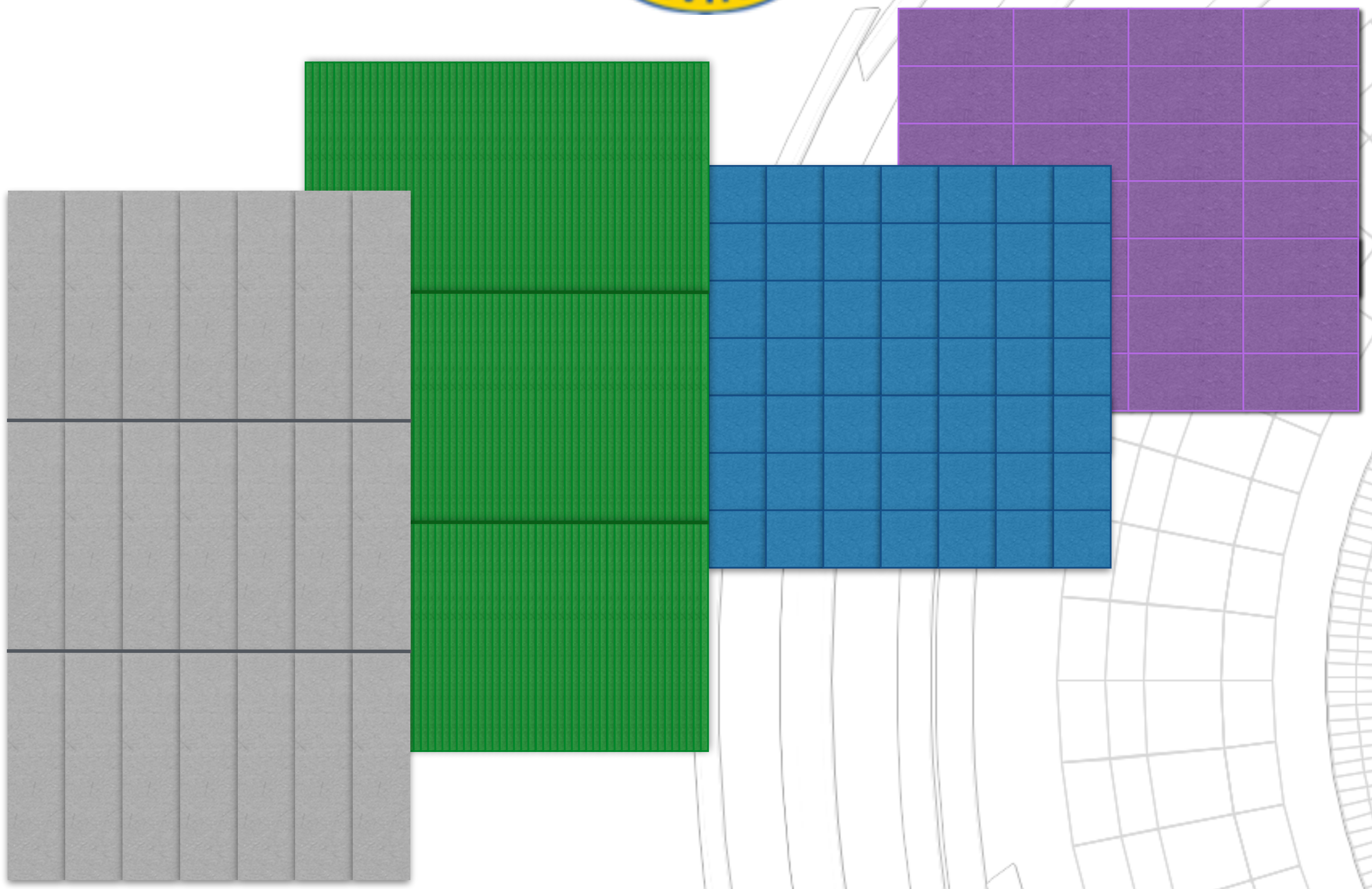
Uncertainties in the era of ML

Aishik Ghosh

ML4FP School

14 August 2024



@Aishik_Ghosh_

Uncertainties, the bedrock of experimental science

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$m_H = 125.25 \pm 0.17$ GeV

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How sure am I ? How can I reduce my uncertainty ?

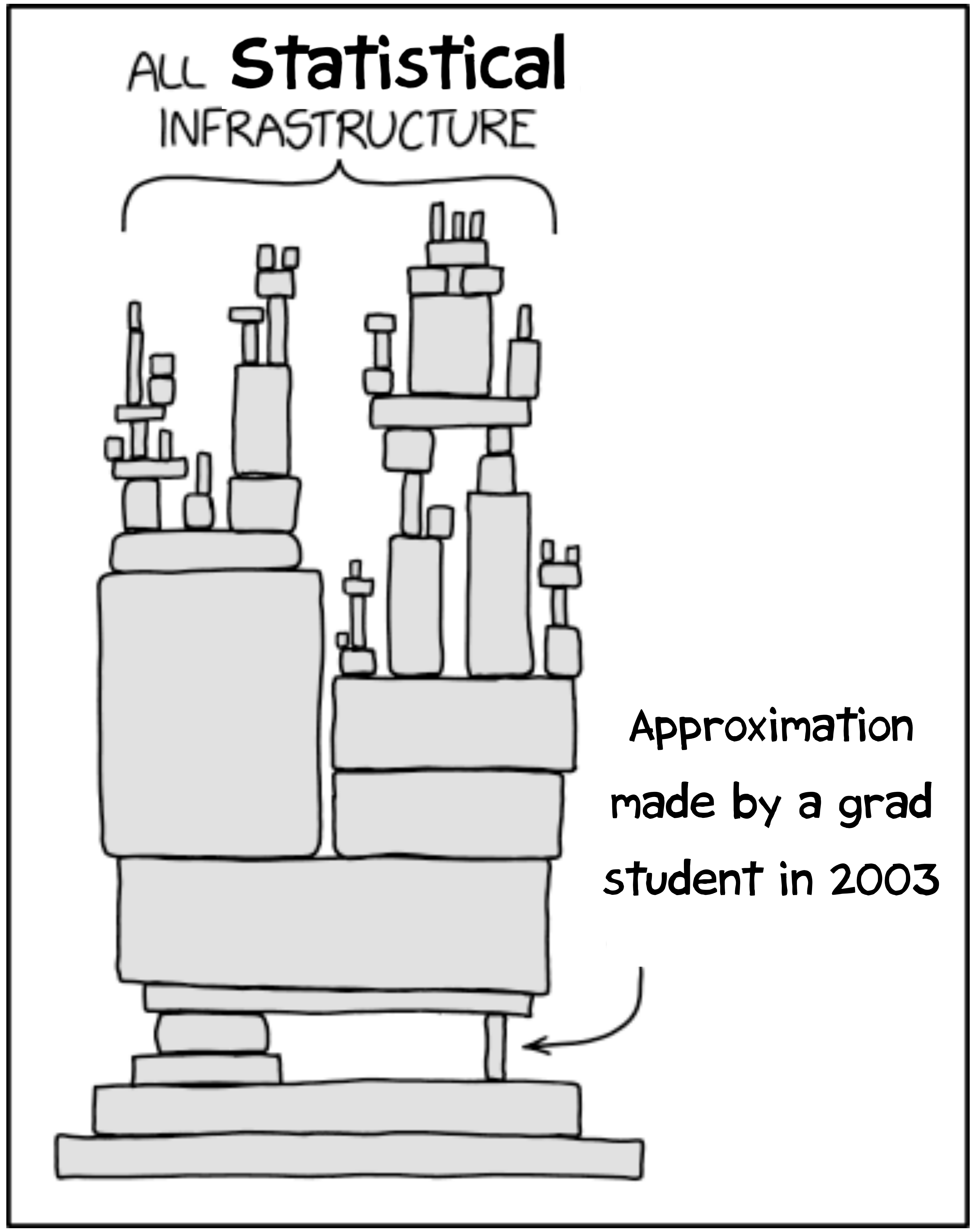
Uncertainties, the bedrock of experimental science

mH = 125.25 ± 0.17 GeV

{statistical, detector systematic, theory systematic, epistemic, ….}

How sure am I ? How can I reduce my uncertainty ?

Nuisance Parameter Infrastructure



Stolen from Daniel Whiteson
Inspired by XKCD

Time to re-examine
some of the
underlying pieces

Are they up to the
task of the precision era?

The four stages of ML adoption

Fear: Will ML exacerbate uncertainties in a way human-designed strategies naturally avoid ?

Solution: Find ML equivalents of uncertainty mitigation tricks we implicitly use in classical methods. Understand good and bad ways to use ML

Opportunity: ML *for* uncertainty – Realising that ML unlocks completely new interpretability tools and methods to tackle uncertainties in a way classical methods couldn’t

Revolution: Novel uncertainty quantification & mitigation methods developed for ML have wider applications, also back-ported to classical (non-ML) algorithms

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We are here

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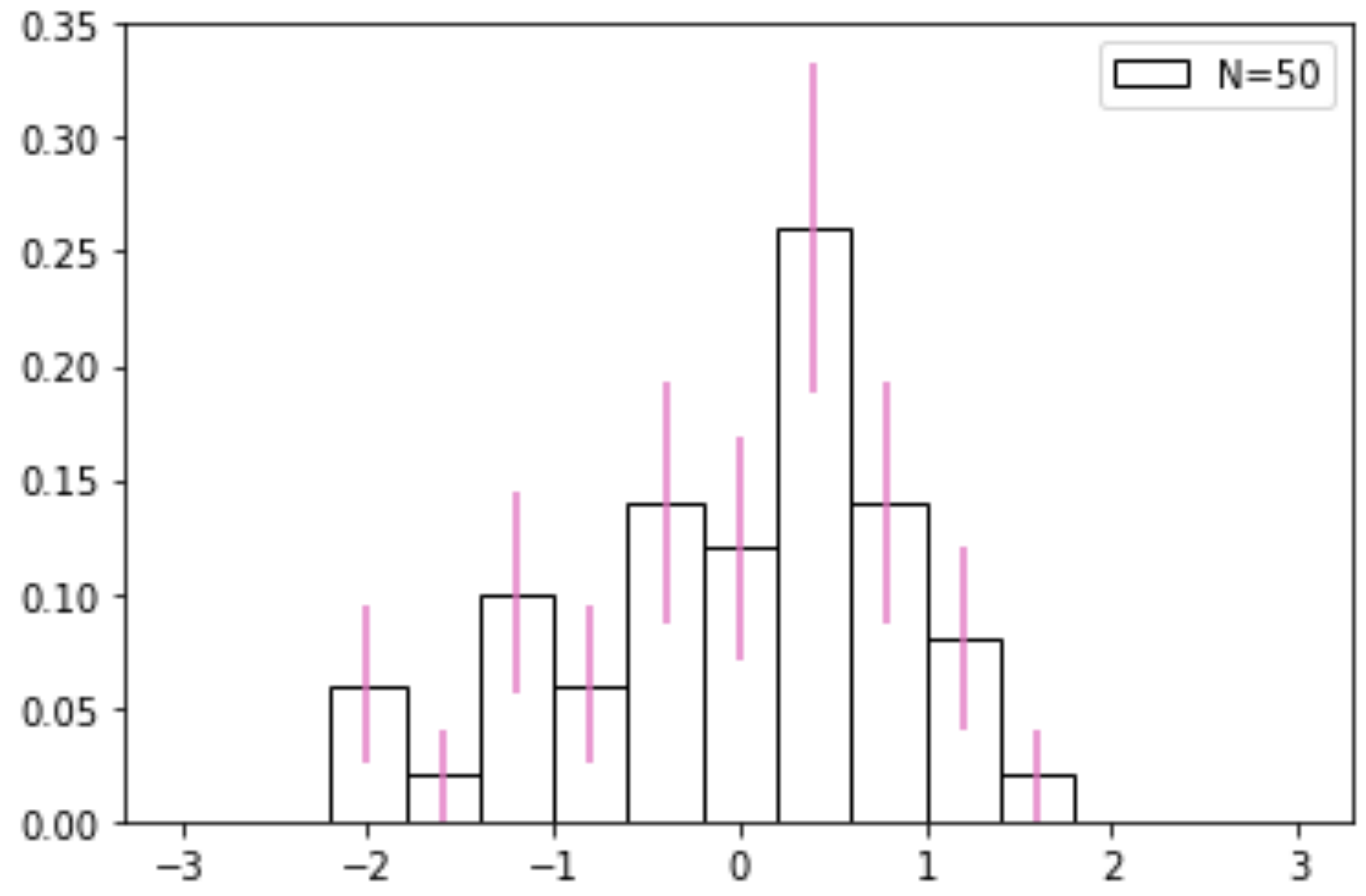
Typical Uncertainties in HEP

Statistical Uncertainty



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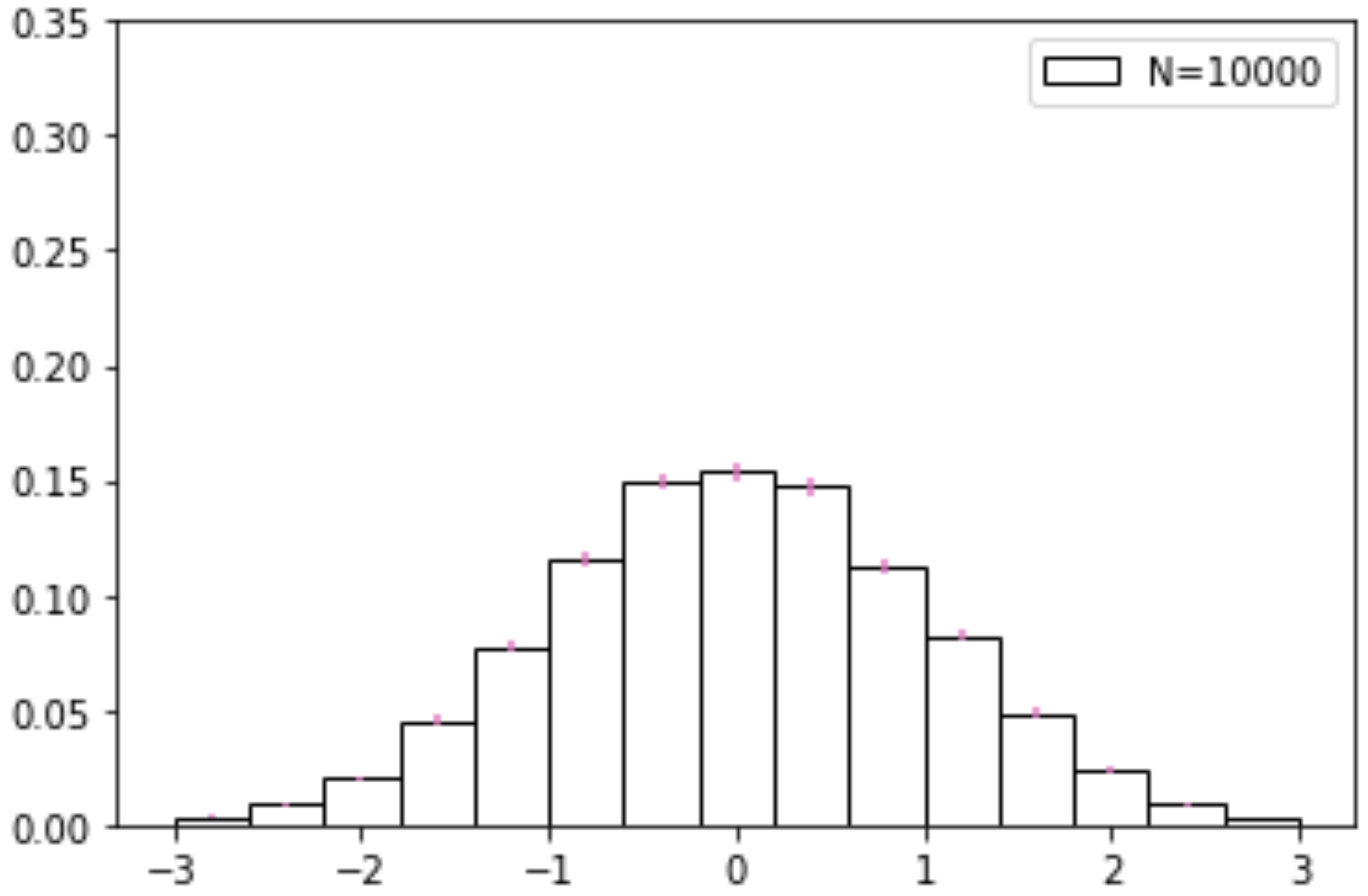

