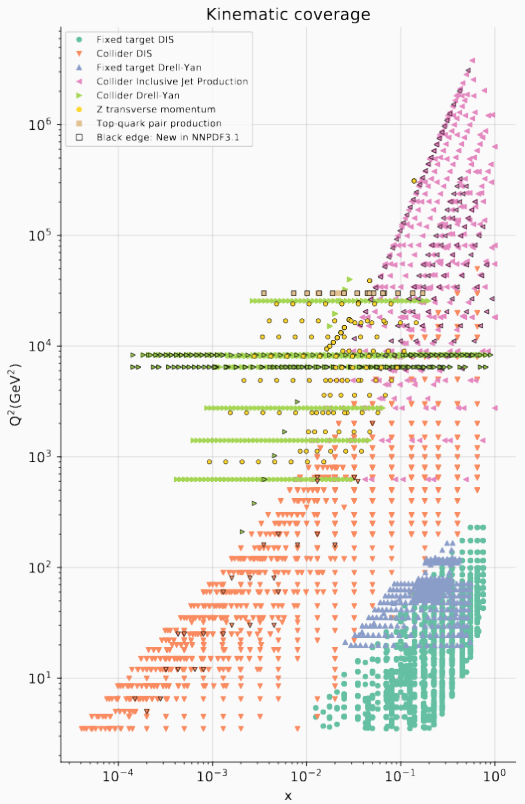

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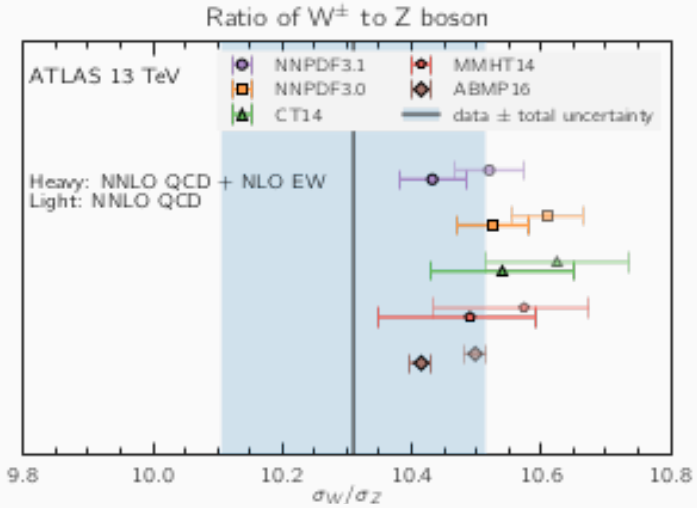

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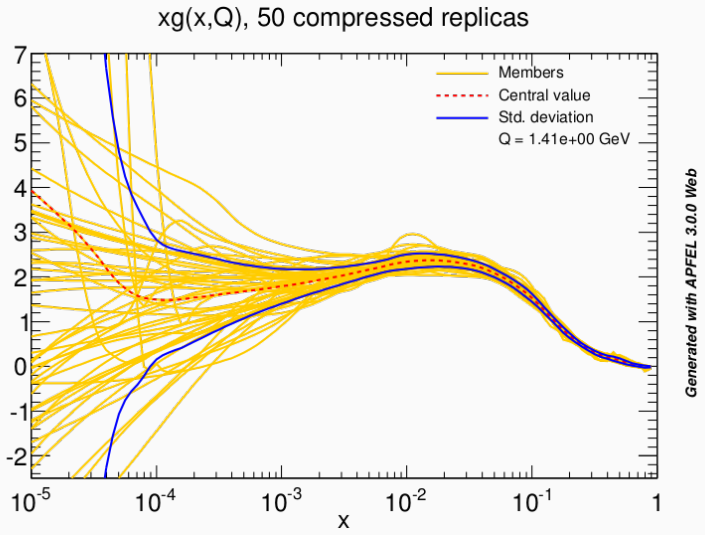
Methodology

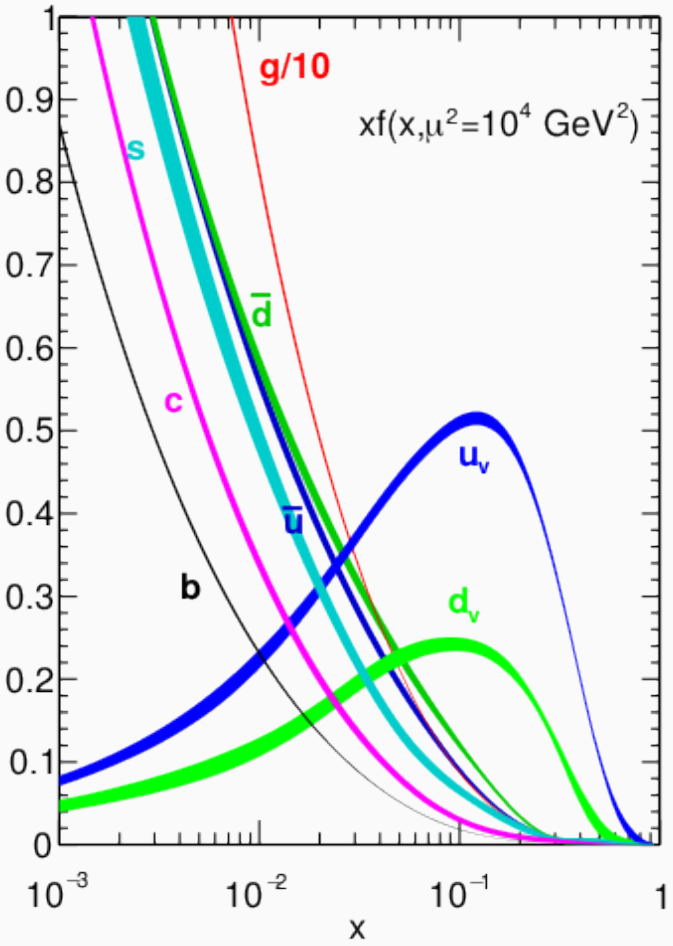
Define an optimized regression models for the PDF fits.



