Methodological improvements in PDF determination

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in collaboration with: S. Carrazza, J. Urtasun-Elizari, E. Villa

hep-ph/1907.05075

N3PDF

Machine Learning • PDFs • QCD

James Stirling Memorial Conference, Durham (2019)

European Research Council

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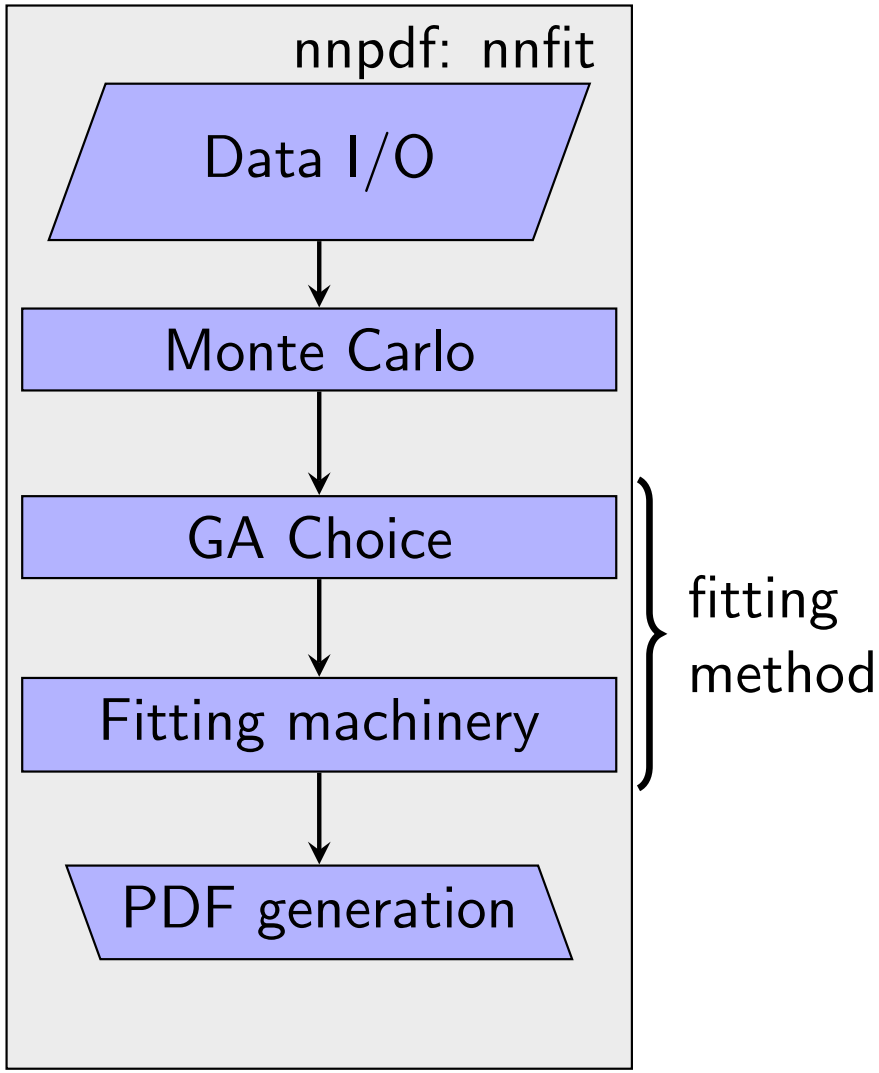
Outline

1. A new methodology, codename `n3fit`
   - Motivation: speed & flexibility $\rightarrow$ more physics
   - Design choices

2. Codename `n3fit`
   - In detail
   - Hyperoptimization: fitting the methodology
   - Result examples

3. Accelerating the fit
   - Handcrafting operations
   - Hardware acceleration

The goal: towards new methodologies



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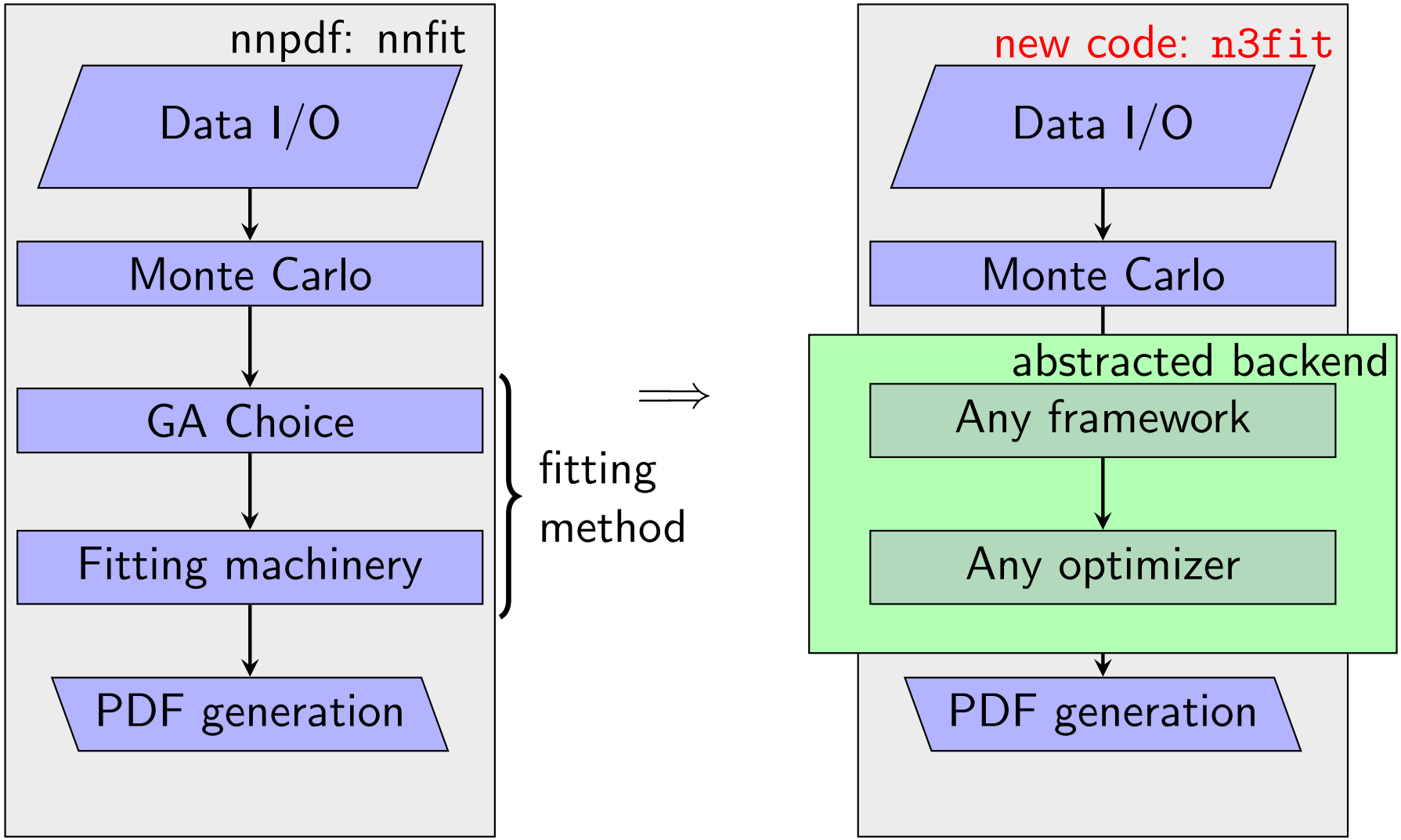
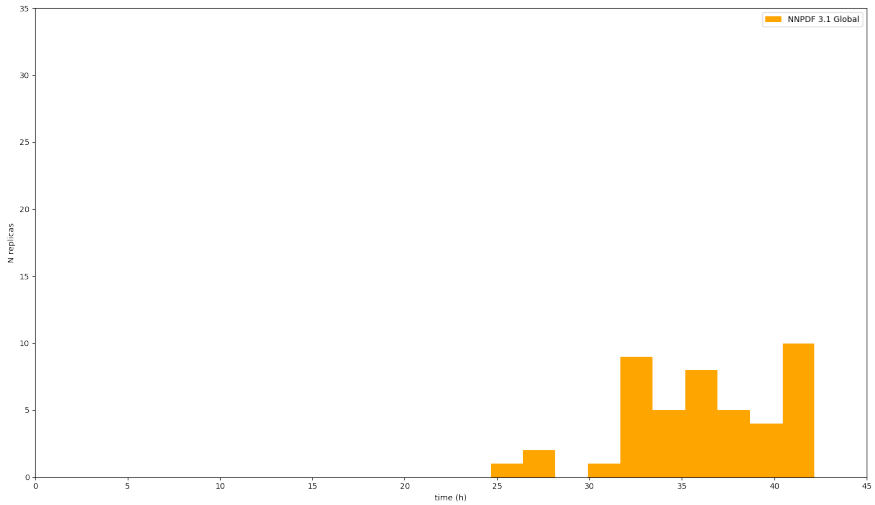


Motivation: more studies available

✓ Rationalization of development
- Easier and faster development
- OOP: full freedom and flexibility



✓ Gains on speed and efficiency:
- Less CPU hours for a fit
- Usage of new technologies
  - ✓ GPU/FPGA
  - ✓ ML libraries

✓ Consequences
- **Speed-up of research**
- **More studies available**
- **Example: fitting the methodology**

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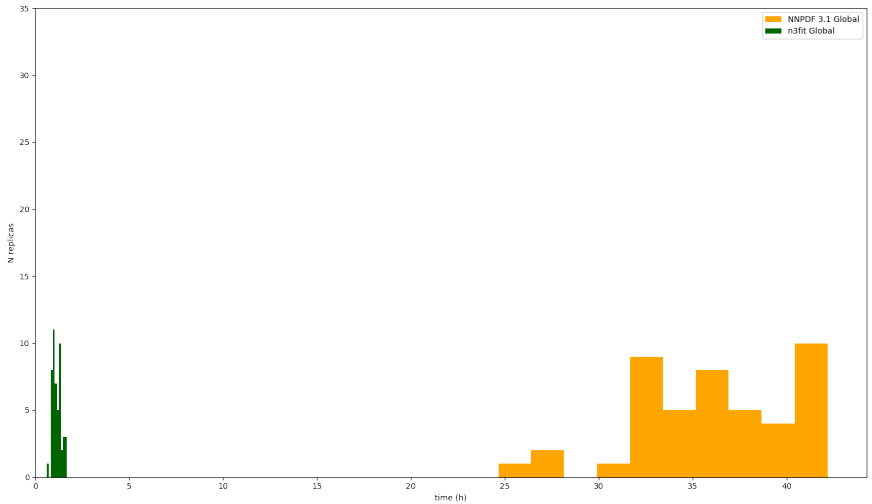

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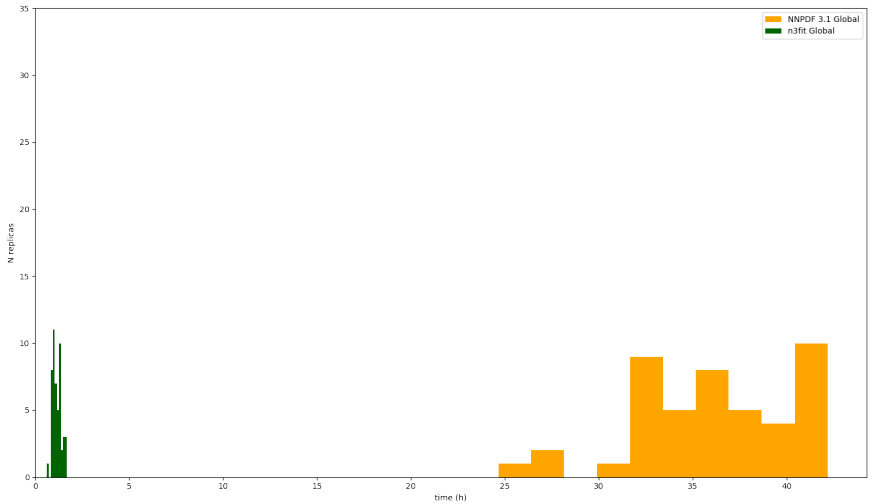

