

How Good is the Standard Model?

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Based on:

D'Agnolo, AW, 2018

D'Agnolo, Grosso, Pierini, AW, Zanetti, 2019

D'Agnolo, Grosso, Pierini, AW, Zanetti, 2021

Goodness of Fit

The major concern of any scientist:

Am I doing **everything** right?

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What could be **wrong?**
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Cross-checks are more easy the more specifically we characterise the possible failure. But also less powerful

easy/partial

- did I turn QED showering on, in my PYTHIA simulation?
- is the power plug of my detector connected?
- ...
-
-
-

hard/complete

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- did I turn QED showering on, in my PYTHIA simulation?
- is the power plug of my detector connected?
- ...
- is my detector system working “normally”?
- ...
- is my state-of-the-art knowledge of fundamental interactions (the **SM**) **correct**, or it **fails** to describe the LHC data?

hard/complete

Goodness of Fit

Statisticians formulate the problem as **g.o.f.***

Be \mathcal{D} a set of data, and \mathcal{R} a stat. hyp. for their distribution

Does \mathcal{R} provide the **right description** of \mathcal{D} ?

*often question emerges after optimising distribution free parameters on the data, as a way to assess fit quality. But the problem is more general

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Again, answer more easy the more restrictive assumptions we make on how the true distribution, if not \mathcal{R} , can look like

But, more partial as well.

Goodness of Fit

Statisticians formulate the problem as **g.o.f.**

Be \mathcal{D} a set of data, and R a stat. hyp. for their distribution

Does R provide the **right description** of \mathcal{D} ?

Again, answer more easy the more restrictive assumptions we make on how the true distribution, if not R , can look like

But, more partial as well.

G.o.f. is a “ill-posed” problem: no **optimal** solution exists.

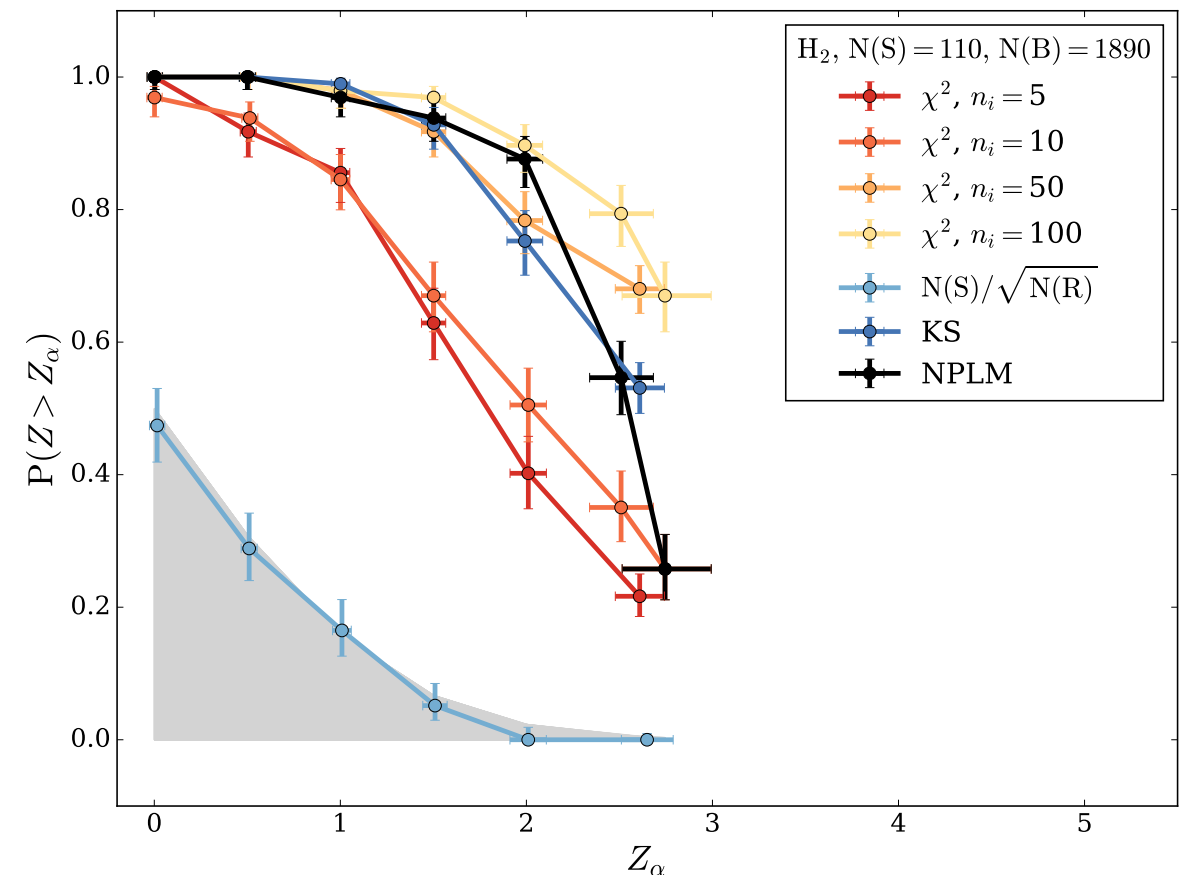
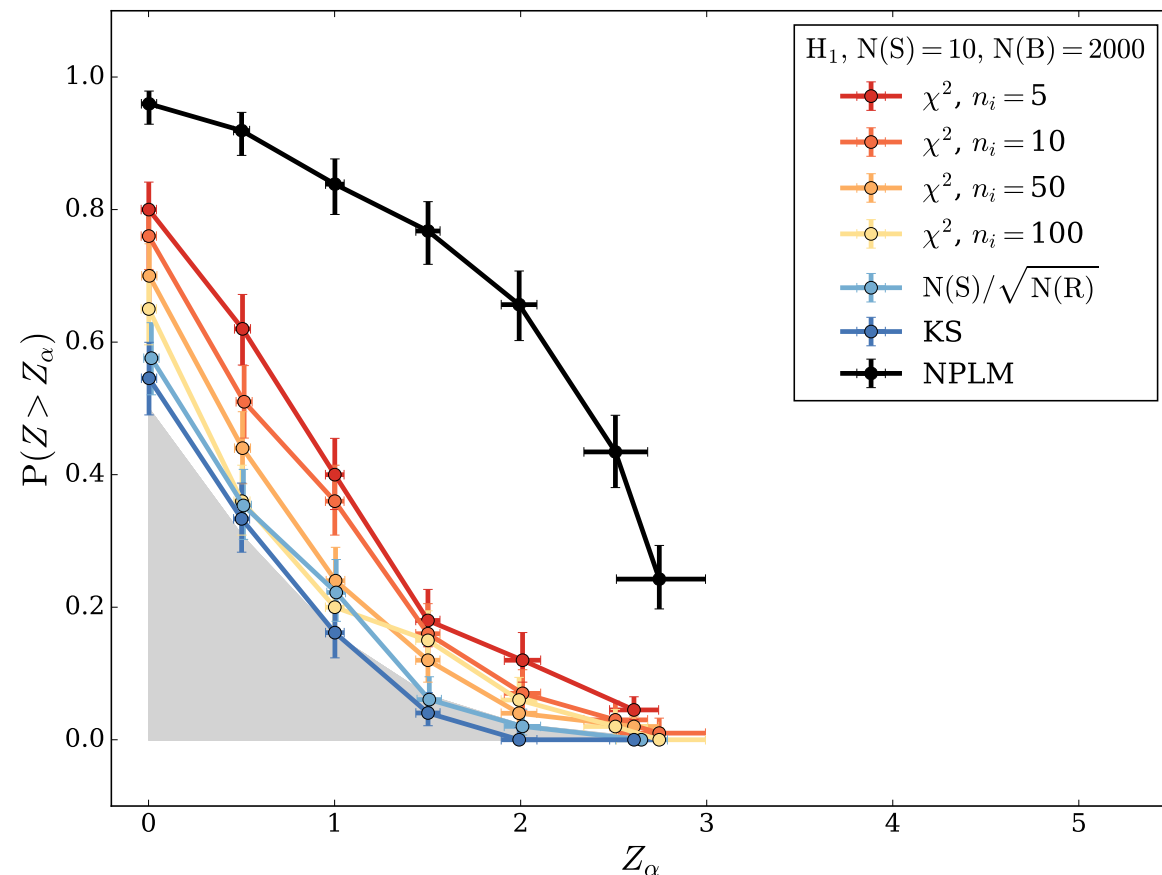
But plenty of **good** solutions exist, especially (only?) in 1d *

We can search for **better** solutions, perhaps even in 1d

*For instance, students quickly learn to plot **binned histograms** with their data, because this **often** allow them to find mistakes

Goodness of Fit

Probability to find evidence of \mathcal{R} being wrong at some level of confidence.
True data distribution departs from \mathcal{R} in different ways, in the two plots.



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The LHC g.o.f. challenge

By analysing the LHC data, we would like to find evidence of **failure of the SM theory**, suggesting need of **BSM**.

