

NPLM: an *Imperfect* Machine to search for New Physics

Dealing with uncertainties in a ML-based model-independent signal extraction

R.T. d'Agnolo¹, G. Grosso^{2,3}, M. Pierini³, A. Wulzer², M. Zanetti²

¹ Université Paris-Saclay and CEA, ² Università degli Studi di Padova and INFN, ³ CERN experimental department

In this talk

- **What is NPLM and how does it work?**

Complete analysis strategy testing the data for departures from SM expectations (from data to a p -value for discovery, taking care of systematic uncertainties in the process).

- main concept (neglecting systematic uncertainties) [1, 2]
- including systematic uncertainties [3]

- **What is NPLM good for?**

Multivariate, unbinned analysis, towards model independence (released constraints, lower level information, simultaneously sensitive to multiple signal patterns).

- 5D analysis of a di-body final state at the LHC [3]

Link to related papers:

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

NPLM algorithm

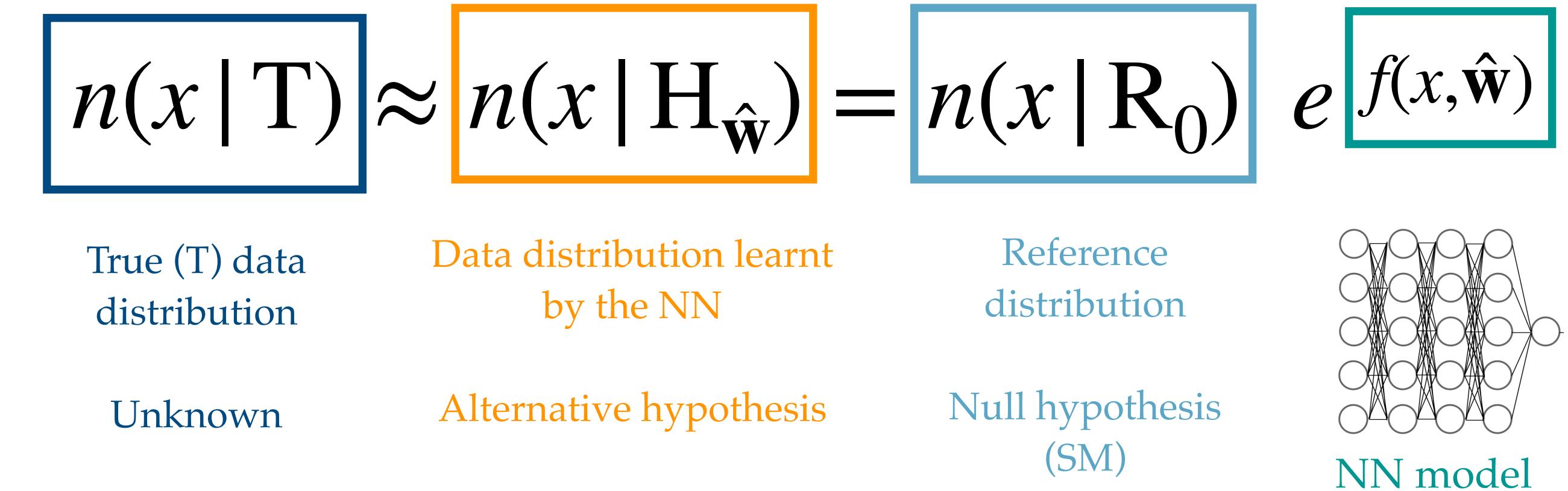
New Physics Learning Machine (NPLM)

Main Concepts (negligible uncertainties)

- Goal: performing a **log-likelihood-ratio hypothesis test**
(End-to-end strategy, from the data to a *p*-value for the discovery)
- Exploiting a Neural Network (NN) to **parametrize** the data distribution in terms of a Reference distribution (R_0)
- **Signal-model-independent**: reduced assumptions on the signal hypothesis

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

R_0 : reference (null) hypothesis
 H_w : alternative hypothesis



New Physics Learning Machine (NPLM)

Main Concepts (negligible uncertainties)

Maximum Likelihood from minimal loss:

Test statistic

$$\bar{t}(\mathcal{D}) = 2 \max_{\mathbf{w}} \log \left[\frac{\mathcal{L}(\mathbf{H}_{\mathbf{w}} | \mathcal{D})}{\mathcal{L}(\mathbf{R}_0 | \mathcal{D})} \right] = -2 \min_{\mathbf{w}} \{ \bar{L}[f(\cdot; \mathbf{w})] \}$$

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

\mathcal{D} : data sample

\mathcal{R} : reference sample (built according to the R_0 hypothesis); could be weighted (w_x)

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 $\sum_{x \in \mathcal{R}} w_x = N(R_0)$

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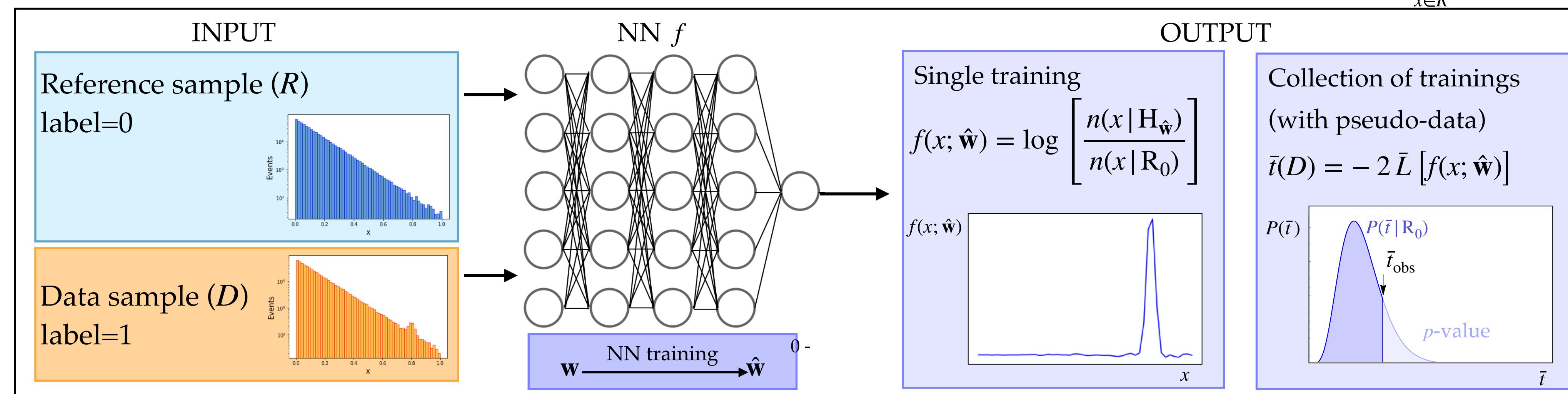
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New Physics Learning Machine (NPLM)

Dealing with multivariate problems (negligible uncertainties)

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

Wilks' 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 $df \leq |\mathbf{w}|$.

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

→ a **NN REGULARIZATION** can solve this problem!

New Physics Learning Machine (NPLM)

Dealing with multivariate problems (negligible uncertainties)

BSM-NN regularization :

Weight clipping parameter:

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

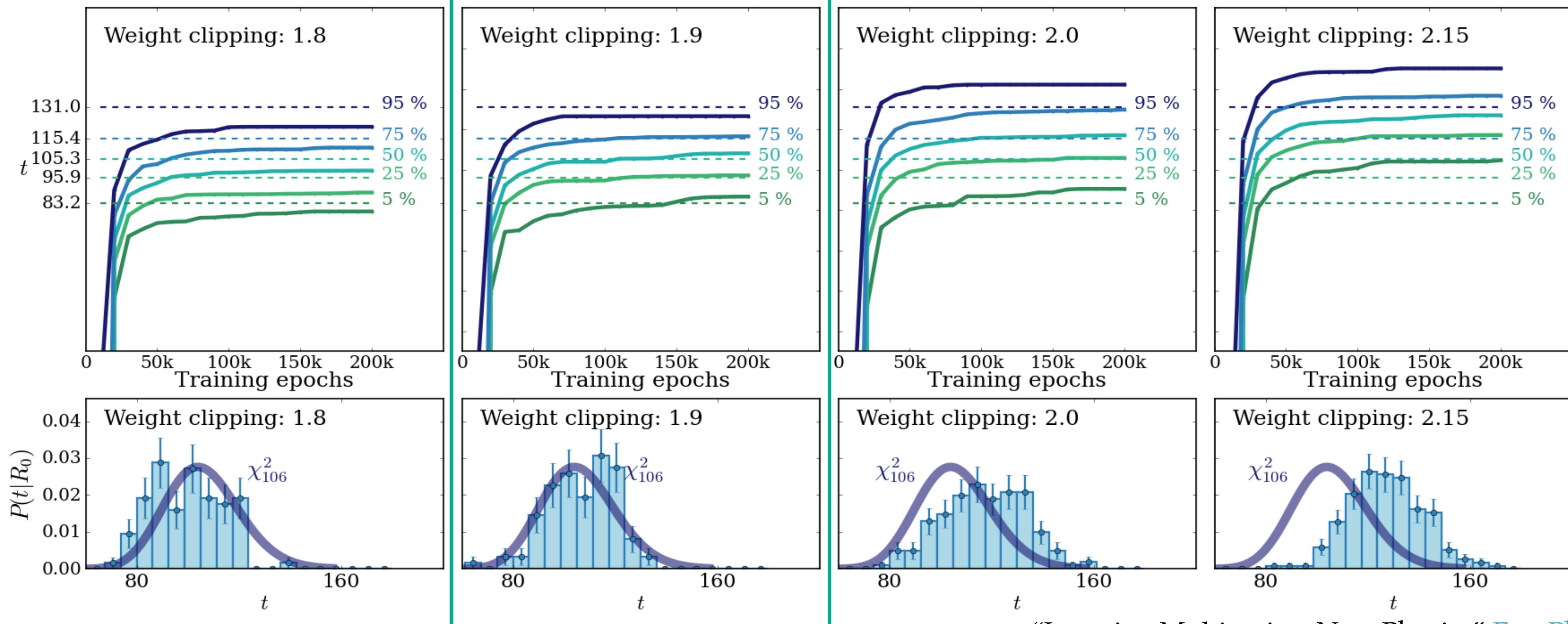
For a chosen NN architecture, **tuning the weight clipping** allows to recover a good agreement of the empirical distribution of \bar{t} under R_0 with a **target $\chi^2_{|w|}$** distribution.