The NNPDF methodology

The technology used in **NNPDF3.1**:

- Neural Networks optimized with Genetic Algorithms
- Custom implementation in C++
- Tuning performed manually



PDF challenges

Challenges:

- How to increase **fit performance speed**?
  - faster fits $\Rightarrow$ more fits
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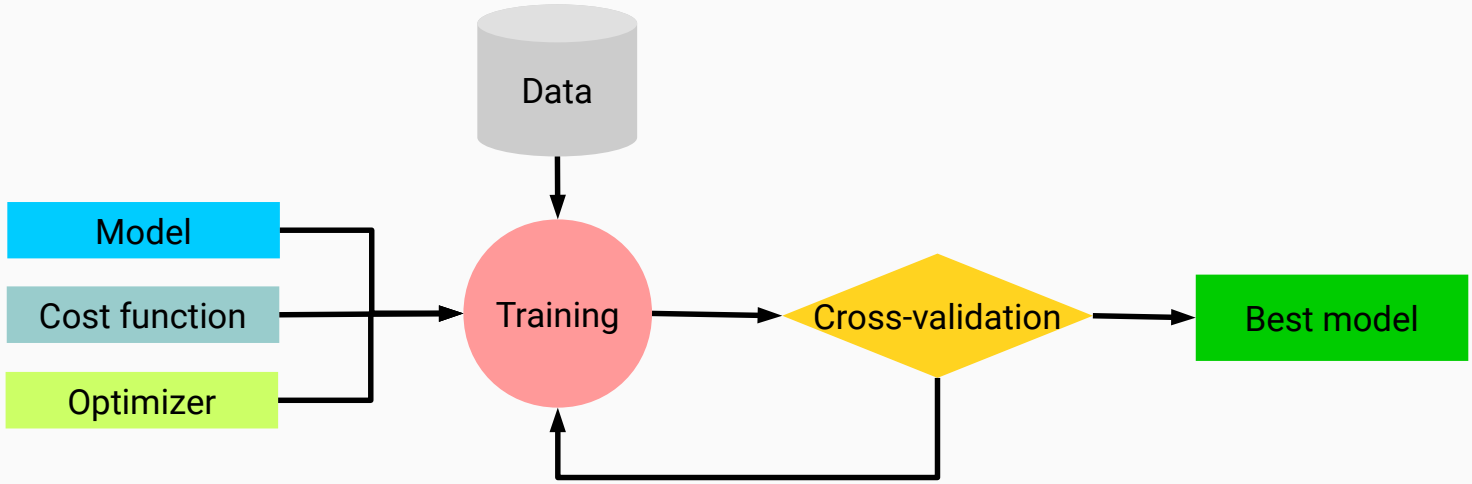
Solution $\Rightarrow$ move towards **deep learning**

- in terms **software/technology**
- in terms of **methodology**

Towards a DL approach

Deep learning pipeline

PDF determination is a supervised learning problem thus we need to provide review for the following sectors:



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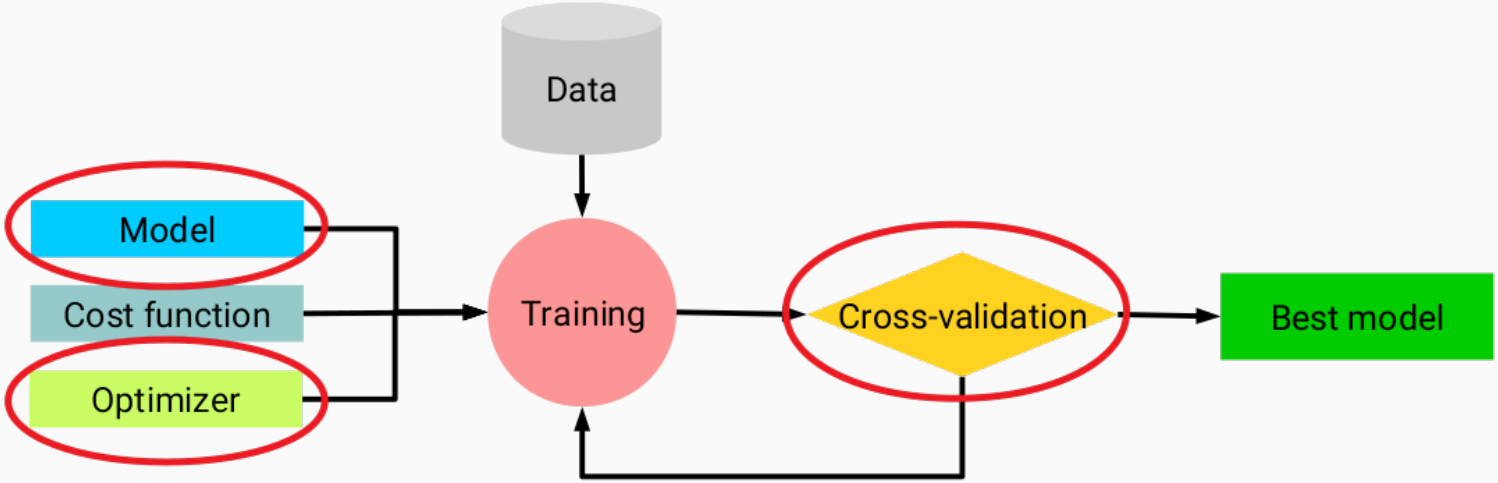
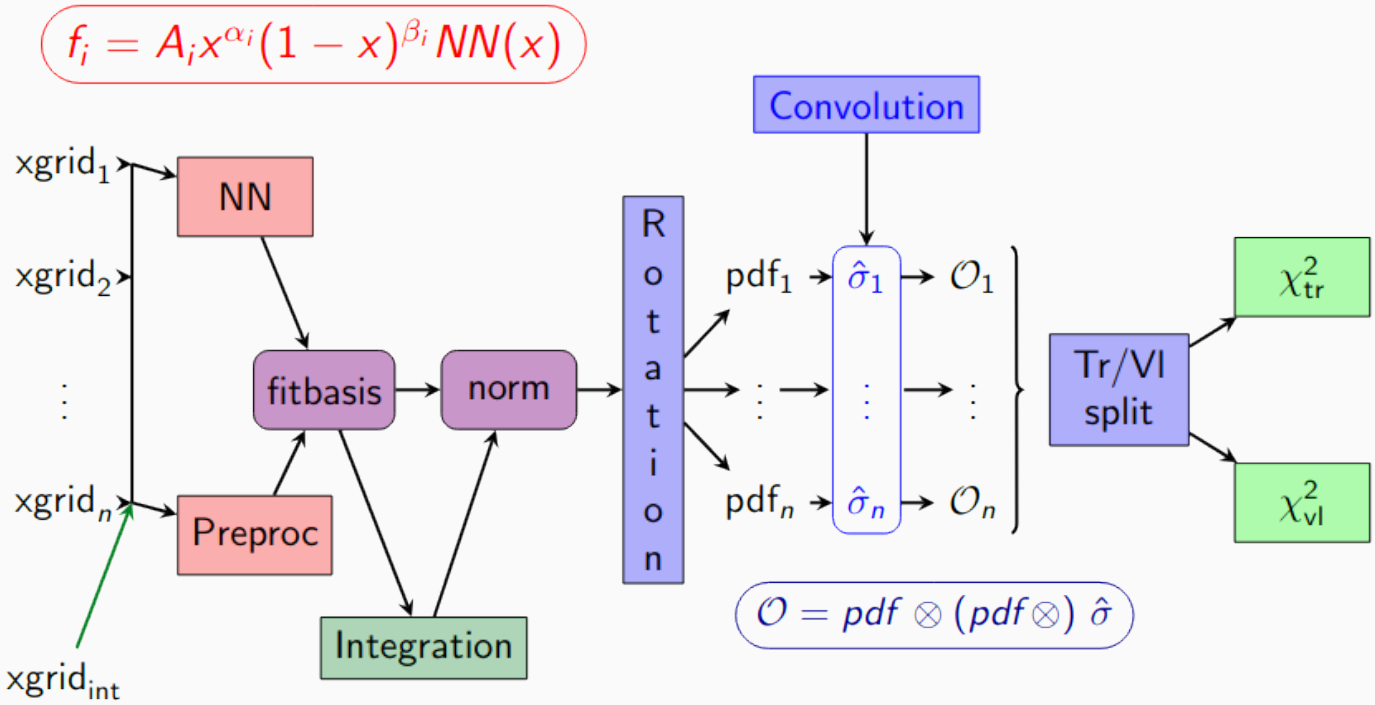


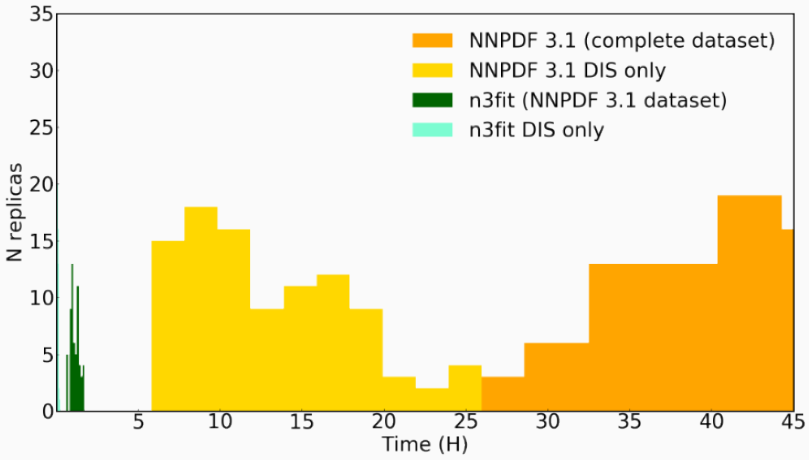
The `n3fit` model

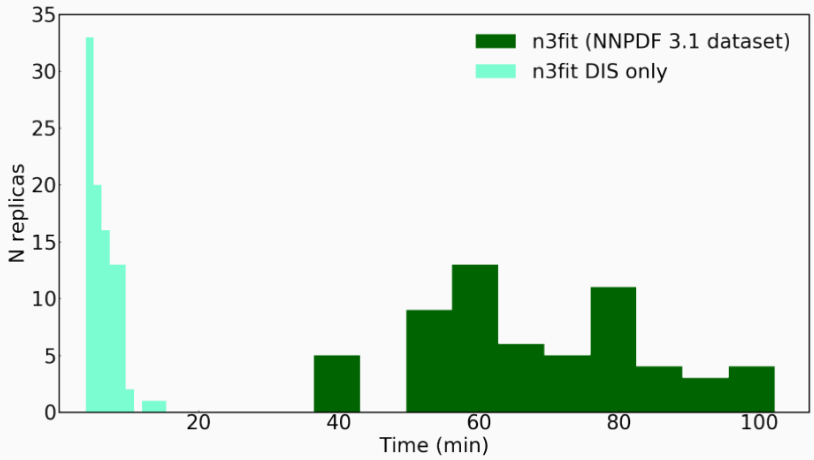


New features:

- `Python/C++` implementation using **TensorFlow**
- Modular approach $\Rightarrow$ easier and faster development
- Can vary all aspects of the methodology

Performance benefits - time per replica





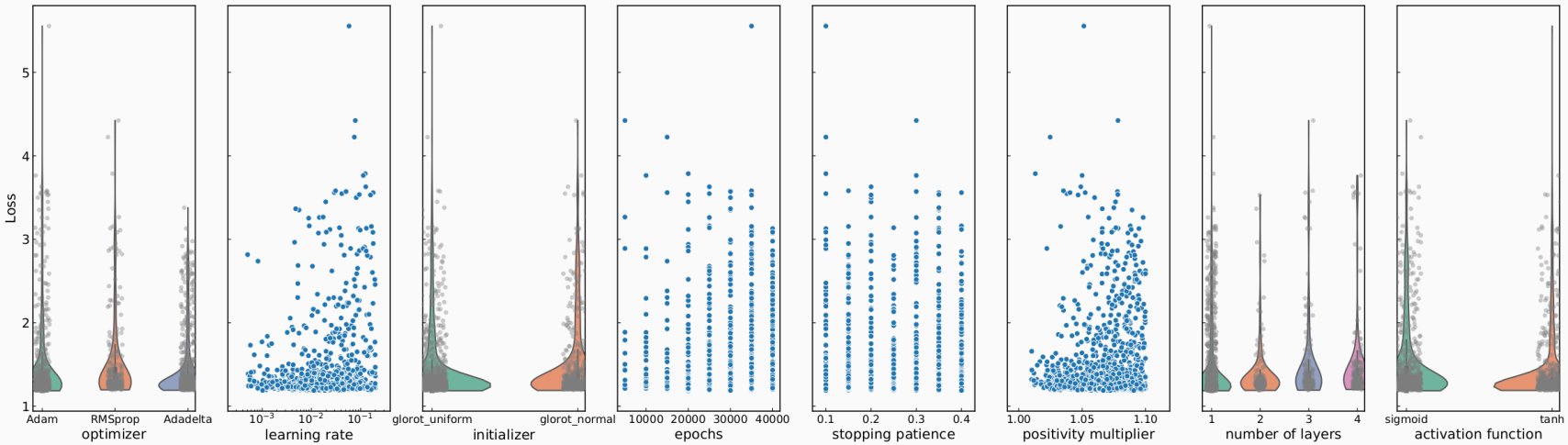
Benefits

- Gain on speed and efficiency, less **CPU hours for a fit**
- Usage of new technologies $\rightarrow$ hardware, libraries
- Usage of **gradient descent** optimization methods

$\Rightarrow$ **Possibility to learn and tune the methodology**

Learning the methodology

How to determine the best methodology?



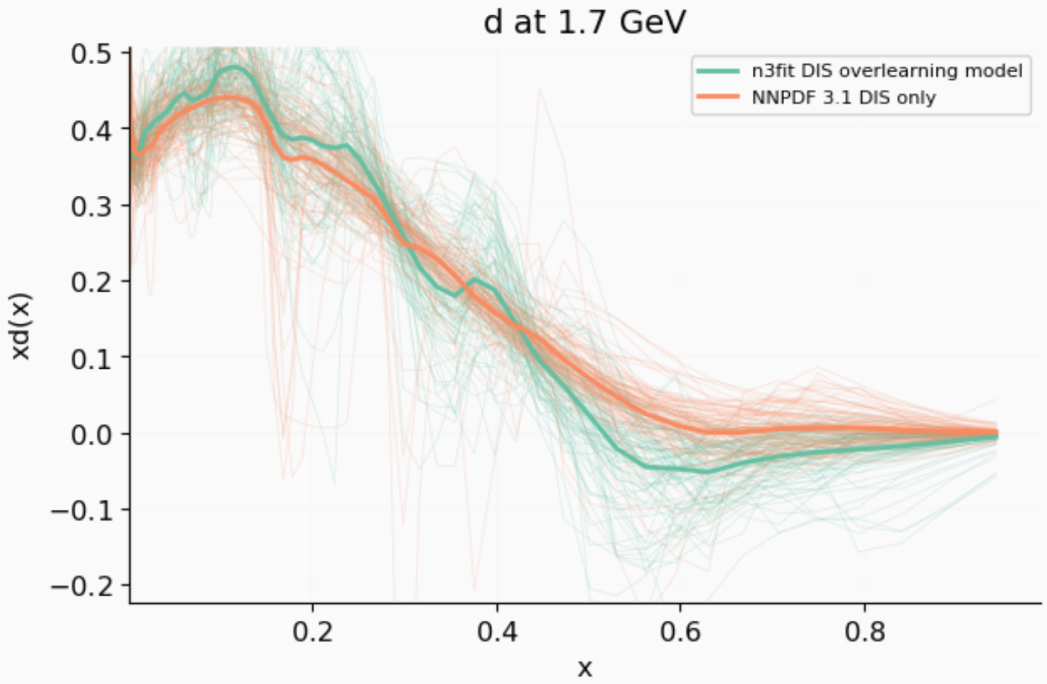
Perform **hyperoptimization scans**:

Neural Network	Fit options
Number of layers (*)	Optimizer (*)
Size of each layer	Initial learning rate (*)
Dropout	Maximum number of epochs (*)
Activation functions (*)	Stopping Patience (*)
Initialization functions (*)	Positivity multiplier (*)

- Optimize figure of merit: validation χ^2
- Use bayesian updating (`hyperopt`)

The overfitting problem

Using validation set χ^2:



The choice of the **right figure of merit** is important:

- **NNPDF** wiggles $\rightarrow$ finite size , goes away as $N_{\rm rep}$ grows
- **N3PDF** wiggles $\rightarrow$ **overfitting**, correlations training-validation data!