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Affecting few (unknown) observables over ∞ many we can measure

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Choose observables sensitive to **one BSM model**

This observable in general **not** sensitive to **another BSM model**

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We call this strategy a “**Model-Dependent**” search

The LHC g.o.f. challenge

What if* the **RIGHT BSM model** has not been formulated?
*very likely

Most likely, **we will not see the SM fail to describe data**



We must design **Model Independent** searches
aimed at detecting “generic” data departures from SM
SM = “Reference Model”, to be compared with data
without reference to alternative physics model

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“Regular” Model-Independence:

weaken hypothesis on BSM nature, e.g.

- Simplified Model (of, say, SUSY, or DM, or HVT, ...)
- Effective Field Theories
- Bump Hunt

“Machine-Learner” Model-Independence:

eliminate phenomenological modelling altogether

G.o.f. from Maximum Likelihood

Data: $\mathcal{D} = \{x_i\}, i = 1, \dots, \mathcal{N}_{\mathcal{D}}$

I.i.d. measurements of, e.g., reconstructed particle momenta in a region of interest

G.o.f. from Maximum Likelihood

Data: $\mathcal{D} = \{x_i\}, i = 1, \dots, \mathcal{N}_{\mathcal{D}}$

Reference Distribution: $n(x|\mathbf{R})$

Alternative Distribution: $n(x|\mathbf{w})$
depending on **parameters** (composite)

$$n(x) = N P(x)$$

$$N = \int dx n(x)$$

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Model Dependent Strategy

$$n(x|\mathbf{w}) = n(x|\mathbf{NP})$$

Alternative as predicted by “NP” model.

Few, or no, free parameters

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This is what regularly done at the LHC:
target sensitivity to manifestations of one
specific theoretical **New Physics Model**

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$$n(x|\mathbf{w}) = n(x|\mathbf{R}) e^{f(x;\mathbf{w})}$$

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 $f(x;\mathbf{w})$ is flexible function approximant

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 $f(x;\mathbf{w})$ is flexible function approximant

If $f(x;\mathbf{w})$ is **piece-wise constant**



Binned Histogram Test
(AKA, Baker-Cousins test)
(used by ATLAS and CMS for Model-
Independent New Physics Searches)

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If $f(x;\mathbf{w})$ is a **neural network**



Our Proposal

G.o.f. from Maximum Likelihood

Data: $\mathcal{D} = \{x_i\}, i = 1, \dots, \mathcal{N}_{\mathcal{D}}$

Basic idea: $f(x; \mathbf{w}) = \text{NN}$
replace histograms with NN, literally!

Highly motivated attempt:

- NN “effective” flexible but smooth function approx.
- Often “sold” as **alternative to hist.** to fit distributions
- Better dimensionality scaling
- Using other models also possible

$$\frac{1}{N} \sum_{i=1}^N P(x)$$

$$\int dx n(x)$$

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Our Proposal

Maximum Likelihood Loss

Turn the evaluation of “t” into supervised training problem:

$$n(x|\mathbf{w}) = n(x|\mathbf{R}) e^{f(x;\mathbf{w})}$$
$$t(\mathcal{D}) = 2 \operatorname{Max}_{\mathbf{w}} \left\{ \log \left[\frac{e^{-N(\mathbf{w})}}{e^{-N(\mathbf{R})}} \prod_{i=1}^{\mathcal{N}_{\mathcal{D}}} \frac{n(x_i|\mathbf{w})}{n(x_i|\mathbf{R})} \right] \right\} \stackrel{\downarrow}{=} -2 \operatorname{Min}_{\mathbf{w}} \left[N(\mathbf{w}) - N(\mathbf{R}) - \sum_{i=1}^{\mathcal{N}_{\mathcal{D}}} f(x_i; \mathbf{w}) \right]$$

We need a **Reference Sample**, distributed according to Reference Model

$$\mathcal{R} = \{x_i\}, \quad i = 1, \dots, \mathcal{N}_{\mathcal{R}}$$

Approximate integral as Monte Carlo sum:

$$N(\mathbf{w}) = \int dx \, n(x|\mathbf{R}) e^{f(x;\mathbf{w})} = \frac{N(\mathbf{R})}{\mathcal{N}_{\mathcal{R}}} \sum_{x \in \mathcal{R}} e^{f(x;\mathbf{w})}$$

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In order to read this as “equal”, we need

$$\mathcal{N}_{\mathcal{R}} \gg N(\mathbf{R})$$

Like saying that $n(x|\mathbf{R})$ is “known”, as it is infinitely samplable

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Get **t = -2 * minimal loss. Trained net is fit to distribution log ratio**

$$t(\mathcal{D}) = -2 \operatorname{Min}_{\{\mathbf{w}\}} \left[\frac{N(\mathcal{R})}{\mathcal{N}_{\mathcal{R}}} \sum_{x \in \mathcal{R}} (e^{f(x;\mathbf{w})} - 1) - \sum_{x \in \mathcal{D}} f(x; \mathbf{w}) \right] \equiv -2 \operatorname{Min}_{\{\mathbf{w}\}} L[f(\cdot, \mathbf{w})]$$

$$L[f] = \sum_{(x,y)} \left[(1-y) \frac{N(\mathcal{R})}{\mathcal{N}_{\mathcal{R}}} (e^{f(x)} - 1) - y f(x) \right]$$

The Algorithm

We compute “t” by supervised training using “ML-Loss”

- Observed (or Toy) **Data are class “1”**

- Class “0” is a **Reference Sample**

SM-distributed * synthetic instances of the features “x”

Can come from **Monte Carlo**, or **Data Driven**

Nothing different from “**background sample**” in regular searches

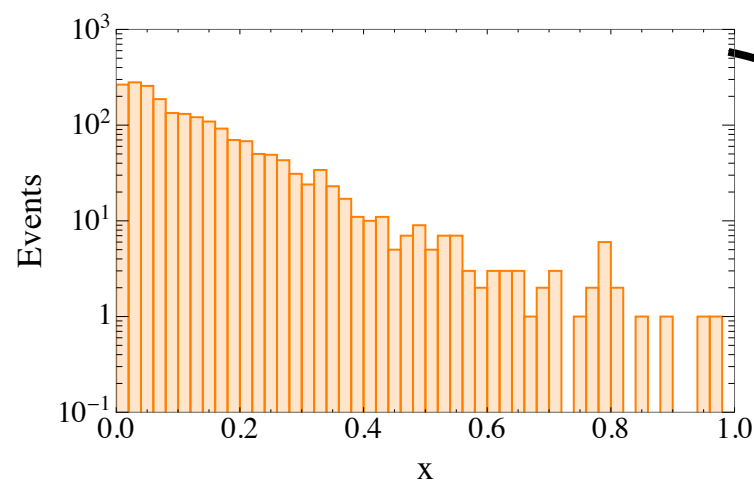
Preferably, more abundant than the data: $\mathcal{N}_{\mathcal{R}} \gg N(\mathcal{R})$

*It must be SM-distributed **if the SM is true**. If BSM in Reference Sample, this generically does not harm our ability to see tension.

