

Overcoming challenges of quantum interference at LHC with neural simulation-based inference and a full implementation in ATLAS

Aishik Ghosh

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04 December 2024



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What's to come

Statistical inference methods developed for LHC analyses
Option to follow technical details or intuitive explanations

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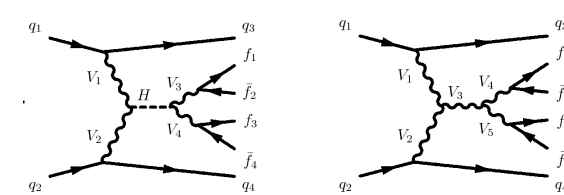
Measuring quantum interference in the off-shell Higgs to four leptons process with Machine Learning

Aishik Ghosh

Université Paris-Saclay, CNRS/IN2P3, IJCLab, 91405 Orsay, France

Abstract — The traditional machine learning approach to optimize a particle physics measurement breaks down in the presence of quantum interference between the signal and background processes. A recently developed family of physics-aware machine learning techniques that rely on the extraction of additional information from the particle physics simulator to train the neural network could be adapted to a signal strength measurement problem. The networks are trained to directly learn the likelihood or likelihood ratio between the test hypothesis and null hypothesis values of the theory parameters being measured. We apply this idea to a signal strength measurement in the off-shell Higgs to four leptons analysis for the Vector Boson Fusion production mode from simulations of the high energy proton-proton collisions at the Large Hadron Collider. Promising initial results indicate that a model trained on simulated data at different values of the signal strength outperforms traditional approaches in the presence of quantum interference.

1 Introduction



(a) Signal: Higgs from Vector Boson Fusion (b) Background: Vector Boson Scattering

Figure 1: Feynman Diagrams of the processes under study. (a) signal Higgs diagram, (b) interfering background diagram

The Heisenberg uncertainty principle of quantum mechanics ($\sigma_E \sigma_t \geq \frac{\hbar}{2}$) allows particles to become “virtual”, with a mass going far away from the one described by special relativity’s mass-energy equivalence formula $E^2 - |\vec{p}|^2 c^2 = m_0^2 c^4$ (where the energy E is given in terms of the rest mass m_0 and momentum \vec{p} of the particle and c is the speed of light in vacuum). They are and are referred to as “off-shell” particles. Quantum mechanics also prescribes that given an initial and final state, all possible intermediate states can and will occur, and they may interfere with one another.

A study of the off-shell Higgs boson decaying to two Z bosons that decay to four leptons (henceforth referred to as “offshell h4l”), such the 2018 study [2] in the ATLAS Collaboration [1] is one of the most interesting studies in high energy particle physics because it allows to break certain degeneracies between the Higgs couplings, and constrain the Higgs width (under certain model dependent assumptions) that cannot be disentangled by an on-shell measurement alone. An update to the previous ATLAS study using the entire Run2

data will have develop innovative methodology to deal with quantum interference between the Higgs Feynman diagram (referred to as “signal”) and other standard model processes (referred to as “background”). While the previous round used simple cuts to define the region of interest, we investigate a recently developed family of physics-aware machine learning techniques to improve the sensitivity of such an analysis. The two main diagrams studied here are shown in Figure 1. Other signal and background processes will be included in future studies. The objective of the analysis is to measure the “signal strength”, μ , of the signal, which is a proxy for measuring how strongly the Higgs interacts with other fields. Interestingly, the usual notion that the signal strength corresponds to the ratio of the observed in data to the expected in Monte Carlo simulation signal yield breaks down in the presence of quantum interference.

This study is performed with data simulated with MadGraph5_aMC [3], Pythia 8 [4] and Delphes 3 [5].

2 Machine Learning in a signal strength measurement

Traditionally, in analyses without quantum interference, one can train a machine learning classifier (such as a Boosted Decision Tree) to separate the signal and background samples (referred to as “events”) that are simulated separately, and under the assumption that it is an optimal classifier, due to the Neyman-Pearson lemma [6], one can get the likelihood ratio [7] between a test hypothesis and the null hypothesis from the output of the classifier. The output of the classifier can be used for a fit to measure the signal strength, μ , optimally. In the presence of quantum interference, this strategy is no longer optimal. Figure 2 shows how a physics variable (the invariant mass of the four leptons) that is

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Abstract — The traditional machine learning approach to optimize a particle physics analysis in the presence of quantum interference between the signal and background processes is limited. Physics-aware machine learning techniques that rely on the extraction of additional information from a physics simulator to train the neural network could be adapted to a signal and background analysis. We apply this idea to the off-shell Higgs to four leptons analysis for the Vector Boson Fusion process at the high energy proton-proton collisions at the Large Hadron Collider. The model trained on simulated data at different values of the signal strength captures the presence of quantum interference.

1 Introduction

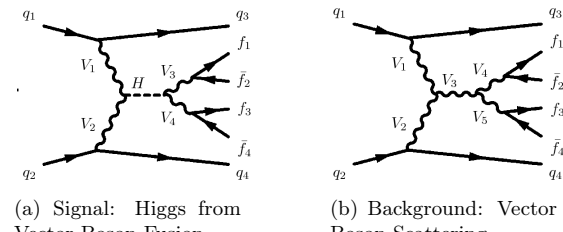




Figure 1: Feynman Diagrams of the processes under study, (a) signal Higgs diagram, (b) interfering background diagram

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A study of the off-shell Higgs boson decaying to two Z bosons that decay to four leptons (henceforth referred to as “offshell h4l”), such the 2018 study [2] in the ATLAS Collaboration [1] is one of the most interesting studies in high energy particle physics because it allows to break certain degeneracies between the Higgs couplings, and constrain the Higgs width (under certain model dependent assumptions) that cannot be disentangled by an on-shell measurement alone. An update to the previous ATLAS study using the entire Run2

EUROPEAN ORGANISATION FOR NUCLEAR RESEARCH (CERN)

Submitted to: Rep. Prog. Phys. CERN-EP-2024-305
December 3, 2024

An implementation of neural simulation-based inference for parameter estimation in ATLAS

The ATLAS Collaboration

Neural simulation-based inference is a powerful class of machine-learning-based methods for statistical inference that naturally handles high-dimensional parameter estimation without the need to bin data into low-dimensional summary histograms. Such methods are promising for a range of measurements, including at the Large Hadron Collider, where no single observable may be optimal to scan over the entire theoretical phase space under consideration, or where binning data into histograms could result in a loss of sensitivity. This work develops a neural simulation-based inference framework for statistical inference, using neural networks to estimate probability density ratios, which enables the application to a full-scale analysis. It incorporates a large number of systematic uncertainties, quantifies the uncertainty due to the finite number of events in training samples, develops a method to construct confidence intervals, and demonstrates a series of intermediate diagnostic checks that can be performed to validate the robustness of the method. As an example, the power and feasibility of the method are assessed on simulated data for a simplified version of an off-shell Higgs boson couplings measurement in the four-lepton final states. This approach represents an extension to the standard statistical methodology used by the experiments at the Large Hadron Collider, and can benefit many physics analyses.

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arXiv:2412.01600v1 [hep-ex] 2 Dec 2024

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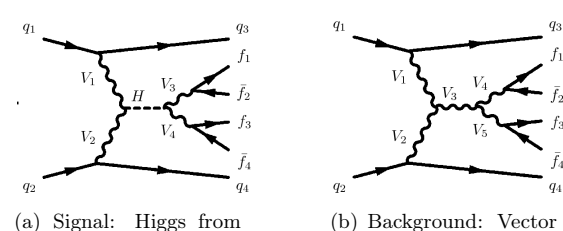



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CERN-EP-2024-298
December 3, 2024

Measurement of off-shell Higgs boson production in the $H^* \rightarrow ZZ \rightarrow 4\ell$ decay channel using a neural simulation-based inference technique in 13 TeV pp collisions with the ATLAS detector

The ATLAS Collaboration

A measurement of off-shell Higgs boson production in the $H^* \rightarrow ZZ \rightarrow 4\ell$ decay channel is presented. The measurement uses 140 fb⁻¹ of proton-proton collisions at $\sqrt{s} = 13$ TeV collected by the ATLAS detector at the Large Hadron Collider and supersedes the previous result in this decay channel using the same dataset. The data analysis is performed using a neural simulation-based inference method, which builds per-event likelihood ratios using neural networks. The observed (expected) off-shell Higgs boson production signal strength in the $ZZ \rightarrow 4\ell$ decay channel at 68% CL is $0.87^{+0.75}_{-0.54}$ ($1.00^{+1.04}_{-0.95}$). The evidence for off-shell Higgs boson production using the $ZZ \rightarrow 4\ell$ decay channel has an observed (expected) significance of 2.5σ (1.3σ). The expected result represents a significant improvement relative to that of the previous analysis of the same dataset, which obtained an expected significance of 0.5σ . When combined with the most recent ATLAS measurement in the $ZZ \rightarrow 2\ell 2\nu$ decay channel, the evidence for off-shell Higgs boson production has an observed (expected) significance of 3.7σ (2.4σ). The off-shell measurements are combined with the measurement of on-shell Higgs boson production to obtain constraints on the Higgs boson total width. The observed (expected) value of the Higgs boson width at 68% CL is $4.3^{+2.7}_{-1.9}$ ($4.1^{+3.5}_{-3.4}$) MeV.

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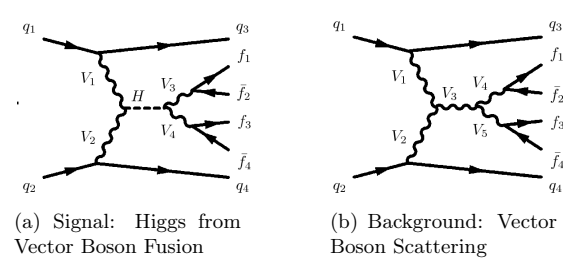



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Similar story for neutron star astrophysics

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An IOP and SISSA journal

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Neural simulation-based inference of the neutron star equation of state directly from telescope spectra

Len Brandes^a, Chirag Modi^{b,c}, Aishik Ghosh^{d,e}, Delaney Farrell^f, Lee Lindblom^g, Lukas Heinrich^h, Andrew W. Steiner^{h,i}, Fridolin Weber^{f,g} and Daniel Whiteson^d

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^ePhysics Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, U.S.A.
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ABSTRACT: Neutron stars provide a unique opportunity to study strongly interacting matter under extreme density conditions. The intricacies of matter inside neutron stars and their equation of state are not directly visible, but determine bulk properties, such as mass and radius, which affect the star’s thermal X-ray emissions. However, the telescope spectra of these emissions are also affected by the stellar distance, hydrogen column, and effective surface temperature, which are not always well-constrained. Uncertainties on these nuisance parameters must be accounted for when making a robust estimation of the equation of state. In this study, we develop a novel methodology that, for the first time, can infer the full posterior distribution of both the equation of state and nuisance parameters directly from

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Brandes et al (incl. Ghosh): JCAP 09(2024)009

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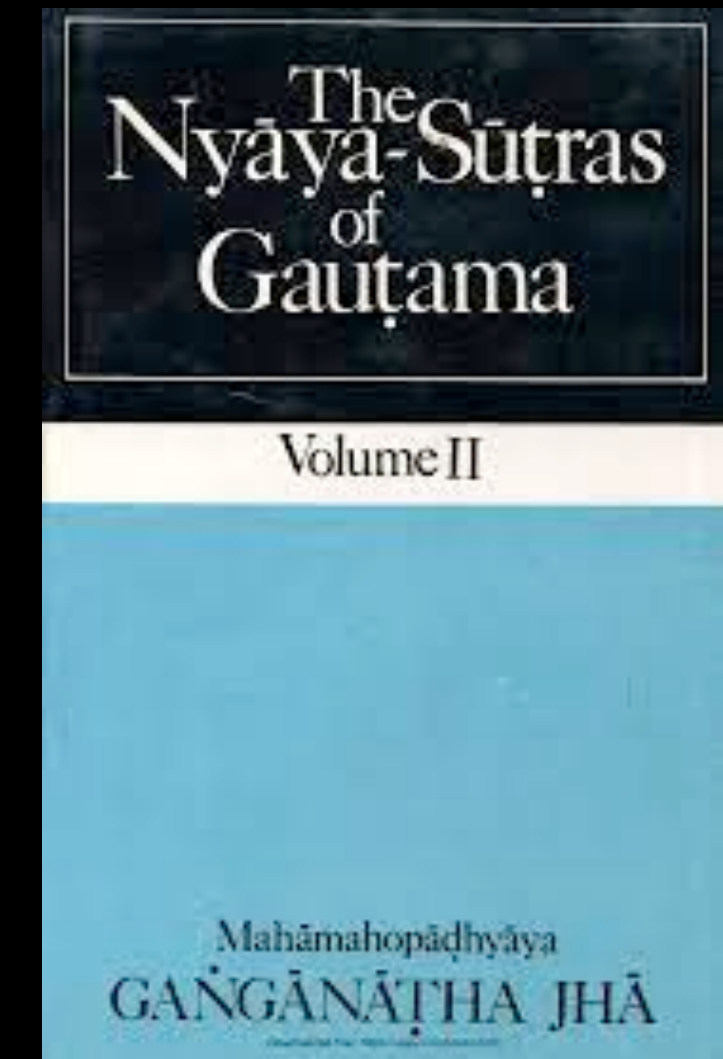
Some of the oldest questions

What elements make up the universe ?
(5 century BCE)



Image: DALL-E

How sure are we?
Theory of Errors & Empirical Knowledge
(6 century BCE)



Some of the oldest questions



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What elements make up the universe ?
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Theorists

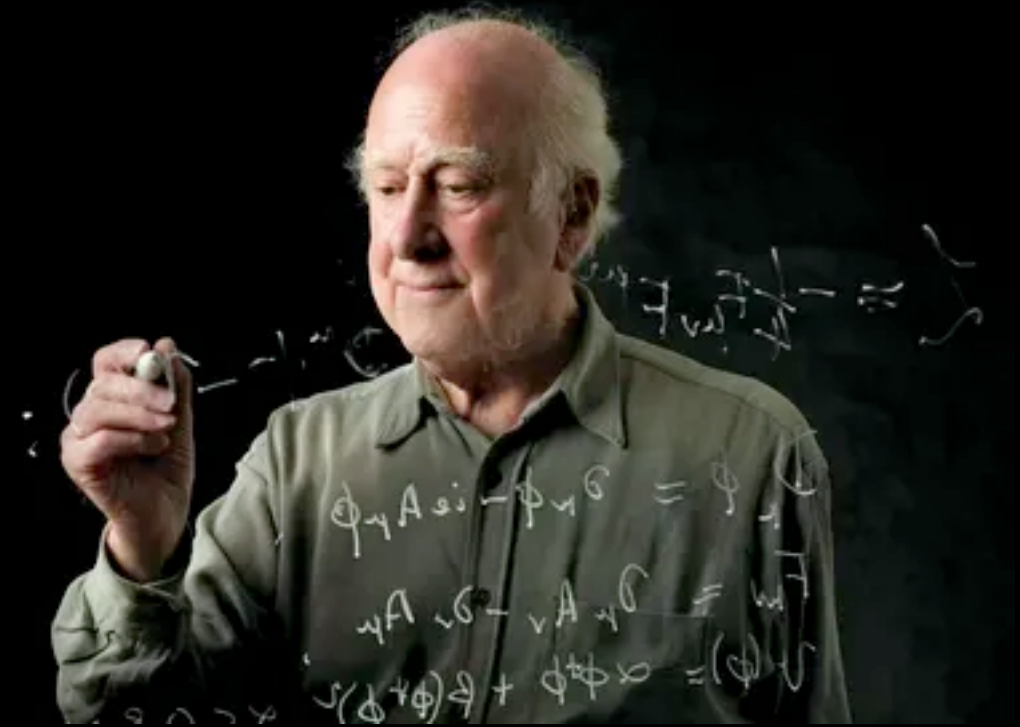
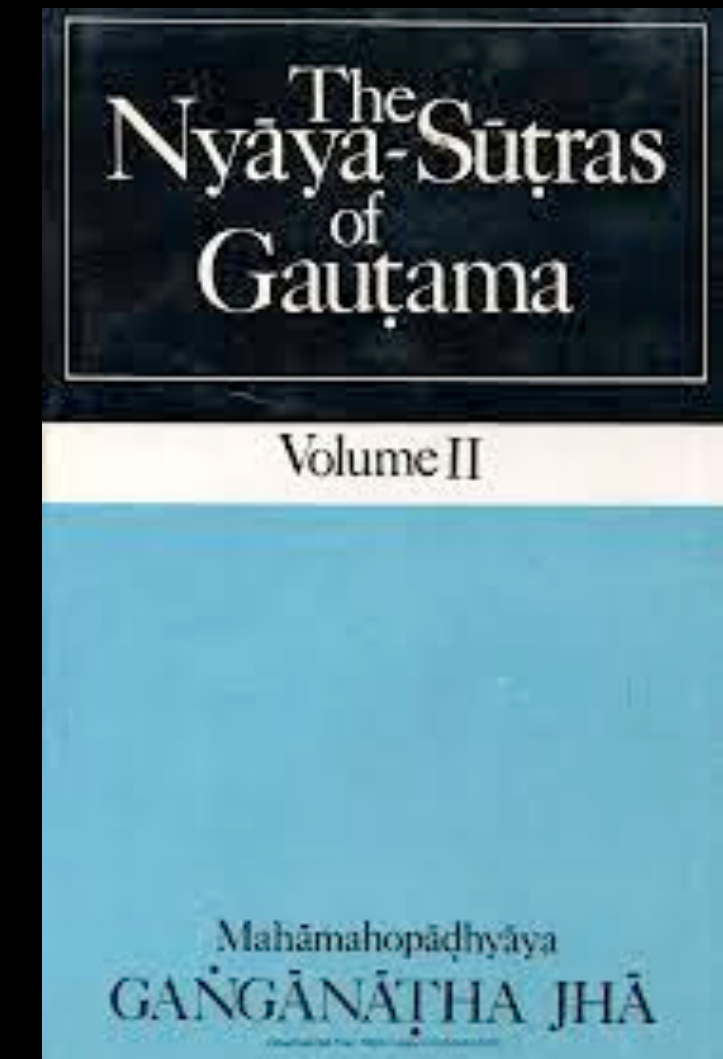


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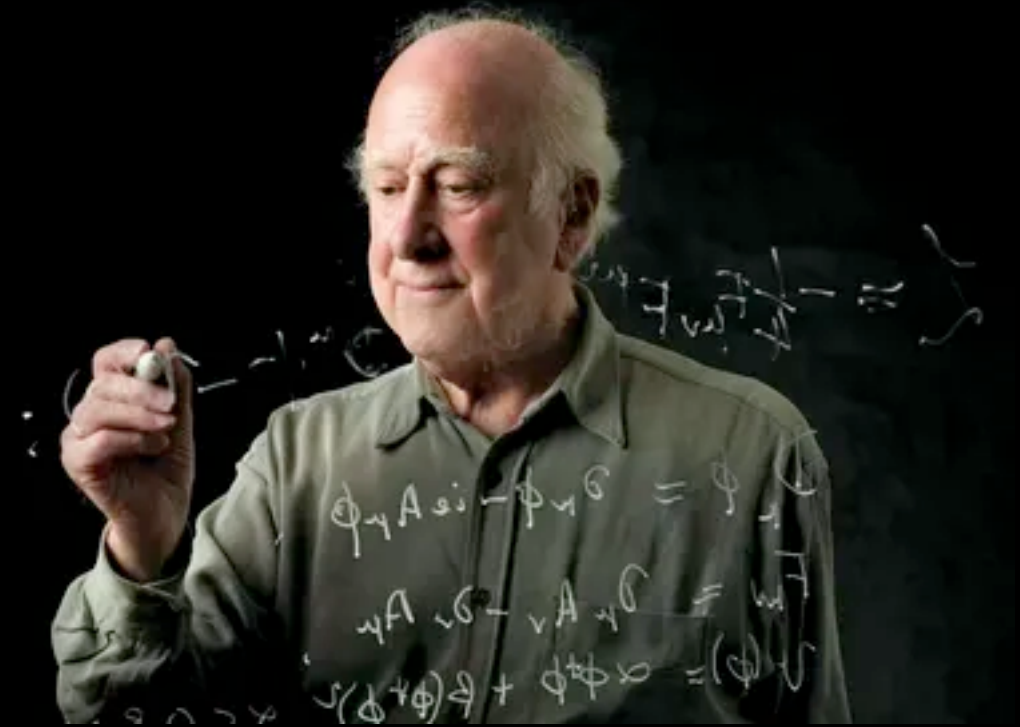


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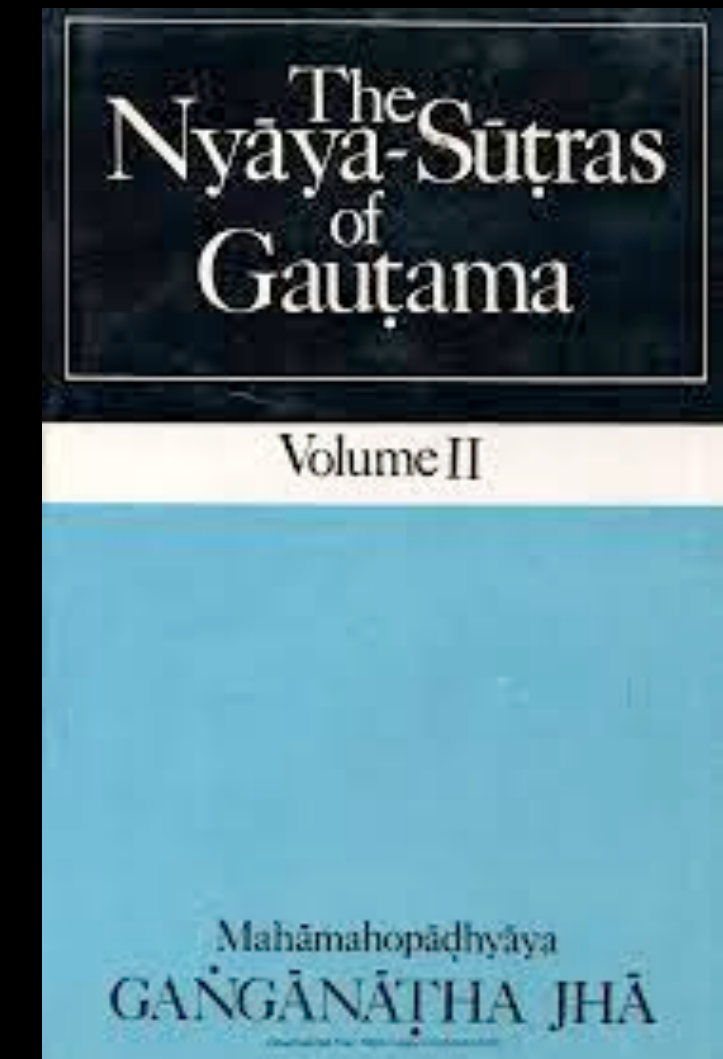


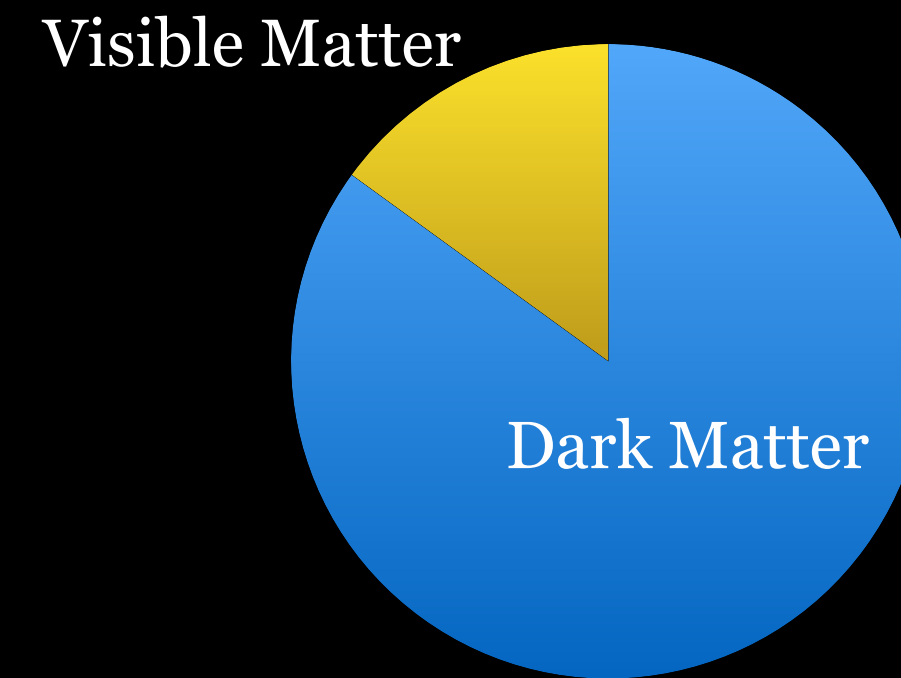
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Experimentalists

Questions about the universe ...

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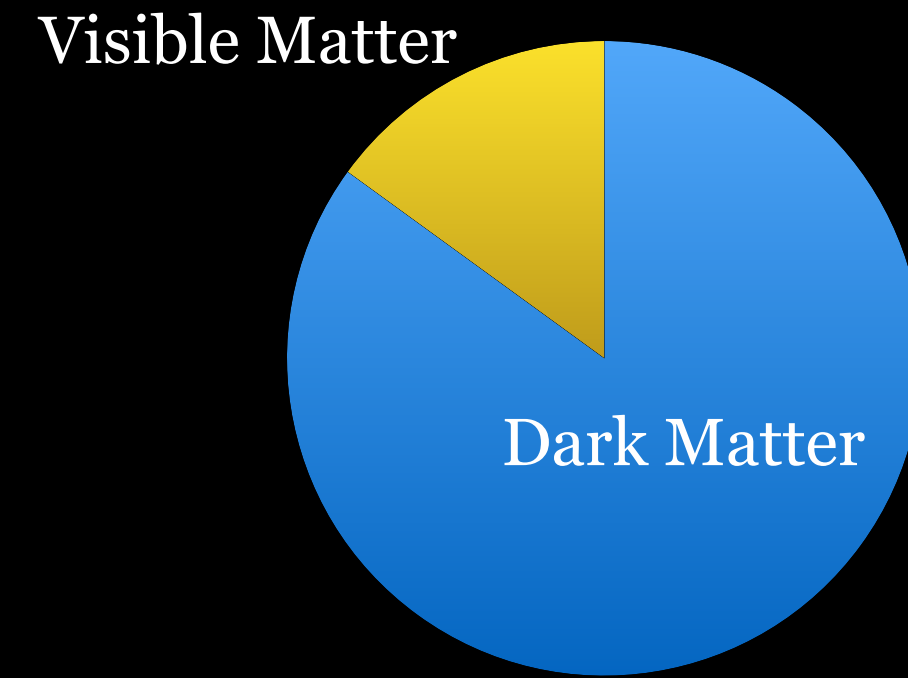


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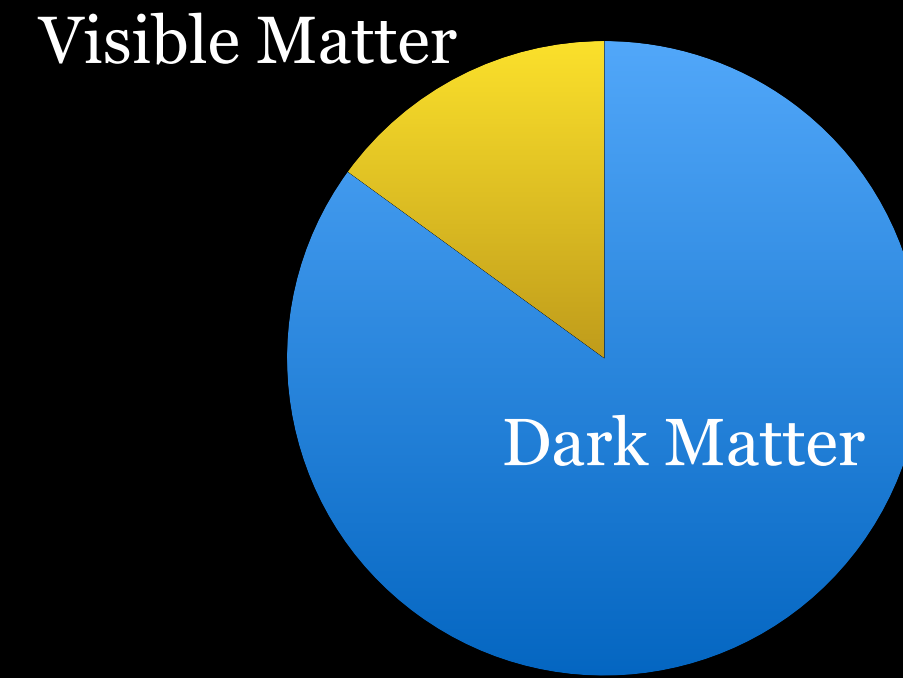


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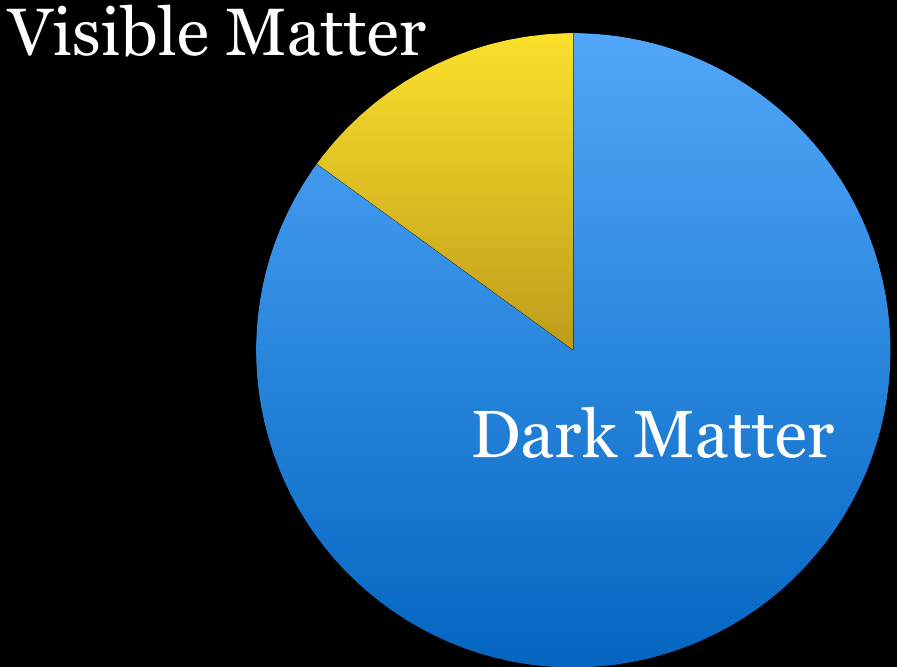


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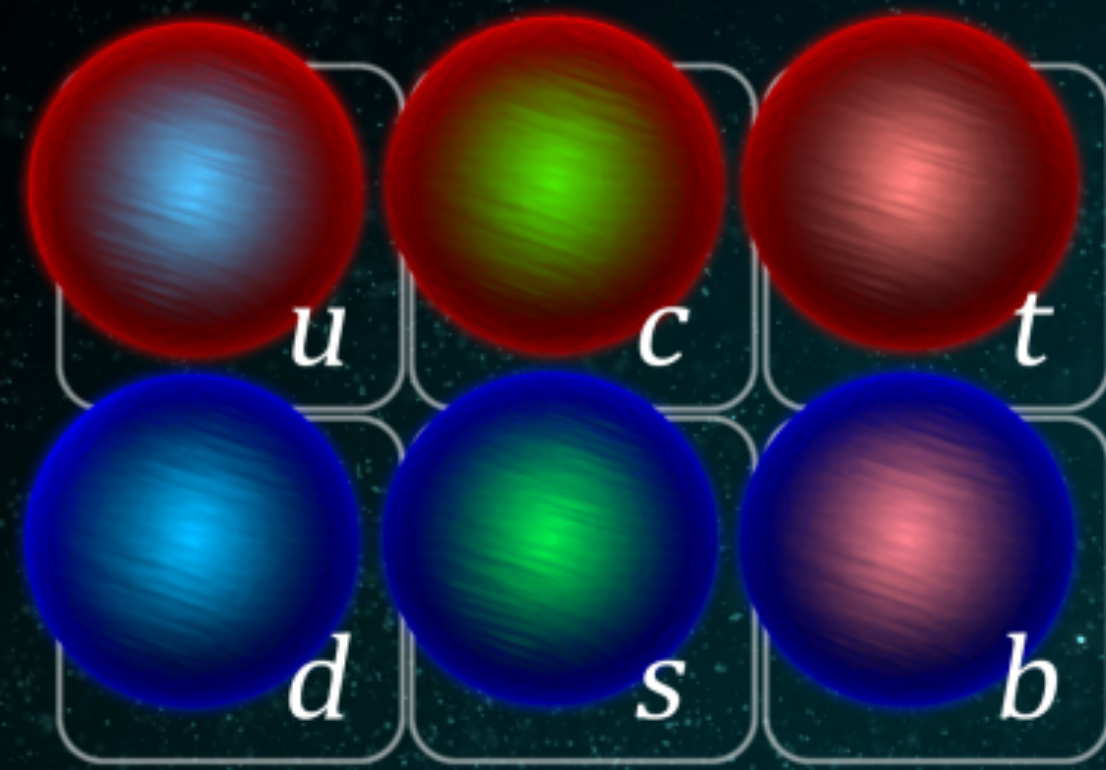
Are there new forces ?

New theories often predict new particles yet to be discovered

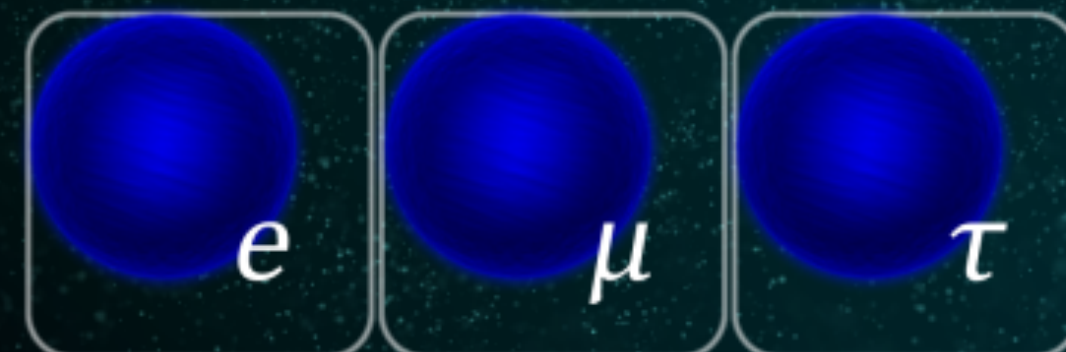


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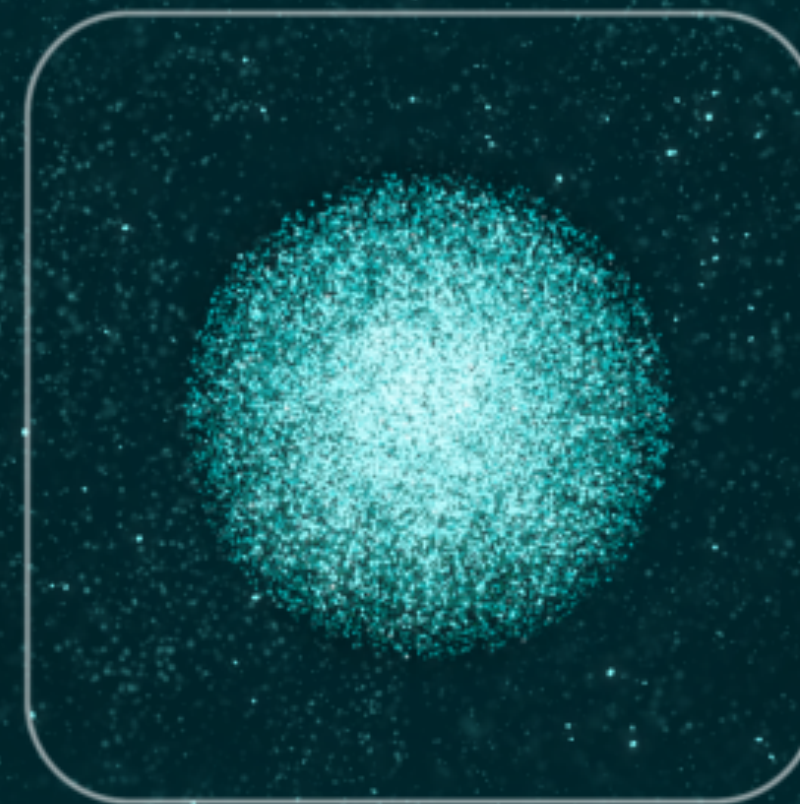
The most fundamental constituents of matter (that we know of...)



Quarks



Leptons



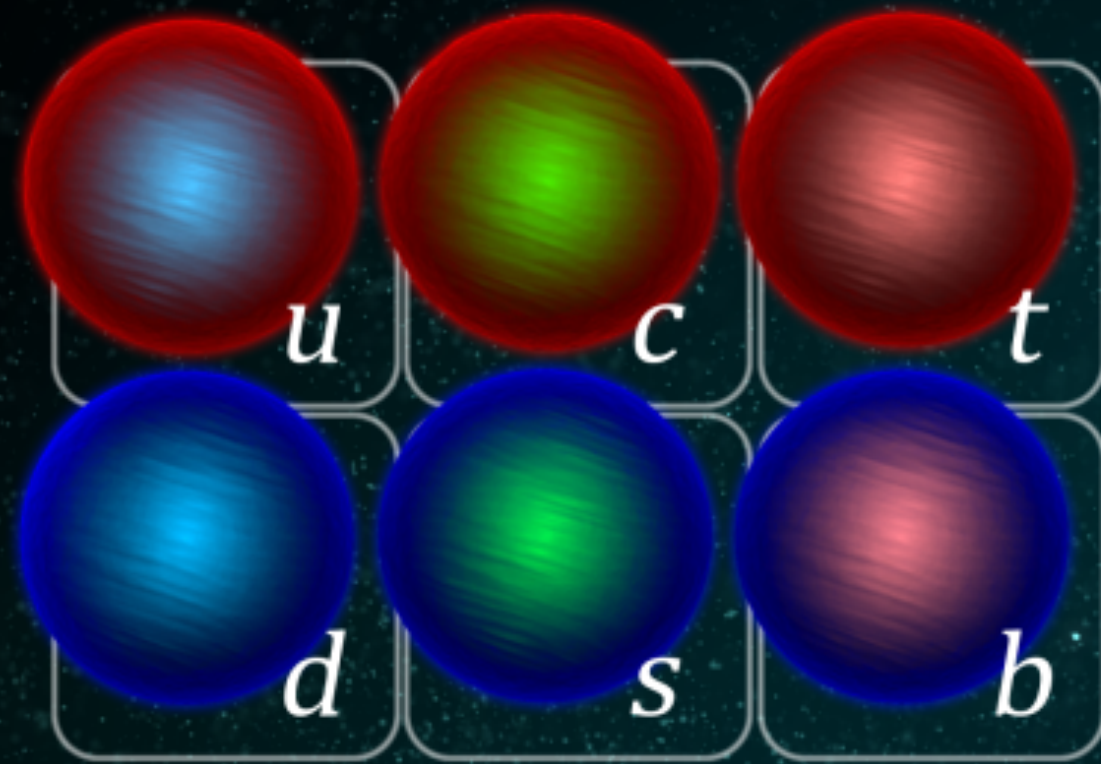
Higgs boson



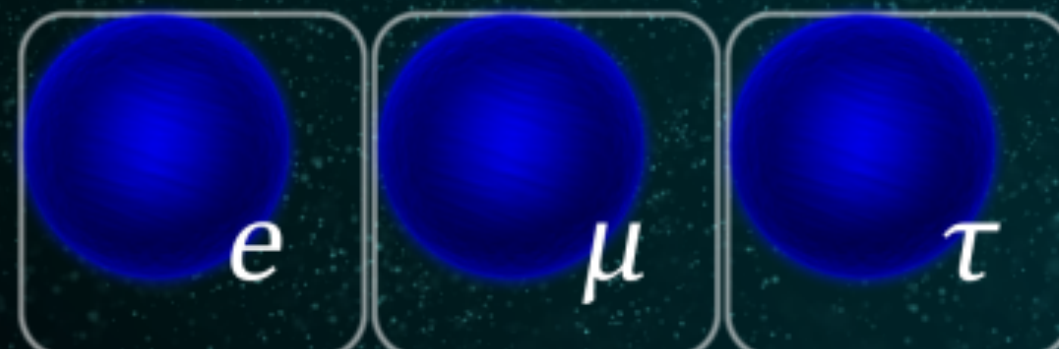
Forces

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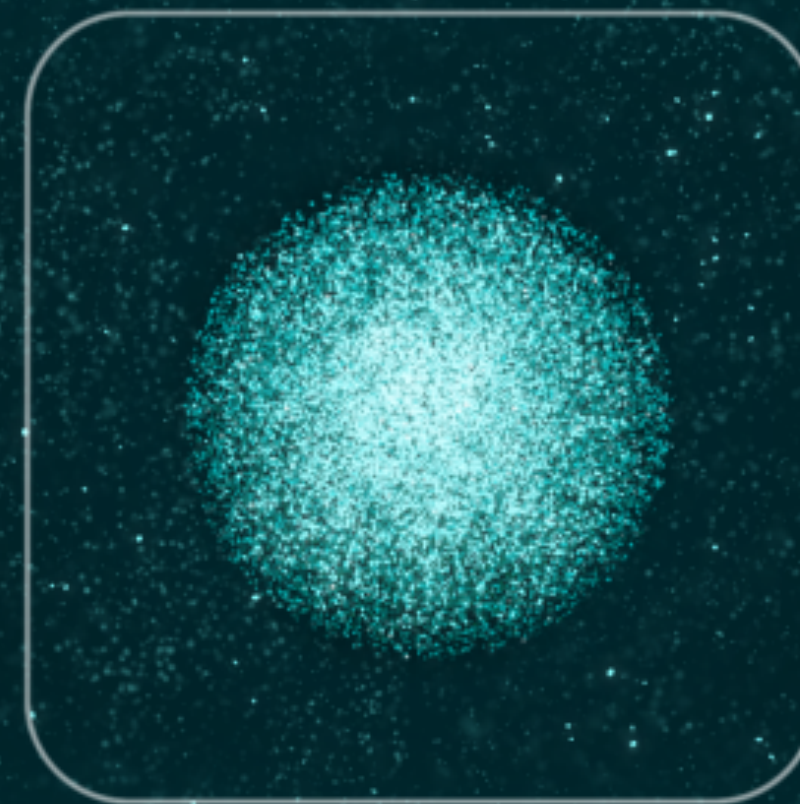
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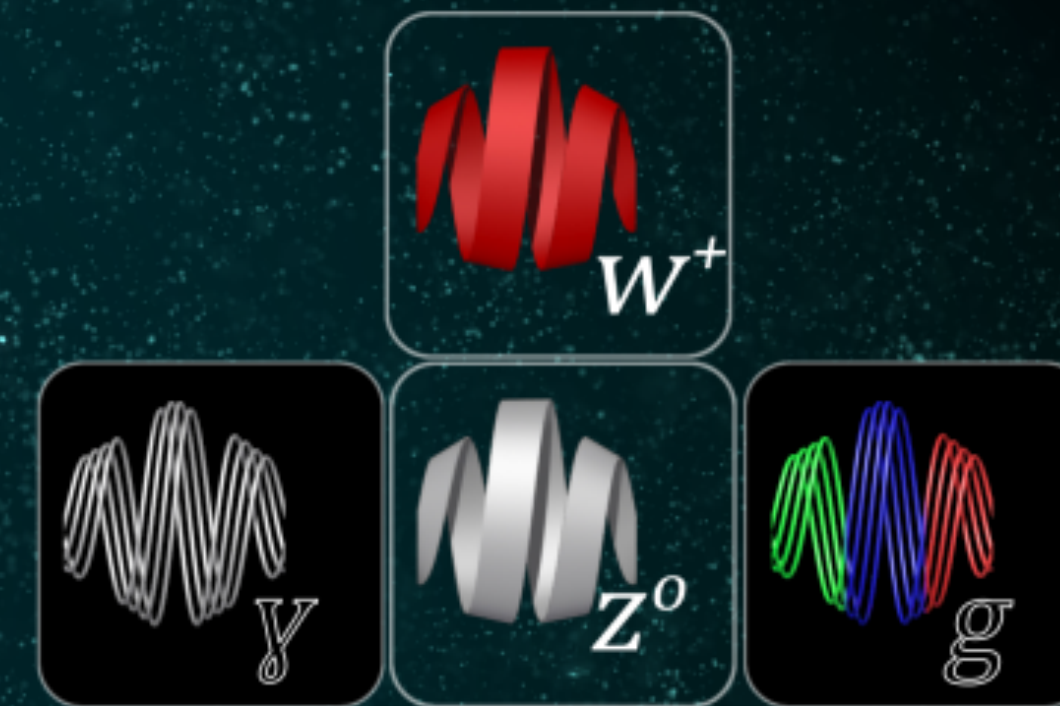
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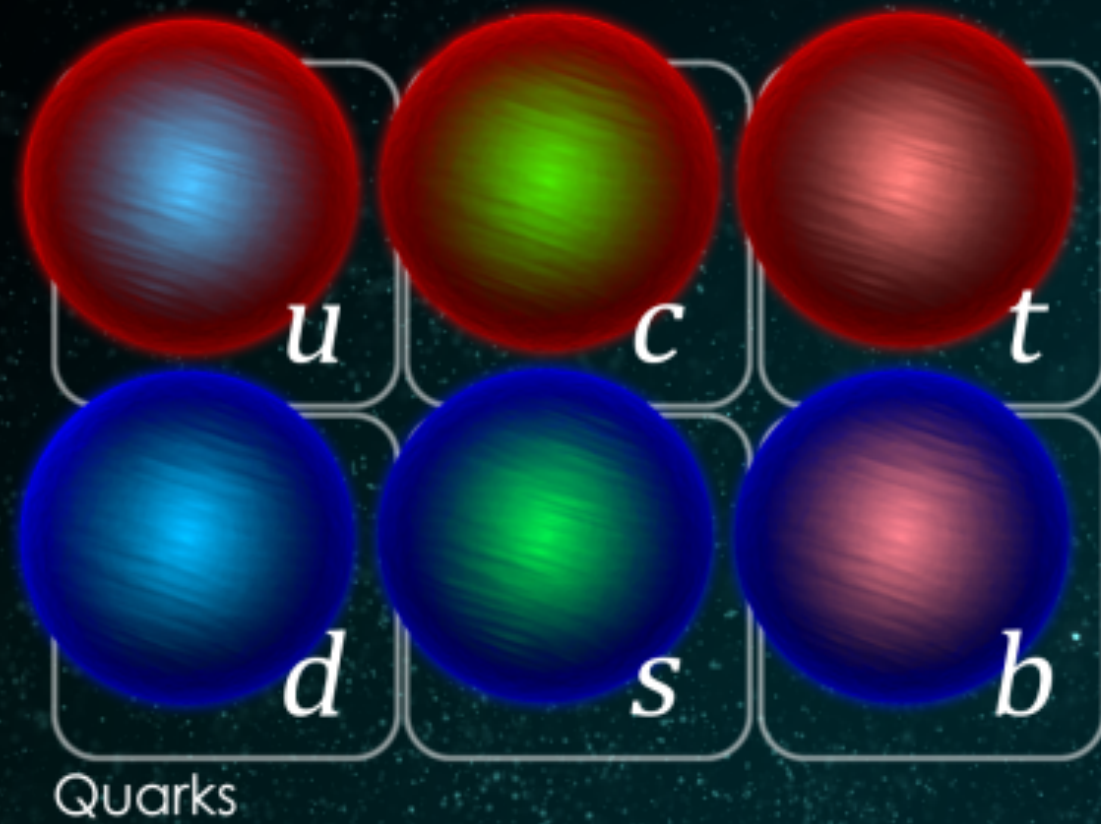
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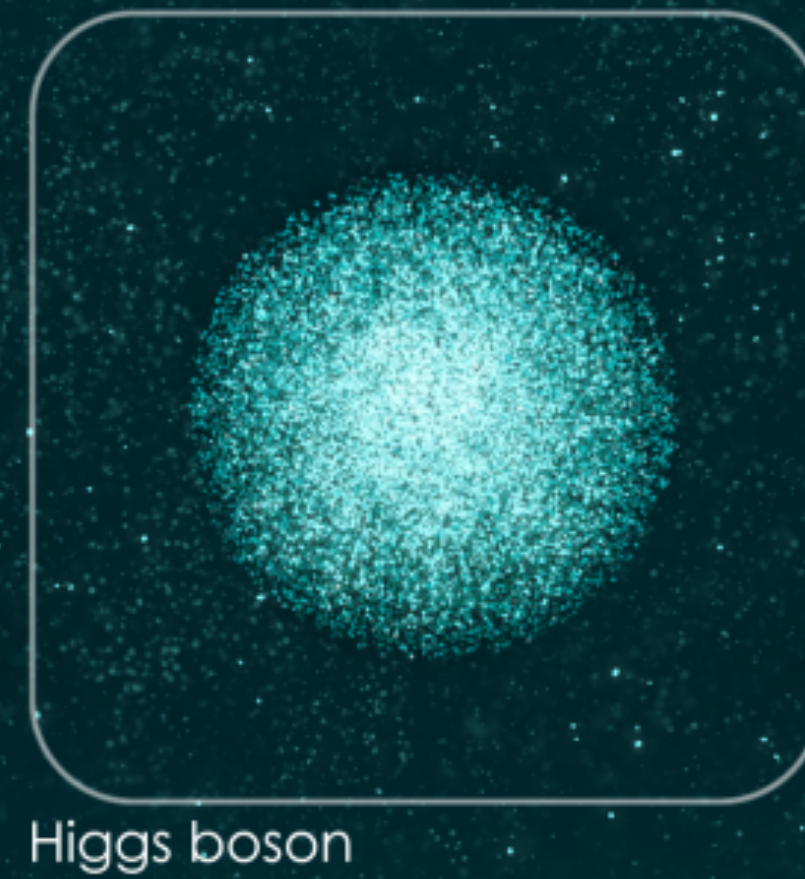
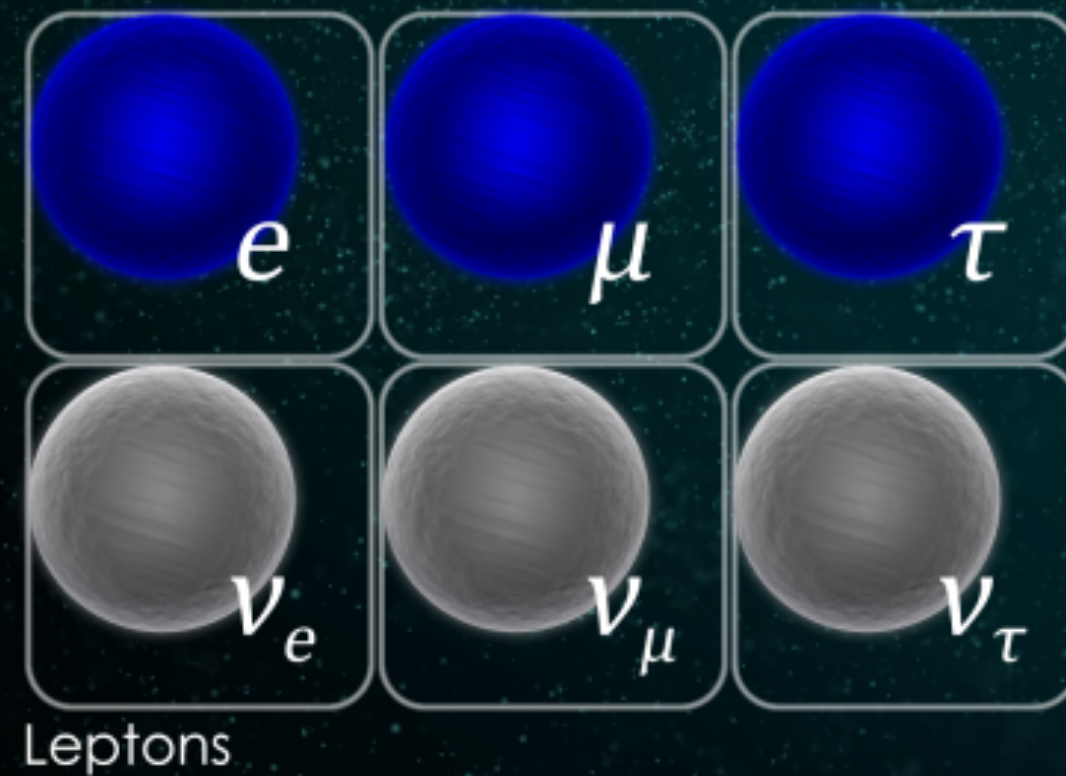
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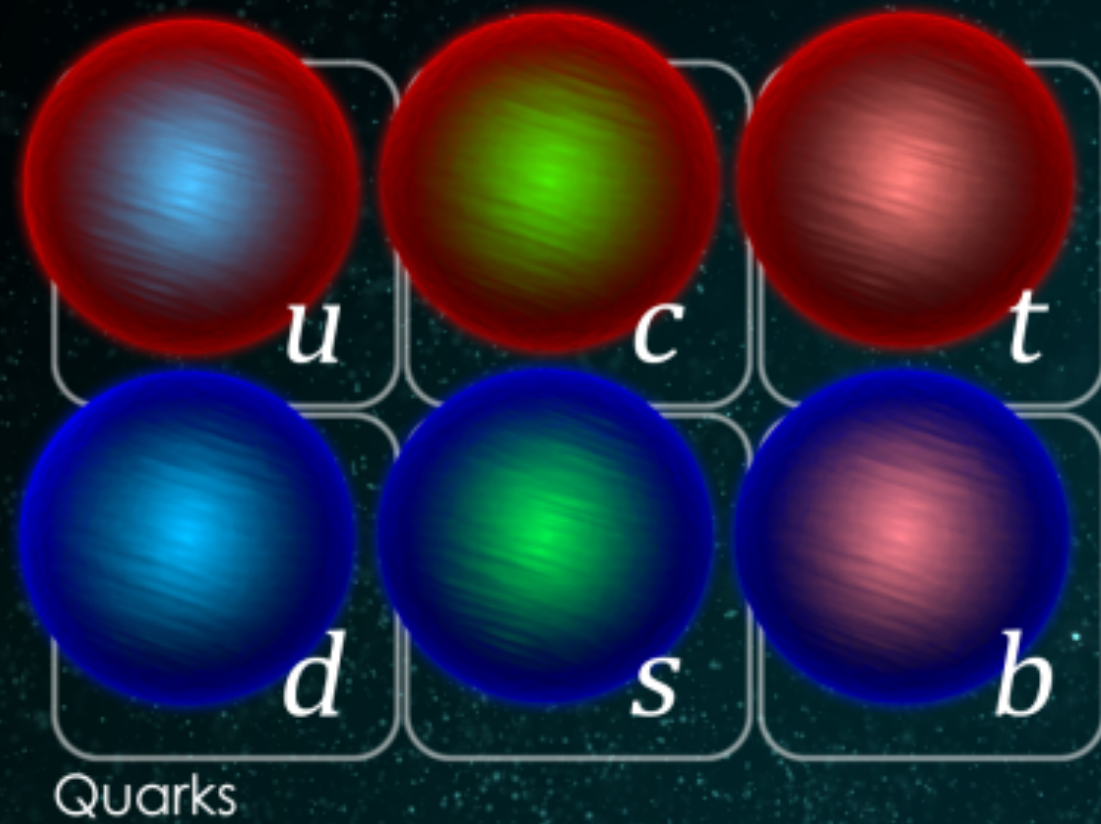


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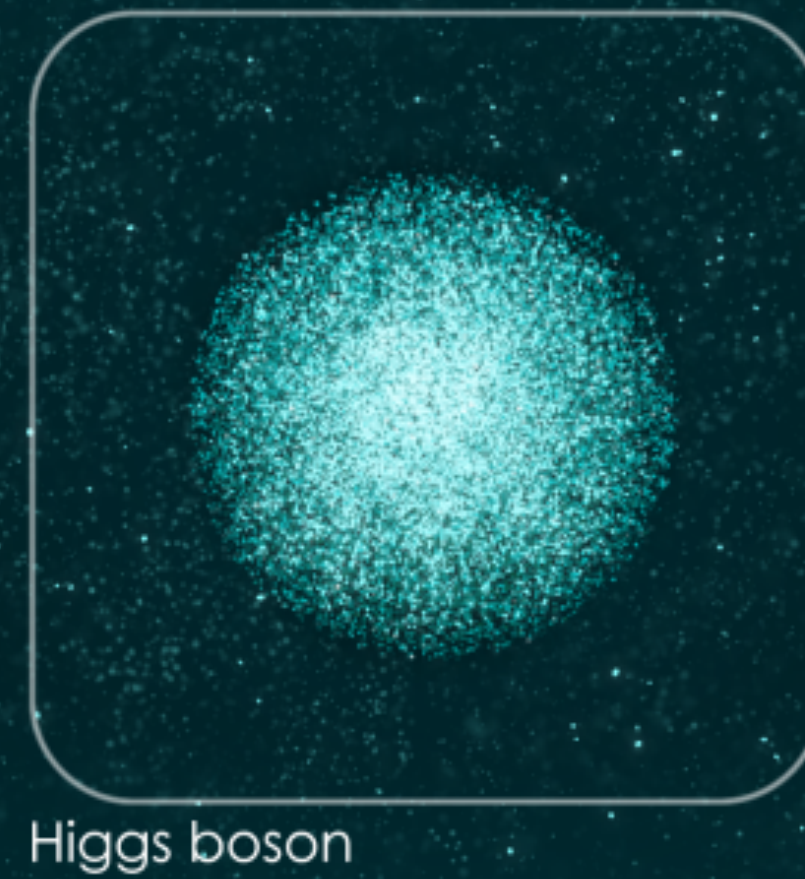
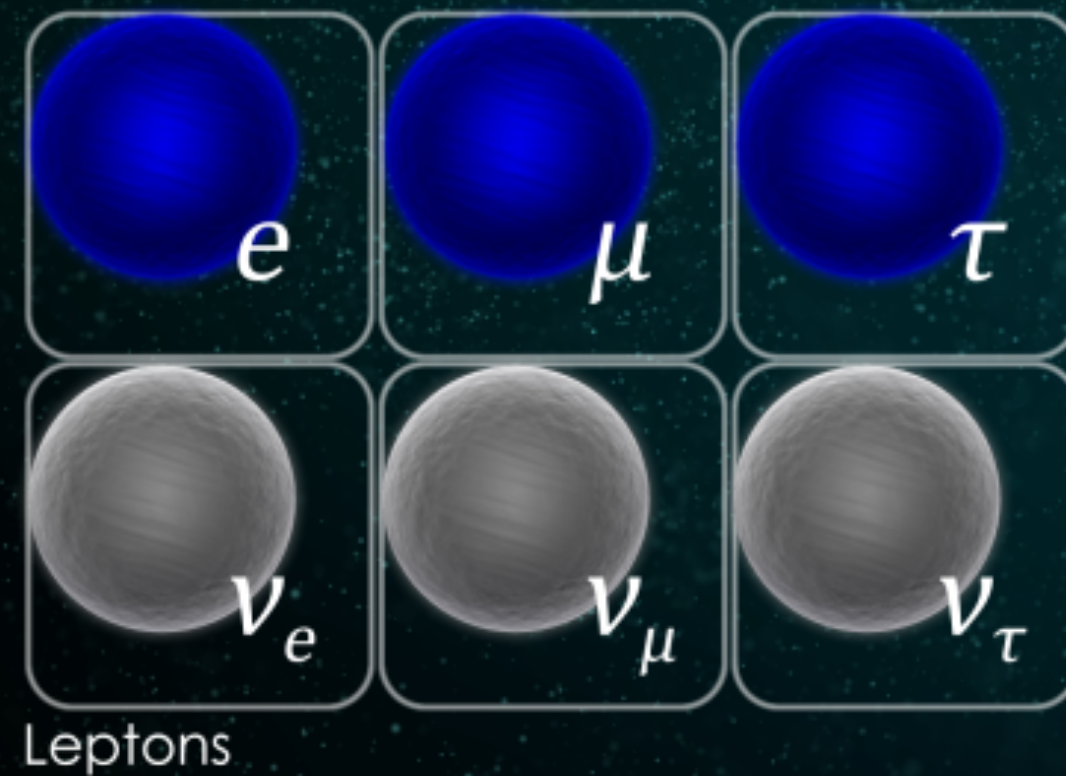


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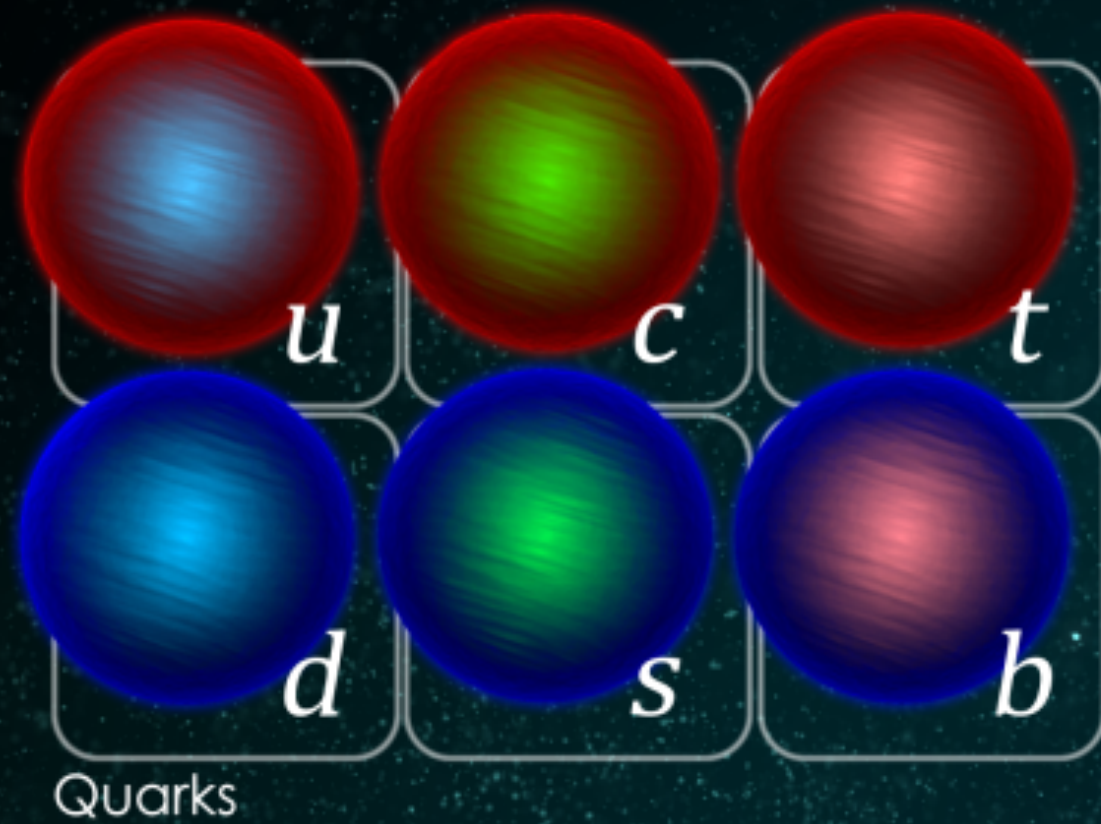


Force
carrier
particles

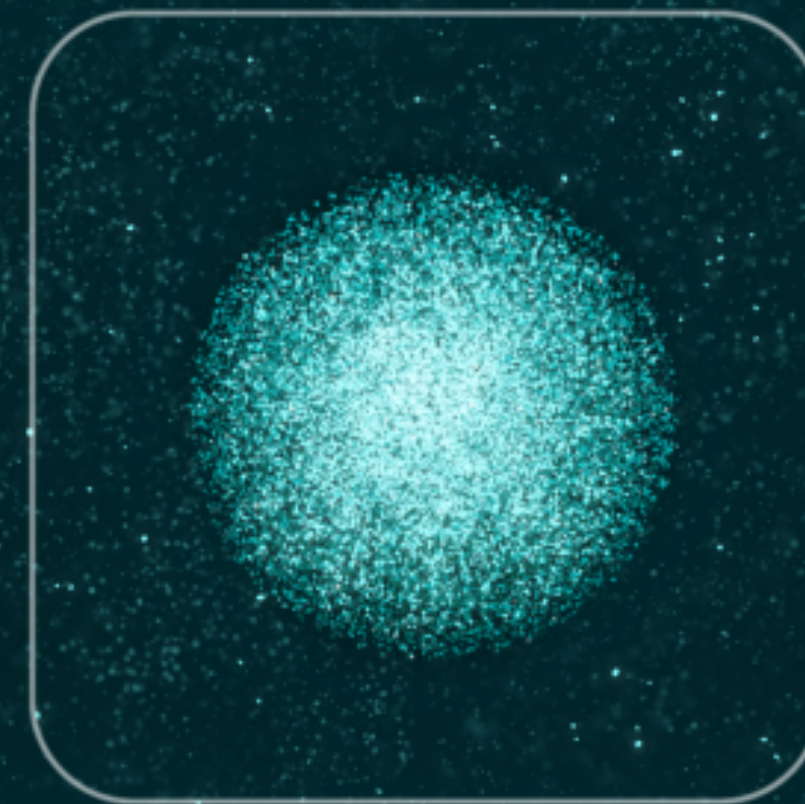
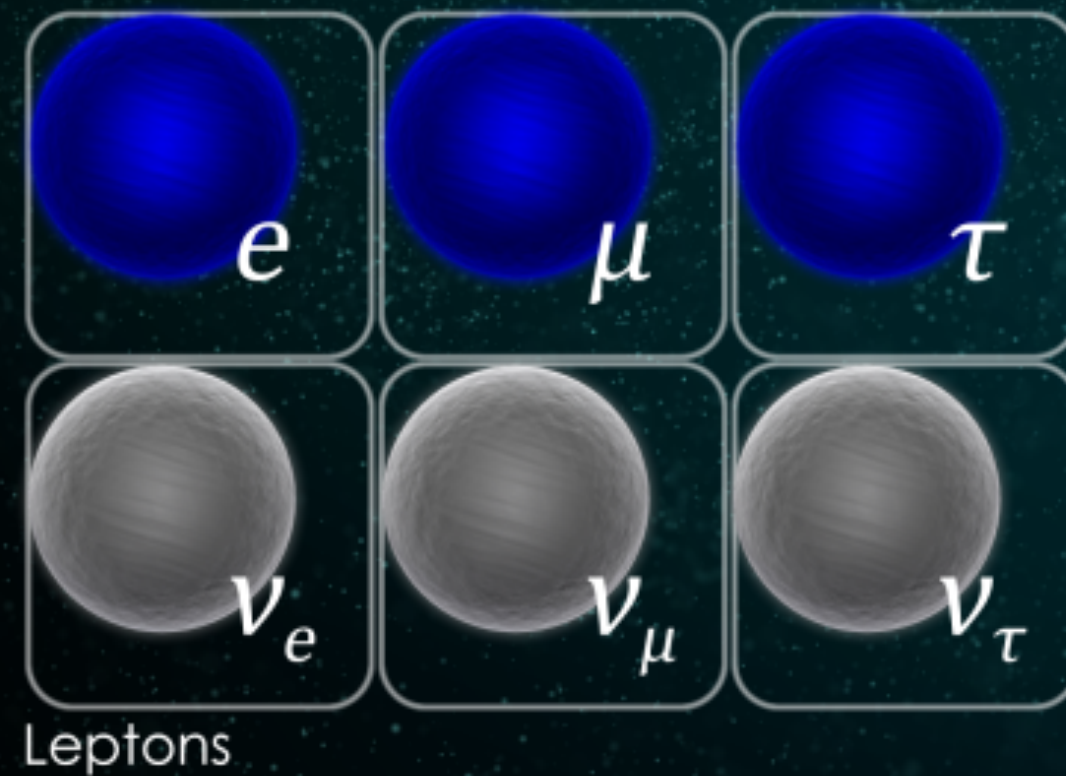


The most fundamental constituents of matter (that we know of...)

Protons
are made
up of u
and d



That's the
electron
and its
cousins

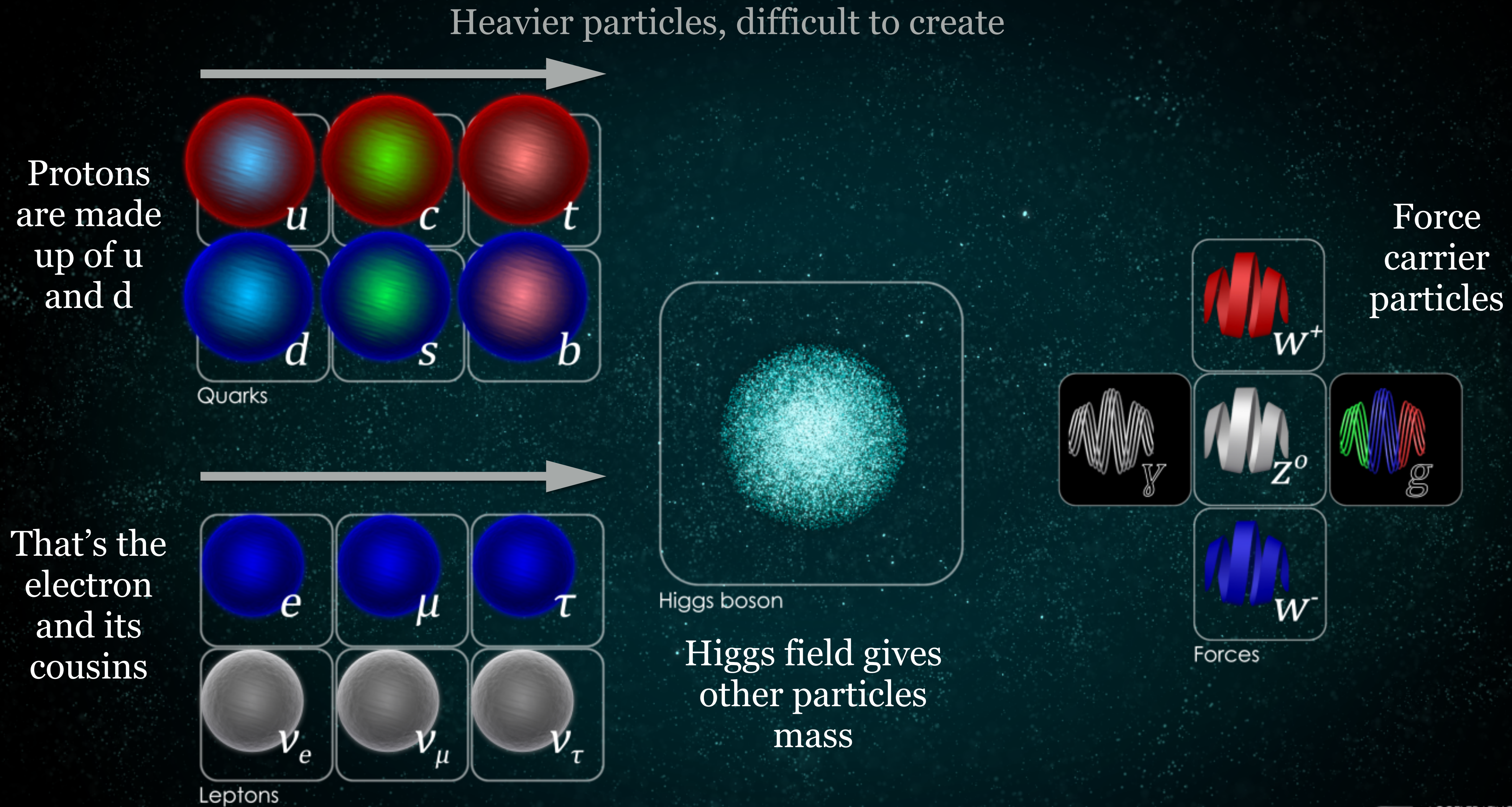


Higgs field gives
other particles
mass

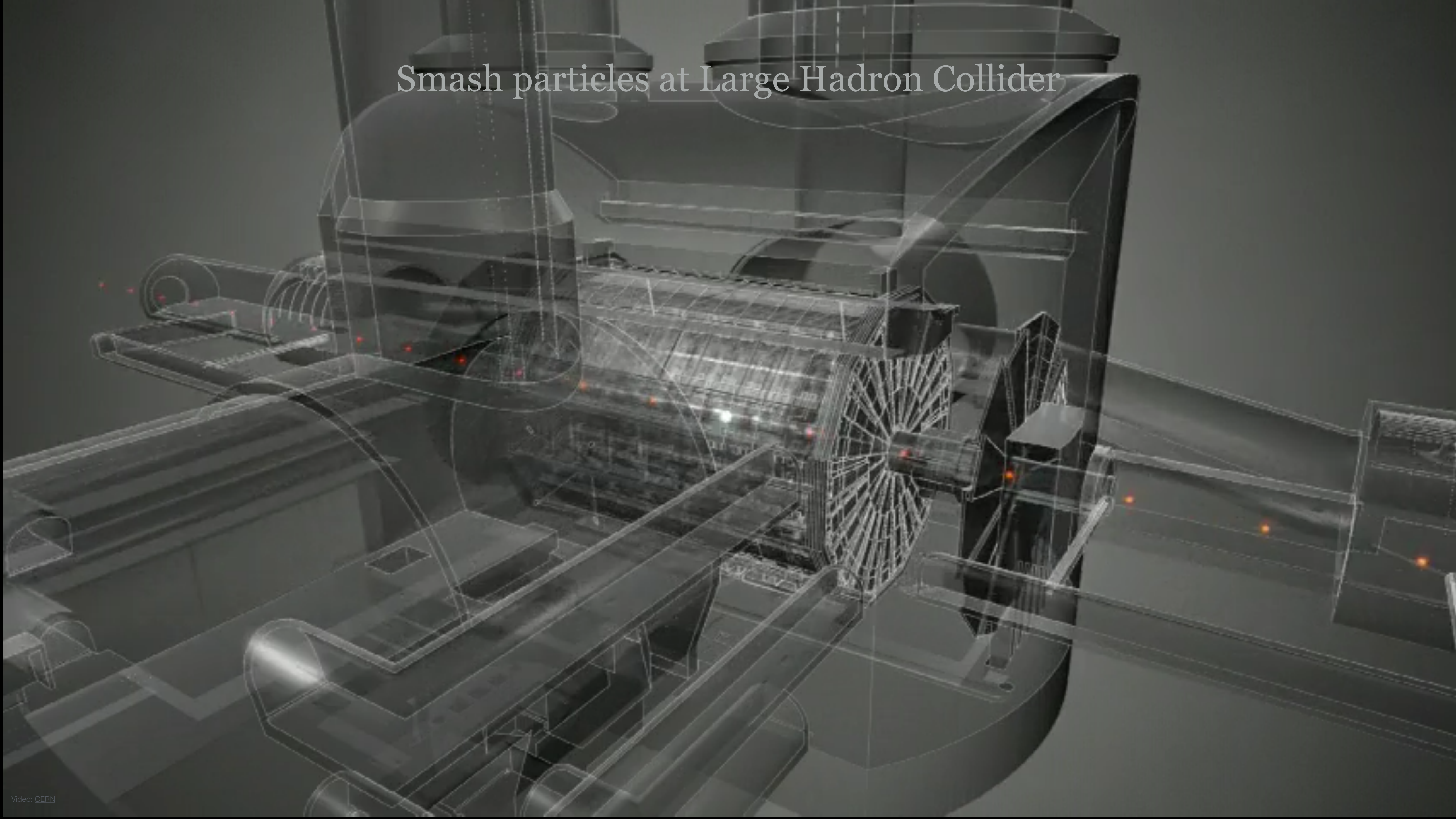
Force
carrier
particles



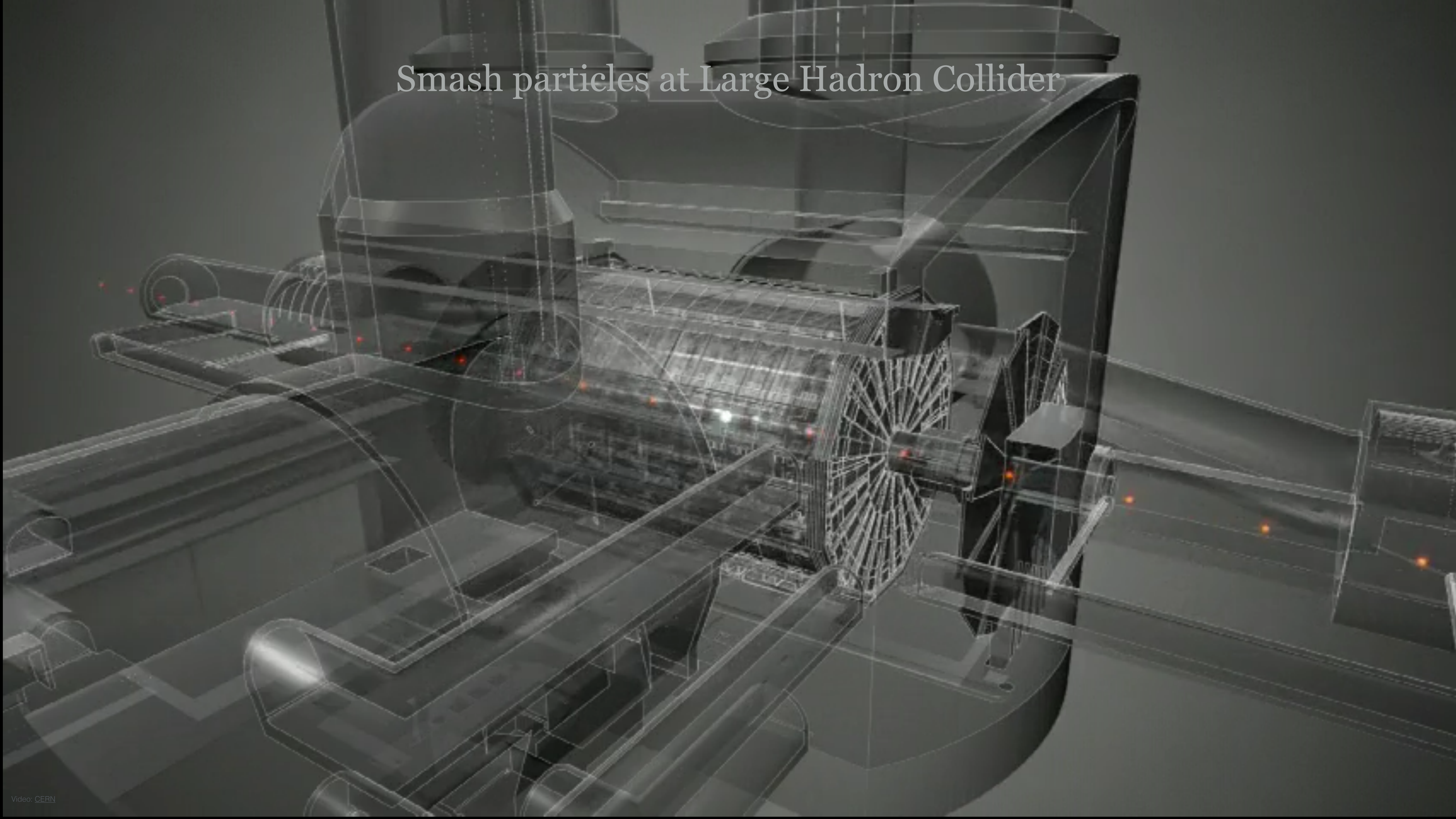
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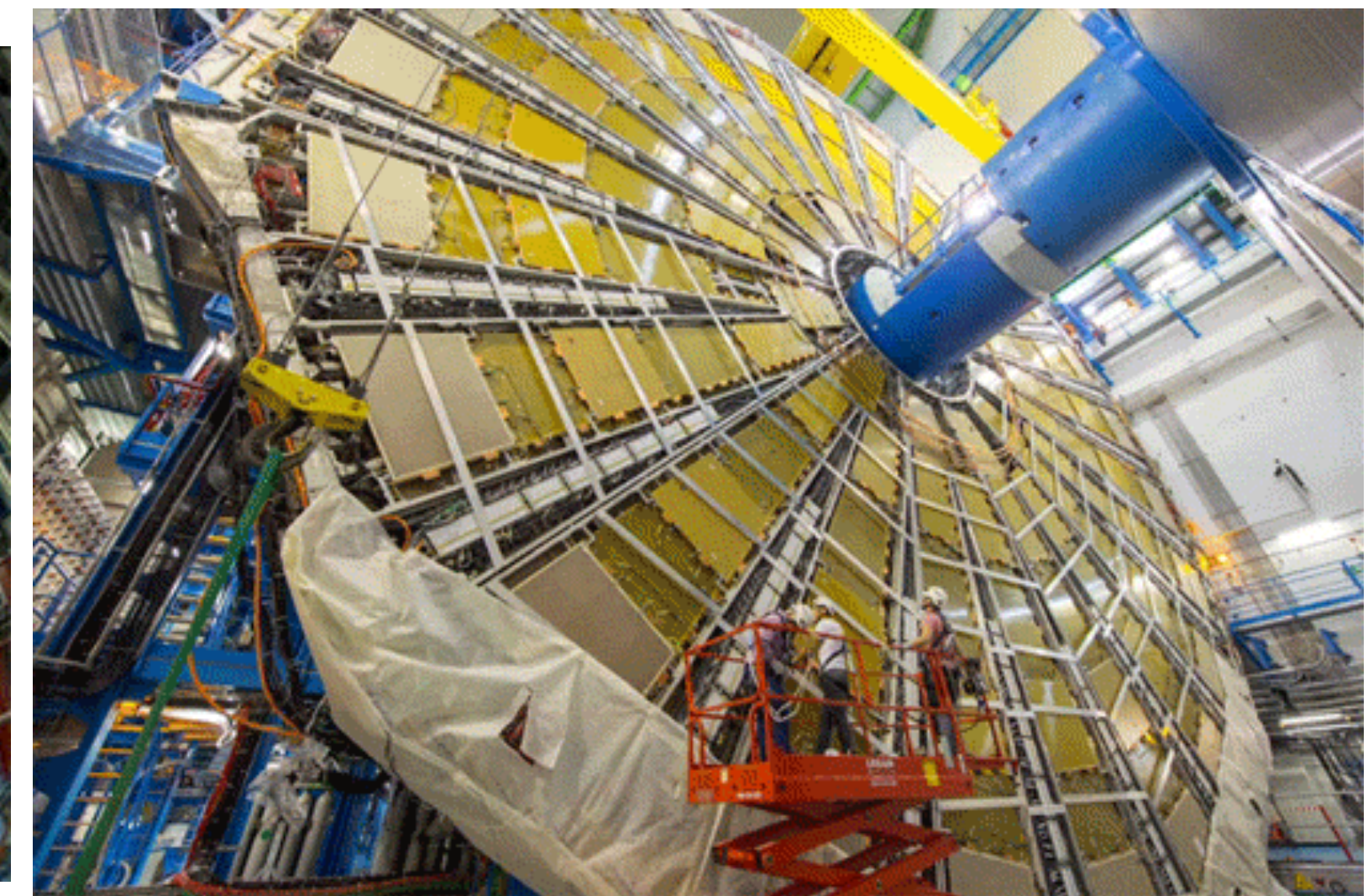
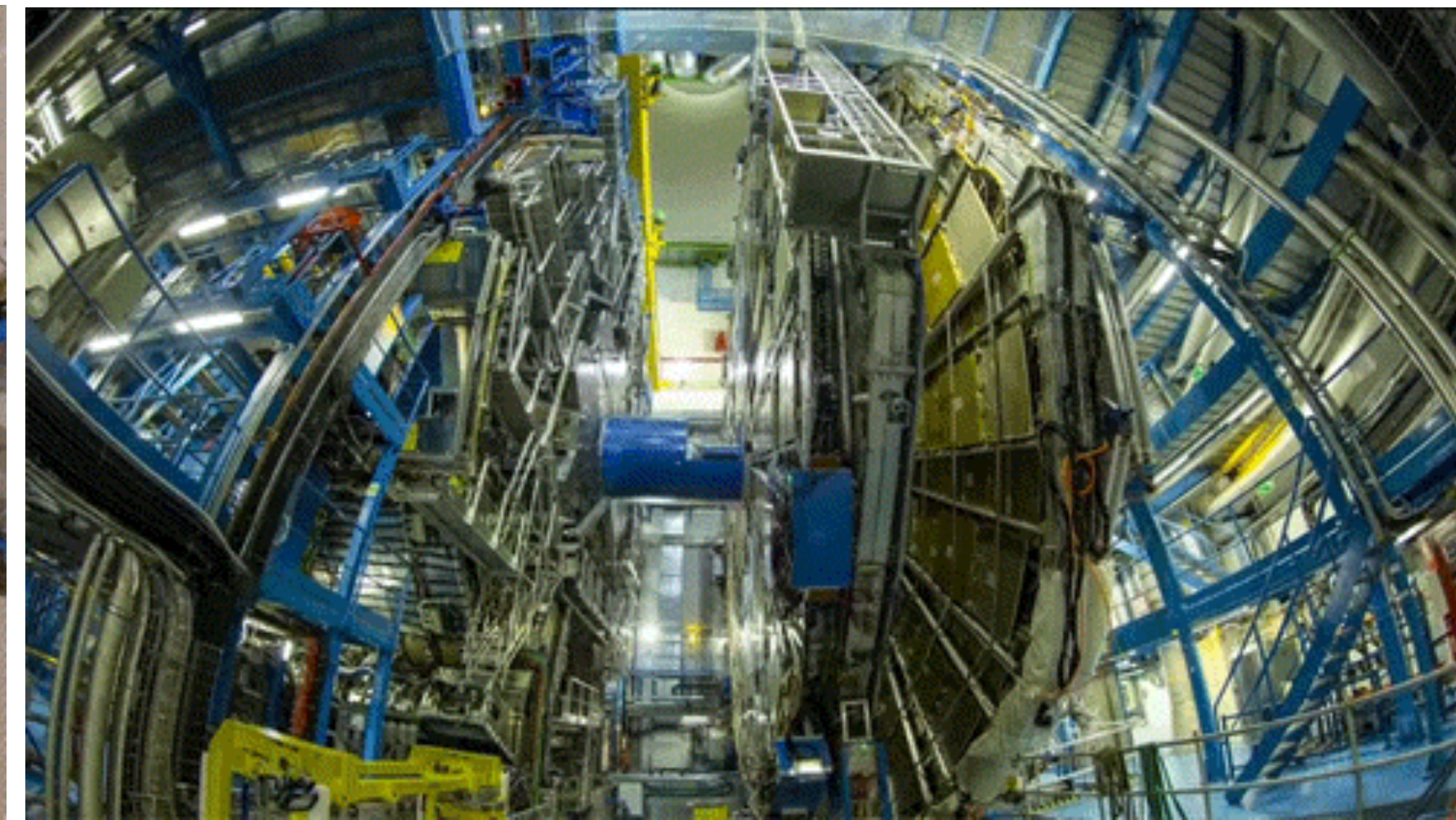
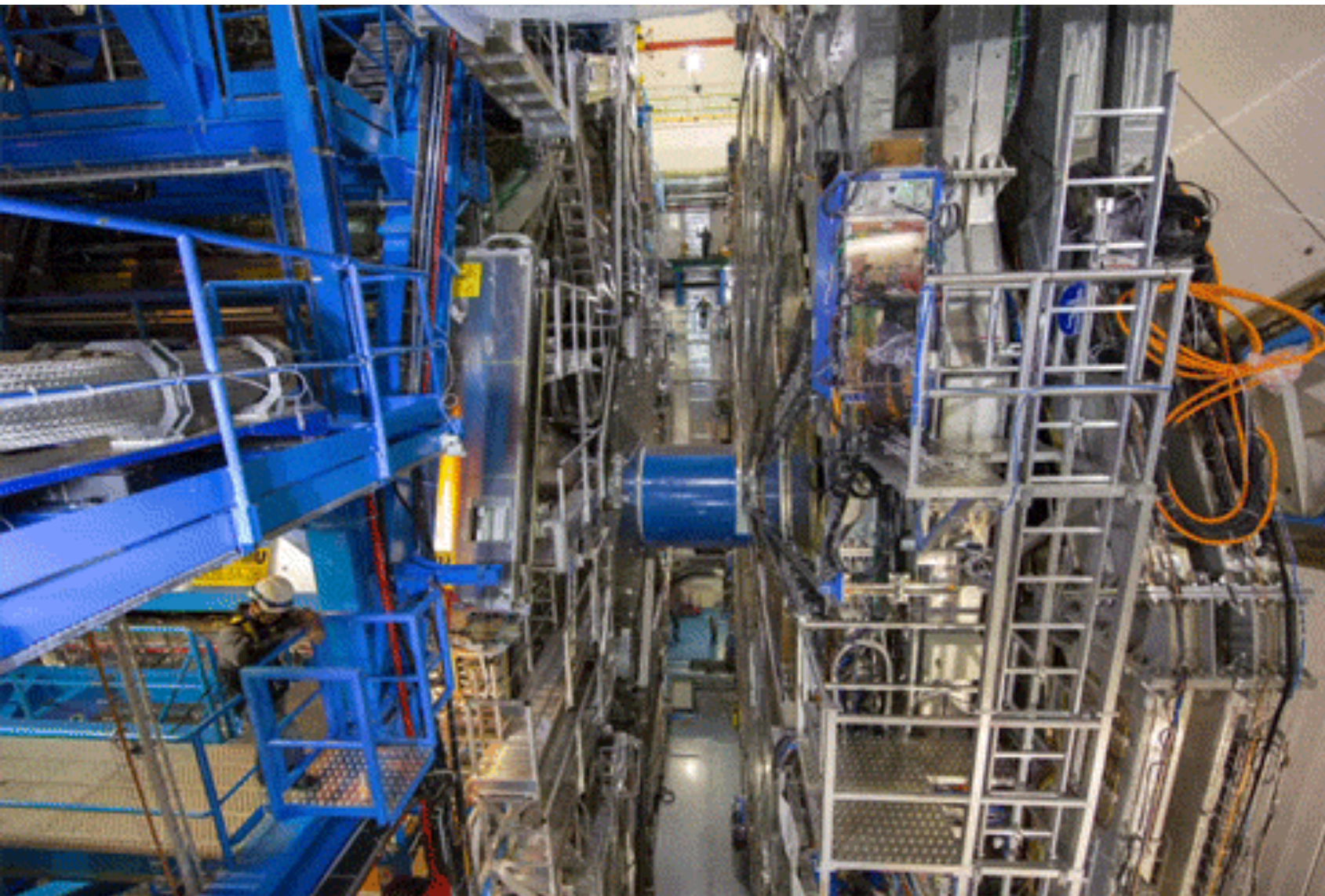
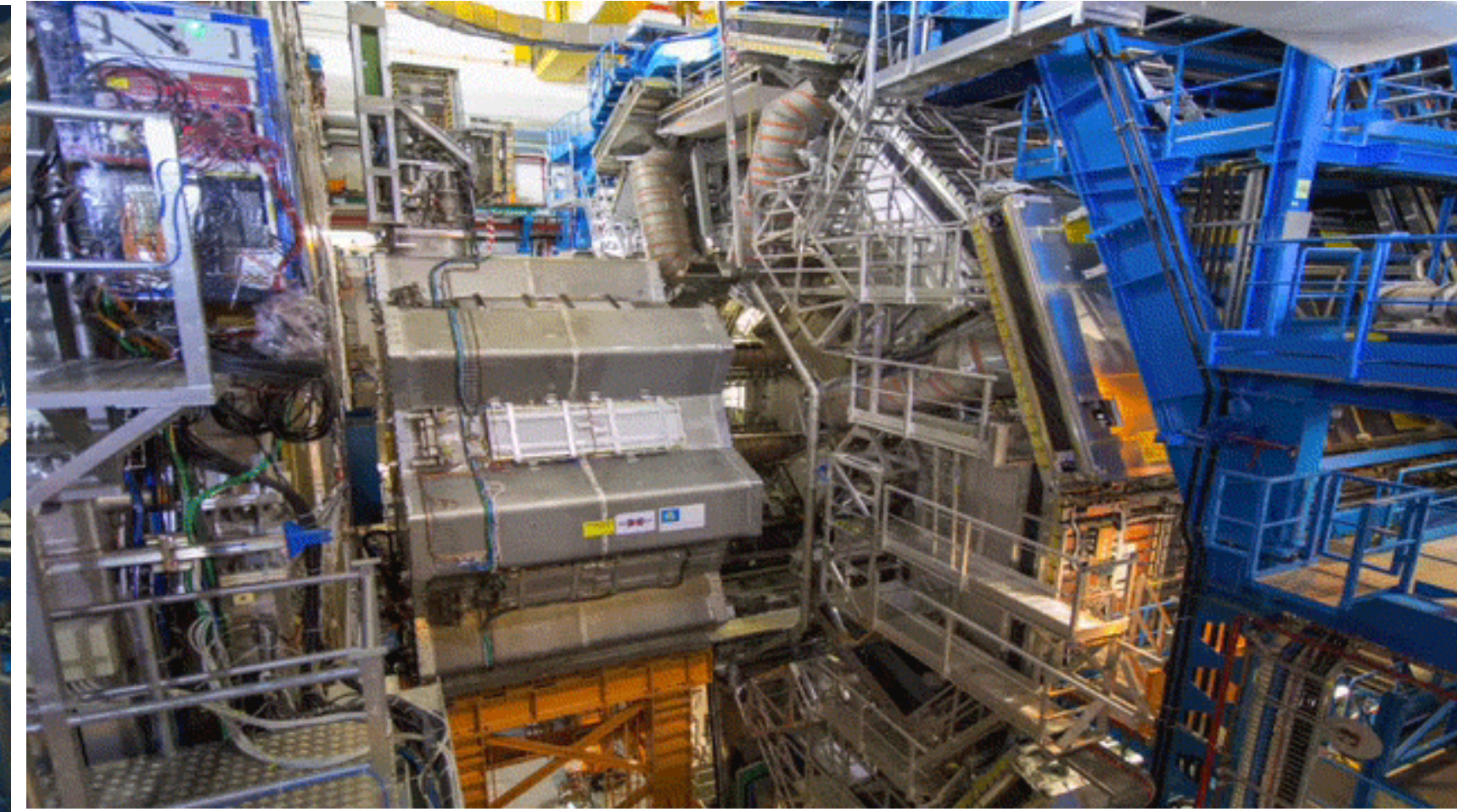
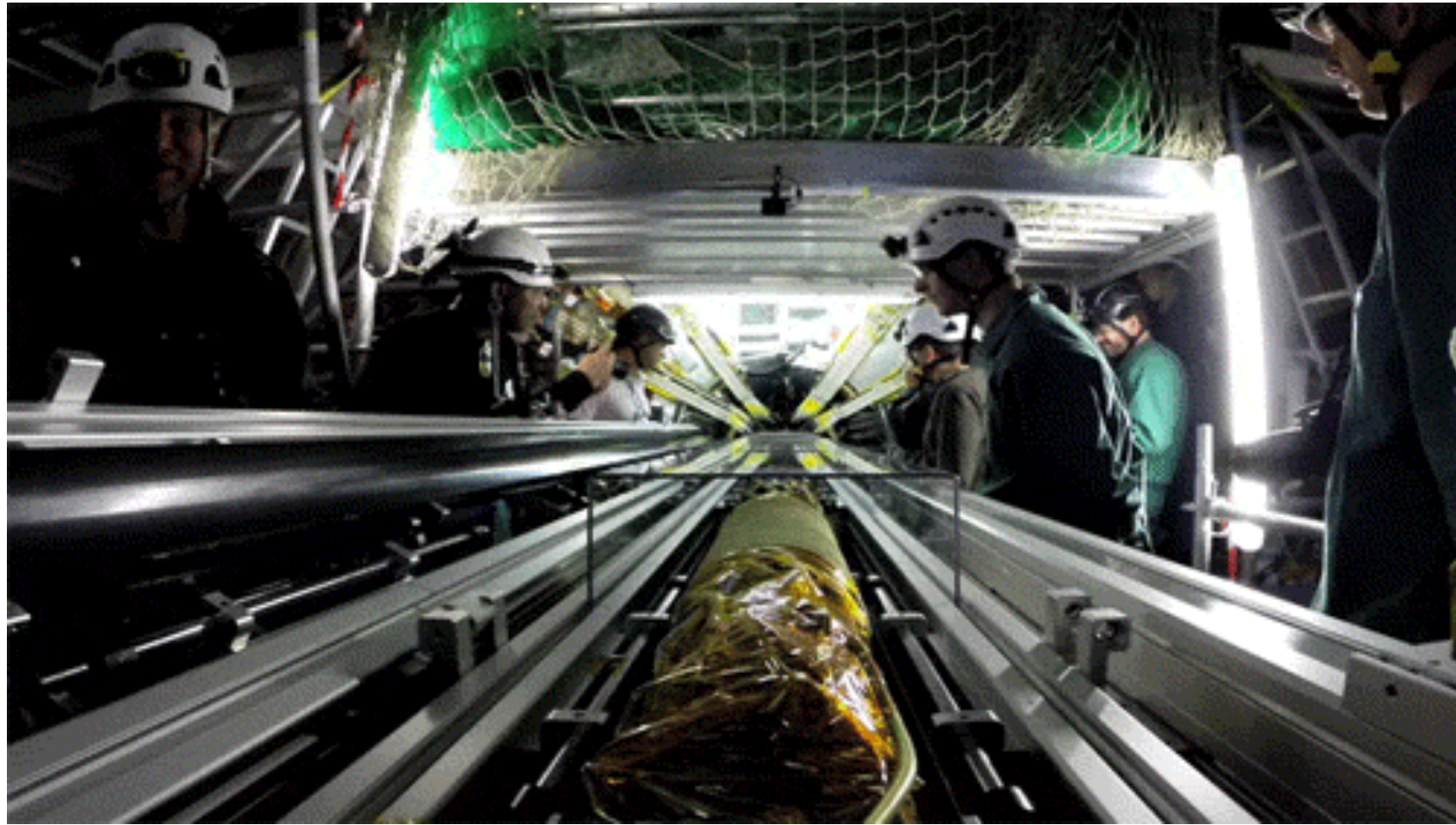
Smash particles at Large Hadron Collider