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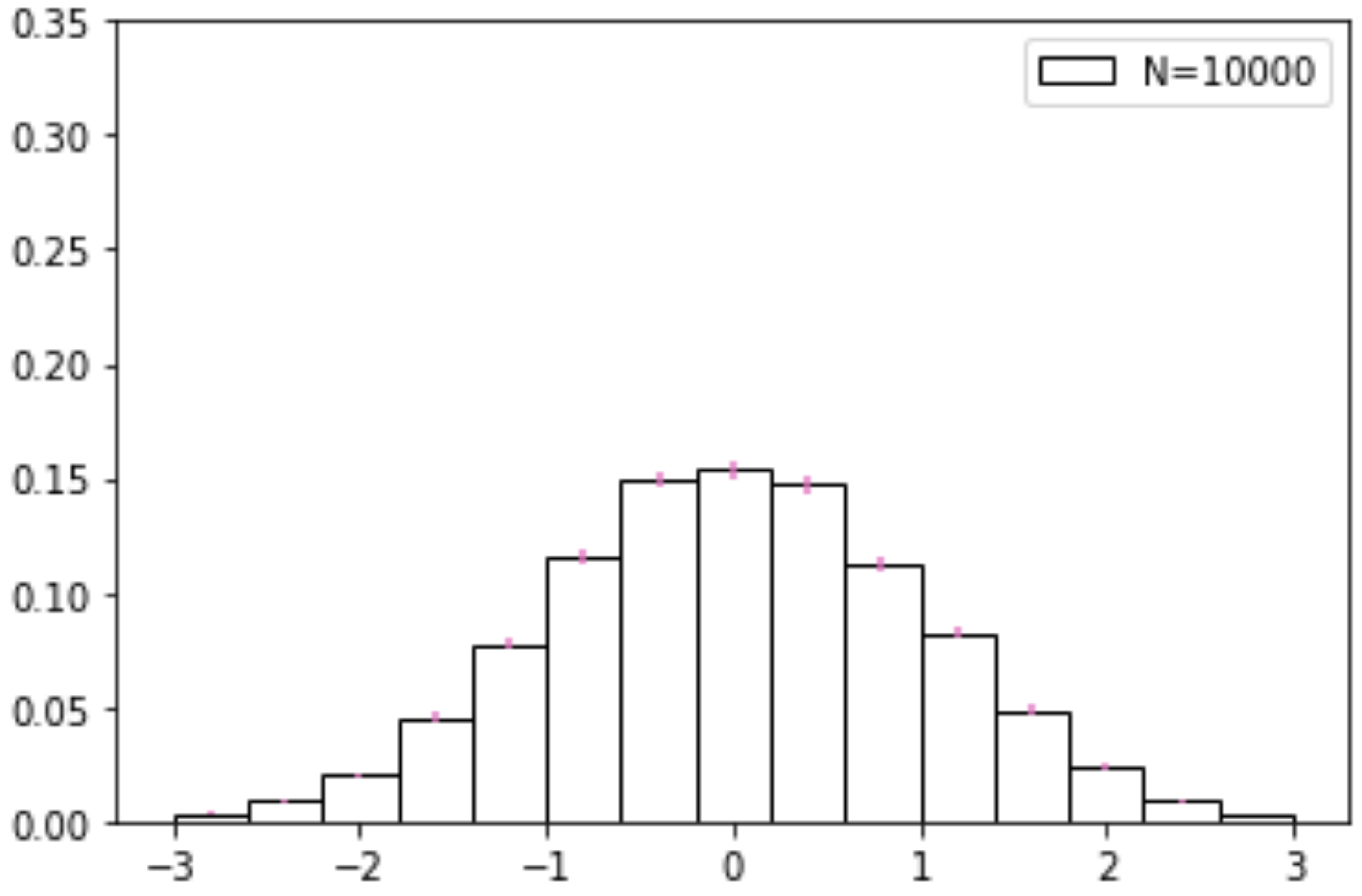
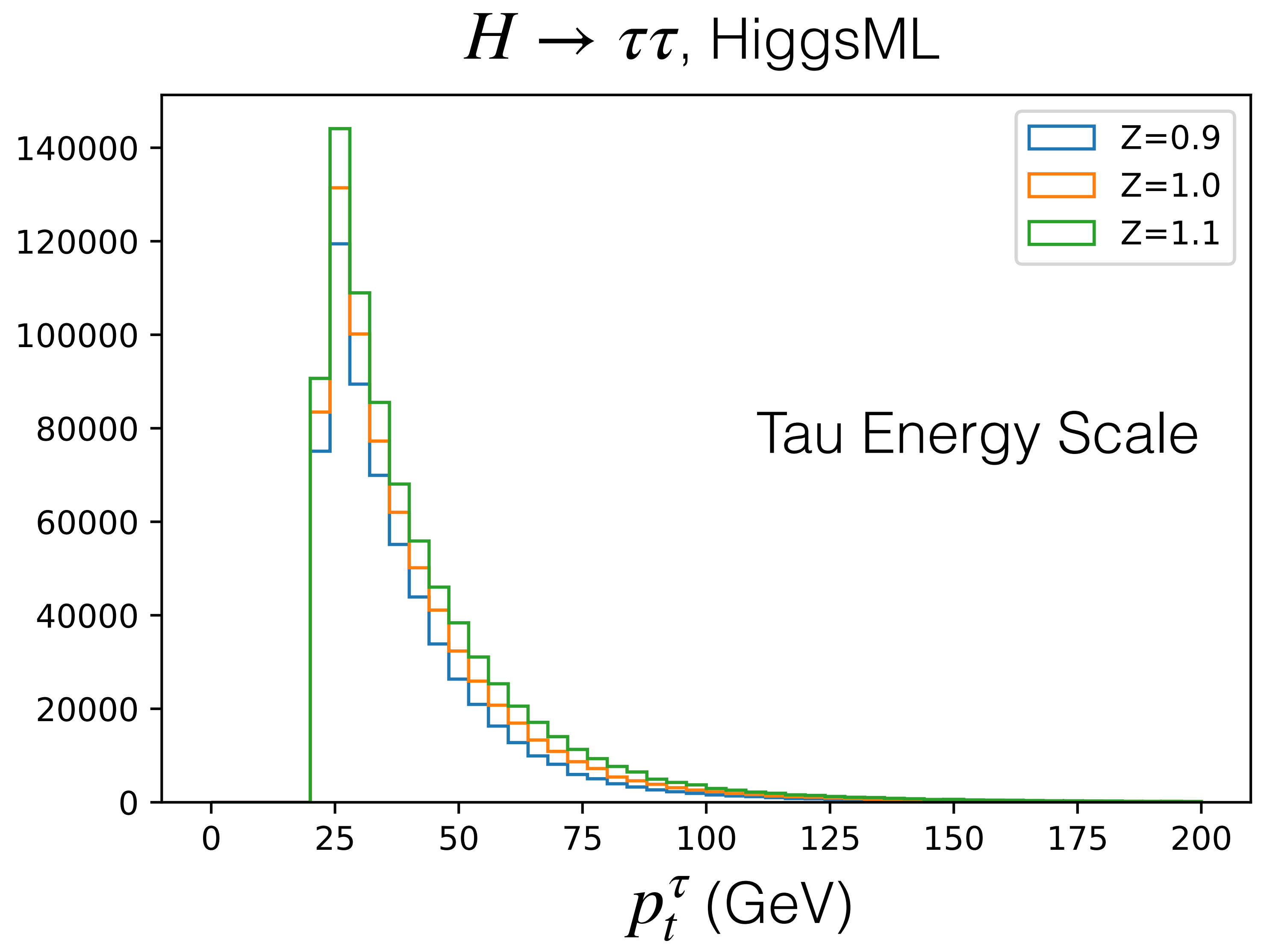


Systematic Experimental Uncertainty



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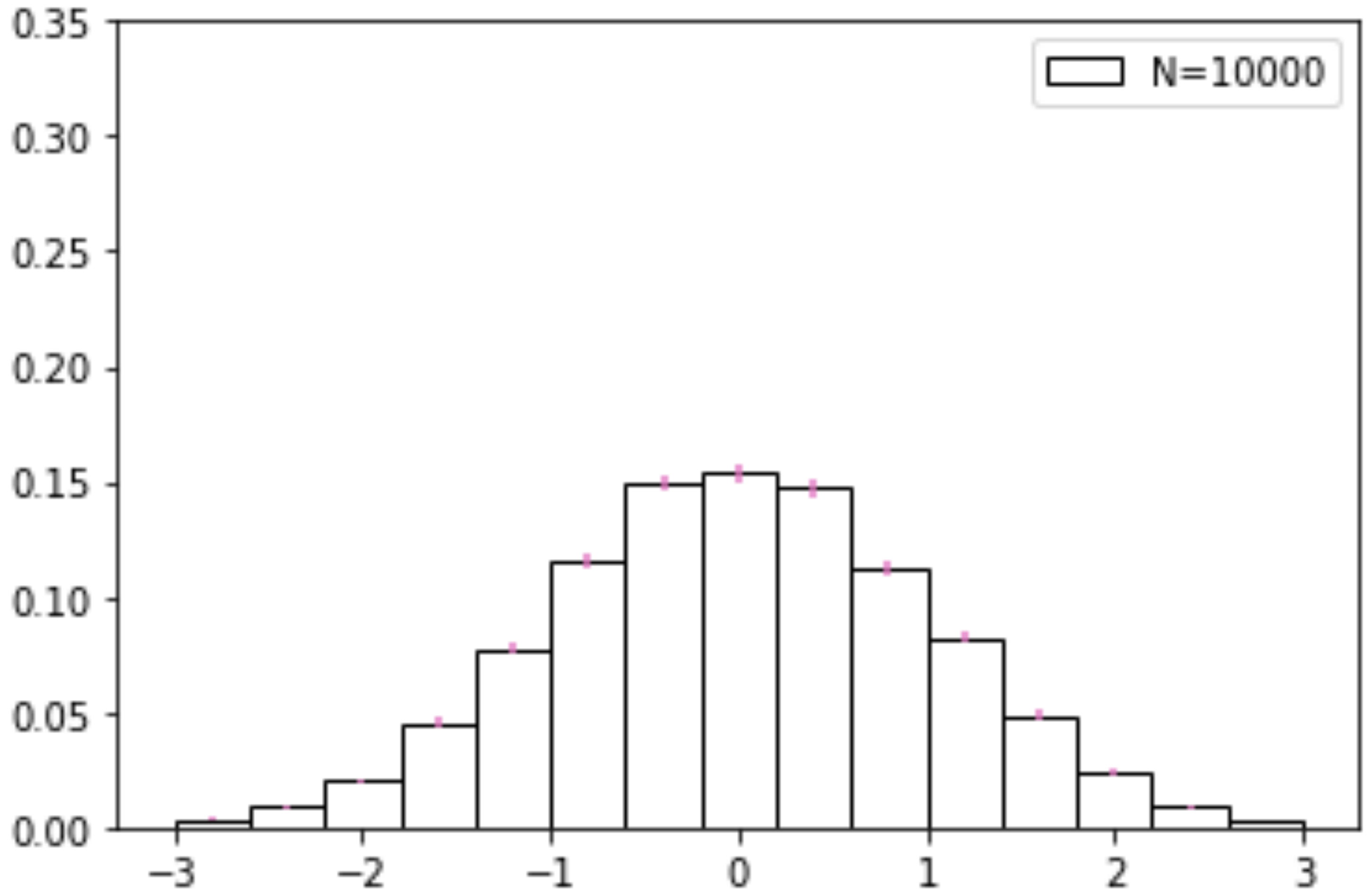

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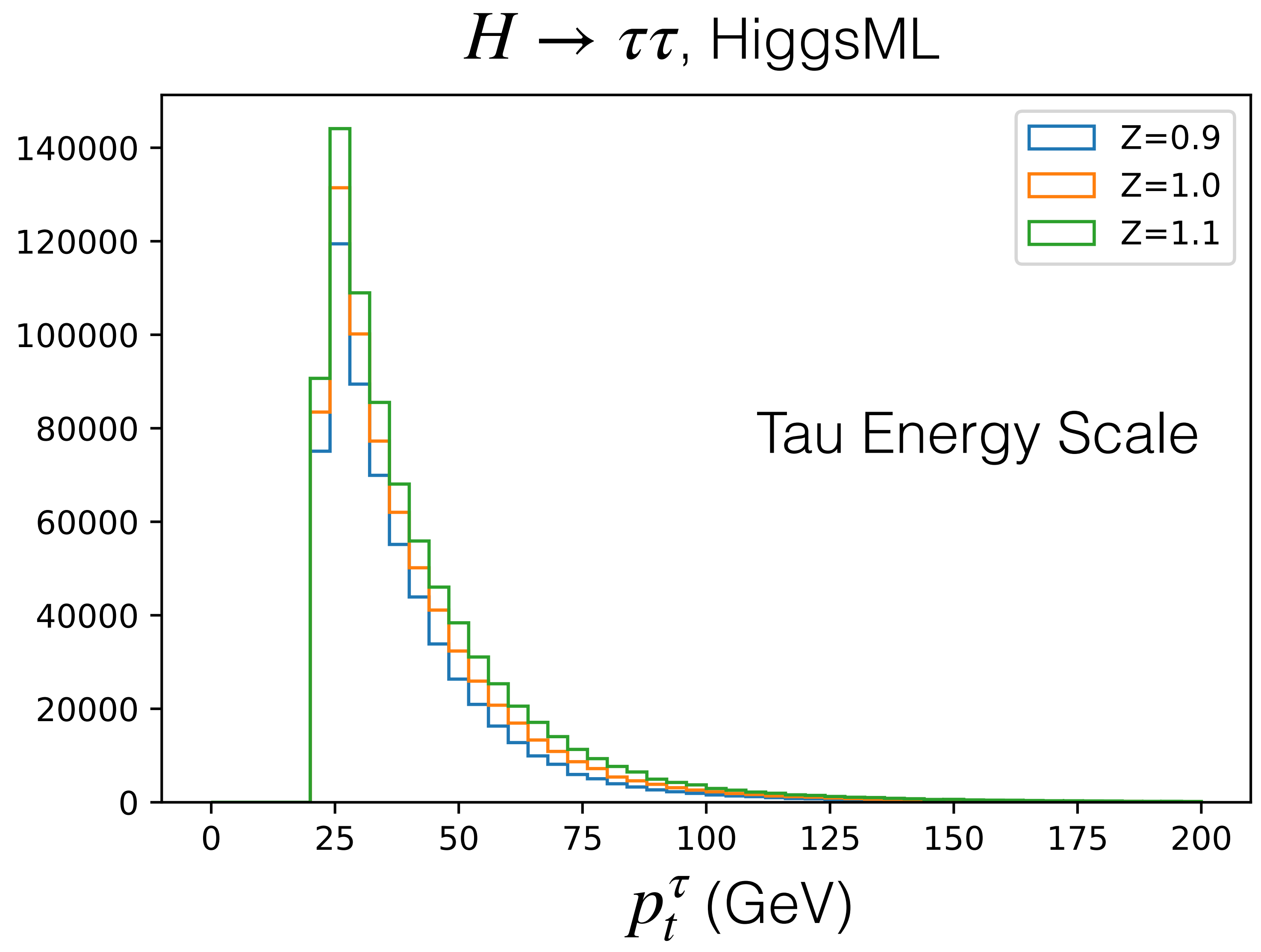
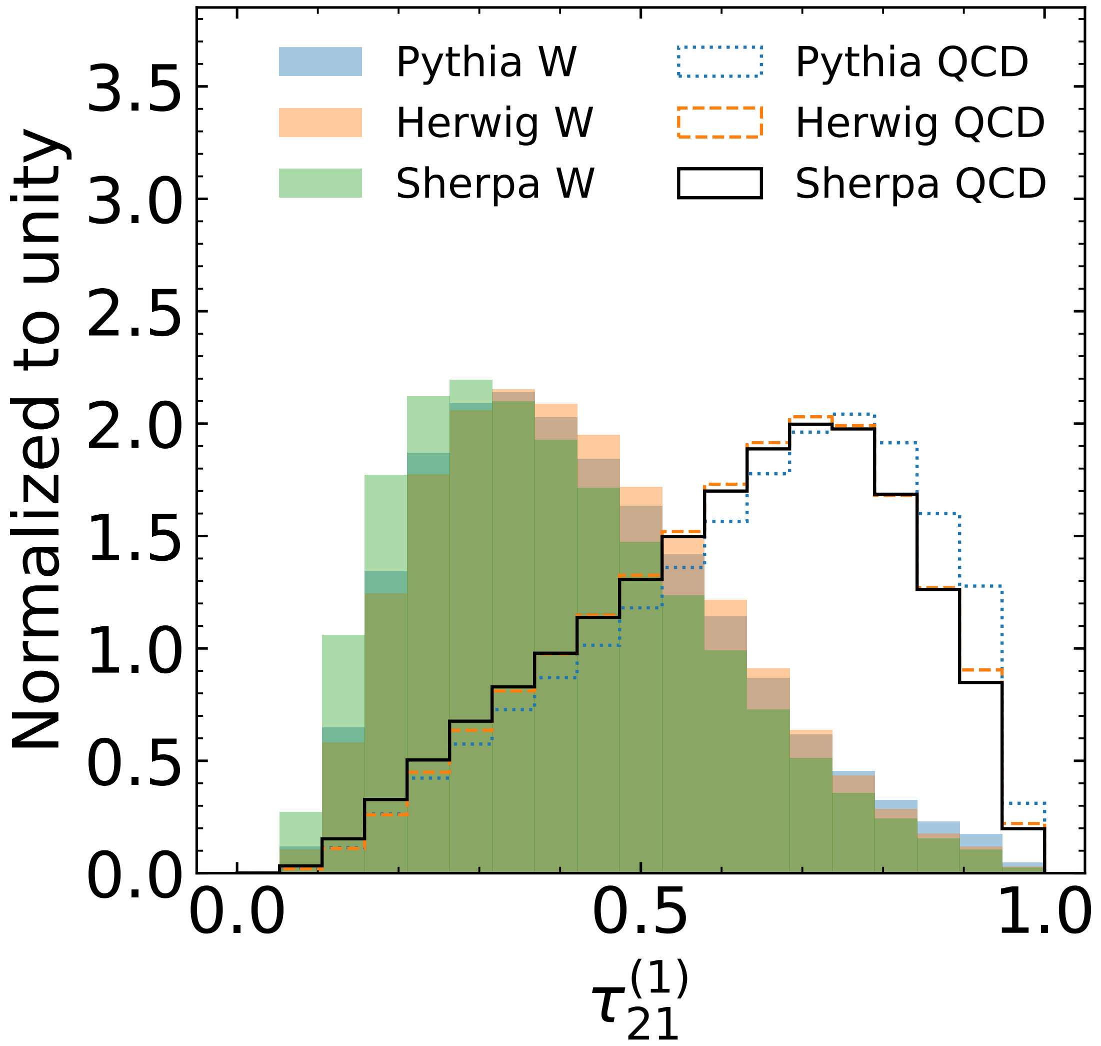