Example:

NN model: 5-7-7-1,
 $|w| = 106$

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 $\chi^2_{|w|}$



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

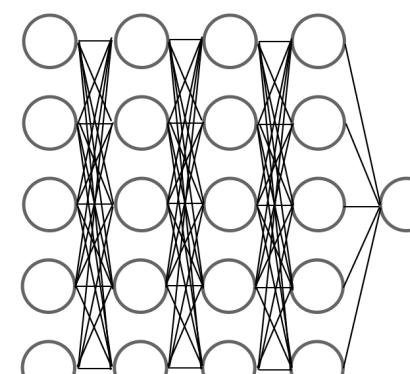
$\boldsymbol{\nu}$: set of nuisance parameters modelling the uncertainties effects

\mathcal{D} : data sample

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

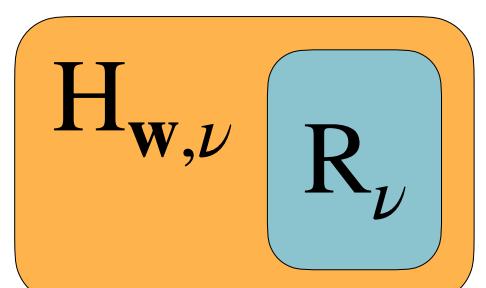
New parametrization

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

True (T) data distribution	Data distribution learnt by the NN	Reference distribution	New term containing the dependence on $\boldsymbol{\nu}$	NN model
Unknown	Alternative hypothesis	Null hypothesis	$r(x; \boldsymbol{\nu})$	

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

Validation of the $(\tau - \Delta)$ procedure

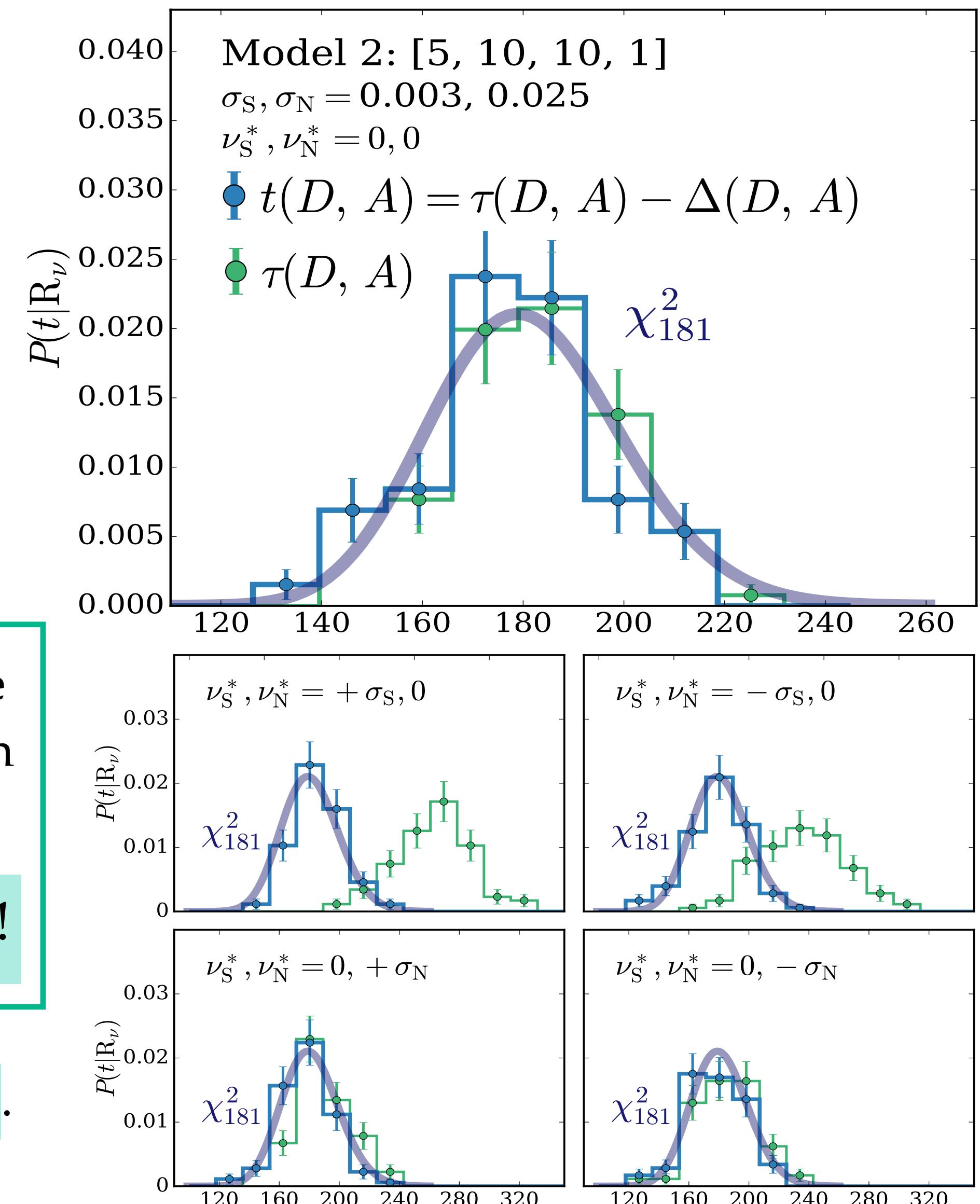
“Toy Data” : test the procedure on simulated toys following the Reference (SM) hypothesis with generation value for the nuisance parameters $\nu^* = \pm \sigma_\nu$:

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

The \bar{t} distribution under the reference hypothesis R_{ν^*} is **compatible with the target $\chi^2_{|w|}$** for values of the true nuisance parameters within the uncertainty ($\nu^* = \pm \sigma_\nu$).

\bar{t} is **independent** of the true value of the nuisance parameters!

We can build a *frequentistic* test statistic relying on the asymptotic $\chi^2_{|w|}$.



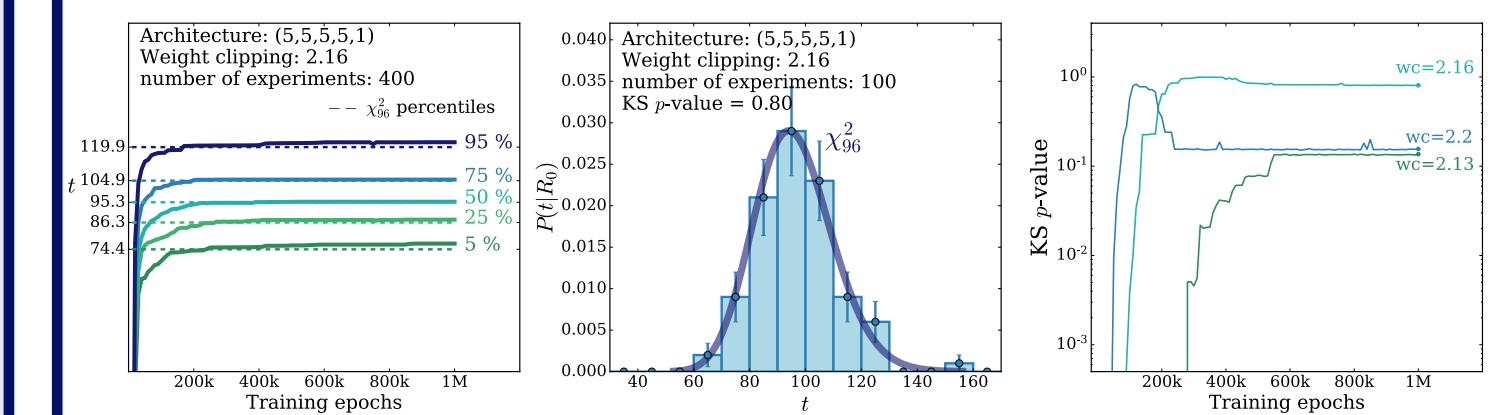
New Physics Learning Machine (NPLM)

Including systematic uncertainties

Final procedure in steps:

1. NN (f) REGULARIZATION:

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



2. NUISANCE TAYLOR'S EXPANSION LEARNING:

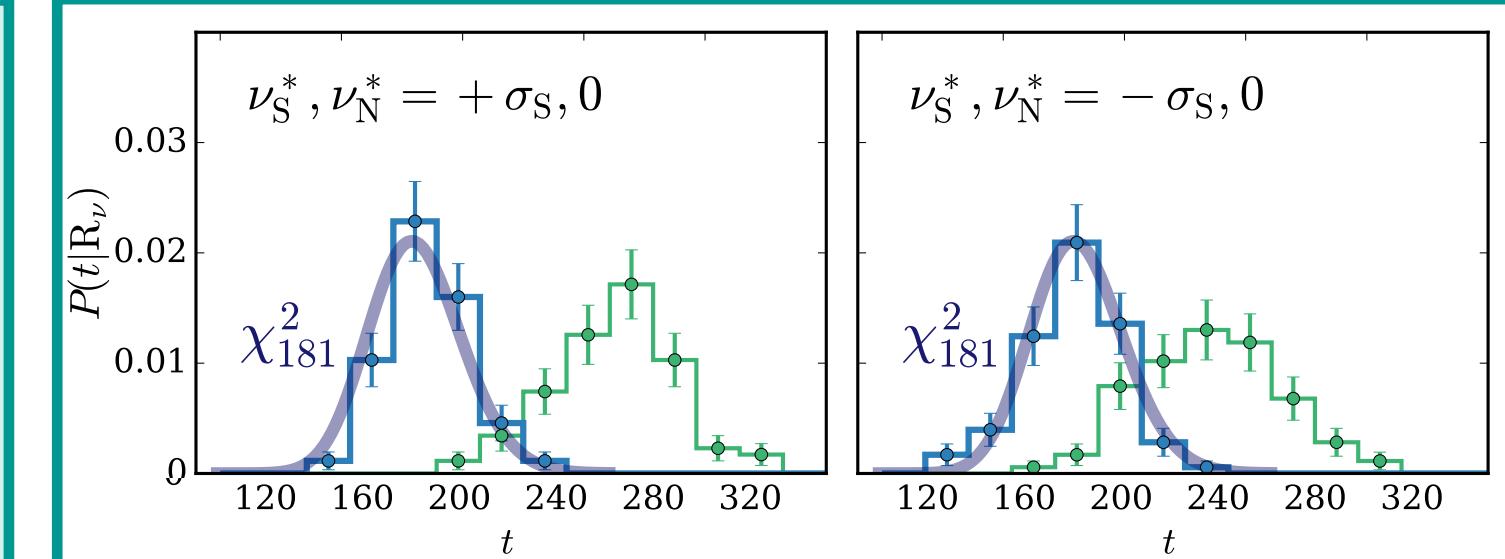
modelling $\hat{r}(x; \nu) = \exp \left[\hat{\delta}_1(x) \nu + \hat{\delta}_2(x) \nu^2 + \dots \right]$;

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

3. $\tau - \Delta$ VALIDATION:

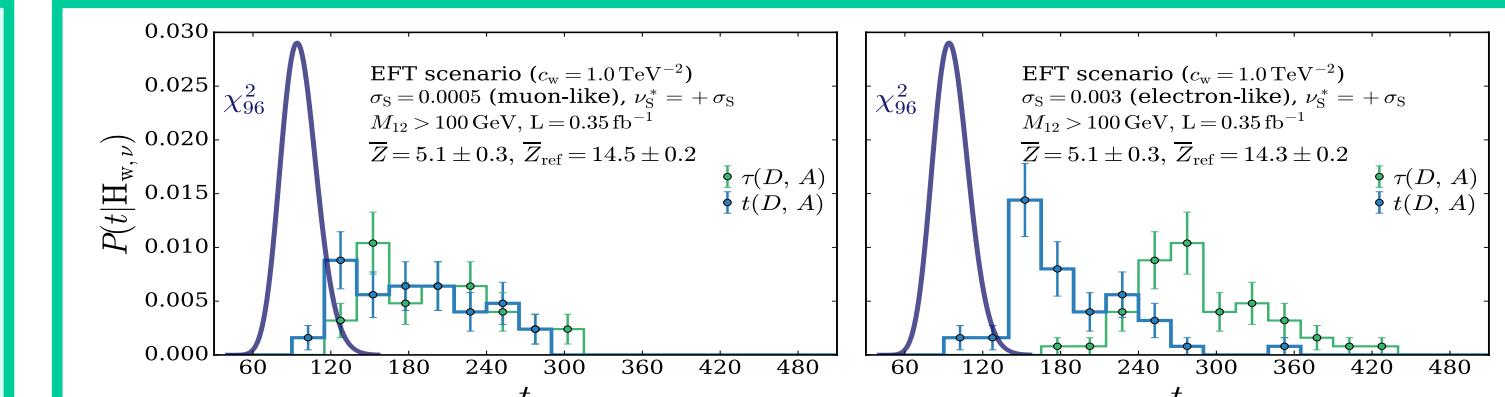
$$\mathcal{D} \sim R_{\nu^*}, \quad \nu^* = \pm \sigma_\nu$$

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



4. TESTING THE DATA:

running the procedure on real data.