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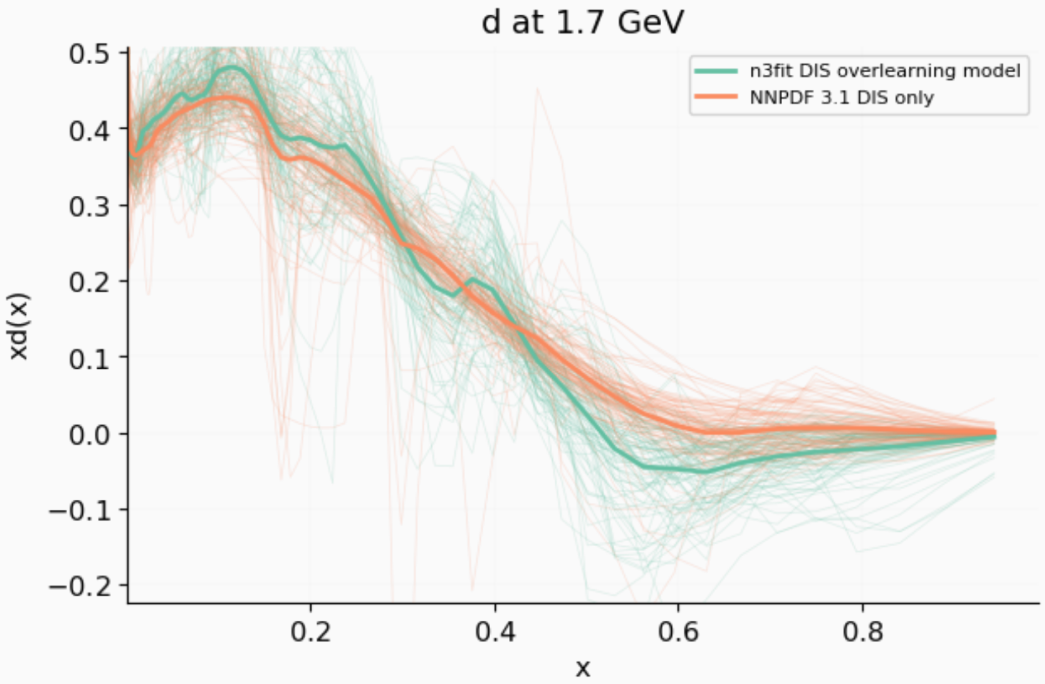

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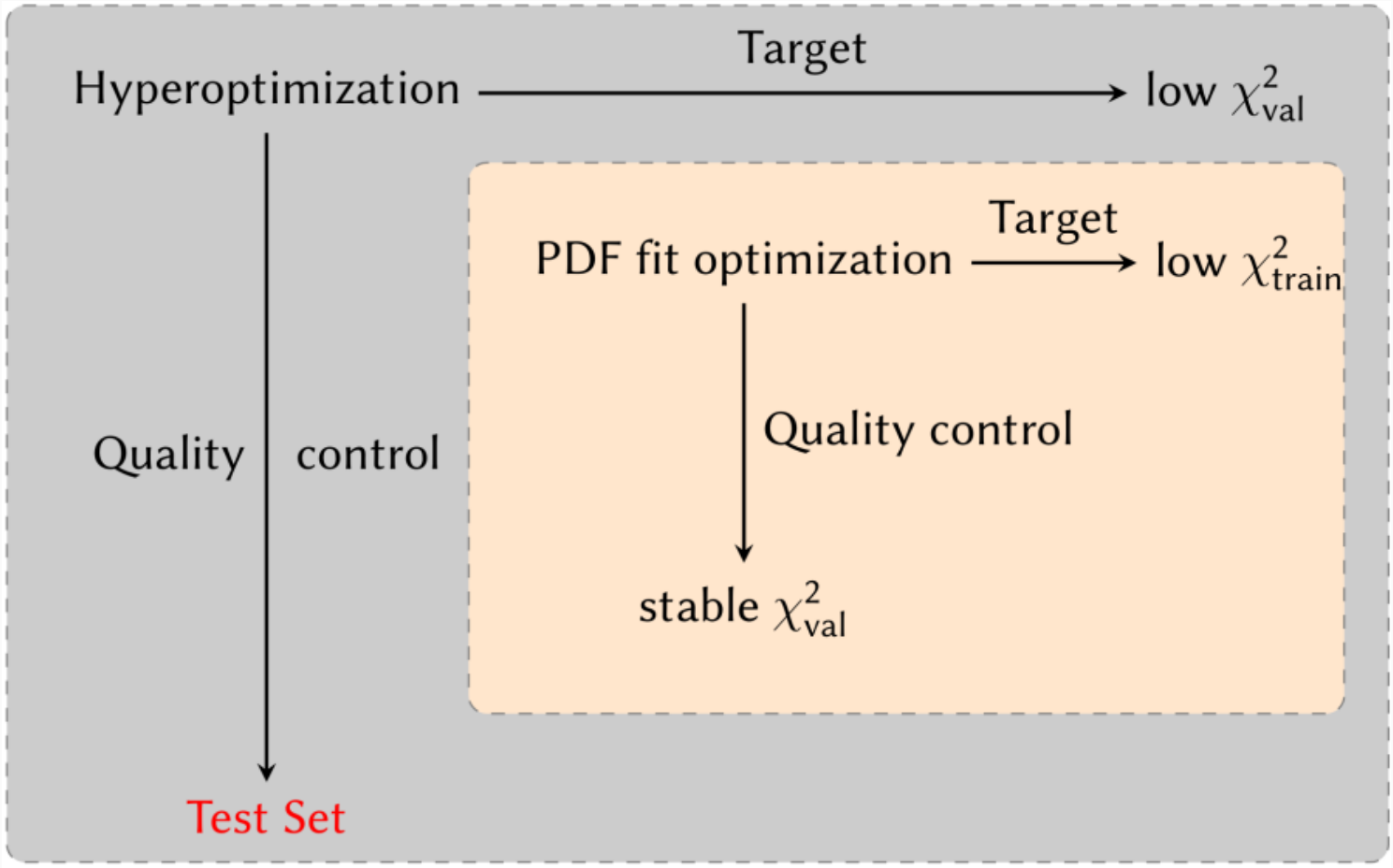
$\Rightarrow$ **define a proper quality control criterion**