Systematic Theory Uncertainty



SHERPA 2.2

Essential terminology

Parameter of Interest (PoI): Parameter we want to measure from data
Eg. **signal strength μ** that describes the strength of a physics process we care about

Nuisance Parameter (NP): Parameters we actually don't want to care about, but they influence our measurement, so we need to account for their impact
Eg. **Jet energy scale**, background normalisation

Essential terminology

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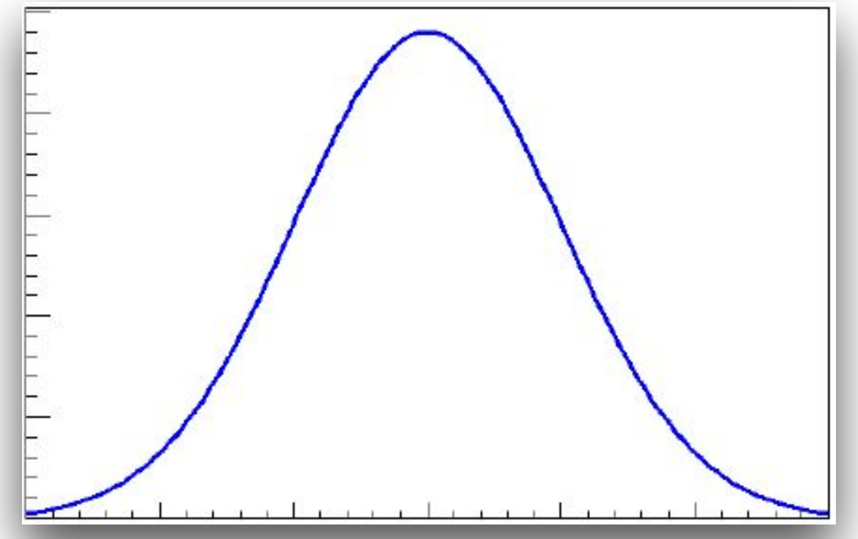
Eg. **Jet energy scale**, background normalisation

We often make auxiliary measurement of NP and use that as a ~~prior~~ constraint in final fit

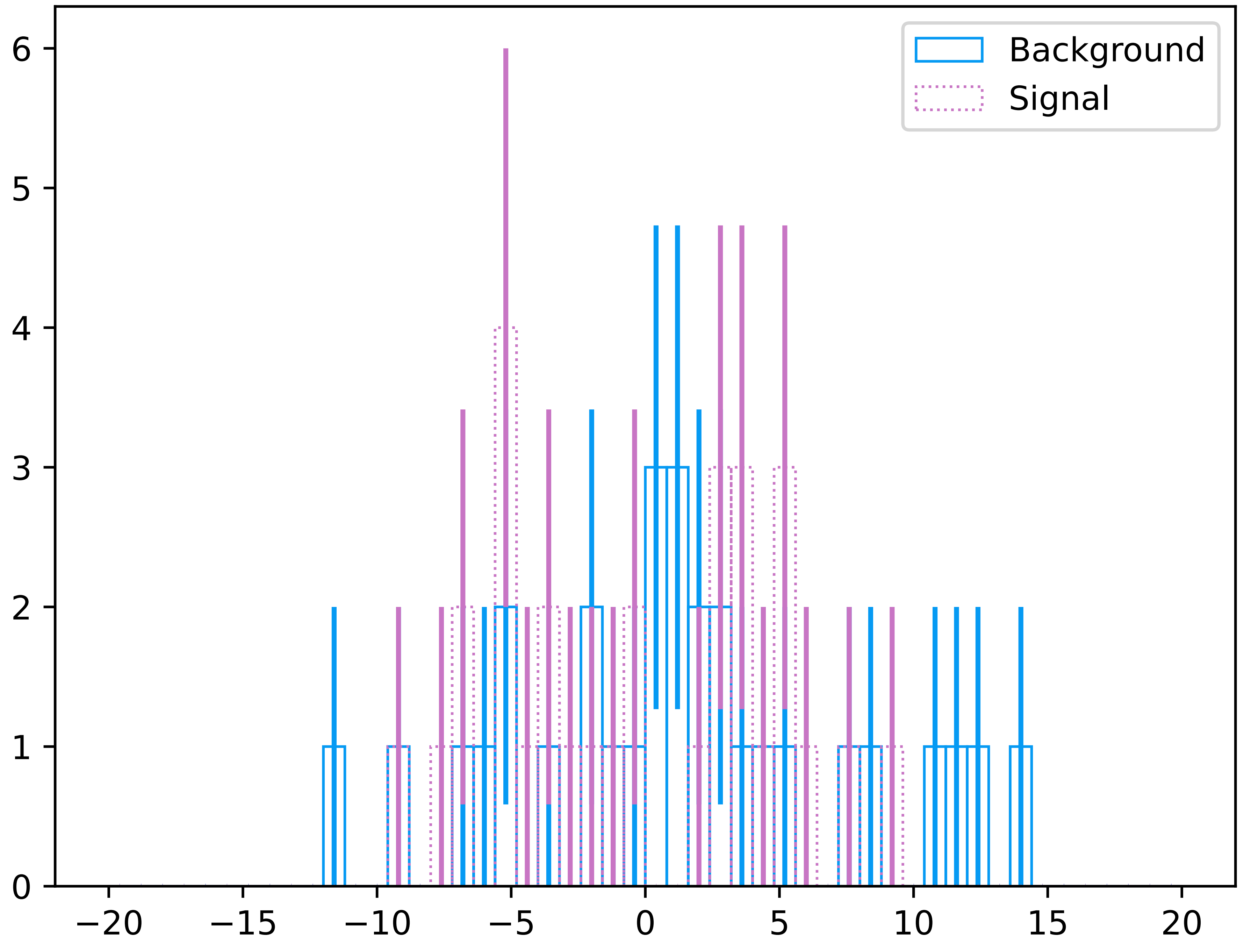
Could also do simultaneous fit in signal and control regions

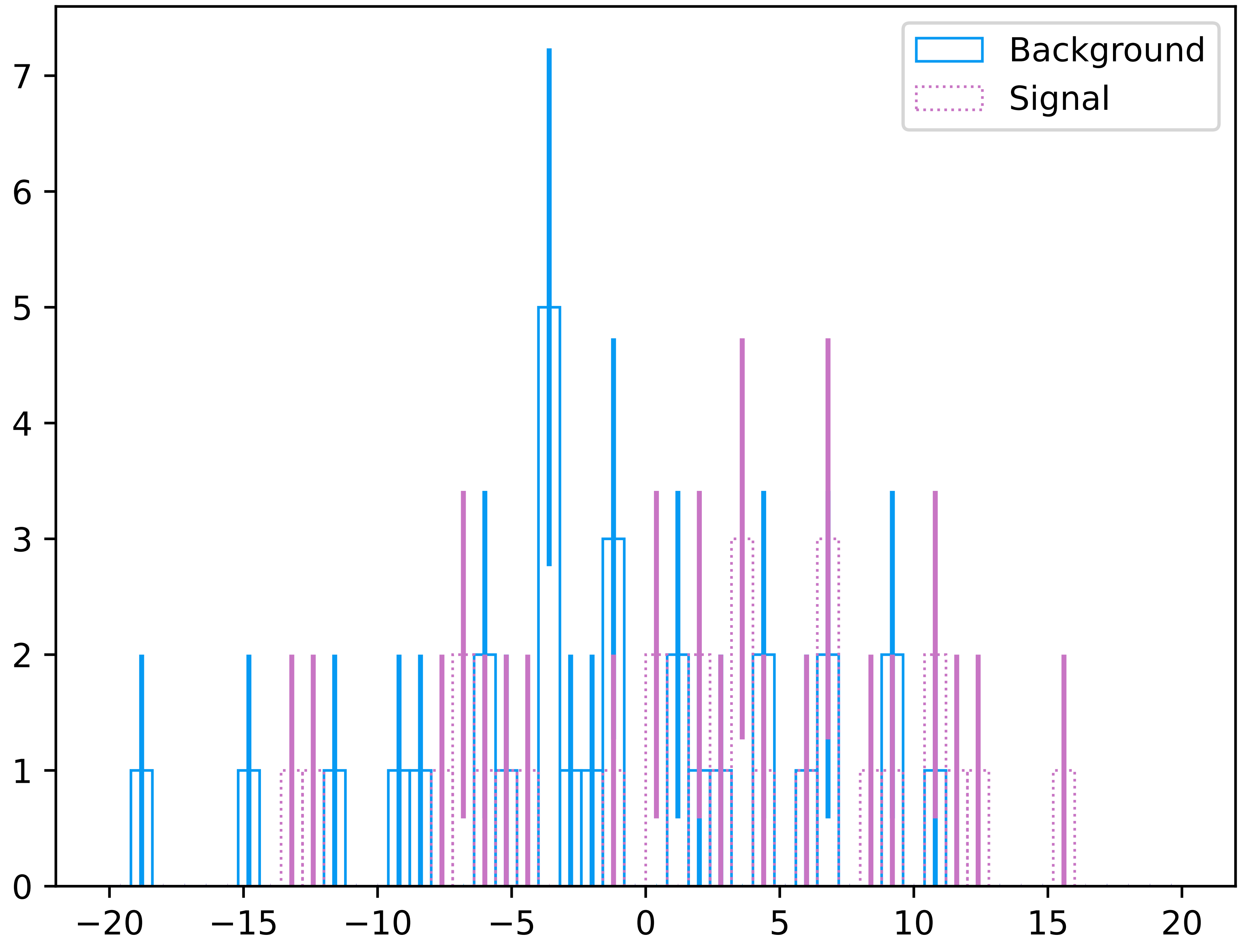


z = Nuisance Parameter
Prior

Uncertainties discussed in ML: Aleatoric Uncertainty

60 samples





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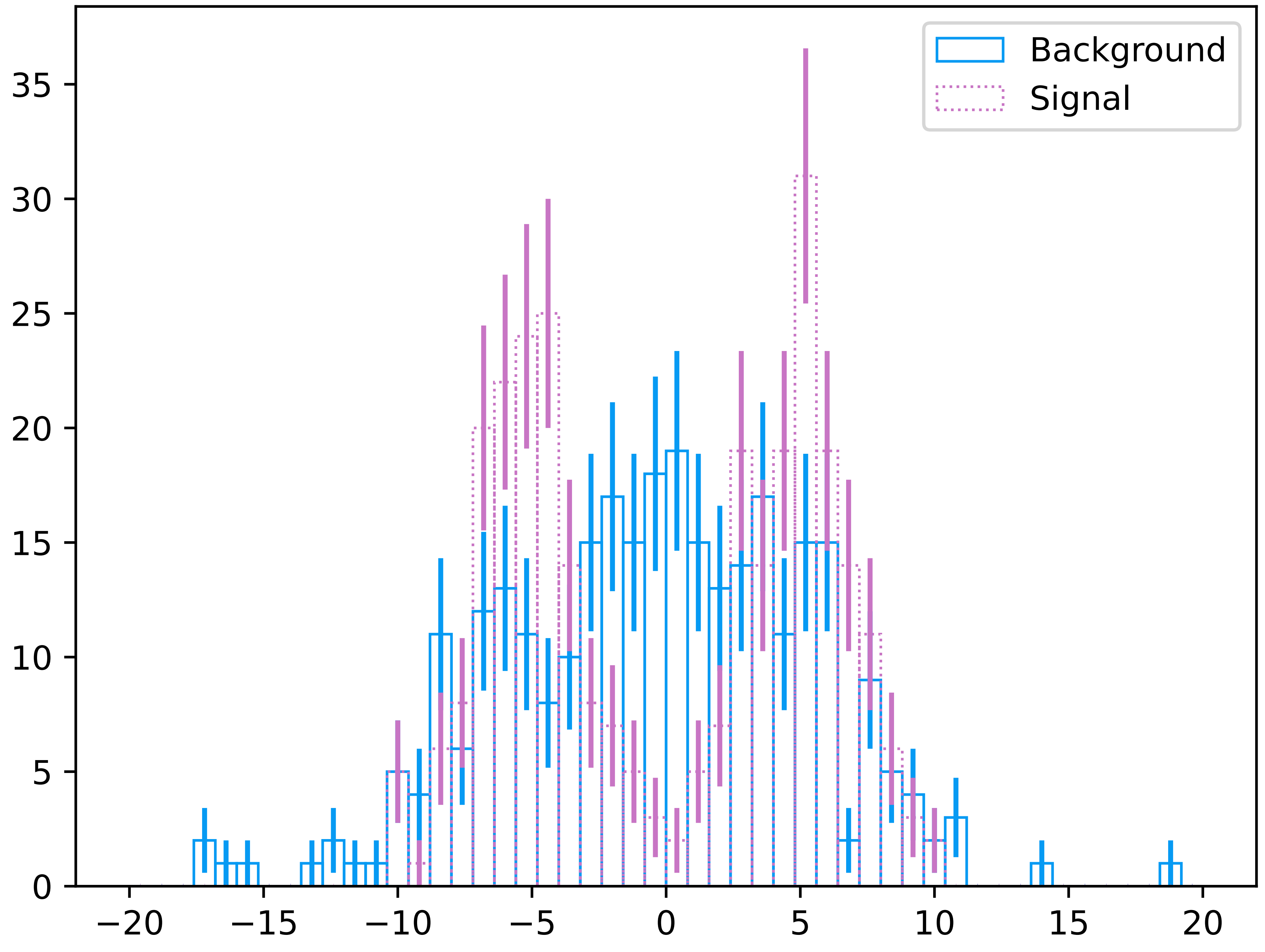