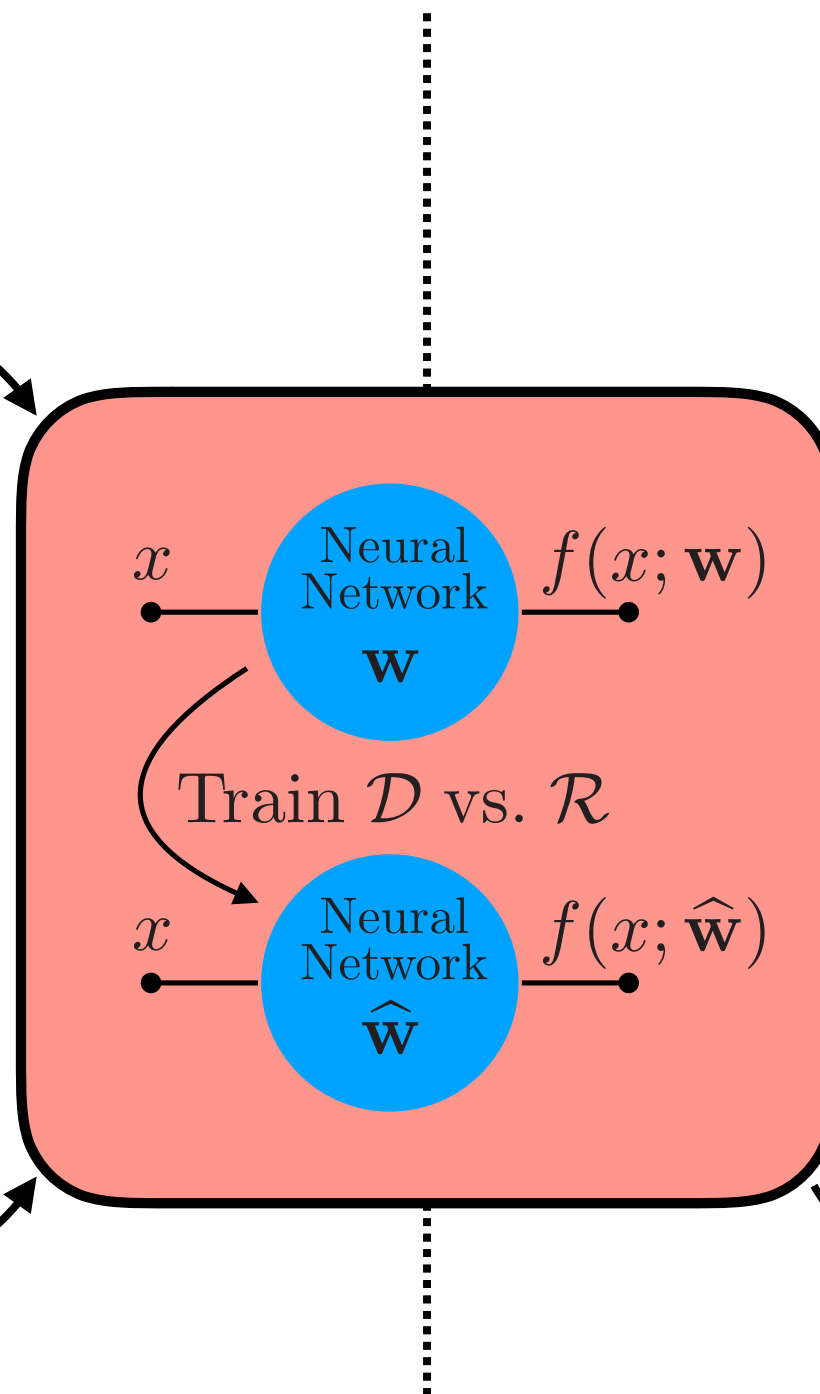
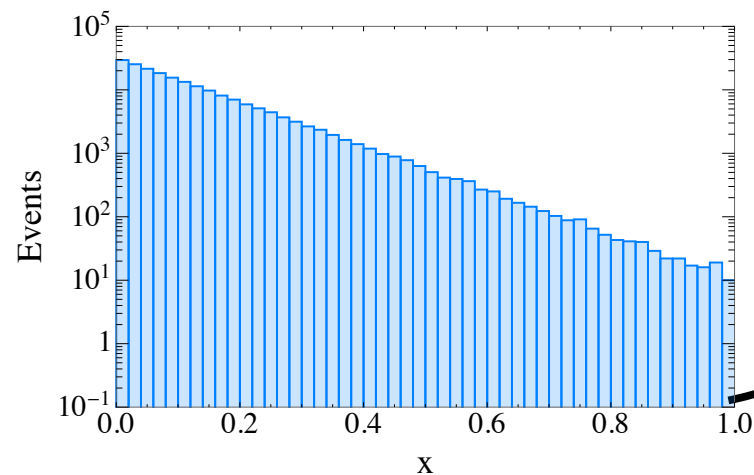
The Algorithm

INPUT

Data sample \mathcal{D}

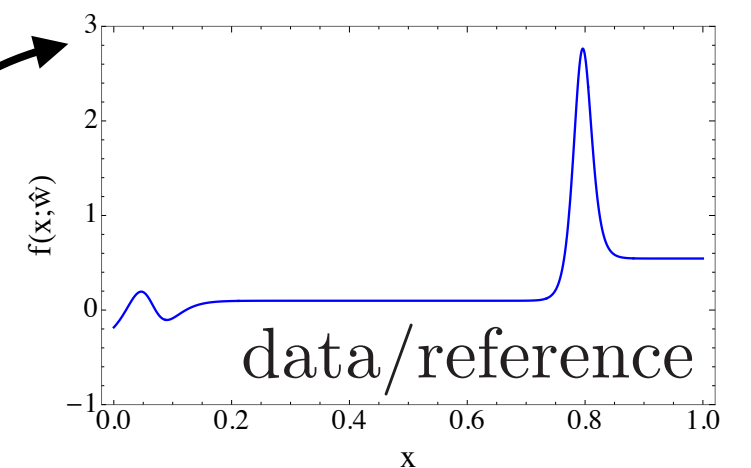


Reference sample \mathcal{R}



OUTPUT

Dist. log ratio



$$f(x; \hat{\mathbf{w}}) \simeq \log \left[\frac{n(x|\mathcal{T})}{n(x|\mathcal{R})} \right]$$

Test statistic t
computed on the
data sample \mathcal{D}

$$t(\mathcal{D}) = -2 \operatorname{Min}_{\{\mathbf{w}\}} L[f]$$

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Preferably, more abundant than the data: $\mathcal{N}_{\mathcal{R}} \gg N(\mathcal{R})$

We generate Toy Datasets in Reference Hypothesis, train on each and compute empirical $P(t|\mathcal{R})$

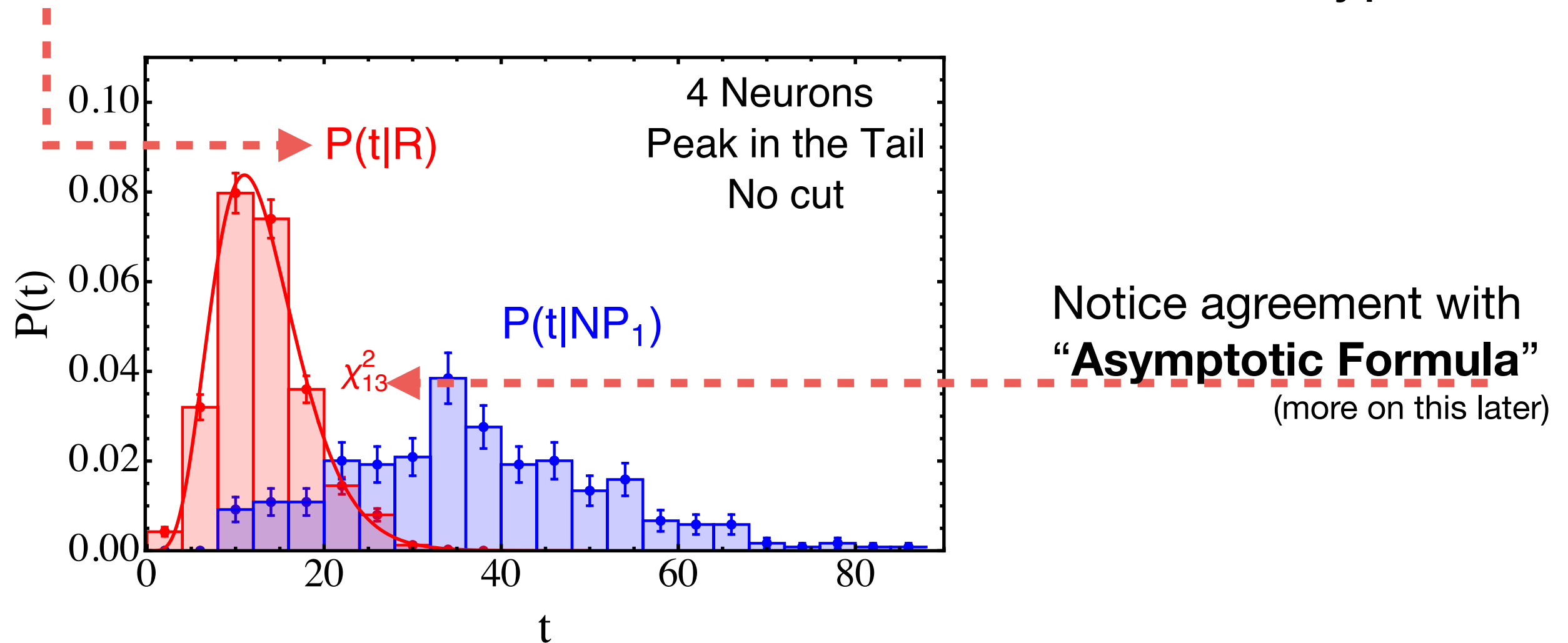
This will give us the observed p-value:

$$p = \int_{t_{\text{obs}}} P(t|\mathcal{R})$$

Illustrating Performances

(Simple 1d example with exponential Reference)