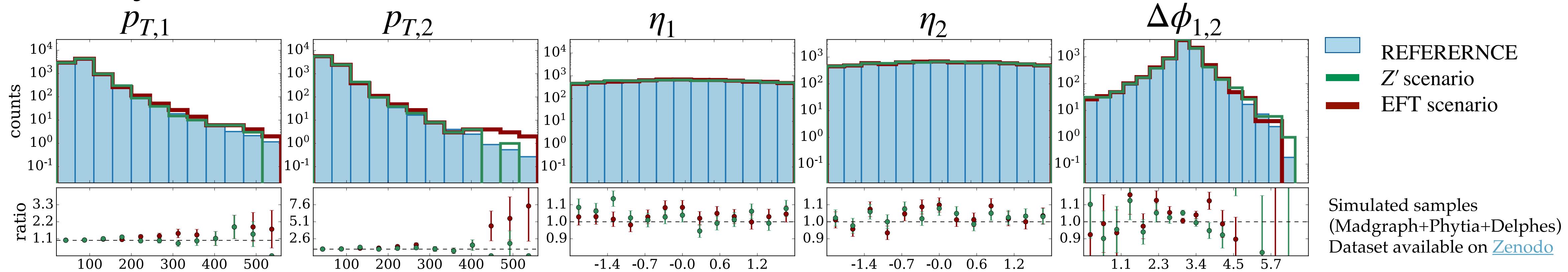


Application: 5D analysis of a di-lepton final state at the LHC

Di-body final state at the LHC

Dataset

5D analysis — Input variables:



Uncertainties on the reference sample (SM):

- Global normalization effect: $\sigma_N = 2.5 \%$

- Momentum scale effect:

$$p_{T1,2}^{(b,e)} = \exp \left[\nu_s \sigma_s^{(b,e)} / \sigma_s^{(b)} \right] p_{T1,2}^{(b,e)} \quad (\text{b}) \text{ barrel region } |\eta| < 1.2, \quad (\text{e}) \text{ endcaps region } |\eta| \geq 1.2$$

- Muon-like regime: $\sigma_S^{(b)} = 0.05 \%$, $\sigma_S^{(e)} = 0.15 \%$
- Electron-like regime: $\sigma_S^{(b)} = 0.3 \%$, $\sigma_S^{(e)} = 0.9 \%$
- Tau-like regime: $\sigma_S^{(b)} = \sigma_S^{(e)} = 3 \%$

Di-body final state at the LHC

Dataset

New Physics benchmarks:

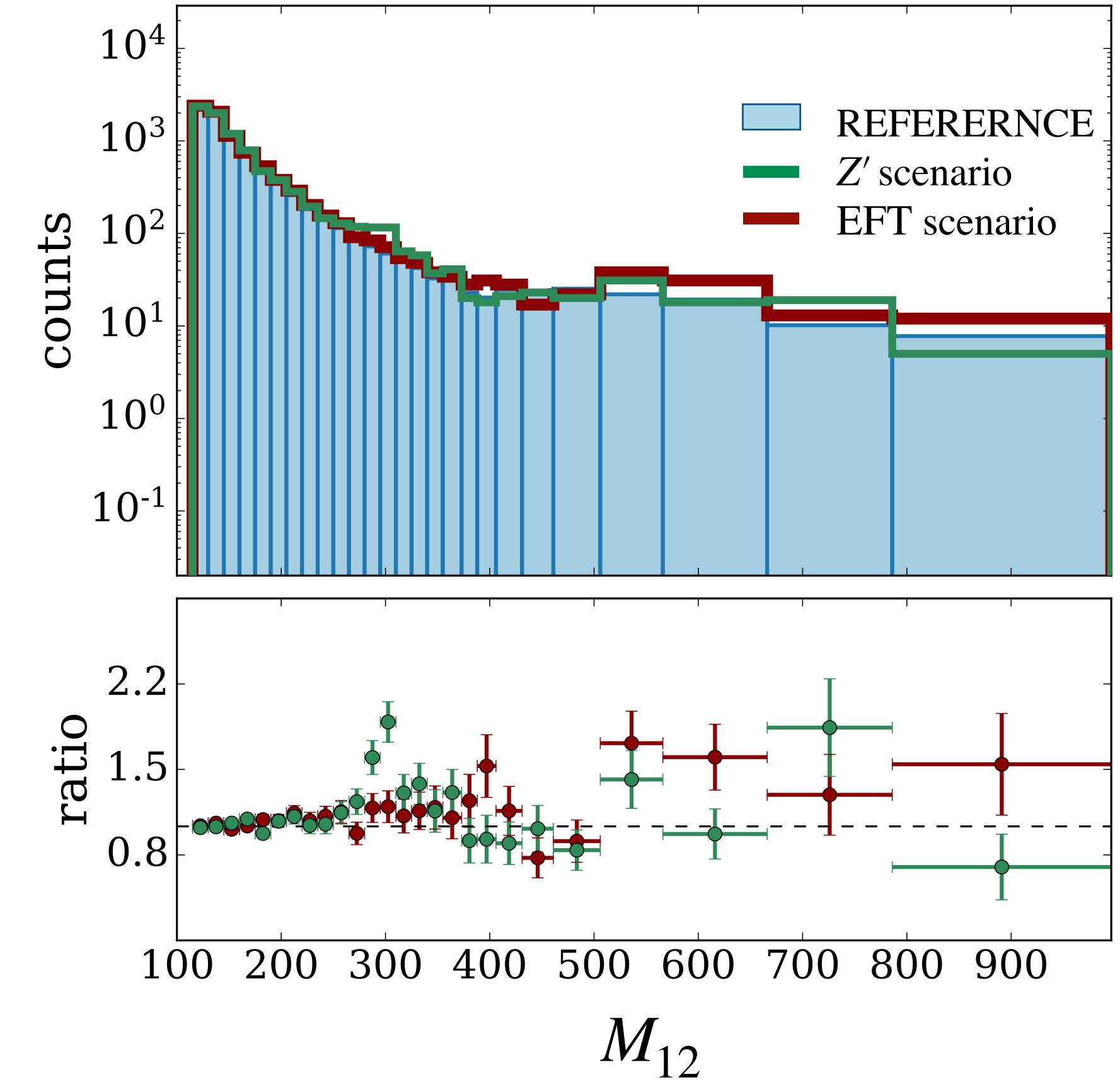
Resonance in the two-body invariant mass

- **Z' scenario:** new vector boson with the same SM coupling as the Z boson and mass of 300 GeV.
 - Muon-like, electron-like regimes:
 $M_{12} > 100 \text{ GeV}, L = 0.35 \text{ fb}^{-1}, N(S) = 120$
 - Tau-like regime:
 $M_{12} > 120 \text{ GeV}, L = 1.1 \text{ fb}^{-1}, N(S) = 210$

Non resonant excess in the tail of the two-body invariant mass

- **EFT scenario:** dimension-6 4-contact operator:
$$\frac{c_W}{\Lambda} J_{L\mu}^a J_{La}^\mu.$$
- Muon-like, electron-like regimes:
 $M_{12} > 100 \text{ GeV}, L = 0.35 \text{ fb}^{-1}, c_W = 1.0 \text{ TeV}^{-2}$
- Tau-like regime:
 $M_{12} > 120 \text{ GeV}, L = 1.1 \text{ fb}^{-1}, c_W = 0.25 \text{ TeV}^{-2}$

Example:
Tau-like regime

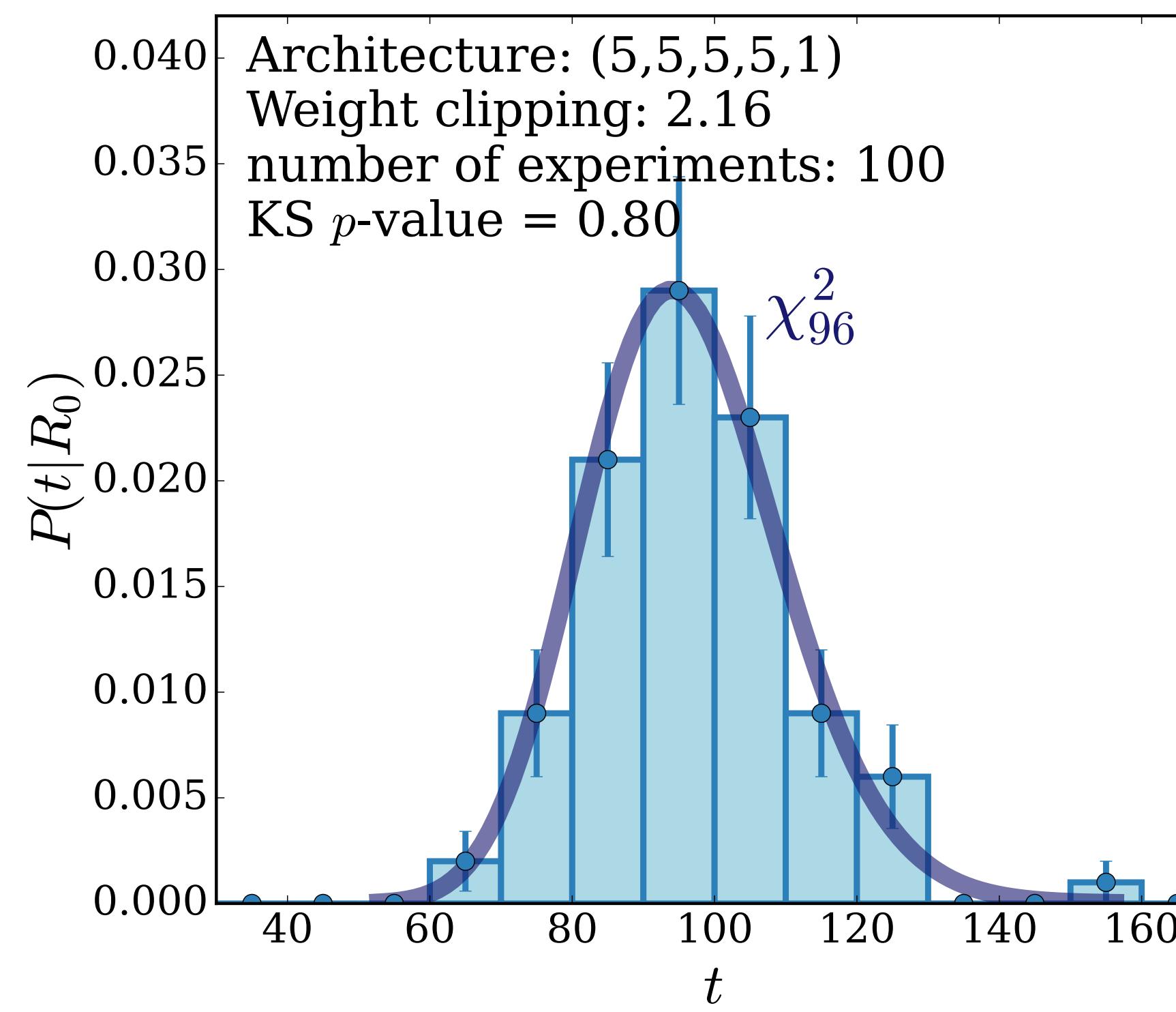


NOTE:
 M_{12} is **not** given as an input to the algorithm!