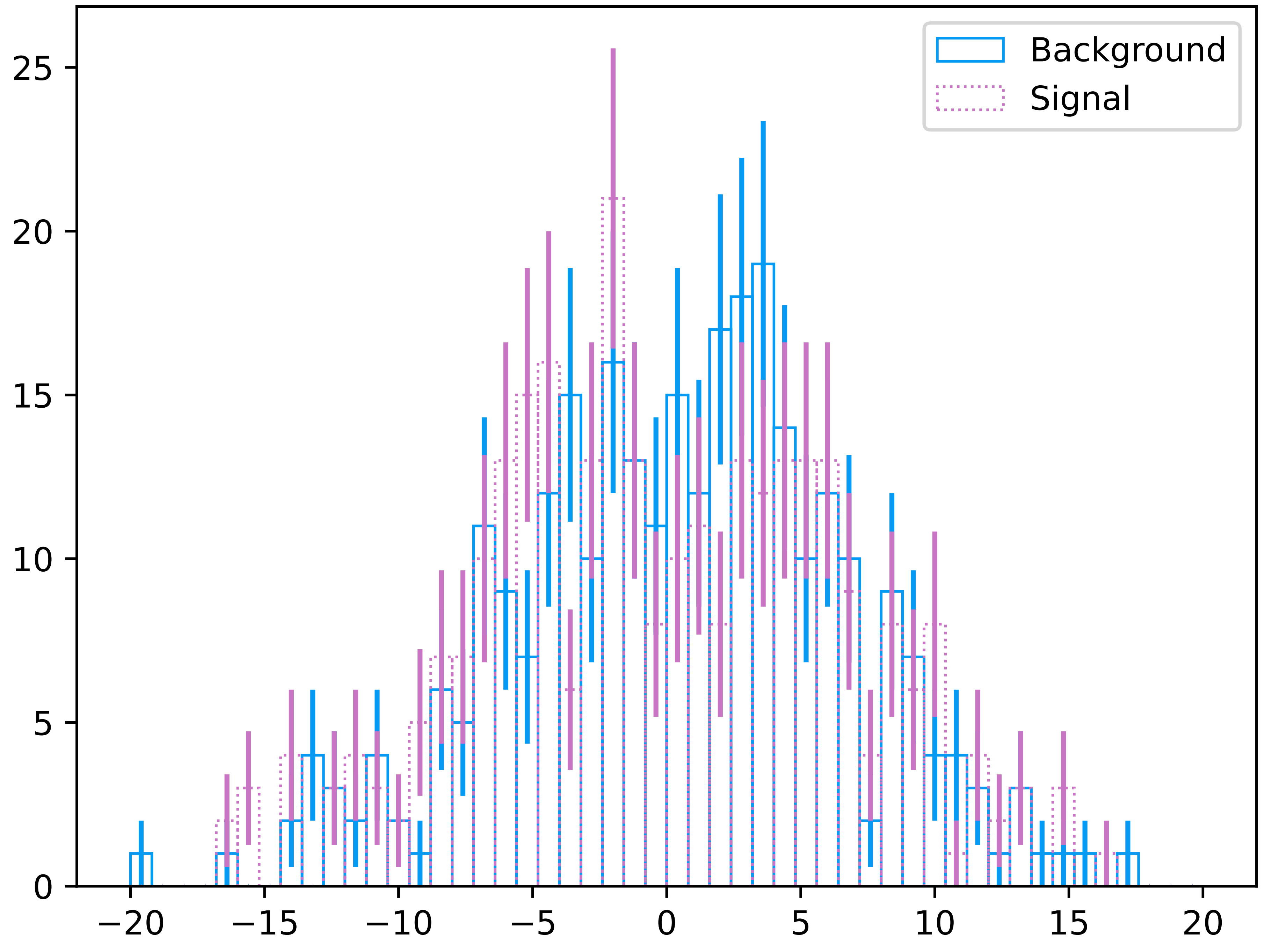

Uncertainties discussed in ML: Aleatoric Uncertainty

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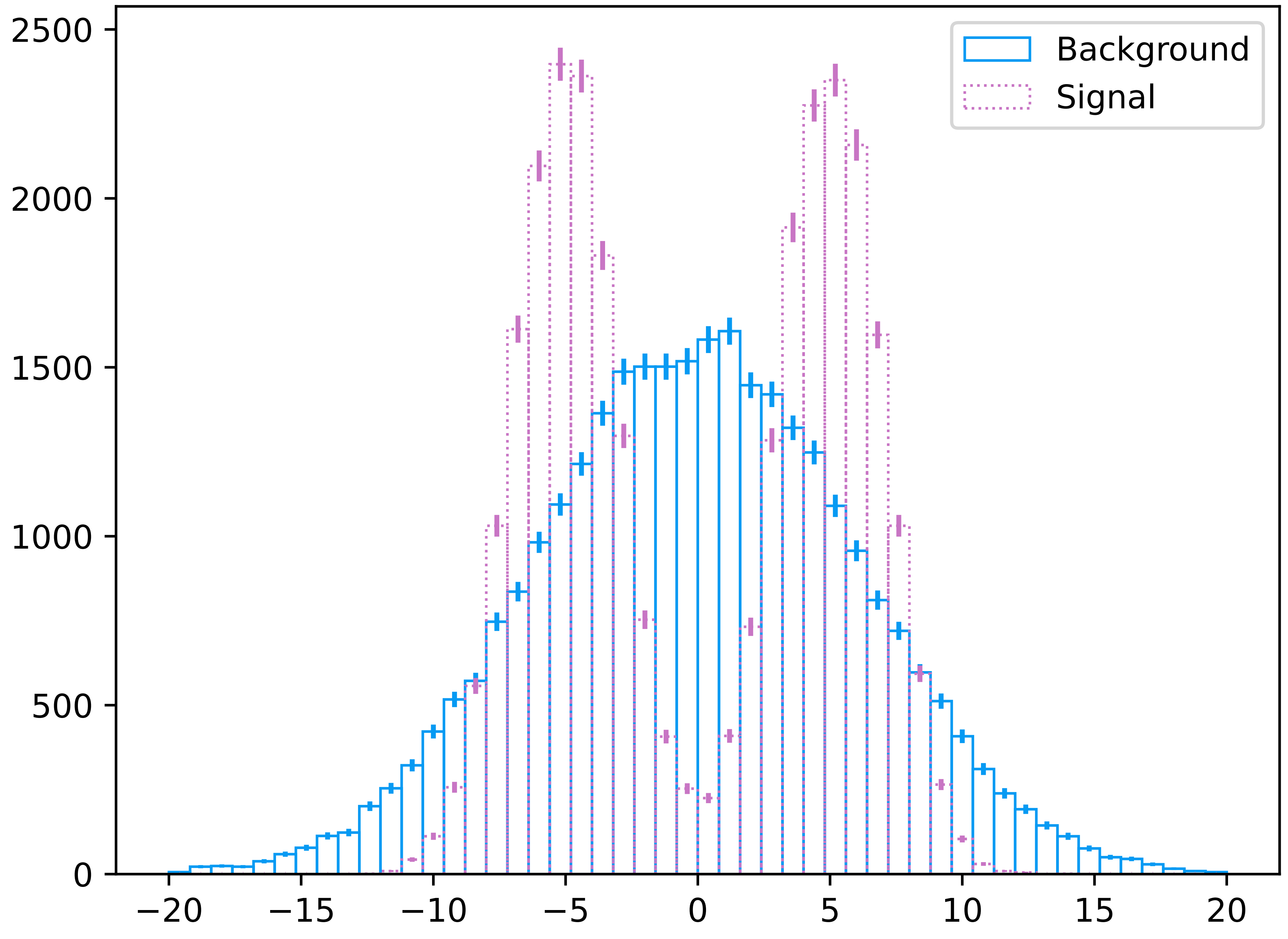

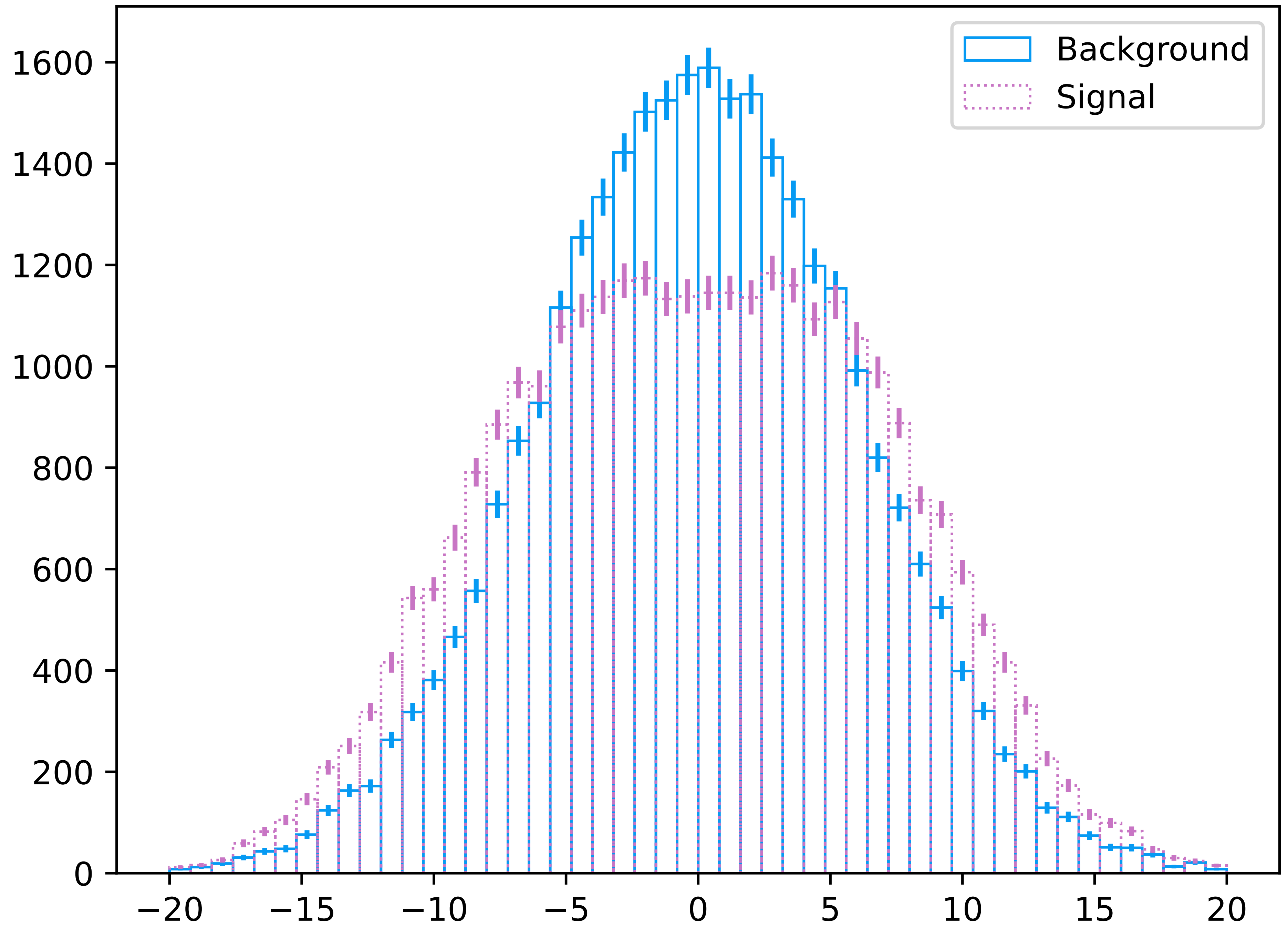

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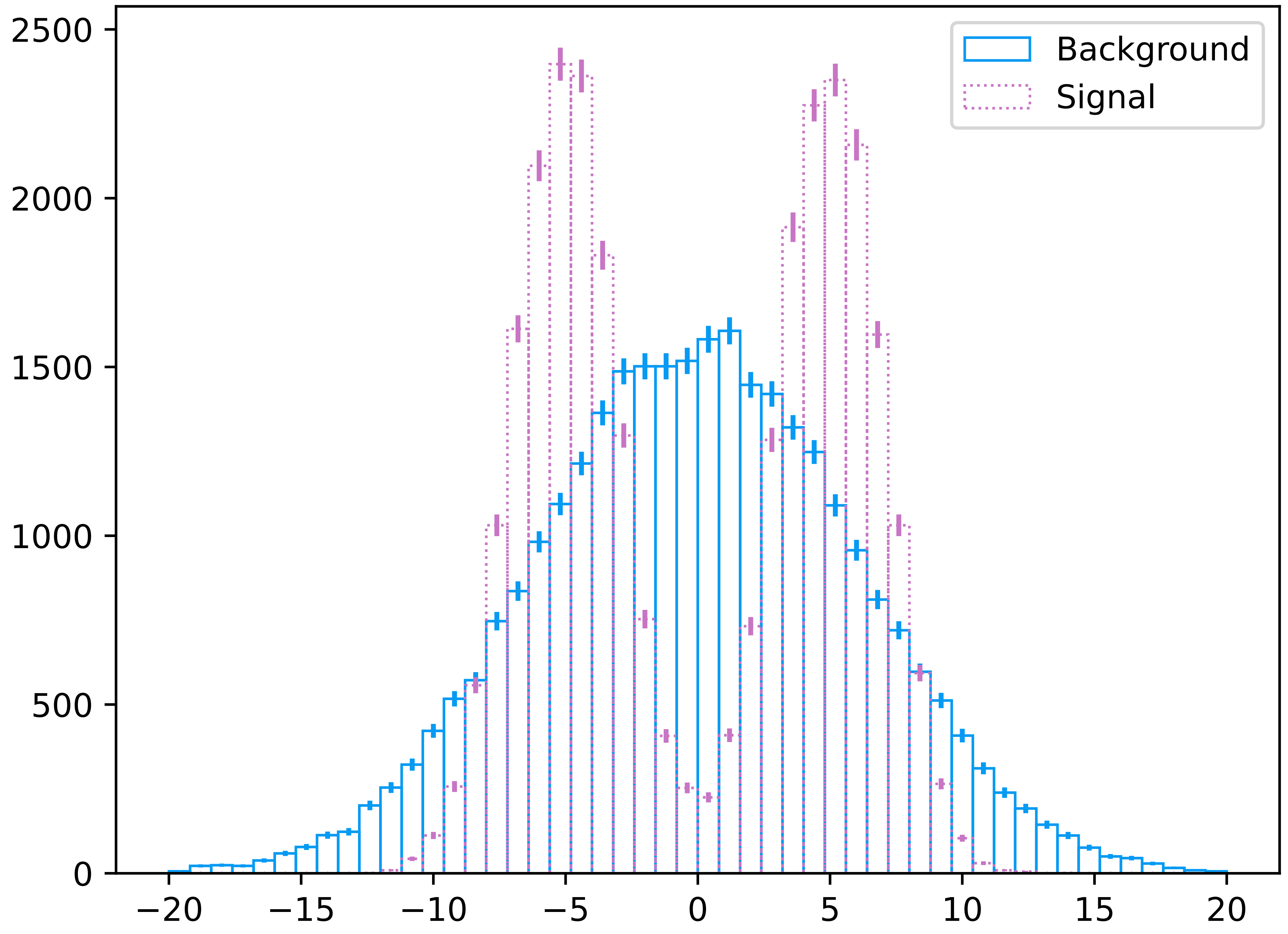
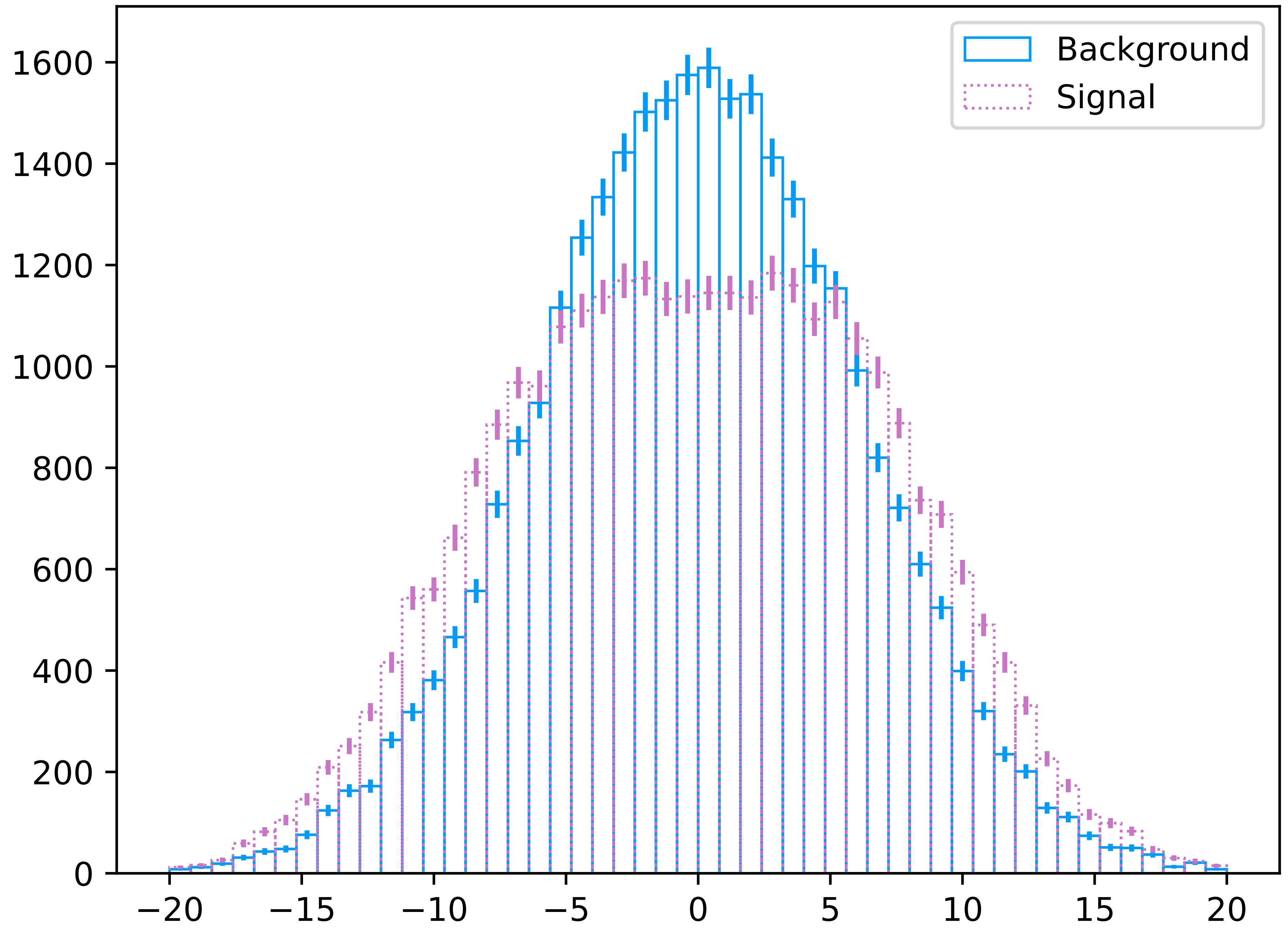
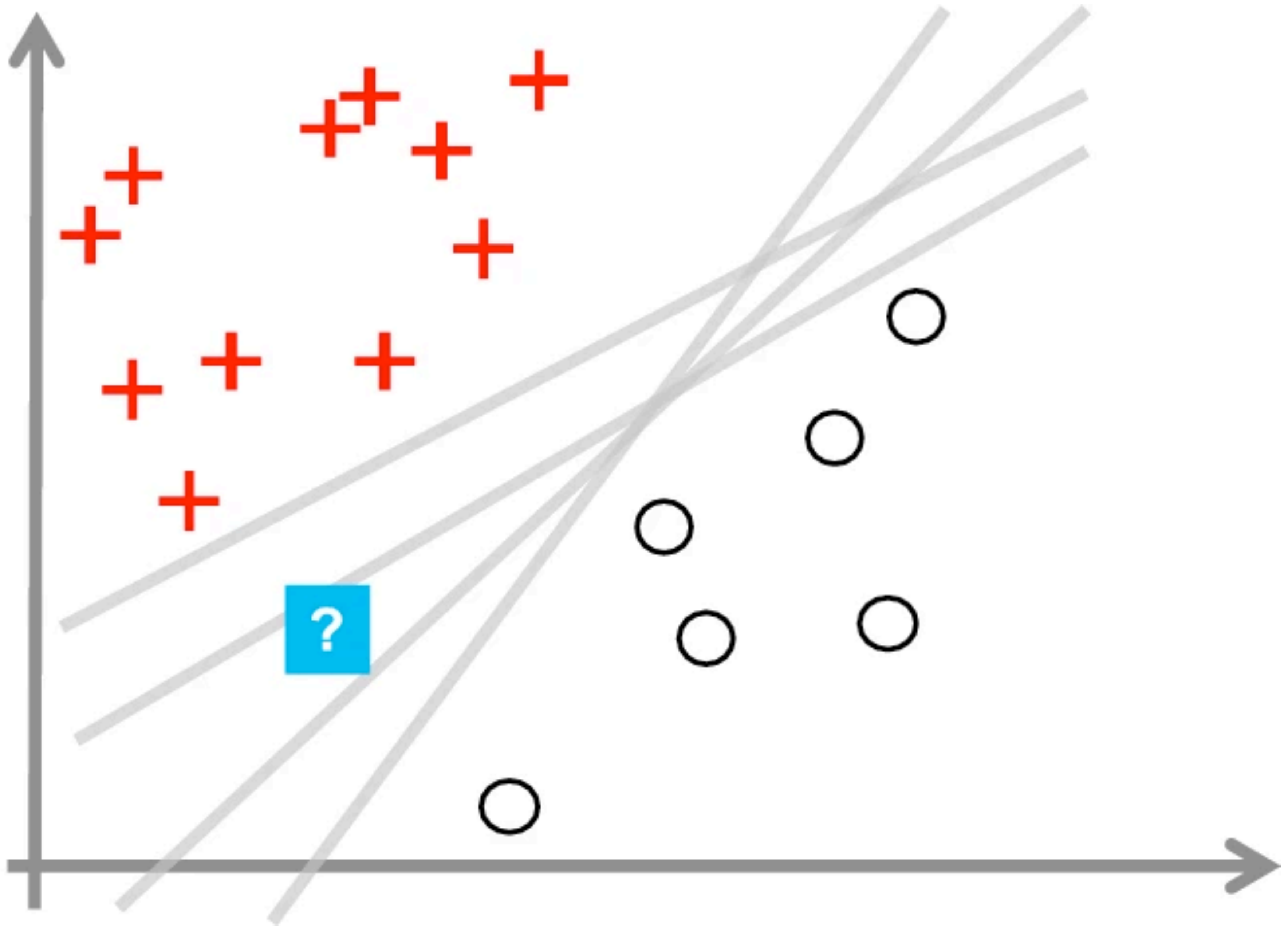