Cross-Validation vs hyperoptimization

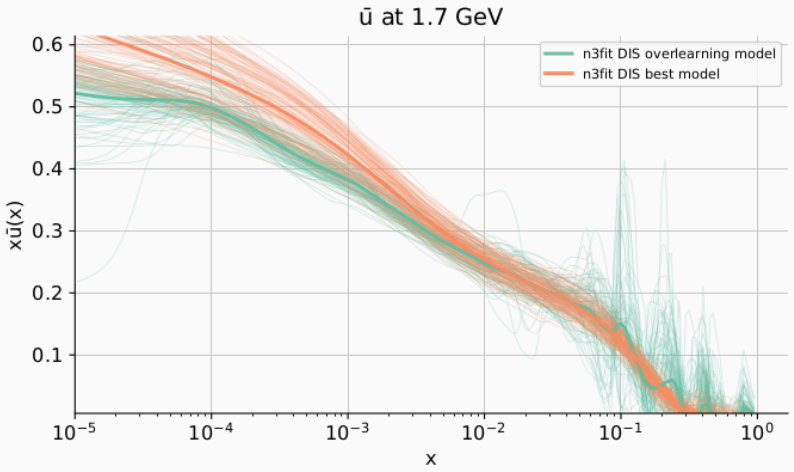
Define a completely uncorrelated **Test Set**

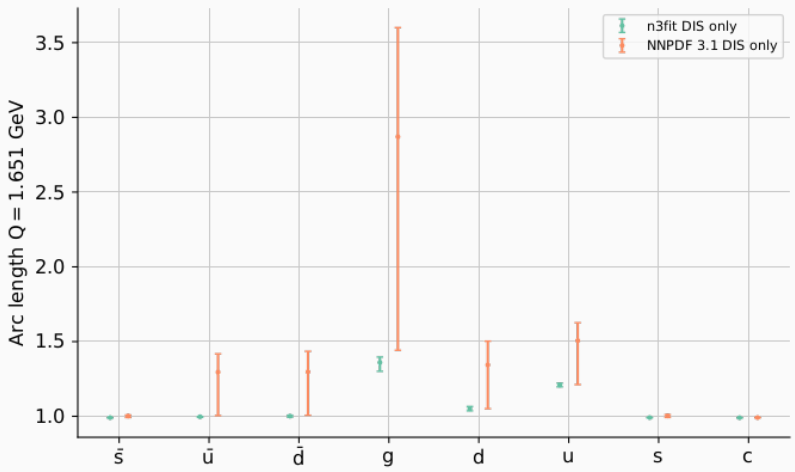


Optimize on weighted average of validation and test.

Removing overfitting

Using test-validation set χ^2:





- No **overfitting**
- Greater **stability**
- Reduced uncertainties

	DIS only	Global
`n3fit` (new)	1.10	1.15
`nnfit` (old)	1.13	1.16

Quality control

Chronological fits

Idea:

1. Take a pre-HERA dataset
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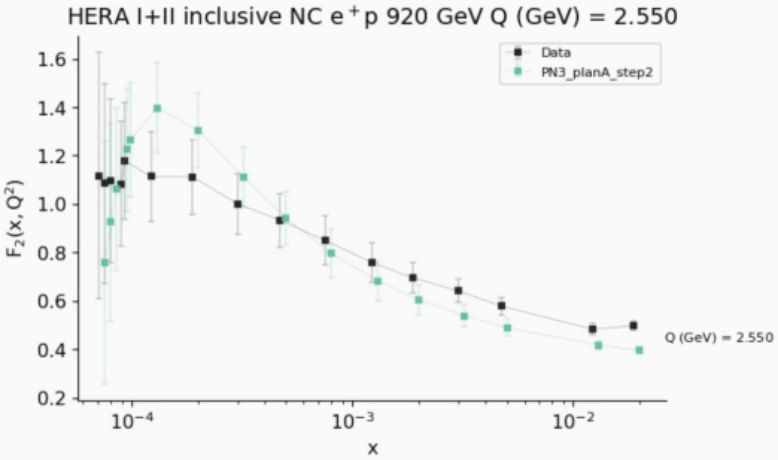
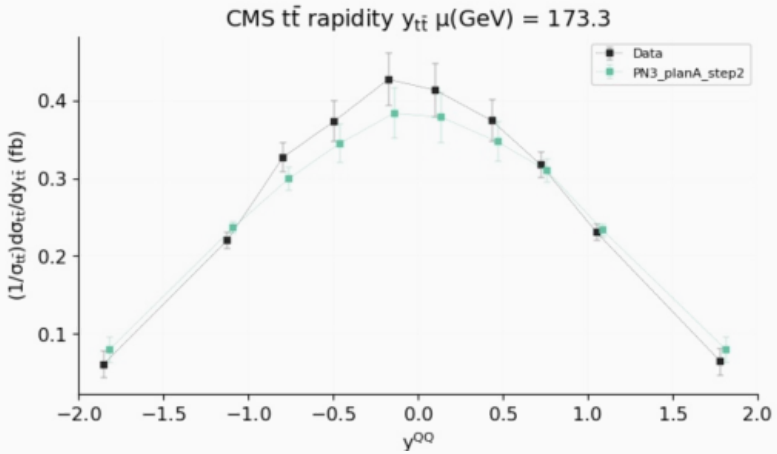
Examples:





⇒ **Results within PDF uncertainty!**

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$\Rightarrow$ **Potential solution:** use k-fold cross-validation.

