

New Physics Learning Machine (NPLM)

Gaia Grosso^{1,2}

¹University and INFN of Padova, ²CERN



Istituto Nazionale di Fisica Nucleare
SEZIONE DI PADOVA
Servizio Fondi Esterini



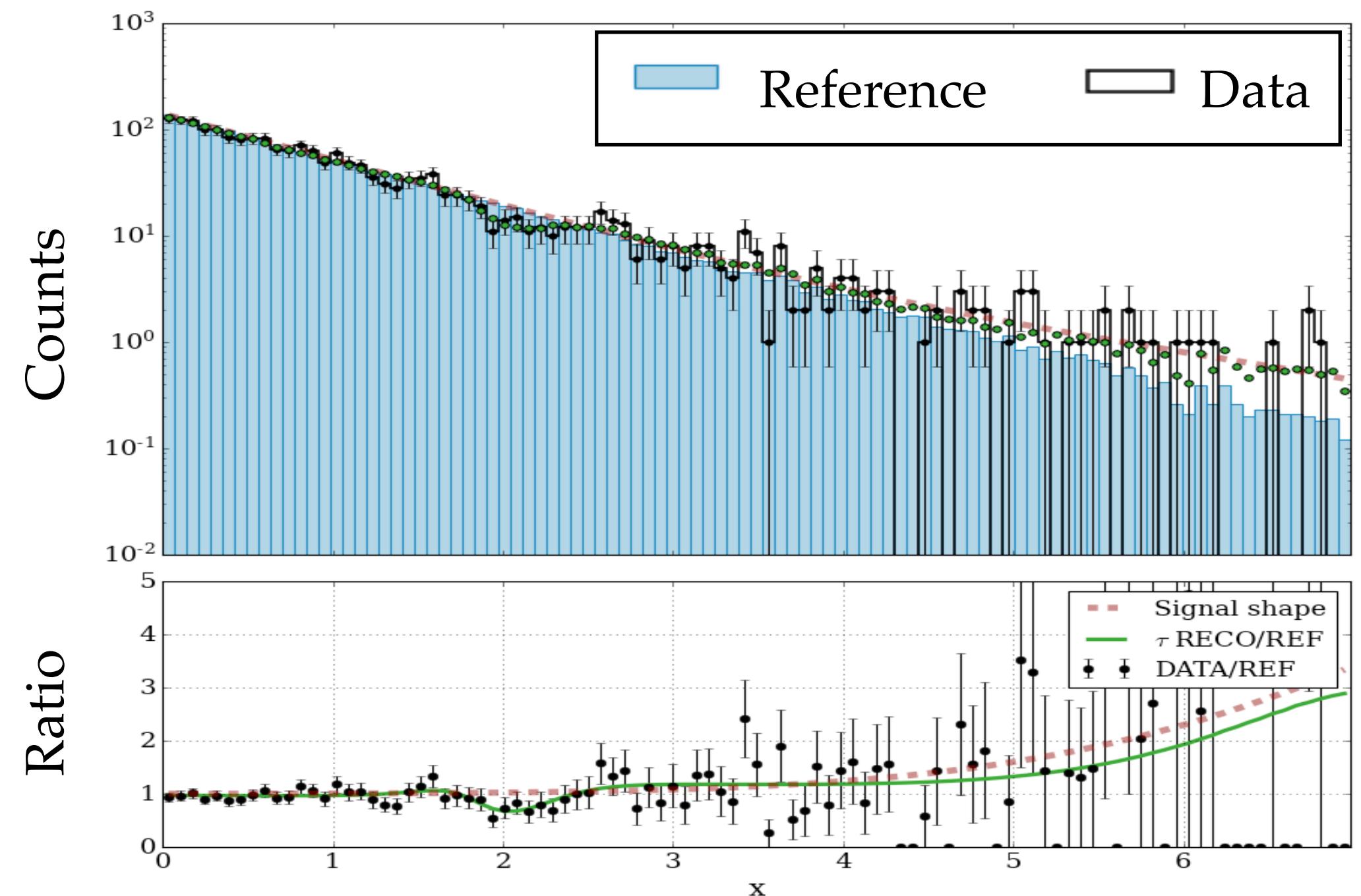
Dipartimento
di Fisica
e Astronomia
Galileo Galilei

In this talk

What is NPLM?

tool for **goodness-of-fit** tests, based on the principle of maximum-likelihood-ratio.

- Signal agnostic
- Multivariate
- Unbinned



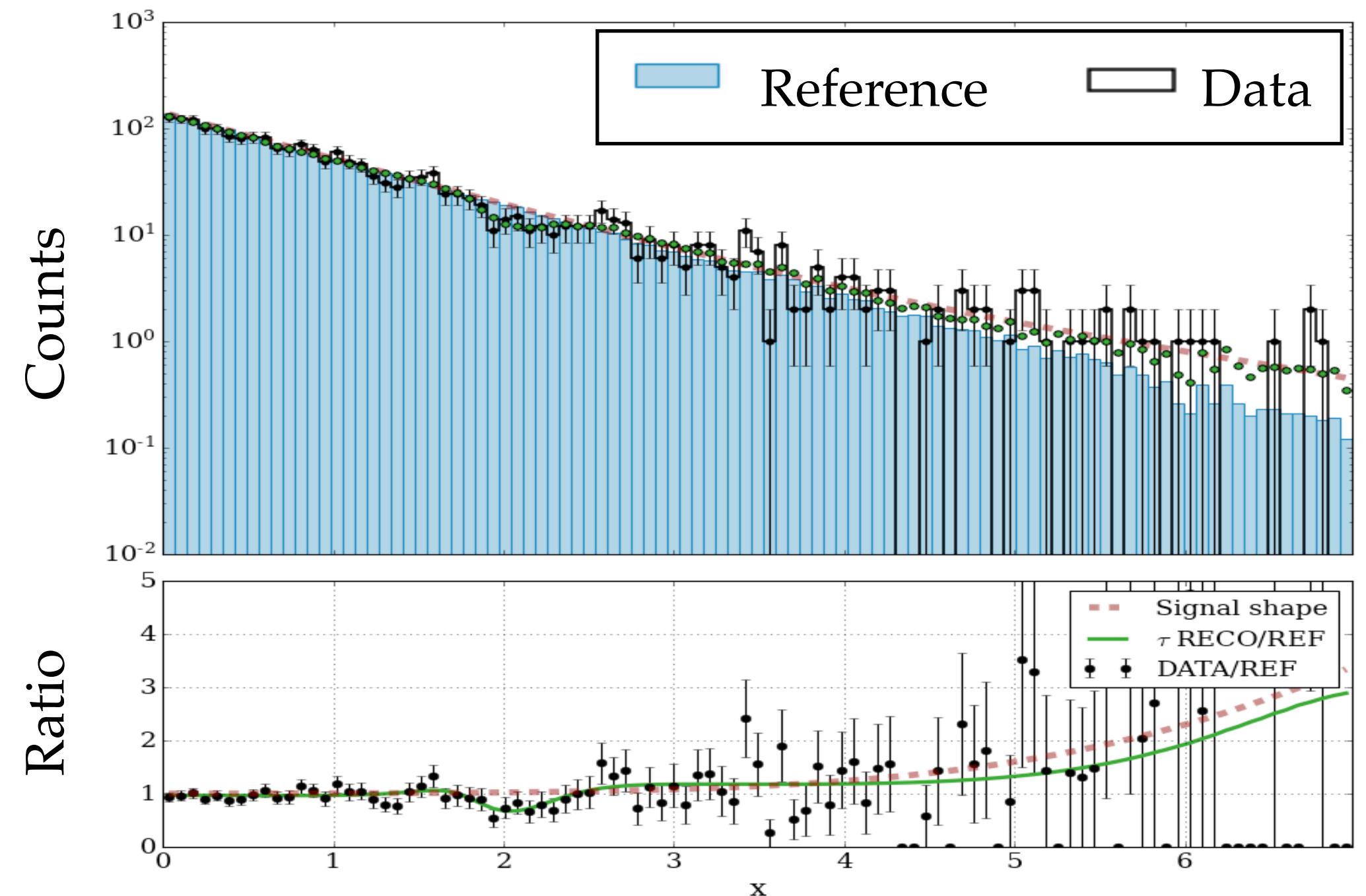
How well does the Reference model describe the data?

In this talk

What is NPLM *for*?

tool for **goodness-of-fit** tests, based on the principle of maximum-likelihood-ratio.

- Model-independent New Physics searches at collider experiments
- Data quality monitor (DQM)
- Generator validation



How well does the Reference model describe the data?

In this talk

How does it work?

Complete analysis strategy to test the data for departures from a Reference model (from the data to a p -value, taking care of systematic uncertainties if needed).

- Main concepts and implementation using NN

“Learning New Physics from a Machine” - d’Agnolo, Wulzer, [Phys. Rev. D \(2018\)](#)

“Learning Multivariate New Physics” - d’Agnolo, Grosso, Pierini, Wulzer, Zanetti, [Eur. Phys. J. C 81, 89 \(2021\)](#)

- Systematic uncertainties

“Learning New Physics from an Imperfect Machine” - d’Agnolo, Grosso, Pierini, Wulzer, Zanetti [Eur. Phys. J. C 82, 275 \(2022\)](#)

- Hands on a 1D toy model (material for Q&A)

NPLM main concepts and NN implementation

New Physics Learning Machine (NPLM)

Main Concepts (negligible uncertainties)

- Goal: performing a **maximum-likelihood-ratio hypothesis test**

End-to-end strategy, from the data to a p -value for the discovery (frequentist approach)

$$t(\mathcal{D}) = \max_{\mathbf{w}} \left[2 \log \frac{\mathcal{L}(\mathcal{D} | H_w)}{\mathcal{L}(\mathcal{D} | R_0)} \right]$$

R_0 : null hypothesis
 H_w : alternative hypothesis

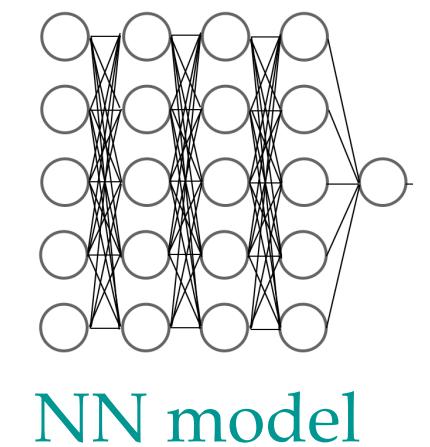
- Exploiting a Neural Network (NN) to **parametrize** the data distribution in terms of a Reference distribution (R_0)

$$n(x | T) \approx n(x | H_{\hat{w}}) = n(x | R_0) e^{f(x, \hat{w})}$$

True (T) data distribution
Unknown

Data distribution learnt by the NN
Alternative hypothesis

Reference distribution
Null hypothesis (SM)



- Signal-model-independent**: reduced assumptions on the signal hypothesis

New Physics Learning Machine (NPLM)

Main Concepts (negligible uncertainties)

Maximum Likelihood from minimal loss:

Test statistic

$$\bar{t}(\mathcal{D}) = 2 \max_{\mathbf{w}} \log \left[\frac{\mathcal{L}(\mathcal{D} | H_{\mathbf{w}})}{\mathcal{L}(\mathcal{D} | R_0)} \right] = -2 \min_{\mathbf{w}} \{ \bar{L}[f(\cdot; \mathbf{w})] \}$$

\mathbf{w} : trainable parameters on the NN model

D : data sample

R : reference sample (built according to the R_0 hypothesis); could be weighted (w)

Loss function

$$\bar{L}[f(x; \mathbf{w})] = - \sum_{x \in \mathcal{D}} [f(x; \mathbf{w})] + \sum_{x \in \mathcal{R}} w_x [e^{f(x; \mathbf{w})} - 1]$$

Assumptions:

- $N_R \gg N_D$ the statistical fluctuations of the reference sample are negligible.
- the weights of the reference sample (w) are such that the reference sample is normalised to match the data sample luminosity $\sum_{x \in \mathcal{R}} w_x = N(R_0)$

New Physics Learning Machine (NPLM)

Main Concepts (negligible uncertainties)

Maximum Likelihood from minimal loss:

Test statistic

$$\bar{t}(\mathcal{D}) = 2 \max_{\mathbf{w}} \log \left[\frac{\mathcal{L}(\mathcal{D} | H_{\mathbf{w}})}{\mathcal{L}(\mathcal{D} | R_0)} \right] = -2 \min_{\mathbf{w}} \{ \bar{L}[f(\cdot; \mathbf{w})] \}$$

Loss function

$$\bar{L}[f(x; \mathbf{w})] = - \sum_{x \in \mathcal{D}} [f(x; \mathbf{w})] + \sum_{x \in \mathcal{R}} w_x [e^{f(x; \mathbf{w})} - 1]$$

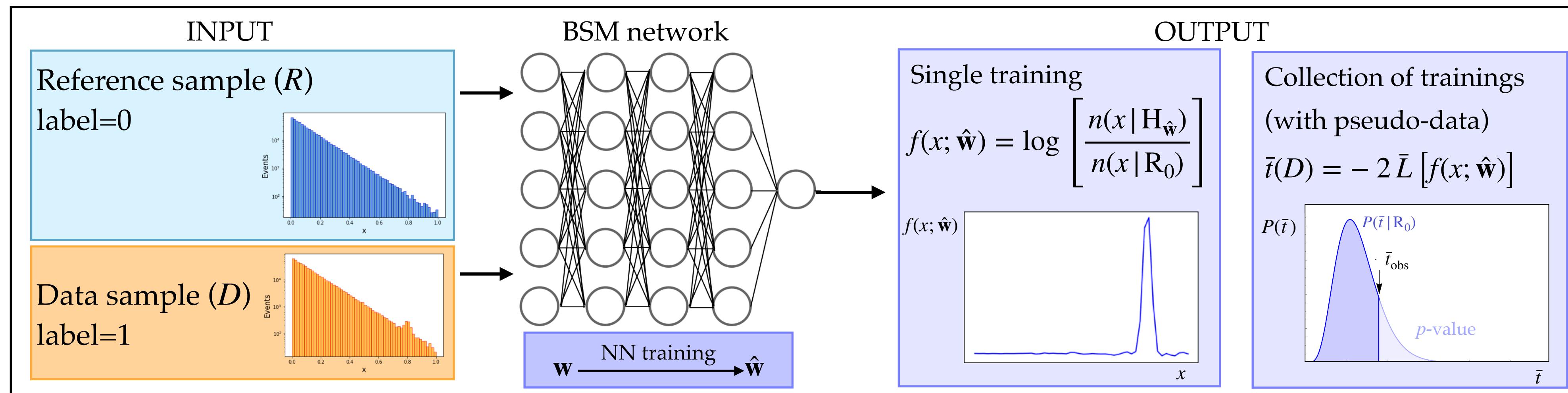
\mathbf{w} : trainable parameters on the NN model

D : data sample

R : reference sample (built according to the R_0 hypothesis); could be weighted (w)

Assumptions:

- $N_R \gg N_D$ the statistical fluctuations of the reference sample are negligible.
- the weights of the reference sample (w) are such that the reference sample is normalised to match the data sample luminosity $\sum_{x \in R} w_x = N(R_0)$

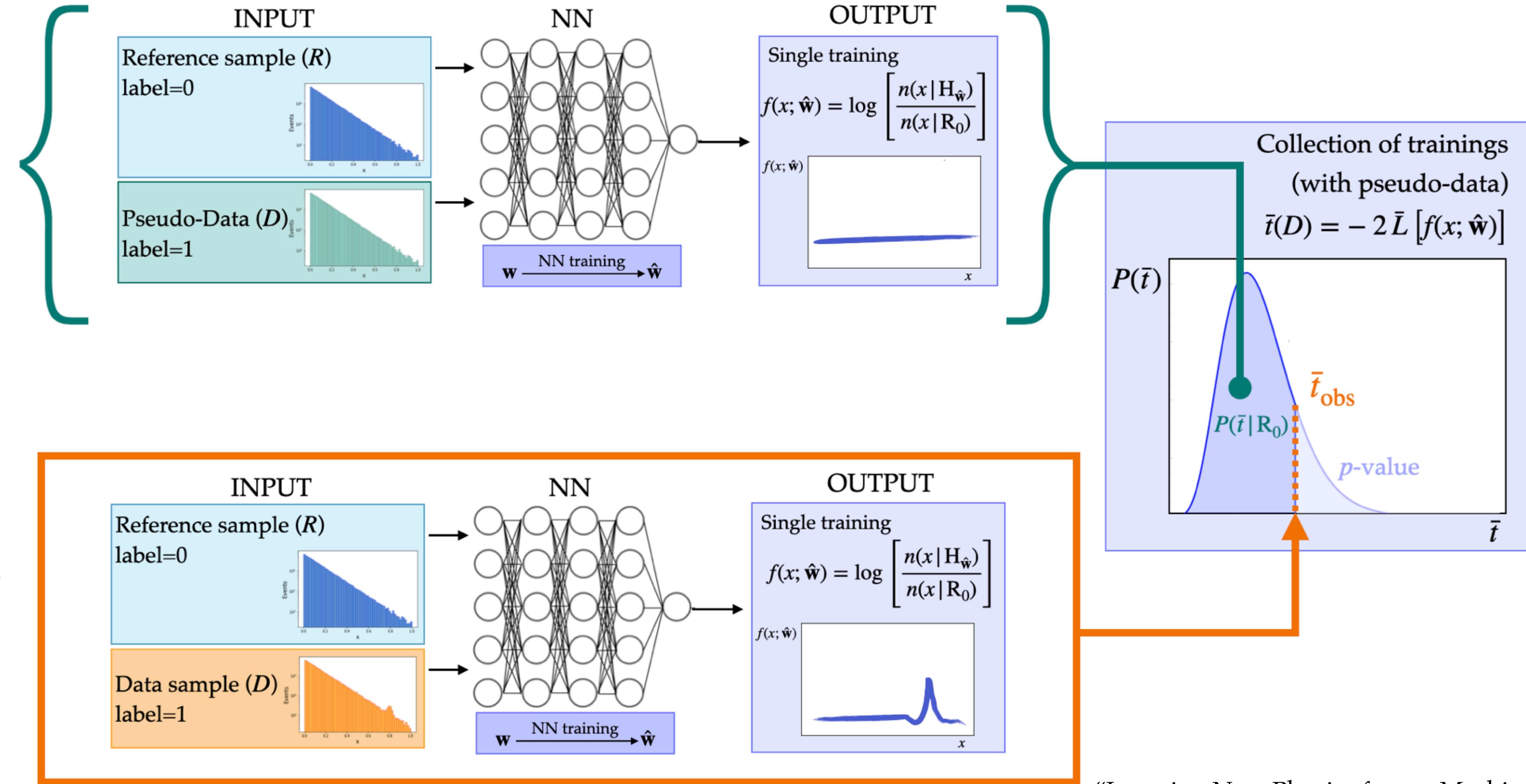


"Learning New Physics from a Machine" [Phys. Rev. D](#)

New Physics Learning Machine (NPLM)

Main Concepts (negligible uncertainties)

1. Run NPLM on toy experiments to simulated the response under the null hypothesis



New Physics Learning Machine (NPLM)

Main Concepts (negligible uncertainties)

Asymptotic formula for the \bar{t} distribution under R_0 :

Wilks-Wald theorem:

Θ_0 : set of parameters describing H_0

Θ_1 : set of parameters describing H_1

If $H_0 \subseteq H_1$, then under the H_0 hypothesis the test statistic

$$t(\mathcal{D}) = 2 \log \frac{\mathcal{L}(H_1 | \mathcal{D})}{\mathcal{L}(H_0 | \mathcal{D})}$$

asymptotically follows a χ^2_{df} distribution with $df = |\Theta_1| - |\Theta_0|$



If the Wilks' theorem hold, the target distribution for \bar{t} under the R_0 hypothesis is a χ^2_{df} with $df = |\mathbf{w}|$.