Intrinsic randomness leads to a per-event uncertainty that cannot be reduced by taking more data

Uncertainties discussed in ML: Epistemic Uncertainty

Could reduce by gathering more data, possibly focused on different parts of parameter space
Eg. Simulations at another value of JES, different particle energies



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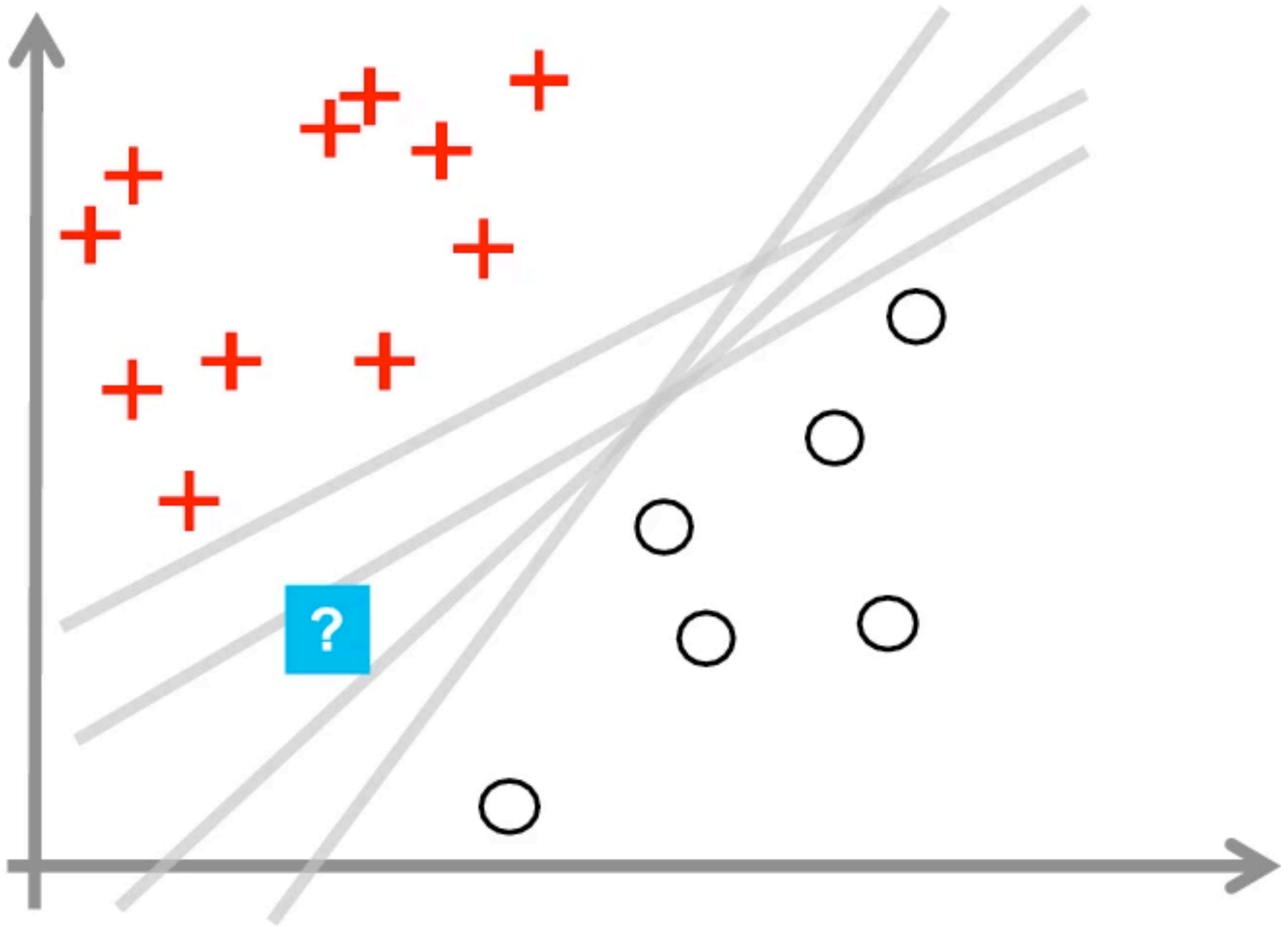

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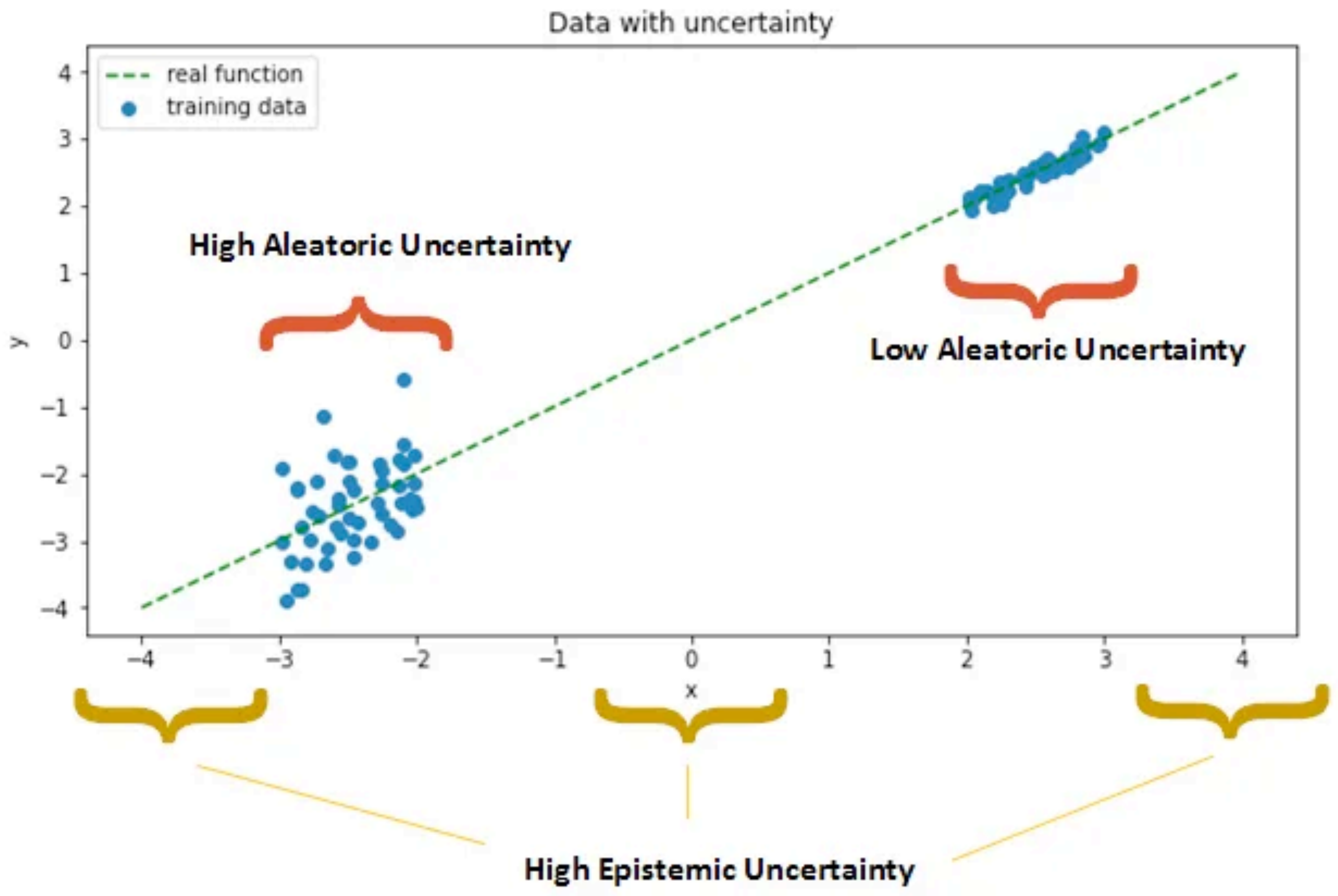

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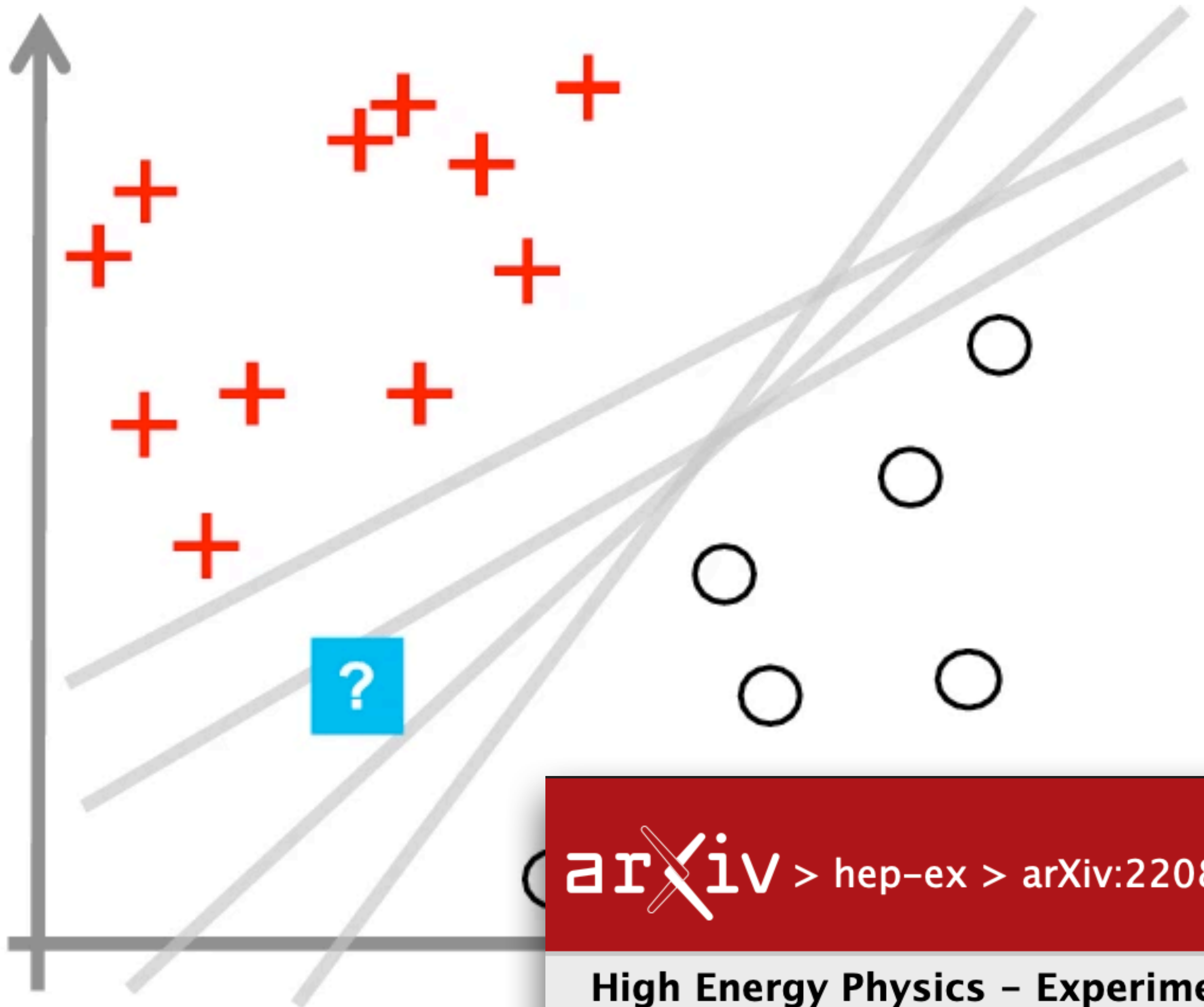

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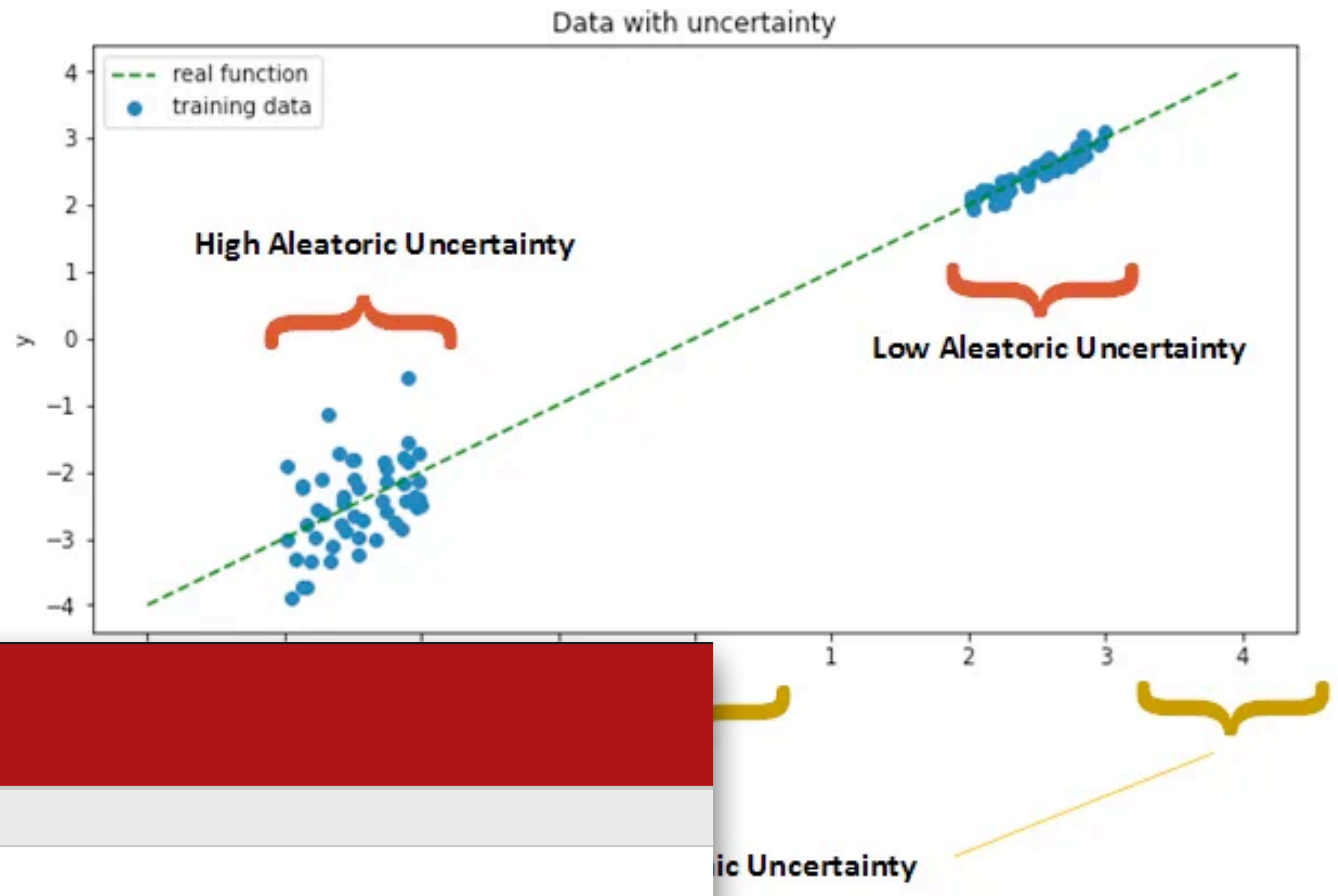

Image: [Source]()

arXiv > hep-ex > arXiv:2208.03284

High Energy Physics – Experiment

[Submitted on 5 Aug 2022 (v1), last revised 6 Sep 2022 (this version, v3)]

Interpretable Uncertainty Quantification in AI for HEP

Thomas Y. Chen, Biprateep Dey, Aishik Ghosh, Michael Kagan, Brian Nord, Nesar Ramachandra

Snowmass 2021: Advocate to build common language between fields

ML uncertainties are relevant in HEP !