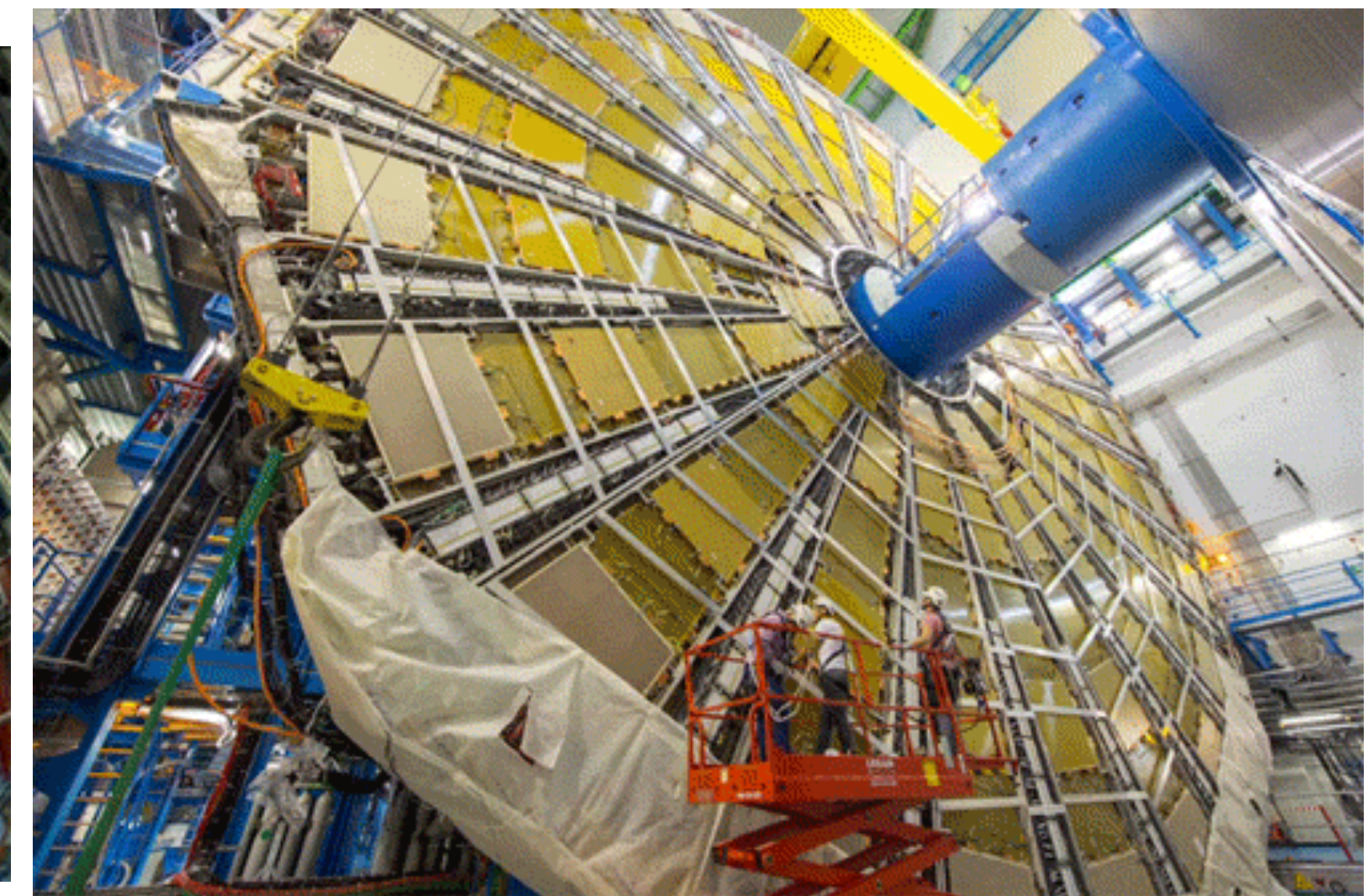
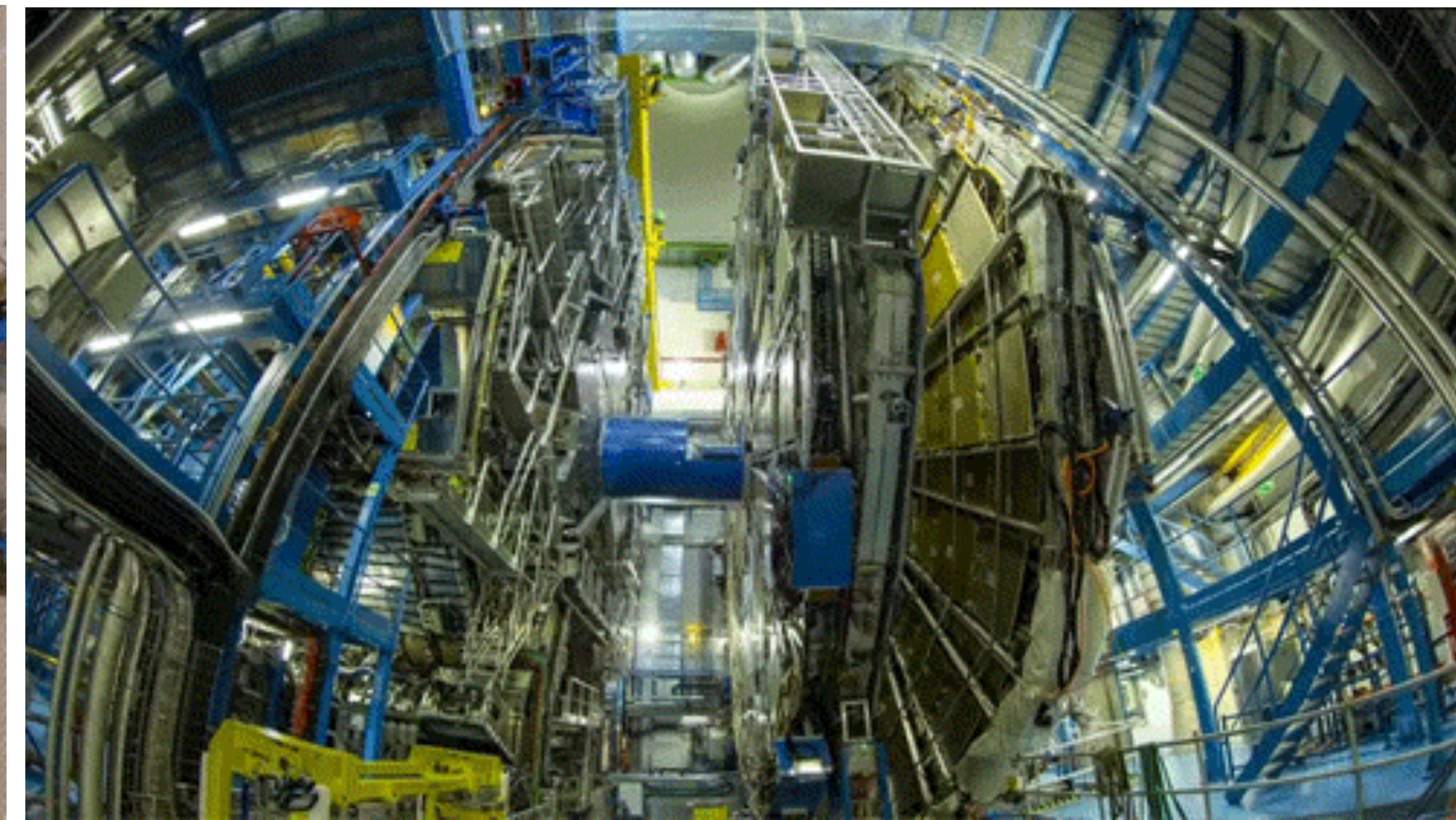
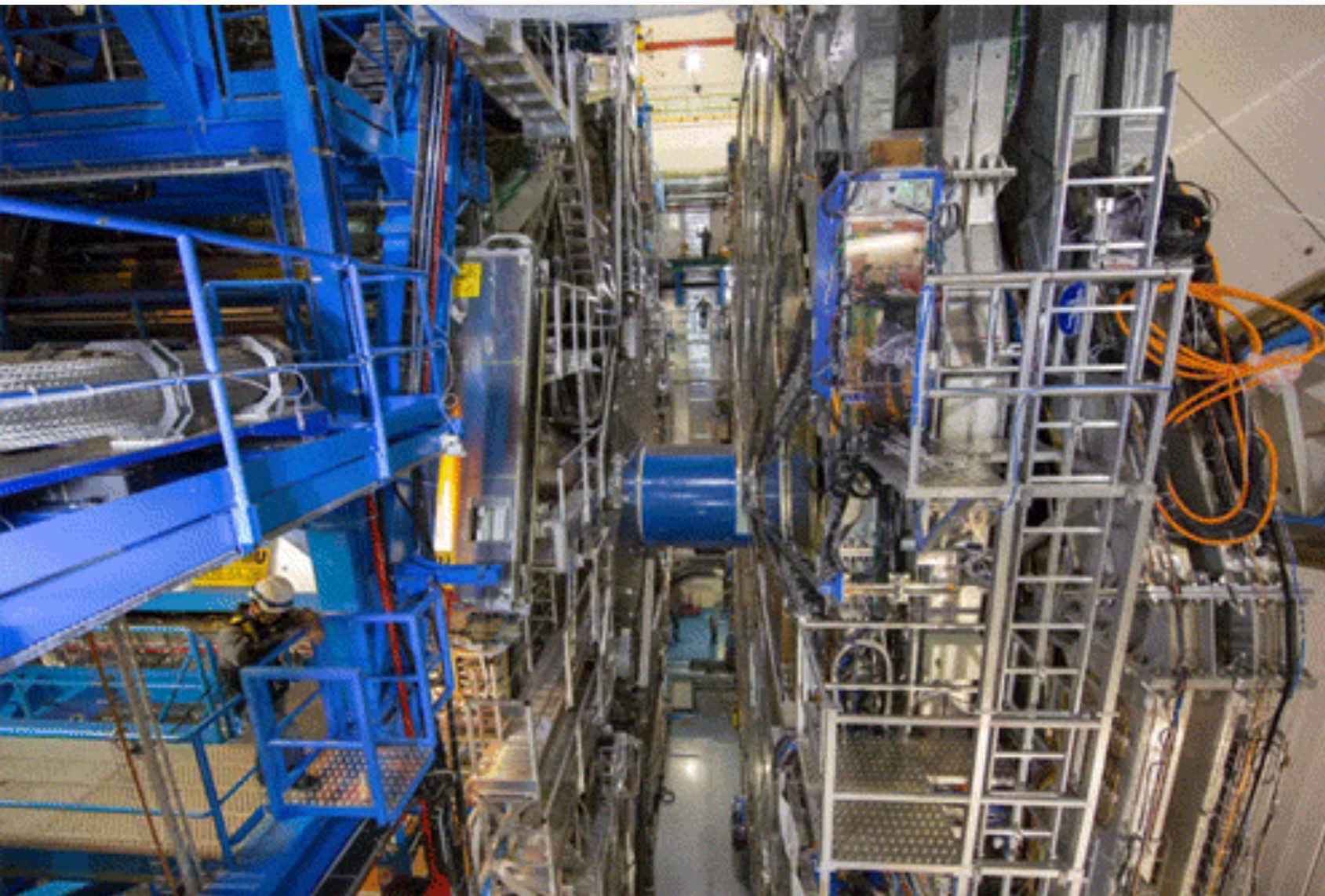
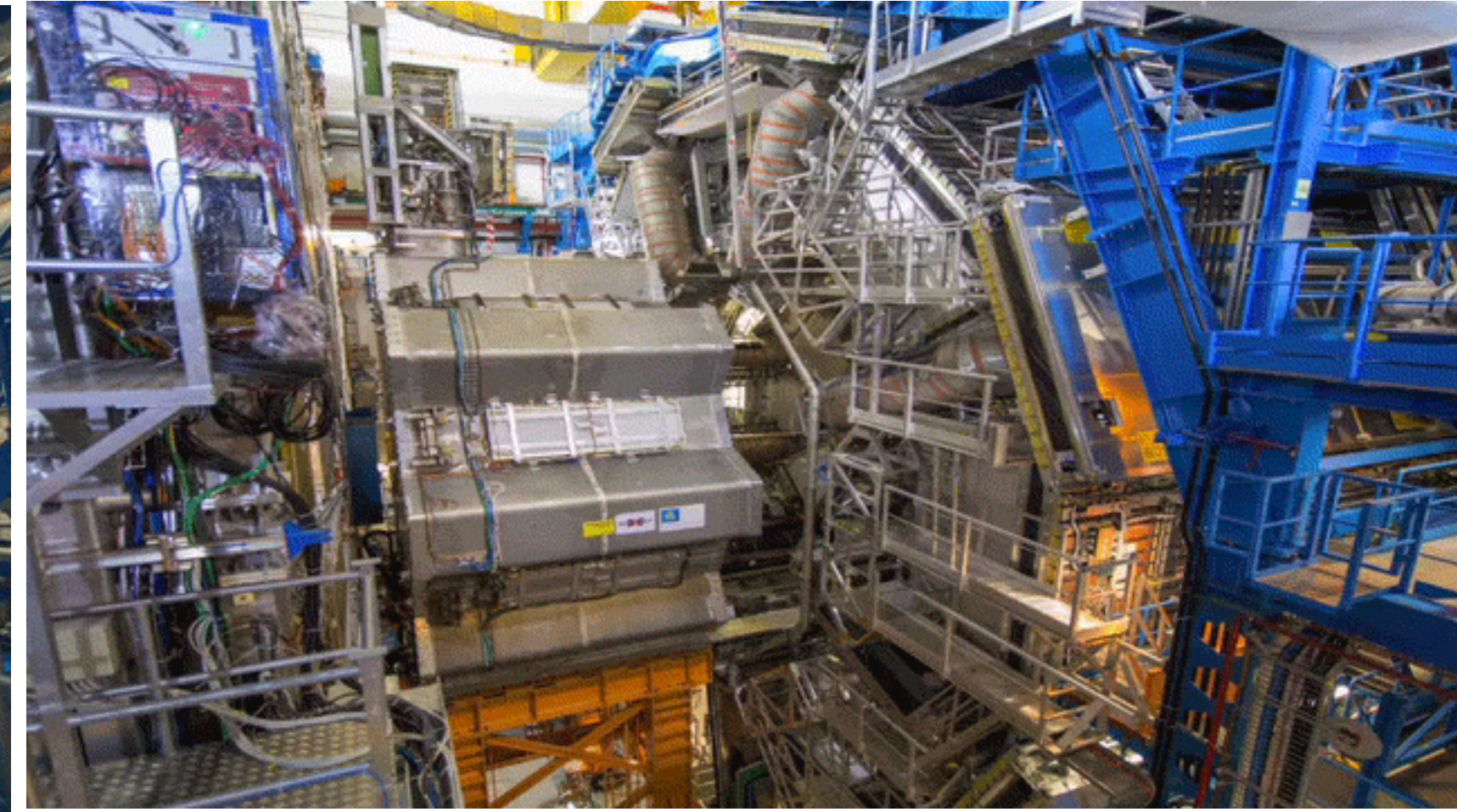
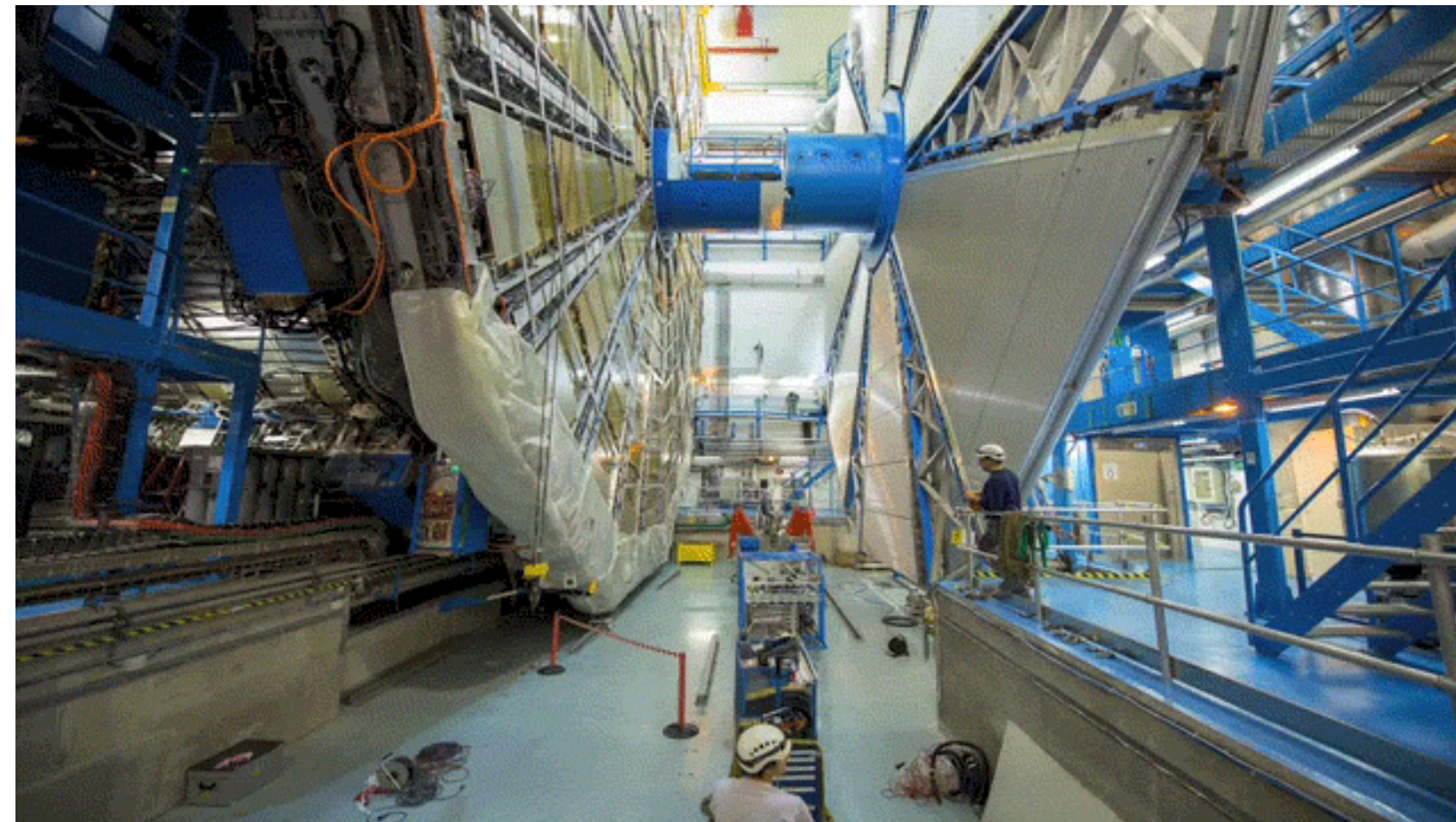
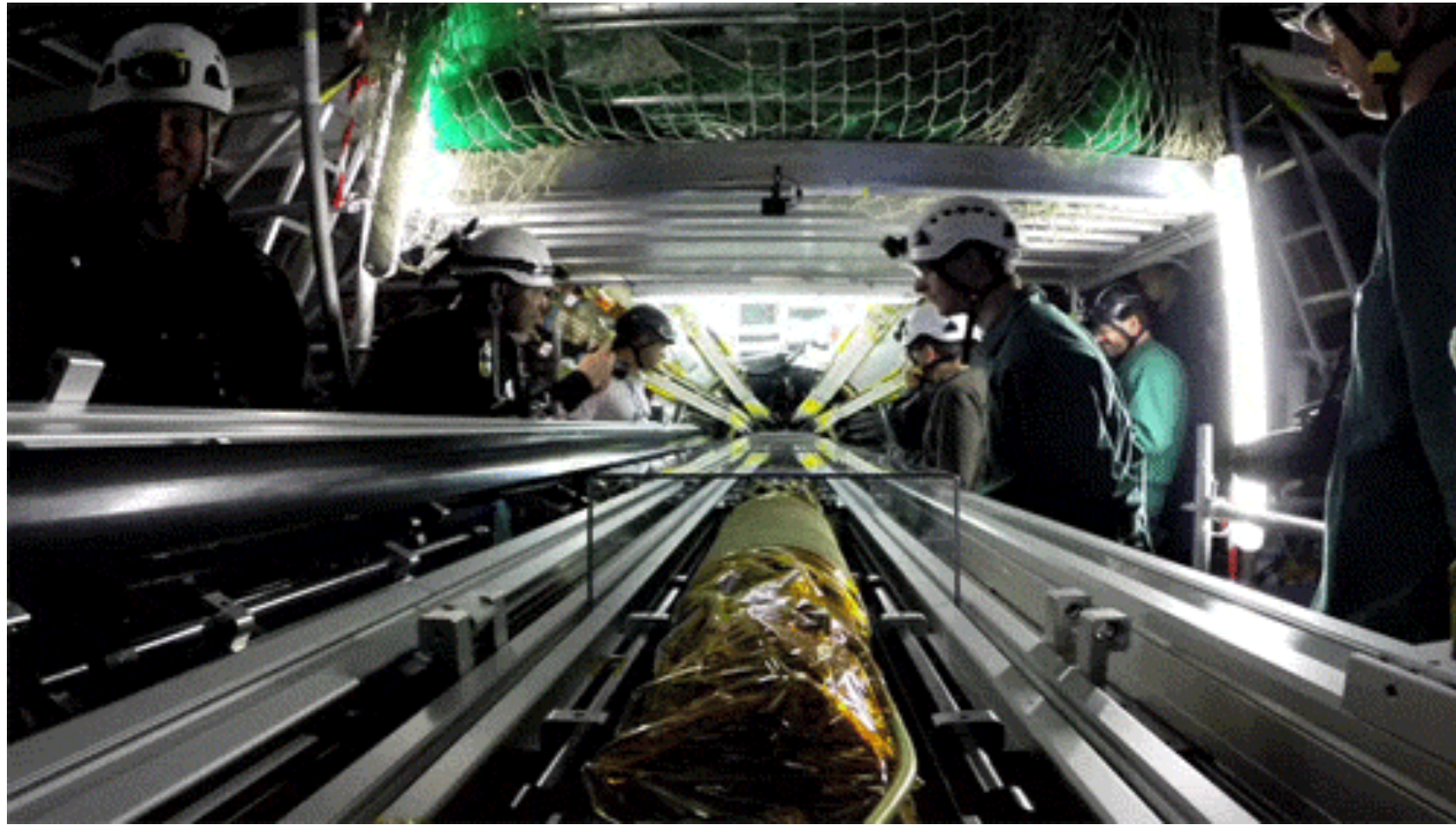
Smash particles at Large Hadron Collider



The detectors

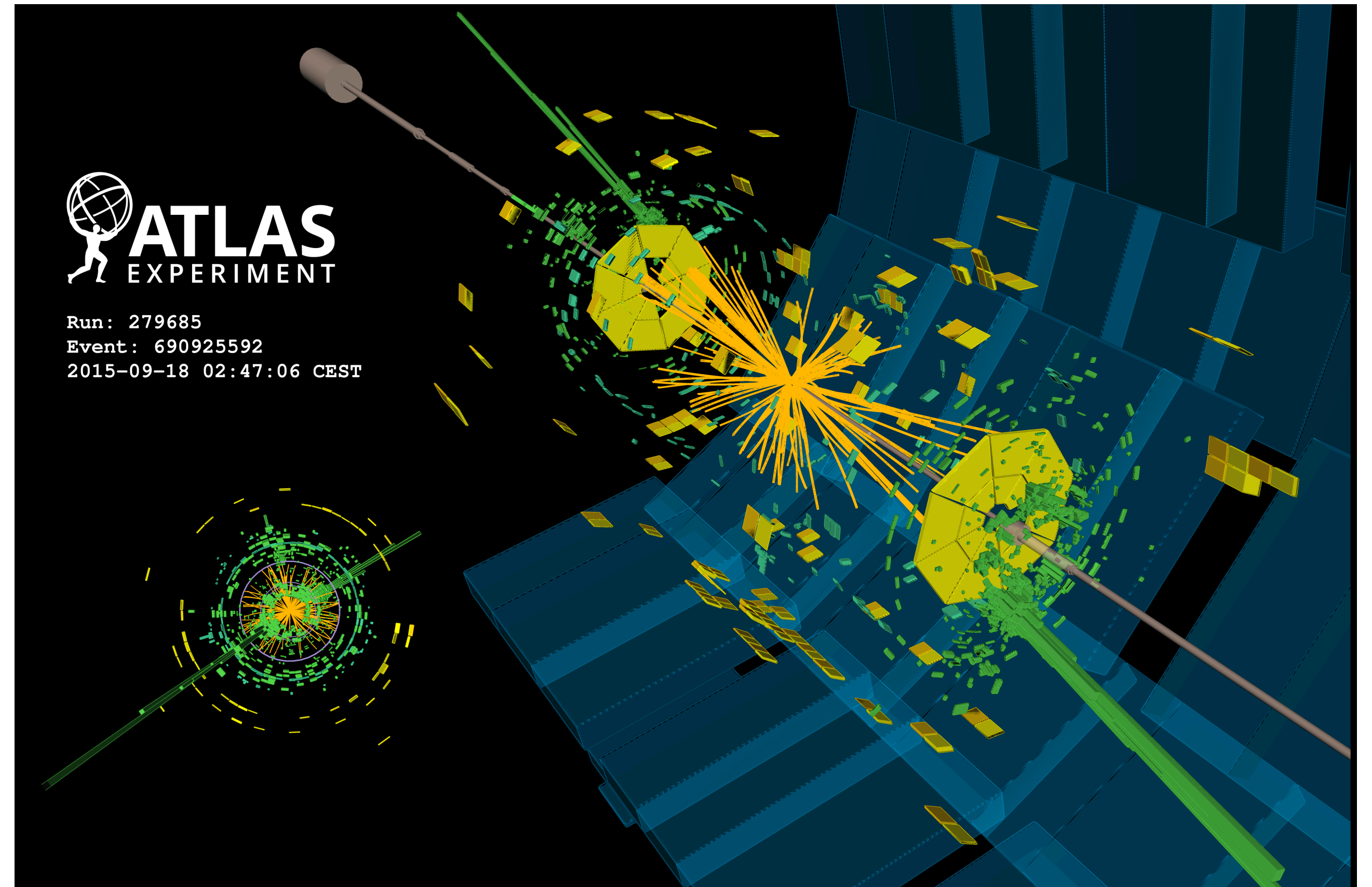


The detectors



Summarise in low dimensions

- Detector has $O(100 \text{ million})$ sensors
- Can't build 100M dimensional histogram
- ▶ Reconstruction pipeline, event selection
- ▶ Design sensitive one-dimensional observable



Summarise in low dimensions

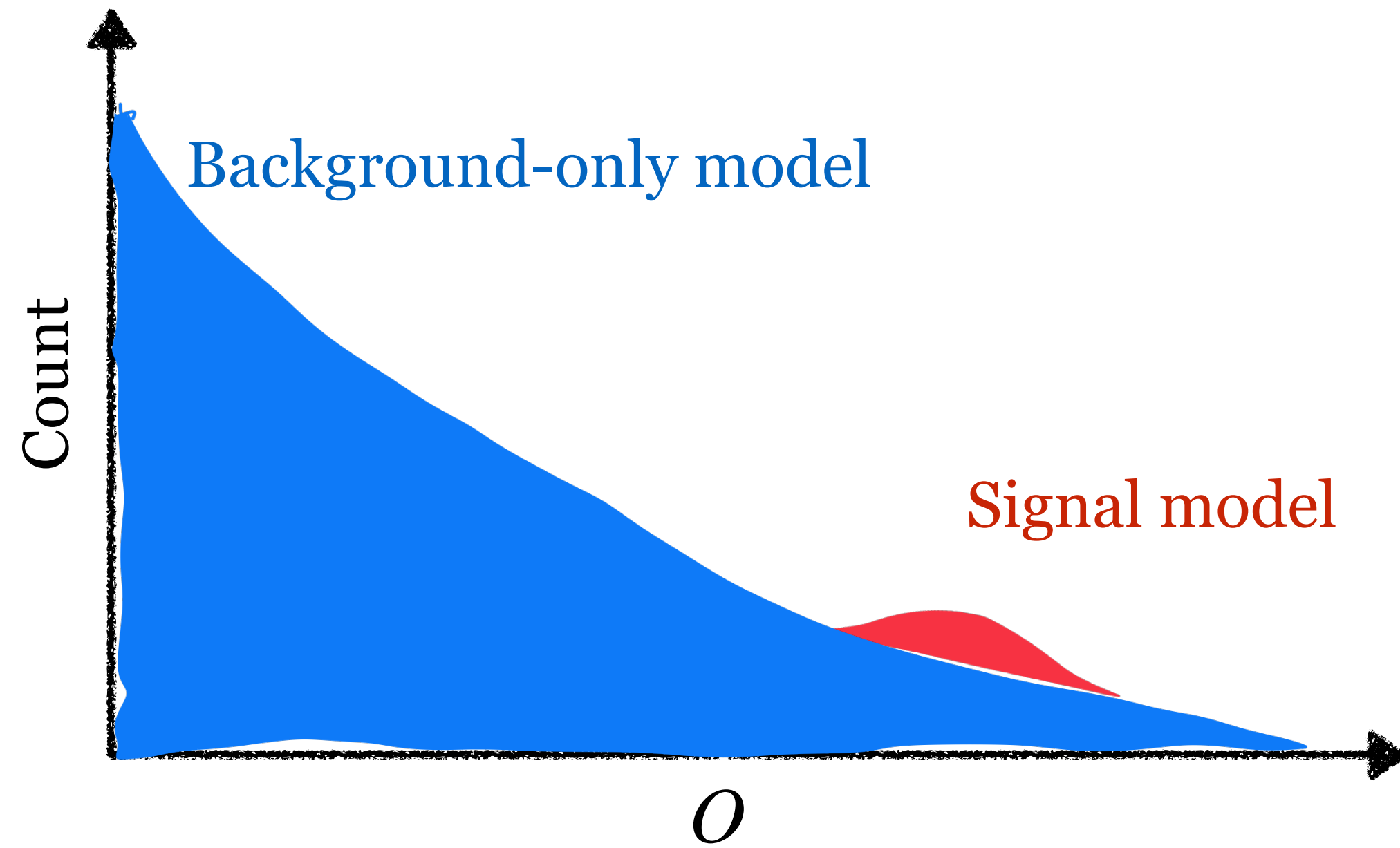
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1 number

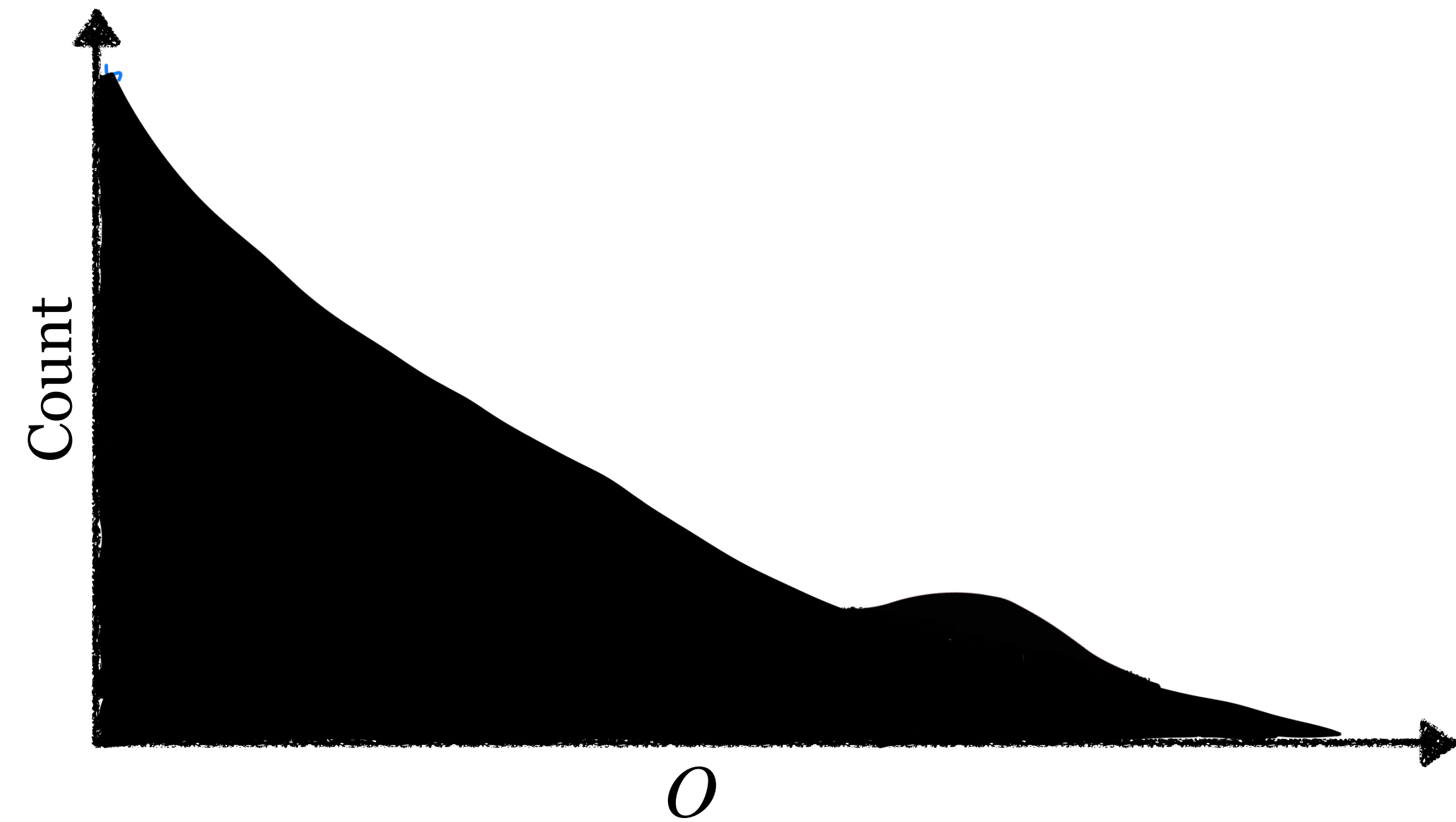


Probability Density Estimation: What we're used to doing..

Theory Predictions

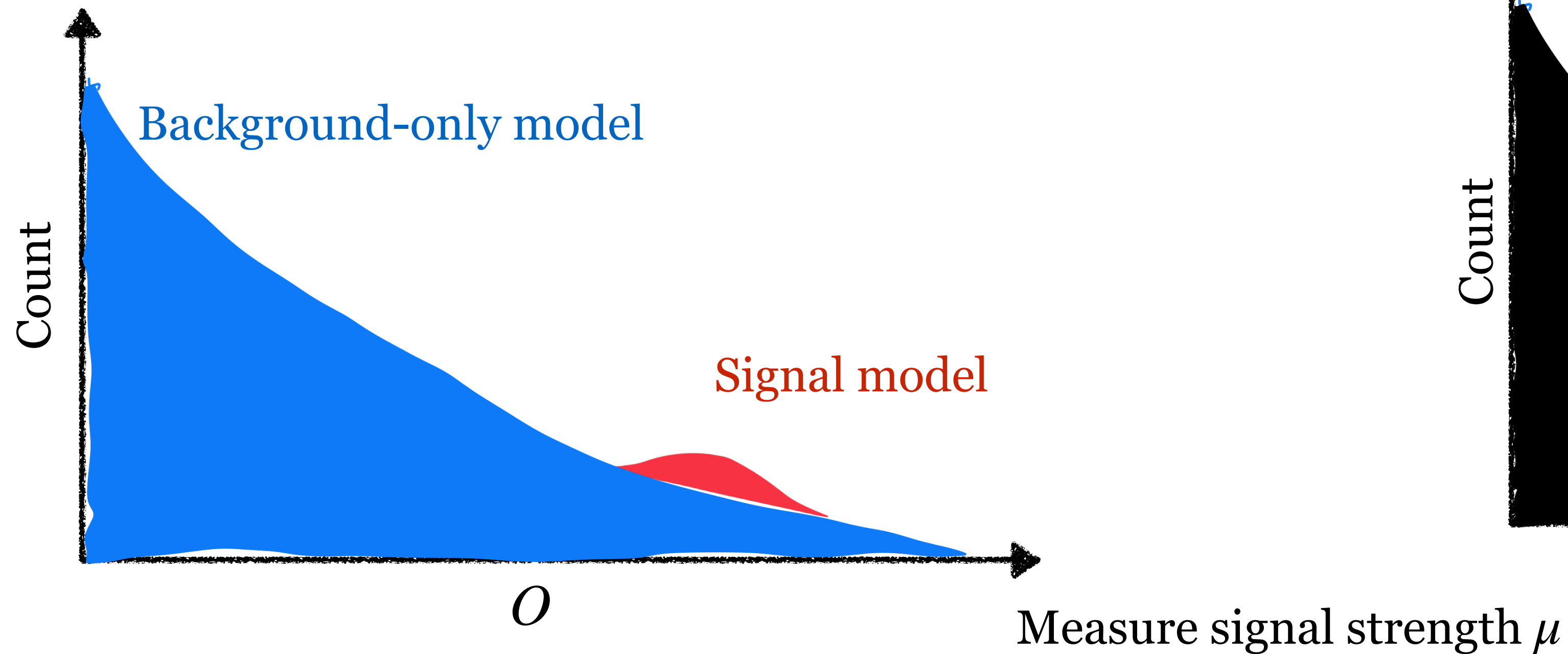


Data

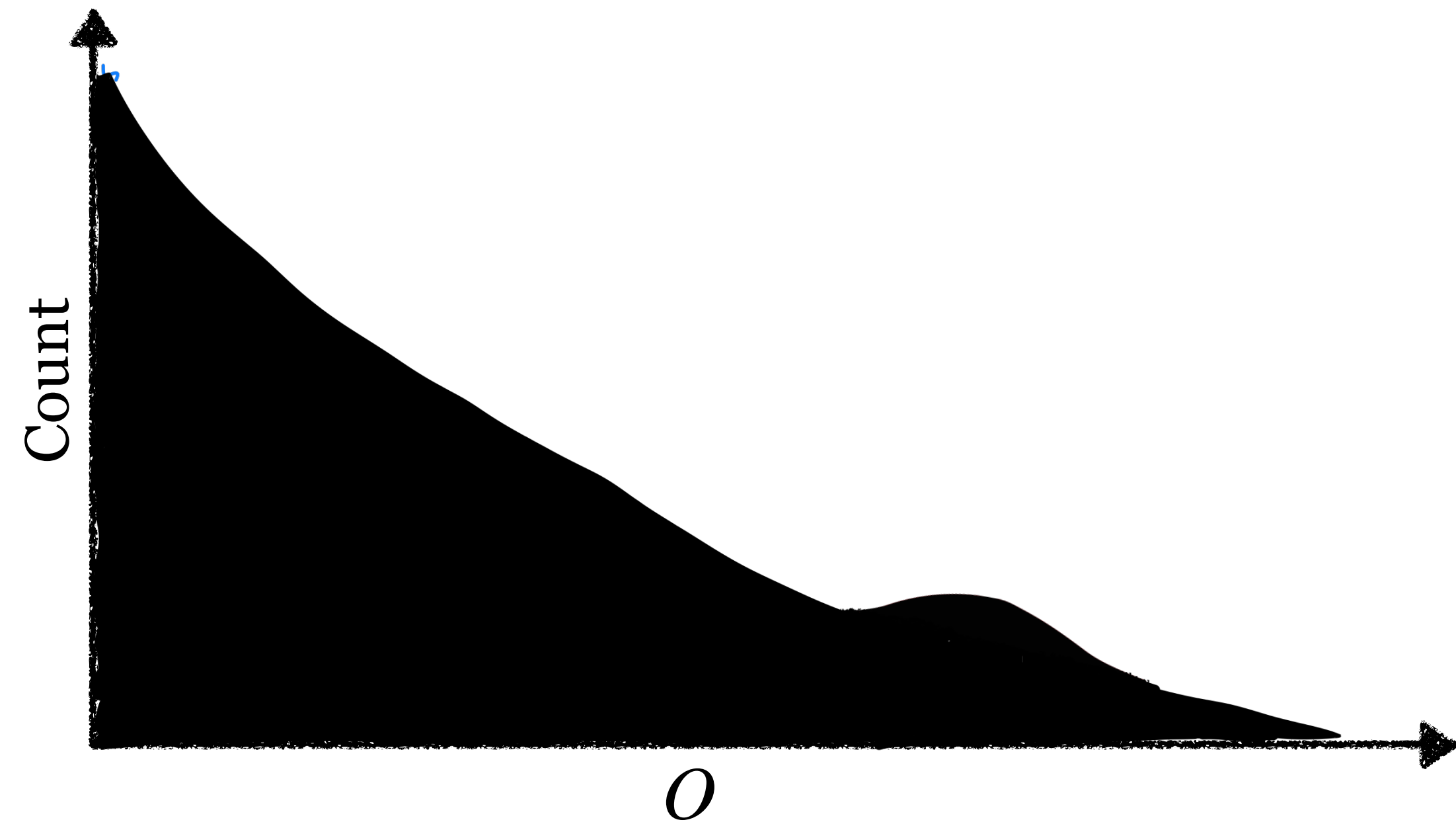


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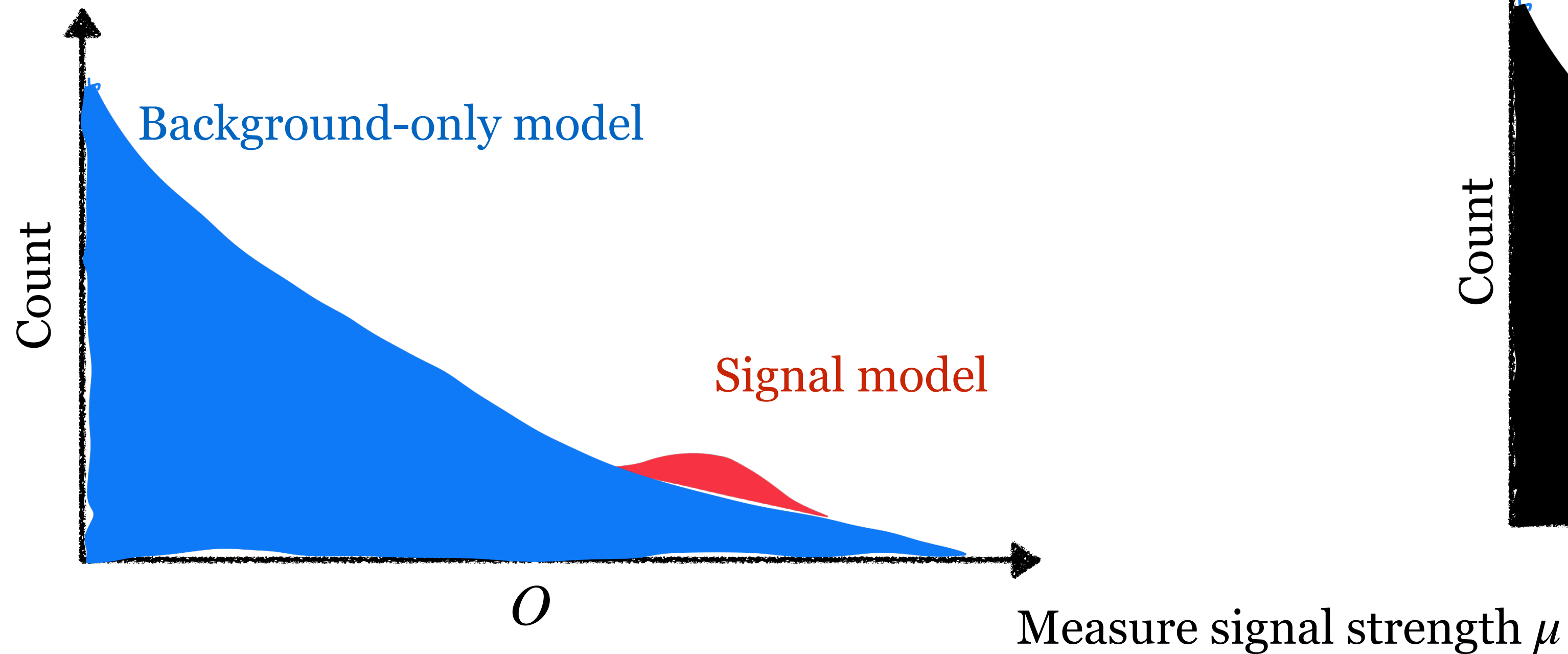
Data



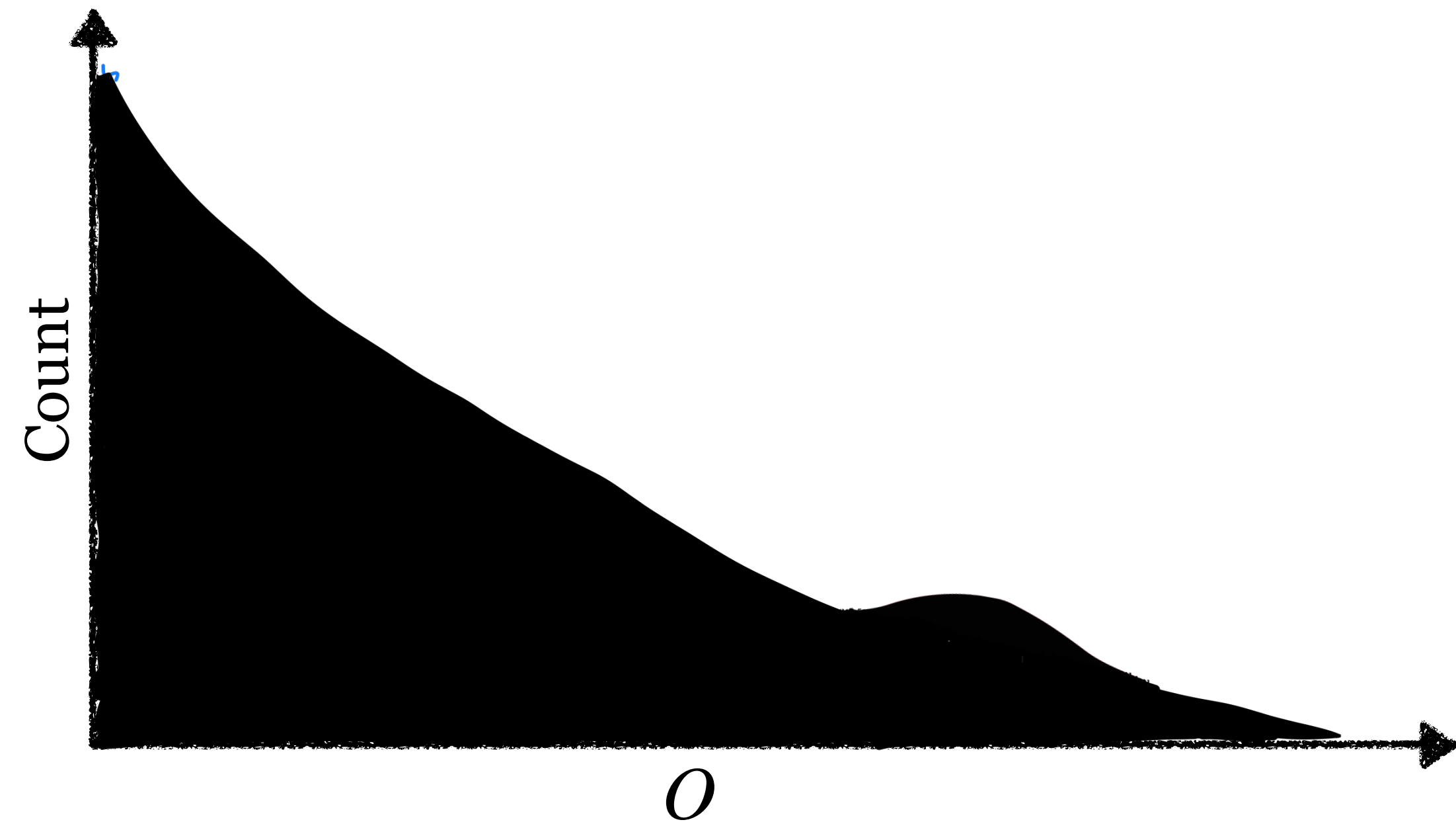
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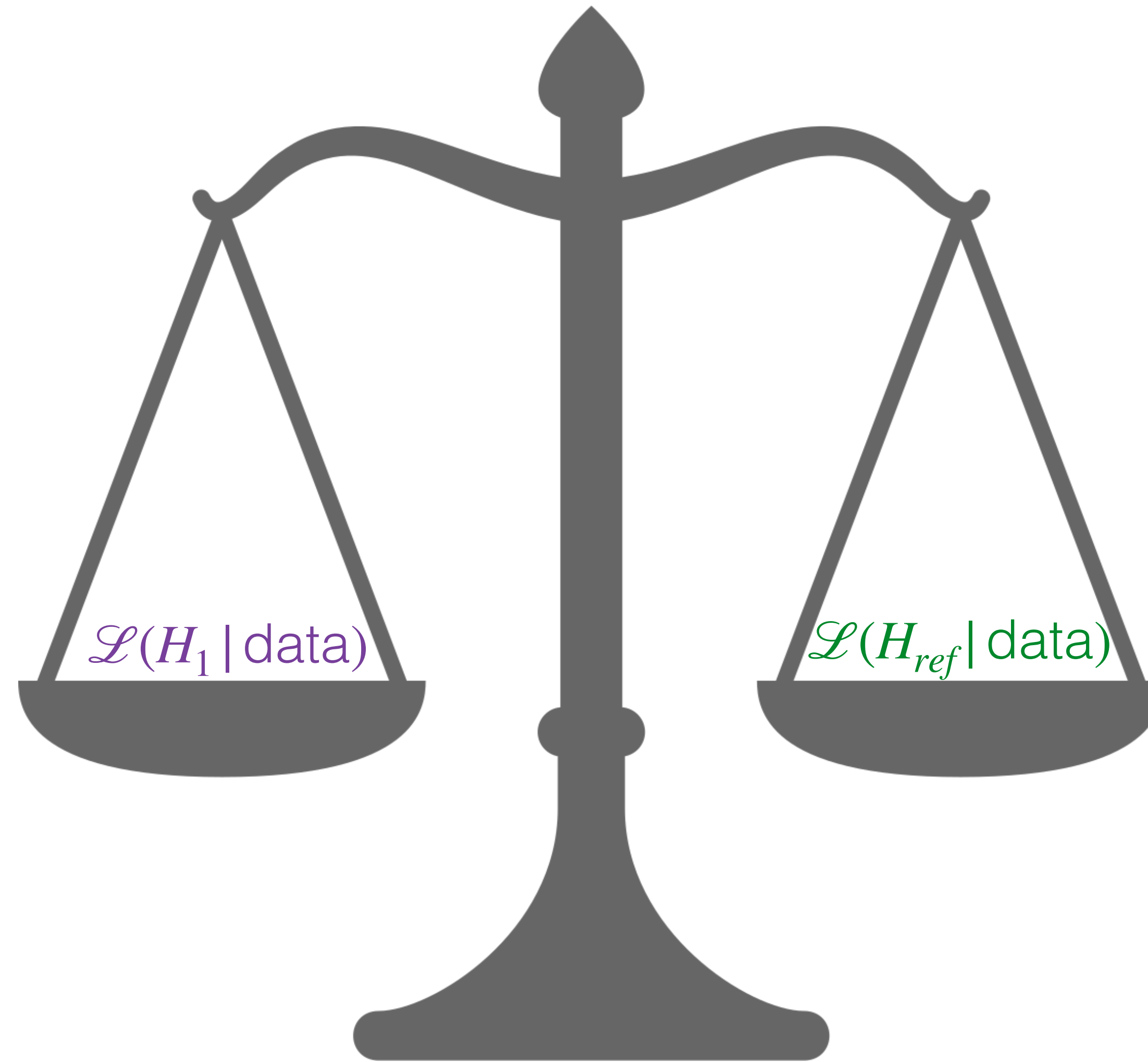


Data



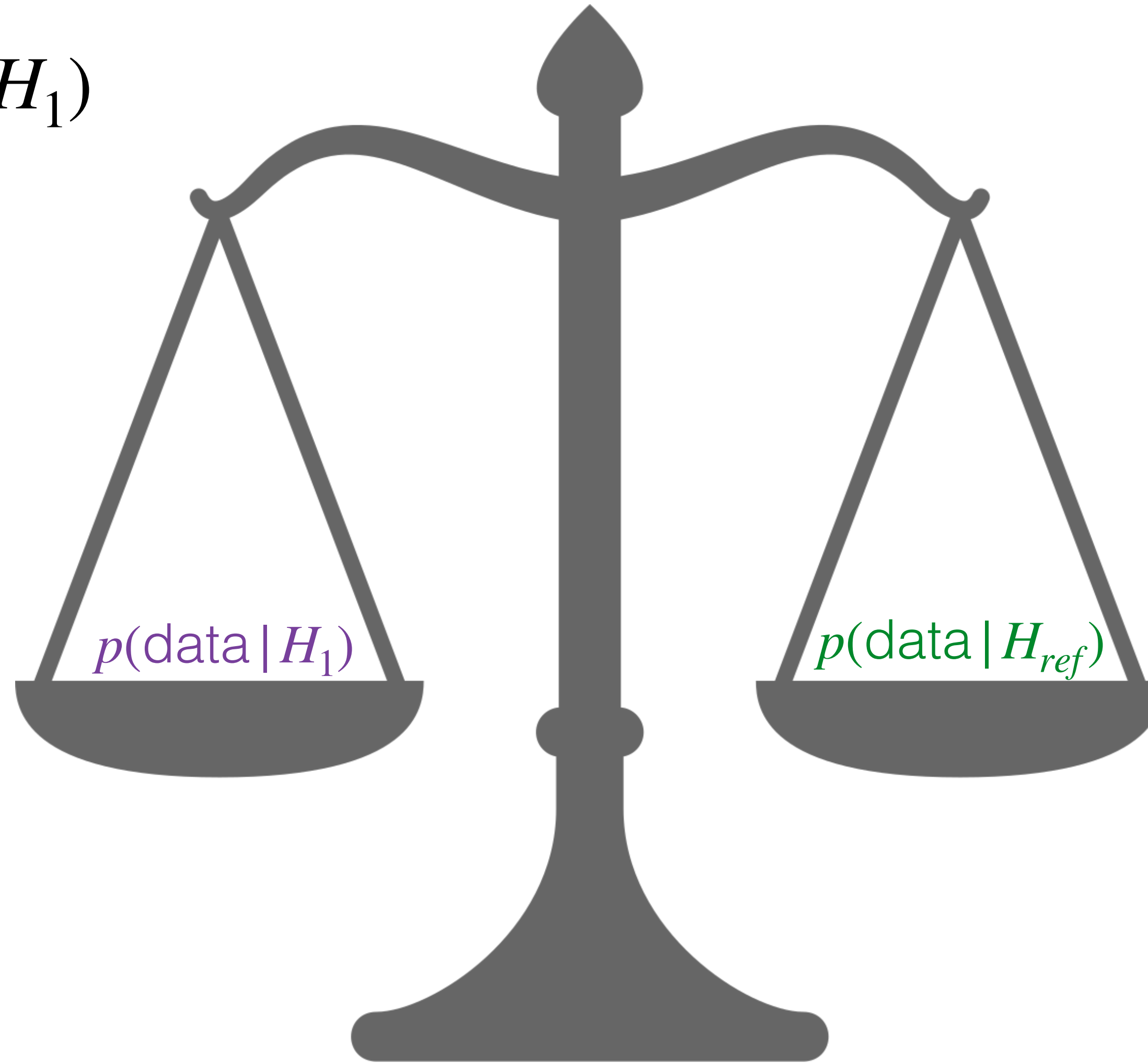
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(Frequentist) Hypothesis tests



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$$\mathcal{L}(H_1 | \text{data}) = p(\text{data} | H_1)$$



Why we can summarise data down to a single observable for typical analysis

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$$\mathcal{L}(\mu | \mathcal{D}) = p(\mathcal{D} | \mu)$$

Neyman–Pearson lemma: Likelihood ratio is the most powerful test statistic

We want to compare likelihoods:

$$\frac{p(\mathcal{D} | \mu)}{p(\mathcal{D} | \mu_0)}$$

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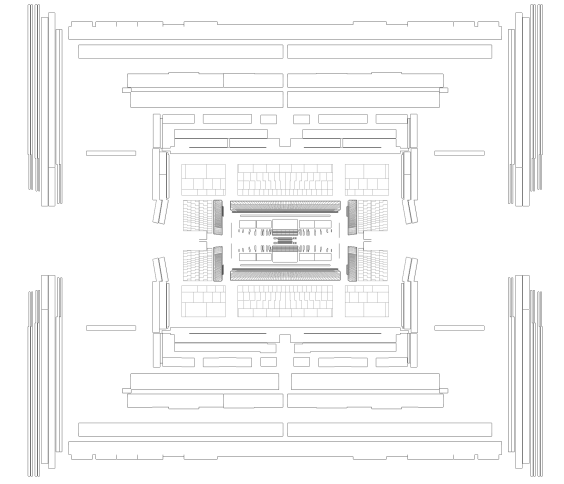
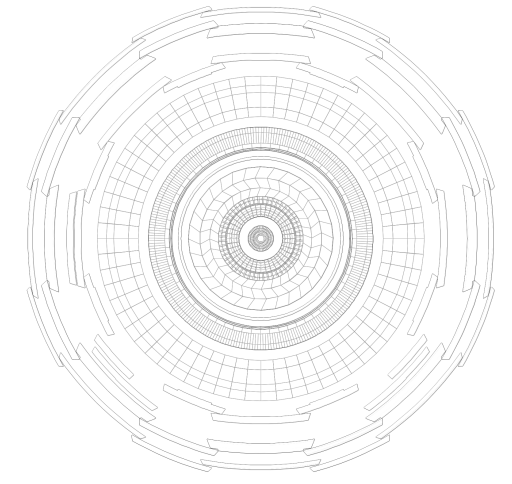
Which contains all the information required for the likelihood ratio:

$$\frac{p(x_i | \mu)}{p(x_i | \mu = 0)} = \frac{1}{\mu \cdot \nu_S + \nu_B} \frac{\mu \cdot \nu_S p(x_i | S) + \nu_B p(x_i | B)}{p(x_i | B)} = \frac{\mu}{\mu \cdot \nu_S + \nu_B} \cdot \left(\frac{s(x_i)}{1 - s(x_i)} + \nu_B \right)$$

Same observable s is optimal to test all μ hypotheses!

No need to develop separate analysis per hypothesis μ

* Equal class weights



A measurement of the Higgs width

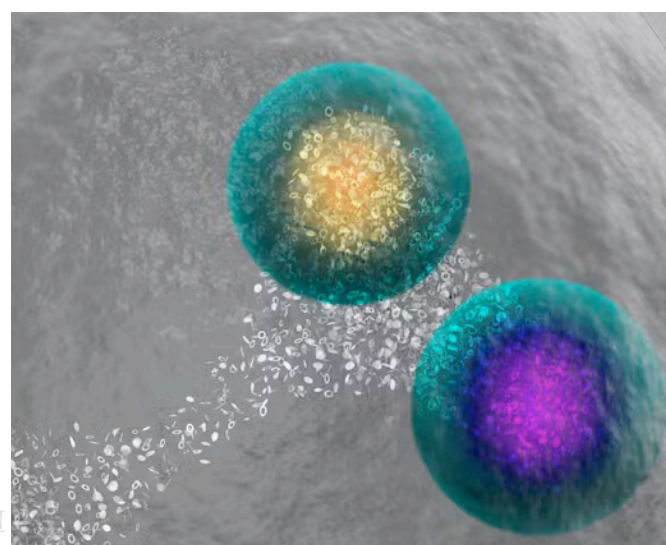
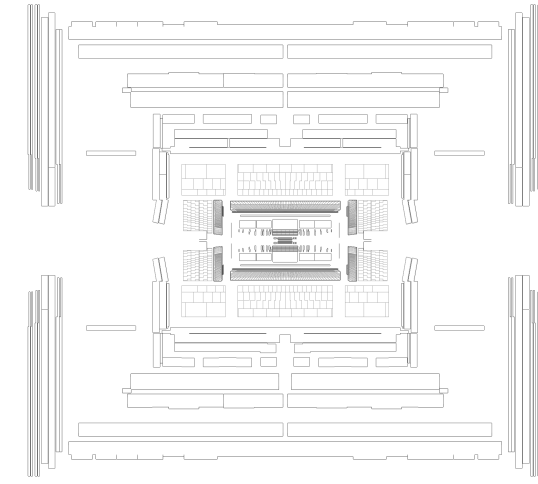
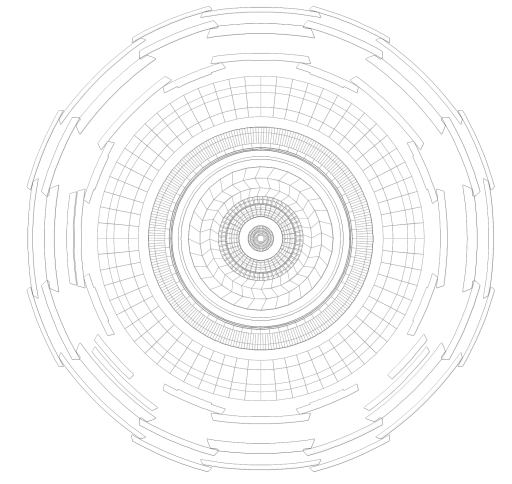


Image: CERN



Undiscovered massive particles



A measurement of the Higgs width

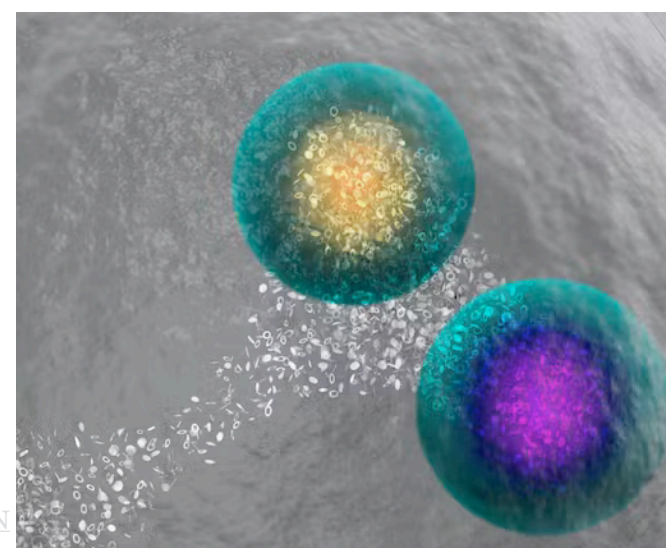
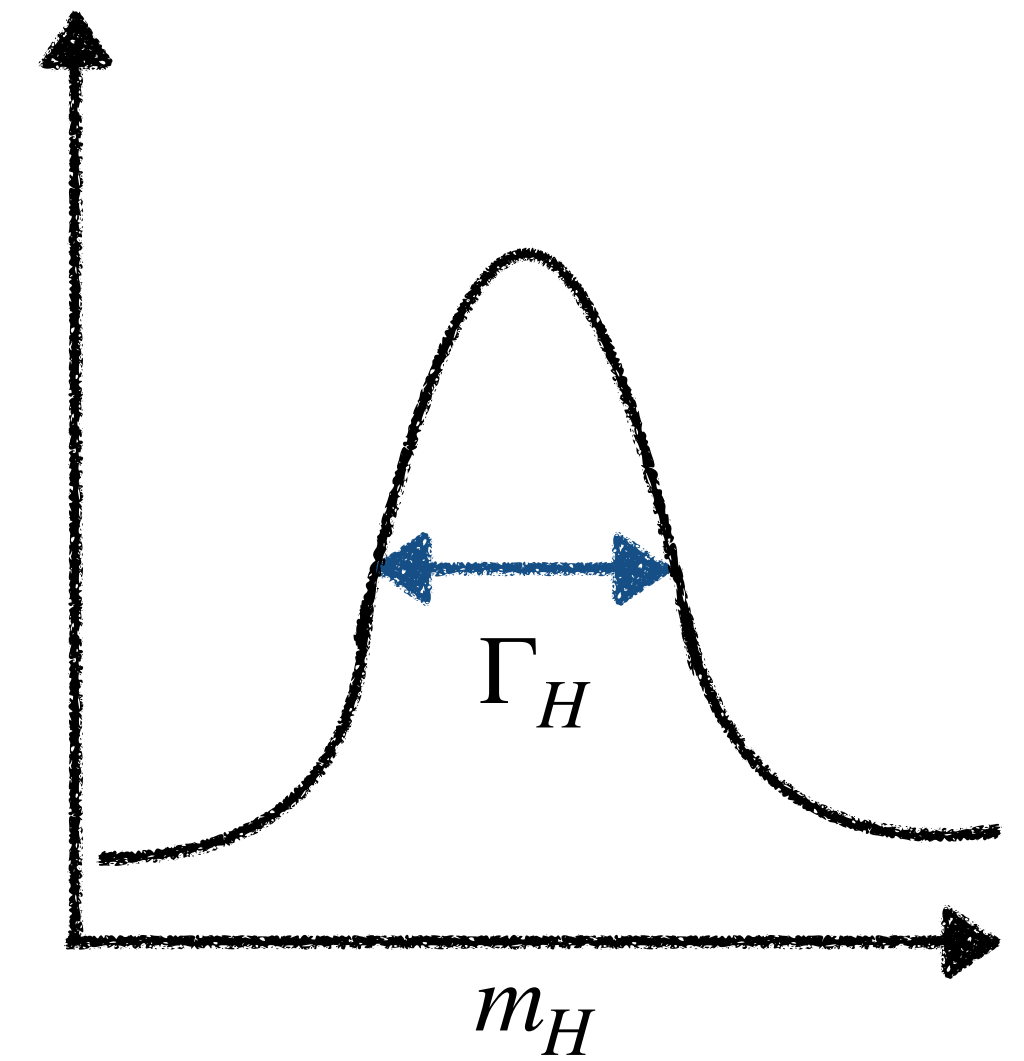
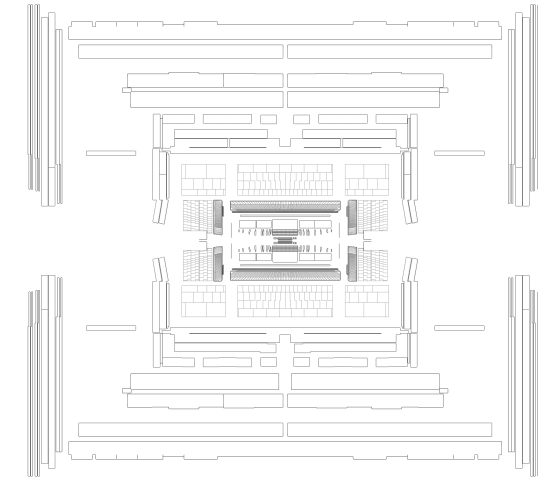
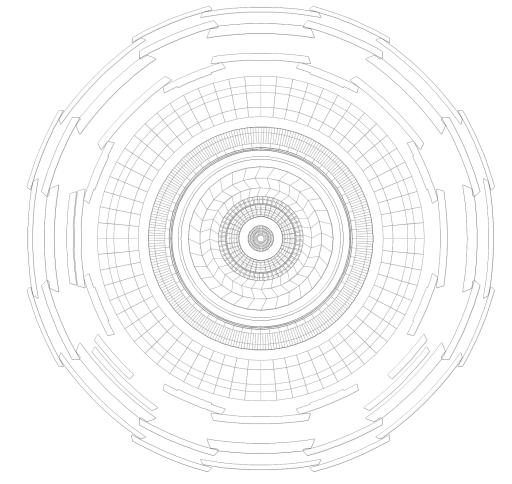


Image: CERN



Undiscovered massive particles



A measurement of the Higgs width

- Enables the probe of a wide variety of new massive particles, other new physics
- Can't measure directly: SM Higgs width ~ 4 MeV, resolution of detector ~ 1 GeV
- Central topic for future colliders

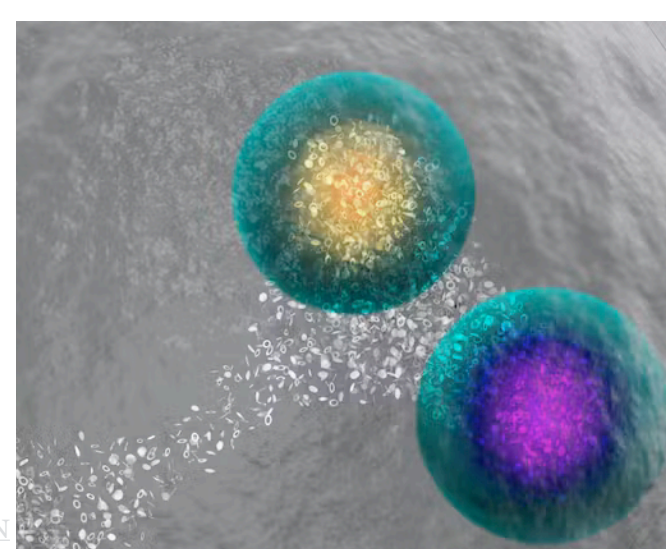
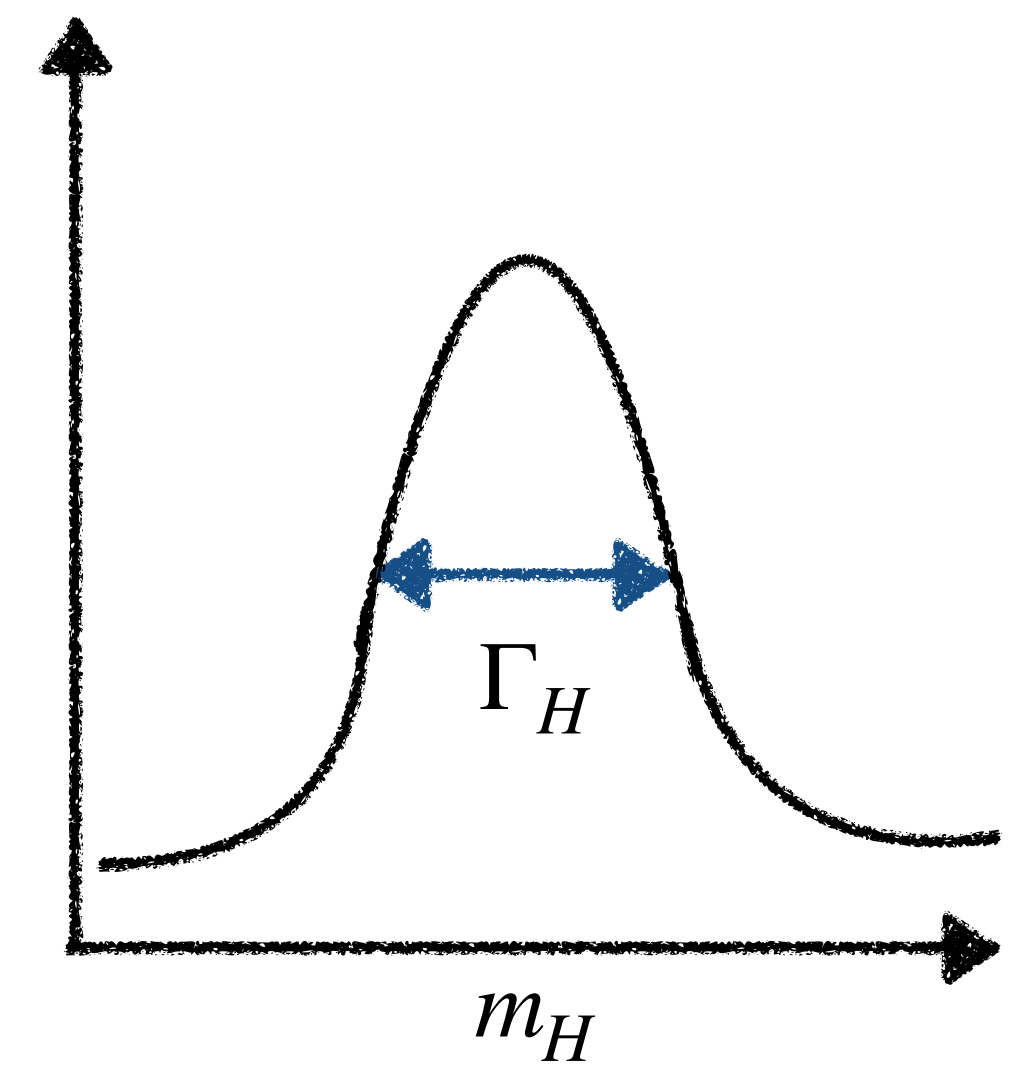
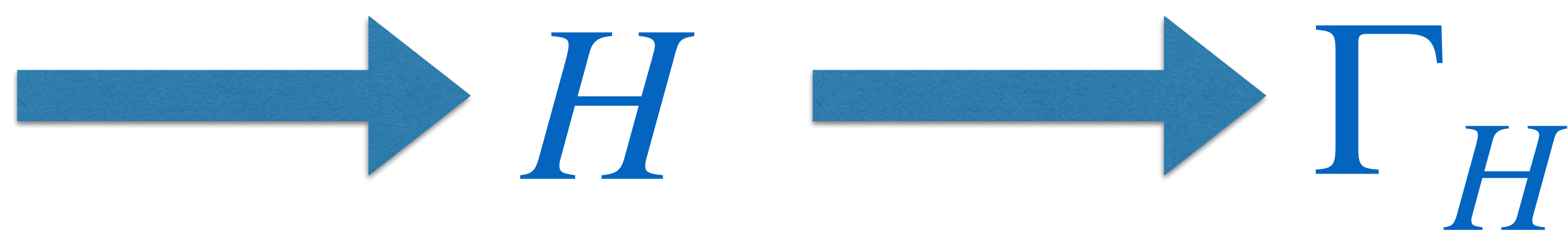
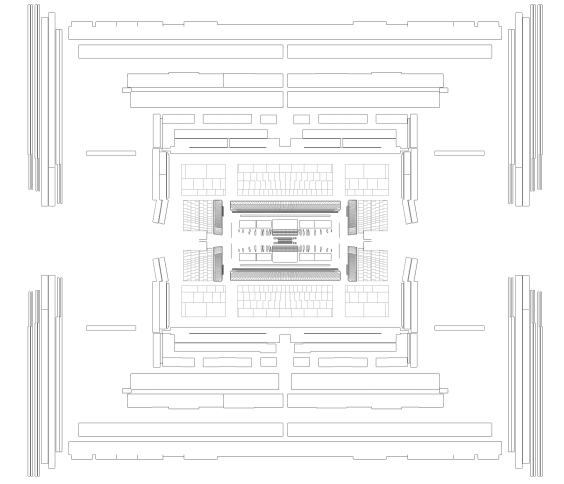
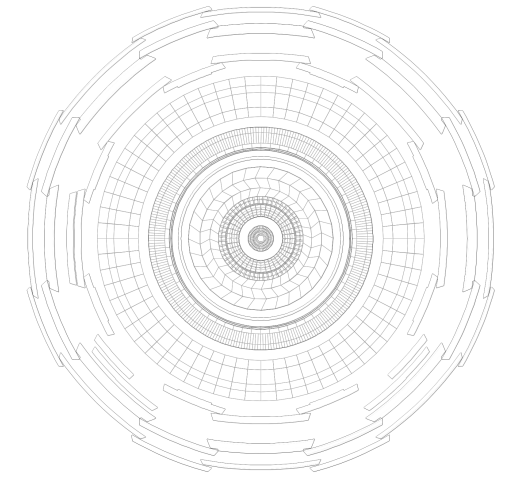