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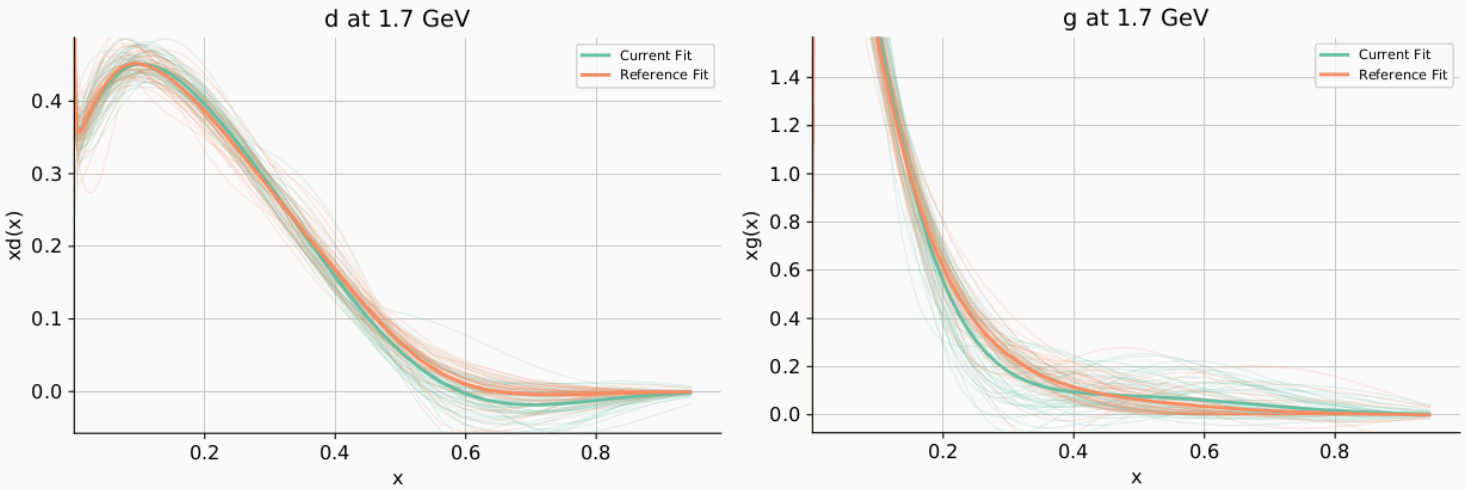

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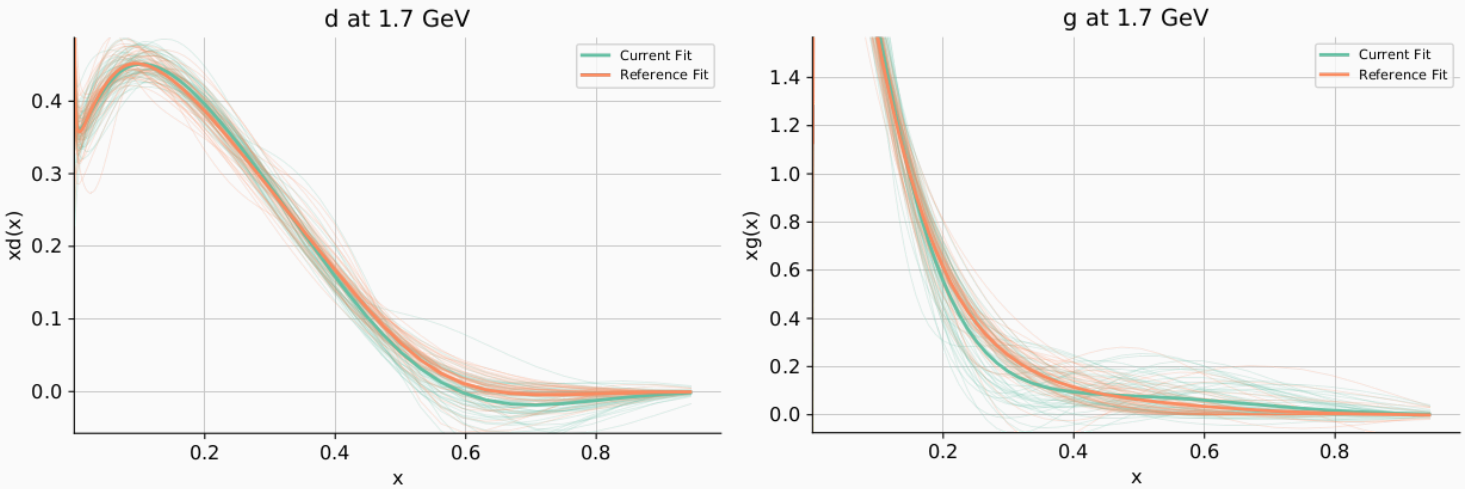