Language and framework

```
Language:  python
      > version:  3.7
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- ✓ Widely used and easy to learn
- ✓ Supported by most ML libraries:
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Framework:  Keras
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- ✓ High level of abstraction
- ✓ Powerful features of Tensorflow
- ✓ Trivially change between (supported) libraries

- ✓ CPU parallelization
- ✓ GPU parallelization
- ✓ FPGA support

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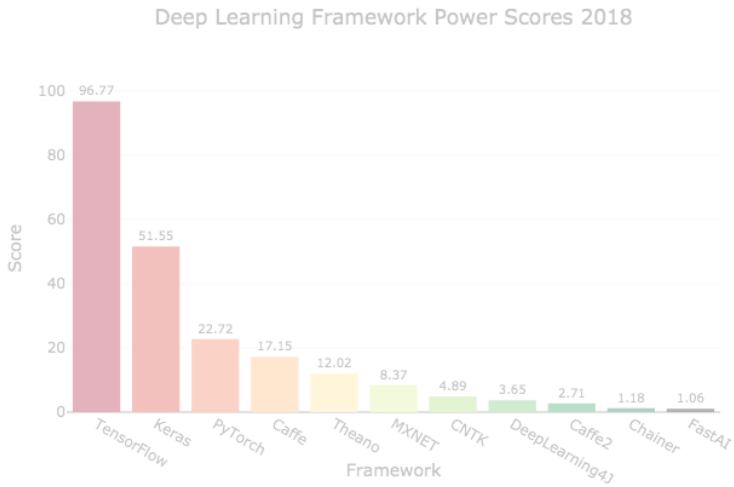

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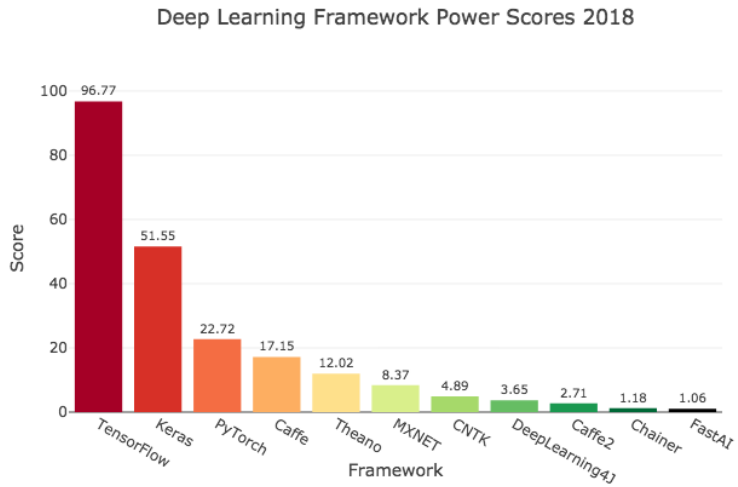

Plot Source

- ✓ CPU parallelization
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Note: the metric in the figure includes GitHub activity and ArXiv articles: Research and development.

The Loss Function

The fitting strategy is based on the minimization of the χ^2,

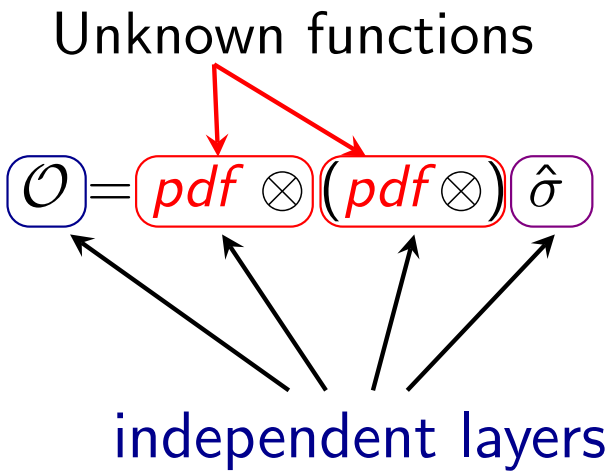
$$\chi^2 = \frac{1}{N} \sum \left(\mathcal{O}^i - \mathcal{D}^i\right) \sigma_{ij}^{-1} \left(\mathcal{O}^j - \mathcal{D}^j\right)$$

