

Goodness-of-fit by Neyman-Pearson Testing: The NPLM Method

Andrea Wulzer



Based on:

D'Agnolo, AW, 2018

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

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

Grosso, Letizia, AW, et. al., 2022

Grosso, Letizia, AW, Zanetti, et. al., 2023

Grosso, Letizia, Pierini, AW, 2023

Grosso, 2024

Grosso, Letizia, 2024

Cappelli, Grosso, Letizia, Reyes-González, Zanetti, to appear

Goodness of Fit

Statisticians formulate an interesting problem: **g.o.f.***

Be $\mathcal{D}$ some data, and R **one hypothesis** for their distribution

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

Not a problem of Hypothesis testing, as only one hyp. involved.

But, it can be addressed by performing an HT, with $H_0 = R$.

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

Goodness of Fit

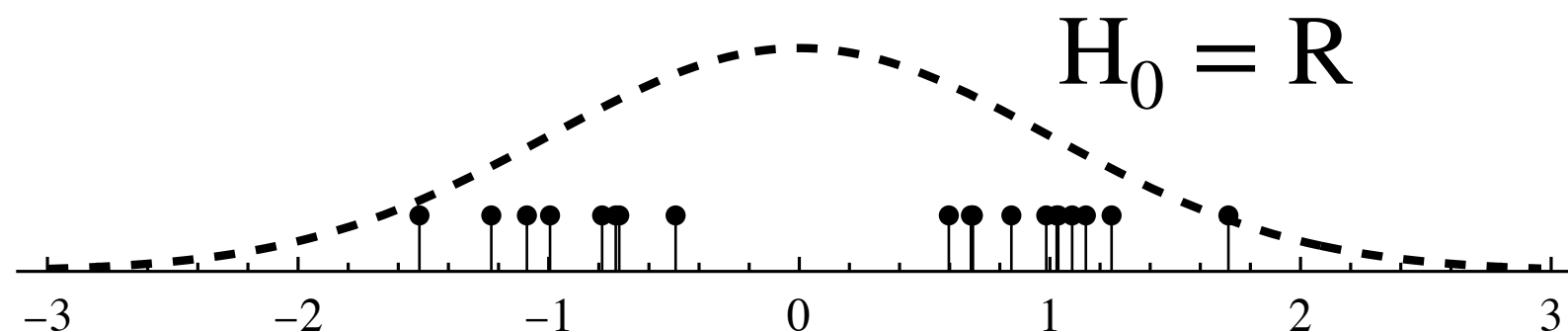
Statisticians formulate an interesting problem: **g.o.f.**

Be $\mathcal{D}$ some data, and **R one hypothesis** for their distribution

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

Example: are these data described by a Standard Gaussian?

We try to answer by comparing the SG with some **Alternative Hypothesis** H_1 . If H_1 works much better, **R** is in trouble.



Goodness of Fit

Statisticians formulate an interesting problem: **g.o.f.**

Be $\mathcal{D}$ some data, and R **one hypothesis** for their distribution

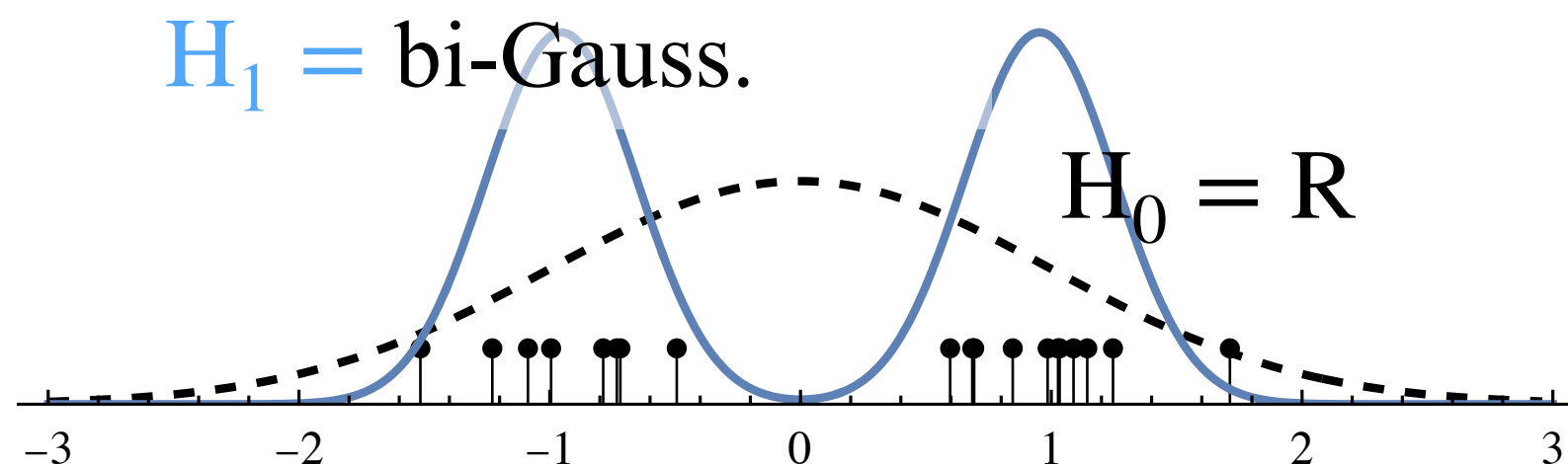
Does R provide the **right description** of $\mathcal{D}$?

Example: are these data described by a Standard Gaussian?

We try to answer by comparing the SG with some **Alternative Hypothesis** H_1 . If H_1 works much better, R is in trouble.

Conclusion strongly depends on which H_1 we try:

- If $H_1 = H_T$ is **true** distribution, very likely we see **tension** of R (low p-value)



Goodness of Fit

Statisticians formulate an interesting problem: **g.o.f.**

Be $\mathcal{D}$ some data, and R **one hypothesis** for their distribution

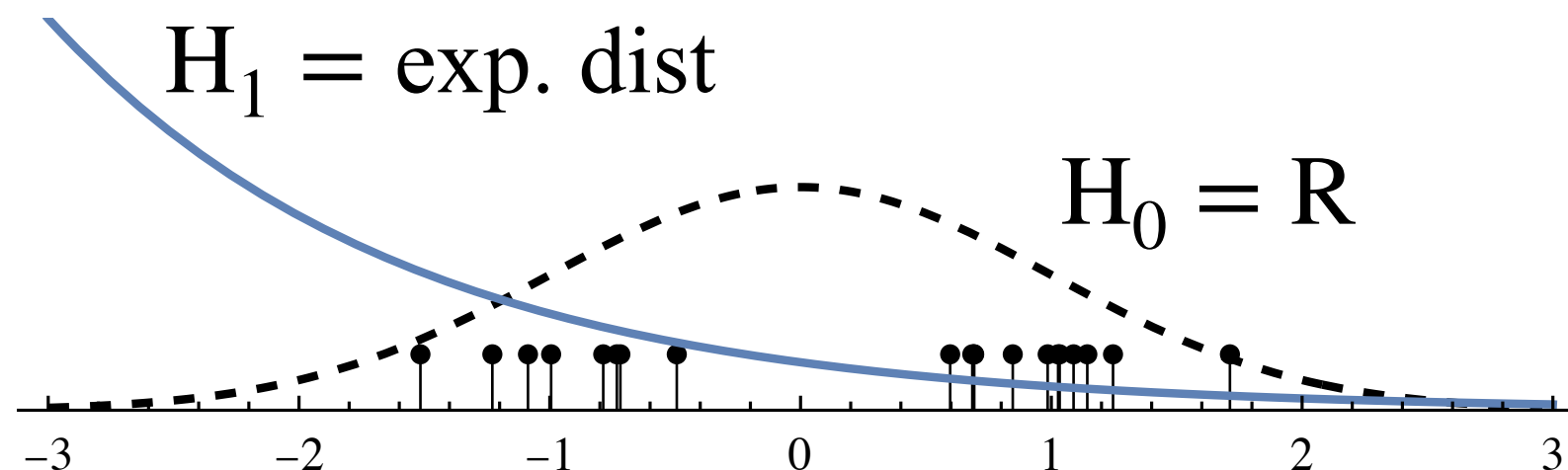
Does R provide the **right description** of $\mathcal{D}$?

Example: are these data described by a Standard Gaussian?

We try to answer by comparing the SG with some **Alternative Hypothesis** H_1 . If H_1 works much better, R is in trouble.

Conclusion strongly depends on which H_1 we try:

- If $H_1 = H_T$ is **true** distribution, very likely we see **tension** of R (low p-value)
- If $H_1 \neq H_T$, we are likely to conclude that R is “good” (high p-value)



Goodness of Fit

Statisticians formulate an interesting problem: **g.o.f.**

Be $\mathcal{D}$ some data, and R **one hypothesis** for their distribution

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

Answering is more **easy** the more **restrictive** assumptions we make on how the true distribution, if not R , can look like.

But, more **partial** as well.

Goodness of Fit

Statisticians formulate an interesting problem: **g.o.f.**

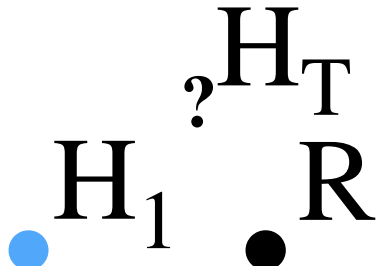
Be $\mathcal{D}$ some data, and R **one hypothesis** for their distribution

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

Answering is more **easy** the more **restrictive** assumptions we make on how the true distribution, if not R , can look like.

But, more **partial** as well.

Simple vs Simple
hypothesis test



H_1 H_T R

- Optimal approach provided by **Neyman–Pearson Lemma:**

$$use: \quad t = \log \frac{\mathcal{L}(H_1)}{\mathcal{L}(H_0)}$$

- Optimal answer to very specific question: **test has no or very limited power if truth $\neq H_1$**

Goodness of Fit

Statisticians formulate an interesting problem: **g.o.f.**

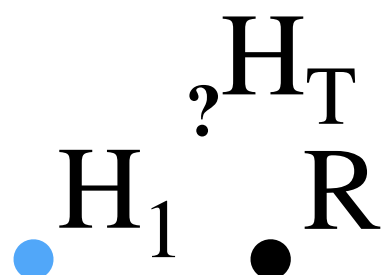
Be $\mathcal{D}$ some data, and R **one hypothesis** for their distribution

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

Answering is more **easy** the more **restrictive** assumptions we make on how the true distribution, if not R , can look like.

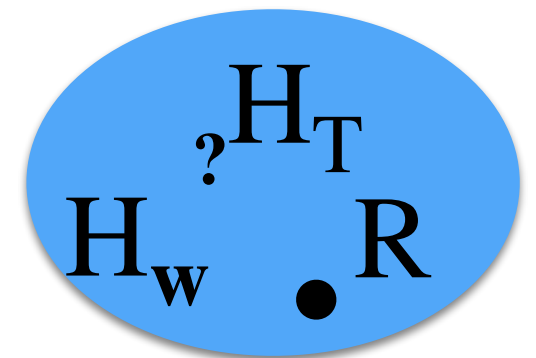
But, more **partial** as well.

Simple vs Simple hypothesis test



- Optimal approach provided by **Neyman–Pearson Lemma**:
$$use: \quad t = \log \frac{\mathcal{L}(H_1)}{\mathcal{L}(H_0)}$$
- Optimal answer to very specific question: **test has no or very limited power if truth $\neq H_1$**

Simple vs Composite hypothesis test

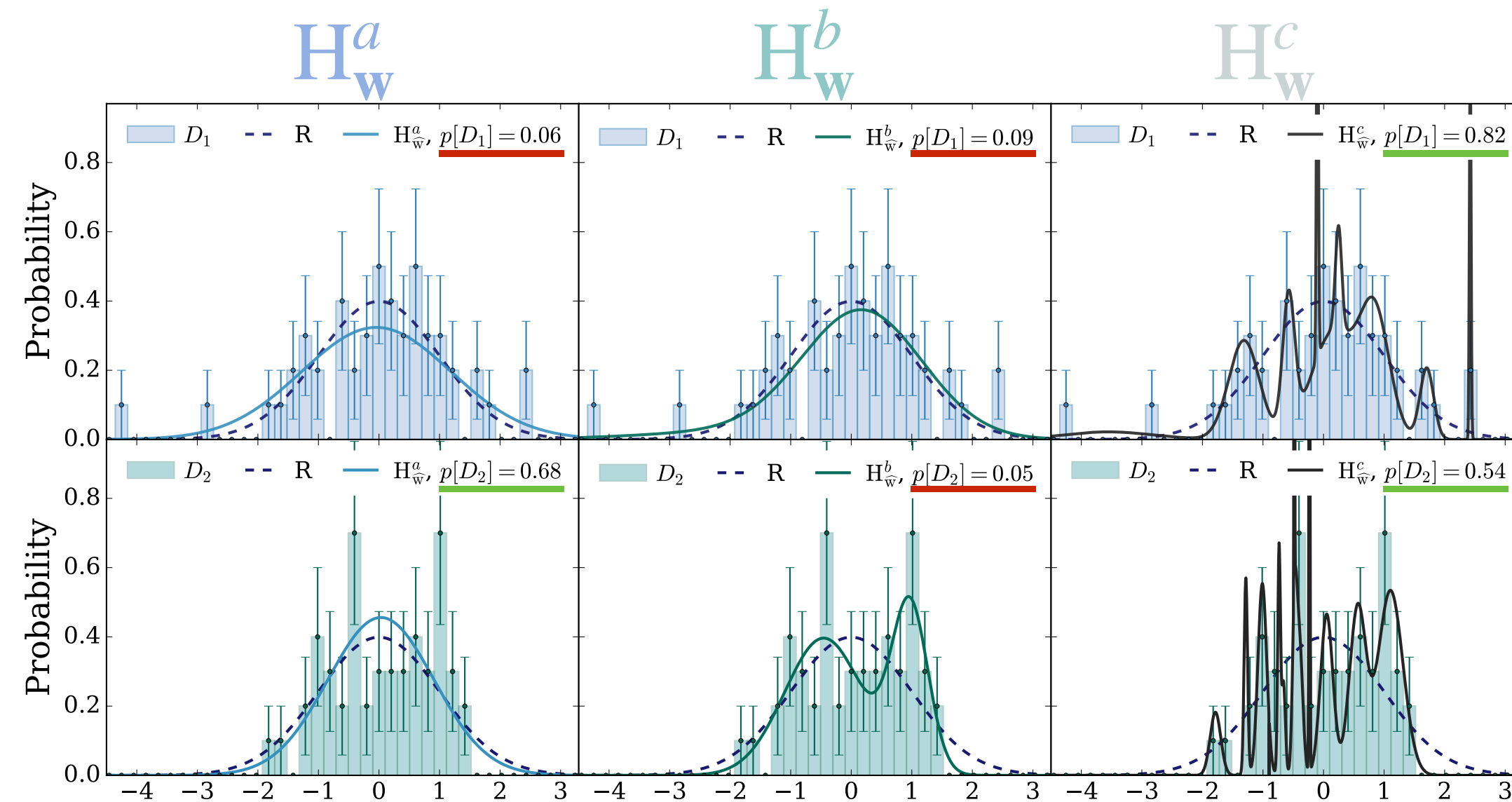


- No Optimal solution. But, **Maximum Likelihood Ratio** is **Good solution**
$$t_{ML} = \log \frac{\mathcal{L}(H_{\hat{w}})}{\mathcal{L}(H_0)} = \max_w \log \frac{\mathcal{L}(H_w)}{\mathcal{L}(H_0)}$$
- Answers a more general question.
It has **some power if truth is in H_w** .
But, larger H_w = less power

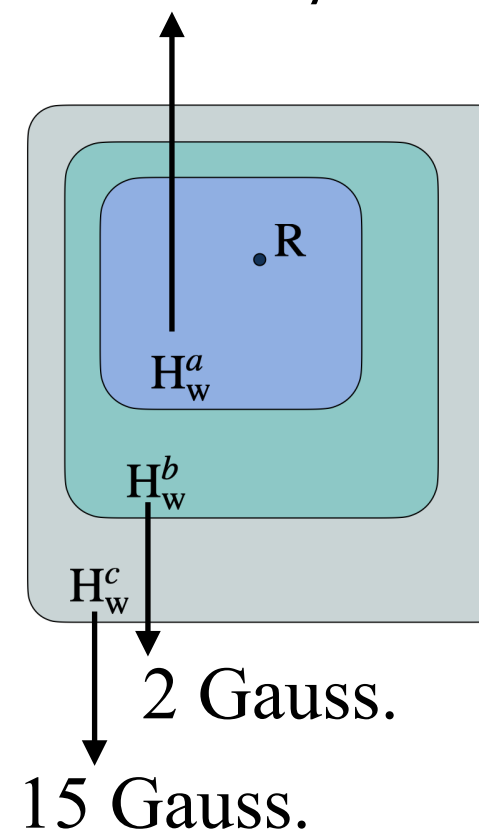
Goodness of Fit

Toy example: 2 datasets, not from R, tested with 3 different H_w 's.