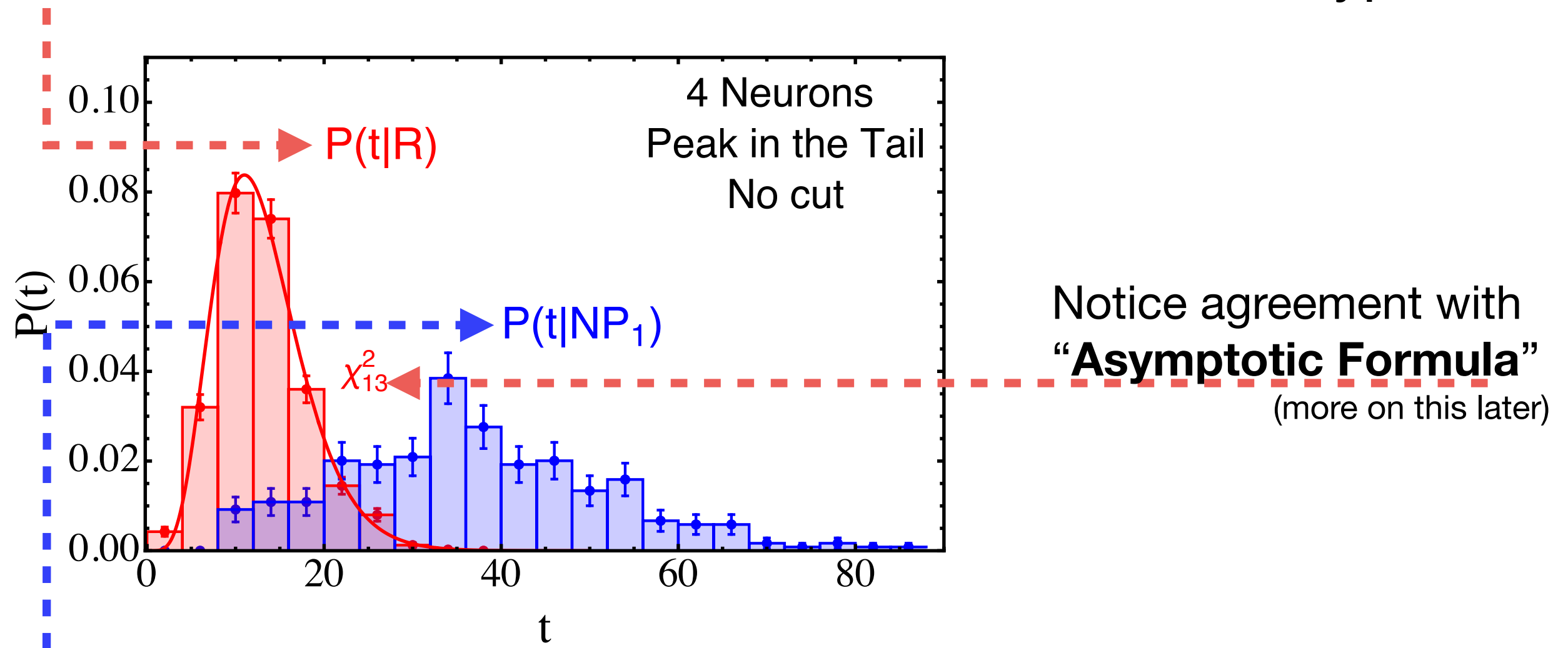
Distribution of the test statistic “t” in Reference Hypothesis



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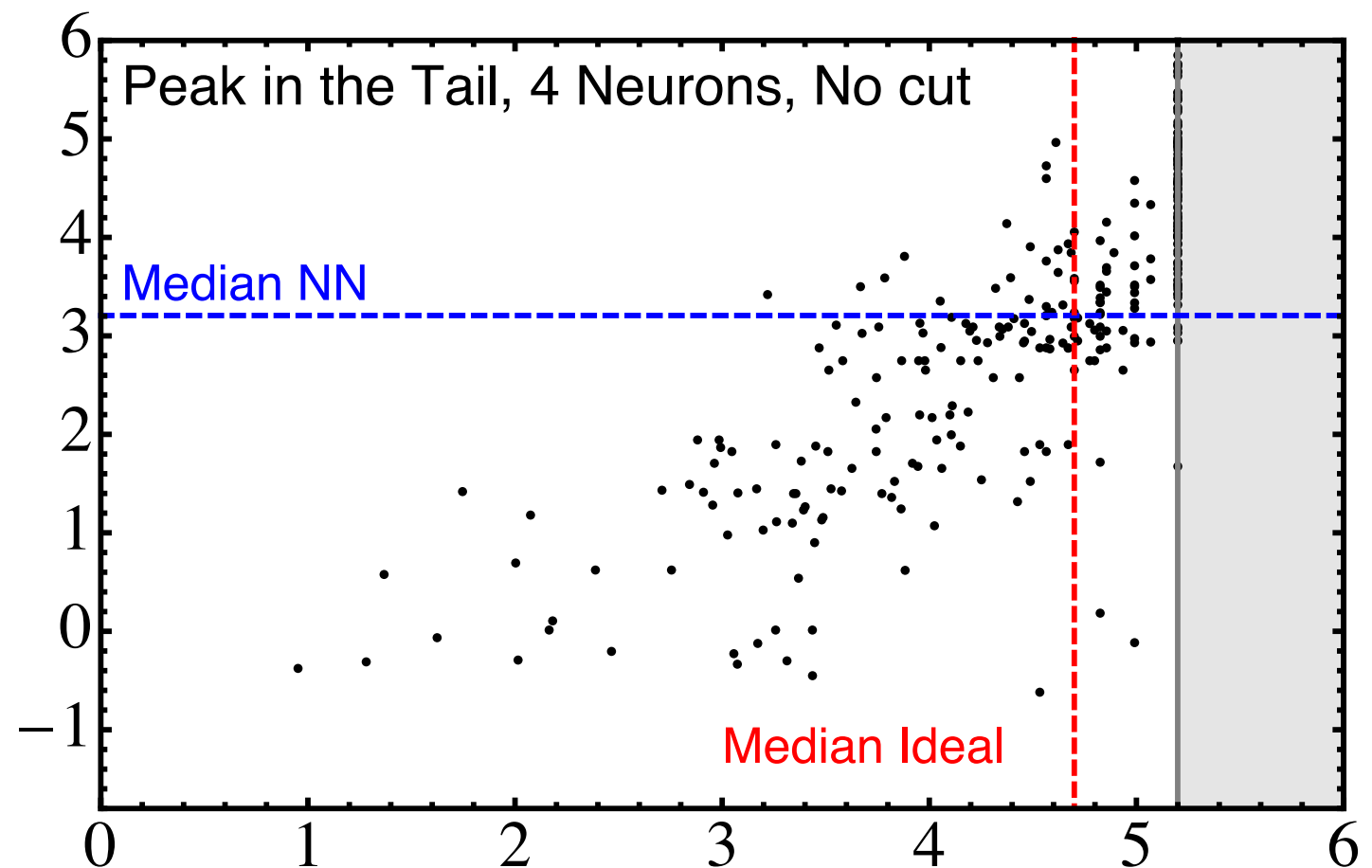
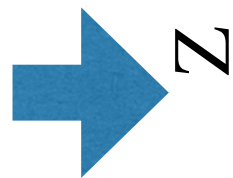
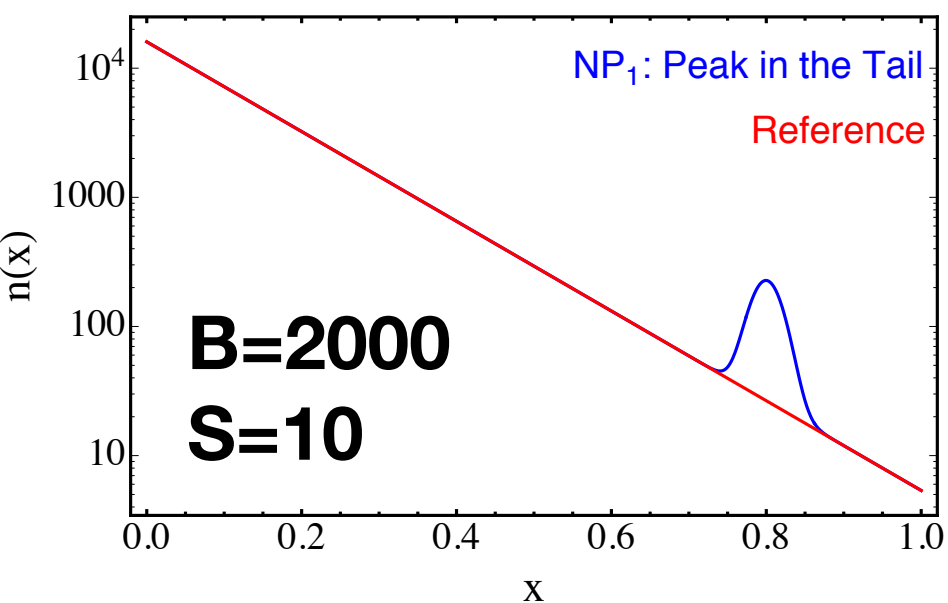


Distribution of “t” in one New Physics Model Hypothesis

$t \rightarrow p \rightarrow Z\text{-score}$ (we use $Z = \Phi^{-1}(1 - p)$)

Quantifying Performances

(Simple 1d example with exponential Reference)