Di-body final state at the LHC

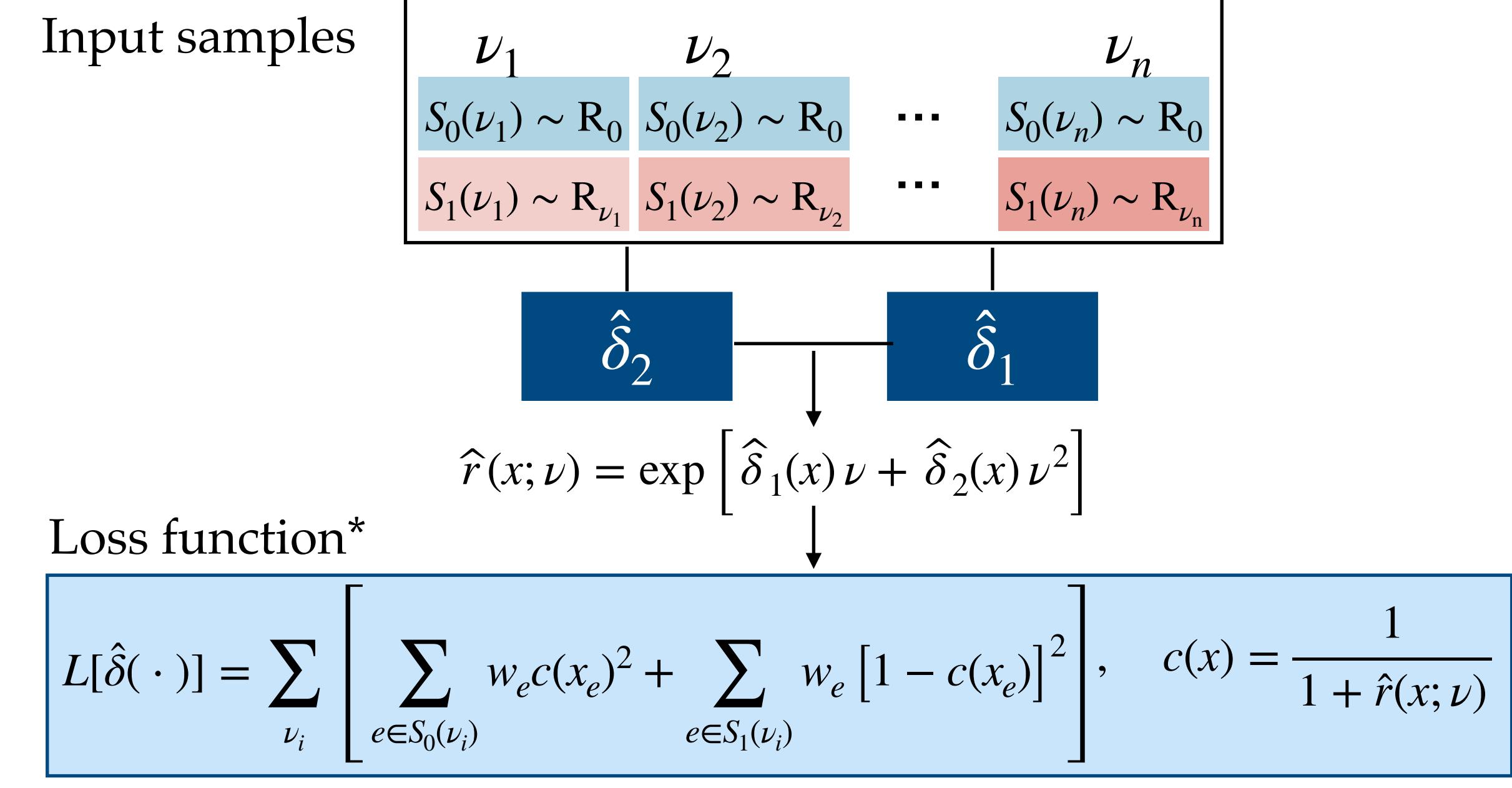
1) NN setup for the τ term:

- Data sample $N(D) \sim 8500$ events
- Reference sample $N(R) = 5 \times N(D) \sim 42\,500$
- Regularised DNN (weight clipping tuning)



2) Taylor's expansion learning for $r(x, \nu)$:

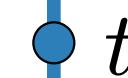
Training a neural network model to learn each coefficient of the Taylor's expansion of $r(x; \nu) = \frac{n(x|R_\nu)}{n(x|R_0)}$
(Parametrized classifier)

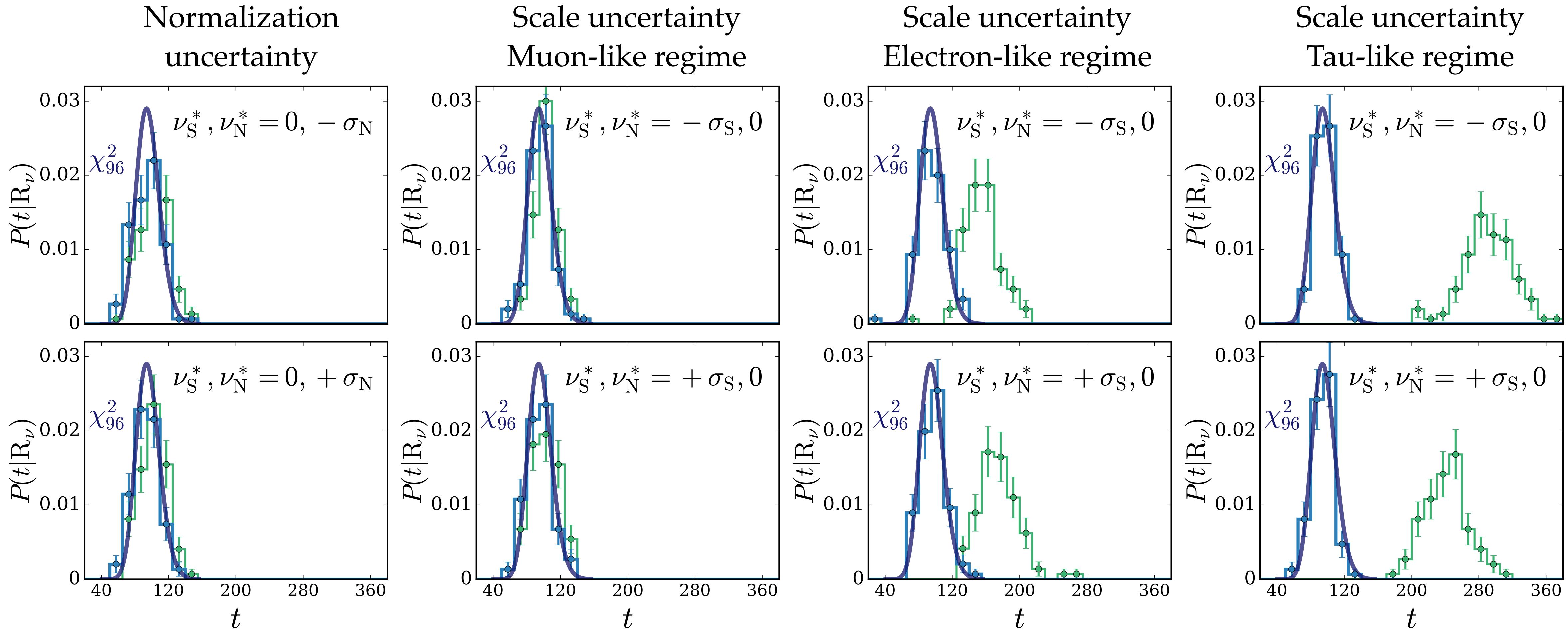


* Parametrized classifiers for optimal EFT sensitivity [arXiv:2007.10356](https://arxiv.org/abs/2007.10356)

Di-body final state at the LHC

$\tau - \Delta$ validation

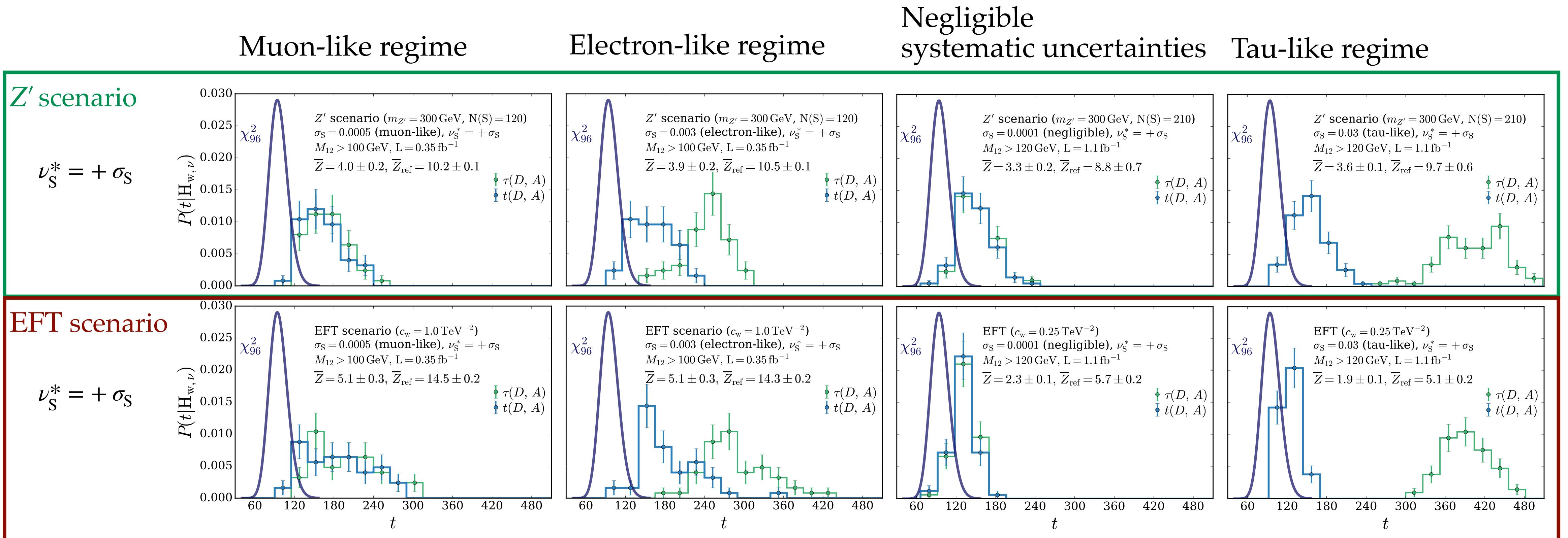
 $t(D, A) = \tau(D, A) - \Delta(D, A)$
 $\tau(D, A)$



DNN [5-5-5-5-1], #trainable parameters = 96, weight clipping = 2.16

Di-body final state at the LHC

Sensitivity to New Physics scenarios



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

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

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

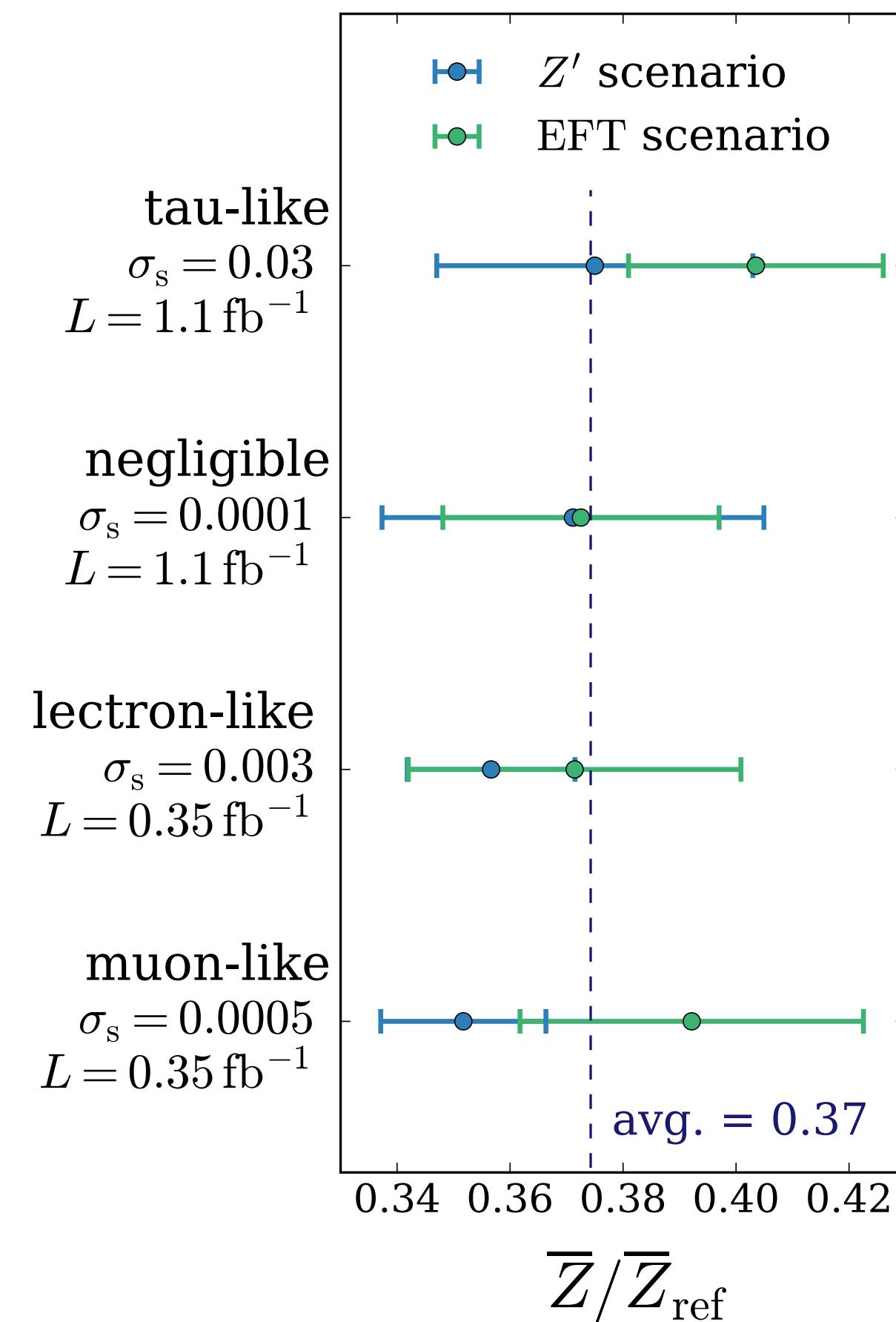
$\tau(D, A)$

Di-body final state at the LHC

Sensitivity to New Physics scenarios

Summary of the results:

- Comparable performances in the resonant and non-resonant scenarios:
 - NPLM is **simultaneously sensitive to any source of New Physics**;
- Comparable performances at different systematic uncertainties regimes:
 - NPLM is robust against the presence of systematic uncertainties;
 - the presence of systematic uncertainties affects NPLM in the same measure as any other hypothesis test;
- **No information** about the New Physics **signal** has been provided to the algorithm at any step of its implementation:
 - The performances of NPLM are lower than any model-dependent strategy by construction ($\bar{Z}/\bar{Z}_{\text{ref}} = 0.37$);



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

- \bar{Z} : Z-score from NPLM

- \bar{Z}_{ref} : Z-score from a model-dependent (optimized) test statistics

Di-body final state at the LHC

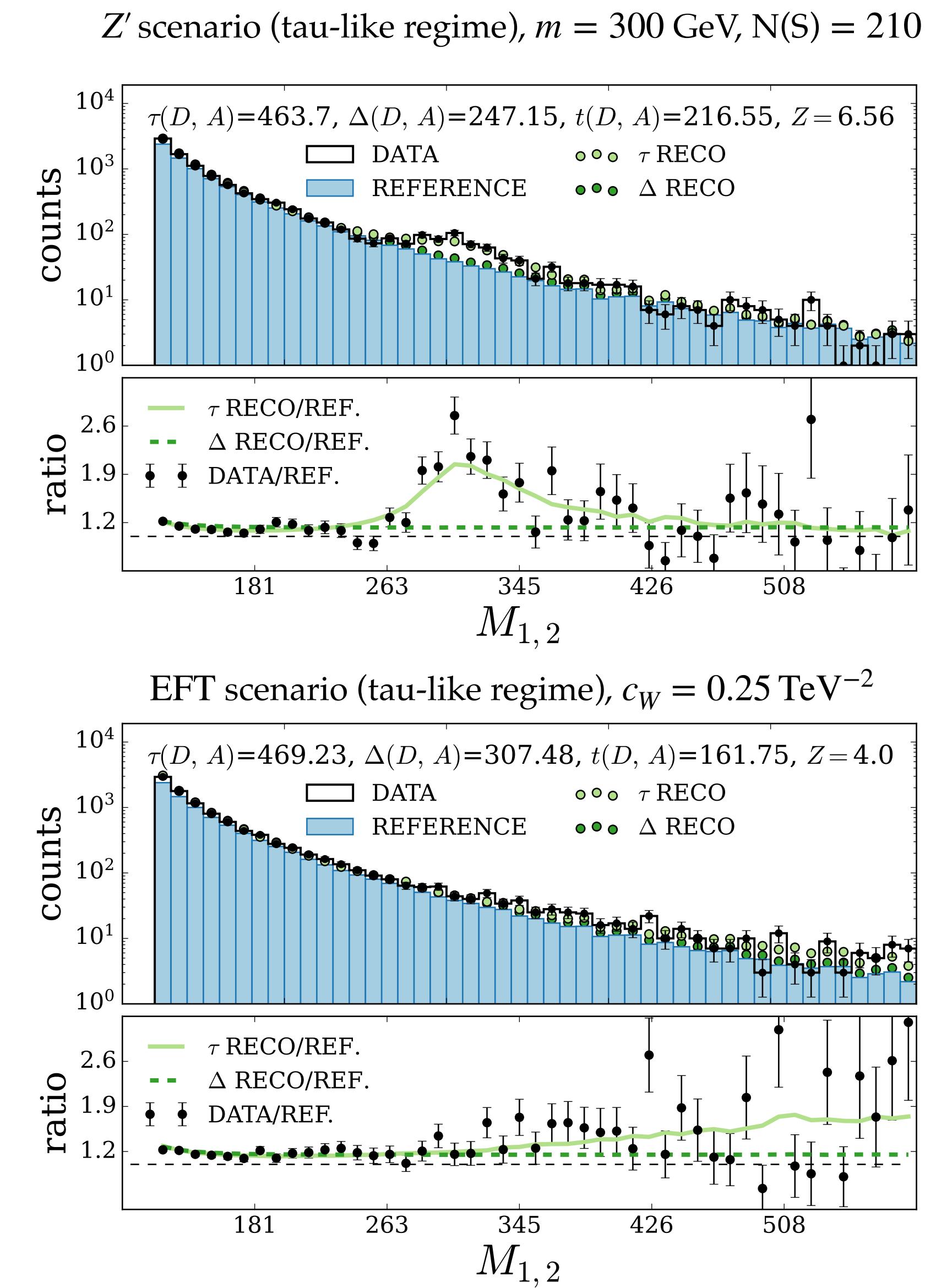
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- Comparable performances at different systematic uncertainties regimes:
 - NPLM is robust against the presence of systematic uncertainties;
 - the presence of systematic uncertainties affects NPLM in the same measure as any other hypothesis test;
- No information about the New Physics signal has been provided to the algorithm at any step of its implementation:
 - The performances of NPLM are lower than any model-dependent strategy by construction ($\bar{Z}/\bar{Z}_{\text{ref}} = 0.37$);
- NPLM is able to *learn* non trivial combinations of the input variables and point to the source of the significant discrepancy.

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

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



Conclusions

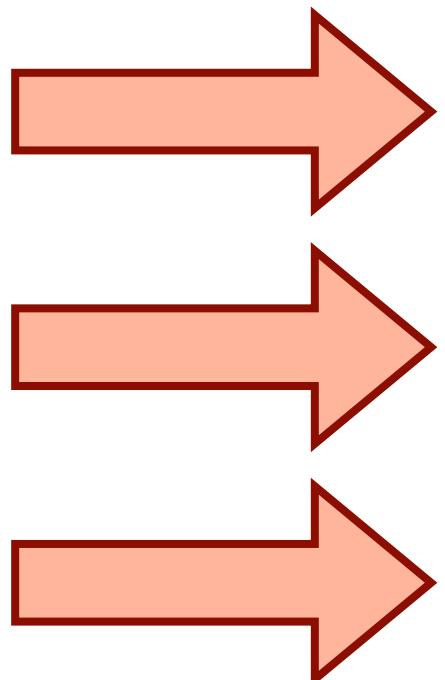
Outlook on future perspectives

Current limitations and future developments:

- Accuracy and size of the Reference sample
- Accuracy in the (multivariate) modelling of the nuisance effects
- Training time

A solution from Kernel Methods (“Learning new physics efficiently with nonparametric methods” [2204.02317](#))

- Optimisation of NPLM sensitivity performances:
how do we choose the NN architecture? Is the regularization heuristic optimal?



Set a **limit** on the actual **luminosity** that we are allowed to inspect, but do not obstacle the applicability of NPLM.

NPLM is ready to be performed on a real analysis at the LHC!

- ✓ Heuristic method to setup **multivariate** analysis
- ✓ Strategy to account for **systematic uncertainties**

Outlook on future perspectives

Getting started with NPLM

- [NPLM package](#): python-based package to run the NPLM analysis strategy
- [Tutorial](#) on 1D toy model for getting started

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

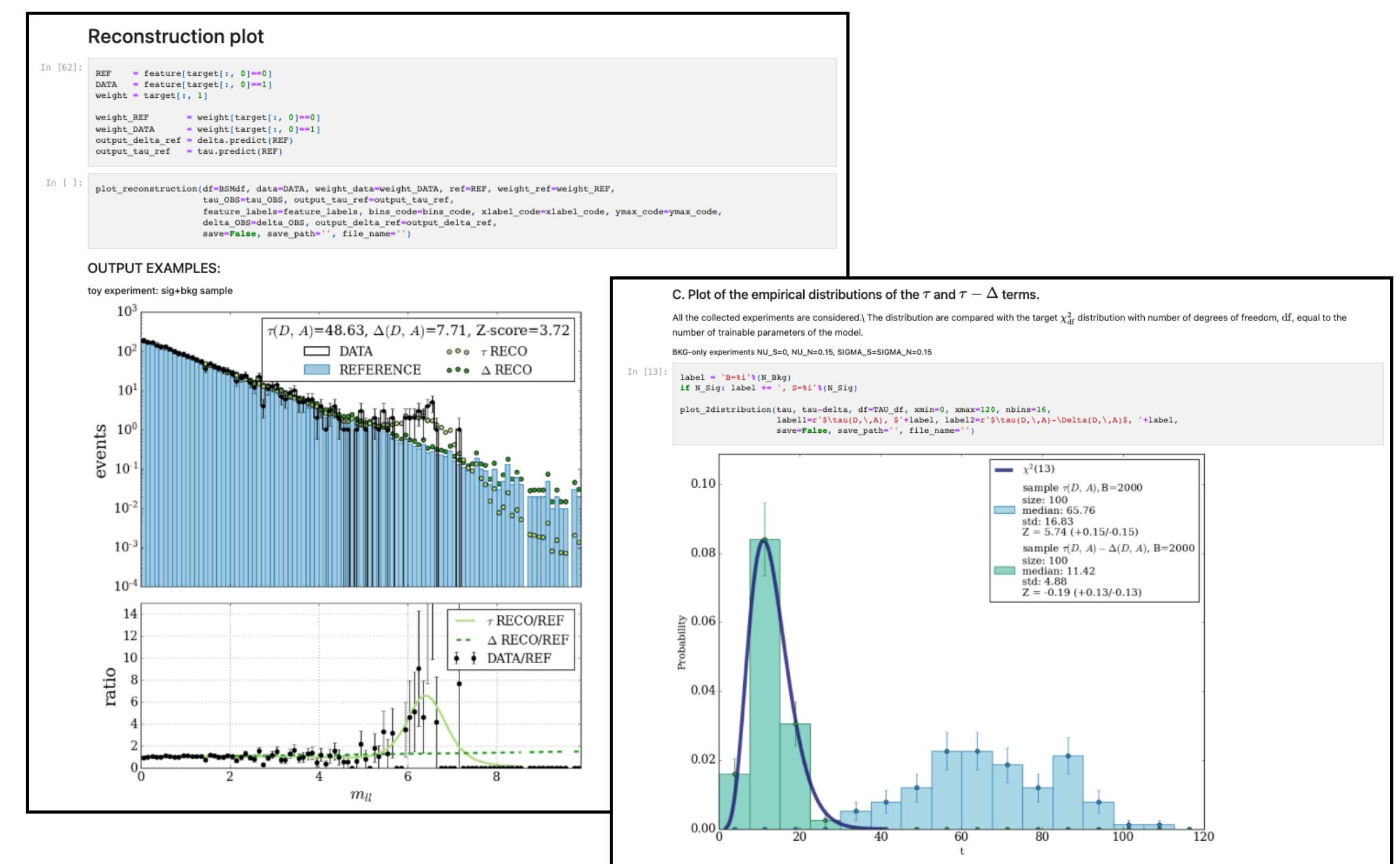
Short description:

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](#).