Image: CERN



Undiscovered massive particles



Higgs Width from off-shell Higgs production

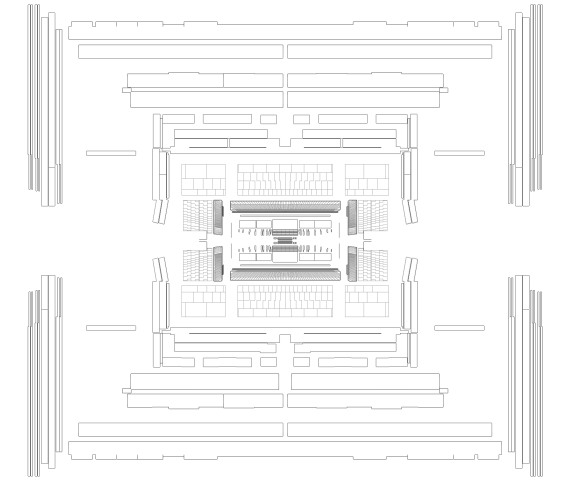
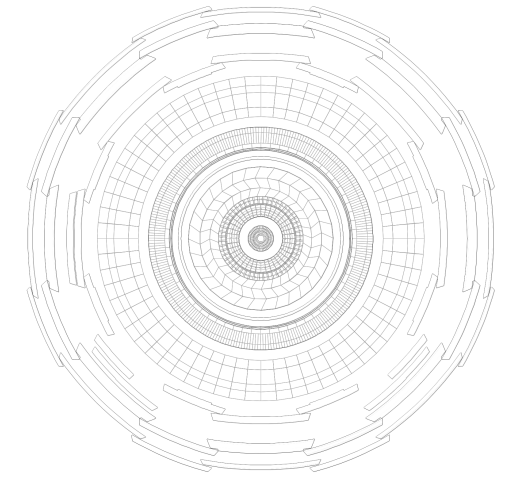
[arXiv:1405.0285](https://arxiv.org/abs/1405.0285) [arXiv:1406.1757](https://arxiv.org/abs/1406.1757)

- Off-shell production helps probe Higgs width

$$\frac{\mu_{\text{off-shell}}}{\mu_{\text{on-shell}}} = \frac{\Gamma_H}{\Gamma_H^{SM}}.$$

$$\sigma_{\text{on-shell}}^{gg \rightarrow H \rightarrow ZZ} \sim \frac{g_f^2 g_V^2}{m_H \Gamma_H}$$

$$\frac{d\sigma_{\text{off-shell}}^{gg \rightarrow H \rightarrow VV}}{dm_{VV}} \propto \frac{g_f^2 g_V^2}{(m_{VV}^2 - m_H^2)^2 + m_H^2 \Gamma_H^2} \simeq \frac{g_f^2 g_V^2}{m_{VV}^4}$$



Higgs Width from off-shell Higgs production

[arXiv:1405.0285](https://arxiv.org/abs/1405.0285) [arXiv:1406.1757](https://arxiv.org/abs/1406.1757)

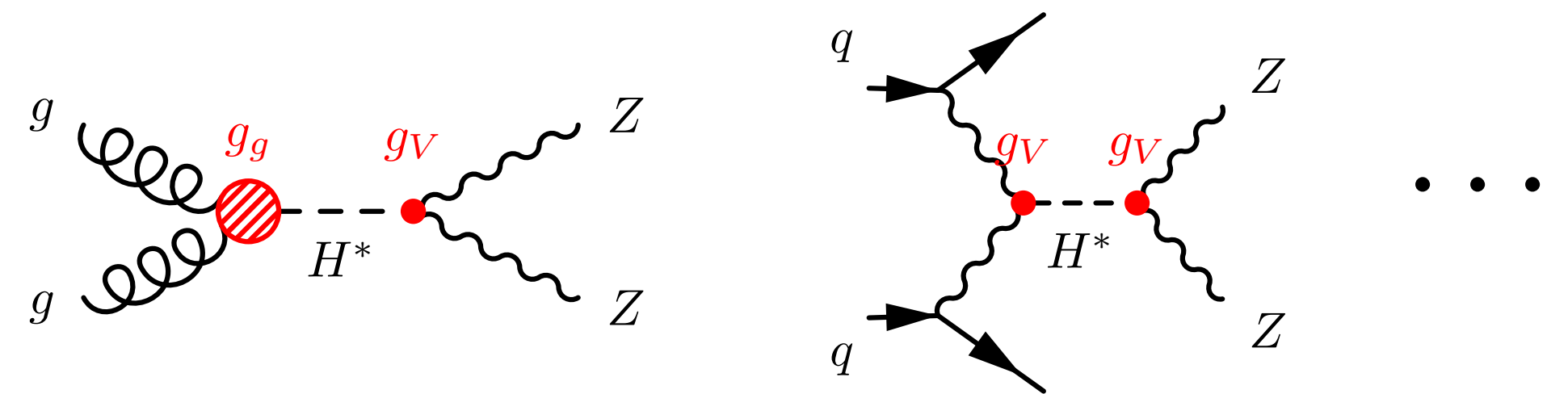
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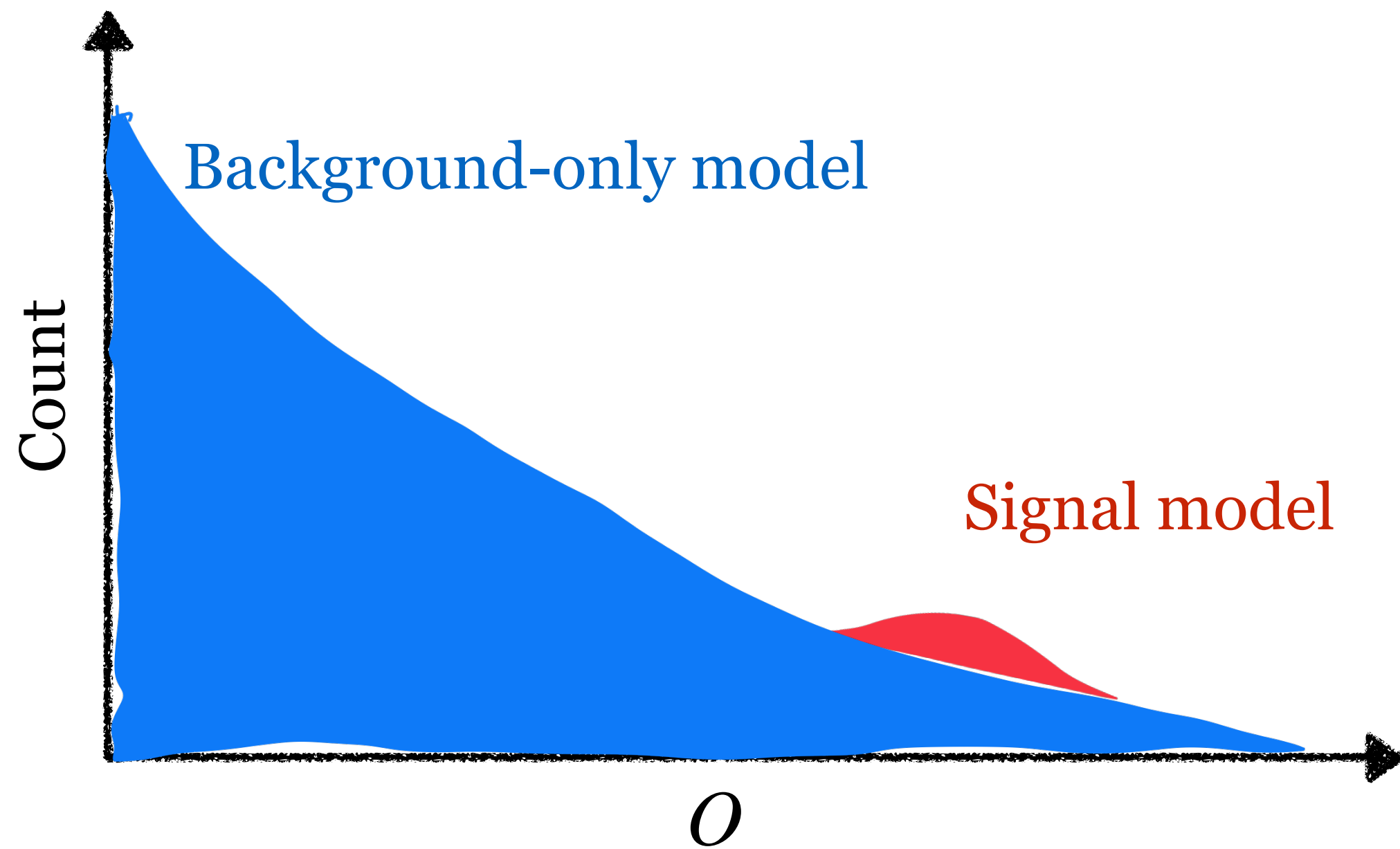
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- Interpretation assumes no new physics
- Essential to measure independently in multiple production modes (ggF, VBF) and final states to verify consistent results



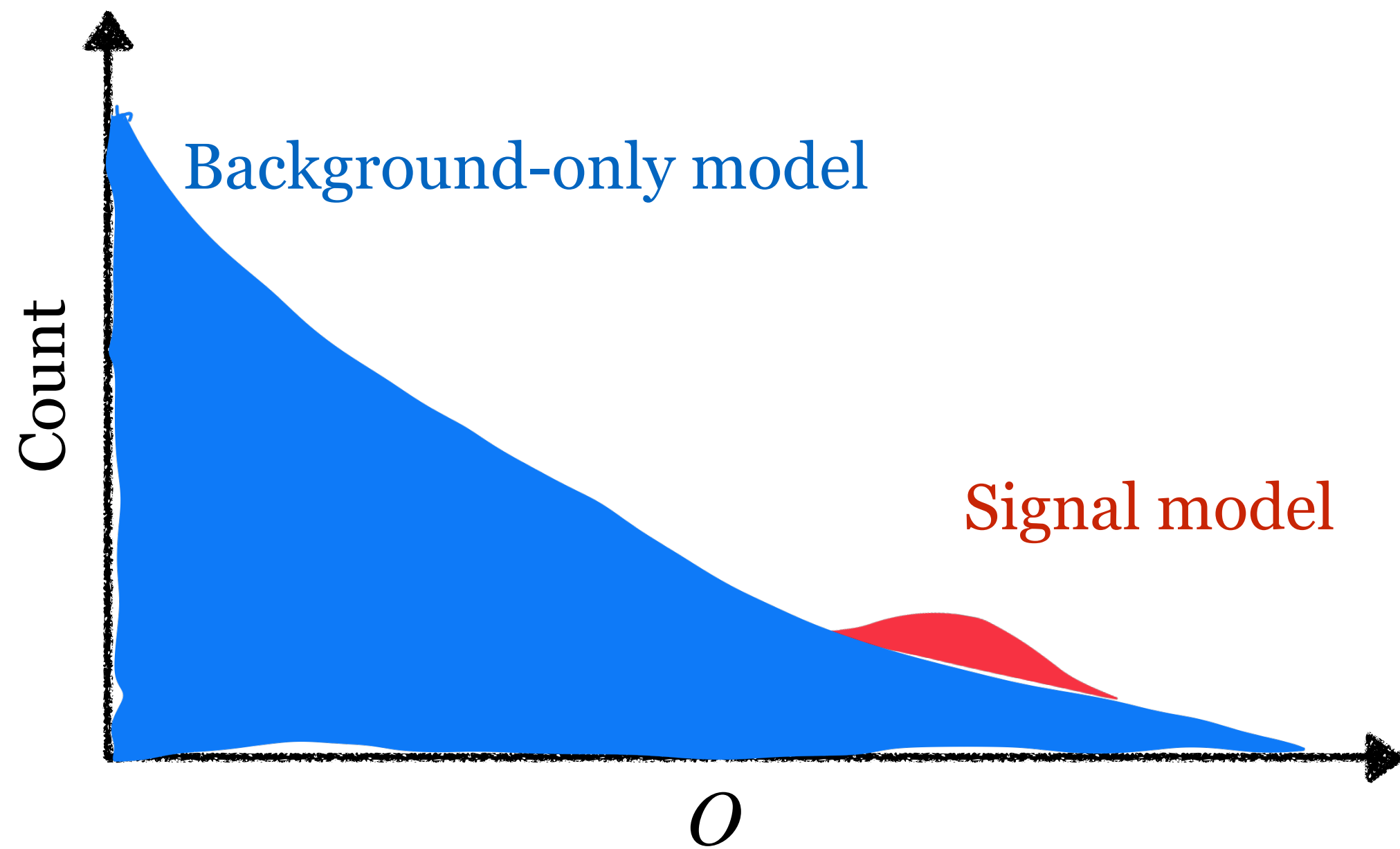
New challenge: Quantum interference Non-linear changes in kinematics



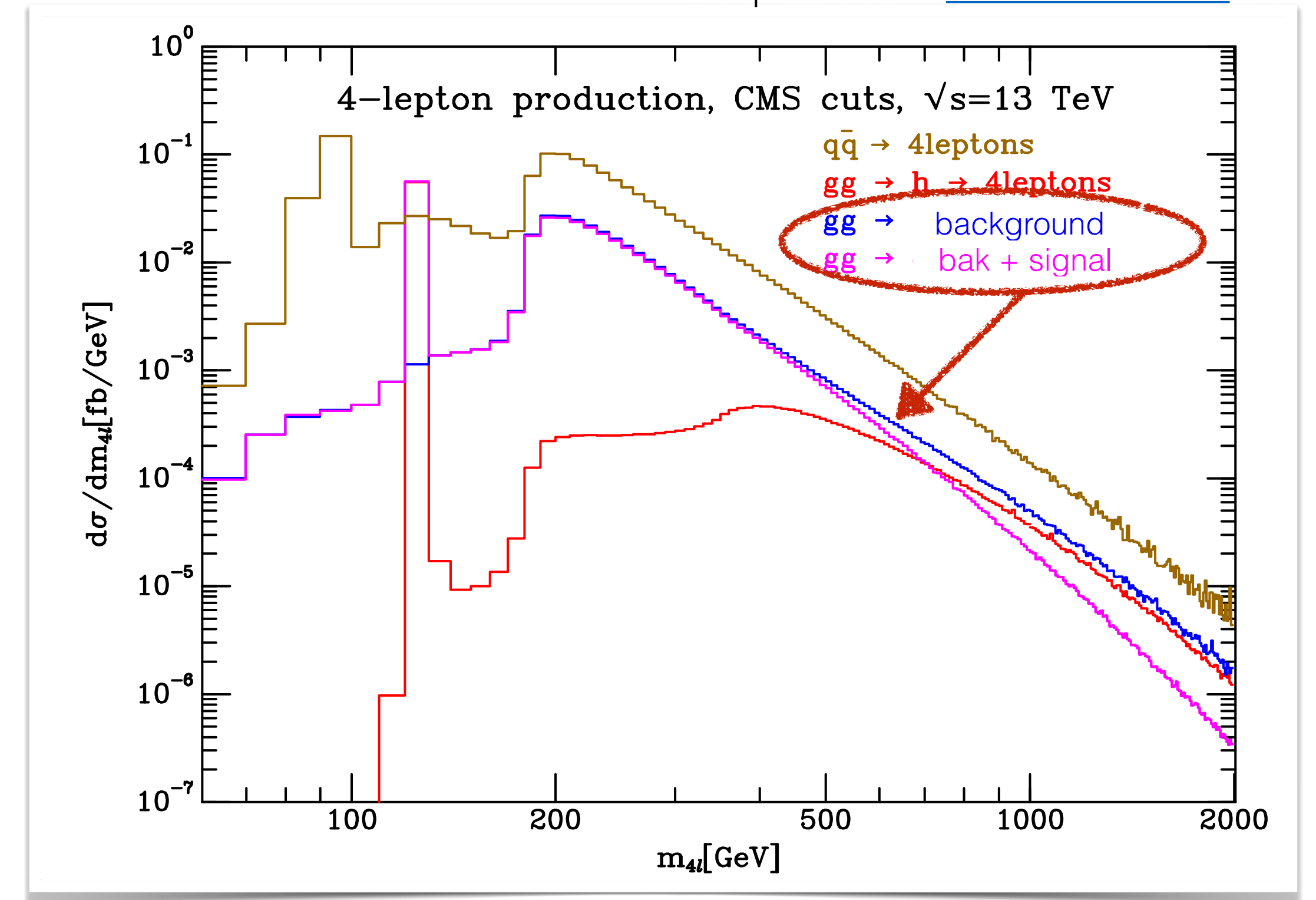
Data can no longer be summarised in 1D histogram (see Ghosh et al: [hal-02971995\(p172\)](https://arxiv.org/abs/1907.09752)) !

New challenge: Quantum interference

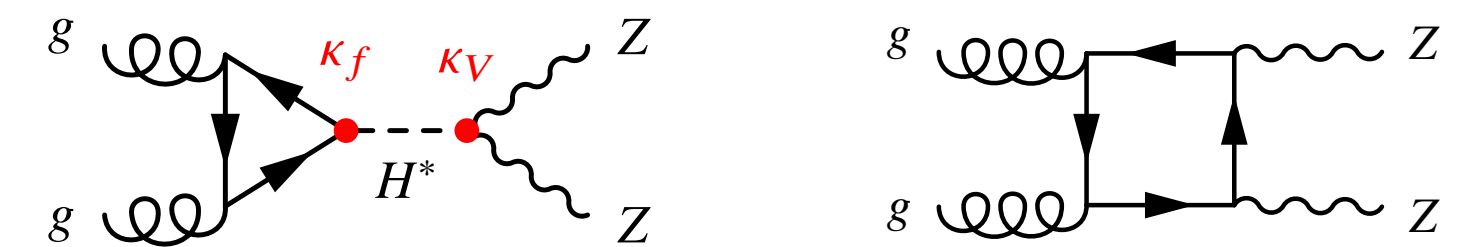
Non-linear changes in kinematics



Campbell et al: [arXiv:1311.3589](https://arxiv.org/abs/1311.3589)



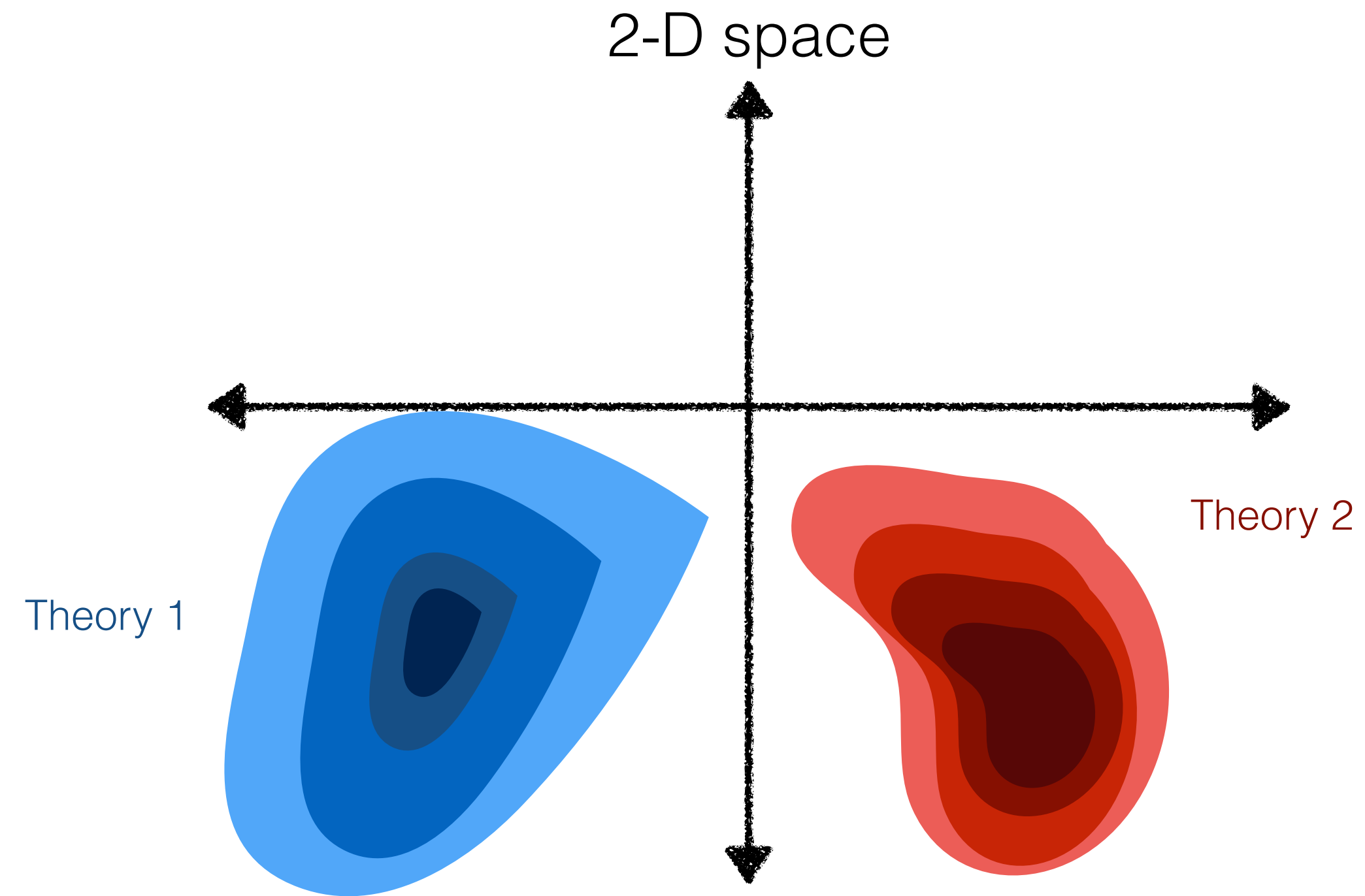
Quantum interference:



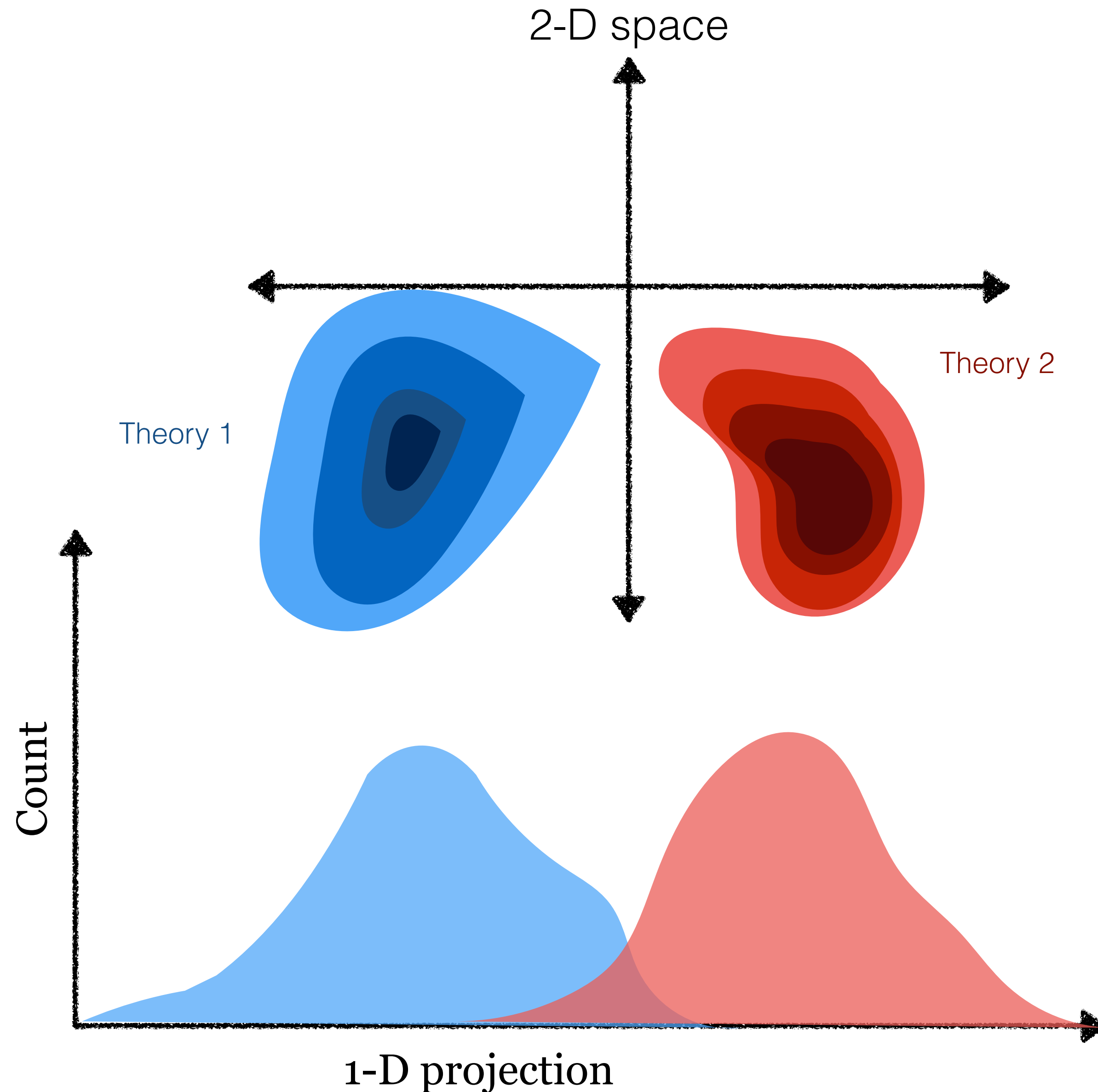
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The problem with one-dimensional summaries...

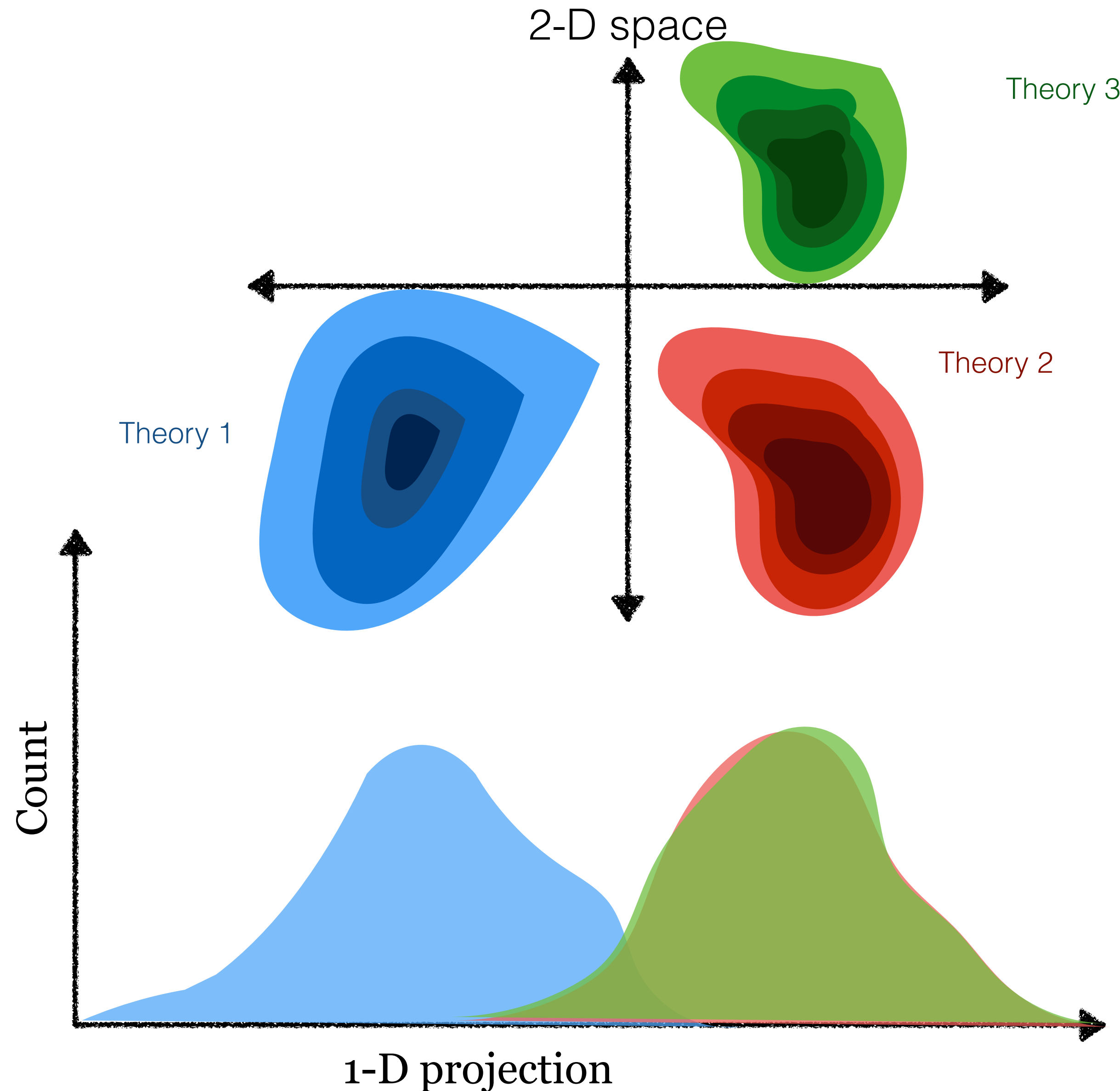
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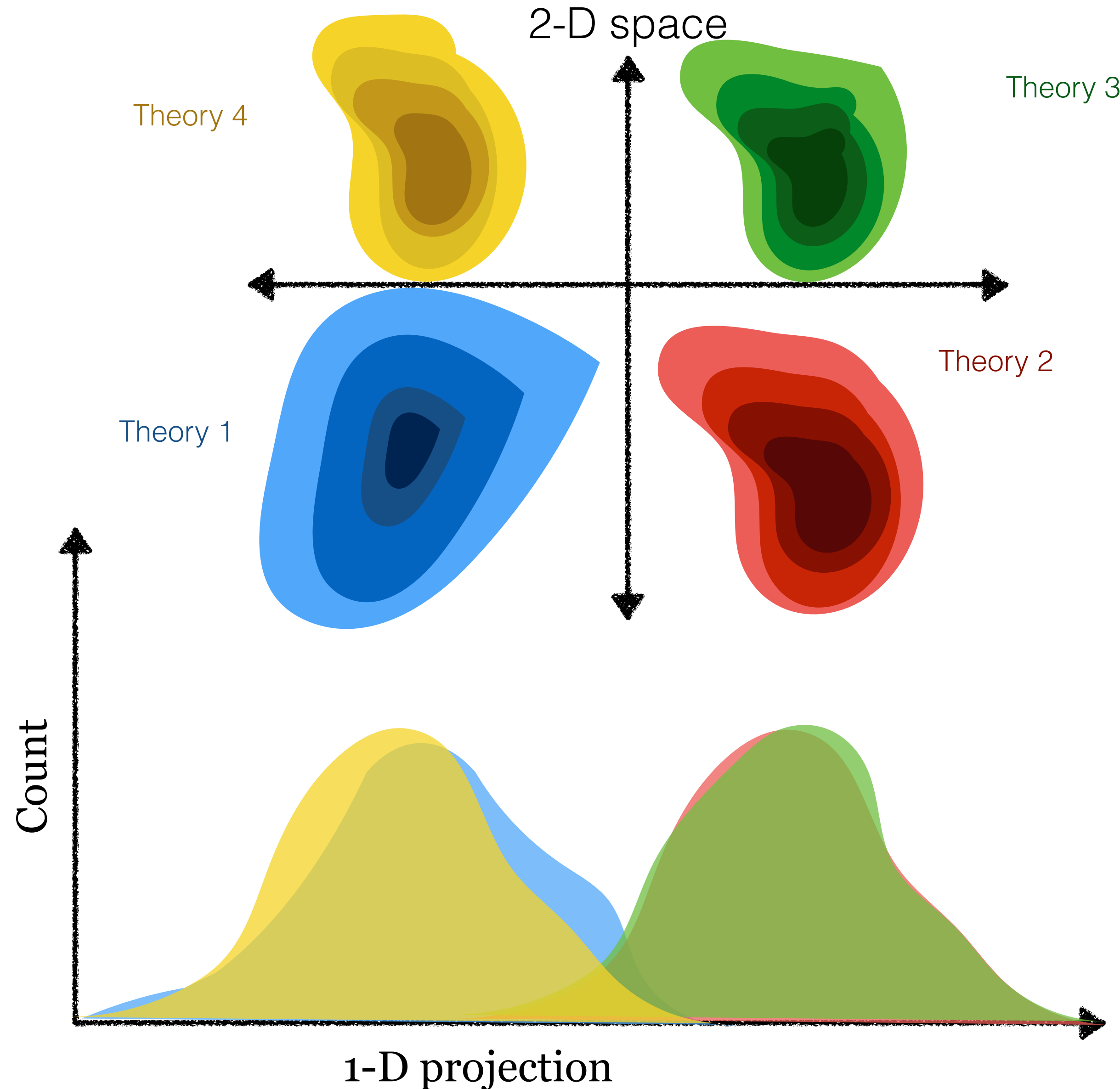
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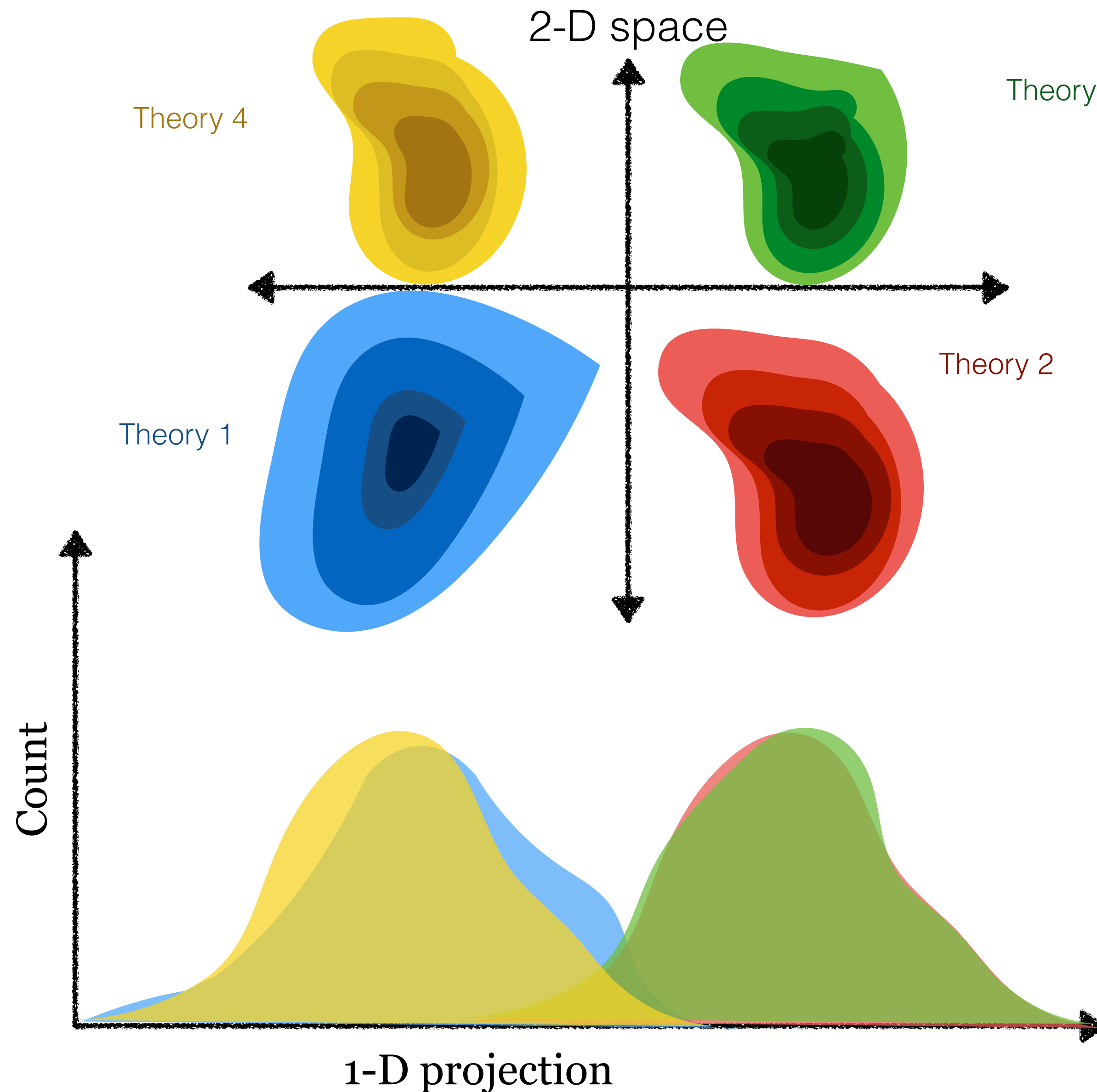
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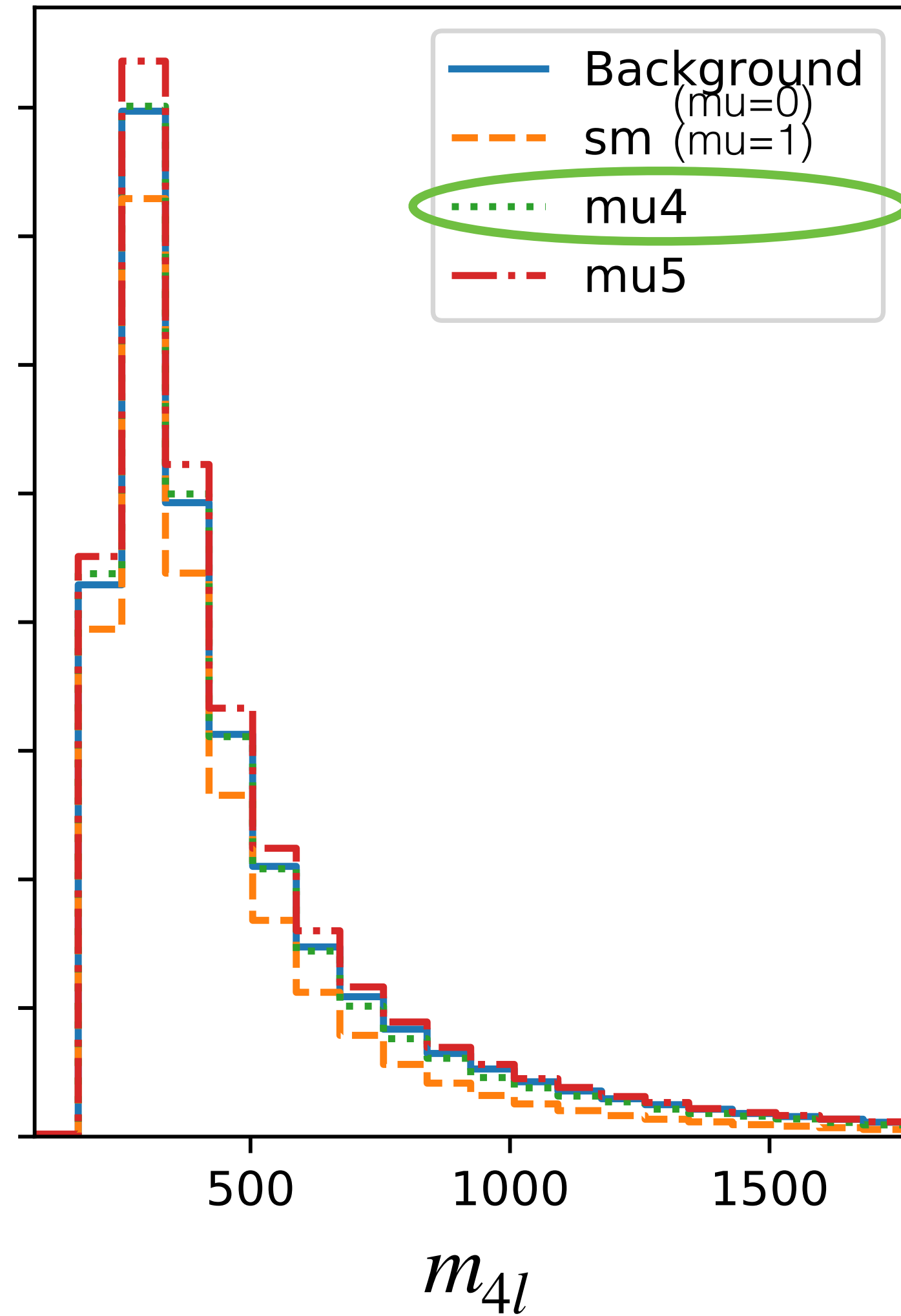
- Clearly separable in 2-D
- No 1-D summary statistic may contain all the information needed to optimally test all theory hypotheses!
- Valuable to have high-dimensional view of data

No single observable captures all information in Higgs width study

Signal-background-inference simulations: MG + Pythia

No single observable captures all information in Higgs width study

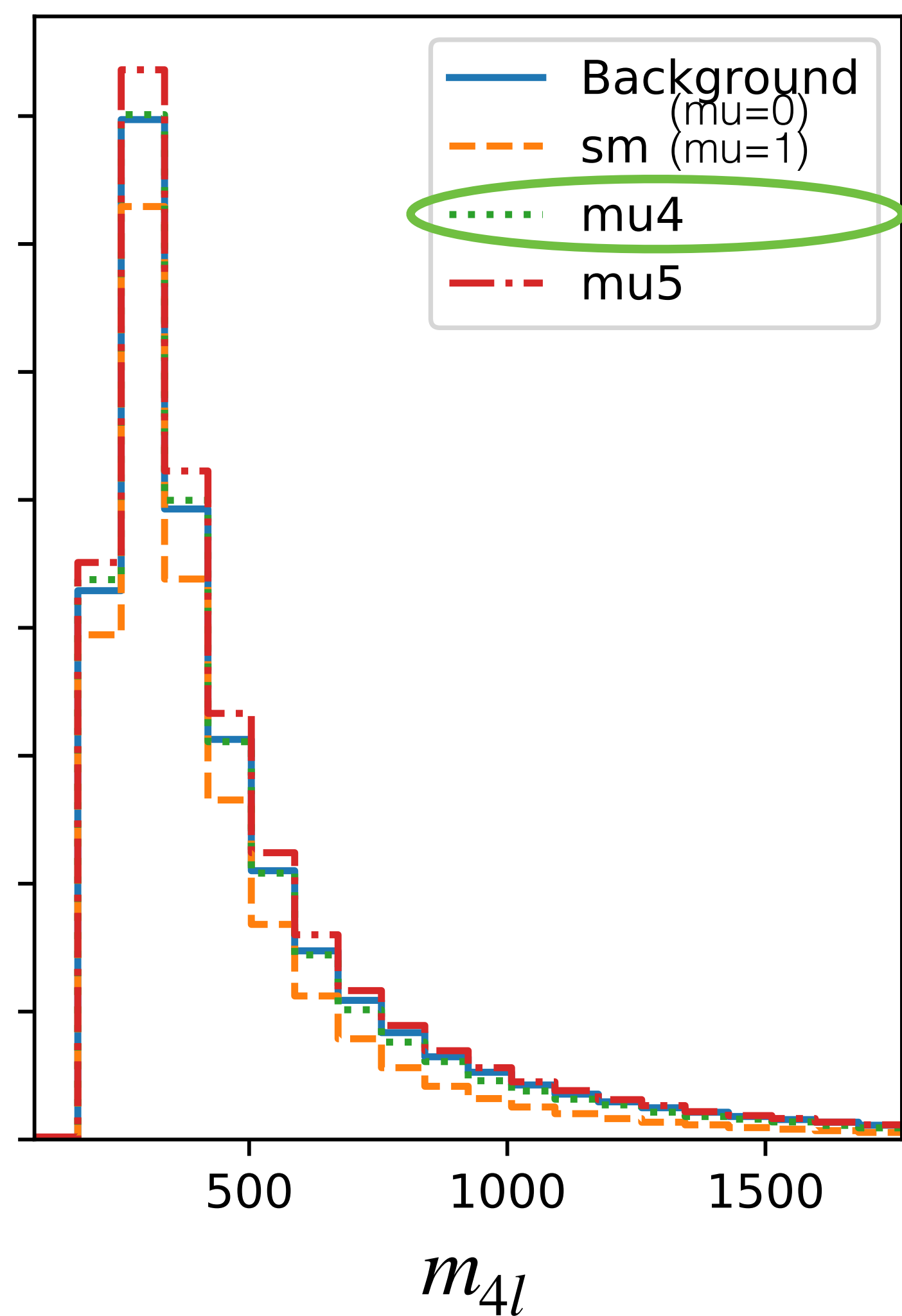
Signal-background-inference simulations: MG + Pythia



Can you spot the green plot?

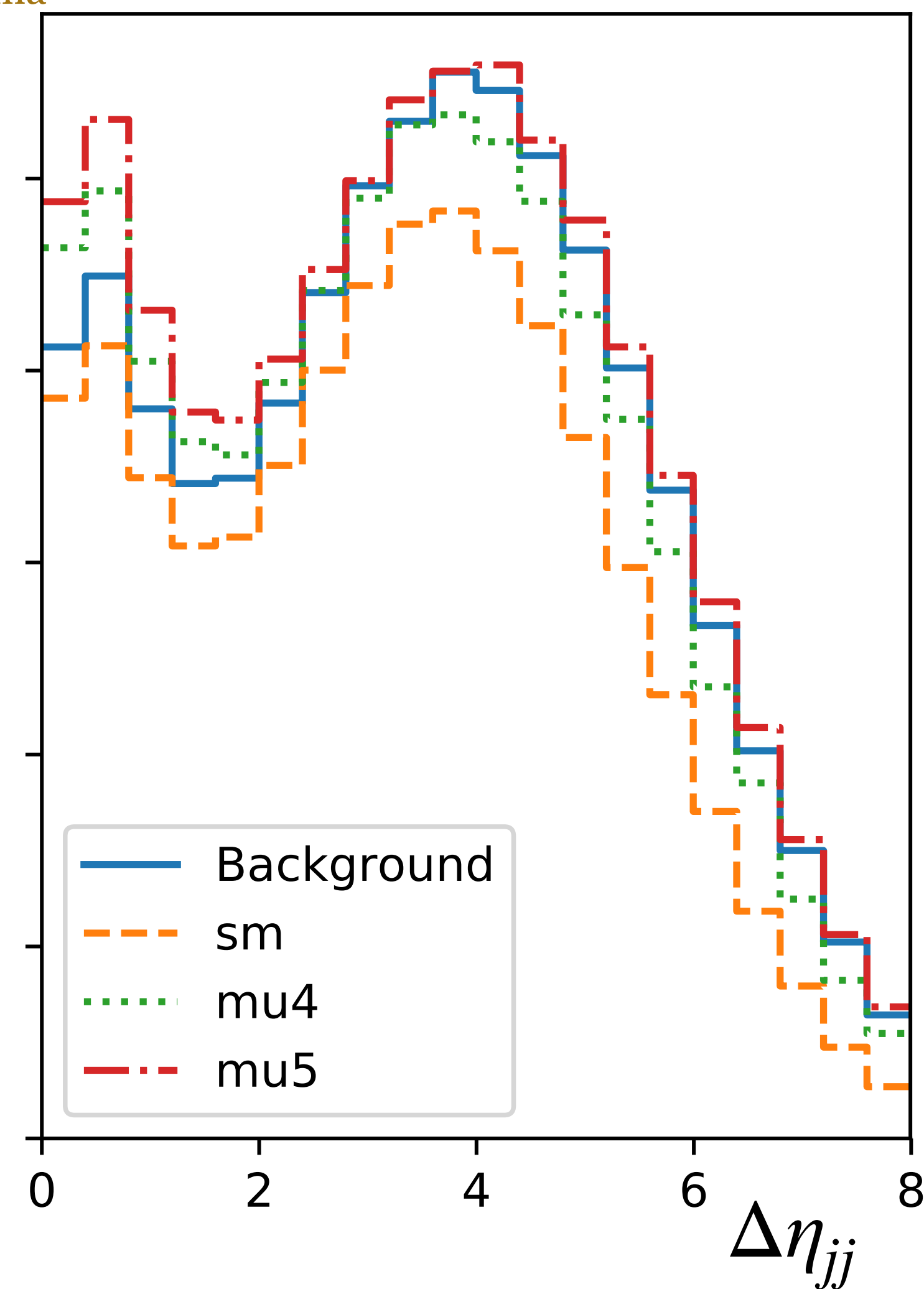
No single observable captures all information in Higgs width study

Signal-background-inference simulations: MG + Pythia



Can you spot the green plot?

$\mu=4$ indistinguishable from $\mu=0$
but other observables can break
the degeneracy



Optimal observable now changes as a function of μ : Cannot collapse problem to 1 dimension

What breaks down?

$$P(X) = |M_s(X) + M_b(X)|^2 = \underbrace{|M_s(X)|^2}_{P_s(X)} + \underbrace{|M_b(X)|^2}_{P_b(X)} + \underbrace{2 \operatorname{Re}(\overline{M_s(X)} M_b(X))}_{P_i(X)}$$

$$N_{exp} = \mu \cdot S + B + \sqrt{\mu} \cdot I$$

A neural network classifier trained on S vs B, estimates the decision function*: $s(x_i) = \frac{p(x_i|S)}{p(x_i|S) + p(x_i|B)}$

Which contains all the information required for the likelihood ratio:

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Same observable s is optimal to test all μ hypotheses!

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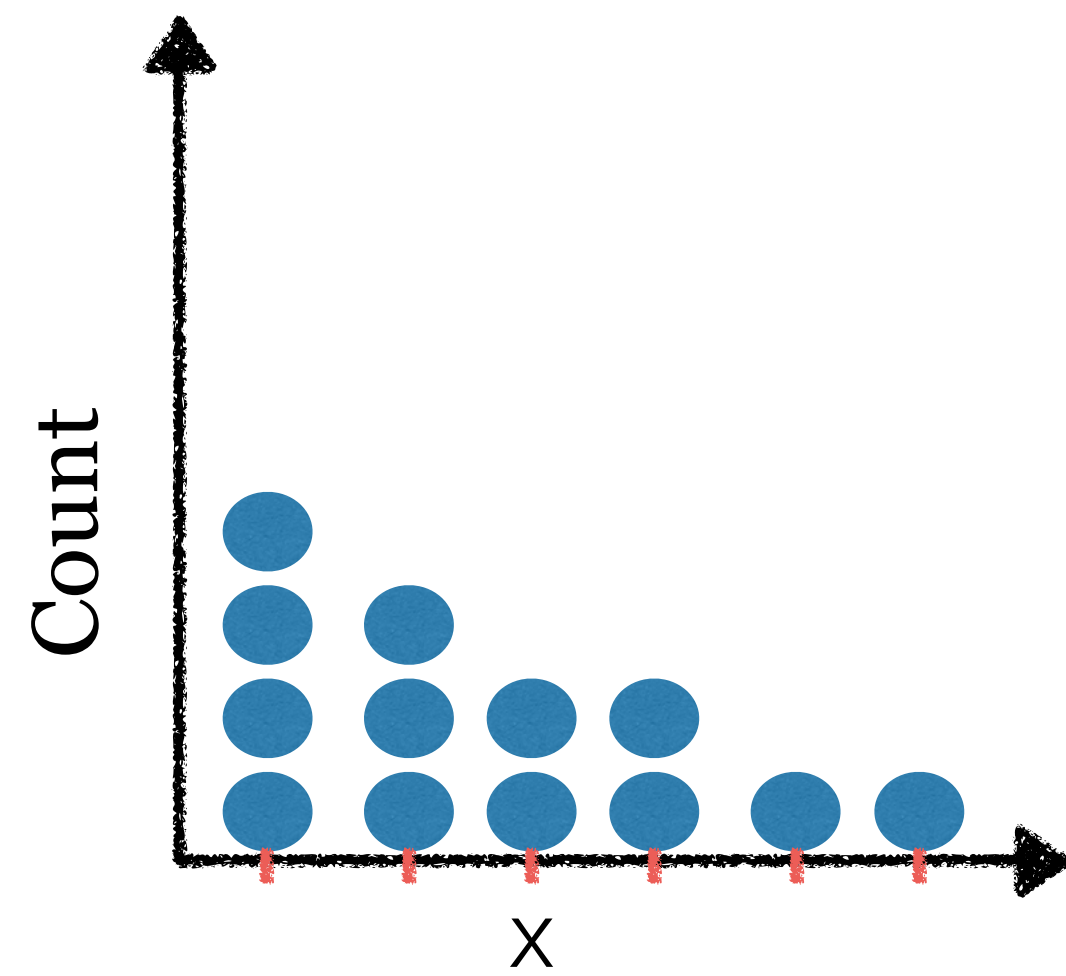
11

No longer in this convenient special case: The same observable no longer optimal due to non-linear effects coming from quantum interference

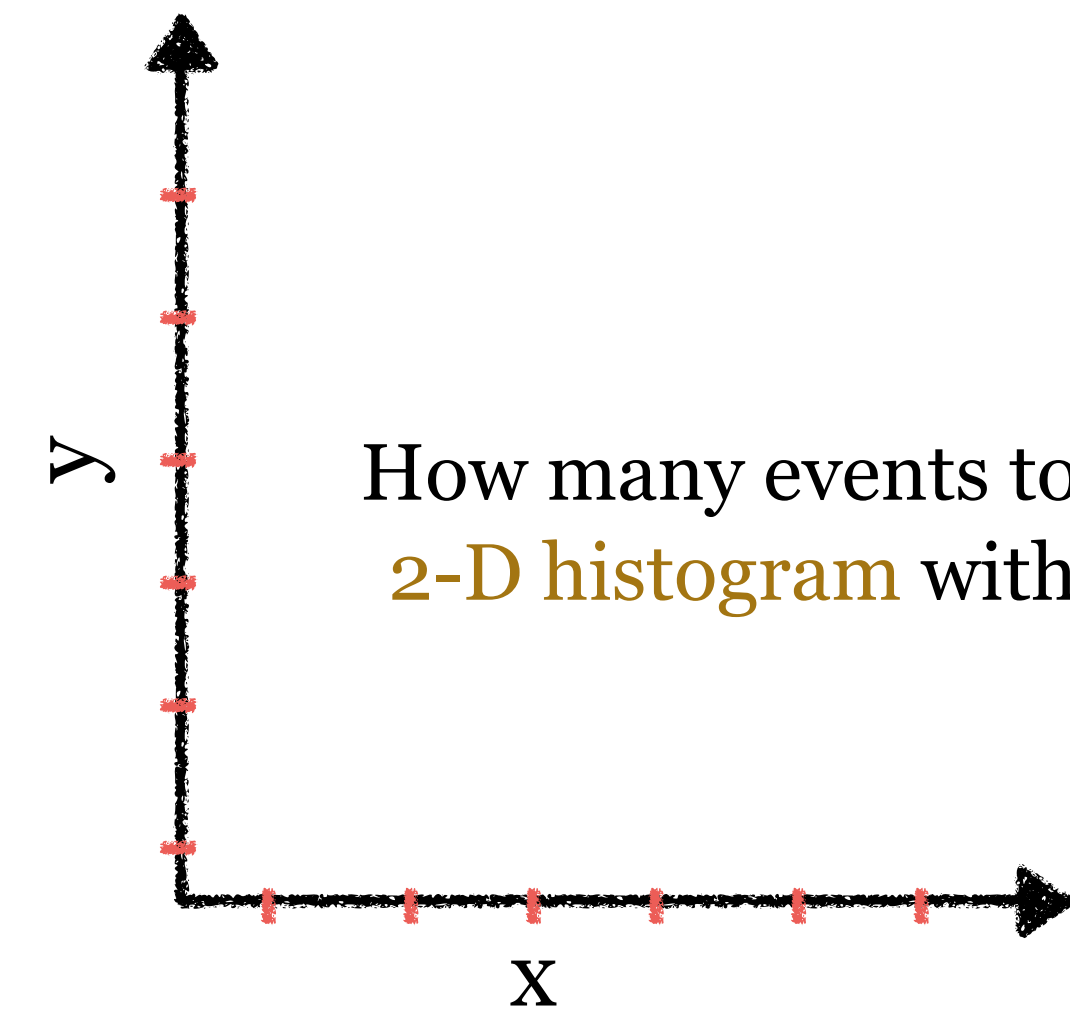
Also does not generalise to an arbitrary theory parameter θ , (eg. Effective Field Theory parameters)

Can we modify the LHC analysis methodology to design near-optimal analyse for the general case?

But probability density estimation in higher dimensions is hard...

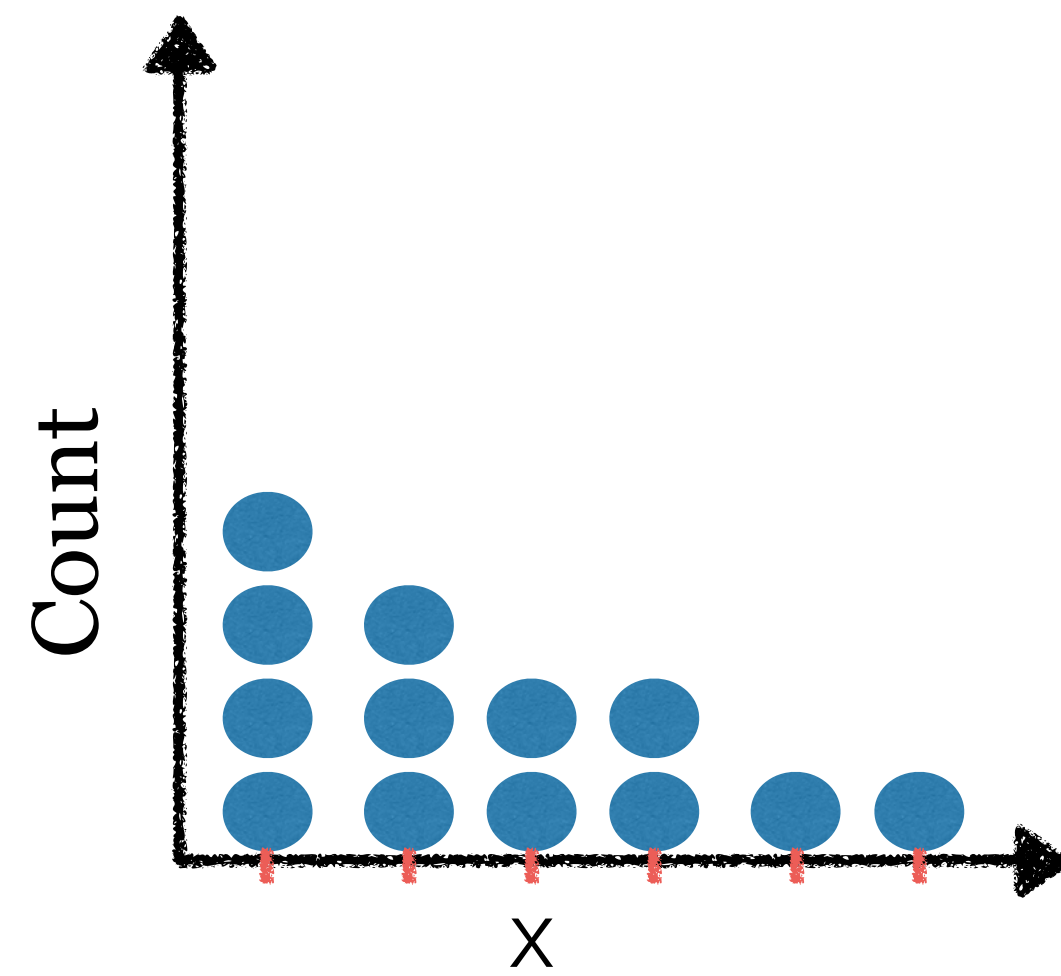


1-D histogram with 6 bins: few events enough to populate it

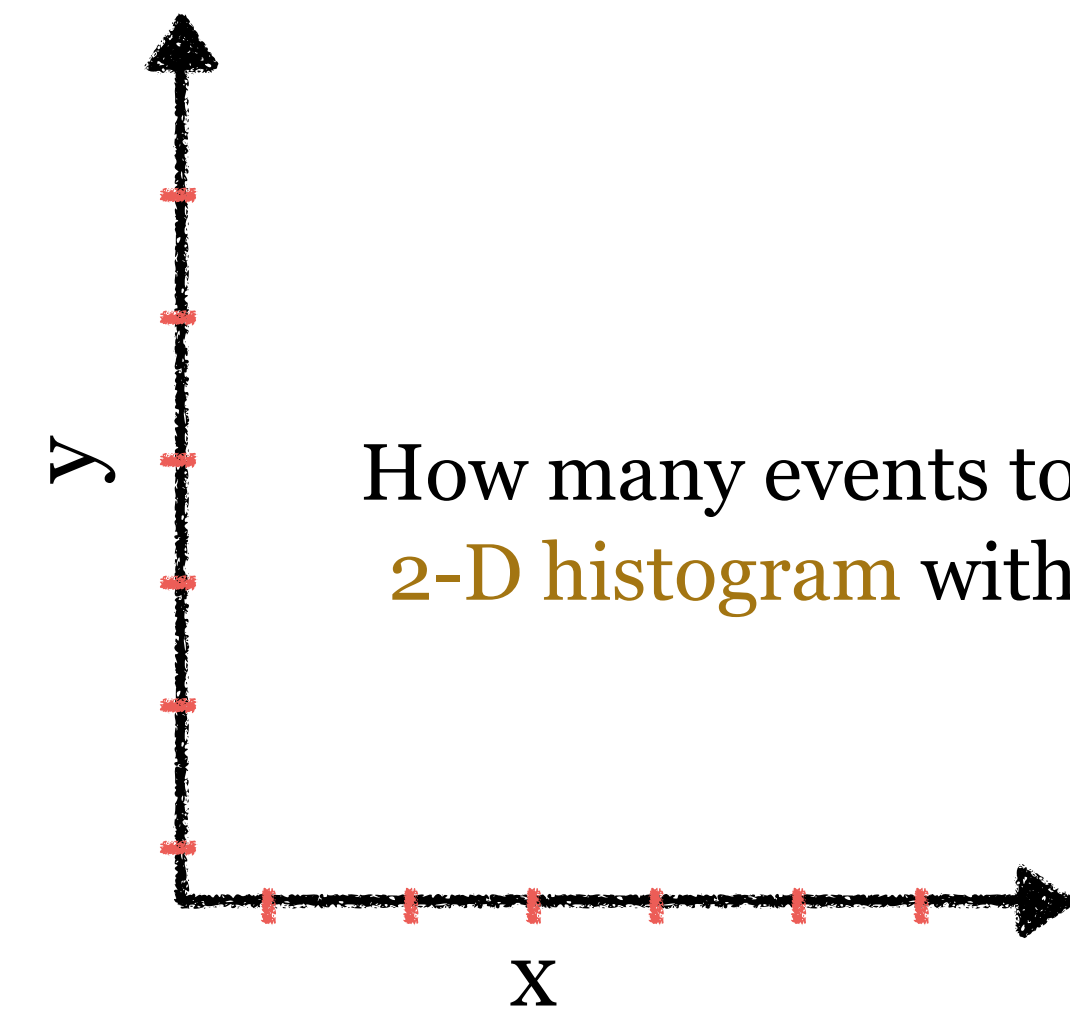


How many events for 50-D histogram
with 6^{50} bins ?

But probability density estimation in higher dimensions is hard...



1-D histogram with 6 bins: few events enough to populate it



How many events to populate 2-D histogram with 6^2 bins ?

Curse of dimensionality

How many events for 50-D histogram with 6^{50} bins ?

Neural networks can give us the likelihood ratios we need

Approximating Likelihood Ratios with Calibrated Discriminative Classifiers

Kyle Cranmer¹, Juan Pavez², and Gilles Louppe¹

¹New York University

²Federico Santa María University

March 21, 2016

Abstract

In many fields of science, generalized likelihood ratio tests are established tools for statistical inference. At the same time, it has become increasingly common that a simulator (or generative model) is used to describe complex processes that tie parameters θ of an underlying theory and measurement apparatus to high-dimensional observations $\mathbf{x} \in \mathbb{R}^p$. However, simulator often do not provide a way to evaluate the likelihood function for a given observation \mathbf{x} , which motivates a new class of likelihood-free inference algorithms. In this paper, we show that likelihood ratios are invariant under a specific class of dimensionality reduction maps $\mathbb{R}^p \mapsto \mathbb{R}$. As a direct consequence, we show that discriminative classifiers can be used to approximate the generalized likelihood ratio statistic when only a generative model for the data is available. This leads to a new machine learning-based approach to likelihood-free inference that is complementary to Approximate Bayesian Computation, and which does not require a prior on the model parameters. Experimental results on artificial problems with known exact likelihoods illustrate the potential of the proposed method.

Keywords: likelihood ratio, likelihood-free inference, classification, particle physics, surrogate model

arXiv:1506.02169v2 [stat.AP] 18 Mar 2016

Neural networks can give us the likelihood ratios

$$\mathcal{L}(\mu | \mathcal{D}) = p(\mathcal{D} | \mu)$$

Neyman–Pearson lemma: Likelihood ratio is the most powerful test statistic

We want to compare likelihoods:

$$\frac{p(\mathcal{D} | \mu)}{p(\mathcal{D} | ref)}$$

A neural network classifier trained on **simulated samples from μ_1** vs **simulated samples from ref** , estimates the decision function:

$$s(x_i) = \frac{p(x_i | \mu_1)}{p(x_i | \mu_1) + p(x_i | ref)}$$

Which contains all the information required for the likelihood ratio:

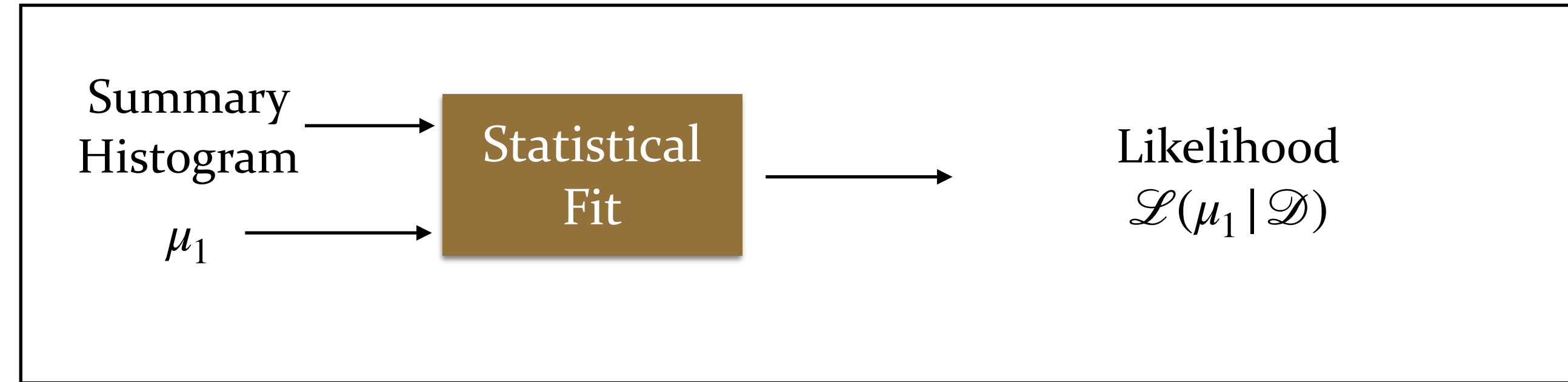
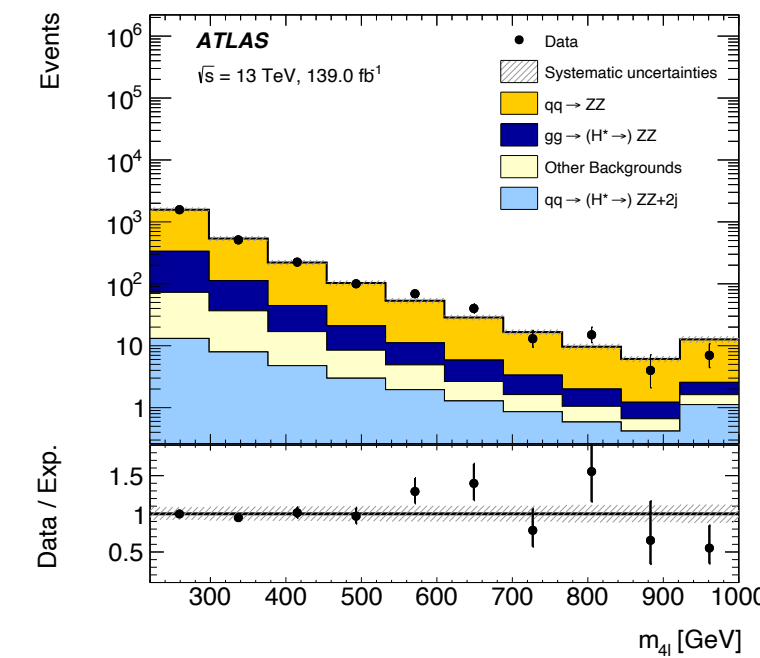
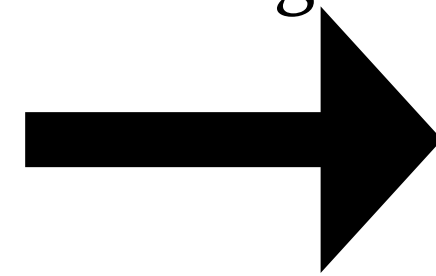
$$\frac{p(x_i | \mu_1)}{p(x_i | ref)} = \frac{s(x_i)}{1 - s(x_i)}$$

- * Optimal statistic to test each value of μ
- * We get the LR *per event* (unbinned)

A new paradigm: Neural simulation-based inference (NSBI)

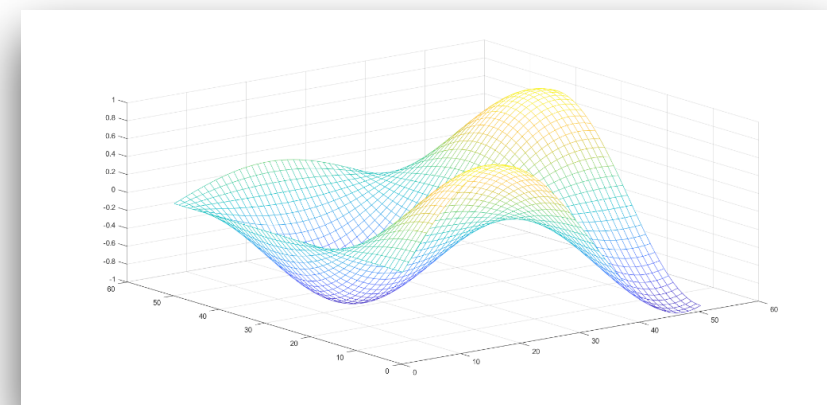
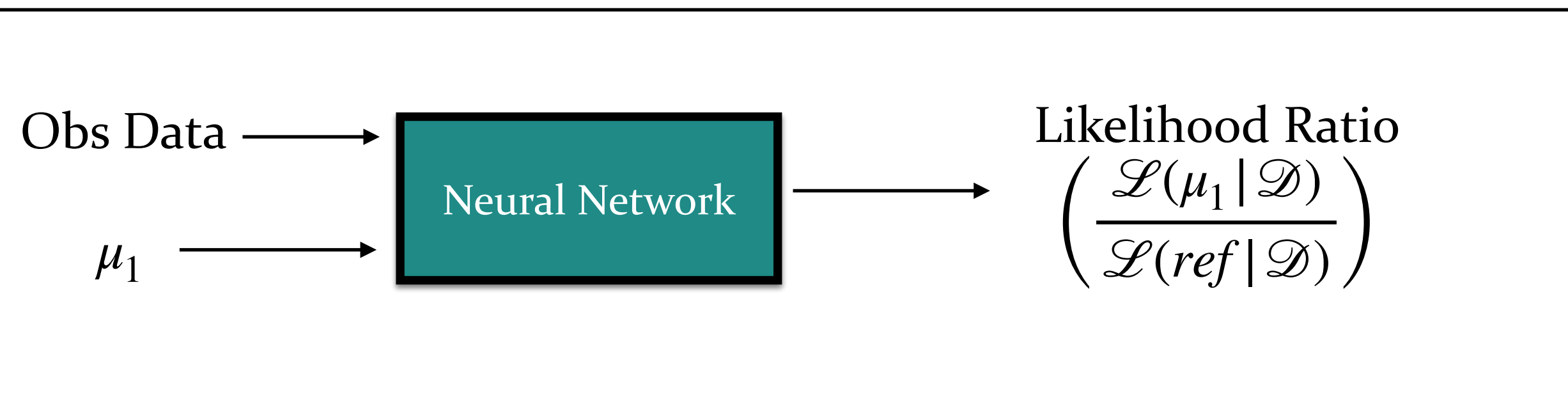
Traditional framework:

Summarisation
to histogram

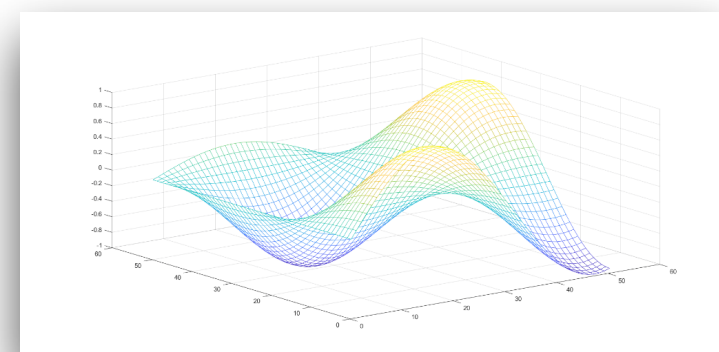


μ is now arbitrary parameter of interest(s)

Neural simulation-based inference framework:



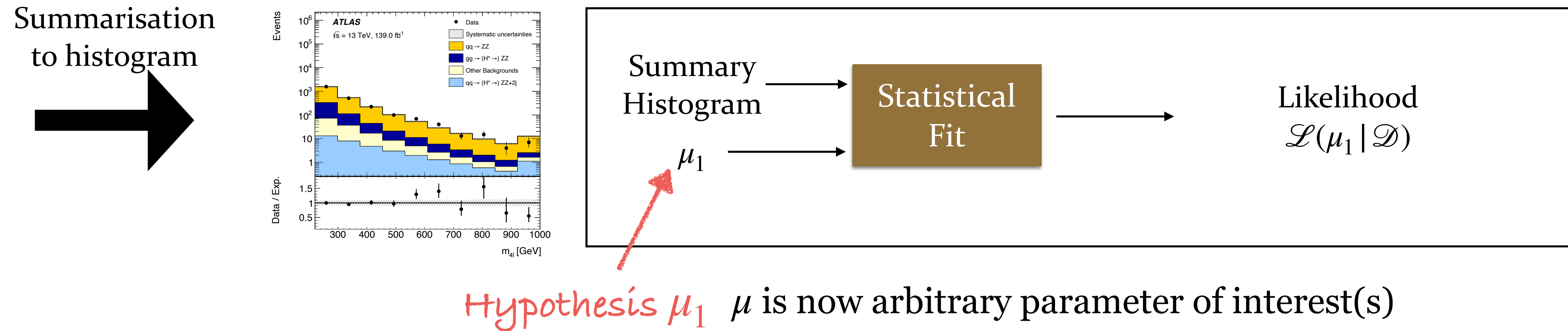
High-dim data



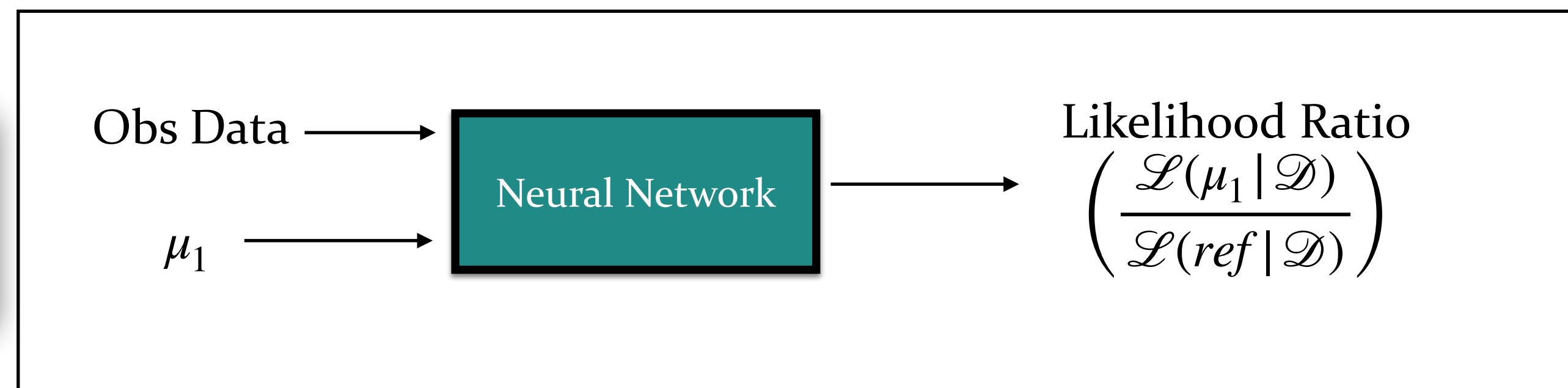
High-dim data

A new paradigm: Neural simulation-based inference (NSBI)

Traditional framework:

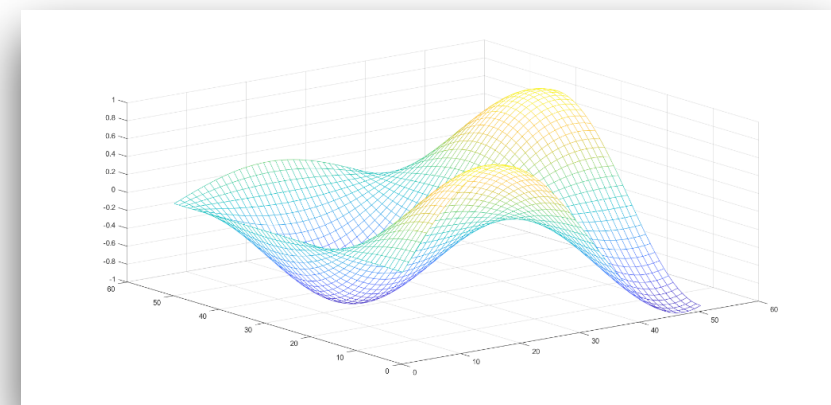


Neural simulation-based inference framework:

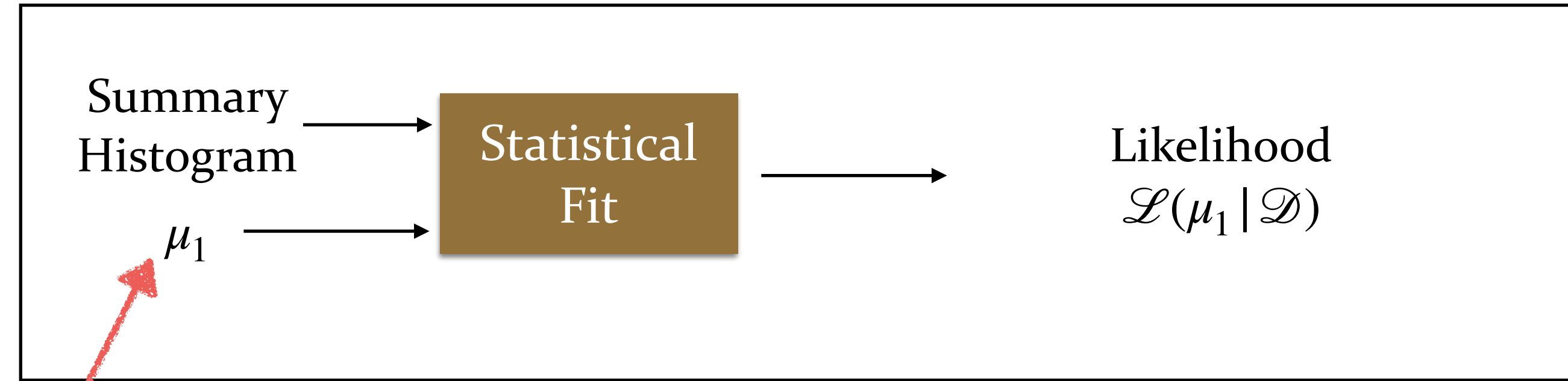
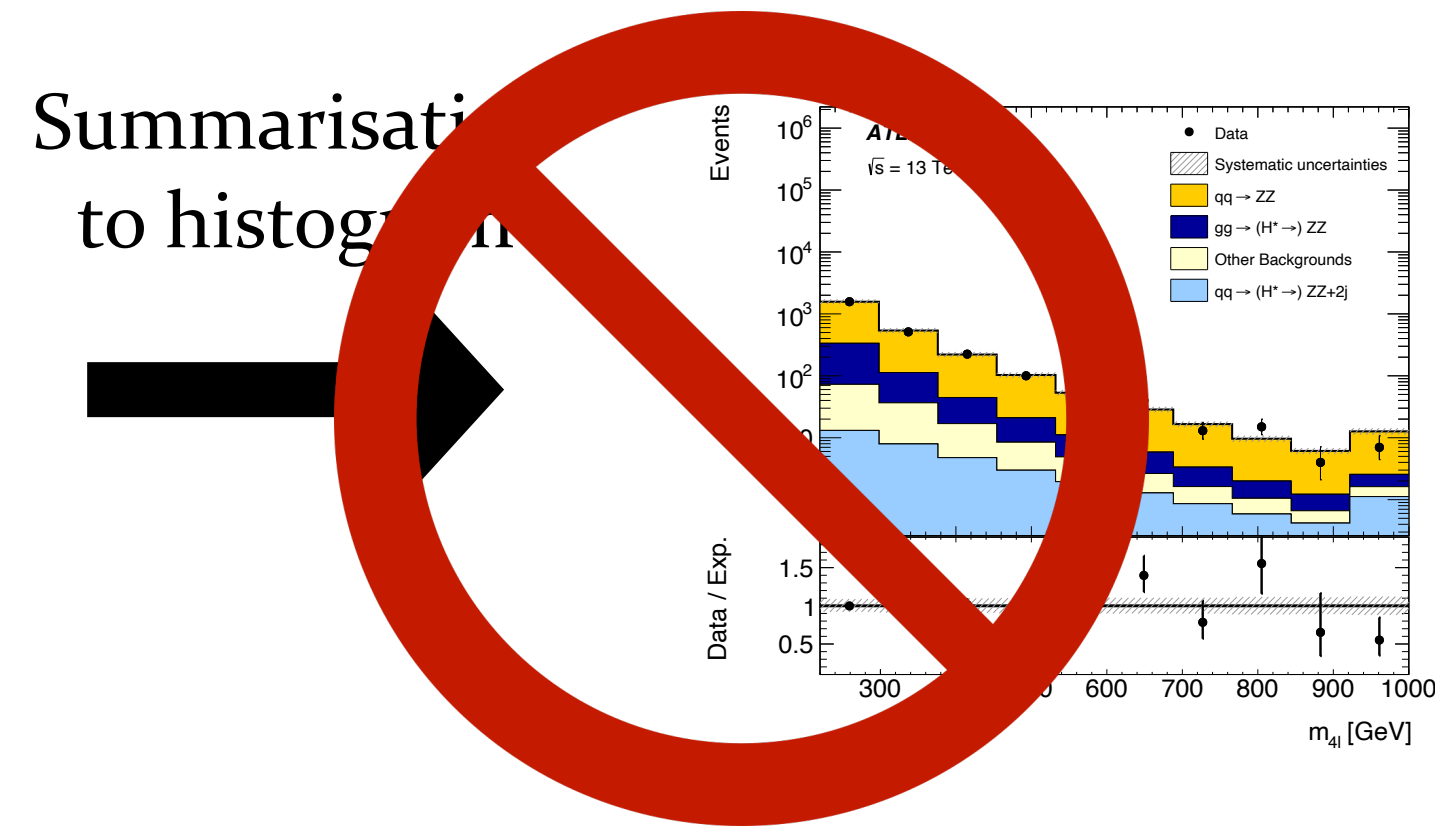


A new paradigm: Neural simulation-based inference (NSBI)

Traditional framework:

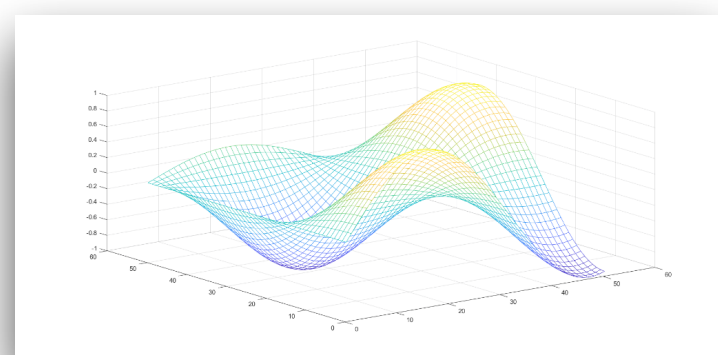


High-dim data

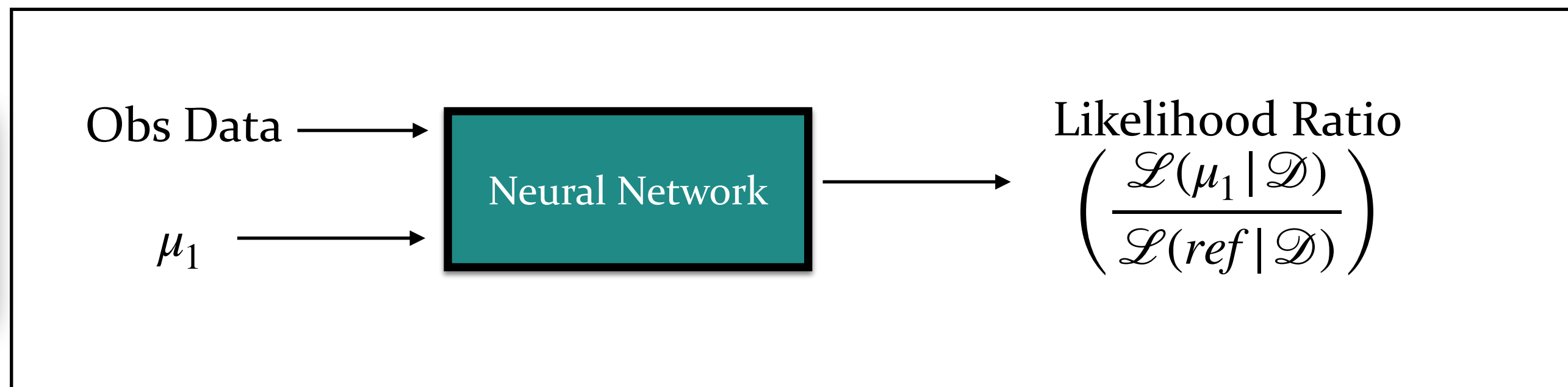


Hypothesis μ_1 μ is now arbitrary parameter of interest(s)

Neural simulation-based inference framework:

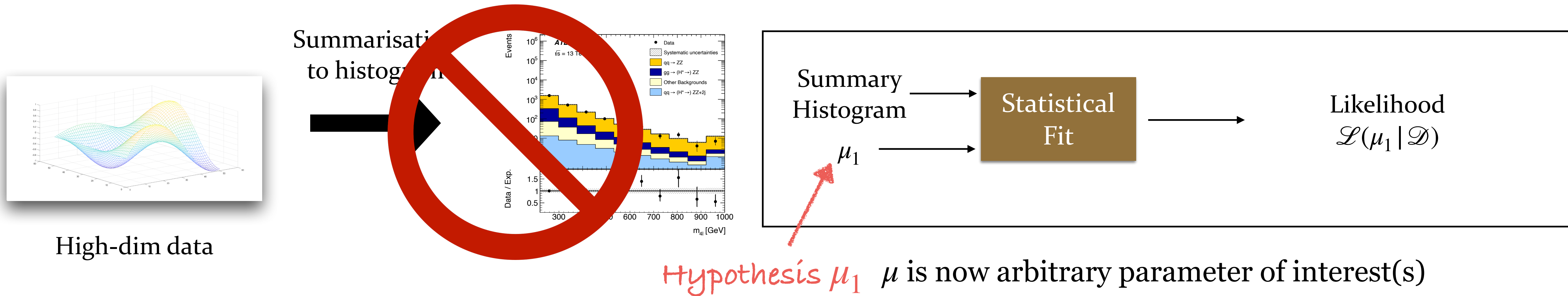


High-dim data

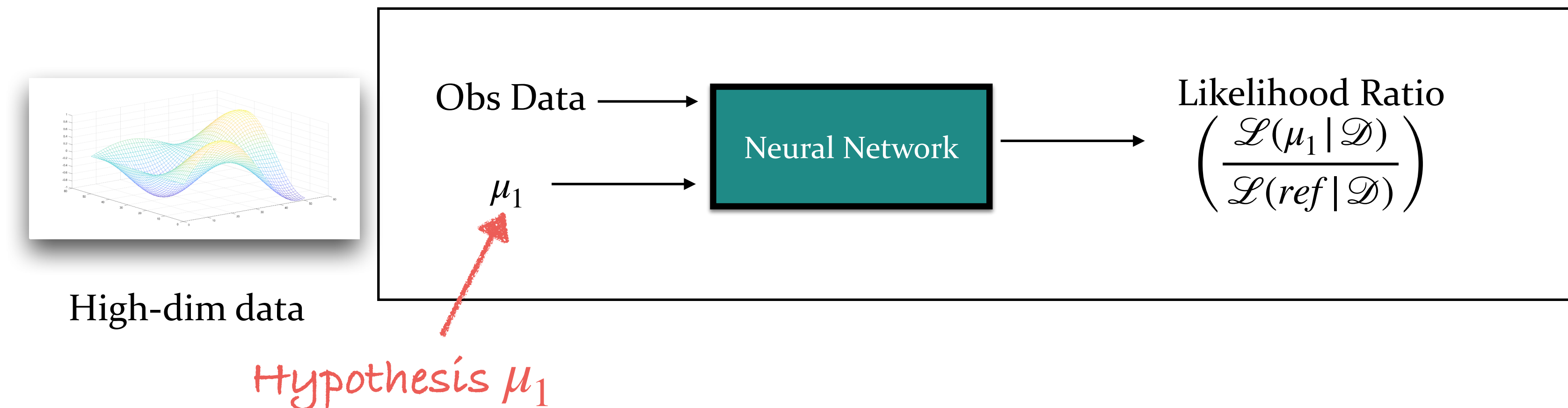


A new paradigm: Neural simulation-based inference (NSBI)

Traditional framework:

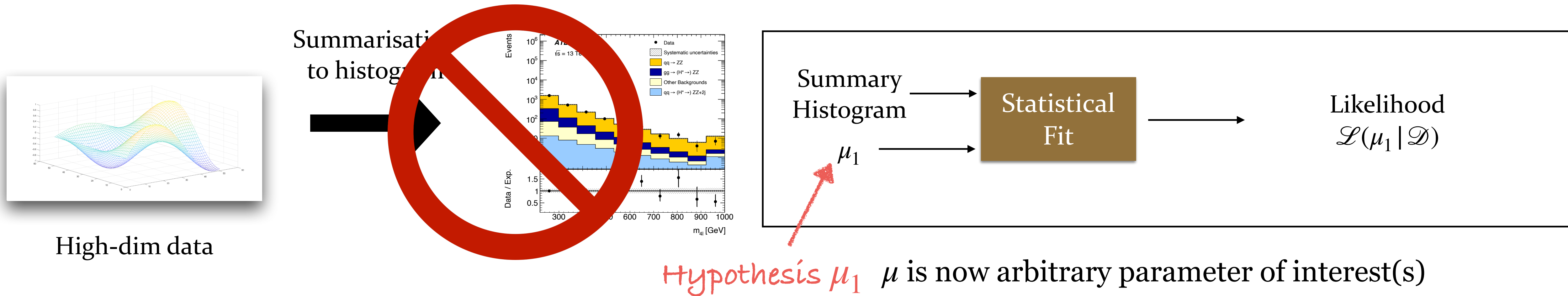


Neural simulation-based inference framework:

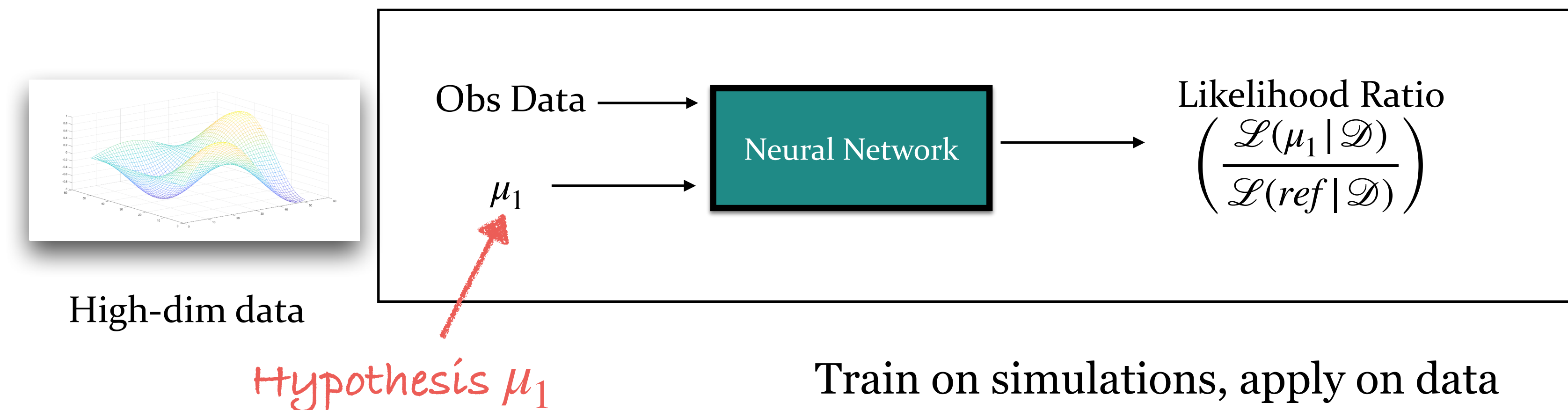


A new paradigm: Neural simulation-based inference (NSBI)

Traditional framework:



Neural simulation-based inference framework:

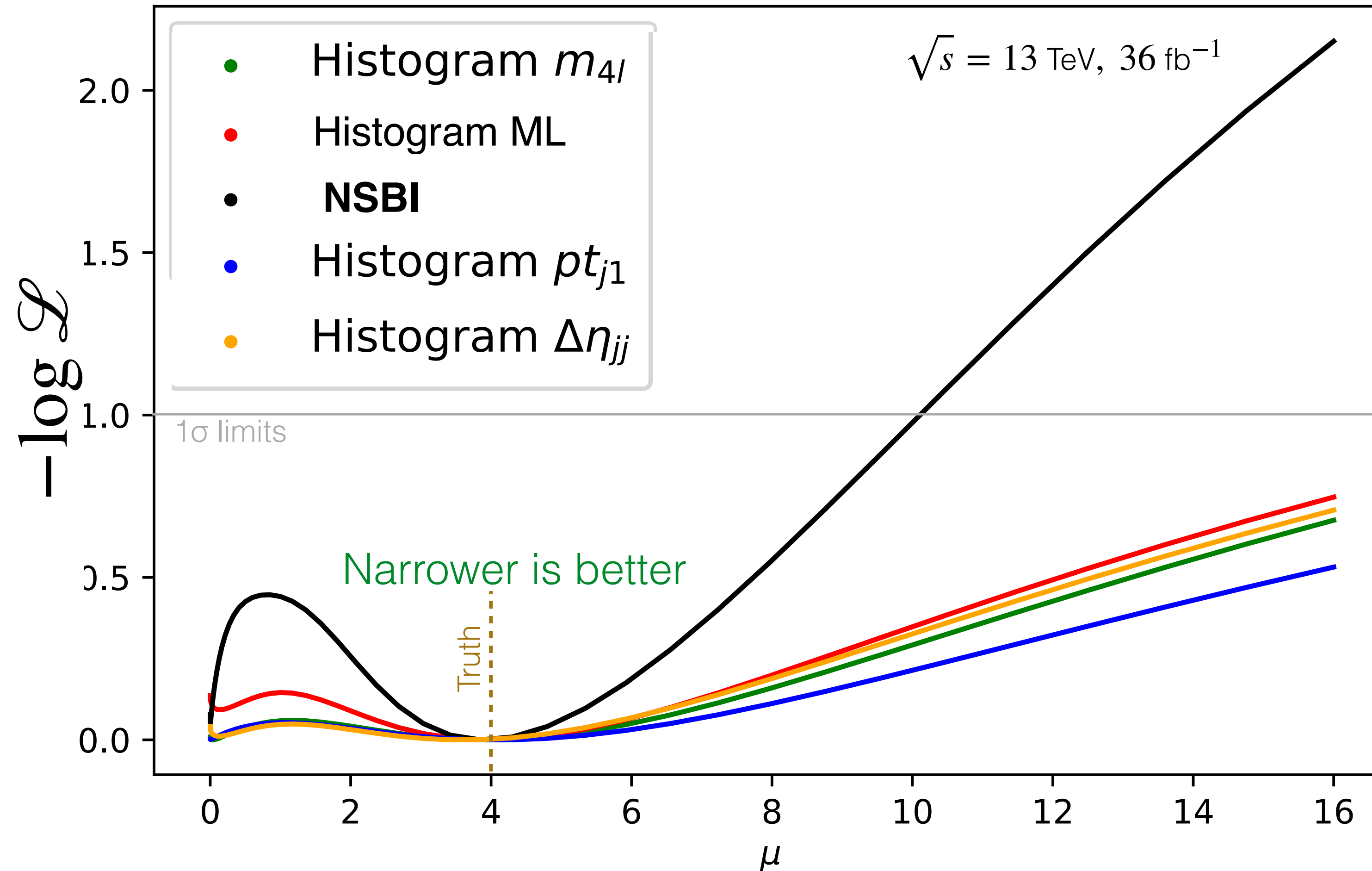


NSBI for Higgs width in proof-of-concept phenomenology study

Expected sensitivity [hal-02971995v3](#) (p172): Ghosh & Rousseau, [Thesis](#): Ghosh

NSBI for Higgs width in proof-of-concept phenomenology study

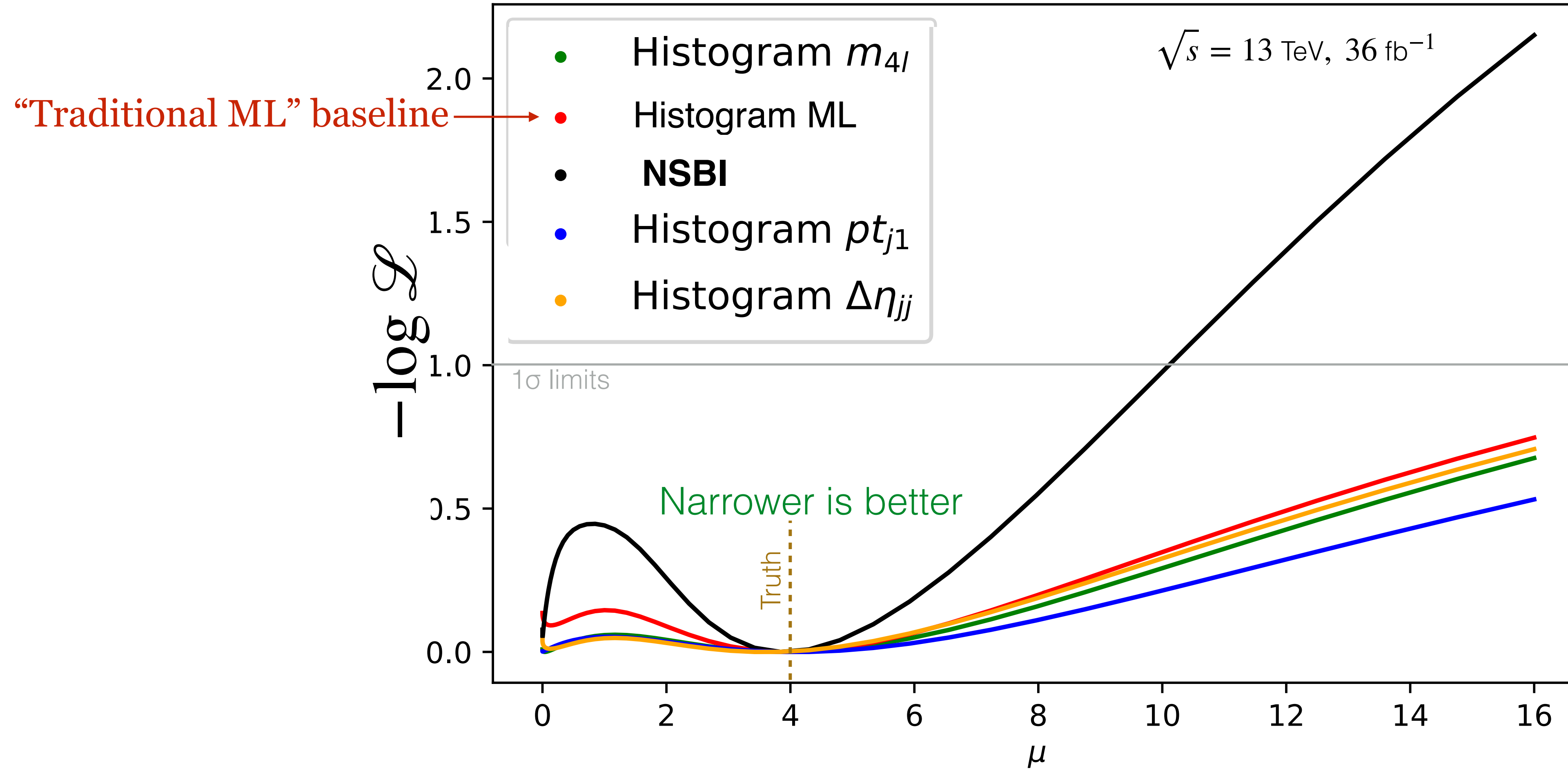
Expected sensitivity [hal-02971995v3](#) (p172): Ghosh & Rousseau, [Thesis](#): Ghosh



(Beyond Standard Model value) $\mu = 4$, without rate

NSBI for Higgs width in proof-of-concept phenomenology study

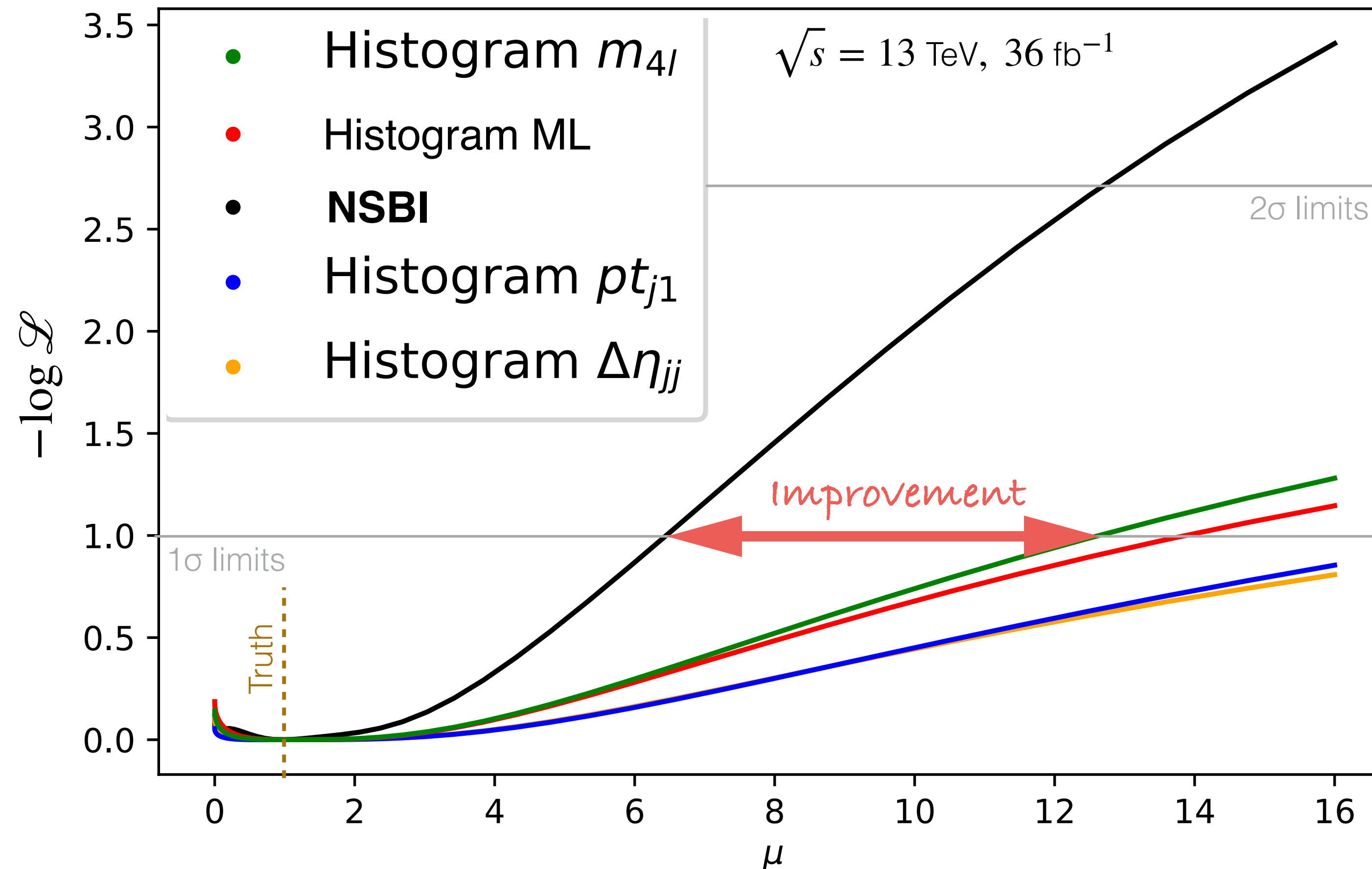
Expected sensitivity [hal-02971995v3](#) (p172): Ghosh & Rousseau, [Thesis](#): Ghosh



(Beyond Standard Model value) $\mu = 4$, without rate

Expected improvement for Standard Model

[hal-02971995v3](#) (p172): Ghosh & Rousseau, [Thesis](#): Ghosh



Exciting gains promised!

SM, without rate

Open problems to extend to full ATLAS analysis:

- Robustness: Design and validation
- Systematic Uncertainties: Incorporate them in likelihood (ratio) model
- Neyman Construction: Throwing toys in a per-event analysis

Open problems to extend to full ATLAS analysis:

- Robustness: Design and validation
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- Neyman Construction: Throwing toys in a per-event analysis

How frequentists ensure coverage



Open problems to extend to full ATLAS

Solved!



arXiv:2412.01600v1 [hep-ex] 2 Dec 2024

An implementation of neural simulation-based inference for parameter estimation in ATLAS

The ATLAS Collaboration

Neural simulation-based inference is a powerful class of machine-learning-based methods for statistical inference that naturally handles high-dimensional parameter estimation without the need to bin data into low-dimensional summary histograms. Such methods are promising for a range of measurements, including at the Large Hadron Collider, where no single observable may be optimal to scan over the entire theoretical phase space under consideration, or where binning data into histograms could result in a loss of sensitivity. This work develops a neural simulation-based inference framework for statistical inference, using neural networks to estimate probability density ratios, which enables the application to a full-scale analysis. It incorporates a large number of systematic uncertainties, quantifies the uncertainty due to the finite number of events in training samples, develops a method to construct confidence intervals, and demonstrates a series of intermediate diagnostic checks that can be performed to validate the robustness of the method. As an example, the power and feasibility of the method are assessed on simulated data for a simplified version of an off-shell Higgs boson couplings measurement in the four-lepton final states. This approach represents an extension to the standard statistical methodology used by the experiments at the Large Hadron Collider, and can benefit many physics analyses.

Solved!

Open problems to extend to full ATLAS

Applied on Run2 data, superseding previous ATLAS paper on same data !

EUROPEAN ORGANISATION FOR NUCLEAR RESEARCH (CERN)



Submitted to: Rep. Prog. Phys.



CERN-EP-2024-305
December 3, 2024

EUROPEAN ORGANISATION FOR NUCLEAR RESEARCH (CERN)



Submitted to: Rep. Prog. Phys.



CERN-EP-2024-298
December 3, 2024

Measurement of off-shell Higgs boson production in the $H^* \rightarrow ZZ \rightarrow 4\ell$ decay channel using a neural simulation-based inference technique in 13 TeV pp collisions with the ATLAS detector

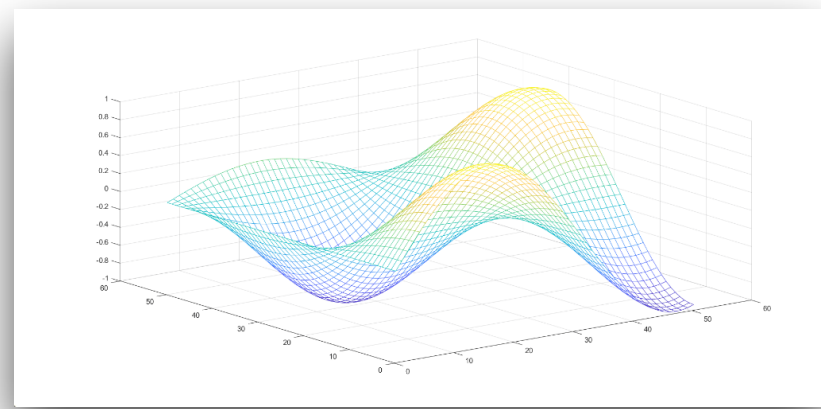
The ATLAS Collaboration

A measurement of off-shell Higgs boson production in the $H^* \rightarrow ZZ \rightarrow 4\ell$ decay channel is presented. The measurement uses 140 fb^{-1} of proton–proton collisions at $\sqrt{s} = 13 \text{ TeV}$ collected by the ATLAS detector at the Large Hadron Collider and supersedes the previous result in this decay channel using the same dataset. The data analysis is performed using a neural simulation-based inference method, which builds per-event likelihood ratios using neural networks. The observed (expected) off-shell Higgs boson production signal strength in the $ZZ \rightarrow 4\ell$ decay channel at 68% CL is $0.87_{-0.54}^{+0.75}$ ($1.00_{-0.95}^{+1.04}$). The evidence for off-shell Higgs boson production using the $ZZ \rightarrow 4\ell$ decay channel has an observed (expected) significance of 2.5σ (1.3σ). The expected result represents a significant improvement relative to that of the previous analysis of the same dataset, which obtained an expected significance of 0.5σ . When combined with the most recent ATLAS measurement in the $ZZ \rightarrow 2\ell 2\nu$ decay channel, the evidence for off-shell Higgs boson production has an observed (expected) significance of 3.7σ (2.4σ). The off-shell measurements are combined with the measurement of on-shell Higgs boson production to obtain constraints on the Higgs boson total width. The observed (expected) value of the Higgs boson width at 68% CL is $4.3_{-1.9}^{+2.7}$ ($4.1_{-3.4}^{+3.5}$) MeV.

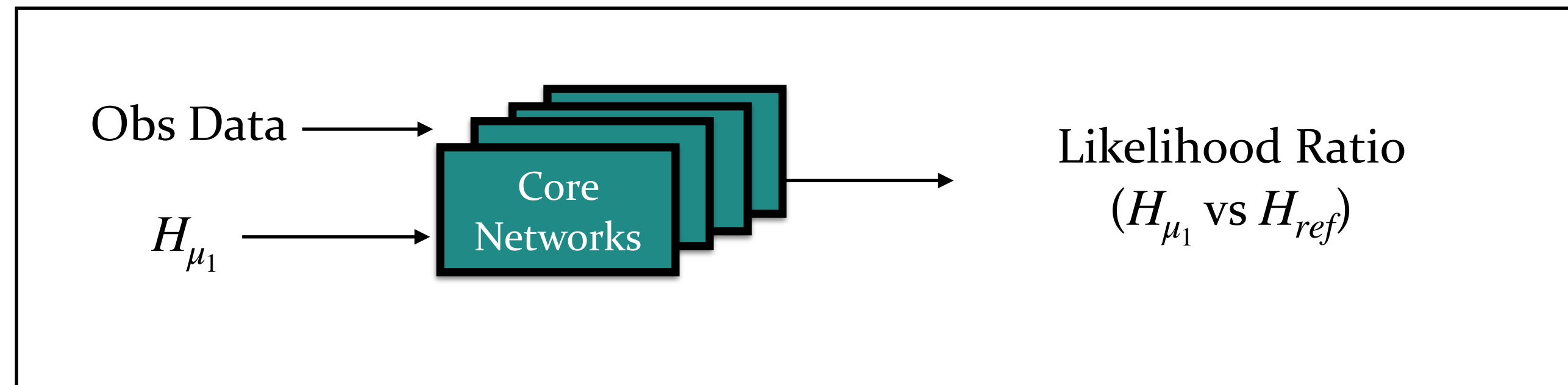
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arXiv:2412.01548v1 [hep-ex] 2 Dec 2024

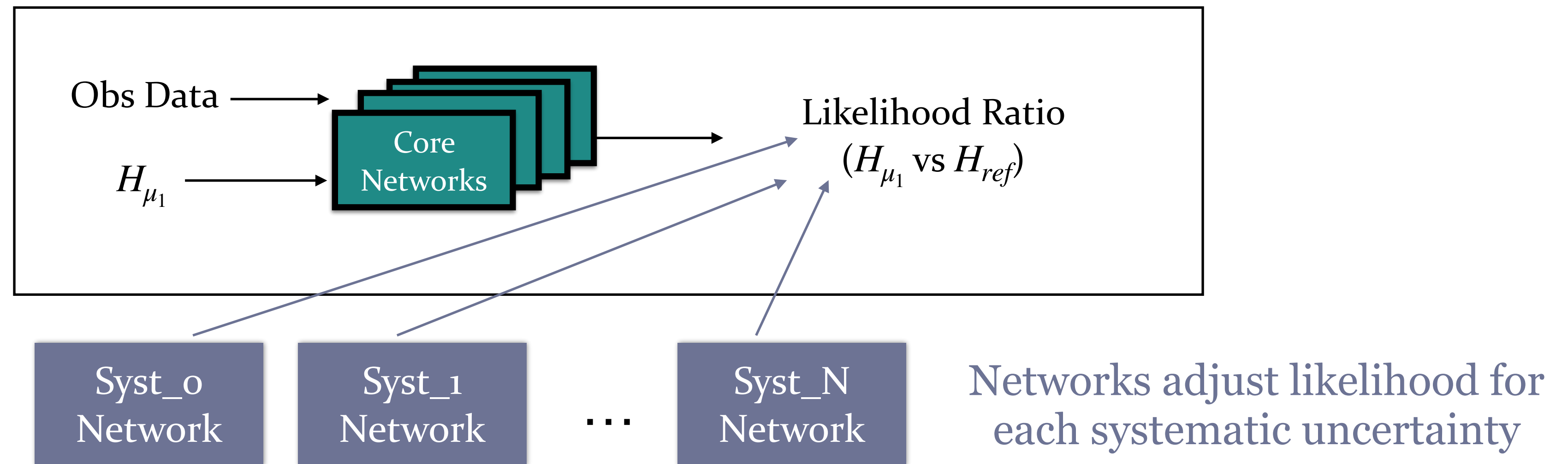
Big picture of full solution developed in ATLAS



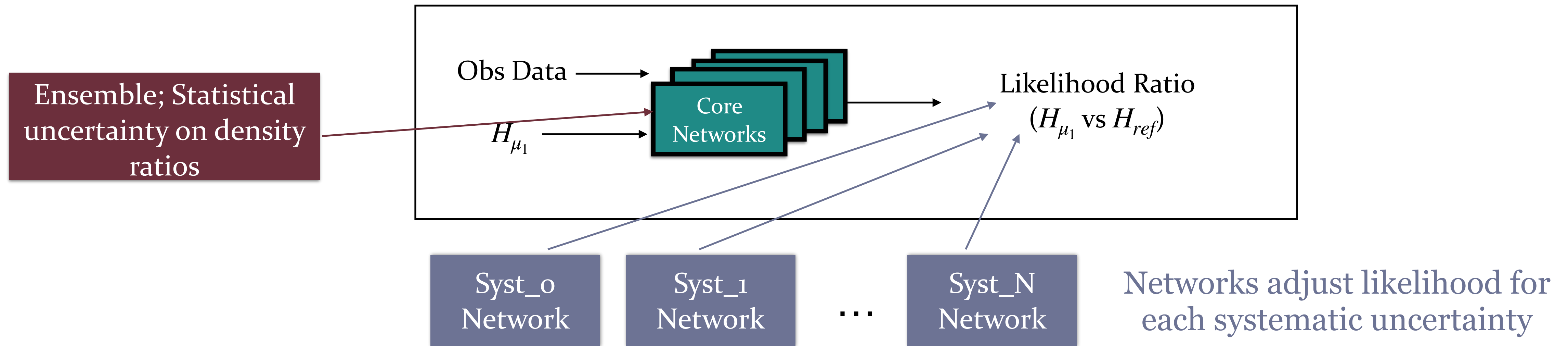
$O(16)$ observables



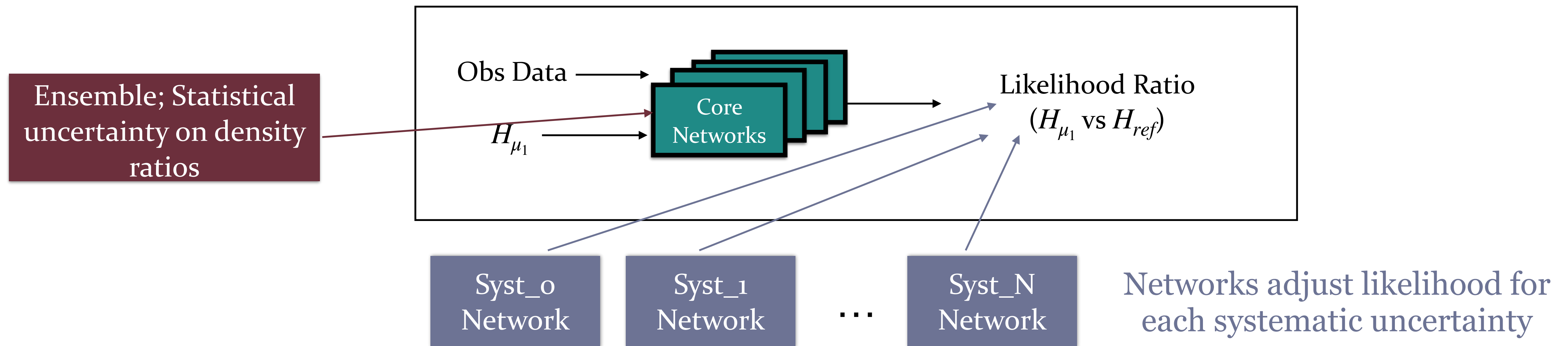
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Big picture of full solution developed in ATLAS

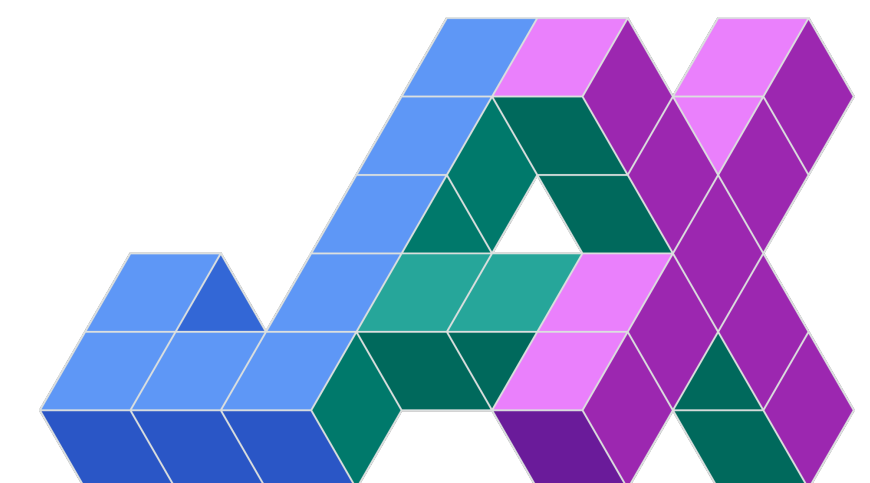


Big picture of full solution developed in ATLAS



Training details

- ◆ Train $O(10^4)$ networks on TensorFlow
- ◆ Computing resources provided by Google, SMU, other HPC clusters
- ◆ Fits with JAX



Open problems to extend to full ATLAS analysis:

- **Robustness: Design** and validation
- **Systematic Uncertainties:** Incorporate them in likelihood (ratio) model
- **Neyman Construction:** Throwing toys in a per-event analysis

Next 2 slides gets a bit technical

Search-Oriented Mixture Model

x_i is one individual event

General Formula

$$p(x_i|\mu) = \frac{1}{\nu(\mu)} \sum_j^{\mathcal{C}} f_j(\mu) \cdot \nu_j p_j(x_i)$$

j runs over different physics process
(Eg. $gg \rightarrow H^* \rightarrow 4l$, $gg \rightarrow ZZ \rightarrow 4l$)

Example use case

Search-Oriented Mixture Model

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Example use case

$$p_{\text{ggF}}(x|\mu) = \frac{1}{\nu_{\text{ggF}}(\mu)} \left[(\mu - \sqrt{\mu}) \nu_S p_S(x) + \sqrt{\mu} \nu_{\text{SBI}_1} p_{\text{SBI}_1}(x) + (1 - \sqrt{\mu}) \nu_B p_B(x) \right]$$

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Comes from theory model chosen to interpret data

Example use case

$$p_{ggF}(x|\mu) = \frac{1}{\nu_{ggF}(\mu)} \left[\underline{(\mu - \sqrt{\mu})} \nu_S p_S(x) + \underline{\sqrt{\mu}} \nu_{SBI_1} p_{SBI_1}(x) + \underline{(1 - \sqrt{\mu})} \nu_B p_B(x) \right]$$

Search-Oriented Mixture Model

x_i is one individual event

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$$p(x_i|\mu) = \frac{1}{v(\mu)} \sum_j^C f_j(\mu) \cdot v_j p_j(x_i)$$

Event rates estimated from simulations

Comes from theory model chosen to interpret data

j runs over different physics process
(Eg. $gg \rightarrow H^* \rightarrow 4l$, $gg \rightarrow ZZ \rightarrow 4l$)

Example use case

$$p_{ggF}(x|\mu) = \frac{1}{v_{ggF}(\mu)} \left[(\mu - \sqrt{\mu}) v_S p_S(x) + \sqrt{\mu} v_{SBI_1} p_{SBI_1}(x) + (1 - \sqrt{\mu}) v_B p_B(x) \right]$$

Search-Oriented Mixture Model

x_i is one individual event

General Formula

$$p(x_i|\mu) = \frac{1}{v(\mu)} \sum_j^C f_j(\mu) \cdot v_j p_j(x_i) \quad ?$$

Event rates estimated from simulations

Comes from theory model chosen to interpret data

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(Eg. $gg \rightarrow H^* \rightarrow 4l$, $gg \rightarrow ZZ \rightarrow 4l$)

Example use case

$$p_{ggF}(x|\mu) = \frac{1}{v_{ggF}(\mu)} \left[(\mu - \sqrt{\mu}) v_S p_S(x) + \sqrt{\mu} v_{SBI_1} p_{SBI_1}(x) + (1 - \sqrt{\mu}) v_B p_B(x) \right]$$

Search-Oriented Mixture Model

x_i is one individual event

General Formula

$$p(x_i|\mu) = \frac{1}{v(\mu)} \sum_j^C f_j(\mu) \cdot v_j p_j(x_i) \quad ? \quad \longrightarrow \quad \frac{p(x_i|\mu)}{p_{\text{ref}}(x_i)} = \frac{1}{v(\mu)} \sum_j^C f_j(\mu) \cdot v_j \frac{p_j(x_i)}{p_{\text{ref}}(x_i)}$$

Event rates estimated from simulations

Reference hypothesis j runs over different physics process
(Eg. $gg \rightarrow H^* \rightarrow 4l, gg \rightarrow ZZ \rightarrow 4l$)

Comes from theory model chosen to interpret data

Example use case

$$p_{\text{ggF}}(x|\mu) = \frac{1}{v_{\text{ggF}}(\mu)} \left[(\mu - \sqrt{\mu}) v_S p_S(x) + \sqrt{\mu} v_{\text{SBI}_1} p_{\text{SBI}_1}(x) + (1 - \sqrt{\mu}) v_B p_B(x) \right]$$

Search-Oriented Mixture Model

x_i is one individual event

General Formula

$$p(x_i|\mu) = \frac{1}{\nu(\mu)} \sum_j^C f_j(\mu) \cdot \nu_j p_j(x_i) \quad ?$$

$\frac{p(x_i|\mu)}{p_{\text{ref}}(x_i)} = \frac{1}{\nu(\mu)} \sum_j^C f_j(\mu) \cdot \nu_j \frac{p_j(x_i)}{p_{\text{ref}}(x_i)}$

Event rates estimated from simulations Reference hypothesis j runs over different physics process
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Comes from theory model chosen to interpret data

Example use case

$$p_{\text{ggF}}(x|\mu) = \frac{1}{\nu_{\text{ggF}}(\mu)} \left[(\mu - \sqrt{\mu}) \nu_S p_S(x) + \sqrt{\mu} \nu_{\text{SBI}_1} p_{\text{SBI}_1}(x) + (1 - \sqrt{\mu}) \nu_B p_B(x) \right]$$

$$\rightarrow \frac{p(x|\mu)}{p_S(x)} = \frac{1}{\nu(\mu)} \left[(\mu - \sqrt{\mu}) \nu_S + \sqrt{\mu} \nu_{\text{SBI}_1} \frac{p_{\text{SBI}_1}(x)}{p_S(x)} + (1 - \sqrt{\mu}) \nu_B \frac{p_B(x)}{p_S(x)} \right]$$

Search-Oriented Mixture Model

x_i is one individual event

General Formula

$$p(x_i|\mu) = \frac{1}{\nu(\mu)} \sum_j^C f_j(\mu) \cdot \nu_j p_j(x_i) \quad ? \quad \xrightarrow{\text{Estimated using an ensemble of networks}} \quad \frac{p(x_i|\mu)}{p_{\text{ref}}(x_i)} = \frac{1}{\nu(\mu)} \sum_j^C f_j(\mu) \cdot \nu_j \frac{p_j(x_i)}{p_{\text{ref}}(x_i)}$$

Event rates estimated from simulations

Reference hypothesis

j runs over different physics process
(Eg. $gg \rightarrow H^* \rightarrow 4l, gg \rightarrow ZZ \rightarrow 4l$)

Comes from theory model chosen to interpret data

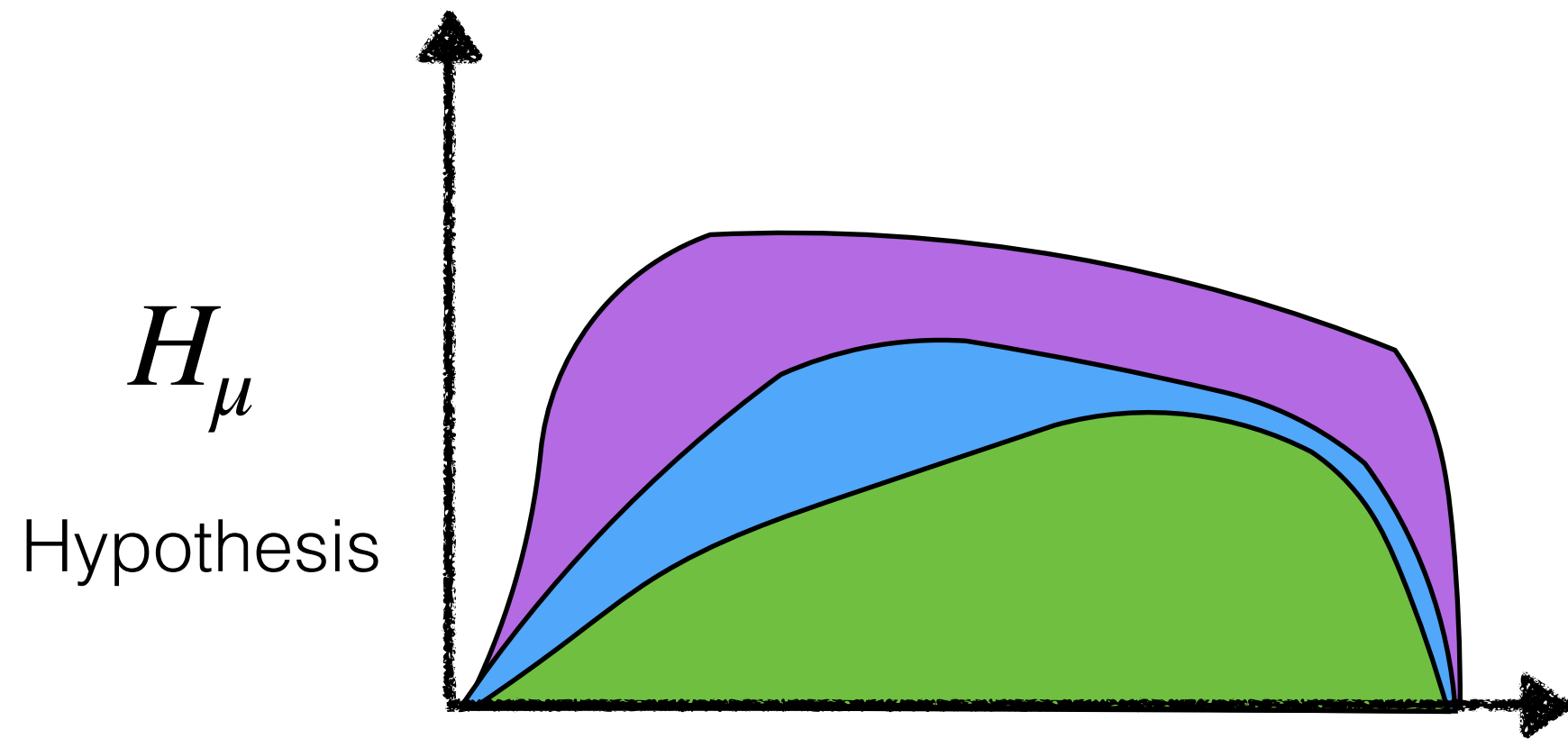
Example use case

$$p_{\text{ggF}}(x|\mu) = \frac{1}{\nu_{\text{ggF}}(\mu)} \left[(\mu - \sqrt{\mu}) \nu_S p_S(x) + \sqrt{\mu} \nu_{\text{SBI}_1} p_{\text{SBI}_1}(x) + (1 - \sqrt{\mu}) \nu_B p_B(x) \right]$$

$$\xrightarrow{\text{Reference hypothesis}} \quad \frac{p(x|\mu)}{p_S(x)} = \frac{1}{\nu(\mu)} \left[(\mu - \sqrt{\mu}) \nu_S + \sqrt{\mu} \nu_{\text{SBI}_1} \frac{p_{\text{SBI}_1}(x)}{p_S(x)} + (1 - \sqrt{\mu}) \nu_B \frac{p_B(x)}{p_S(x)} \right]$$

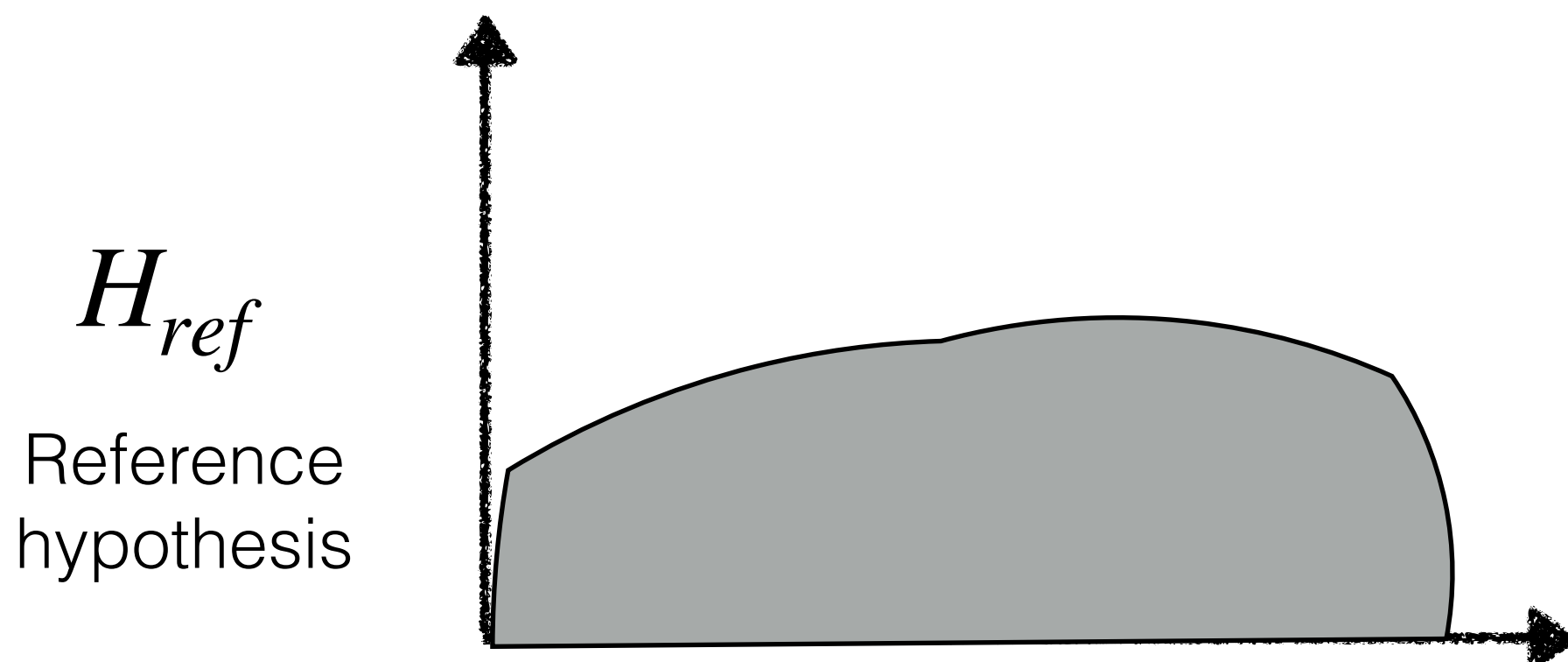
Robust, parameterised classifier without parameterising

H_{ref} : Reference hypothesis



$$\frac{p(x_i|\mu)}{p_{ref}(x_i)} = \frac{1}{v(\mu)} \sum_j^C f_j(\mu) \cdot v_j \frac{p_j(x_i)}{p_{ref}(x_i)}$$

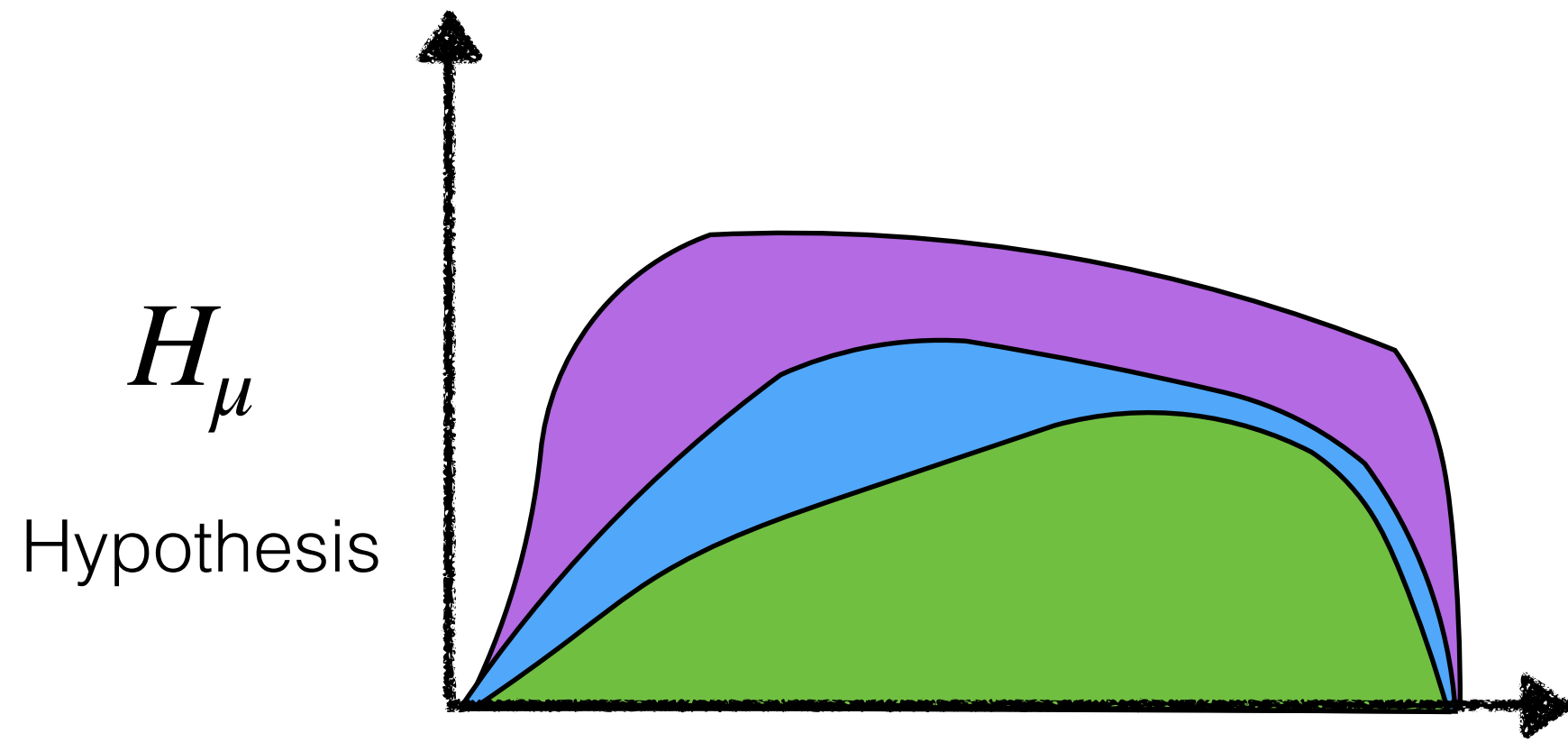
VS



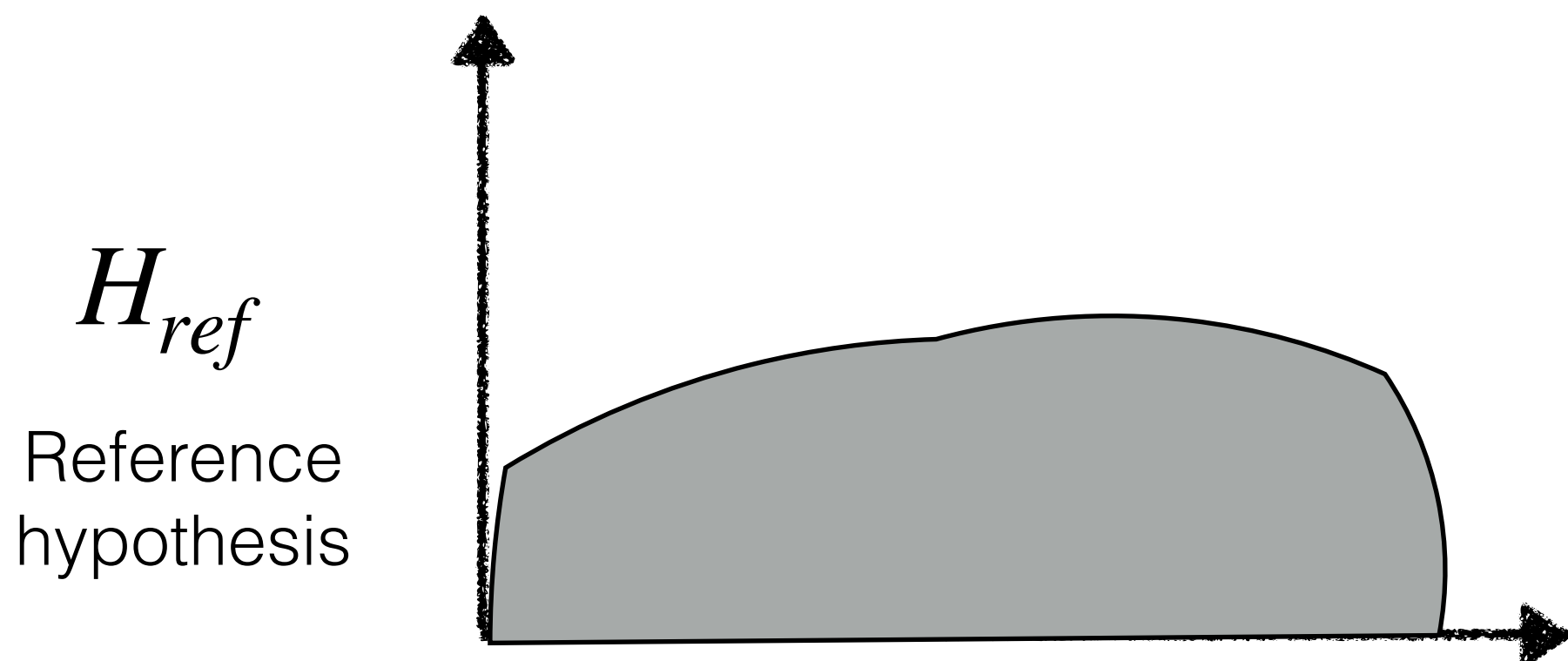
A separate classifier per physics process j
(Eg. $gg \rightarrow H^* \rightarrow 4l$, $gg \rightarrow ZZ \rightarrow 4l$)

Robust, parameterised classifier without parameterising

H_{ref} : Reference hypothesis



VS

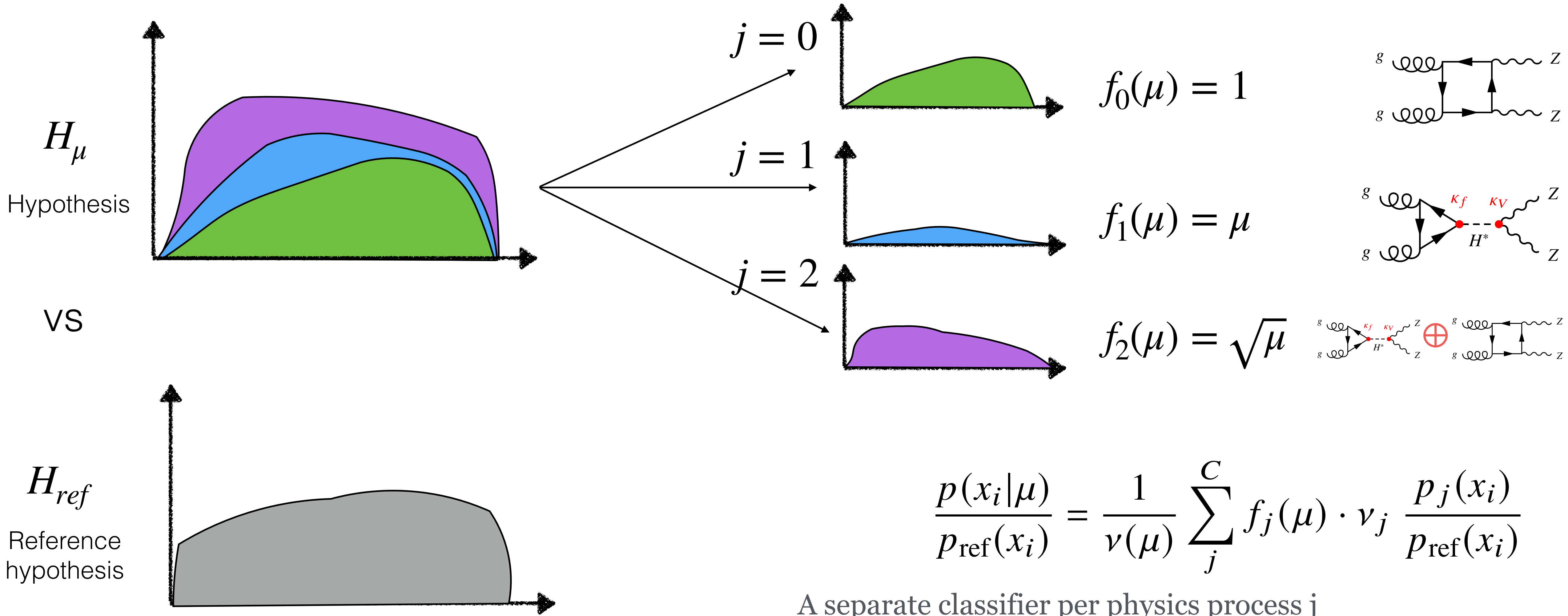


$$\frac{p(x_i|\mu)}{p_{ref}(x_i)} = \frac{1}{v(\mu)} \sum_j^C f_j(\mu) \cdot v_j \frac{p_j(x_i)}{p_{ref}(x_i)}$$

A separate classifier per physics process j
 (Eg. $gg \rightarrow H^* \rightarrow 4l, gg \rightarrow ZZ \rightarrow 4l$)

Robust, parameterised classifier without parameterising

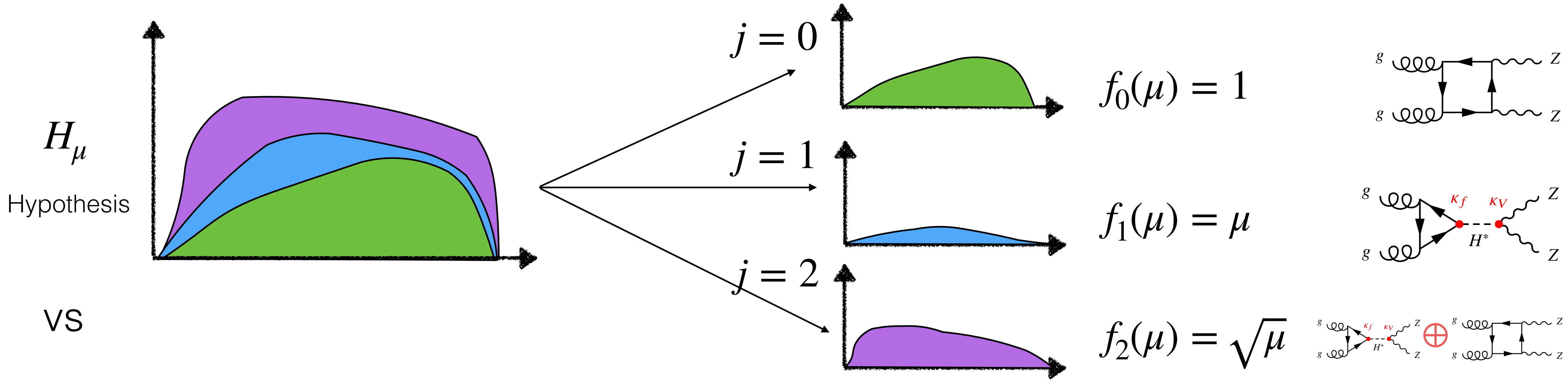
H_{ref} : Reference hypothesis



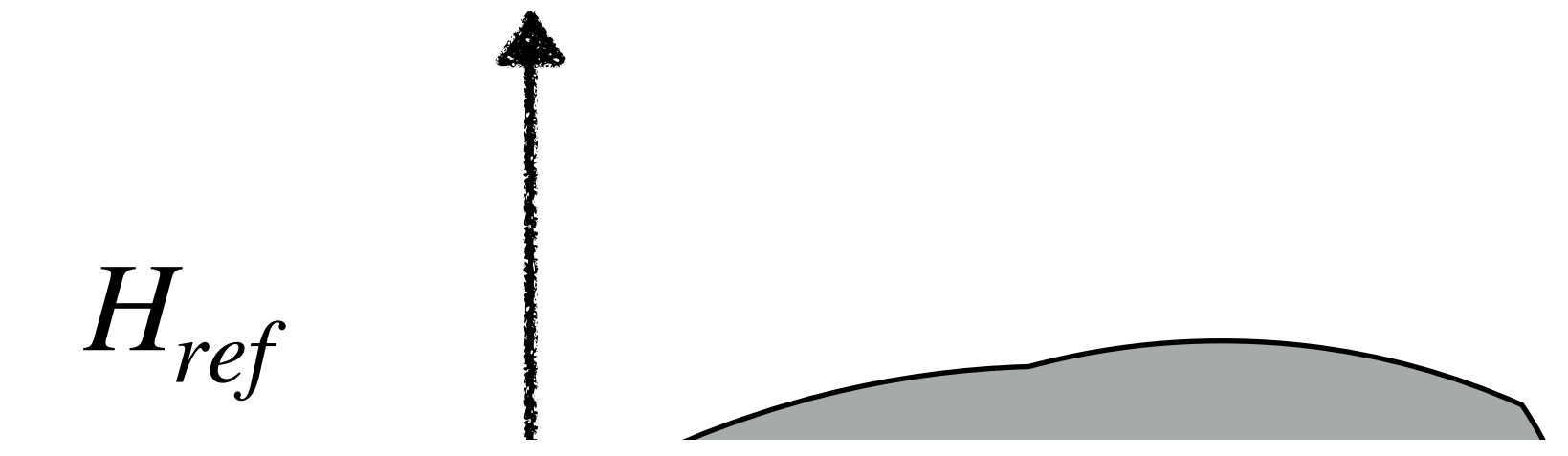
A separate classifier per physics process j
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Robust, parameterised classifier without parameterising

H_{ref} : Reference hypothesis



VS



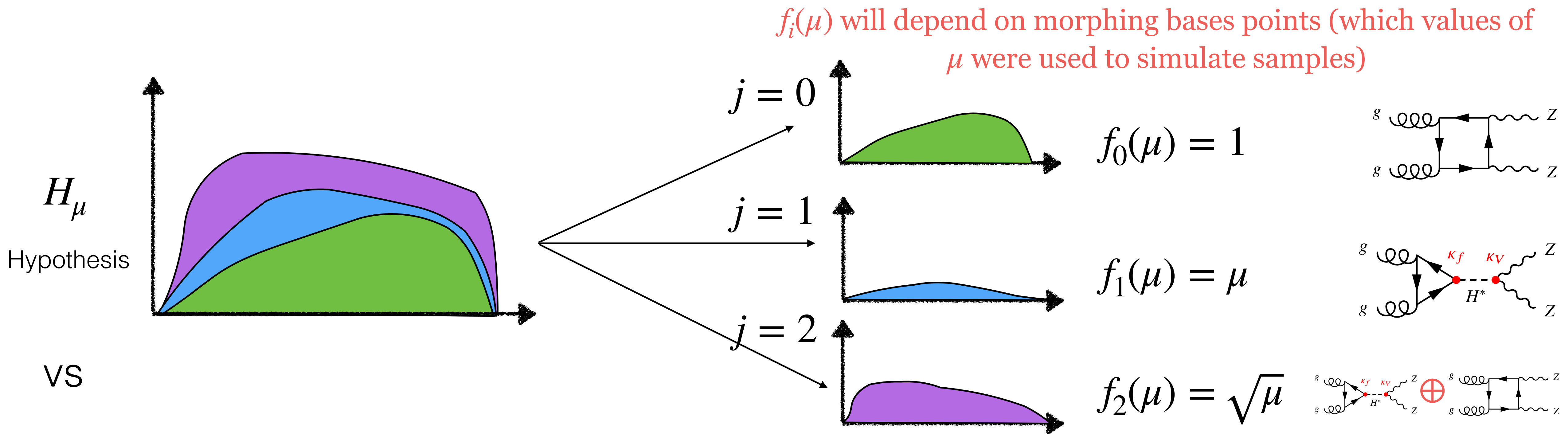
Analytically parameterised in μ , allows to get LR for any hypothesis μ without training parameterised networks!

$$\frac{p(x_i|\mu)}{p_{ref}(x_i)} = \frac{1}{v(\mu)} \sum_j^C f_j(\mu) \cdot v_j \frac{p_j(x_i)}{p_{ref}(x_i)}$$

A separate classifier per physics process j
(Eg. $gg \rightarrow H^* \rightarrow 4l, gg \rightarrow ZZ \rightarrow 4l$)

Robust, parameterised classifier without parameterising

H_{ref} : Reference hypothesis



F_h **Analytically parameterised in μ** , allows to get LR for any hypothesis μ without training parameterised networks !

$$\frac{p(x_i|\mu)}{p_{ref}(x_i)} = \frac{1}{v(\mu)} \sum_j^C f_j(\mu) \cdot v_j \frac{p_j(x_i)}{p_{ref}(x_i)}$$

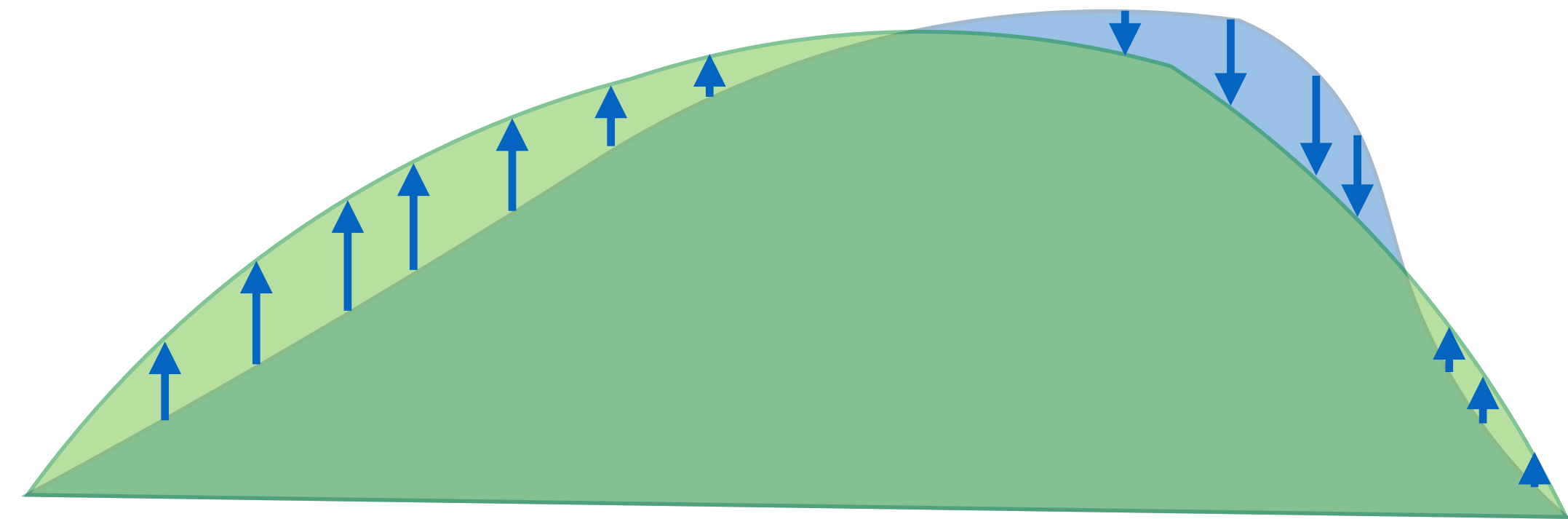
A separate classifier per physics process j
(Eg. $gg \rightarrow H^* \rightarrow 4l$, $gg \rightarrow ZZ \rightarrow 4l$)

Open problems to extend to full ATLAS analysis:

- **Robustness:** Design and validation
- **Systematic Uncertainties:** Incorporate them in likelihood (ratio) model
- **Neyman Construction:** Throwing toys in a per-event analysis


Validate quality of LR estimation with re-weighting task

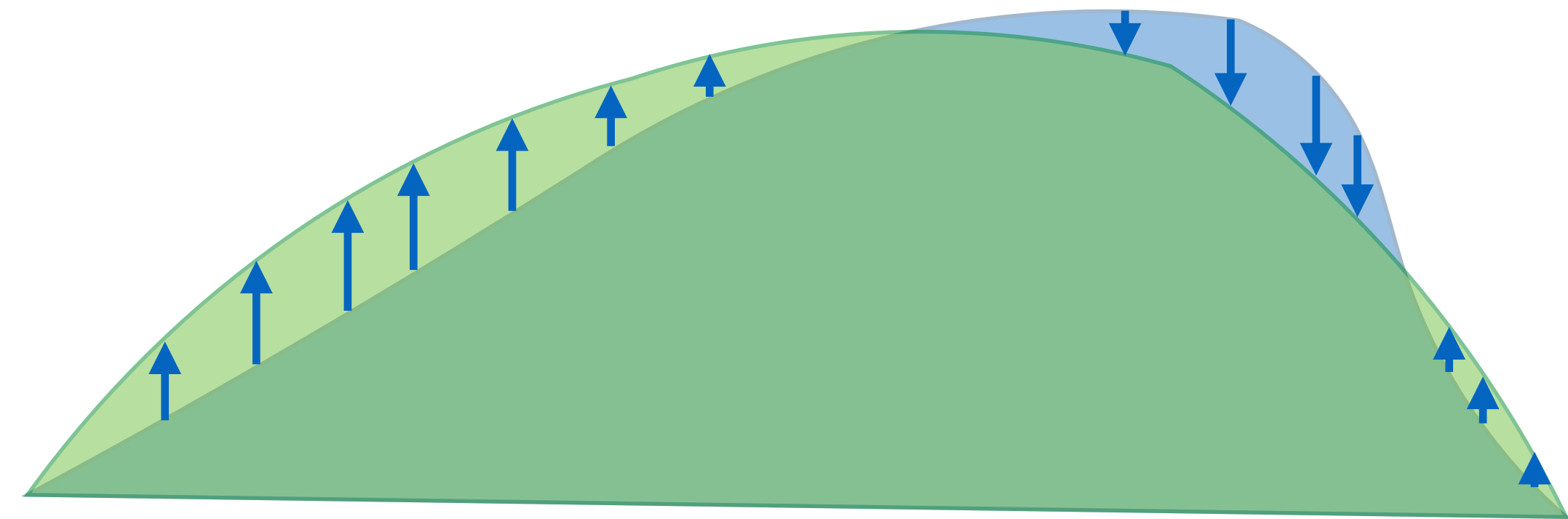
Reweighting: Calculate weights w_i for events x_i in **blue sample** to match **green sample**



Validate quality of LR estimation with re-weighting task

Reweighting: Calculate weights w_i for events x_i in **blue sample** to match **green sample**

$$w_i = r(x_i, \mu_0, \mu_1) = \frac{p(x_i | \mu_0)}{p(x_i | \mu_1)}$$




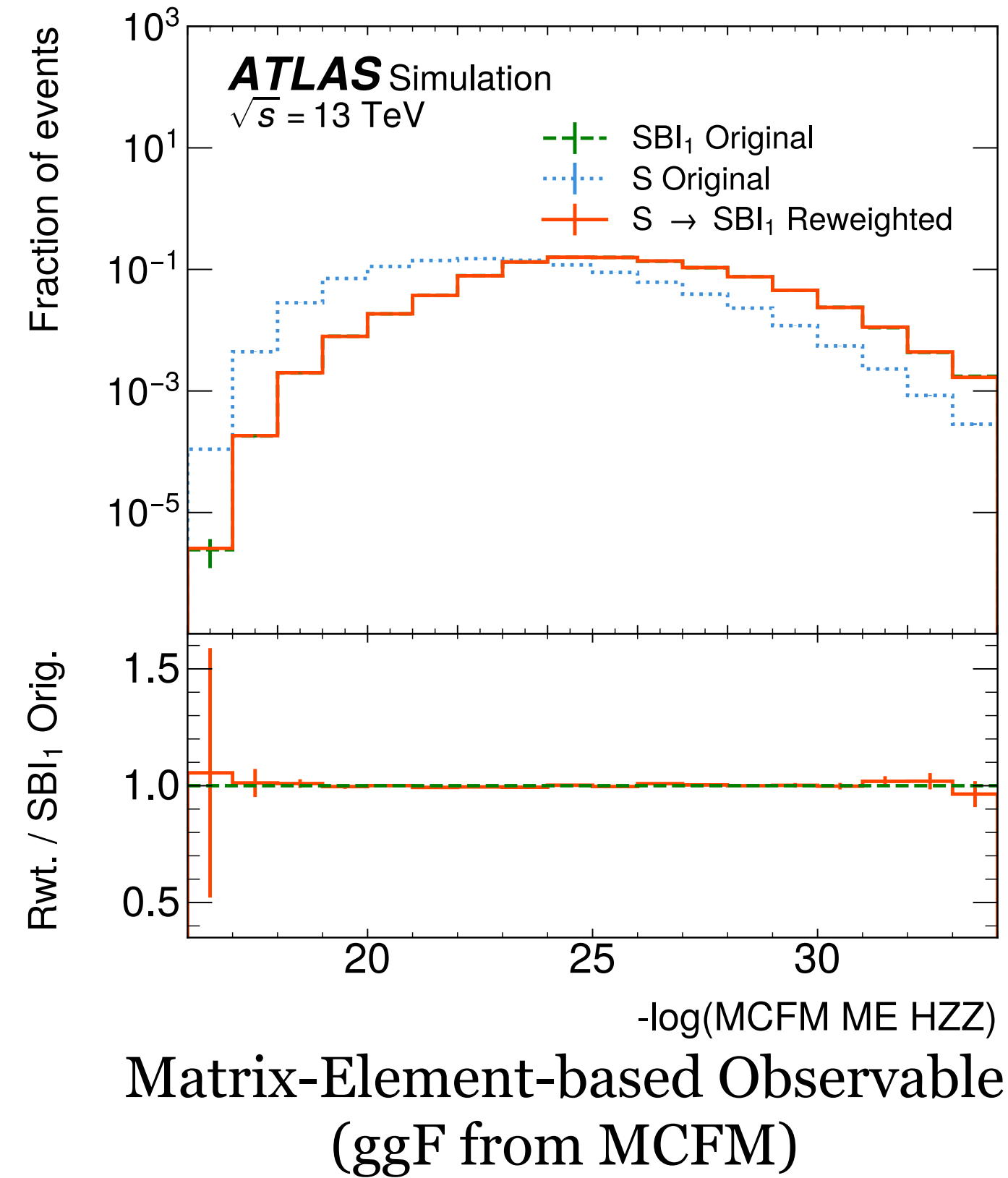
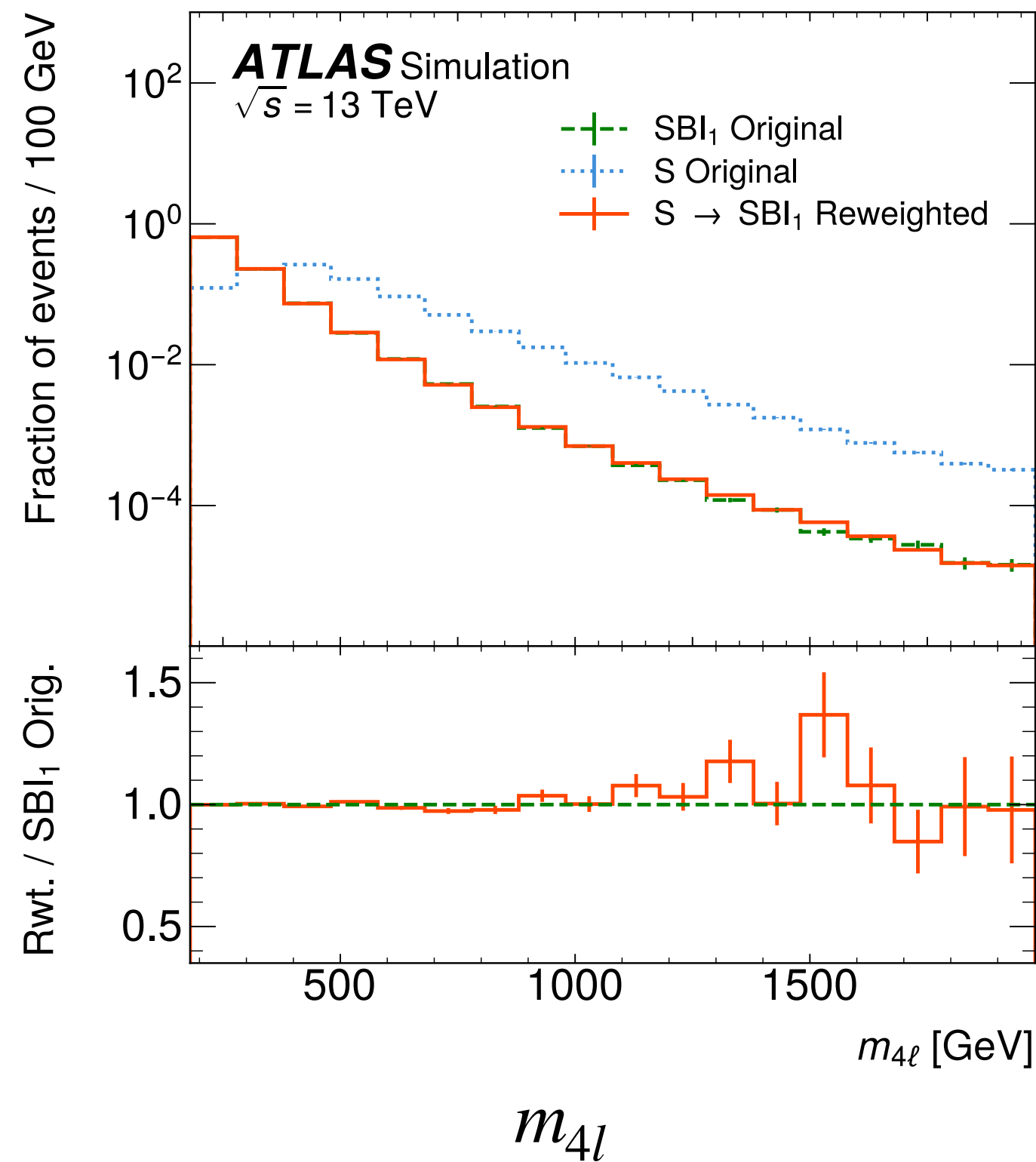
Already estimated using an ensemble of networks

Re-weight closures

Variable used in training

Source
Target
RW

High-level variable
never used in training



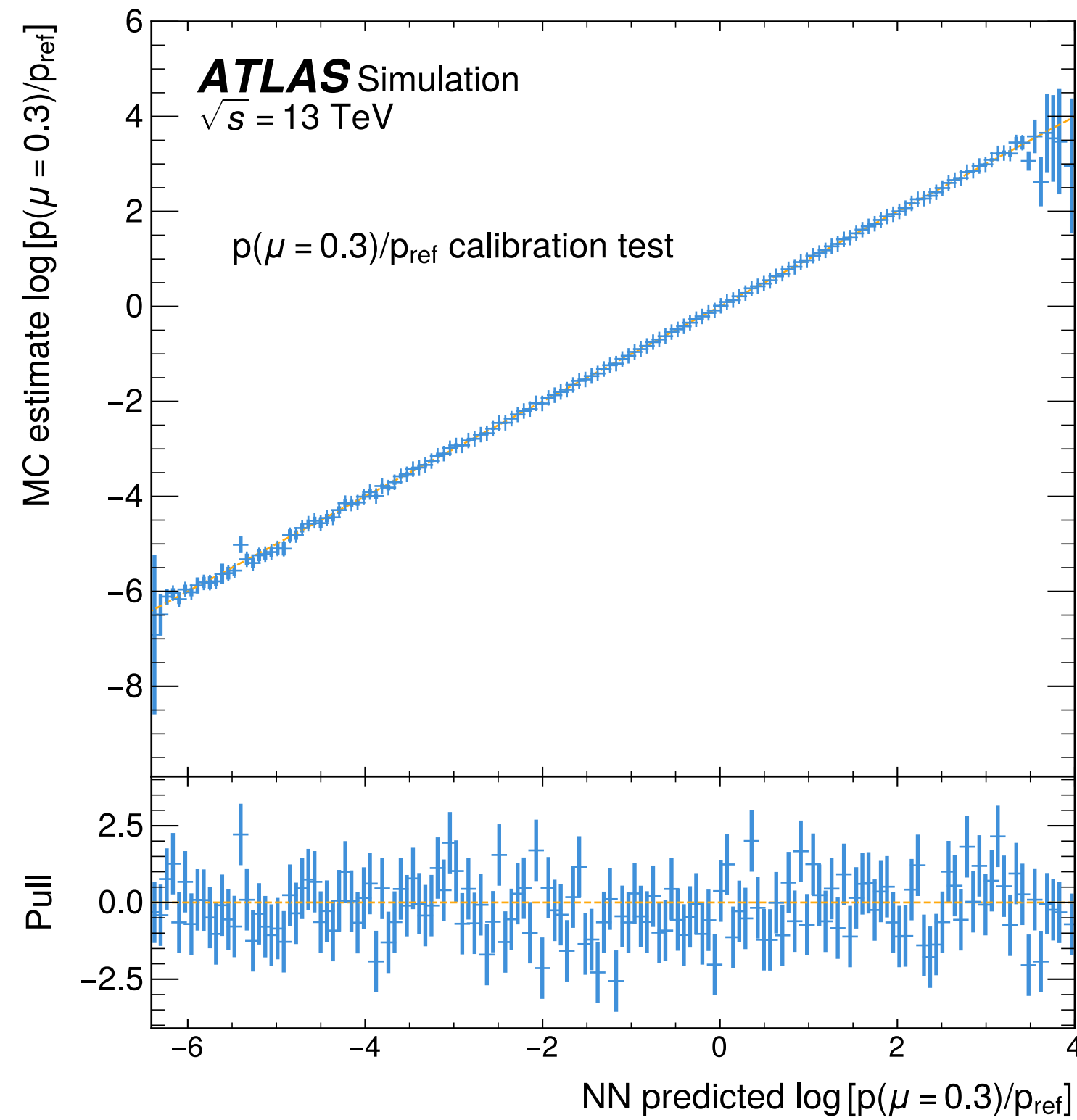
High-Dim Classifier Test:
Train independent classifier on RW vs Target,
AUC=0.5 \Rightarrow LRs well estimated