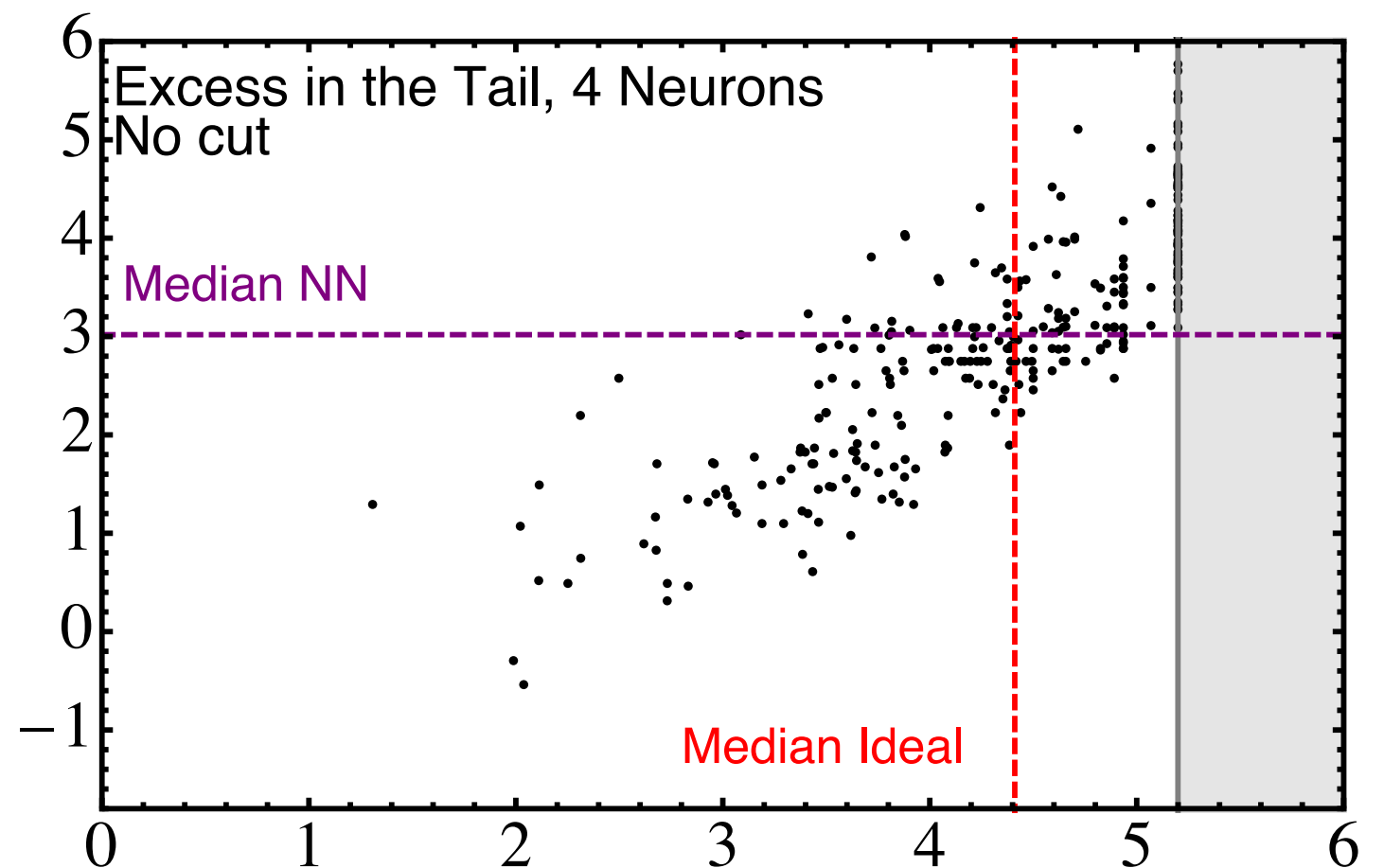
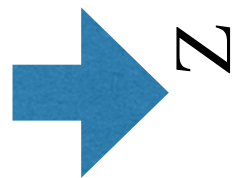
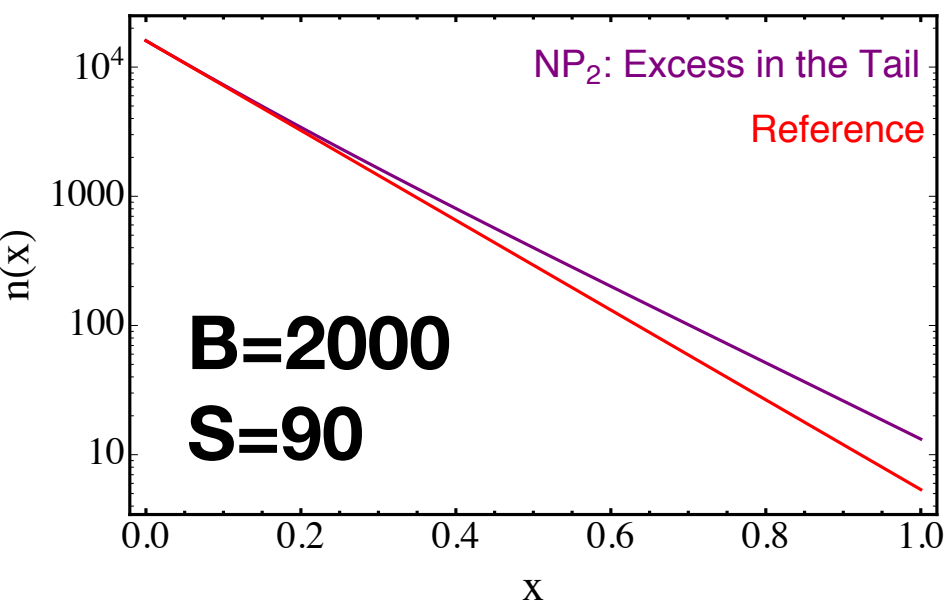


“Ideal Z-score”: Z_{id}

A “measure of dataset discrepancy”
(the Z-score of optimal test for NP1 model)

Quantifying Performances

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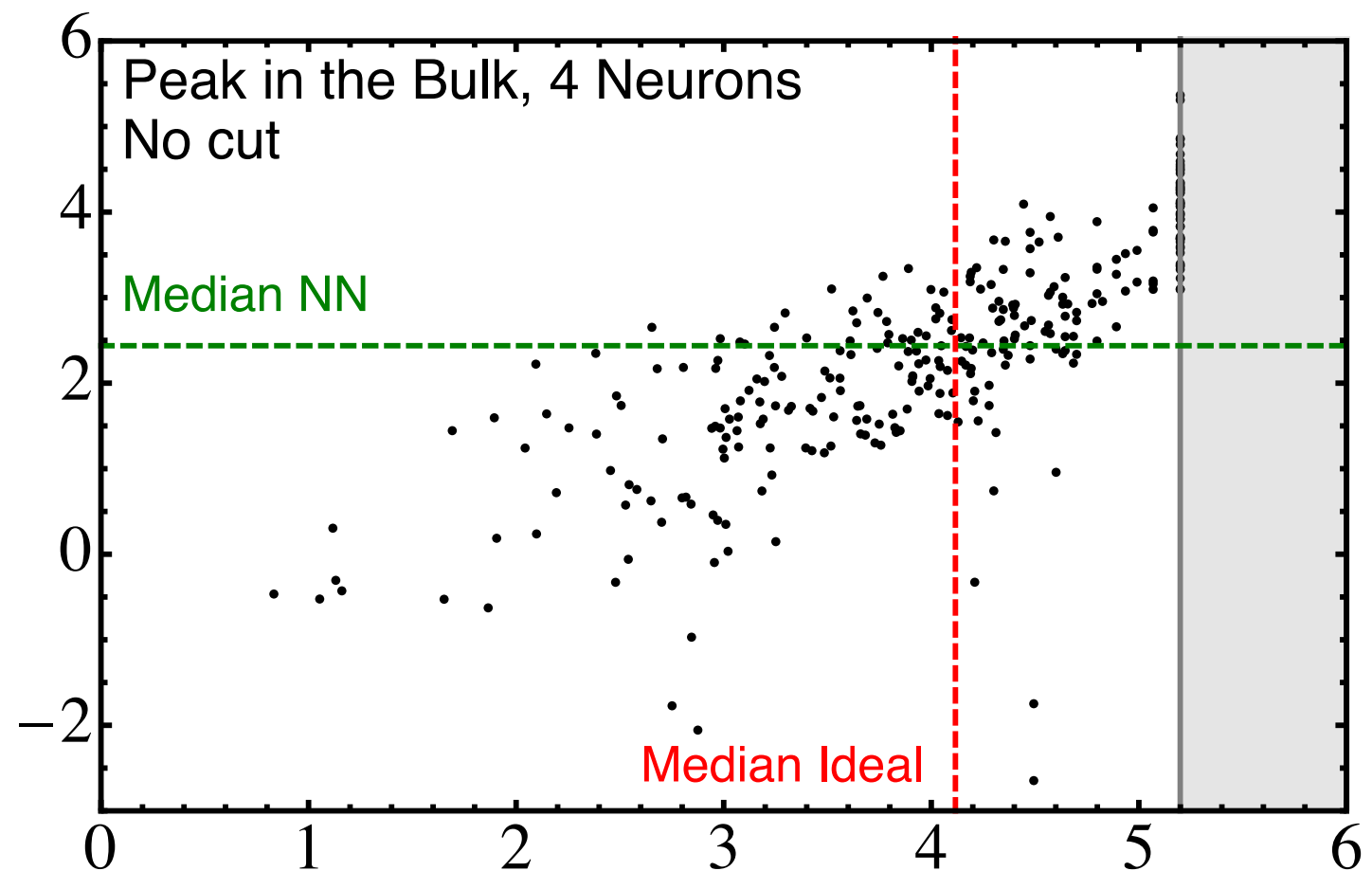
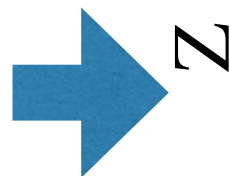
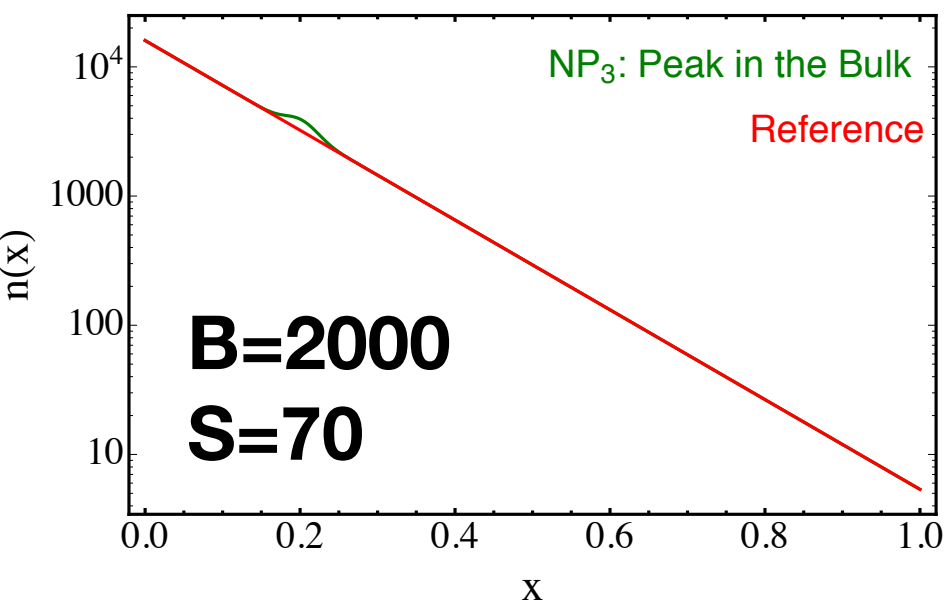