Backup

New Physics Learning Machine (NPLM)

Main Concepts (negligible uncertainties)

Maximum Likelihood from minimal loss:

Test statistic

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

\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_x)

$$= 2 \log \left[\frac{e^{-N(\hat{\mathbf{w}})}}{e^{-N(R)}} \prod_{x \in \mathcal{D}} \frac{n(x | \hat{\mathbf{w}})}{n(x | R)} \right] = -2 \underset{\{\mathbf{w}\}}{\text{Min}} \left[N(\mathbf{w}) - N(R) - \sum_{x \in \mathcal{D}} f(x; \mathbf{w}) \right]$$

$$= -2 \min_{\mathbf{w}} \{ \bar{L}[f(\cdot; \mathbf{w})] \}$$

$$N(\mathbf{w}) = \frac{N(R)}{\mathcal{N}_R} \sum_{x \in \mathcal{R}} e^{f(x; \mathbf{w})}$$

Loss function

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

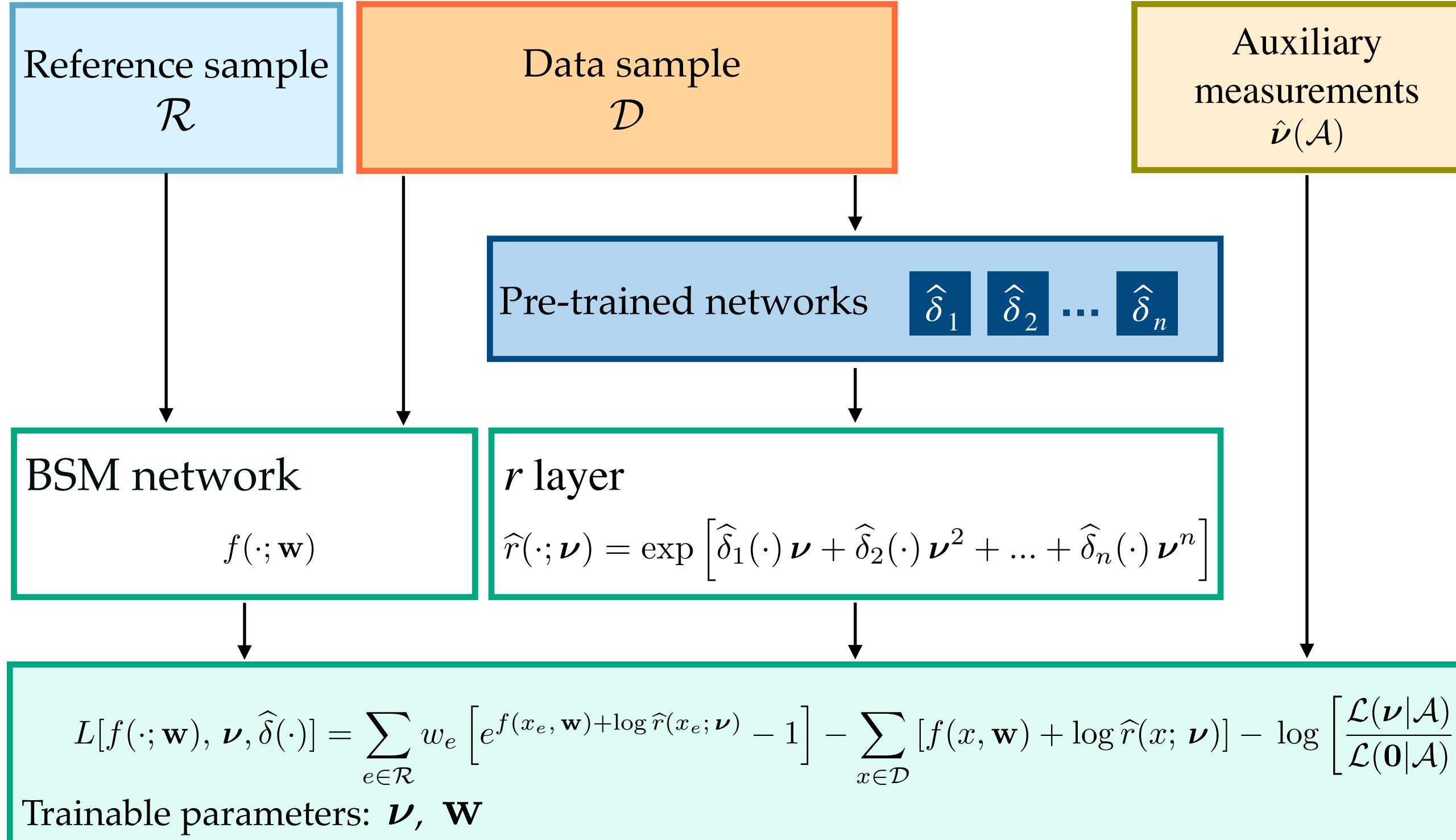
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New Physics Learning Machine (NPLM)

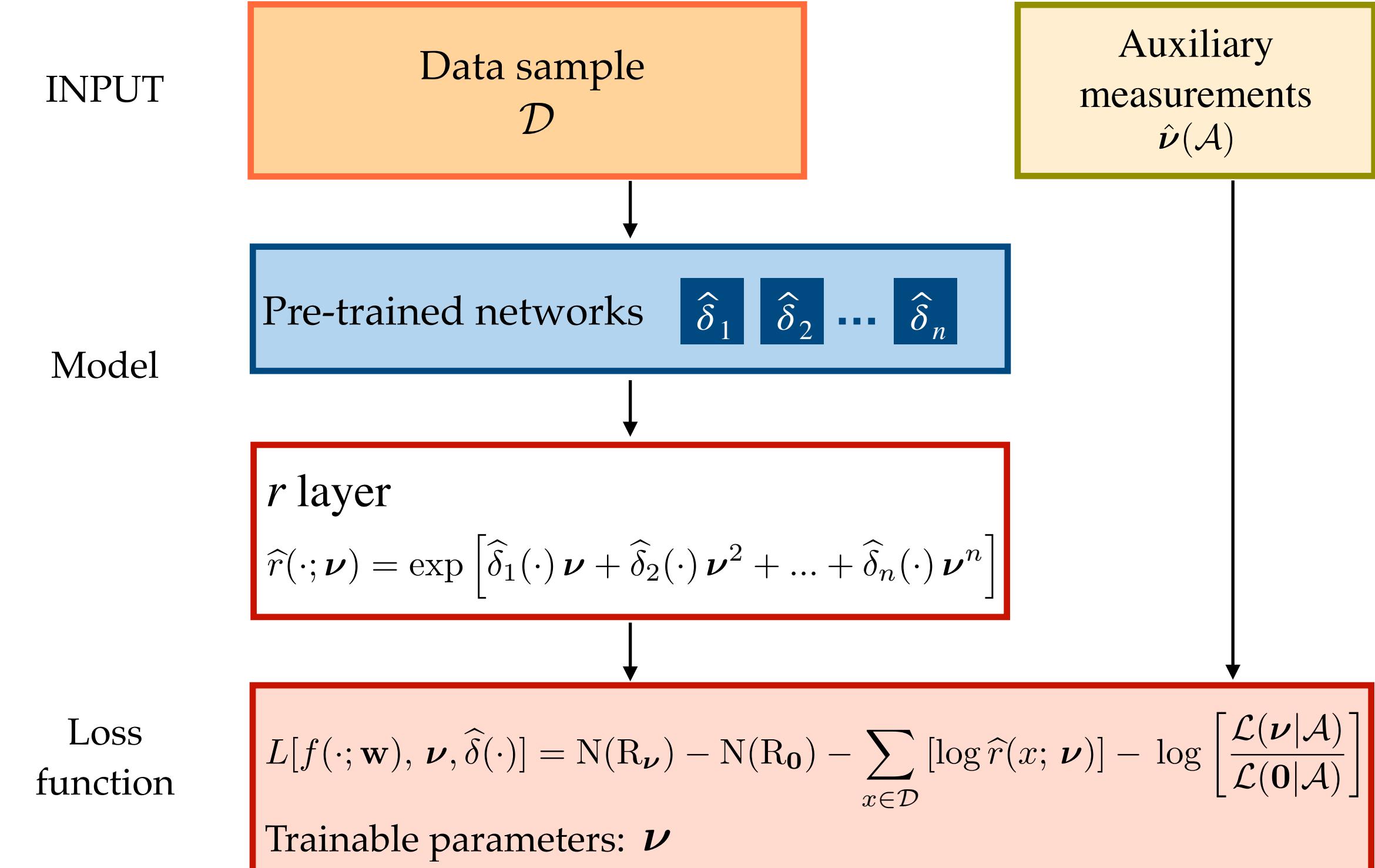
Including systematic uncertainties

τ term



$$\tau(\mathcal{D}, \mathcal{A}) = -2 \min_{\mathbf{w}, \boldsymbol{\nu}} L \left[f(\cdot, \mathbf{w}), \boldsymbol{\nu}; \hat{\delta}(\cdot) \right]$$

Δ term



$$\Delta(\mathcal{D}, \mathcal{A}) = -2 \min_{\boldsymbol{\nu}} L \left[\boldsymbol{\nu}; \hat{\delta}(\cdot) \right]$$