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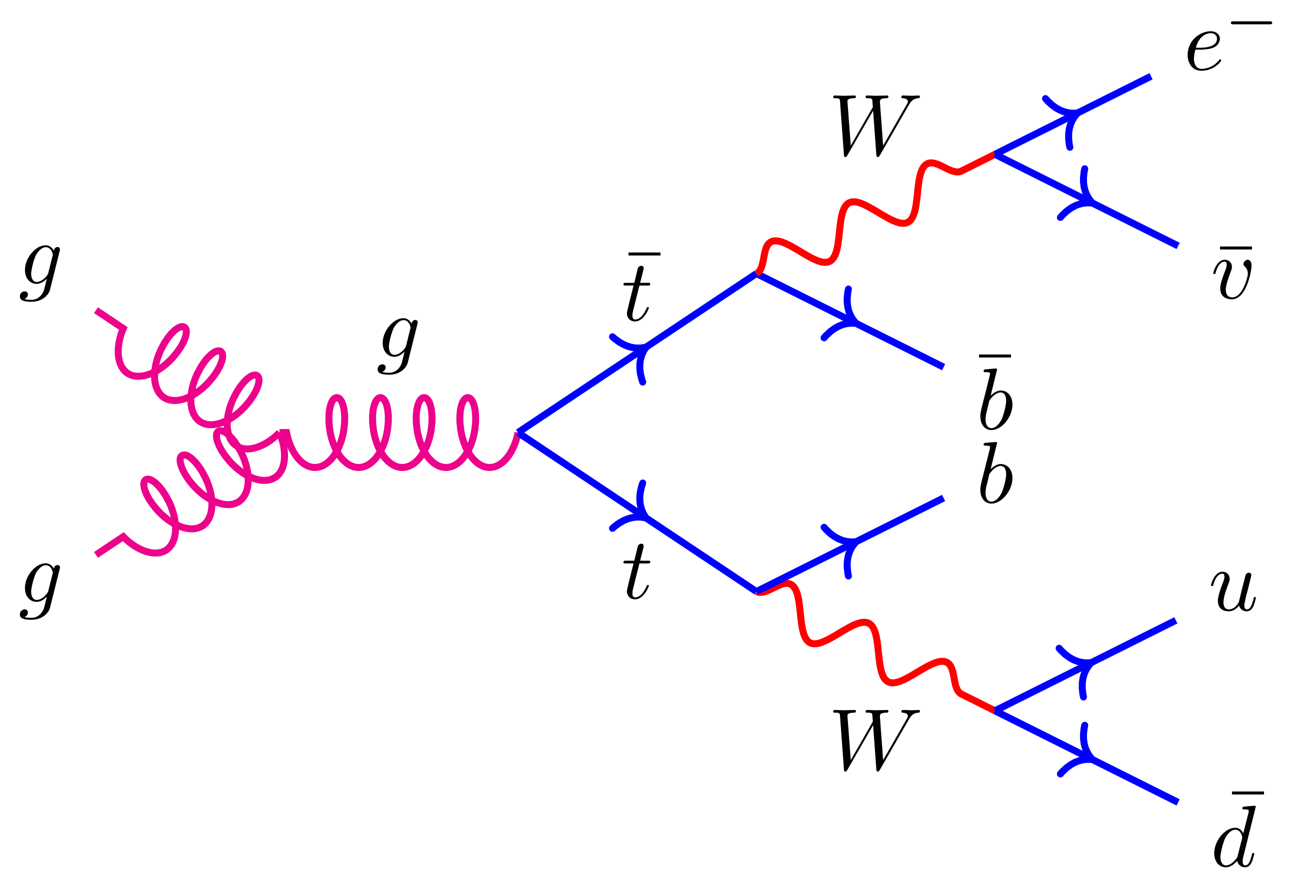
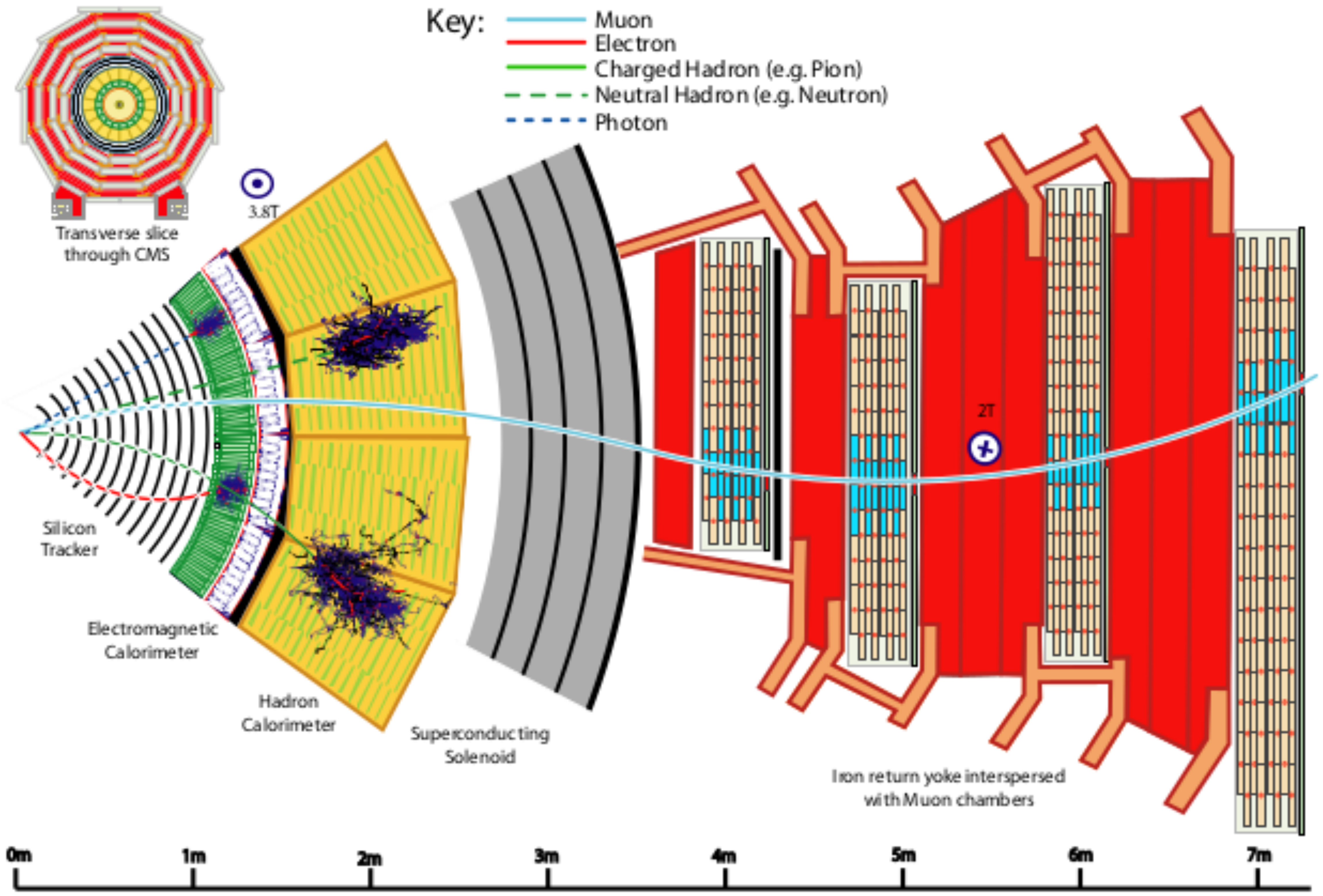
Eg. Estimating likelihoods directly with neural networks

OmniFold: Anderson et al. (incl. Nachman)

High-dimensional unfolding with neural networks



Fundamental interactions



Detector effects on measurement

OmniFold: Anderson et al. (incl. Nachman)

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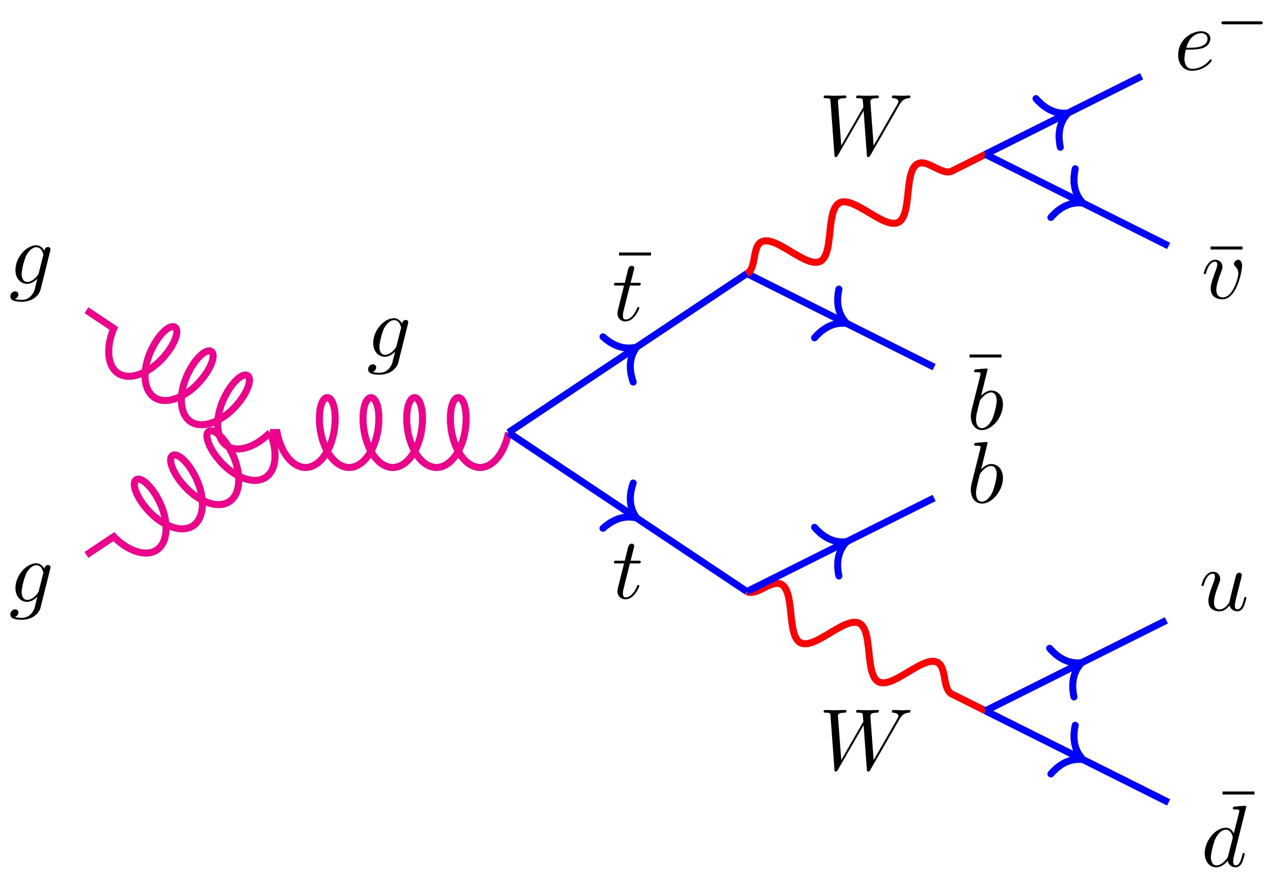

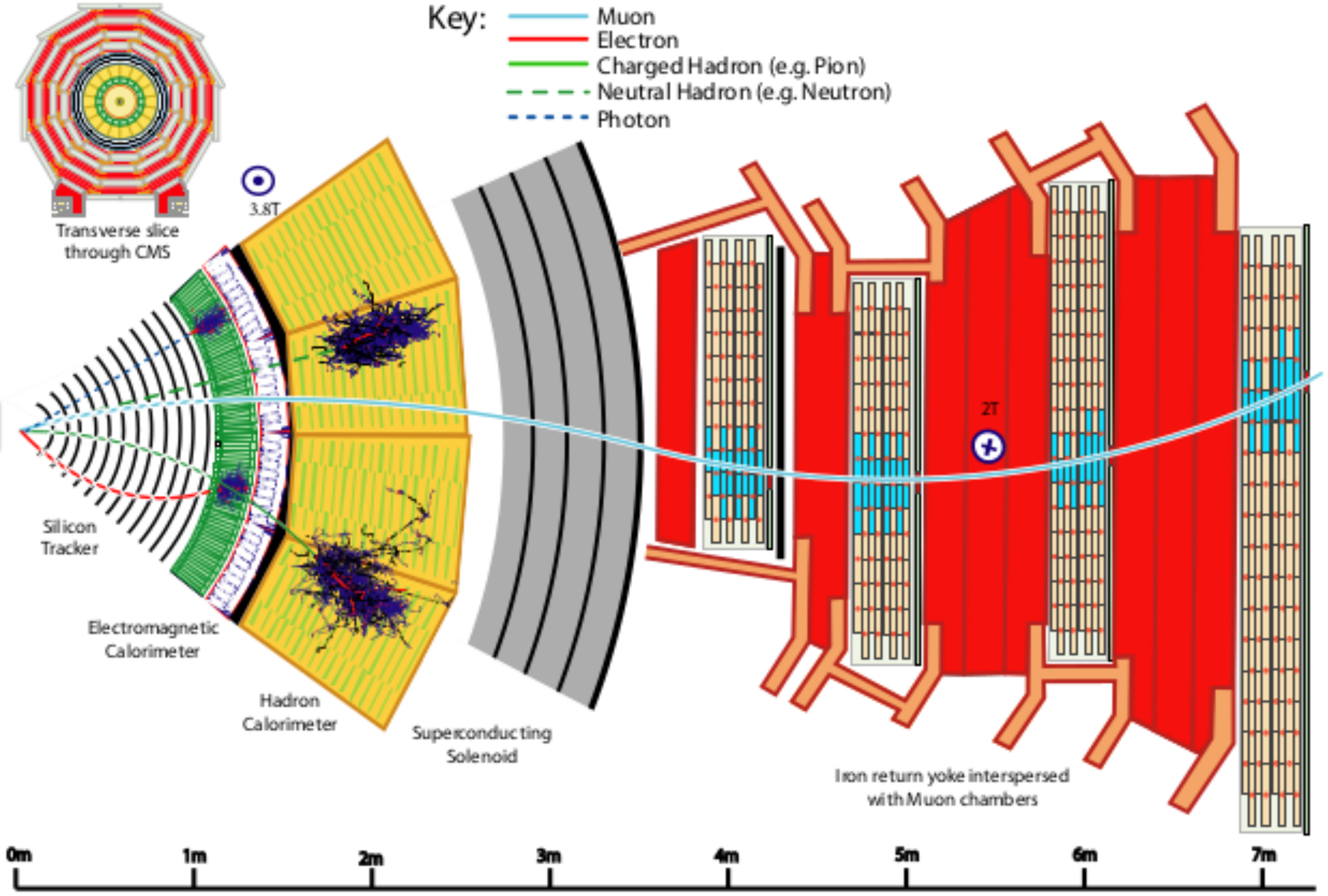

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Detector effects on measurement