“Ideal Z-score”: Z_{id}

A “measure of dataset discrepancy”
(the Z-score of optimal test for NP2 model)

Quantifying Performances

(Simple 1d example with exponential Reference)

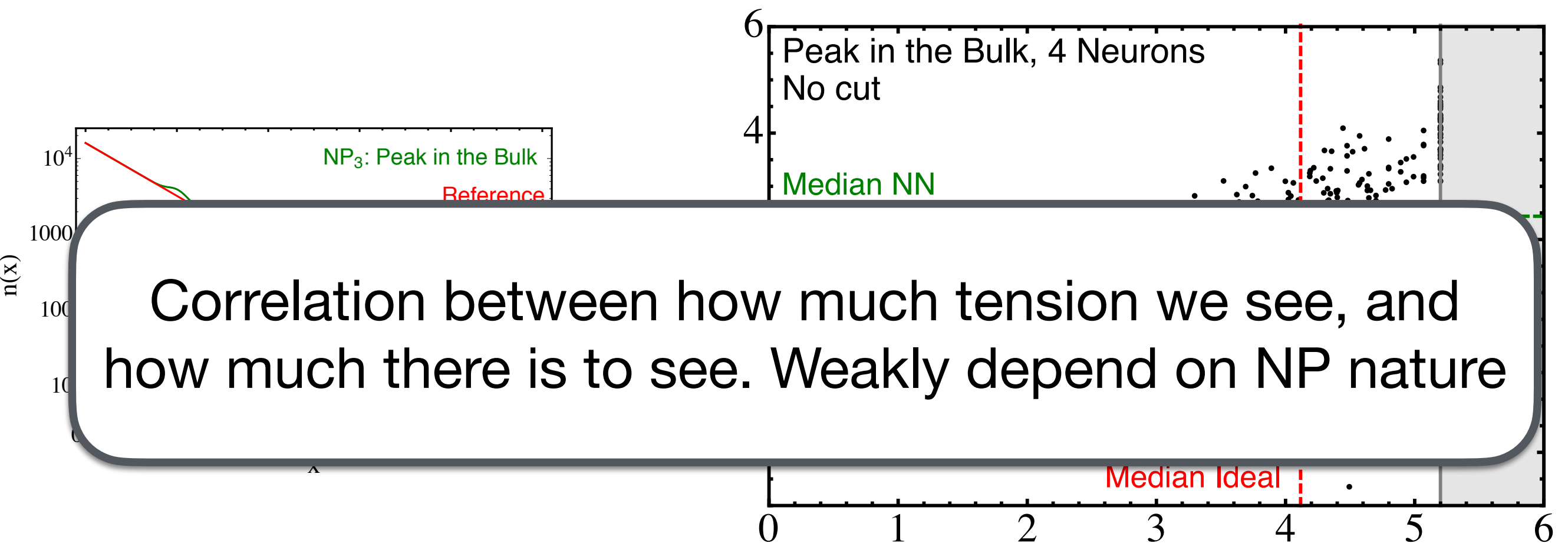


“Ideal Z-score”: Z_{id}

A “measure of dataset discrepancy”
(the Z-score of optimal test for NP3 model)

Quantifying Performances

(Simple 1d example with exponential Reference)



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An **Imperfect** Machine

Reference Model Predictions are unavoidably imperfect
e.g., PDF/Lumi/Detector Modeling ...

Imperfections are **Nuisance Parameters**

Constrained by **Auxiliary Measurements**
Define a **composite** Reference hypothesis

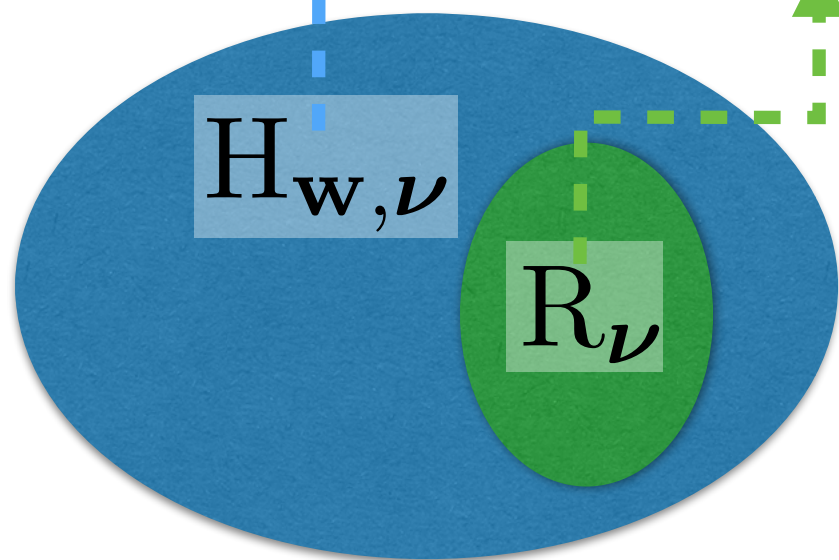
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$$t(\mathcal{D}, \mathcal{A}) = 2 \log \frac{\max_{\mathbf{w}, \nu} [\mathcal{L}(H_{\mathbf{w}, \nu} | \mathcal{D}) \cdot \mathcal{L}(\nu | \mathcal{A})]}{\max_{\nu} [\mathcal{L}(R_{\nu} | \mathcal{D}) \cdot \mathcal{L}(\nu | \mathcal{A})]}$$



Just like in no-nuisance case:

$$n(x | H_{\mathbf{w}, \nu}) = e^{f(x; \mathbf{w})} n(x | R_{\nu})$$

Beyond-Reference effects
parametrised by NN

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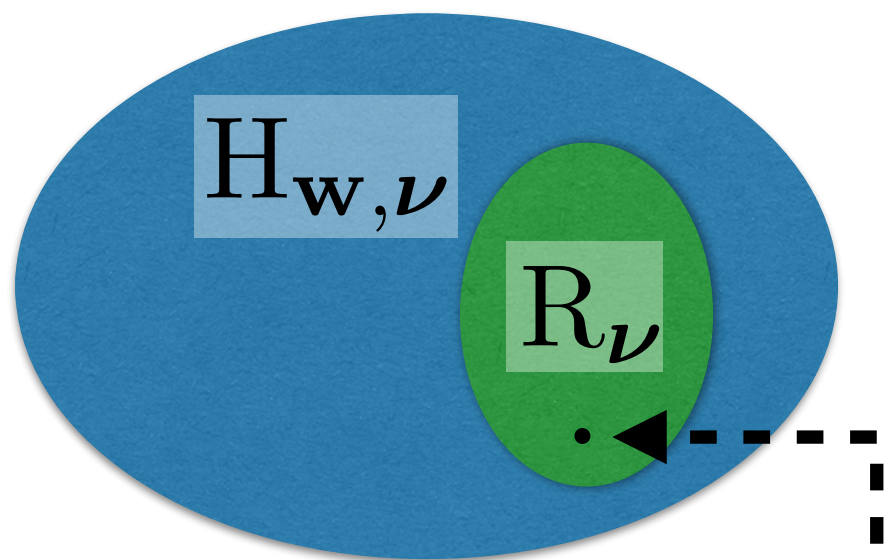
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Define a **composite** Reference hypothesis