Red is good: means R in trouble — **Green** is bad: means that R looks OK



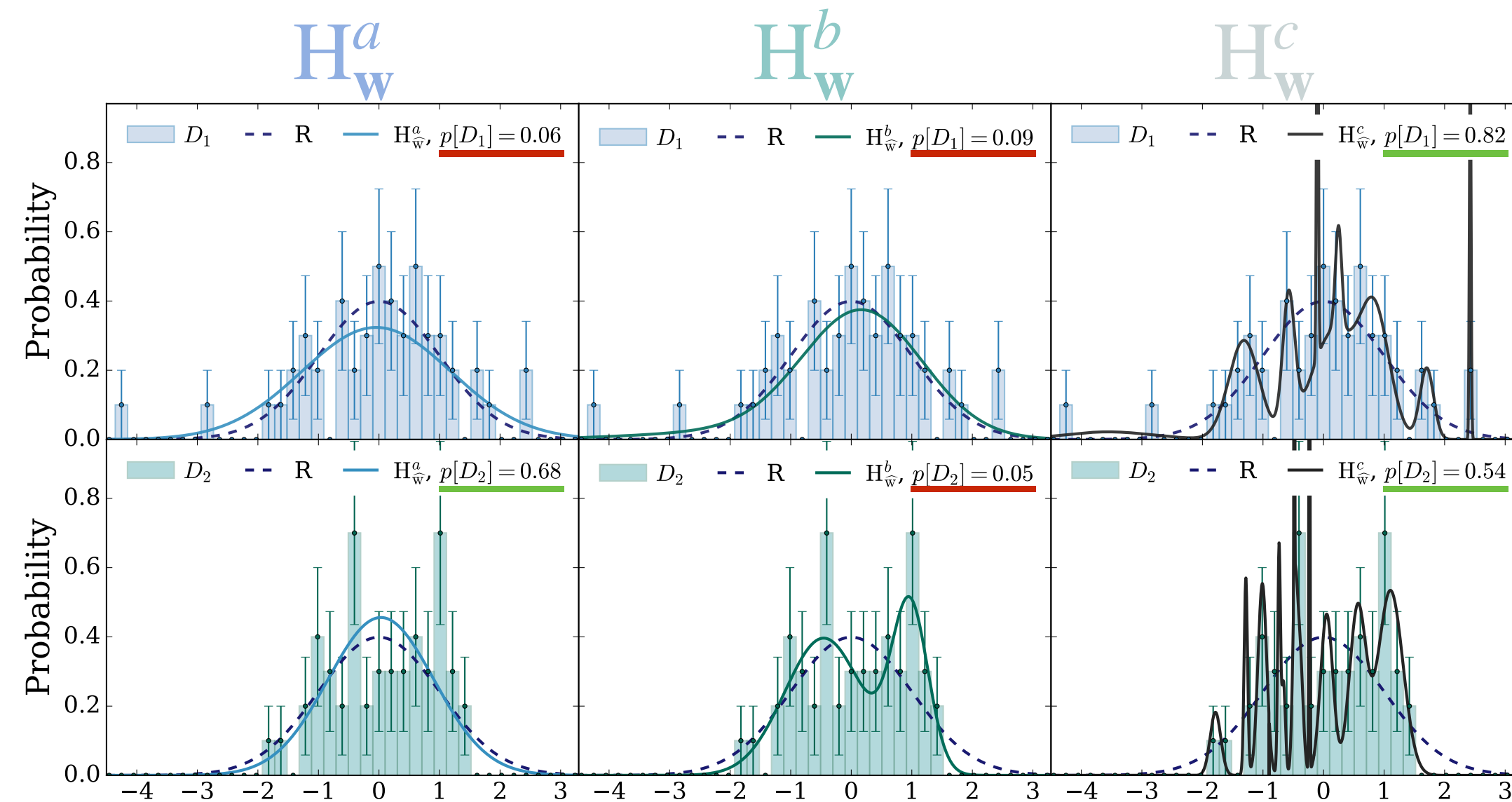
One Gaussian with free μ, σ



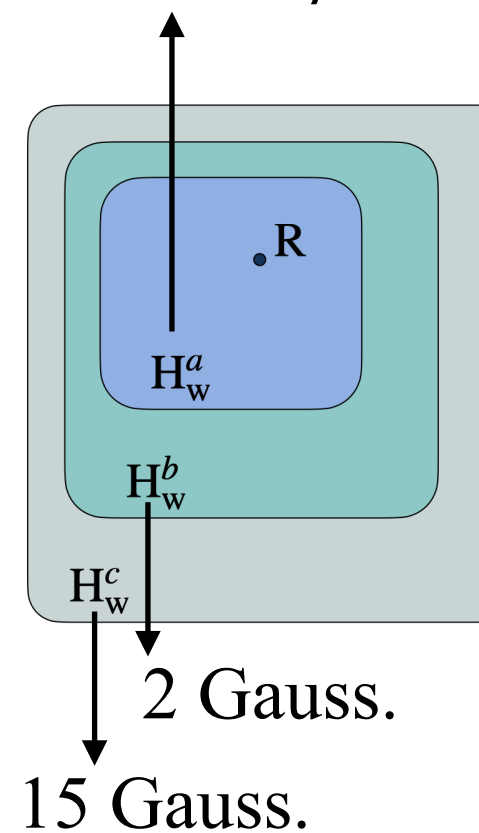
Goodness of Fit

Toy example: 2 datasets, not from R , tested with 3 different H_w 's.

Red is good: means R in trouble — **Green** is bad: means that R looks OK



One Gaussian with free μ, σ



We need large H_w but avoid overfitting

New Physics Learning Machine (NPLM)

[D'Agnolo, AW, 2018]

Data: i.i.d. measurements of feature vector x (e.g., particle mom.)

$$\mathcal{D} = \{x_i\}_{i=1}^{\mathcal{N}}$$

In LHC, number of points is Poisson variable with expected N

Hypotheses: number density in x space (in LHC, $d\sigma \times \text{lumi.}$.)

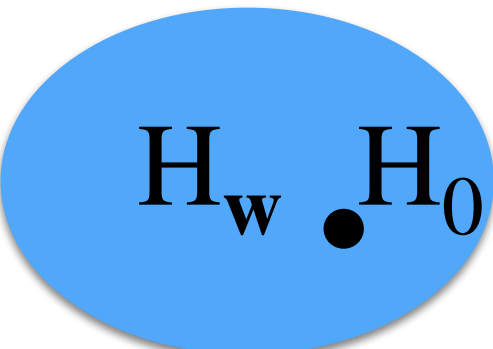
$$n(x) = N \cdot P(x), \quad N = \int dx n(x)$$

Reference Hypothesis: $n(x | R)$

In LHC, the **SM prediction**

Alternative Hypothesis:

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



$H_{\mathbf{w}} \bullet H_0$

New Physics Learning Machine (NPLM)

[D'Agnolo, AW, 2018]

Data: i.i.d. measurements of feature vector x (e.g., particle mom.)

$$\mathcal{D} = \{x_i\}_{i=1}^{\mathcal{N}}$$

In LHC, number of points is Poisson variable with expected N

Hypotheses: number density in x space (in LHC, $d\sigma \times \text{lumi.}$.)

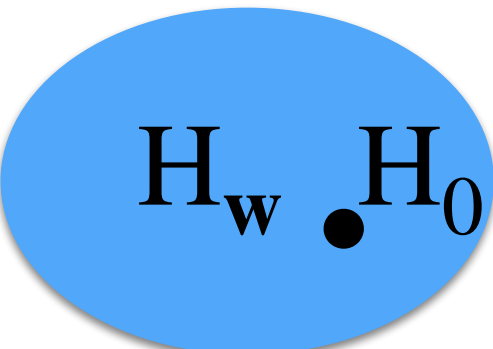
$$n(x) = N \cdot P(x), \quad N = \int dx n(x)$$

Reference Hypothesis: $n(x | R)$

In LHC, the **SM prediction**

Alternative Hypothesis:

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



$H_{\mathbf{w}} \bullet H_0$

In NPLM, set of functions $f(x; \mathbf{w})$ that defines the Alternatives is **Neural Network** or other approximant good in many dimensions, like **kernels**

New Physics Learning Machine (NPLM)

[D'Agnolo, AW, 2018]

NPLM computes the Maximum Likelihood test statistic

$$t_{\text{ML}}(\mathcal{D}) = 2 \log \frac{\mathcal{L}(H_{\hat{\mathbf{w}}}; \mathcal{D})}{\mathcal{L}(R; \mathcal{D})} = 2 \log \frac{e^{-N(\hat{\mathbf{w}})}}{e^{-N(R)}} \prod_{x \in \mathcal{D}} \frac{n(x | H_{\hat{\mathbf{w}}})}{n(x | R)}$$

Using (since $n(x | R)$ not available) a **Reference Sample**

$$\mathcal{R} = \{x_i\}_{i=1}^{N_R}$$

$\mathcal{R}$ is made of instances of x that follow the R distribution

New Physics Learning Machine (NPLM)

[D'Agnolo, AW, 2018]

NPLM computes the Maximum Likelihood test statistic

$$t_{\text{ML}}(\mathcal{D}) = 2 \log \frac{\mathcal{L}(H_{\hat{\mathbf{w}}}; \mathcal{D})}{\mathcal{L}(R; \mathcal{D})} = 2 \log \frac{e^{-N(\hat{\mathbf{w}})}}{e^{-N(R)}} \prod_{x \in \mathcal{D}} \frac{n(x | H_{\hat{\mathbf{w}}})}{n(x | R)}$$

Using (since $n(x | R)$ not available) a **Reference Sample**

$$\mathcal{R} = \{x_i\}_{i=1}^{N_R}$$

$\mathcal{R}$ is made of instances of x that follow the R distribution

The Likelihood Ratio Trick:

*“ A continuous-output classifier approximates “
the ratio between the p.d.f.s of the training data*

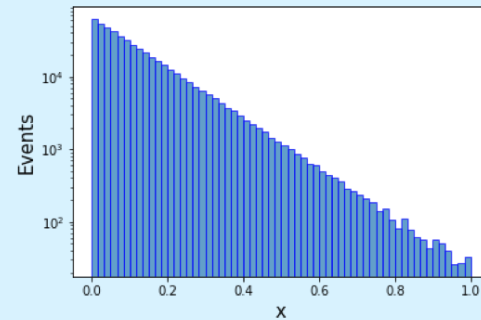
Computation of t by **supervised training** $\mathcal{D}$ vs $\mathcal{R}$

In **NN** implementation, using special loss function that gives $t = -2 \min[\text{loss}]$

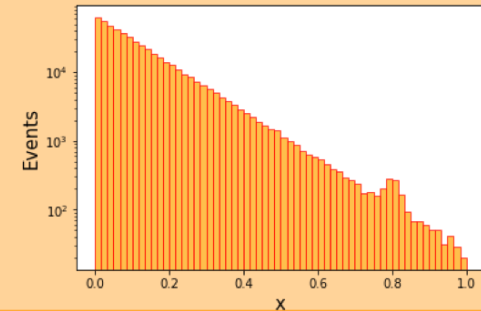
In **kernel** implementation, by learning “ $\hat{\mathbf{w}}$ ” and plugging in

INPUT

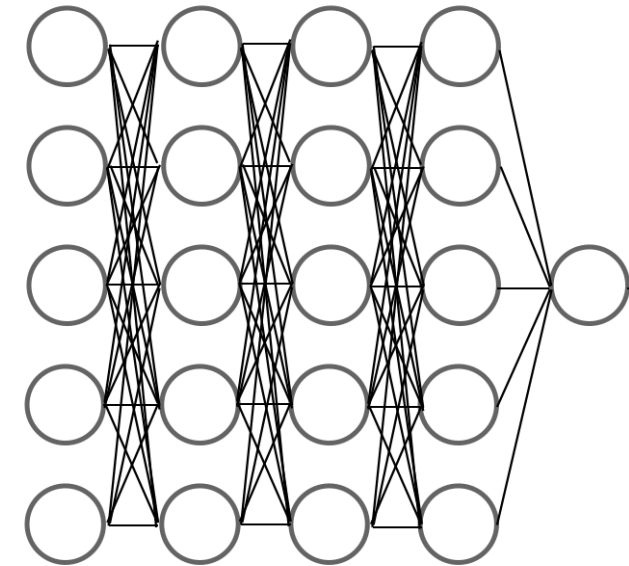
Reference sample (R)
label=0



Data sample (D)
label=1



BSM network



$\mathbf{w}$ $\xrightarrow{\text{NN training}}$ $\hat{\mathbf{w}}$

Unbinned training samples!

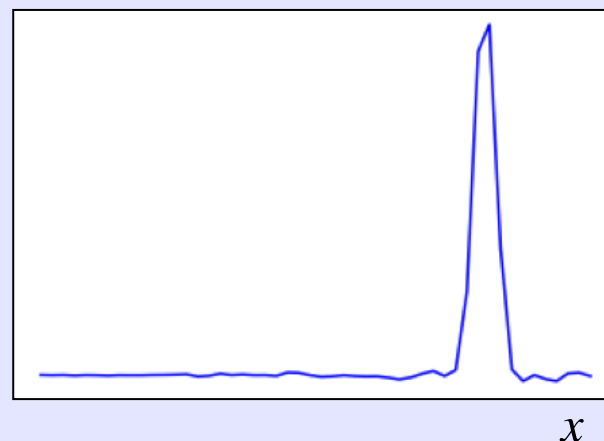
OUTPUT

Single training

$$t(D) = -2L[f(x; \hat{\mathbf{w}})]$$

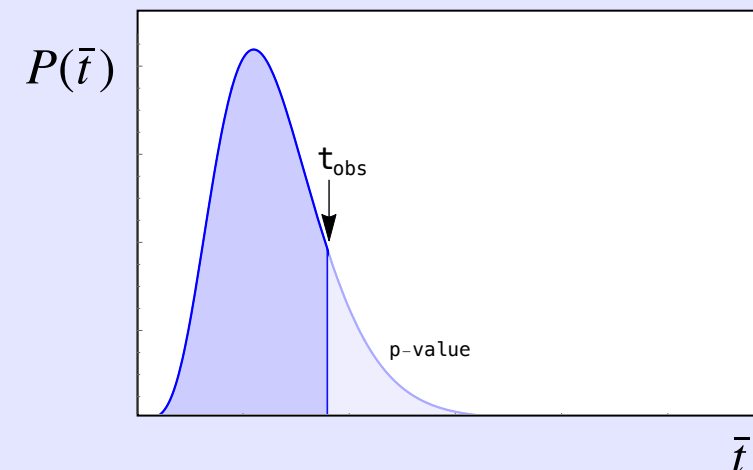
$$f(x; \hat{\mathbf{w}}) = \log \left[\frac{n(x | H_{\hat{\mathbf{w}}})}{n(x | R_0)} \right]$$

$f(x; \hat{\mathbf{w}})$



Many trainings
(with pseudo-data)

Empirical distribution of t
 $\rightarrow$ p-value for new datasets



Comparing Performances

[Grosso, Letizia, Pierini, AW, 2023]

Many classical methods for g.o.f. with one-dimensional data:

- χ^2 : Bin data and compare with expected in each bin
- **EDF tests**: Compare EDF with CDF. Variants are KS, CvM, AD.
- **Spacing tests**: Spacings of CDF(points). Variants are Moran, RPS

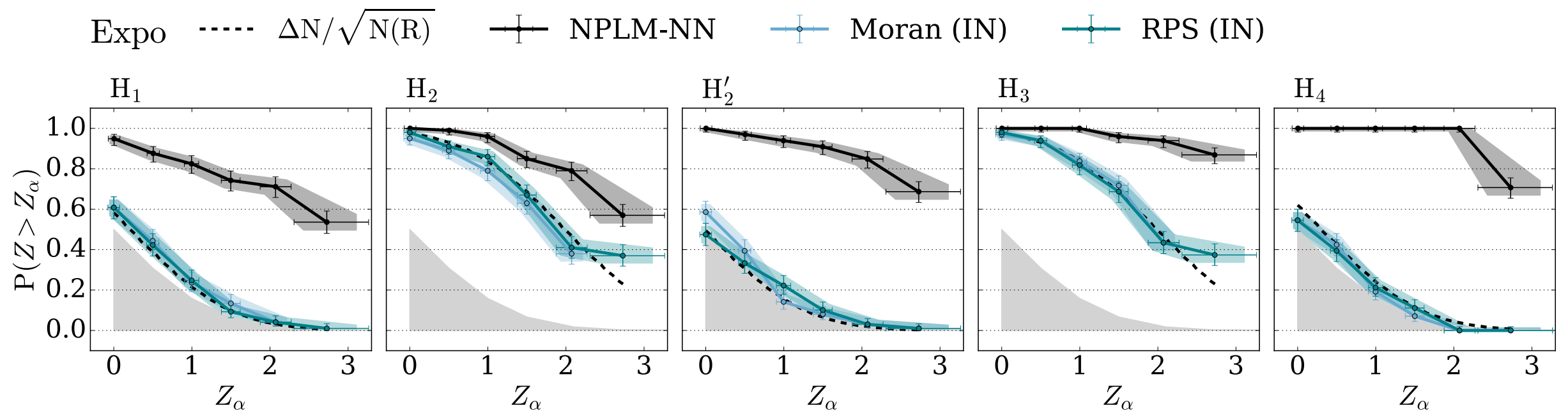
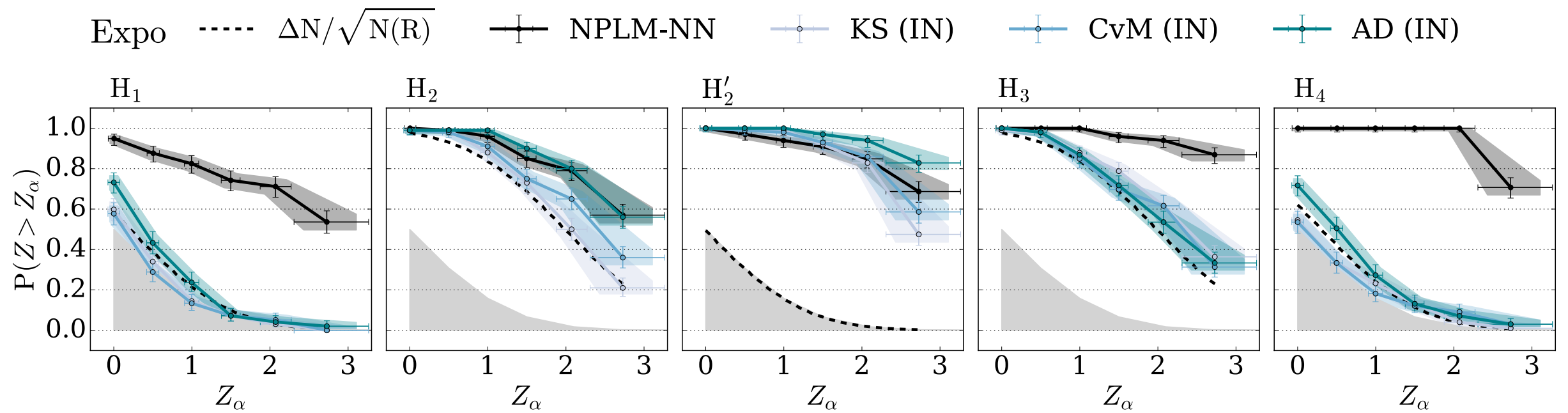
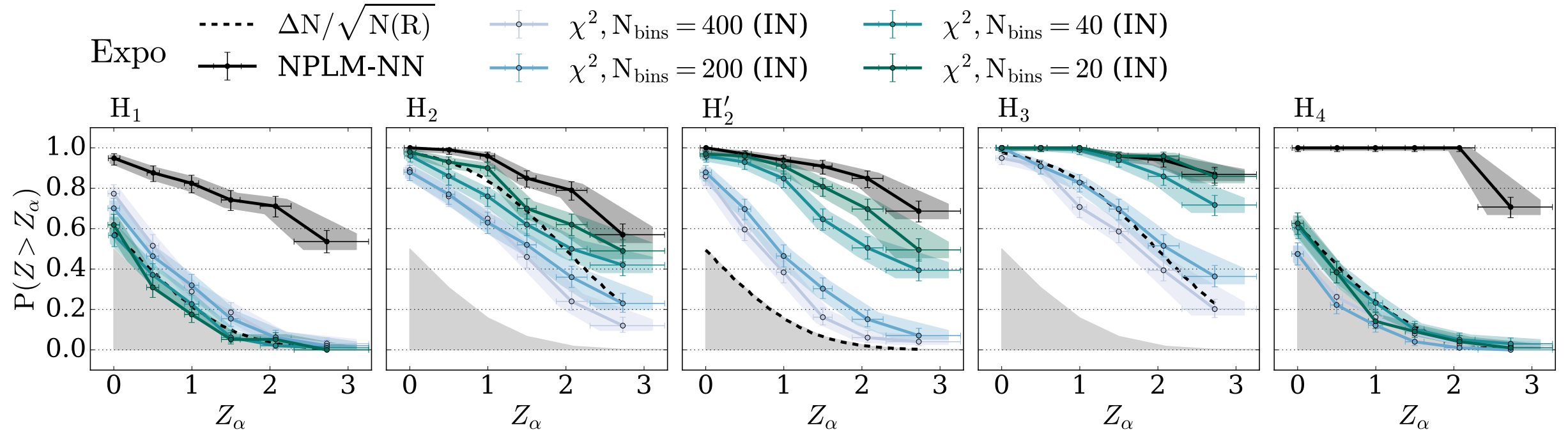
Comparing Performances

[Grosso, Letizia, Pierini, AW, 2023]

Many classical methods for g.o.f. with one-dimensional data:

- χ^2 : Bin data and compare with expected in each bin
- **EDF tests**: Compare EDF with CDF. Variants are KS, CvM, AD.
- **Spacing tests**: Spacings of CDF(points). Variants are Moran, RPS

While $d = 1$ g.o.f. is considered a “solved problem”, and $d > 1$ is what we care, interesting that **NPLM works better**.