Due to the **finite size** of the training samples, the **sparsity** of the data (especially in multivariate problems) and the **approximation** errors, the distribution of $\bar{t}(D)$ under R_0 does not follow the target $\chi^2_{|\mathbf{w}|}$ by default.

→ a **(NN) MODEL REGULARIZATION** procedure can solve this problem!

New Physics Learning Machine (NPLM)

Main Concepts (negligible uncertainties)

NN Model regularization:

Weight clipping parameter:

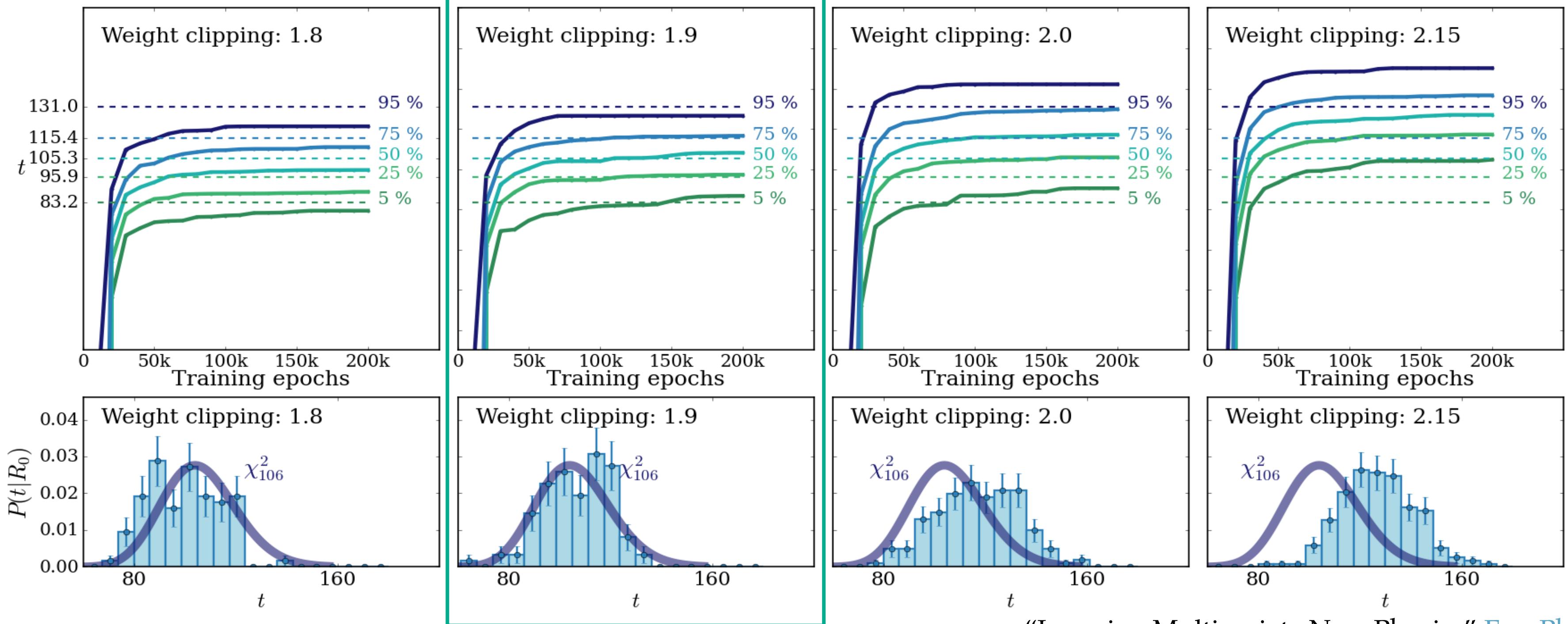
Upper boundary to the magnitude that each trainable parameter can assume during the training.

For a chosen NN architecture, tuning the weight clipping allows to recover a good agreement of the empirical distribution of \bar{t} under R_0 with the target $\chi^2_{|w|}$ distribution.

Example:
NN model: 5-7-7-1,
Number of parameters: 106

Legend:

- Percentiles of the empirical \bar{t} distribution under R_0
- Percentiles of the target $\chi^2_{|w|}$
- Empirical \bar{t} distribution under R_0
- Target $\chi^2_{|w|}$



NPLM systematic uncertainties

New Physics Learning Machine (NPLM)

Including systematic uncertainties

Test statistic

$$t(\mathcal{D}, \mathcal{A}) = 2 \log \left[\frac{\max_{\mathbf{w}, \boldsymbol{\nu}} \mathcal{L}(H_{\mathbf{w}}, \boldsymbol{\nu} | \mathcal{D}, \mathcal{A})}{\max_{\boldsymbol{\nu}} \mathcal{L}(R_{\boldsymbol{\nu}} | \mathcal{D}, \mathcal{A})} \right] = 2 \log \left[\frac{\max_{\mathbf{w}, \boldsymbol{\nu}} \mathcal{L}(H_{\mathbf{w}}, \boldsymbol{\nu} | \mathcal{D}) \mathcal{L}(\boldsymbol{\nu} | \mathcal{A})}{\max_{\boldsymbol{\nu}} \mathcal{L}(R_{\boldsymbol{\nu}} | \mathcal{D}) \mathcal{L}(\boldsymbol{\nu} | \mathcal{A})} \right]$$

\mathbf{w} : trainable parameters on the NN model

$\boldsymbol{\nu}$: set of nuisance parameters modelling the uncertainties effects

\mathcal{D} : data sample

\mathcal{A} : auxiliary sample (used to constrain $\boldsymbol{\nu}$)

New parametrization

$$n(x | T) \approx n(x | H_{\hat{\mathbf{w}}, \hat{\boldsymbol{\nu}}}) = n(x | R_0) \frac{n(x | R_{\hat{\boldsymbol{\nu}}})}{n(x | R_0)} e^{f(x; \hat{\mathbf{w}})}$$

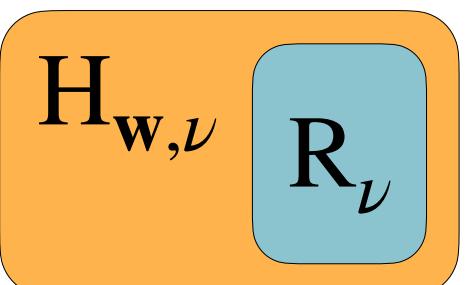
New term containing the dependence on $\boldsymbol{\nu}$

$r(x; \boldsymbol{\nu})$

True (T) data distribution	Data distribution learnt by the NN	Reference distribution	
Unknown	Alternative hypothesis	Null hypothesis	NN model

Note:

This parametrization choice guarantees $R_{\boldsymbol{\nu}} \subseteq H_{\mathbf{w}, \boldsymbol{\nu}}$
 $(R_{\boldsymbol{\nu}} = H_{\mathbf{w}, \boldsymbol{\nu}} \text{ for } f(\cdot; \mathbf{w}) \equiv 0)$



New Physics Learning Machine (NPLM)

Including systematic uncertainties

Maximum Likelihood from minimal loss:

Test statistic

$$t(\mathcal{D}, \mathcal{A}) = 2 \log \left[\frac{\max_{\mathbf{w}, \boldsymbol{\nu}} \mathcal{L}(\mathbf{H}_{\mathbf{w}}, \boldsymbol{\nu} | \mathcal{D}, \mathcal{A})}{\max_{\boldsymbol{\nu}} \mathcal{L}(\mathbf{R}_{\boldsymbol{\nu}} | \mathcal{D}, \mathcal{A})} \right] = 2 \log \left[\frac{\max_{\mathbf{w}, \boldsymbol{\nu}} \mathcal{L}(\mathbf{H}_{\mathbf{w}}, \boldsymbol{\nu} | \mathcal{D}) \mathcal{L}(\boldsymbol{\nu} | \mathcal{A})}{\max_{\boldsymbol{\nu}} \mathcal{L}(\mathbf{R}_{\boldsymbol{\nu}} | \mathcal{D}) \mathcal{L}(\boldsymbol{\nu} | \mathcal{A})} \right]$$

$$= \tau(\mathcal{D}, \mathcal{A}) - \Delta(\mathcal{D}, \mathcal{A})$$

Tau term:

$$\tau(\mathcal{D}, \mathcal{A}) = 2 \max_{\mathbf{w}, \boldsymbol{\nu}} \log \left[\frac{\mathcal{L}(\mathbf{H}_{\mathbf{w}}, \boldsymbol{\nu} | \mathcal{D}) \mathcal{L}(\boldsymbol{\nu} | \mathcal{A})}{\mathcal{L}(\mathbf{R}_0 | \mathcal{D}) \mathcal{L}(\mathbf{0} | \mathcal{A})} \right] = -2 \min_{\mathbf{w}, \boldsymbol{\nu}} L \left[f(x, \mathbf{w}), \boldsymbol{\nu}; \hat{\delta}(x) \right]$$

Delta term:

$$\Delta(\mathcal{D}, \mathcal{A}) = 2 \max_{\boldsymbol{\nu}} \log \left[\frac{\mathcal{L}(\mathbf{R}_{\boldsymbol{\nu}} | \mathcal{D}) \mathcal{L}(\boldsymbol{\nu} | \mathcal{A})}{\mathcal{L}(\mathbf{R}_0 | \mathcal{D}) \mathcal{L}(\mathbf{0} | \mathcal{A})} \right] = -2 \min_{\boldsymbol{\nu}} L \left[\boldsymbol{\nu}; \hat{\delta}(x) \right]$$

\mathbf{w} : trainable parameters on the NN model

$\boldsymbol{\nu}$: set of nuisance parameters modelling the uncertainties effects

\mathcal{D} : data sample

\mathcal{A} : auxiliary sample (used to constrain $\boldsymbol{\nu}$)

Contains the dependence on a NN model

Built on the knowledge of the Reference model (purely SM term)

$$r(x; \boldsymbol{\nu}) = \frac{n(x | \mathbf{R}_{\boldsymbol{\nu}})}{n(x | \mathbf{R}_0)}$$

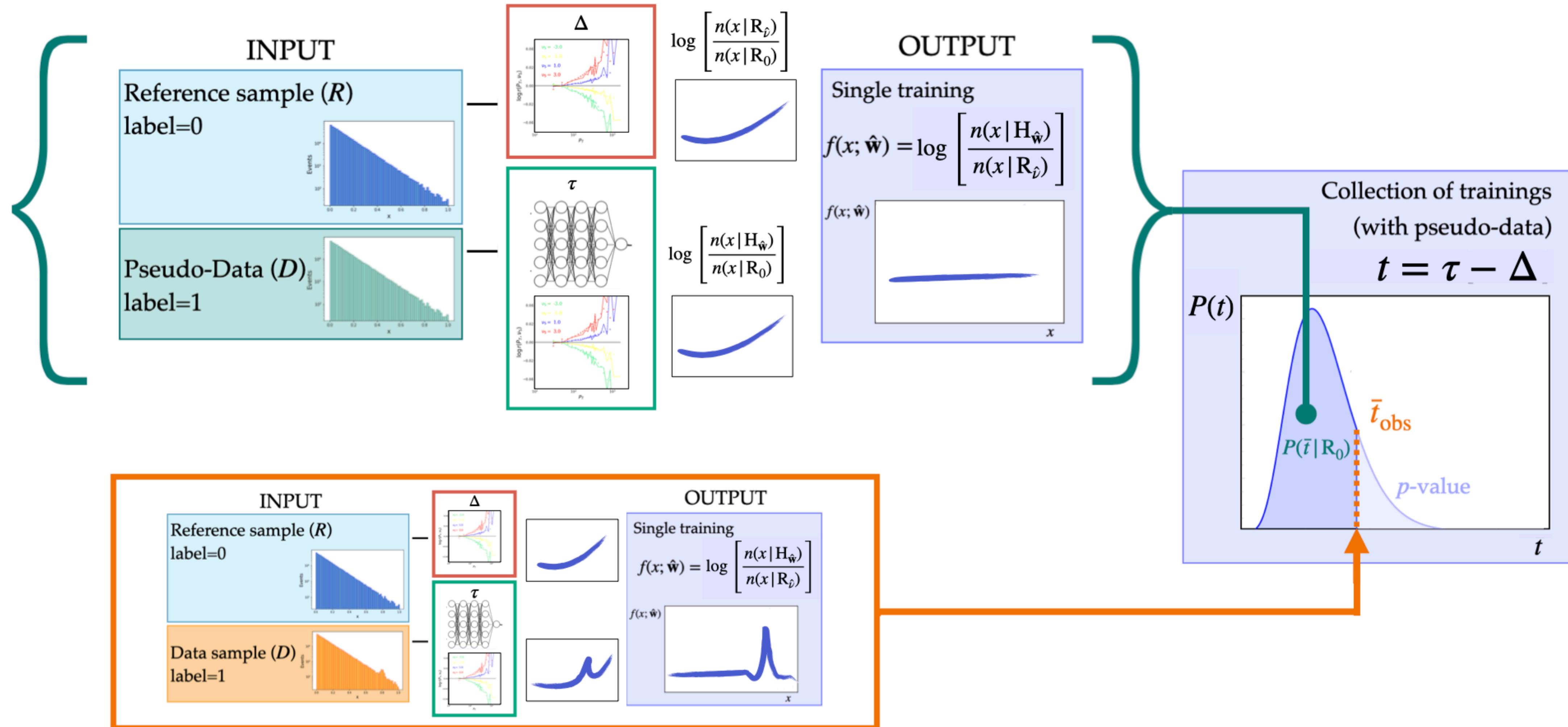
Taylor's expansion learning:

$$\hat{r}(x; \boldsymbol{\nu}) = \exp \left[\hat{\delta}_1(x) \boldsymbol{\nu} + \hat{\delta}_2(x) \boldsymbol{\nu}^2 + \dots \right]$$

NN 1 NN2 ...