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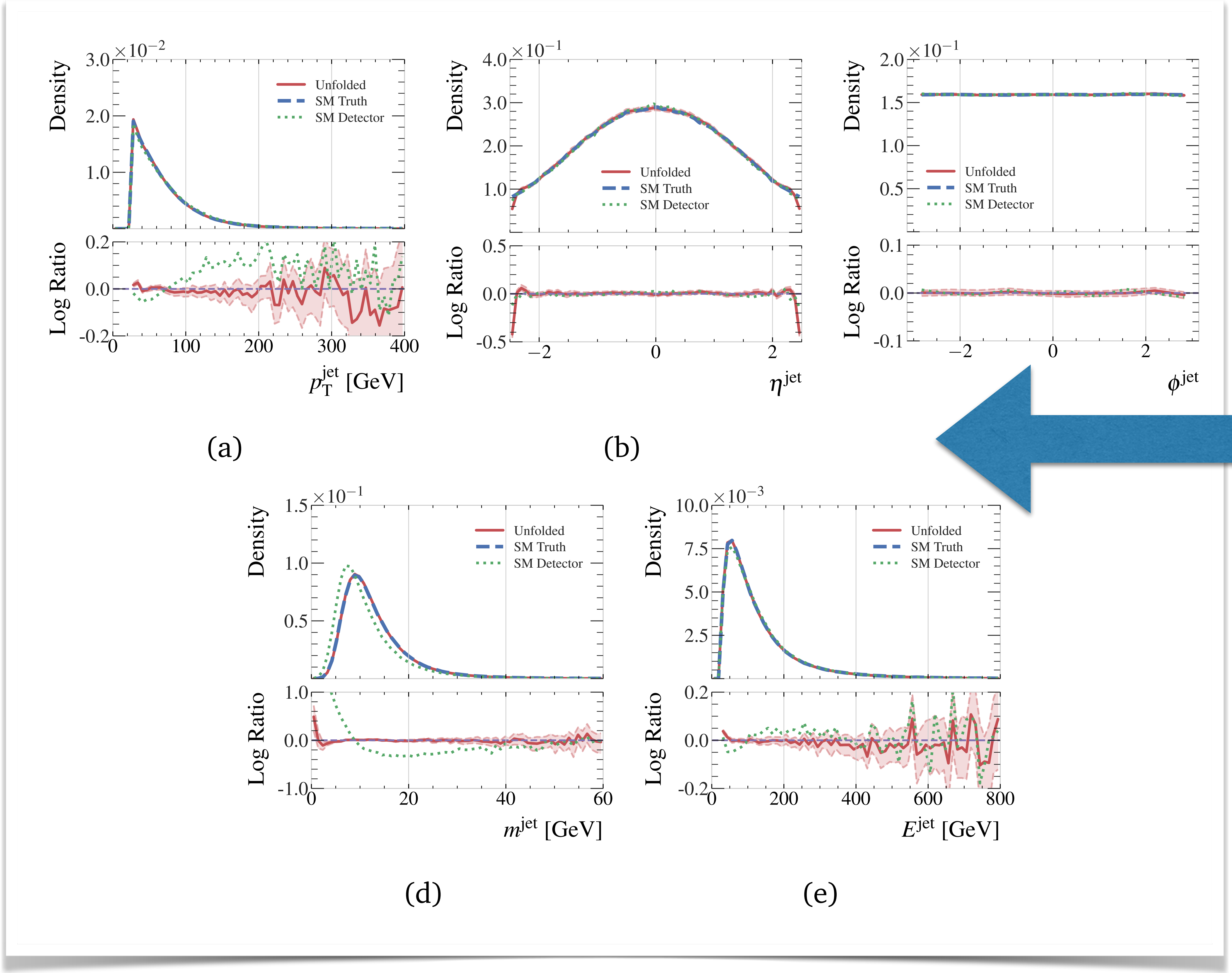
VLD: Shmakov et al. (incl. **Ghosh**, Whiteson)

High-dimensional unfolding with neural networks

cINNs: Backes et al

Many others: Huetsch et al (incl. Shmakov, Diefenbacher, Mikuni, Nachman, Whiteson)



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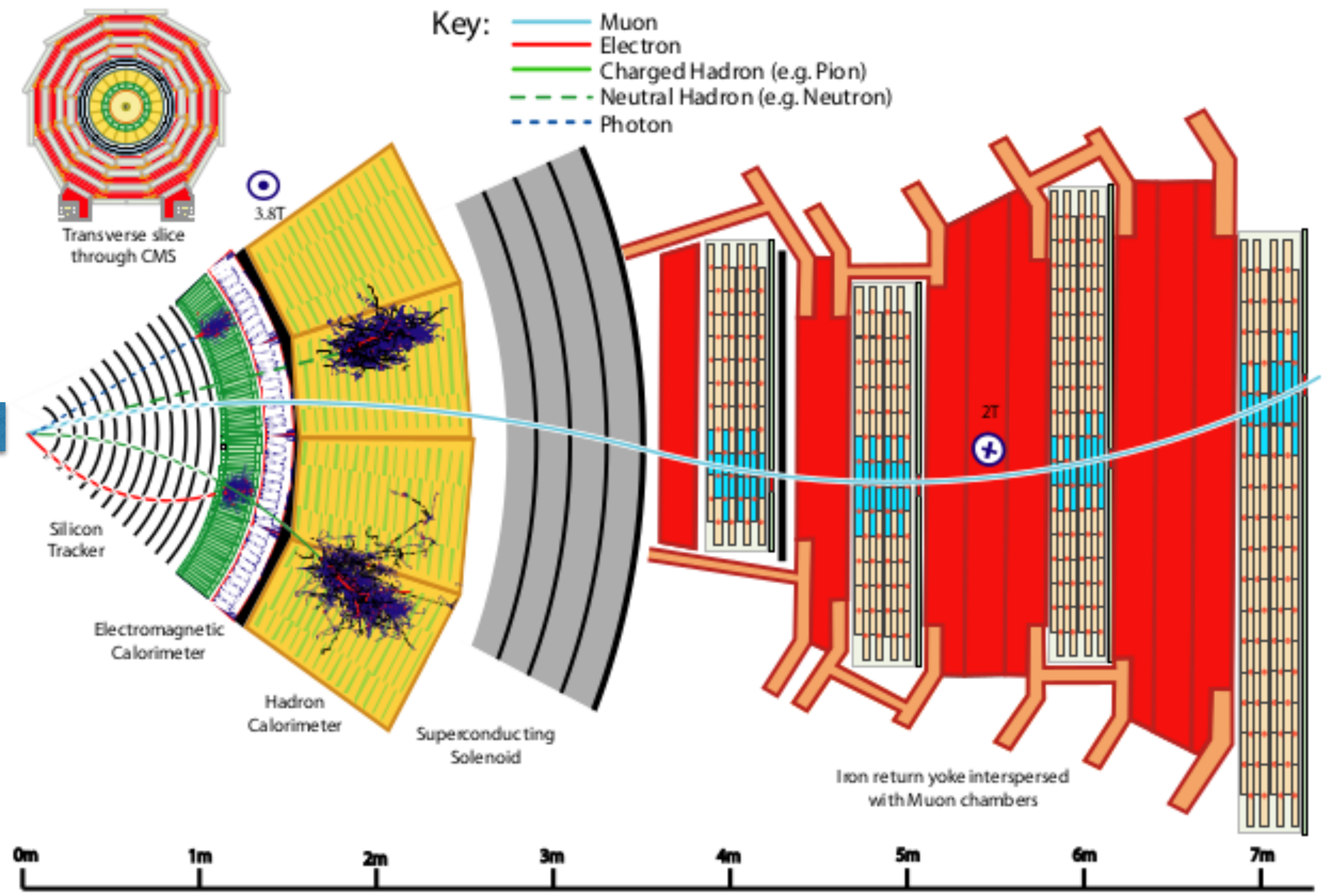

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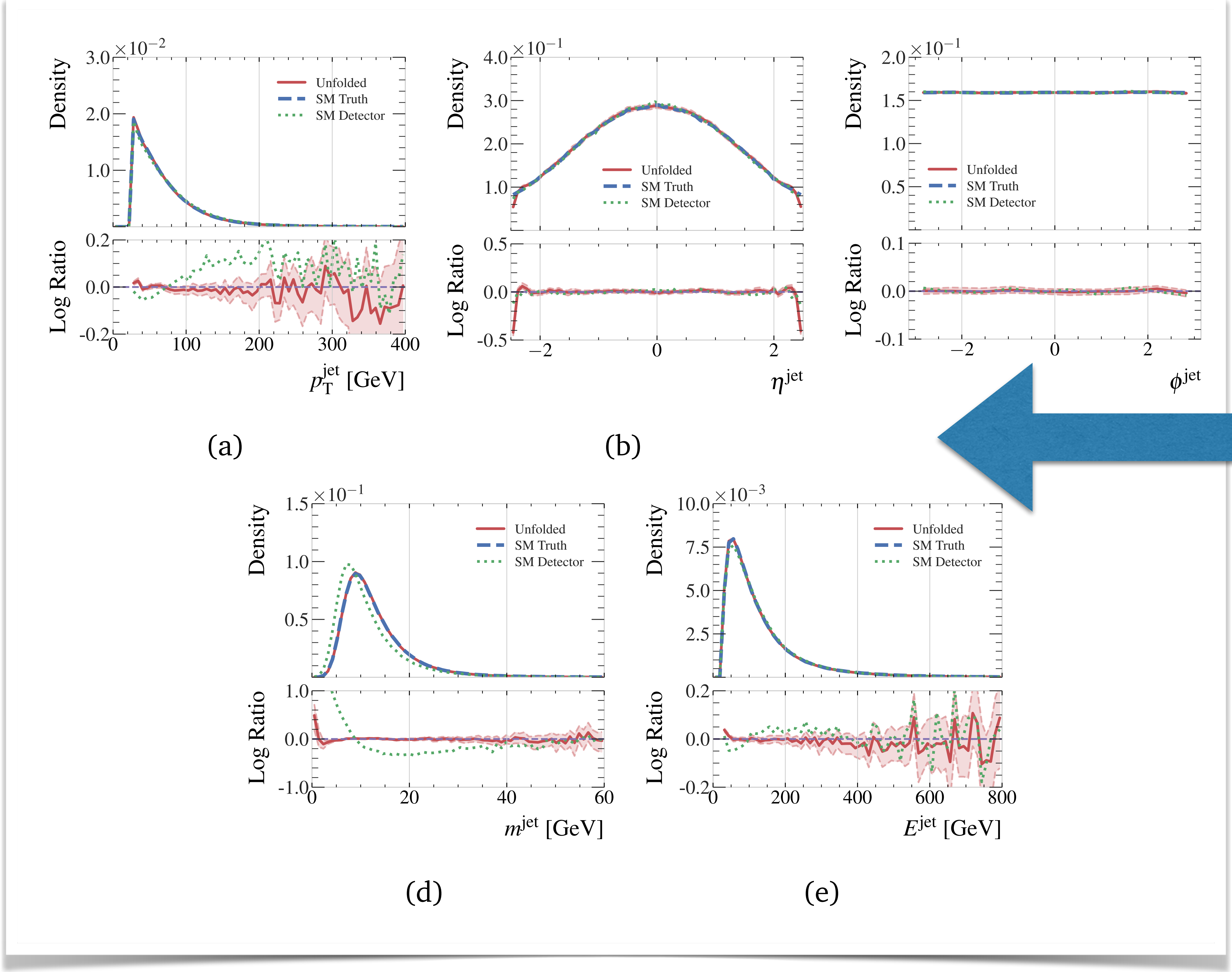

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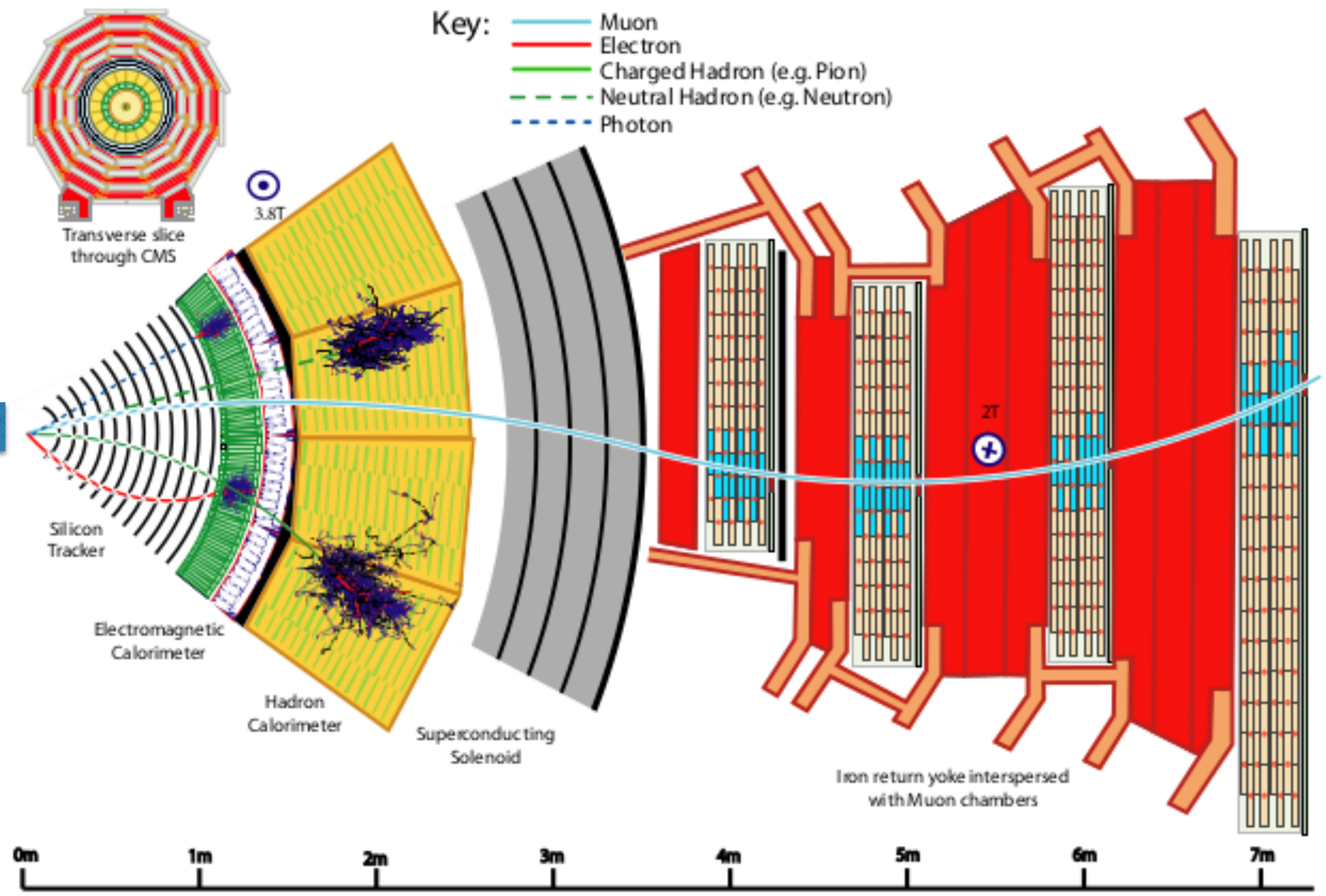
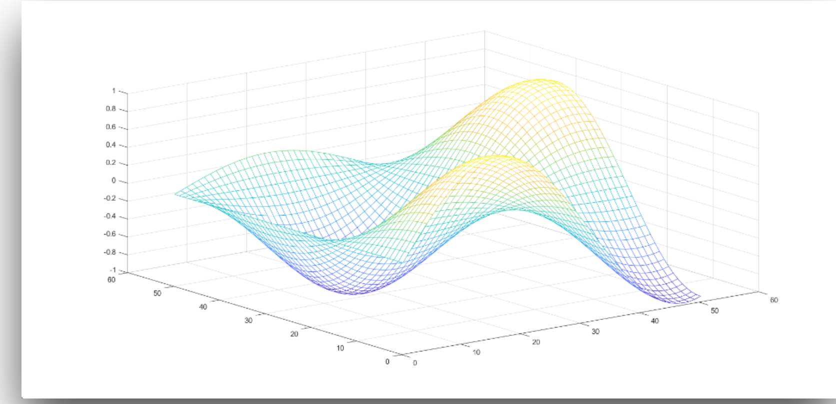