N: number of data points

$\mathcal{O}^i$: theoretical prediction

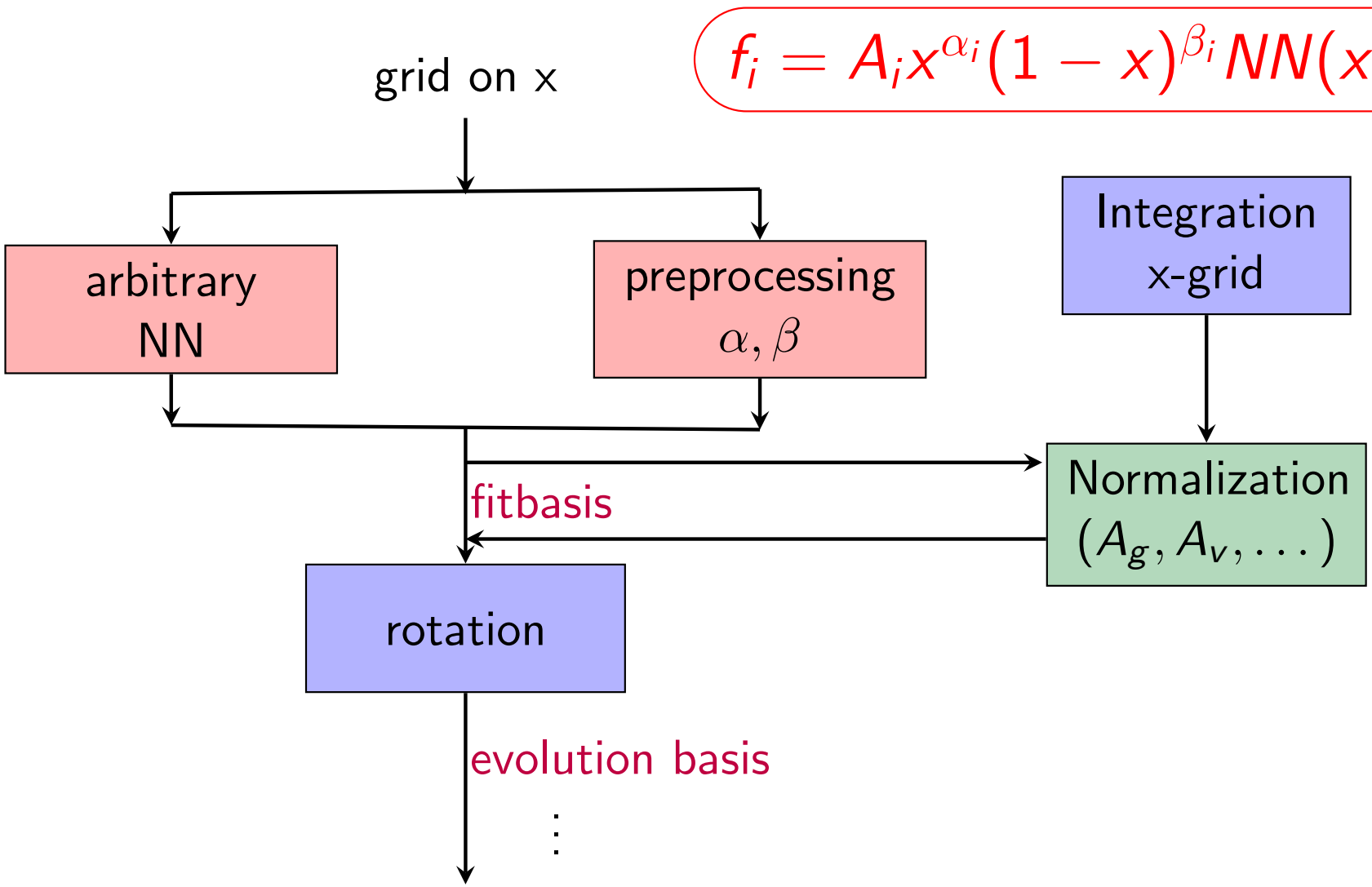
$\mathcal{D}^i$: experimental data point

σ_{ij}: covariance matrix

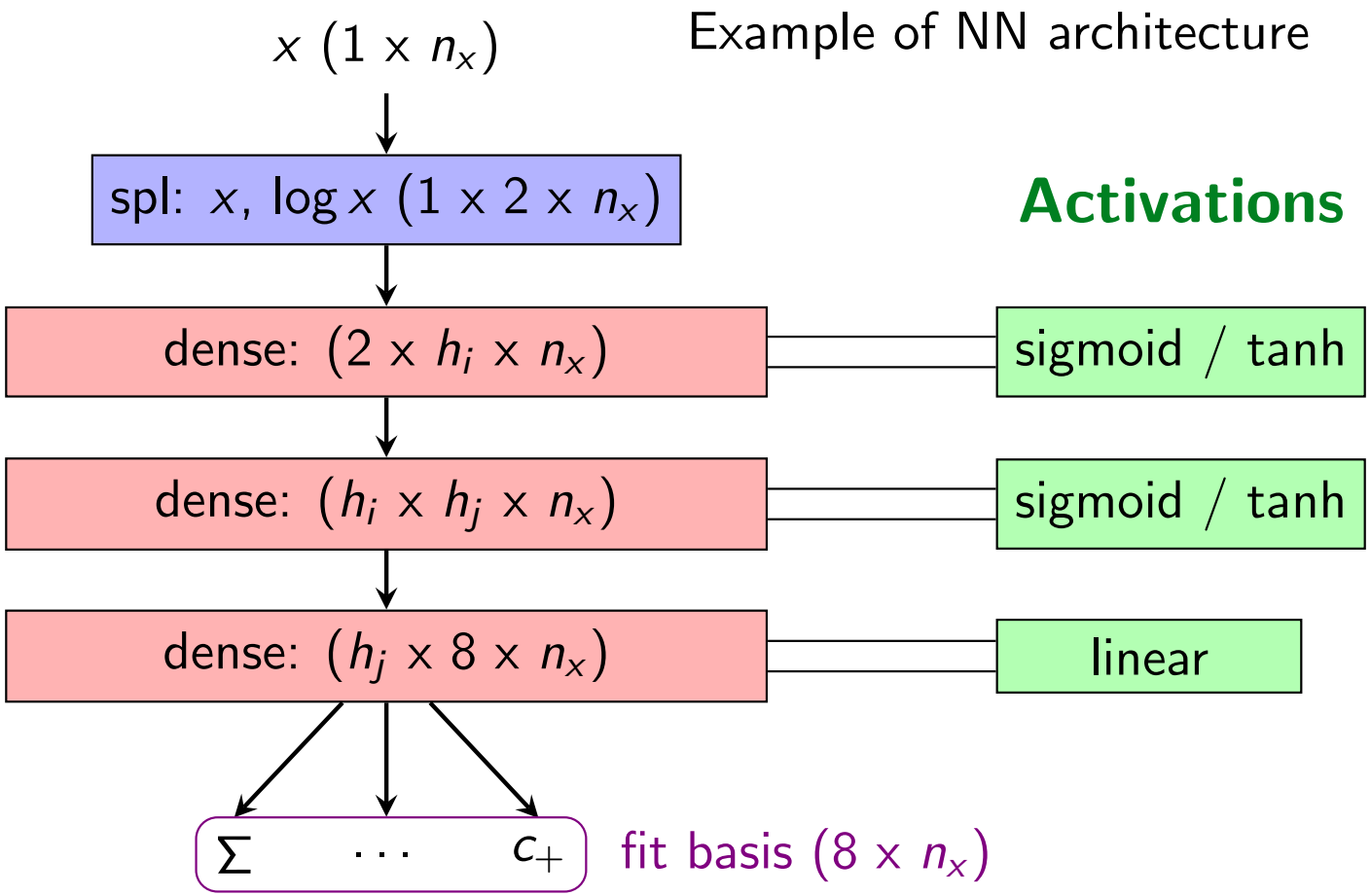


Note: The partonic cross section σ correspond to APFELgrid tables as described in hep-ph/1605.02070

The PDF model

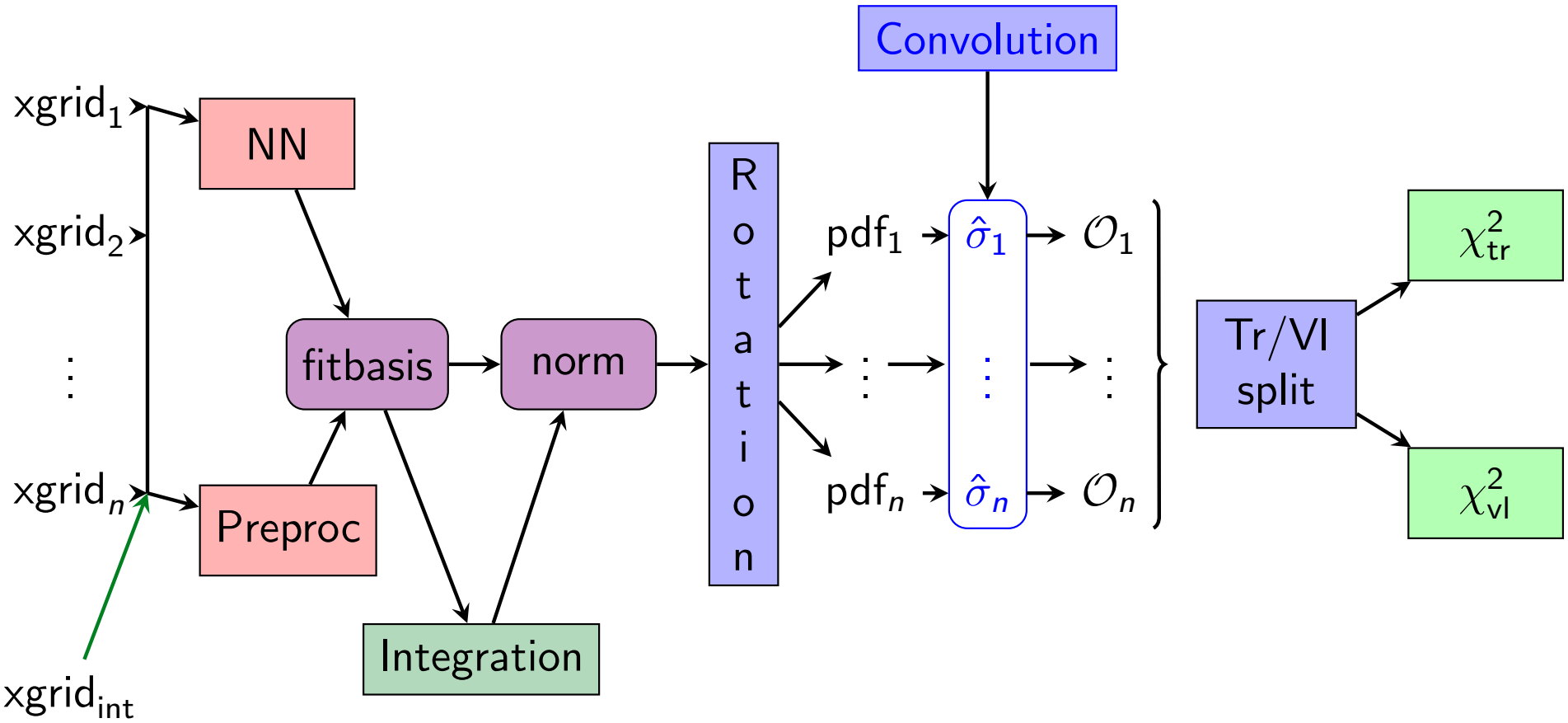


The Neural Network: $NN(x)$



Swapping and testing different network architectures is a matter of seconds: we can systematically scan and find the best model.

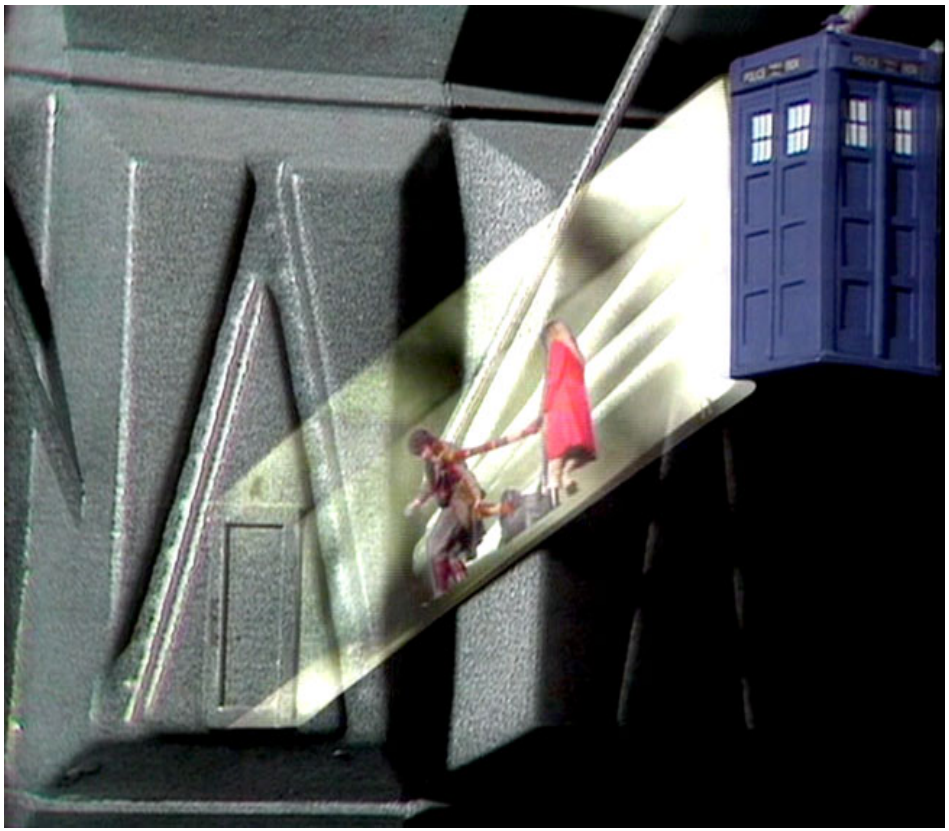
The full model



The art of the hyperparameter selection

With technology, what used to be hand-made can now be computer generated.

1978



2014

We can now let `n3fit` select its own hyperparameters

Scan over hyperparameters: fitting the methodology

The main goal of NNPDF was to reduce the bias introduced in the PDF fits by the choice of the functional form of the PDFs, but...

$\longrightarrow$ NN are defined by set of parameters

$\longrightarrow$ Not clear which is the best choice