New Physics Learning Machine (NPLM)

Including systematic uncertainties

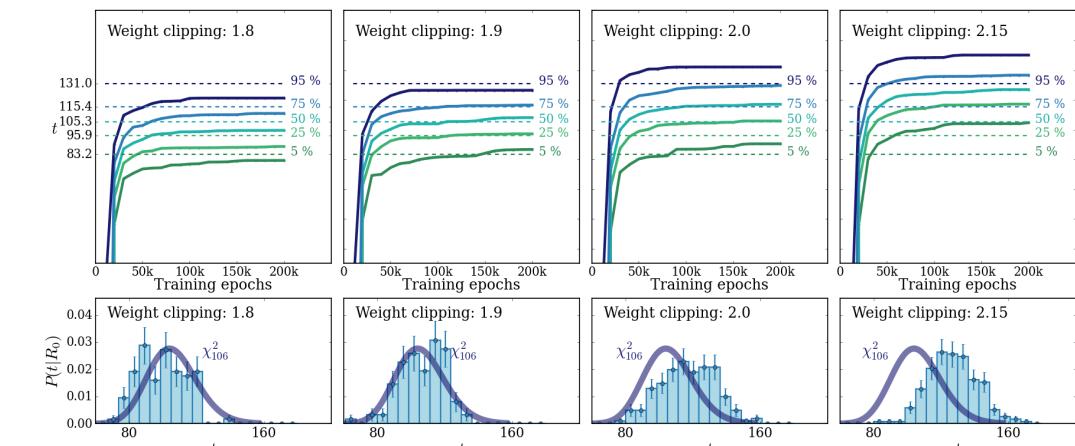


"Learning New Physics from an Imperfect Machine" [Eur. Phys. J. C](#)

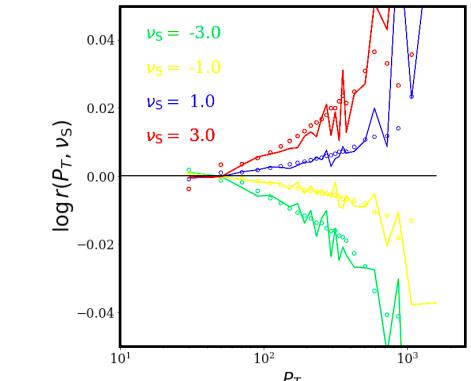
New Physics Learning Machine (NPLM)

Preparation steps (before looking at the data):

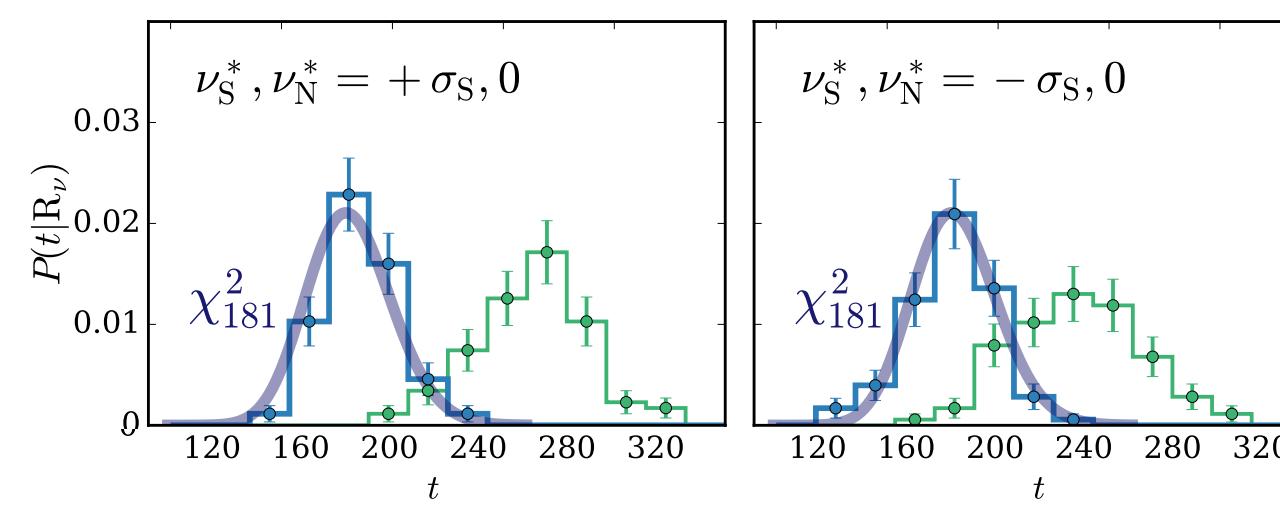
- NN model selection



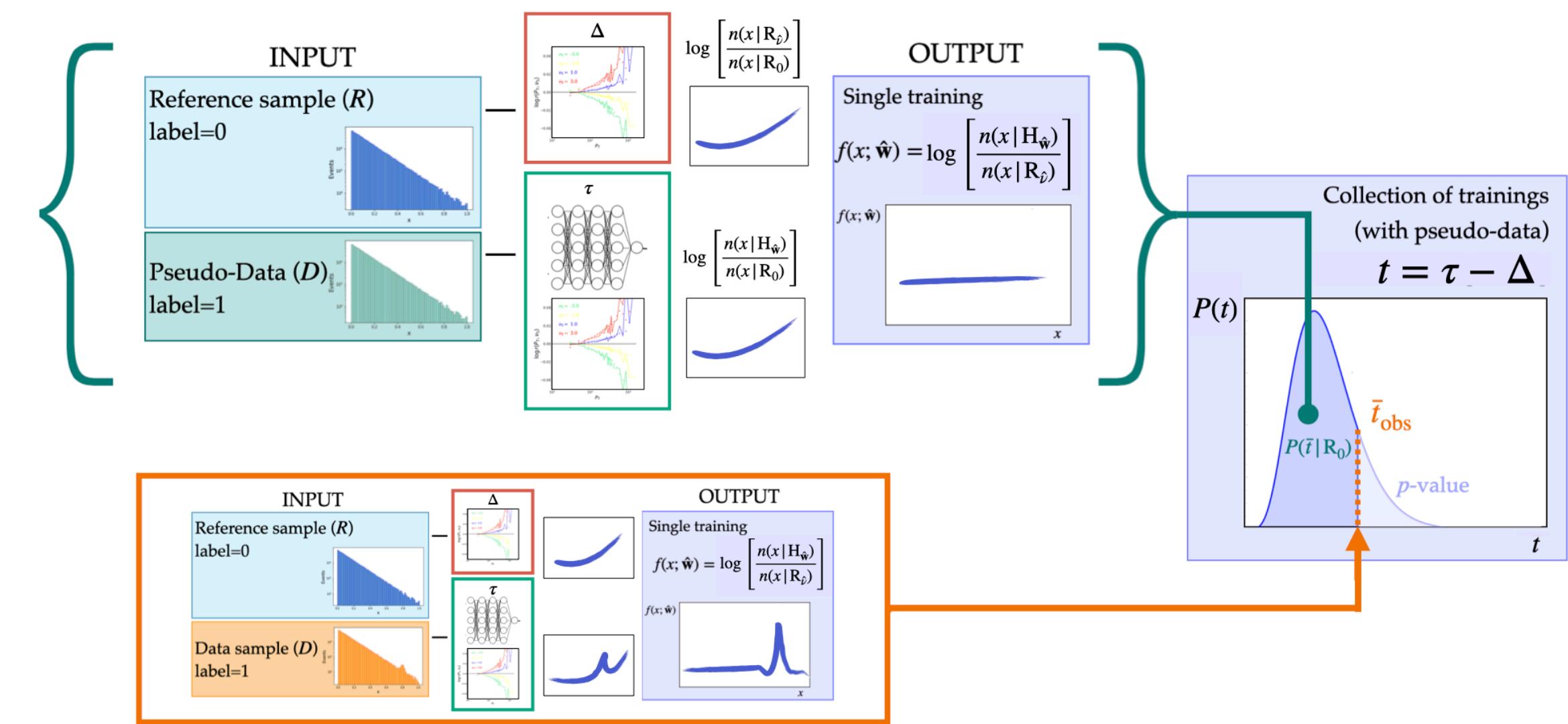
- Parametric NN for Taylor's expansion on ν
- $$\hat{r}(x; \nu) = \exp \left[\hat{\delta}_1(x) \nu + \hat{\delta}_2(x) \nu^2 + \dots \right]$$



- Validation: $\mathcal{D} \sim R_{\nu^*}, \nu^* = \pm \sigma_\nu$



τ
 $\tau - \Delta$



"Learning New Physics from an Imperfect Machine" [Eur. Phys. J. C](#)

Hands on a 1D toy model

Hands on a 1D toy model

Reference model:

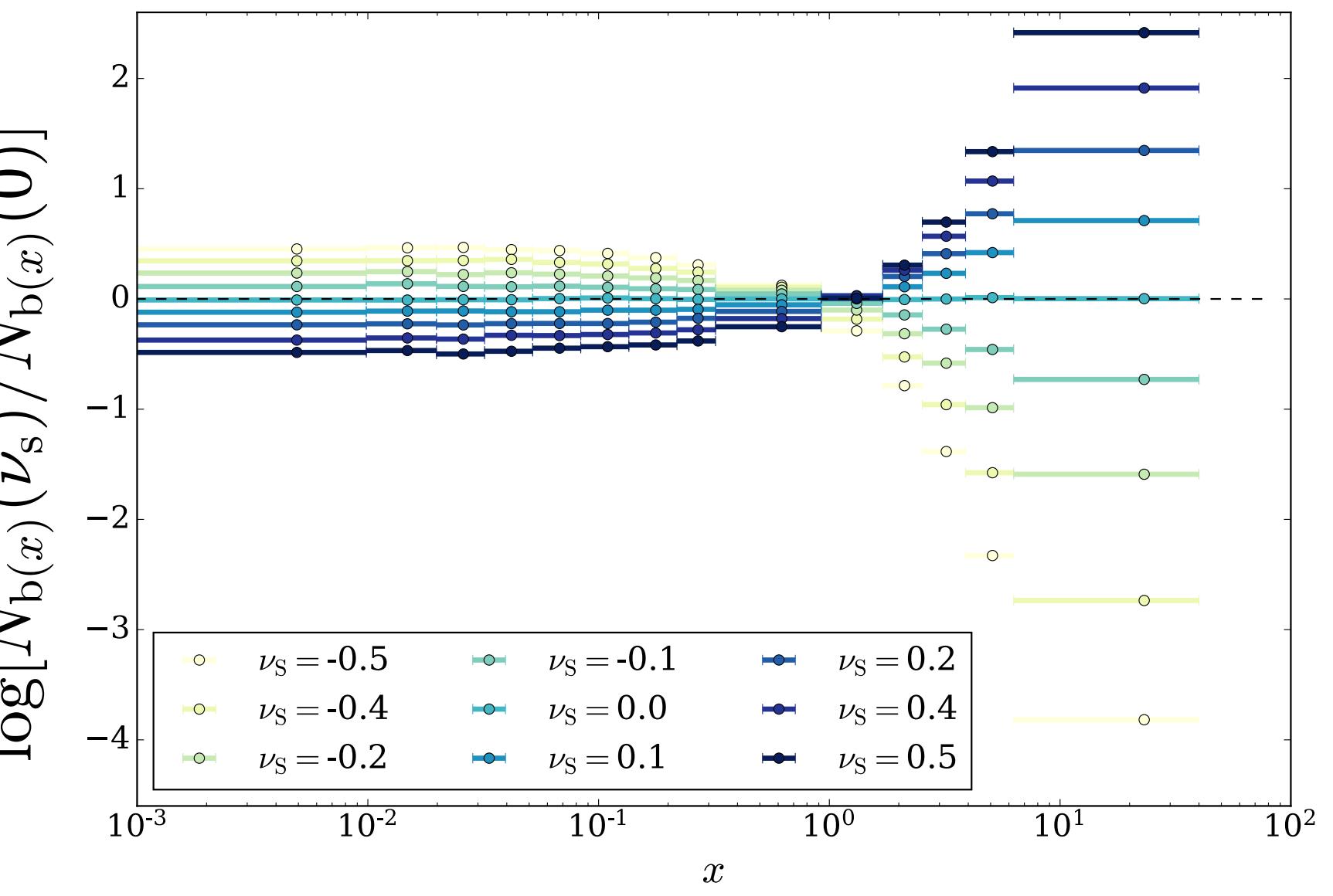
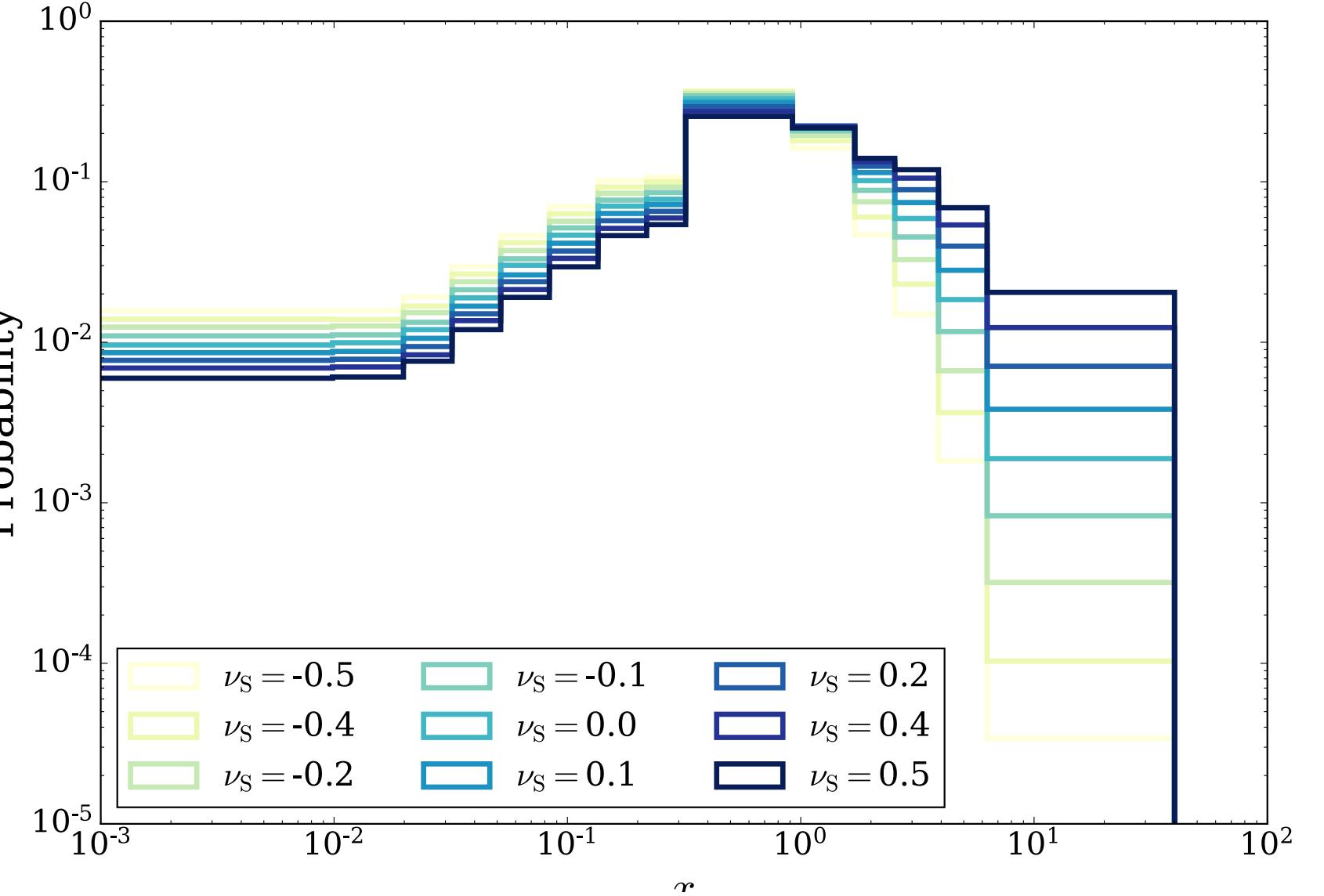
Exponentially falling distribution

affected by:

- a scale uncertainty (ν_S)
- a normalization uncertainty (ν_N)

$$n(x|R_{\nu}) = n(x|R_{\nu_N, \nu_S}) = N(R_0) \exp \left[-x e^{-\nu_S} - \nu_S + \nu_N \right]$$

Scale effect on the distribution

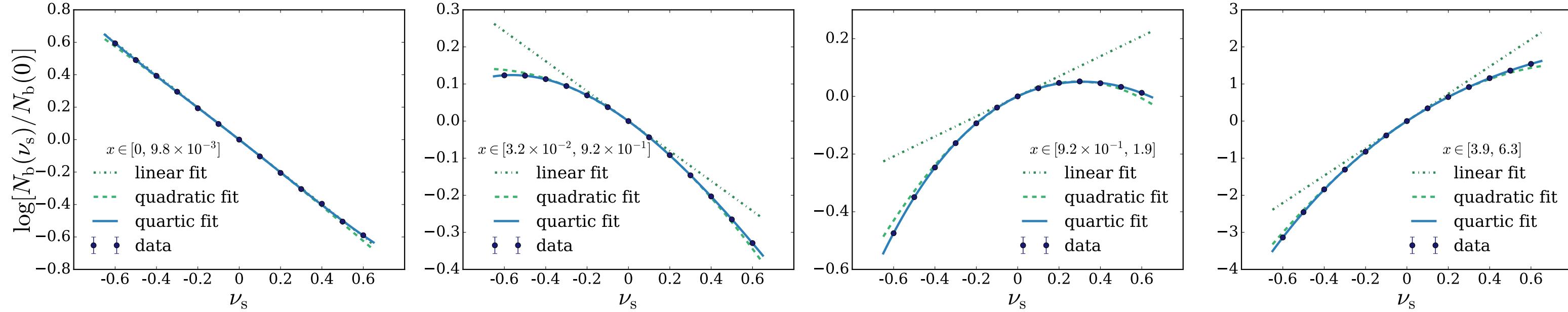


Hands on a 1D toy model

Learning the coefficient of the Taylor Expansion for ν_s :

Preliminary study

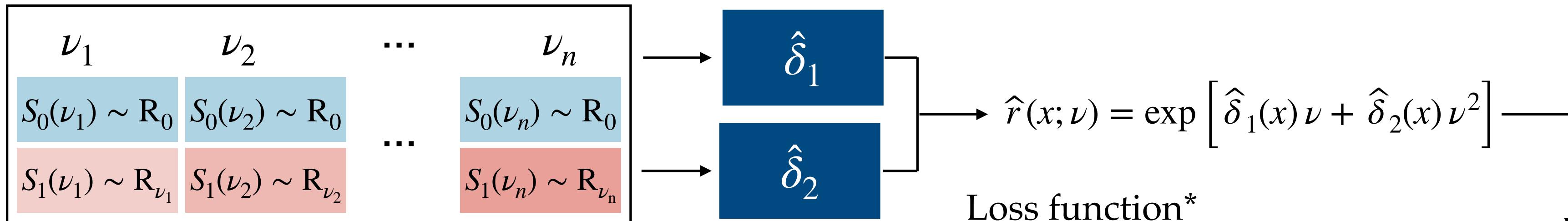
Preliminary binned analysis to determine the proper order for the Taylor's expansion



Taylor's expansion learning

Training a neural network model to learn each coefficient of the Taylor's expansion of $r(x; \nu) = \frac{n(x | R_\nu)}{n(x | R_0)}$