Calibration curves of probability density ratios

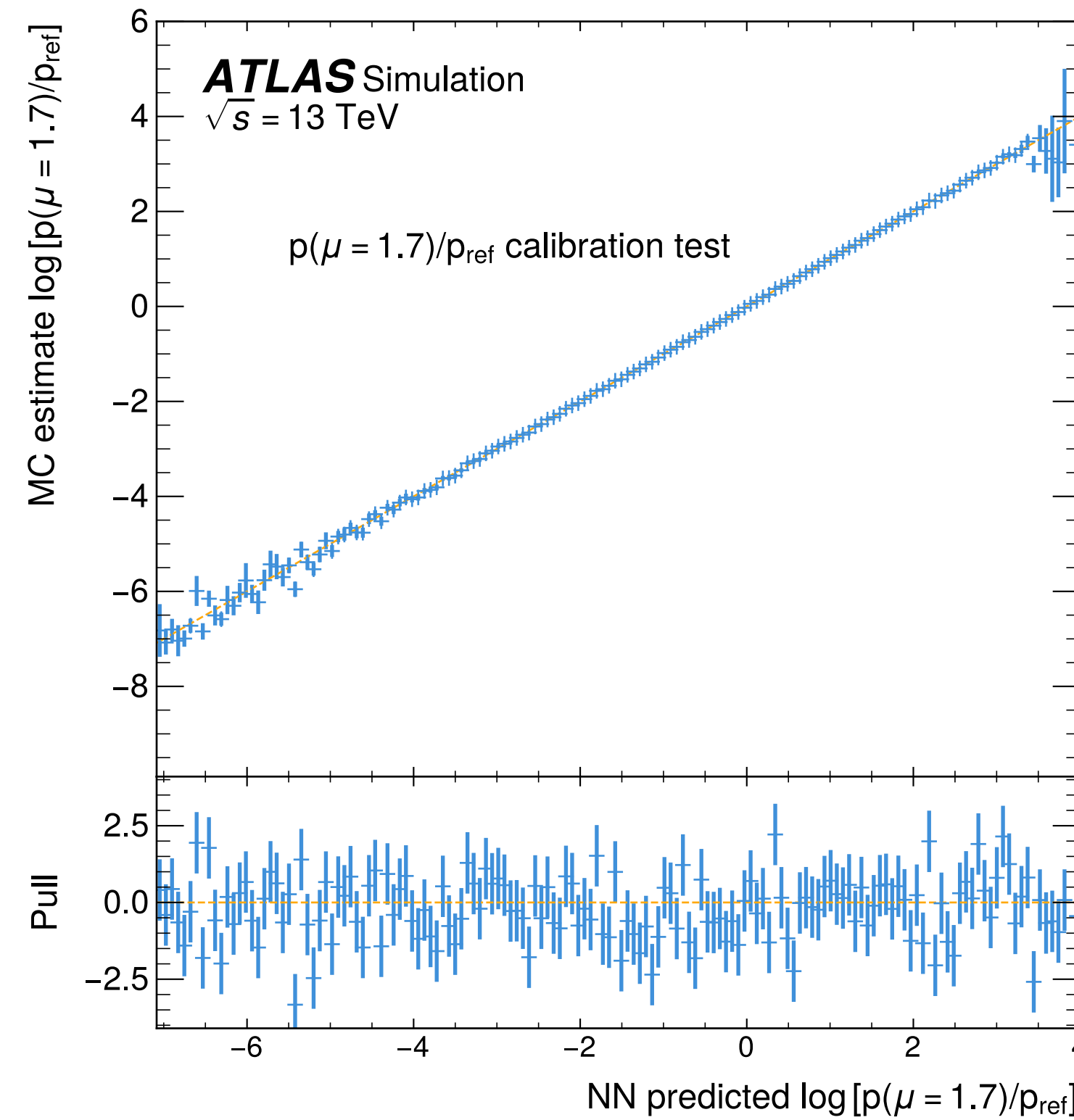
$$\frac{P_{\mu=0.3}(x_i)}{P_{ref}(x_i)}$$

$$\frac{P_{\mu=1.7}(x_i)}{P_{ref}(x_i)}$$

Binned estimate

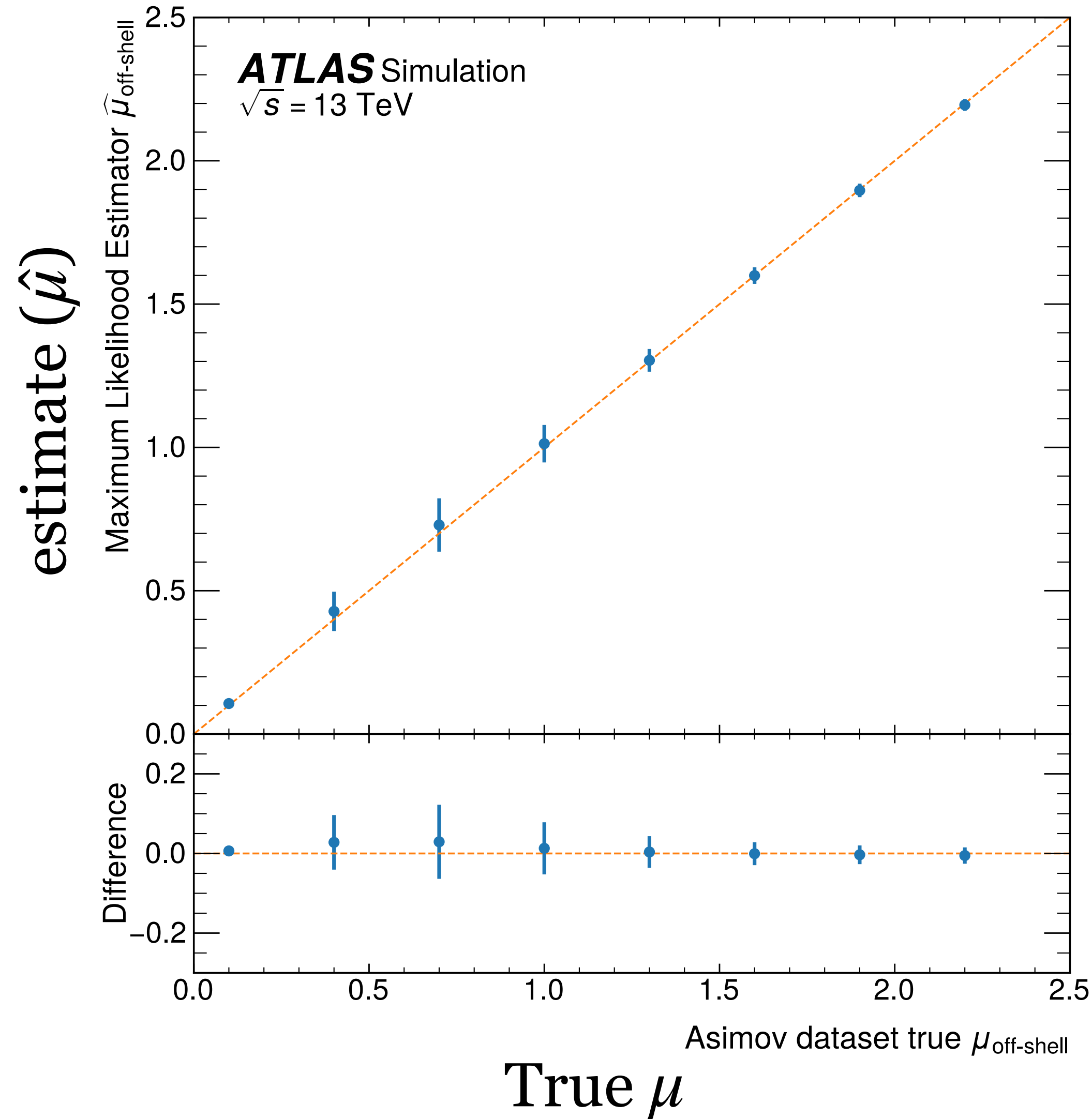


Ensemble prediction



Ensemble prediction

Perfect calibration would give $y = x$

Testing full analysis on samples from different values of μ Maximum likelihood estimate ($\hat{\mu}$)No bias: Method recovers correct value of μ on average

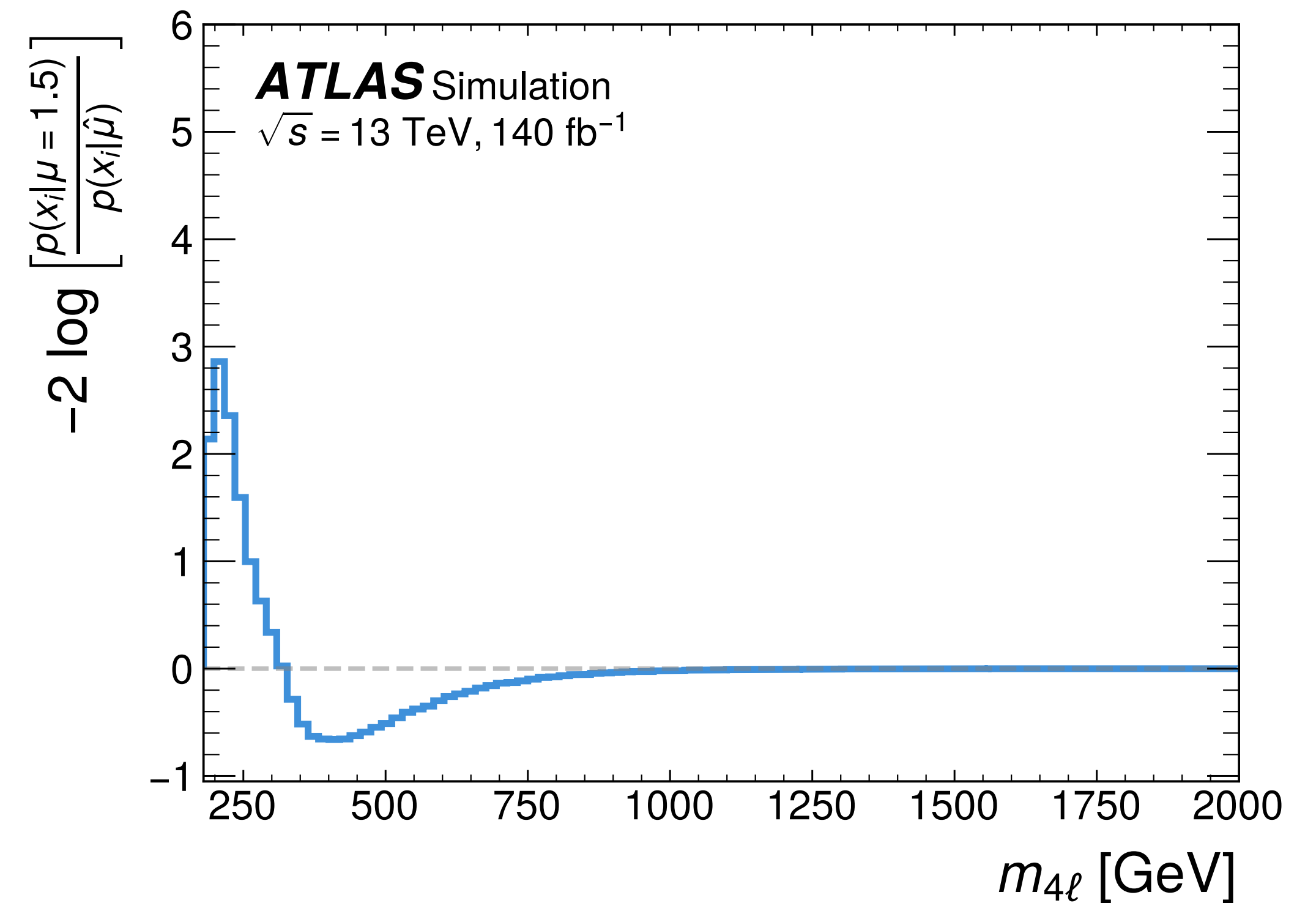
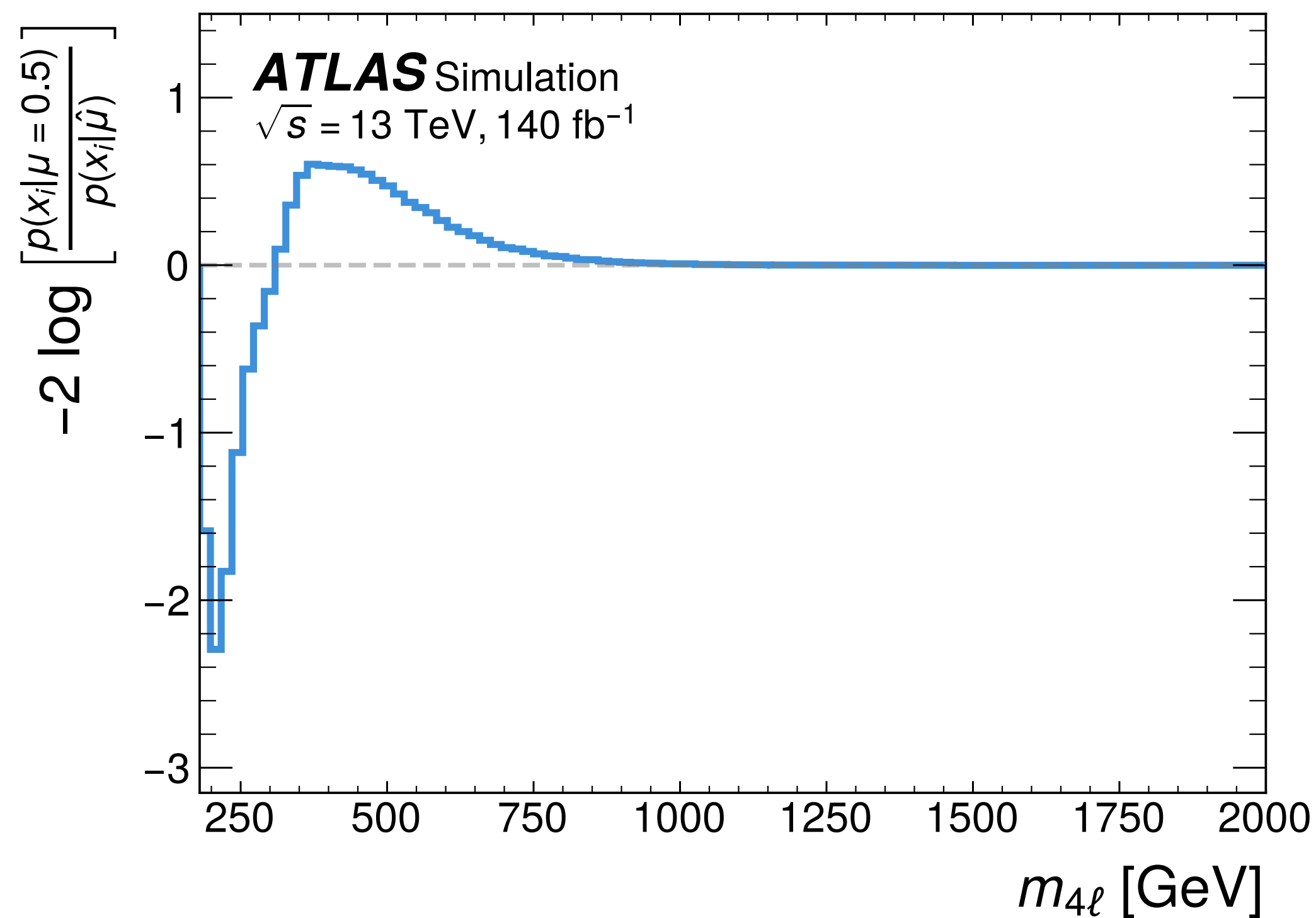
(Correct value when tested on the median 'Asimov dataset')

And many more diagnostics (see [backup](#))

Interpretability: Which phase space favours one hypothesis over another?

$$-2 \cdot \log \frac{P(x_i | \mu = 0.5)}{P(x_i | \mu = 1)}$$

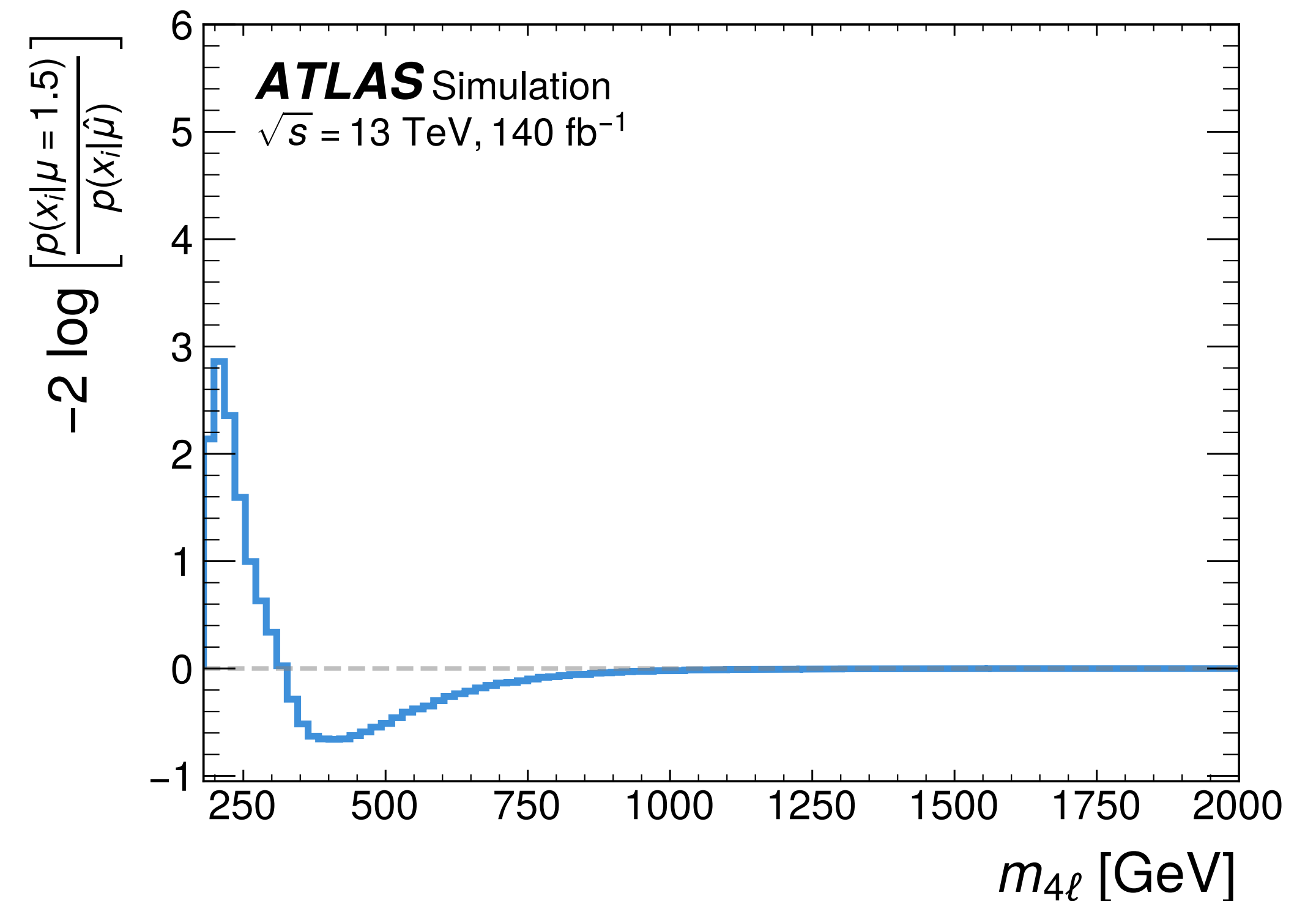
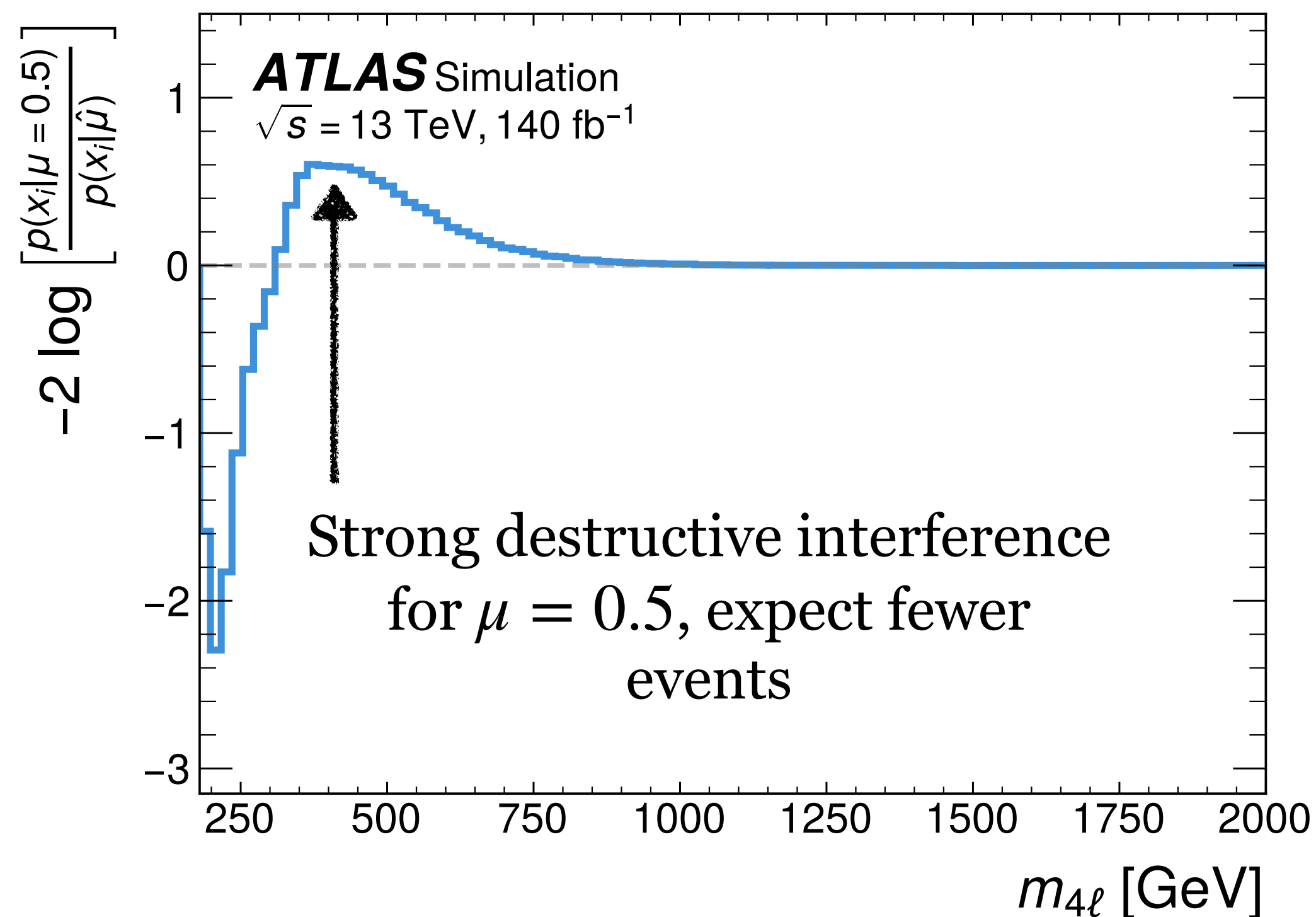
$$-2 \cdot \log \frac{P(x_i | \mu = 1.5)}{P(x_i | \mu = 1)}$$



Interpretability: Which phase space favours one hypothesis over another?

$$-2 \cdot \log \frac{P(x_i | \mu = 0.5)}{P(x_i | \mu = 1)}$$

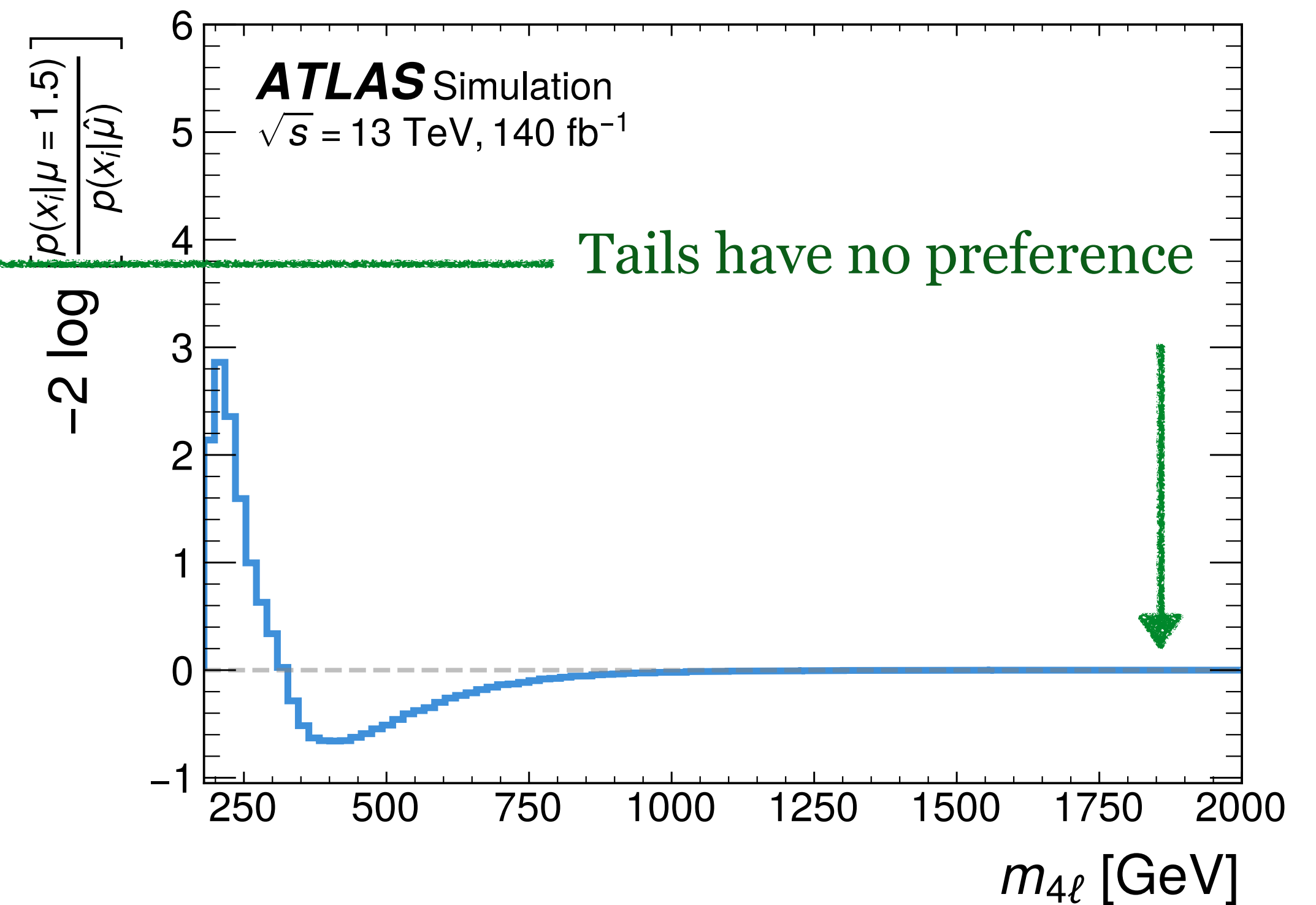
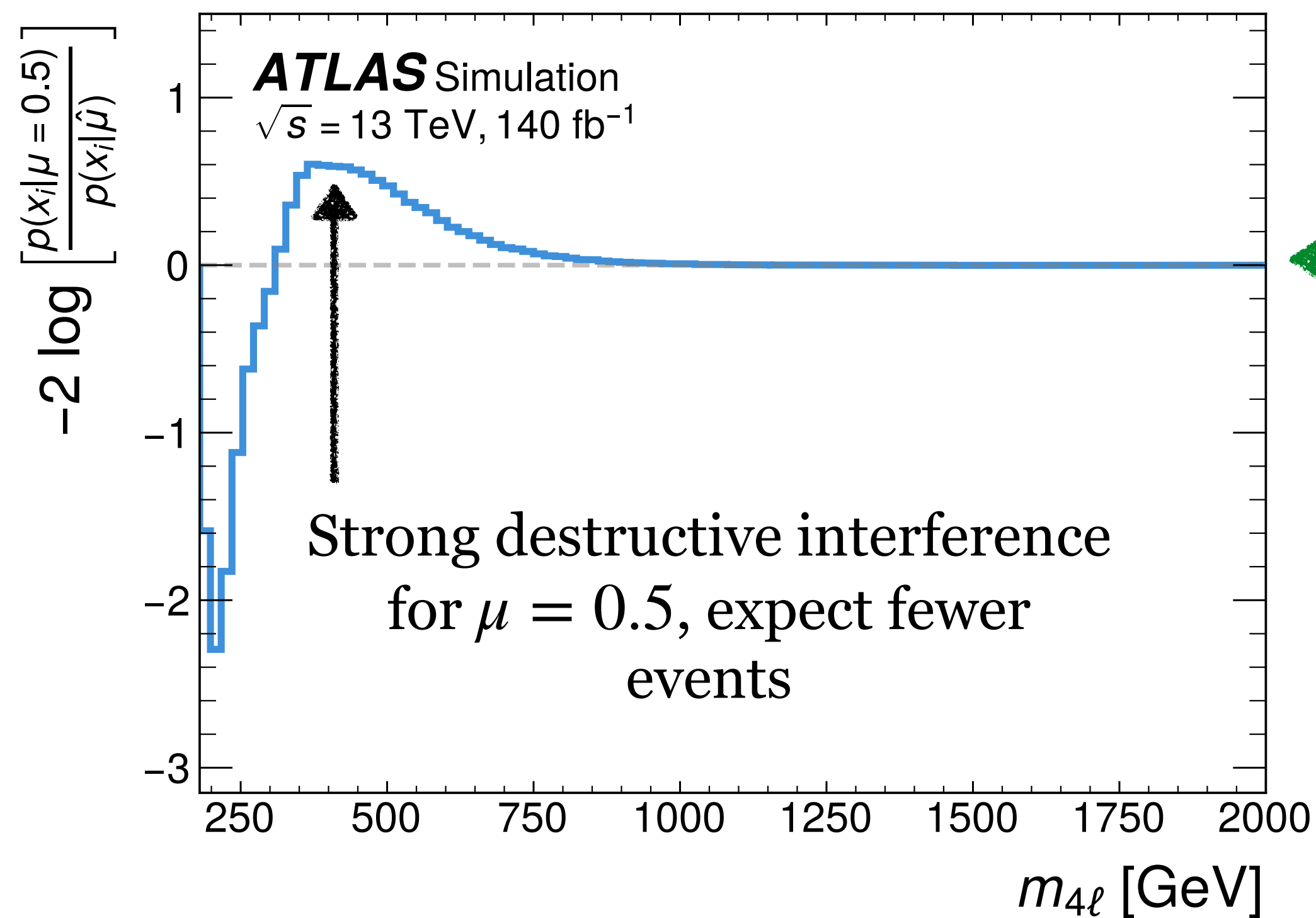
$$-2 \cdot \log \frac{P(x_i | \mu = 1.5)}{P(x_i | \mu = 1)}$$



Interpretability: Which phase space favours one hypothesis over another?

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$$-2 \cdot \log \frac{P(x_i | \mu = 1.5)}{P(x_i | \mu = 1)}$$



Open problems to extend to full ATLAS analysis:

- ✓ Robustness: Design and validation
- ▶ **Systematic Uncertainties: Incorporate them in likelihood (ratio) model**
- Neyman Construction: Throwing toys in a per-event analysis

Systematic uncertainties

Experimental uncertainties:

Eg. Inaccuracies in the calibration of our detector

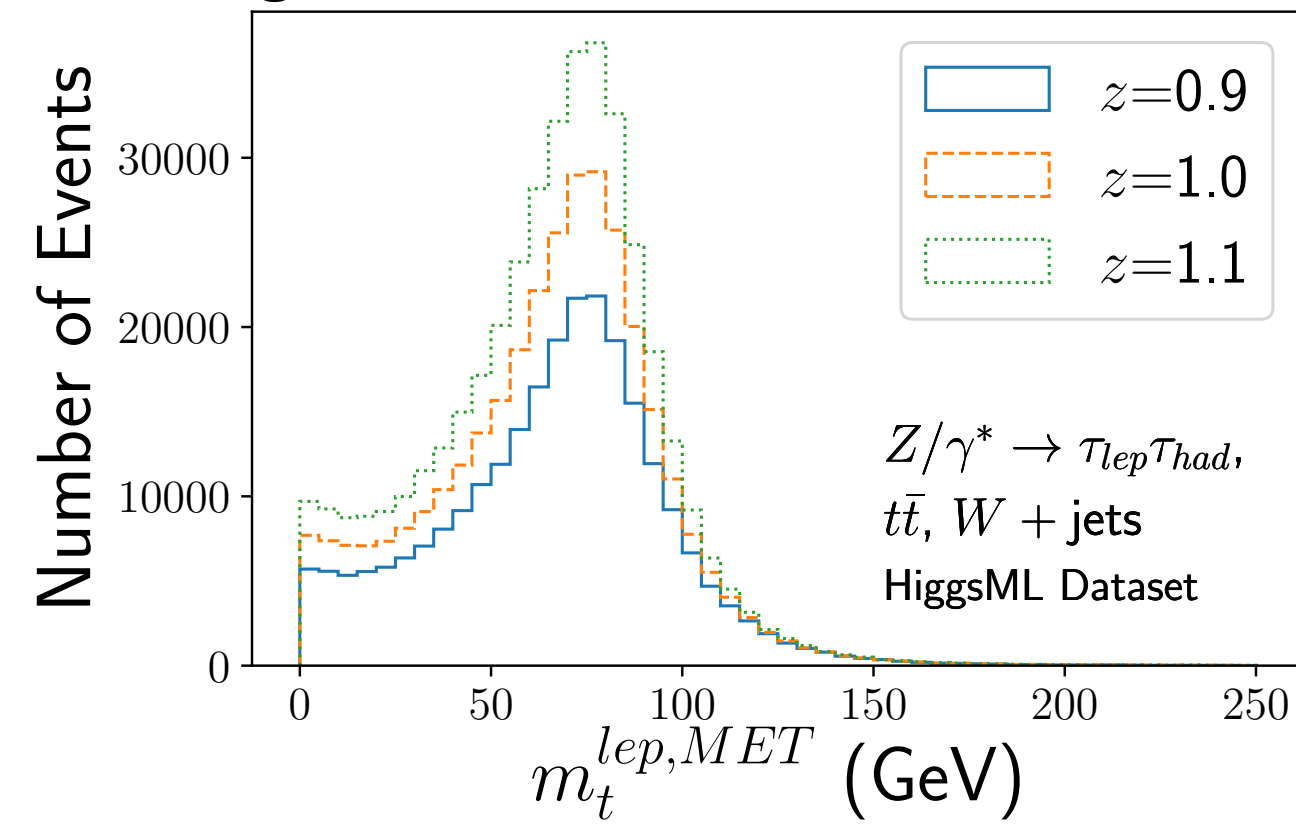


Image: arXiv:2105.08742

Theory uncertainties:

Eg. Inability to compute QFT to infinite order

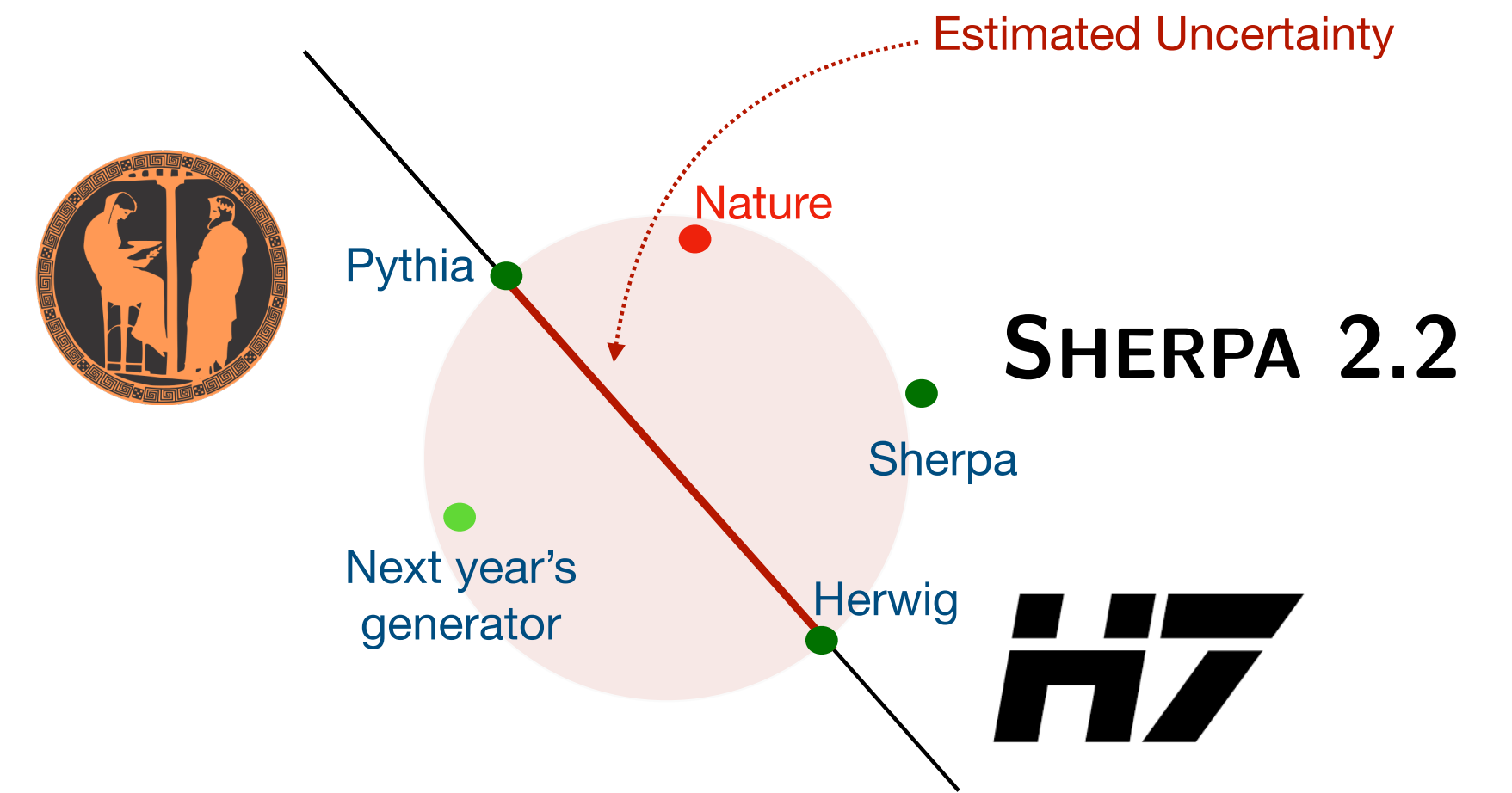


Image: arXiv:2109.08159

Systematic uncertainties

Experimental uncertainties:

Eg. Inaccuracies in the calibration of our detector

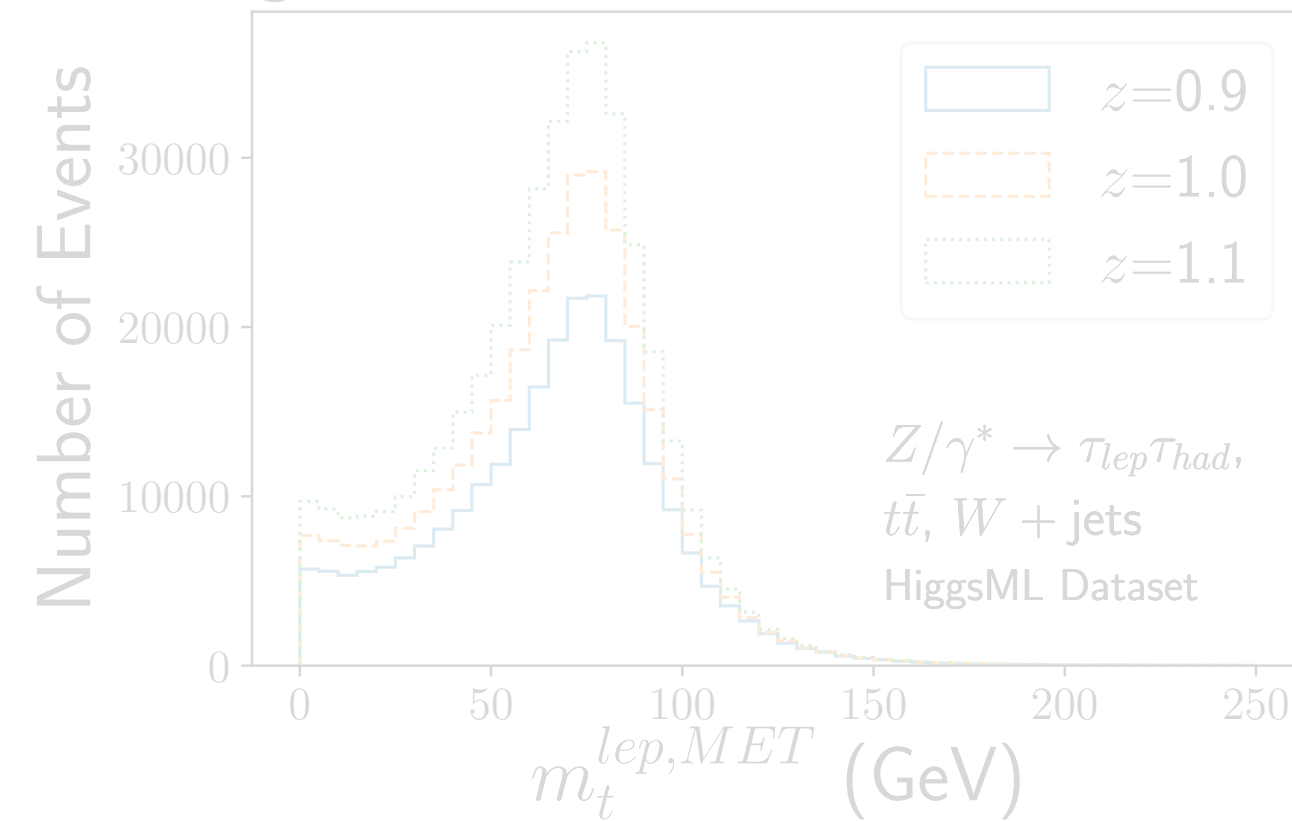


Image: arXiv:2105.08742

Theory uncertainties:

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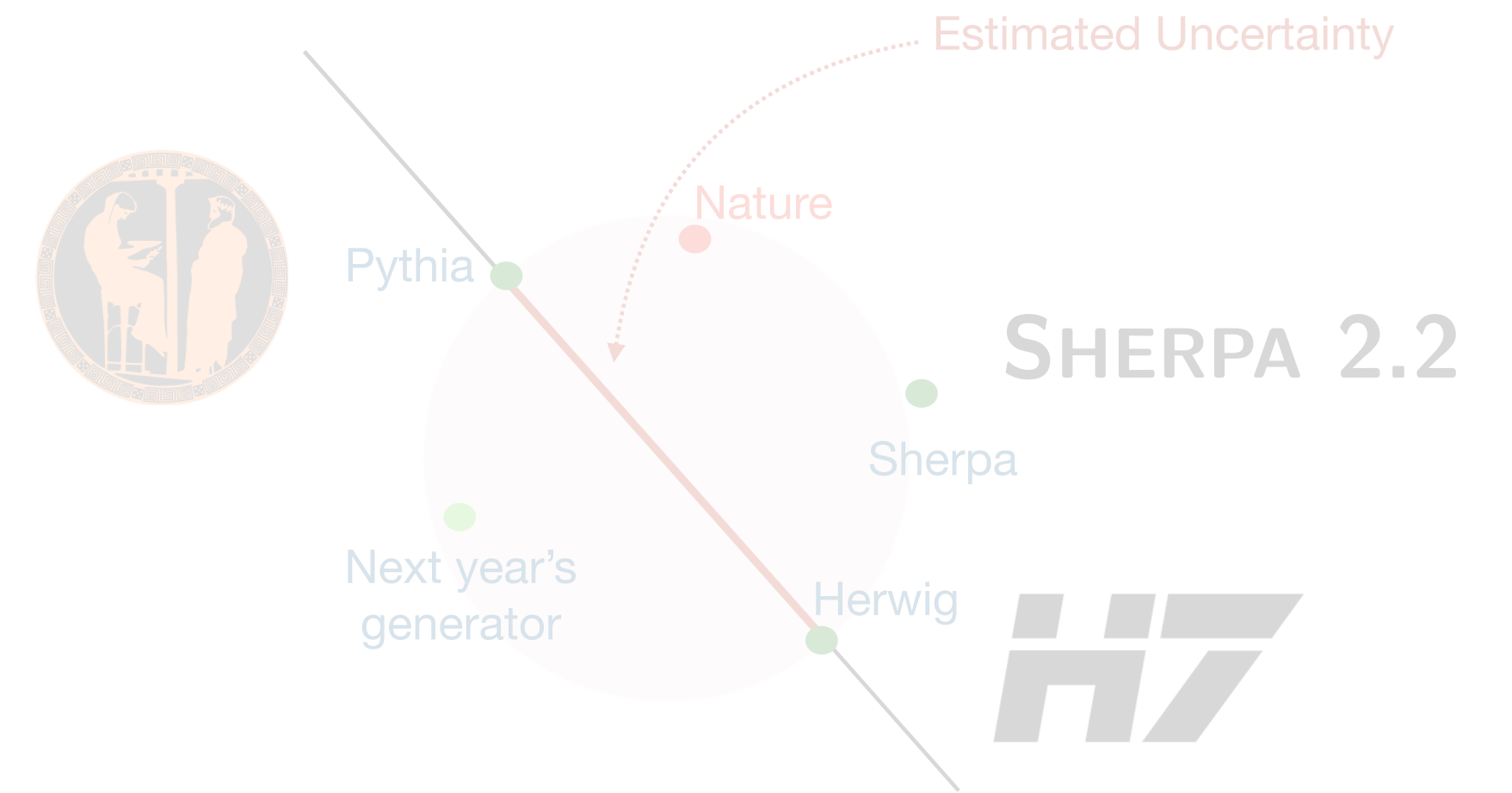
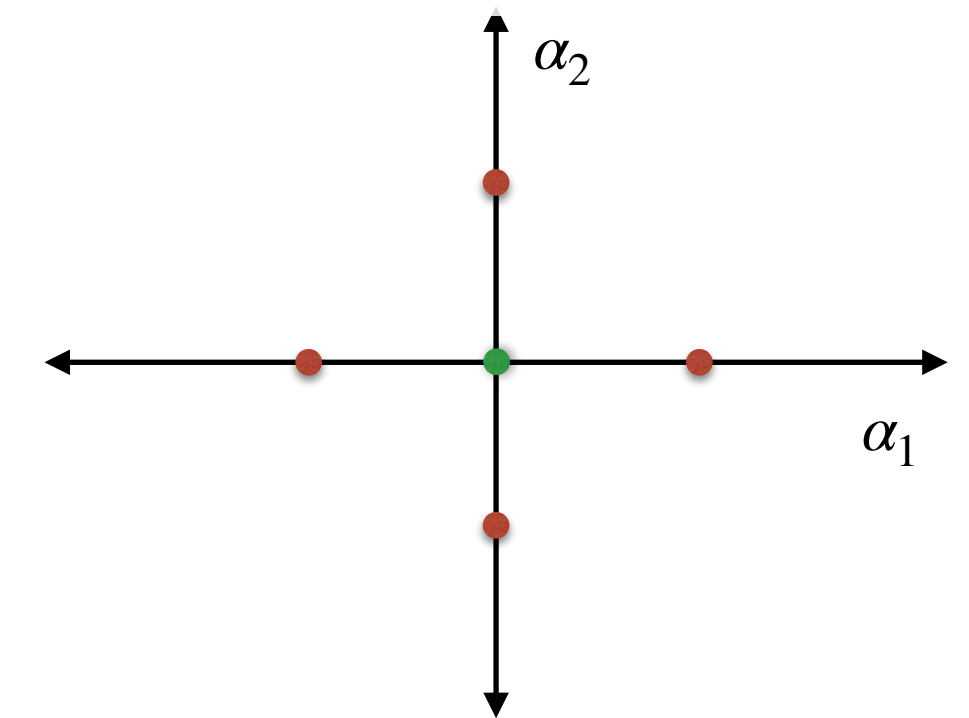


Image: arXiv:2109.08159

- We only have simulations at 3 variations of each nuisance parameter α_k



Known interpolation strategies

See formula used in [backup](#)

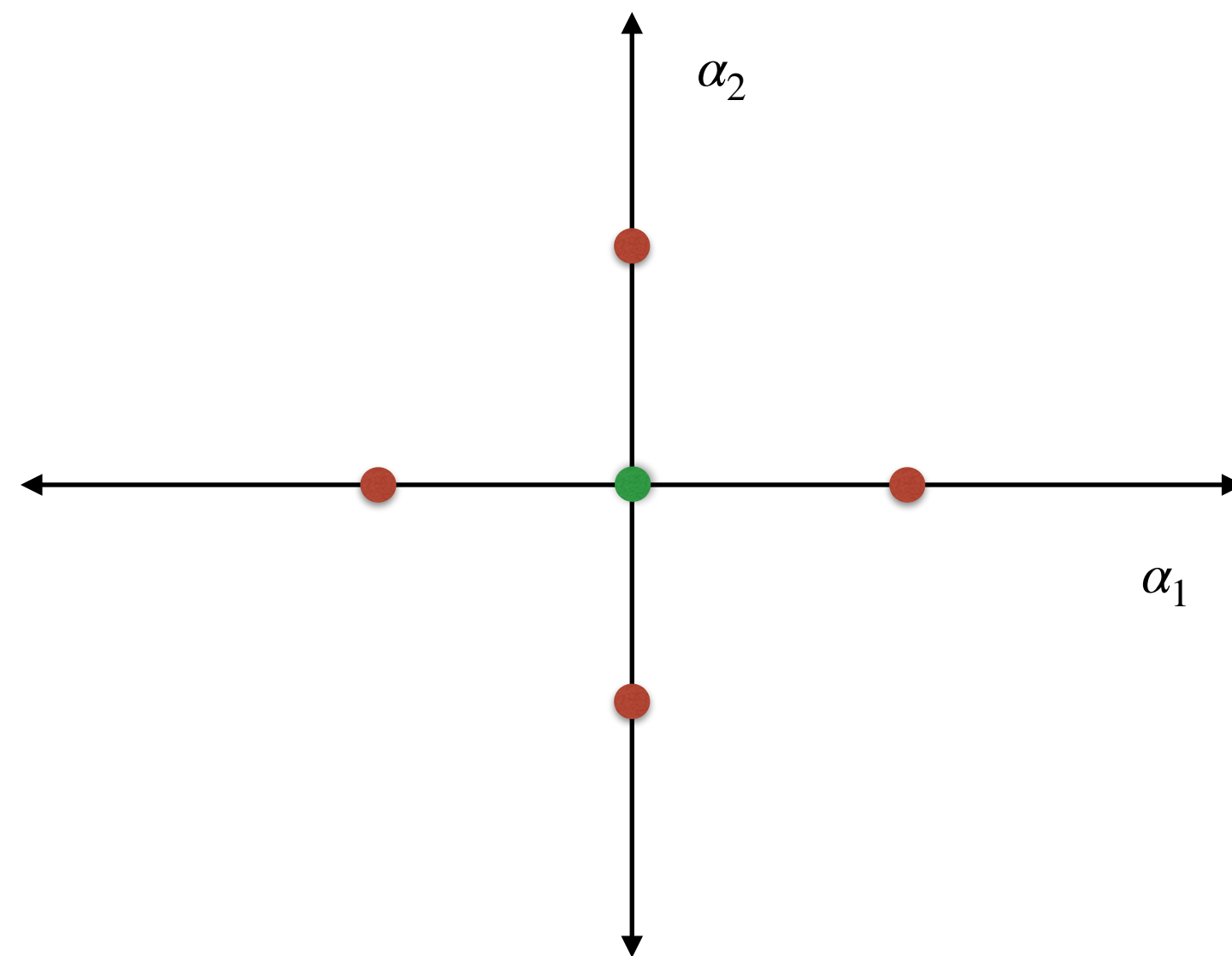
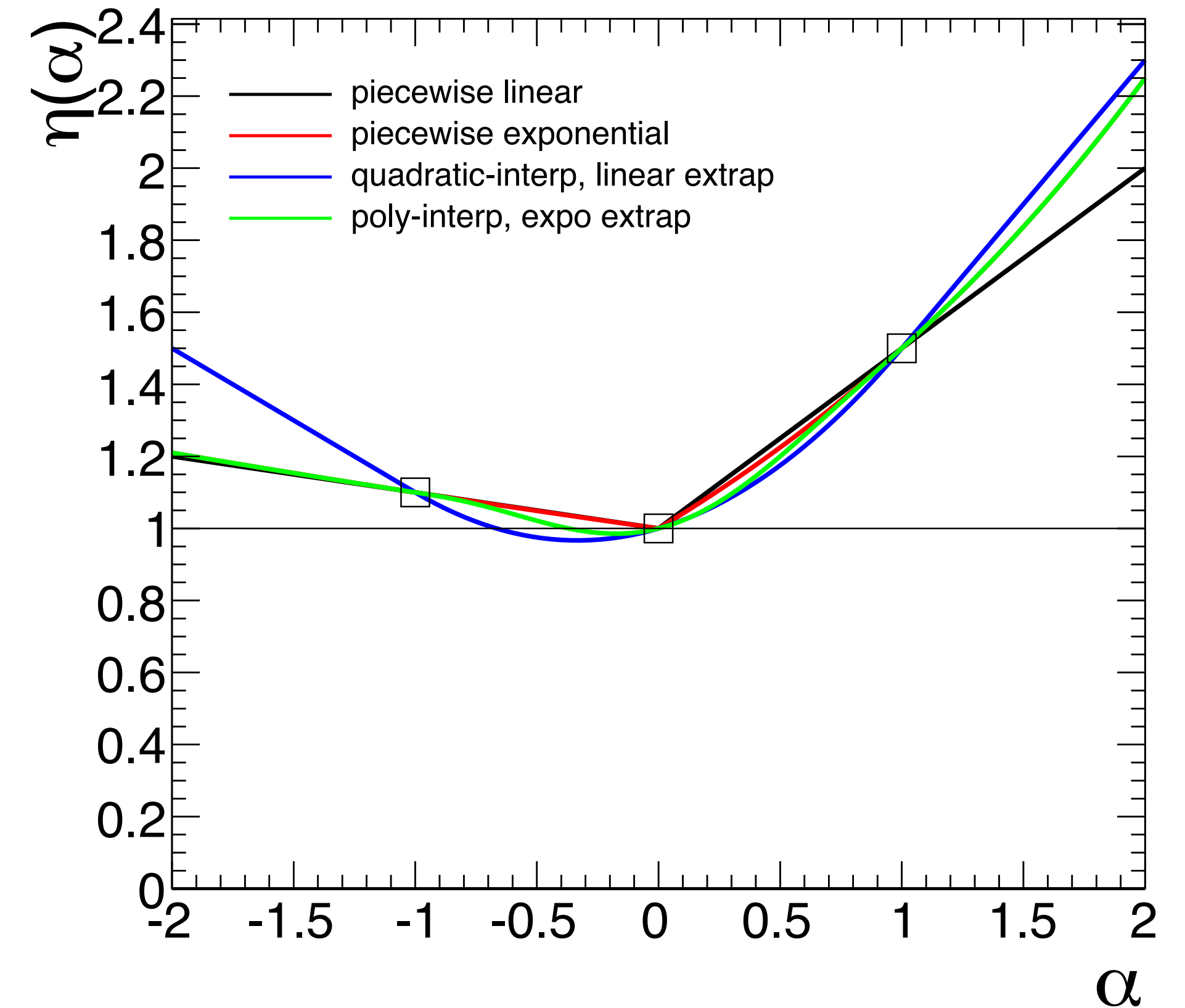


Image: arXiv:1503.07622

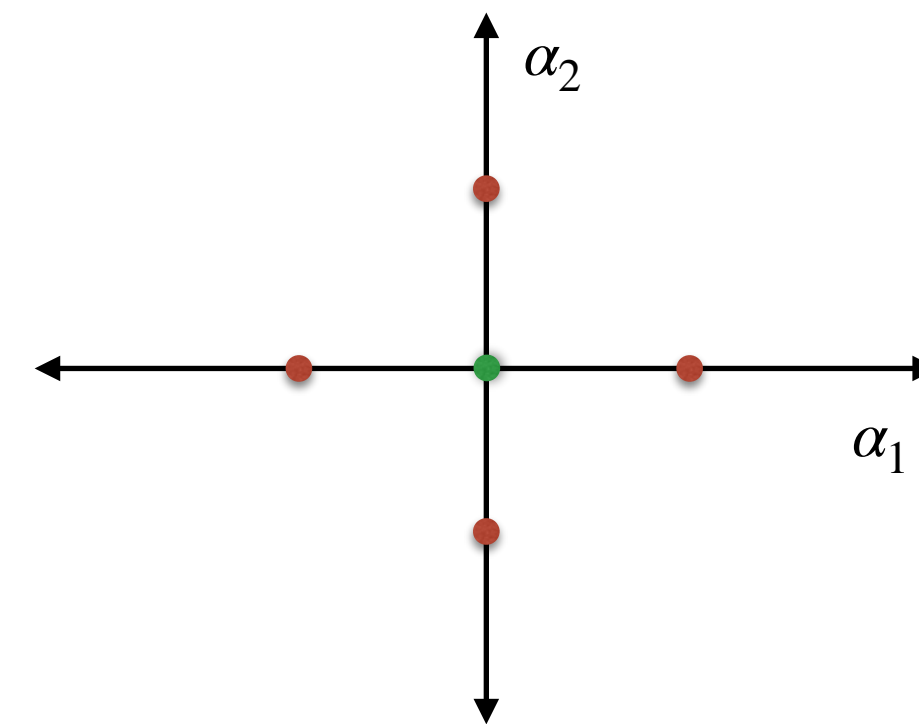


⇒ Combine these traditional interpolation with neural network estimation of per-event likelihood ratios

Probability density ratio including nuisance parameters (α)

x_i is one individual event

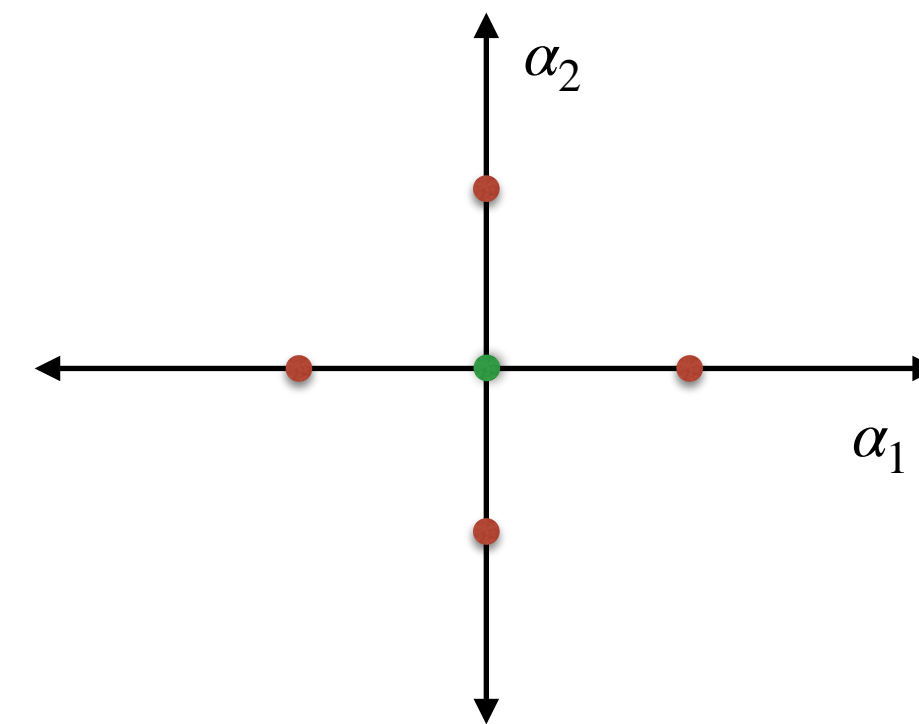
$$\frac{p(x_i | \mu, \alpha)}{p_{ref}(x_i)} =$$



Probability density ratio including nuisance parameters (α)

x_i is one individual event

$$\frac{p(x_i | \mu, \alpha)}{p_{ref}(x_i)} = \frac{1}{\nu(\mu, \alpha)} \sum_j^C f_j(\mu) \cdot \nu_j \cdot \frac{p_j(x_i)}{p_{ref}(x_i)} \cdot \prod_k^{N_{syst}} G_j(\alpha_k) \cdot g_j(x_i, \alpha_k)$$



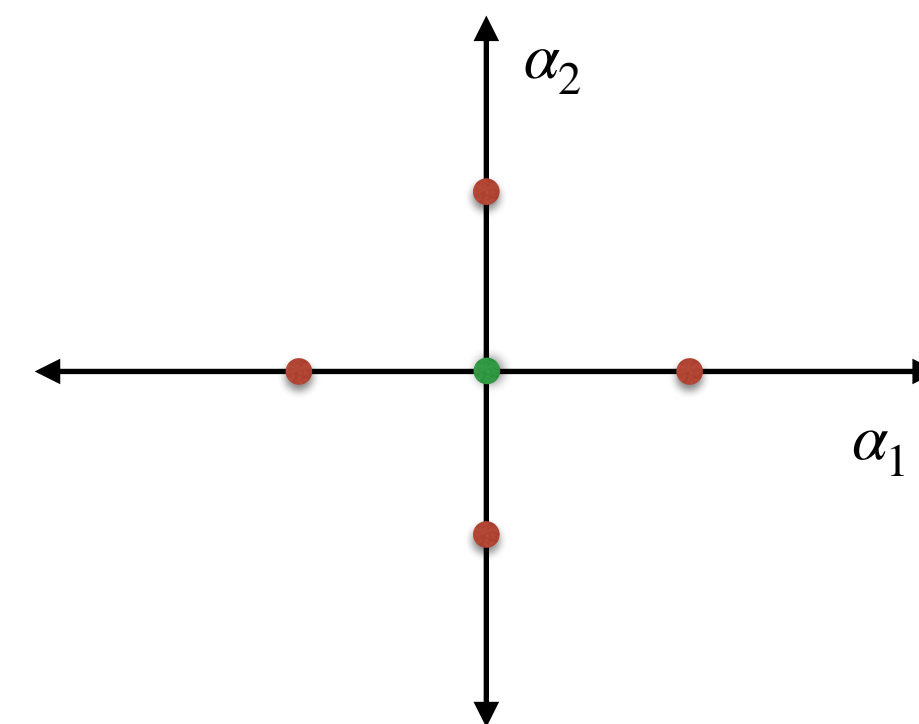
$$g_j(x_i, \alpha_k) = \frac{p_j(x_i, \alpha_k)}{p_j(x_i)}$$

Probability density ratio including nuisance parameters (α)

x_i is one individual event

$$\frac{p(x_i | \mu, \alpha)}{p_{ref}(x_i)} = \frac{1}{\nu(\mu, \alpha)} \sum_j^C \left(f_j(\mu) \cdot \nu_j \cdot \frac{p_j(x_i)}{p_{ref}(x_i)} \right) \cdot \prod_k^{N_{syst}} G_j(\alpha_k) \cdot g_j(x_i, \alpha_k)$$

We have this already



$$g_j(x_i, \alpha_k) = \frac{p_j(x_i, \alpha_k)}{p_j(x_i)}$$

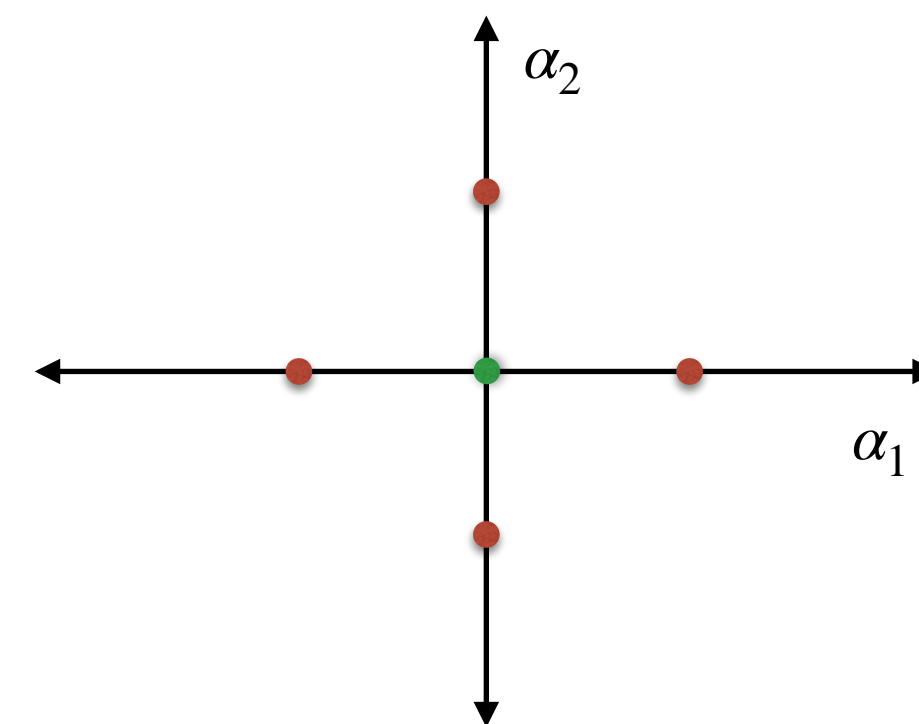
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We have this already

Estimate from simulations and existing interpolation methods



$$g_j(x_i, \alpha_k) = \frac{p_j(x_i, \alpha_k)}{p_j(x_i)}$$

Probability density ratio including nuisance parameters (α)

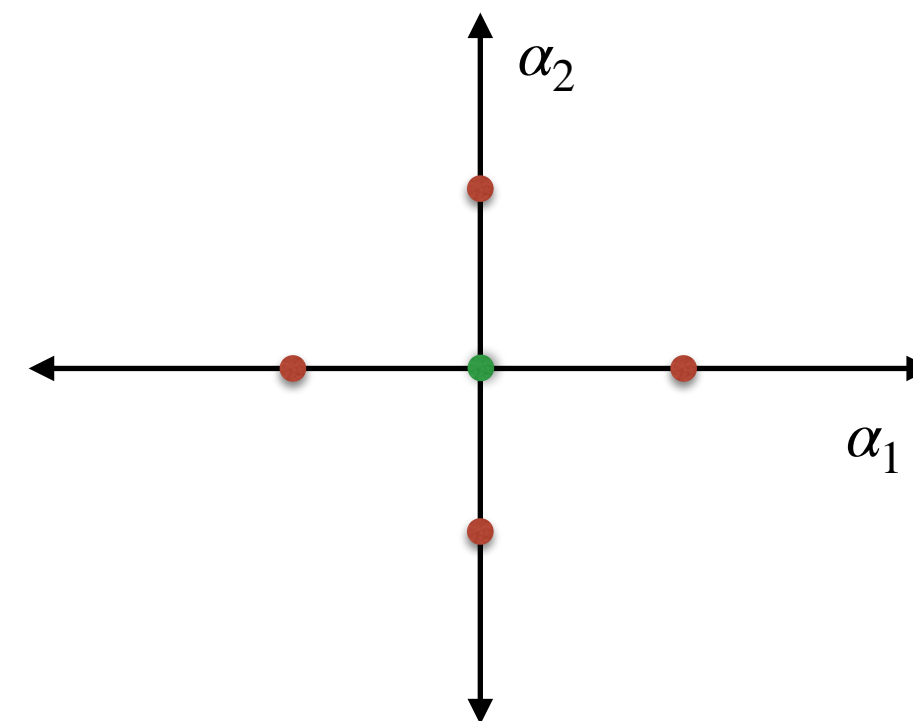
x_i is one individual event

$$\frac{p(x_i | \mu, \alpha)}{p_{ref}(x_i)} = \frac{1}{\nu(\mu, \alpha)} \sum_j^C f_j(\mu) \cdot \nu_j \cdot \frac{p_j(x_i)}{p_{ref}(x_i)} \cdot \prod_k^{N_{syst}} G_j(\alpha_k) \cdot g_j(x_i, \alpha_k)$$

We have this already

Per-event terms estimated using another ensemble of networks and interpolation methods

Estimate from simulations and existing interpolation methods



$$g_j(x_i, \alpha_k) = \frac{p_j(x_i, \alpha_k)}{p_j(x_i)}$$

Final test statistic

x_i is one individual event

$$\frac{L_{\text{full}}(\mu, \alpha | \mathcal{D})}{L_{\text{ref}}(\mathcal{D})} = \text{Pois}(N_{\text{data}} | \nu(\mu, \alpha)) \prod_i^{N_{\text{data}}} \frac{p(x_i | \mu, \alpha)}{p_{\text{ref}}(x_i)} \prod_k \text{Gaus}(a_k | \alpha_k, \delta_k)$$

Final test statistic

x_i is one individual event

$$\frac{L_{\text{full}}(\mu, \alpha | \mathcal{D})}{L_{\text{ref}}(\mathcal{D})} = \text{Pois}(N_{\text{data}} | \nu(\mu, \alpha)) \prod_i^{N_{\text{data}}} \frac{p(x_i | \mu, \alpha)}{p_{\text{ref}}(x_i)} \prod_k \text{Gaus}(a_k | \alpha_k, \delta_k)$$

From previous slide

Final test statistic

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Prod over events

From previous slide

Final test statistic

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$$\frac{L_{\text{full}}(\mu, \alpha | \mathcal{D})}{L_{\text{ref}}(\mathcal{D})} = \text{Pois}(N_{\text{data}} | \nu(\mu, \alpha)) \prod_i^{N_{\text{data}}} \frac{p(x_i | \mu, \alpha)}{p_{\text{ref}}(x_i)} \prod_k \text{Gaus}(a_k | \alpha_k, \delta_k)$$

Rate term (points to $\text{Pois}(N_{\text{data}} | \nu(\mu, \alpha))$)
Prod over events (points to $\prod_i^{N_{\text{data}}}$)
From previous slide (points to $\frac{p(x_i | \mu, \alpha)}{p_{\text{ref}}(x_i)}$)

Final test statistic

x_i is one individual event

$$\frac{L_{\text{full}}(\mu, \alpha | \mathcal{D})}{L_{\text{ref}}(\mathcal{D})} = \text{Pois}(N_{\text{data}} | \nu(\mu, \alpha)) \prod_i^{N_{\text{data}}} \frac{p(x_i | \mu, \alpha)}{p_{\text{ref}}(x_i)} \prod_k \text{Gaus}(a_k | \alpha_k, \delta_k)$$

Rate term (points to $\text{Pois}(N_{\text{data}} | \nu(\mu, \alpha))$)
Prod over events (points to $\prod_i^{N_{\text{data}}}$)
From previous slide (points to $\frac{p(x_i | \mu, \alpha)}{p_{\text{ref}}(x_i)}$)
Constrain term (points to $\prod_k \text{Gaus}(a_k | \alpha_k, \delta_k)$)

Final test statistic

x_i is one individual event

$$\frac{L_{\text{full}}(\mu, \alpha | \mathcal{D})}{L_{\text{ref}}(\mathcal{D})} = \text{Pois}(N_{\text{data}} | \nu(\mu, \alpha)) \prod_i^{N_{\text{data}}} \frac{p(x_i | \mu, \alpha)}{p_{\text{ref}}(x_i)} \prod_k \text{Gaus}(a_k | \alpha_k, \delta_k)$$

Rate term (points to Poisson term)

Prod over events (points to \prod_i)

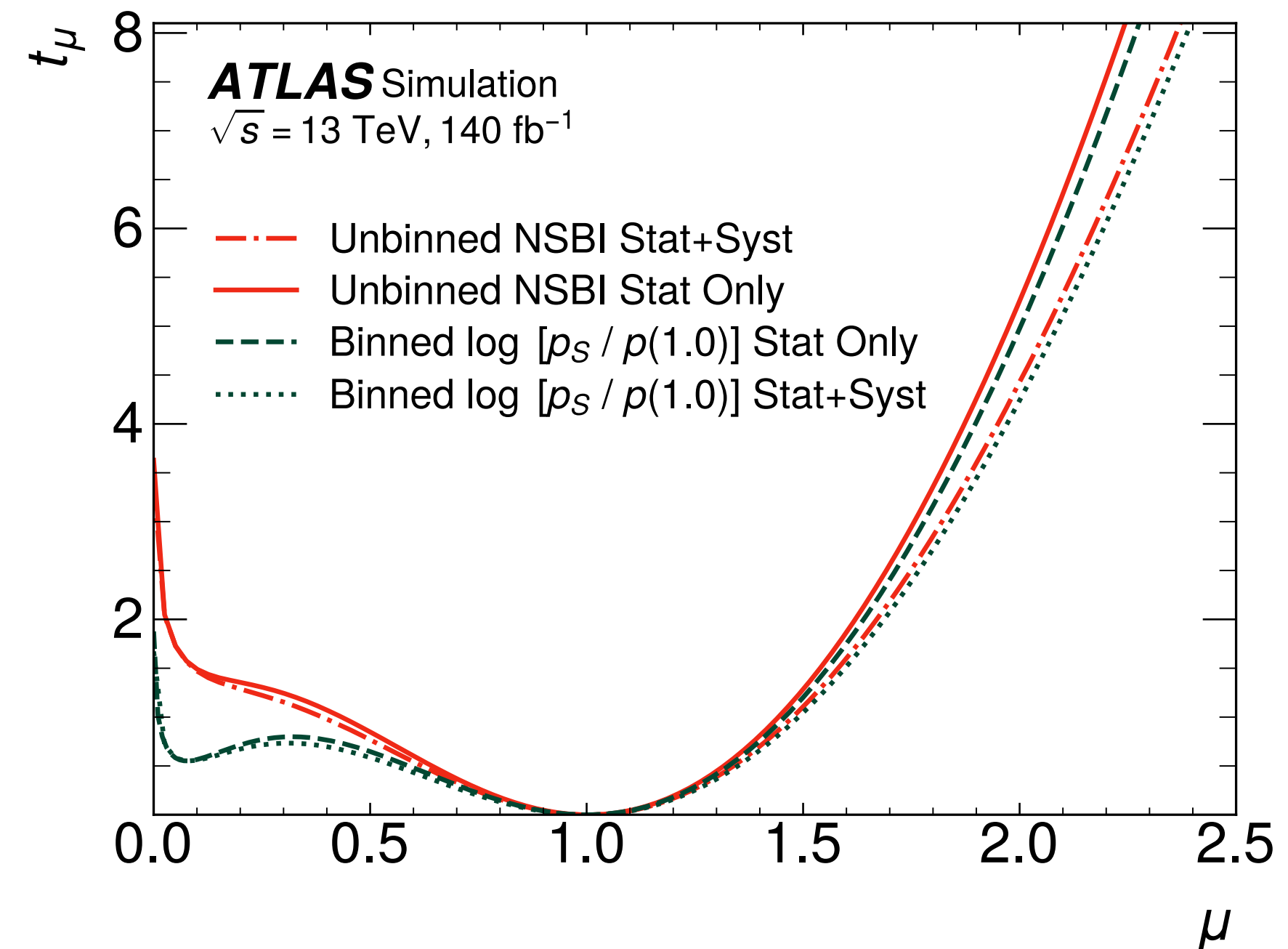
From previous slide (points to $\frac{p(x_i | \mu, \alpha)}{p_{\text{ref}}(x_i)}$)

Constrain term (points to $\prod_k \text{Gaus}(a_k | \alpha_k, \delta_k)$)

Profiling:

$$t_\mu = -2 \ln \left(\frac{L_{\text{full}}(\mu, \hat{\hat{\alpha}}) / L_{\text{ref}}}{L_{\text{full}}(\hat{\mu}, \hat{\alpha}) / L_{\text{ref}}} \right)$$

This is why we define p_{ref} to be independent of μ



Final test statistic

x_i is one individual event

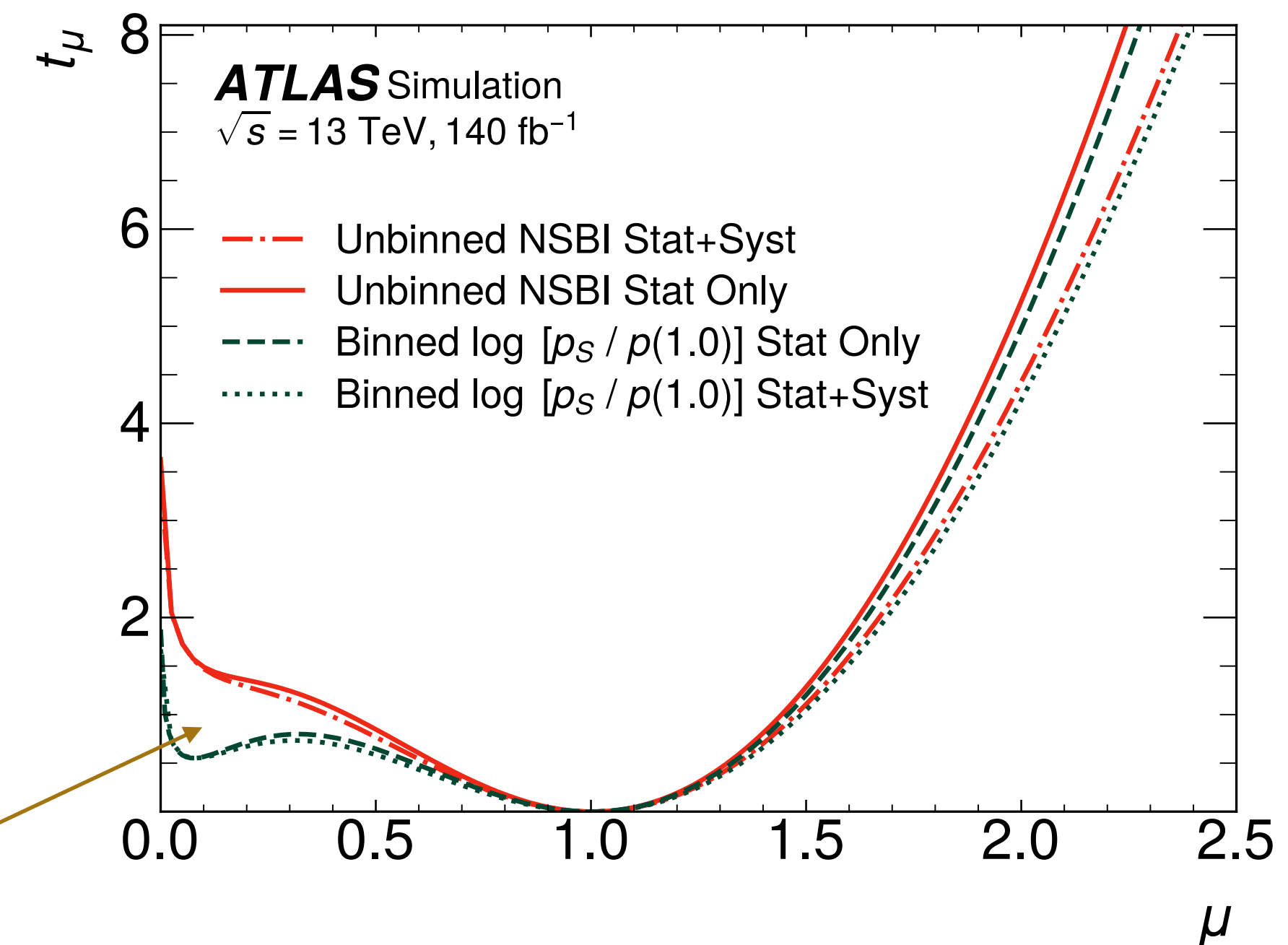
$$\frac{L_{\text{full}}(\mu, \alpha | \mathcal{D})}{L_{\text{ref}}(\mathcal{D})} = \text{Pois}(N_{\text{data}} | \nu(\mu, \alpha)) \prod_i^{N_{\text{data}}} \frac{p(x_i | \mu, \alpha)}{p_{\text{ref}}(x_i)} \prod_k \text{Gaus}(a_k | \alpha_k, \delta_k)$$

Rate term Prod over events From previous slide Constrain term

Profiling:

$$t_\mu = -2 \ln \left(\frac{L_{\text{full}}(\mu, \hat{\hat{\alpha}}) / L_{\text{ref}}}{L_{\text{full}}(\hat{\mu}, \hat{\alpha}) / L_{\text{ref}}} \right)$$

This is why we define p_{ref} to be independent of μ

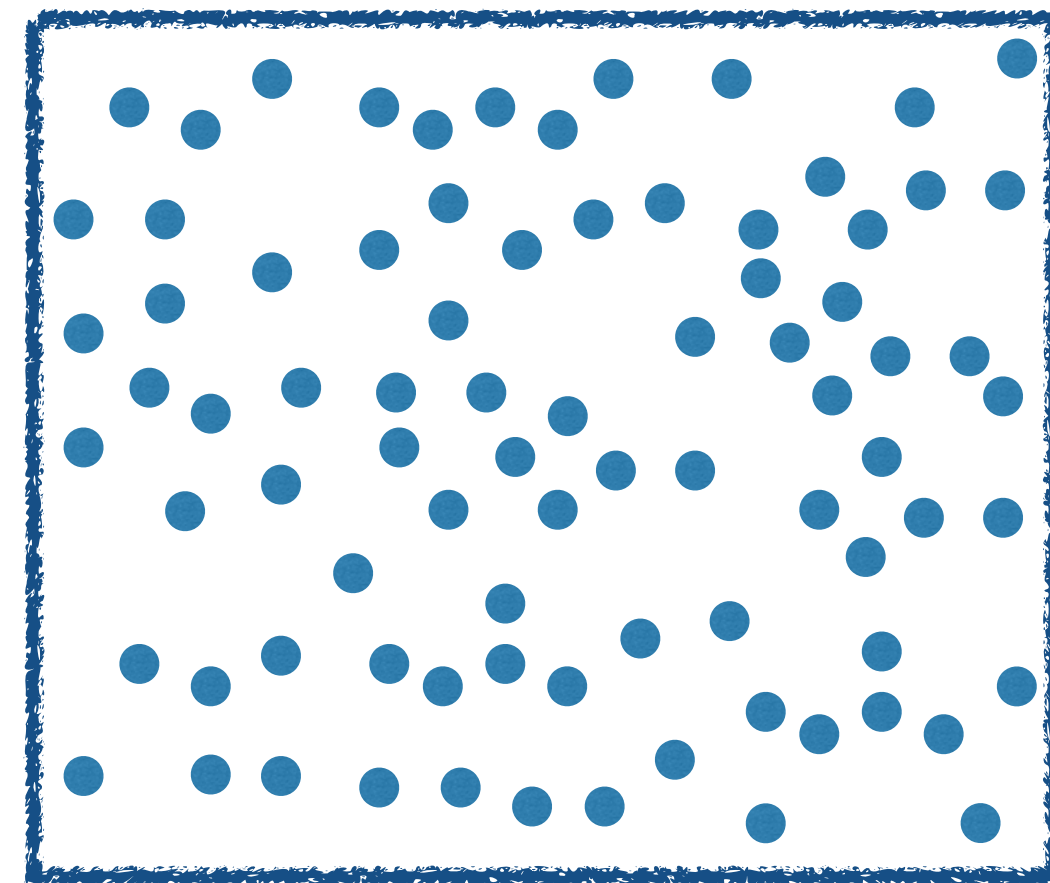


Non-parabolic shape due to non-linear effects from quantum interference

Uncertainty from finite training samples

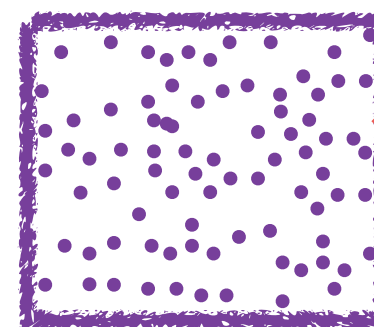
Estimating the variance on mean: Bootstrapping