OUTPUT

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

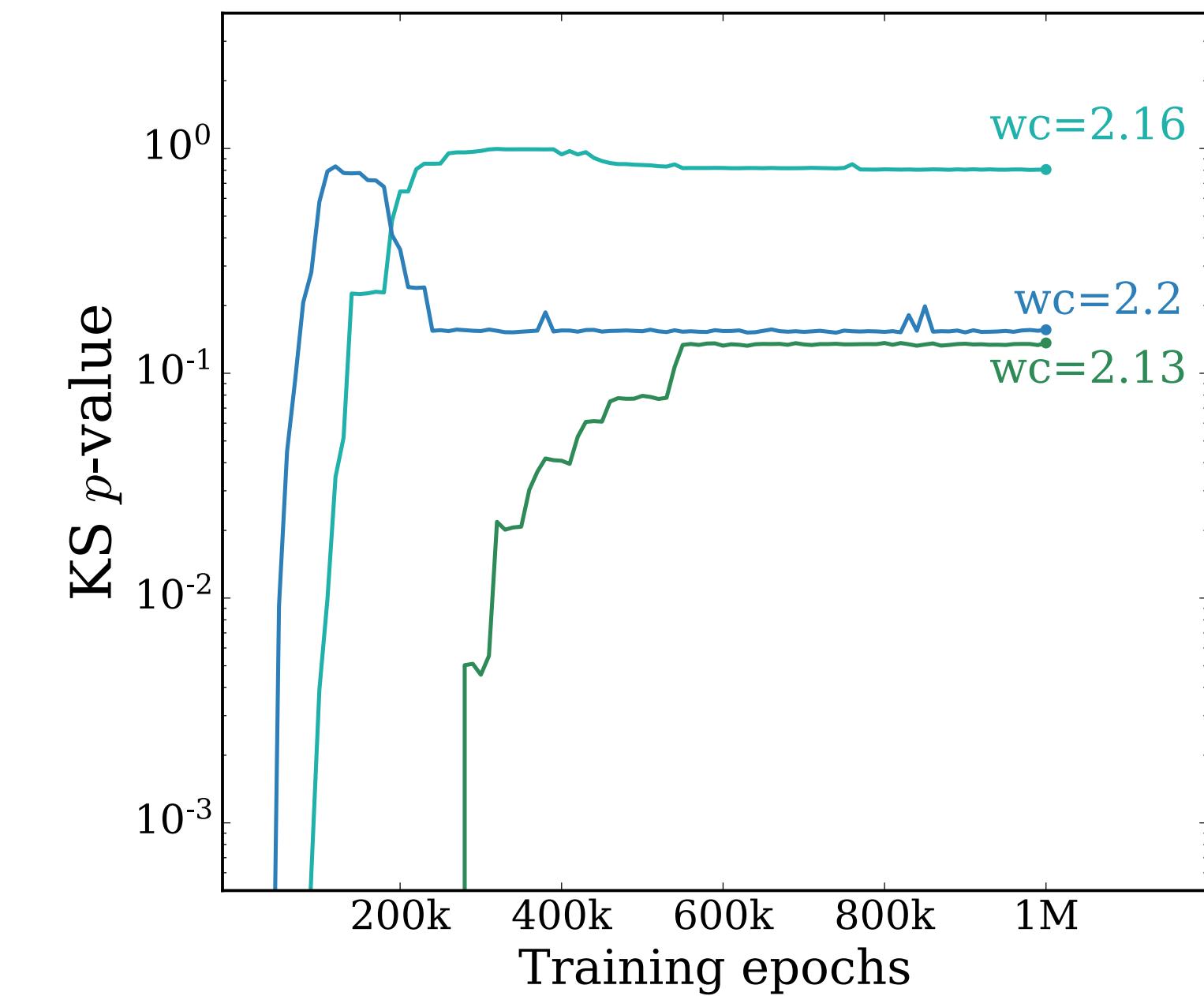
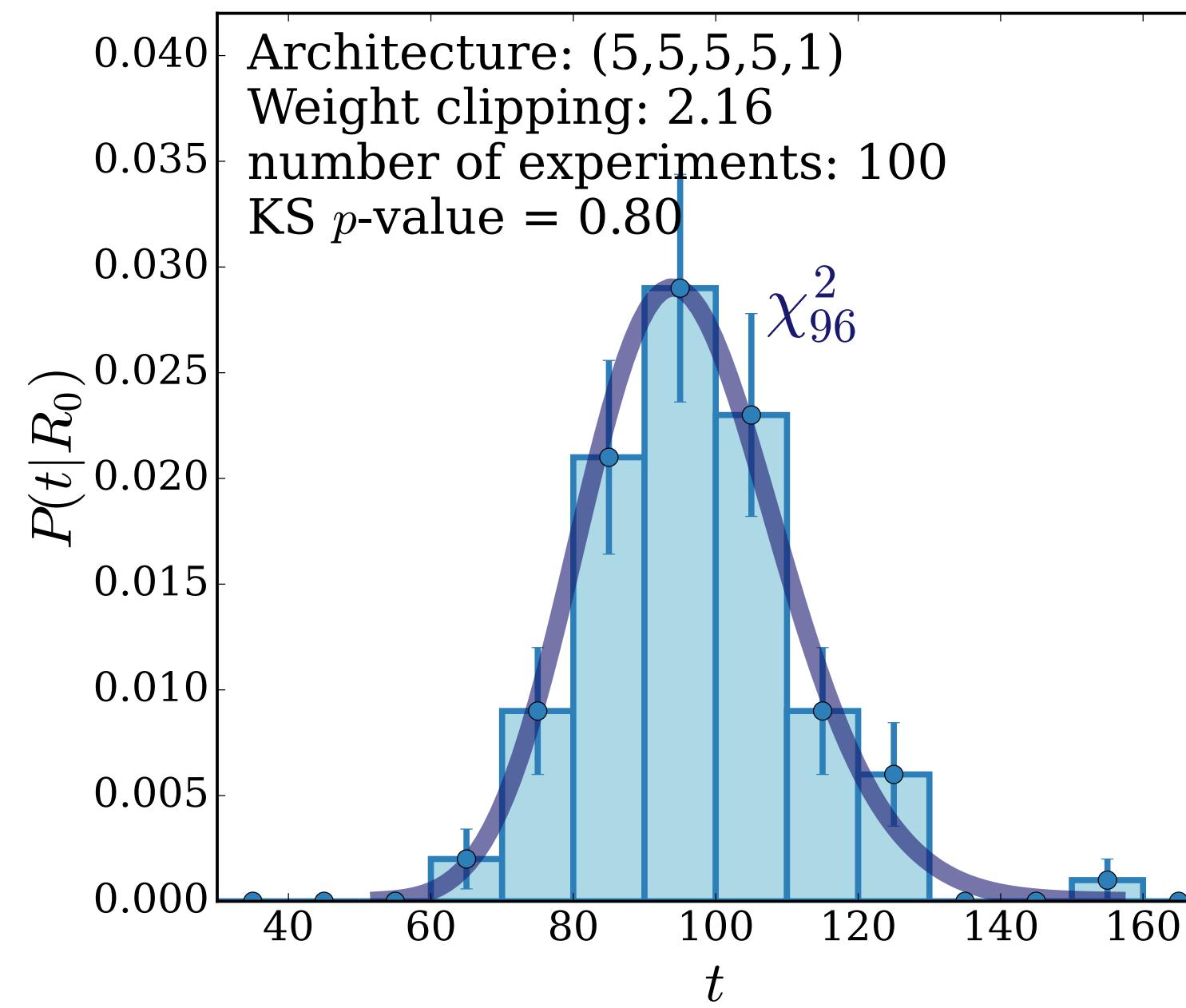
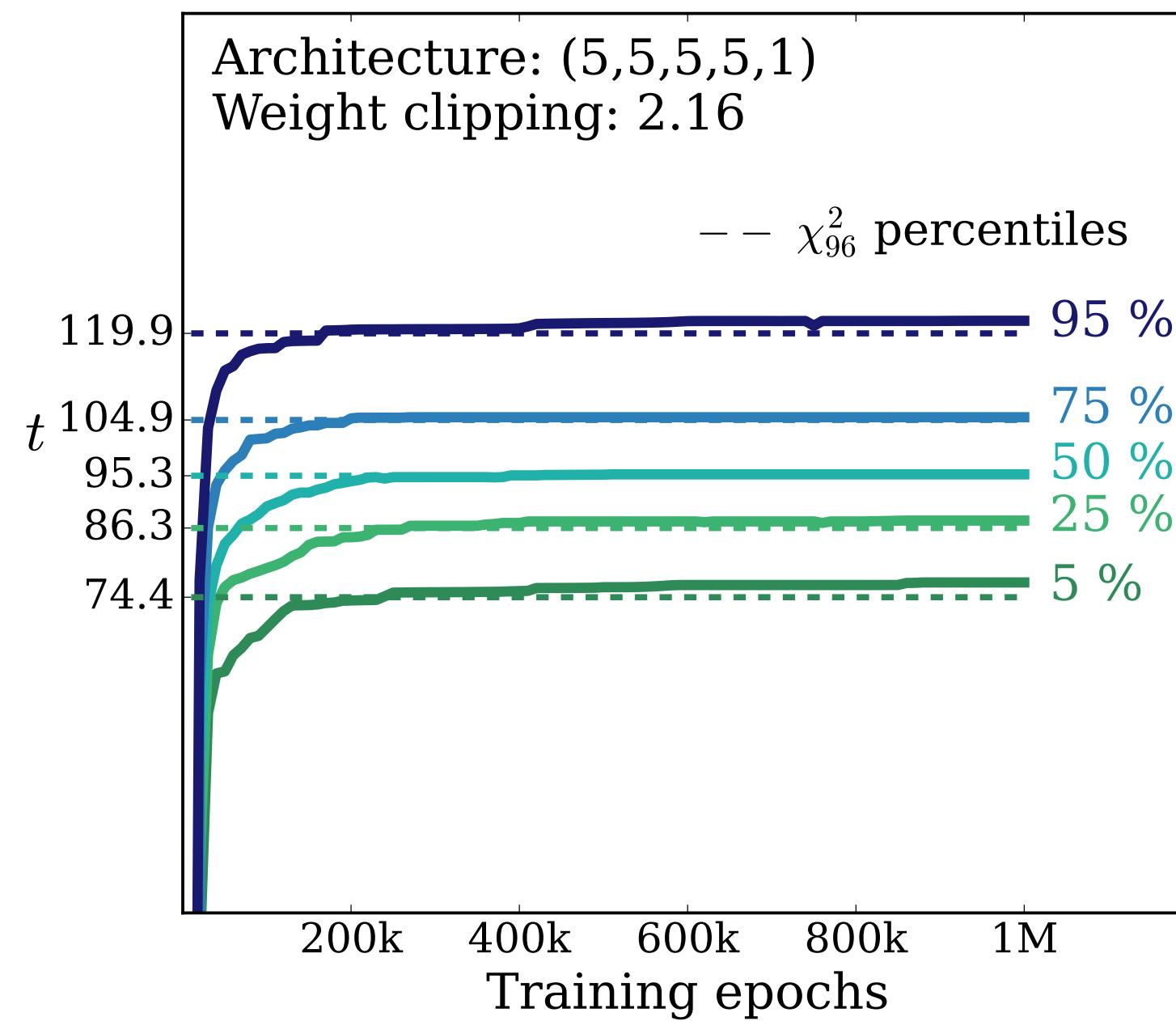
Di-body final state at the LHC

Step 1: Model selection

Training setup:

- Data sample $N(D) \sim 8500$ events
- Reference sample $N(R) = 5 \times N(D) \sim 42500$

Weight clipping tuning:

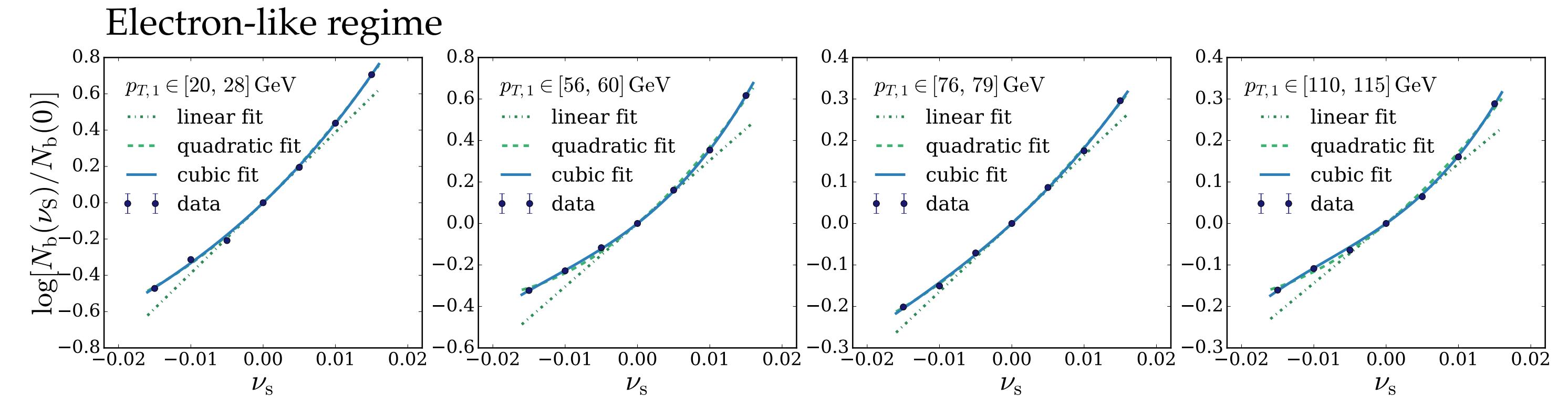


Di-body final state at the LHC

Step 2: Nuisance Taylor's expansion Learning

Preliminary study

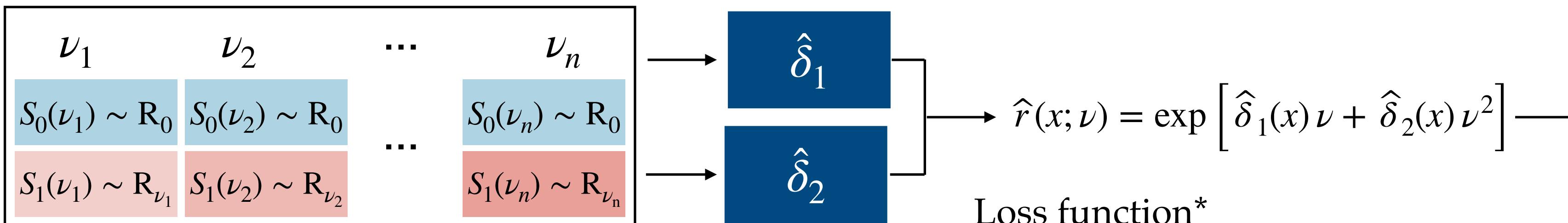
Preliminary binned analysis to determine the proper order for the Taylor's expansion