Comparing Performances

[Grosso, Letizia, Pierini, AW, 2023]

For $d > 1$, most established solution are **Classifier-Based Tests**

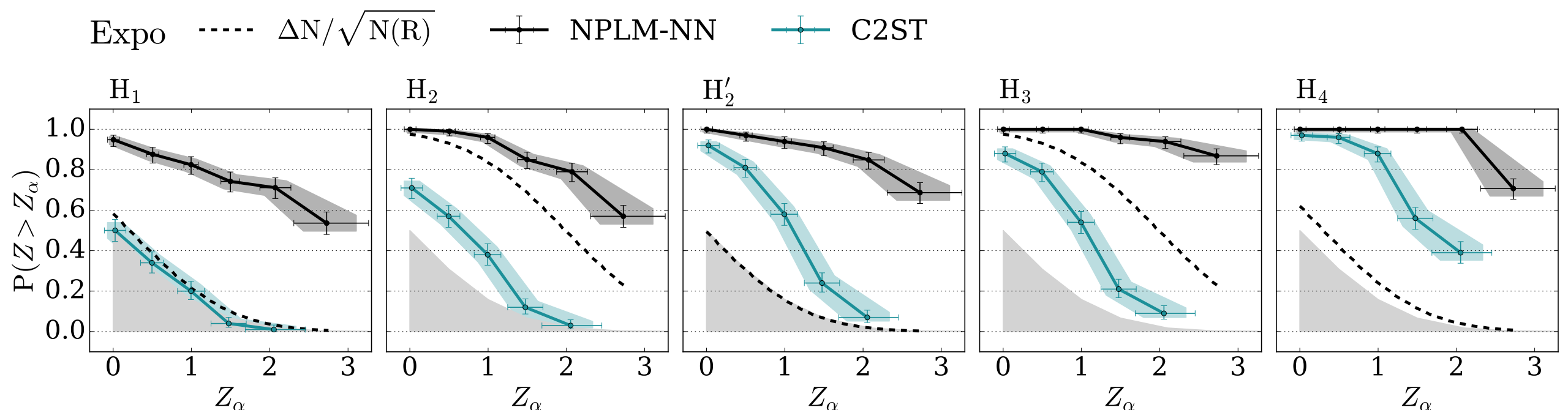
- **General idea:** Train $\mathcal{D}$ vs $\mathcal{R}$. Get more decisive classifier if $\mathcal{D} \approx \mathcal{R}$
Use **some metric** evaluated on trained classifier output for Hypothesis Test.
[Friedman, 2003]

- **C2ST:** Most natural implementation. Uses classification accuracy metric.
[Lopez-Paz, Oquab, 2016]

Employed for generative models validation

- **Variants:** We studied different metric and compared in/out evaluation.

NPLM vs C2ST: $d = 1$



Comparing Performances

[Grosso, Letizia, Pierini, AW, 2023]

For $d > 1$, most established solution are **Classifier-Based Tests**

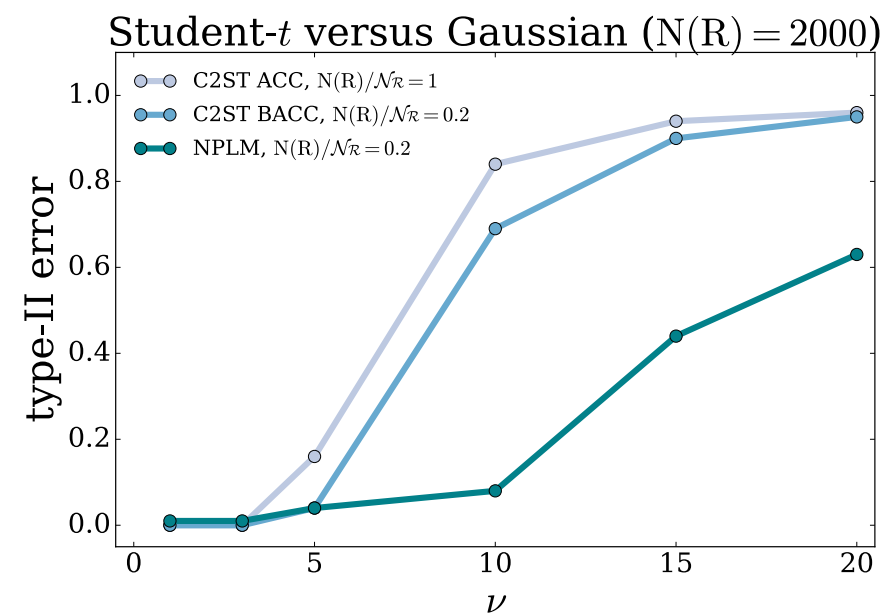
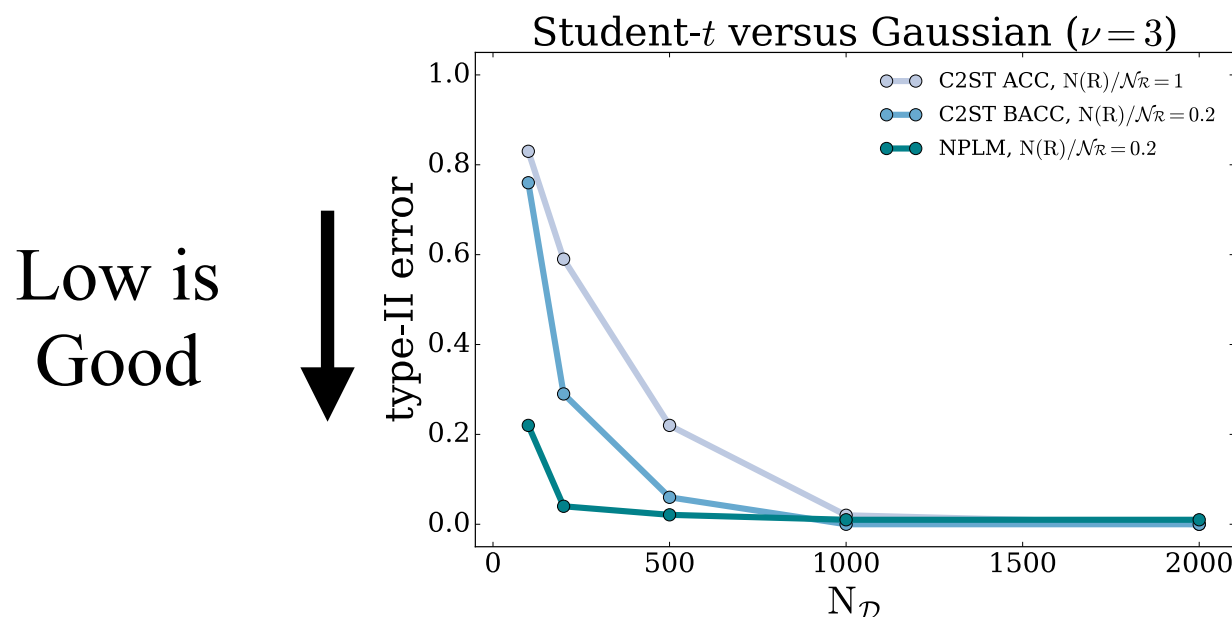
- **General idea:** Train $\mathcal{D}$ vs $\mathcal{R}$. Get more decisive classifier if $\mathcal{D} \approx \mathcal{R}$
Use **some metric** evaluated on trained classifier output for Hypothesis Test.
[Friedman, 2003]

- **C2ST:** Most natural implementation. Uses classification accuracy metric.
[Lopez-Paz, Oquab, 2016]

Employed for generative models validation

- **Variants:** We studied different metric and compared in/out evaluation.

NPLM vs C2ST: $d = 1$



Comparing Performances

[Grosso, Letizia, Pierini, AW, 2023]

For $d > 1$, most established solution are **Classifier-Based Tests**

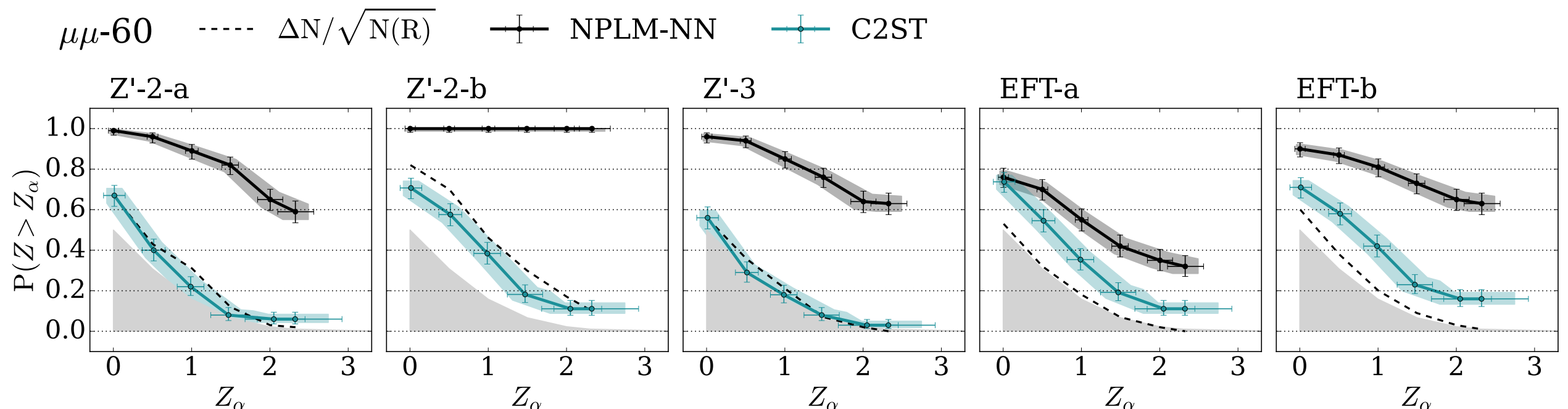
- **General idea:** Train $\mathcal{D}$ vs $\mathcal{R}$. Get more decisive classifier if $\mathcal{D} \approx \mathcal{R}$
Use **some metric** evaluated on trained classifier output for Hypothesis Test.
[Friedman, 2003]

- **C2ST:** Most natural implementation. Uses classification accuracy metric.
[Lopez-Paz, Oquab, 2016]

Employed for generative models validation

- **Variants:** We studied different metric and compared in/out evaluation.

NPLM vs C2ST: $d = 5$



Comparing Performances

[Grosso, Letizia, Pierini, AW, 2023]

For $d > 1$, most established solution are **Classifier-Based Tests**

- **General idea:** Train $\mathcal{D}$ vs $\mathcal{R}$. Get more decisive classifier if $\mathcal{D} \approx \mathcal{R}$
Use **some metric** evaluated on trained classifier output for Hypothesis Test.
[Friedman, 2003]
- **C2ST:** Most natural implementation. Uses classification accuracy metric.
[Lopez-Paz, Oquab, 2016]
Employed for generative models validation
- **Variants:** We studied different metric and compared in/out evaluation.

NPLM is a Classifier-Based Test. Why so much better?

After comparison of many CBT variants, we conclude that the key is using Maximum Likelihood Ratio as metric, and in-sample eval.

Distinctive feature of NPLM is implementing N&P Testing!

Applications

Some of the many applications of g.o.f. are:

- **Model-Agnostic BSM Searches**
- **Data Quality Monitoring:** Tell if apparatus operates “normally”
- **Generative Models:** GM validation and selection

Data Quality Monitoring

[Grosso, Letizia, AW, Zanetti, et. al., 2023]

No Reference uncertainties: $\mathcal{R}$ is data in good operation condition

n D DQM

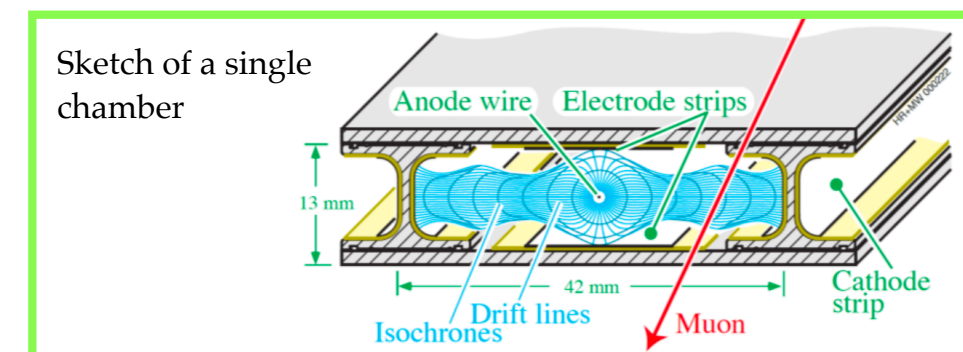
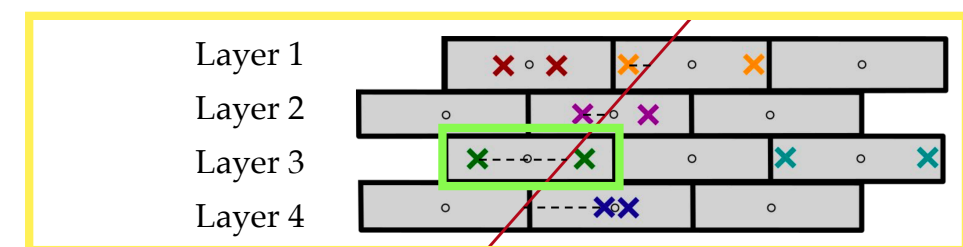
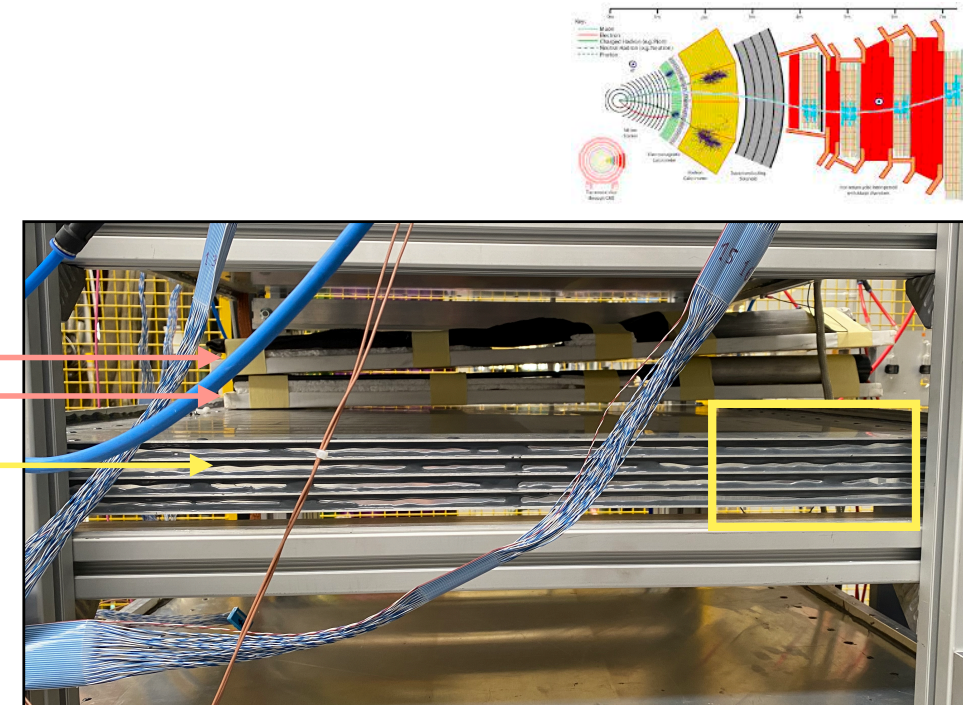
Online monitoring of a DT chamber:

Setup (Legnaro INFN national laboratory):

- 2 scintillators as signal trigger
- 1 drift tube chamber: 4 layers 16 wires each (16x4=64 wires)
- Source of signals: cosmic muons (triggered rate ~ 3 MHz)
- **Event:** muon track reconstructed interpolating 3/4 hits (one per layer)

Observables (6D problem):

- 4 drift times [$t_{\text{drift},1}, t_{\text{drift},2}, t_{\text{drift},3}, t_{\text{drift},4}$]: time for the ionised electrons to reach the wire from the interaction point ($v_{\text{drift}} = \text{cm/s}$).
- θ : reconstructed track angle
- N_{hits} : average number of hits per time window (“orbit”)



Data Quality Monitoring

[Grosso, Letizia, AW, Zanetti, et. al., 2023]