Want to estimate mean of population



Population

Random Sample

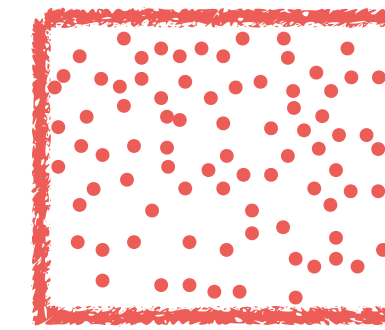


Sample

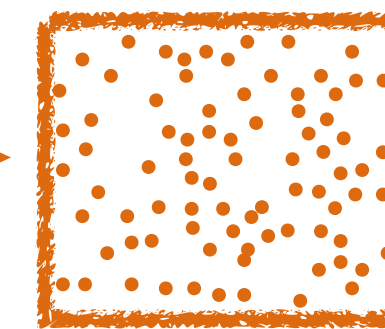


Image: Source

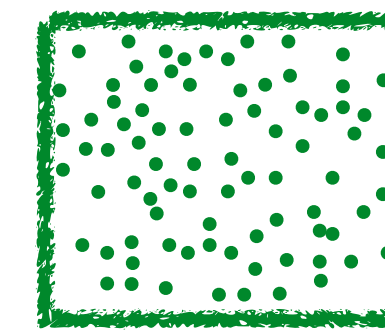
Re-Sample with replacement



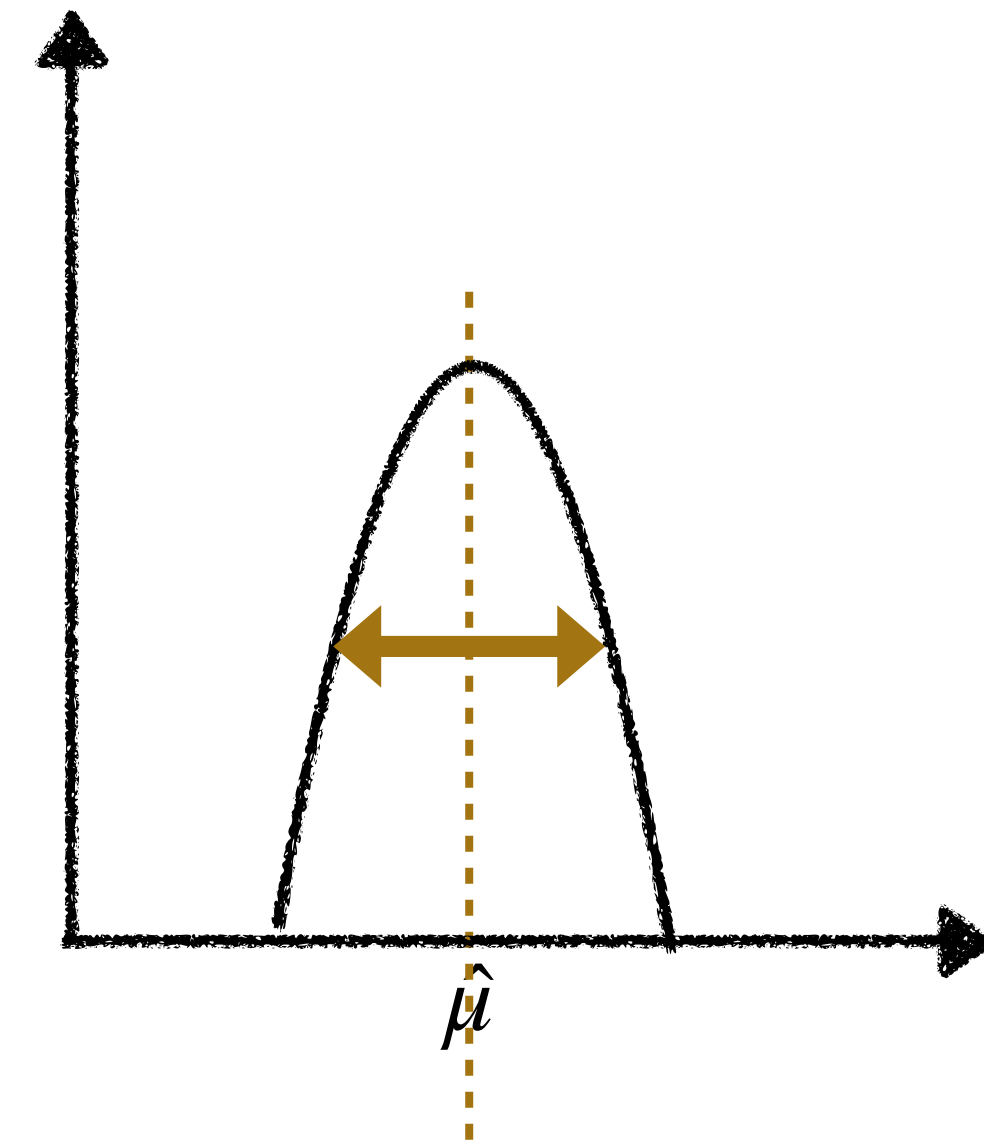
Sample Mean 1



Sample Mean 2



Sample Mean 3

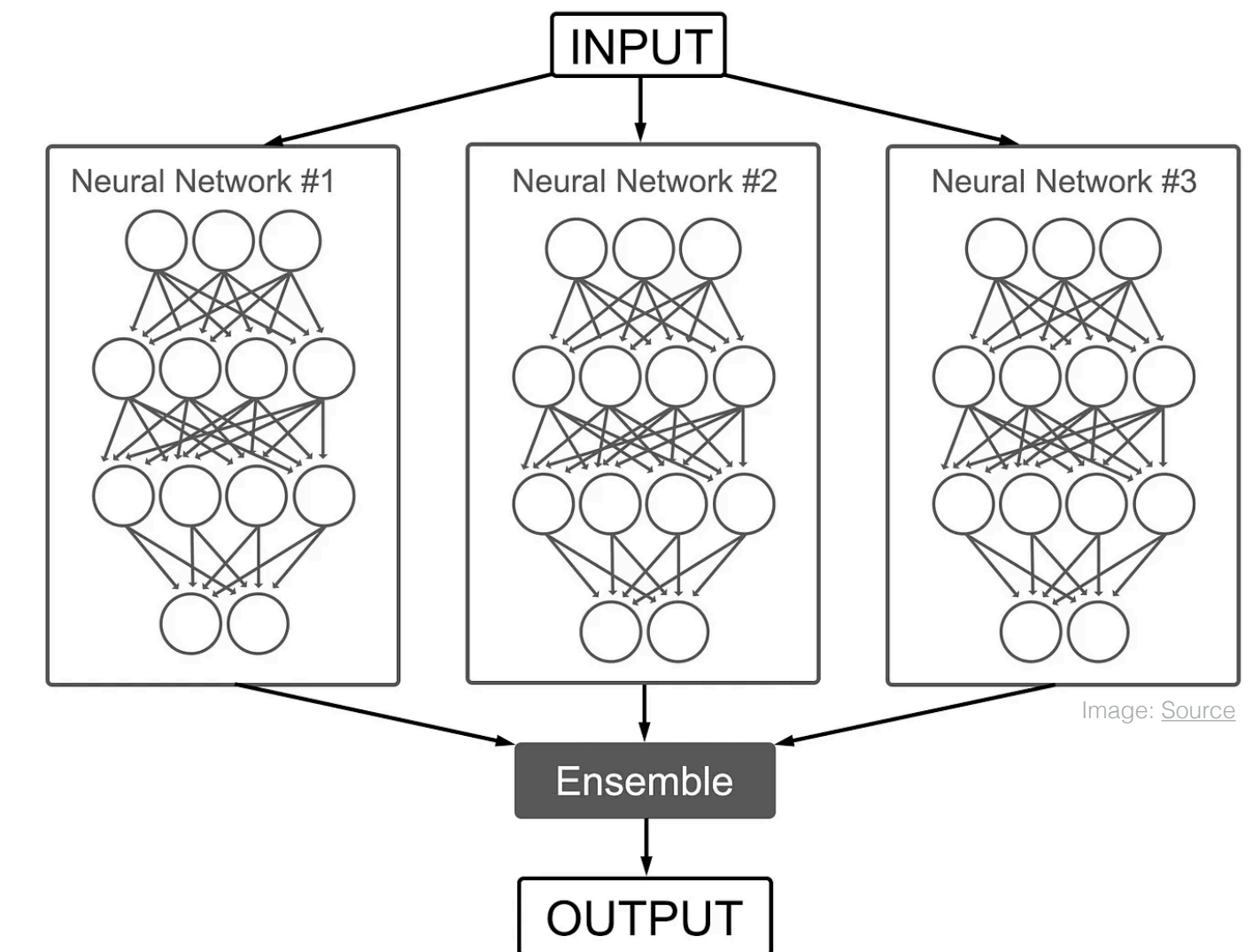


Estimate variance on the mean

Quantifying uncertainty on estimated density ratio

$$w_i \rightarrow w_i \cdot \text{Pois}(1)$$

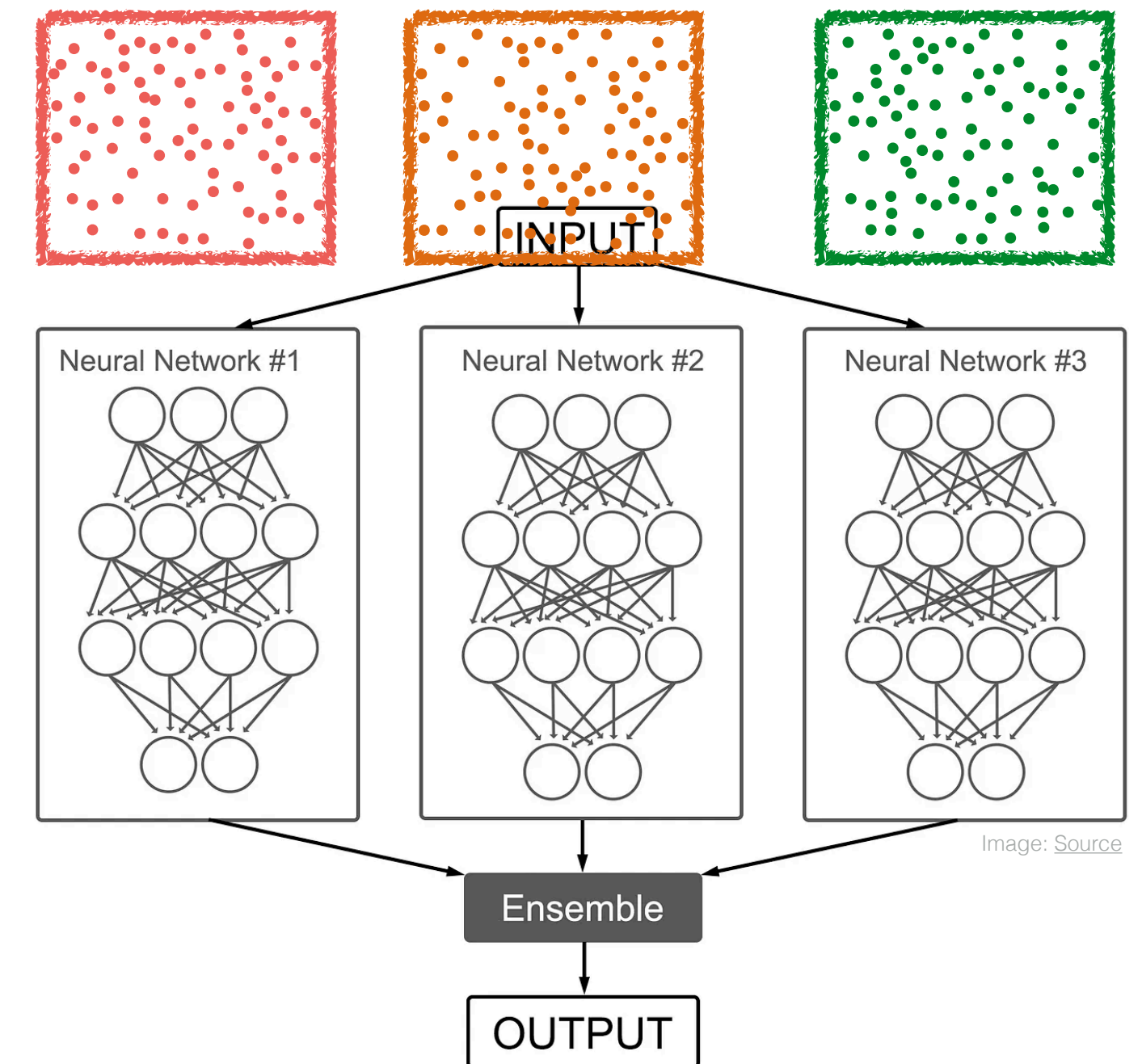
- Train an ensemble of networks, each on a Poisson fluctuated version of the training dataset
- Ensemble average used as final prediction, estimate the variance on mean from bootstrapped ensembles



Quantifying uncertainty on estimated density ratio

$$w_i \rightarrow w_i \cdot \text{Pois}(1)$$

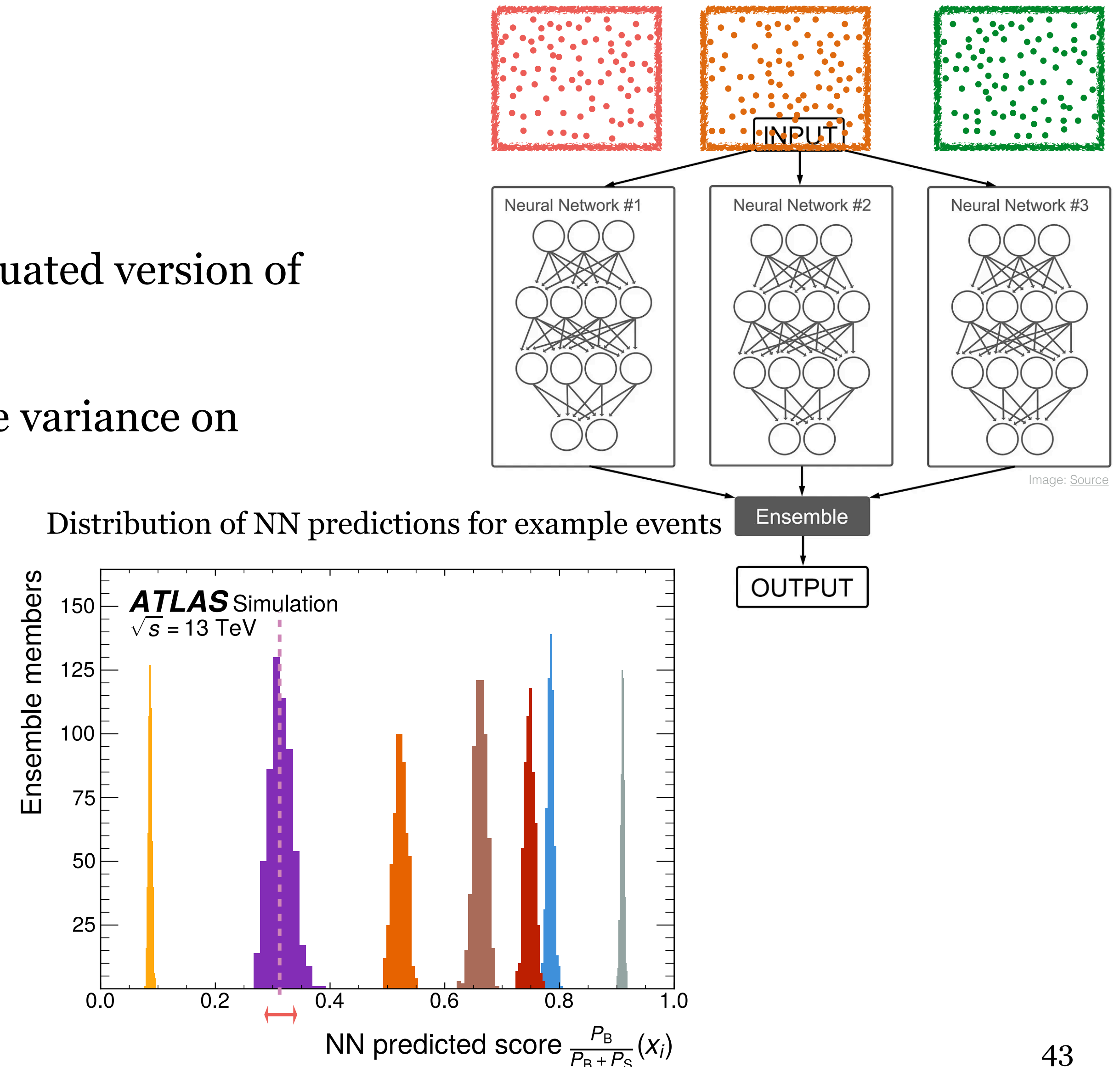
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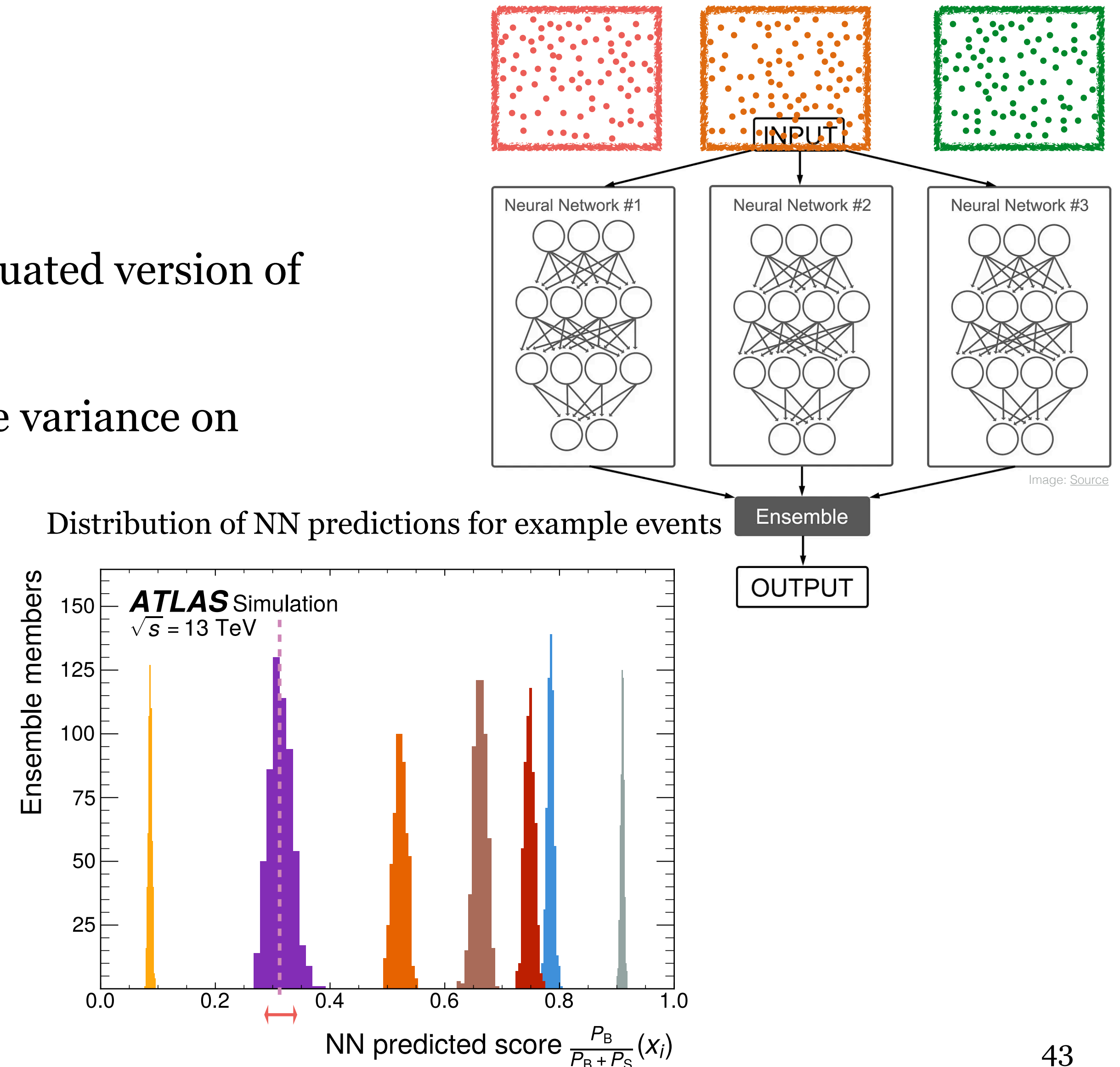
Quantifying uncertainty on estimated density ratio

$$w_i \rightarrow w_i \cdot \text{Pois}(1)$$

- Train an ensemble of networks, each on a Poisson fluctuated version of the training dataset
- Ensemble average used as final prediction, estimate the variance on mean from bootstrapped ensembles
- Propagate with spurious signal method

$$f_j(\mu) \rightarrow f_j(\mu + \alpha \cdot \Delta \hat{\mu}(\mu))$$

Constraint term: $\text{Gauss}(0,1)$



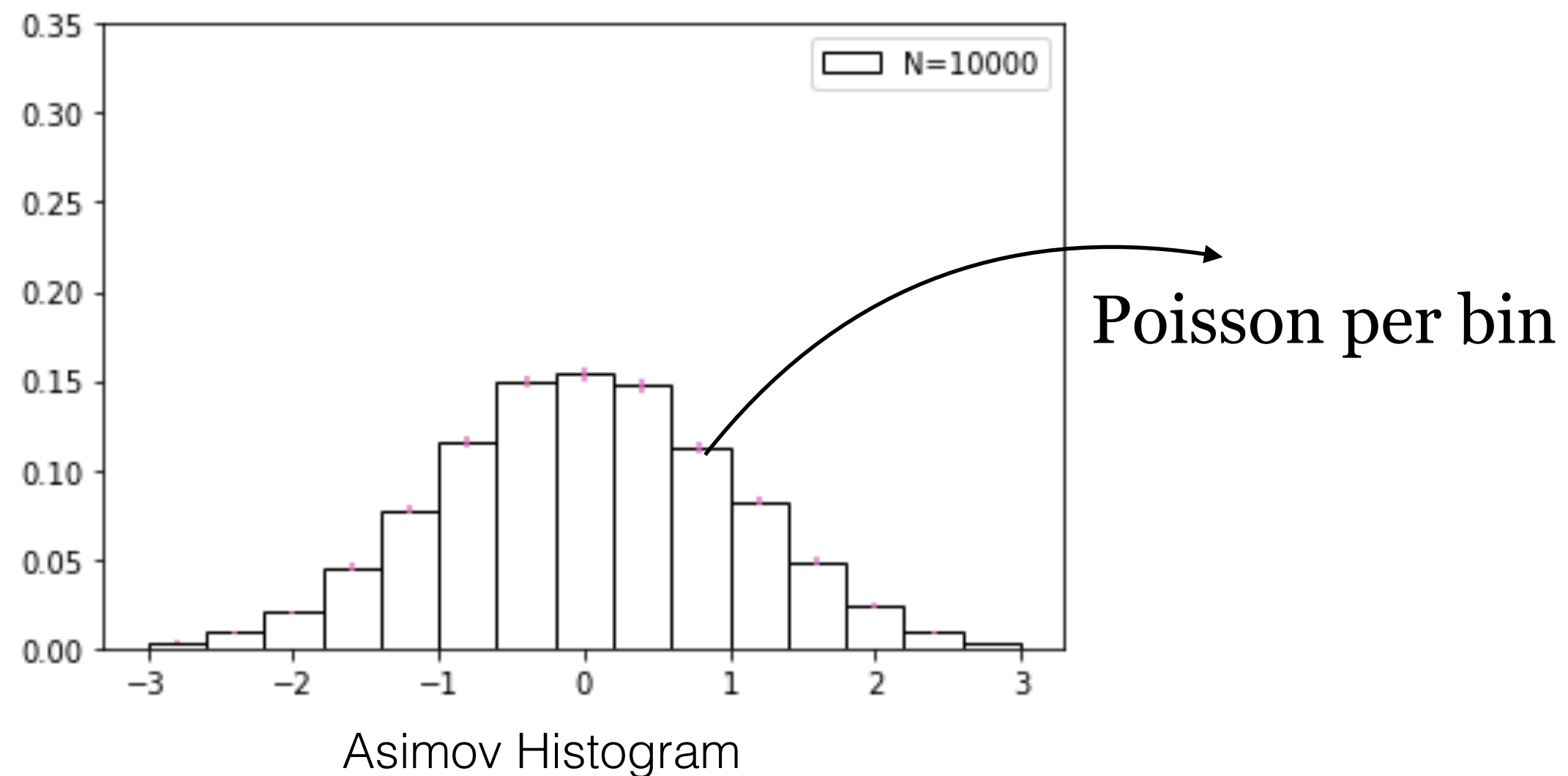
Open problems to extend to full ATLAS analysis:

- ✓ Robustness: Design and validation
- ✓ Systematic Uncertainties: Incorporate them in likelihood (ratio) model
- ▶ **Neyman Construction: Throwing toys in a per-event analysis**

Generating event-level pseudo-experiments

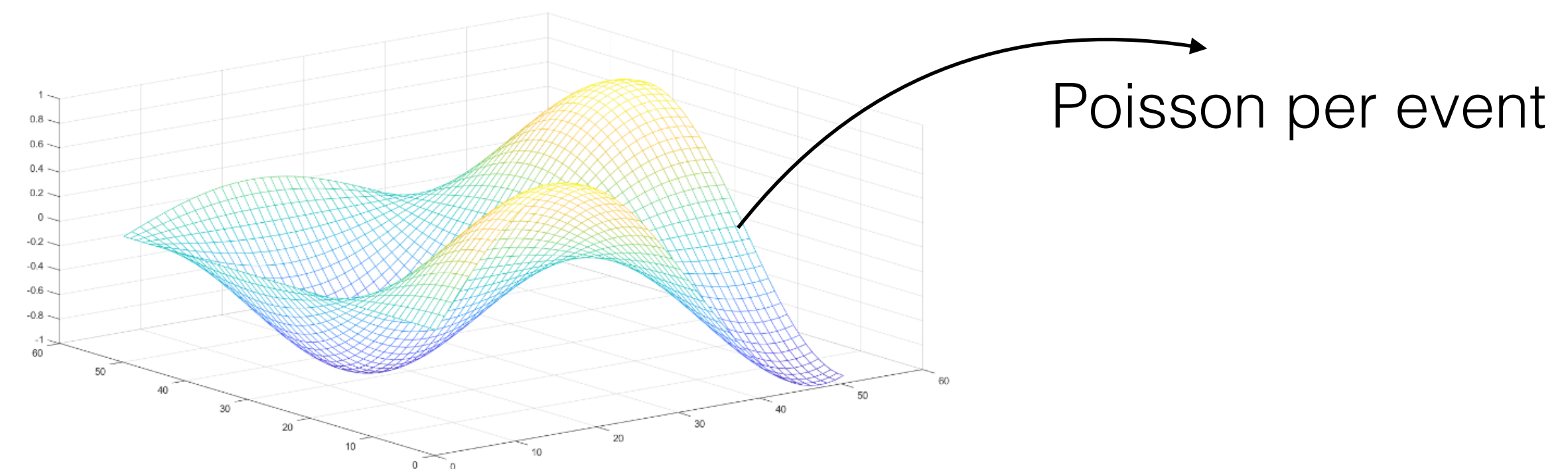
Need to generate random possible datasets we could collect at the LHC

Traditionally:



$$N_i^{toy} = \text{Poisson}(N_i^{Asimov})$$

NSBI:



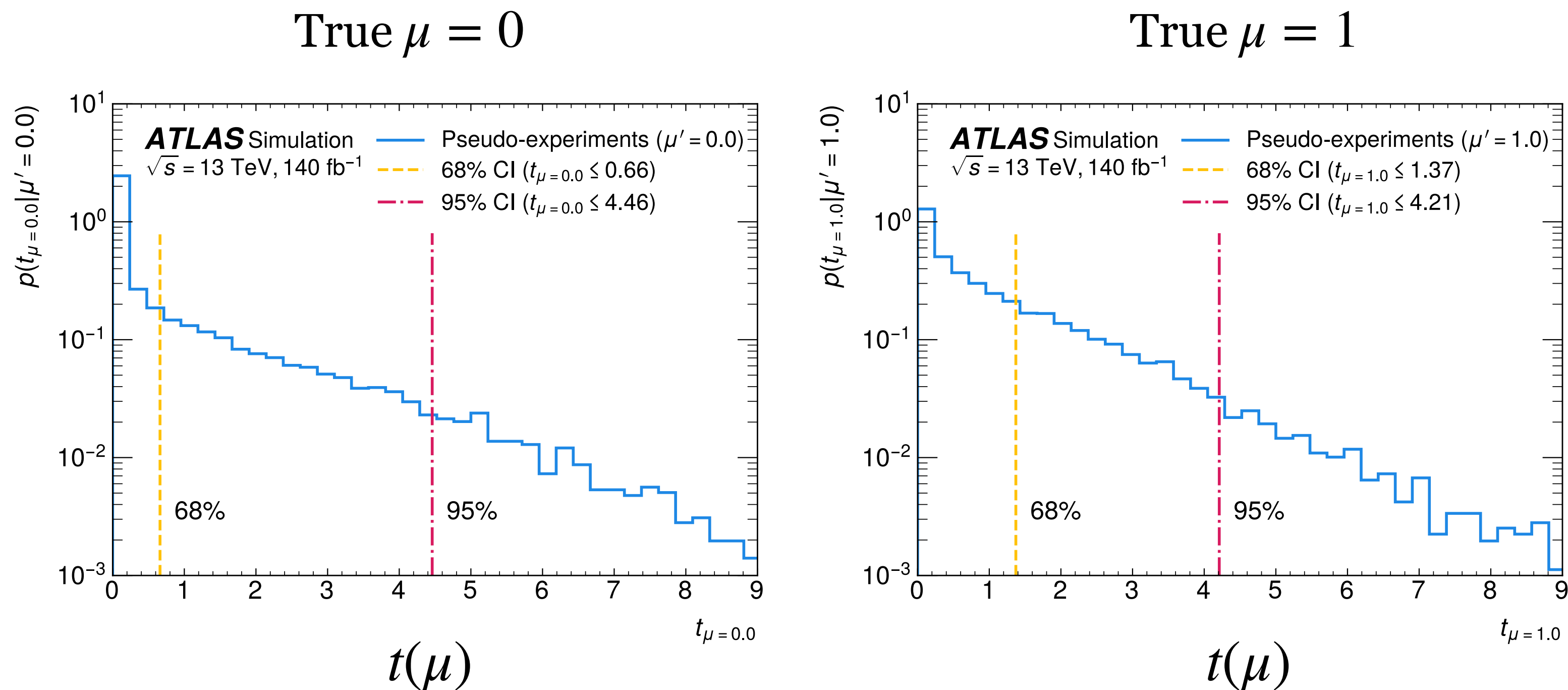
$$w_i^{toy} = \text{Poisson}(w_i^{Asimov})$$

‘Unweighted’ events, i.e. integer weights

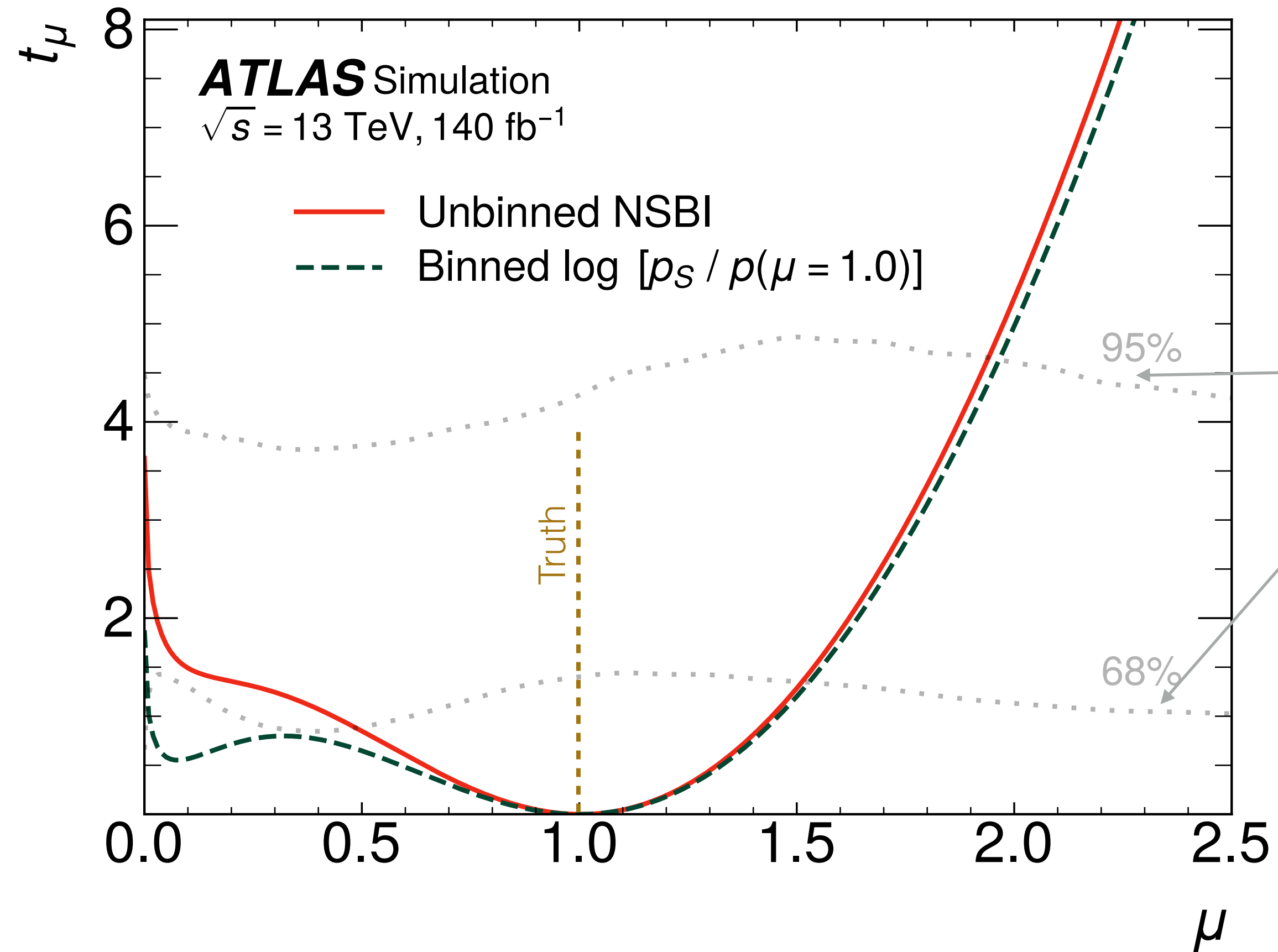
Negative weights? See [backup](#)

Neyman Construction

- To build confidence intervals, we need to ‘invert the hypothesis test’
- Generate pseudo-experiments (‘toys’) and determine 68 % & 95 % CI as a function of parameter of interest

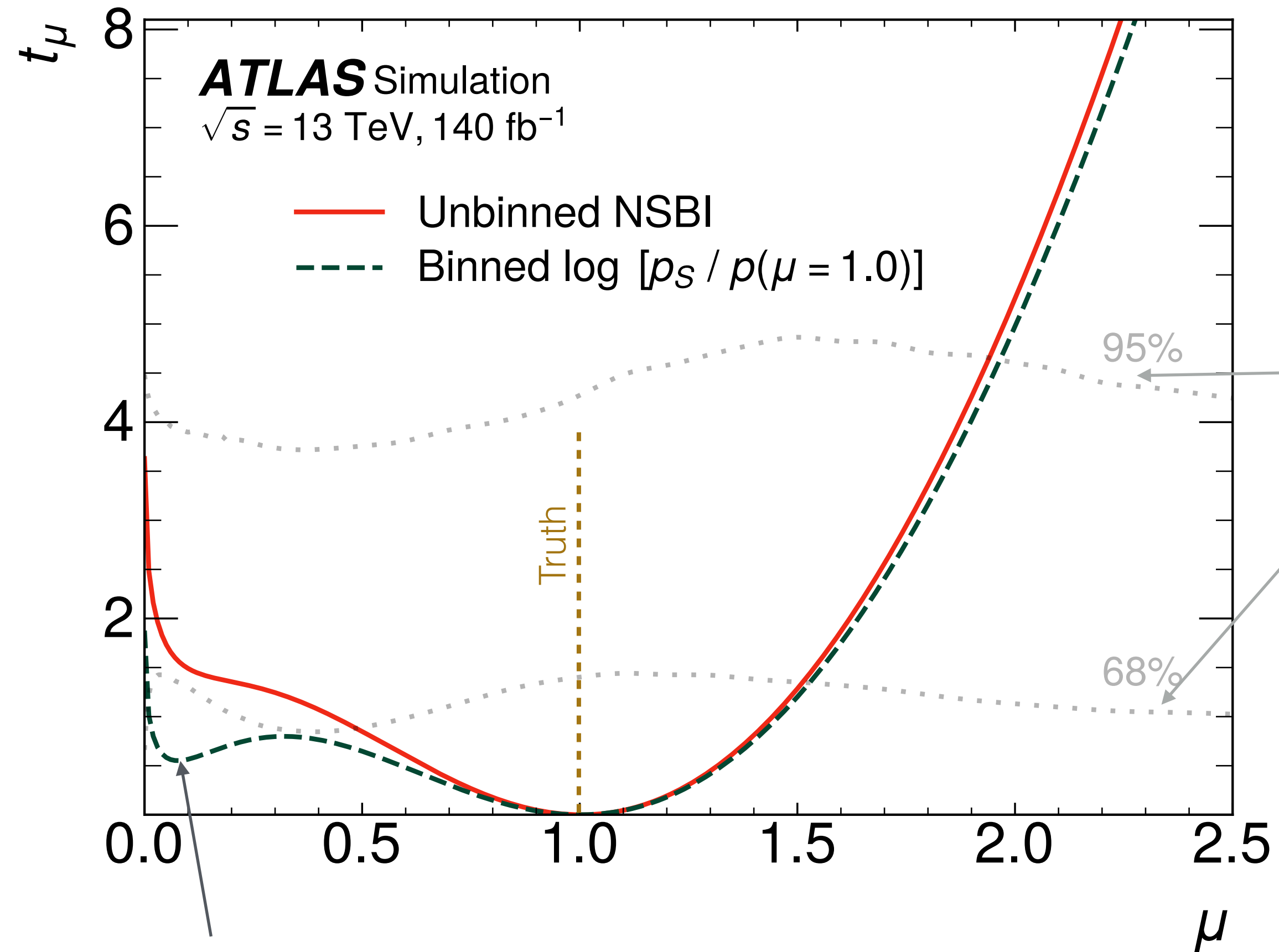


Confidence belts



Similar to structure seen in histogram analysis

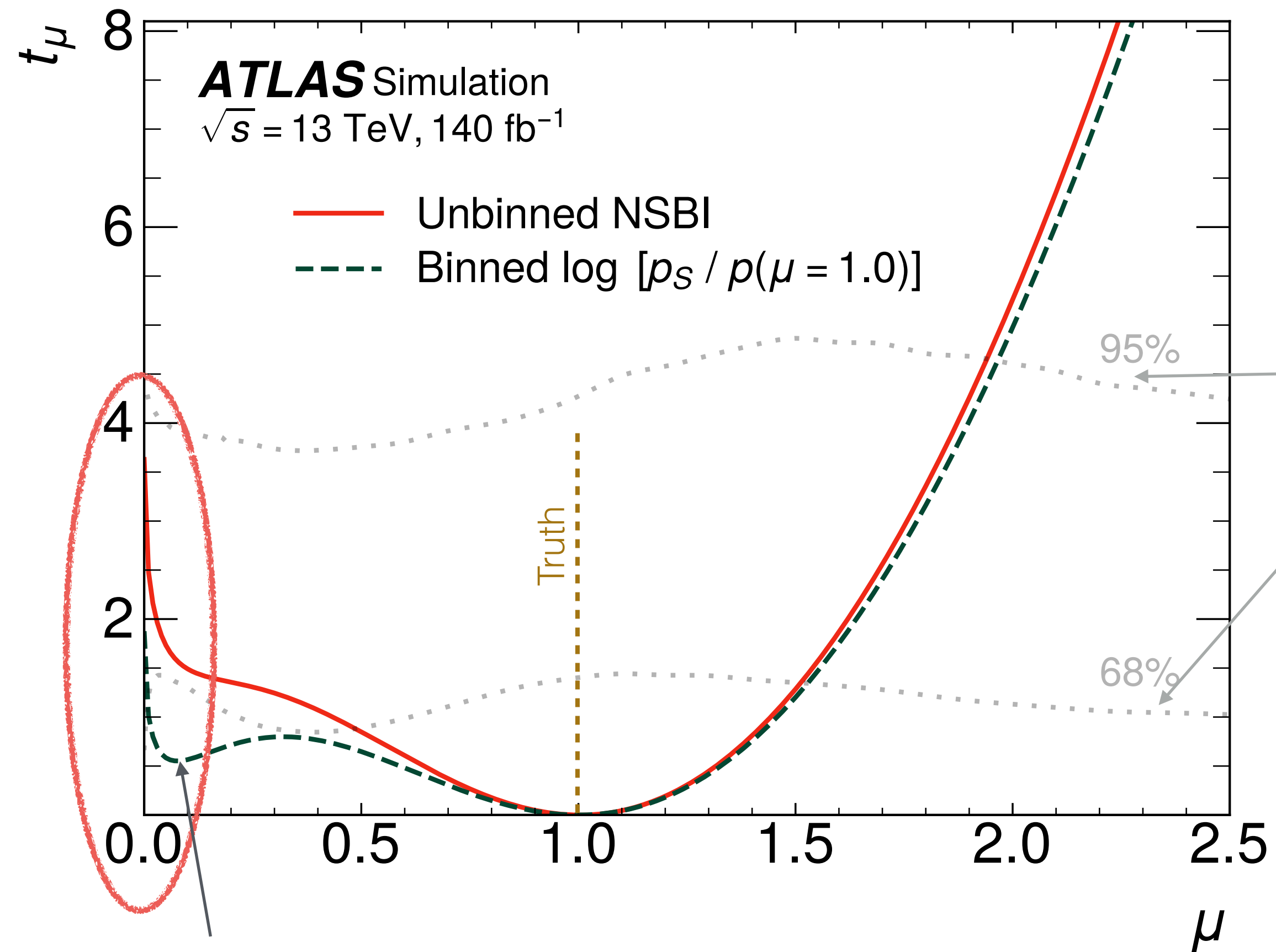
Confidence belts



Similar to structure seen in histogram analysis

Significant improvement in QI impacted region

Confidence belts



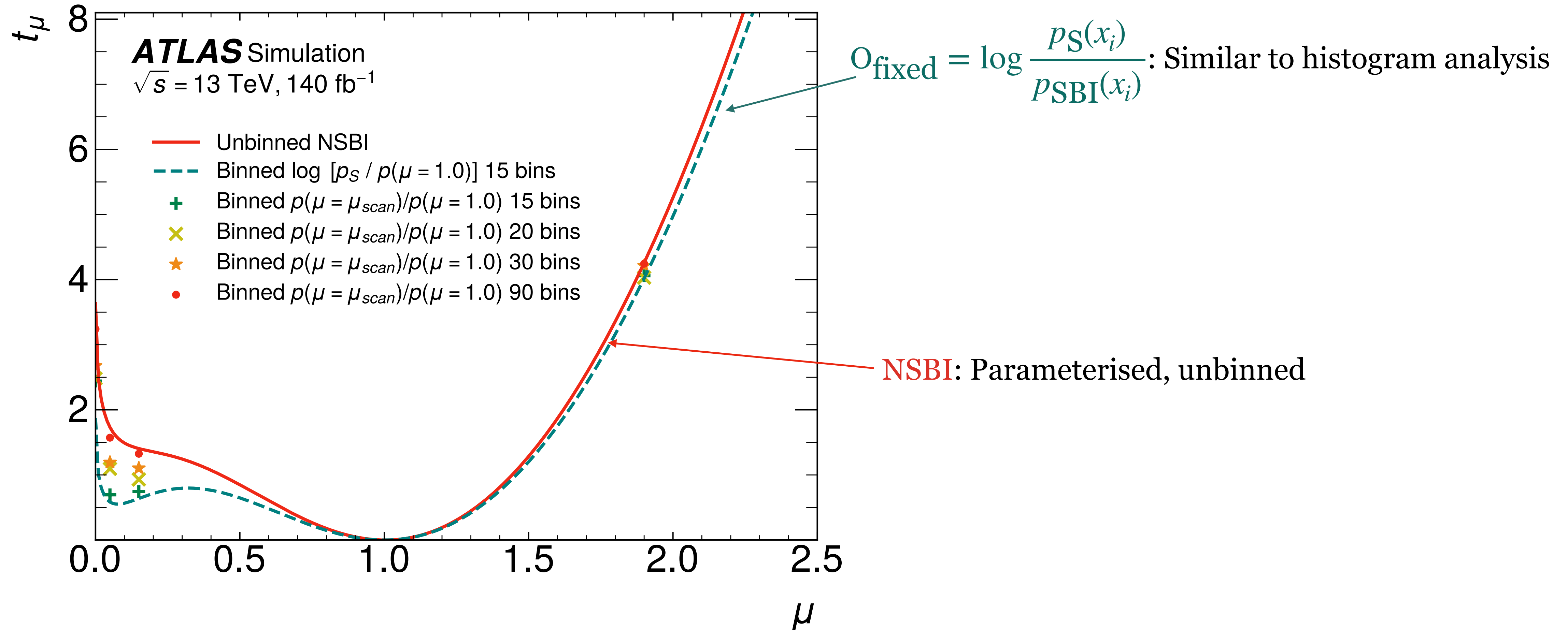
Similar to structure seen in histogram analysis

Significant improvement in QI impacted region

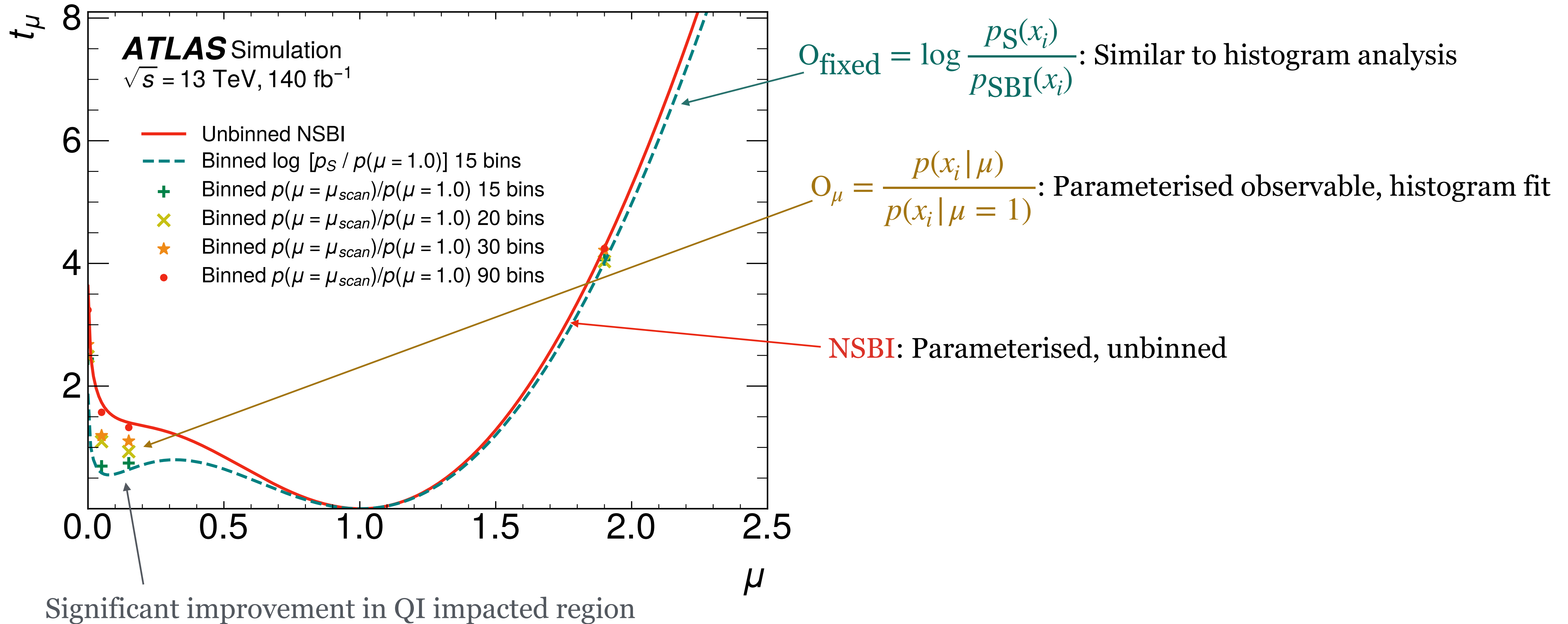
Expect a dramatic improvement in ability to reject null hypothesis

Why does NSBI work better than traditional analyses?

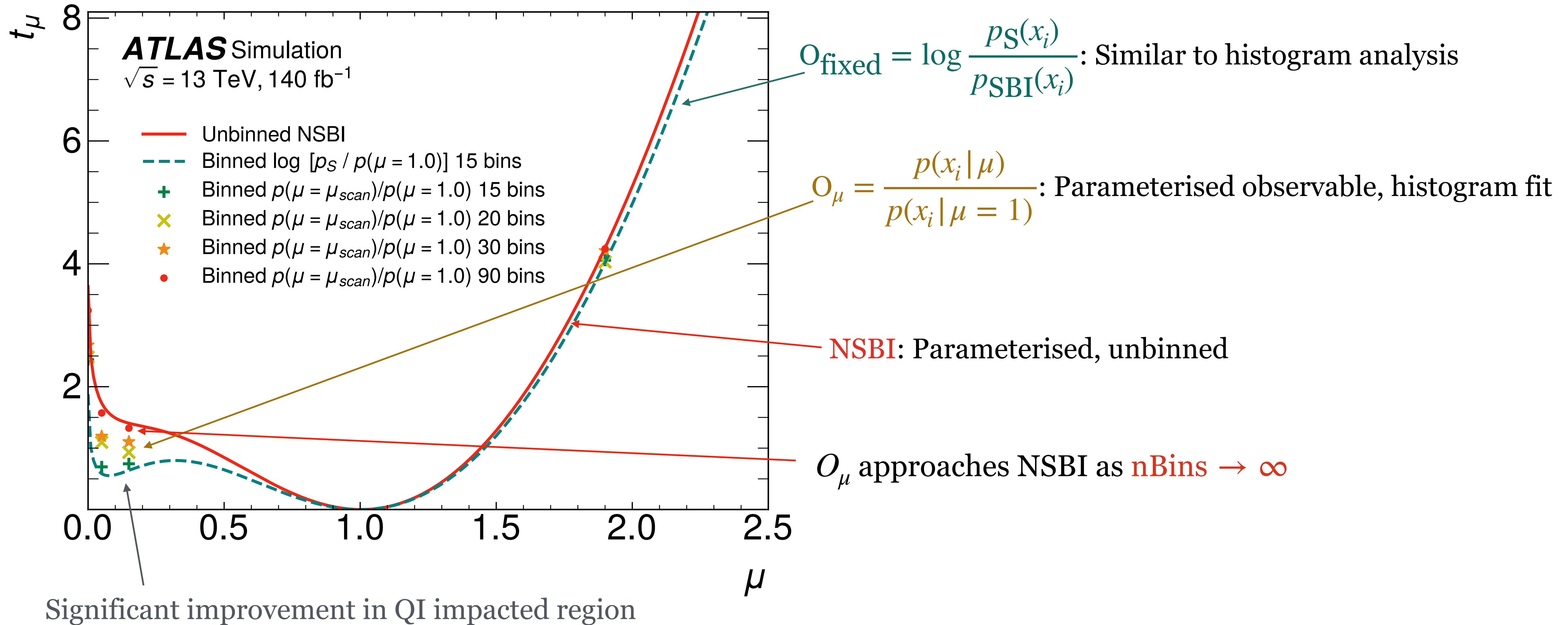
Why does it work better than traditional analyses?



Why does it work better than traditional analyses?

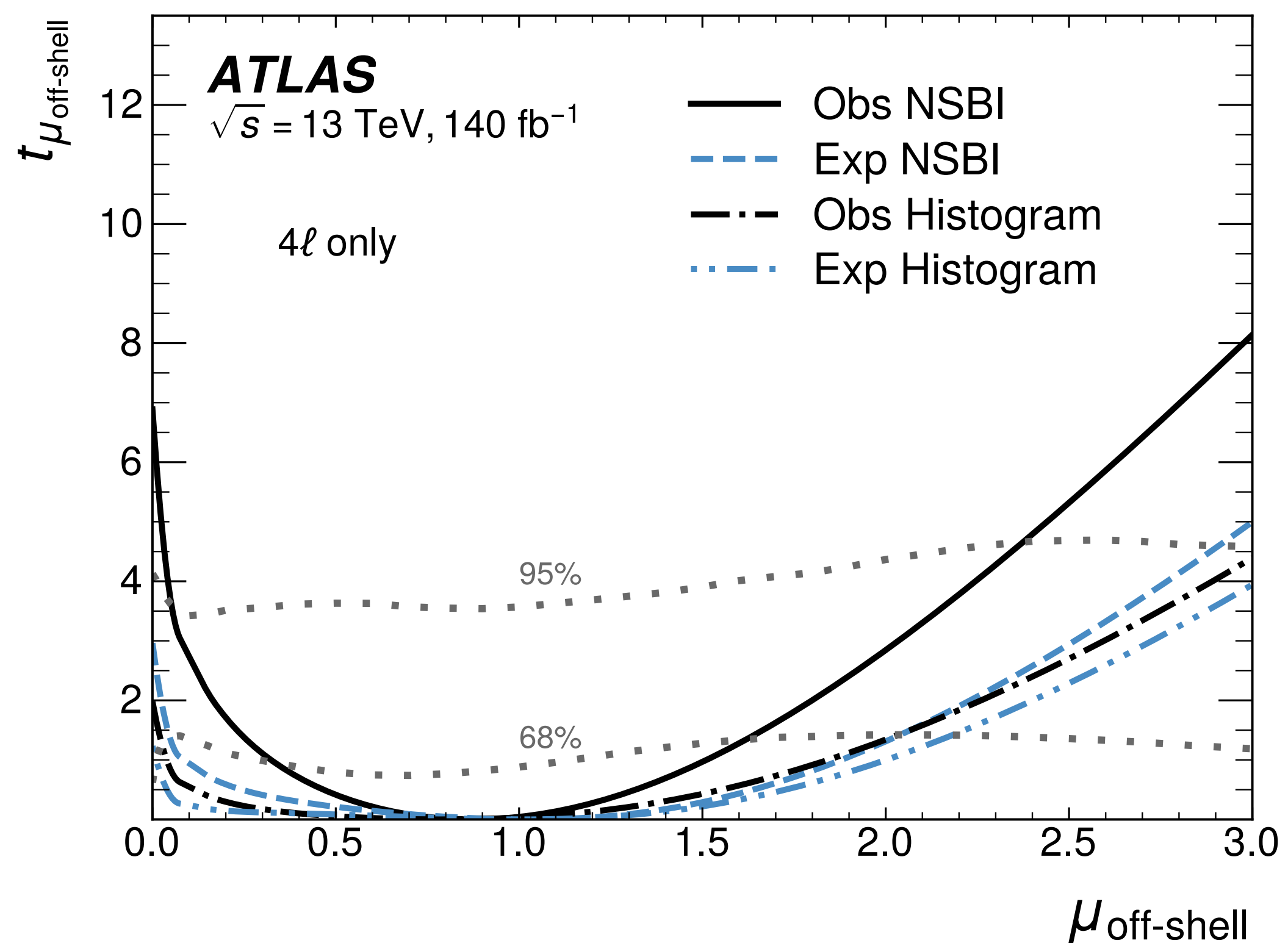


Why does it work better than traditional analyses?



Final results: Apply on real data and supersede previous Run2 paper!

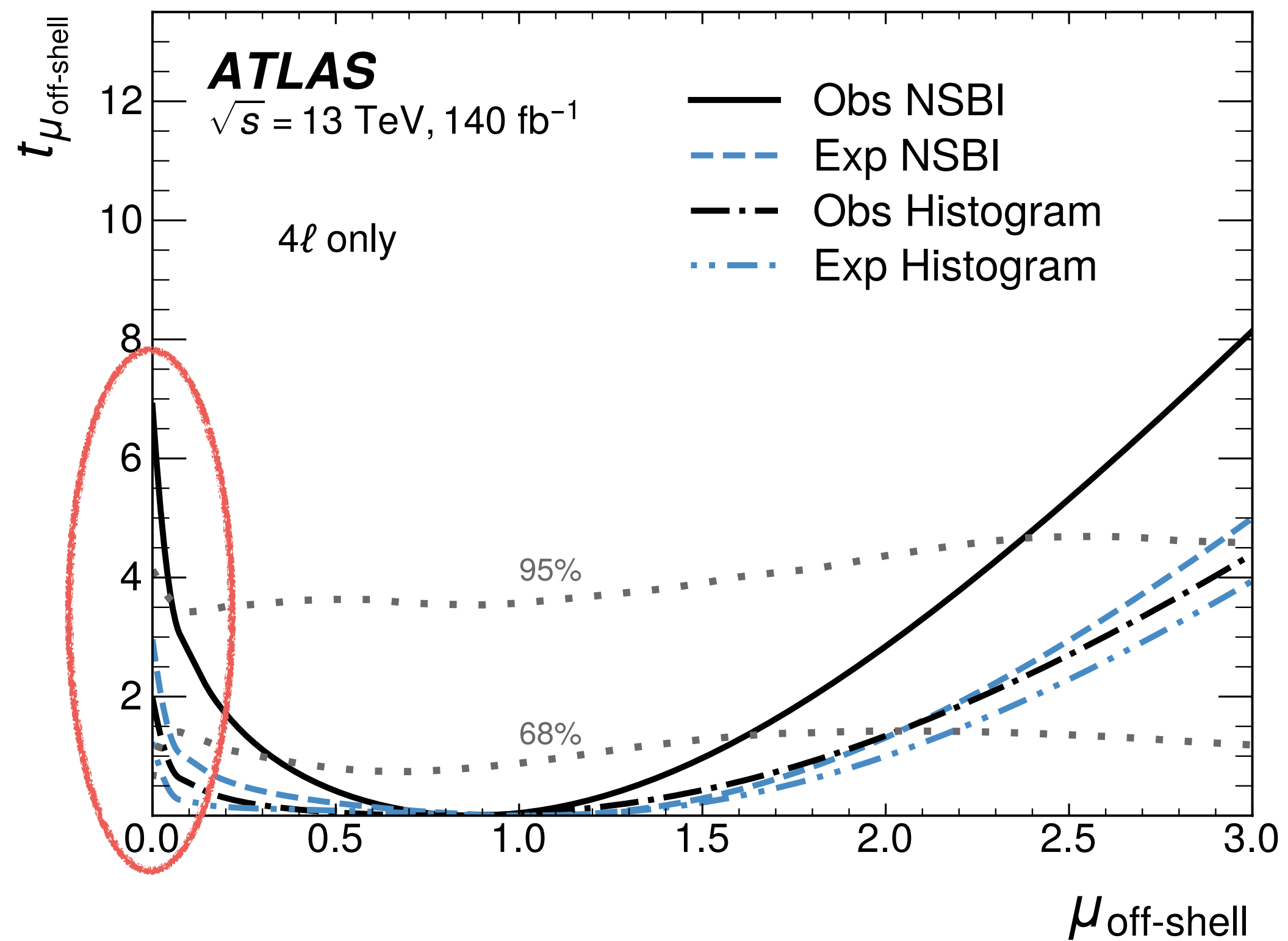
NSBI vs histogram analysis



Observed data happens to provide stronger than expected constrains for both hist and NSBI (consistent)

Final results: Apply on real data and supersede previous Run2 paper!

NSBI vs histogram analysis

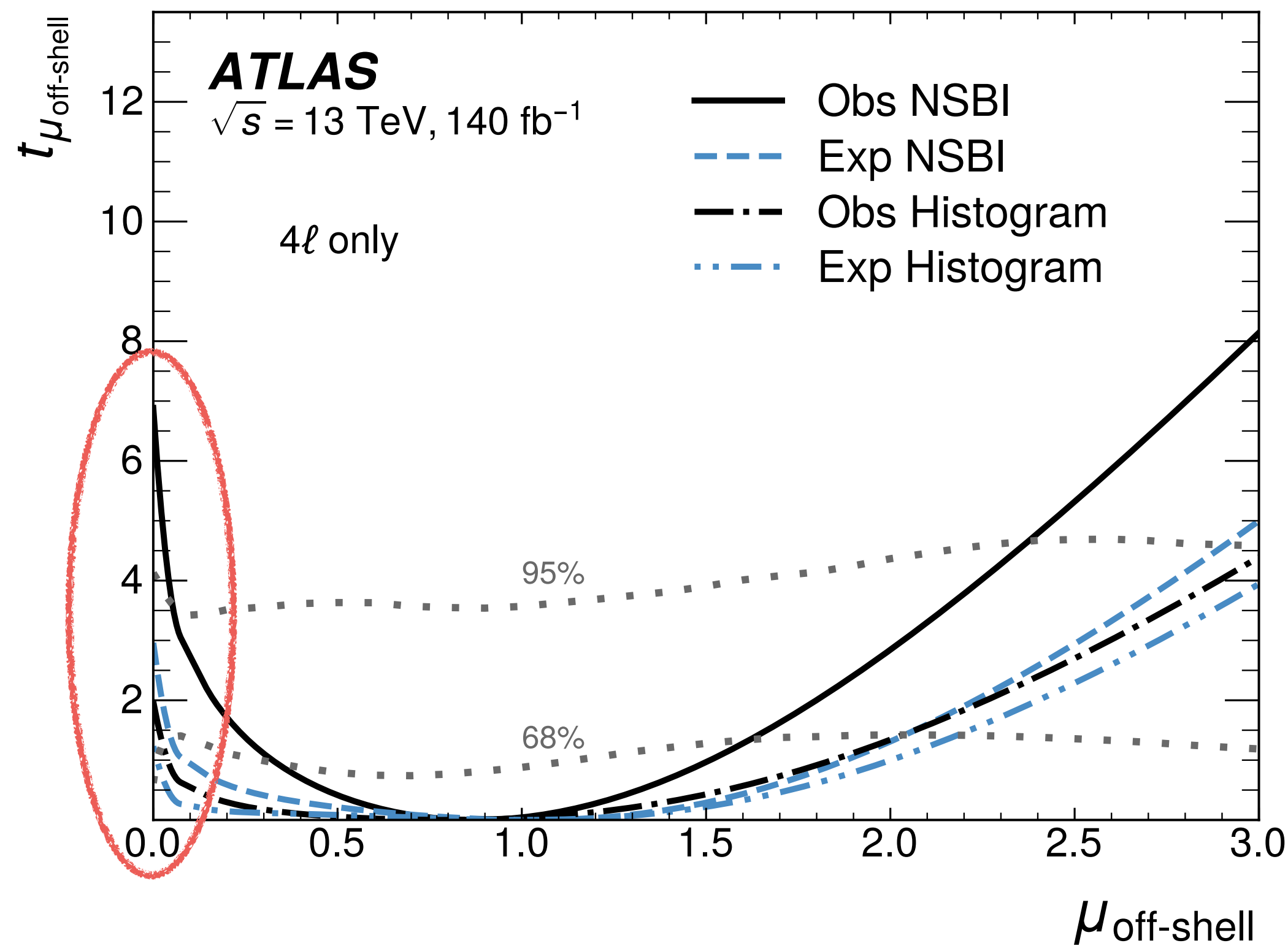


Unprecedented improvement in ability to reject null hypothesis! (2.6x gain over previous method)

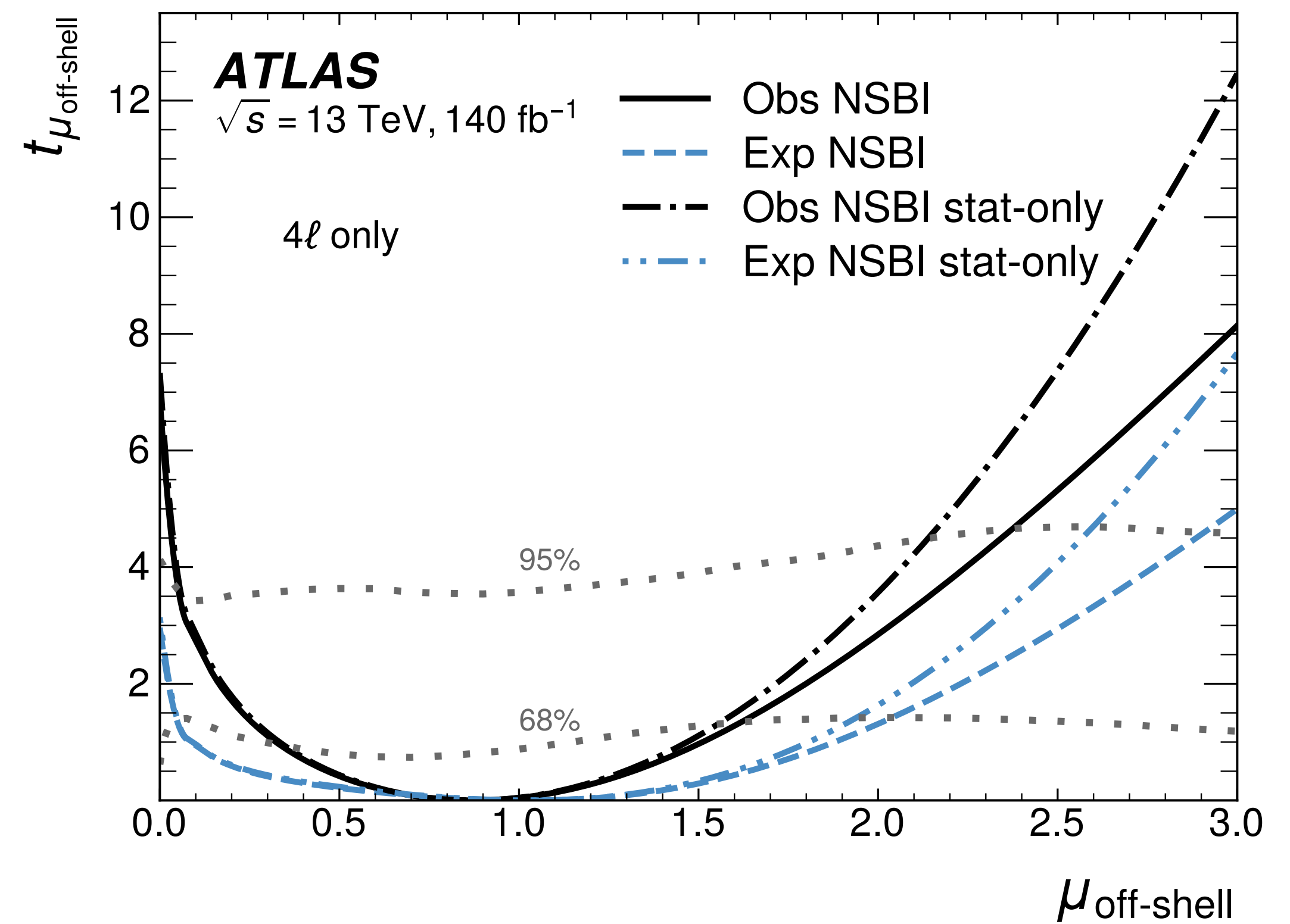
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NSBI vs histogram analysis



Stat-only vs Stat+Syst uncertainties



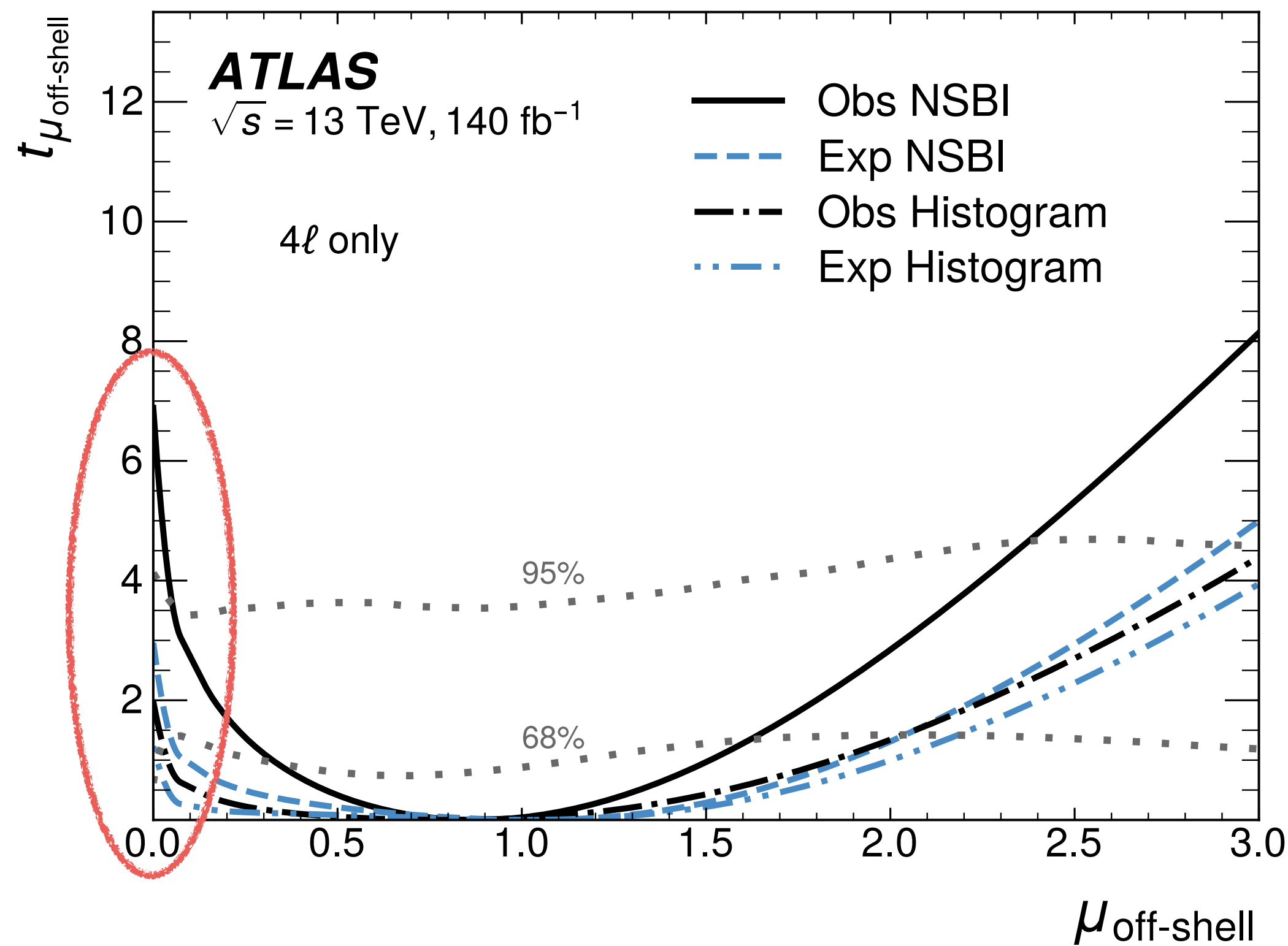
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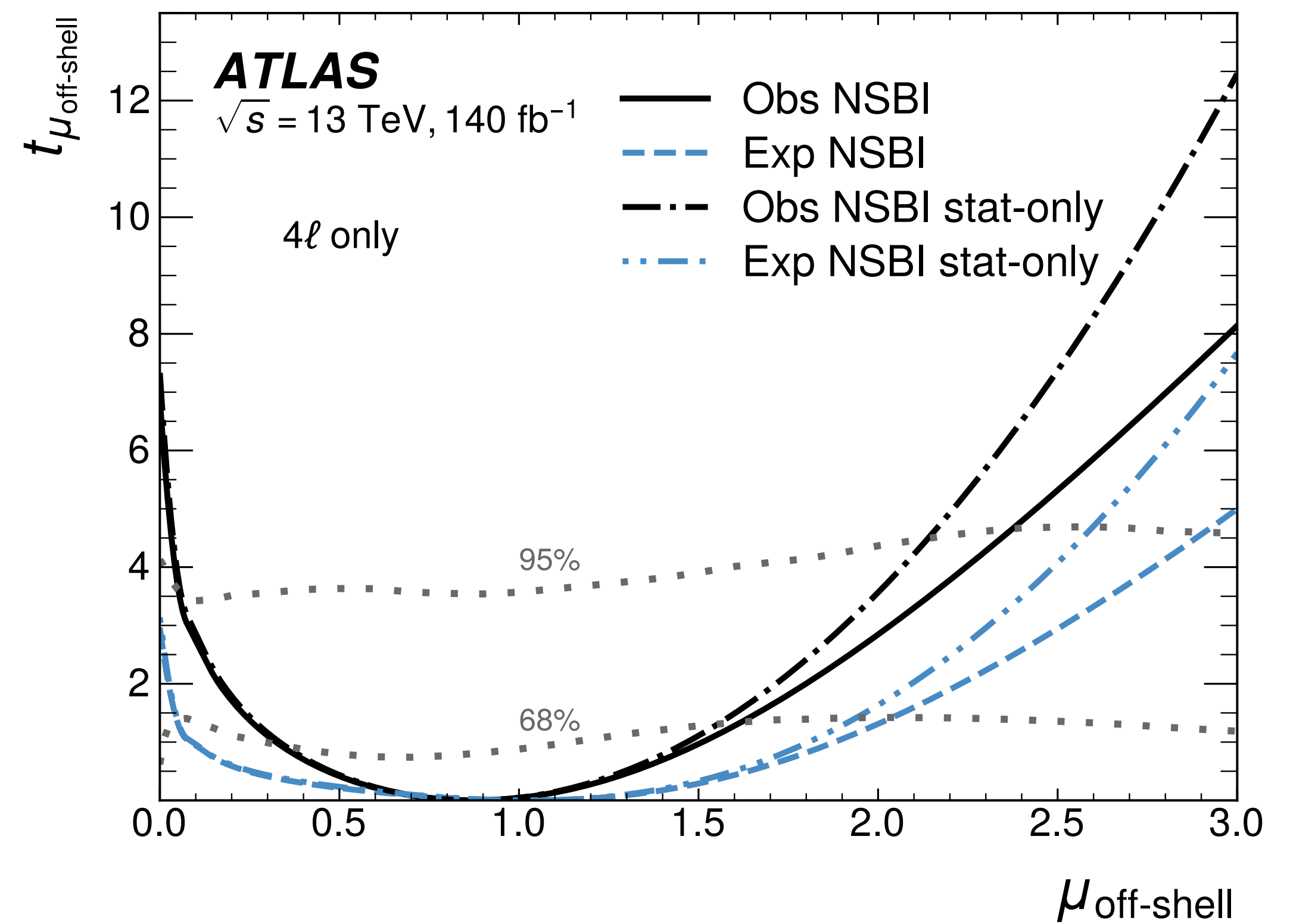
Nuisance parameters decrease sensitivity, as expected

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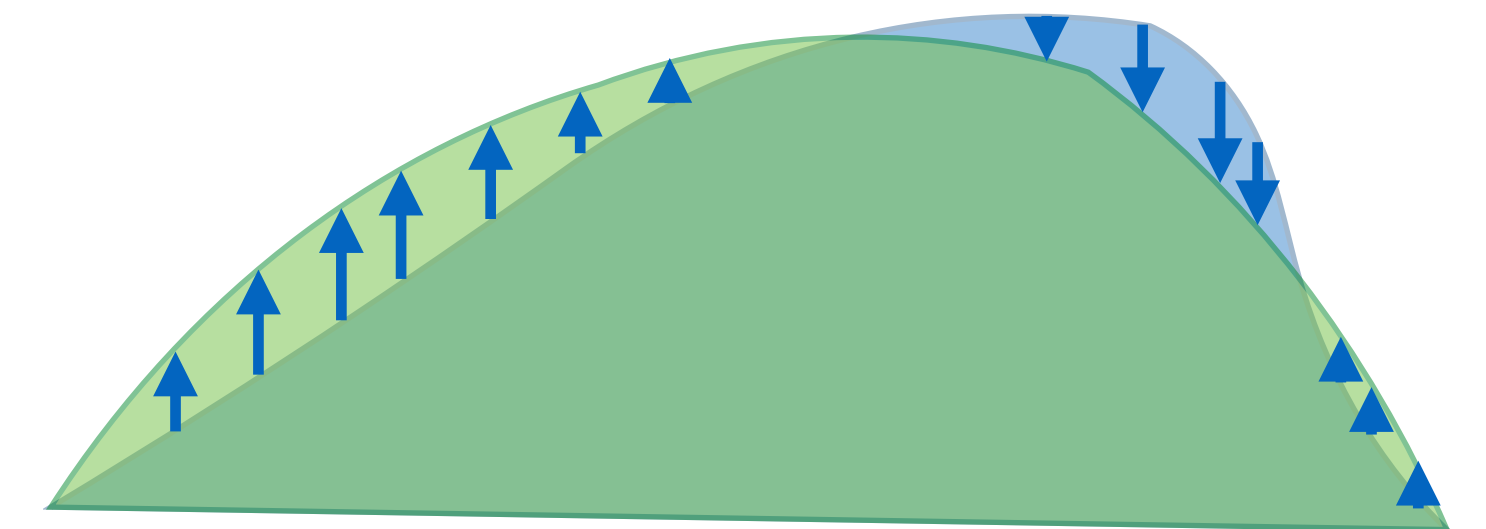
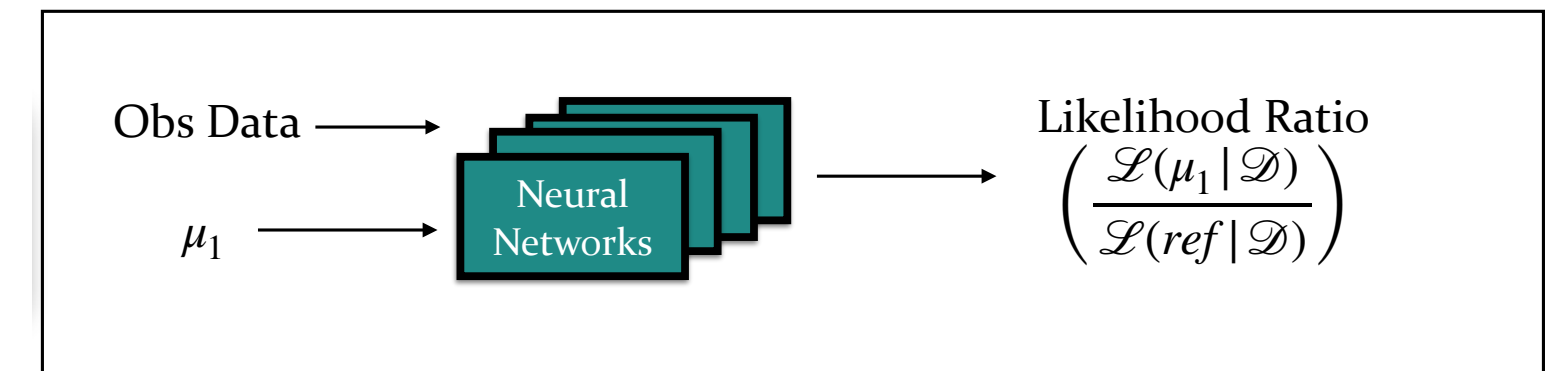
Observed data happens to provide stronger than expected constrains for both hist and NSBI (consistent)

Full results in [backup](#)

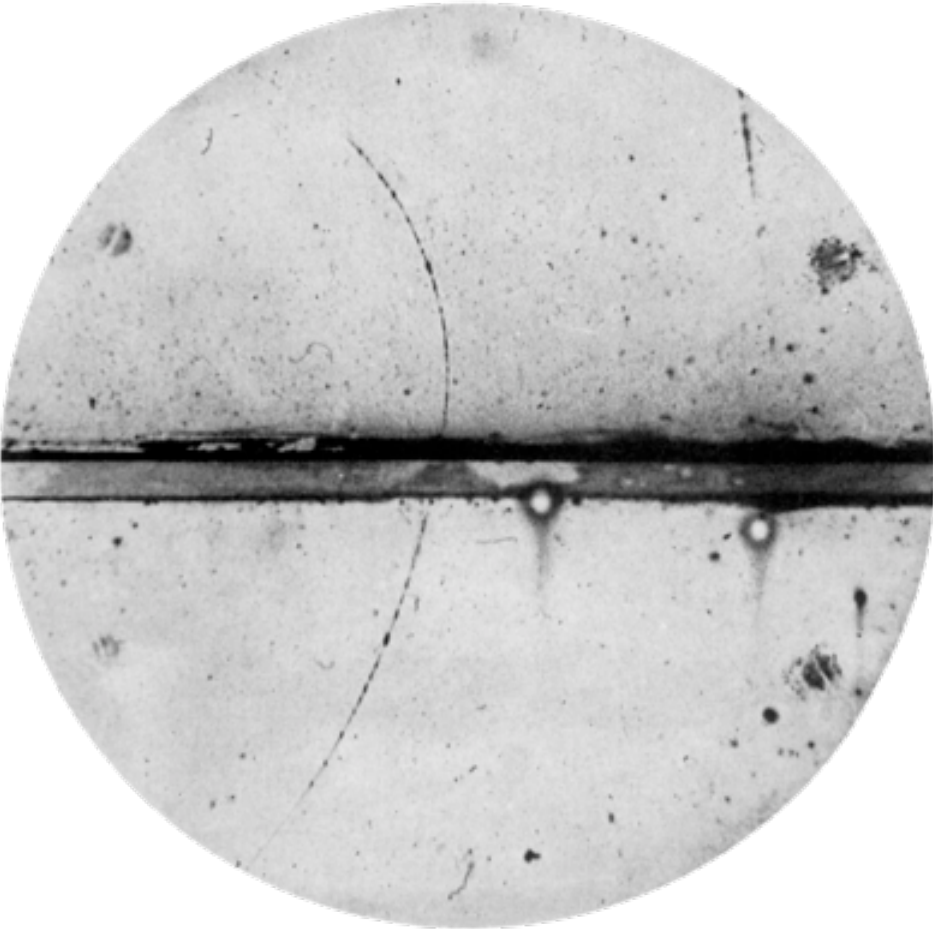
Nuisance parameters decrease sensitivity, as expected

Summary

- Quantum interference breaks assumptions in traditional statistical methods at LHC
- Neural inference can optimally handle these challenges:
 - Shown in phenomenology study
 - ATLAS developed method for deployment including systematics
 - Re-analysed Run 2 data and achieved a dramatic improvement in sensitivity ($H \rightarrow 4l$)
- NSBI has wide-ranging applications, in particle physics, astrophysics and beyond!
- Weaknesses: Same as traditional analyses (systematics, training statistics)
 - Developed diagnostic tools to identify issues



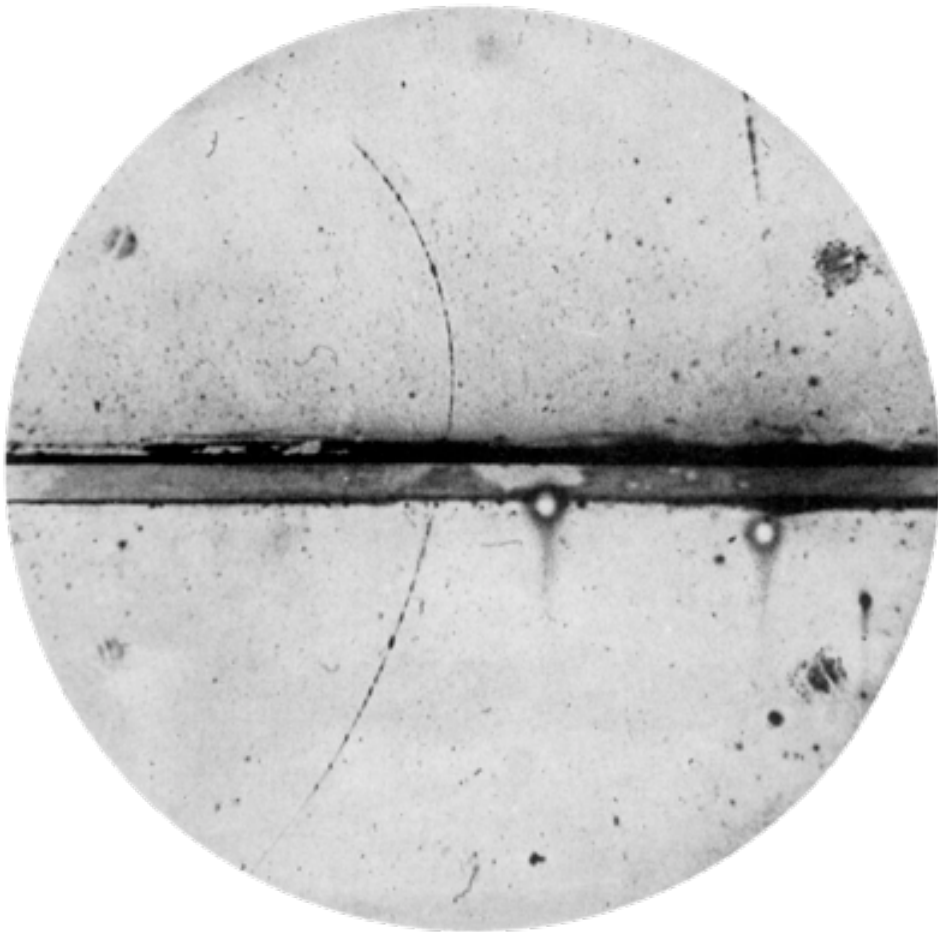
Positron discovery (1930s)



Single event

Positron discovery (1930s)

Top quark discovery (1990s)



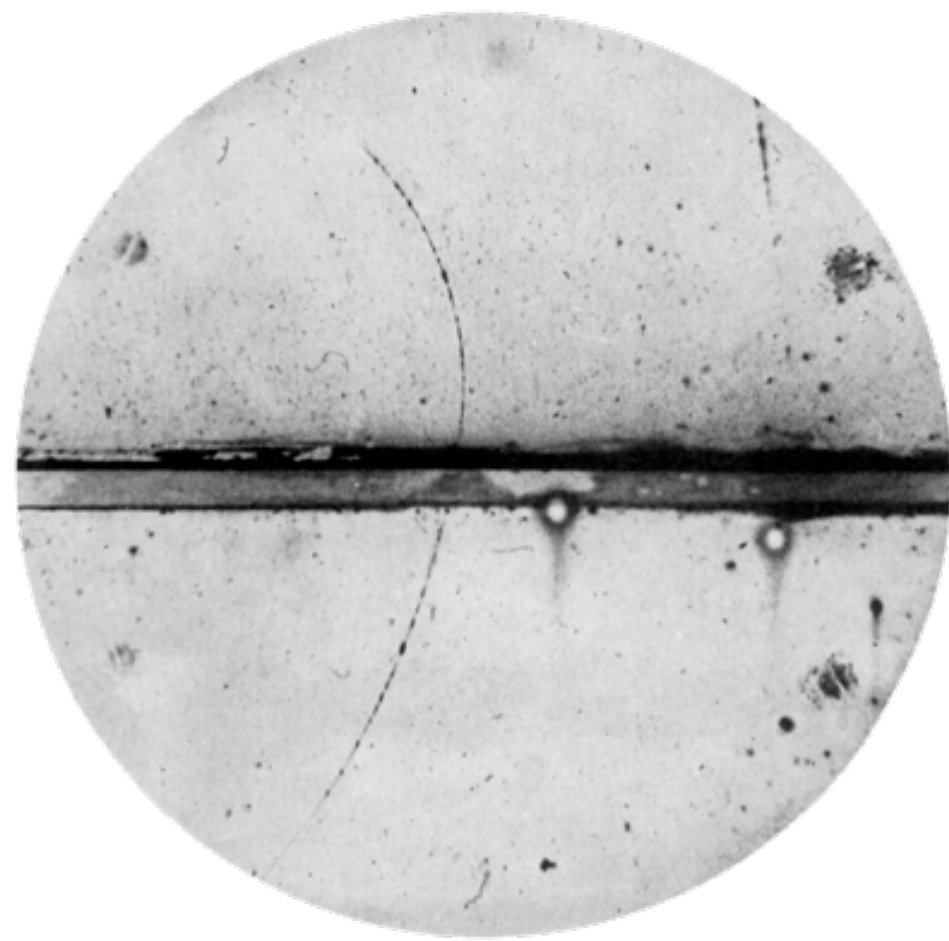
Channel:	SVX
observed	27 tags
expected background	6.7 ± 2.1
background probability	2×10^{-5}

Single event

Multiple events:
Cut-and-count



Positron discovery (1930s)



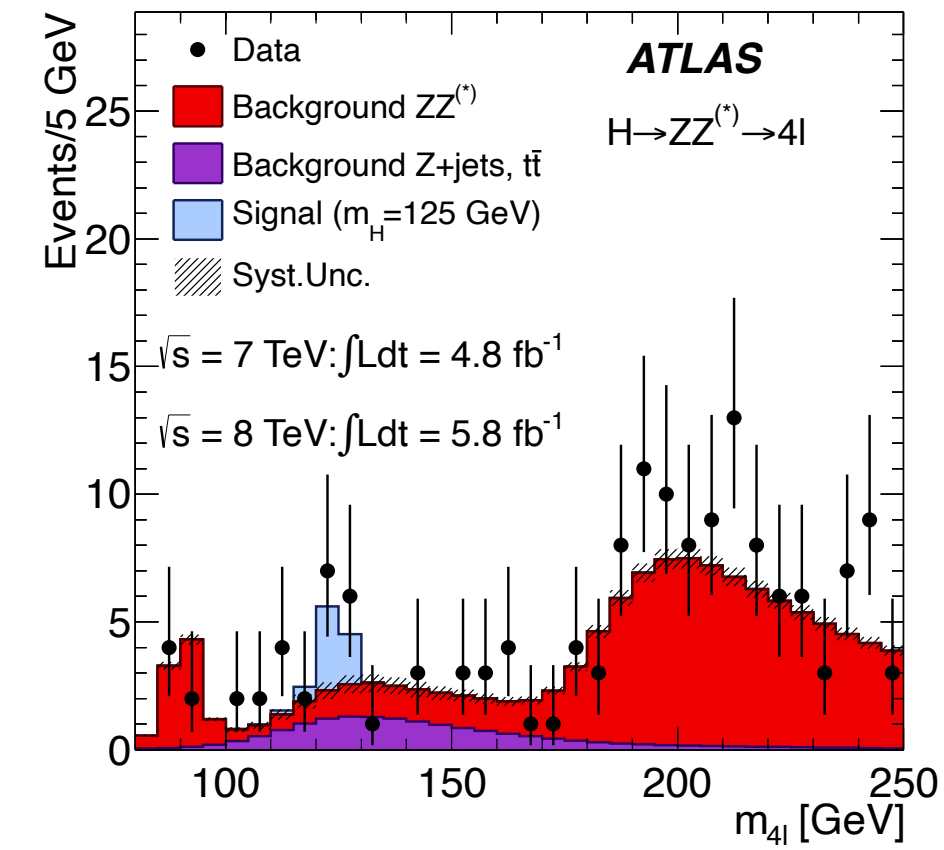
Single event

Top quark discovery (1990s)

Channel:	SVX
observed	27 tags
expected background	6.7 ± 2.1
background probability	2×10^{-5}

Multiple events:
Cut-and-count

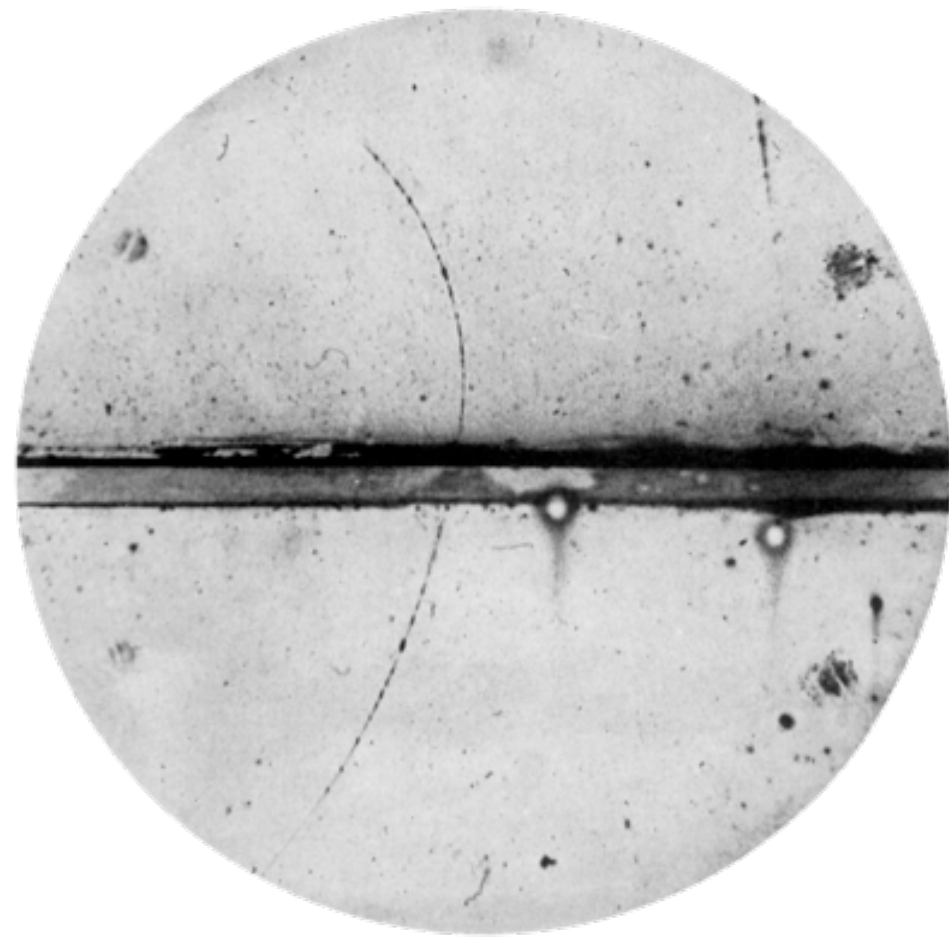
Higgs boson discovery (2010s)



Shape information:
Histogram



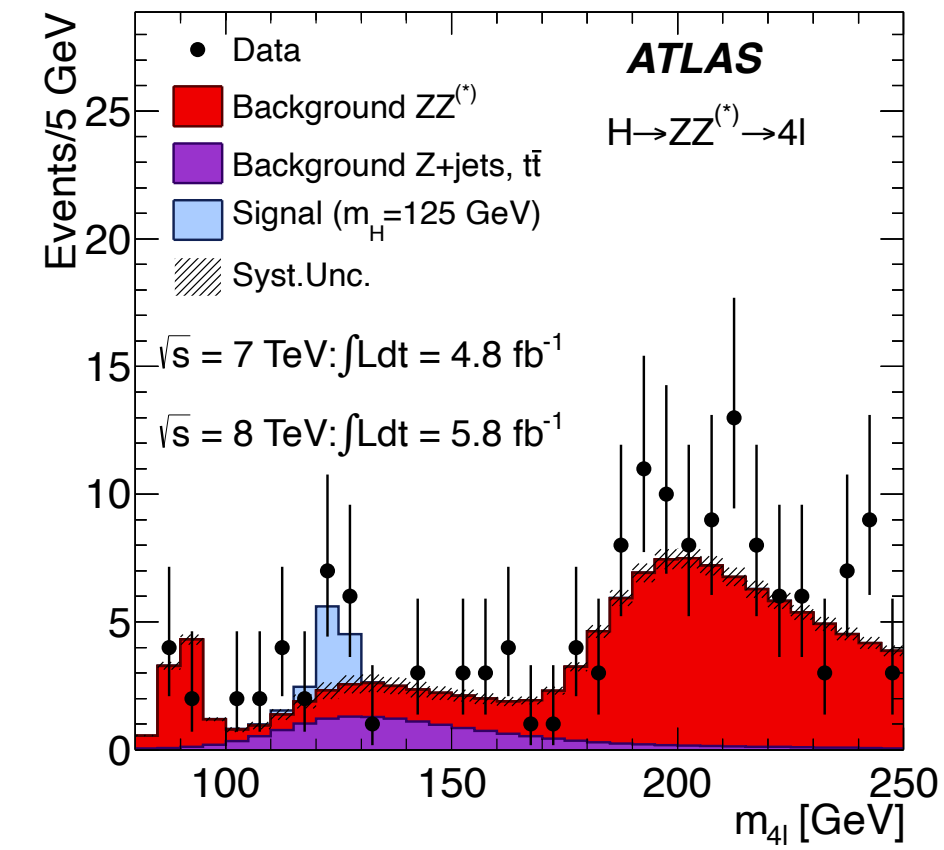
Positron discovery (1930s)



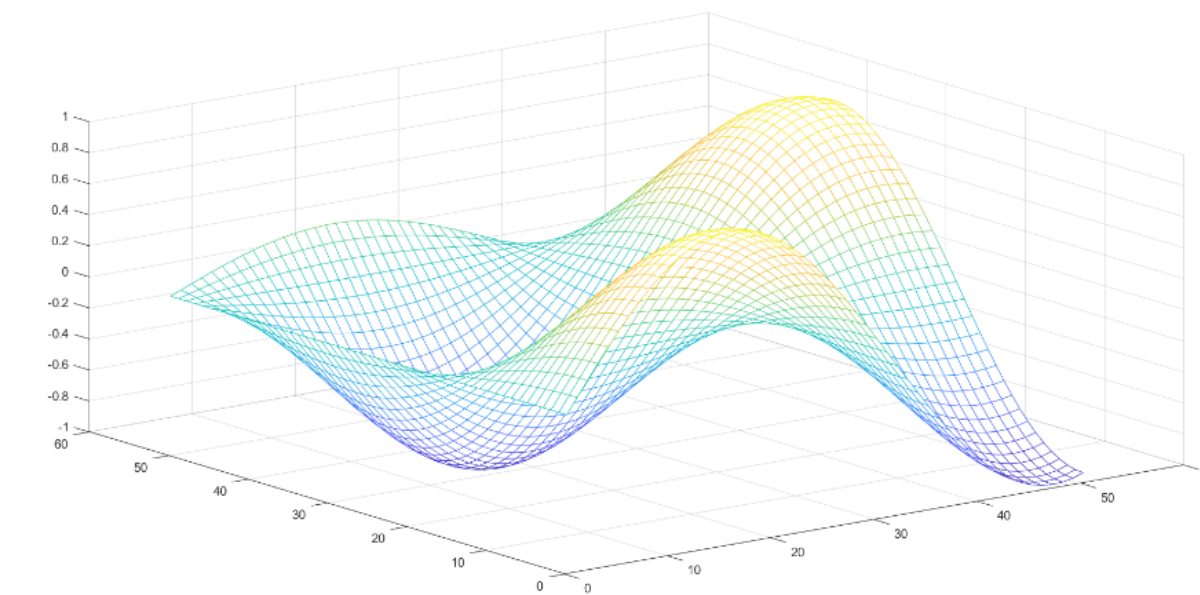
Top quark discovery (1990s)

Channel:	SVX
observed	27 tags
expected background	6.7 ± 2.1
background probability	2×10^{-5}

Higgs boson discovery (2010s)



Future discovery (2020s ?)