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



Central-Value Reference: R_0
Nuisance set to their C-V

An Imperfect Machine

Reference

Imperfect

“Delta” term by direct likelihood maximisation

After **learning the effect of nuisance** locally on distribution

$$r(x; \boldsymbol{\nu}) \equiv \frac{n(x|R_{\boldsymbol{\nu}})}{n(x|R_0)} = \exp \left[\nu \delta_1(x) + \frac{1}{2} \nu^2 \delta_2(x) + \dots \right]$$

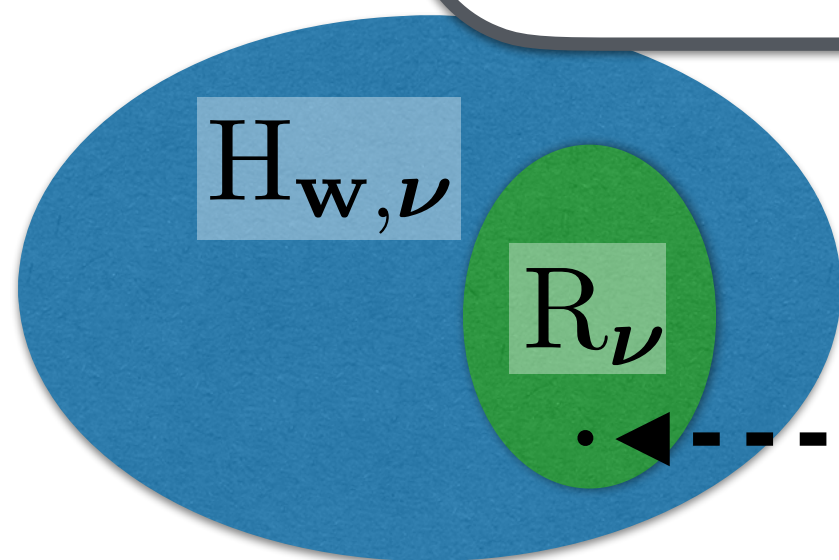
Adaptation of **likelihood-free inference** techniques

Would require dedicated seminar. [See e.g. 1907.10621, 2007.10356, ...]

Just be aware that:

- i) learning requires (enough) R data with non-C-V nuisance
- ii) the **quality** of the reconstruction can play crucial role

$$t(\mathcal{D}, \mathcal{A}) = 2 \log \frac{p(\mathcal{D}|\mathcal{A})}{p(\mathcal{D})}$$



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

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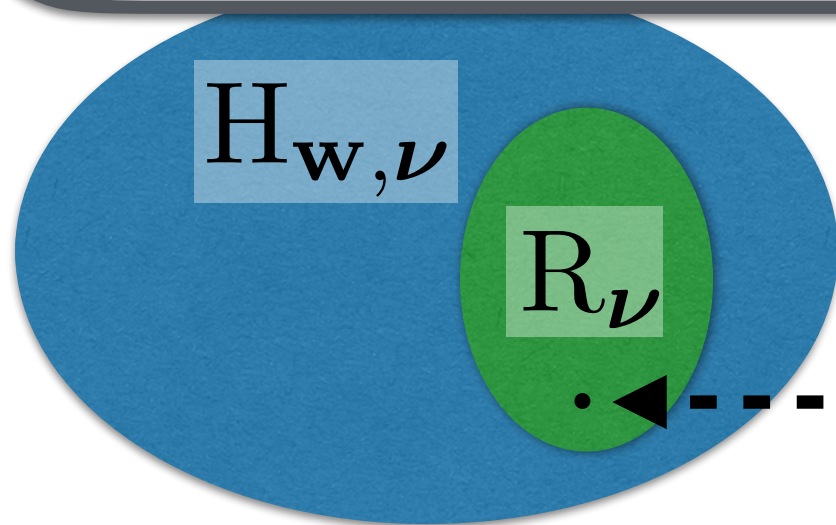
An Imperfect Machine

“Tau” term by training on Data

Almost like for no nuisance, but with modified ML-Loss:

$$L \left[f(\cdot; \mathbf{w}), \boldsymbol{\nu}; \hat{\delta}(\cdot) \right] = - \sum_{x_i \in \mathcal{D}} [f(x_i; \mathbf{w}) + \log(r(x_i; \boldsymbol{\nu}))] + \sum_{e \in \mathcal{R}} w_e \left[e^{f(x_e; \mathbf{w}) + \log(r(x_e; \boldsymbol{\nu}))} - 1 \right] \\ + \log \left[\frac{\mathcal{L}(\boldsymbol{\nu} | \mathcal{A})}{\mathcal{L}(\mathbf{0} | \mathcal{A})} \right]$$

And, with simultaneous **training over the nuisance** parameters
Data trained against **Central-Value Reference** sample **only**



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

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Nuisance set to their C-V

An Imperfect Machine

Reference Model Predictions are unavoidably imperfect
e.g., PDF/Lumi/Detector Modeling ...

Imperfections are **Nuisance Parameters**

Constrained by **Auxiliary Measurements**
Define a **composite** Reference hypothesis

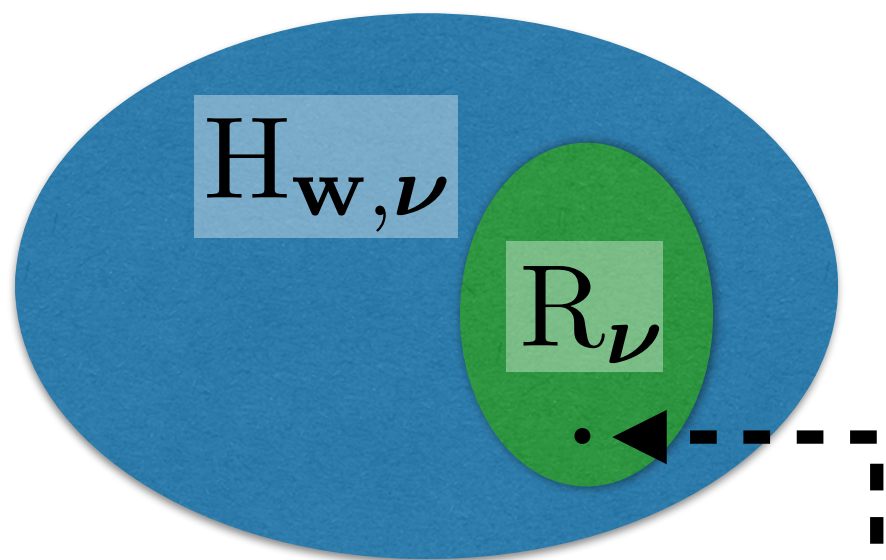
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$$P(t | \mathbf{R}_{\nu}) = P(t | \mathbf{R}_0) = \chi_d^2$$



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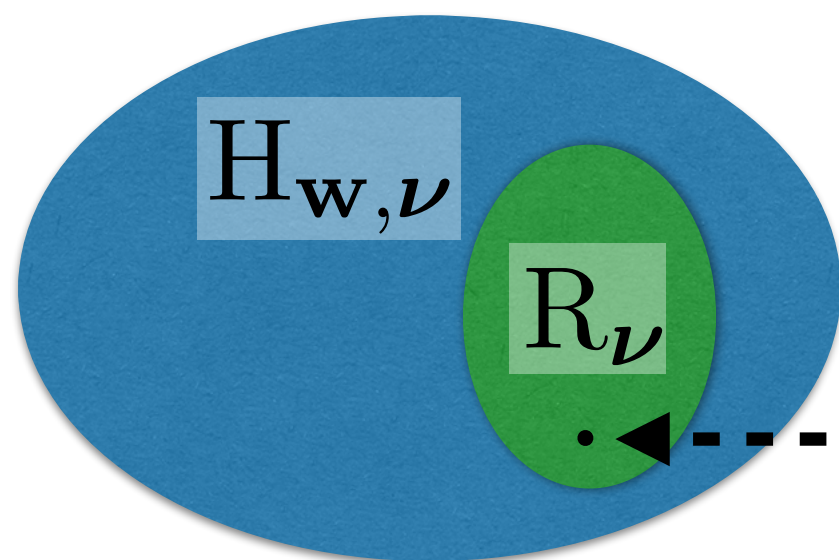