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*

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

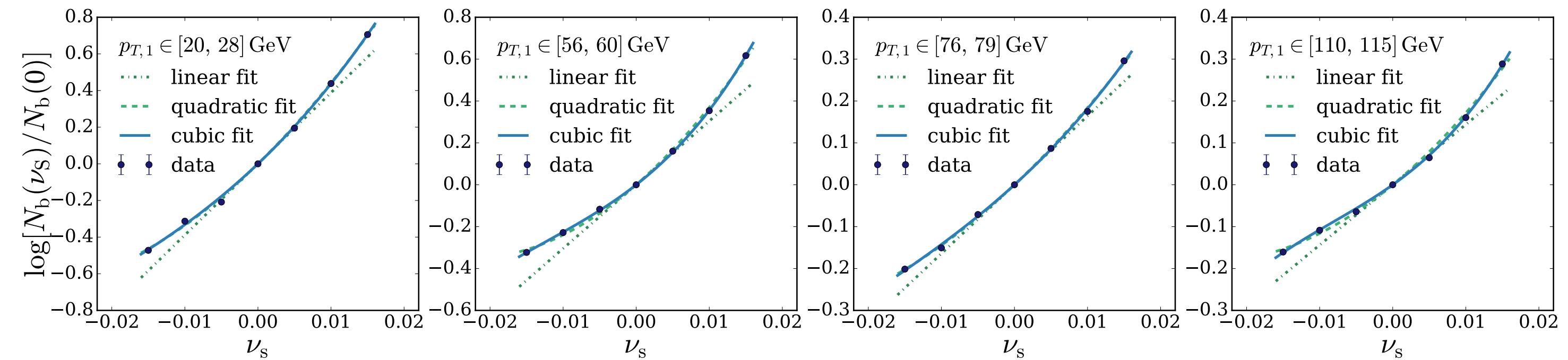
* Parametrized classifiers for optimal EFT sensitivity [arXiv:2007.10356](https://arxiv.org/abs/2007.10356)

Di-body final state at the LHC

Step 2: Nuisance Taylor's expansion Learning

Preliminary study

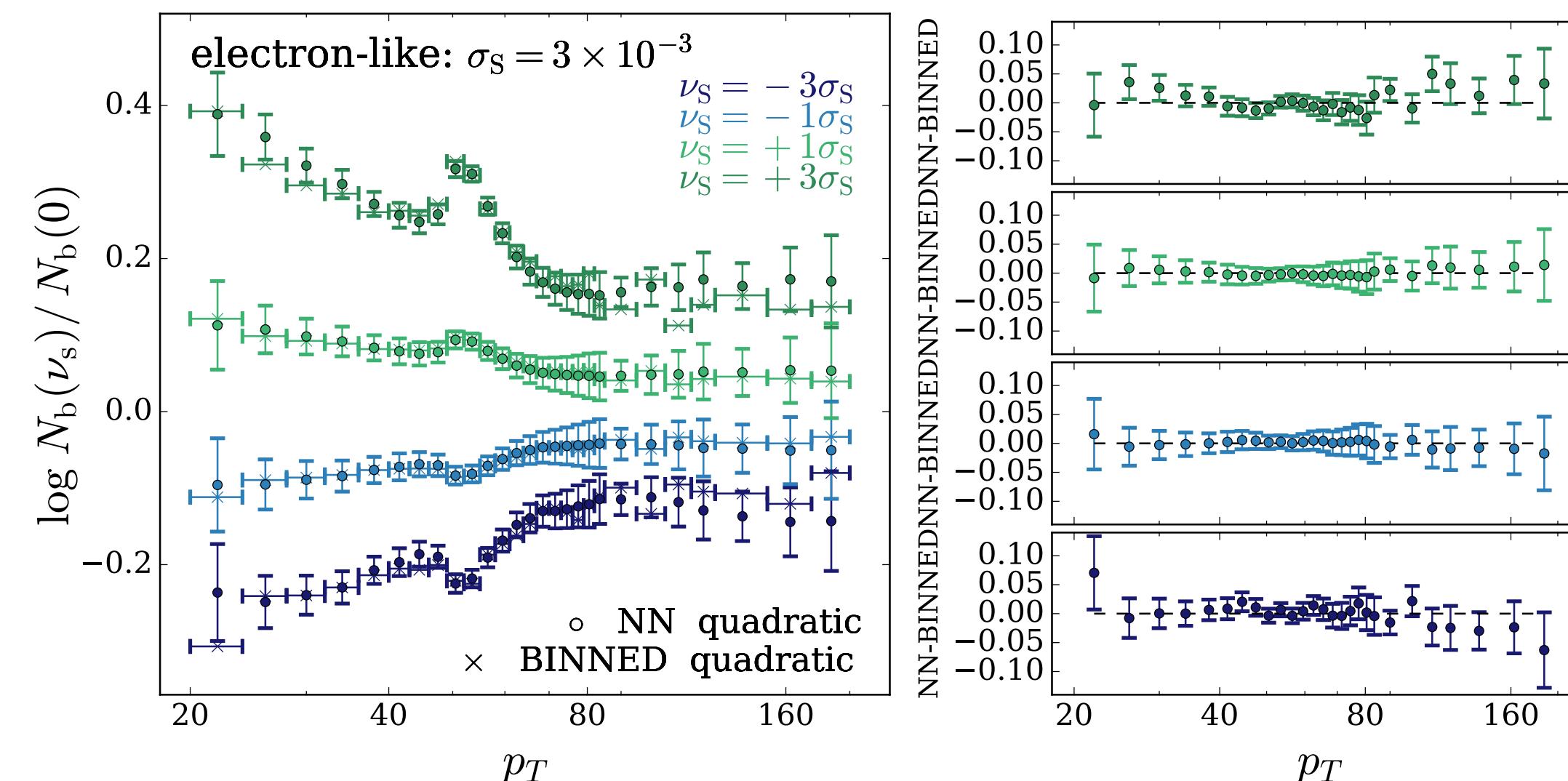
Preliminary binned analysis to determine the proper order for the Taylor's expansion



Taylor's expansion learning

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

Results:



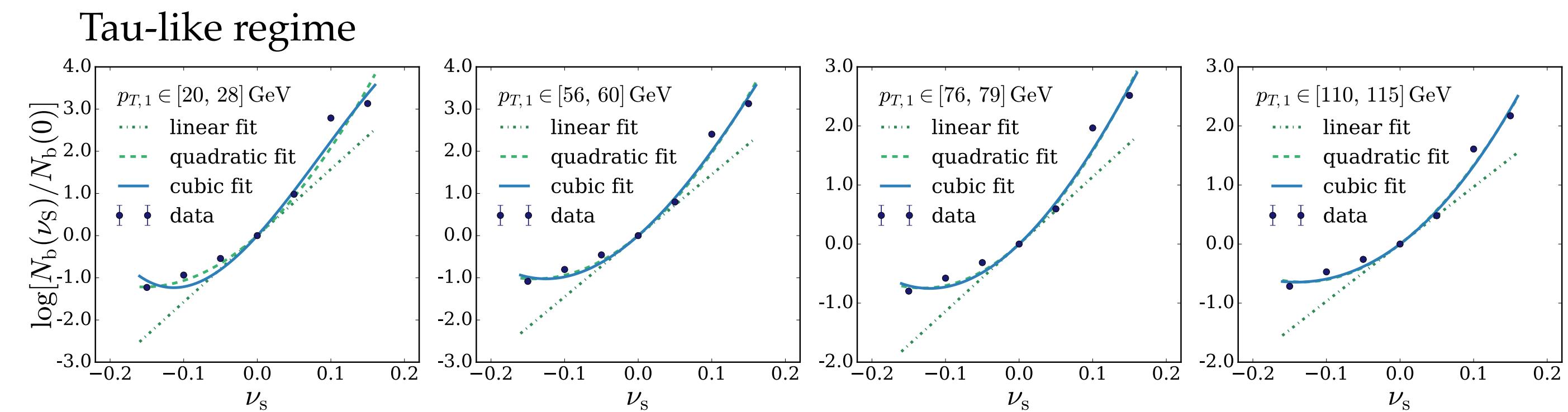
Di-body final state at the LHC

Step 2: Nuisance Taylor's expansion Learning: tau-like regime

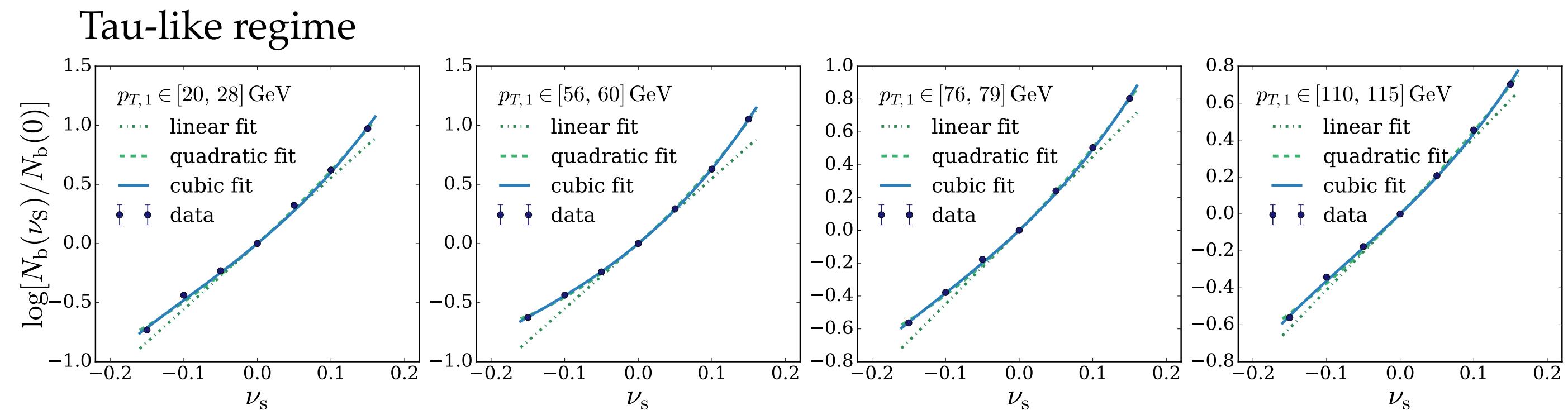
Preliminary study

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

$M_{1,2} > 100 \text{ GeV}$



$M_{1,2} > 120 \text{ GeV}$

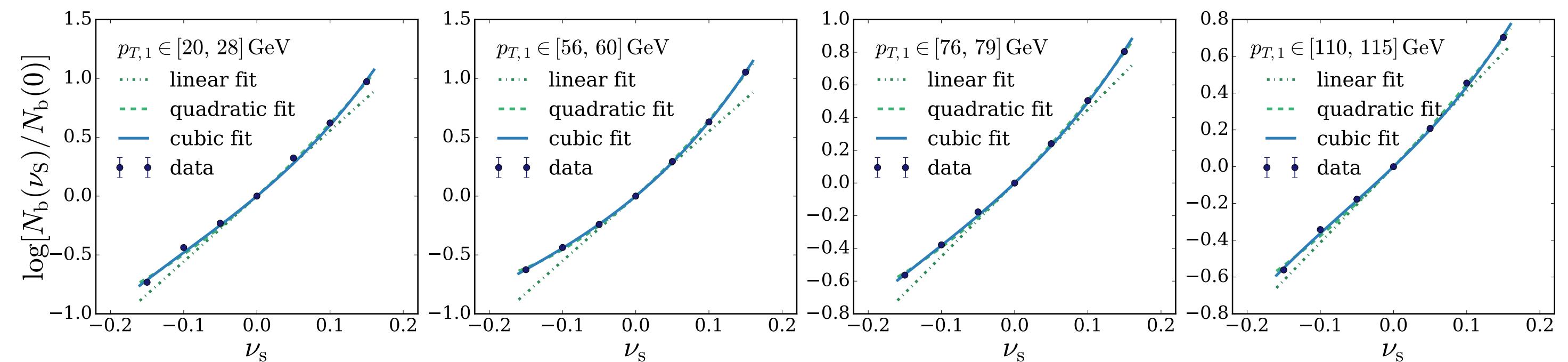


Di-body final state at the LHC

Step 2: Nuisance Taylor's expansion Learning

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 $r(x; \nu) = \frac{n(x | R_\nu)}{n(x | R_0)}$

Results:

