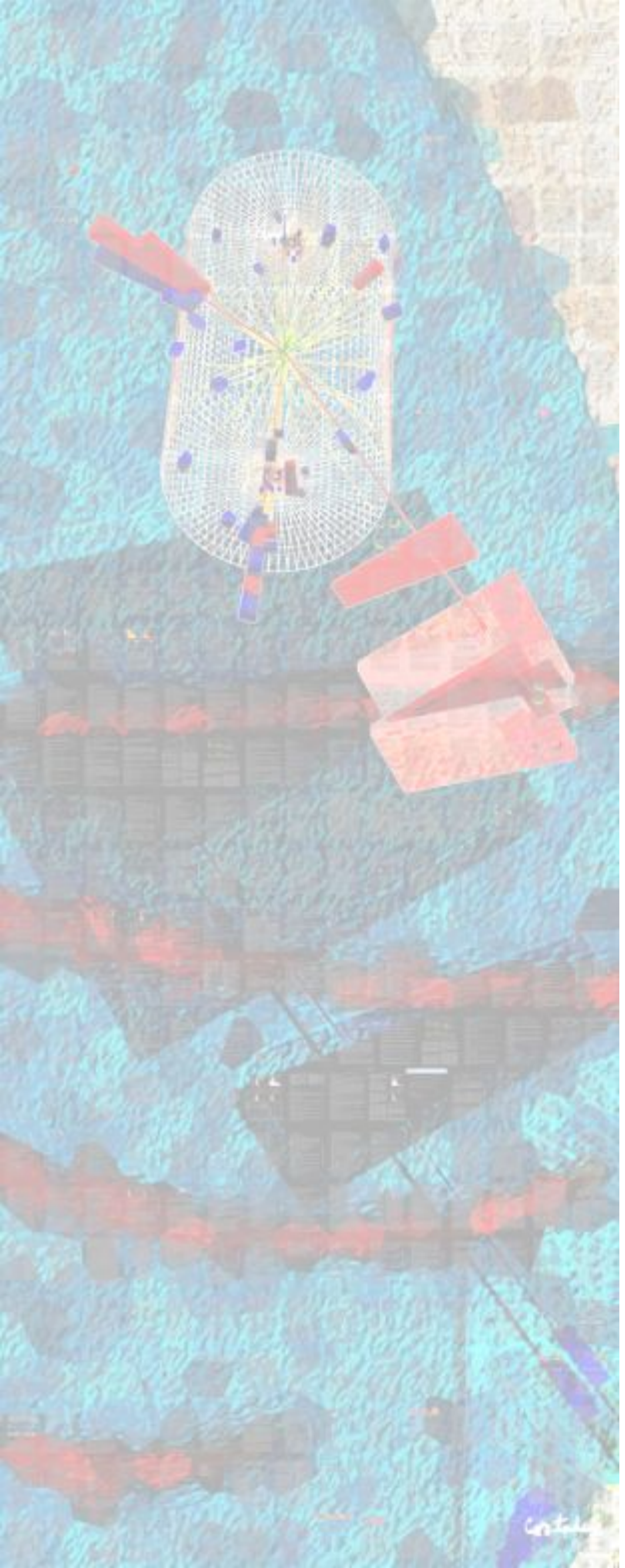


https://github.com/jonathon-langford/aims-inference-2026

→ 2_inference_with_classifiers

Inference with classifiers

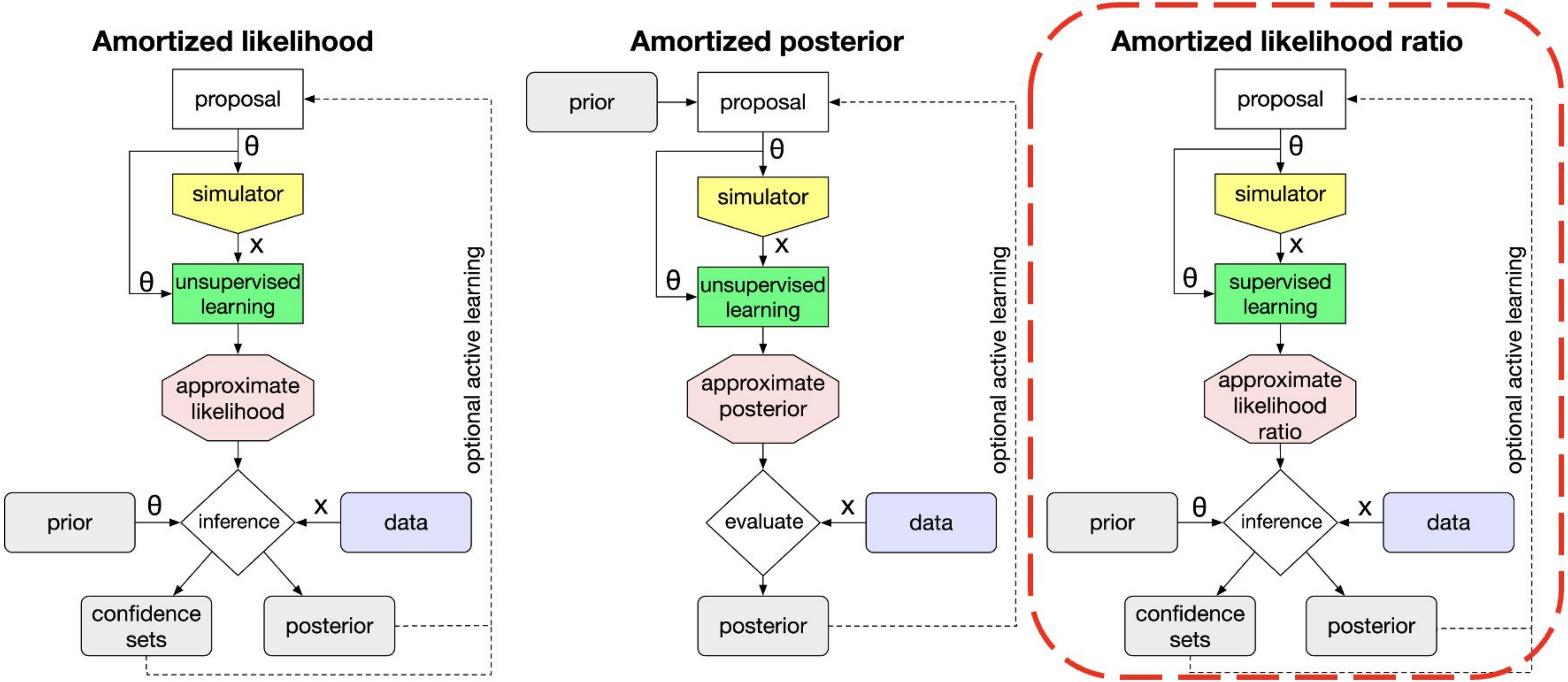
AIMS 2026

Jon Langford

16th Feb 2026

Schmidt Sciences

3 families of amortised inference



Imperial College London

Adapted slide from Callum

Cranmer et al., 2020

Lecture contents & ILOs

This lecture will demonstrate how to use a simple machine learning (ML) classifier for simulation-based inference (SBI). This will help you bridge the gap between ML and some fundamental concepts in statistics.

We will cover the following topics:

- Introduction to frequentist inference and simulation-based inference (SBI)
- Inference with a simple ML classifier
- Hypothesis testing
- Parameter estimation with parametric classifiers

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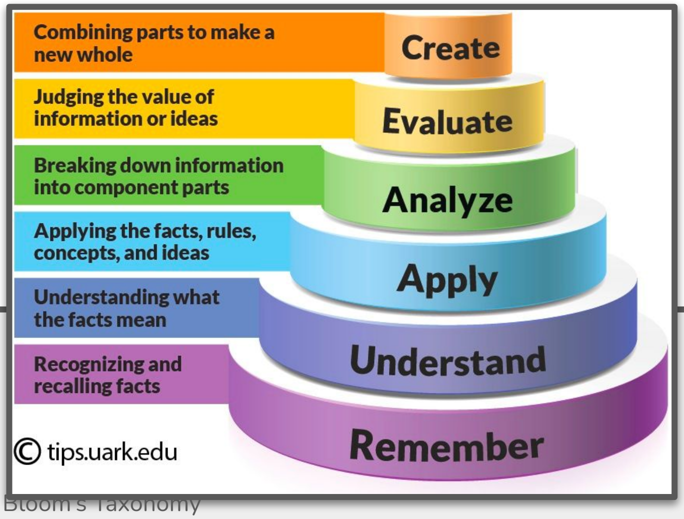

Bloom's Taxonomy

By the end of the lecture you will be able to...

- **Understand** the need for simulation-based inference in the modern era of science
- **Understand** how to use a simple ML classifier to learn the likelihood-ratio and **apply** this knowledge to perform a hypothesis test on a research problem with an unknown likelihood
- Extend the approach to learning the conditional likelihood-ratio via a parametric classifier and **apply** this to a parameter estimation problem. **Evaluate** the performance by comparing to the analytic solution

Likelihoods are key

- Likelihoods ("probability density") hold the key to inference
    - You perform an experiment N_{obs} times and observe the dataset $\mathcal{D} = \{x_i\}_{i=1}^{N_{\text{obs}}}$, where $x \in \mathbb{R}^d$
    - You have a **model** (defined by parameters θ) that describes the data: $p(x|\theta)$

$$\boxed{p(\mathcal{D}|\theta) = \prod_{x_i \in \mathcal{D}}^{N_{\text{obs}}} p(x_i|\theta)}$$

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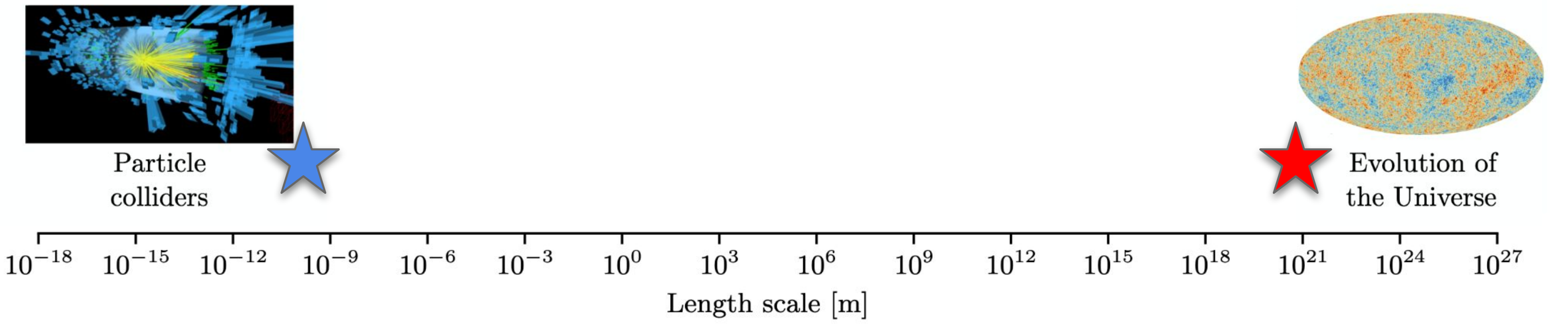
- **Simple example:** x is tossing a coin. Define θ as probability of throwing a HEAD:

$$\boxed{\begin{aligned} p(\text{HEADS}|\theta) &= \theta \\ p(\text{TAILS}|\theta) &= 1-\theta \end{aligned}}$$

- We throw a coin 5 times and get the sequence $\mathcal{D} = \{x_i\}_{i=1}^{N_{\text{obs}}}$ = (H, T, T, H, T)
  - First assume coin is fair (**Null hypothesis**, $\mathcal{H}_0$) i.e. $\theta = 0.5$ $\rightarrow p(\mathcal{D}|\theta = 0.5) = 0.5 \cdot (1-0.5) \cdot (1-0.5) \cdot 0.5 \cdot (1-0.5) = 0.5^5 \approx 0.031$
  - **Alternative hypothesis** ($\mathcal{H}_1$) for a biased coin e.g. $\theta = 0.7 \rightarrow p(\mathcal{D}|\theta = 0.7) = 0.7 \cdot (1-0.7) \cdot (1-0.7) \cdot 0.7 \cdot (1-0.7) \approx 0.013$
  - Our data prefers $\mathcal{H}_0$ to $\mathcal{H}_1$ i.e. **we have used the likelihood to infer something about θ**
- Comparison (ratio) of likelihoods is a key concept in statistical inference…

Inference paradigms

- How to use likelihood $p(\mathcal{D}|\theta)$ to infer parameters θ ?



Frequentist inference

$$t = -2\ln\left(\frac{p(\mathcal{D}|\theta)}{p(\mathcal{D}|\theta_0)}\right)$$

Bayesian inference

$$p(\theta|\mathcal{D}) = \frac{p(\mathcal{D}|\theta)p(\theta)}{p(\mathcal{D})}$$

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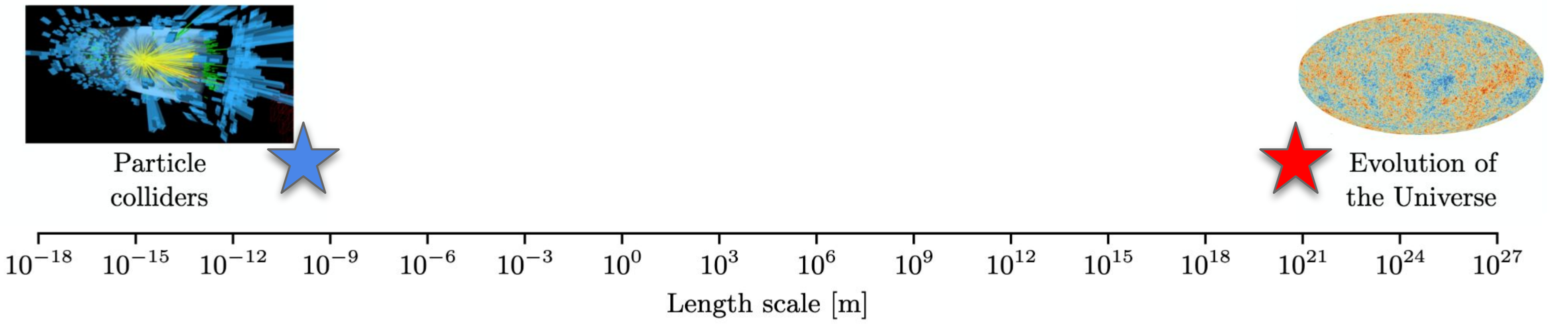

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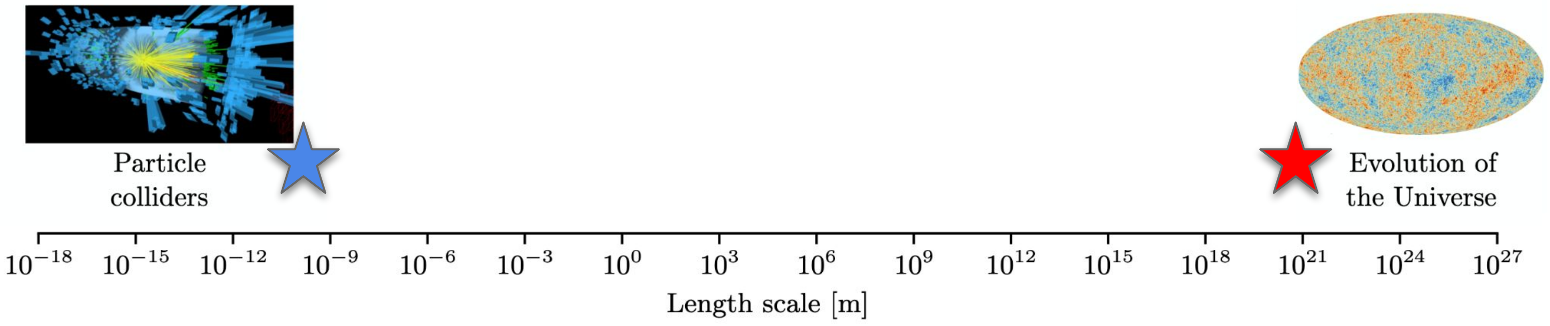

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- Interpretation over hypothetical repetitions of the experiment

- Key takeaways:
  - Define a **test-statistic (t)** = a number (score) to summarise **how compatible the data is with $\boldsymbol{\theta}$ (vs $\boldsymbol{\theta}_0$)**
  - Neyman Pearson Lemma: **"likelihood ratio is the most powerful test-statistic"**
    - Log-likelihood ratio: $\prod_{x_i\in\mathcal{D}}^{N_{\text{obs}}} p(x_i|\theta) \longrightarrow \sum_{x_i\in\mathcal{D}}^{N_{\text{obs}}} \ln p(x_i|\theta)$. Factor of -2 for Wilks' Theorem (see later)

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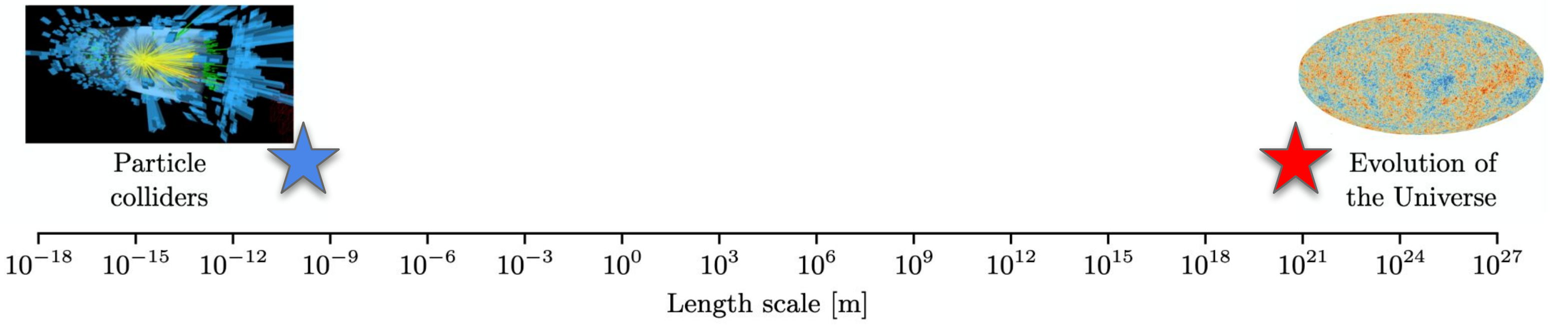

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- Let's see this in action for the simple hypothesis test example on the previous slide...

Frequentist hypothesis testing

- Simple two-class hypothesis test: $\boxed{t = -2\ln\left(\frac{p(\mathcal{D}|\mathcal{H}_1)}{p(\mathcal{D}|\mathcal{H}_0)}\right)}$ where $\mathcal{H}_0 : \theta = 0.5\,(\text{fair})$, $\mathcal{H}_1 : \theta = 0.7\,(\text{biased})$

- Interpretation over hypothetical repetitions of the experiment:
  - We need to build up distributions of the test-statistic under each hypothesis
  - Simulate the experiment (N=5 tosses) assuming $\mathcal{H}_0$ is true → Calculate t
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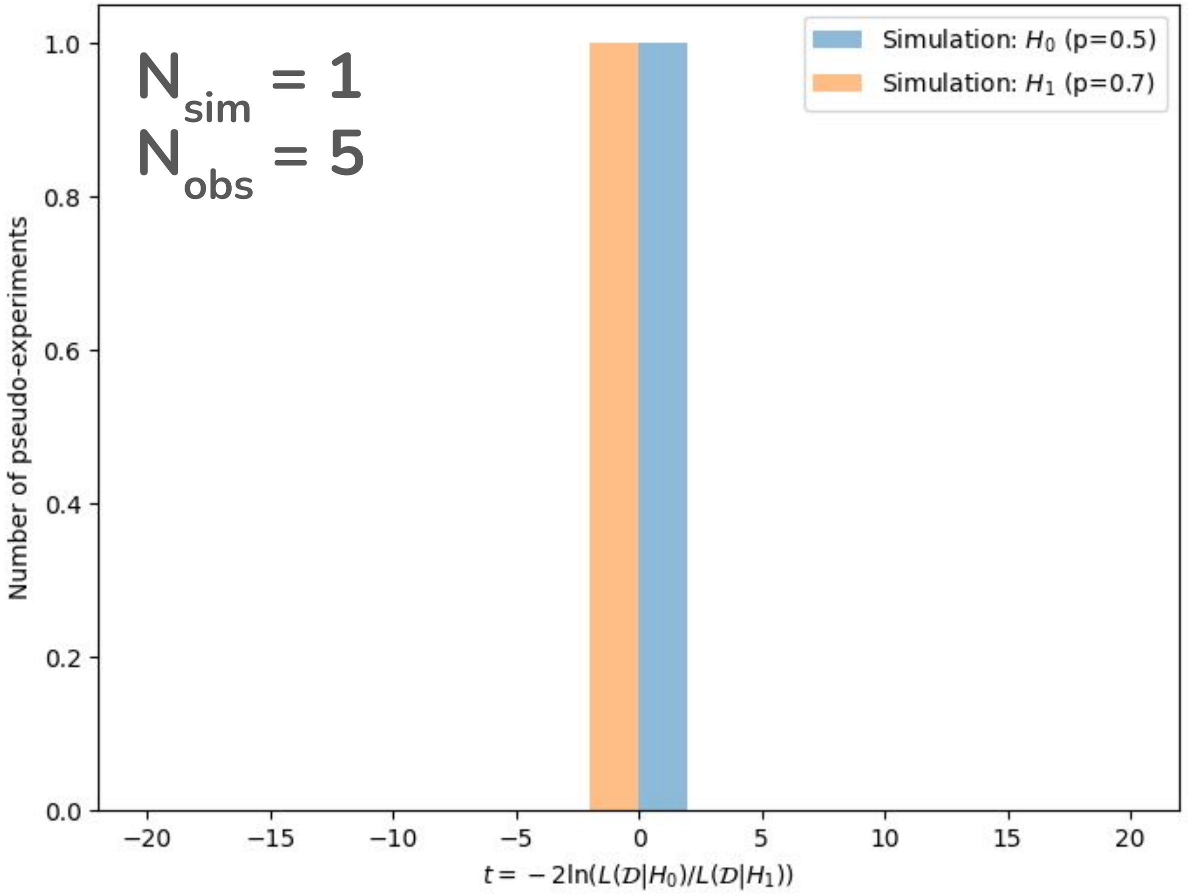

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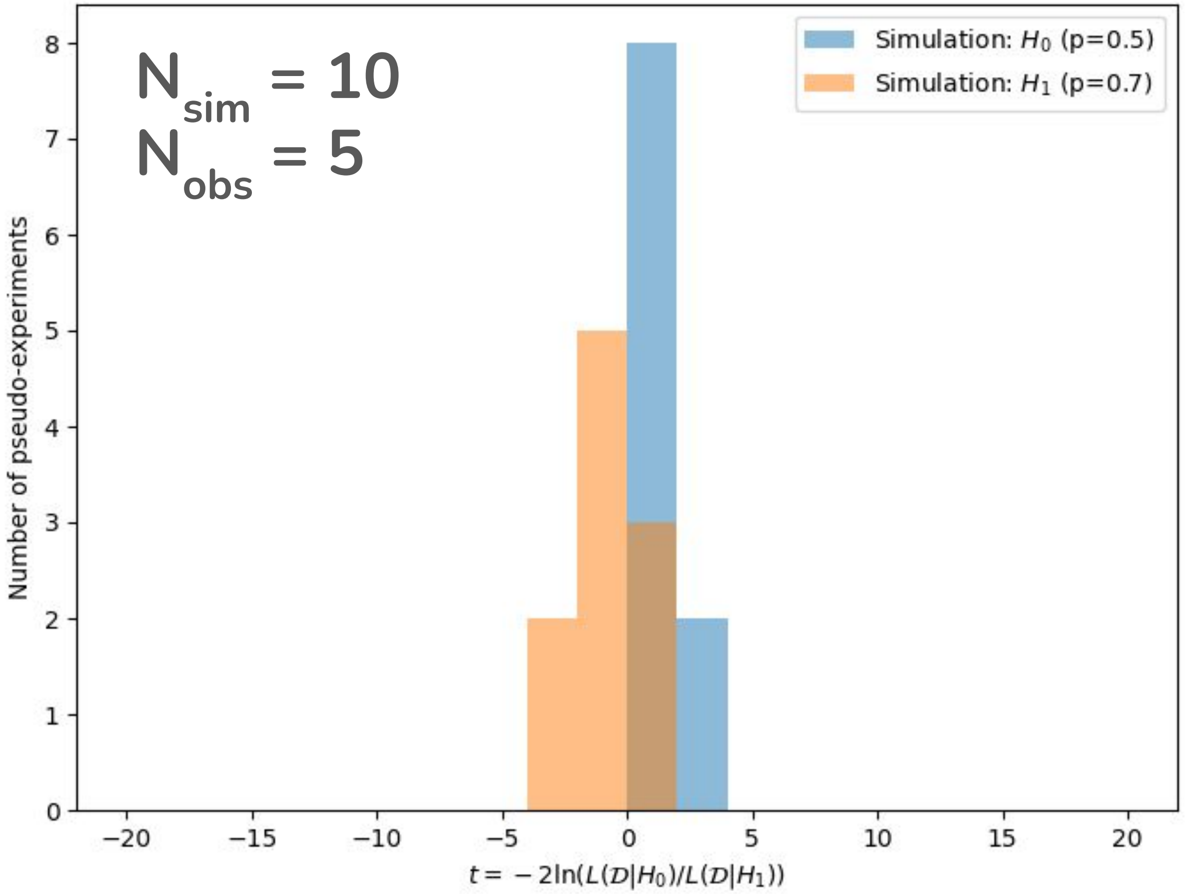

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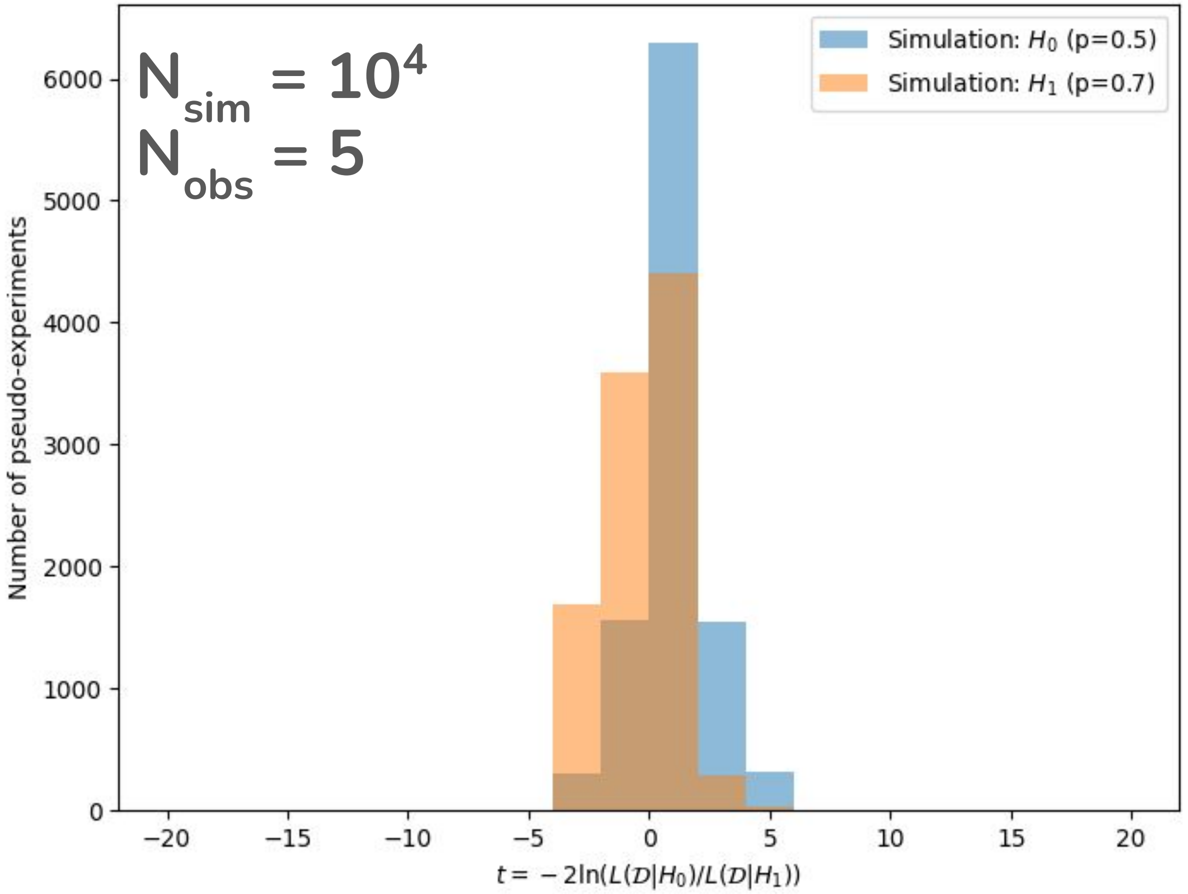

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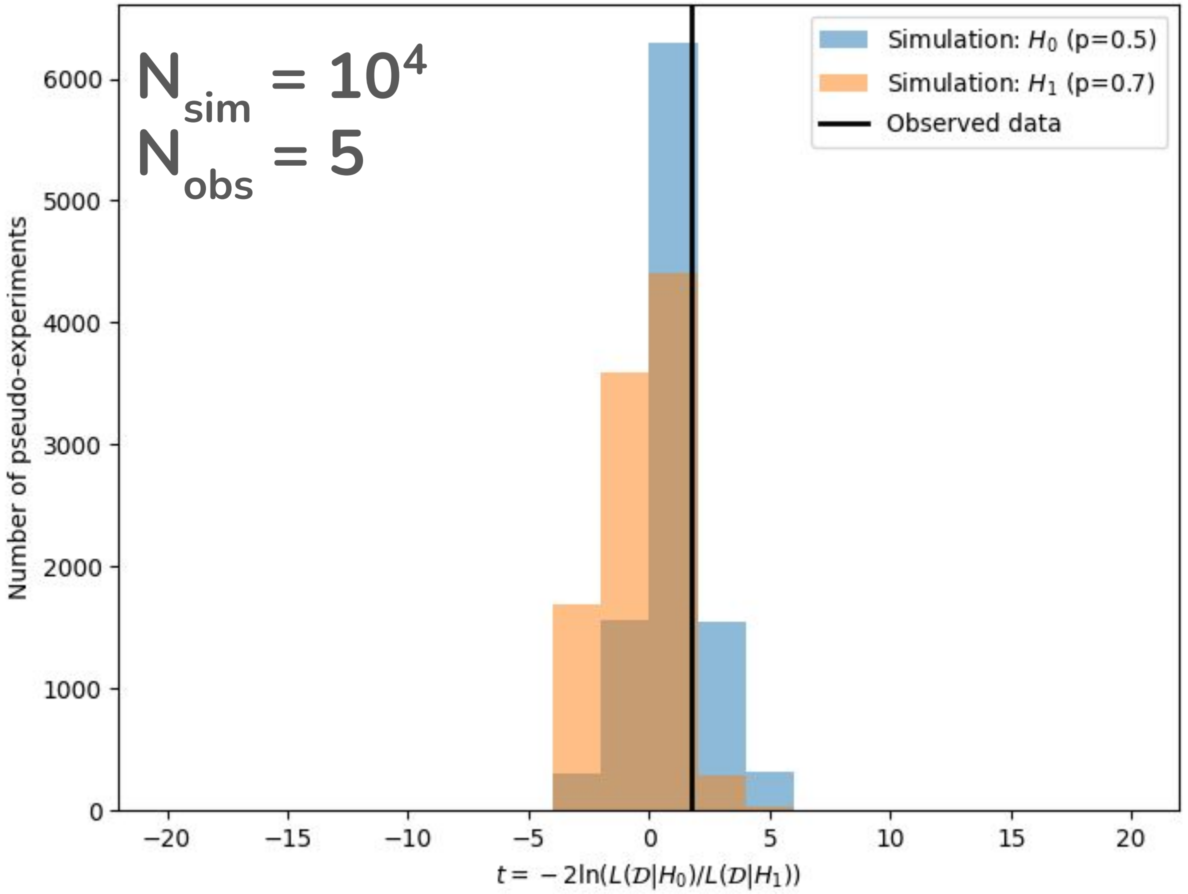

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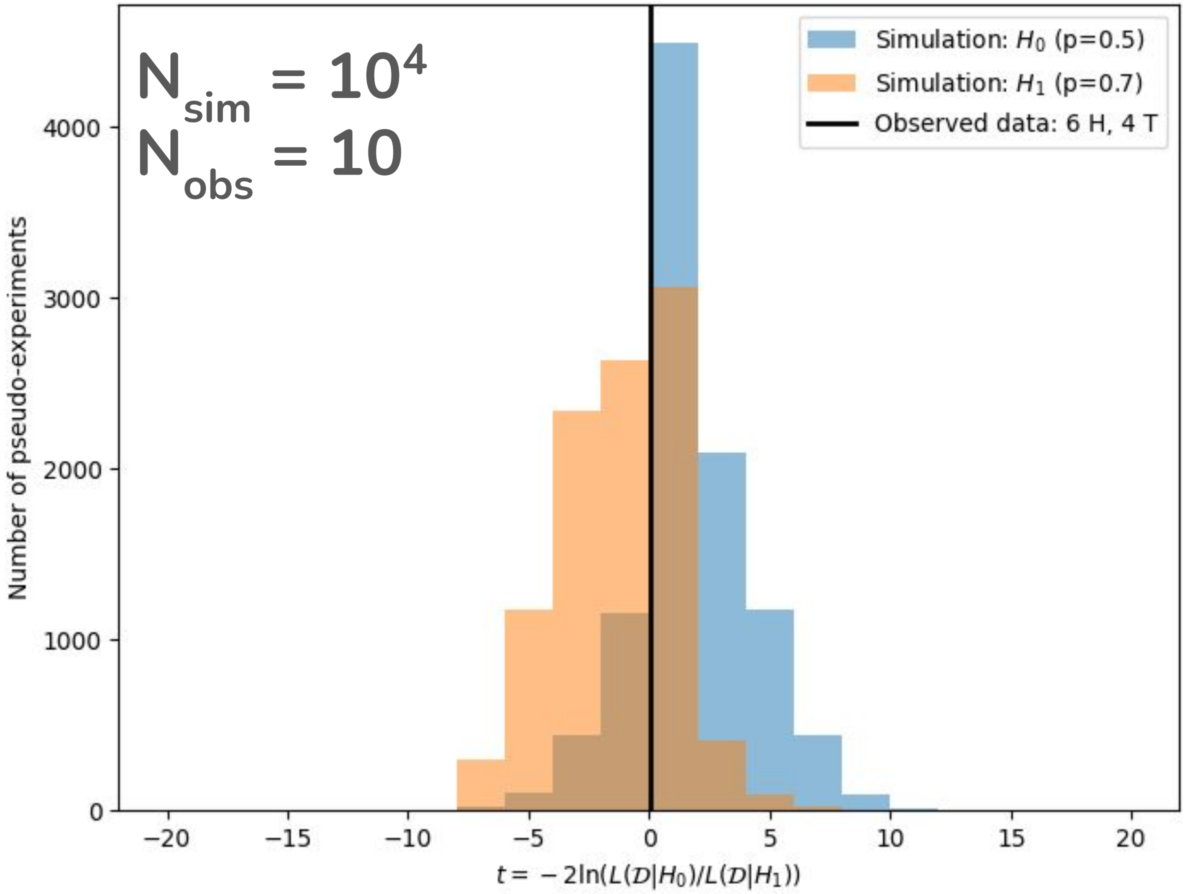
- What happens when we toss more coins e.g. N_{obs} = 10?



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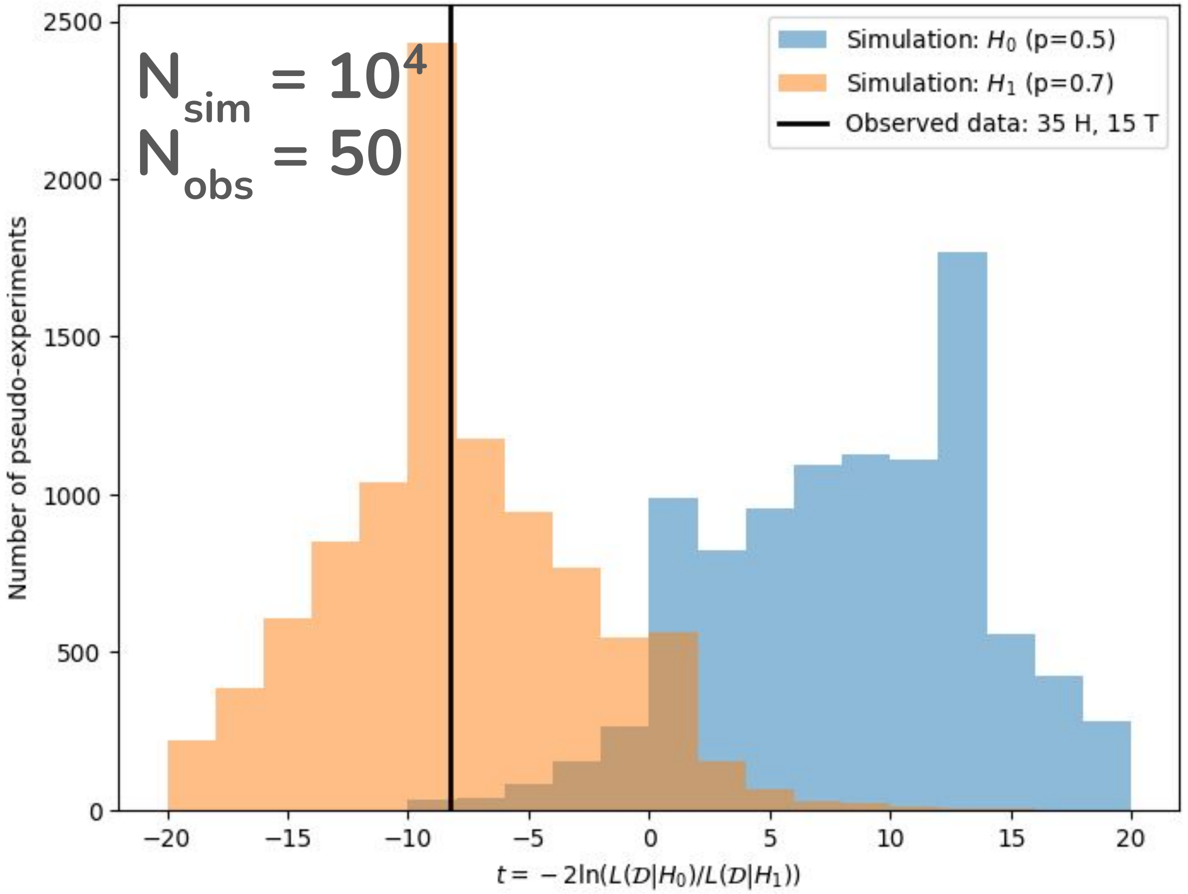

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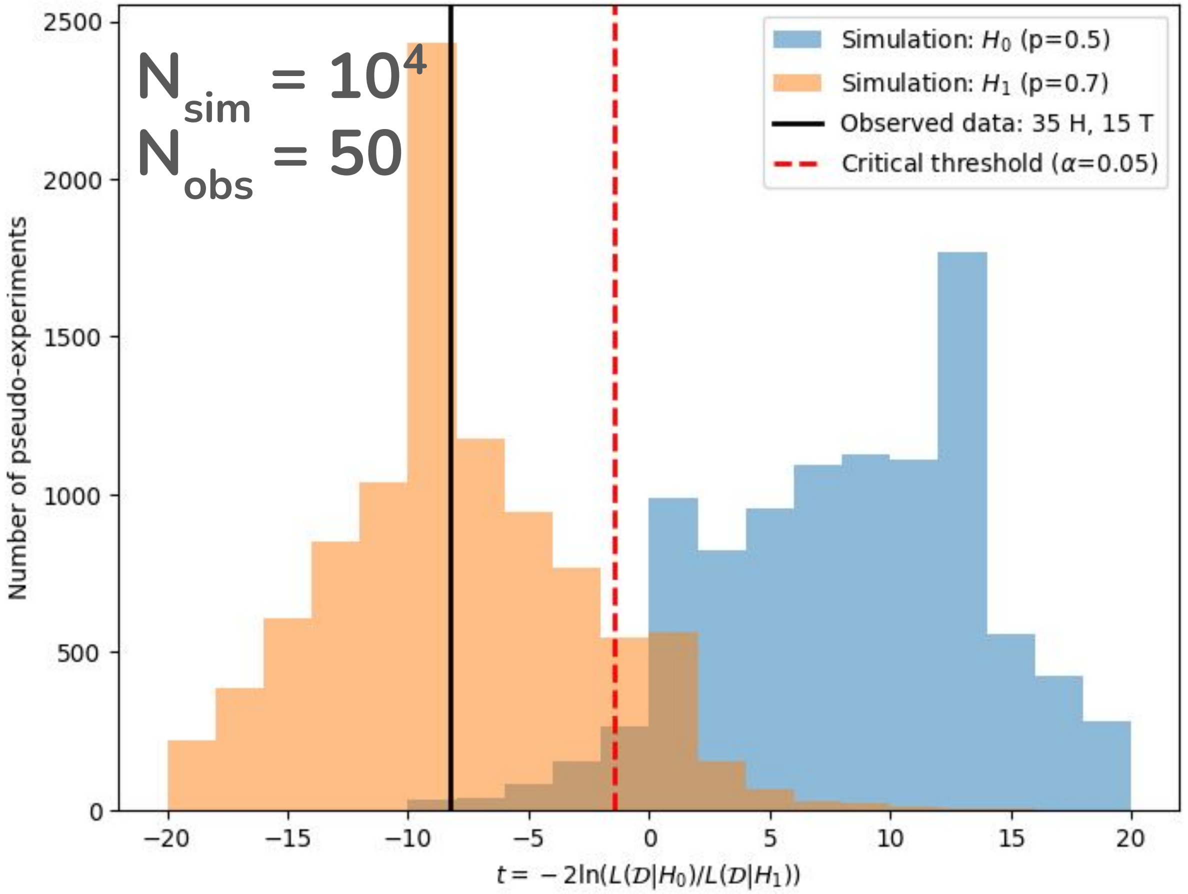

- Calculate t = t_{obs} for the observed data and compare to the distributions → which hypothesis does our data support?
- What happens when we toss more coins e.g. N_{obs} = 50?
- Eventually t_{obs} passes critical threshold → reject the null hypothesis and **conclude that our coin is biased!**
  - We will extend this technique to parameter estimation (infer θ and associated confidence intervals) later

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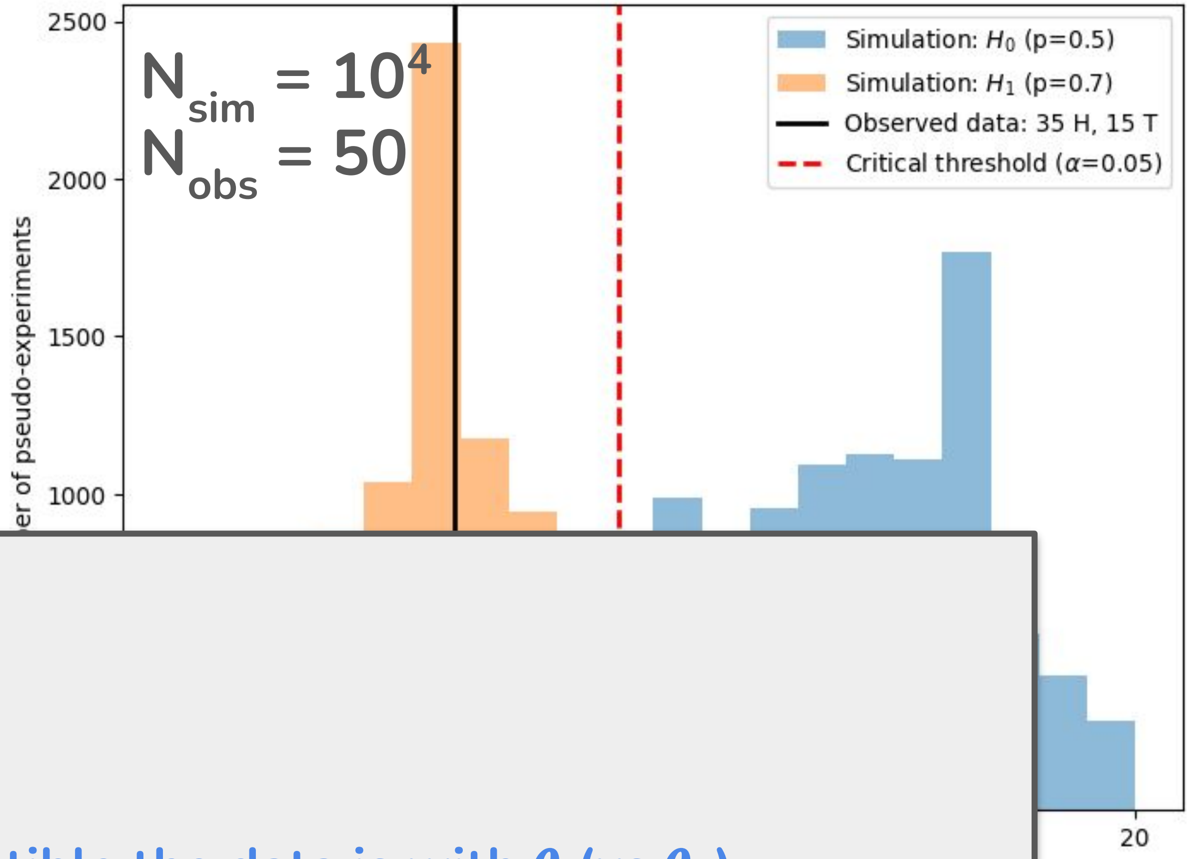
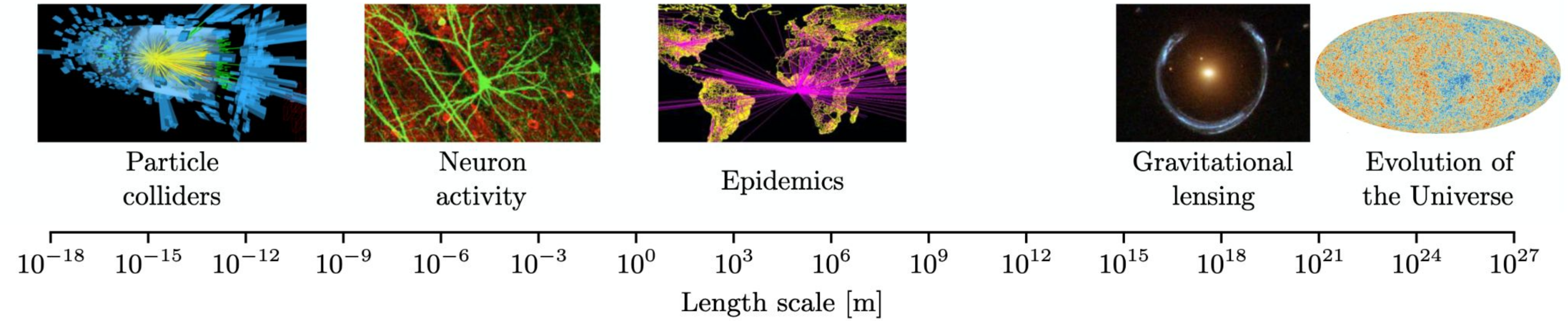


- Key takeaways:
  - Likelihood holds the key to inference
  - Define a **test-statistic (t)** = a number (score) to summarise **how compatible the data is with θ (vs θ_0)**
  - Neyman Pearson Lemma: **"likelihood ratio is the most powerful test-statistic"**
- Research ≠ tossing coins… **can we learn the log-likelihood-ratio test-statistic for more complex problems?**

Scientific era of simulations

Figure taken from [arXiv:1911.01429]



- Incredible complexity across all experimental length scales
  - Impossible to calculate likelihoods (intractable)

$$p(\mathcal{D}|\theta) = \prod_{x_i \in \mathcal{D}}^{N_{obs}} \int dz\, p(x_i|\theta, z)$$

Latent features

Model parameters

θ

Inference *Difficult*

$\mathcal{D} = \{x_i\}_{i=1}^{N_{\mathrm{obs}}}$

Experimental data

Scientific era of simulations

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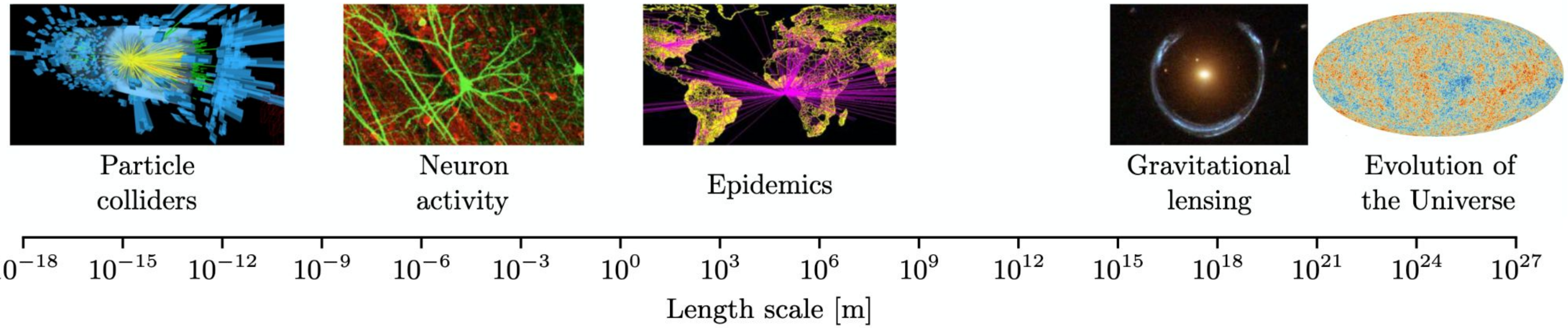

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- But we have access to **high-fidelity simulations**

Model parameters

θ

Inference

Available $\longrightarrow$

Difficult $\longleftarrow$

Simulation

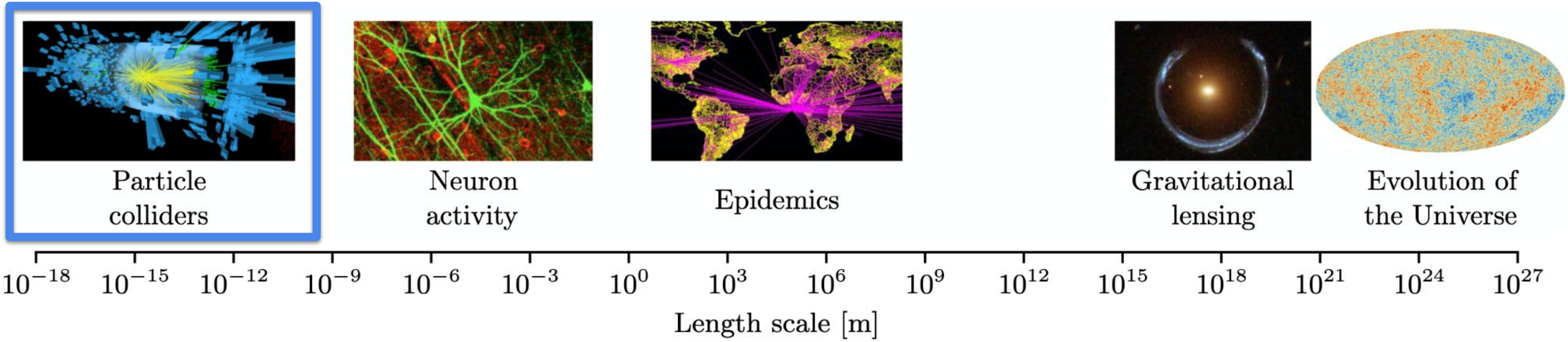
$x_i^{\text{sim}} \sim p(x|\theta)$

$\mathcal{D} = \{x_i\}_{i=1}^{N_{\text{obs}}}$

Experimental data

Scientific era of simulations

Figure taken from [arXiv:1911.01429]



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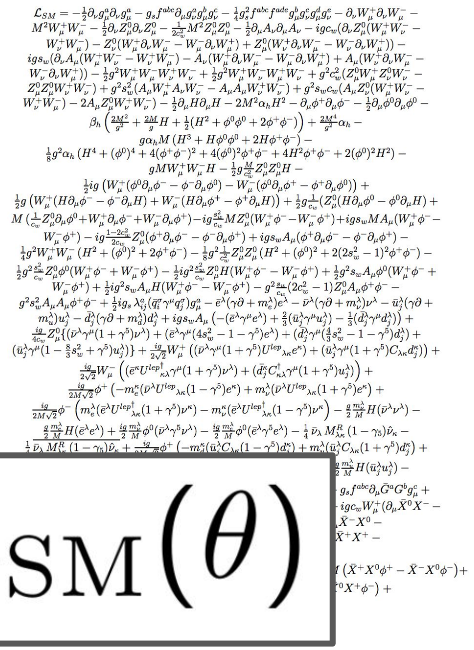
Inference

Difficult

Experimental data

Scientific era of simulations

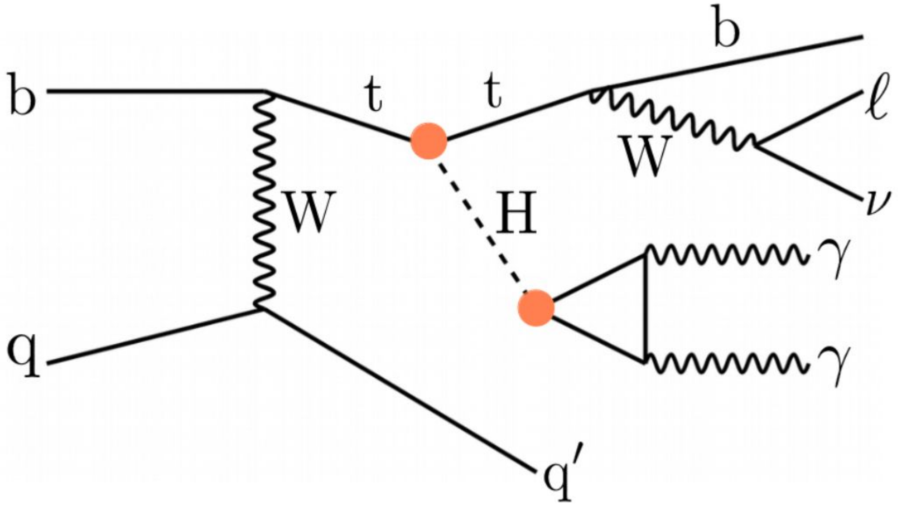
$$p(x \mid \theta) = \int \mathrm{d}z_d \int \mathrm{d}z_s \int \mathrm{d}z_p p(x|z_d)p(z_d|z_s)p(z_s|z_p)p(z_p|\theta)$$



$$\boxed{\mathcal{L}_{\mathrm{SM}}(\theta)}$$

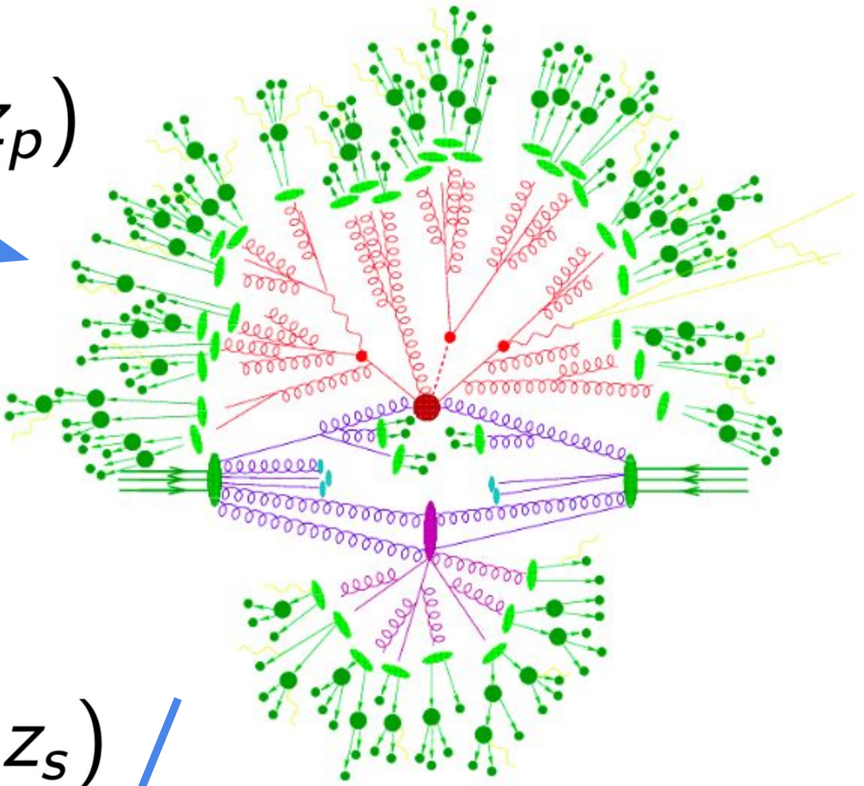
Model Lagrangian
(underlying theory)

$p(z_p|\theta)$



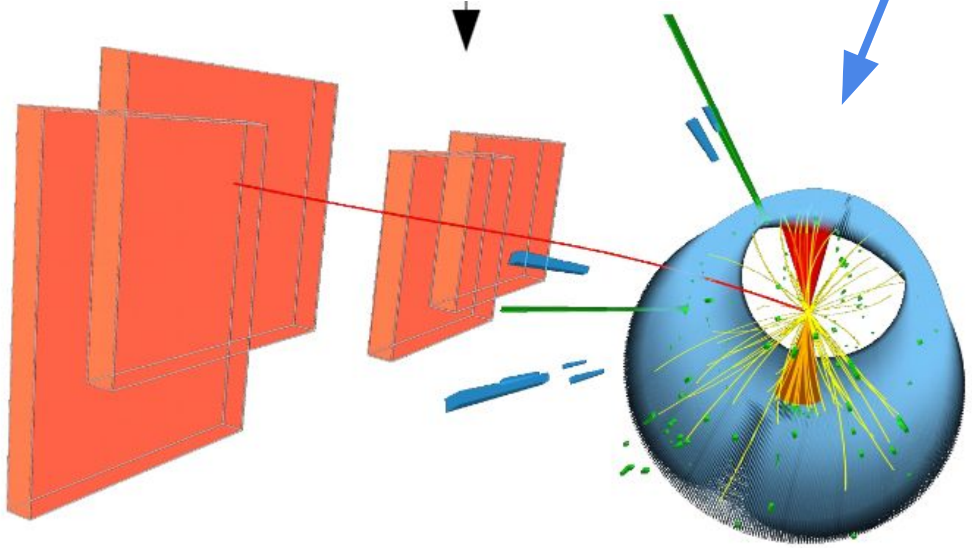
Hard scatter

$p(z_s|z_p)$



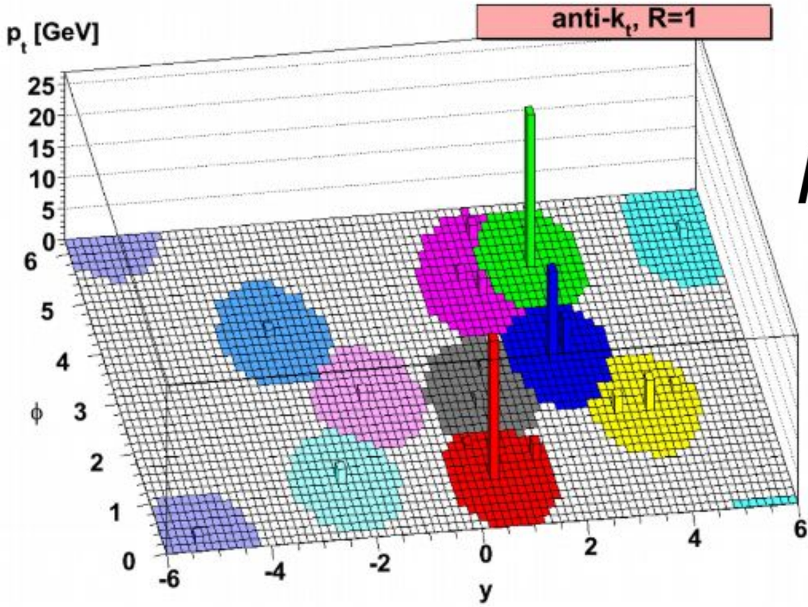
Parton shower and hadronisation

$p(z_d|z_s)$



Interaction of particles with detector material

$p(x|z_d)$



Reconstruction from electronic signals

X

Simulated Data

Scientific era of simulations

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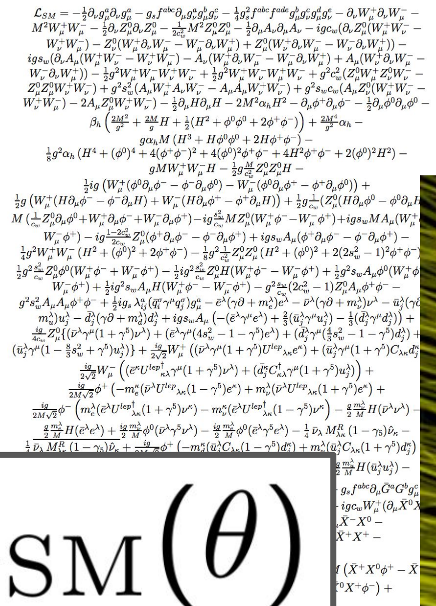

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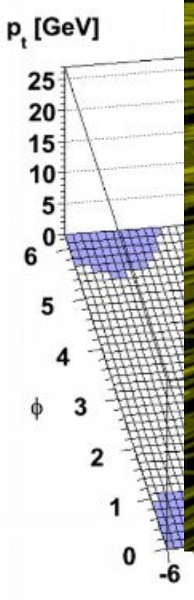

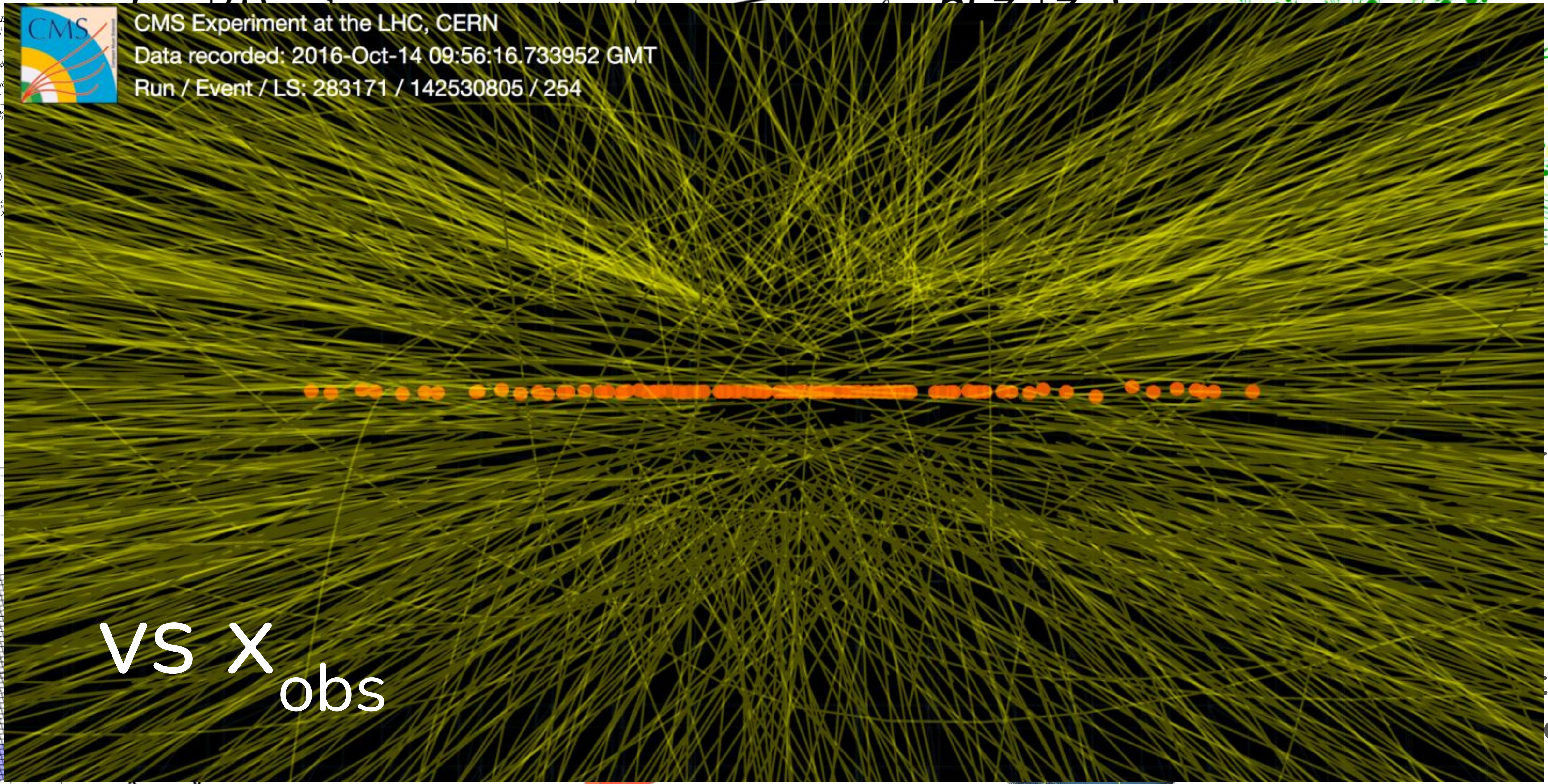

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X ←
Simulated Data

Reconstruction from electronic signals

Scientific era of simulations

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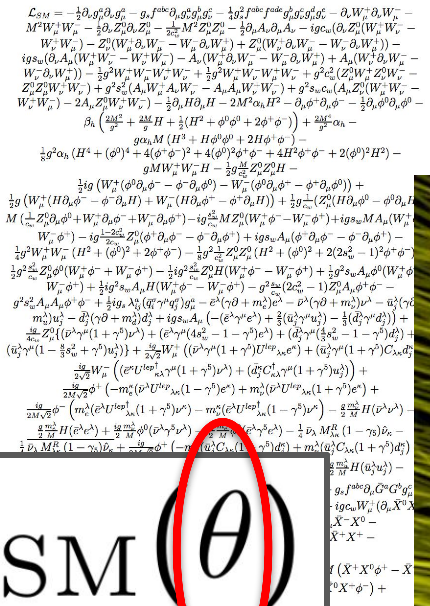

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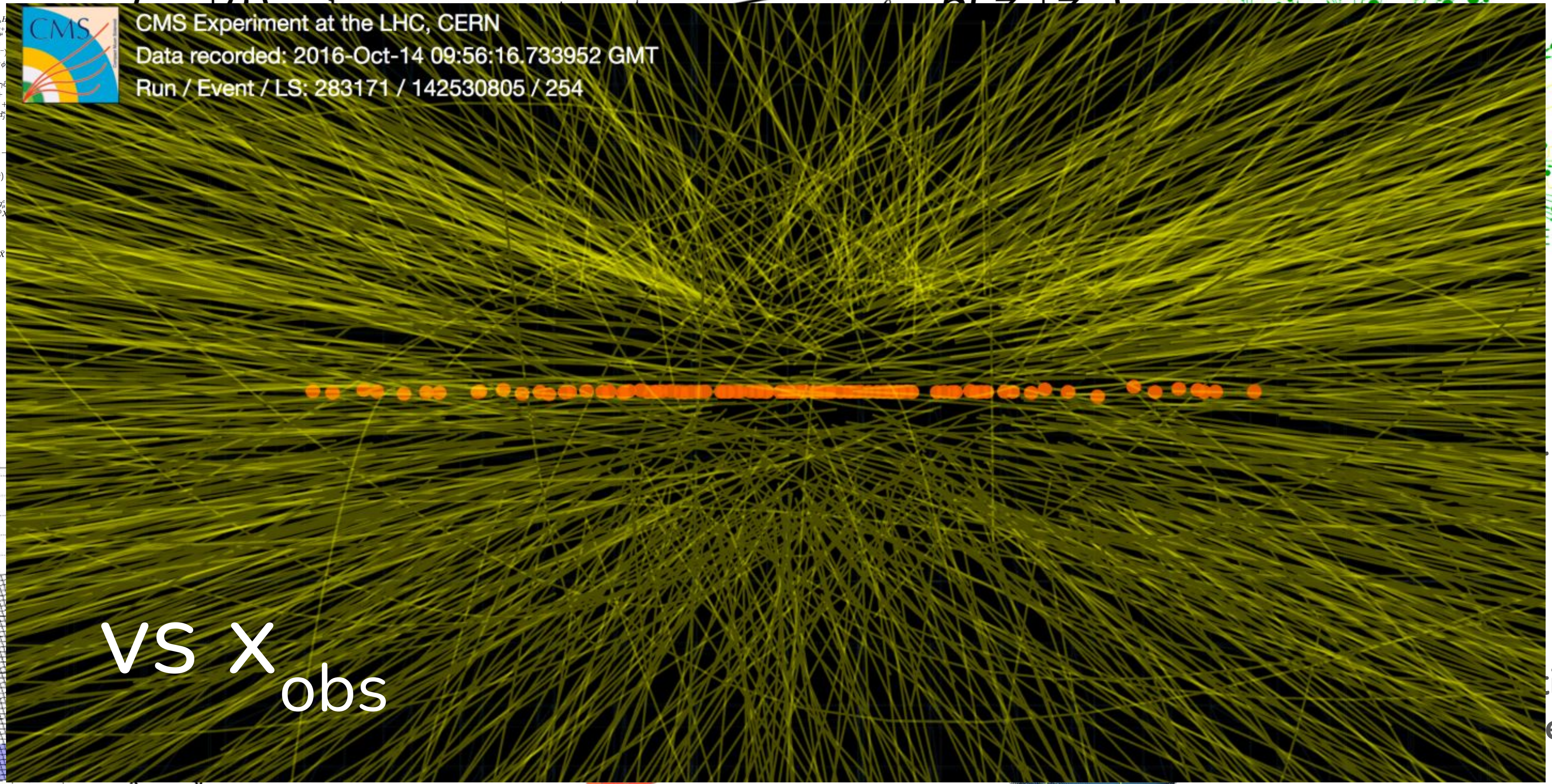
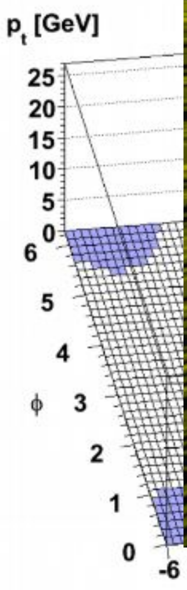


VS X_{obs}

$X \leftarrow$

Simulated Data



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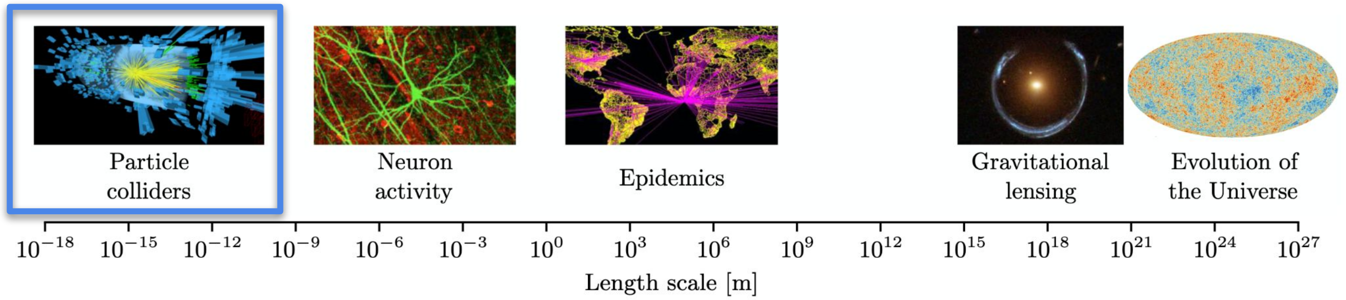
Reconstruction from electronic signals

Simulation-based inference (SBI)



- Traditional approaches to SBI
  - Approximate Bayesian Computation (ABC)
  - (Probability) density estimation via histogramming/kernels

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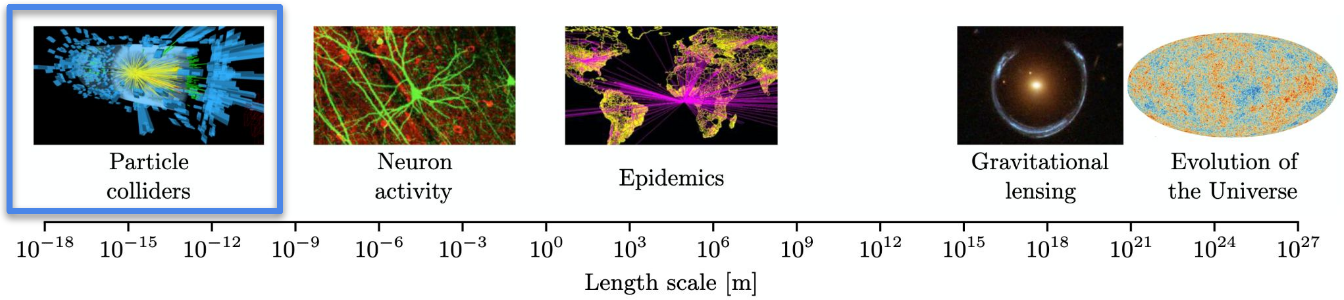

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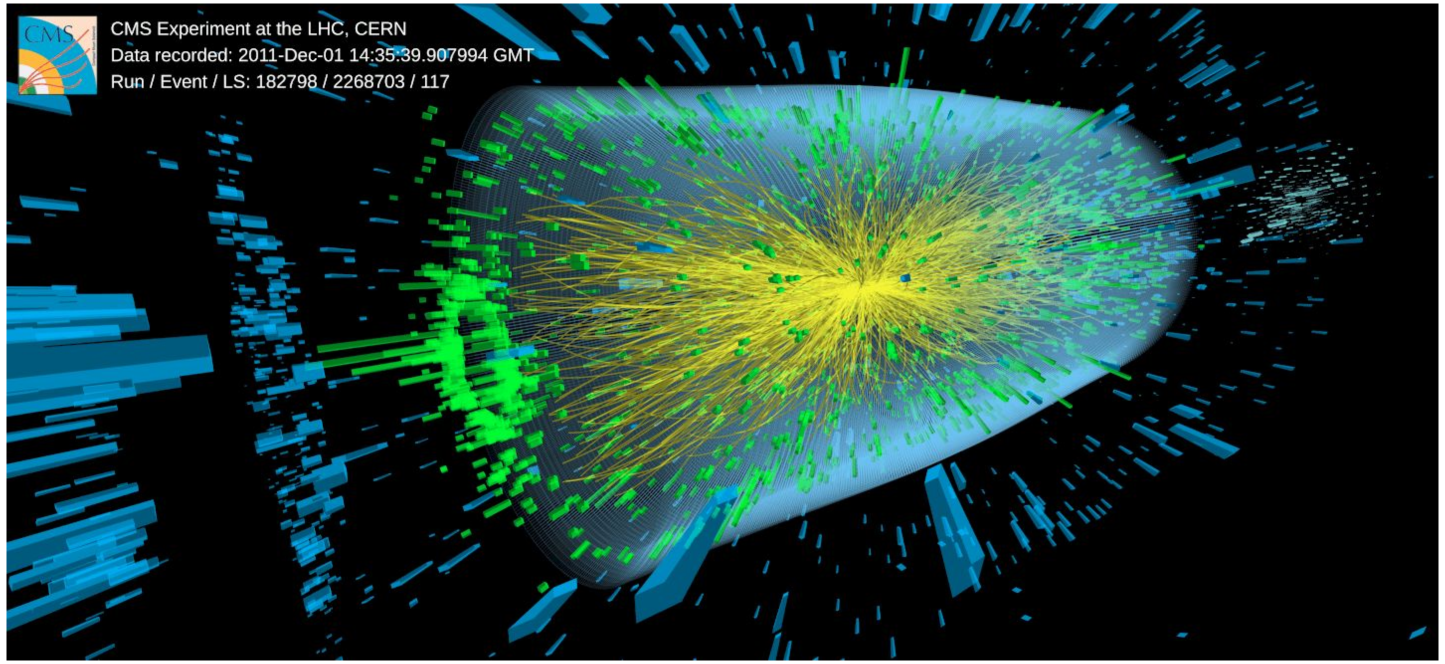
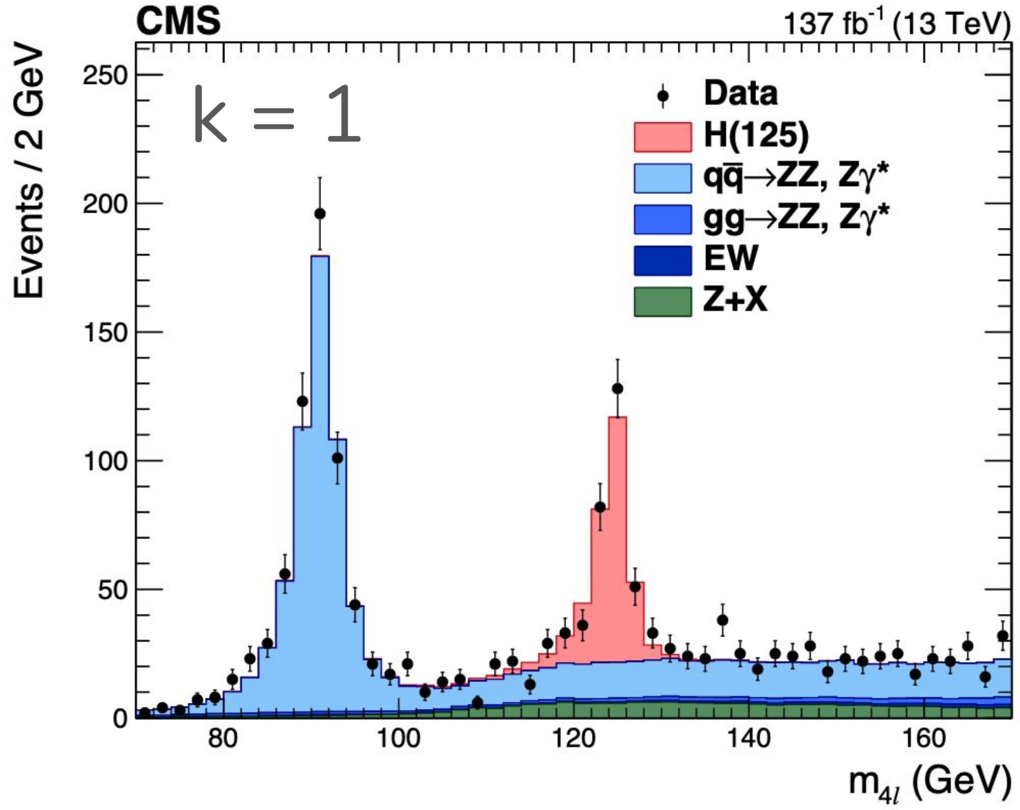
$$f(x) \in \mathbb{R}^k, \quad k \ll d$$

- Data is often high-dimensional: $x \in \mathbb{R}^d$ → construct low-dimensional summary statistic for inference



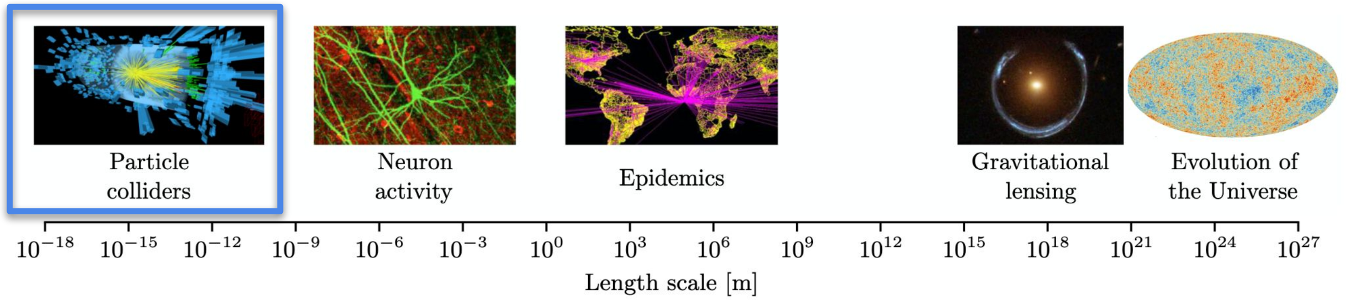
e.g. energy & momentum of O(100) particles produced in each LHC collision



$$\hat{p}(f(x)|\theta) = \frac{N_b}{N_{\text{tot}}\Delta_b}$$

Bin the simulation in summary statistic and estimate the density
→ Compare to observed data

Simulation-based inference (SBI)



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  - Approximate Bayesian Computation (ABC)
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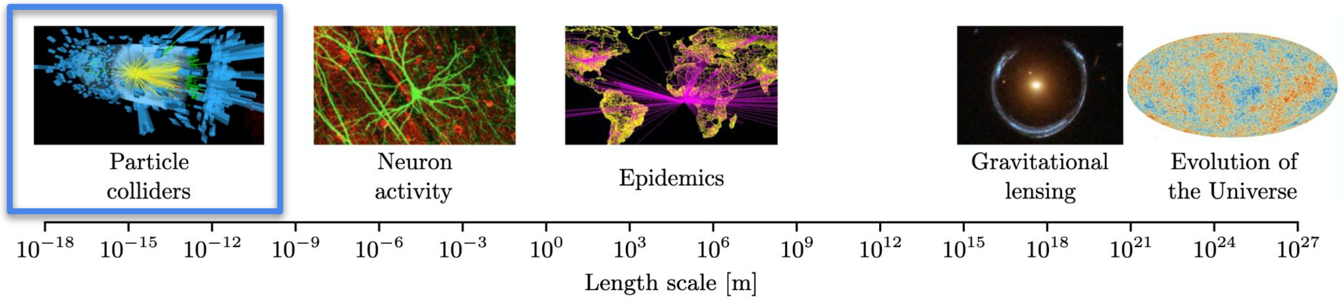

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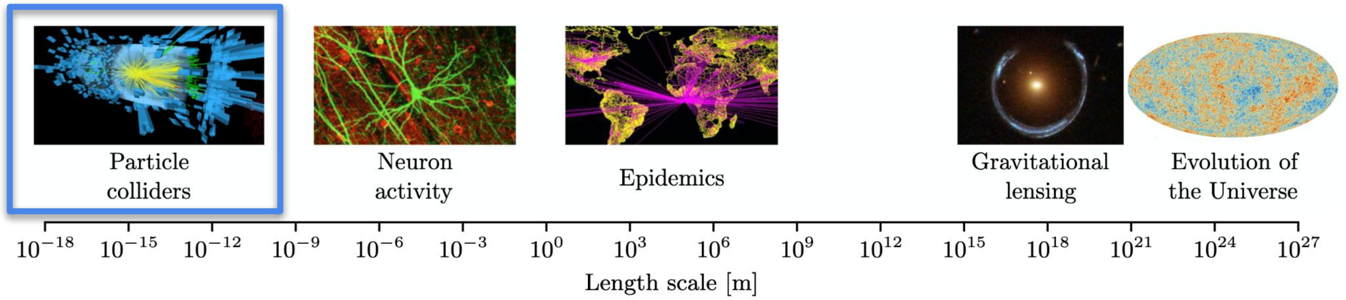

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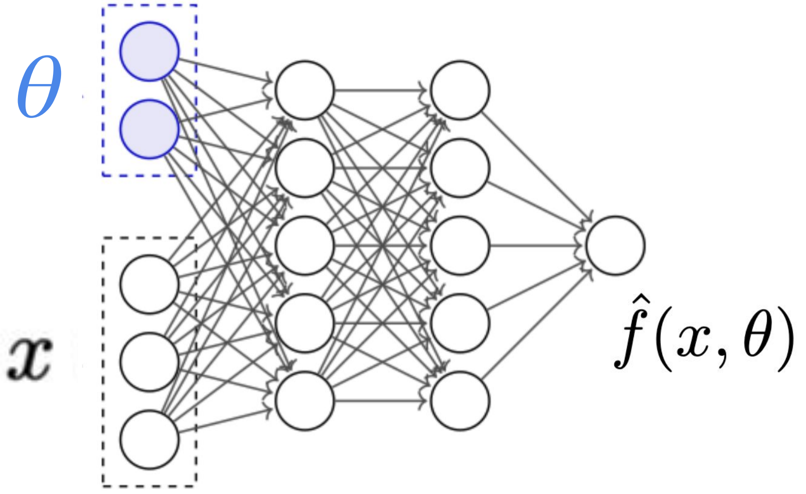

A: use Machine-Learning (ML) → retain maximum sensitivity to θ

- Deep learning models can be effective surrogates for the likelihood-ratio
- Function of the (full) multivariate input space → No need for low-dimensional summaries that lose statistical power

"Neural SBI" will help us squeeze every drop of information out of the data

Learning the log-likelihood ratio

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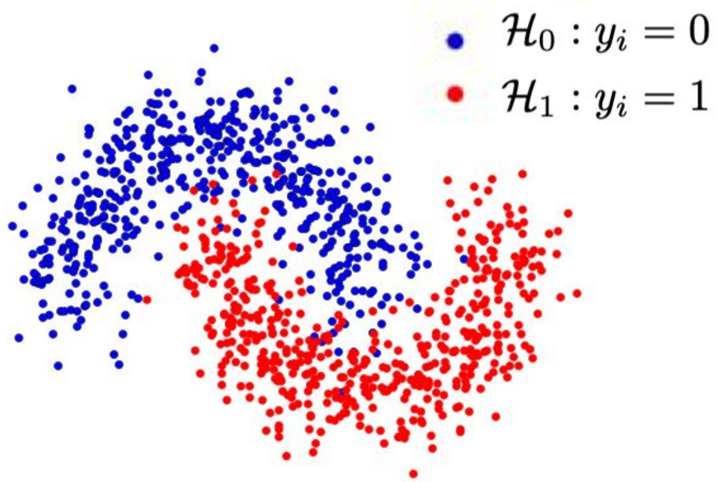

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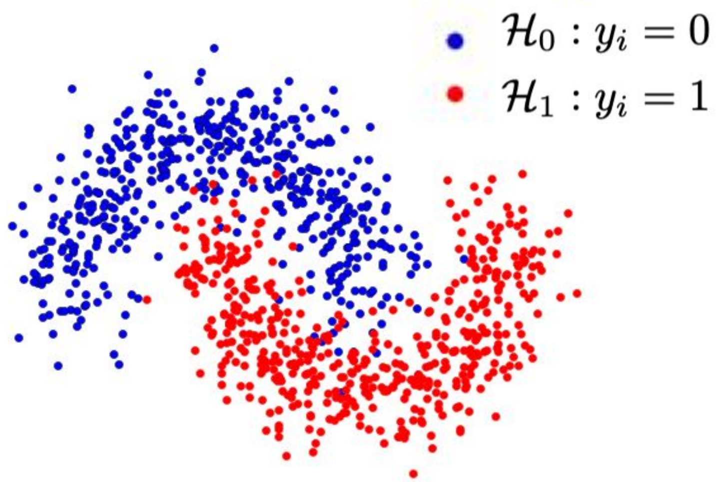

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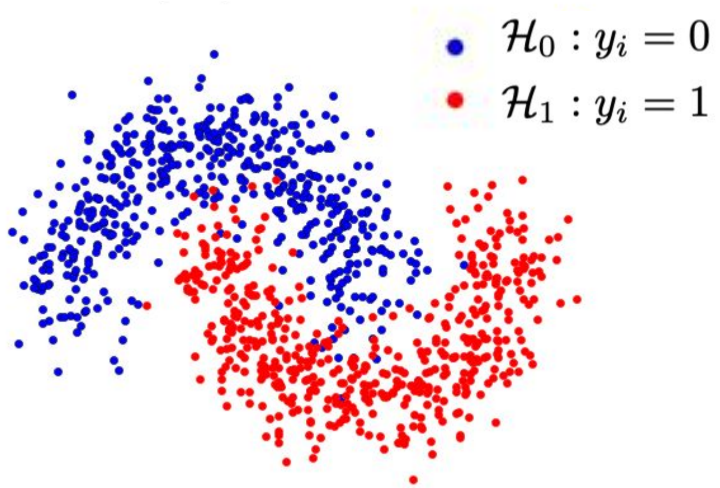

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  - Assuming "balanced classes" → optimal decision function (i.e. f(x) which minimizes the loss) is...

$$f(x_i) = \frac{p(x_i|\mathcal{H}_1)}{p(x_i|\mathcal{H}_0) + p(x_i|\mathcal{H}_1)}$$

  - In reality (finite training samples, finite architecture), our trained classifier will be an estimator of optimal decision function

$$\hat{f}(x_i) \approx f(x_i) = \frac{p(x_i|\mathcal{H}_1)}{p(x_i|\mathcal{H}_0) + p(x_i|\mathcal{H}_1)}$$

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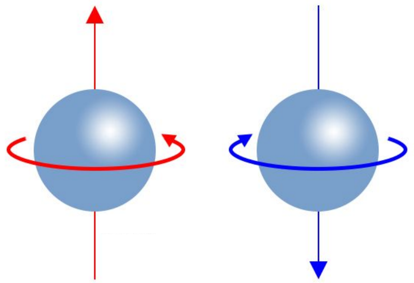
- **Key takeaway:** we can use output of binary classifier trained with simulation to approximate log-likelihood ratio test-statistic

Hypothesis testing example

- `hypothesis_test_particle_spin.ipynb`
- Two-class hypothesis test where **analytic likelihood is not known (intractable)**… but we have a faithful simulator

Hypothesis testing example



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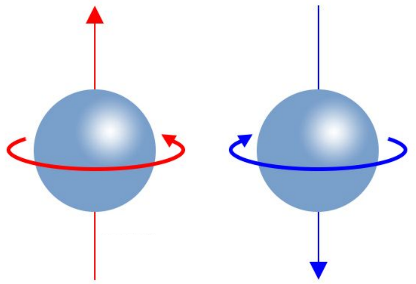

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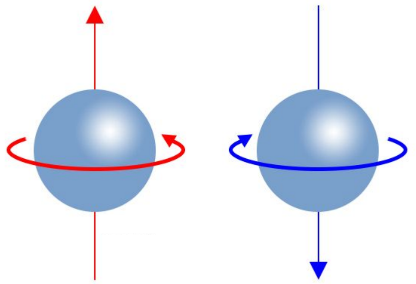

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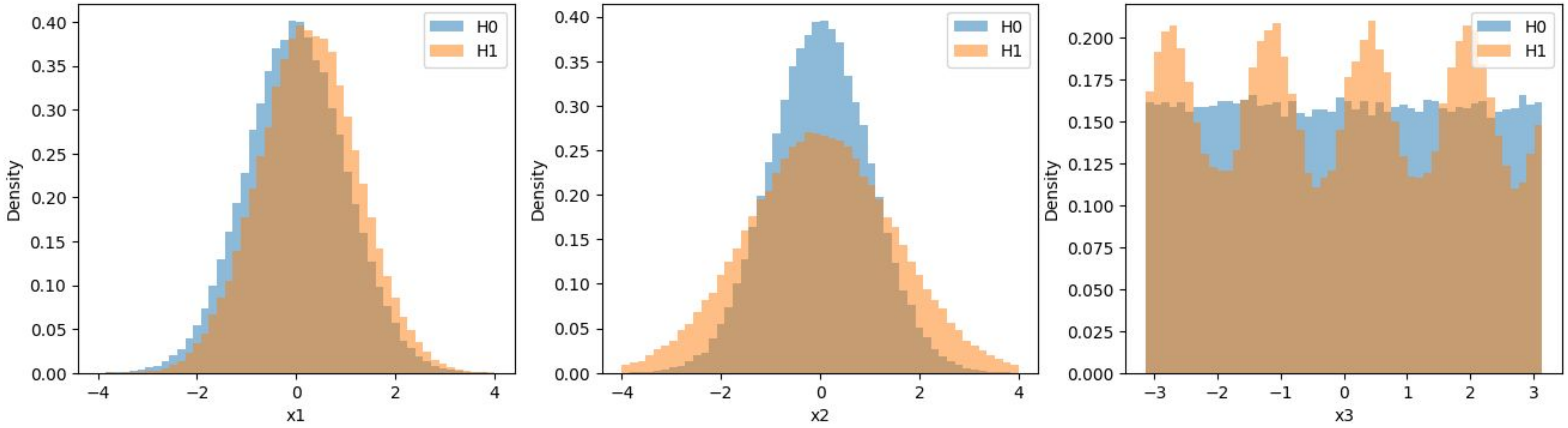

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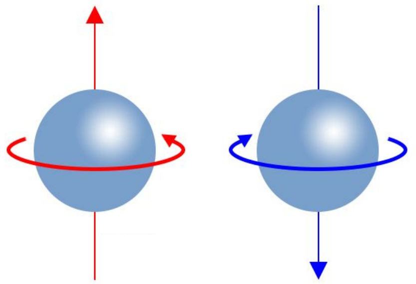

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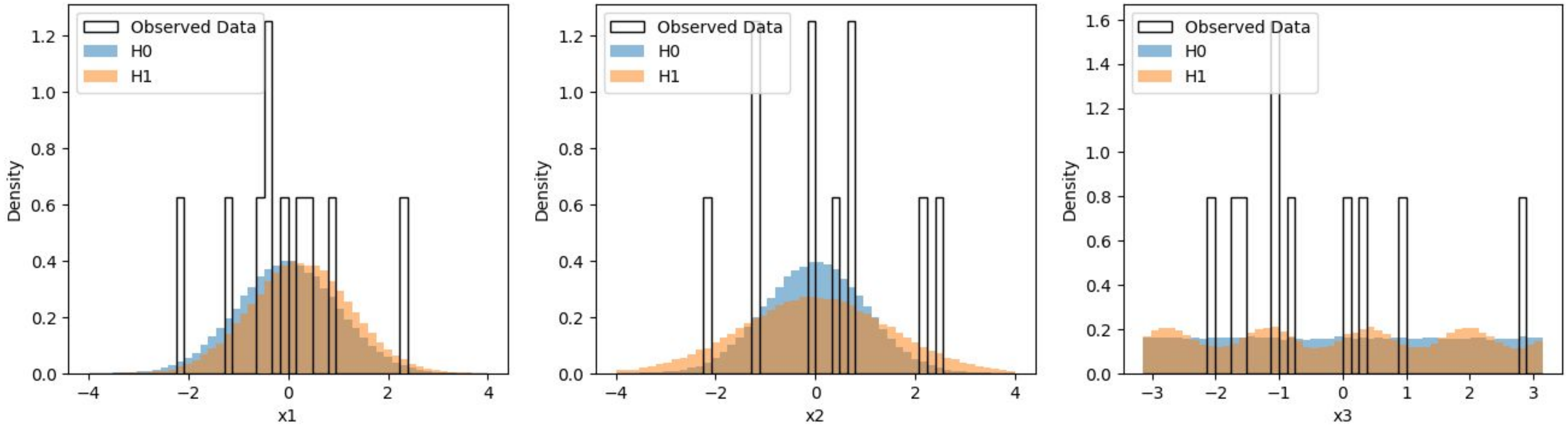

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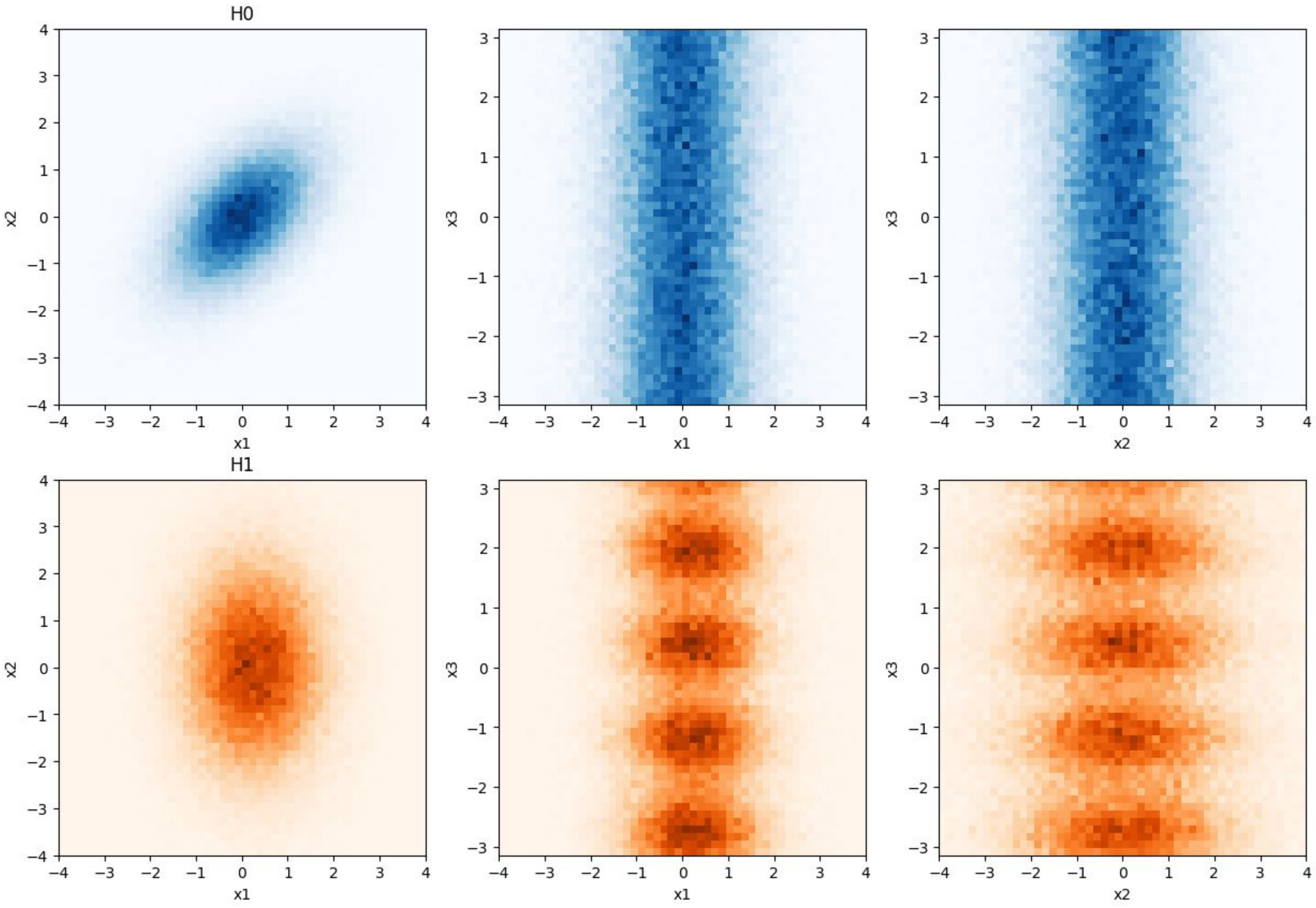

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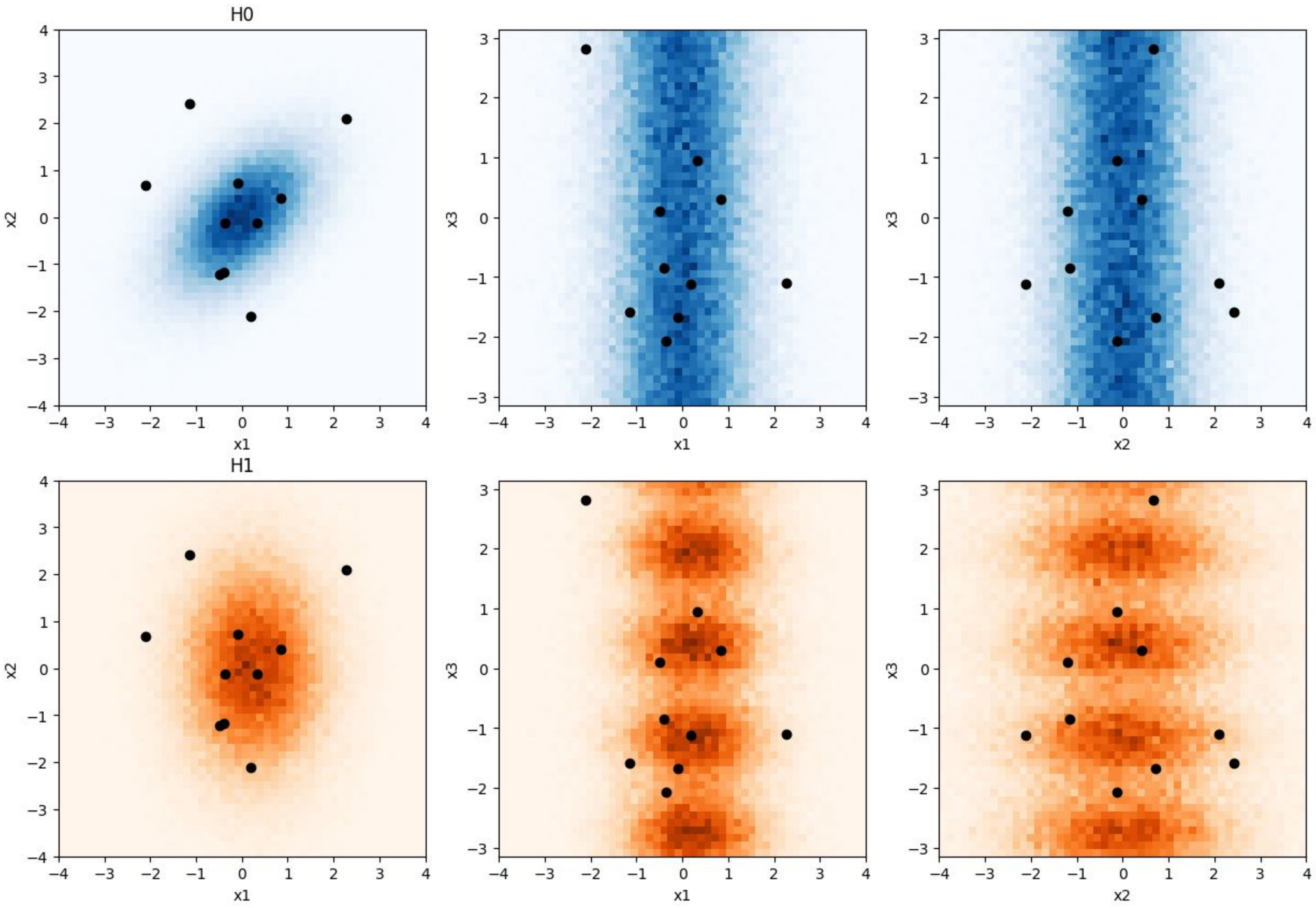
$\mathcal{H}_0$

$\mathcal{H}_1$



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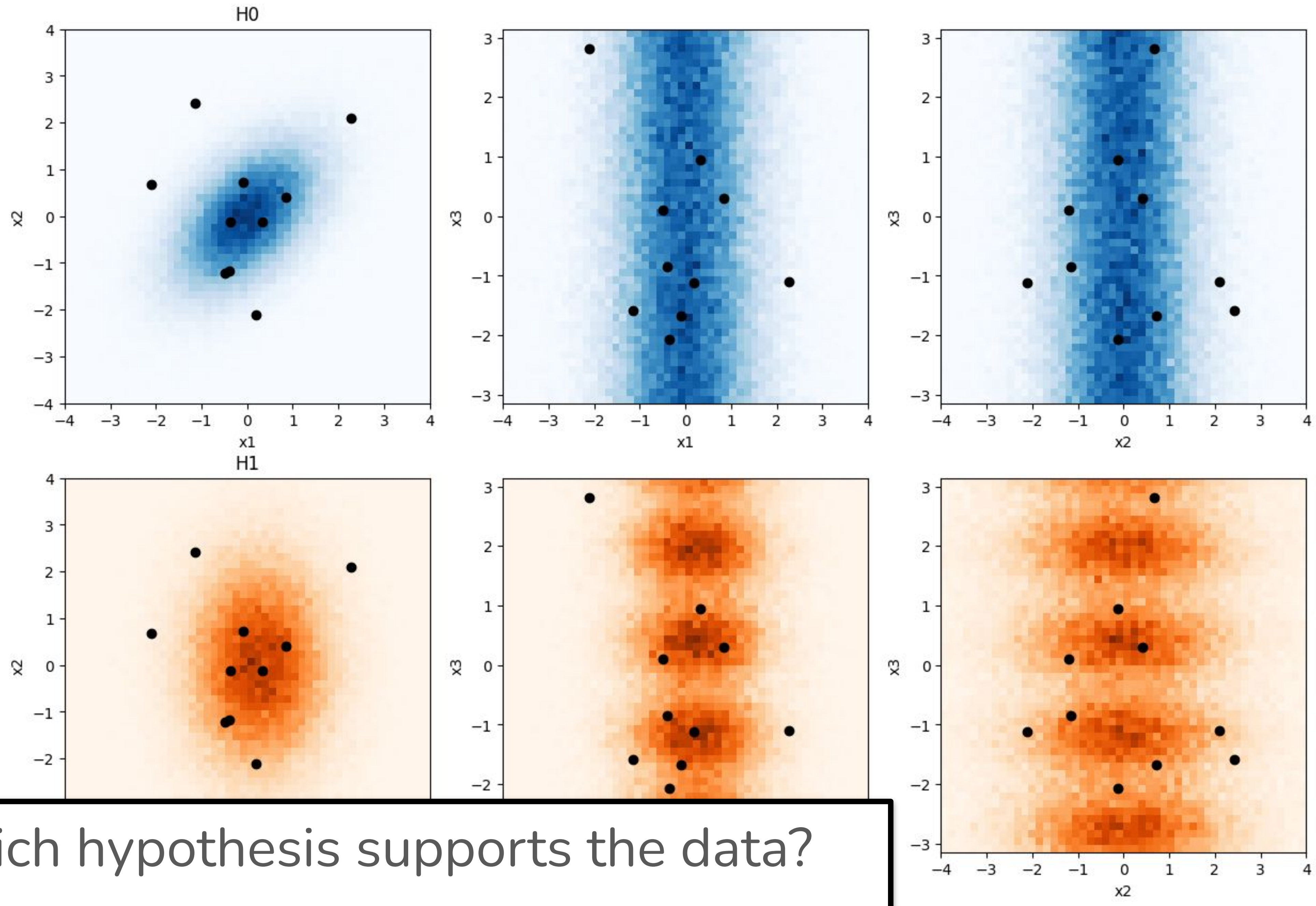
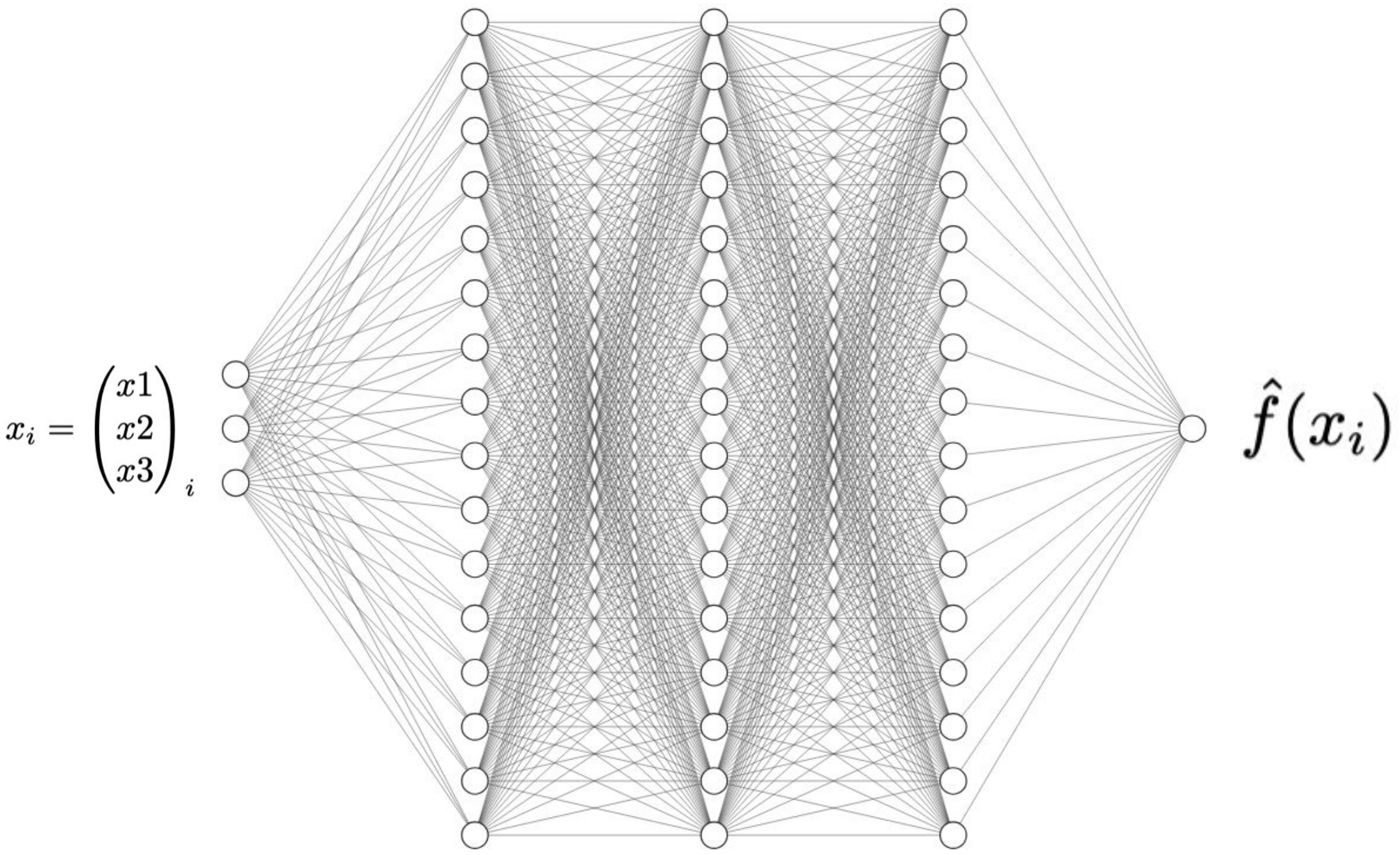
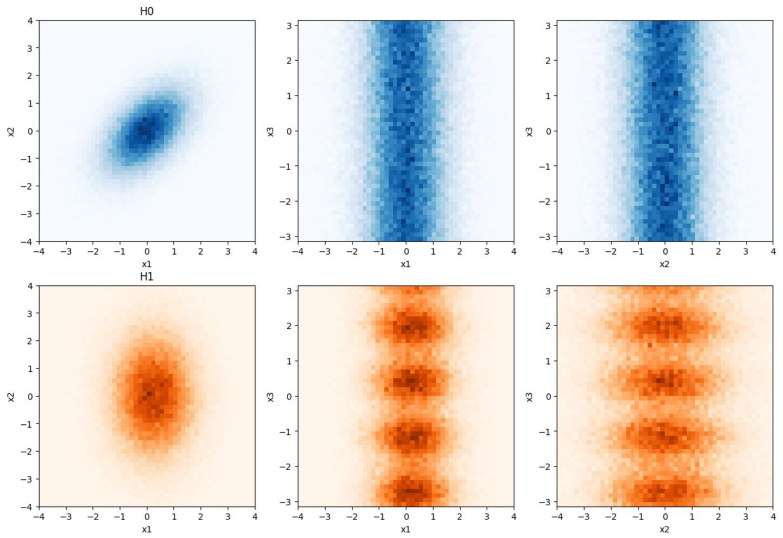


Can you tell by eye which hypothesis supports the data?

Classifier training

- We train a simple multi-layer perceptron (MLP) with **`torch.nn`** to classify between simulated samples: $\mathcal{H}_0$ vs $\mathcal{H}_1$





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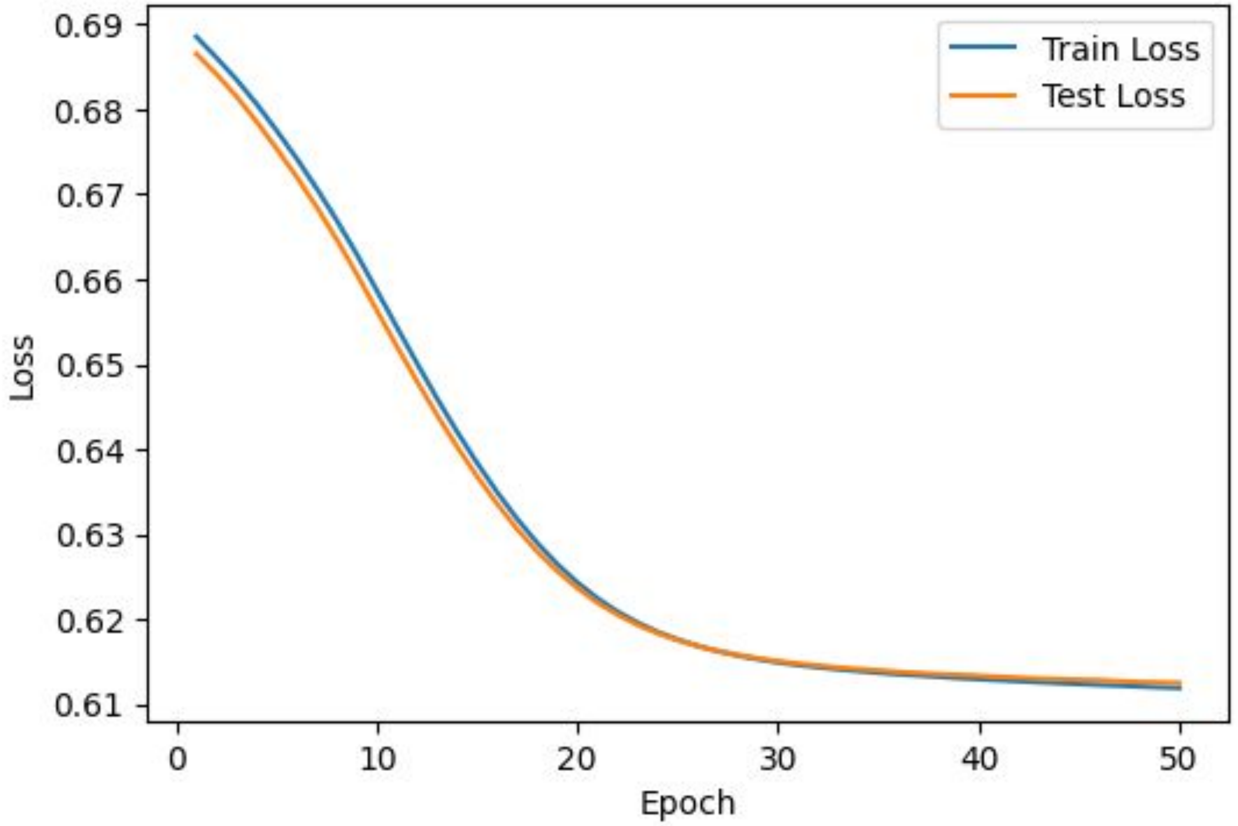

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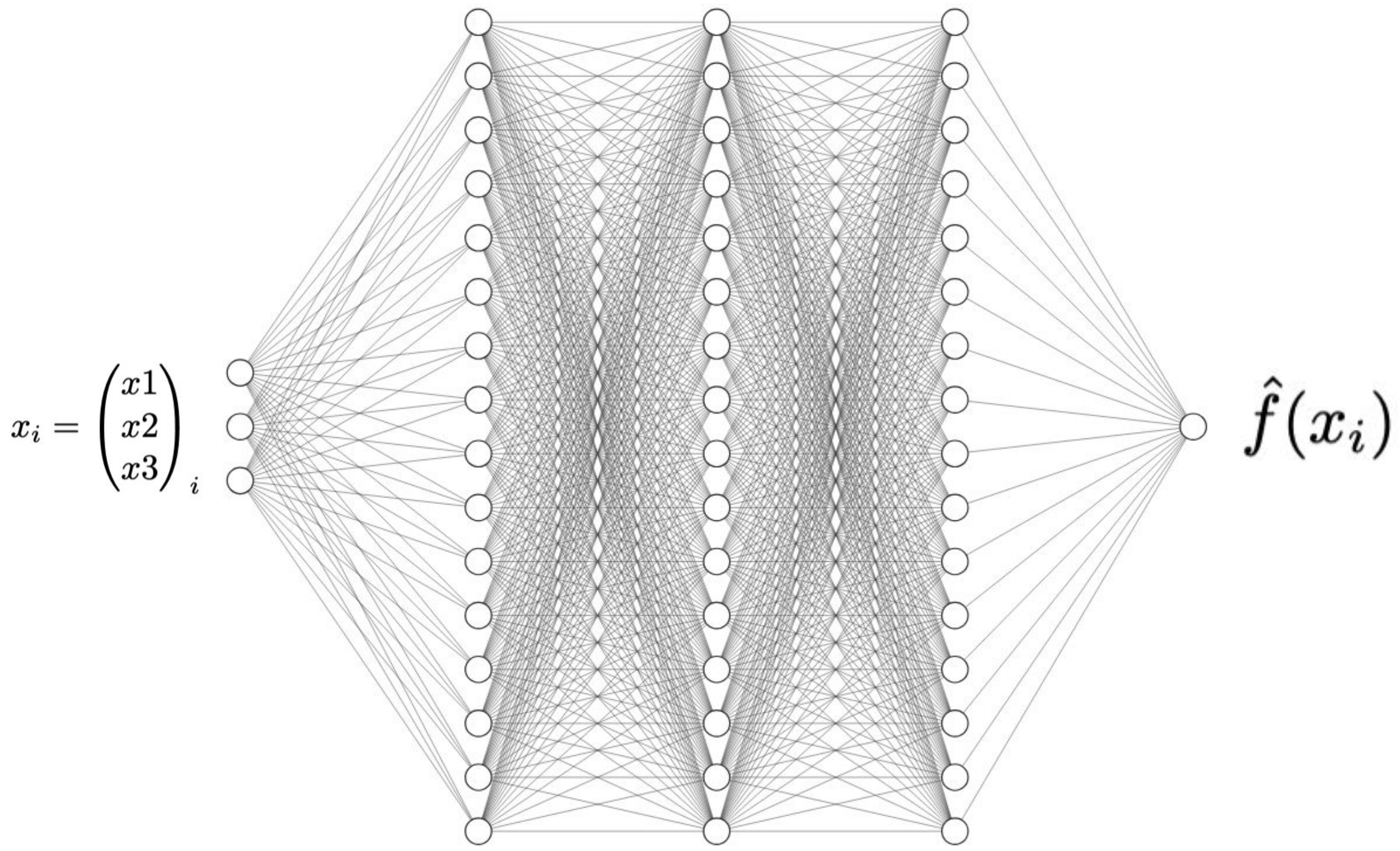
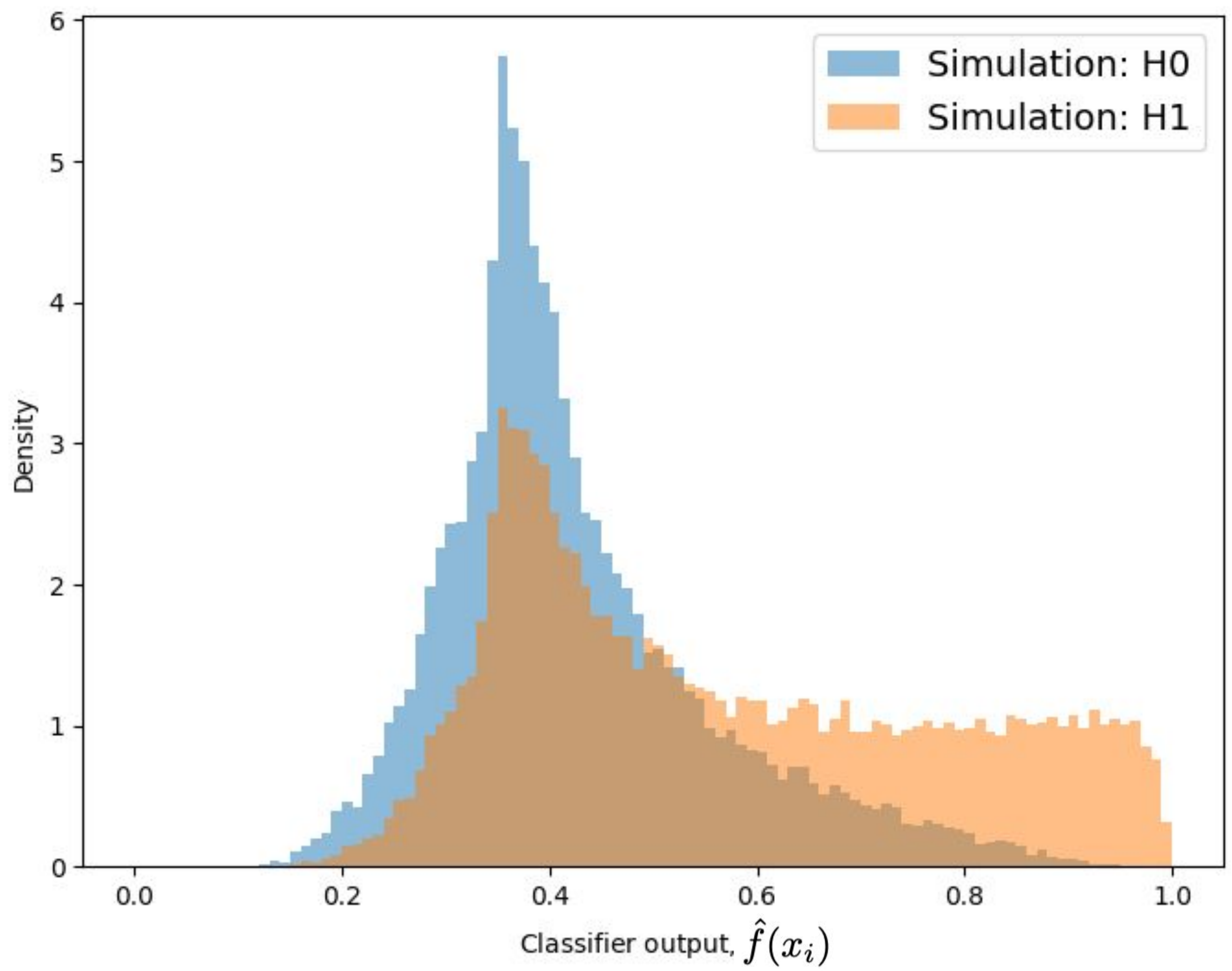
- After training we can evaluate the network (on an independent test sample) and plot the classifier output: $\hat{f}(x_i)$





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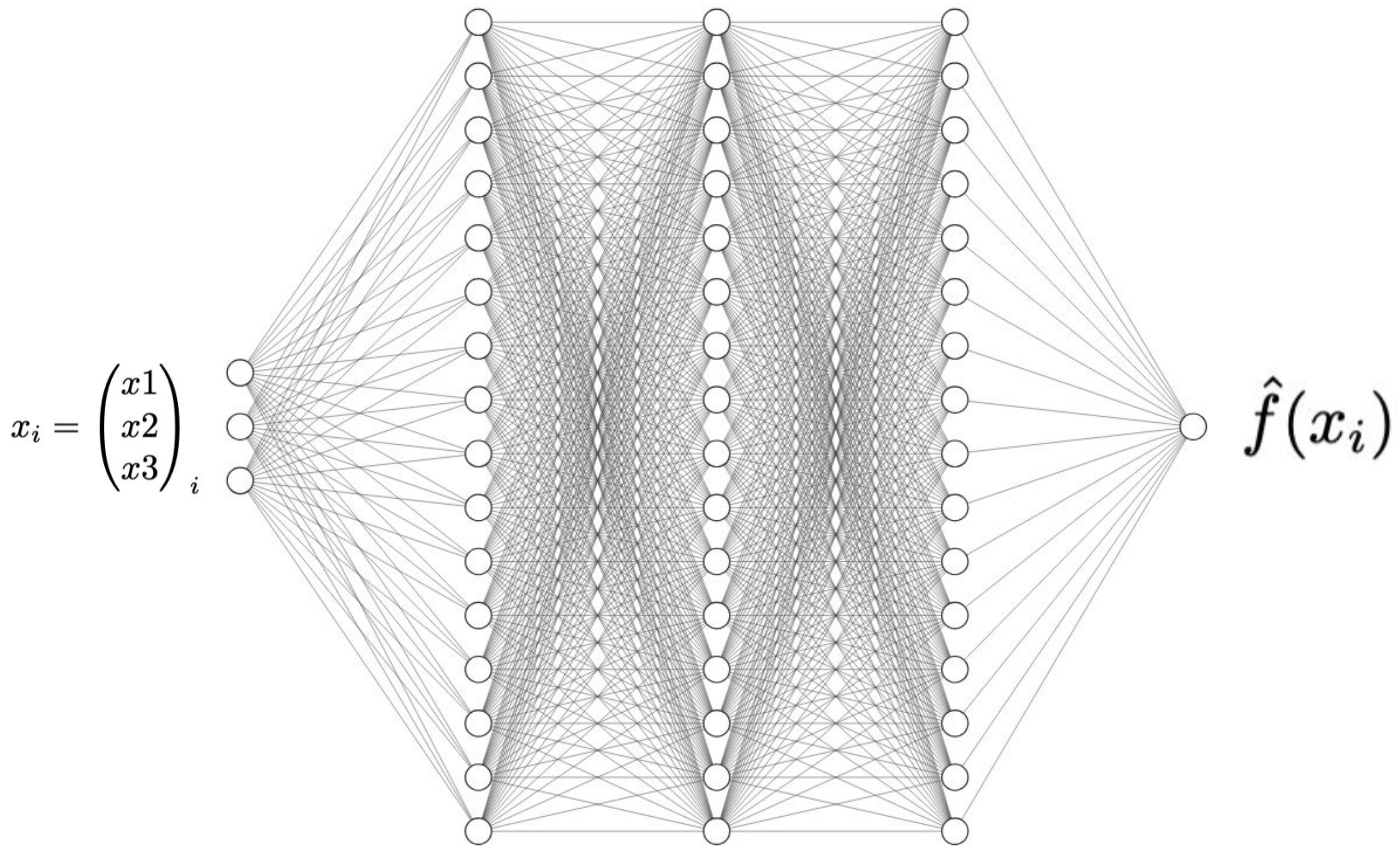

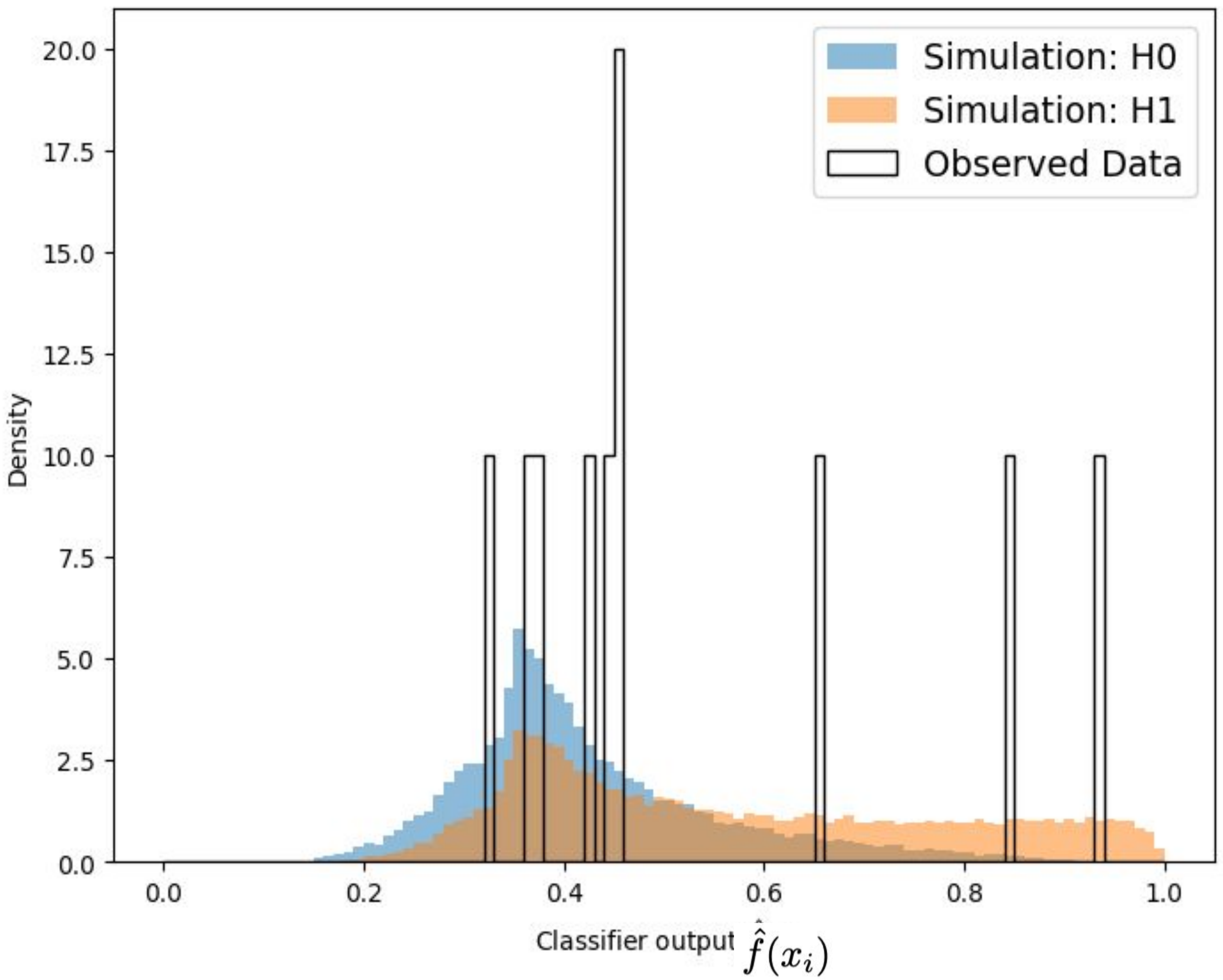

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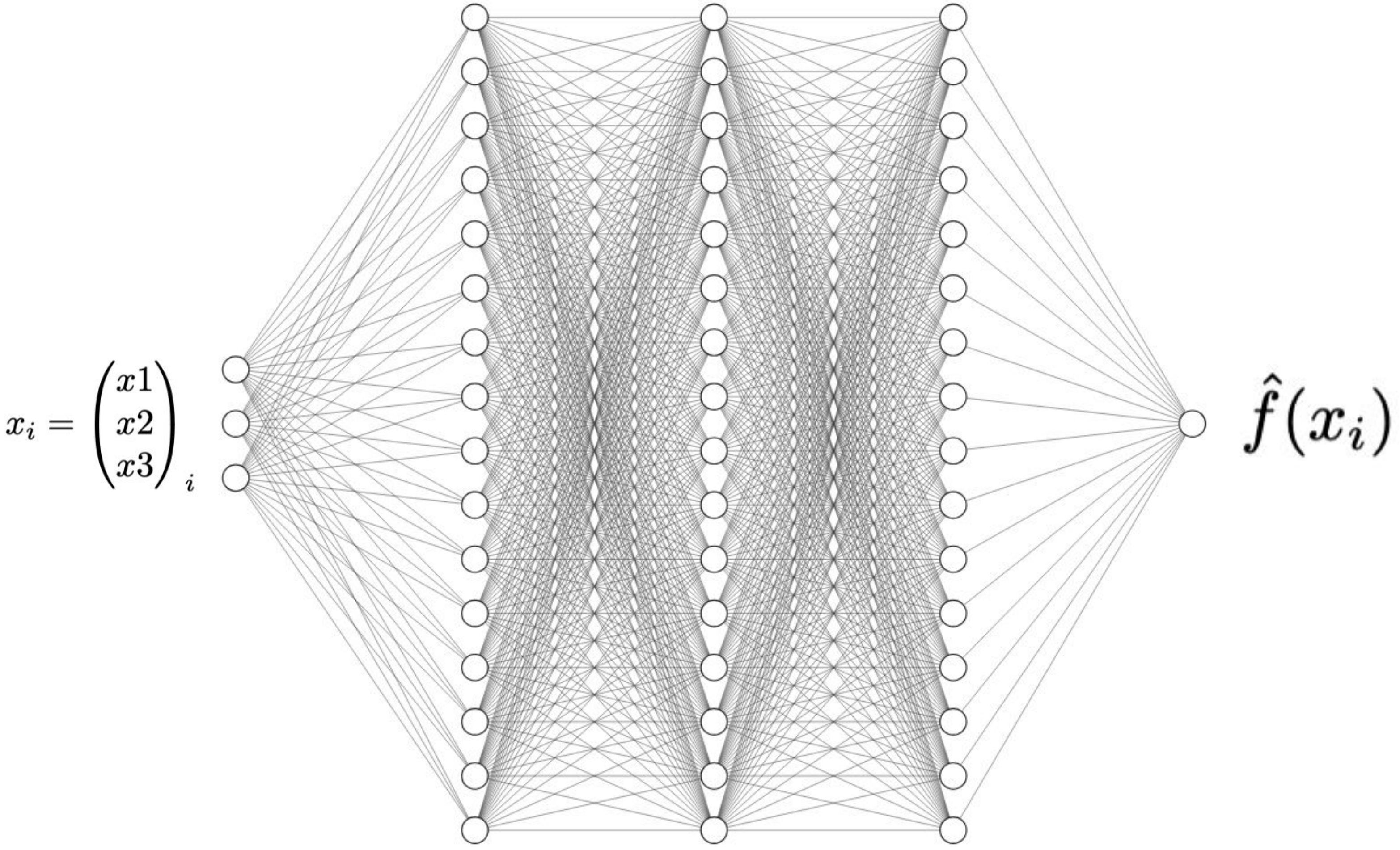

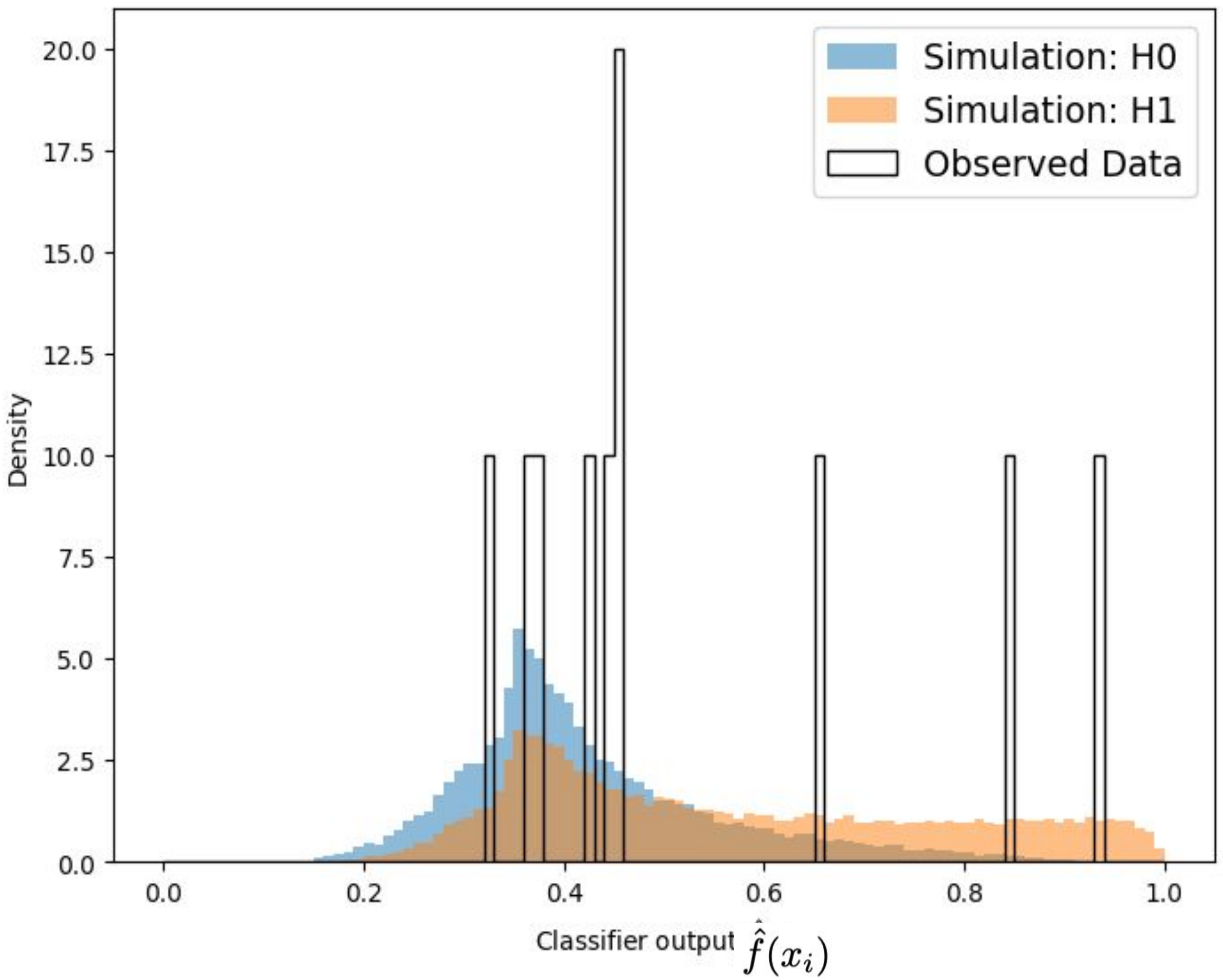

$$\boxed{\mathcal{L}[f] = -\frac{1}{N}\sum_{i=1}^{N} y_i \ln f(x_i) + (1-y_i)\ln(1-f(x_i))}$$

- Good discrimination between $\mathcal{H}_0$ and $\mathcal{H}_1$
- Observed data (10 samples) $\rightarrow$ shows a preference for $\mathcal{H}_1$

Inference with a classifier

Frequentist inference

$$t_\theta = -2\ln\left(\frac{p(\mathcal{D}|\theta)}{p(\mathcal{D}|\theta_0)}\right)$$

$$\frac{\hat{f}(x_i)}{1-\hat{f}(x_i)} \approx \frac{p(x_i|\mathcal{H}_1)}{p(x_i|\mathcal{H}_0)}$$

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Frequentist inference is defined over (hypothetical) repetitions of the experiment

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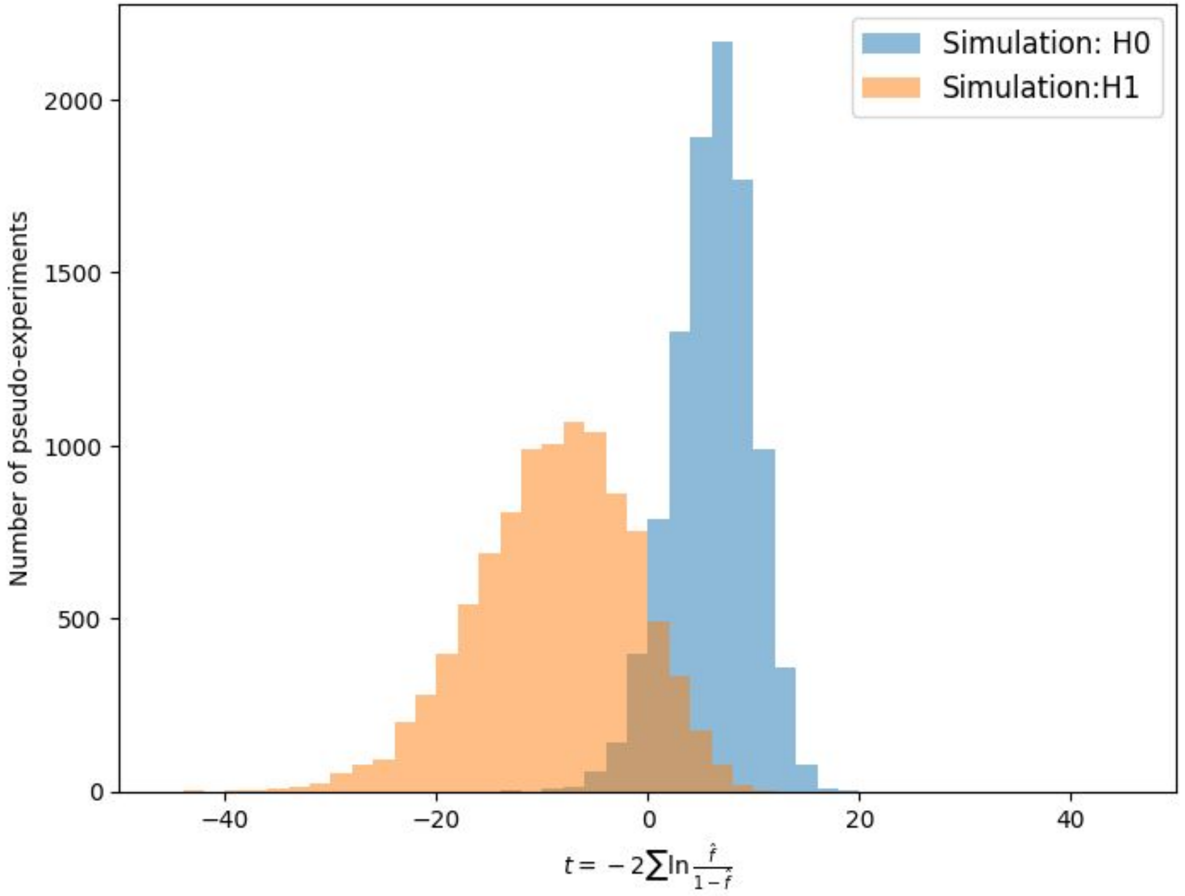

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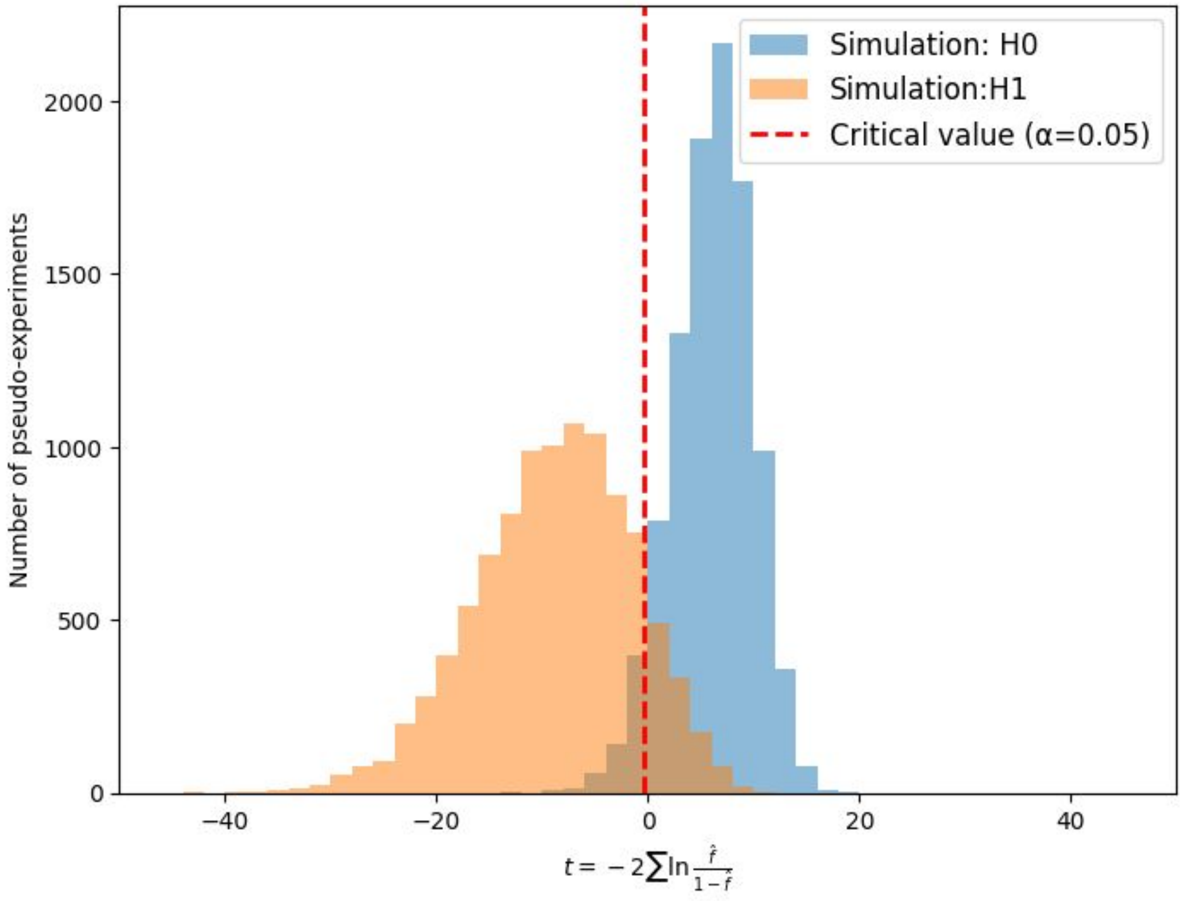

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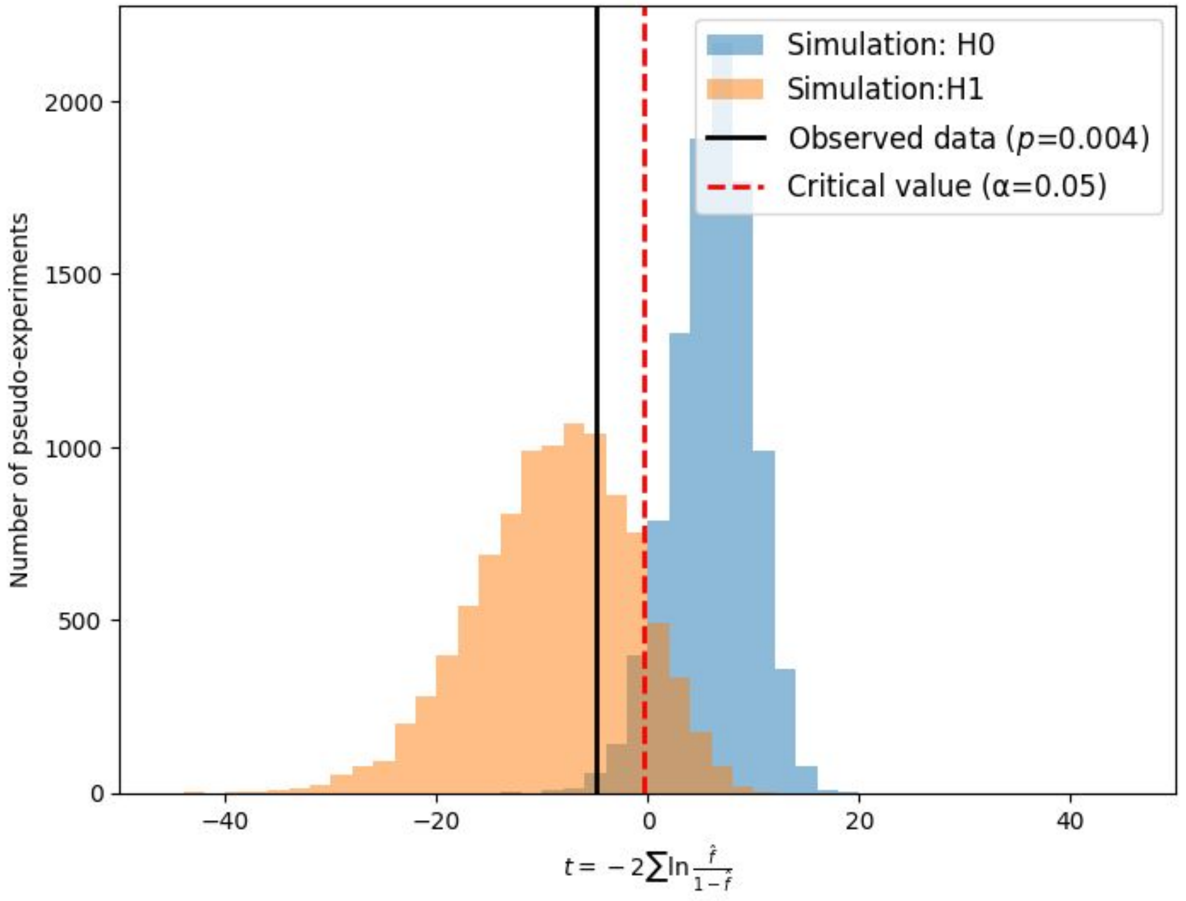

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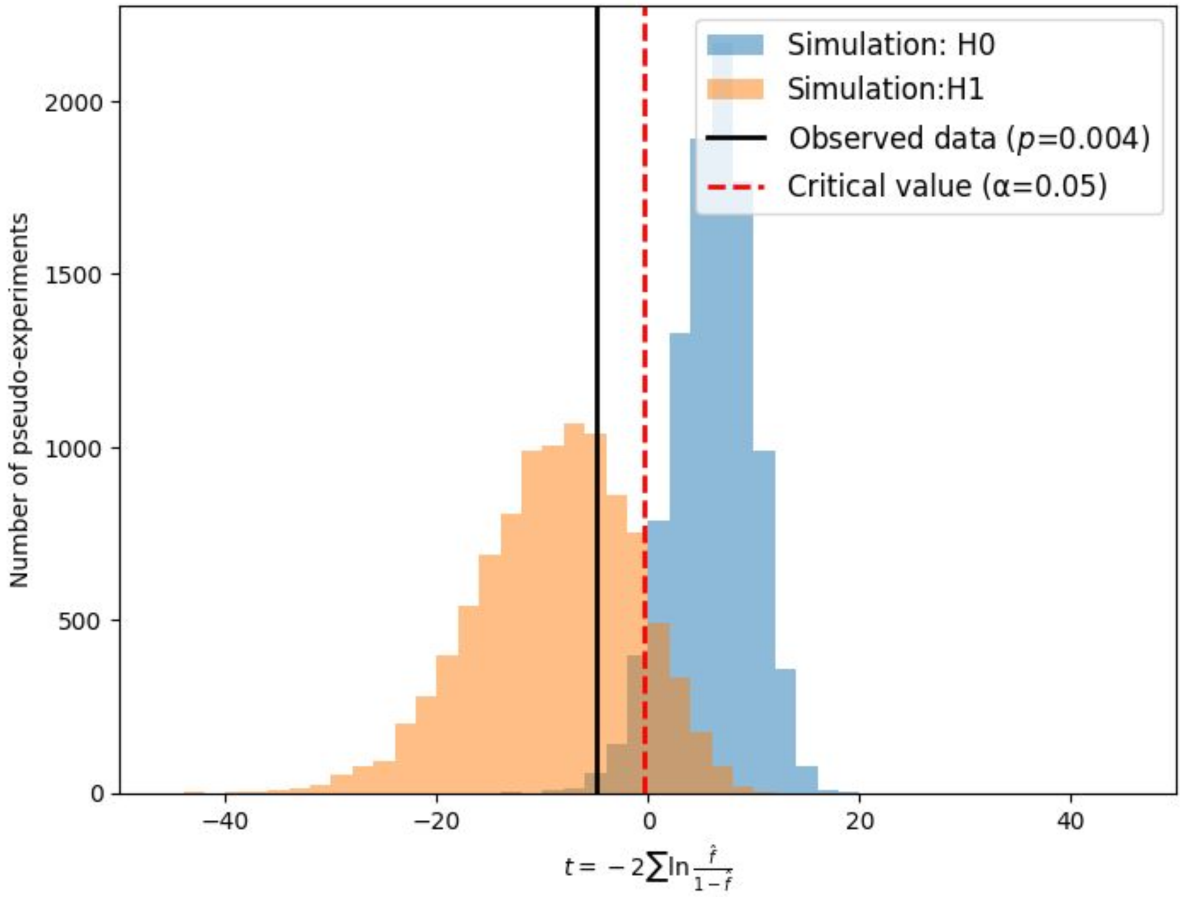

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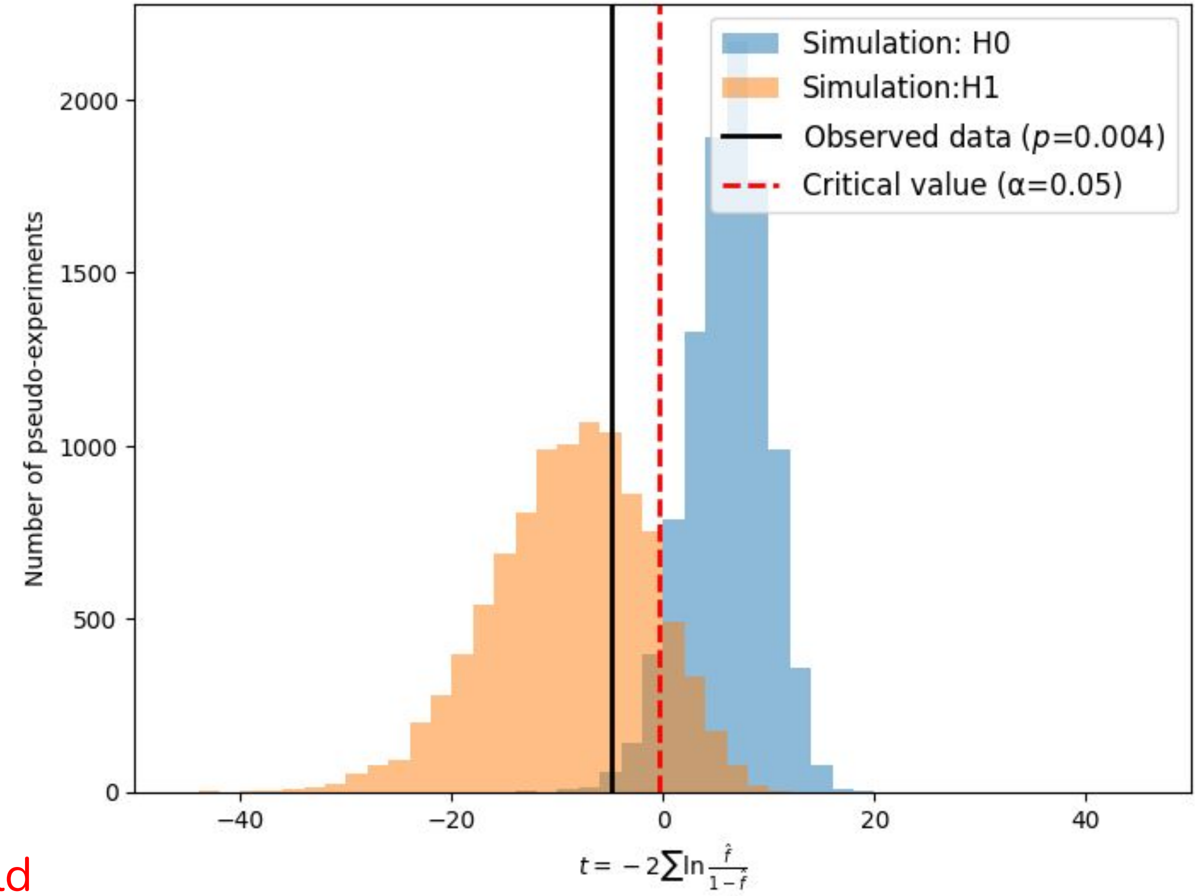

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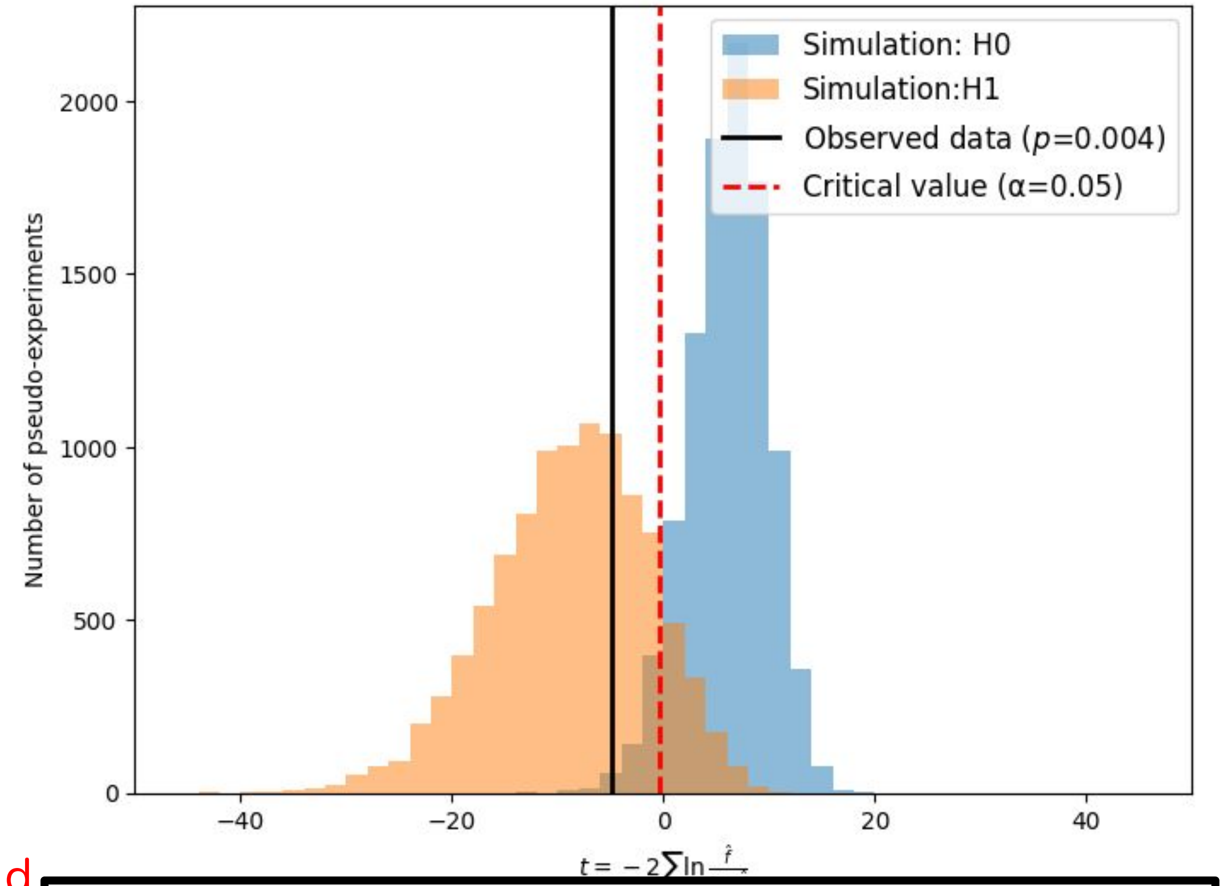

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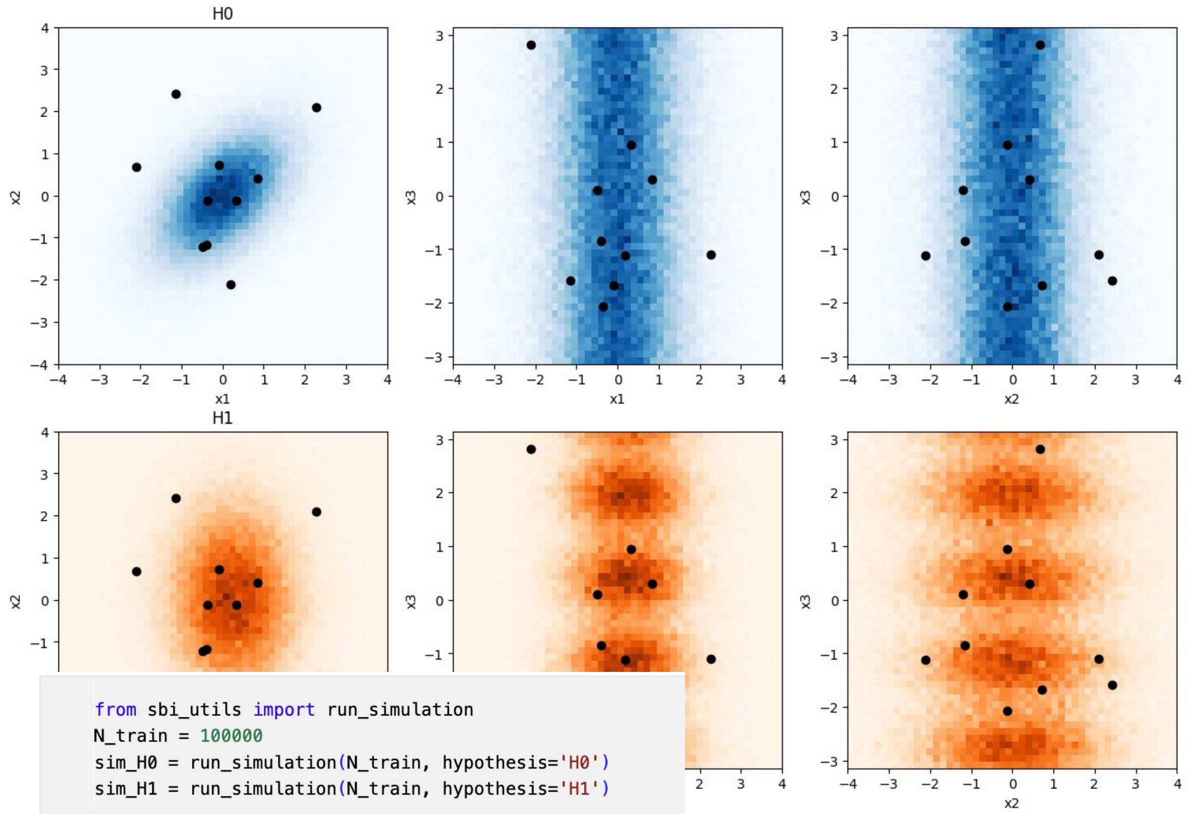
Lear

Particle A is spin-1

Summary: hypothesis testing

- We were presented with a research problem with 10 data samples and an unknown (intractable) likelihood: $p(x|\theta)$
- Nevertheless, we had access to a faithful simulation of the data: $x_i^{\text{sim}} \sim p(x|\theta)$
- We trained a binary classifier over full (3D) feature space to distinguish $\mathcal{H}_0$ (spin-0) from $\mathcal{H}_1$ (spin-1)
- Use output of classifier to approximate log-likelihood-ratio test-statistic → compare observed data to pseudo-experiments
- Our data was inconsistent with $\mathcal{H}_0$ with a p-value of 0.004 → We reject the null hypothesis and conclude A is spin-one!

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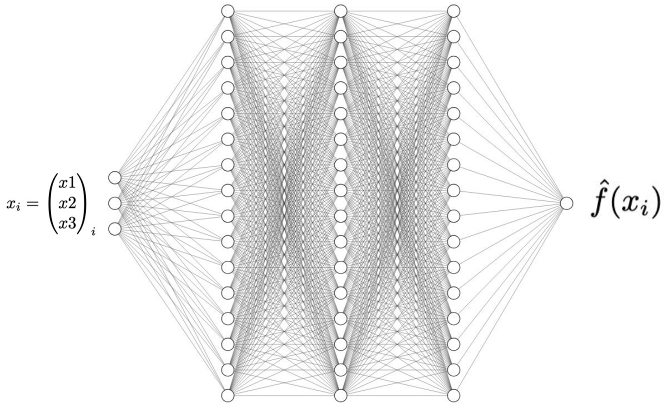
```
[15] ✓ 0.3s



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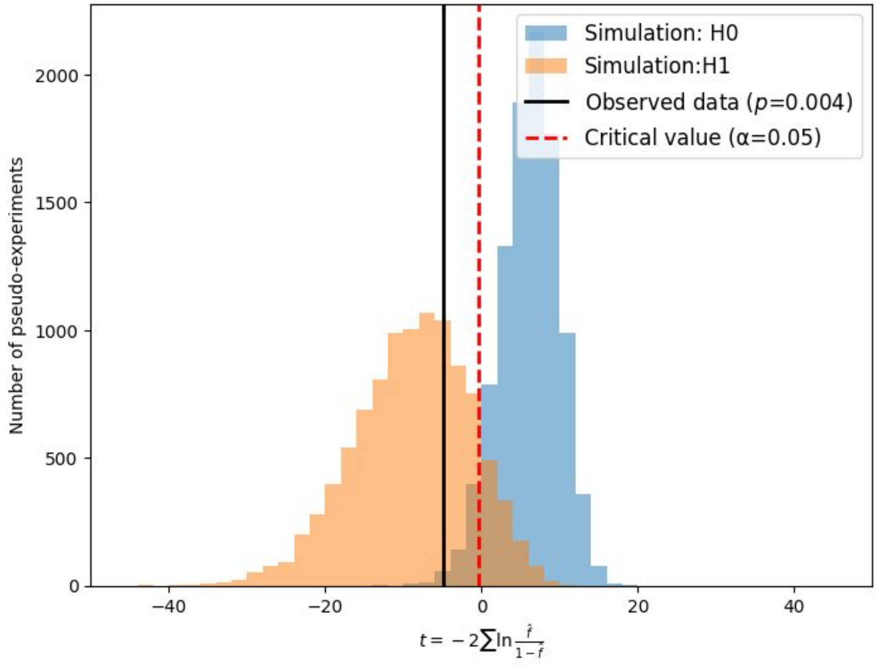

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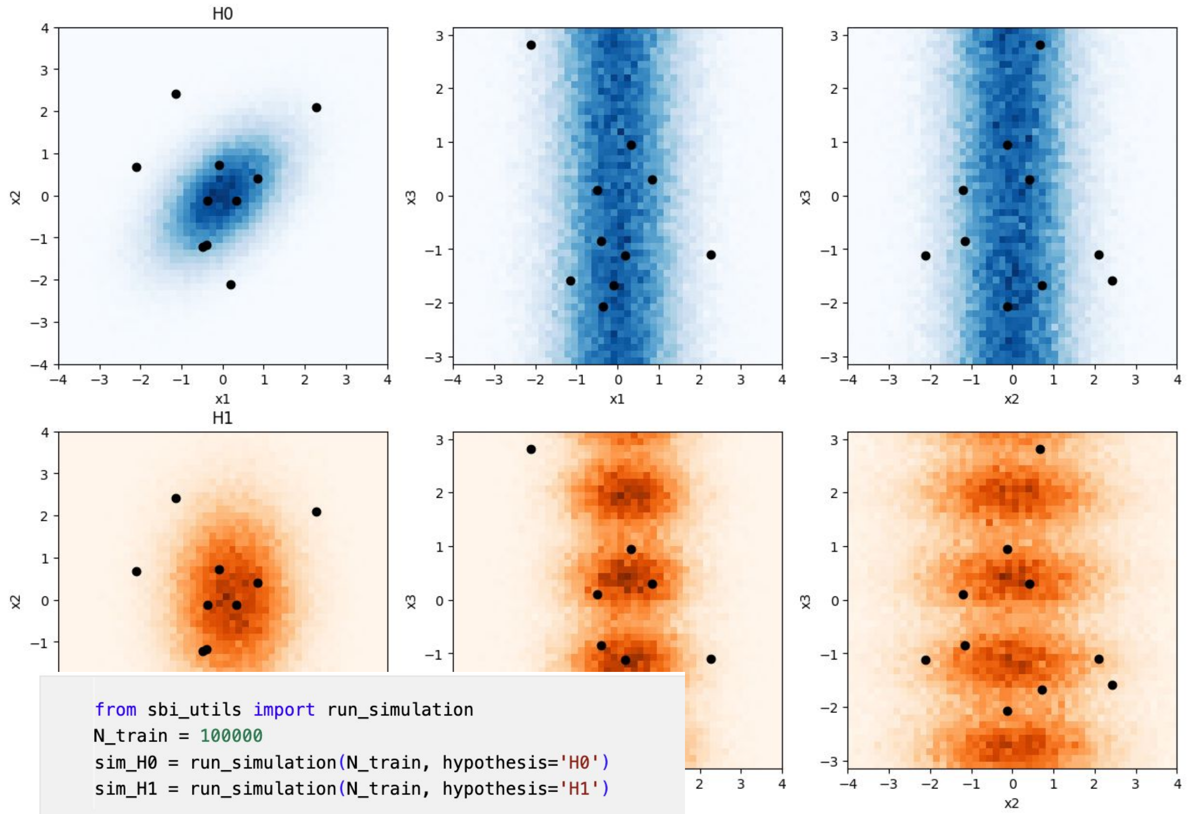


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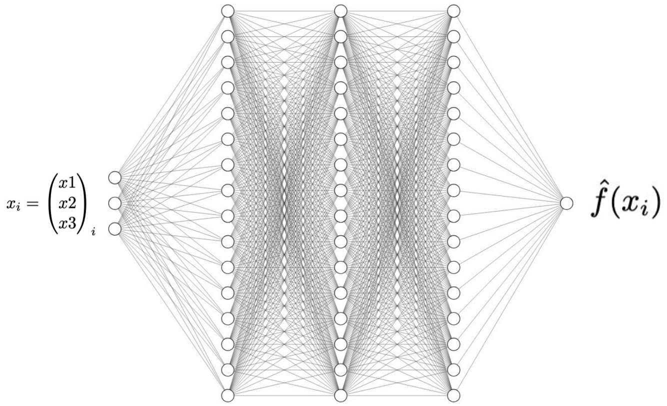

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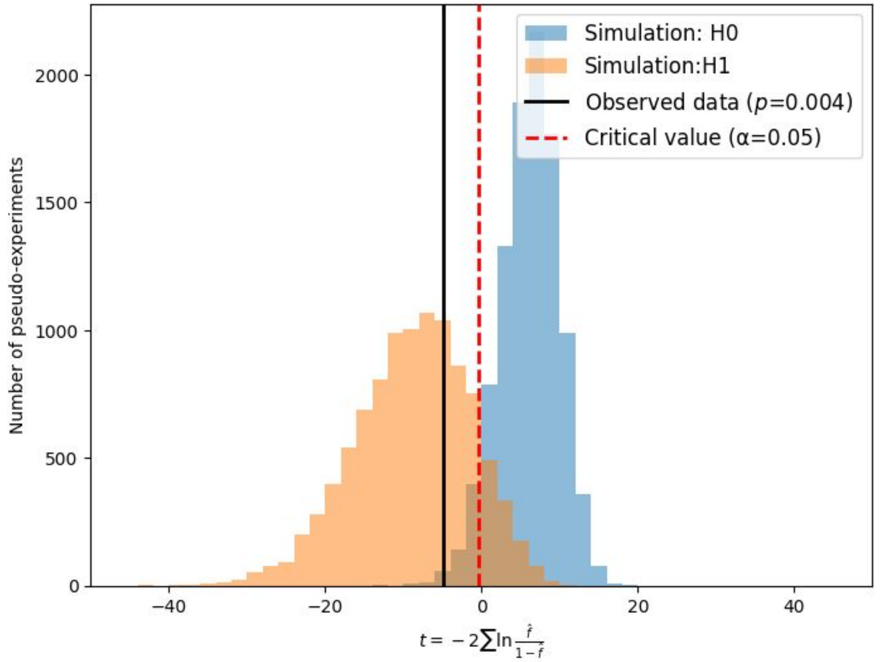
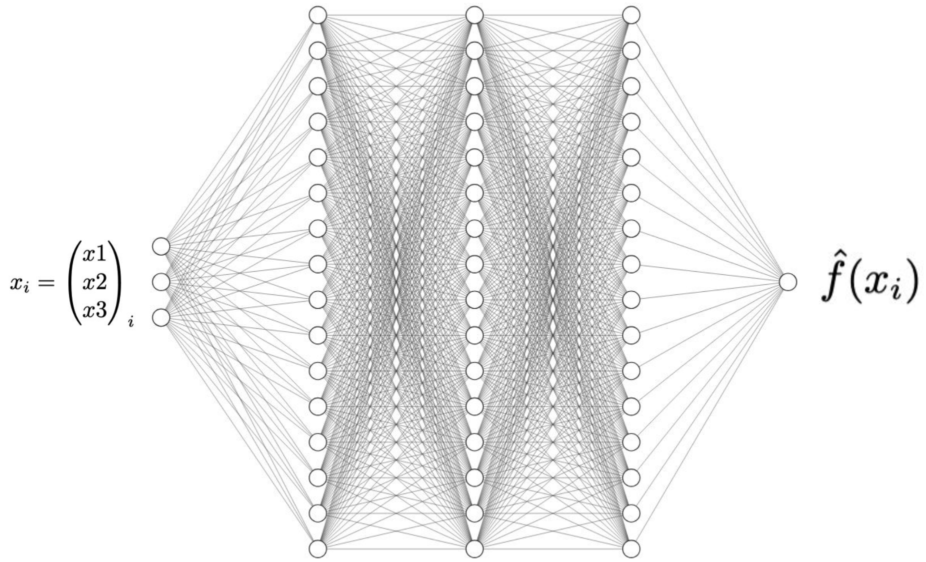


- End-to-end example of using a ML classifier for SBI (hypothesis testing)!
  - **Key: This is not architecture specific and generalises to more complex data**

Amortized inference

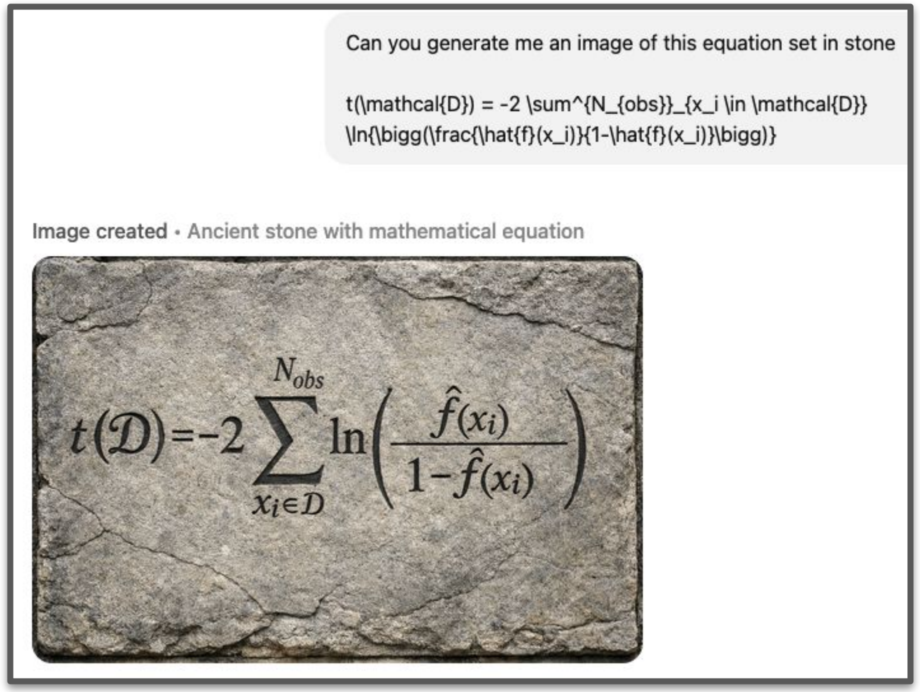


- Classifier output is just a function defined over the feature space: $\hat{f}(x_i)$

- Assuming that the experimental conditions remain the same (i.e. the probability density does not change), we can simply re-calculate the test-statistic for any new observations:

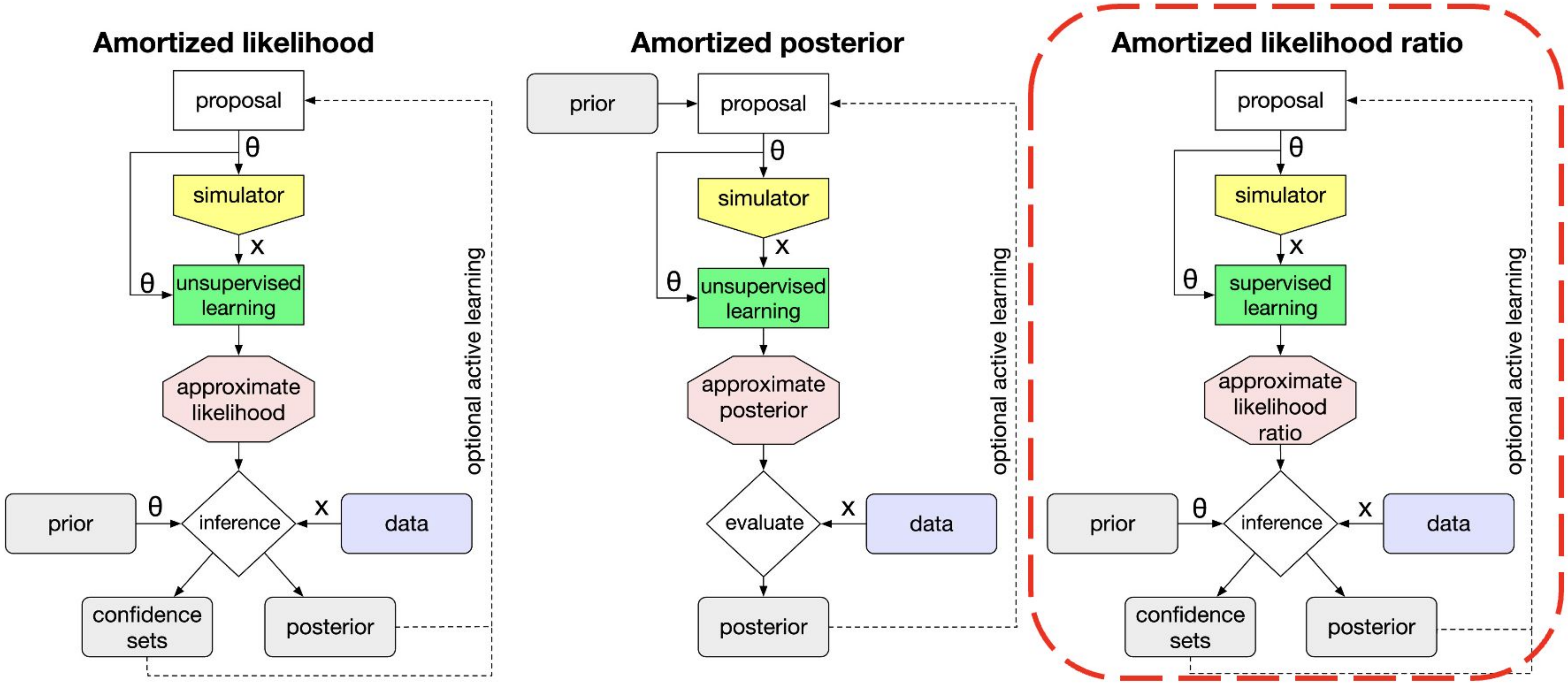
$$t \equiv t(\mathcal{D}) = -2 \sum_{x_i \in \mathcal{D}}^{N_{obs}} \ln\left(\frac{\hat{f}(x_i)}{1 - \hat{f}(x_i)}\right)$$

- **Inference procedure is “amortized” for future experiments:**
  - We do not need to retrain the classifier
  - Very useful when dealing with problems with extremely complicated likelihoods



Credit: ChatGPT

3 families of amortised inference

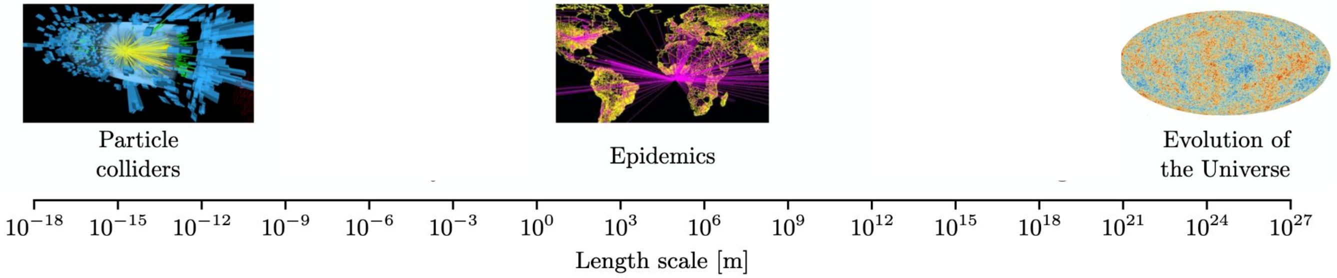


Imperial College London

Adapted slide from Callum

Cranmer et al., 2020

Parameter estimation



- We have shown how to use a classifier for a simple hypothesis test
- More common problem: **parameter estimation**
  - We have a model $p(x|\theta)$ that describes data, where θ is a parameter of the model
  - Use observed data to infer θ i.e. extract best fit value and confidence intervals
  - θ is e.g. mass of a new particle produced at LHC, R_0 of a new infectious disease, Hubble constant governing Universe expansion
- For this inference task, we need to learn the conditional probability density ratio: $$\boxed{\frac{p(x|\theta)}{p(x|\theta_0)}}$$
- *N.B. extending previous idea to "composite hypothesis testing" over ensemble of hypotheses* $\frac{p(x|\mathcal{H}_1)}{p(x|\mathcal{H}_0)} \longrightarrow \frac{p(x|\{\mathcal{H}_1\}_\theta)}{p(x|\mathcal{H}_0)}$
- Log-likelihood ratio test-statistic becomes conditional on the parameter θ: $$\boxed{t(\mathcal{D}|\theta) = -2\sum_{x_i \in \mathcal{D}}^{N_{obs}} \ln \frac{p(x_i|\theta)}{p(x_i|\theta_0)}}$$
  - This is what we will use for inference!

Frequentist parameter estimation

c.f. maximum likelihood estimate $t(\mathcal{D}|\hat{\theta}) = \min[t(\mathcal{D}|\theta)] \equiv t_{\min}$

- For a fixed dataset, $\mathcal{D}$, the point in parameter space $\hat{\theta}$ which minimizes the test-statistic is the best-fit value

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- What about confidence interval (CI) estimation i.e. the uncertainty in θ ?
  - Frequentist interpretation: e.g. 68% CI = a range in θ that covers the true parameter value in 68% of repeated experiments
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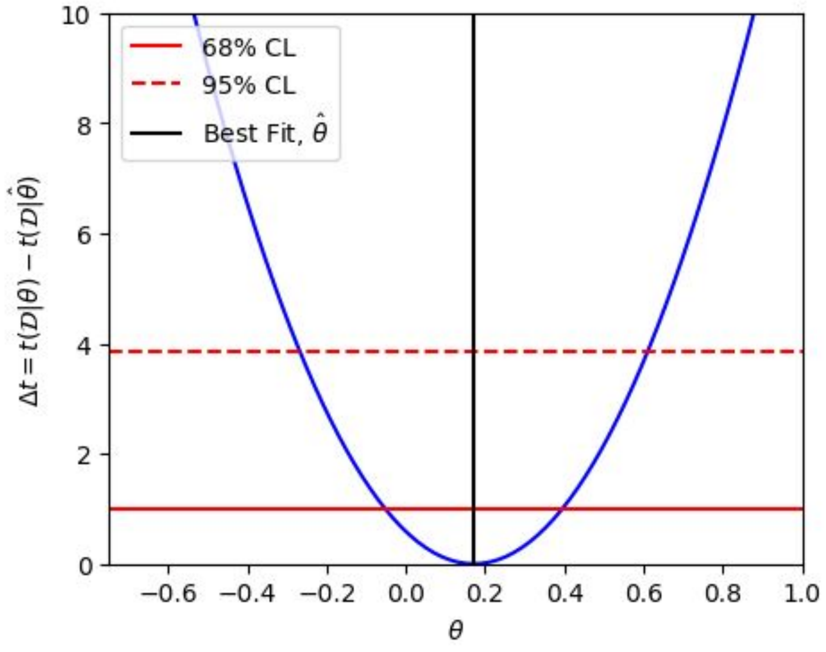
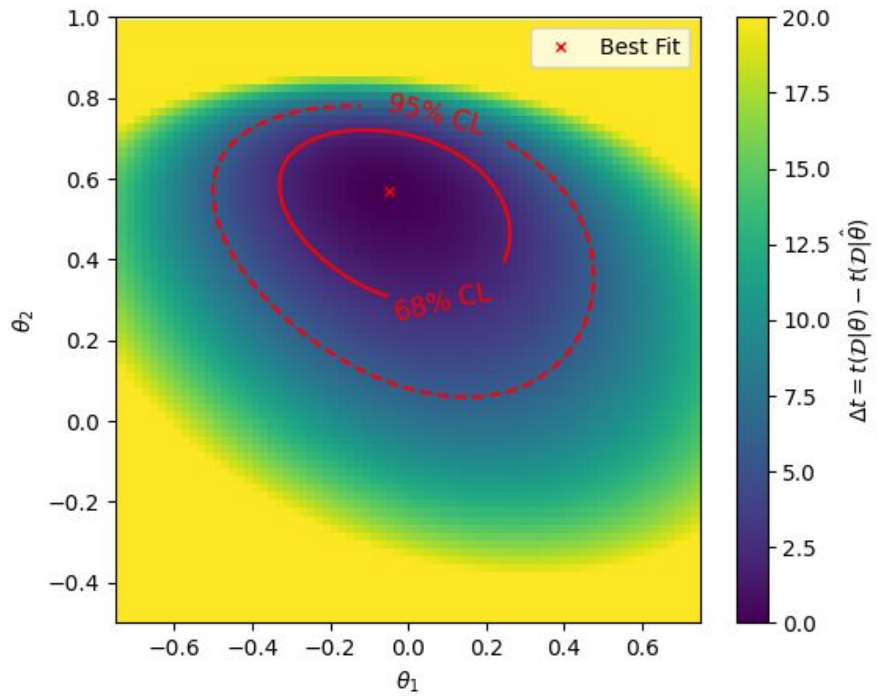
  - (Most cases) use Wilks' Theorem: "(delta) log-likelihood ratio test statistic asymptotically ($N_{obs} \rightarrow \infty$) approaches the χ^2 distribution with *n* degrees of freedom, where *n* is the dimensionality of θ (under the null hypothesis)"
    - In a nutshell: calculate $\boxed{\Delta t(\mathcal{D}|\theta) = t(\mathcal{D}|\theta) - t(\mathcal{D}|\hat{\theta})}$ and use properties of the χ^2 distribution to infer confidence intervals



1D parameter example



2D parameter example

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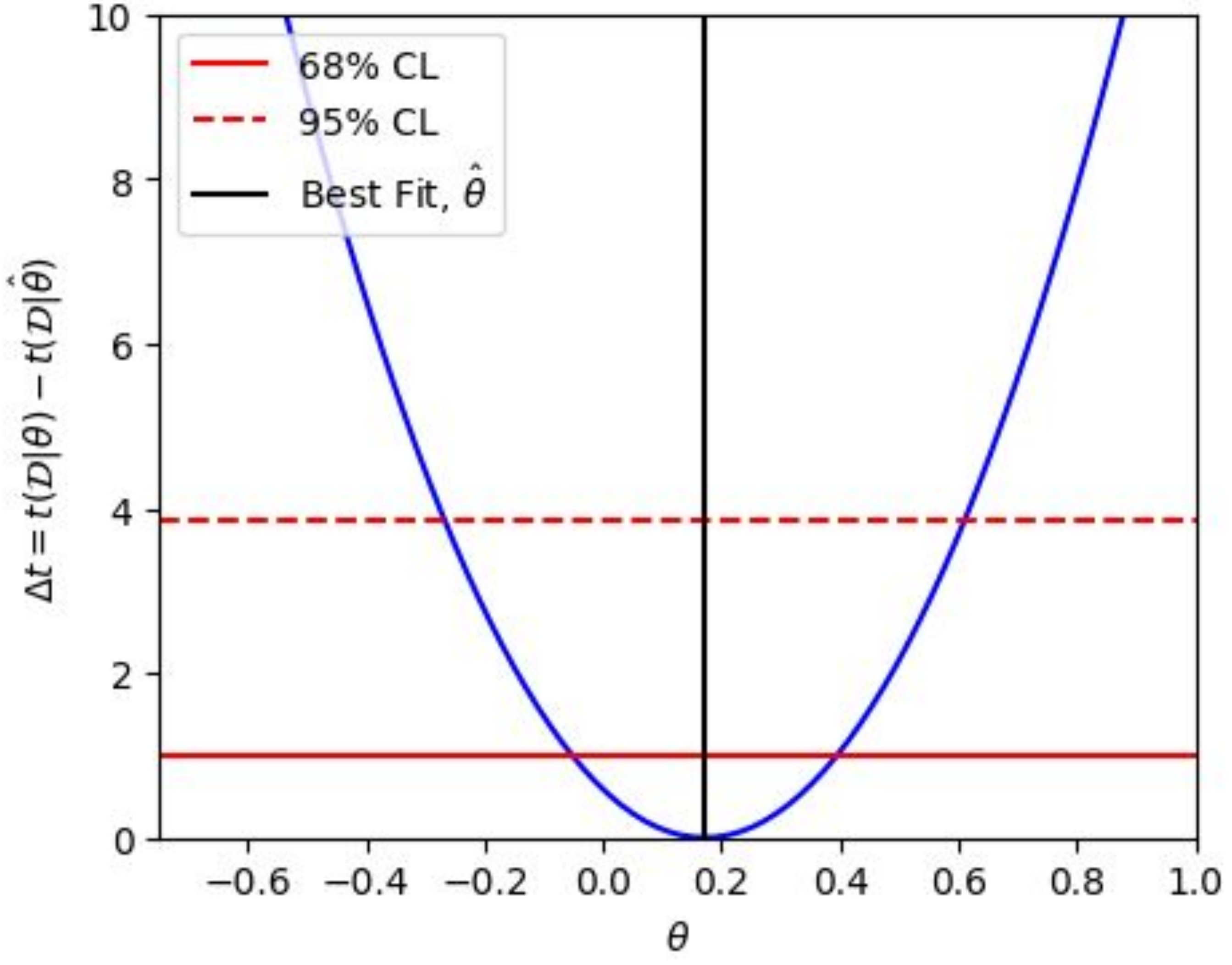

1D example:

- 68% CL is region defined by $\Delta t < 1$
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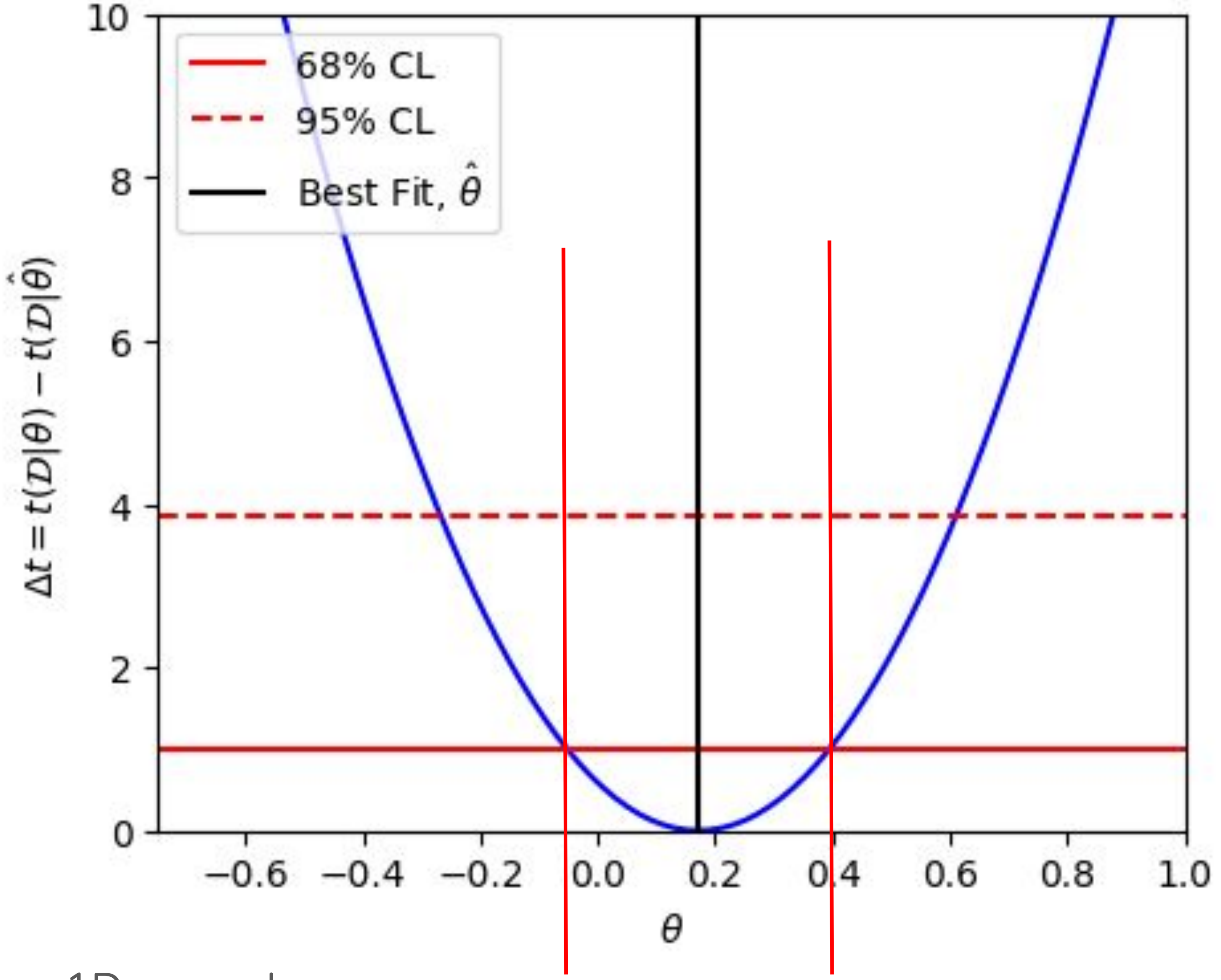

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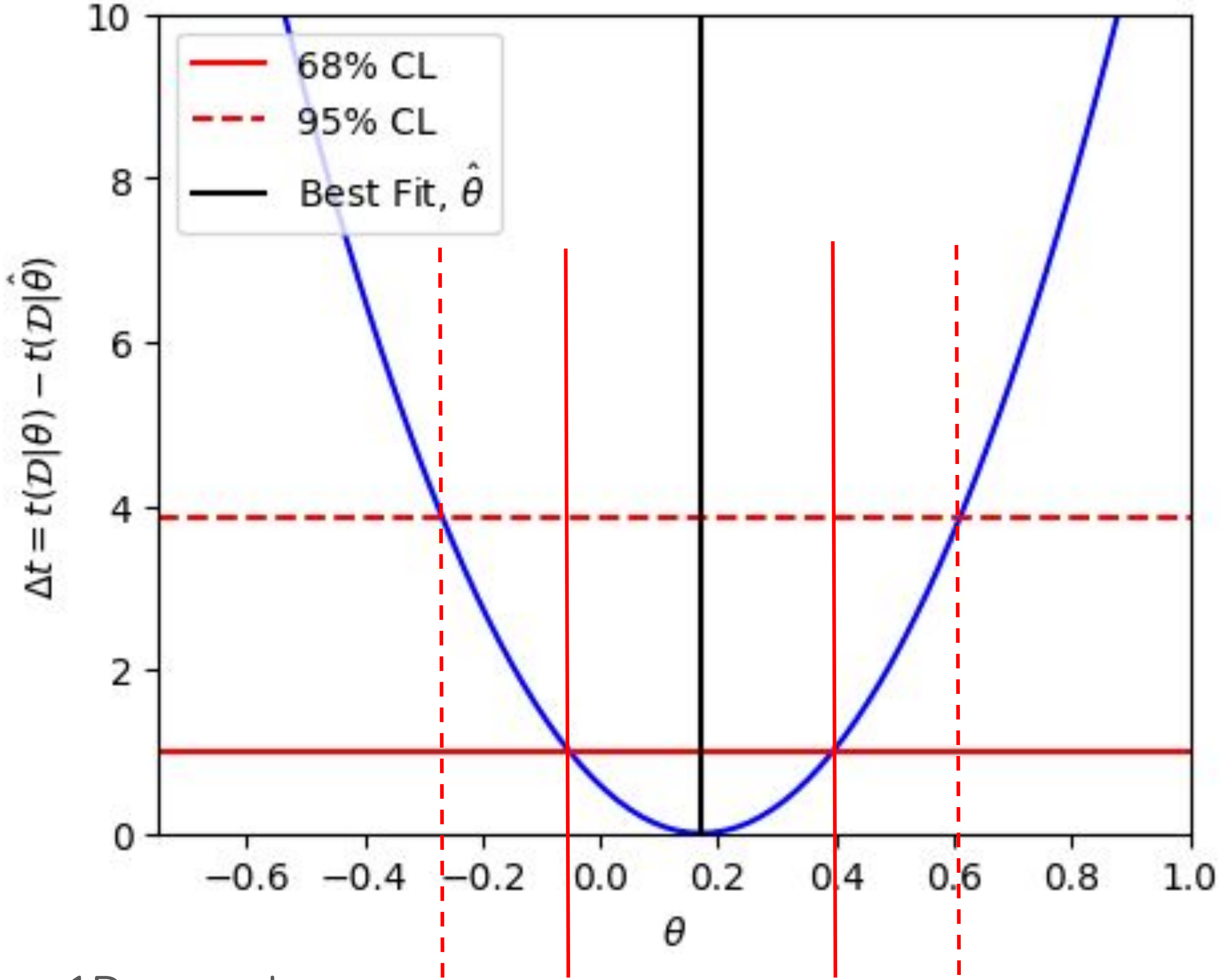

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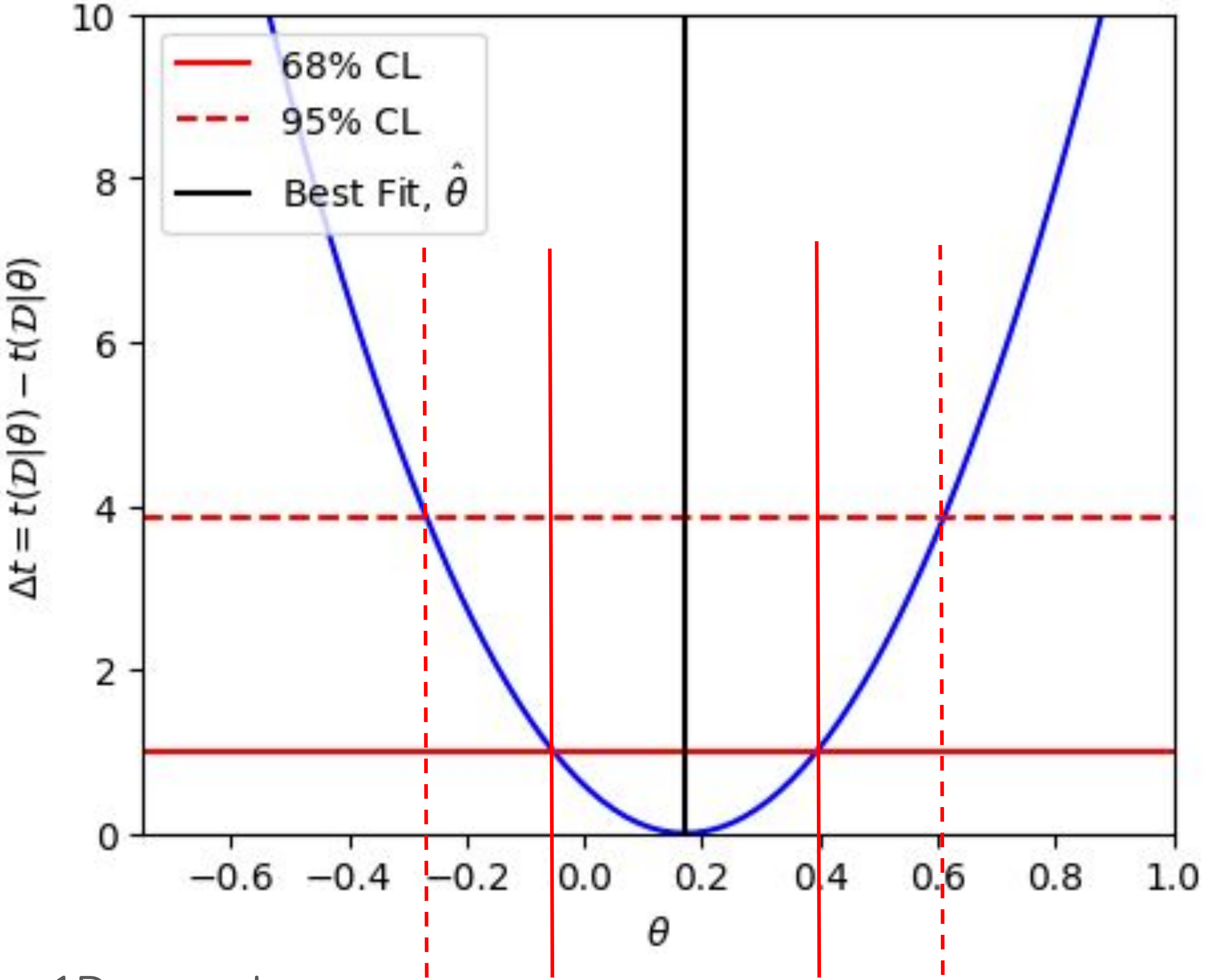

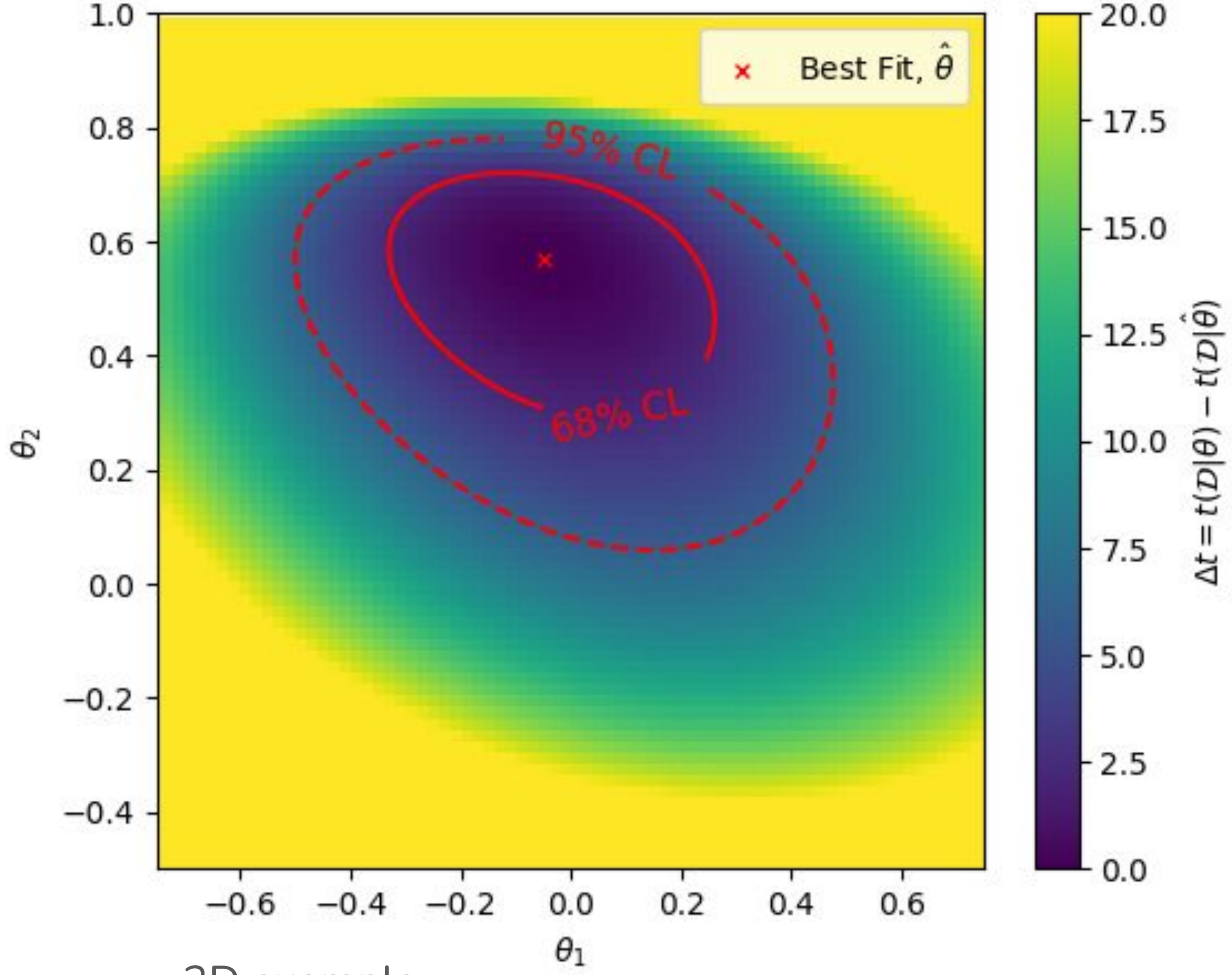

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2D example:

- 68% CL is region defined by $\Delta t < 2.30$
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Parameter estimation with classifiers

$$\frac{p(x_i|\theta)}{p(x_i|\theta_0)}$$

- How to use Machine Learning to estimate the <u>conditional</u> log-likelihood ratio test-statistic for inference?

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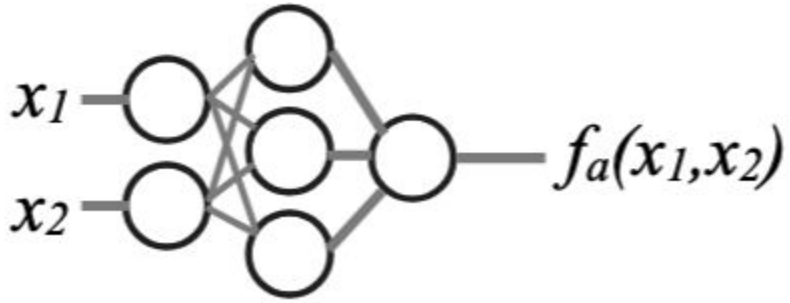

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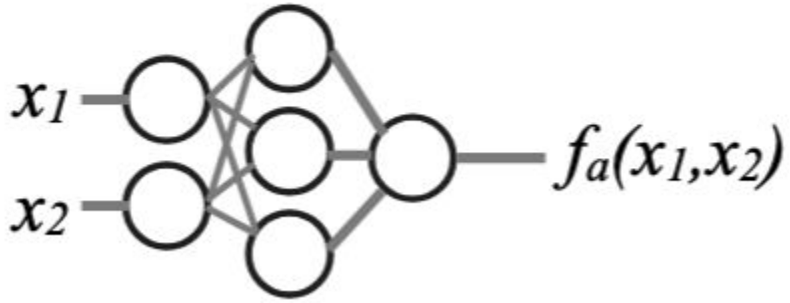
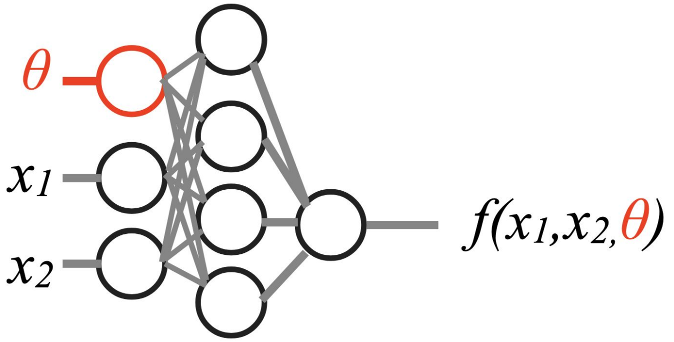


- Parametric classifier is a function of both input features and parameters: $\hat{f}(x_i, \theta_i)$
  - Result that is parameterized in terms of θ
  - Different output values for different values of the parameters θ

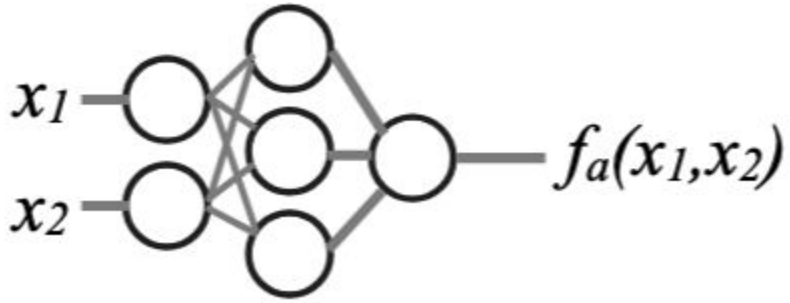


Parameter estimation with classifiers

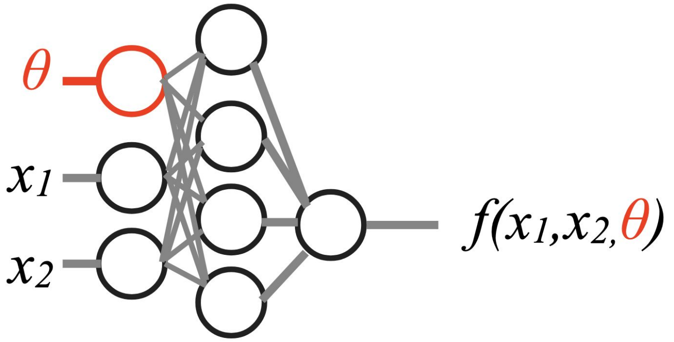
$$\frac{p(x_i|\theta)}{p(x_i|\theta_0)}$$

- **How to use Machine Learning to estimate the conditional log-likelihood ratio test-statistic for inference?**
  - Parametric classifier. simple idea of extending input feature space from $x \longrightarrow x, \theta$

    - Standard classifier is a function of the input features: $\hat{f}(x_i)$
      - Evaluates to a (single) real number



    - Parametric classifier is a function of both input features and parameters: $\hat{f}(x_i, \theta_i)$
      - Result that is parameterized in terms of θ
      - Different output values for different values of the parameters θ



- **But how do we train these classifiers for inference?**

Parameter estimation with classifiers

$$\frac{p(x_i|\theta)}{p(x_i|\theta_0)}$$

- **How to use Machine Learning to estimate the conditional log-likelihood ratio test-statistic for inference?**
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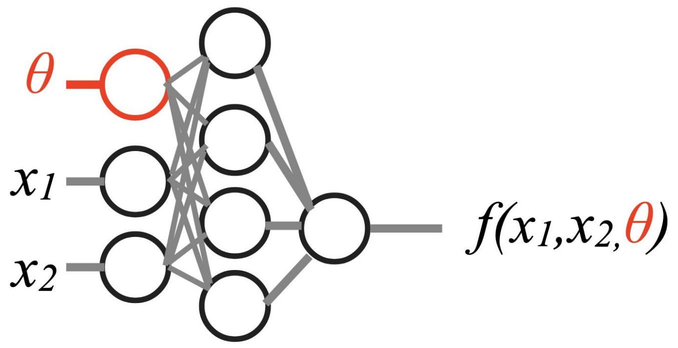

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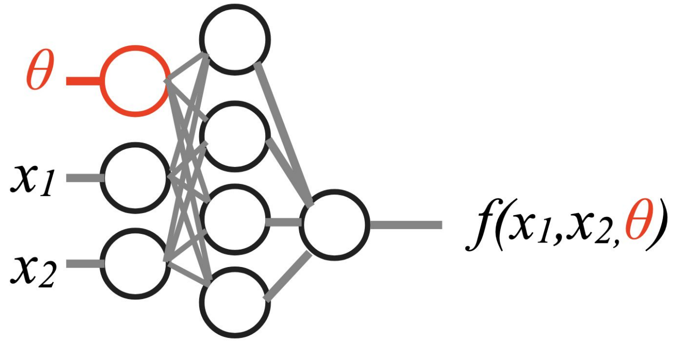
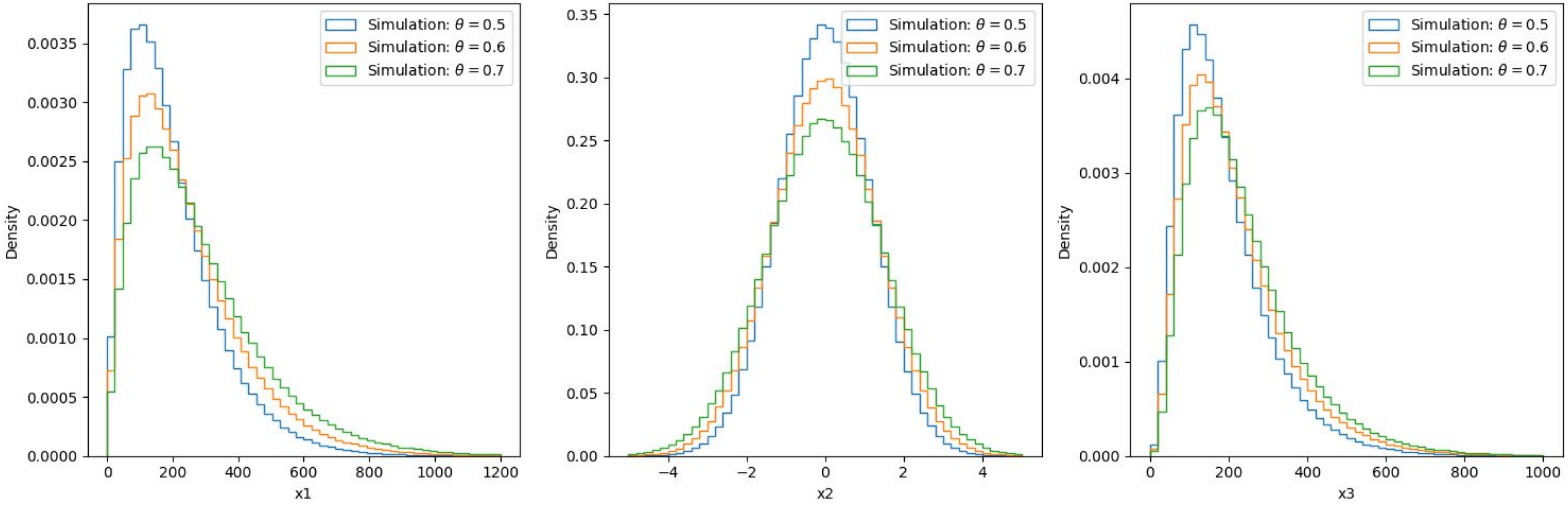
    - e.g. 3D input feature space (`x1,x2,x3`) with one parameter θ





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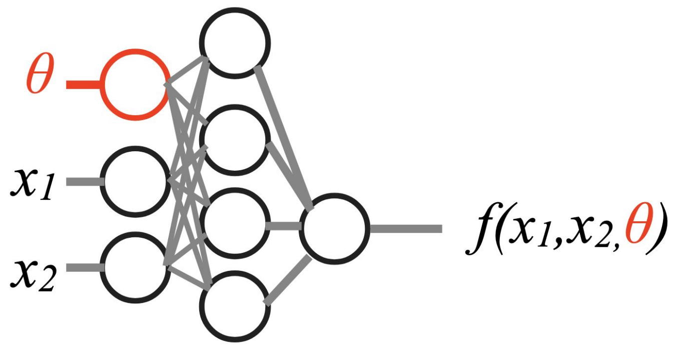
  - Use simulation to train a binary classifier, $f(x_i, \theta_i)$, by minimizing BCE loss:



$$\mathcal{L}[f] = -\frac{1}{N}\sum_{i=1}^{N} y_i \ln f(x_i, \theta_i) + (1 - y_i)\ln\left(1 - f(x_i, \theta_i)\right)$$

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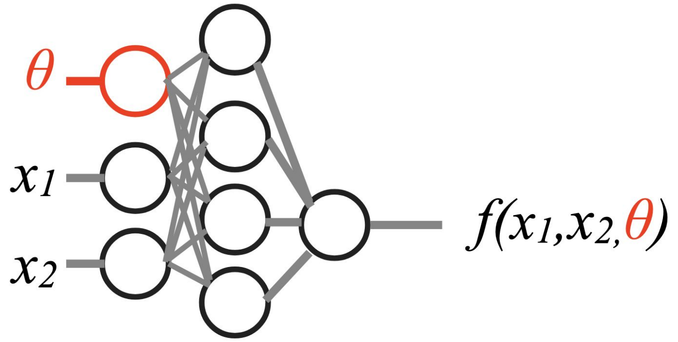

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$\mathcal{H}_0 : y_i = 0$

$\mathcal{H}_1 : y_i = 1$

  - Reference class 0 ($\mathcal{H}_0$): draw samples from simulator with fixed $\theta = \theta_0$: $\boxed{x_i^{\mathcal{H}_0} \sim p(x|\theta_0)}$
    - θ_0 = reference hypothesis. Final parameter estimation is independent of this value, but it helps to pick something sensible
  - Ensemble class 1 ($\{\mathcal{H}_1\}_\theta$): draw samples from simulator with various θ values: $\boxed{x_i^{\mathcal{H}_1}, \theta_i^{\mathcal{H}_1} \sim p(x|\theta)}$
    - If possible, generate samples to be continuous in θ e.g. sampled from uniform distribution over *sensible* range
    - In practice, often simpler to generate sub-samples with discrete steps in θ (interpolates if steps are *sufficiently fine-grained*)

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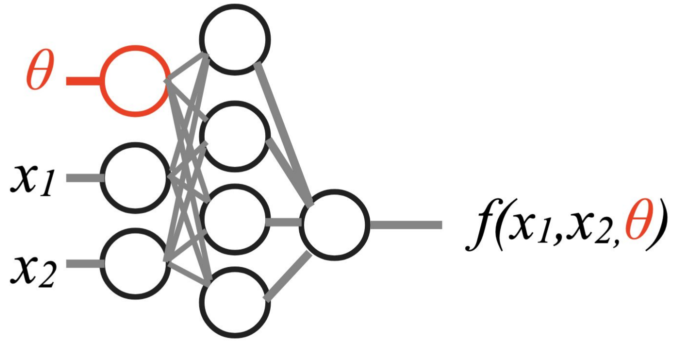

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    - In practice, often simpler to generate sub-samples with discrete steps in θ (interpolates if steps are *sufficiently fine-grained*)
  - Assuming "balanced classes", our trained classifier approximates:

$$\hat{f}(x_i, \theta_i) \approx f(x_i, \theta_i) = \frac{p_{\mathcal{H}_1}(x_i, \theta_i)}{p_{\mathcal{H}_0}(x_i, \theta_0) + p_{\mathcal{H}_1}(x_i, \theta_i)}$$

Likelihood-ratio trick

$$\boxed{\frac{\hat{f}(x_i, \theta_i)}{1 - \hat{f}(x_i, \theta_i)} \approx \frac{p_{\mathcal{H}_1}(x_i, \theta_i)}{p_{\mathcal{H}_0}(x_i, \theta_0)}}$$

Parameter estimation with classifiers

- **How to use Machine Learning to estimate the conditional log-likelihood ratio test-statistic for inference?**
  - We have arrived at an estimator for the "joint" probability density using parametric classifier: $\frac{\hat{f}(x_i, \theta_i)}{1 - \hat{f}(x_i, \theta_i)} \approx \frac{p_{\mathcal{H}_1}(x_i, \theta_i)}{p_{\mathcal{H}_0}(x_i, \theta_0)}$

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    - **Probability theory:** $\boxed{\begin{array}{c} \textit{joint} \quad = \textit{conditional x marginal} \\ p(A, B) = p(A|B) \times p(B) \end{array}}$ $p(B) = \int p(A, B)\, \mathrm{d}A$

$$\boxed{\frac{\hat{f}(x_i, \theta_i)}{1 - \hat{f}(x_i, \theta_i)} \approx \frac{p(x_i|\theta_i) p_{\mathcal{H}_1}(\theta_i)}{p(x_i|\theta_0) p_{\mathcal{H}_0}(\theta_0)}}$$

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  - Now comes the key training "trick" - align the marginal of $\mathcal{H}_0$ with $\{\mathcal{H}_1\}_\theta$

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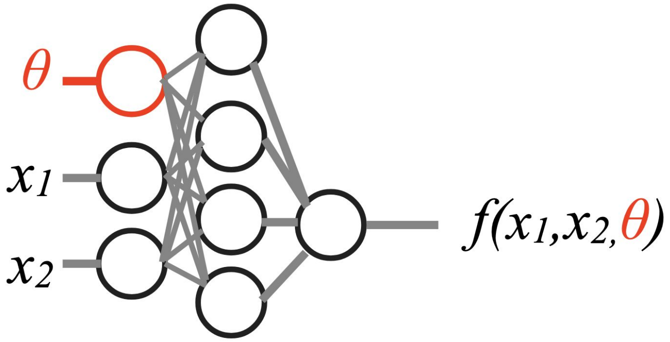
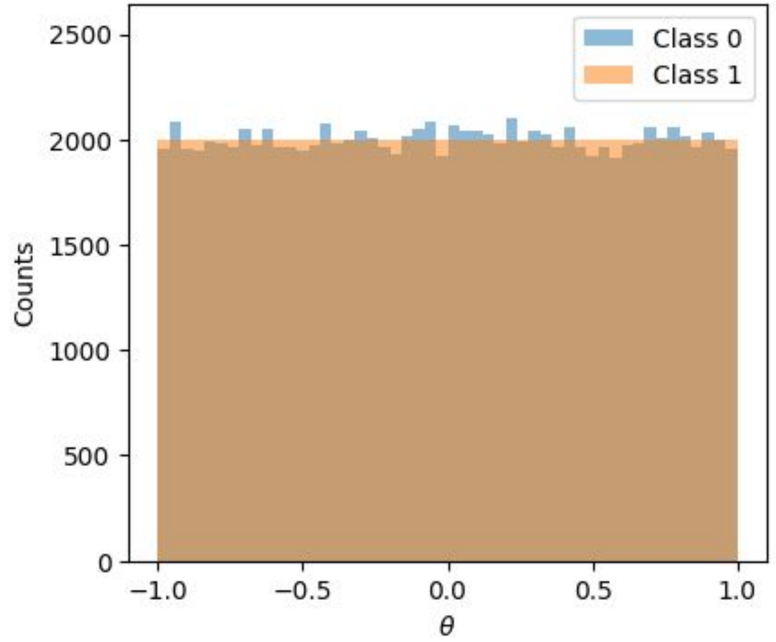
    - When training the network, rather than using $\theta = \theta_0$ for Class 0 samples, you must pair each $x_i^{\mathcal{H}_0}$ with a randomly sampled value of $\theta_i^{\mathcal{H}_0} \sim p_{\mathcal{H}_1}(\theta)$
    - Enforces $p(\theta)$ to be the same between Class 0 and Class 1





e.g. simple 1D parameter example

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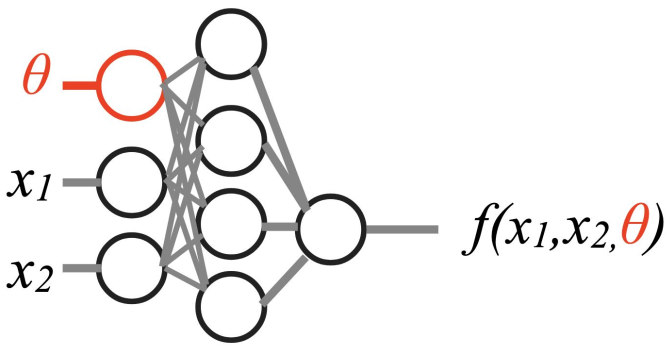

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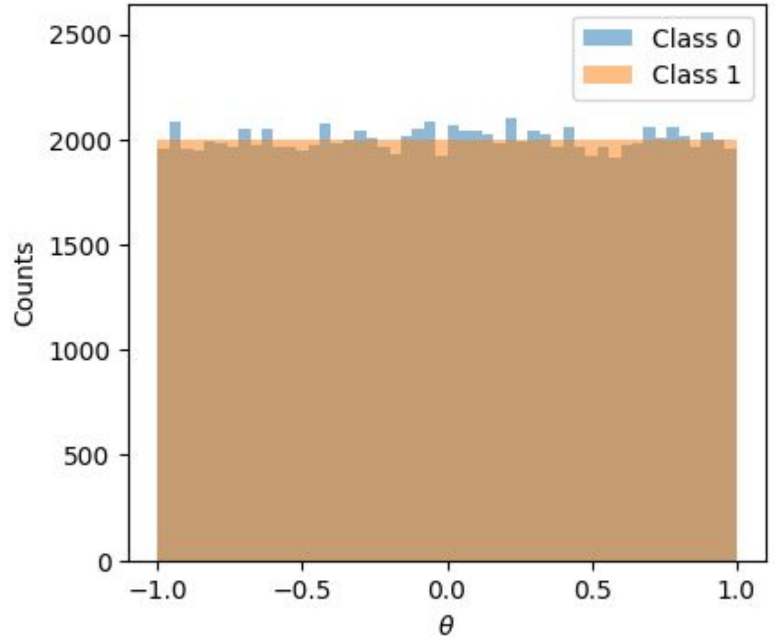

e.g. simple 1D parameter example

- Use output of parametric binary classifier trained in this way to approximate conditional likelihood ratio

Parameter estimation with classifiers

- **How to use Machine Learning to estimate the conditional log-likelihood ratio test-statistic for inference?**

$$\boxed{\frac{\hat{f}(x_i,\theta_i)}{1-\hat{f}(x_i,\theta_i)} \approx \frac{p(x_i|\theta_i)}{p(x_i|\theta_0)}}$$

$$\boxed{t(\mathcal{D}|\theta) = -2\sum_{x_i\in\mathcal{D}}^{N_{obs}} \ln\frac{p(x_i|\theta)}{p(x_i|\theta_0)} \approx -2\sum_{x_i\in\mathcal{D}}^{N_{obs}} \ln\frac{\hat{f}(x_i,\theta_i)}{1-\hat{f}(x_i,\theta_i)}}$$

Key takeaway: we can use output of parametric binary classifier trained with simulation to approximate conditional log-likelihood ratio test-statistic

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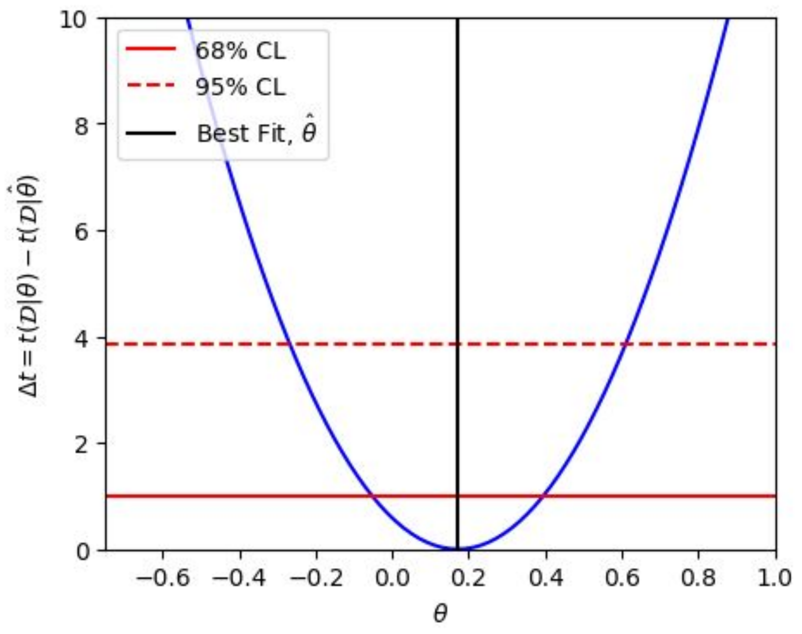
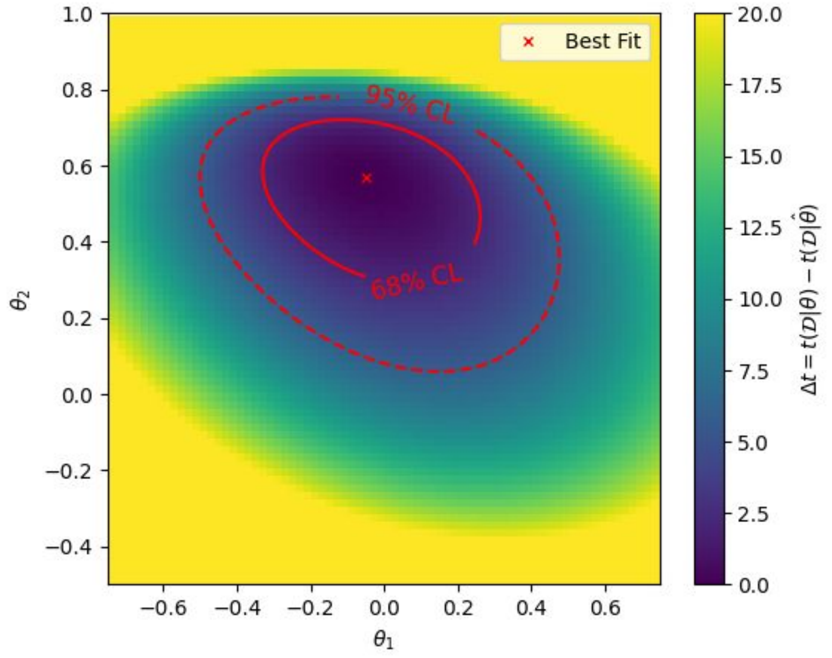
- For a given dataset $\mathcal{D}$, we evaluate the classifier (and subsequently the approximate test-statistic) over θ parameter space
- **Use $\Delta t(\mathcal{D}|\theta)$ to infer best-fit values and confidence intervals**





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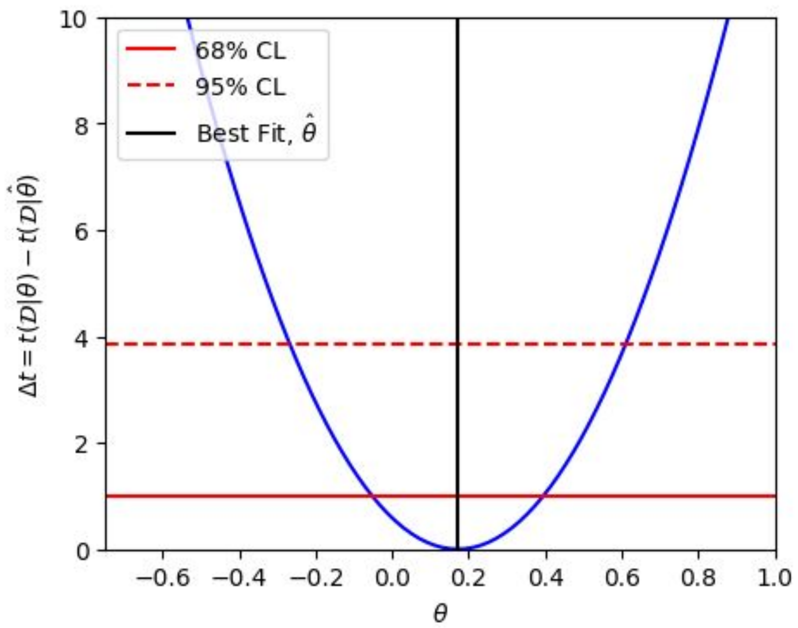
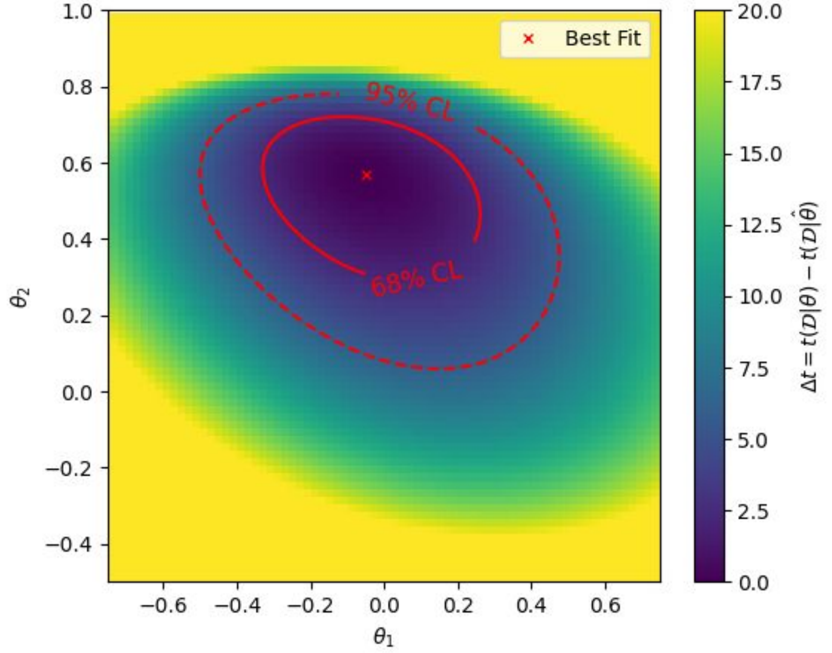
- Function of the full input feature (x) space





"Neural SBI" helps us squeeze every drop of information out of the data

Parameter estimation example

- parameter_estimation.ipynb
- 2D parameter estimation task: in this example the analytic likelihood **is** known (**2D Gaussian**)
    - We will use a simulator to learn the test-statistic and then compare to the analytic solution
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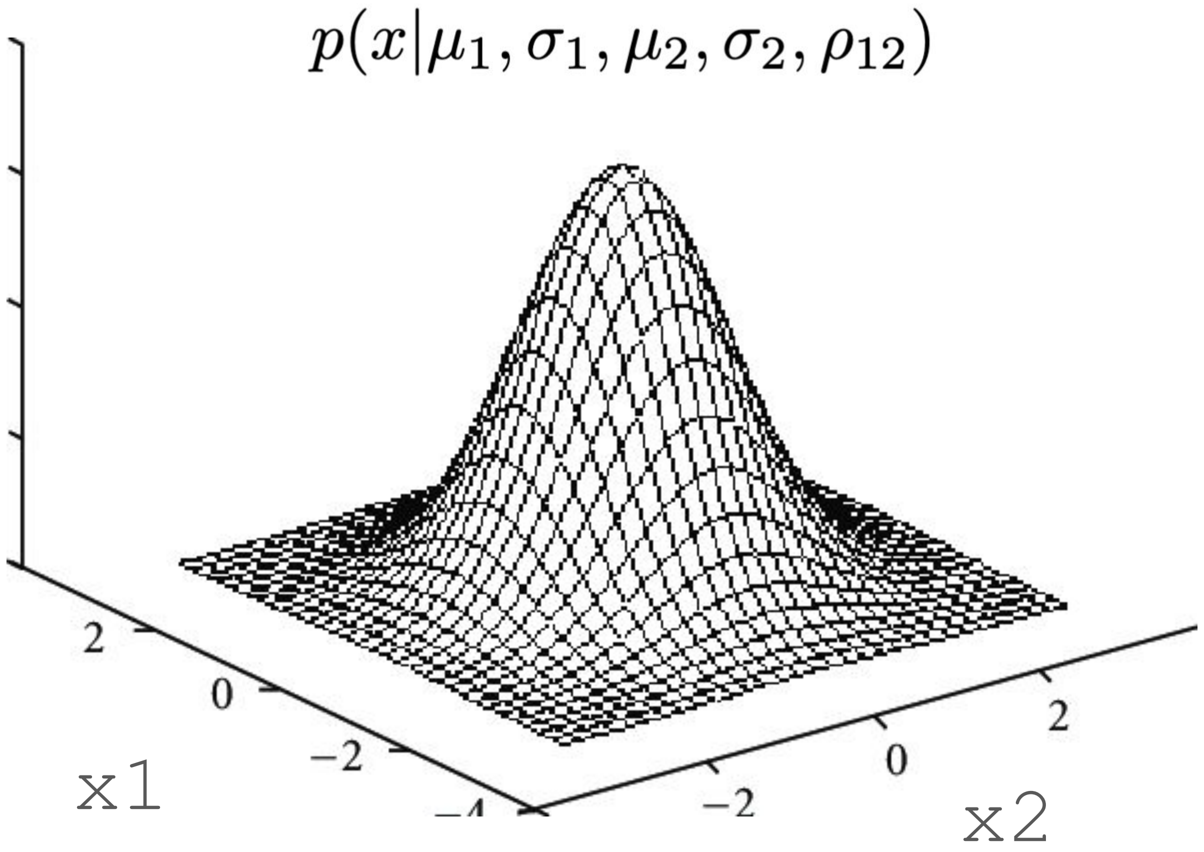

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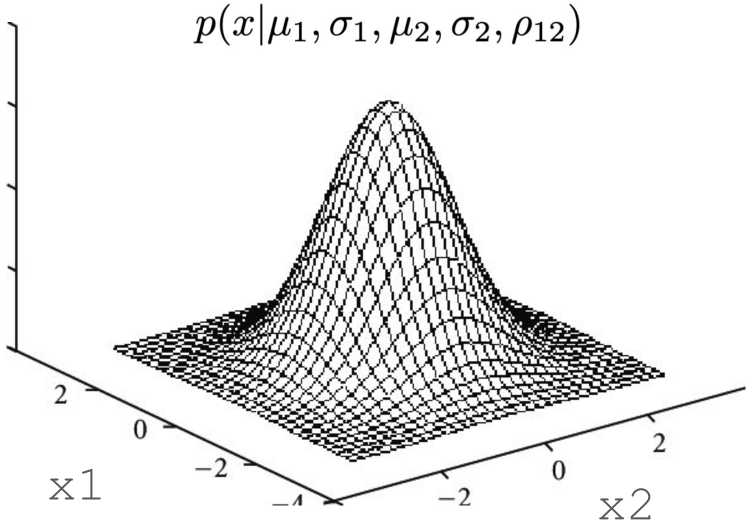
  - Two observables x = (x1, x2) are measured and we have N_{obs} = 20 data points



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  - Mean μ_1 and stdevs σ_1, σ_2 of the 2D Gaussian are already known (= 0, 1, 1)
  - Analytic probability density:

$$\boxed{p(x|\mu_2, \rho_{12}) = \frac{1}{2\pi\sqrt{1-\rho_{12}^2}} \exp\left(-\frac{1}{2(1-\rho_{12}^2)}\left[x_1^2 + (x_2-\mu_2)^2 - 2\rho_{12}x_1(x_2-\mu_2)\right]\right)}$$

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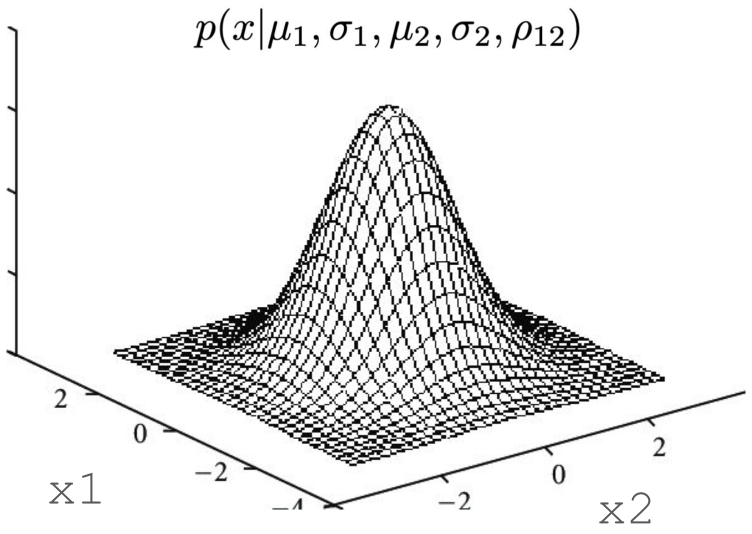

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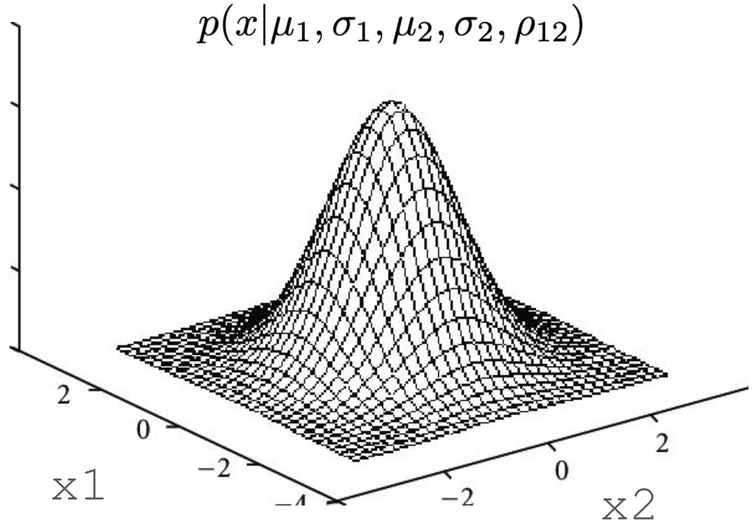

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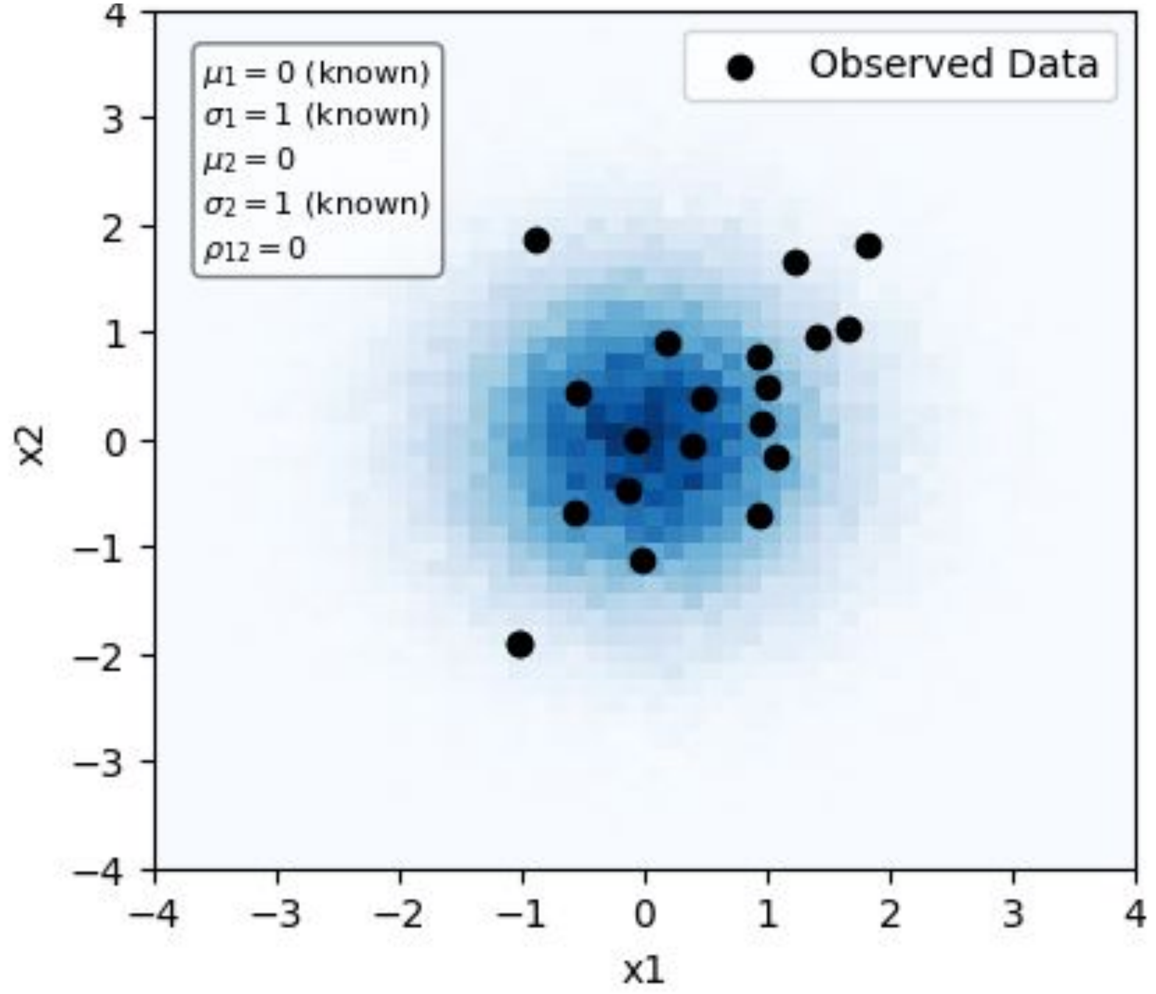
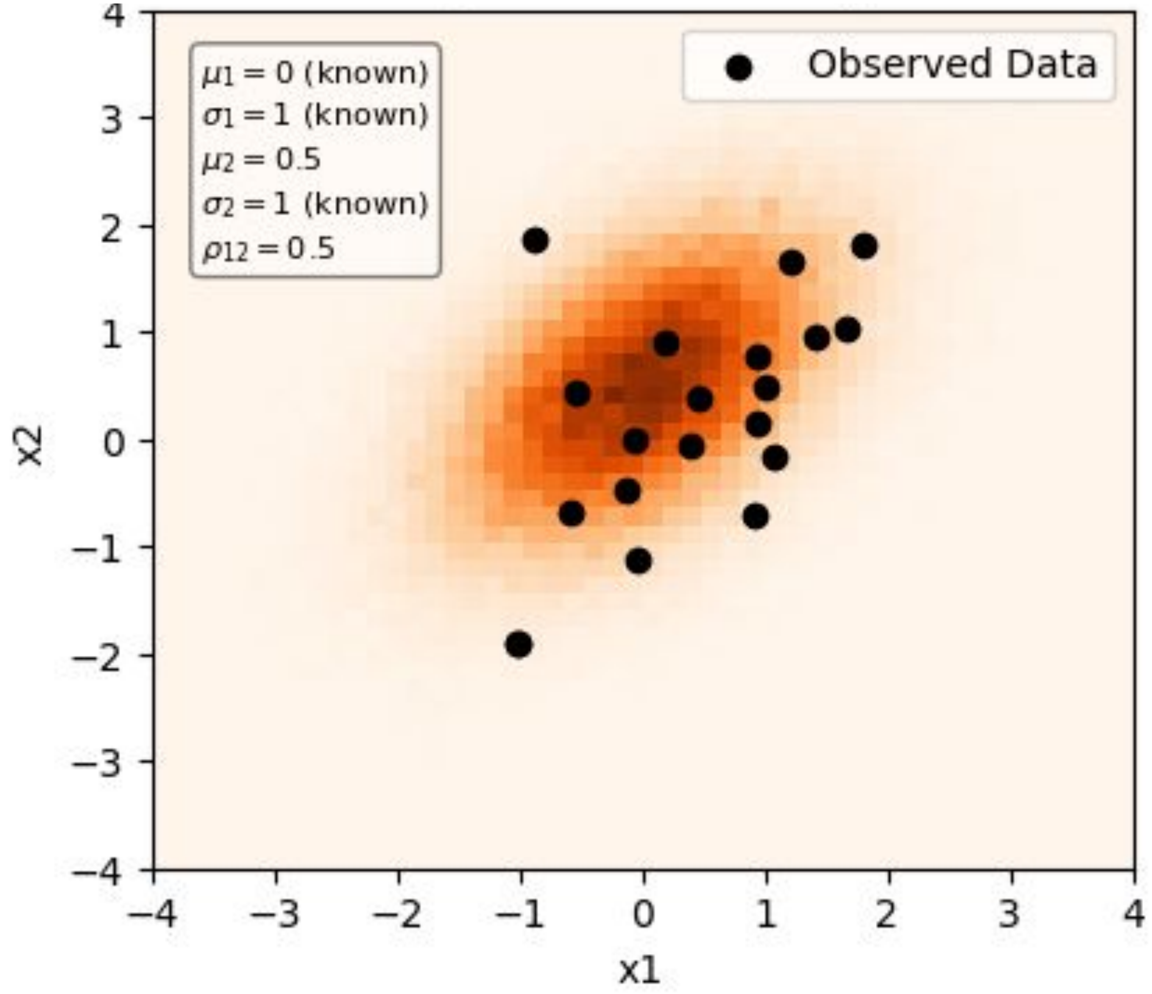
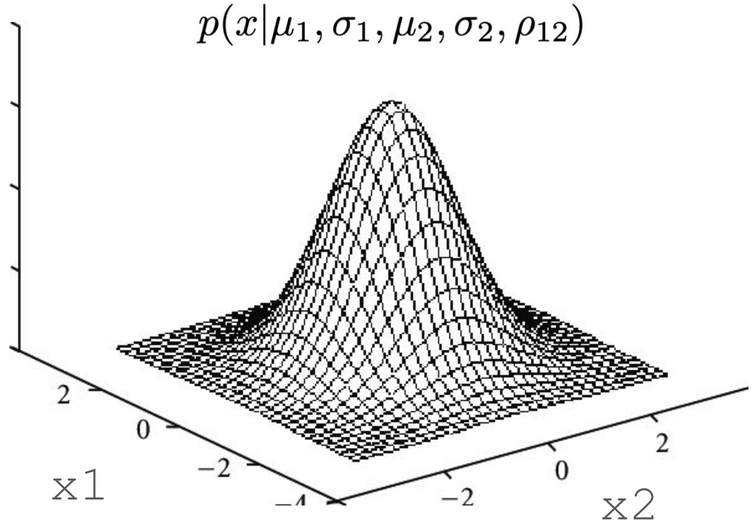
14	-1.013156	-1.897984
15	0.998487	0.492797
16	0.392428	-0.049023
17	-0.131662	-0.484124
18	-0.032107	-1.135443
19	-0.572507	-0.682939

We will use the simulation to approximate the <u>conditional log-likelihood ratio test-statistic</u> for inference

Parameter estimation example







	x1	x2
0	-1.010586	-1.910270
1	1.808325	1.808219
2	-0.873411	1.869261
3	0.471487	0.392625
4	1.220651	1.658730
5	1.411832	0.942164
6	0.185869	0.893841
7	0.949642	0.160108
8	1.068799	-0.175526
9	0.933053	0.773940
10	1.666441	1.042463
11	0.922885	-0.706301
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$$\boxed{p(x|\mu_2, \rho_{12}) = \frac{1}{2\pi\sqrt{1-\rho_{12}^2}} \exp\left(-\frac{1}{2(1-\rho_{12}^2)}\left[x_1^2 + (x_2-\mu_2)^2 - 2\rho_{12}x_1(x_2-\mu_2)\right]\right)}$$

- We can simulate data for any values of $\theta = (\mu_2, \rho_{12})$: $x_i^{\text{sim}} \sim p(x|\mu_2, \rho_{12})$

We will use the simulation to approximate the <u>conditional log-likelihood ratio test-statistic</u> for inference

Analytic solution

- Analytic probability density: $p(x|\mu_2, \rho_{12}) = \frac{1}{2\pi\sqrt{1-\rho_{12}^2}} \exp\left(-\frac{1}{2(1-\rho_{12}^2)}\left[x_1^2 + (x_2-\mu_2)^2 - 2\rho_{12}x_1(x_2-\mu_2)\right]\right)$

- Define test-statistic with respect to some reference hypothesis: $\theta_0 = (0,0)$

$$t(\mathcal{D}|\mu_2, \rho_{12}) = -2\sum_{x_i \in \mathcal{D}}^{N_{obs}} \ln \frac{p(x_i|\mu_2, \rho_{12})}{p(x_i|0,0)} \longrightarrow \Delta t(\mathcal{D}|\mu_2, \rho_{12}) = t(\mathcal{D}|\mu_2, \rho_{12}) - t(\mathcal{D}|\hat{\mu}_2, \hat{\rho}_{12})$$

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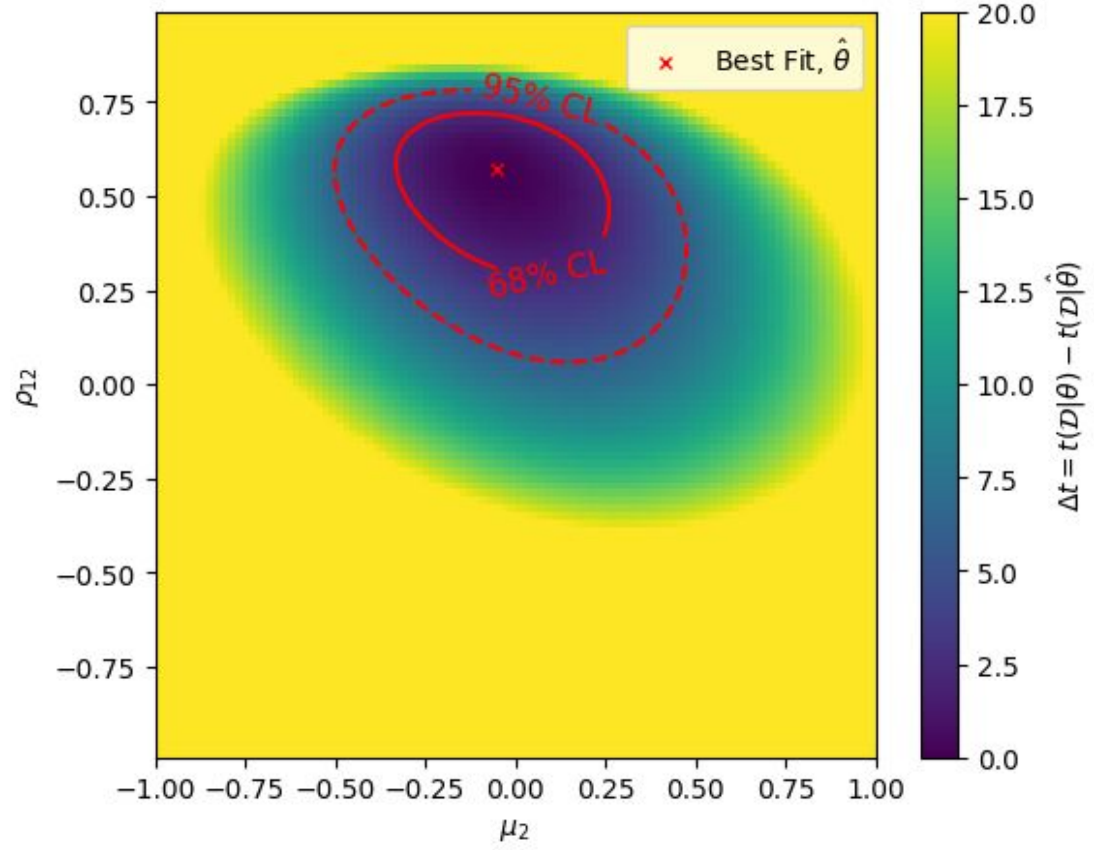
- Scan over $\theta = (\mu_2, \rho_{12})$ parameter space and calculate $\Delta t(\mathcal{D}|\mu_2, \rho_{12})$



Analytic solution

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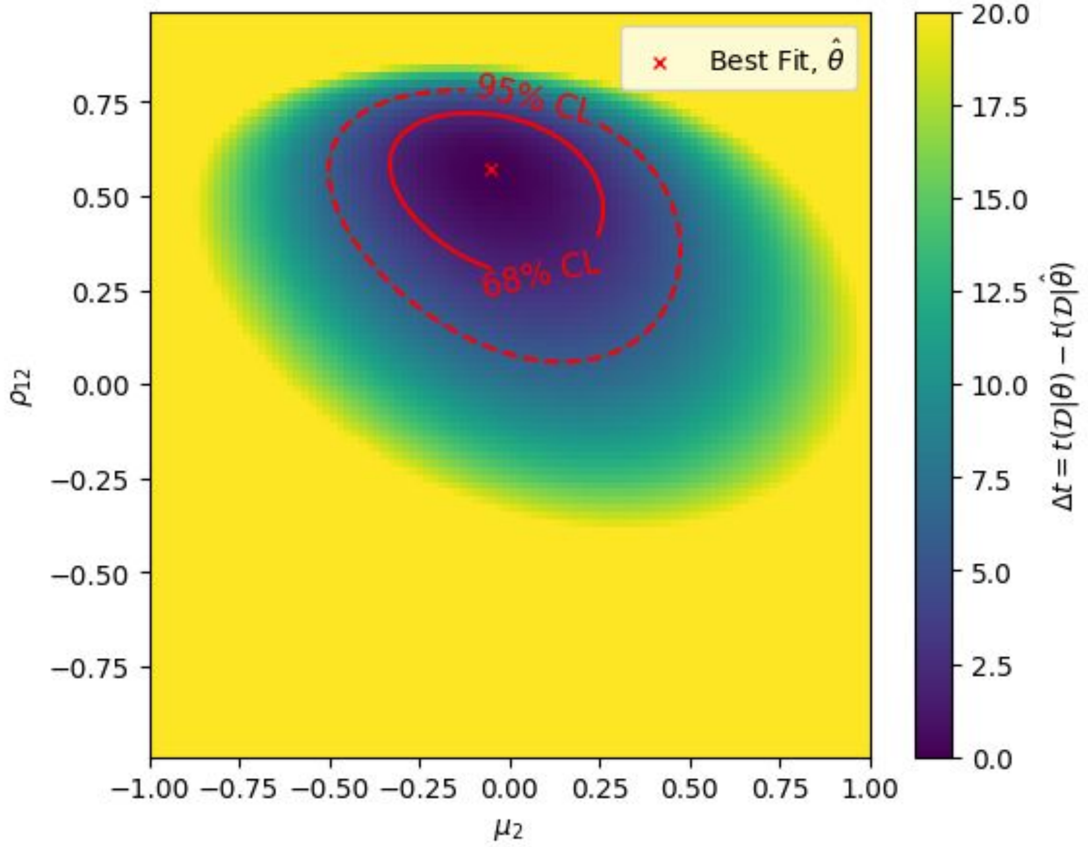

Use Wilks' Theorem to estimate confidence intervals:

- 68% CL is region defined by $\Delta t < 2.30$
- 95% CL is region defined by $\Delta t < 5.99$

Analytic solution

- Analytic probability density: $p(x|\mu_2, \rho_{12}) = \frac{1}{2\pi\sqrt{1-\rho_{12}^2}} \exp\left(-\frac{1}{2(1-\rho_{12}^2)}\left[x_1^2 + (x_2-\mu_2)^2 - 2\rho_{12}x_1(x_2-\mu_2)\right]\right)$

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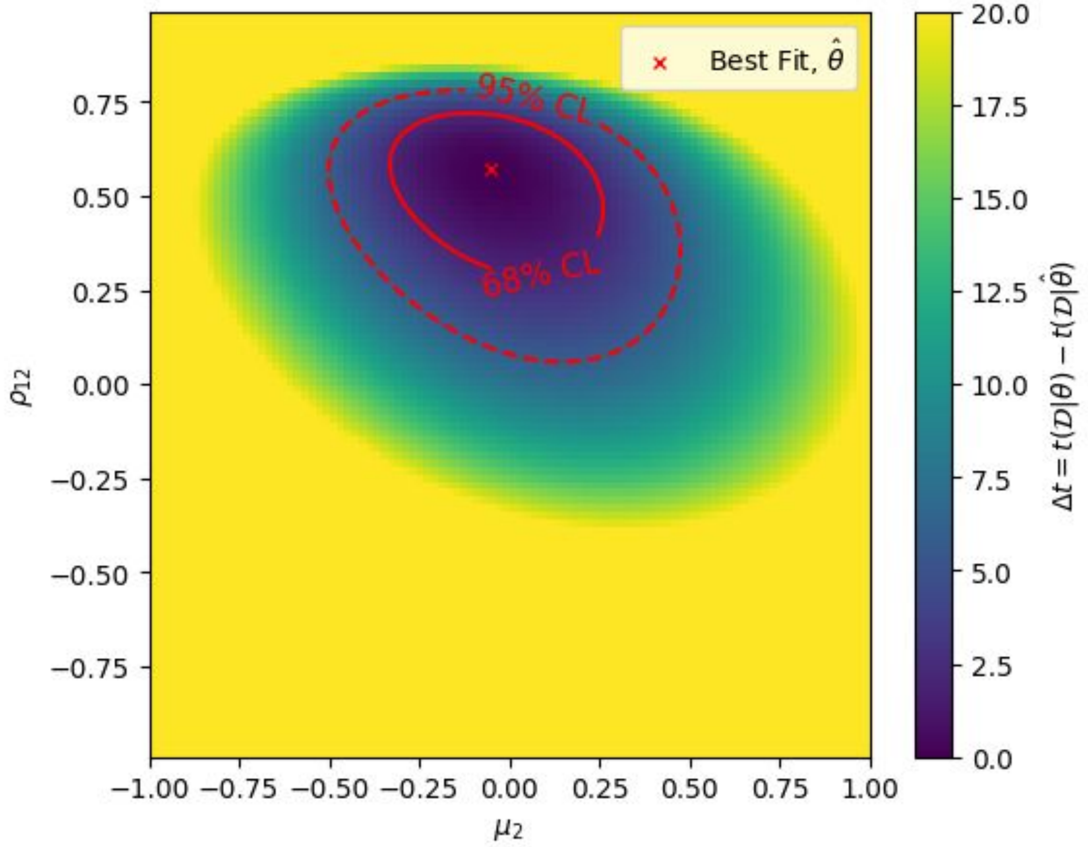


Use Wilks' Theorem to estimate confidence intervals:

- 68% CL is region defined by $\Delta t < 2.30$
- 95% CL is region defined by $\Delta t < 5.99$

Can we approximate the test-statistic using our neural SBI methods?

Parametric classifier training

1) Simulate training data

```
sim_H0 = run_simulation(num_train_per_class, mu1=0, sigma1=1, mu2=0, sigma2=1, rho12=0)
```

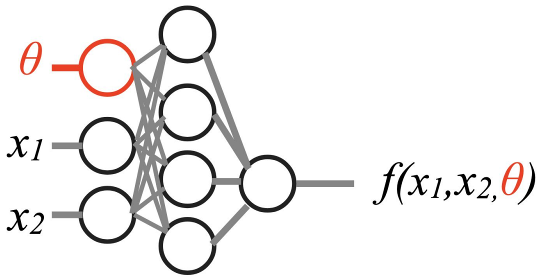
- Class 0: simulate N samples from reference $\theta_0 = (0, 0)$
- Class 1: simulate N samples with different $\theta = (\mu_2, \rho_{12})$ values
  - Define grid of points in $\theta = (\mu_2, \rho_{12})$ space (50x50 *over sensible range*)
  - Simulate N/2500 samples at each point and concatenate

```
N = 100000
sim_H1_ensemble = []
mu2_train_vals = np.linspace(-1,1,50)
rho12_train_vals = np.linspace(-0.9999,0.9999,50)

# Calculate the number of training samples per parameter point to keep total = num_train_per_class
num_train_per_subsample = N // (len(mu2_train_vals) * len(rho12_train_vals))
for mu2 in mu2_train_vals:
    for rho12 in rho12_train_vals:
        sim_subsample = run_simulation(num_train_per_subsample, mu1=0, sigma1=1, mu2=mu2, sigma2=1, rho12=rho12)
        sim_subsample['mu2'] = mu2
        sim_subsample['rho12'] = rho12
        sim_H1_ensemble.append(sim_subsample)

# Concatenate all subsamples into a single dataframe and add label
sim_H1 = pd.concat(sim_H1_ensemble, ignore_index=True)
sim_H1['label'] = 1
```

Parametric classifier training

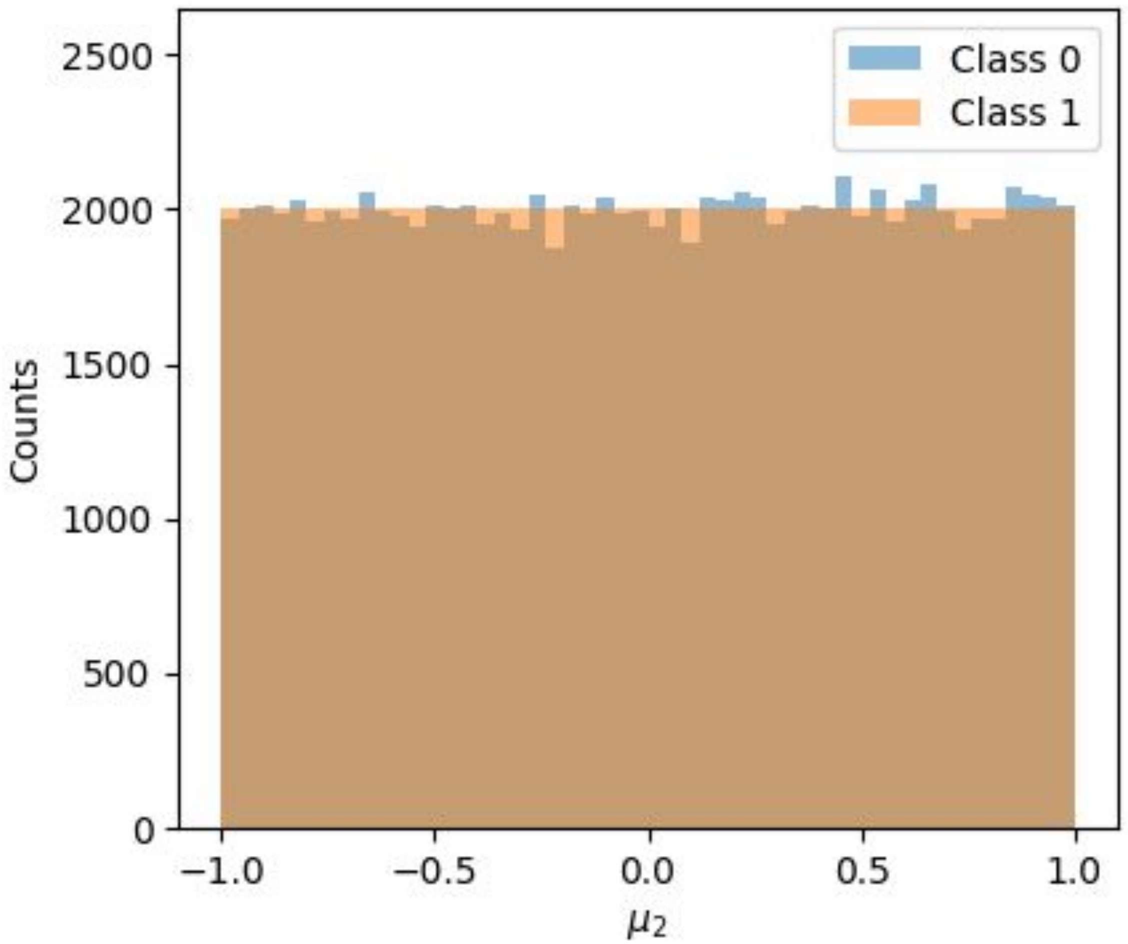


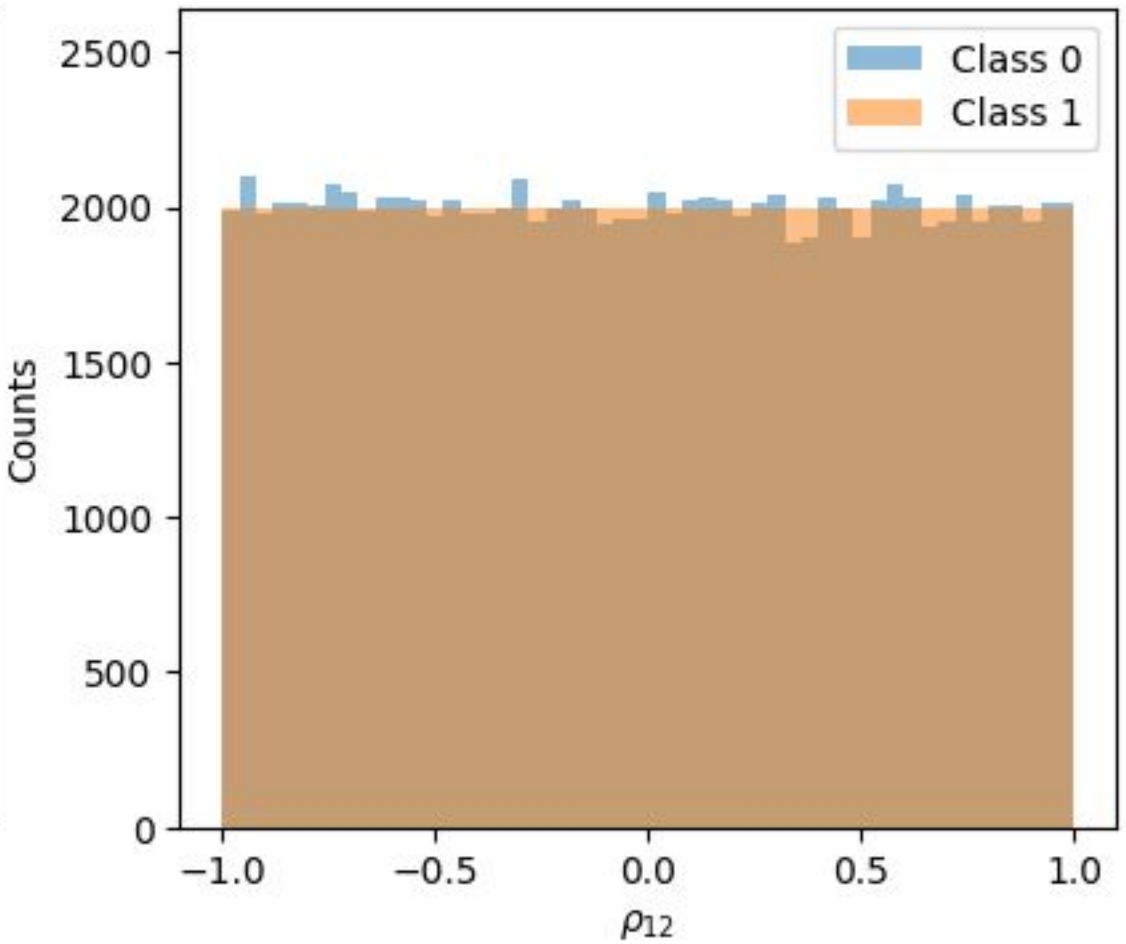
1) Simulate training data

2) Align marginal distribution of Class 0 with Class 1 i.e. pair each $x_i^{\mathcal{H}_0}$ with randomly sampled $\mu_2^{\mathcal{H}_0}, \rho_{12}^{\mathcal{H}_0} \sim p_{\mathcal{H}_1}(\mu_2, \rho_{12})$

```
sim_H0['mu2'] = np.random.choice(mu2_train_vals, size=len(sim_H0))
sim_H0['rho12'] = np.random.choice(rho12_train_vals, size=len(sim_H0))

# Add label for H0
sim_H0['label'] = 0
```





Parametric classifier training

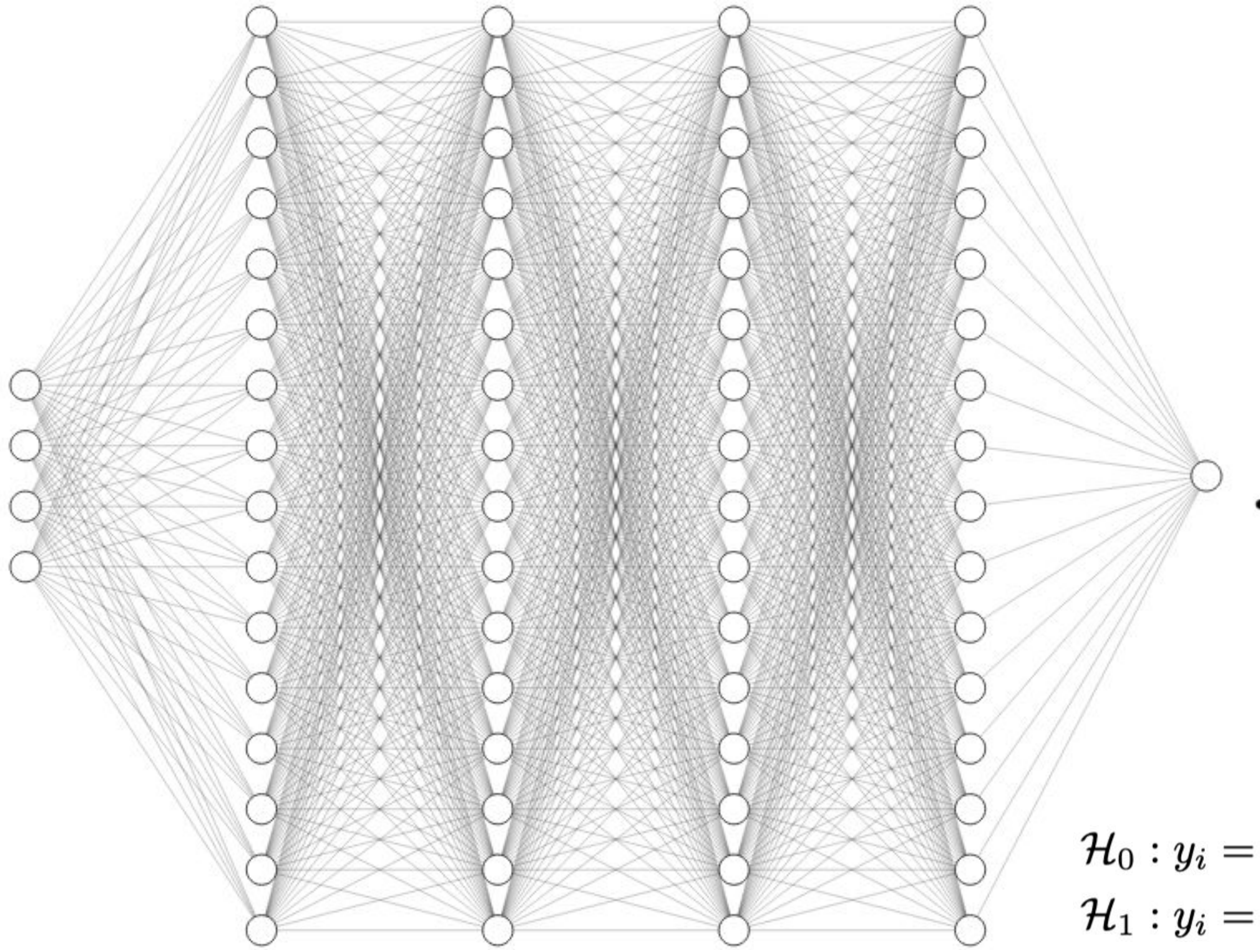
1) Simulate training data

2) Align marginal distribution of Class 0 with Class 1 i.e. pair each $x_i^{\mathcal{H}_0}$ with randomly sampled $\mu_2^{\mathcal{H}_0}, \rho_{12}^{\mathcal{H}_0} \sim p_{\mathcal{H}_1}(\mu_2, \rho_{12})$

3) Train parametric classifier with **`torch.nn`** to classify between Class 0 (reference) and Class 1 (ensemble)

$$\boxed{\theta_i = \begin{pmatrix} \mu_2 \\ \rho_{12} \end{pmatrix}_i}$$

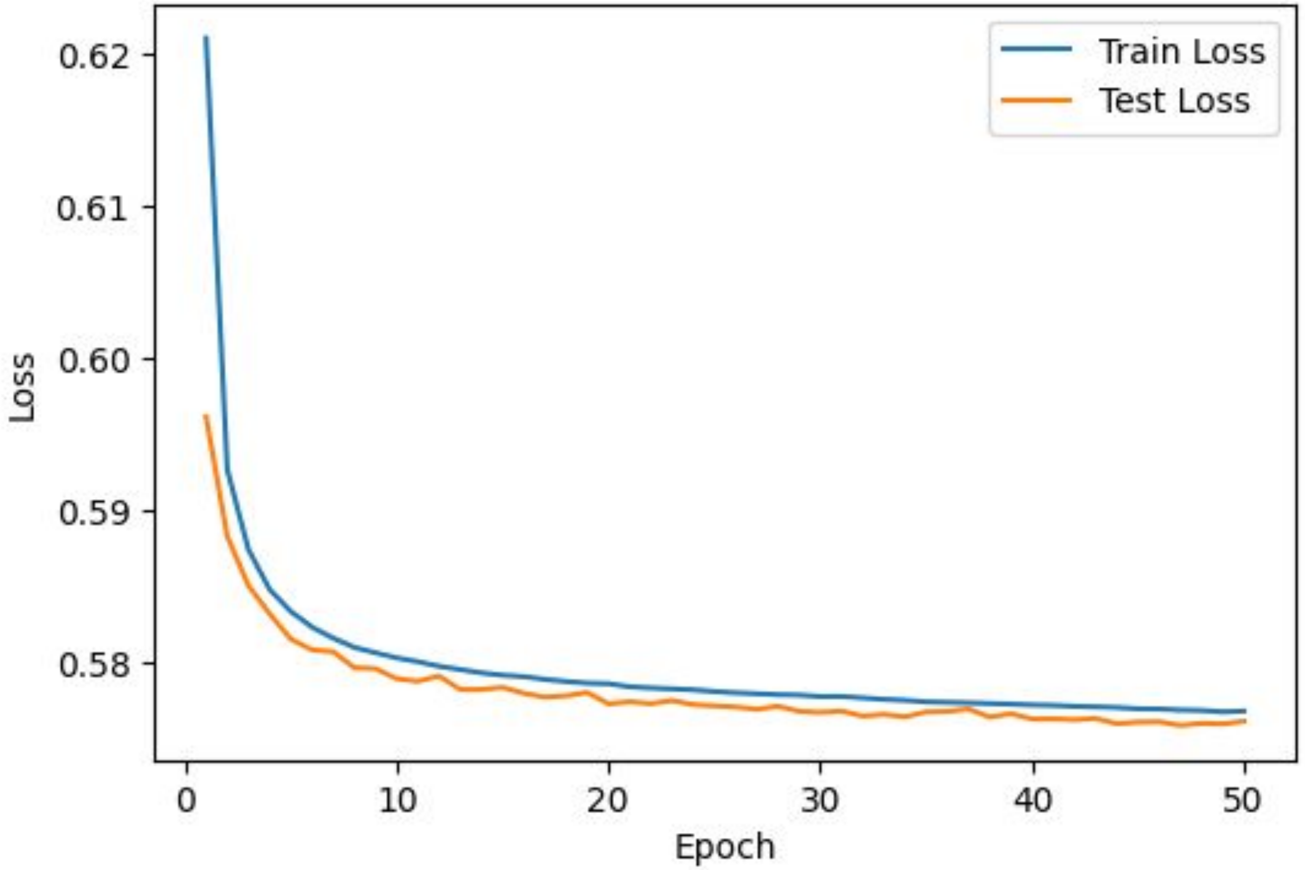
$$x_i = \begin{pmatrix} x1 \\ x2 \end{pmatrix}_i$$



$$\hat{f}(x_i, \theta_i)$$

$$\mathcal{H}_0 : y_i = 0$$
$$\mathcal{H}_1 : y_i = 1$$

$$\mathcal{L}[f] = -\frac{1}{N} \sum_{i=1}^{N} y_i \ln f(x_i, \theta_i) + (1 - y_i) \ln (1 - f(x_i, \theta_i))$$



Parameter estimation with classifier

1) Simulate training data

2) Align marginal distribution of Class 0 with Class 1 i.e. pair each $x_i^{\mathcal{H}_0}$ with randomly sampled $\mu_2^{\mathcal{H}_0}, \rho_{12}^{\mathcal{H}_0} \sim p_{\mathcal{H}_1}(\mu_2, \rho_{12})$

3) Train parametric classifier with **`torch.nn`** to classify between Class 0 (reference) and Class 1 (ensemble)

4) Evaluate classifier for observed data $\mathcal{D}$ over $\theta = (\mu_2, \rho_{12})$ parameter space → calculate learned test-statistic

	x1	x2
0	-1.010586	-1.910270
1	1.808325	1.808219
2	-0.873411	1.869261
3		
4		
5		
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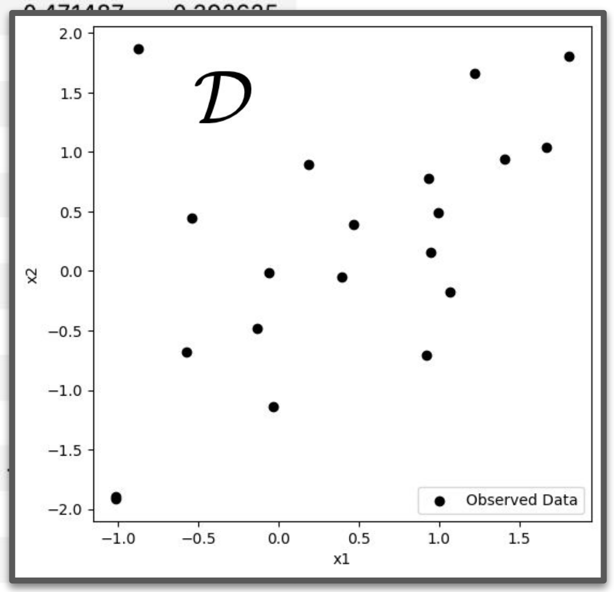

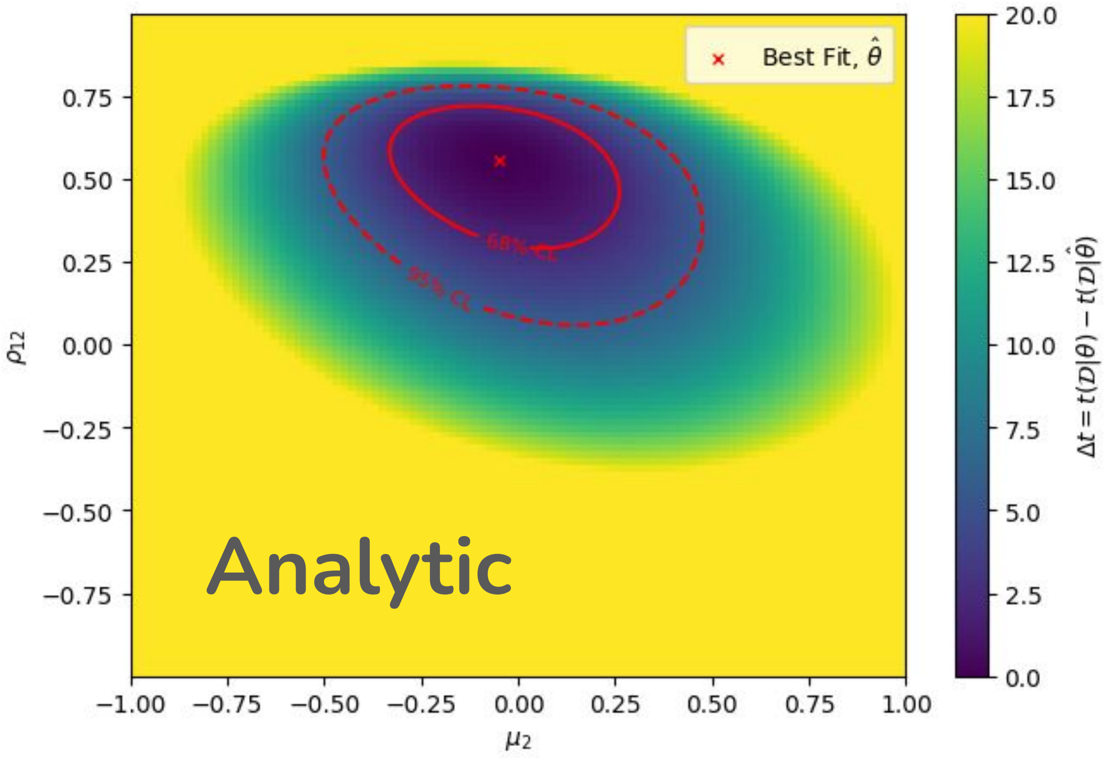

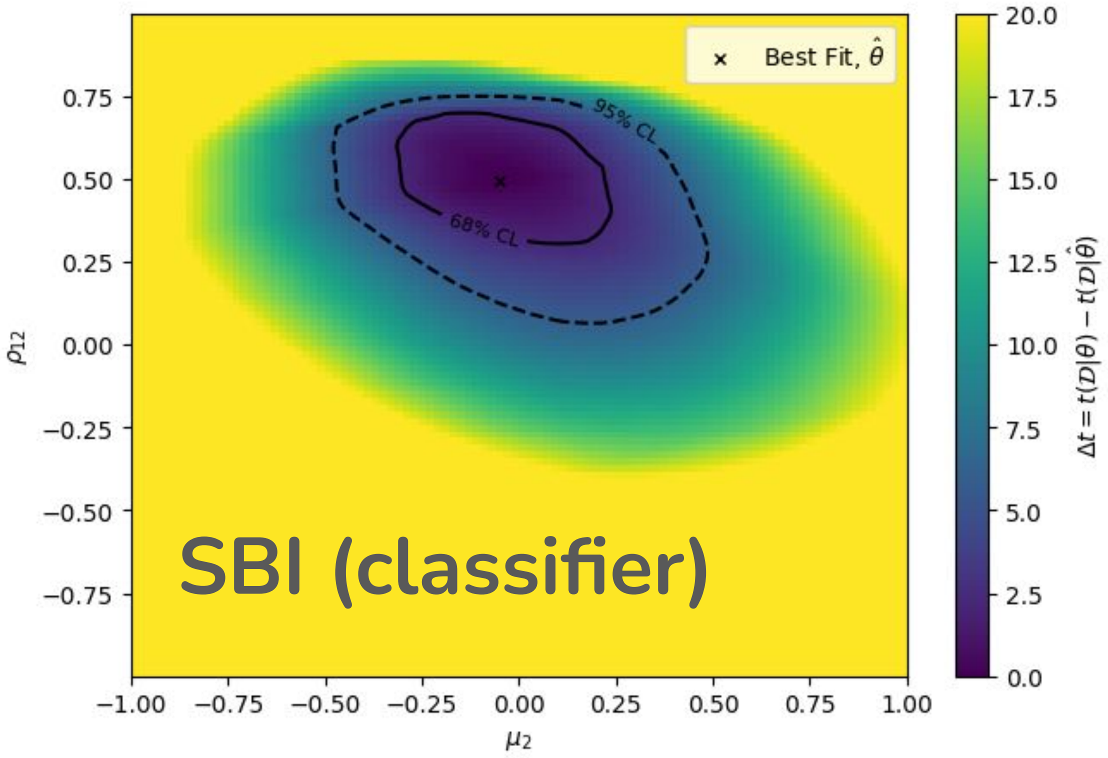

$$t(\mathcal{D}|\mu_2, \rho_{12}) = -2 \sum_{x_i \in \mathcal{D}}^{N_{obs}} \ln \frac{p(x_i|\mu_2, \rho_{12})}{p(x_i|0,0)}$$

$$t(\mathcal{D}|\mu_2, \rho_{12}) = -2 \sum_{x_i \in \mathcal{D}}^{N_{obs}} \ln \frac{\hat{f}(x_i, \mu_2, \rho_{12})}{1 - \hat{f}(x_i, \mu_2, \rho_{12})}$$

Parameter estimation with classifier

1) Simulate training data
2) Align marginal distribution of Class 0 with
3) Train parametric classifier with **`torch.nn`**
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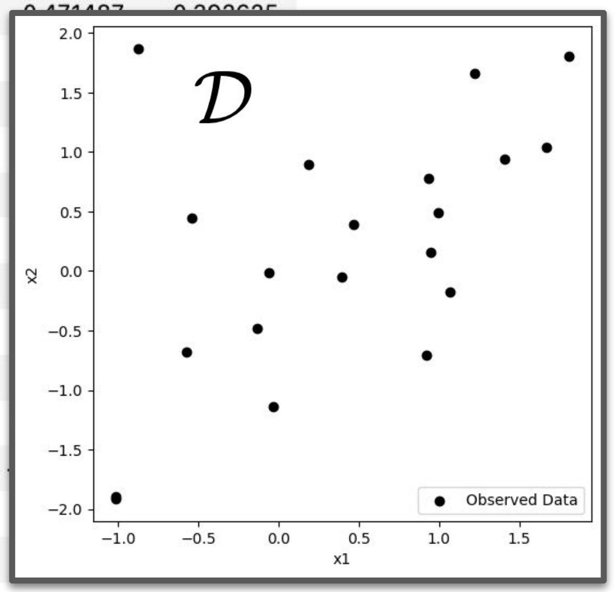
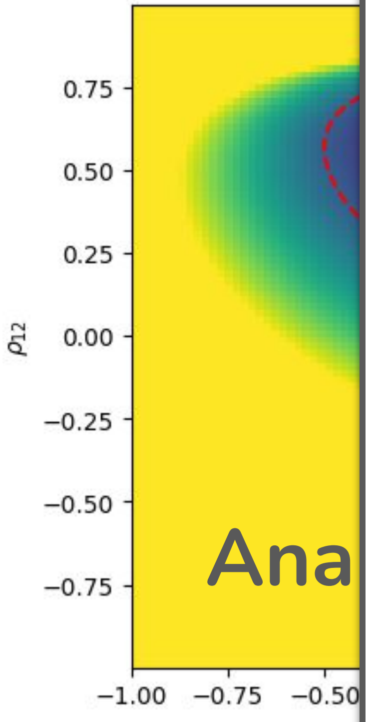
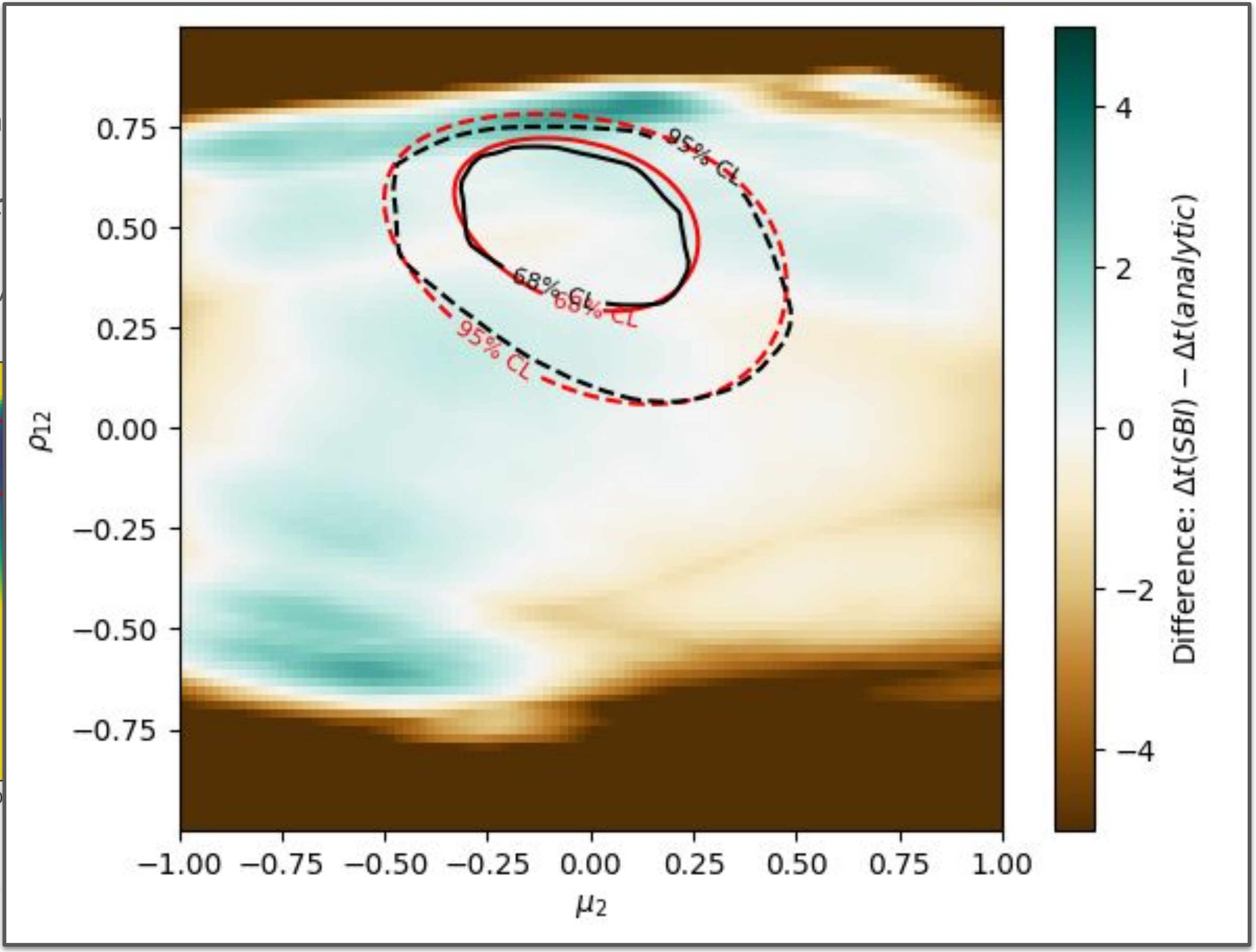
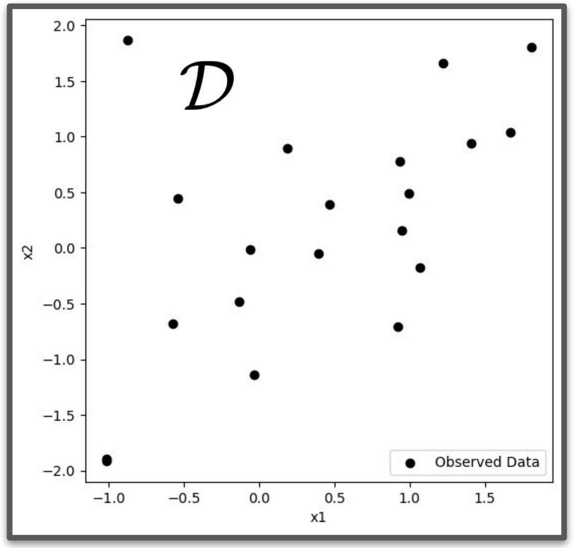




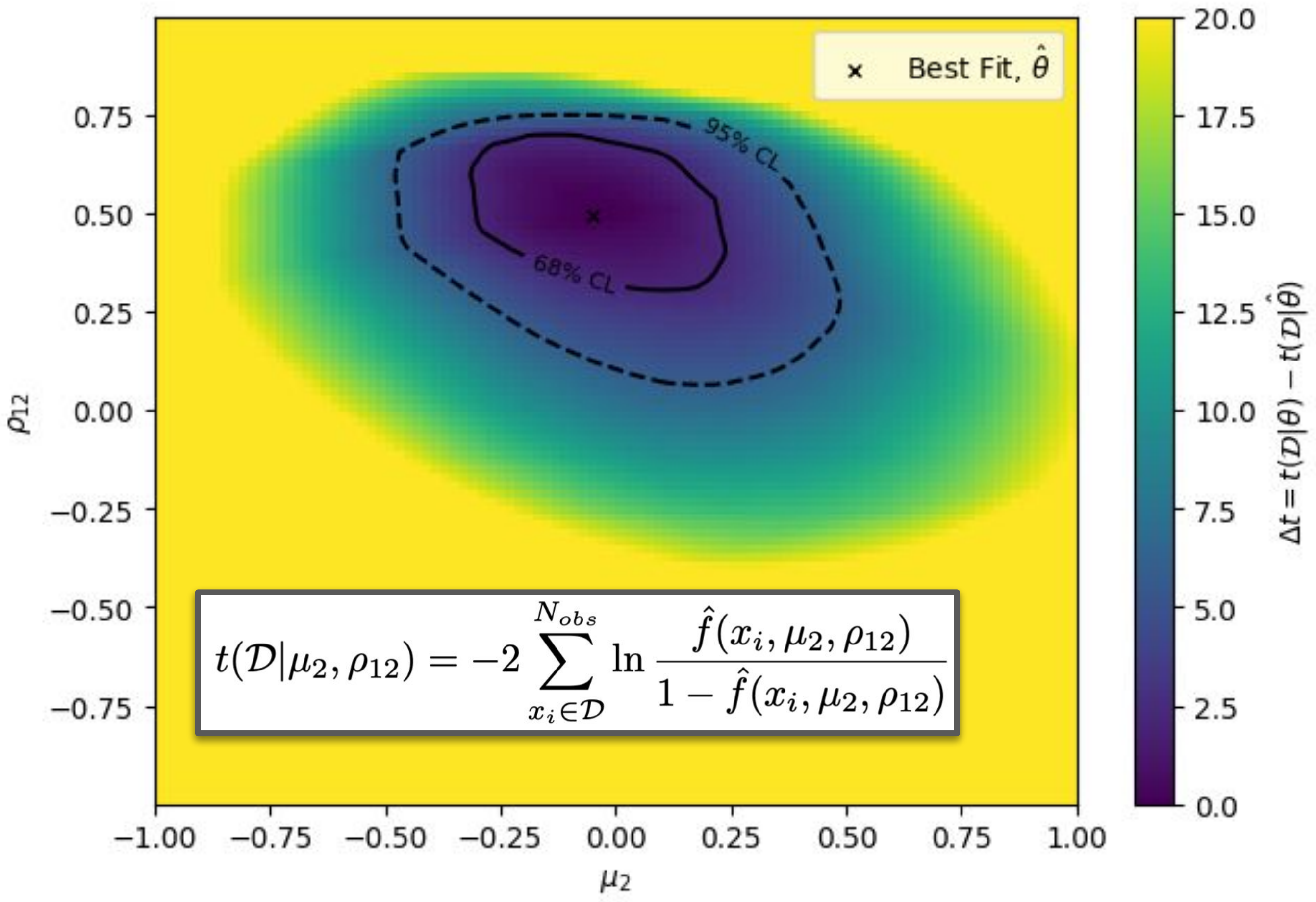
$t(\mathcal{D}|\mu_2, \rho_{12})$



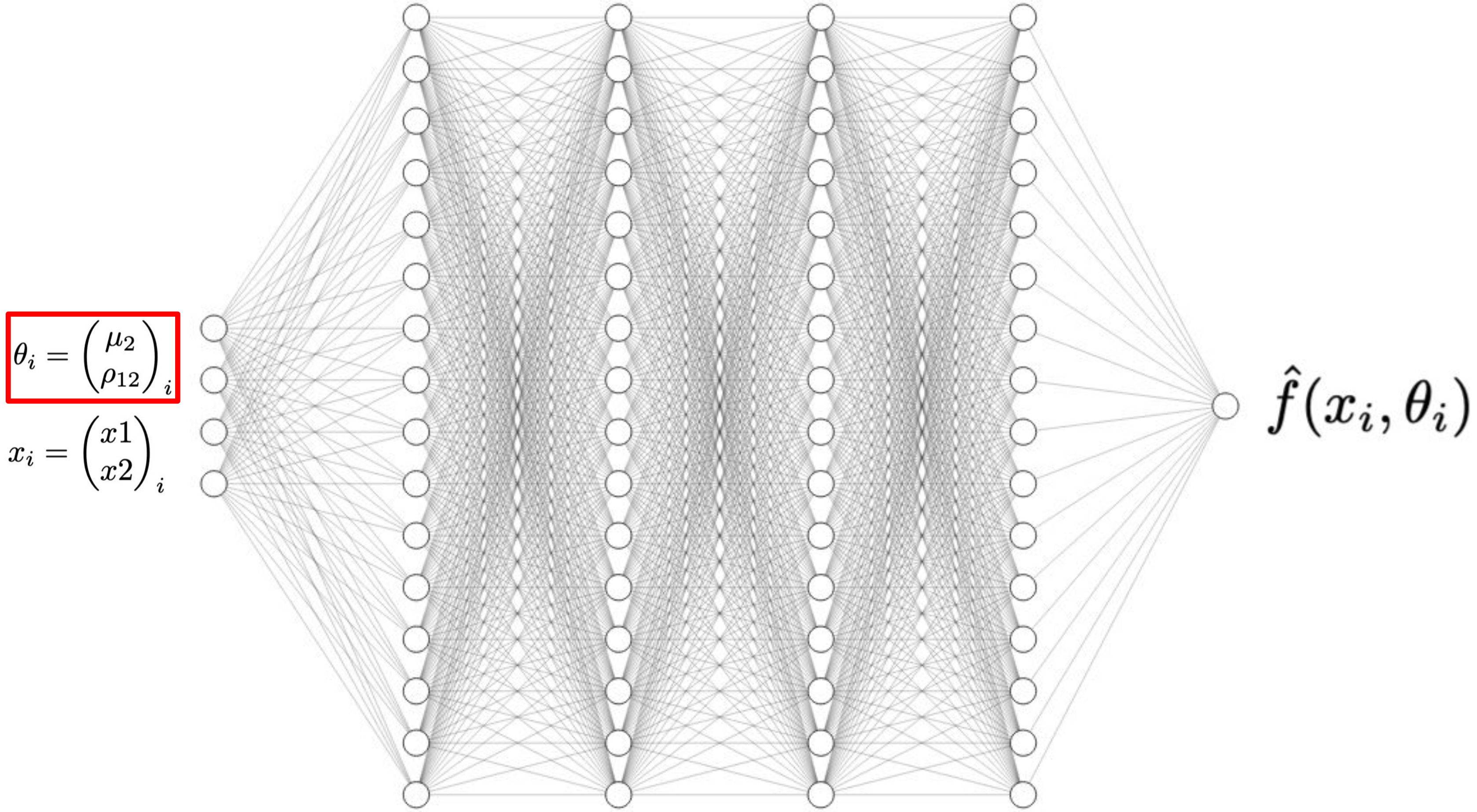
Summary: parameter estimation



- We were presented with a research problem to estimate two parameters for a dataset (N_{obs} = 20)
- Our simulator could generate data for different parameter values: $x_i, \theta_i \sim p(x|\theta)$
- We trained a <u>binary parametric classifier</u> to distinguish Class 0 (reference) from Class 1 (ensemble)
- Use output of classifier to approximate **<u>conditional</u> log-likelihood-ratio test-statistic**



$$t(\mathcal{D}|\mu_2, \rho_{12}) = -2 \sum_{x_i \in \mathcal{D}}^{N_{obs}} \ln \frac{\hat{f}(x_i, \mu_2, \rho_{12})}{1 - \hat{f}(x_i, \mu_2, \rho_{12})}$$



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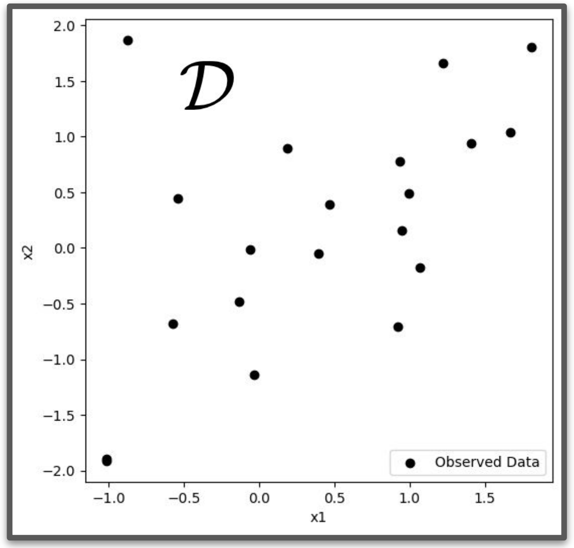

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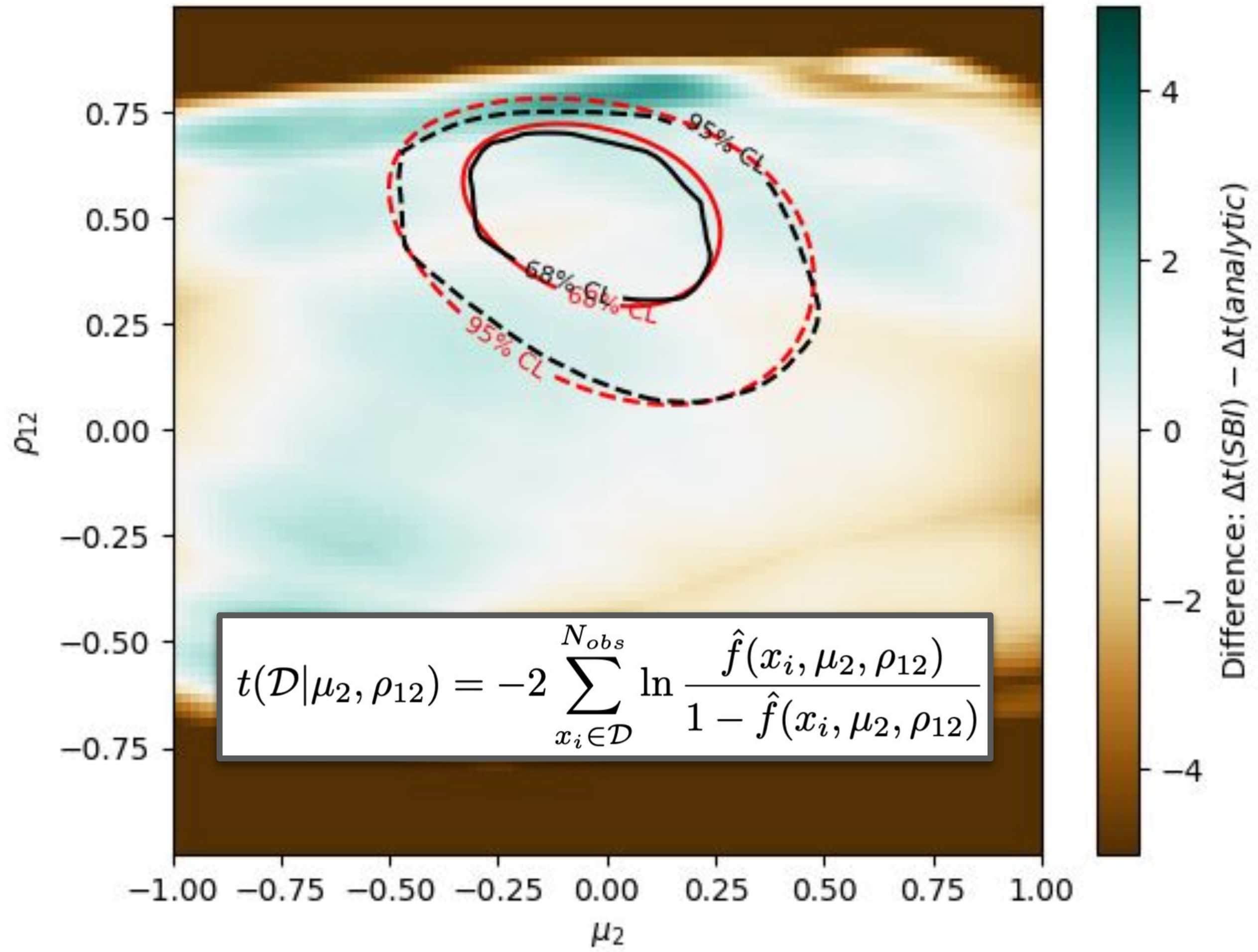
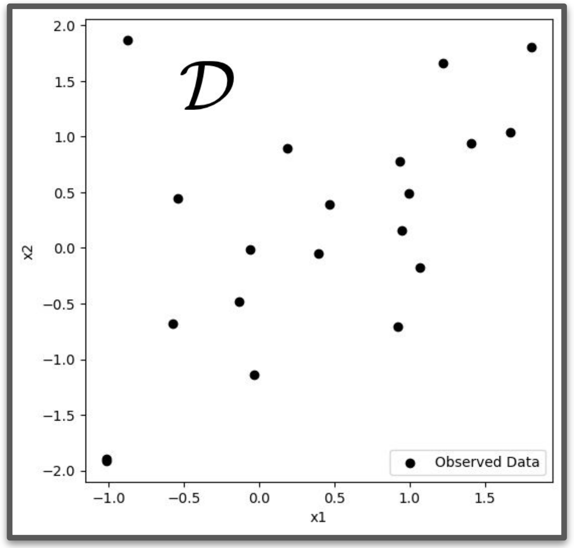


$$t(\mathcal{D}|\mu_2, \rho_{12}) = -2 \sum_{x_i \in \mathcal{D}}^{N_{obs}} \ln \frac{\hat{f}(x_i, \mu_2, \rho_{12})}{1 - \hat{f}(x_i, \mu_2, \rho_{12})}$$

- We were able to accurately reproduce the analytic solution!
  - Scope for improvement: slight bias in the estimator
    - Increasing amount of training data?
    - Increasing granularity of $\theta = (\mu_2, \rho_{12})$ training grid?
    - More complex classifier architecture?
- Inference is amortized (same classifier for new data)

Summary: parameter estimation



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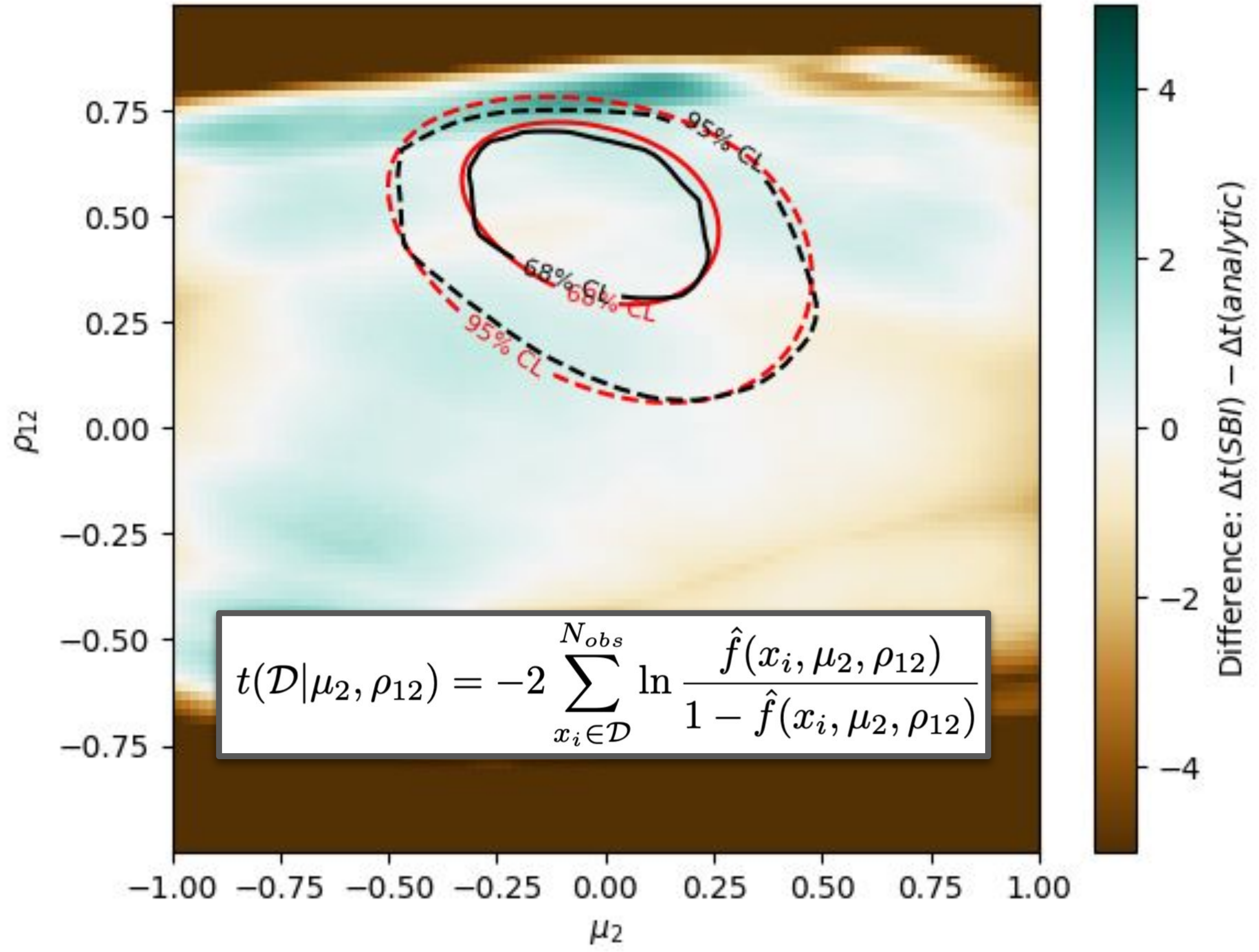
- We trained a binary parametric classifier to distinguish Class 0 (reference) from Class 1 (ensemble)
- Use output of classifier to approximate **conditional log-likelihood-ratio test-statistic**



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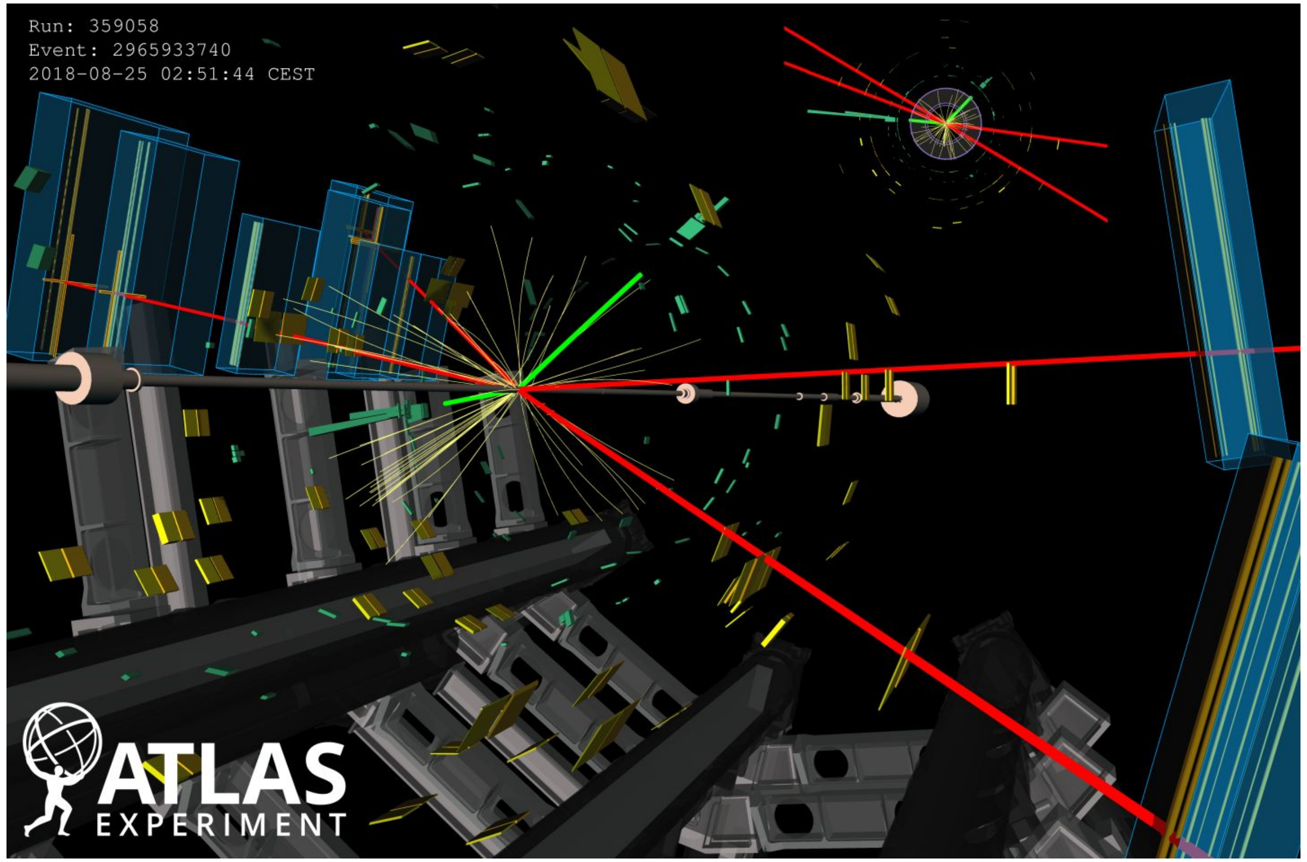
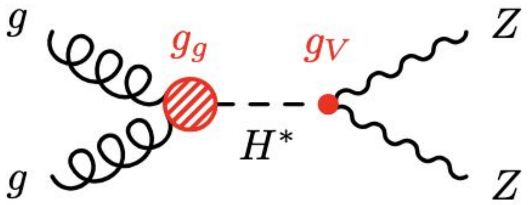
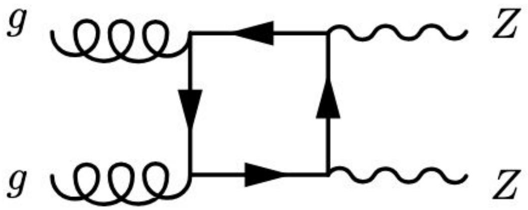
- Inference is amortized (same classifier for new data)
- End-to-end example of using a ML classifier for SBI (parameter est.)
  - **Extends to real-world problems with no analytic solution!**

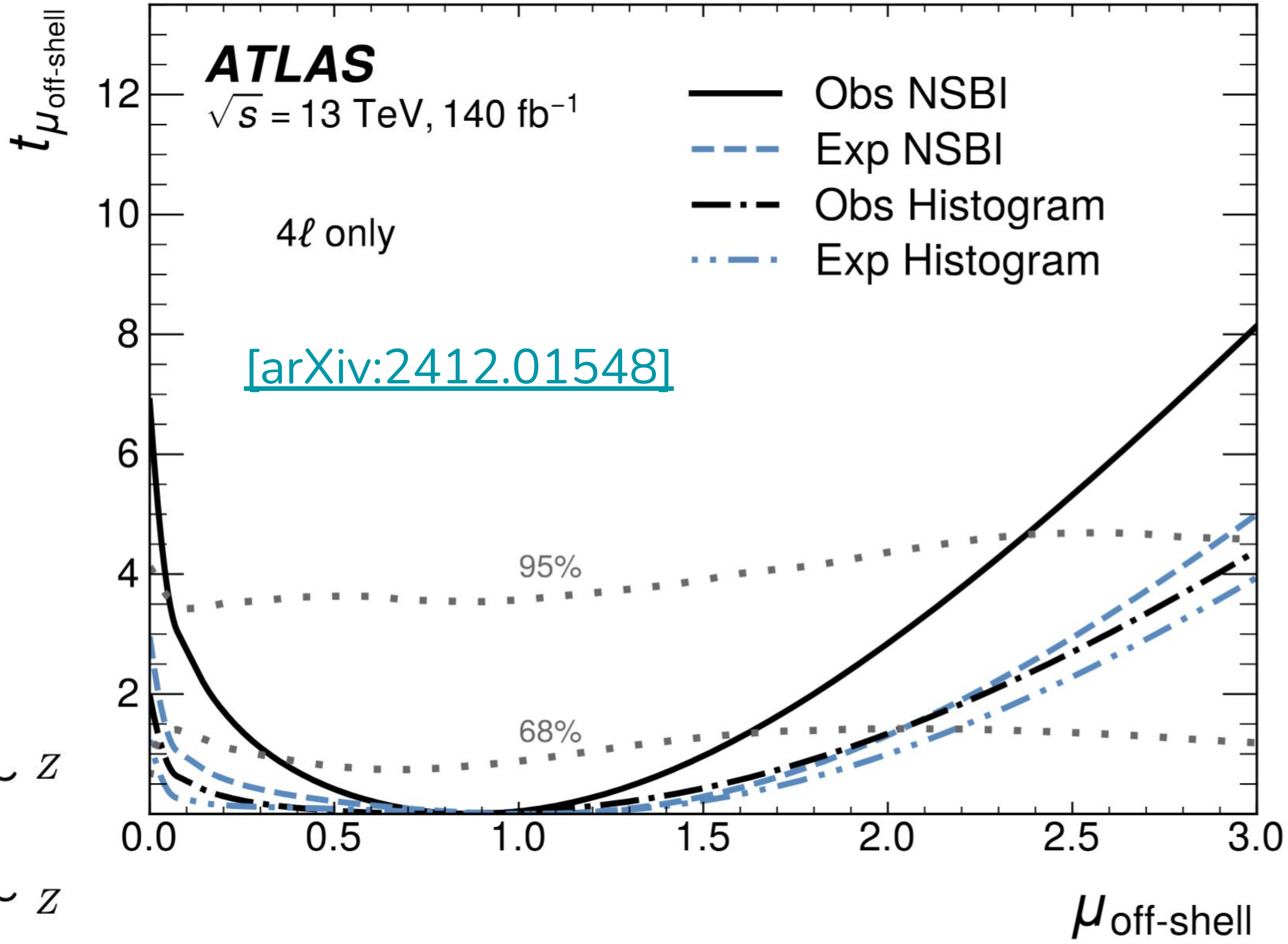
Neural SBI in physics

- Neural SBI is a **new tool** in the field → only recently reached a mature enough state for complex physics analyses









[arXiv:2412.01548]

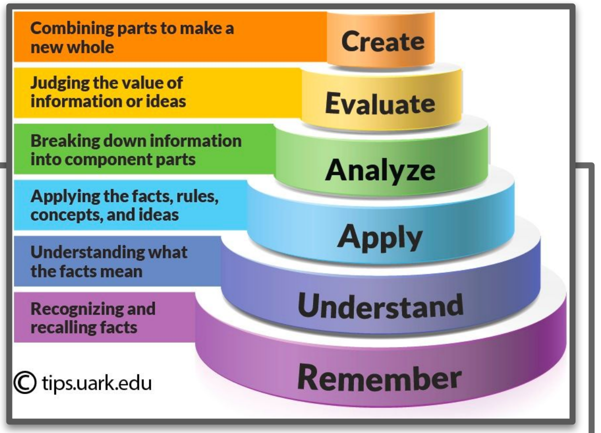
- We are starting to use neural SBI to **better understand fundamental properties of the Universe**

Further reading

- **General overview of SBI with ML: [arXiv:1911.01429]**

- **What if we do not have a "faithful" simulator?**
  - i.e. systematic differences between observed data and synthetic (simulated) data
  - Leads to systematic uncertainties in the measurements
  - Incorporate "nuisance parameters" into the classifier training → profile/marginalize in the inference step
  - [arXiv:1506.02169], [arXiv:2105.08742]
- **Validating and calibrating the classifier**
  - Sub-optimal training may lead to a biased estimator for the likelihood ratio, which could (in principle) lead to wrong conclusions!
  - Crucial to perform diagnostic checks on SBI model to validate output is what we expect
  - Without the analytic solution we must use (independent) simulation samples for validation
  - [arXiv:2412.01600] (Section 4)
- **Learning the likelihood**
  - Using ML classifiers is just one (simple) approach for SBI, where we learn the likelihood-ratio
  - Modern ML techniques can be used to learn the likelihood directly e.g. conditional normalising flows [JMLR 22 (2021)]
- **Bayesian approach to SBI: neural posterior estimation**
  - This lecture presented SBI in a frequentist paradigm but of course this extends to Bayesian inference
  - Many applications look at learning the posterior directly
  - [arXiv:2011.05991], [arXiv:2106.12594]

Lecture summary

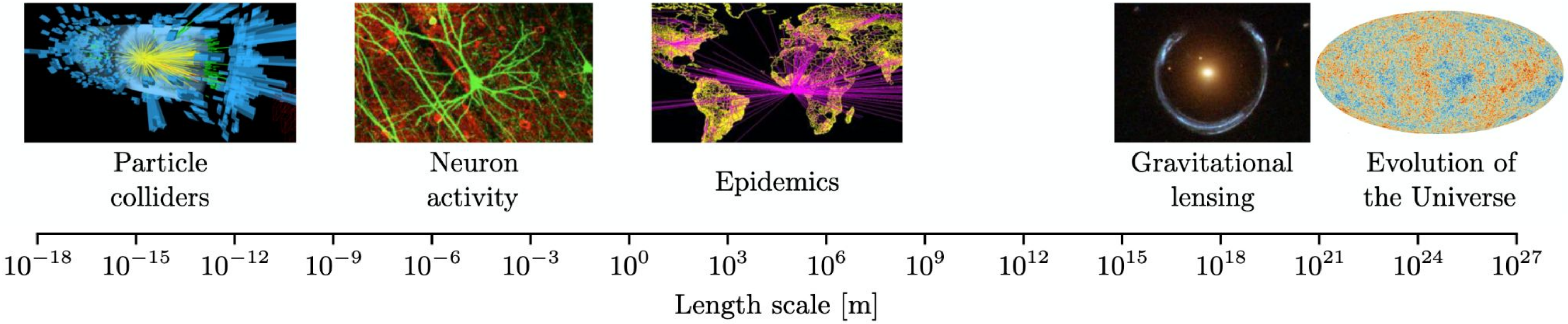


Intended Learning Outcomes

- **Understand** the need for simulation-based inference in the modern era of science
- **Understand** how to use a simple ML classifier to learn the likelihood-ratio and **apply** this knowledge to perform a hypothesis test on a research problem with an unknown likelihood
- Extend the approach to learning the conditional likelihood-ratio via a parametric classifier and **apply** this to a parameter estimation problem. **Evaluate** the performance by comparing to the analytic solution

I hope this lecture has helped bridge the gap between ML and some core concepts in statistics!

Remember, these techniques generalise to complex data → Use ML classifiers to perform SBI for more interesting problems!

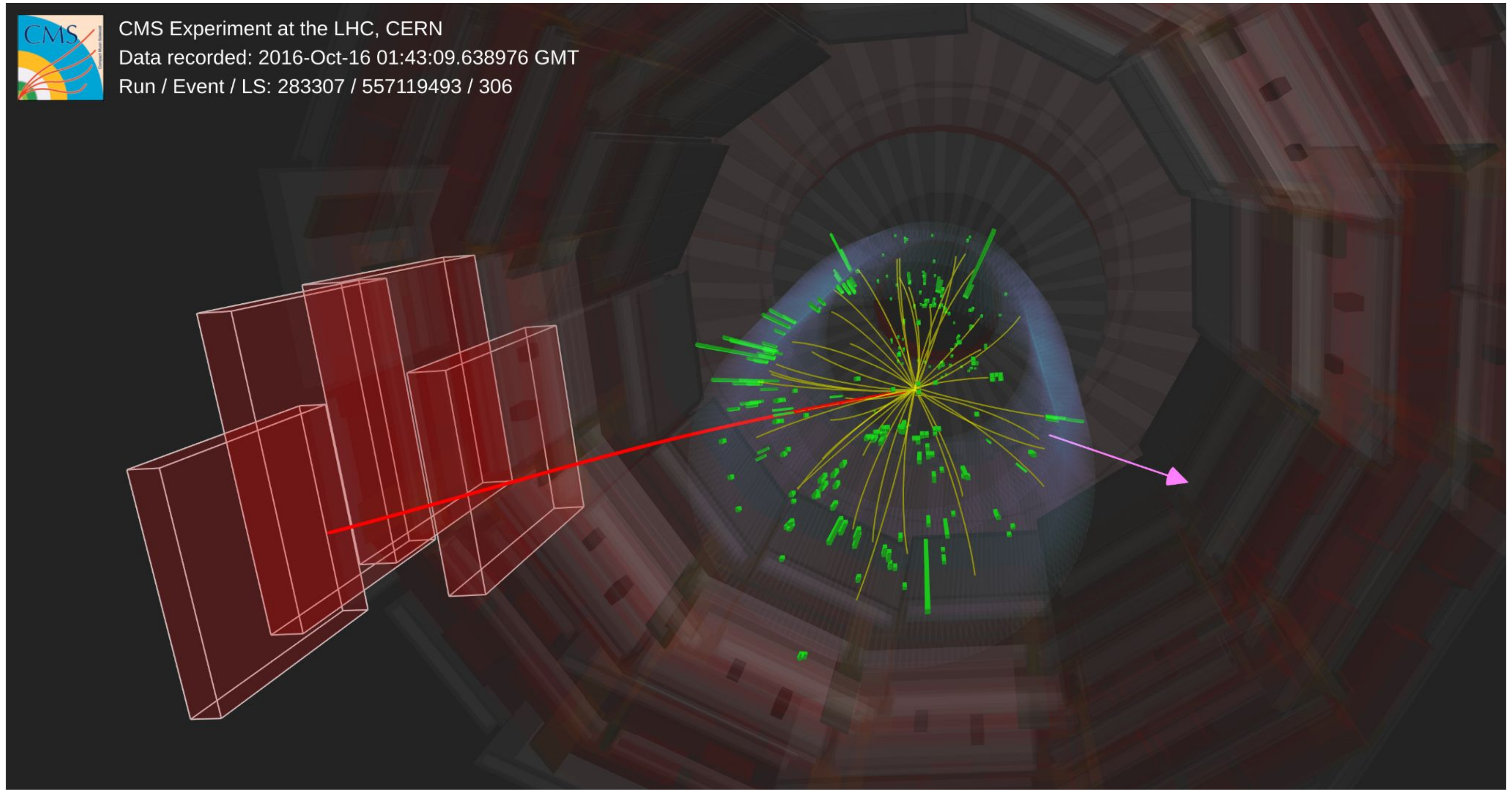


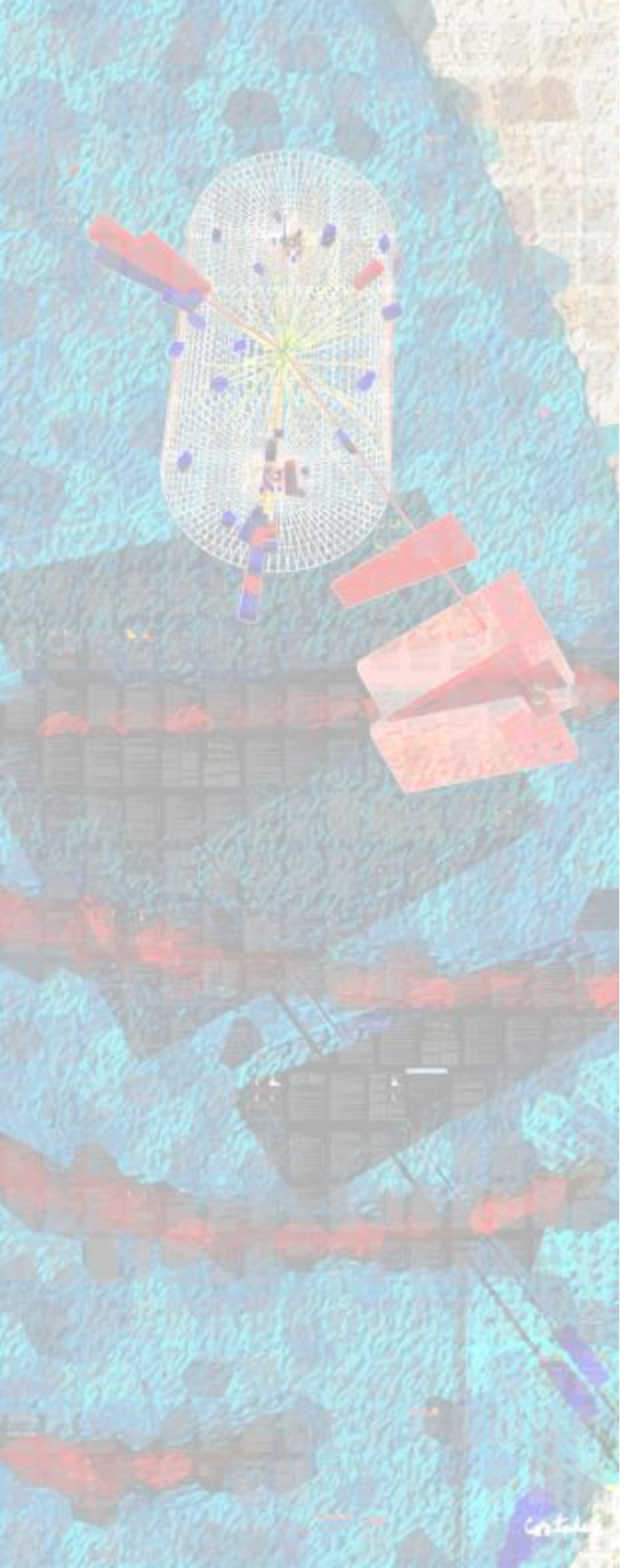
The project

	lepton_pt	lepton_eta	lepton_phi	MET	MET_phi
0	552.738053	-2.693822	3.070057	389.872251	-0.626361
1	407.853875	-0.745842	-0.146834	208.253263	-1.244364
2	207.347397	-0.450228	-1.180252	165.012537	1.492187
3	77.556986	-0.149318	0.036112	102.431505	-2.749619
4	258.979666	1.273499	0.618953	120.369223	-2.912761
5	283.114789	0.804300	-1.495211	273.862677	1.040215
6	37.932233	1.674090	-2.913335	91.038384	0.636168
7	691.113212	-1.402575	-1.345433	432.995845	3.084805
8	508.449227	0.002224	0.225774	277.623512	-2.114758
9	50.517533	-0.078815	1.446648	66.547468	-2.701350

- You will use neural SBI to infer the properties of a new particle (A) discovered at the LHC
  - You are provided with a dataset of N_{obs} = 10 samples: $A \rightarrow \mu + \nu$ decays
  - 5D kinematic observables related to muon (μ) and neutrino (ν)
- A decays instantaneously → we need to infer properties of particle A from its decay products
- Inference tasks:
  - Quantum spin (spin 0 vs spin 1)
    - Hypothesis Test
  - Mass of particle A
    - Parameter estimation
- We can (faithfully) simulate the A decays

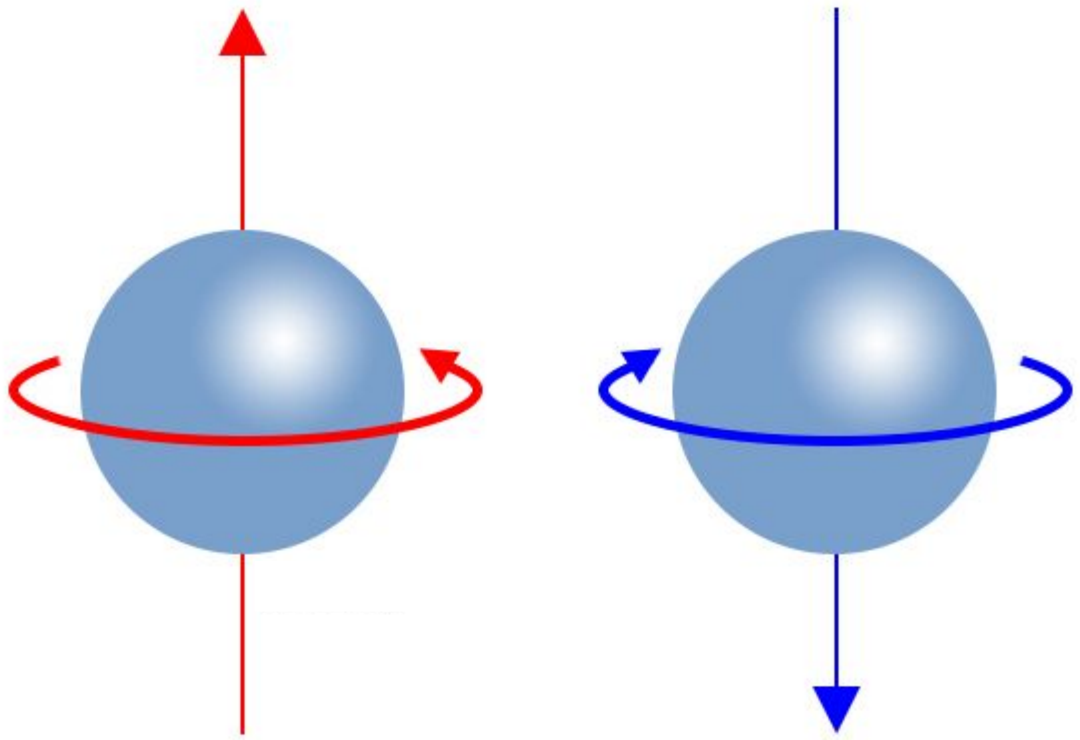
```
from simulator import simulate_collisions
data = simulate_collisions(num_events, spin, mass)
```





Back-Up

What is a particle's spin?



- Spin is a purely quantum mechanical property of an elementary particle
- It is an intrinsic form of angular momentum
  - Unlike everyday (classical) spinning objects
  - Does not correspond to any literal rotation in space
- Instead quantum spin influences how a particle behaves, decays, and how it interacts with forces
- This makes is possible to distinguish between different types of particles by their spin values
  - Bosons - integer spins
  - Fermions - spin-½ particles
  - These have very different properties...