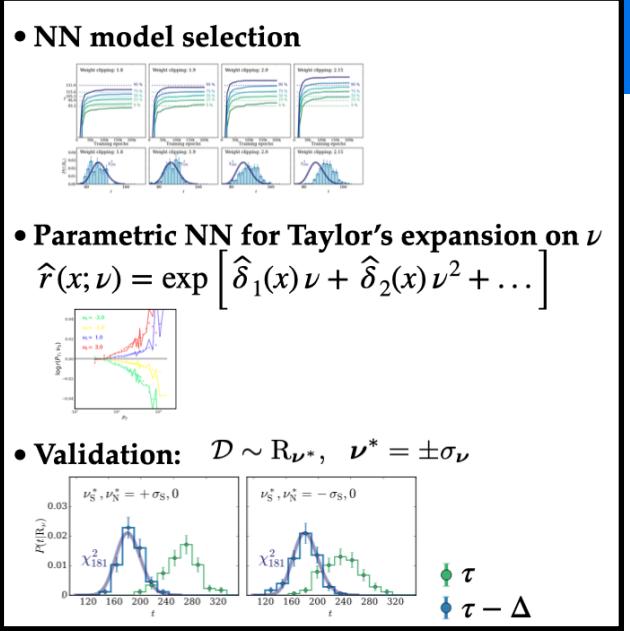
Input samples



Loss function*

$$L[\hat{\delta}(\cdot)] = \sum_{\nu_i} \left[\sum_{e \in S_0(\nu_i)} w_e c(x_e)^2 + \sum_{e \in S_1(\nu_i)} w_e [1 - c(x_e)]^2 \right], \quad c(x) = \frac{1}{1 + \hat{r}(x; \nu)}$$

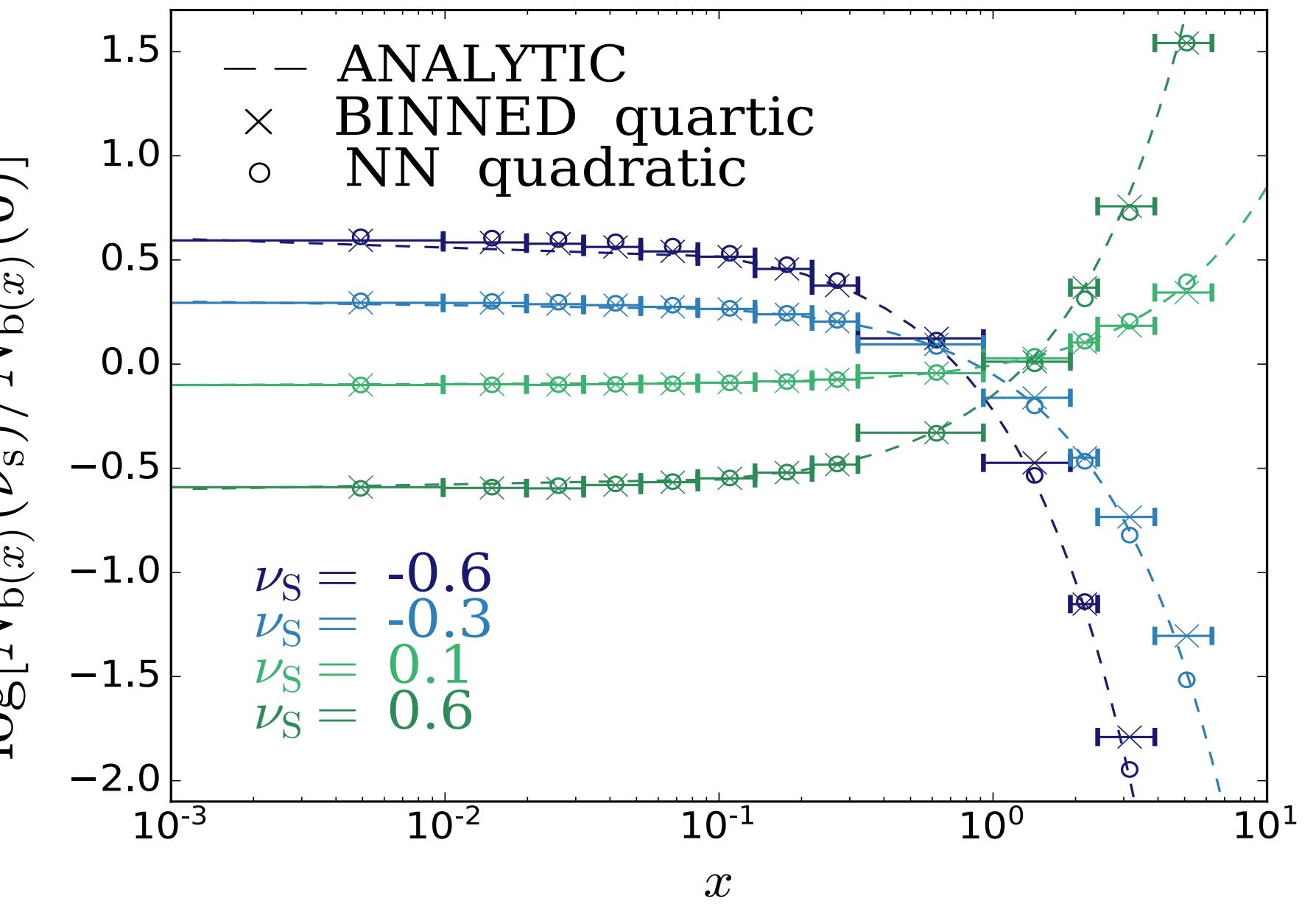
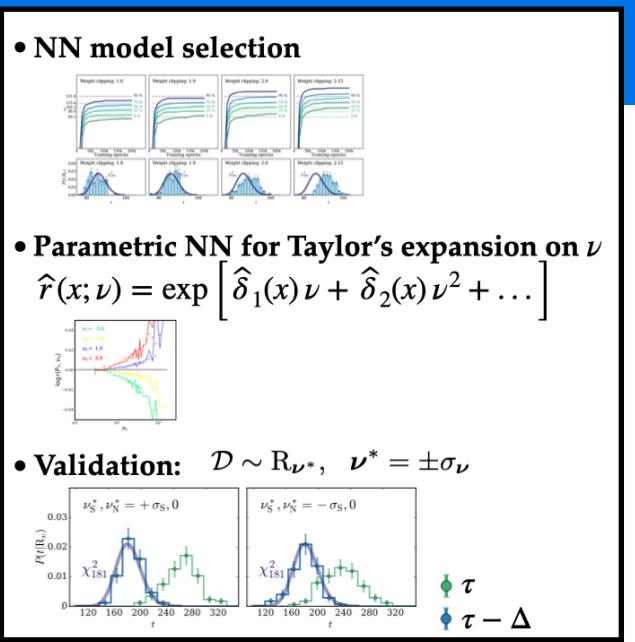
* Parametrized classifiers for optimal EFT sensitivity [arXiv:2007.10356](https://arxiv.org/abs/2007.10356)



Hands on a 1D toy model

Learning the coefficient of the Taylor Expansion for ν_S :

$$\log r_{b_i}(\boldsymbol{\nu}) = \nu_N + \nu_S \hat{\delta}_{1,b_i} + \frac{1}{2} \nu_S^2 \hat{\delta}_{2,b_i} \quad \forall i \in [1, \dots N_{bins}]$$



Hands on a 1D toy model

NN model selection:

Weight clipping tuning

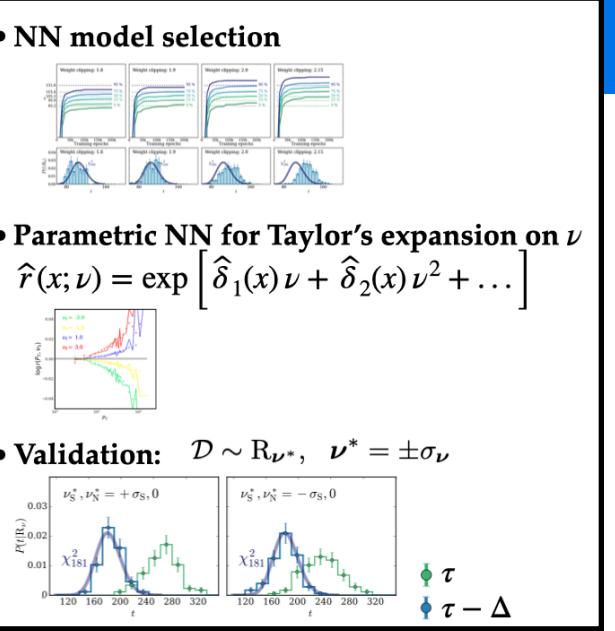
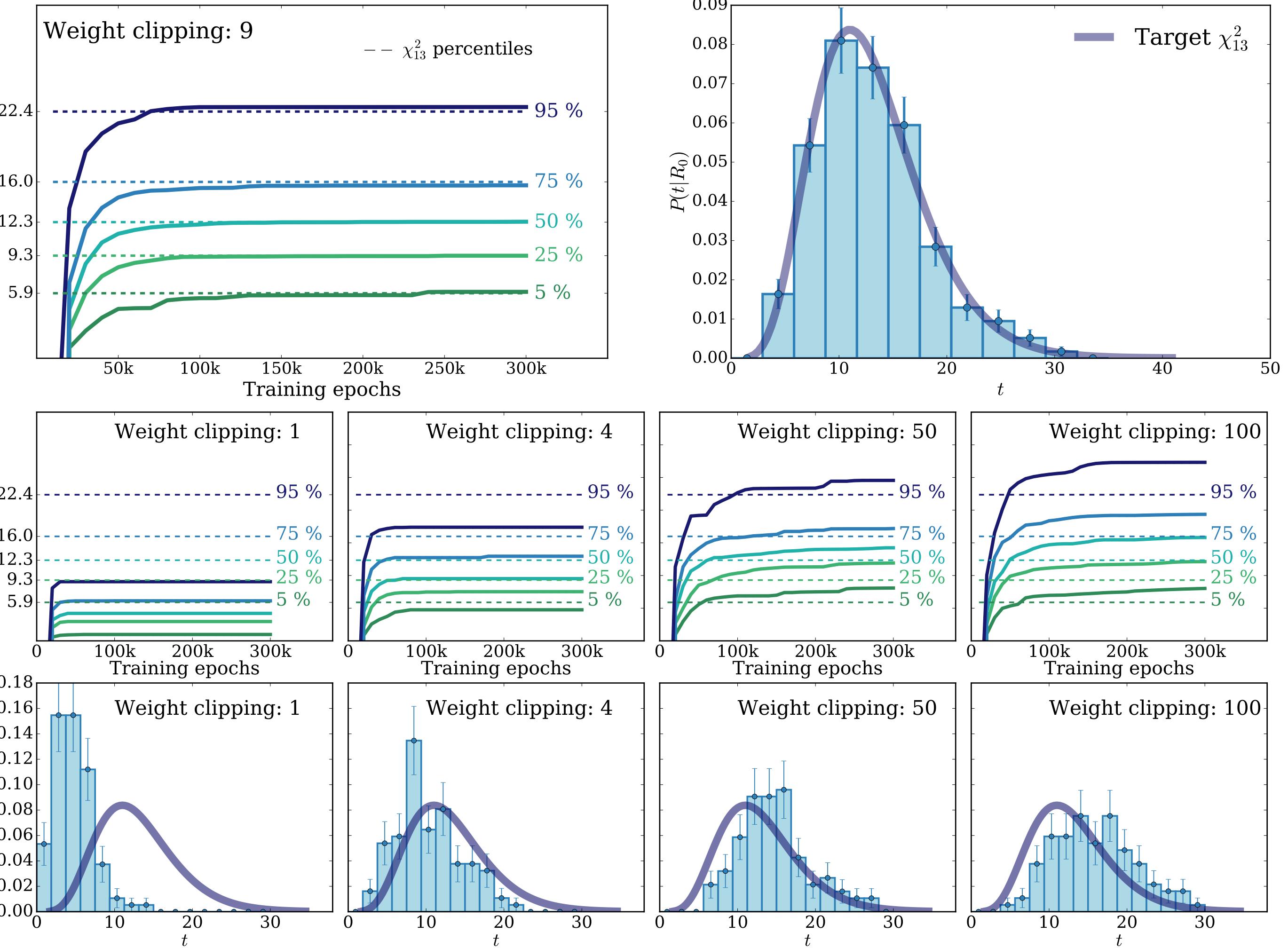
(In the R_0 hypothesis)

Here we used:

- 2000 data
- 200 000 reference (R_0)
- Architecture 1-4-1 (9 dof, very simple!)

Legend:

-  Percentiles of the empirical \bar{t} distribution under R_0
-  Percentiles of the target $\chi^2_{|w|}$
-  Empirical \bar{t} distribution under R_0
-  Target $\chi^2_{|w|}$

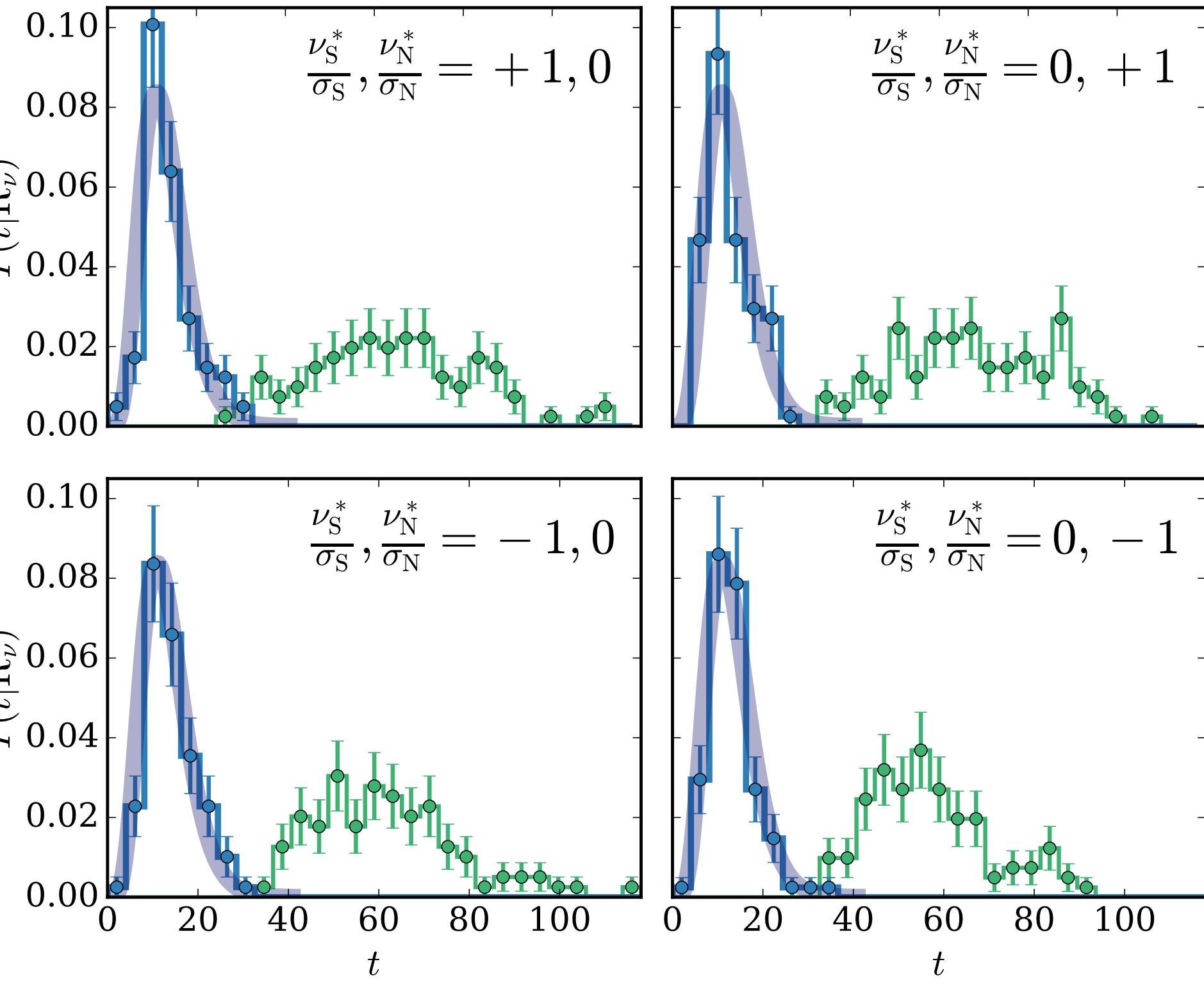
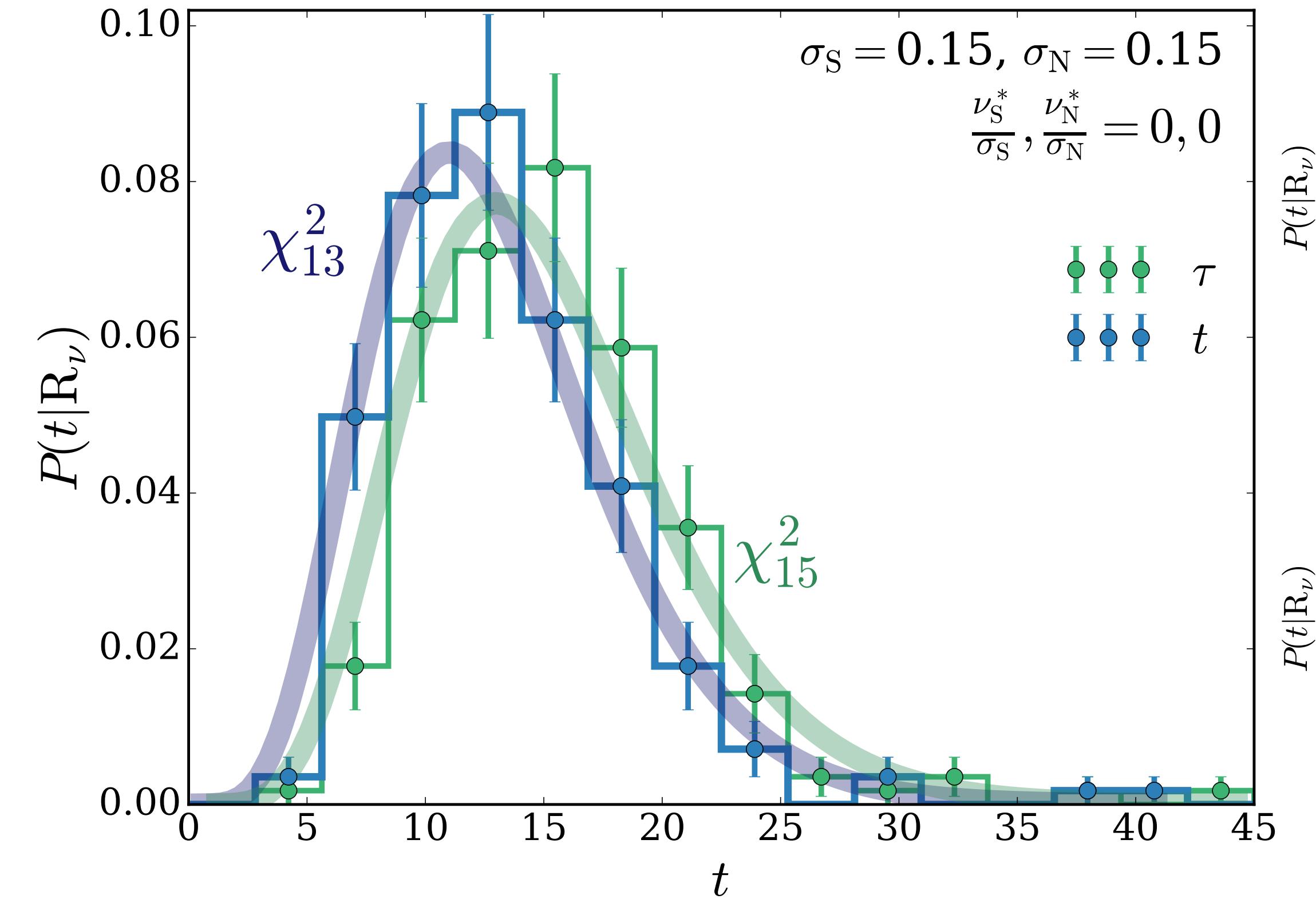
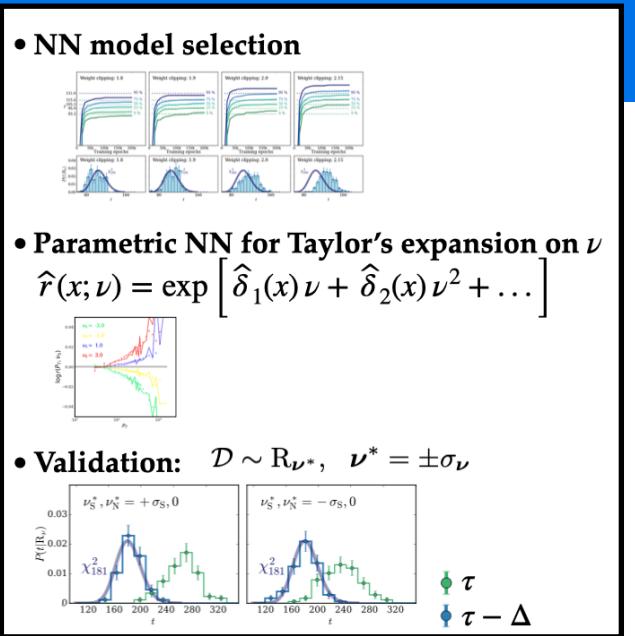