Single event

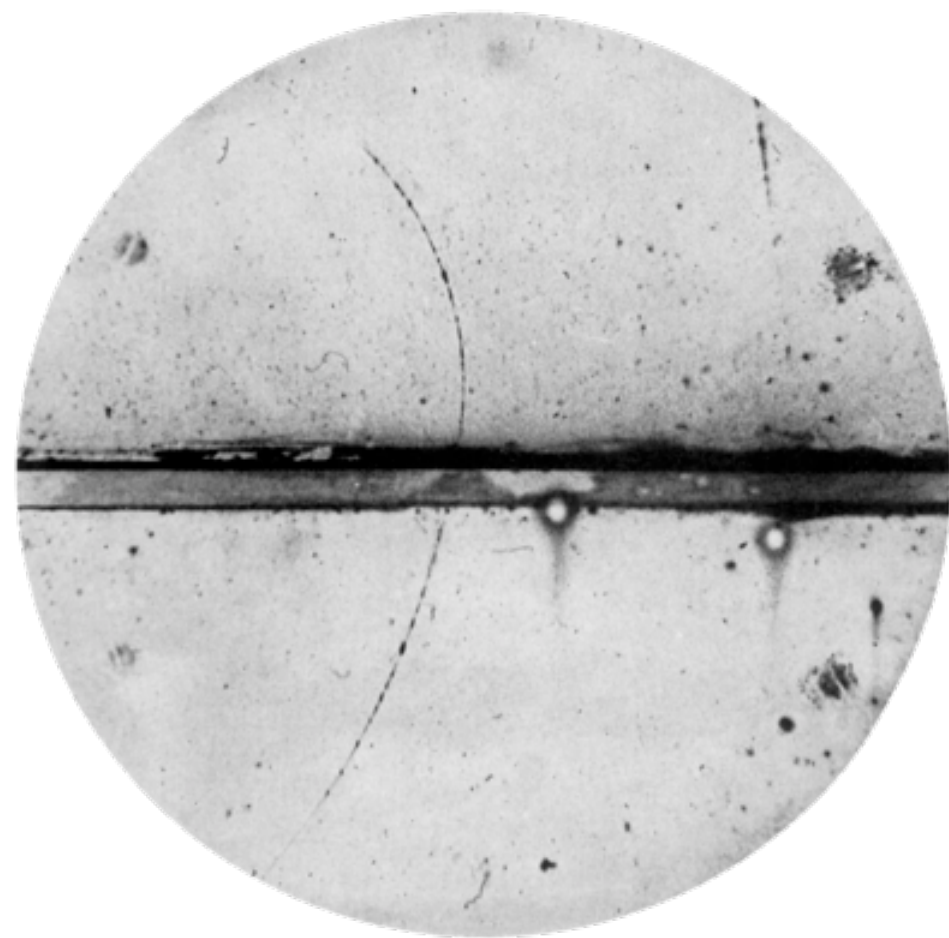
Multiple events:
Cut-and-count

Shape information:
Histogram

High-dim shape information,
continuous (i.e. unbinned):
Neural inference



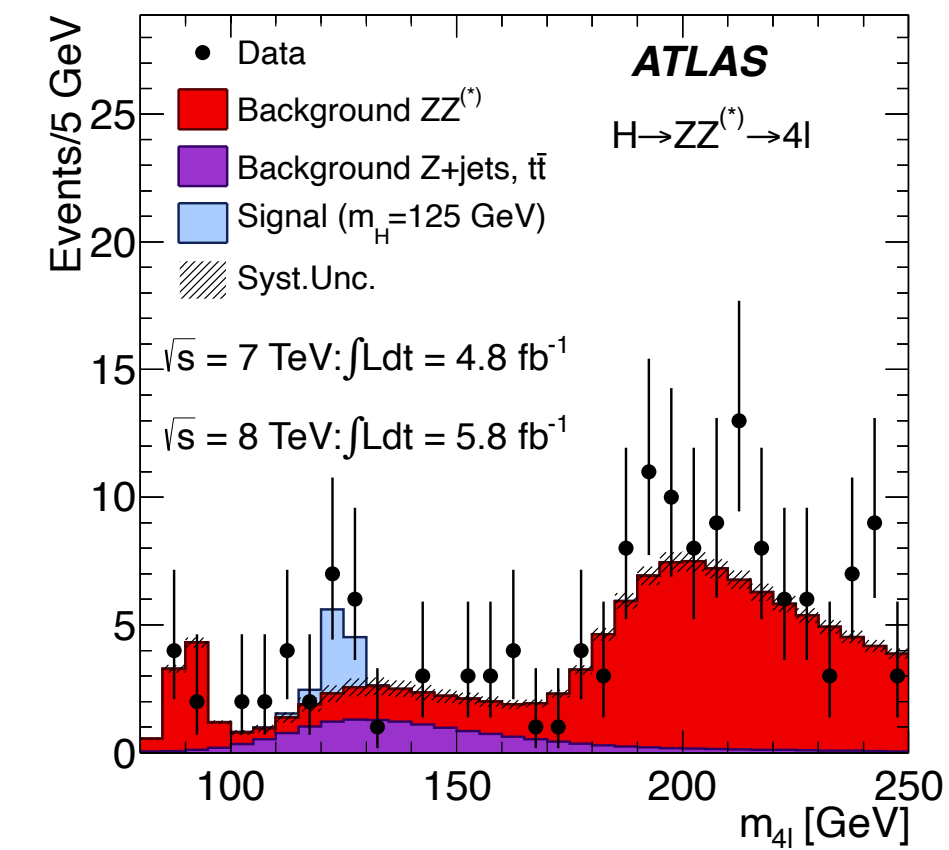
Positron discovery (1930s)



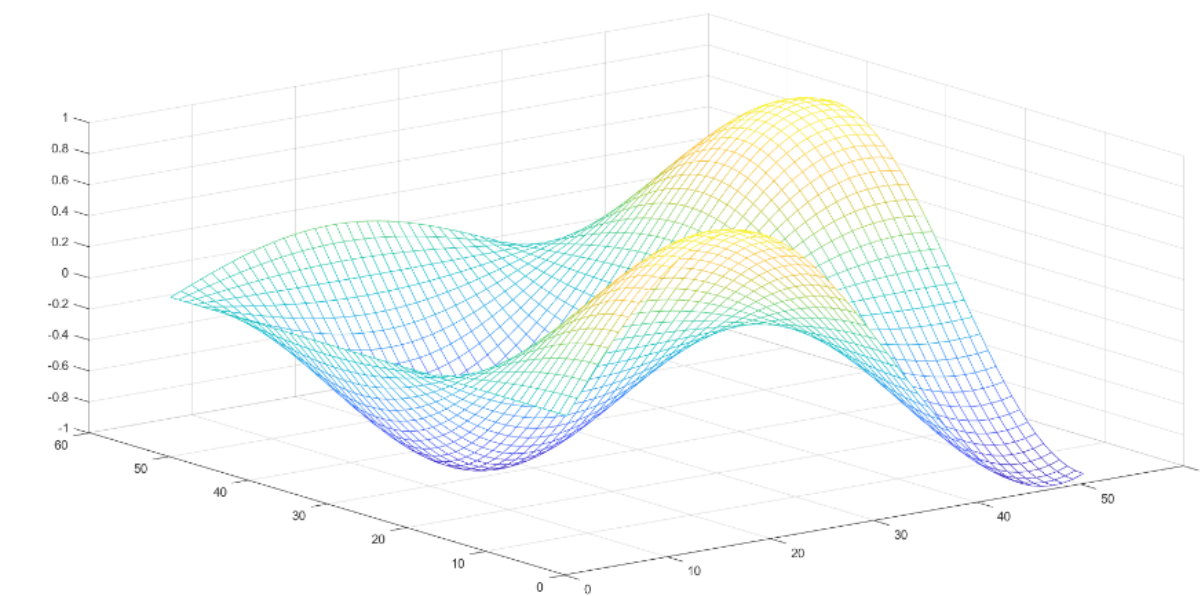
Top quark discovery (1990s)

Channel:	SVX
observed	27 tags
expected background	6.7 ± 2.1
background probability	2×10^{-5}

Higgs boson discovery (2010s)



Future discovery (2020s ?)



Single event

Multiple events:
Cut-and-count

Shape information:
Histogram

High-dim shape information,
continuous (i.e. unbinned):
Neural inference

Thank you !

Reference Sample

A combination of signal samples, to ensure non-zero probability in entire region of analysis
Does not have to be physical!

$$p_{\text{ref}}(x_i) = \frac{1}{\sum_k v_k} \sum_k^{C_{\text{signals}}} v_k \cdot p_k(x_i)$$

\Rightarrow In our dataset, $p_{\text{ref}}(\cdot) = p_S(\cdot)$

Choice of $p_{\text{ref}}(\cdot)$ can be made purely on numerical stability of training, as it drops out in profile step

$$t_\mu = -2 \ln \left(\frac{L_{\text{full}}(\mu, \hat{\alpha}) / \cancel{L_{\text{ref}}}}{L_{\text{full}}(\hat{\mu}, \hat{\alpha}) / \cancel{L_{\text{ref}}}} \right)$$

Dealing with negative weighted events

$$w_i^{toy} = \text{Poisson}(w_i^{Asimov})$$

Simulated samples include events with negative weights due to the way we calculate QFT higher order effects

Use a positive weighted sample instead:

1. Start from a positive weighted reference sample
2. Re-weight it to intended parameter point in μ, α
3. Throw toys from this sample

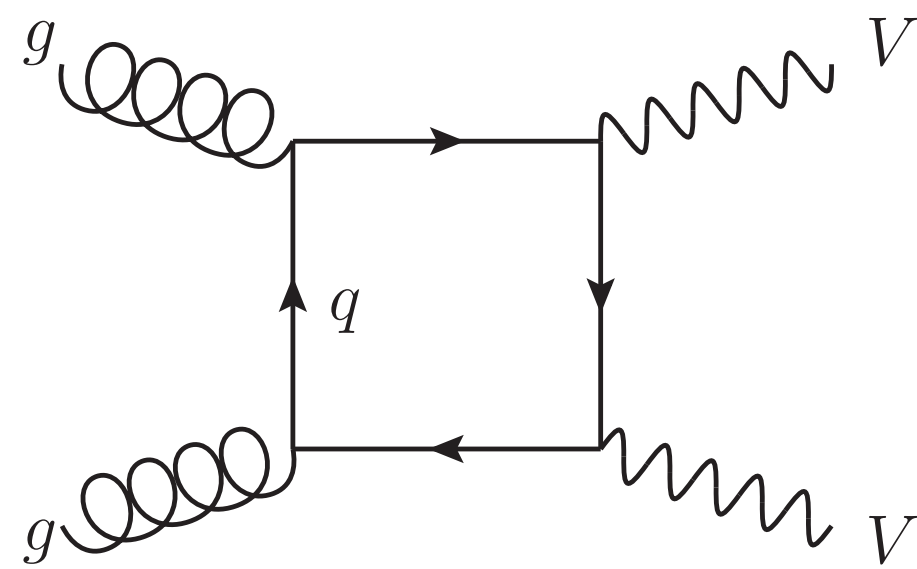
$$w_i^{\text{rwt-ref}} \rightarrow w_i^{\text{Asimov}}(\mu, \alpha) = \frac{v(\mu, \alpha)}{v_{\text{rwt-ref}}} \cdot \frac{p(x_i | \mu, \alpha)}{p_{\text{rwt-ref}}(x_i)} \cdot w_i^{\text{rwt-ref}}$$

Non-linear problem

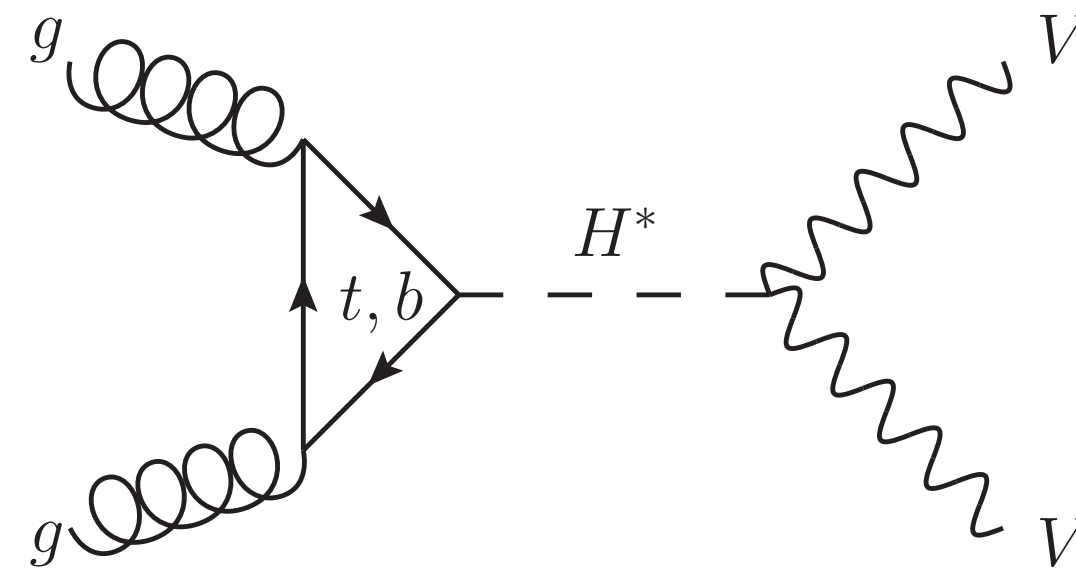
hal-02971995v3: Ghosh et al.

$$P(X) = |M_s(X) + M_b(X)|^2 = \underbrace{|M_s(X)|^2}_{P_s(X)} + \underbrace{|M_b(X)|^2}_{P_b(X)} + \underbrace{2 \operatorname{Re}(\overline{M_s(X)} M_b(X))}_{P_i(X)}$$

This term is negative



gg Background



ggF Signal

Scale by signal strength μ :

$$|M_s(X)|^2 \rightarrow |\sqrt{\mu} \cdot M_s(X)|^2,$$

$$P_{\text{scaled}}(X) = \mu \cdot P_s(X) + P_b(X) + \sqrt{\mu} \cdot P_i(X).$$

Combination with histogram analyses

$$\frac{L_{\text{comb}}(\mu, \alpha)}{L_{\text{ref}}} = \frac{L_{\text{full}}(\mu, \alpha)}{L_{\text{ref}}} L_{\text{hist}}(\mu, \alpha)$$

Calculating pulls and impacts in JAX

Hessian:

$$C_{nm} = \left[\frac{1}{2} \frac{\partial^2 \lambda}{\partial \alpha_n \partial \alpha_m} (\hat{\mu}, \hat{\alpha}) \right]^{-1}$$

$$\lambda(\mu, \alpha) = -2 \ln(L_{full}(\mu, \alpha) / L_{ref})$$

Pulls:

$$\frac{\hat{\alpha}_k - \alpha_k^0}{\sqrt{C_{kk}}}$$

Post-fit Impact:

$$\begin{aligned} \Gamma_k &= \frac{\partial \hat{\mu}}{\partial \alpha_k} \times \sqrt{C_{kk}} \\ &= - \left[\frac{\partial^2 \lambda}{\partial^2 \mu} (\hat{\mu}, \hat{\alpha}) \right]^{-1} \frac{\partial^2 \lambda}{\partial \mu \partial \alpha_k} (\hat{\mu}, \hat{\alpha}) \times \sqrt{C_{kk}}, \end{aligned}$$

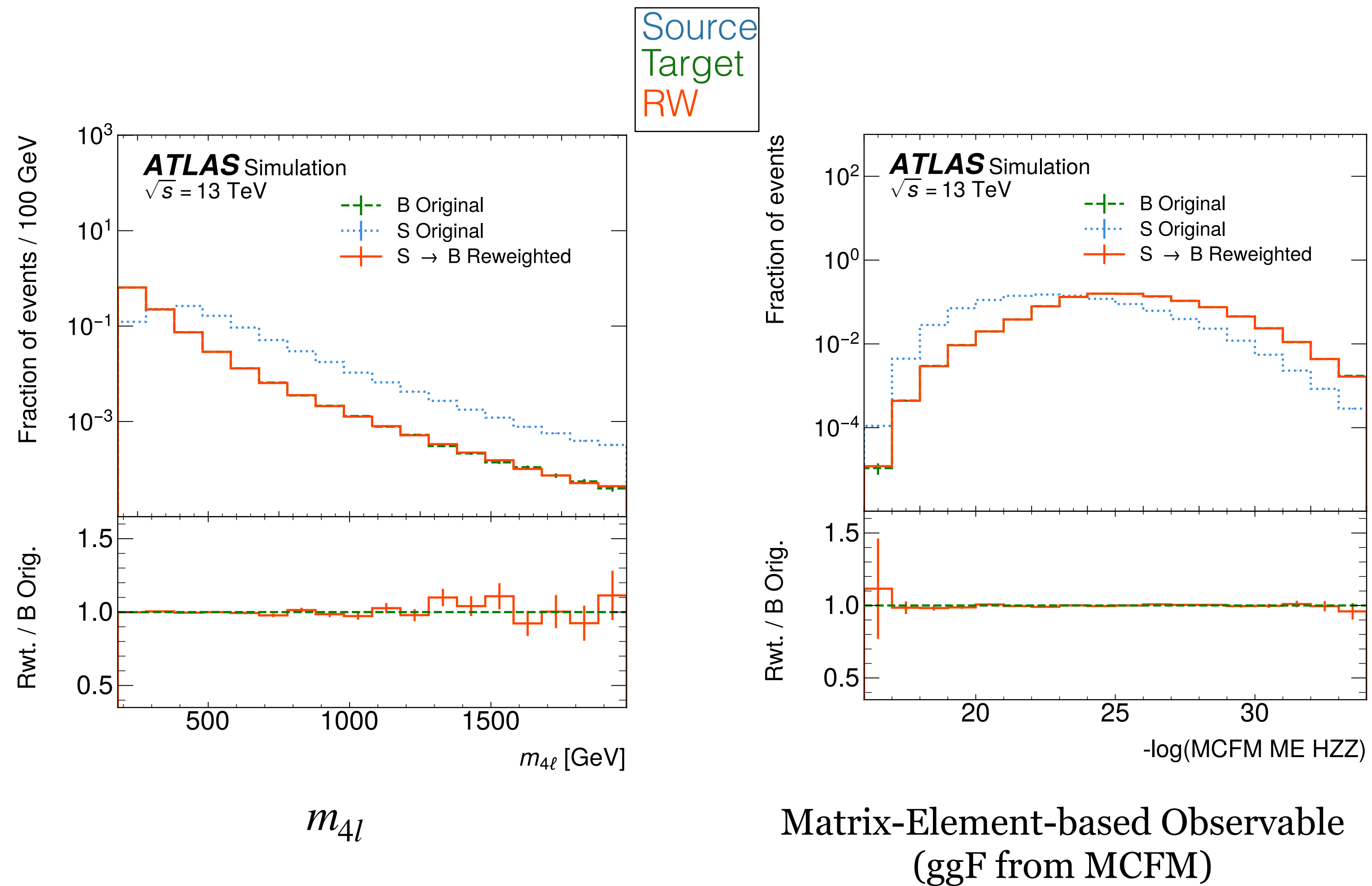
Vertical interpolation

$$G_j(\alpha_k) = \begin{cases} \left(\frac{v_j(\alpha_k^+)}{v_j(\alpha_k^0)} \right)^{\alpha_k} & \alpha_k > 1 \\ 1 + \sum_{n=1}^6 c_n \alpha_k^n & -1 \leq \alpha_k \leq 1 \\ \left(\frac{v_j(\alpha_k^-)}{v_j(\alpha_k^0)} \right)^{-\alpha_k} & \alpha_k < -1 \end{cases} \quad g_j(x_i, \alpha_k) = \begin{cases} (g_j(x_i, \alpha_k^+))^{\alpha_k} & \alpha_k > 1 \\ 1 + \sum_{n=1}^6 c_n \alpha_k^n & -1 \leq \alpha_k \leq 1 \\ (g_j(x_i, \alpha_k^-))^{-\alpha_k} & \alpha_k < -1 \end{cases}$$

With some continuity requirements

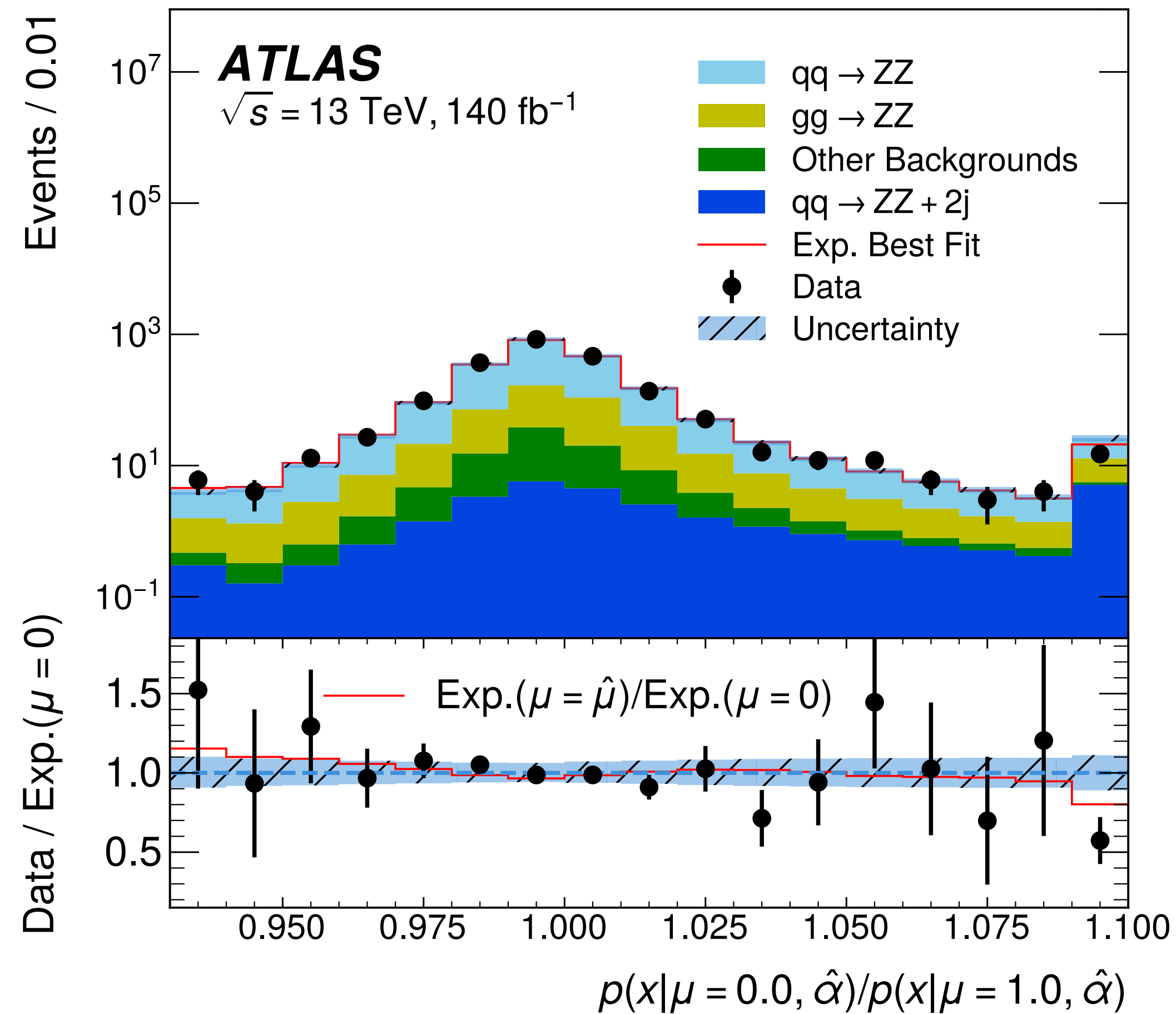
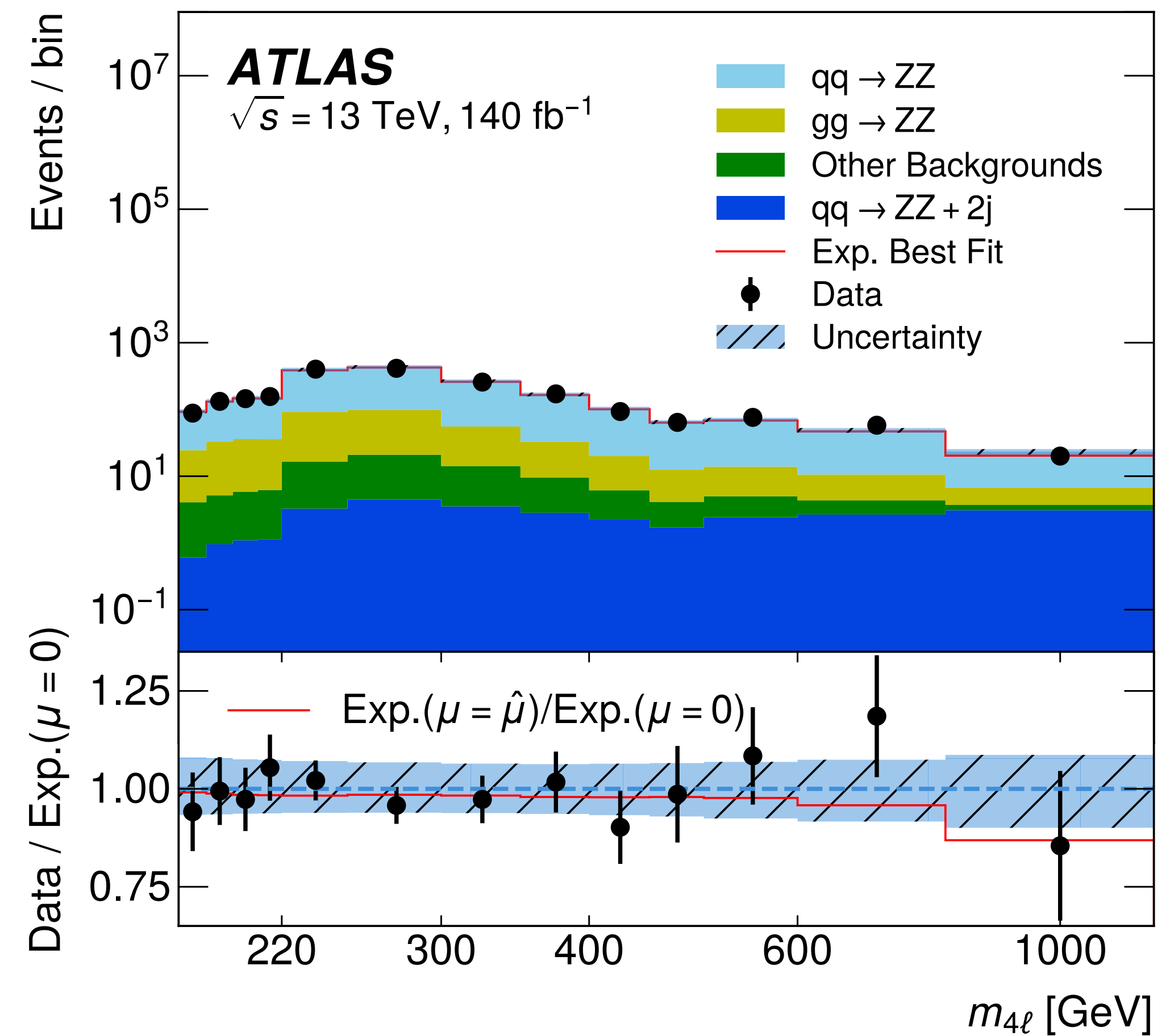
More diagnostics

Re-weight closures for B



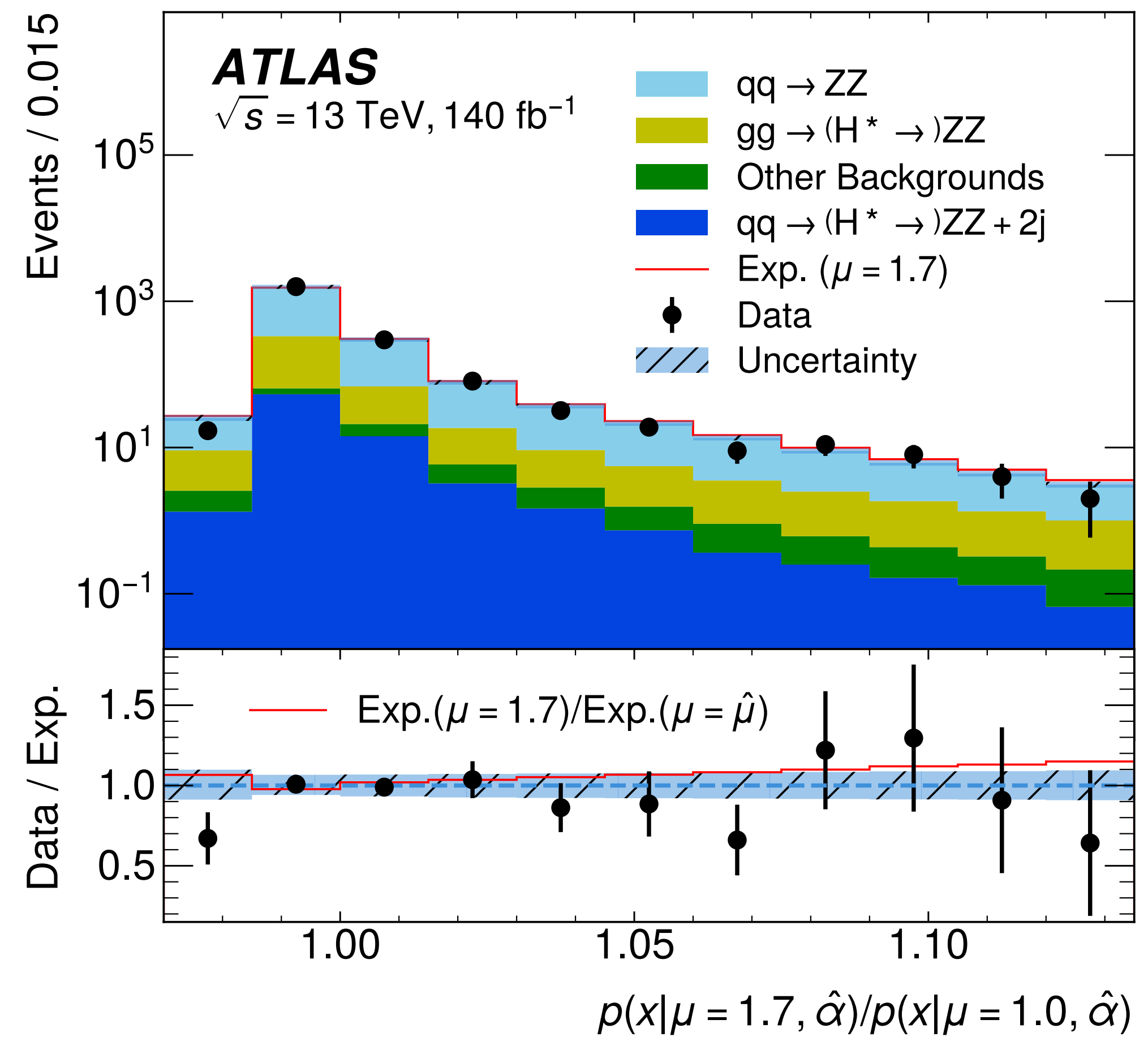
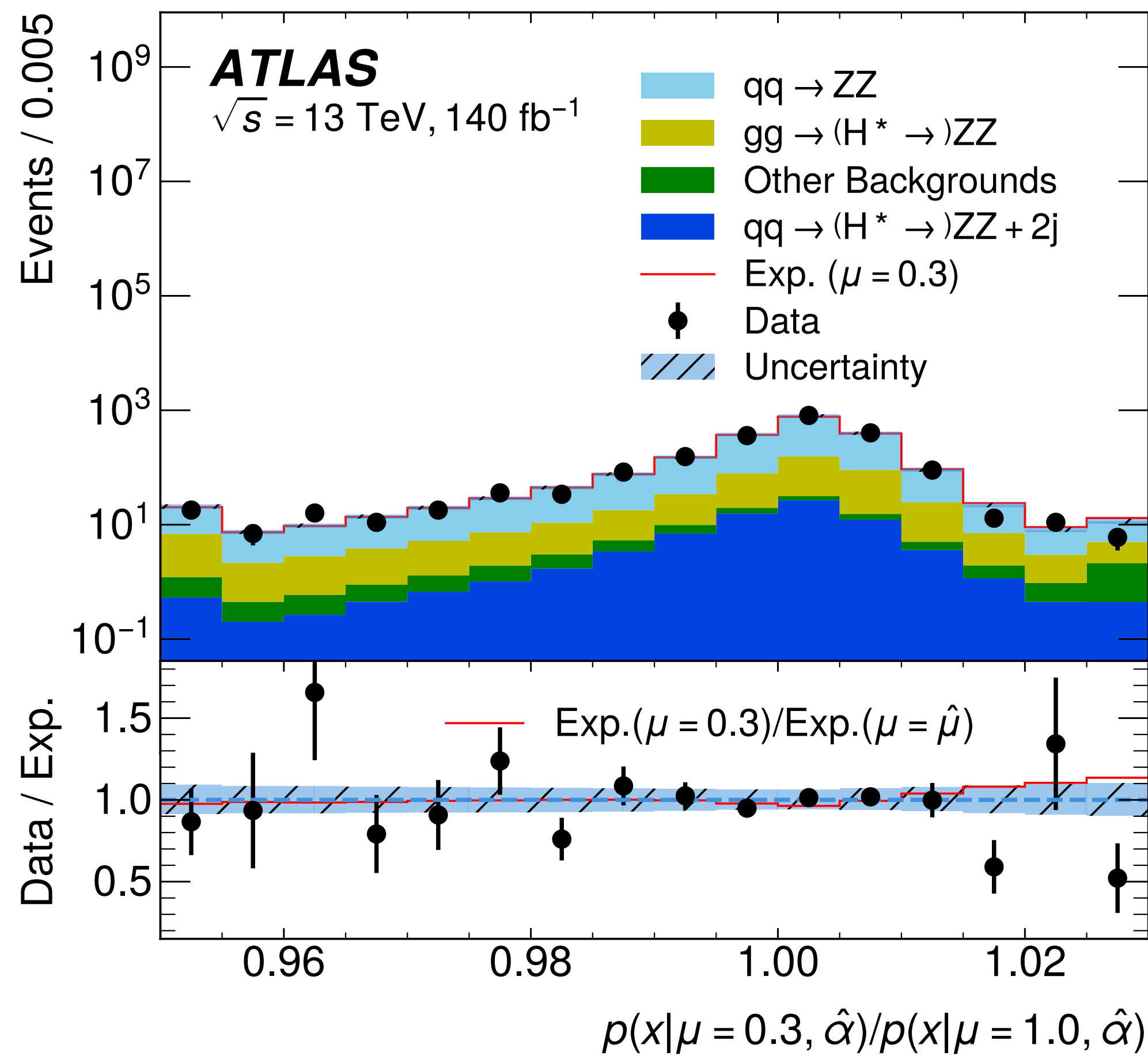
Data-MC validation

NN observable

 m_{4l} 

Data-MC validation

Different NN observables



Physics analysis results

Impact of nuisance parameters

Systematic Uncertainty Fixed	$\mu_{\text{off-shell}}$ Value at which $t_{\mu_{\text{off-shell}}} = 4$	
	NSBI analysis	Histogram-based
All (stat-only)	1.96	2.13
Parton shower uncertainty for $gg \rightarrow ZZ$ (normalization)	2.07	2.26
Parton shower uncertainty for $gg \rightarrow ZZ$ (shape)	2.12	2.29
NLO EW uncertainty for $q\bar{q} \rightarrow ZZ$	2.10	2.27
NLO QCD uncertainty for $gg \rightarrow ZZ$	2.09	2.29
Parton shower uncertainty for $q\bar{q} \rightarrow ZZ$ (shape)	2.12	2.29
Jet energy scale and resolution uncertainty	2.11	2.26
None (full result)	2.12	2.30

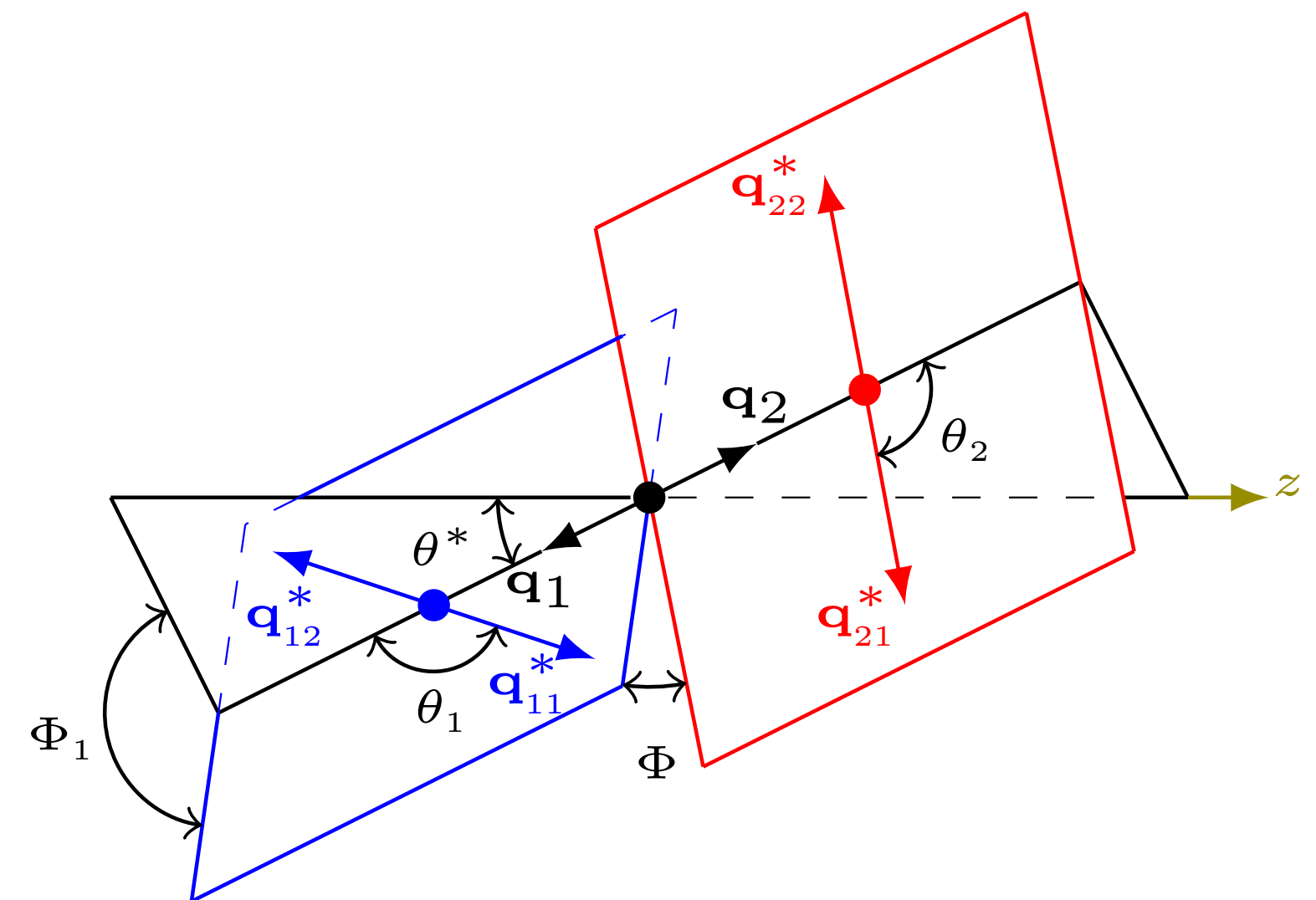
Full probability model, input variables

$$p(x|\mu_{\text{off-shell}}^{\text{ggF}}, \mu_{\text{off-shell}}^{\text{EW}}) = \frac{1}{\nu(\mu_{\text{off-shell}}^{\text{ggF}}, \mu_{\text{off-shell}}^{\text{EW}})} \times$$

$$\left[\mu_{\text{off-shell}}^{\text{ggF}} \nu_{\text{S}}^{\text{ggF}} p_{\text{S}}^{\text{ggF}}(x) + \sqrt{\mu_{\text{off-shell}}^{\text{ggF}}} \nu_{\text{I}}^{\text{ggF}} p_{\text{I}}^{\text{ggF}}(x) + \nu_{\text{B}}^{\text{ggF}} p_{\text{B}}^{\text{ggF}}(x) + \right.$$

$$\left. \mu_{\text{off-shell}}^{\text{EW}} \nu_{\text{S}}^{\text{EW}} p_{\text{S}}^{\text{EW}}(x) + \sqrt{\mu_{\text{off-shell}}^{\text{EW}}} \nu_{\text{I}}^{\text{EW}} p_{\text{I}}^{\text{EW}}(x) + \nu_{\text{B}}^{\text{EW}} p_{\text{B}}^{\text{EW}}(x) + \nu_{\text{NI}} p_{\text{NI}}(x) \right],$$

Variable	Definition
$m_{4\ell}$	quadruplet mass
m_{Z1}	Z_1 mass
m_{Z2}	Z_2 mass
$\cos \theta^*$	cosine of the Higgs boson decay angle [$\mathbf{q}_1 \cdot \mathbf{n}_z / \mathbf{q}_1 $]
$\cos \theta_1$	cosine of the Z_1 decay angle [$-(\mathbf{q}_2) \cdot \mathbf{q}_{11} / (\mathbf{q}_2 \cdot \mathbf{q}_{11})$]
$\cos \theta_2$	cosine of the Z_2 decay angle [$-(\mathbf{q}_1) \cdot \mathbf{q}_{21} / (\mathbf{q}_1 \cdot \mathbf{q}_{21})$]
Φ_1	Z_1 decay plane angle [$\cos^{-1}(\mathbf{n}_1 \cdot \mathbf{n}_{\text{sc}}) (\mathbf{q}_1 \cdot (\mathbf{n}_1 \times \mathbf{n}_{\text{sc}})) / (\mathbf{q}_1 \cdot \mathbf{n}_1 \times \mathbf{n}_{\text{sc}})$]
Φ	angle between Z_1, Z_2 decay planes [$\cos^{-1}(\mathbf{n}_1 \cdot \mathbf{n}_2) (\mathbf{q}_1 \cdot (\mathbf{n}_1 \times \mathbf{n}_2)) / (\mathbf{q}_1 \cdot \mathbf{n}_1 \times \mathbf{n}_2)$]
$p_T^{4\ell}$	quadruplet transverse momentum
$y^{4\ell}$	quadruplet rapidity
n_{jets}	number of jets in the event
m_{jj}	leading dijet system mass
$\Delta\eta_{jj}$	leading dijet system pseudorapidity
$\Delta\phi_{jj}$	leading dijet system azimuthal angle difference



Network architecture

Feed-forward dense networks

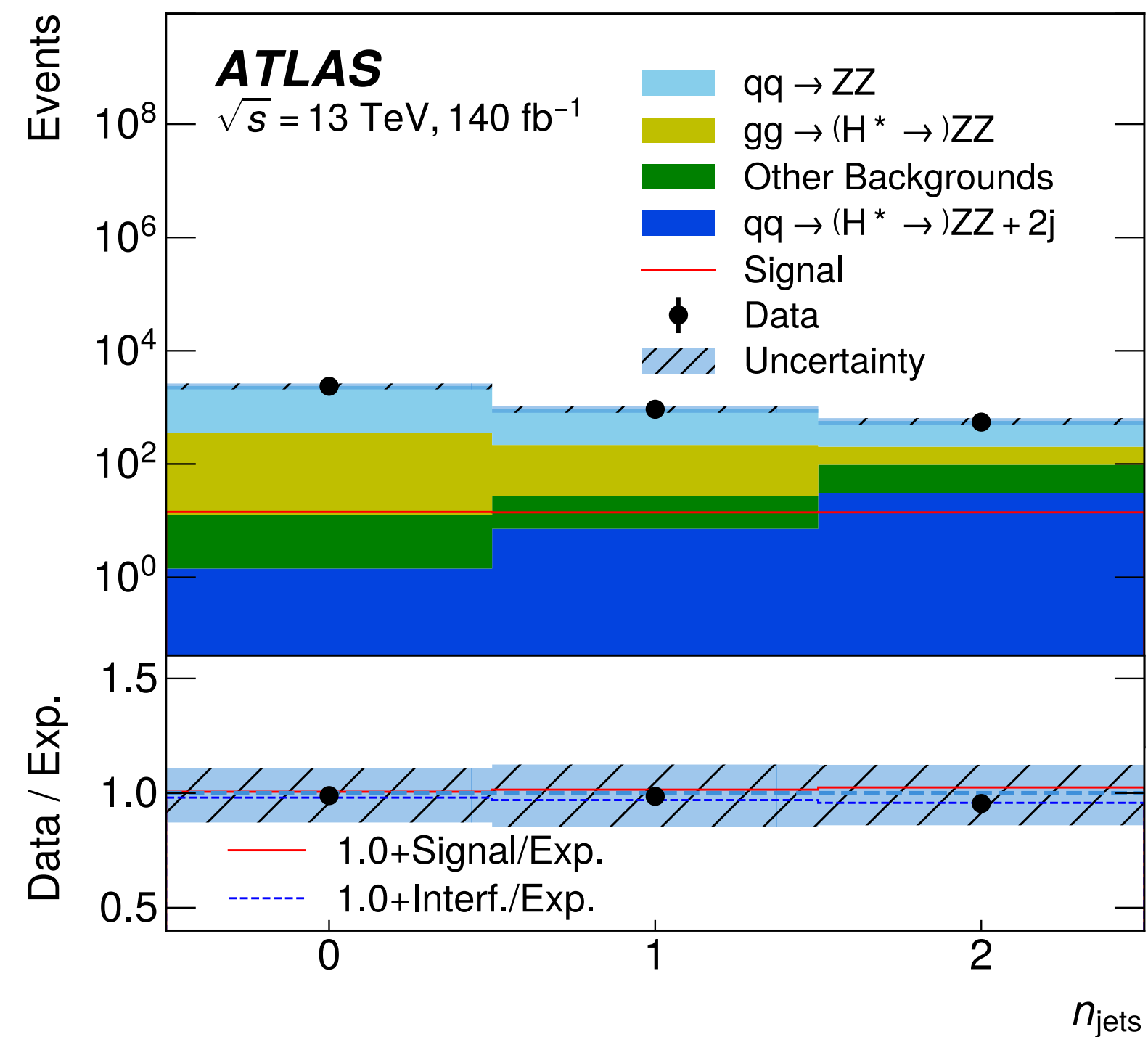
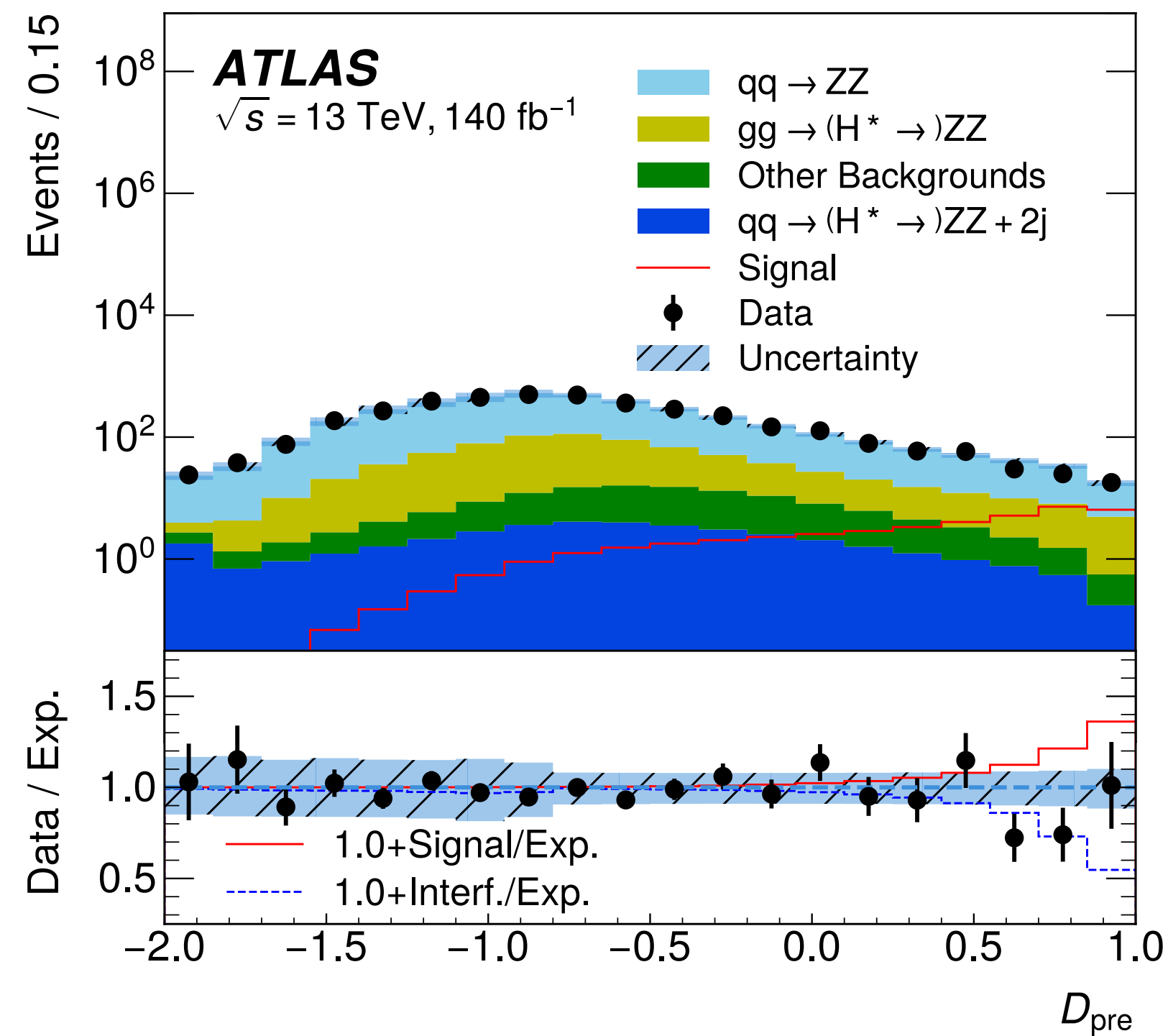
- 5 hidden layers with 1000 nodes
- Swish activation
- Single node output layer with sigmoid activation

Loss: Weighted binary cross-entropy

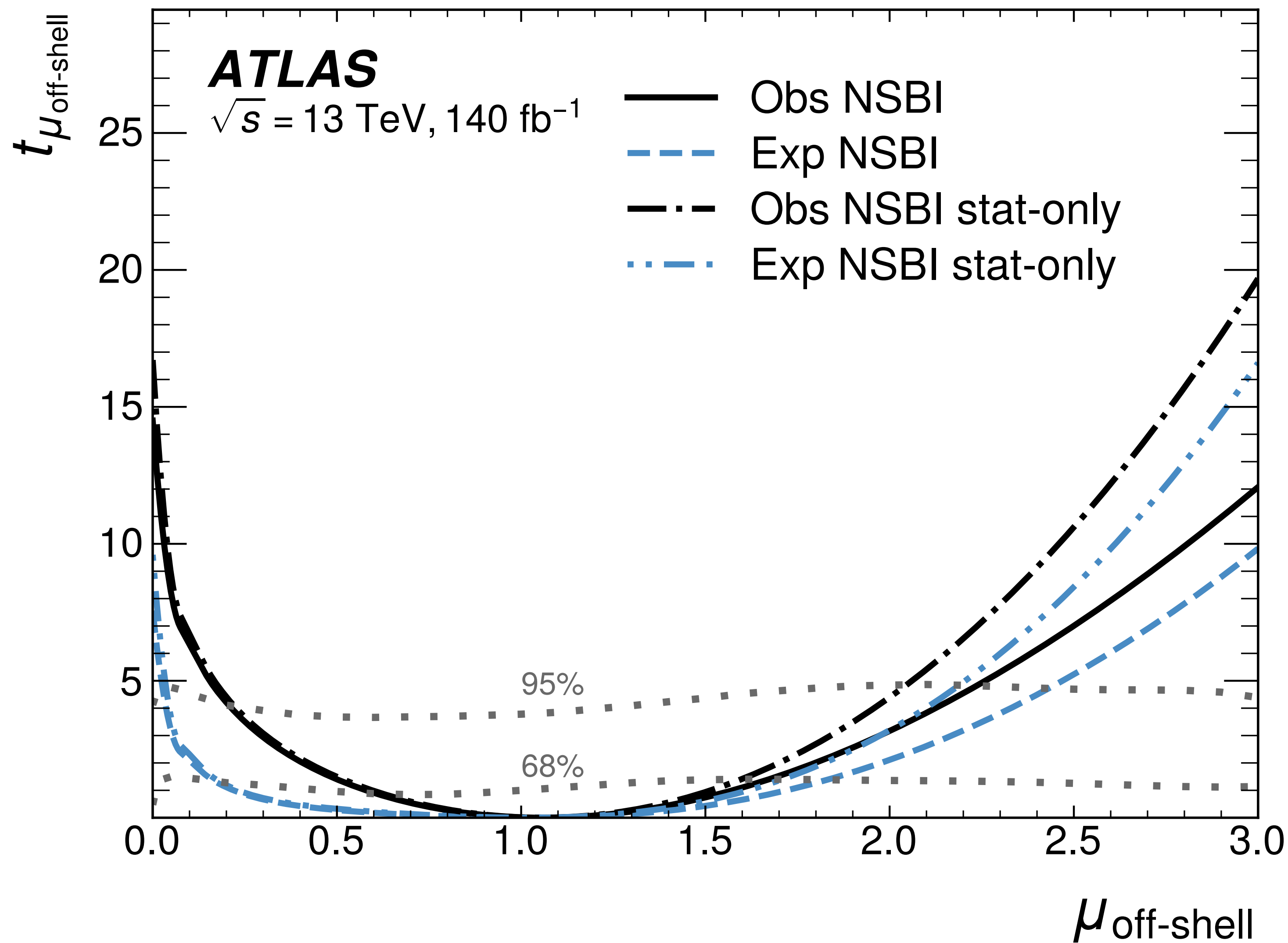
$O(10^4)$ networks takes approx 4000 GPU hours to train

Pre-selection region definition

$$D_{\text{pre}}(x) = \log \frac{s_{\text{pre}, S}^{\text{ggF}}(x) + s_{\text{pre}, S}^{\text{EW}}(x)}{s_{\text{pre}, B}^{\text{ggF}}(x) + s_{\text{pre}, B}^{\text{EW}}(x) + s_{\text{pre}, q\bar{q}ZZ}(x)},$$

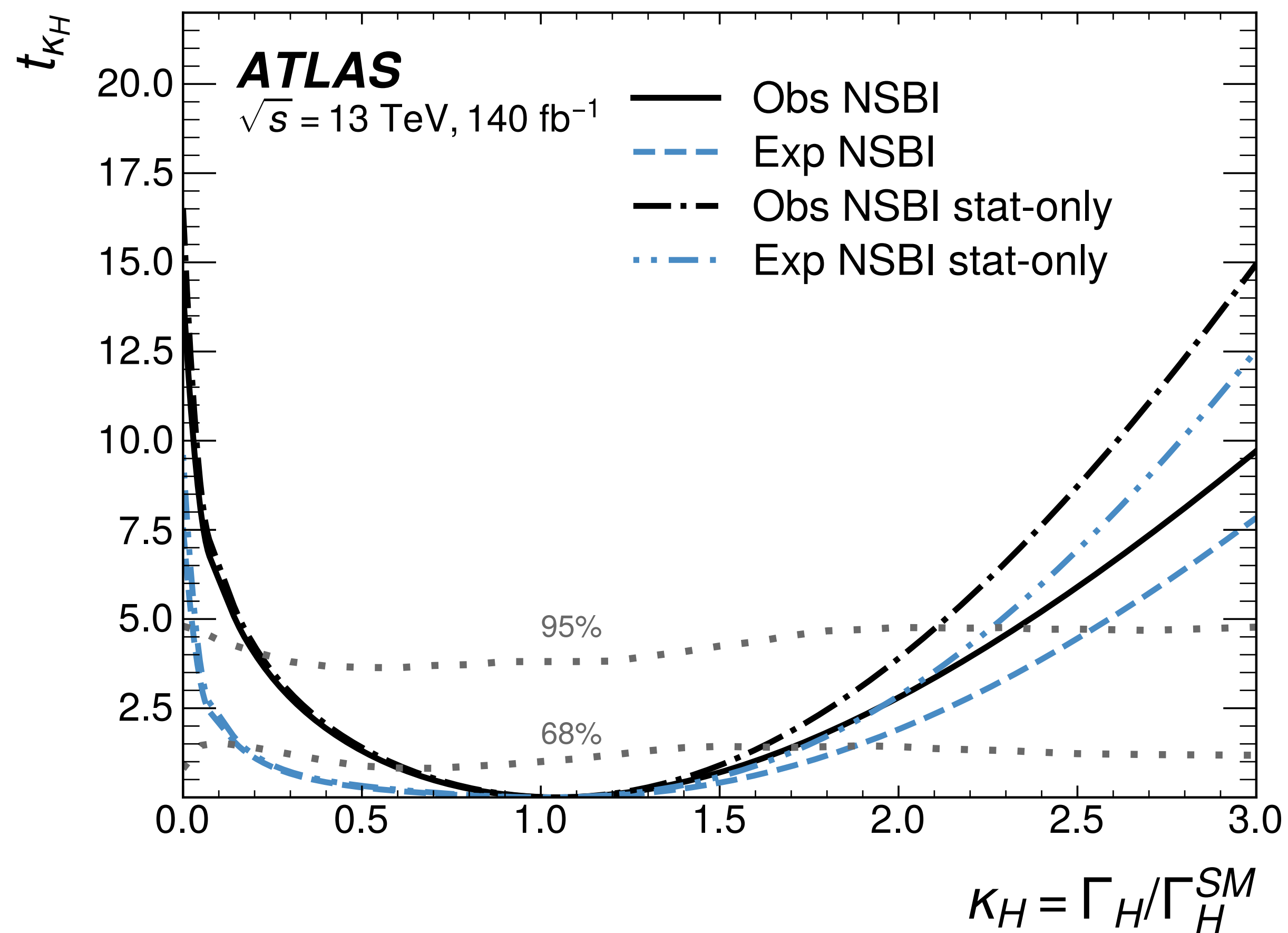


Result after combination with $ll\nu\nu$



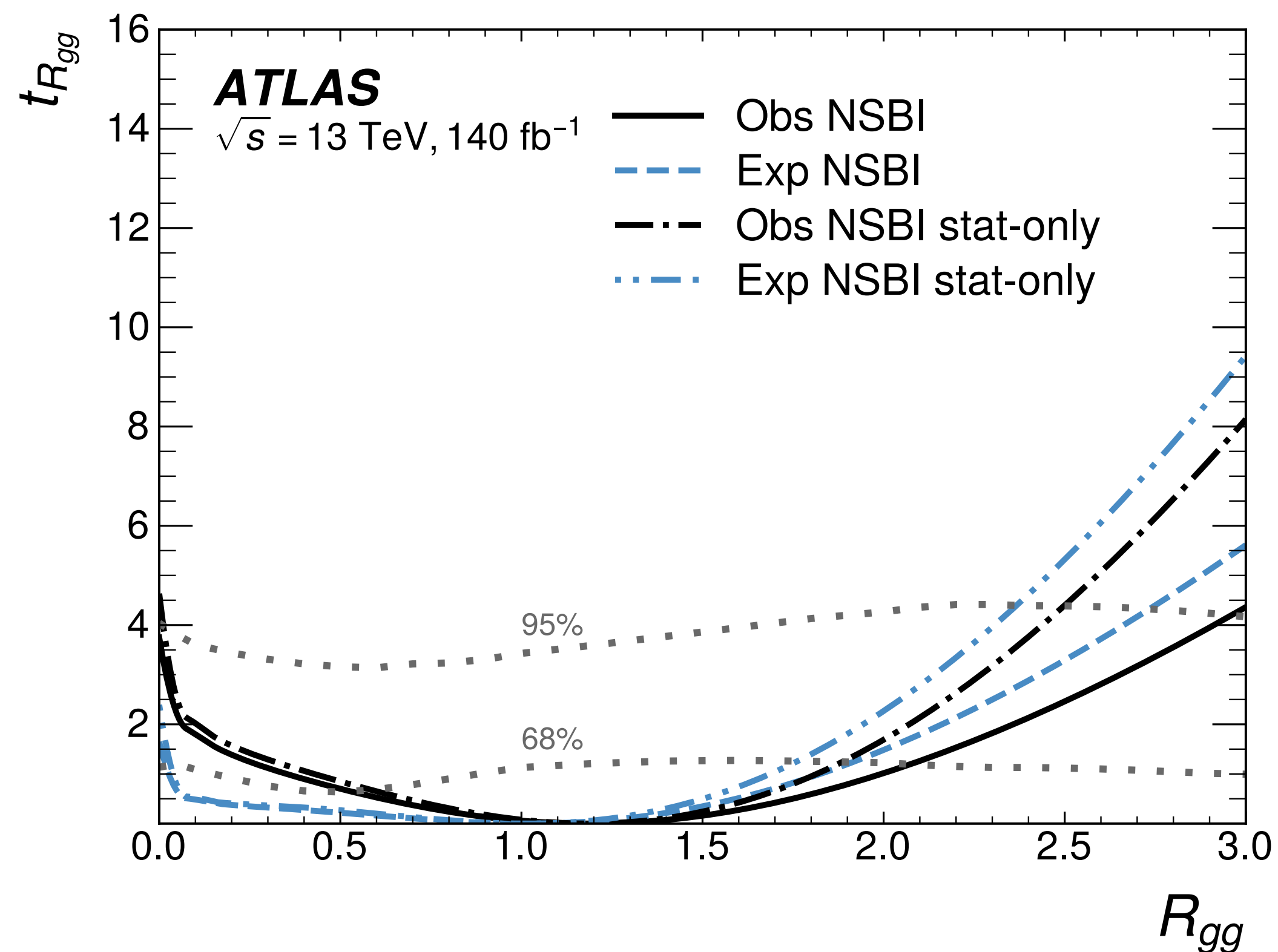
$ll\nu\nu$ dominates sensitivity

Width interpretation

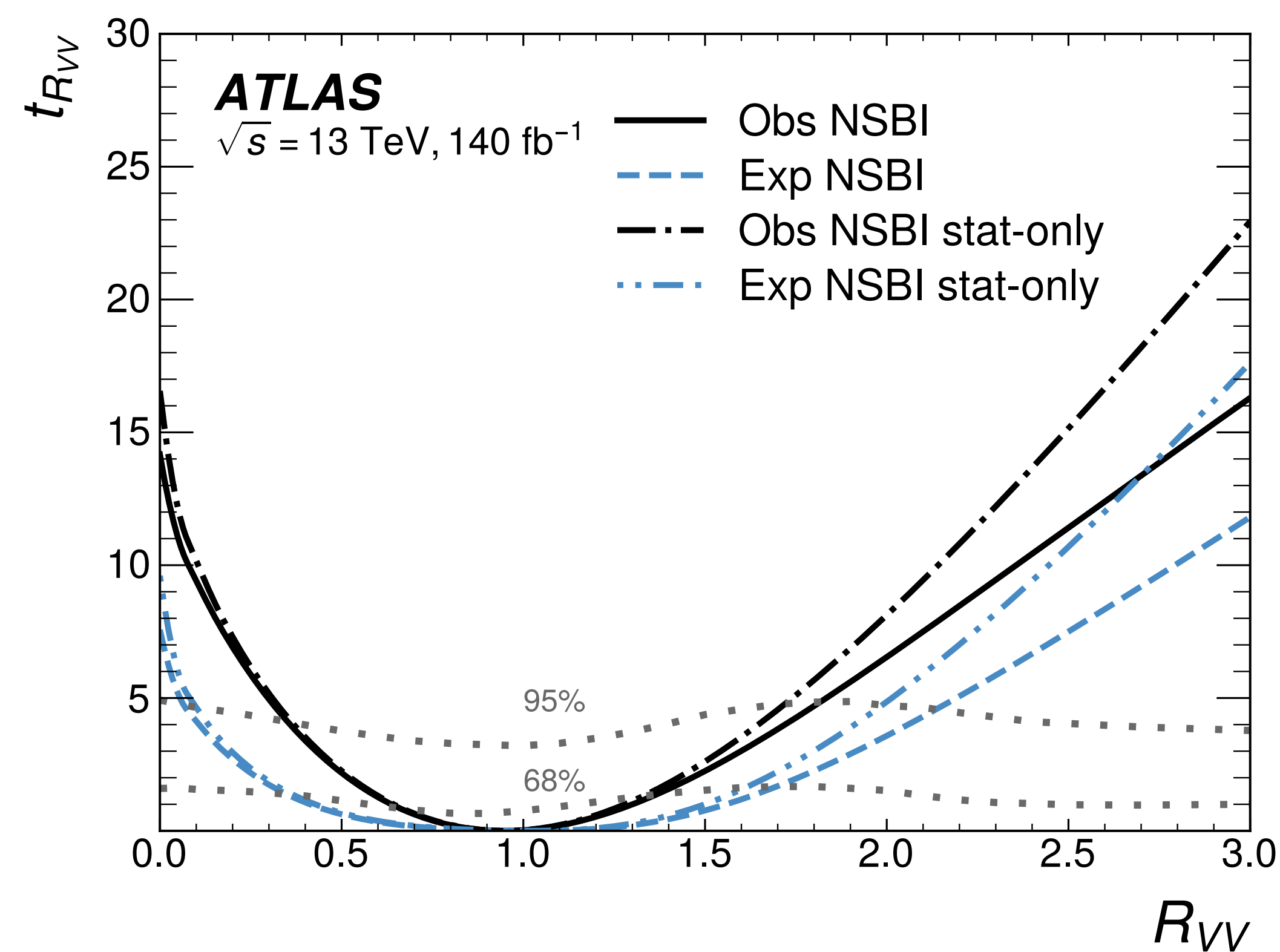


CI obtained from Neyman construction

Width sensitivity in ggF and VBF



$$R_{gg} = \kappa_{g,\text{on-shell}}^2 / \kappa_{g,\text{off-shell}}^2$$



$$R_{VV} = \kappa_{V,\text{on-shell}}^2 / \kappa_{V,\text{off-shell}}^2$$

Comparison to previous result in same data

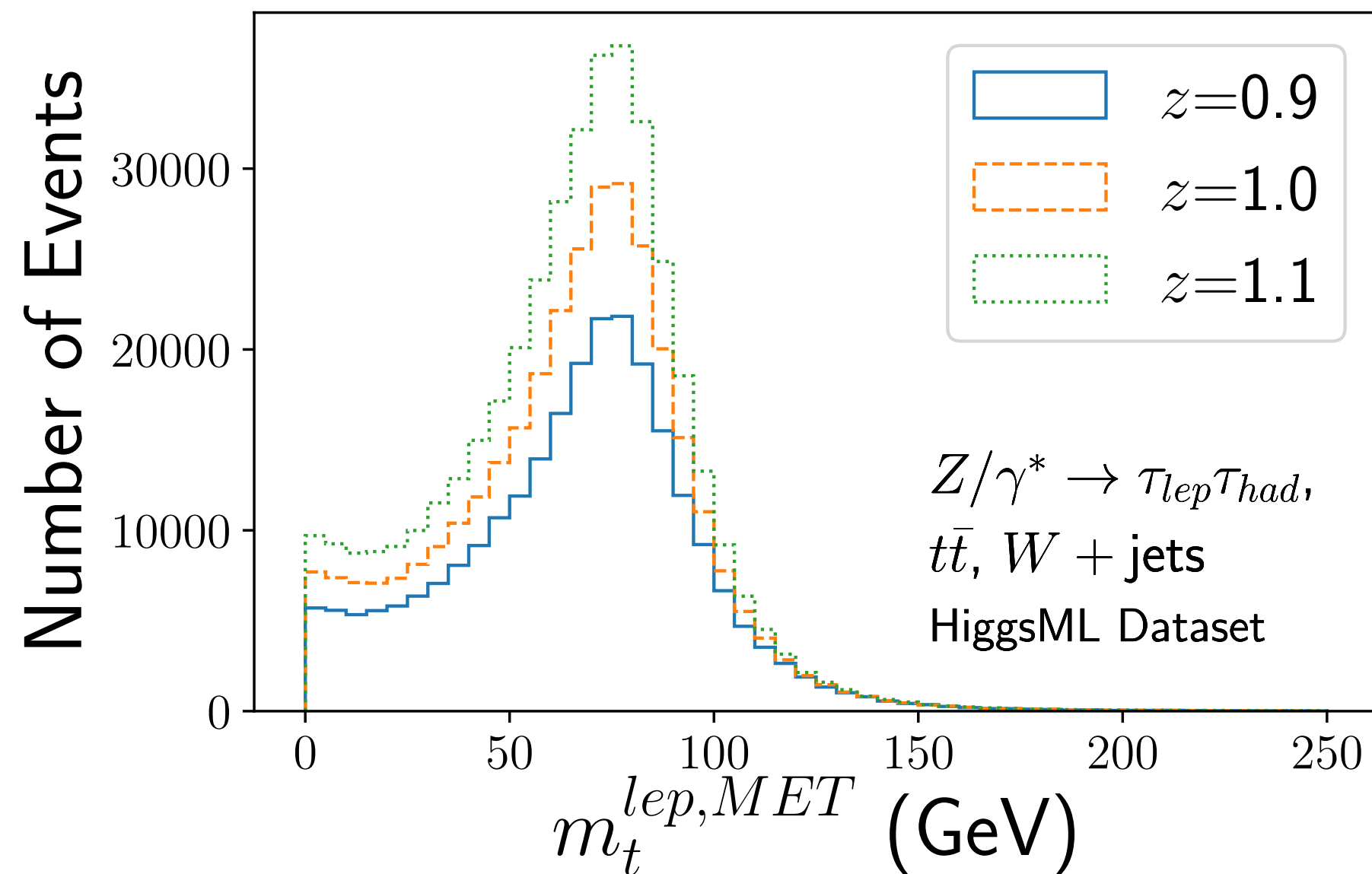
Parameter	Value	68% CL interval		95% CL interval	
		Observed	Expected	Observed	Expected
NSBI analysis					
$\mu_{\text{off-shell}} (4\ell \text{ only})$	0.87	[0.33, 1.62]	[0.05, 2.04]	[0.05, 2.38]	< 2.38
$\mu_{\text{off-shell}}$	1.06	[0.61, 1.67]	[0.17, 1.83]	[0.21, 2.24]	[0.01, 2.42]
Γ_H [MeV] (4ℓ only)	3.43	[1.37, 6.71]	[0.20, 8.25]	[0.18, 9.98]	< 12.09
Γ_H [MeV]	4.29	[2.41, 6.95]	[0.66, 7.61]	[0.76, 9.66]	[0.12, 10.50]
R_{gg}	1.19	[0.53, 2.07]	[0.02, 1.92]	< 2.96	< 2.73
R_{VV}	0.95	[0.61, 1.39]	[0.31, 1.70]	[0.30, 1.86]	[0.06, 2.14]
Histogram-based analysis					
$\mu_{\text{off-shell}} (4\ell \text{ only})$	0.79	[0.02, 2.00]	< 2.14	< 2.97	< 3.10
$\mu_{\text{off-shell}}$	1.09	[0.54, 1.81]	[0.08, 1.90]	[0.10, 2.41]	[0.01, 2.52]
Γ_H [MeV] (4ℓ only)	3.43	[0.10, 8.42]	< 8.89	< 12.48	< 12.89
Γ_H [MeV]	4.37	[2.13, 7.43]	[0.35, 7.94]	[0.39, 10.14]	< 10.79
R_{gg}	1.23	[0.00, 2.20]	< 1.98	< 3.15	< 2.84
R_{VV}	0.95	[0.60, 1.43]	[0.27, 1.74]	[0.26, 1.90]	[0.02, 2.18]

Uncertainty-aware analysis optimisation

[PRD.104.056026](#): Aishik Ghosh, Benjamin Nachman, and Daniel Whiteson

Experimental uncertainties:

Eg. Inaccuracies in the calibration of our detector



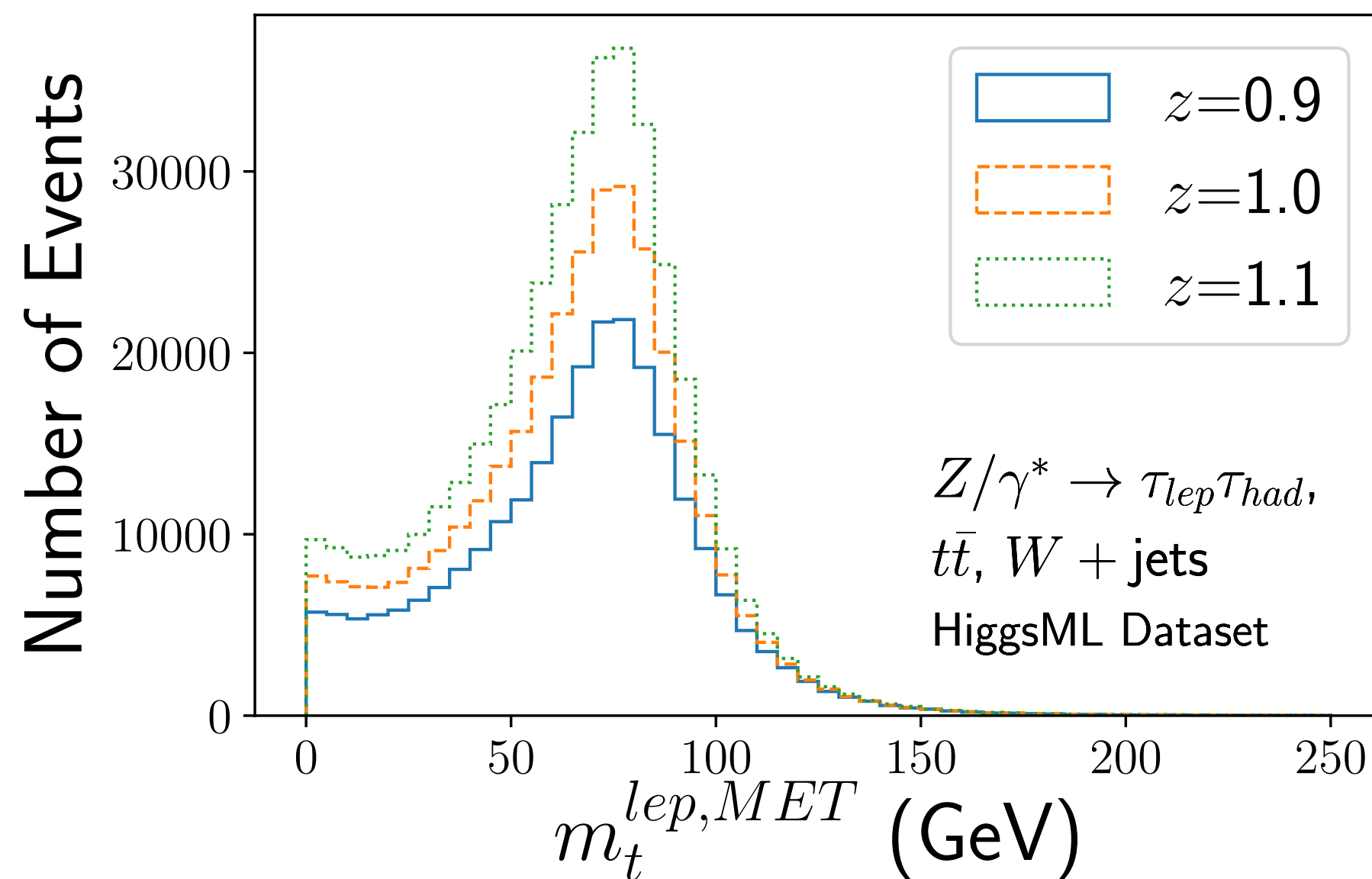
- Current analyses strategies optimised while ignoring systematic uncertainties
- Added in post-facto
- Leads to loss in sensitivity compared to uncertainty-aware optimisation (see details)

Uncertainty-aware analysis optimisation

[PRD.104.056026](#): Aishik Ghosh, Benjamin Nachman, and Daniel Whiteson

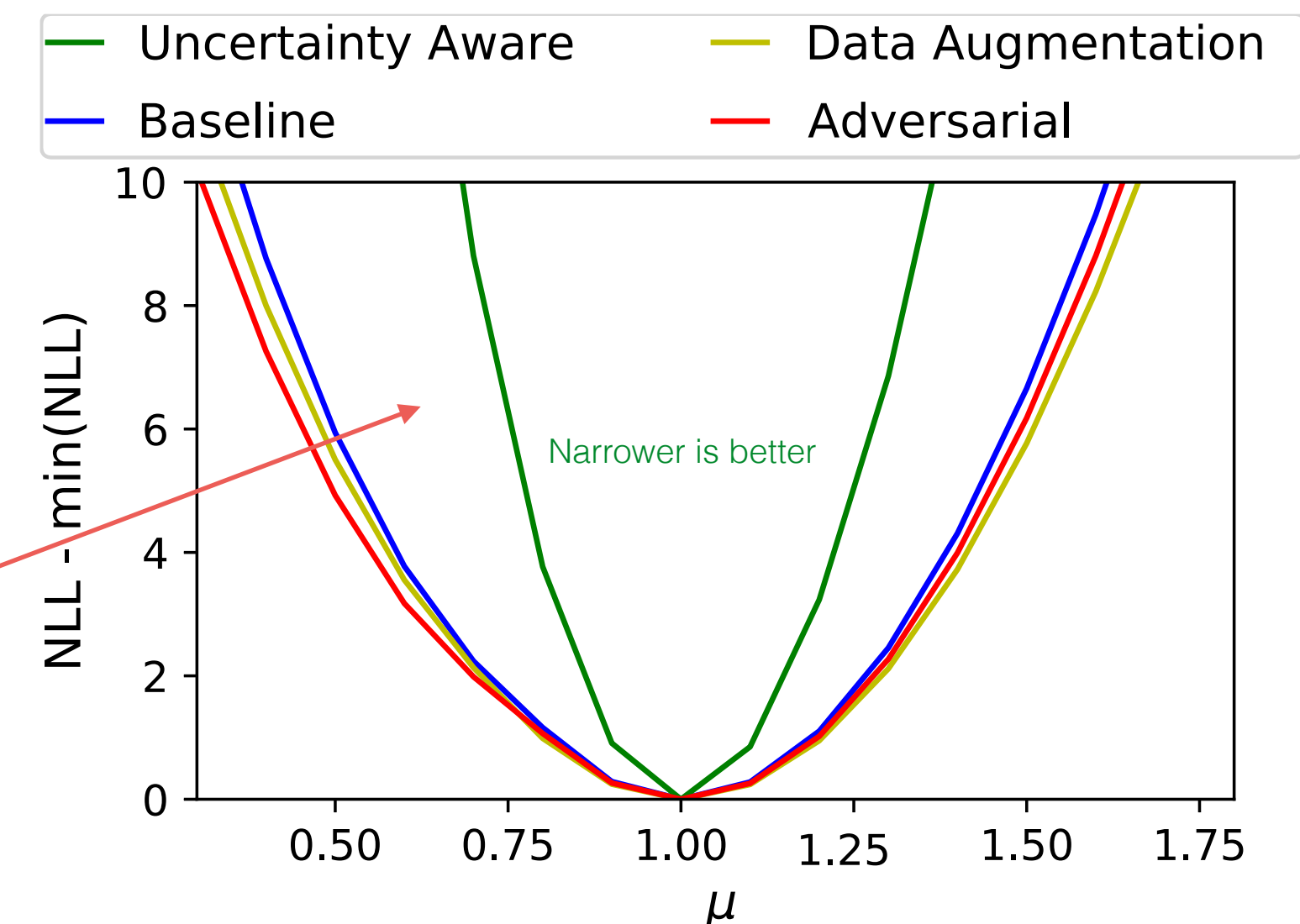
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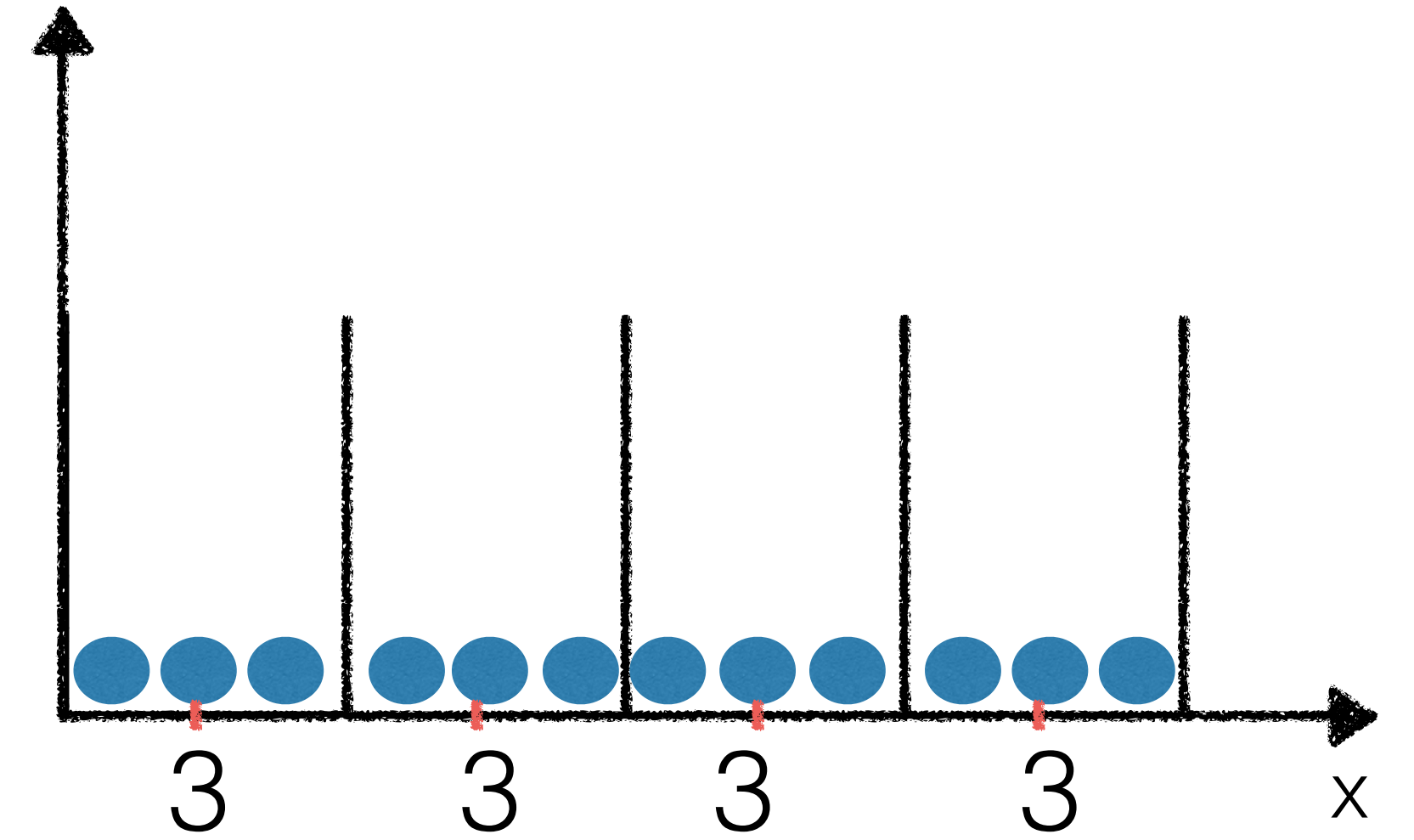
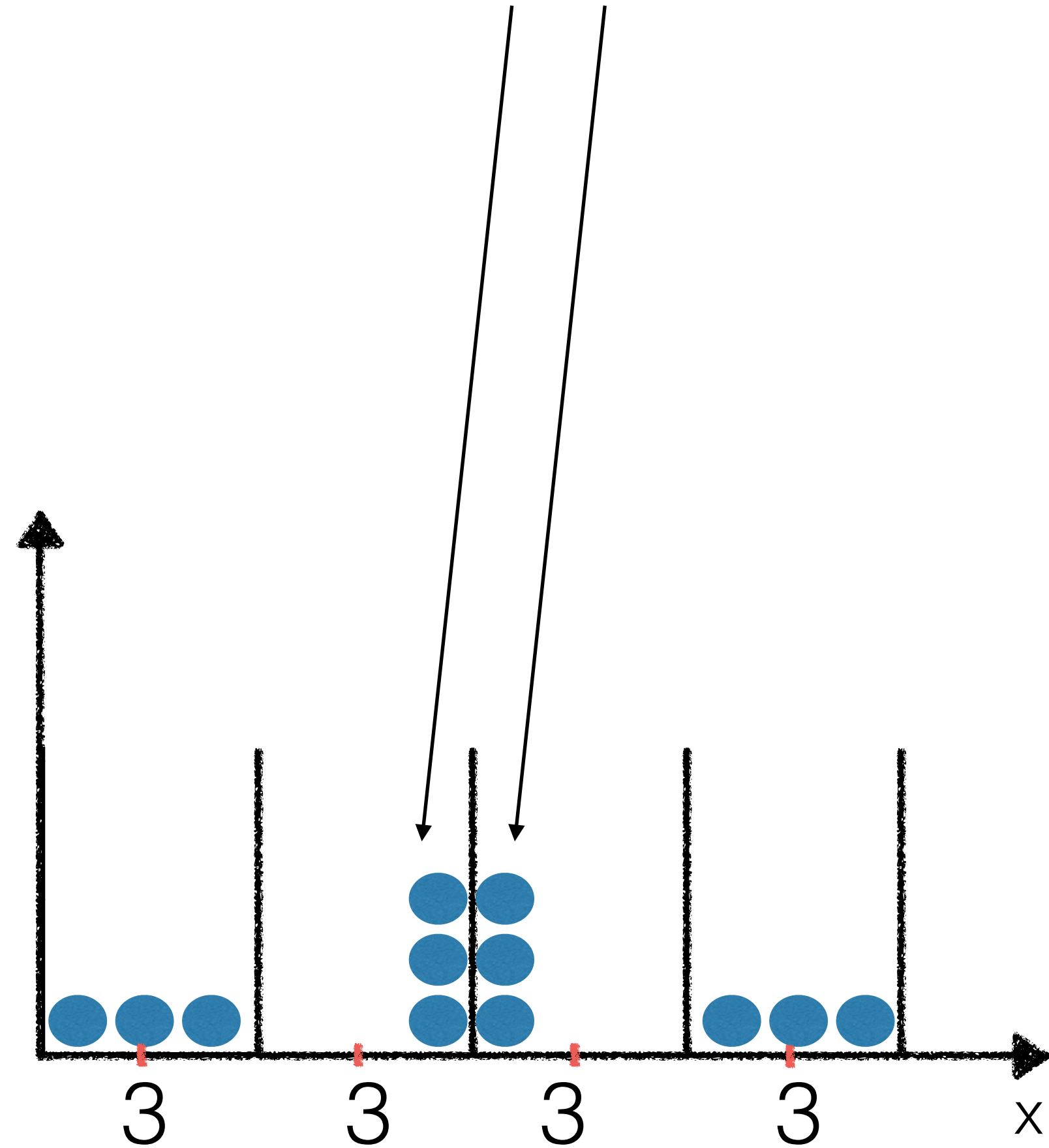
- Current analyses strategies optimised while ignoring systematic uncertainties
- Added in post-facto
- Leads to loss in sensitivity compared to uncertainty-aware optimisation (see details)

Difference b/w post-facto and uncertainty-aware



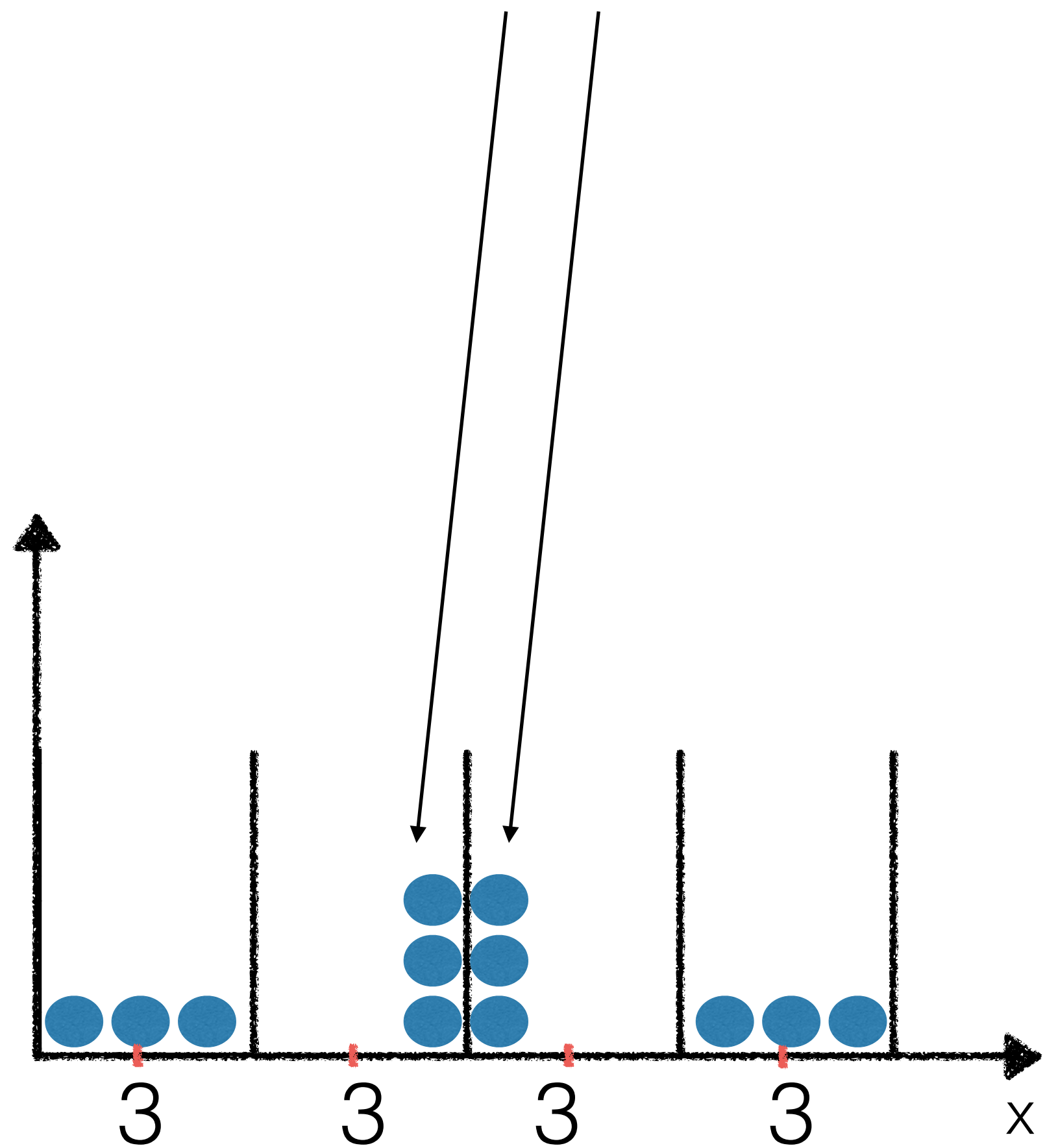
Avoids binning data into histograms, which is another lossy compression

Information on individual events lost!

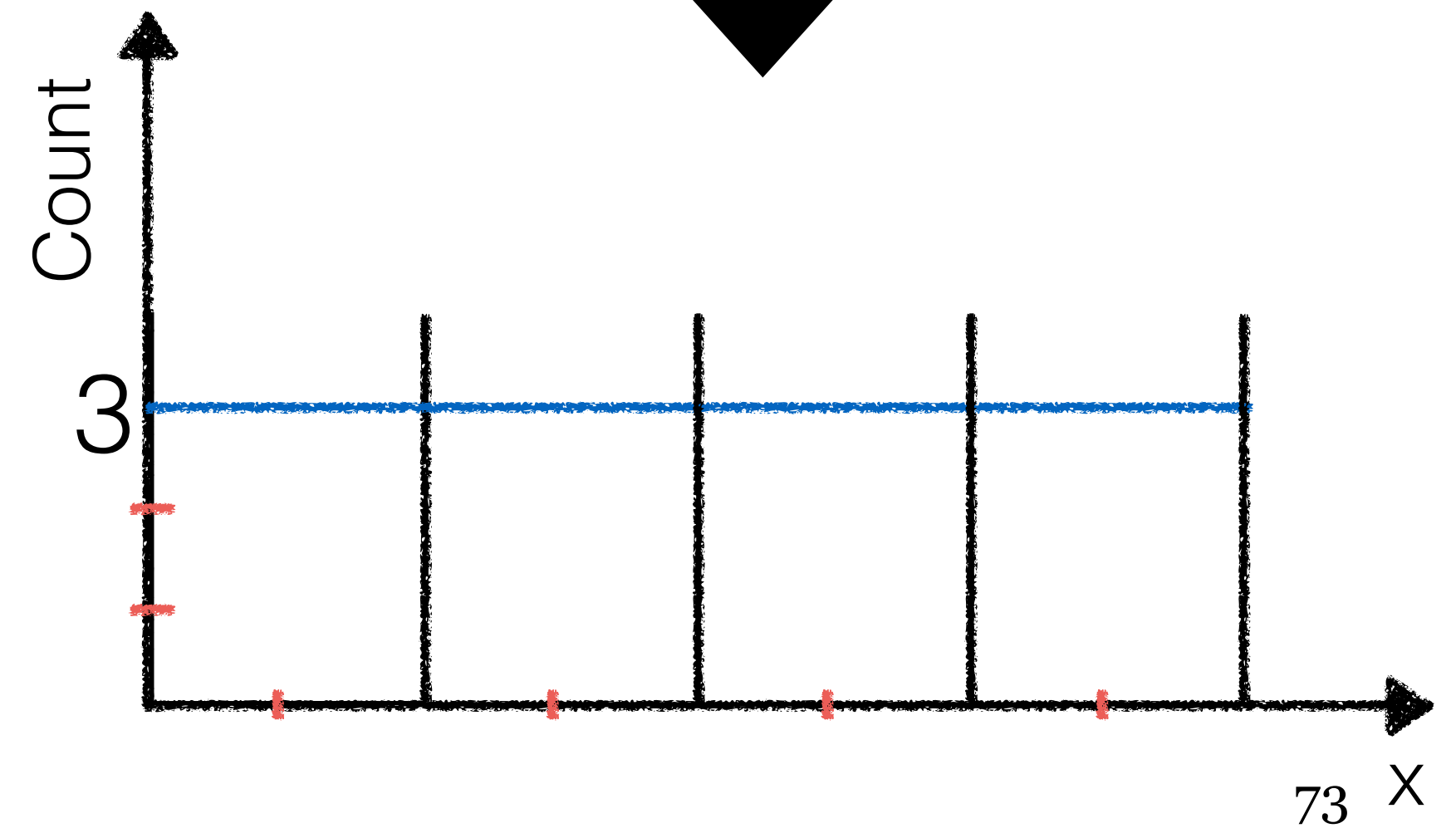
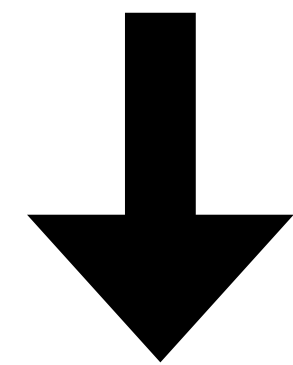
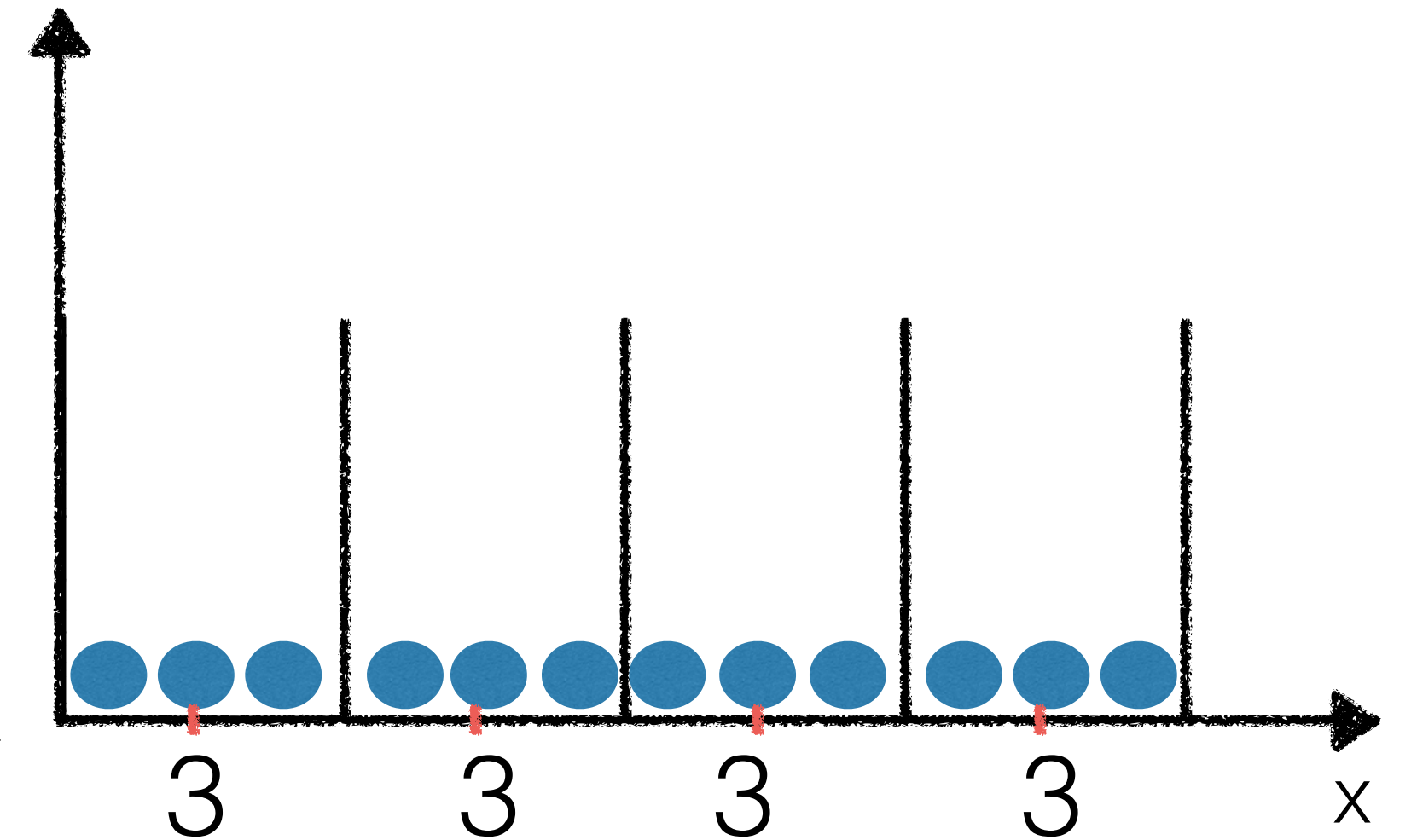


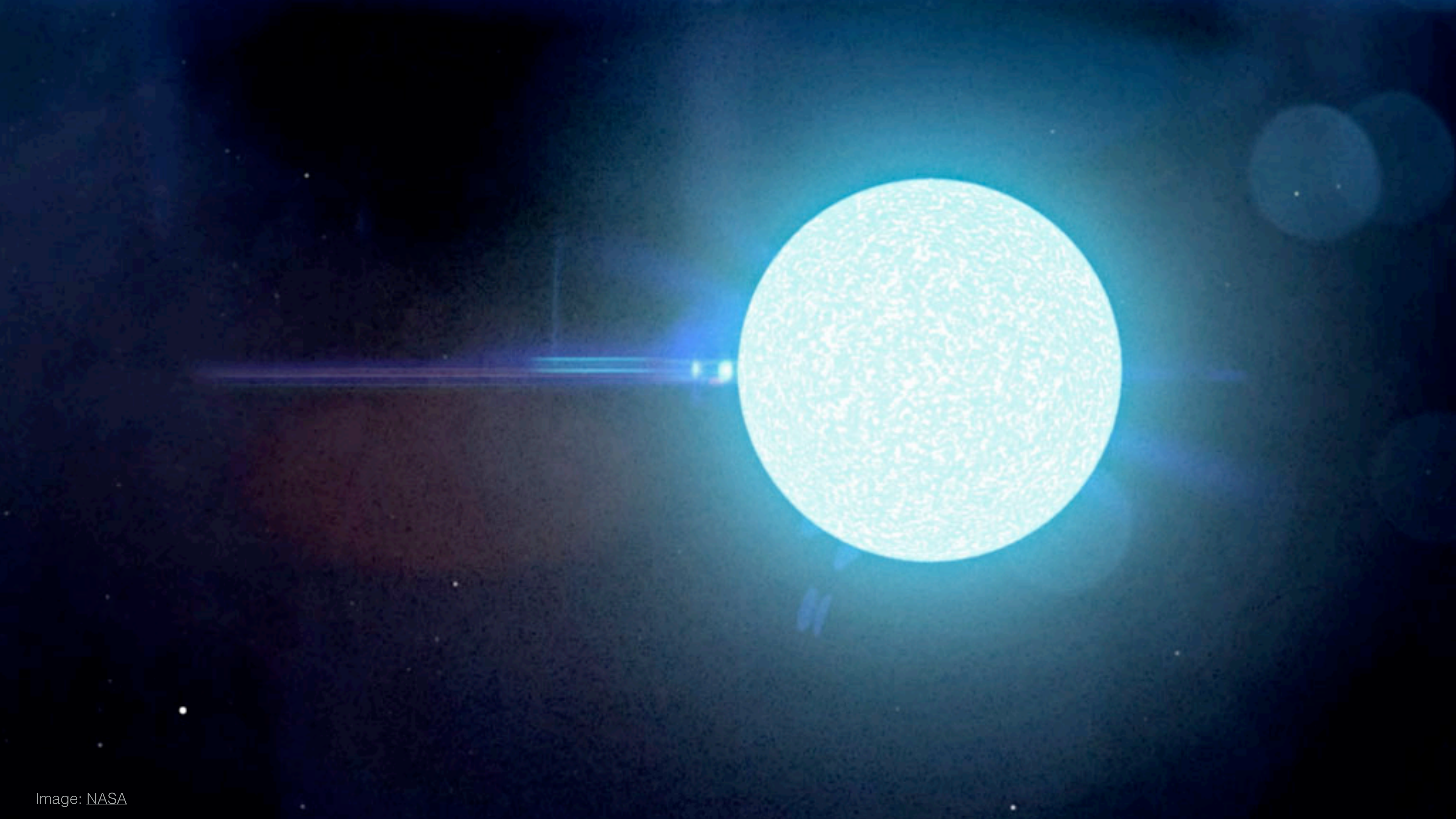
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Information on individual events lost!



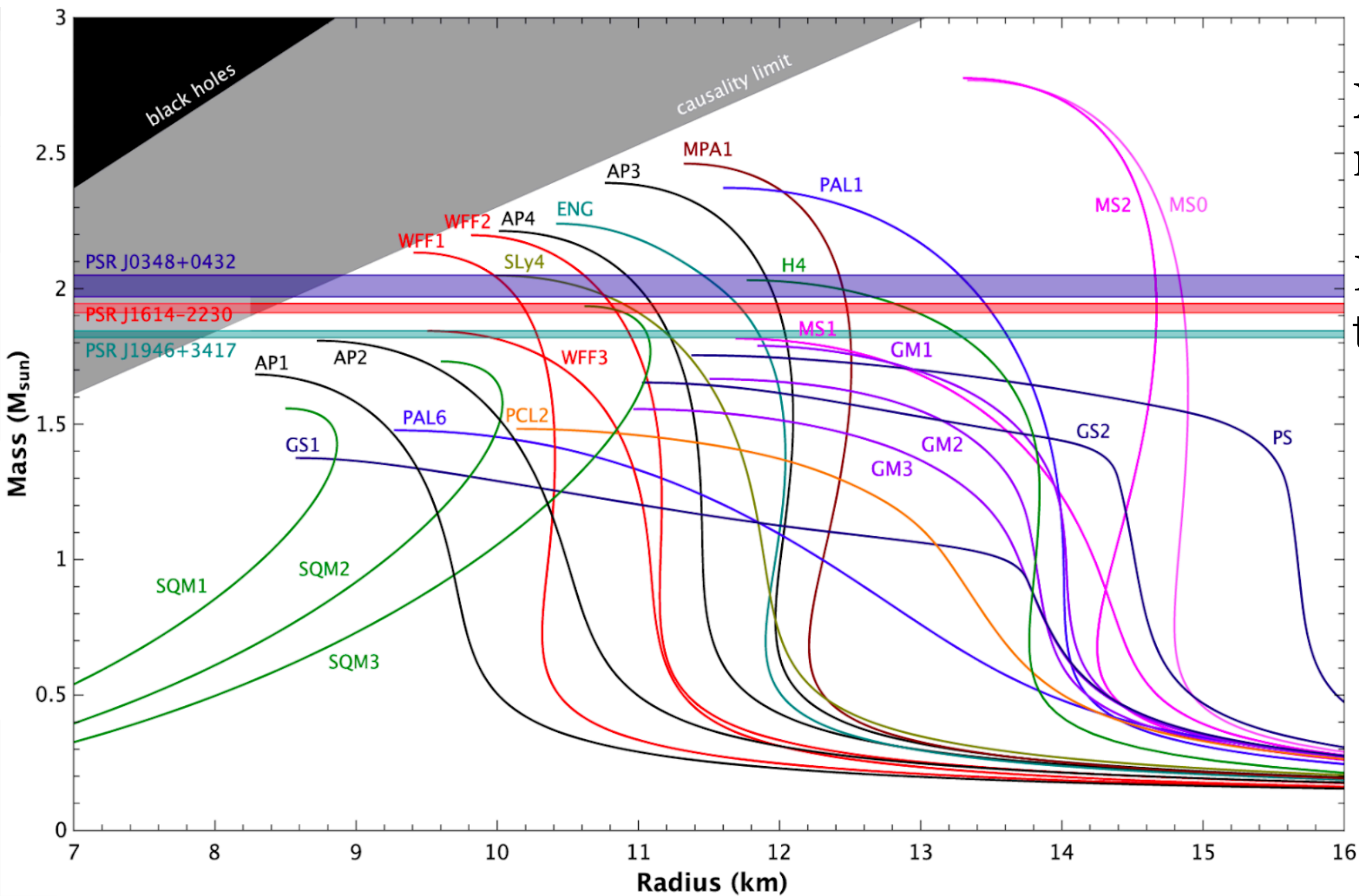
Same representation in histogram







Telescope measurements of energy spectra of neutron stars



Mass-radius curves created by different equation of state (EoS) models

Horizontal bars show massive neutron star observations used to “rule out” EoS models.

Two communities:

- **Astrophysicists** measure mass/radius from telescope
- **Nuclear theorists** measure EoS from mass/radius

Figure from Lattimer J. M., Prakash M., 2001, The Astrophysical Journal, 550, 426–442

Telescope measurements of energy spectra

Probe the interior:
Equation of State parameters

λ_1, λ_2

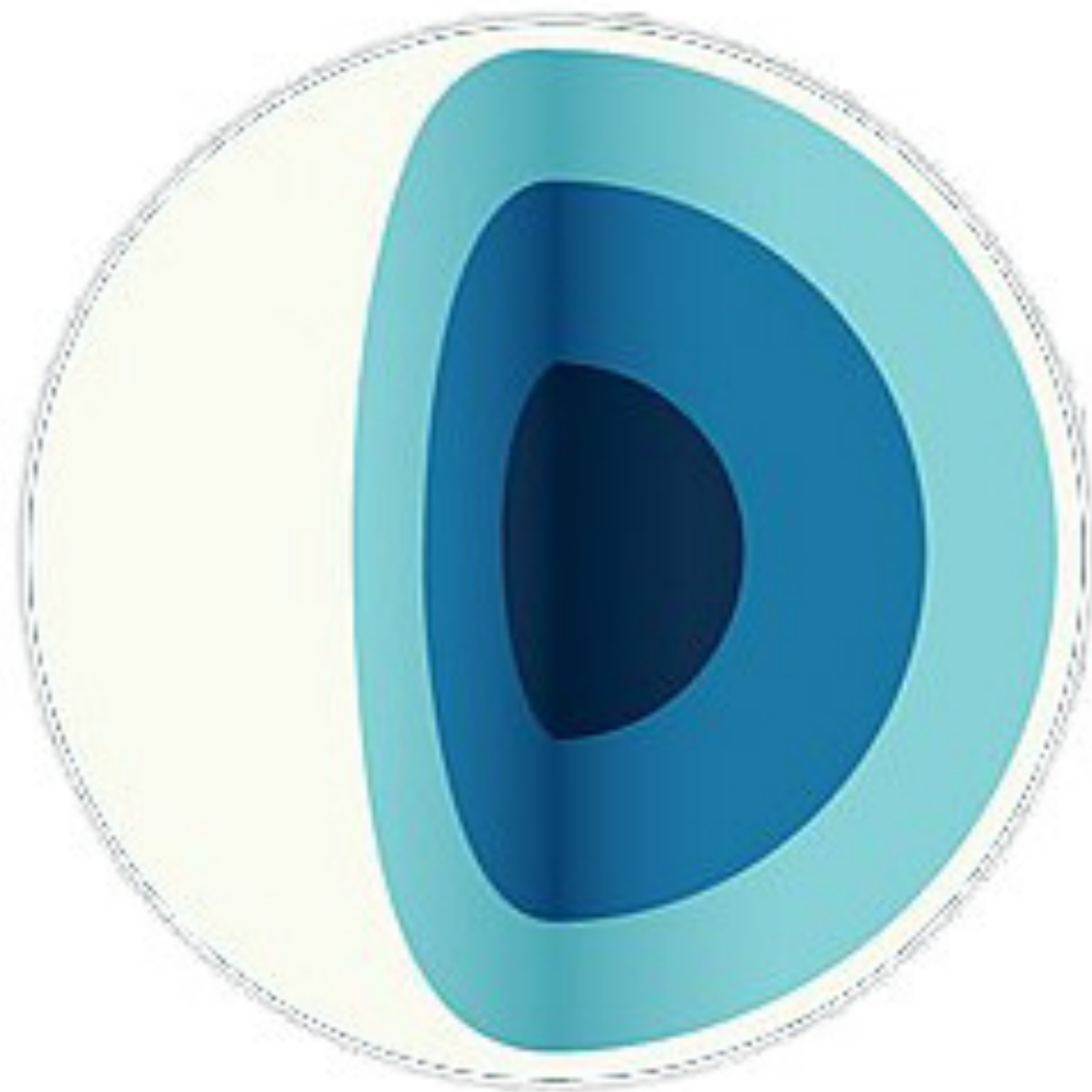
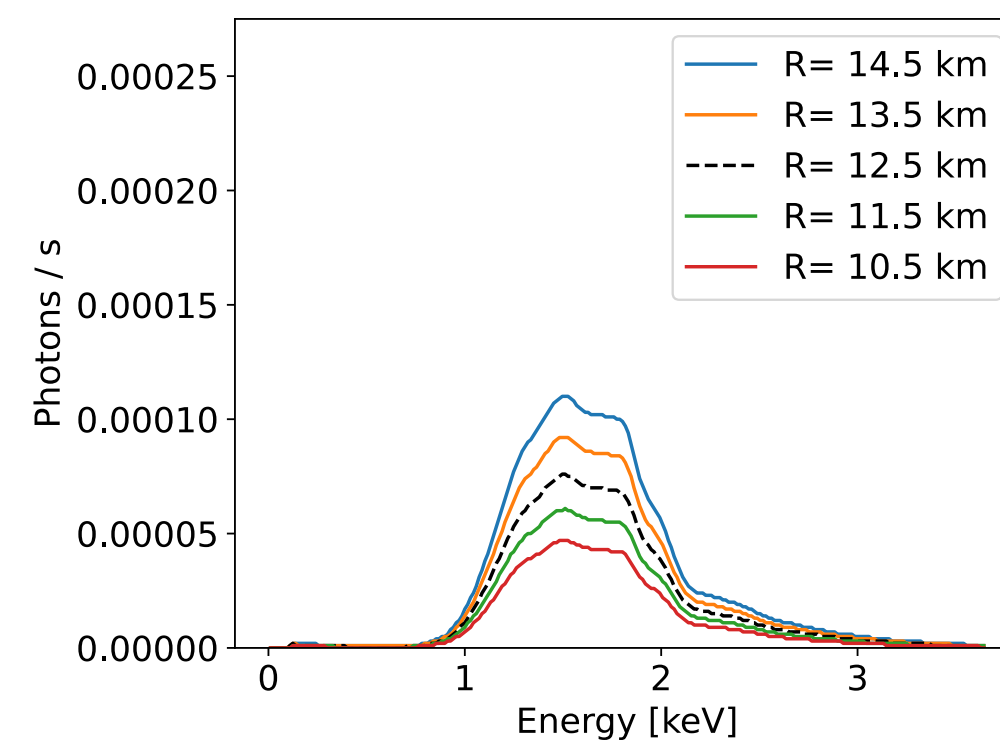
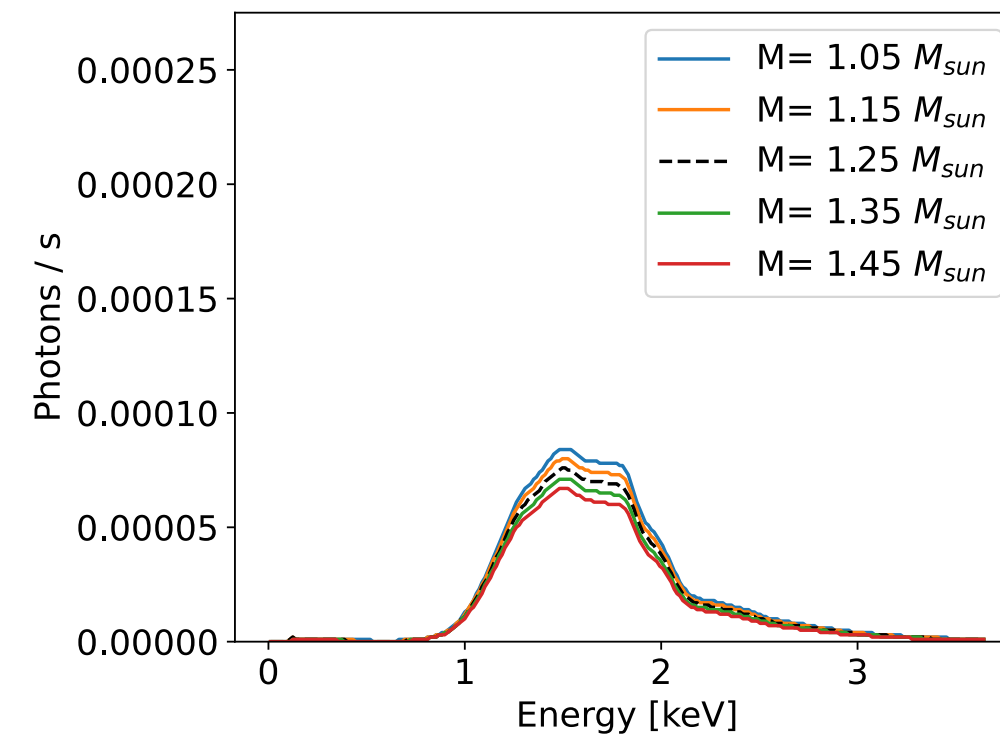


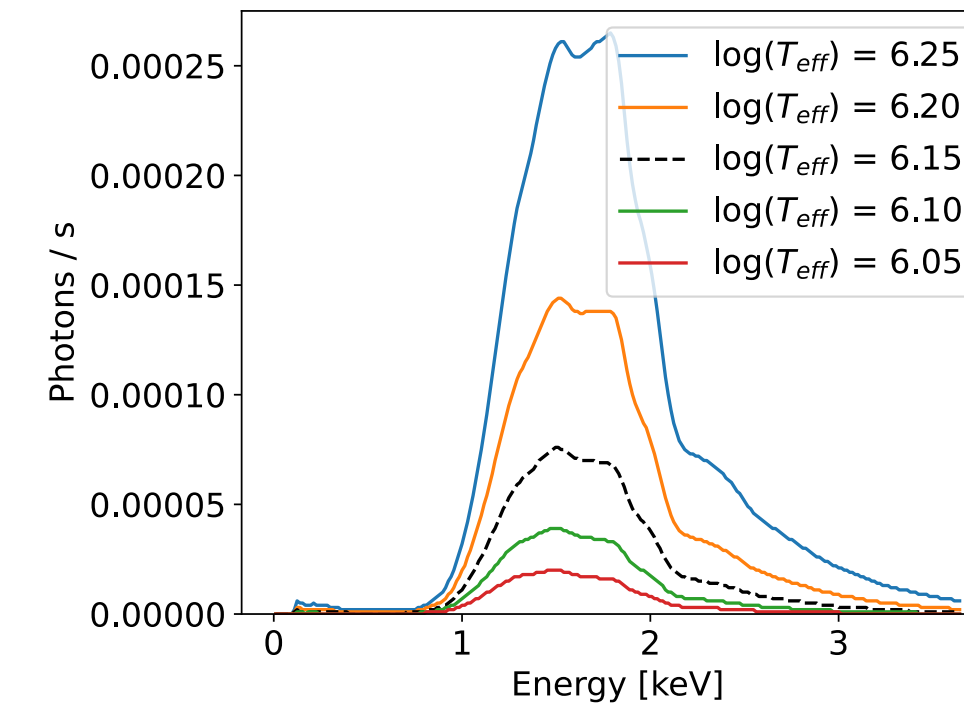
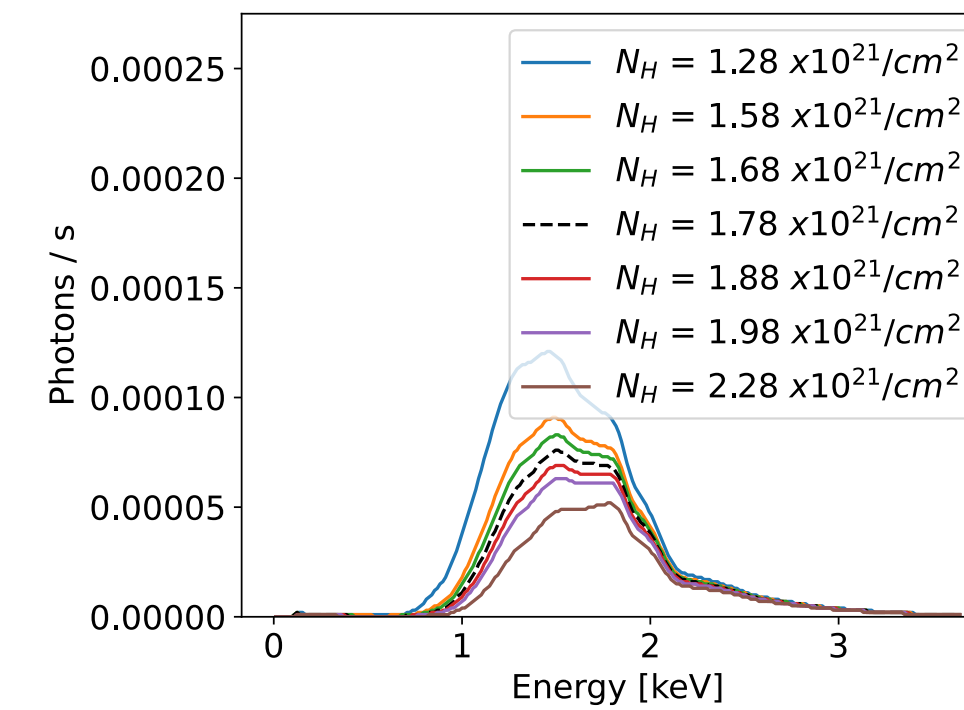
Image: [Wikimedia/NASA](#)

Mass



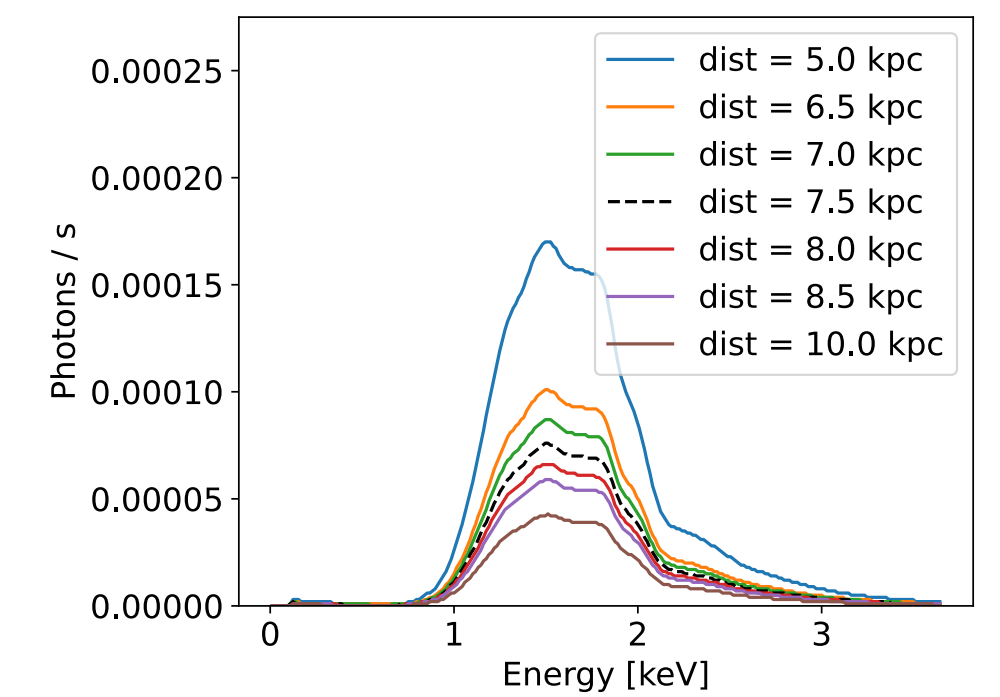
Radius

Hydrogen Column



Effective Temperature

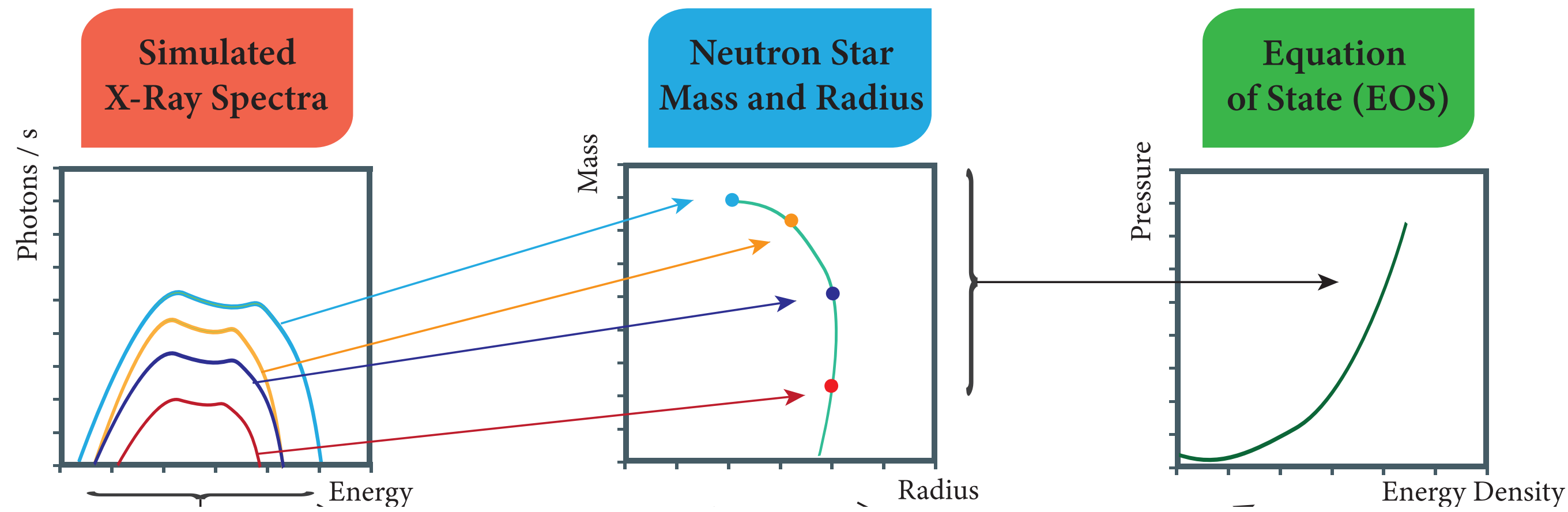
Distance



Traditional method: Two-step inference



Neutron star in sky



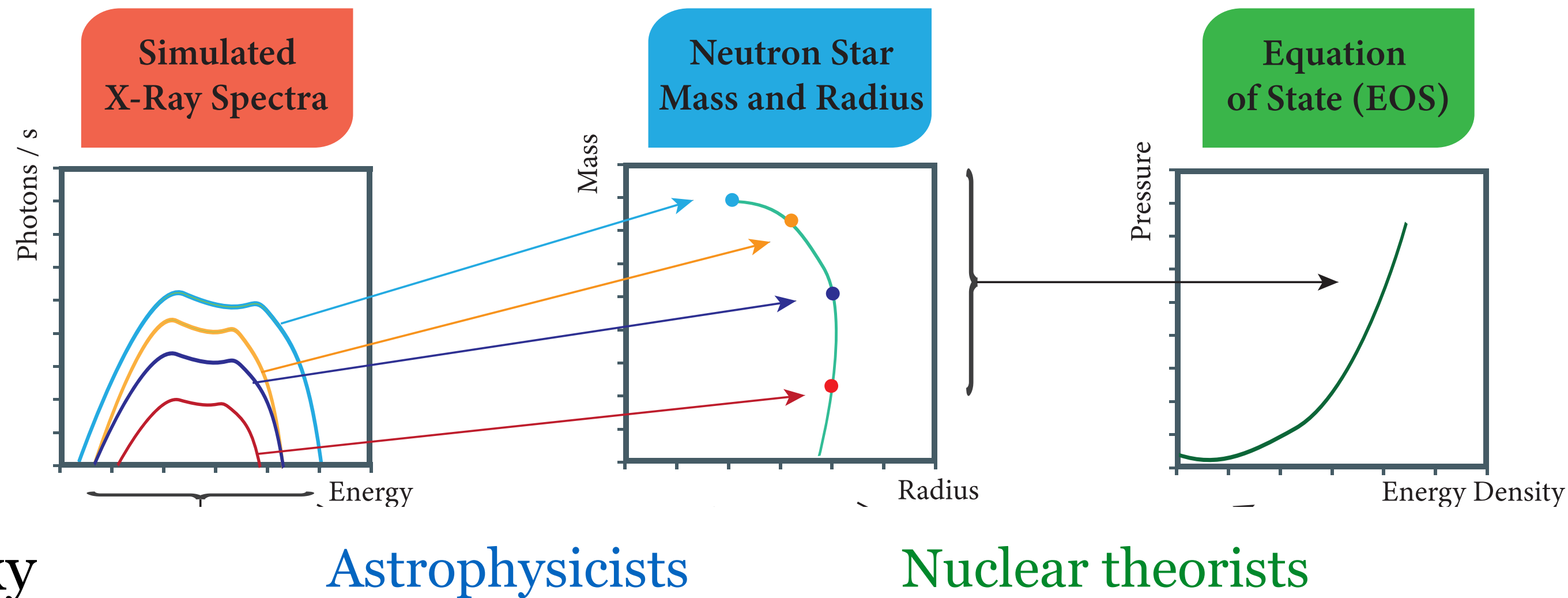
Astrophysicists

Nuclear theorists

Traditional method: Two-step inference

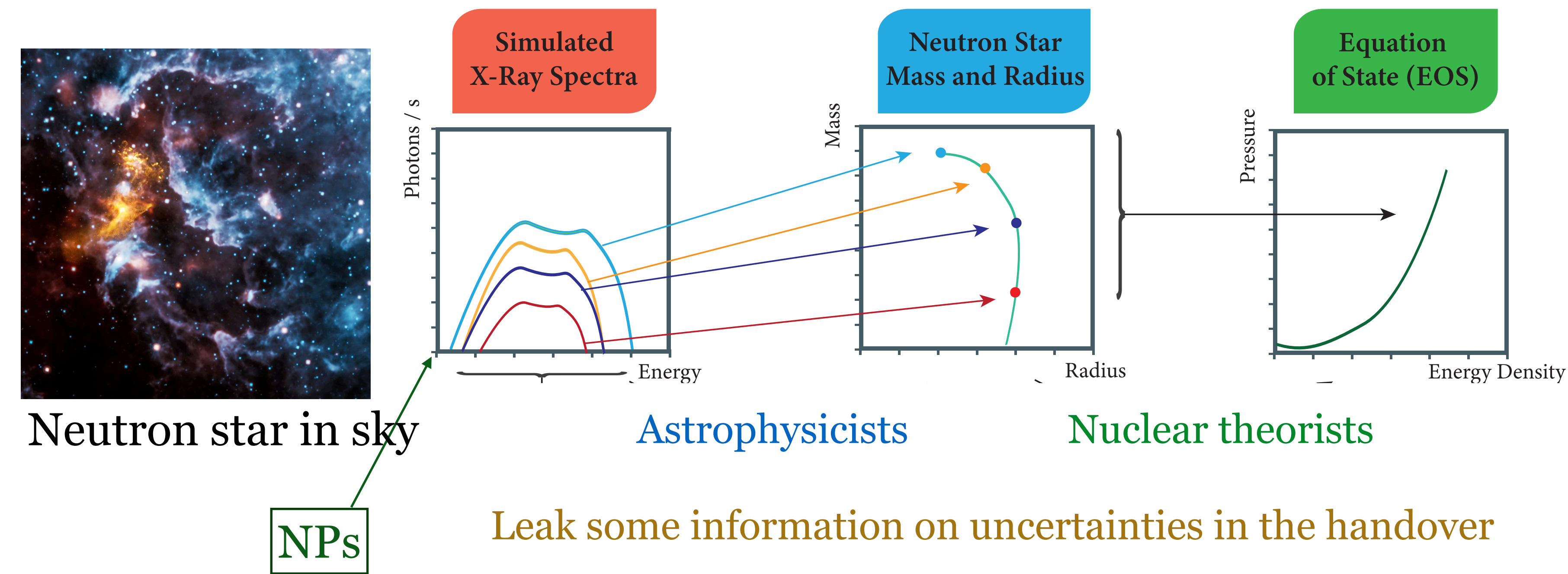


Neutron star in sky



Leak some information on uncertainties in the handover

Traditional method: Two-step inference

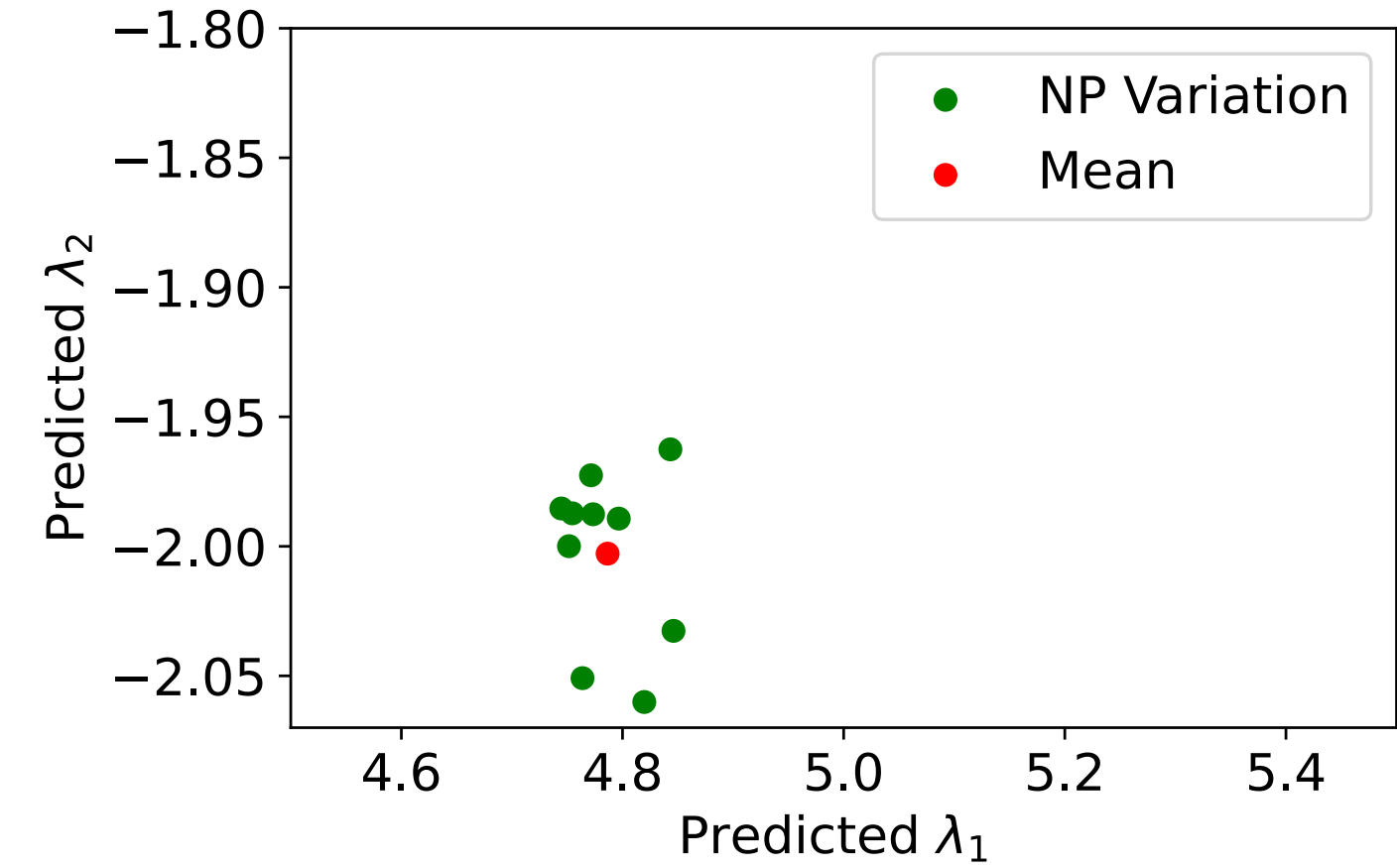
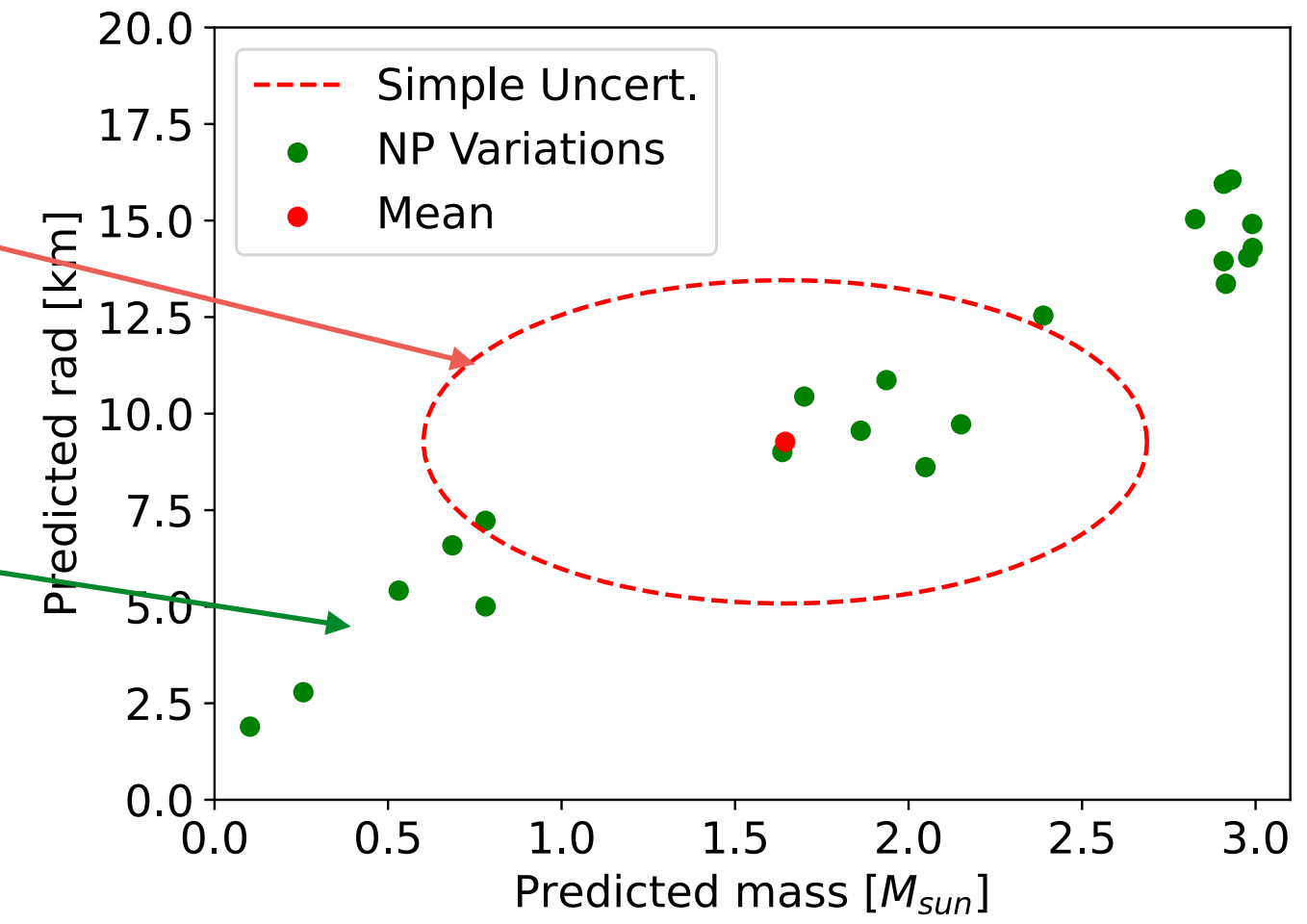


Leak some information on uncertainties in the handover

Traditional method: Two-step inference

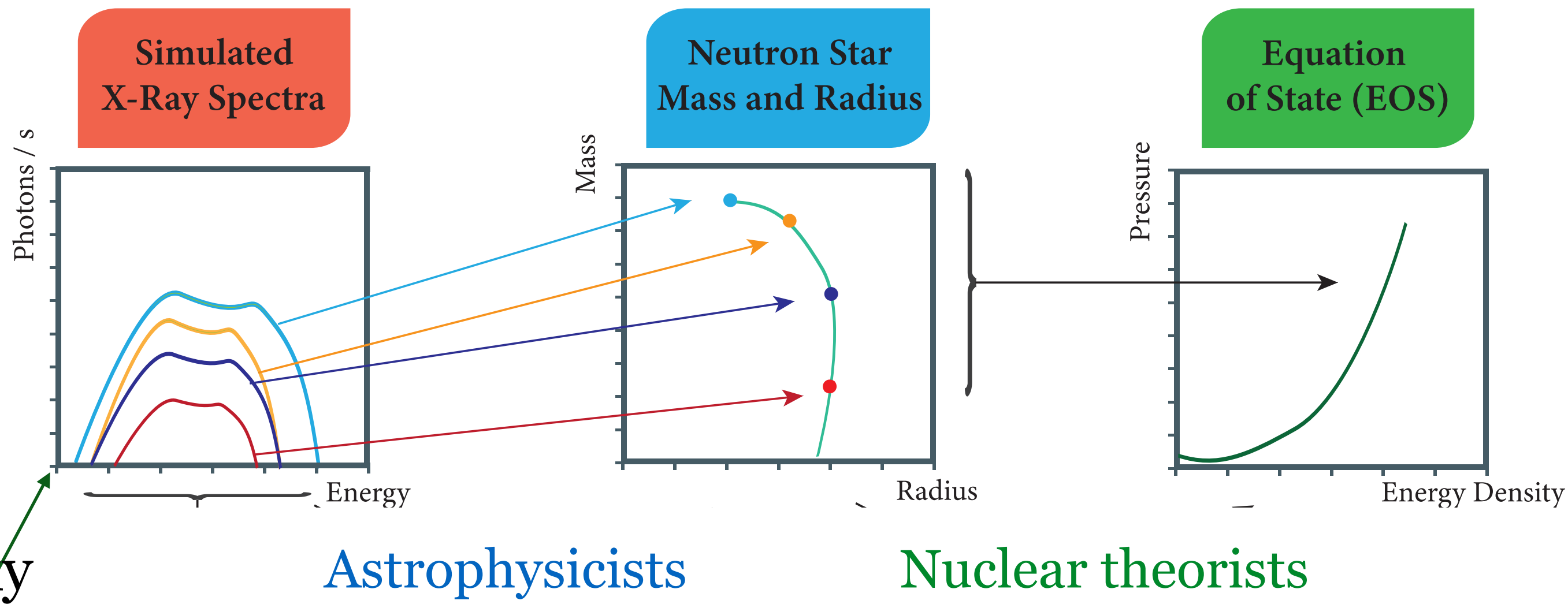
SOTA collapsed information into 2 numbers + assumed uncorrelated Gaussian uncertainties

Real uncertainties look quite different

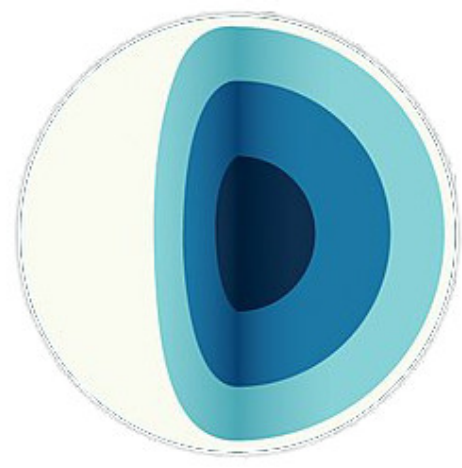


Neutron star in sky

NPs

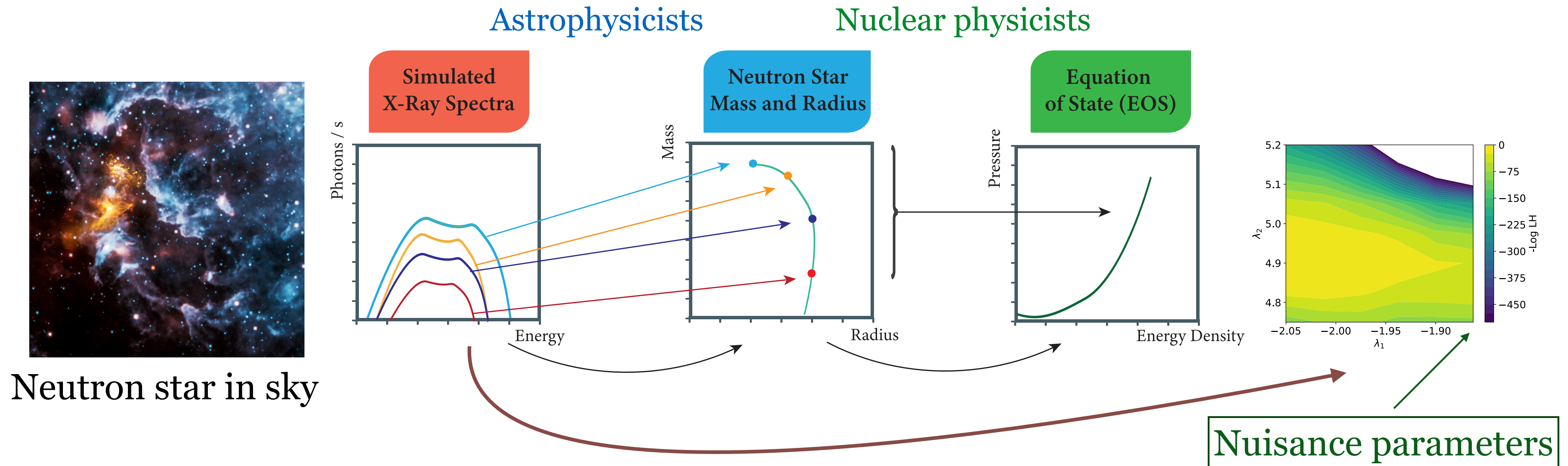


Leak some information on uncertainties in the handover



Inferring neutron star EoS parameters with NSBI

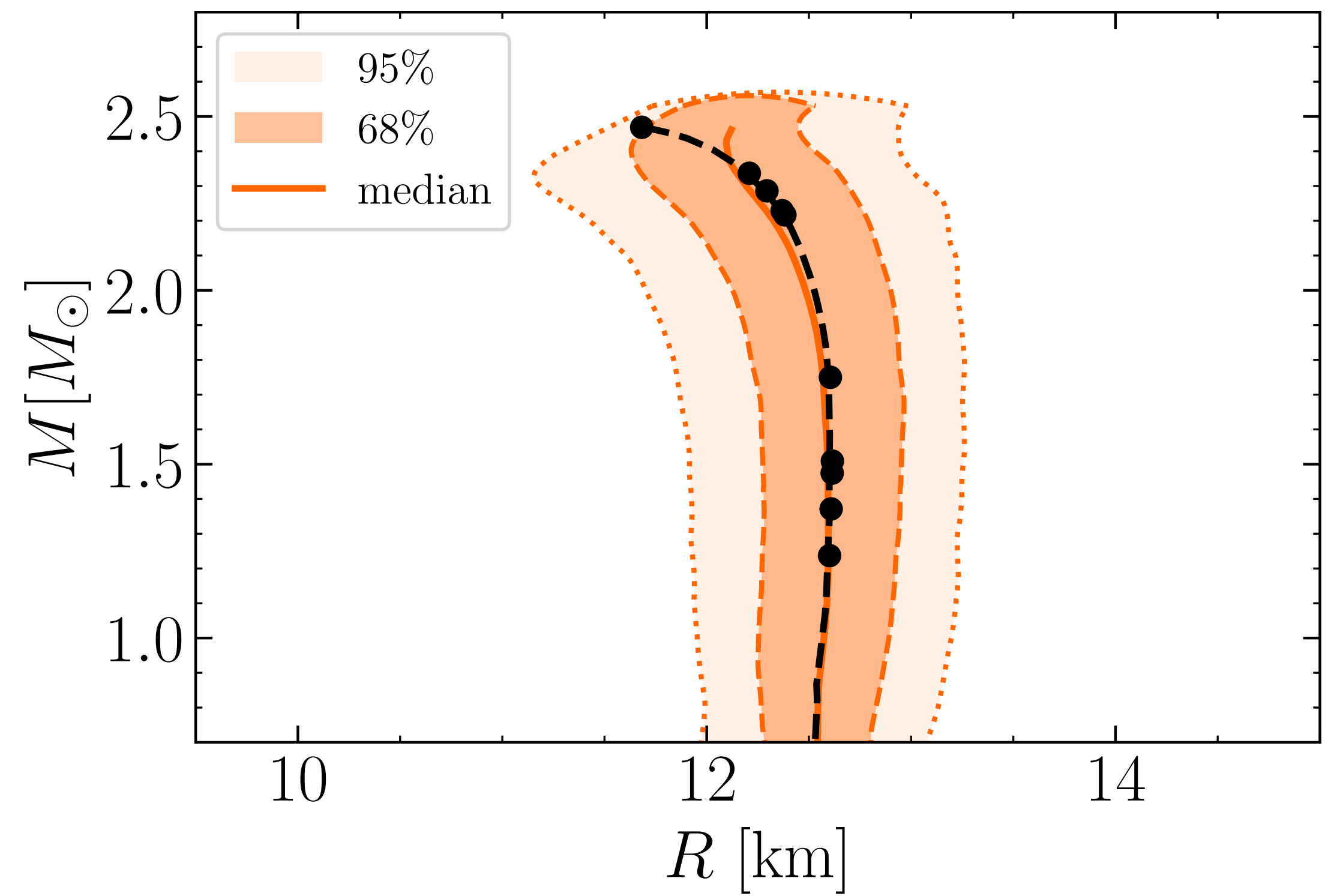
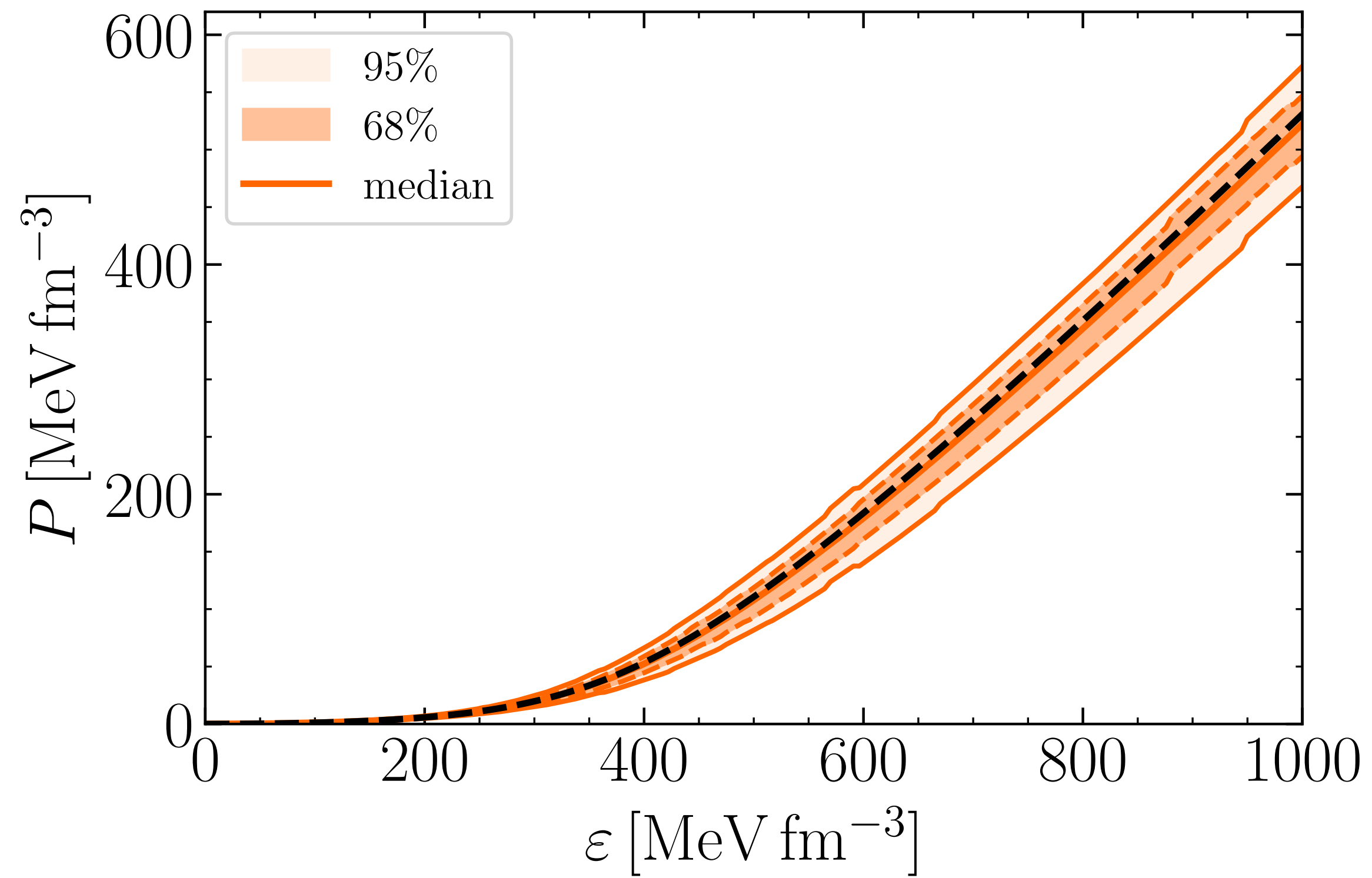
Recover the likelihood of EoS + NPs directly from the raw high-dimensional telescope spectra!



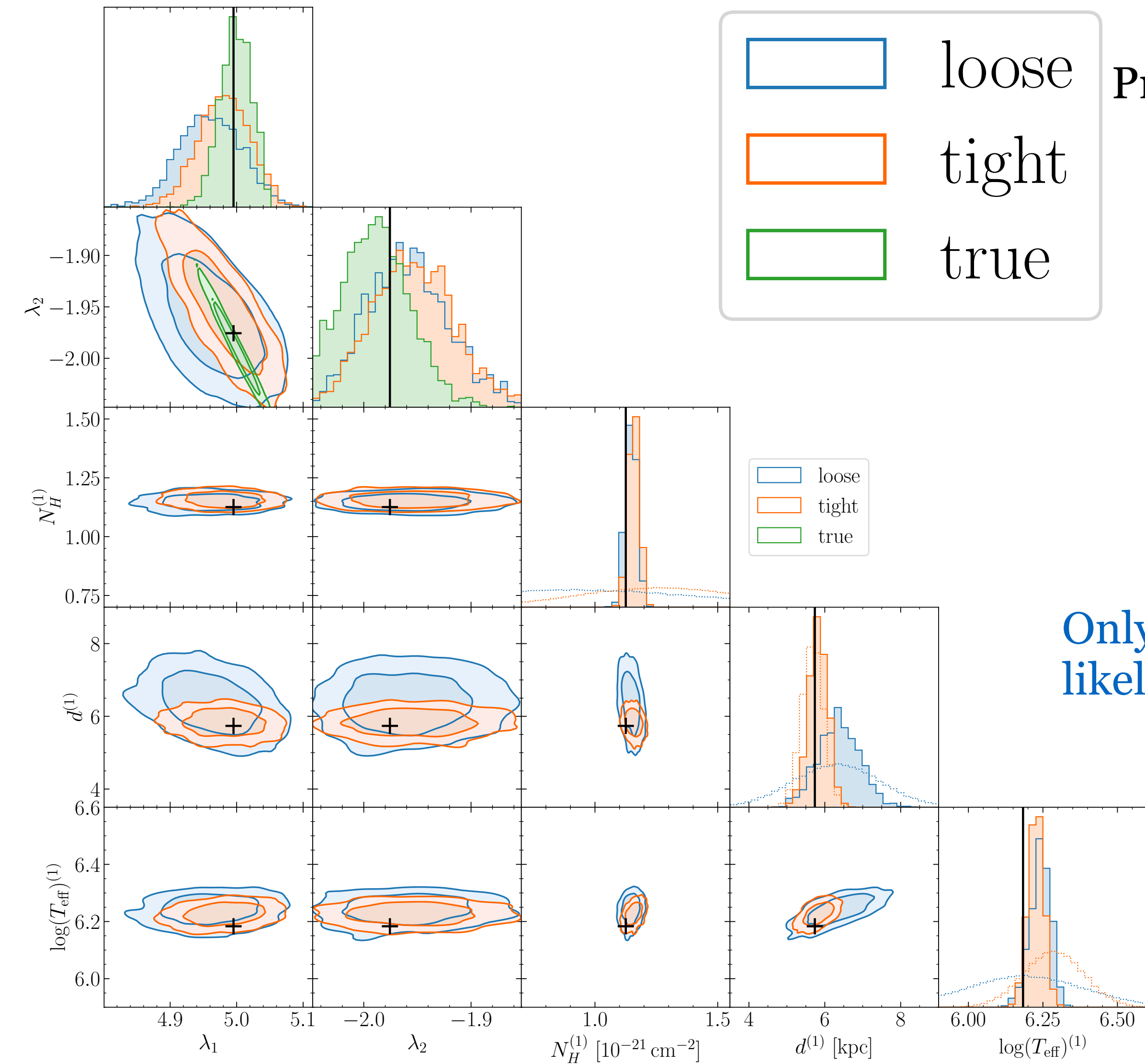
Direct estimation of likelihood from high-dimensional raw data allows more reliable uncertainty propagation and better measurements!

Meaningful posteriors, most sensitive method!

Bayesian Posteriors and credible intervals



Enhanced Interpretability: Effect of nuisance parameters



loose
tight
true

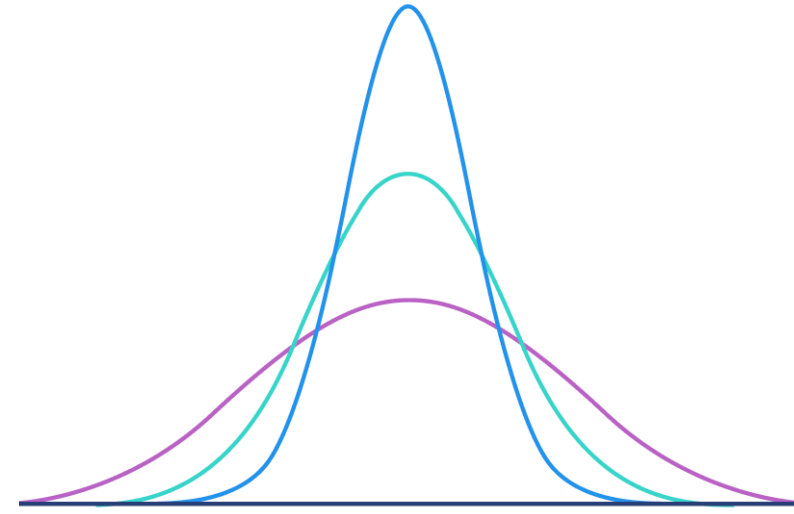
Prior knowledge on nuisance parameters

loose
tight
true

Only possible to visualise these due to the fast and differentiable likelihood from networks

Most sensitive method for EoS inference to date!

[CAPo9\(2024\)009](#): Brandes, Modi, Ghosh, et al



NP priors

NP priors		$\lambda_{1,\text{pred}} - \lambda_{1,\text{truth}}$		$\lambda_{2,\text{pred}} - \lambda_{2,\text{truth}}$		Combined
$p(\nu)$	Method	μ	σ	μ	σ	σ_{tot}
true	ML-Likelihood _{EOS}	-0.02	0.066	0.01	0.070	0.096
	NN(Spectra)	-0.02	0.066	0.01	0.075	0.099
	NN(M, R via XSPEC)	-0.03	0.065	0.01	0.055	0.085
	NLE	0.00	0.056	-0.01	0.070	0.090
tight	ML-Likelihood _{EOS}	-0.02	0.078	0.03	0.081	0.112
	NN(Spectra)	0.02	0.085	-0.02	0.077	0.115
	NN(M, R via XSPEC)	-0.03	0.081	0.01	0.056	0.098
	NLE	0.00	0.066	-0.02	0.071	0.097
loose	ML-Likelihood _{EOS}	-0.04	0.089	0.03	0.081	0.120
	NN(Spectra)	-0.03	0.131	-0.01	0.078	0.152
	NN(M, R via XSPEC)	-0.03	0.123	0.01	0.058	0.136
	NLE	0.00	0.085	-0.01	0.074	0.113

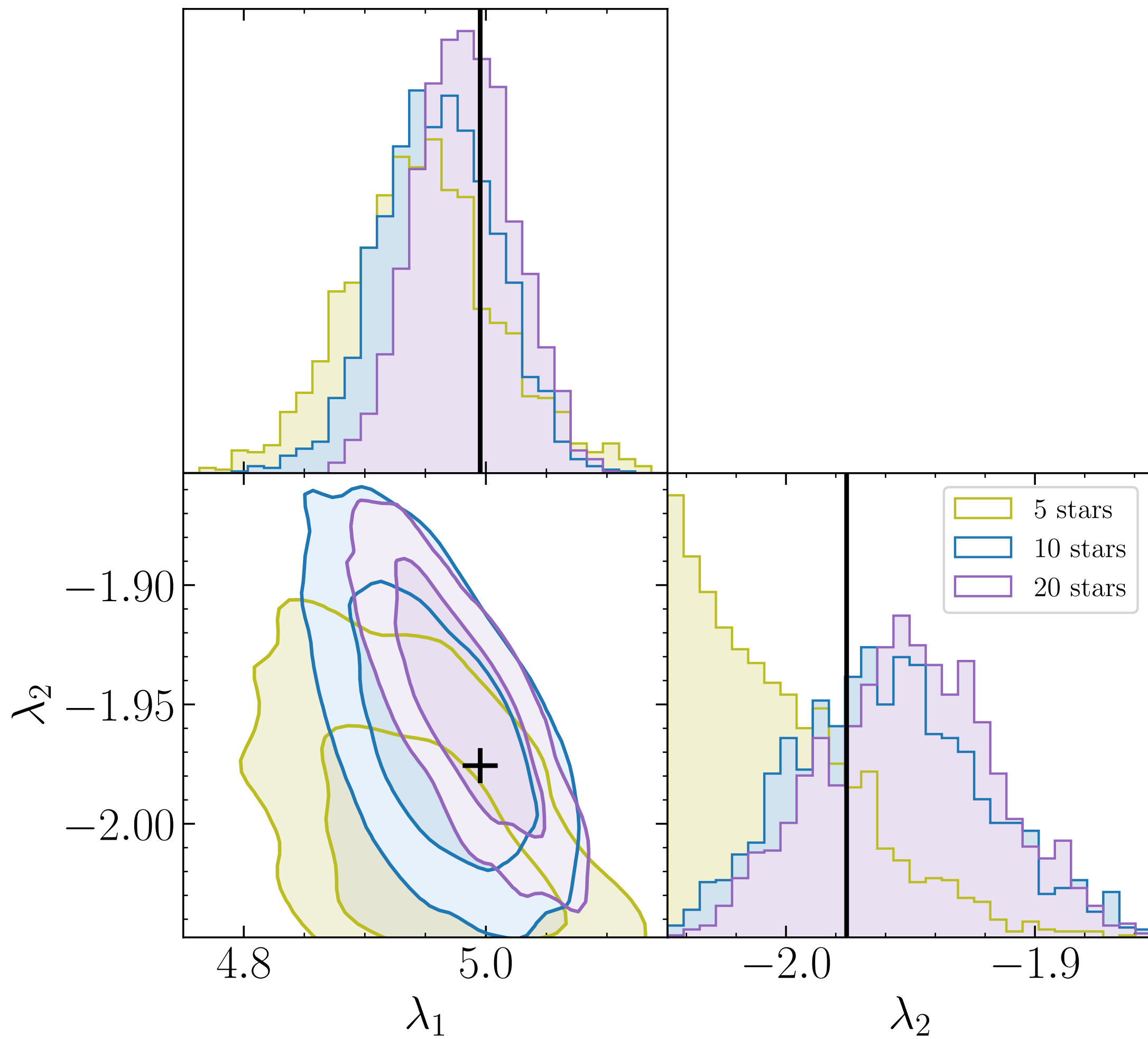
Pretend that nuisance parameters known exactly



Realistic scenarios:



Which neutron stars should we measure next ?



Test potential improvement in sensitivity coming from new measurements

Could inform decisions on which stars to measure next!

$$p(\text{theory} \mid \text{data}) = \frac{p(\text{data} \mid \text{theory})p(\text{theory})}{p(\text{data})}$$

What we all
want
(Posterior)

$$p(\text{theory} \mid \text{data}) = \frac{p(\text{data} \mid \text{theory})p(\text{theory})}{p(\text{data})}$$

What we all
want
(Posterior)

Likelihood

$$p(\text{theory} \mid \text{data}) = \frac{p(\text{data} \mid \text{theory})p(\text{theory})}{p(\text{data})}$$

What we all
want
(Posterior)

Likelihood

Prior

$$p(\text{theory} \mid \text{data}) = \frac{p(\text{data} \mid \text{theory})p(\text{theory})}{p(\text{data})}$$

Evidence