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Independence of t distribution on the **true value of nuisance** is **essential** for feasible test



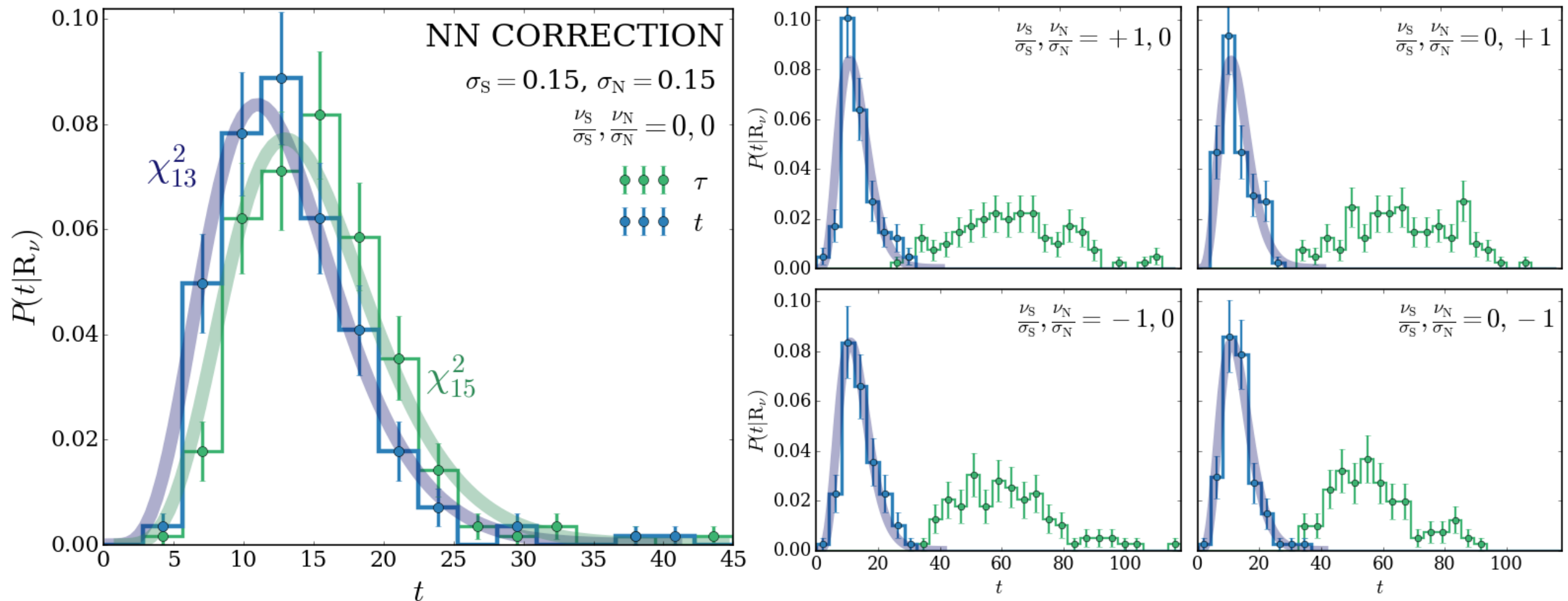
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An Imperfect Machine at Work

(Simple 1d example with exponential Reference)

Tau distribution distorted by non-central value nuisance
if not corrected, produces false positives

t = Tau-Delta independent of nuisance



Remarks/Concerns

Remark #1: By Wilks-Wald Theorem, $P(t|R)$ is a χ^2 , with as many d.o.f. as fit parameters (for us, number of NN pars)...

Provided statistics is large relative to “complexity” of model being fitted

or, which is the same

Provided fit model “simple enough”, for given data stat.



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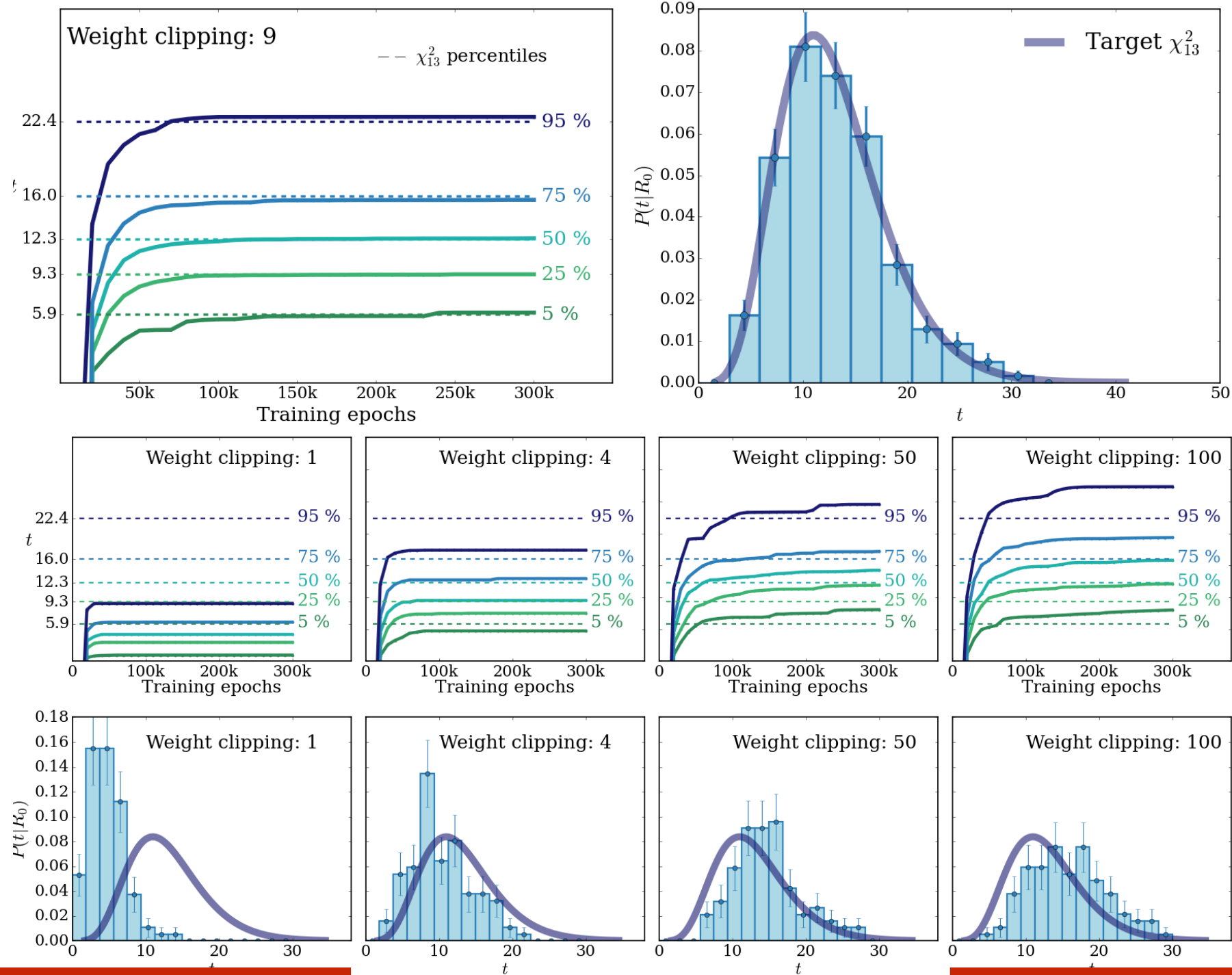
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Criterion used in particular to select **Weight Clipping** regularisation par.

Weight Clipping Selection

(Simple 1d example with exponential Reference)



Asy.For. violation by fit
parameters boundary

Asy.For. violation by sensitivity
to sparse data points

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Concern #1: We do not like Weight Clipping, and we would like better regularization and measure of NN complexity

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The Reference Sample is not of course infinite.

We do empirically check that results weakly depend on the specific Reference sample instance.

Factor few more abundant than Data found enough

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Concern #2:

We have no Analytic/Asymptotic control of the Reference Sample fluctuations effects.

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Remark #3:

Ours is a GoF 2-sample test from classifier training.

[proposed by J.Friedman, 2004 in hep context, but not really studied]

With specific test statistics and loss function choice, dictated by Maximum Likelihood approach.

Maximum Likelihood convenient viewpoint to deal with imperfections as nuisance parameters.

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Concern #3:

No concern here.

But comparative study useful.

[see Chakravarti, Kuusela, Lei, Wasserman, 2021 for a first attempt]

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Strategy has been defined, and applied to problems of the same scale of complexity as LHC analysis

Further progress requires **full-fledged implementation** in **realistic LHC final state** (2 leptons?, 4 leptons?, more exotic?)

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weighted samples

generative models

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Non-NN Models

Kernel Method “Falkon”

[Letizia, Grosso, et. al., 2022]

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Thank You