Hands on a 1D toy model

Validation

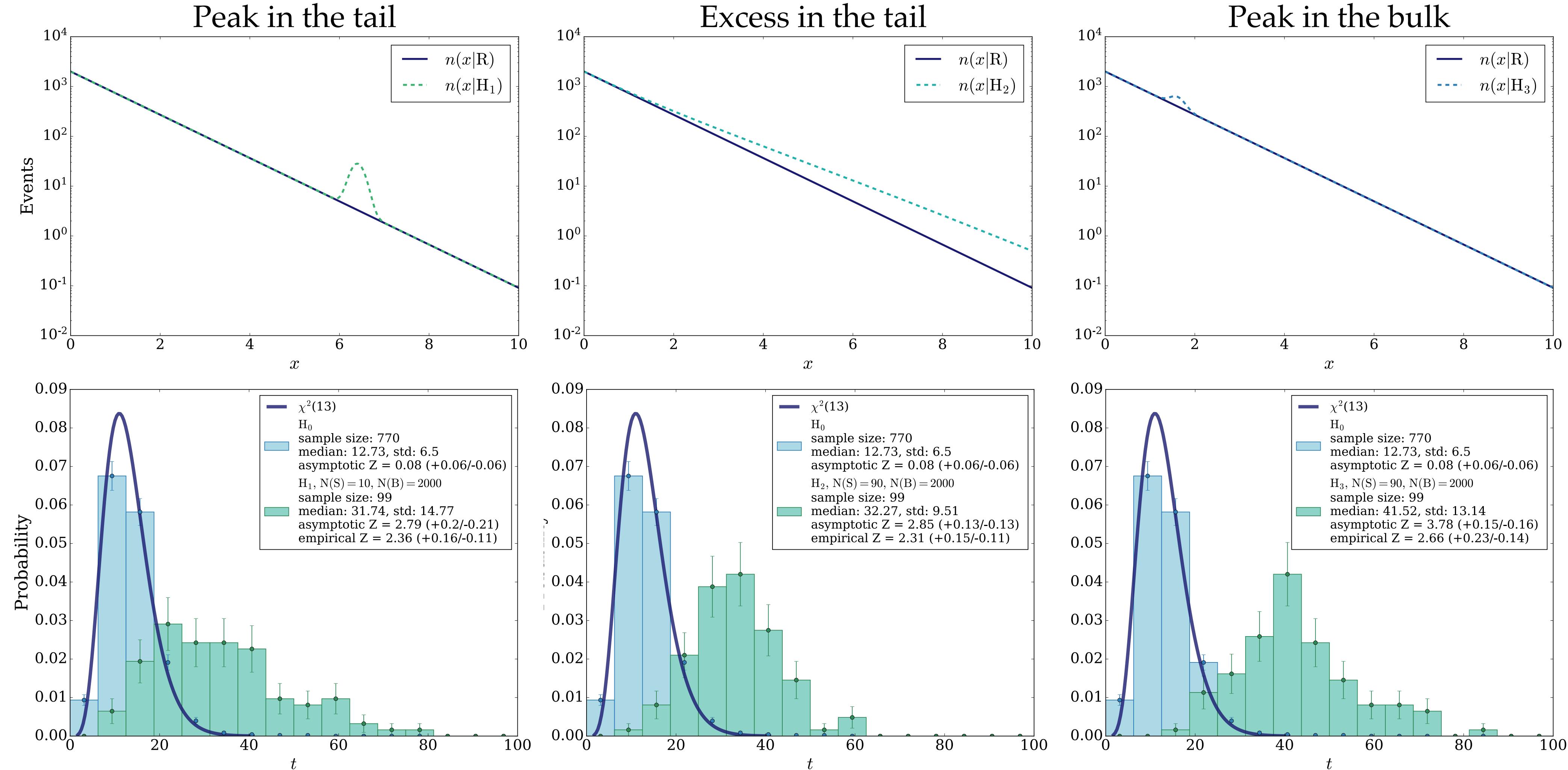
Verifying that the $\chi^2_{|w|}$ is recovered

$$\mathcal{D} \sim R_{\nu^*}, \quad \nu^* = \pm \sigma_\nu$$



Hands on a 1D toy model

Inject signals

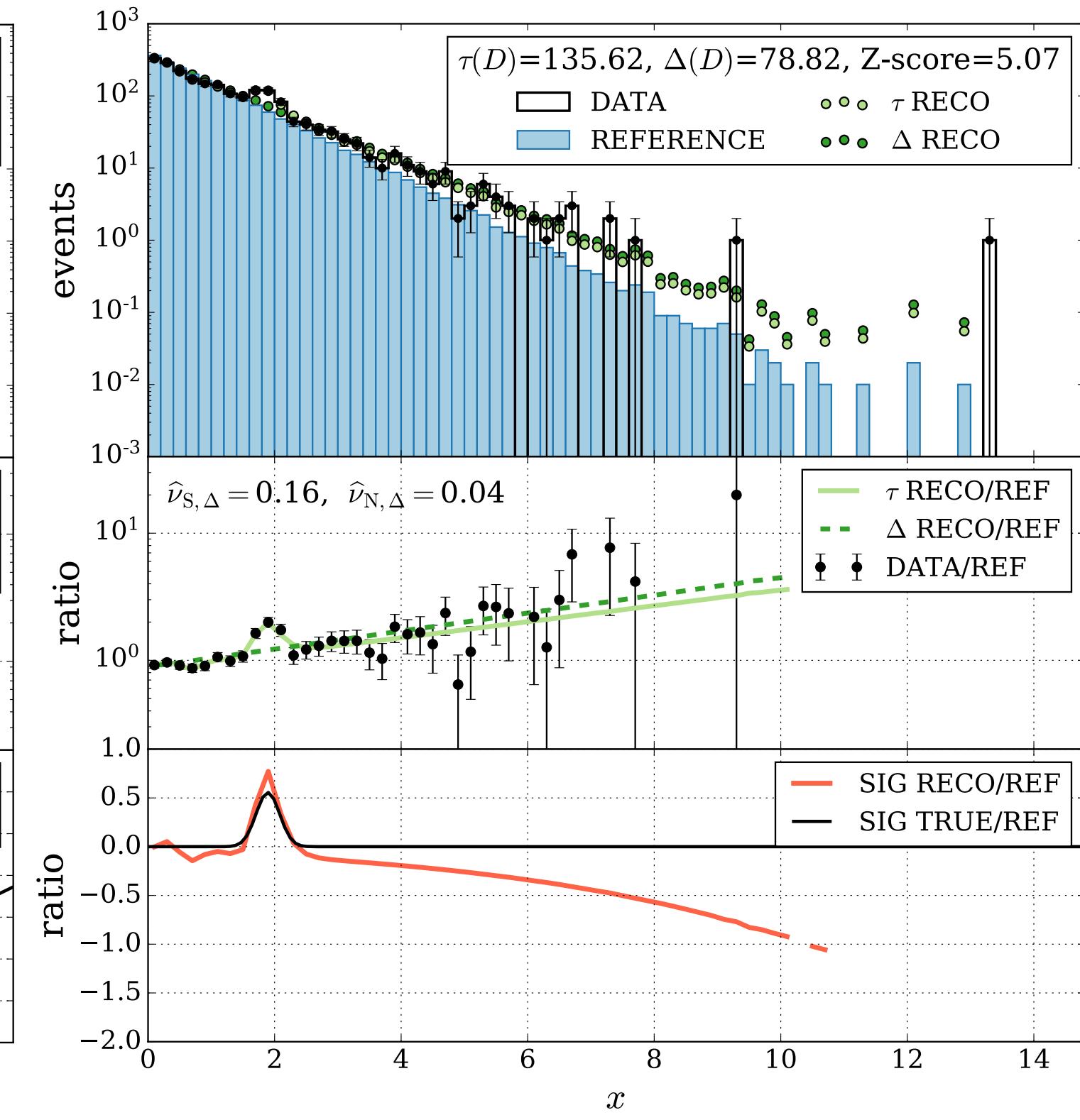
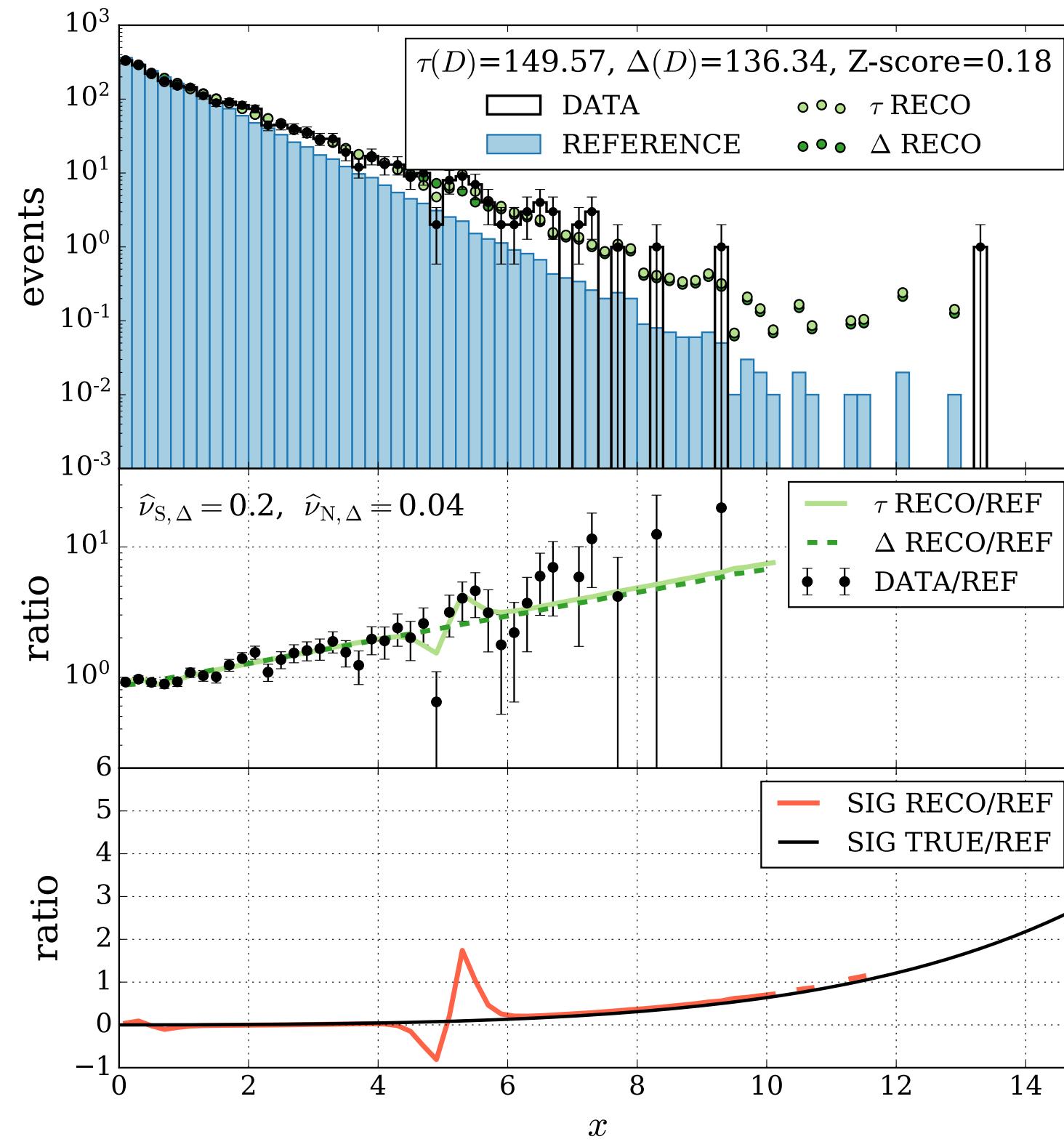
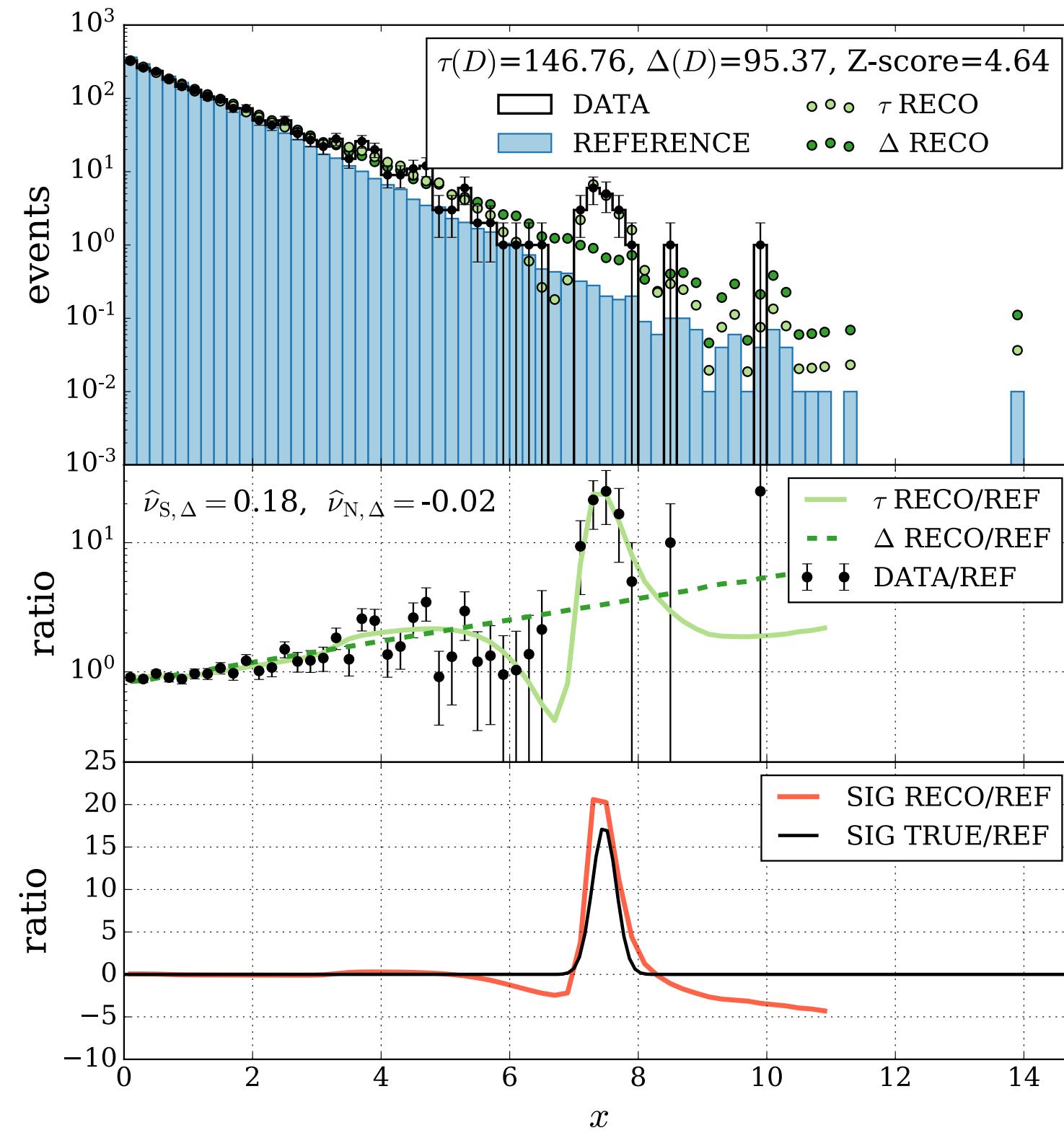


Hands on a 1D toy model

Interpret the result: anomaly characterisation

$$\tau \text{ reconstruction: } n(x | H_{\hat{\mathbf{w}}, \hat{\nu}}) = n(x | R_0) \frac{n(x | R_{\hat{\nu}})}{n(x | R_0)} e^{f(x; \hat{\mathbf{w}})}$$

$$\Delta \text{ reconstruction: } n(x | R_{\hat{\nu}})$$



...to conclude

Code and resources

Getting started with NPLM

- [NPLM package](#): python-based package to run the NPLM analysis strategy

NPLM 0.0.6

`pip install NPLM`

Released: Feb 1, 2022

package to run the New Physics Learning Machine (NPLM) algorithm.

Navigation

- Project description
- Release history
- Download files

Project description

NPLM_package

a package to implement the New Physics Learning Machine (NPLM) algorithm

Short description:

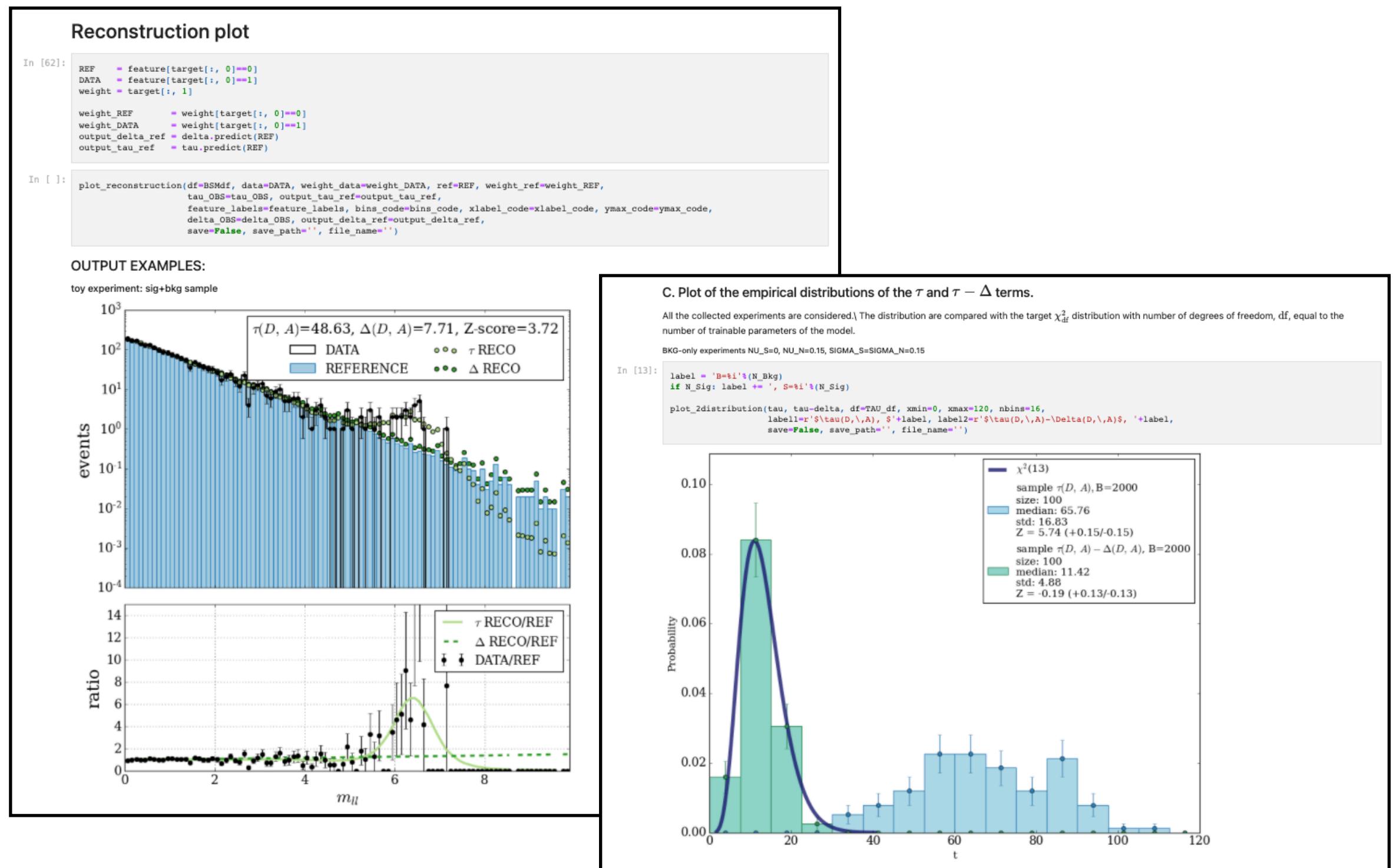
NPLM is a strategy to detect data departures from a given reference model, with no prior bias on the nature of the new physics model responsible for the discrepancy. The method employs neural networks, leveraging their virtues as flexible function approximants, but builds its foundations directly on the canonical likelihood-ratio approach to hypothesis testing. The algorithm compares observations with an auxiliary set of reference-distributed events, possibly obtained with a Monte Carlo event generator. It returns a p-value, which measures the compatibility of the reference model with the data. It also identifies the most discrepant phase-space region of the dataset, to be selected for further investigation. Imperfections due to mis-modelling in the reference dataset can be taken into account straightforwardly as nuisance parameters.

Related works:

- "Learning New Physics from a Machine" ([Phys. Rev. D](#))
- "Learning Multivariate New Physics" ([Eur. Phys. J. C](#))
- "Learning New Physics from an Imperfect Machine" ([arXiv](#))

View statistics for this project via [Libraries.io](#), or by using [our public dataset on Google BigQuery](#).

- [Tutorial](#) on 1D toy model for getting started



Summary

Today's presentation:

- Main concepts and implementation using NN

“Learning New Physics from a Machine” - d’Agnolo, Wulzer, [Phys. Rev. D \(2018\)](#)

“Learning Multivariate New Physics” - d’Agnolo, Grosso, Pierini, Wulzer, Zanetti, [Eur. Phys. J. C 81, 89 \(2021\)](#)

- Systematic uncertainties

“Learning New Physics from an Imperfect Machine” - d’Agnolo, Grosso, Pierini, Wulzer, Zanetti [Eur. Phys. J. C 82, 275 \(2022\)](#)

More about NPLM in a upcoming contribution from Marco Letizia:

- NPLM implementation using kernel methods, DQM application

“Learning New Physics efficiently with non parametric methods” - Letizia, Grosso et al. [Eur. Phys. J. C 82, 879 \(2022\)](#)

“Fast kernel methods for Data Quality Monitoring as a goodness-of-fit test” - Letizia, Grosso et al. [2303.05413](#) (preprint)

Outlook

Ongoing studies and future directions for NPLM

- NPLM as a **goodness-of-fit** tool: comparison with state of the art, pros and cons (contribution at [neurips22 \(ML for physical science workshop\)](#), paper in preparation)
- Exploring alternative methods of **regularisation**

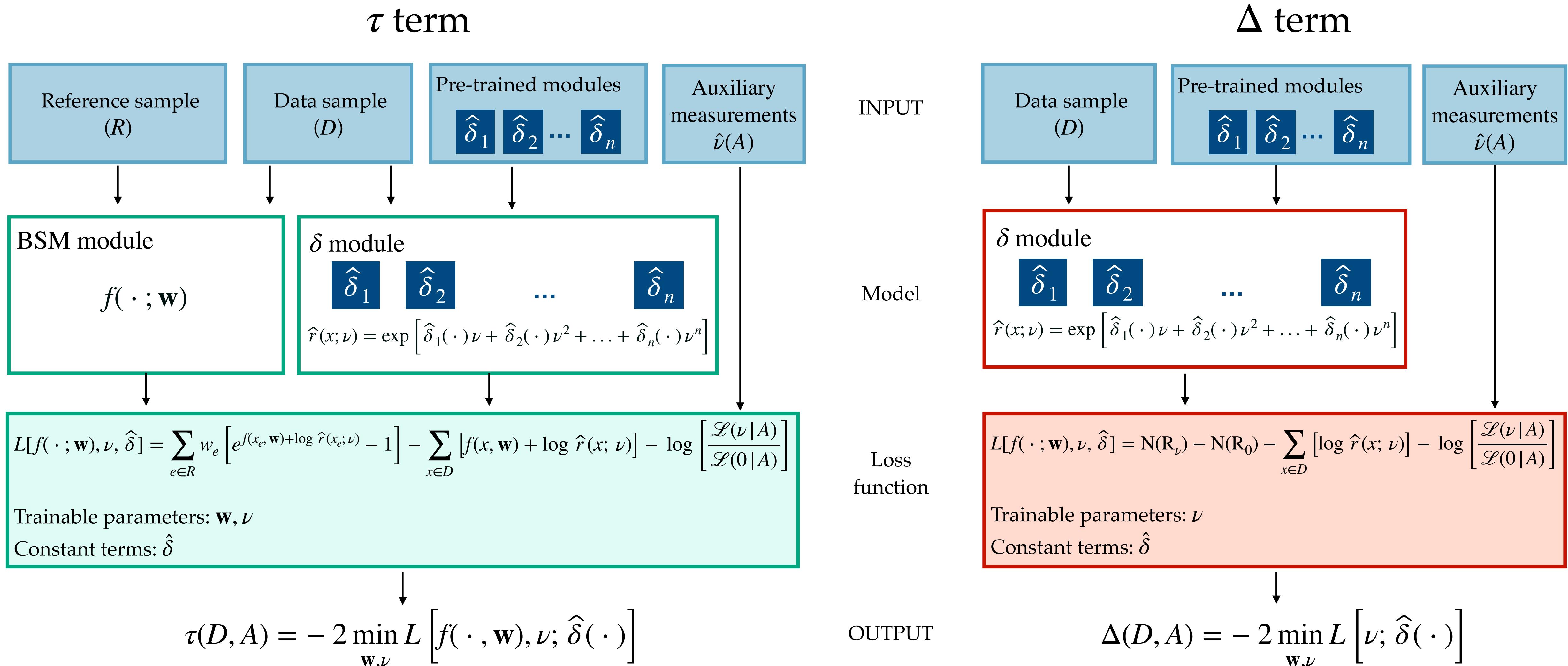
Current applications

- Model-independent search with collider data ([Eur. Phys. J. C 82, 275 \(2022\)](#) + ongoing work)
- Multi-dimensional DQM (preprint [2303.05413](#))
- Multidimensional validation of MC simulators (ongoing work)
- Bank fraud detection (ongoing work)
- **Any idea? :)**

Backup slides

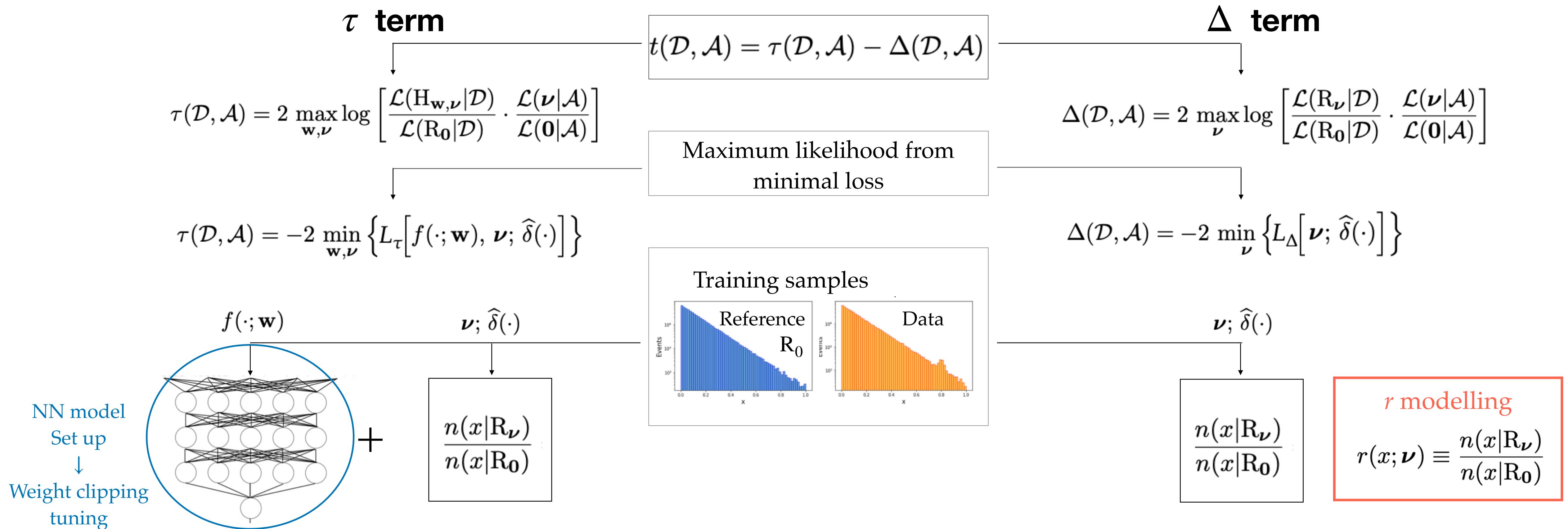
New Physics Learning Machine (NPLM)

Including systematic uncertainties



New Physics Learning Machine (NPLM)

Including systematic uncertainties



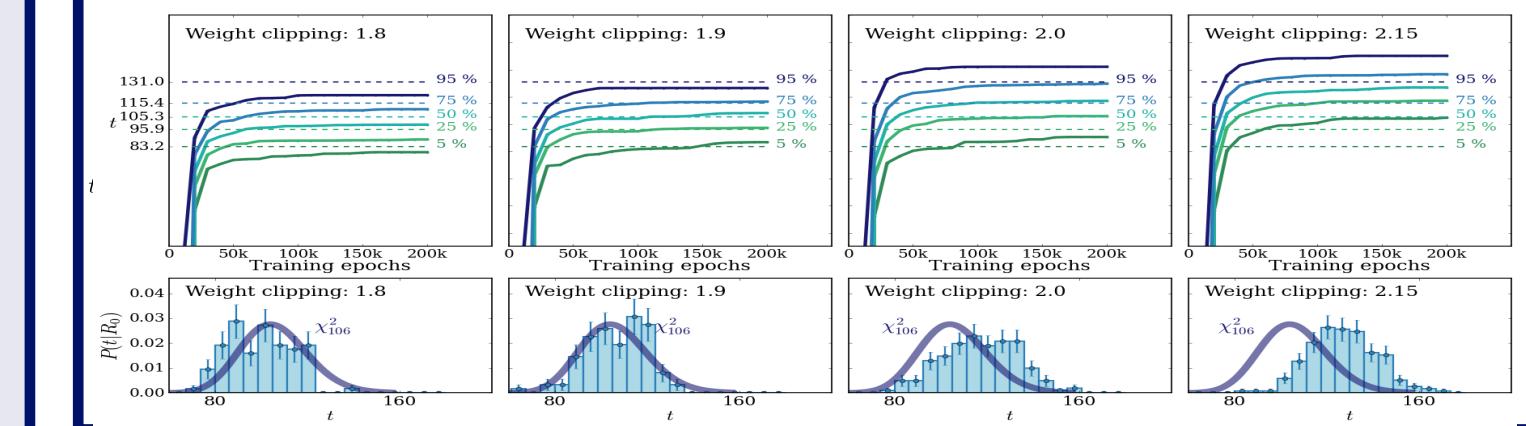
New Physics Learning Machine (NPLM)

Including systematic uncertainties

Final procedure in steps:

1. NN MODEL SELECTION:

weight clipping tuning \rightarrow target $\chi^2_{|\mathbf{w}|}$;



2. NUISANCE TAYLOR'S EXPANSION LEARNING:

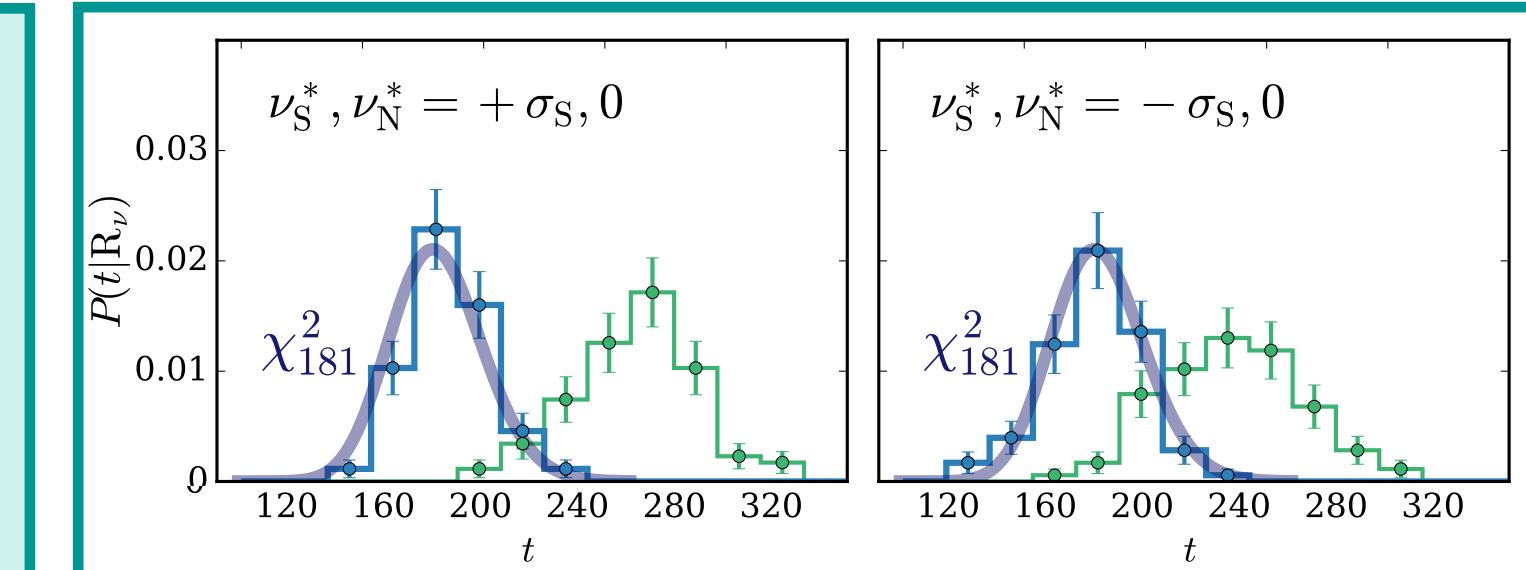
modelling $\hat{r}(x; \nu) = \exp \left[\hat{\delta}_1(x) \nu + \hat{\delta}_2(x) \nu^2 + \dots \right]$;

$$\hat{r}(x; \nu) = \exp \left[\begin{array}{c} \hat{\delta}_1(x) \nu \\ \text{NN 1} \end{array} + \begin{array}{c} \hat{\delta}_2(x) \nu^2 \\ \text{NN2} \end{array} + \dots \right]$$

3. VALIDATION:

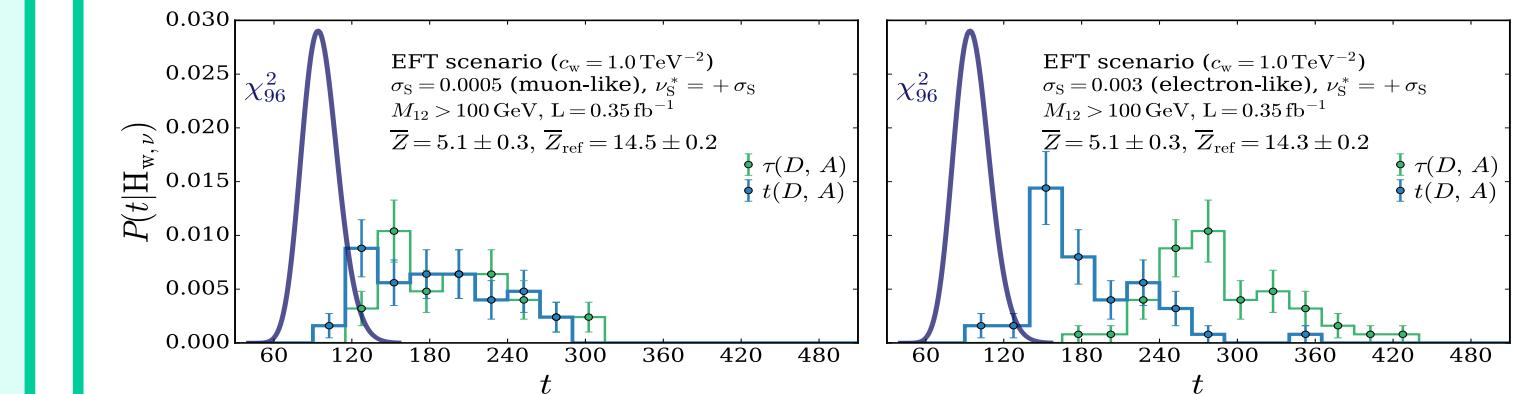
$$\mathcal{D} \sim R_{\nu^*}, \quad \nu^* = \pm \sigma_\nu$$

Verifying that the target $\chi^2_{|\mathbf{w}|}$ is always recovered;

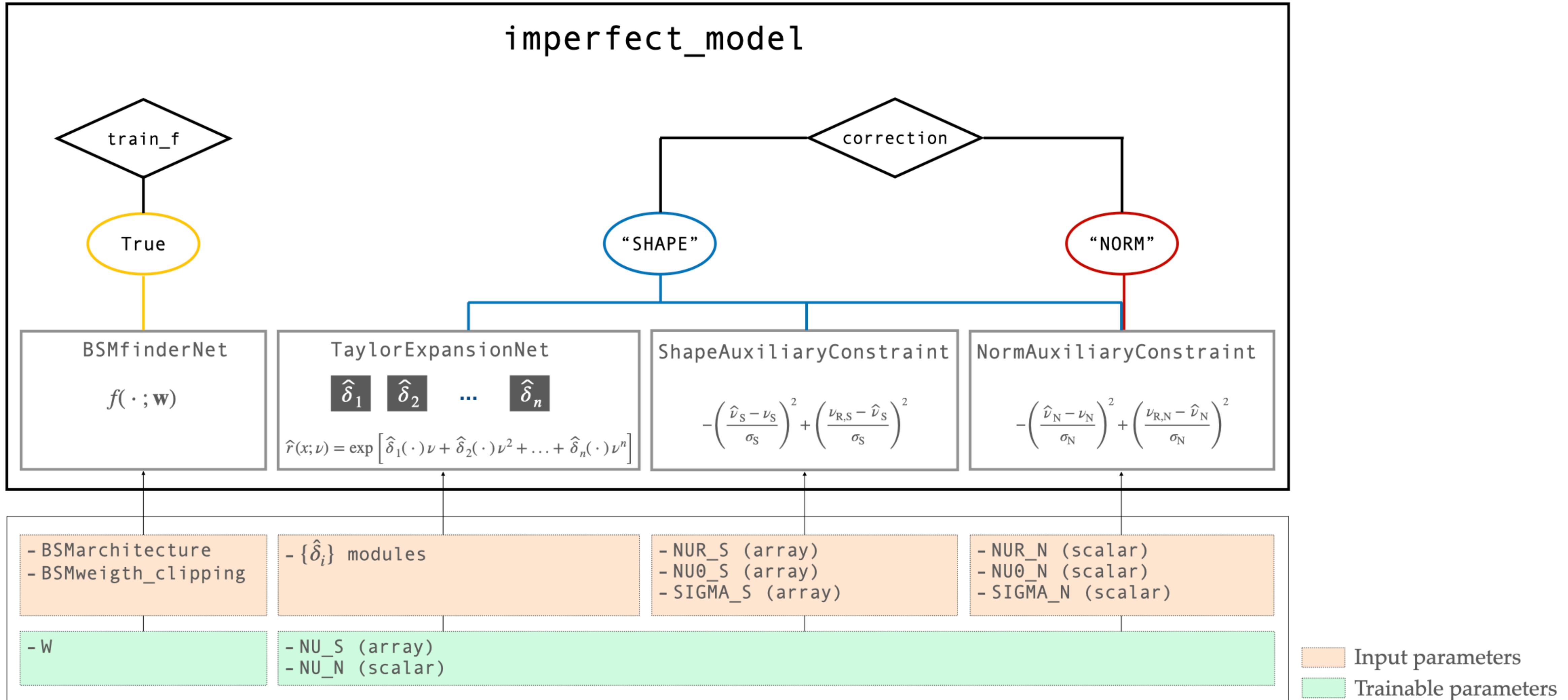


4. TESTING THE DATA:

running the procedure on real data.



The model implementation in Keras + Tensorflow

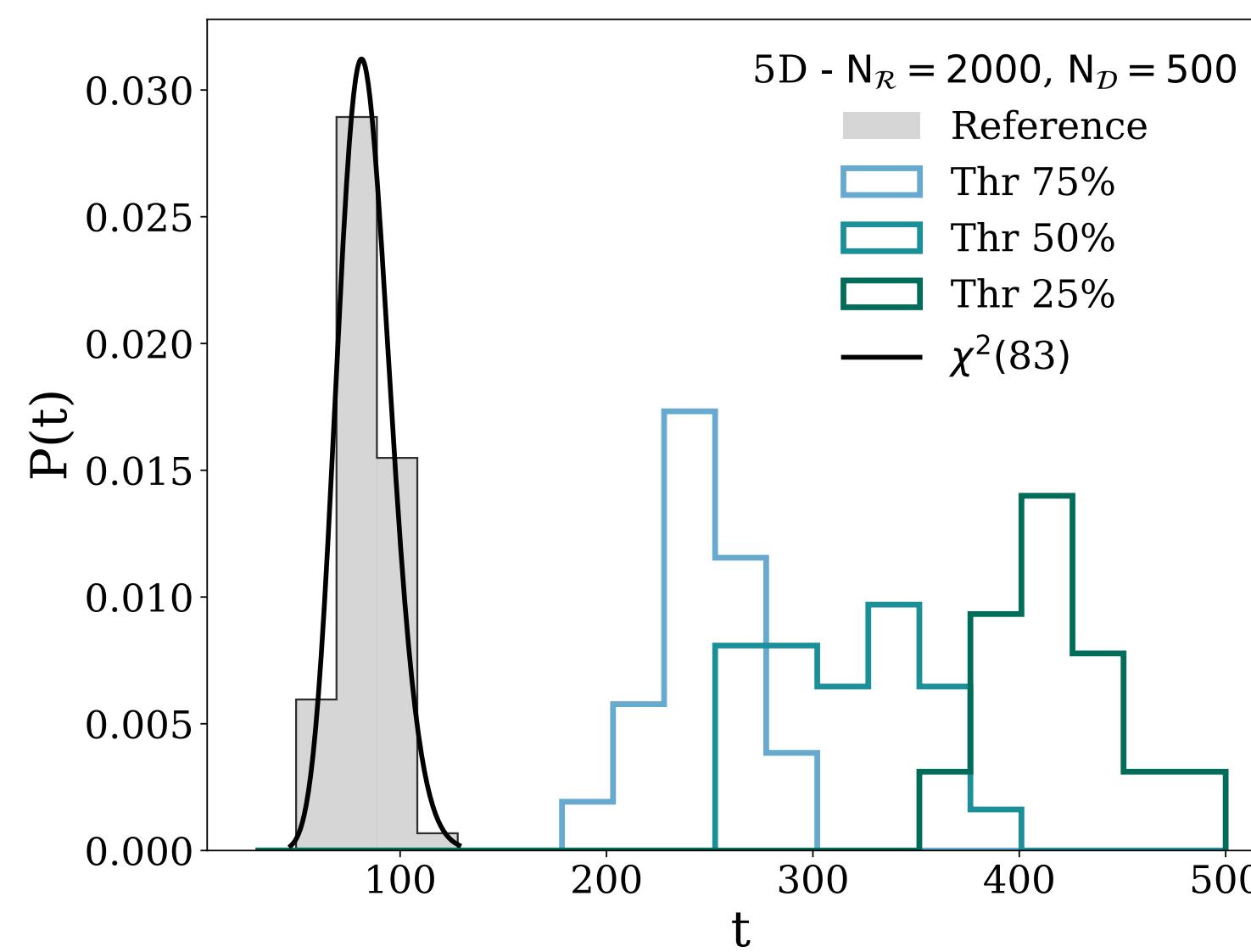


use case :
Validation of generator models
DQM

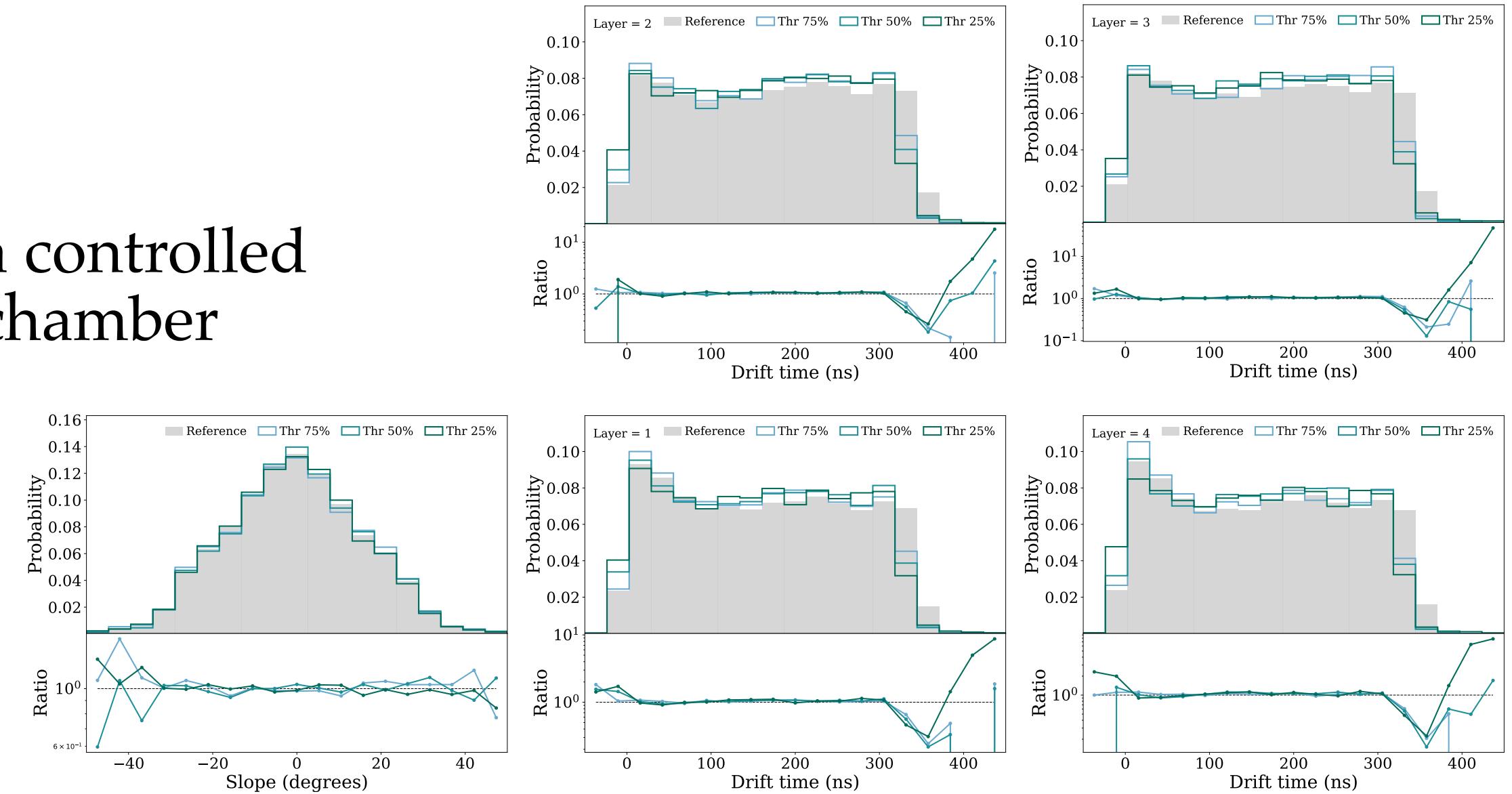
Example: n D DQM

Online monitoring of a DT chamber:

- **Reference sample:** long run in optimal conditions
- **Anomalous samples:** short runs acquired in presence of a controlled anomaly in the value of the **threshold tension** of the DT chamber
- Result of the test statistics
Complete separation of the distributions!



NPLM with kernel methods
 $M = 50, \sigma = 4.84, \lambda = 10^{-7}$
 $N(D) = 5000$
 $N_{\text{ref}} = 200\,000$
Execution time: ~ 1.5 s



Distribution of the observables at different values of the threshold tension

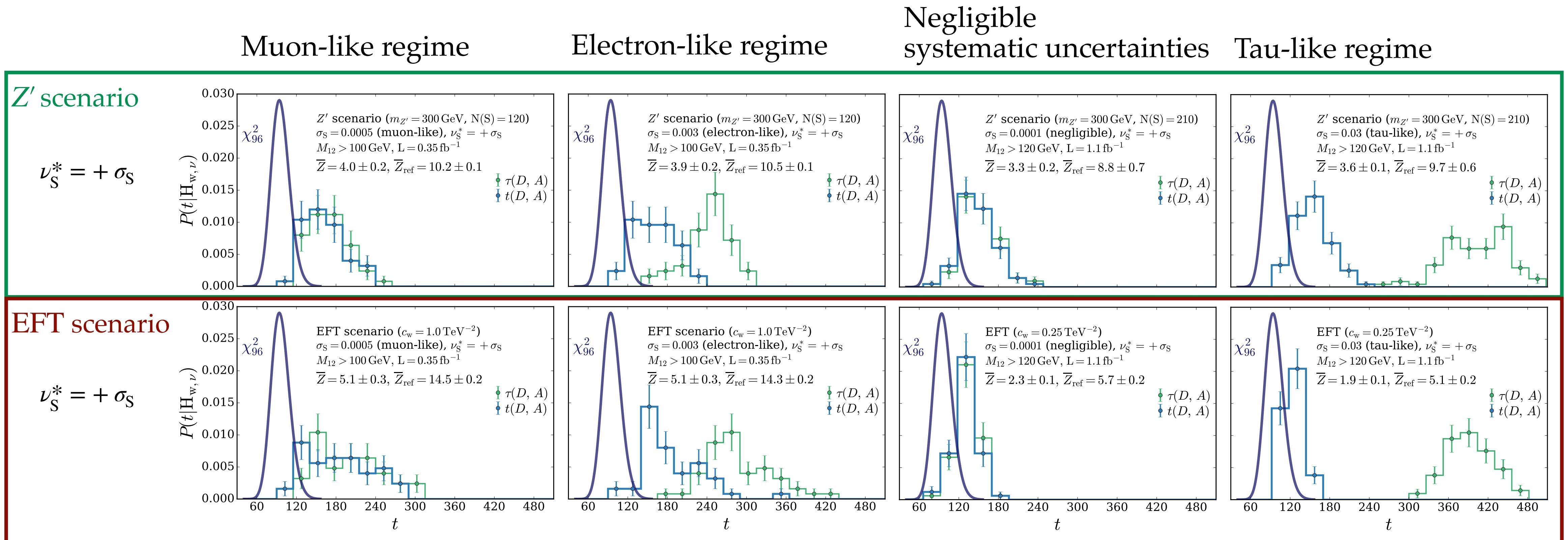
→ more about this in an upcoming follow up talk!