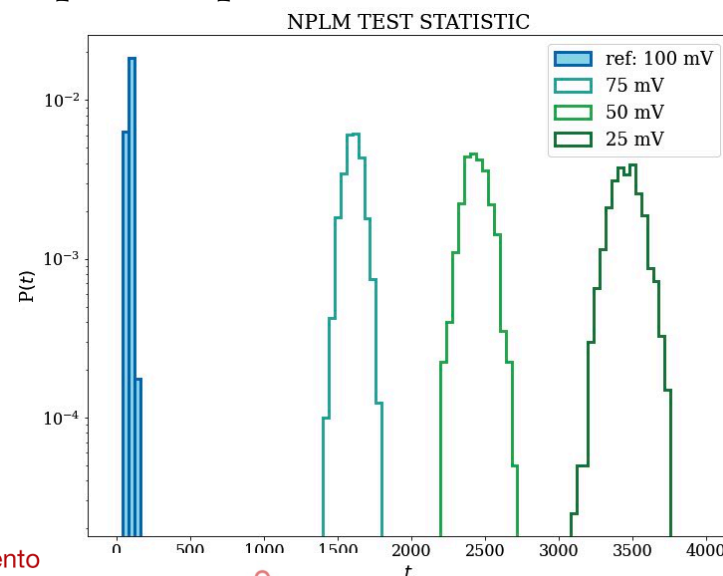
Much better than standard methods, and **fast enough**

n D DQM

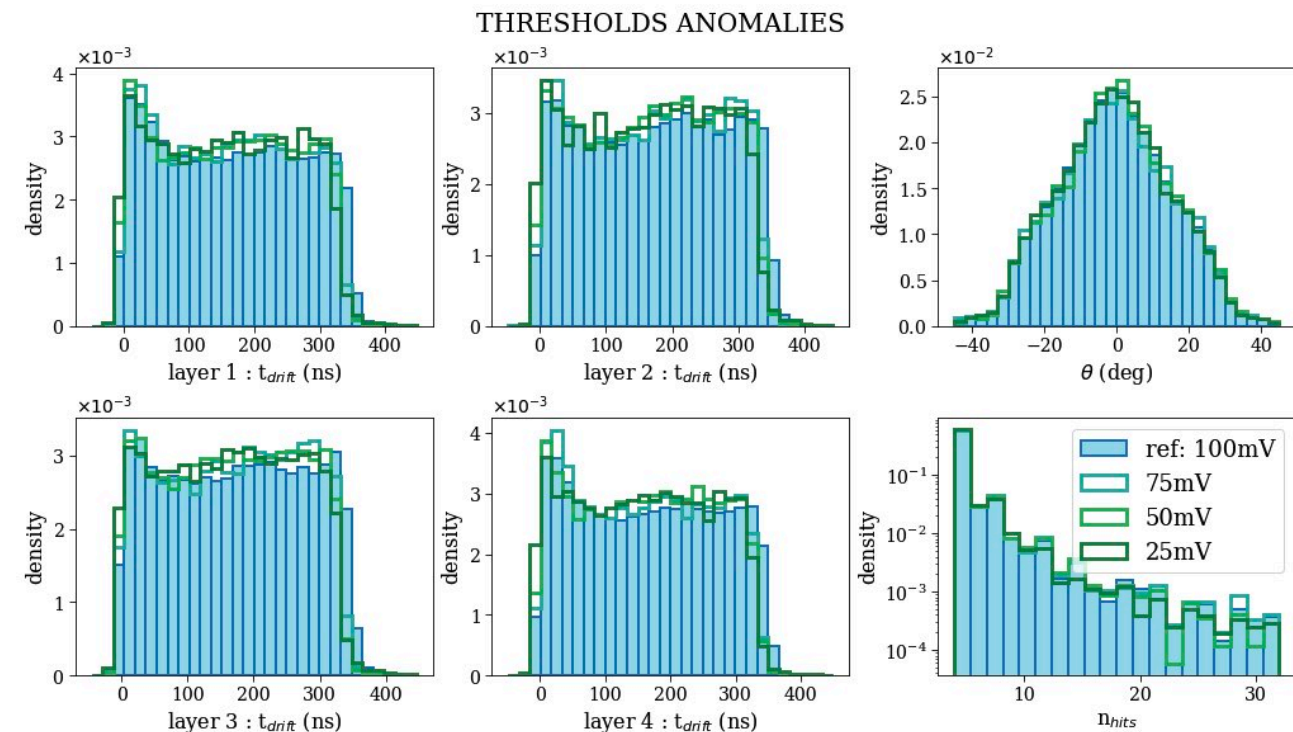
Online monitoring of a DT chamber:

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



Distribution of the observables at different values of the threshold tension

→ more about this in Marco's talk tomorrow!

Generative Models Validation

[To Appear: Cappelli, Grosso, Letizia, Reyes-González, Zanetti]

A mixture of Gaussians in d dimension, vs a Normalising Flow
Tested with NPLM using 10K points, $\ll$ NF training sample size

$N_{tr} \backslash d$	4	8	12	16	20	30
100k	9.88 $^{+1.22}_{-1.29}$	8.88 $^{+1.12}_{-1.19}$	14.73 $^{+1.23}_{-0.94}$	16.81 $^{+1.04}_{-1.06}$	14.46 $^{+1.09}_{-0.84}$	14.97 $^{+1.09}_{-0.84}$
200k	4.79 $^{+1.00}_{-1.07}$	9.90 $^{+0.94}_{-1.05}$	9.56 $^{+1.04}_{-1.04}$	8.34 $^{+0.96}_{-1.09}$	6.45 $^{+0.97}_{-1.07}$	7.32 $^{+0.90}_{-0.81}$
500k	1.93 $^{+1.02}_{-0.99}$	3.01 $^{+0.74}_{-1.13}$	3.16 $^{+1.10}_{-1.02}$	5.05 $^{+1.02}_{-0.99}$	2.07 $^{+0.81}_{-0.97}$	3.06 $^{+1.13}_{-0.86}$

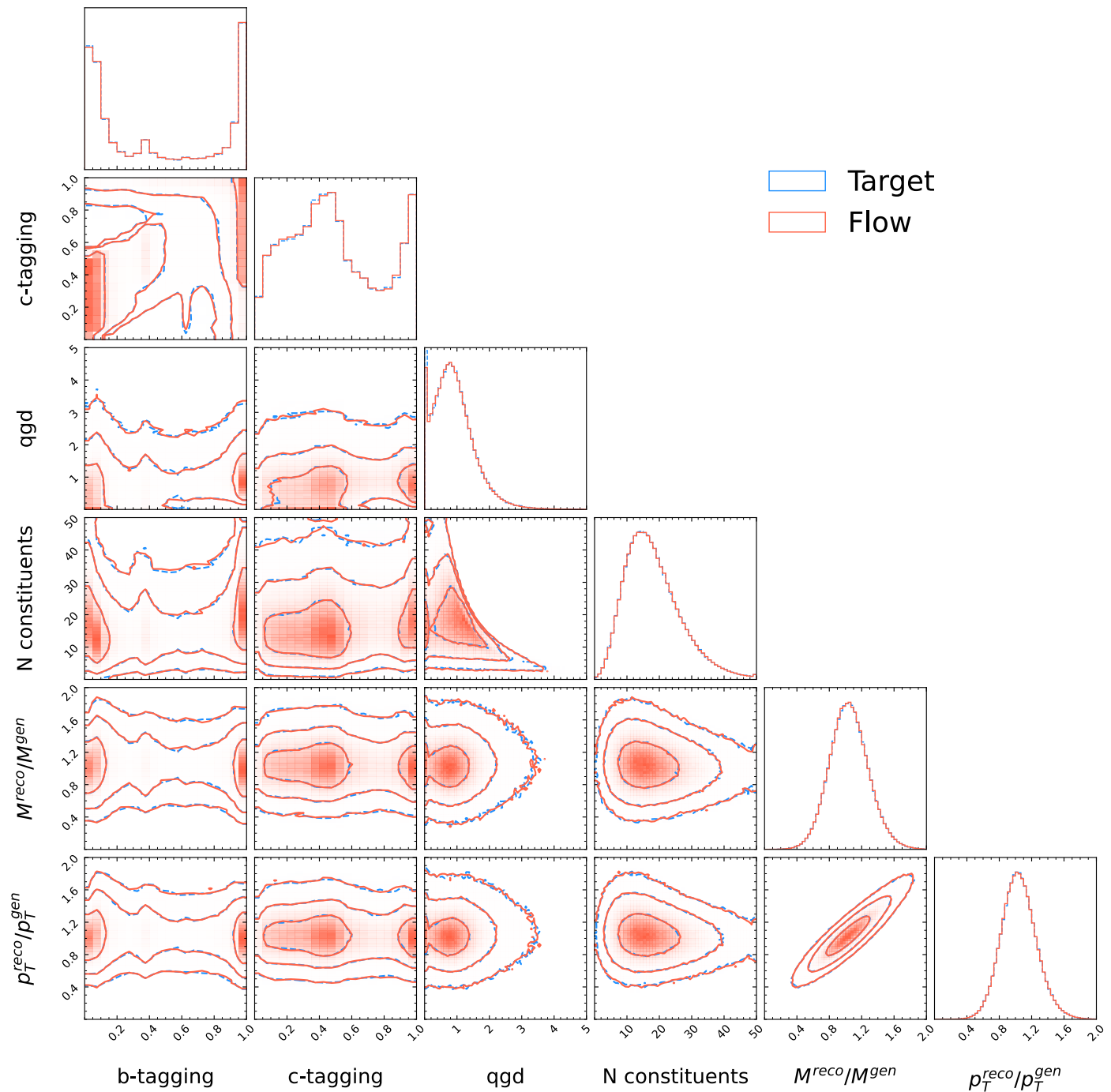
Table 1: Table of median Z-scores obtained with the NPLM method for various NFs models, characterised by training samples of different size (N_{tr}) and different number of dimensions (d). We report errors estimated as the 68% confidence interval, defined symmetrically around the median value.

Very high Z-scores. Consistently go down as N_{tr} increases

Generative Models Validation

[To Appear: Cappelli, Grosso, Letizia, Reyes-González, Zanetti]

Surrogate detector simulator [Vaselli, Cattafesta, Asenov, Rizzi; 2402.13684].
With realistic-looking 2d marginals:



Generative Models Validation

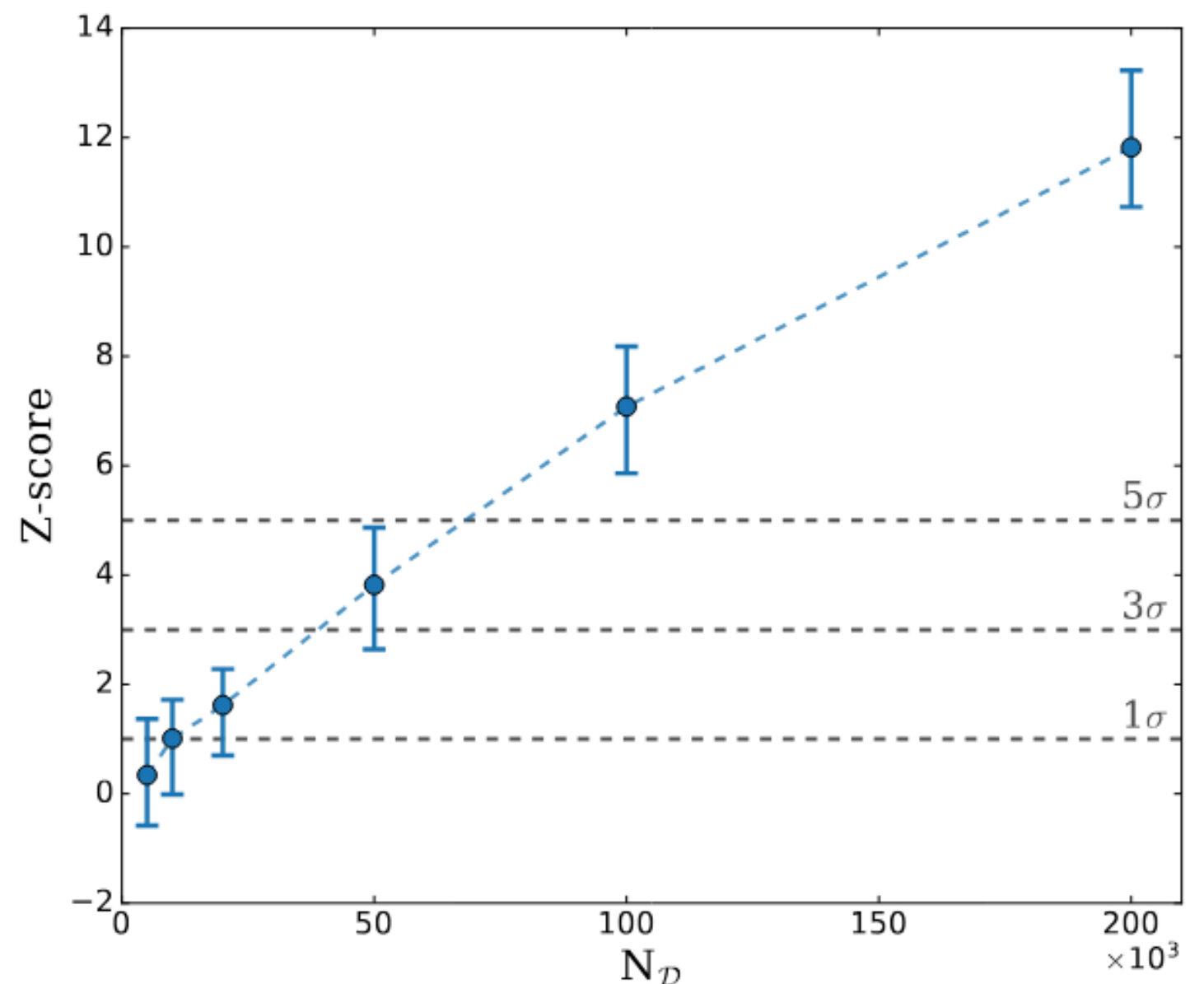
[To Appear: Cappelli, Grosso, Letizia, Reyes-González, Zanetti]

Surrogate detector simulator [Vaselli, Cattafesta, Asenov, Rizzi; 2402.13684].

With realistic-looking 2d marginals:

Tested with NPLM using less data than training size 500K

$N_{\mathcal{D}}$	Z-score
5 k	$0.34^{+1.03}_{-0.92}$
10 k	$1.01^{+0.71}_{-1.02}$
20 k	$1.62^{+0.66}_{-0.92}$
50 k	$3.82^{+1.05}_{-1.18}$
100 k	$7.08^{+1.10}_{-1.22}$
200 k	$11.82^{+1.41}_{-1.09}$



Generative Models Validation

[To Appear: Cappelli, Grosso, Letizia, Reyes-González, Zanetti]

Surrogate detector simulator [Vaselli, Cattafesta, Asenov, Rizzi; 2402.13684].

With realistic-looking 2d marginals:

Tested with NPLM using less data than training size 500K

Personal Conclusions:

- Data augmentation with Generative Models is a **mirage**.
Because NPLM distinguishes small generated sample from true
- Maybe we can augment some marginal. Maybe we need finite accuracy because of systematics mis-modeling.
But please explain/demonstrate why and how

Generative Models Validation

[To Appear: Cappelli, Grosso, Letizia, Reyes-González, Zanetti]

Surrogate detector simulator [Vaselli, Cattafesta, Asenov, Rizzi; 2402.13684].

With realistic-looking 2d marginals:

Tested with NPLM using less data than training size 500K

Personal Conclusions:

- Data augmentation with Generative Models is a **mirage**.
Because NPLM distinguishes small generated sample from true
- Maybe we can augment some marginal. Maybe we need finite accuracy because of systematics mis-modeling.
But please explain/demonstrate why and how

Objective Conclusion:

- NPLM is very sensitive to mis-modelling
- Could be the best metric for generative models selection

Take-home messages

Goodness-of-fit

- A truly profound problem of Science!
- Could serve for model-agnostic BSM searches.
- But also for Data Validation, for DQM, validation of generators including Generative Models
- NPLM in our studies is found better than other methods

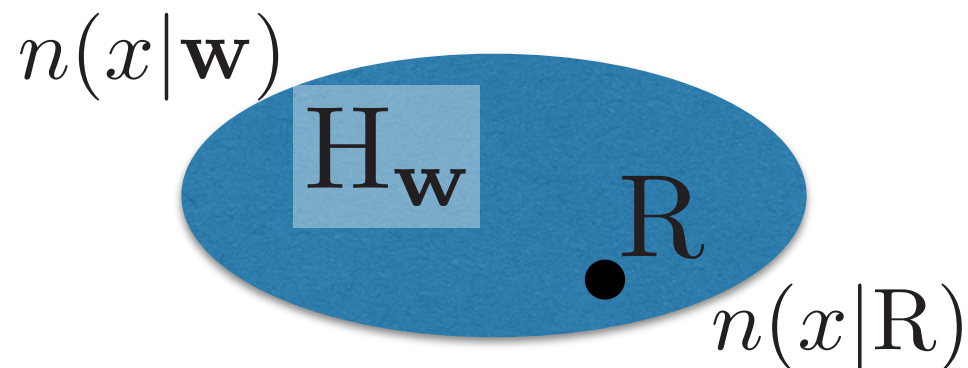
Thank You

New Physics Learning Machine (NPLM)

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

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

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



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

$f(x;\mathbf{w})$ is a **neural network**, or other flexible functional approximant with good properties in many dimensions, like **kernels**

Strategy is to evaluate the classical Likelihood Ratio test statistic

$$t(\mathcal{D}) = 2 \log \frac{\max_{\mathbf{w}} [\mathcal{L}(H_{\mathbf{w}}|\mathcal{D})]}{\mathcal{L}(R|\mathcal{D})} = 2 \max_{\mathbf{w}} \left\{ \log \left[\frac{e^{-N(\mathbf{w})}}{e^{-N(R)}} \prod_{i=1}^{\mathcal{N}_{\mathcal{D}}} \frac{n(x_i|\mathbf{w})}{n(x_i|R)} \right] \right\}$$

by **supervised training Data vs Reference** (background) sample.

Reference = artificial data distributed as predicted by the SM

By using a special loss function:

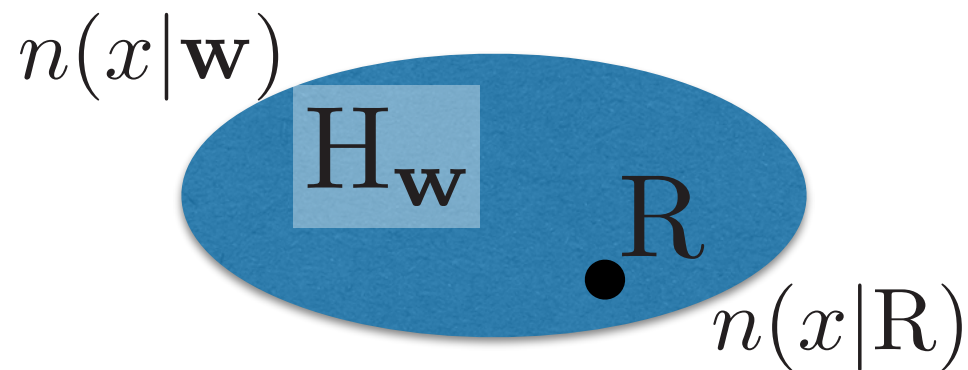
$$L[f] = \sum_{(x,y)} \left[(1-y) \frac{N(R)}{\mathcal{N}_{\mathcal{R}}} (e^{f(x)} - 1) - y f(x) \right] \rightarrow t(\mathcal{D}) = -2 \min_{\{\mathbf{w}\}} L[f(\cdot, \mathbf{w})]$$

New Physics Learning Machine (NPLM)

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

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

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



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

$f(x;\mathbf{w})$ is a **neural network**, or other flexible functional approximant with good properties in many dimensions, like **kernels**

Three-lines derivation:

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

Approximate integral as Monte Carlo sum:

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

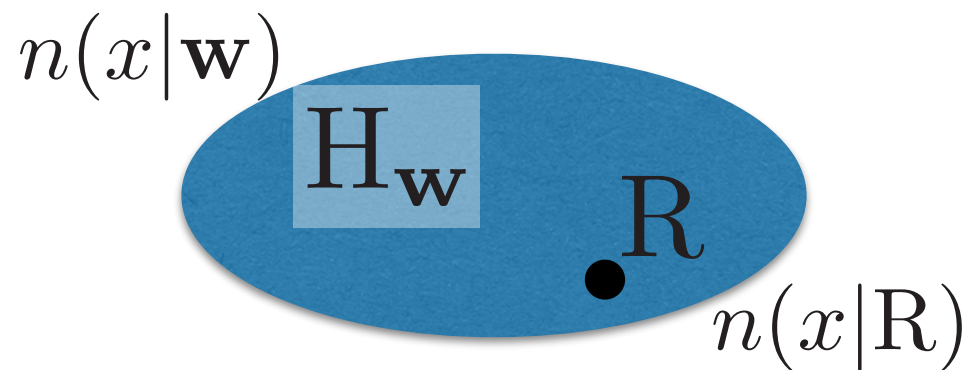
$$t(\mathcal{D}) = -2 \operatorname{Min}_{\{\mathbf{w}\}} \left[\frac{N(R)}{\mathcal{N}_{\mathcal{R}}} \sum_{x \in \mathcal{R}} (e^{f(x;\mathbf{w})} - 1) - \sum_{x \in \mathcal{D}} f(x; \mathbf{w}) \right] \equiv -2 \operatorname{Min}_{\{\mathbf{w}\}} L[f(\cdot, \mathbf{w})]$$

New Physics Learning Machine (NPLM)

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

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

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



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

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

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

Like saying that $n(x|R)$ is “known”, as it is infinitely samplable. Factor few enough.

Three-lines derivation:

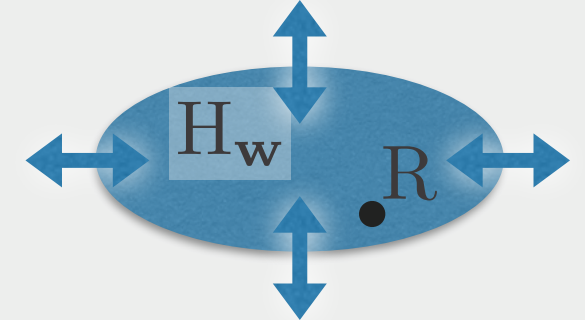
$$t(\mathcal{D}) = 2 \operatorname{Max}_{\mathbf{w}} \left\{ \log \left[\frac{e^{-N(\mathbf{w})}}{e^{-N(R)}} \prod_{i=1}^{\mathcal{N}_{\mathcal{D}}} \frac{n(x_i|\mathbf{w})}{n(x_i|R)} \right] \right\}$$

Approximate integral as Monte Carlo sum:

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

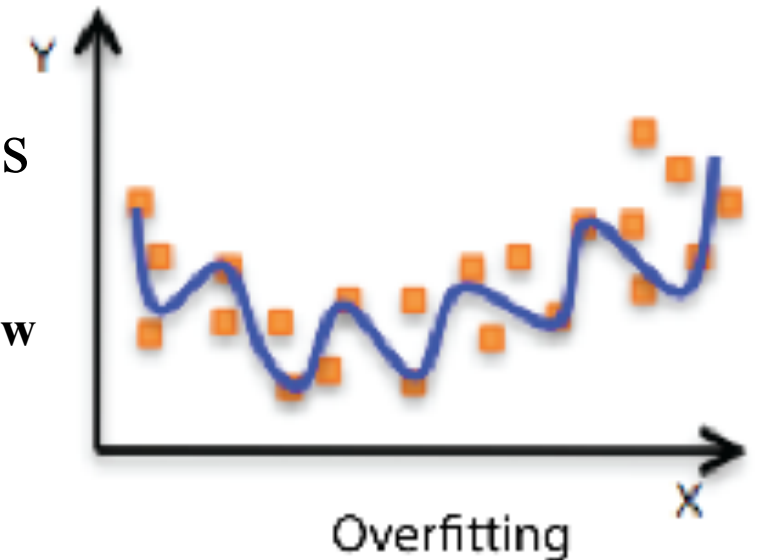
$$t(\mathcal{D}) = -2 \operatorname{Min}_{\{\mathbf{w}\}} \left[\frac{N(R)}{\mathcal{N}_{\mathcal{R}}} \sum_{x \in \mathcal{R}} (e^{f(x;\mathbf{w})} - 1) - \sum_{x \in \mathcal{D}} f(x;\mathbf{w}) \right] \equiv -2 \operatorname{Min}_{\{\mathbf{w}\}} L[f(\cdot, \mathbf{w})]$$

Model Selection



Which hypotheses (distributions) our (statistical) model contains?

- Not “all of them”, otherwise it would fail (overfitting)
- It should contain approximations of all the reasonable ones
- No Statistical Learning notion of model capacity seems reasonable physics measure of volume or boundaries of H_w
- Minimal allowed variation scale would sound reasonable, but no theory developed



Waiting for principled approach, solution is **χ^2 -compatibility**:

- **Naive** Wilks Theorem application:

$P(t|R)$ is χ^2 , with as many d.o.f. as fit parameters (for us, num. of NN par.s)

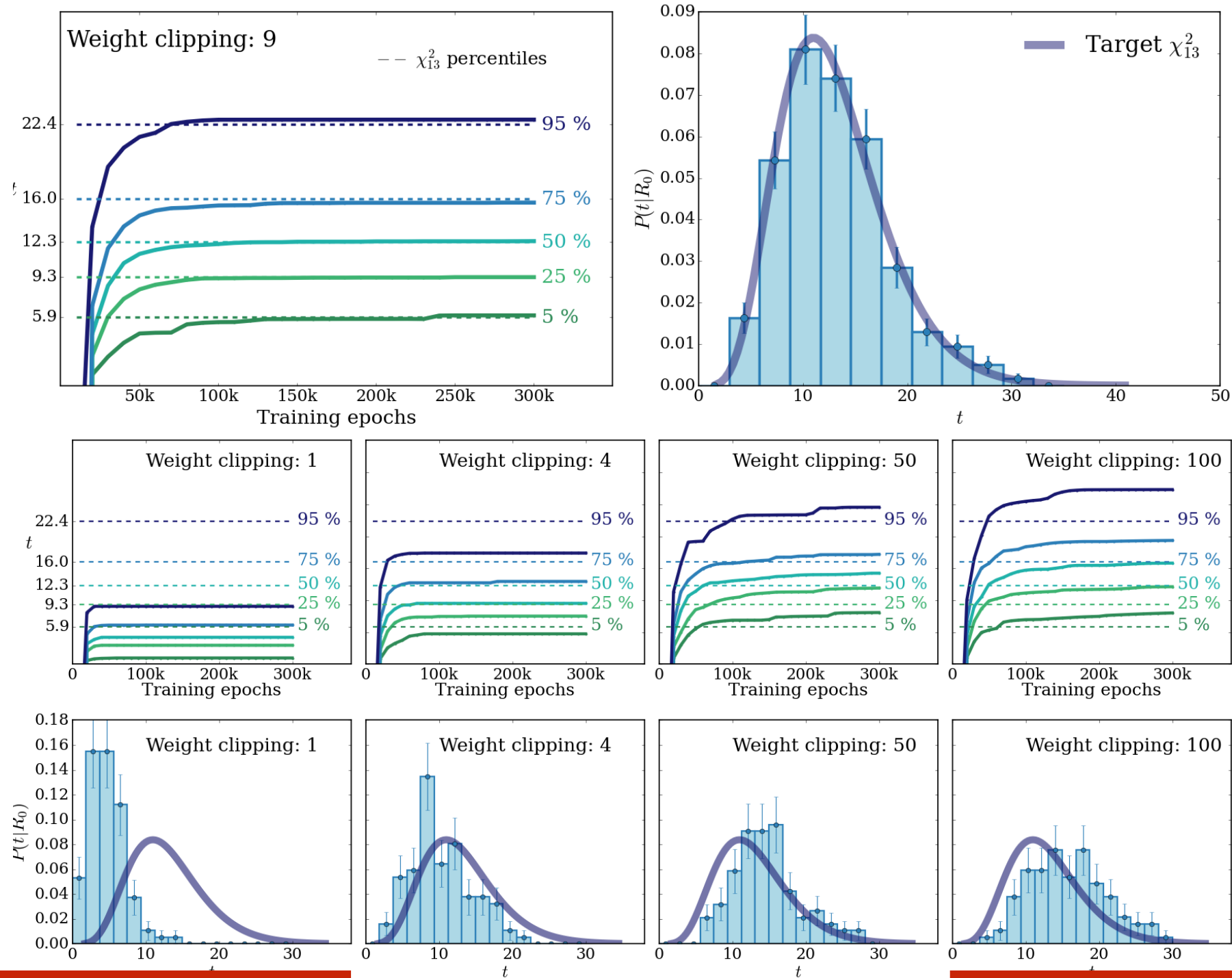
Provided statistics is large relative to fitted model “complexity”

... or, which is the same ...

Provided model is “simple enough”, for given data statistics

- Asy. For. violation = sensitivity to low-statistics portion of dataset = overfitting
- Regularisation by Weight Clipping, that forbids sharp variations
- NN with too many parameters cannot be made χ^2 -compatible. Take largest allowed

Weight Clipping Selection

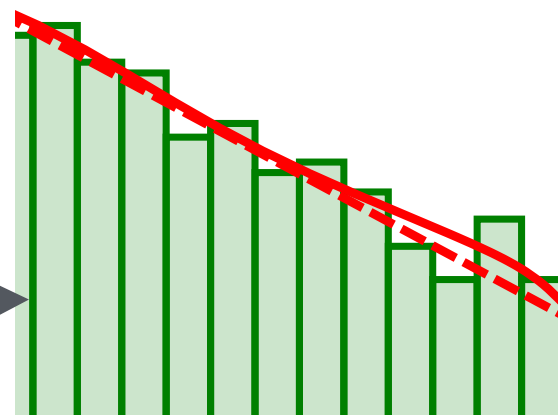
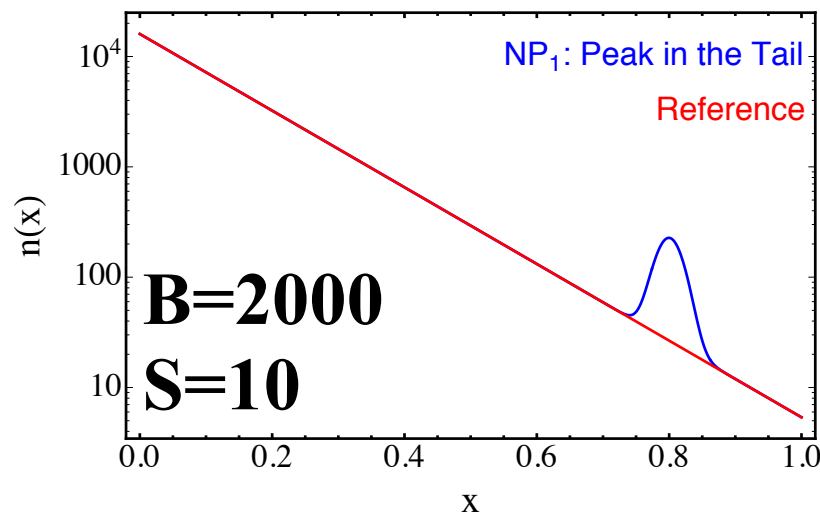


Asy. For. violation by fit
parameters boundary

Asy. For. violation by sensitivity
to sparse data points

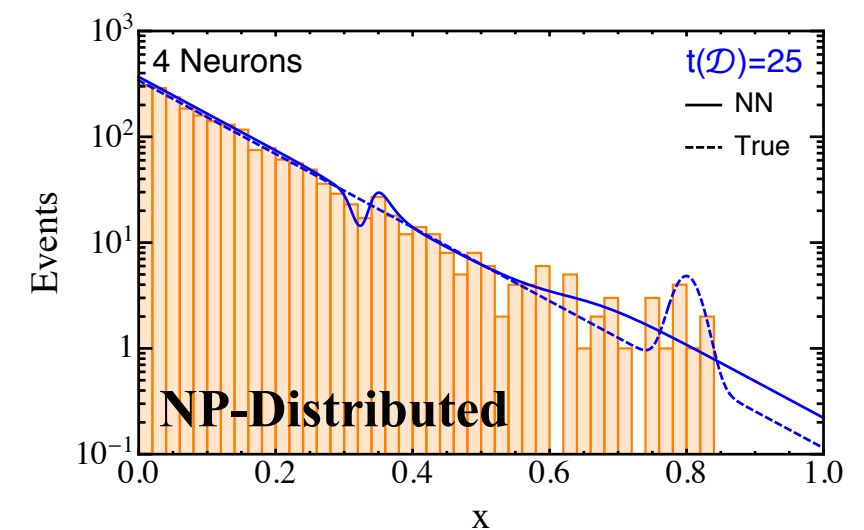
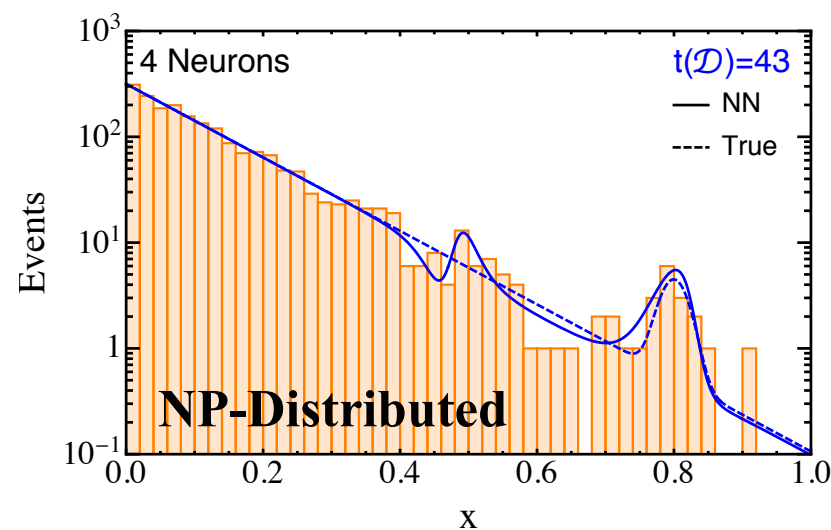
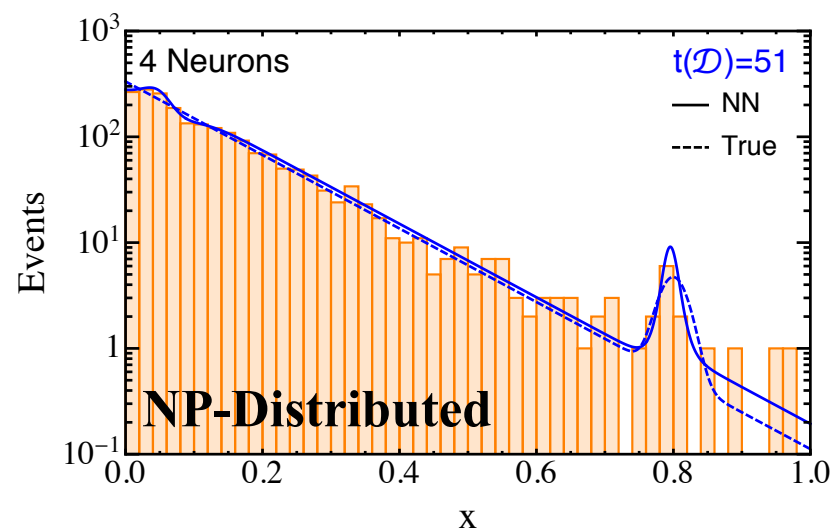
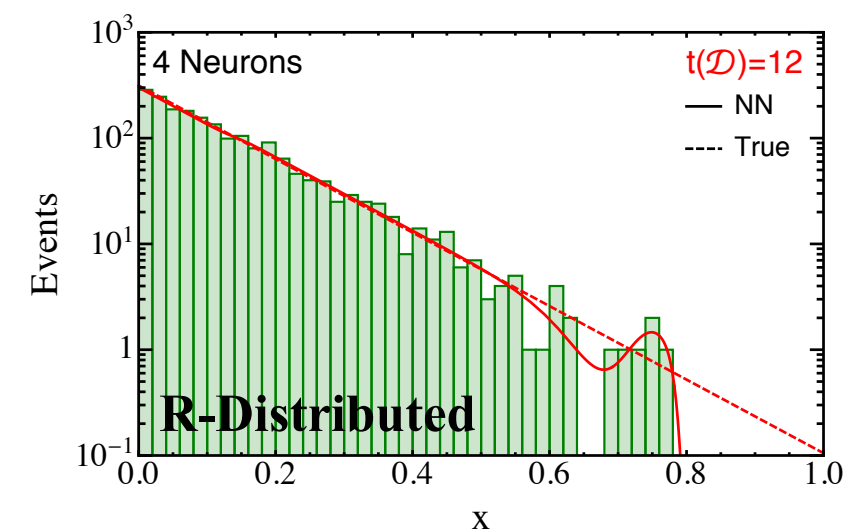
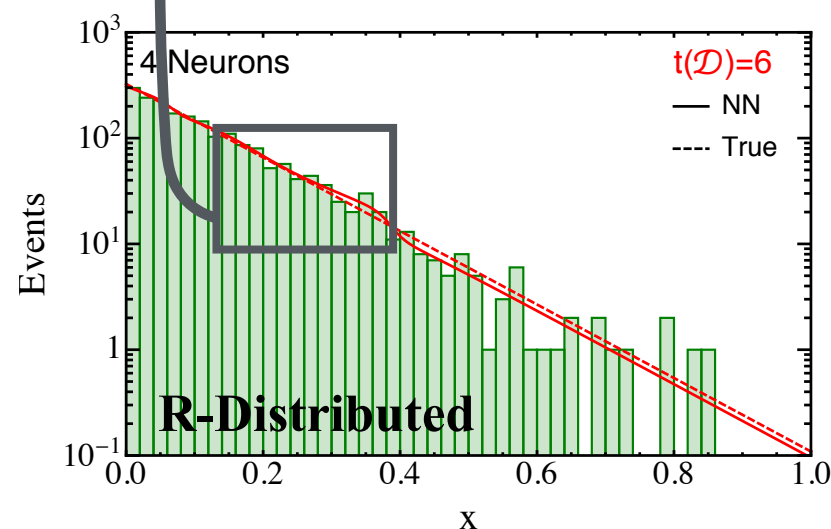
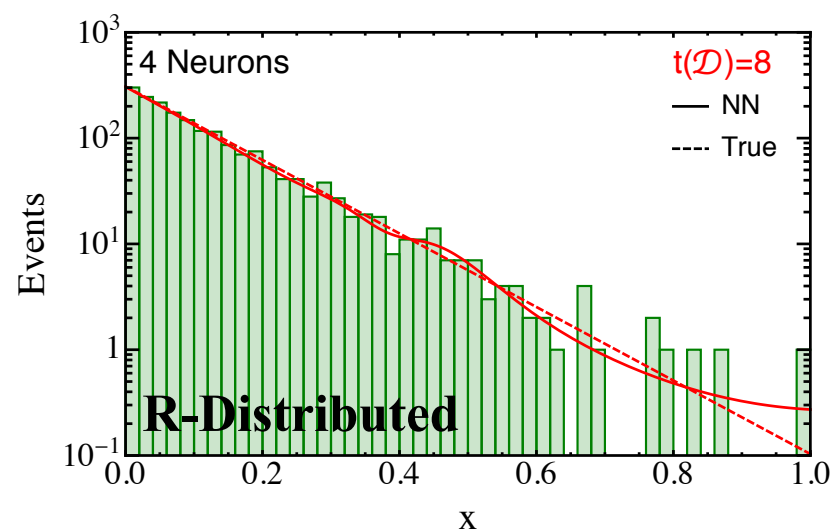
Illustrating Performances

(Simple 1d example with exponential Reference)



Bins: Non-discrepant data fluctuations wash out reach

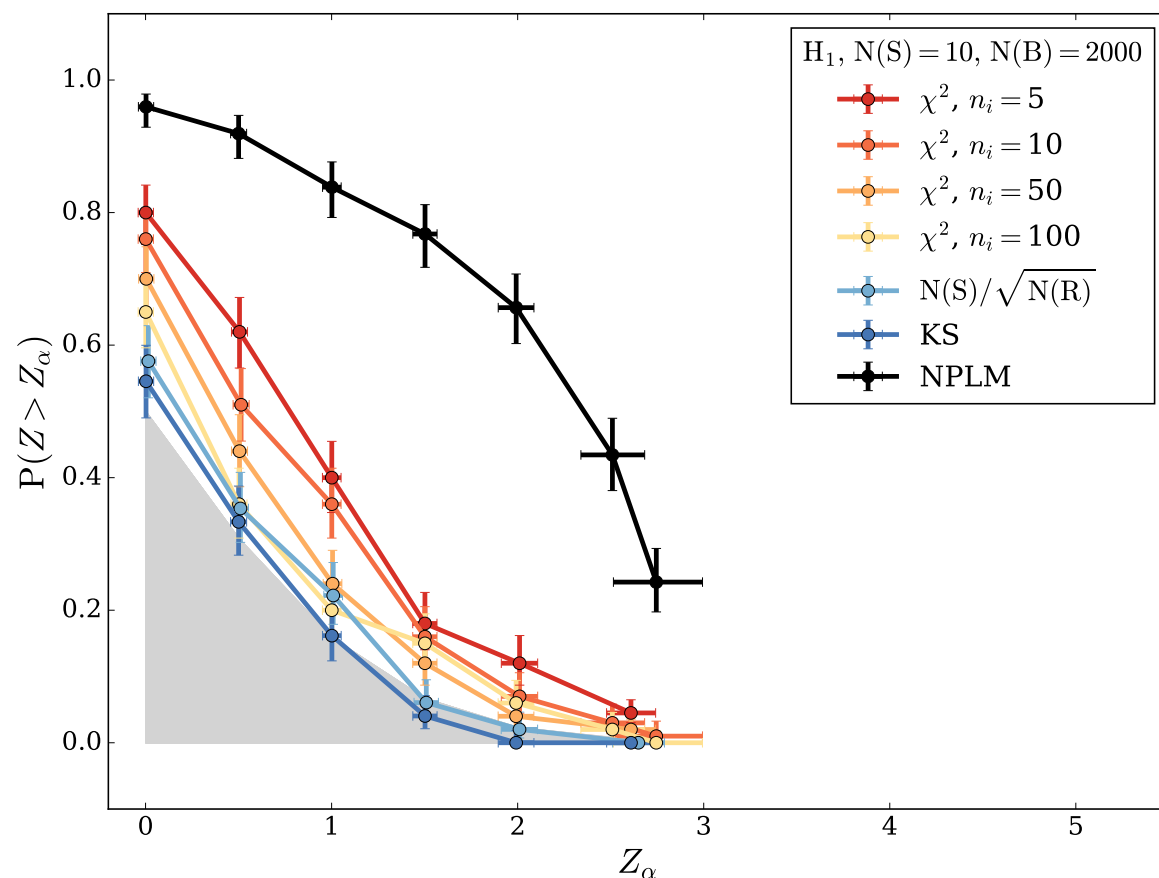
NN: Smooth curve. Can handle non-discrepant data



Illustrating Performances

(Simple 1d example with exponential Reference)

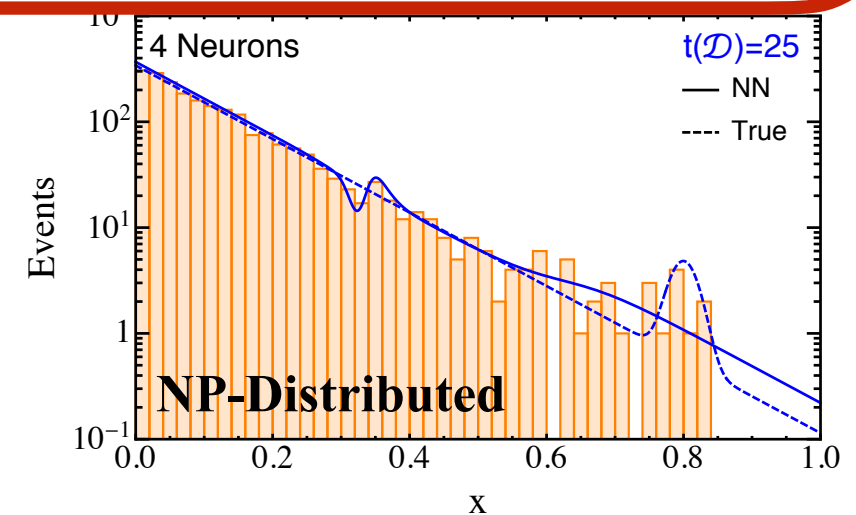
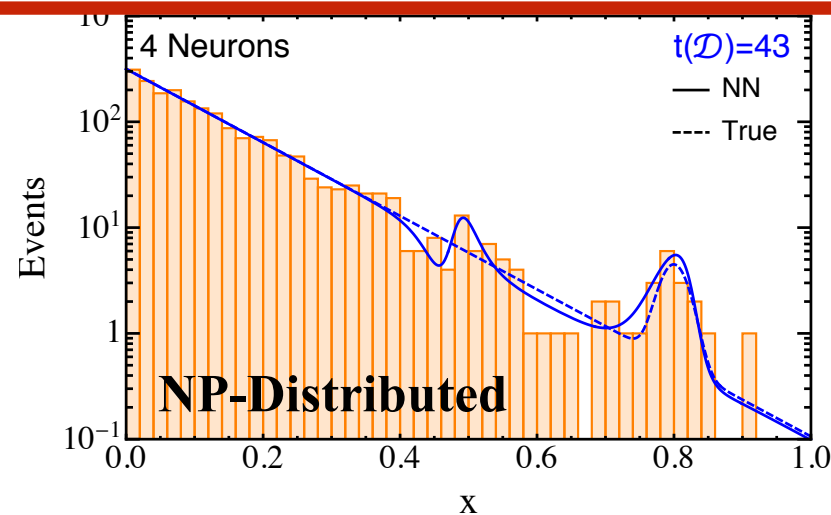
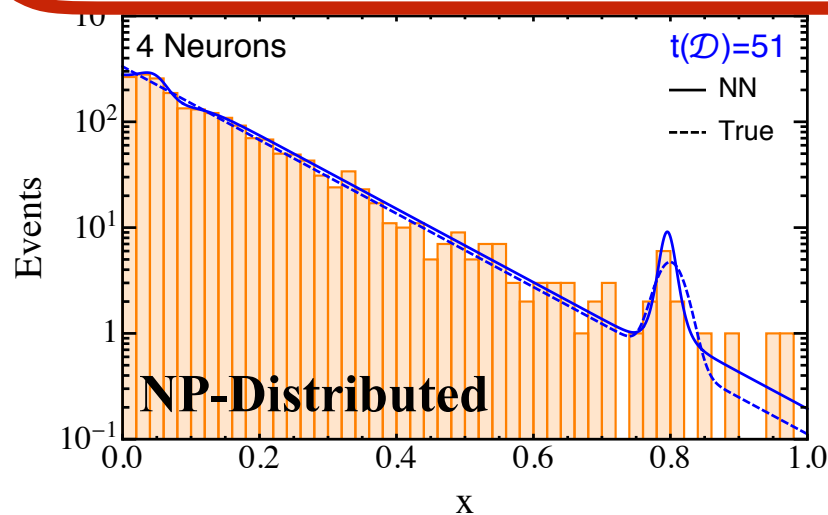
Probability to find evidence of R being wrong at some level of confidence.



We are better than binned χ^2 because our model has less parameters but same effective expressive power.

Same reason why bins are outdated as statistical models.

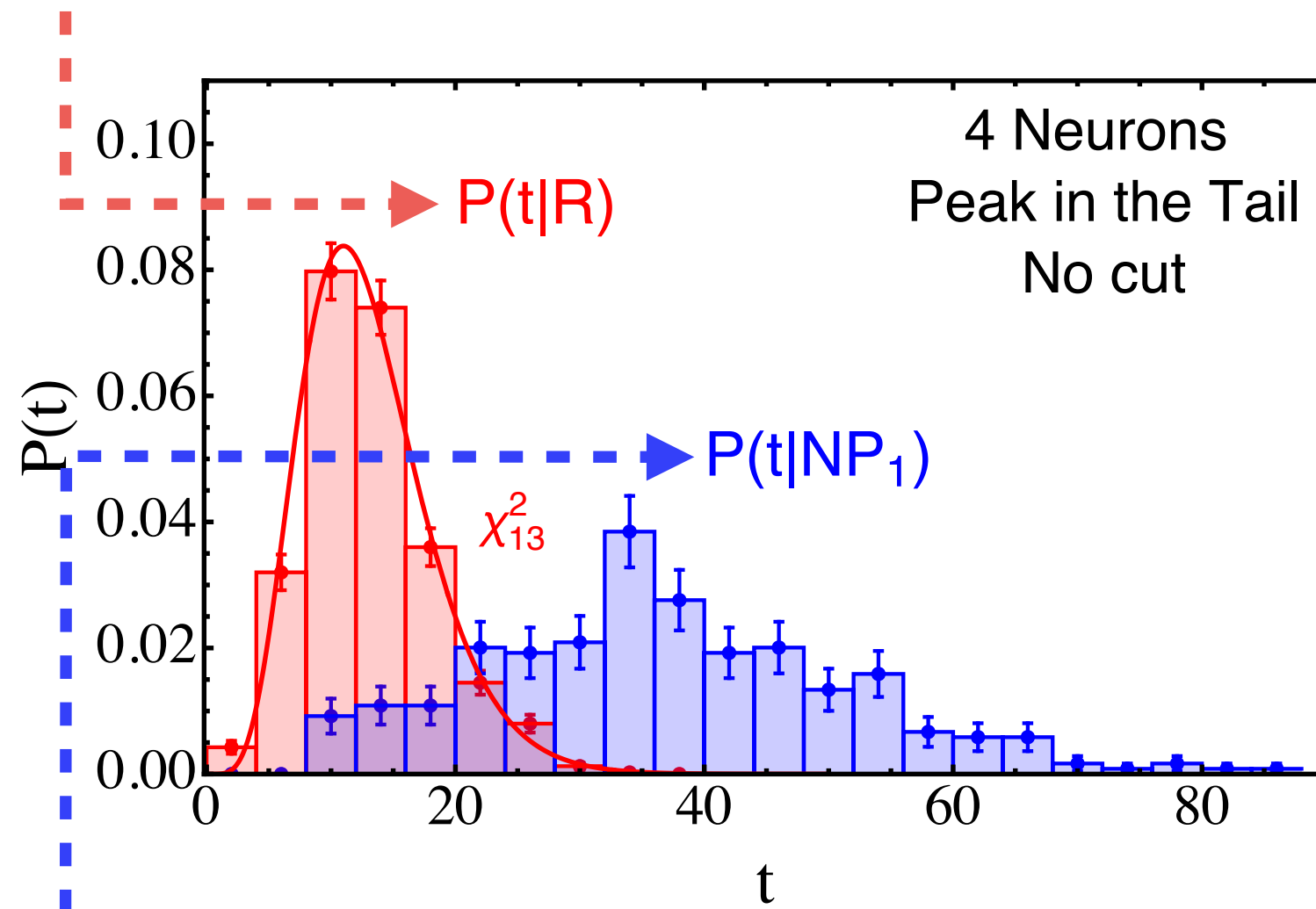
Gap to bins grows (exponentially) with (the curse of) dimensionality.



Illustrating Performances

(Simple 1d example with exponential Reference)

Distribution of the test statistic “t” in Reference Hypothesis



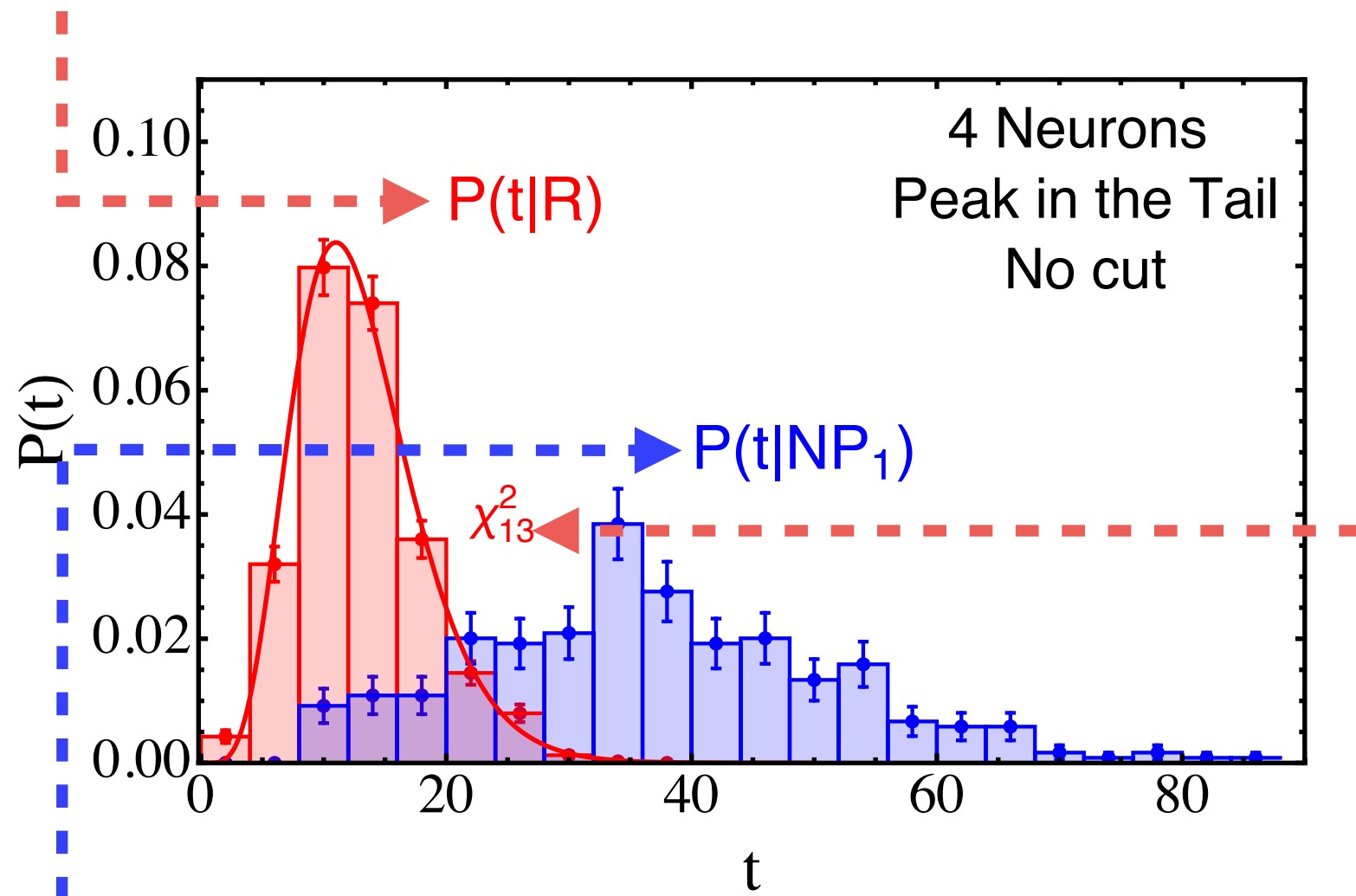
Distribution of “t” in one New Physics Model Hypothesis

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

Illustrating Performances

(Simple 1d example with exponential Reference)

Distribution of the test statistic “t” in Reference Hypothesis



Notice agreement with **Wilks' Formula:**

Sufficiently **regularised networks** found to **behave as if their number of d.o.f. was equal to number of parameters.**

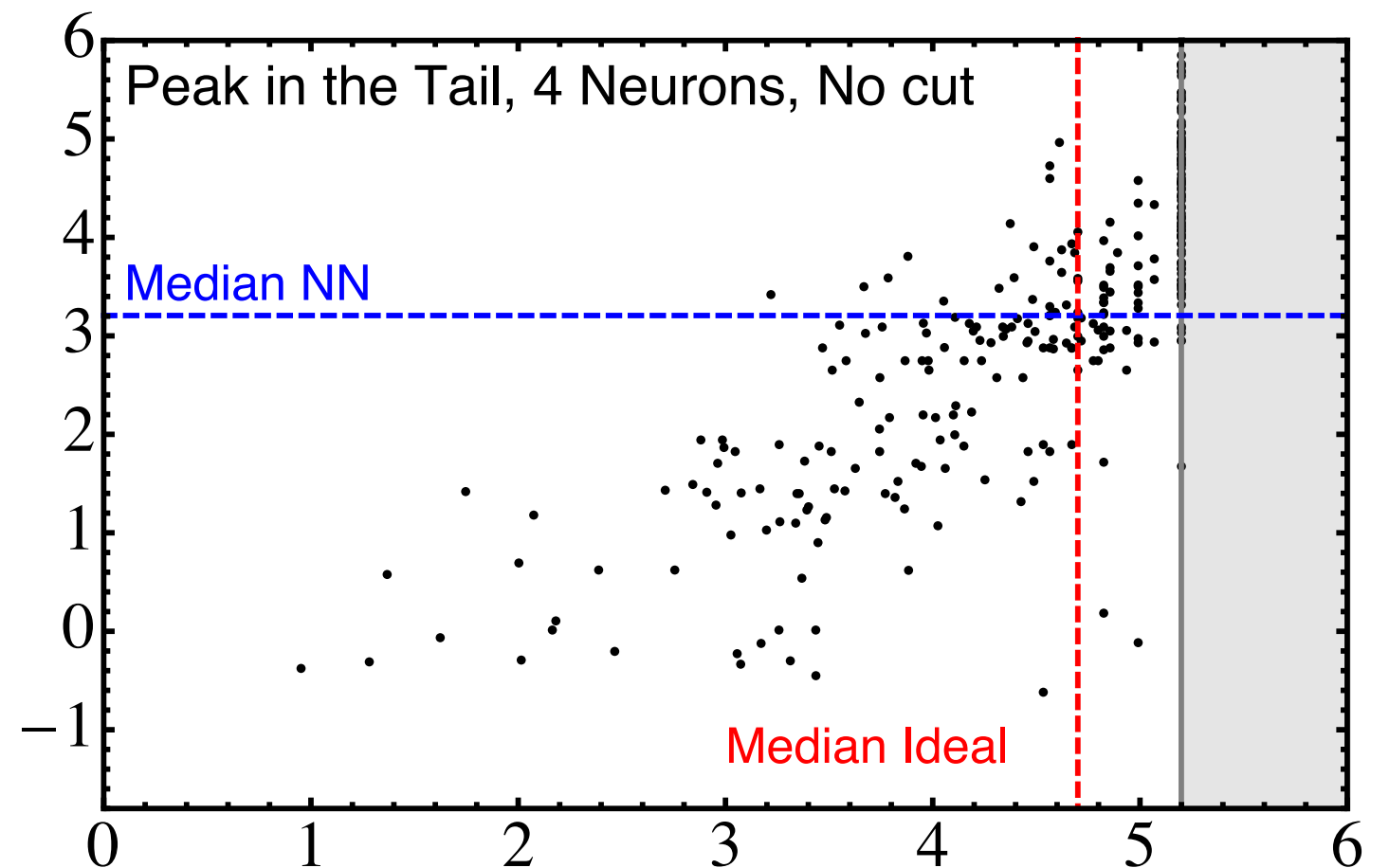
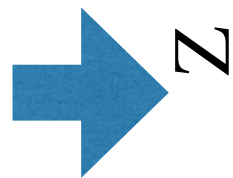
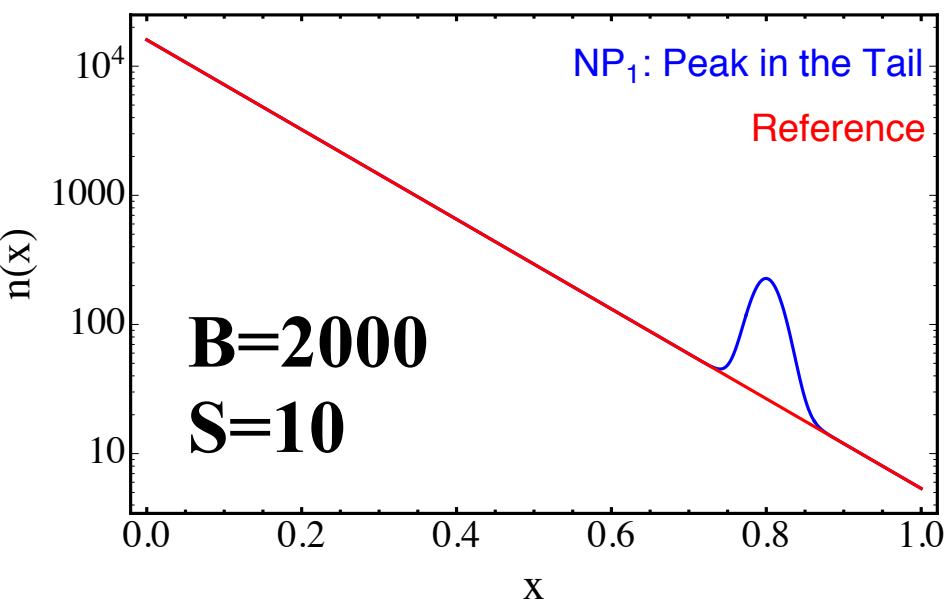
Theoretical reason mysterious

Distribution of “t” in one New Physics Model Hypothesis

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

Illustrating Performances

(Simple 1d example with exponential Reference)



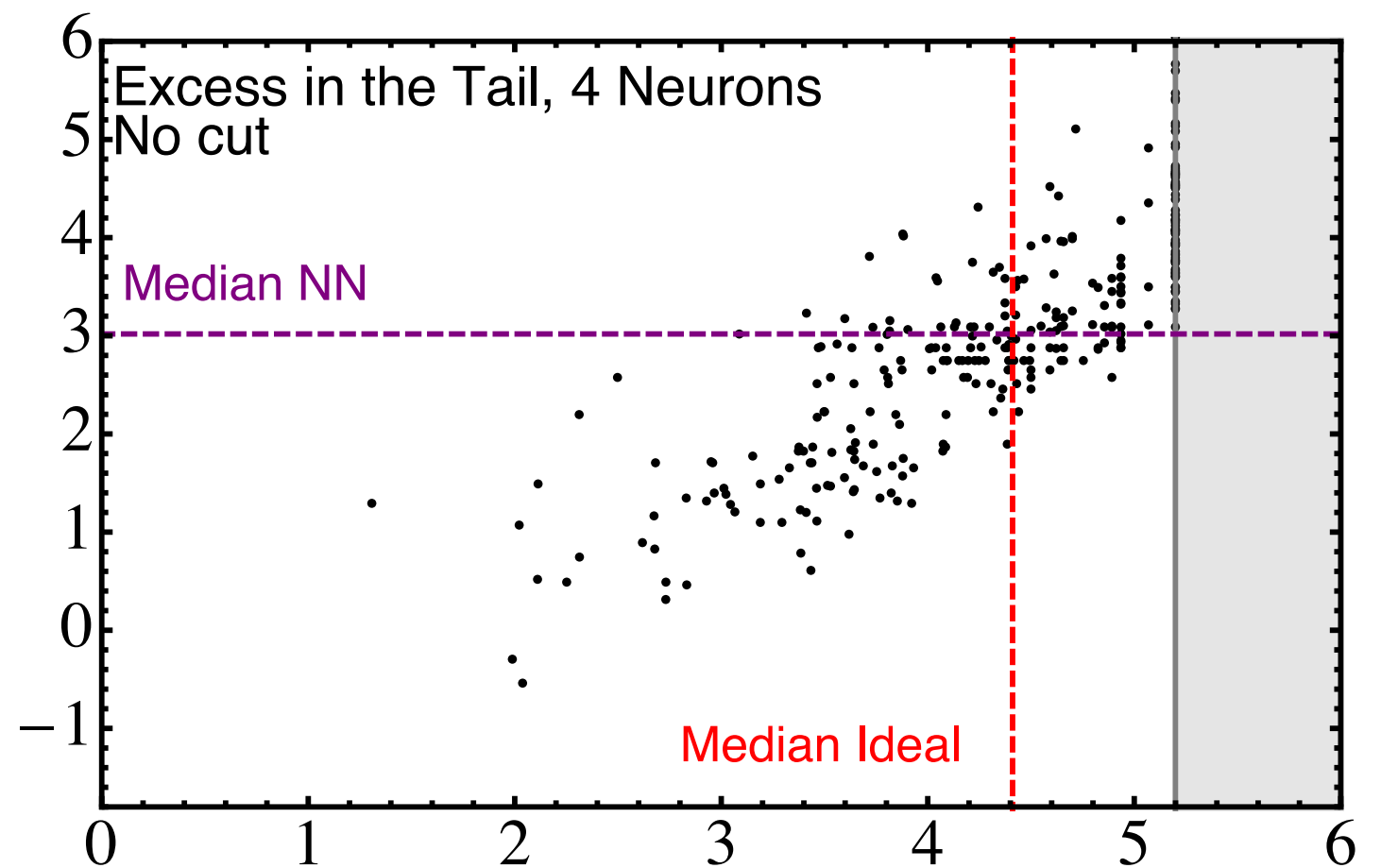
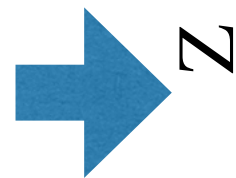
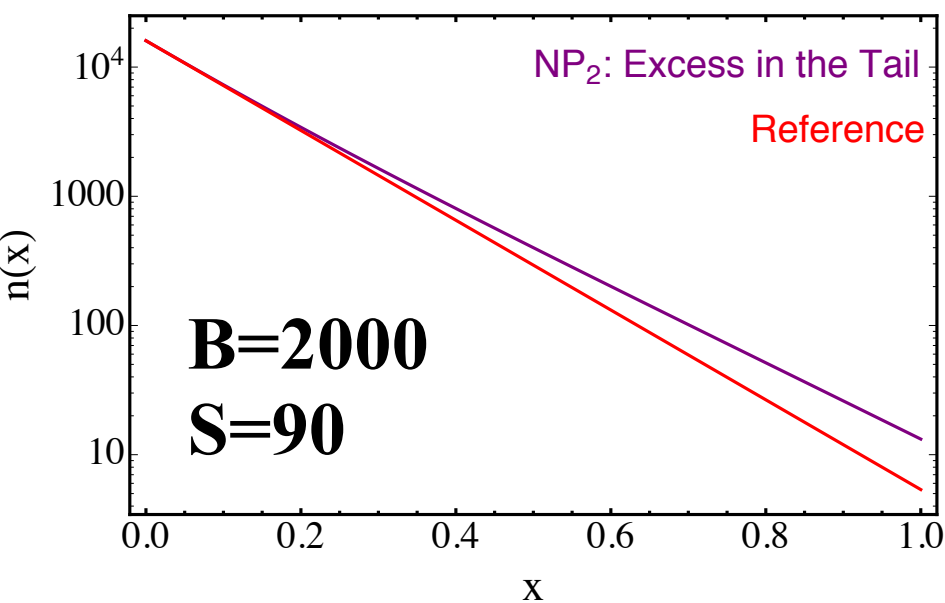
“Ideal Z-score”: Z_{id}

A “measure of dataset discrepancy”:

Z-score of optimal test for **NP1** model

Illustrating Performances

(Simple 1d example with exponential Reference)



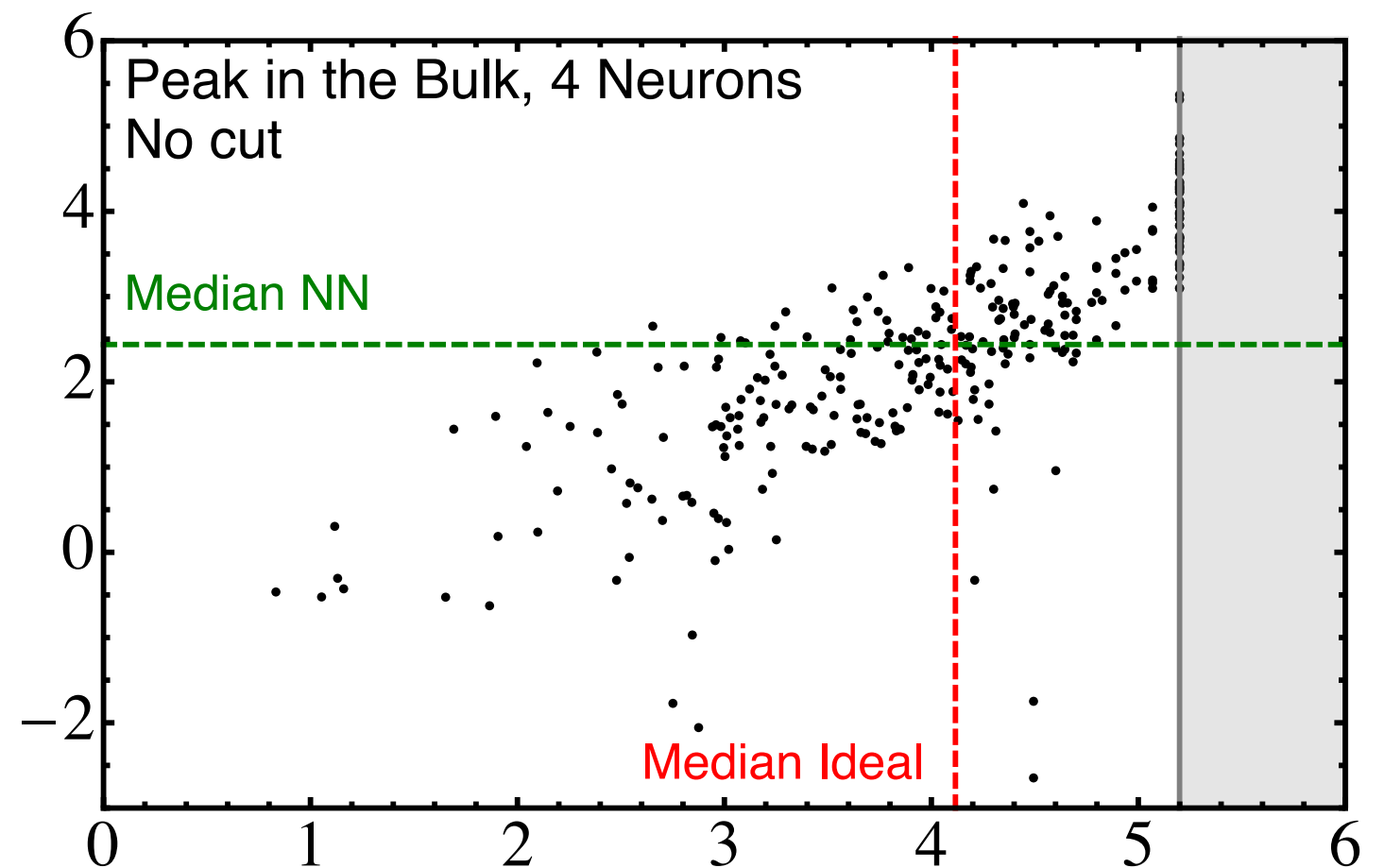
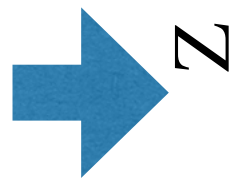
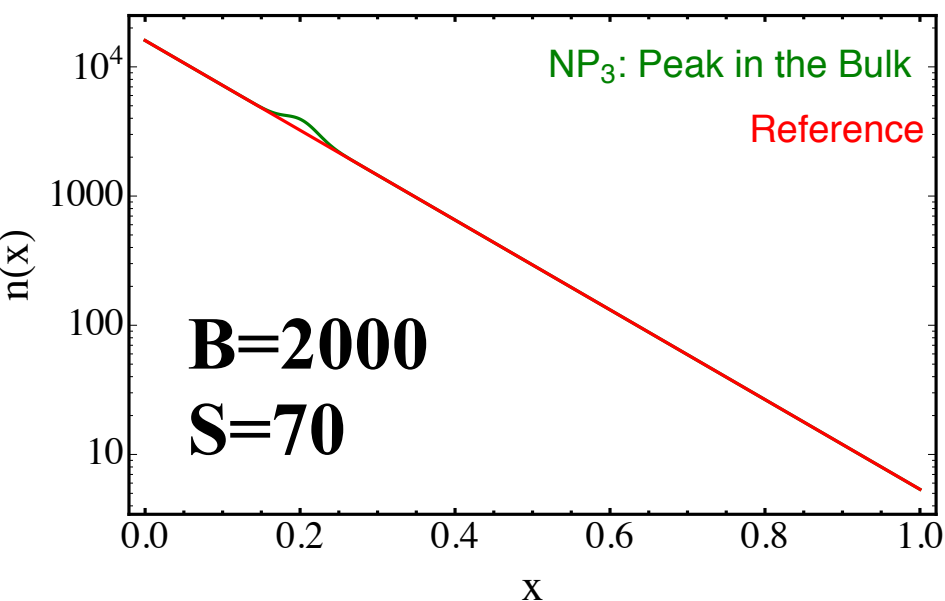
“Ideal Z-score”: Z_{id}

A “measure of dataset discrepancy”:

Z-score of optimal test for **NP2** model

Illustrating Performances

(Simple 1d example with exponential Reference)