$\longrightarrow$ Humans are usually good at recognising patterns

✗ but the wiser decision is not guaranteed

In order to overcome these issues we implement a hyperparameter scan: let the computer decide

✓ Scan over thousands of hyperparameter combinations

✓ Define a reward function to grade the model

The next step: fitting the whole methodology

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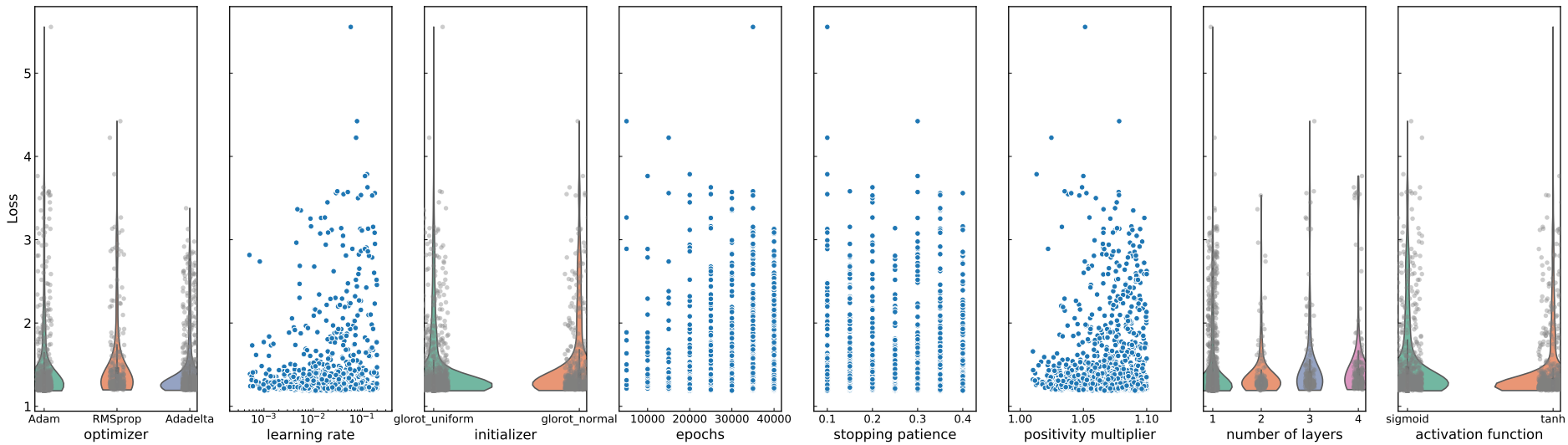
Hyperparameter scan

Each blue dot corresponds to a different set of hyperparameters.

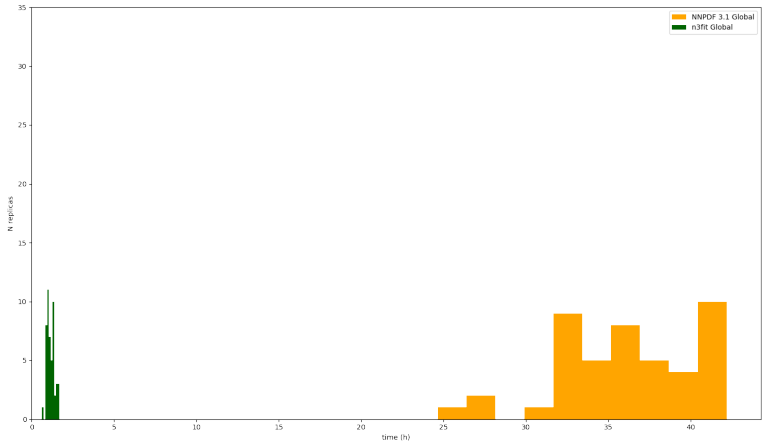


- ✓ Optimizer
- ✓ Initializer
- ✓ Stopping Patience
- ✓ Number of Layers
- ✓ Learning Rate
- ✓ Epochs
- ✓ Positivity Multiplier
- ✓ Activation Function

Results report

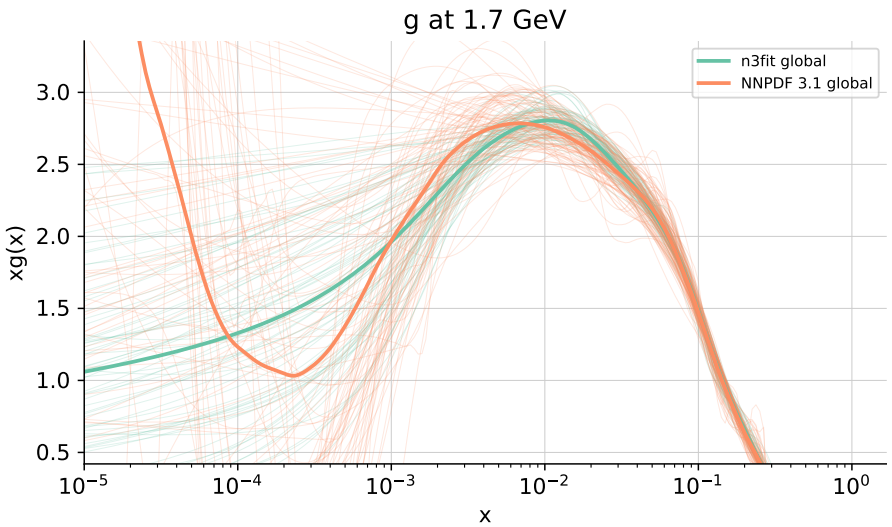
n3fit is fully implemented now and produces results which are compatible with previous releases of NNPDF.

	n3fit	NNPDF 3.1
χ^2	1.149	1.158
Avg time	70 minutes	35 hours
Memory	16 Gb	5 Gb
Stability	95%	70%



As an example we show a comparison using as a baseline a global NNPDF 3.1 NNLO fit against a model created by the hyperoptimization procedure.