In collaboration with **UniGe** | **MaLGa**

use case :
 n D New Physics search

Harder task: n D analysis

Two body final state (5D): sensitivity to NP scenarios



$$\text{Z-score: } Z = \Phi^{-1} [1 - p]$$

\bar{Z} : Z-score from the median of the empirical $t(D, A)$ distribution

$$\bullet \quad t(D, A) = \tau(D, A) - \Delta(D, A)$$

$$\bullet \quad \tau(D, A)$$

Harder task: n D analysis

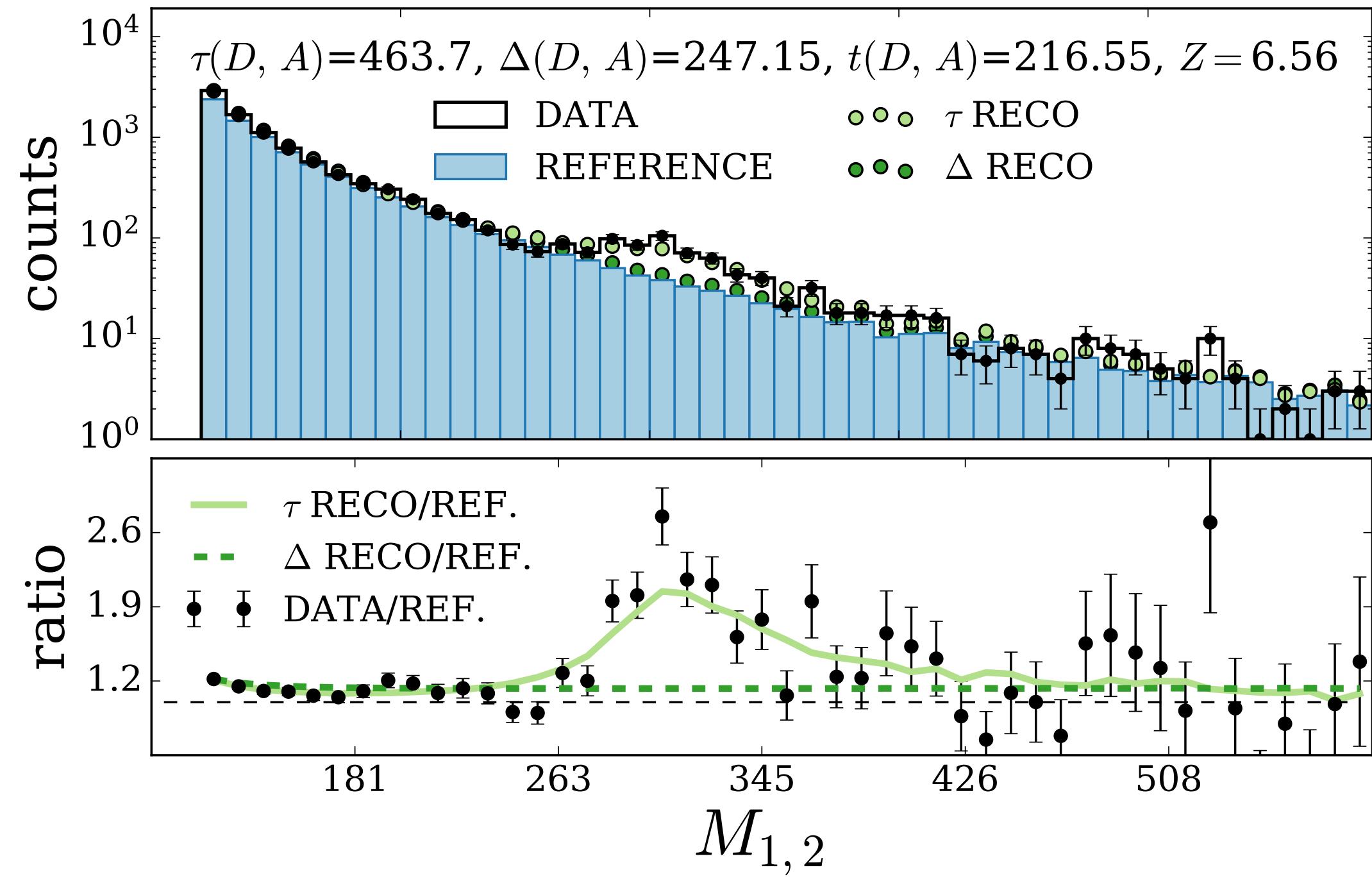
Two bodies final state (5D)

Signal reconstruction with the NN:

Architecture: [5-5-5-5-1] (96 dof), weigh clipping 2.15, $L = 240 \text{ fb}^{-1}$

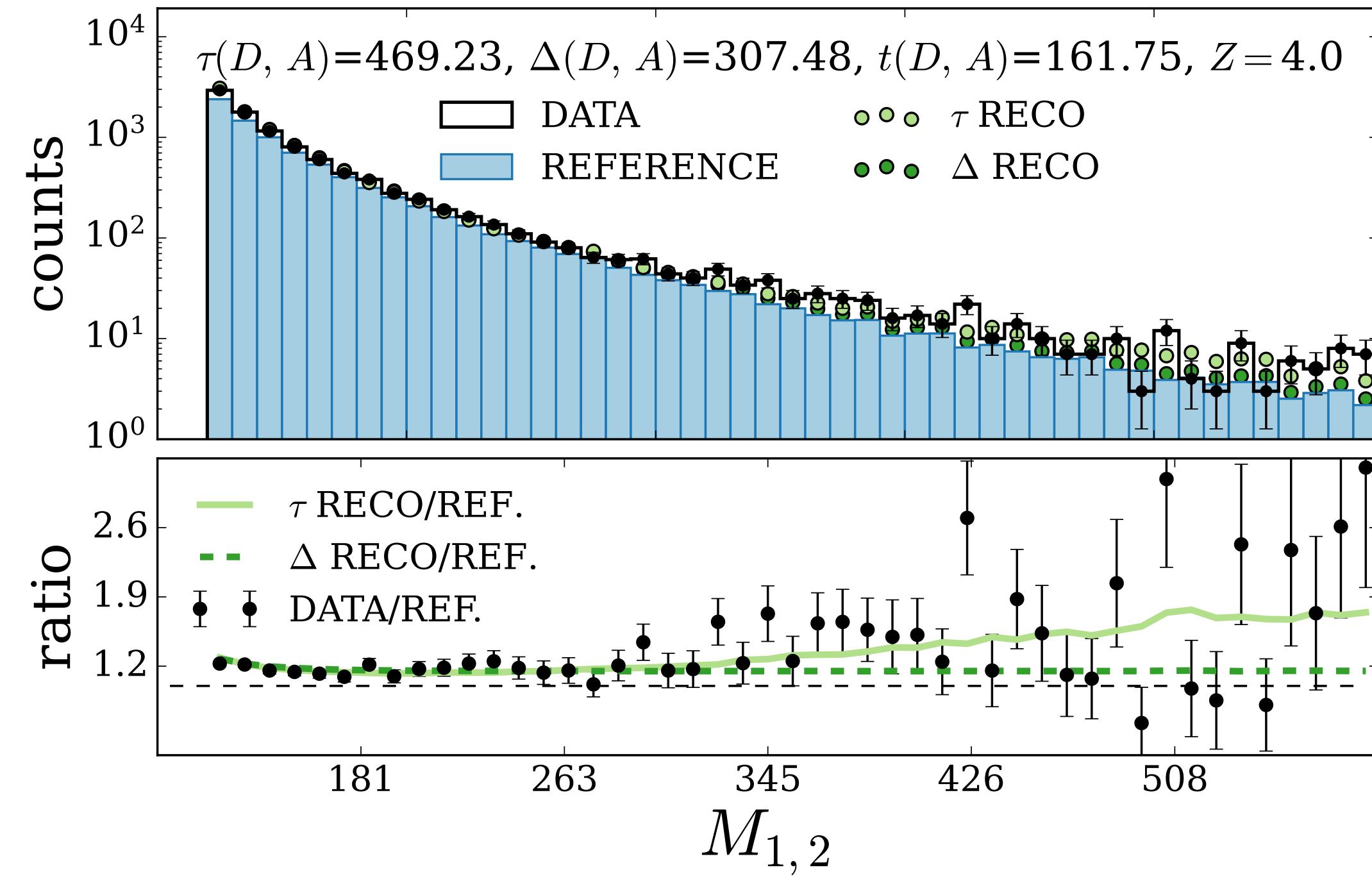
$$\tau \text{ reconstruction: } n(x | H_{\hat{\mathbf{w}}, \hat{\nu}}) = n(x | R_0) \frac{n(x | R_{\hat{\nu}})}{n(x | R_0)} e^{f(x; \hat{\mathbf{w}})}$$

$$\Delta \text{ reconstruction: } n(x | R_{\hat{\nu}})$$



NOTE:

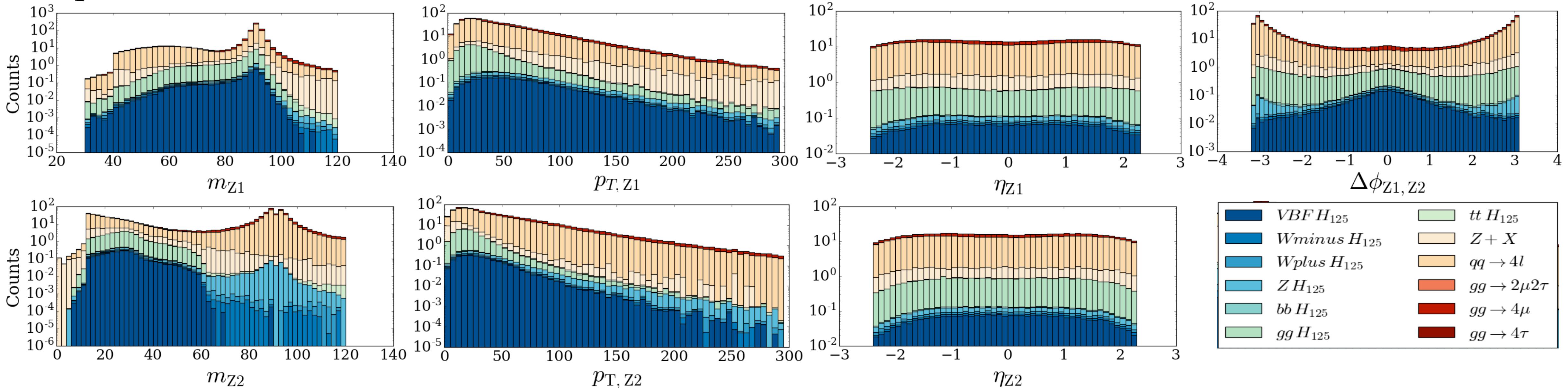
M_{12} is **not** given as an input to the algorithm!



Harder task: n D analysis

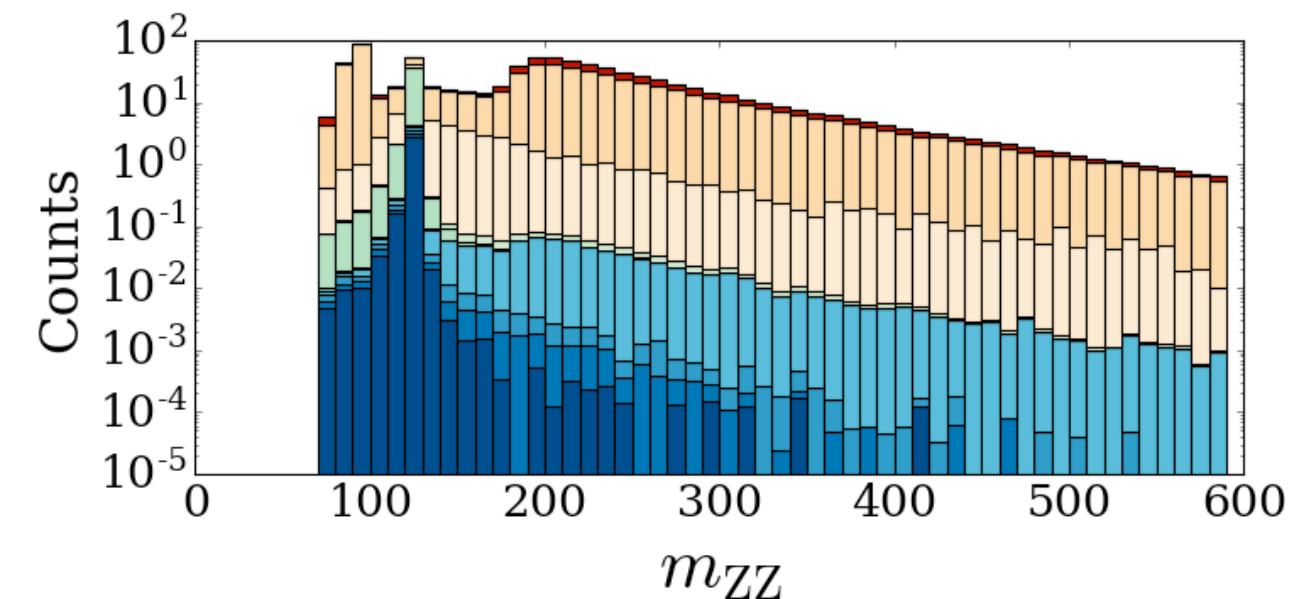
ZZ to 4 muons final state (7D)

Input variables:



Signal benchmarks:

- Higgs boson (as an exercise)



NOTE:

m_{ZZ} is **not** given as an input to the algorithm!

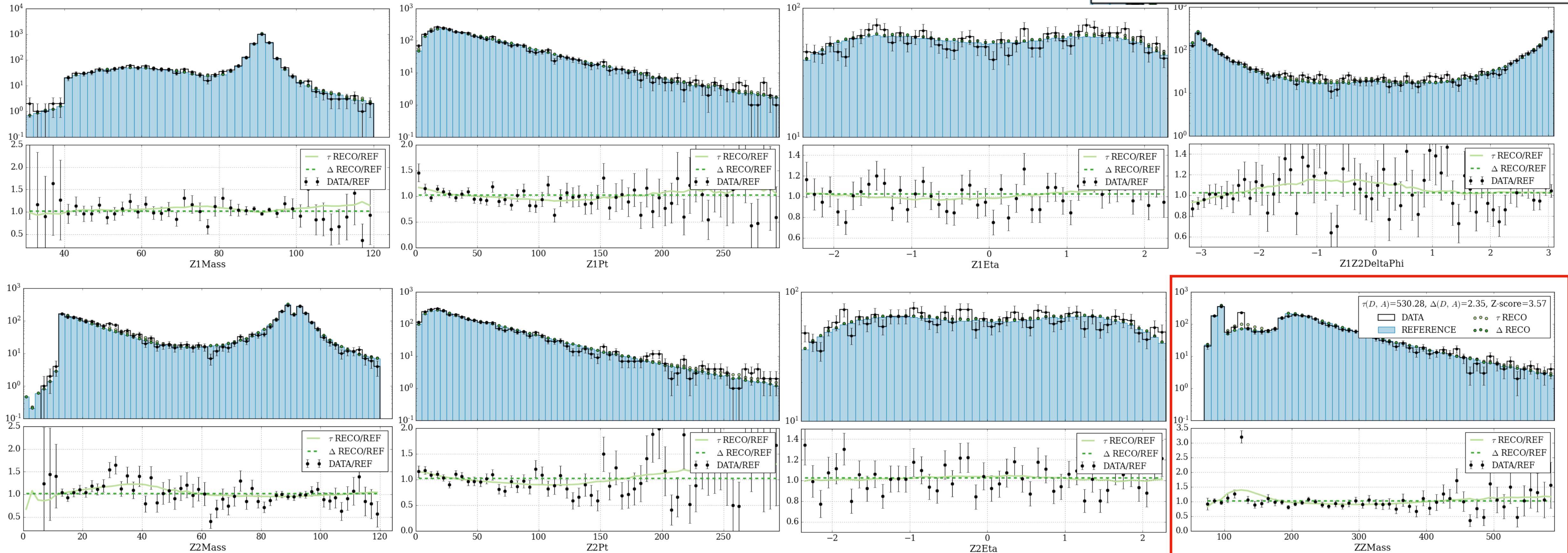
n D analysis

ZZ to 4 leptons final state (7D)

Signal reconstruction with the NN:

Architecture: [7-16-16-1] (417 dof), weigh clipping 1.75

$\tau(D, A) = 530.28, \Delta(D, A) = 2.35, Z\text{-score} = 3.57$
 DATA REFERENCE
 τ RECO Δ RECO



Ongoing work for optimizing NPLM sensitivity in **high dimensional** problems