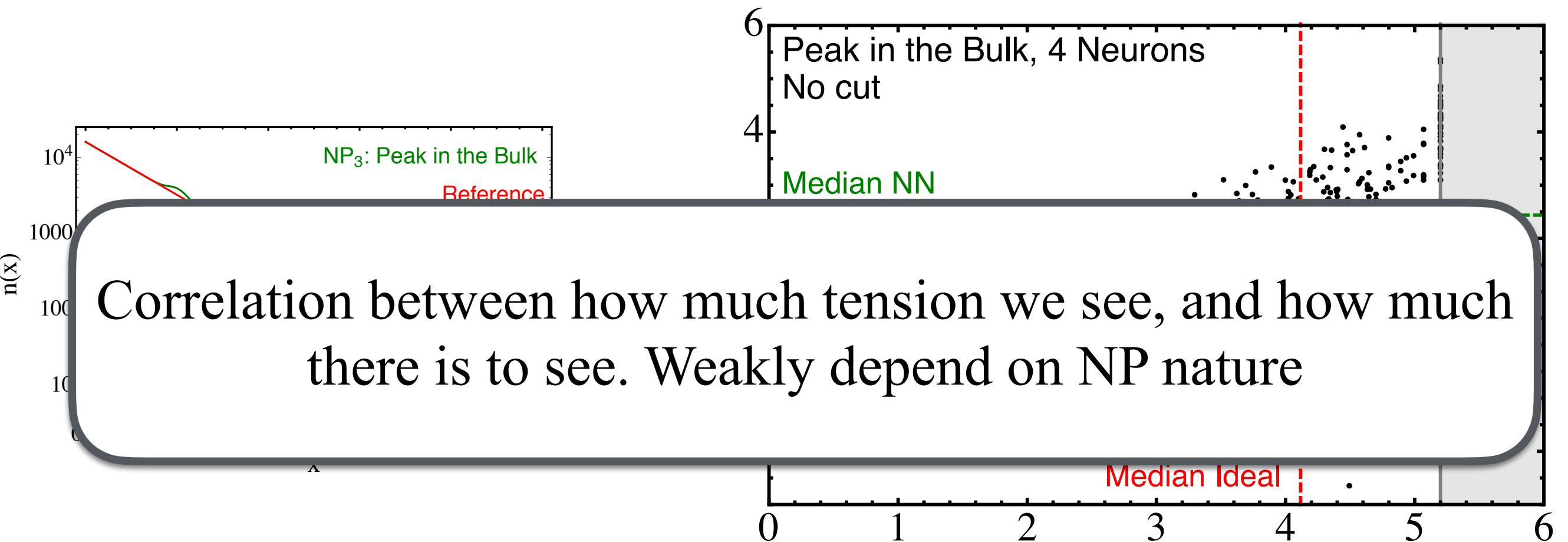
“Ideal Z-score”: Z_{id}

A “measure of dataset discrepancy”:

Z-score of optimal test for **NP3** model

Illustrating Performances

(Simple 1d example with exponential Reference)



“Ideal Z-score”: Z_{id}

A “measure of dataset discrepancy”:

Z-score of optimal test for **NP3** model

Imperfect Machine

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

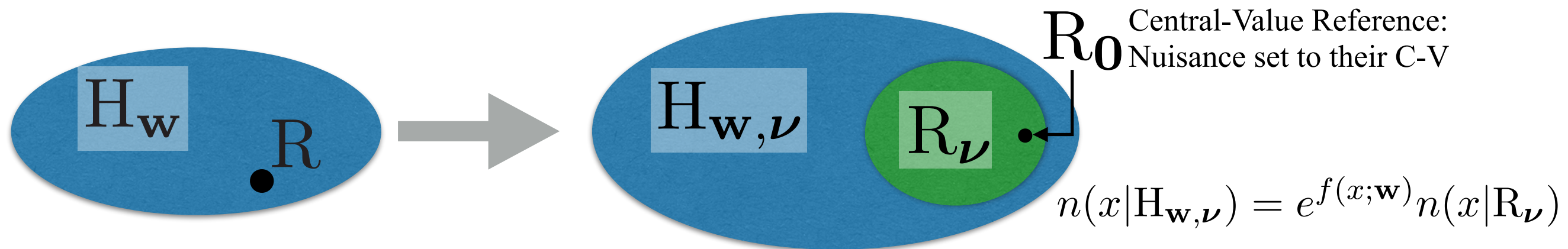
Reference Sample is an **imperfect** representation of SM

e.g., PDF/Lumi/Detector Modeling ...

Imperfections are **Nuisance Parameters**

Constrained by **Auxiliary Measurements**

Define a **composite** Reference hypothesis



Strategy conceptually unchanged.

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

$$= 2 \max_{\mathbf{w}, \nu} \log \left[\frac{\mathcal{L}(H_{\mathbf{w},\nu}|\mathcal{D})}{\mathcal{L}(R_0|\mathcal{D})} \cdot \frac{\mathcal{L}(\nu|\mathcal{A})}{\mathcal{L}(\mathbf{0}|\mathcal{A})} \right] - 2 \max_{\nu} \log \left[\frac{\mathcal{L}(R_{\nu}|\mathcal{D})}{\mathcal{L}(R_0|\mathcal{D})} \cdot \frac{\mathcal{L}(\nu|\mathcal{A})}{\mathcal{L}(\mathbf{0}|\mathcal{A})} \right] = \tau(\mathcal{D}, \mathcal{A}) - \Delta(\mathcal{D}, \mathcal{A})$$

Implementation slightly more complex

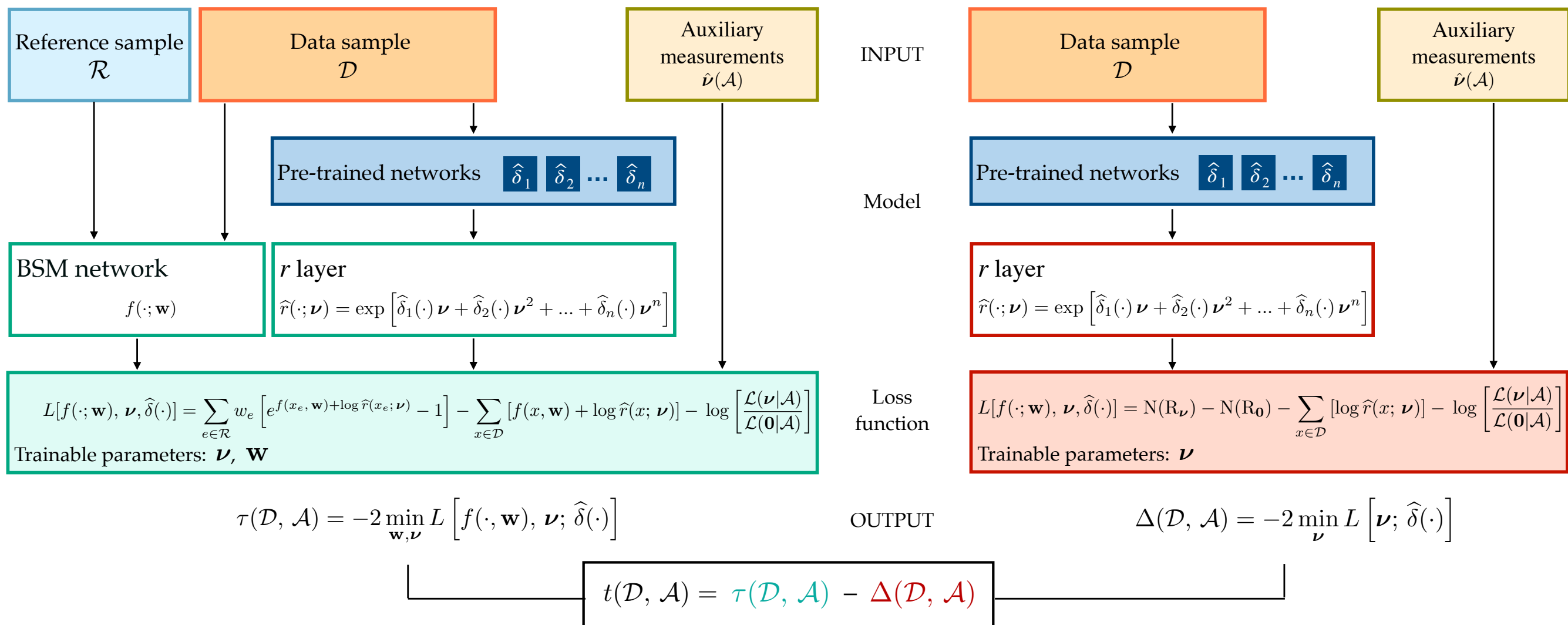
Imperfect Machine

New Physics Learning Machine (NPLM)

Including systematic uncertainties

τ term

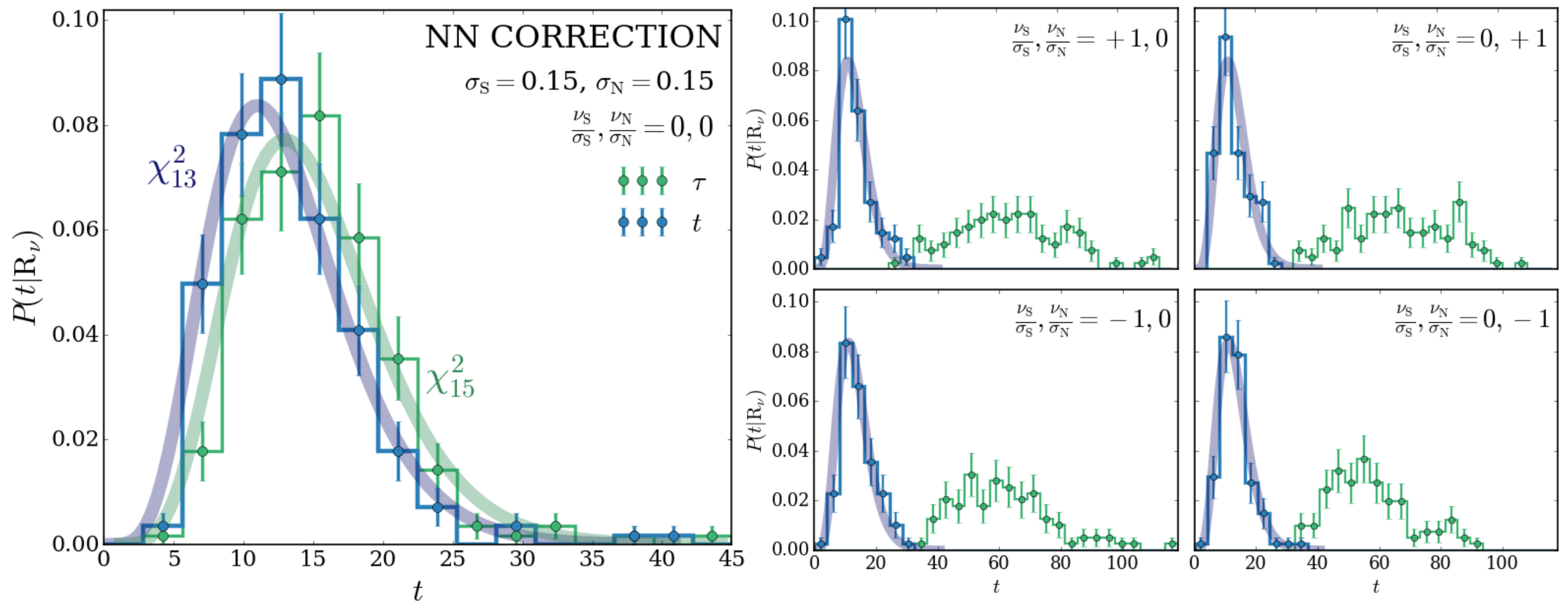
Δ term



An Imperfect Machine at Work

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

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



t = Tau-Delta independent of true nuisance value
this is essential for a feasible test

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**.

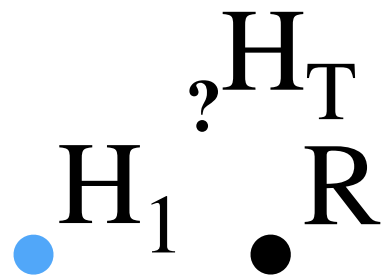
This is a tremendously hard gof problem!

BSM is tiny departure from SM, or large in tiny prob. region

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

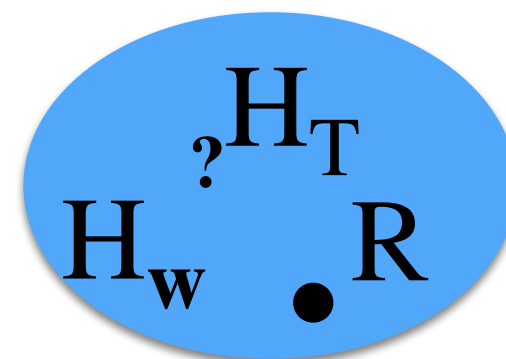
Our generic discussion ...

Simple vs Simple
hypothesis test



- Optimal approach provided by **Neyman–Pearson Lemma**
- Optimal answer to very specific question: **test has no or very limited power if truth $\neq H_1$**

Simple vs Composite
hypothesis test



- No Optimal solution. But, **Maximum Likelihood Ratio** is **Good solution**
- Answers a more general question. It has **some power if truth is in H_w** . But, larger H_w = less power

The LHC g.o.f. challenge

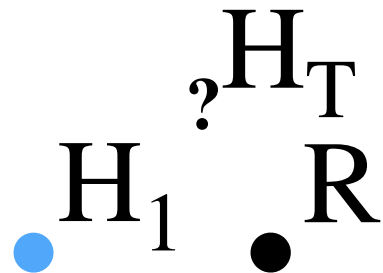
By analysing the LHC data, we would like to find evidence of **failure of the SM theory**, suggesting need of **BSM**.

This is a tremendously hard gof problem!

BSM is tiny departure from SM, or large in tiny prob. region
Affecting few (unknown) observables over ∞ many we can measure

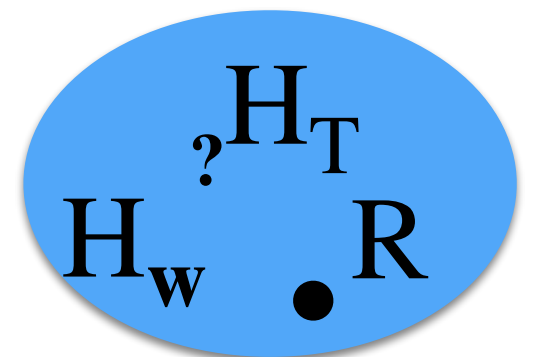
Our generic discussion ... perfectly matches LHC practice:

Model-dependent
BSM searches



- Optimise sensitivity to **one specific BSM model**
- Fail to discover other models.
What if the right theoretical model is not yet formulated?

Model-independent
searches



- Could reveal **truly unexpected** new physical laws.
- No hopes to find Optimal strategy.
But we must aim at a Good strategy

Towards LHC

Our proposed strategy is fully defined, including:

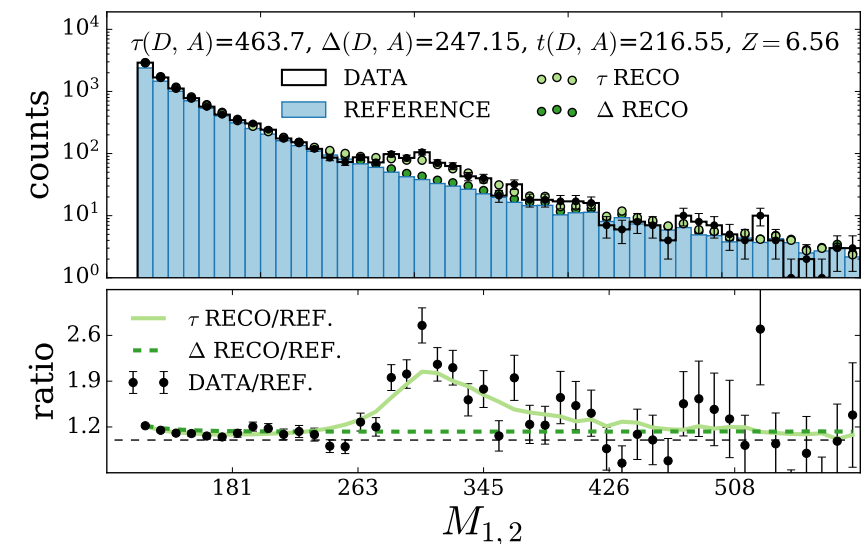
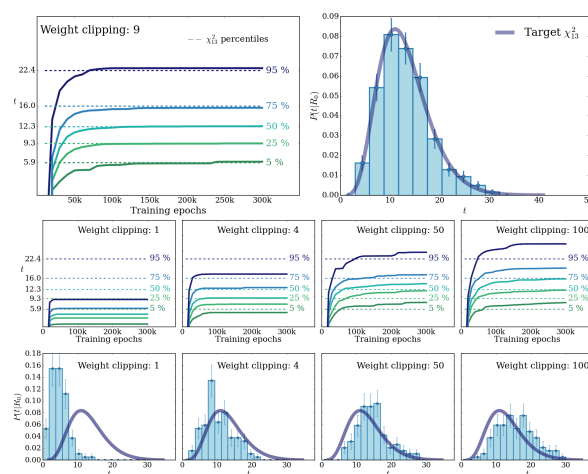
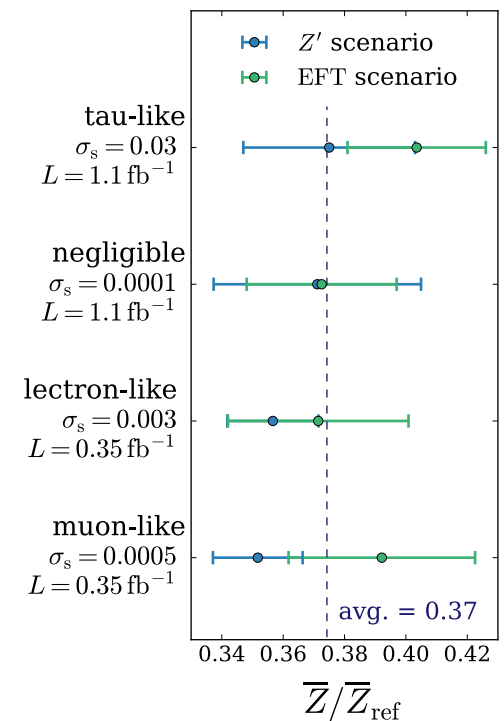
- Hyperparameters and regularisation selection
- Systematic approach to Reference mis-modelling

Validated on problems of realistic scale of complexity:

- 2-body final state with uncertainties ($d = 5$)
- 1l+MET “SUSY” ($d = 8$)
- Heavy Higgs to WWbb ($d = 21$)

Results in summary:

- model-selection strategy converges
- sensitivity to resonant or non-resonant NP
- “uniform” response to NP of different nature
- trained network reconstruct NP



Backup