$\Rightarrow$ **Compatible with our previous Test Set definition.**

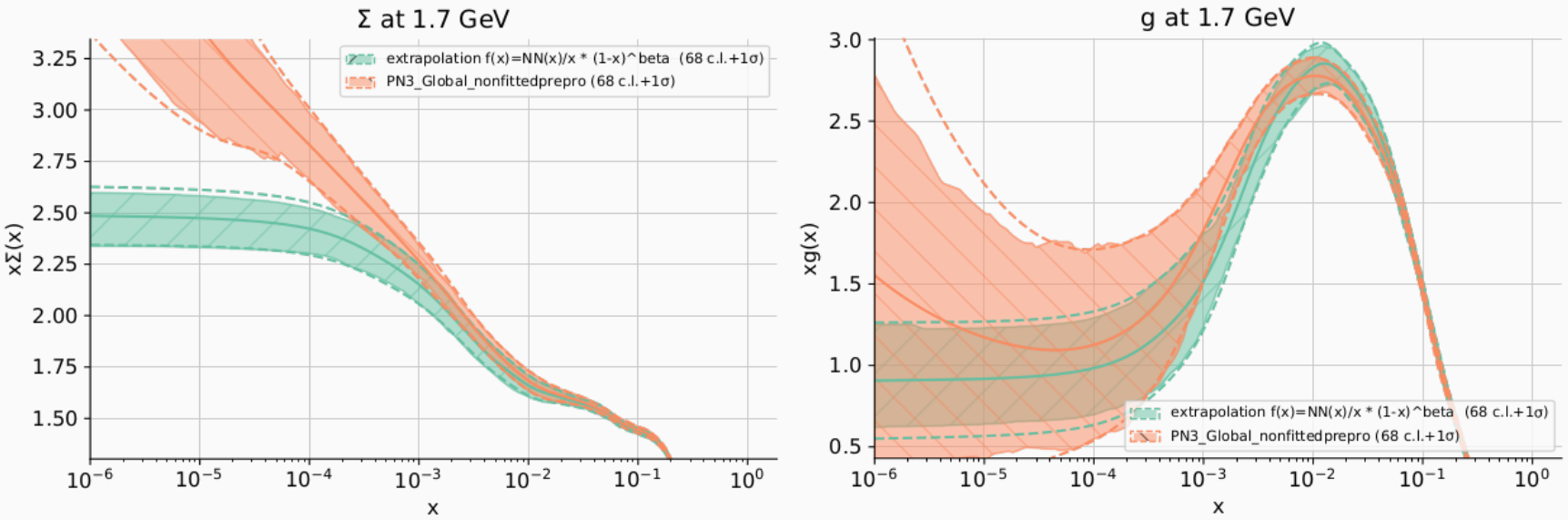
Future challenges

Extrapolation region

The current parametrization uses preprocessing:

$$f(x) = x^{-\alpha}(1-x)^{\beta} NN(x)$$

If preprocessing is removed, we observe saturation at small-x:



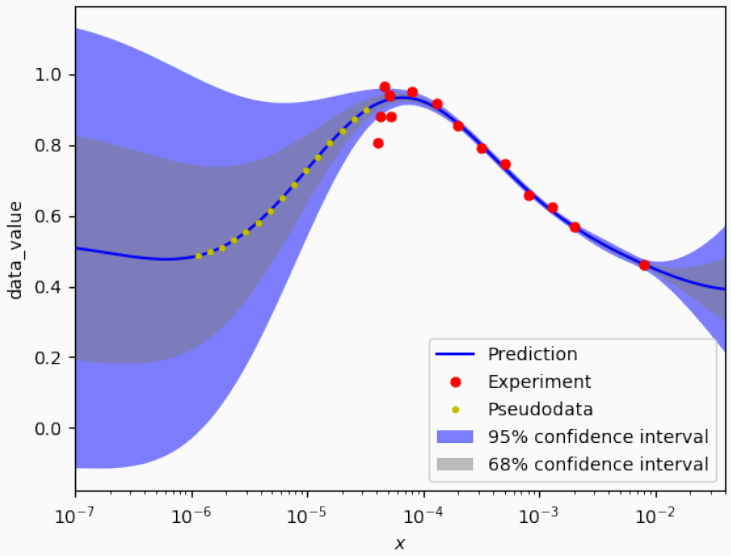
Challenges:

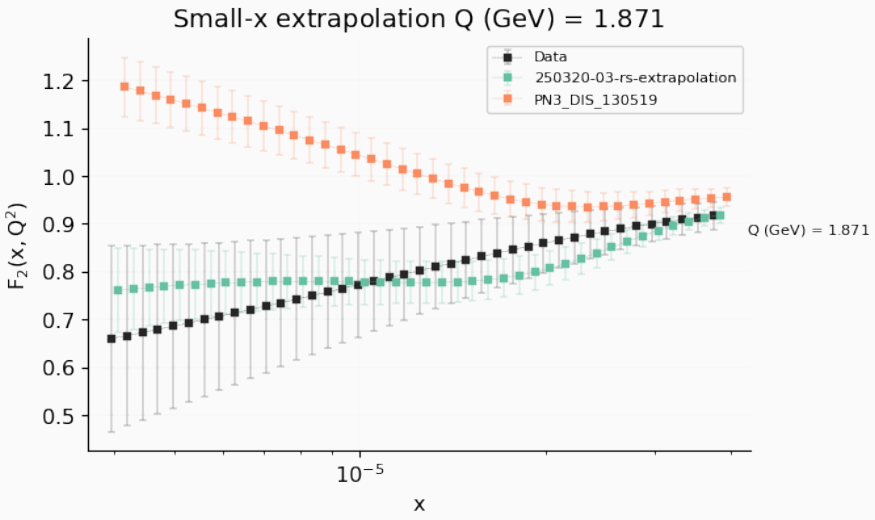
- Modify neural network input architecture
- Generate pseudodata in the extrapolation region

Extrapolation region

Gaussian pseudodata:

- use gaussian process to model DIS observables
- propagate a prior gaussian into extrapolation
- generate gaussian pseudodata and add it to fit





Final comments

Towards the NNPDF4.0 release:

- Faster run times and stable results
- Possibility to learn the methodology
- Quality control, reduced uncertainties
- Better understanding of model behavior

Thank you!