Stability



✓ Better stability replica-by-replica

✓ More replicas satisfy post-fit requirements

Which translates to

✓ Even smaller computing times!

✓ More complete statistical analysis at the same cost

✓✓ More accurate PDF determination!

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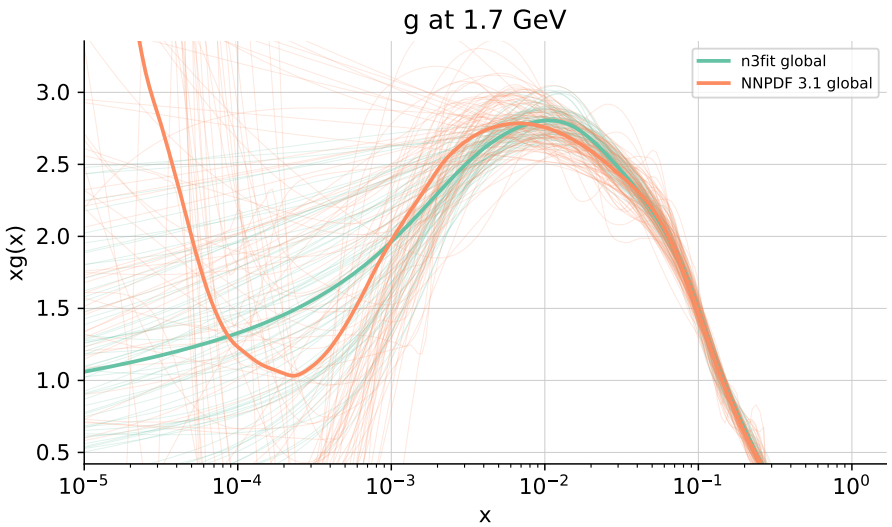

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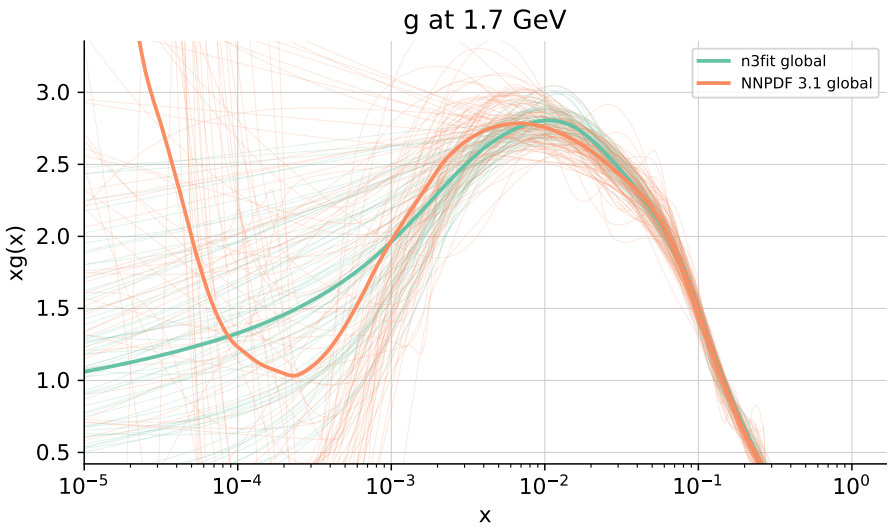

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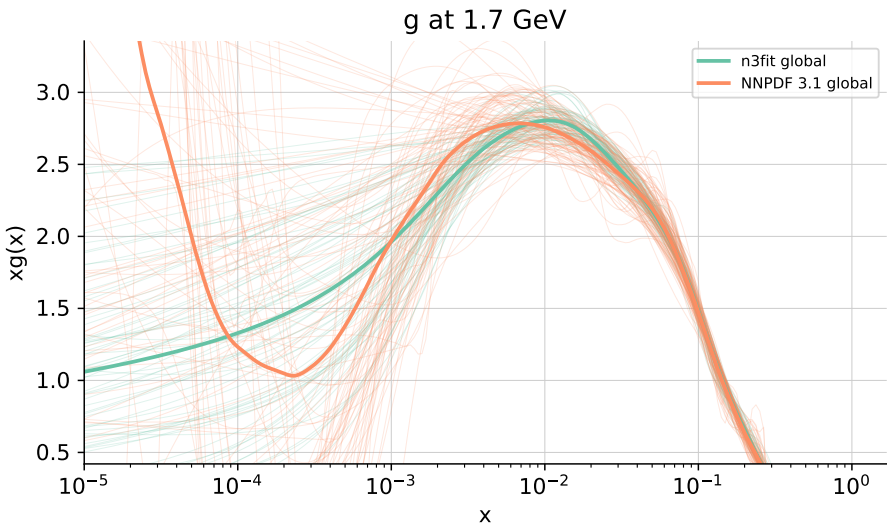

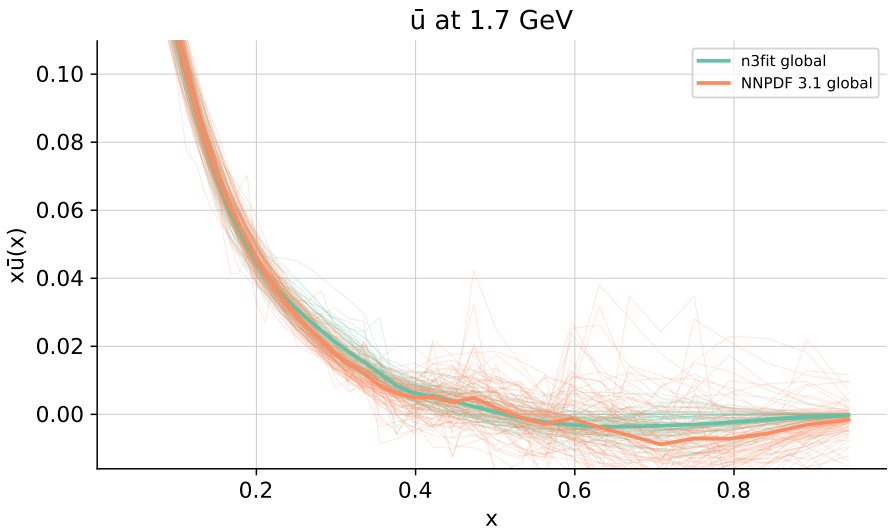

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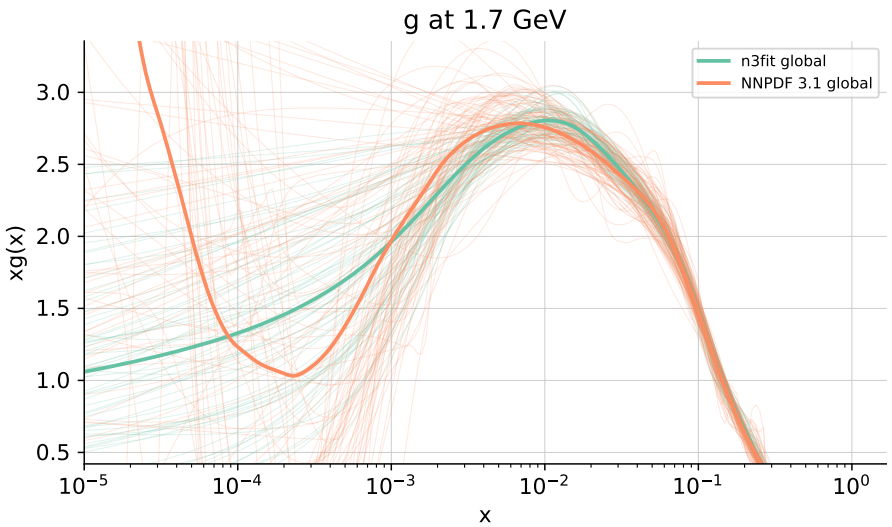

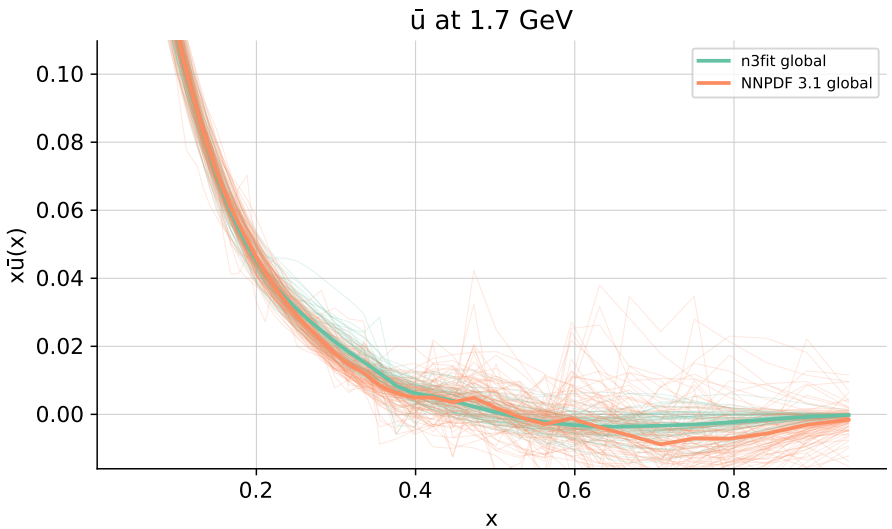

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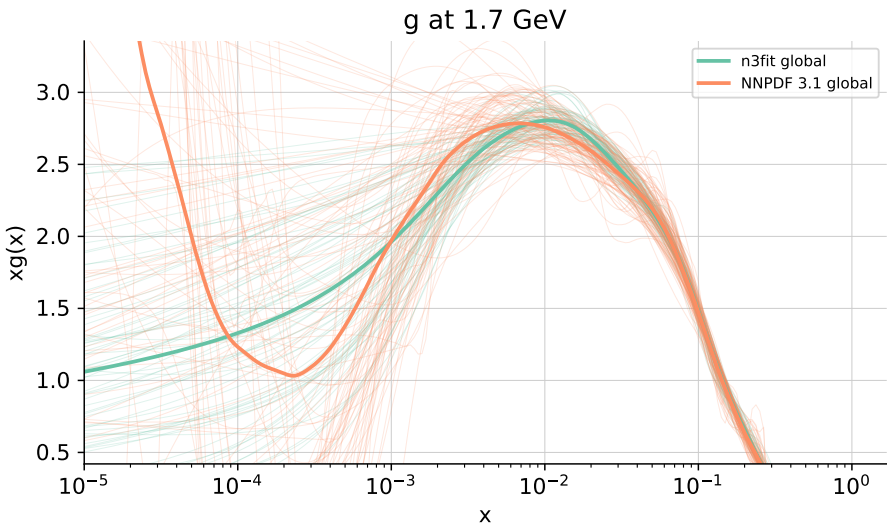

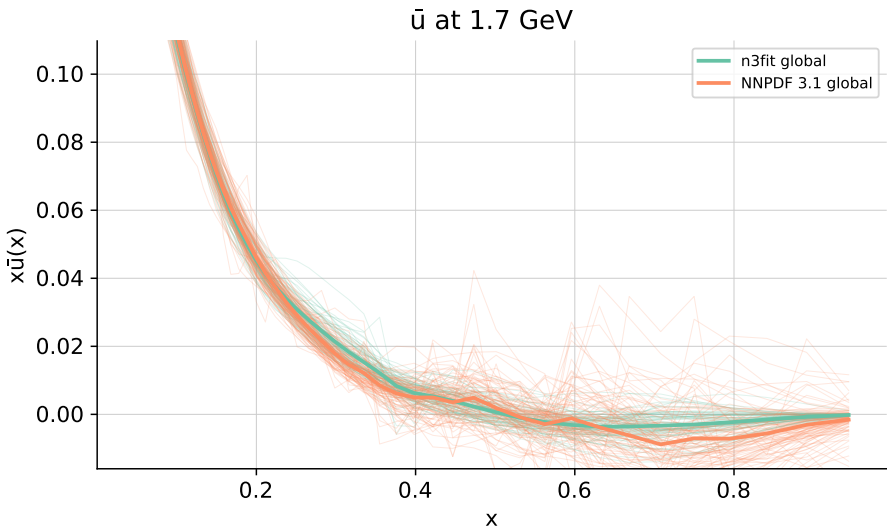

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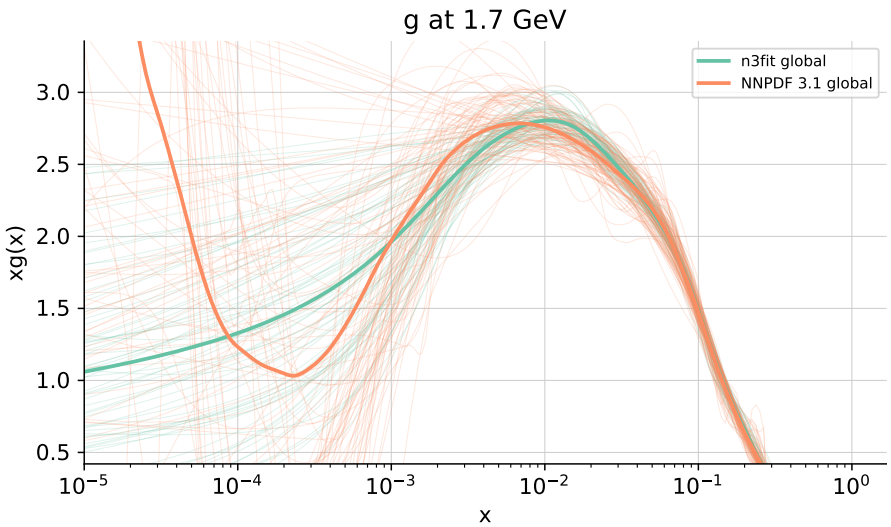

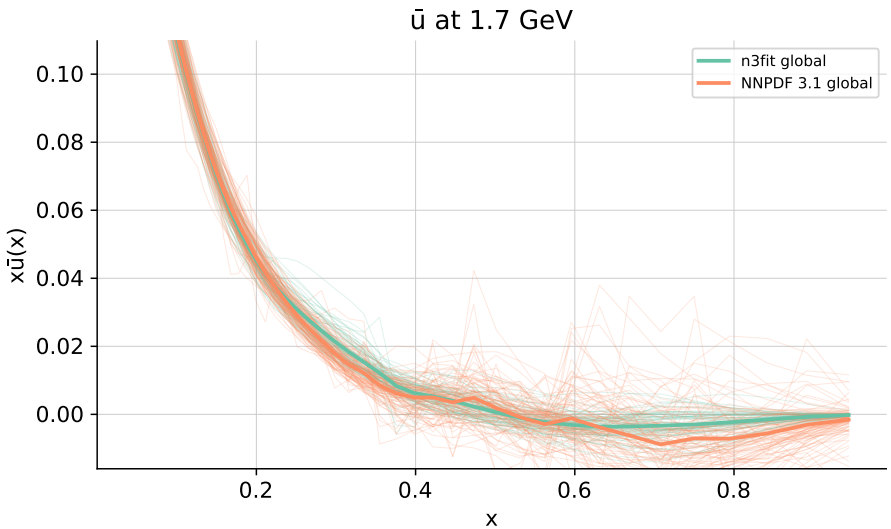

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Fit duration distribution

One of the most obvious improvements
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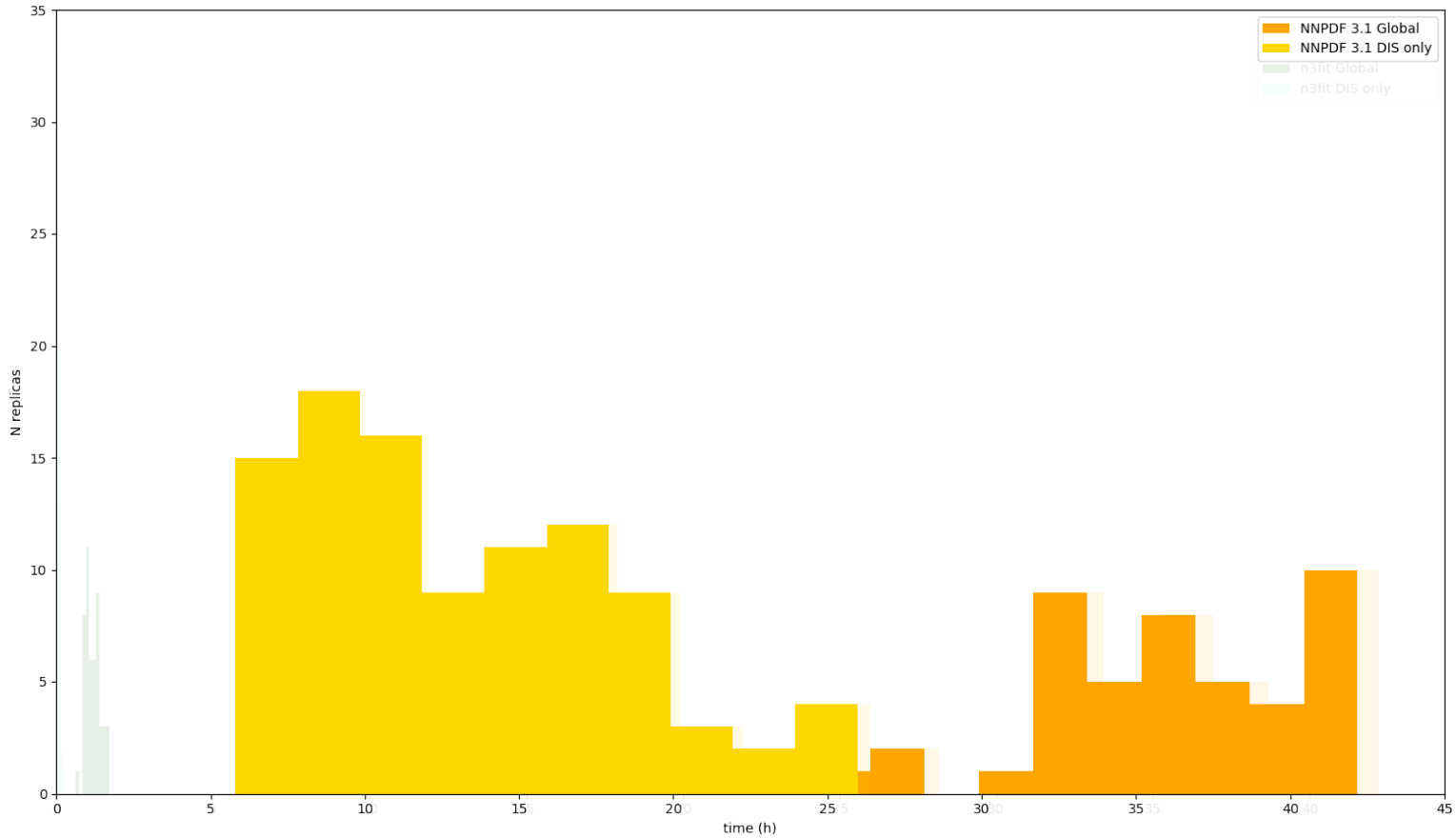

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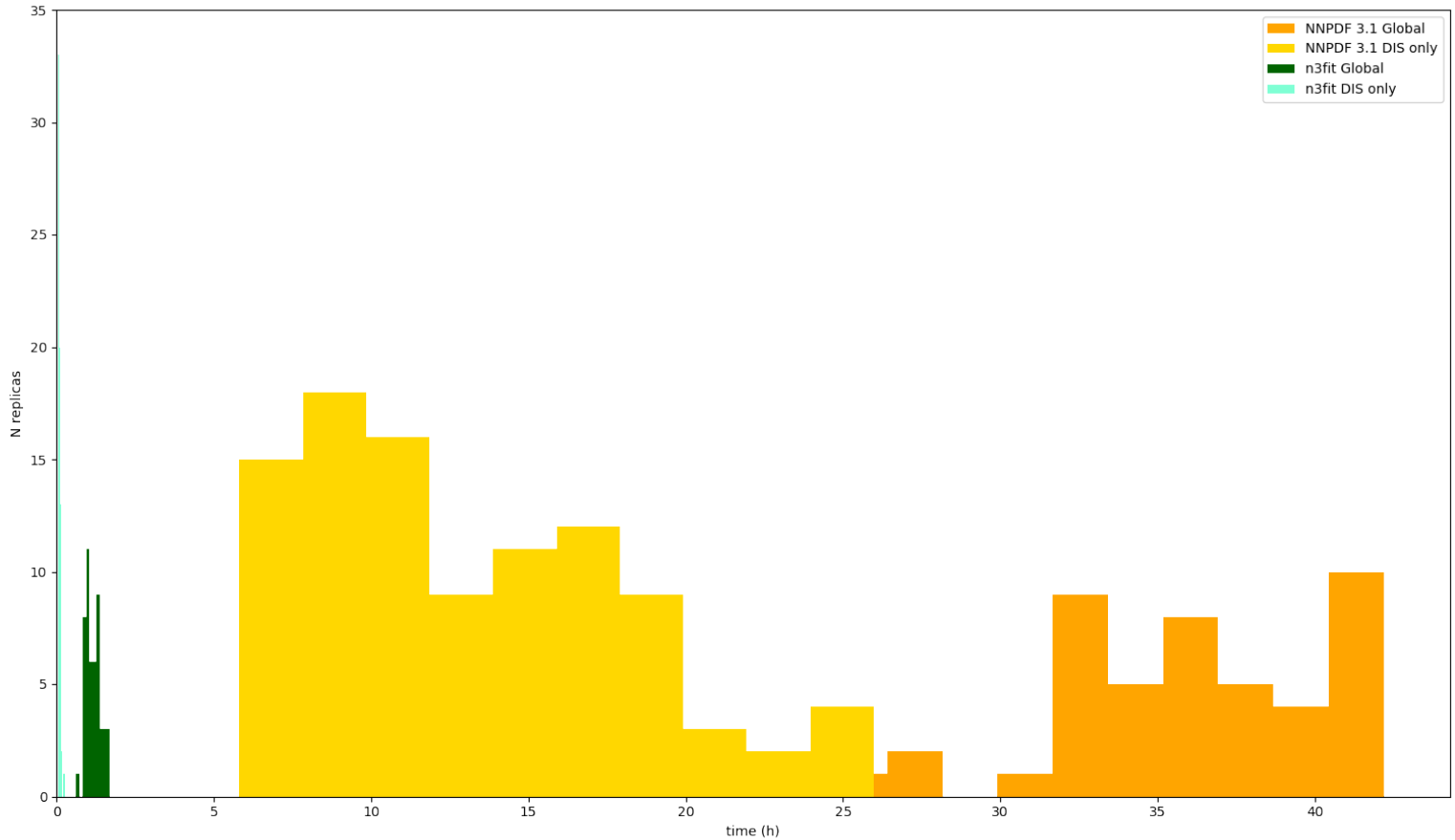
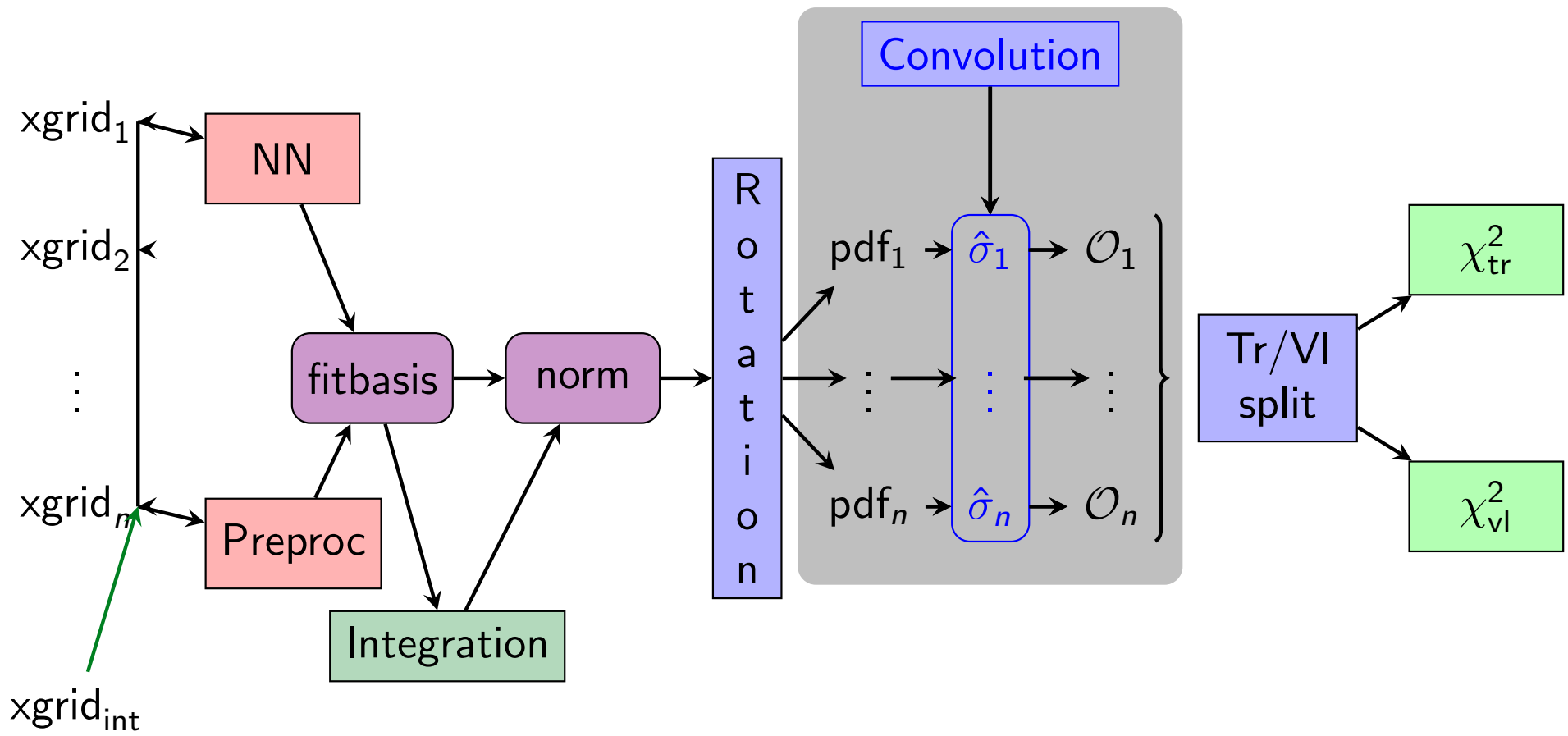


Customizing the operators

Tensorflow is very clever, but we have more information:



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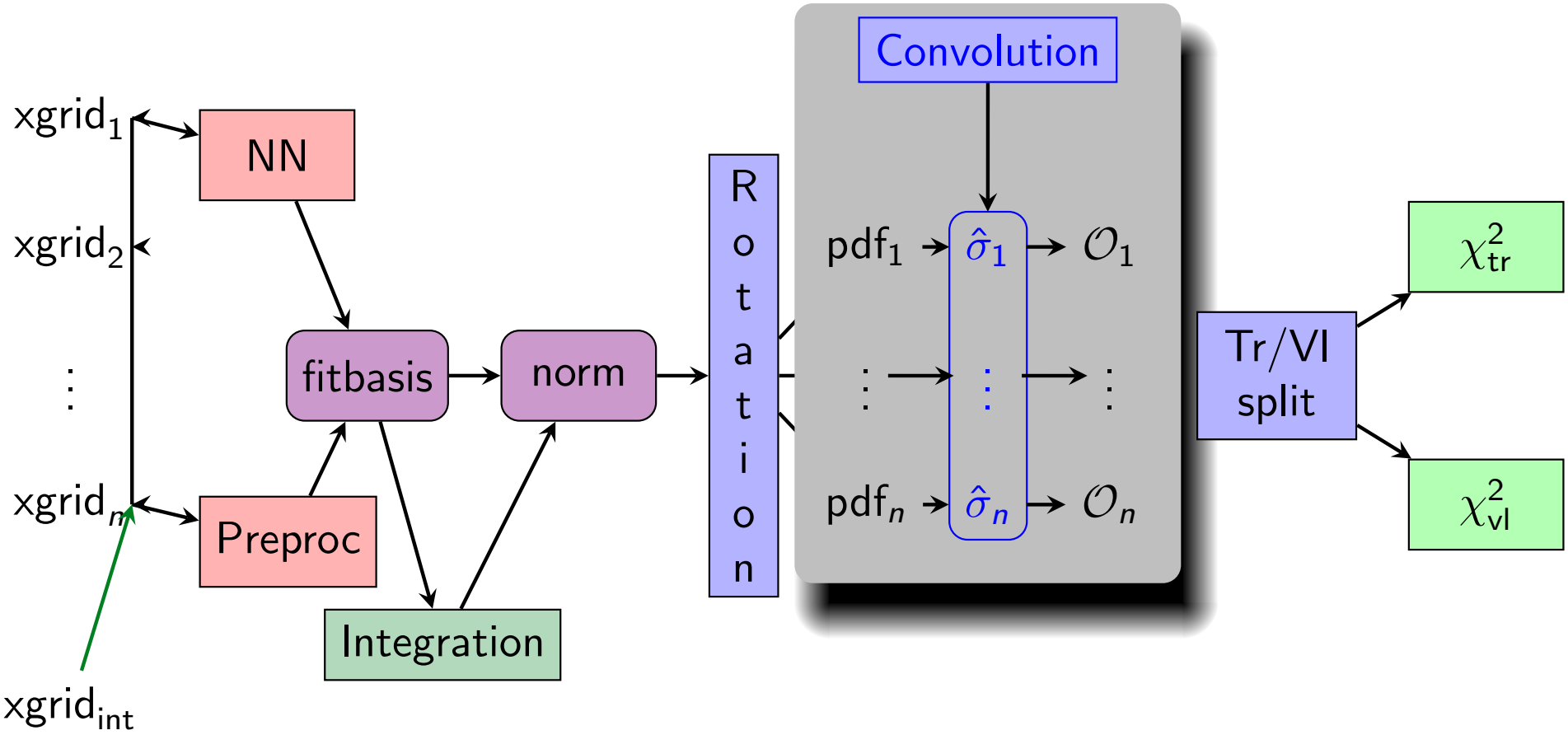

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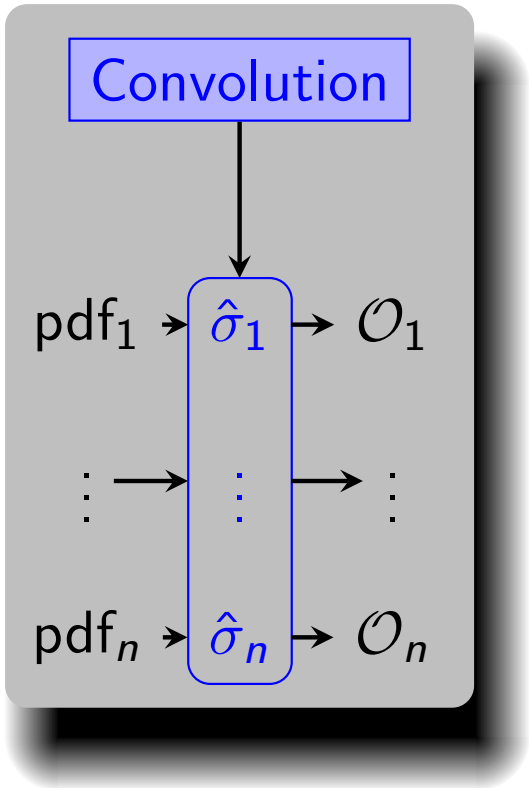
	TensorFlow	Our own
Memory Total	18.4 Gb	12.5 Gb
Memory Fit	16.3 Gb	10.4 Gb
Time/epoch (s)	0.5 s	0.3 s

As the memory is reduced we can "fit" more and more replicas in one single run: time reduction is a function of the memory.



Hardware accelerating the fits

The problem of fitting many replicas is the perfect candidate for GPU parallelization

$\longrightarrow$ Not massively CPU intensive

$\longrightarrow$ Same operations are repeated for all replicas

Example operation, contraction of rank-2 tensors: $z_M^N = x_\alpha^N y_M^\alpha$.

N	M	α	CPU AVX	TF (CPU)	TF (GPU)	OpenCL (GPU)
8	10^3	10^5	0.48	0.44	0.552	1.10
8	10^4	10^5	4.86	4.13	4.68	3.41
$8 \cdot 10^3$	10^4	10^4	48.8	1.89	1.24	15.8

Comparison on the time-cost (in seconds) per operation

CPU in table corresponds to intel i9-9980XE

GPU in table corresponds to nvidia Titan V

Summary

✓ We have achieved a very powerful, flexible and fast machinery for PDF fitting.

✓ Faster run times: iterate over different choices of models or parameters.

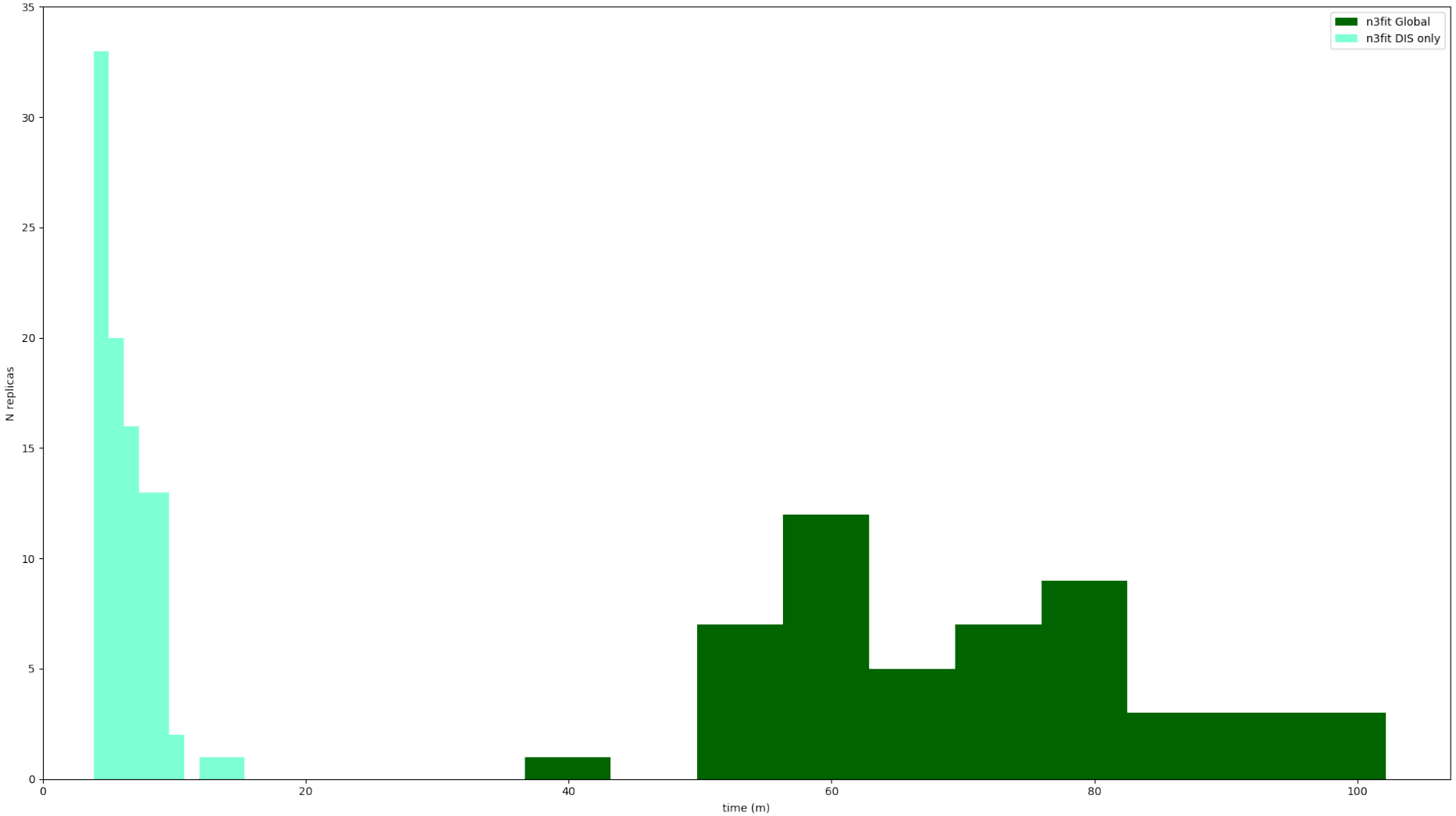
✓ The framework allows full customization *by design*.

⟶ **The cost of doing new studies is reduced, both the development/implementation and the raw computational cost.**

Future: can we also fit using FPGAs?

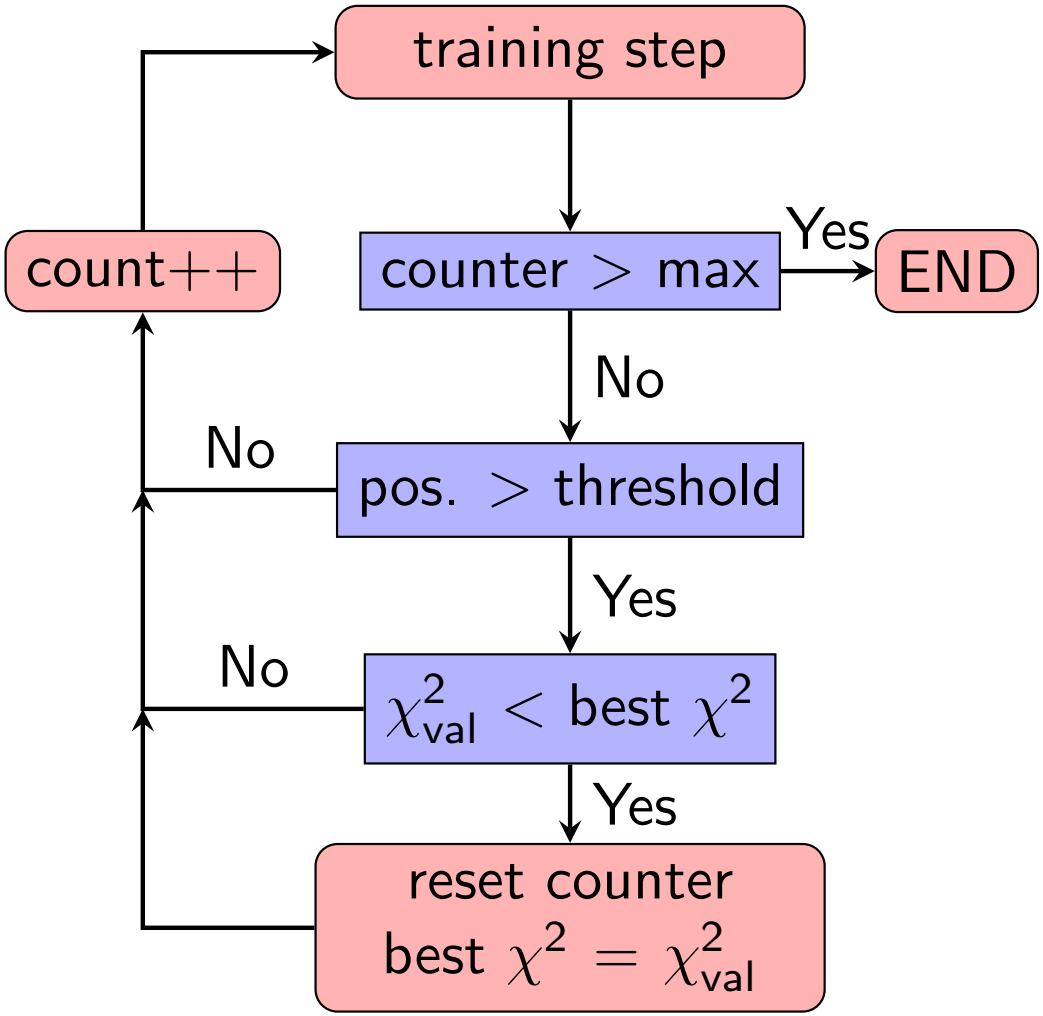
Thanks!

Zoom-in on the timings



Stopping

`Stopping method:` **Look-back method where positivity passes**



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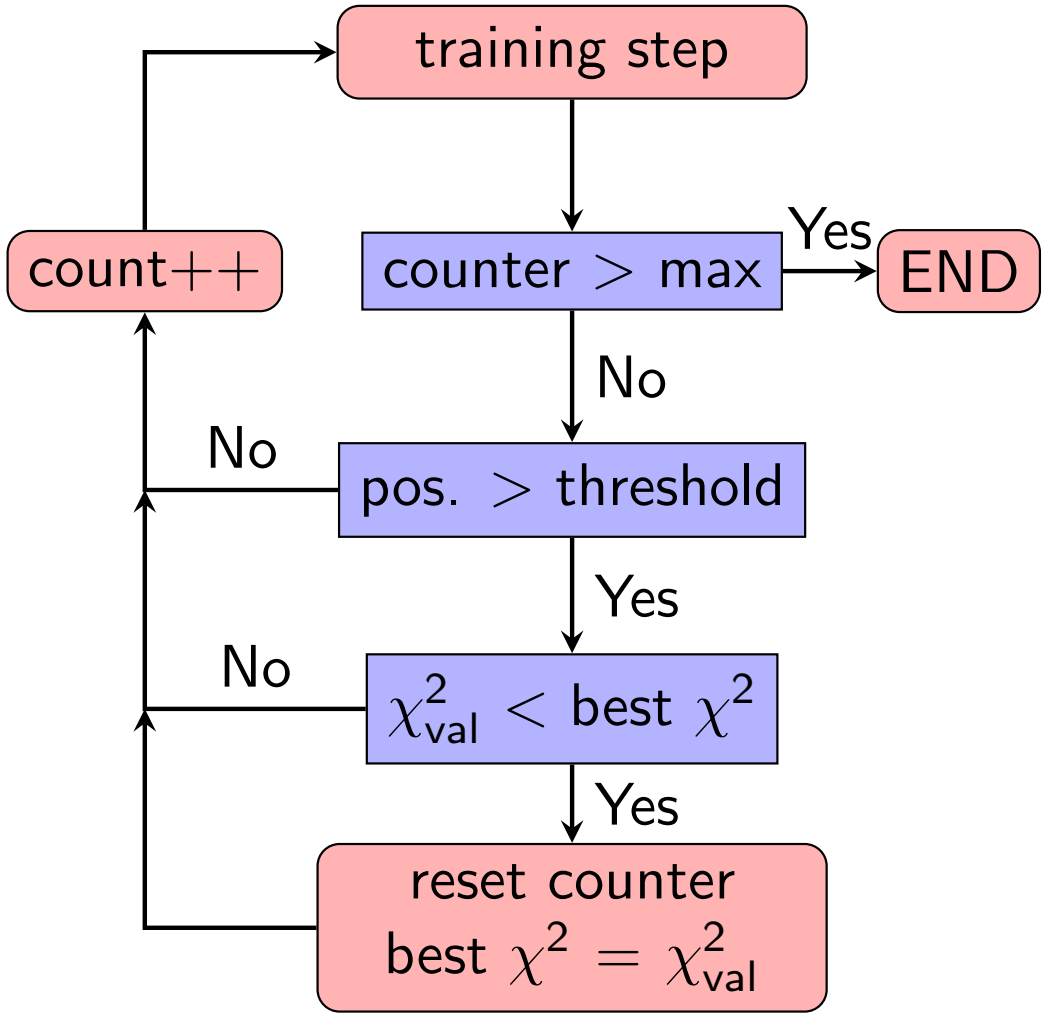

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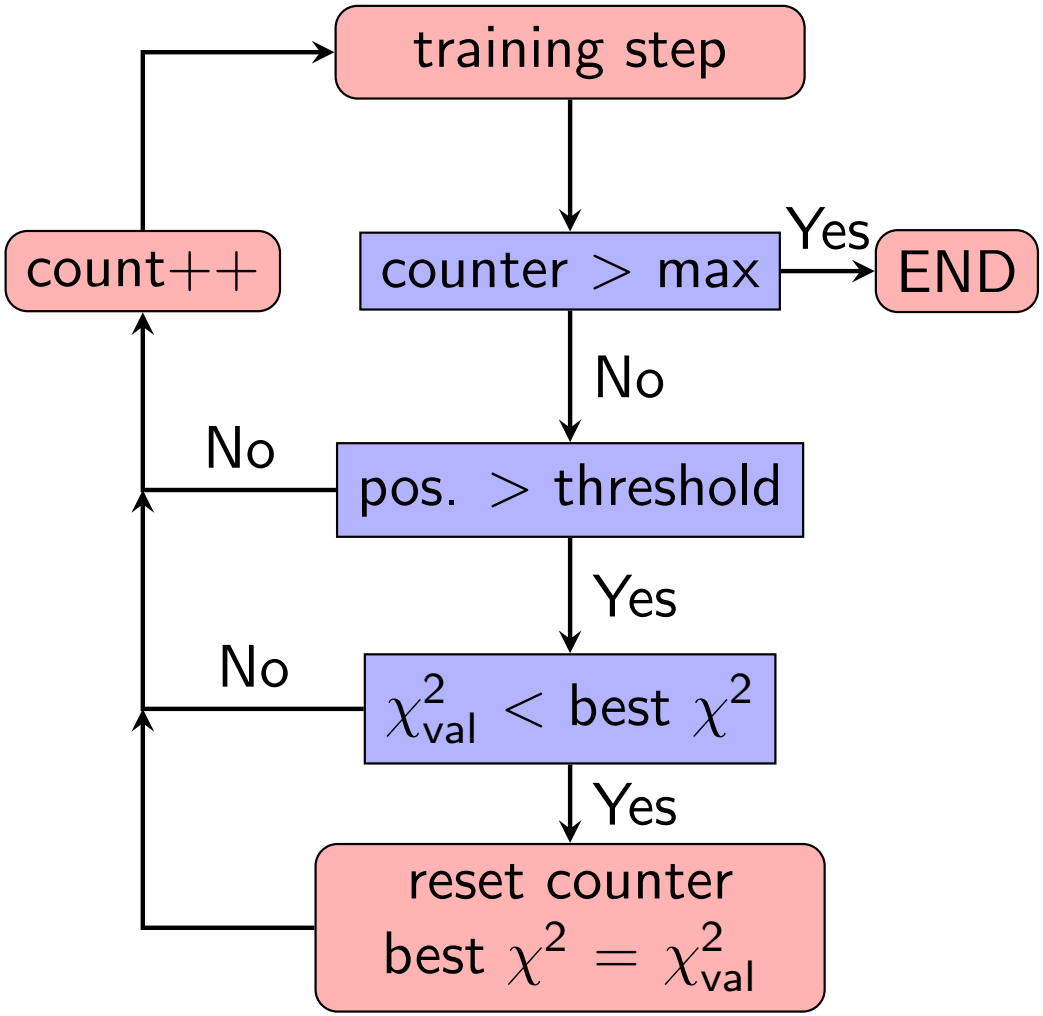

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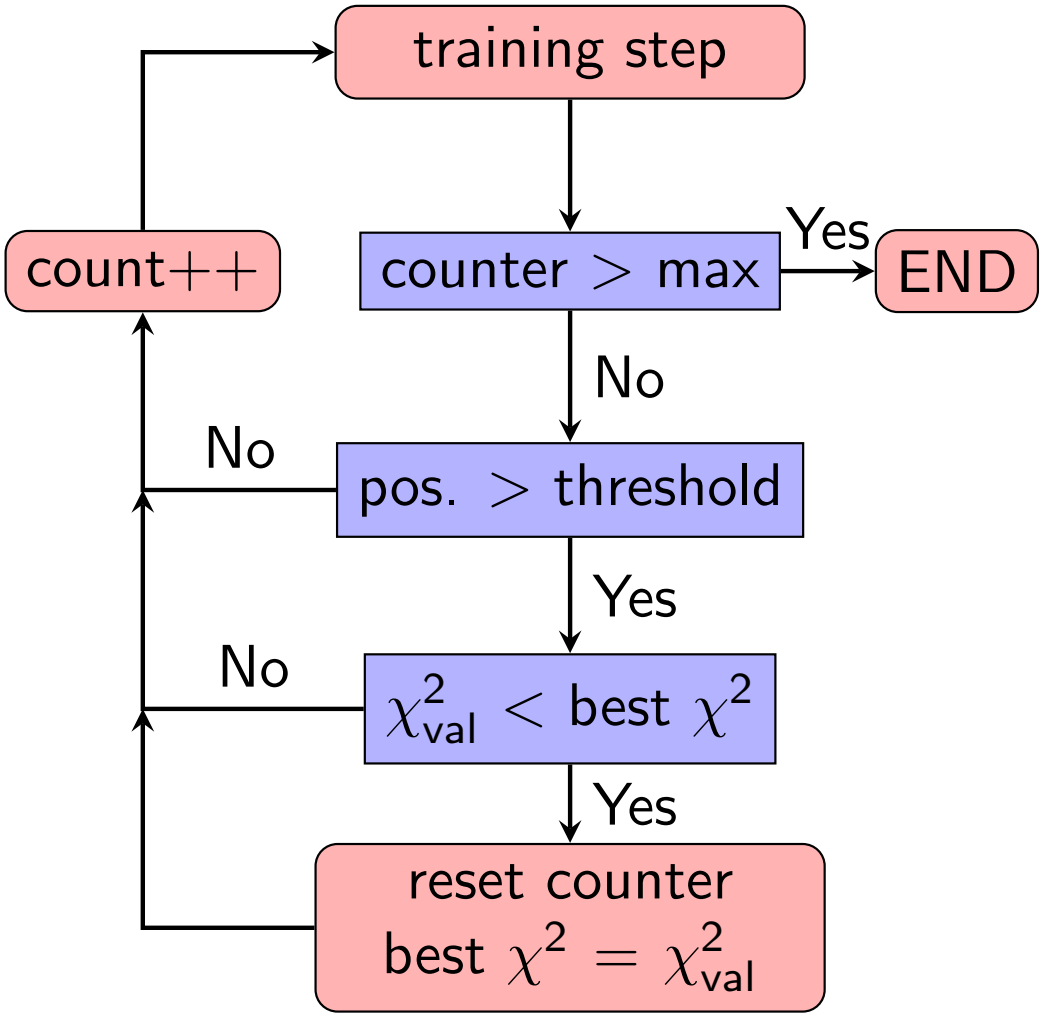
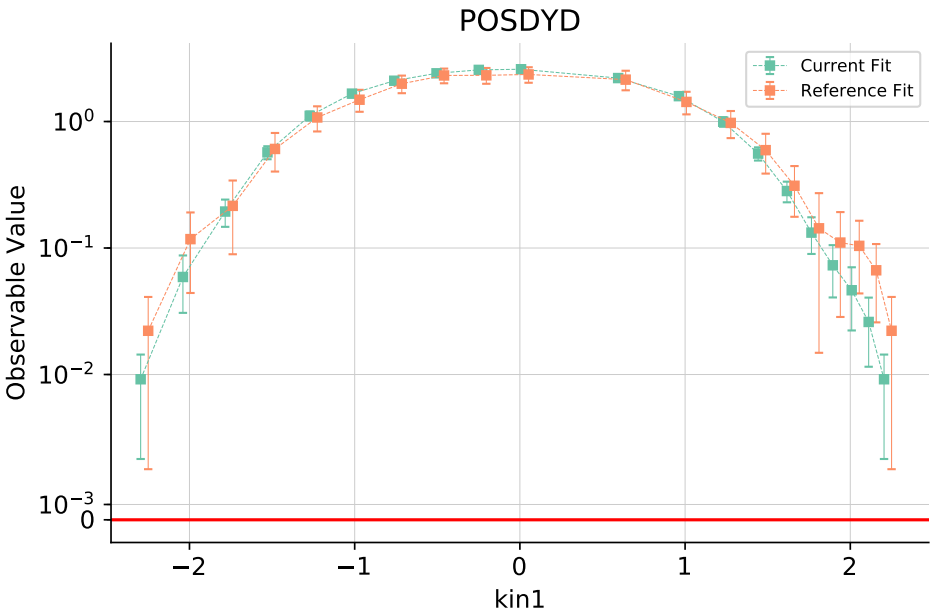
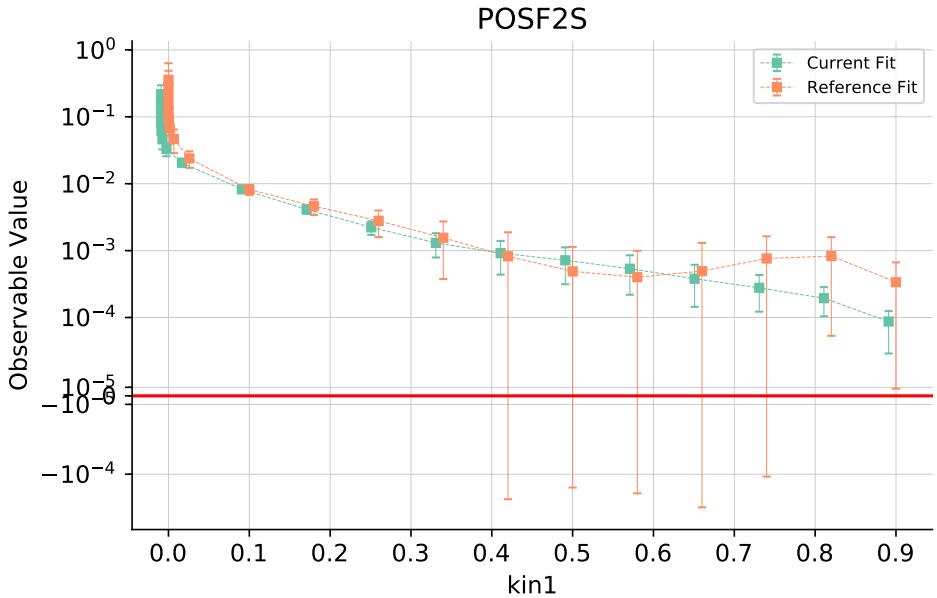
- ✓ Minimize χ^2 of validation sets
- ✓ Enforces positivity constraints



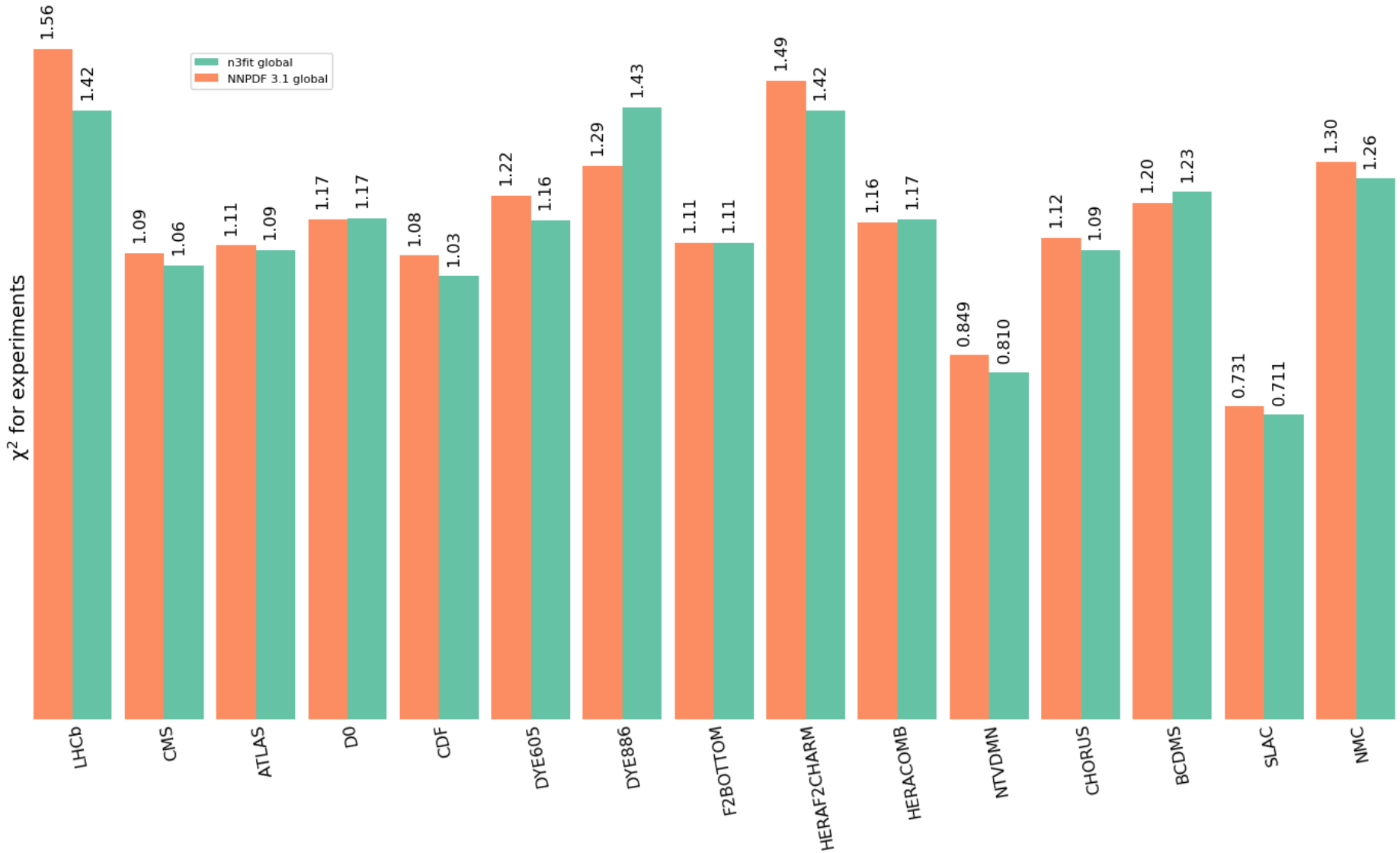
Positivity constrained

Once all these considerations are applied, we obtain no replicas of negative positivity.

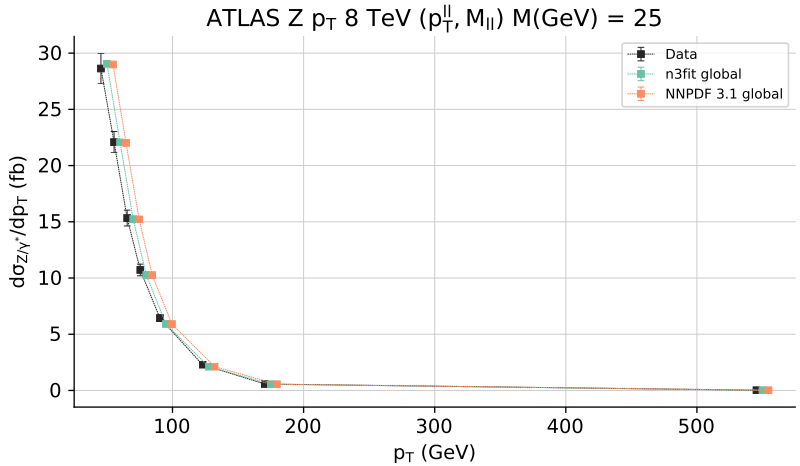


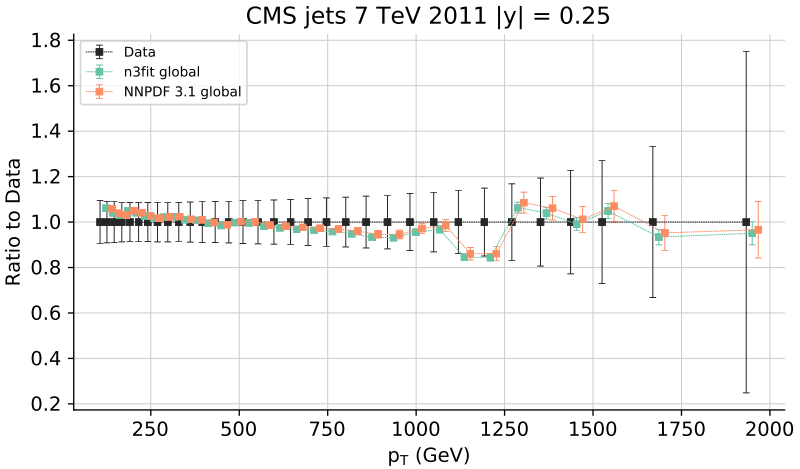


Per-experiment results



Comparison to data





→ Results compatible with NNPDF 3.1

→ Not only a similar χ^2-goodness but also similar per-point results

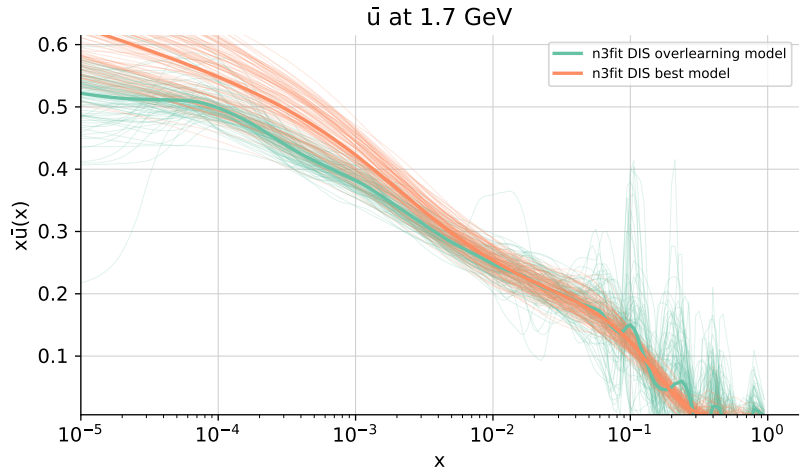
✓ The new methodology is compatible with the previous one!

Warning: overfitting!

With great power comes great responsability.

An unsupervised parameter scan is dangerous: it can find that overfitting is preferable.

- ✗ It did minimise the validation!
- ✗ Hyperopt is able to trick cross-validation when choosing the model.



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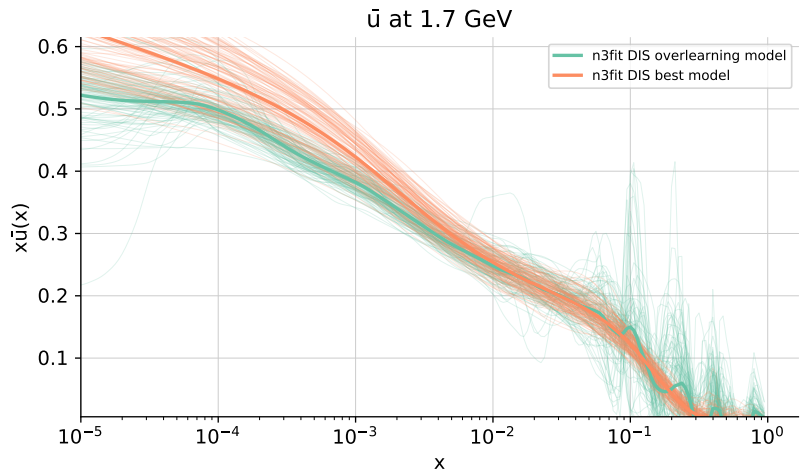

Solution:

- ✓ Create a test-set:

  Take a few experiments out of the hyperparameter scan and use them to probe the generalization power of the network