Detector effects on measurement

See more in ‘Unfolding’ talk later today by Vinicius Mikuni

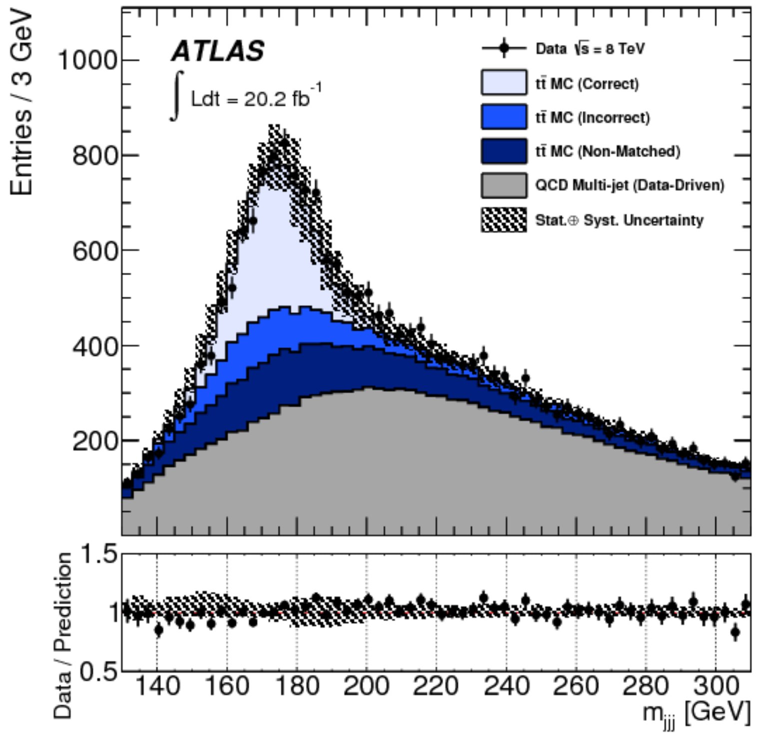
High dimensional hypothesis tests with neural networks

Traditional framework:



High-dim data

Summarisation to histogram



Summary Histogram → Statistical Fit

θ_1 → Statistical Fit

Statistical Fit → Likelihood $\mathscr{L}(\theta_1 | \mathscr{D})$

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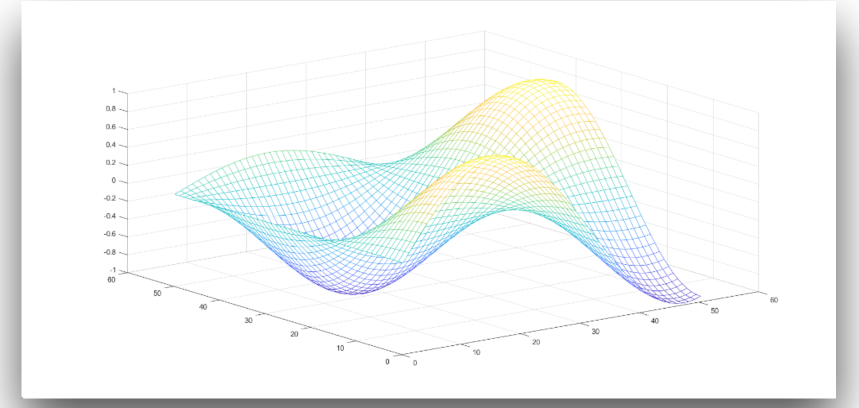
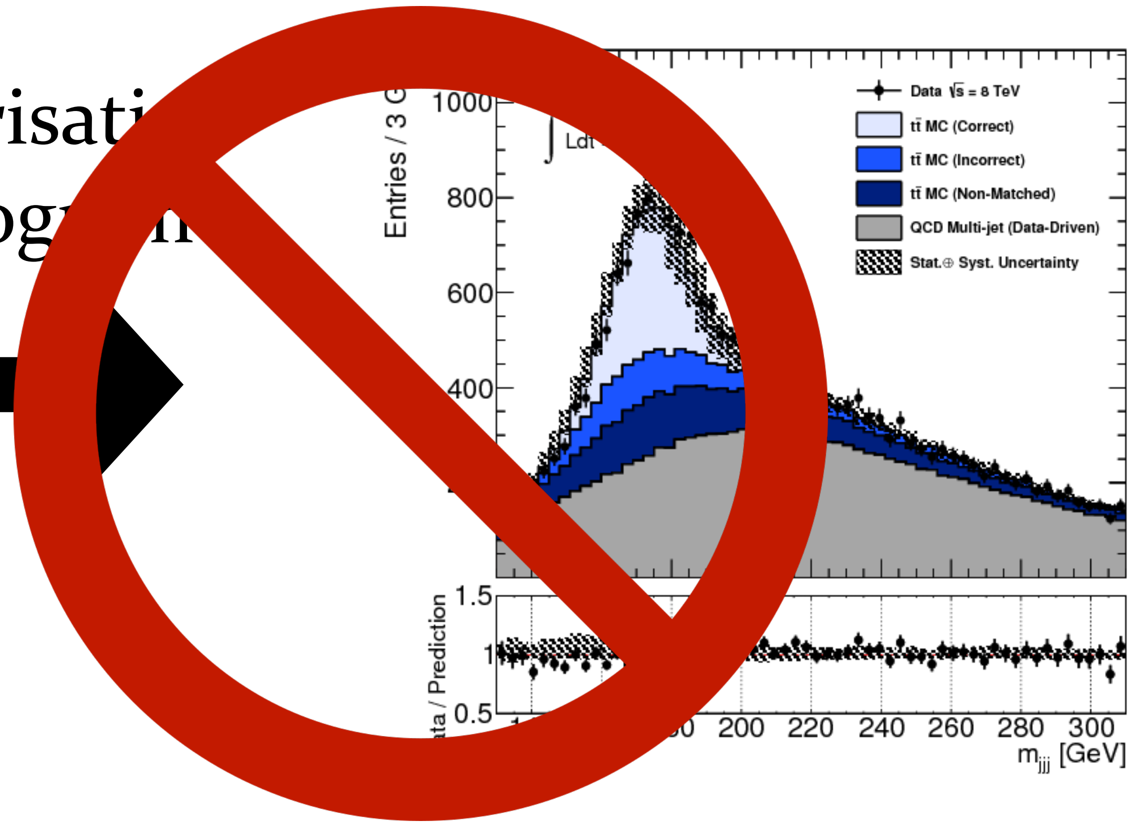


High-dim data

Summarisati
to histog



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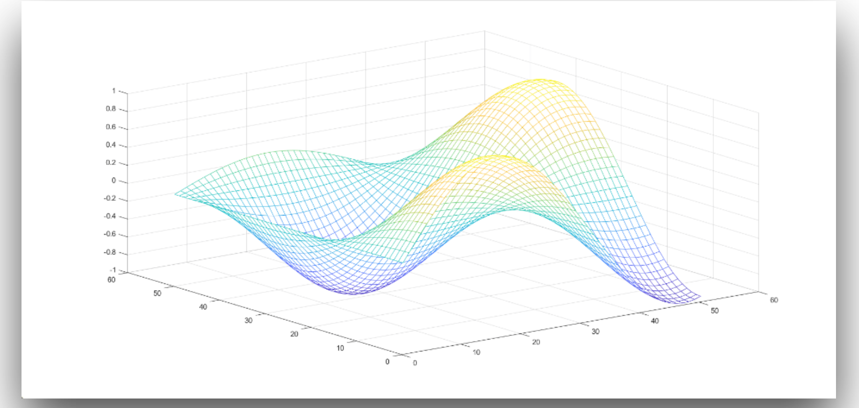

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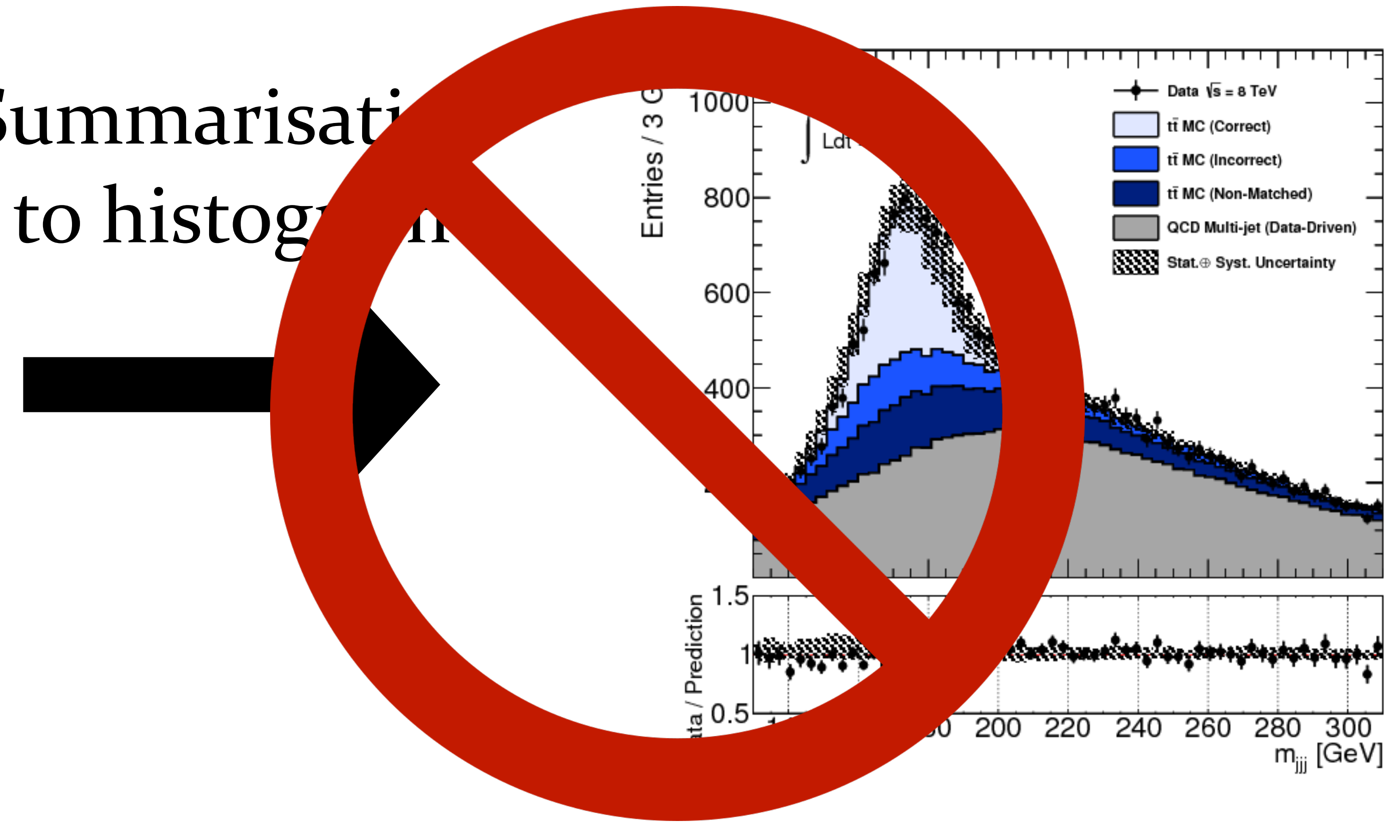

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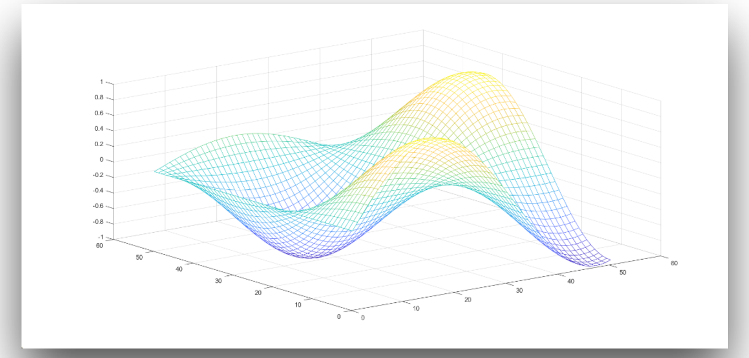
The neural inference framework:



High-dim data
O(16) observables

Obs Data → Neural Networks → Likelihood Ratio

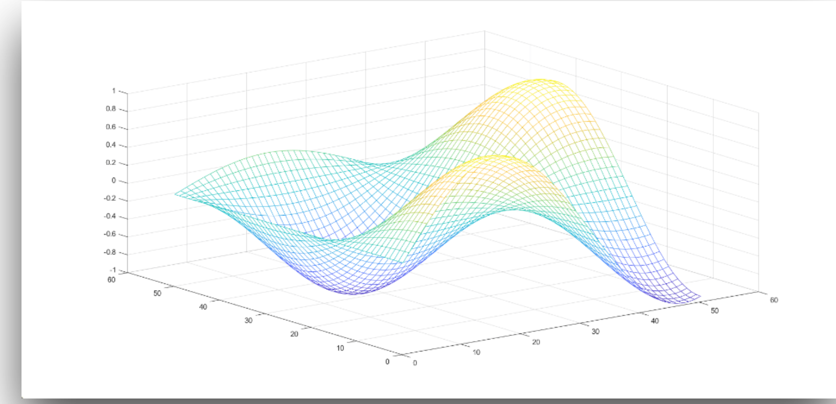
θ_1 → Neural Networks

Likelihood Ratio
$$\left(\frac{\mathscr{L}(\theta_1 | \mathscr{D})}{\mathscr{L}(ref | \mathscr{D})} \right)$$

CARL: Cranmer et al

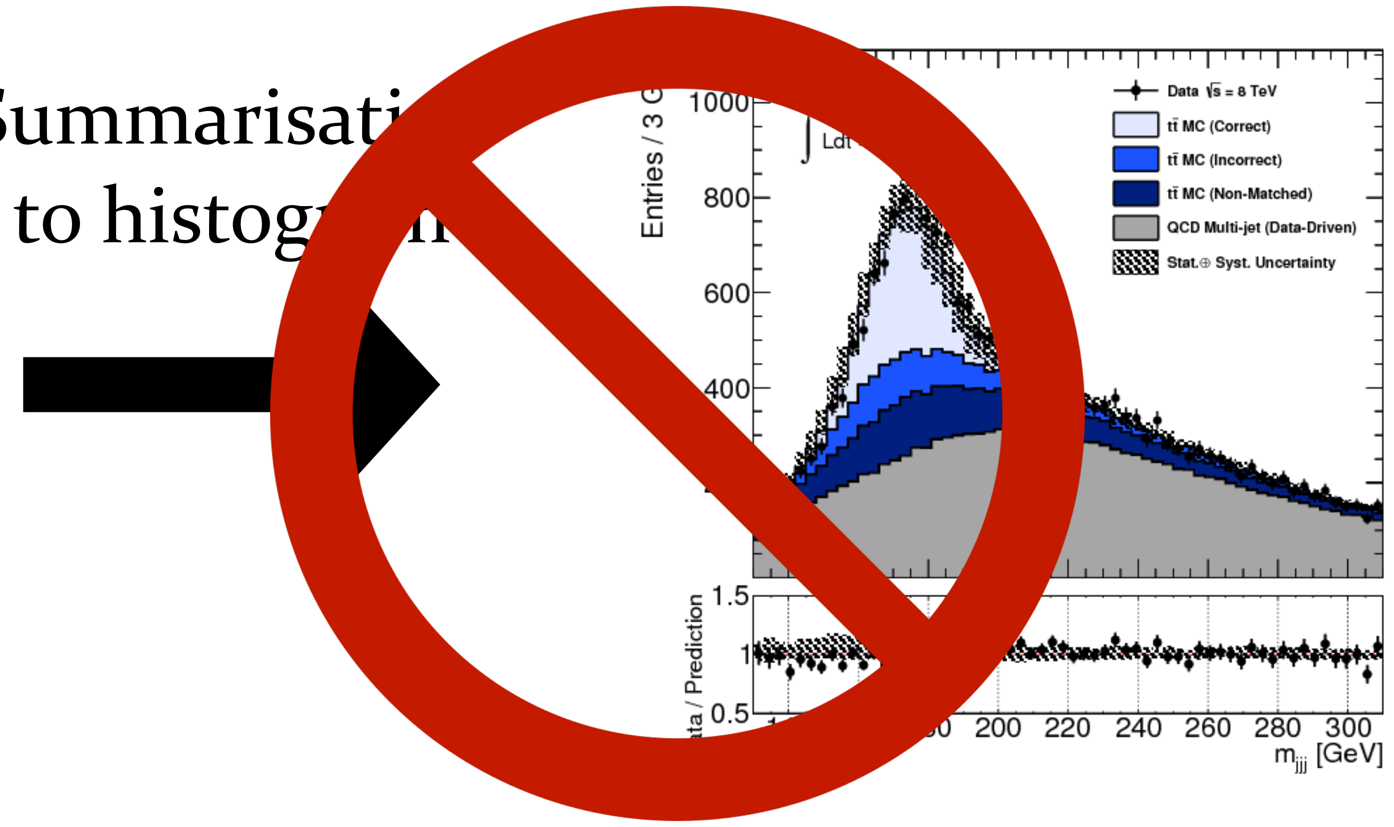
High dimensional hypothesis tests with neural networks

Traditional framework:



High-dim data

Summarisation to histogram



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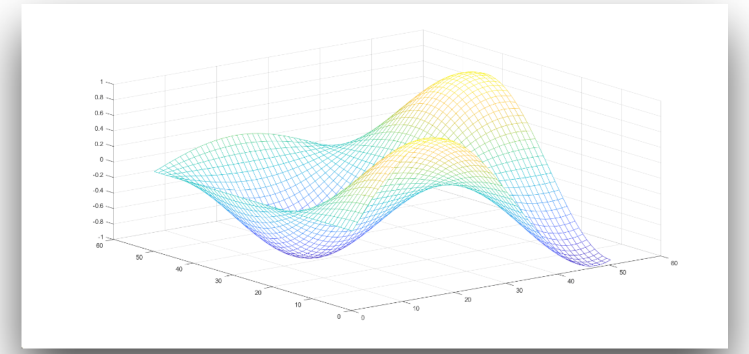

High-dim data
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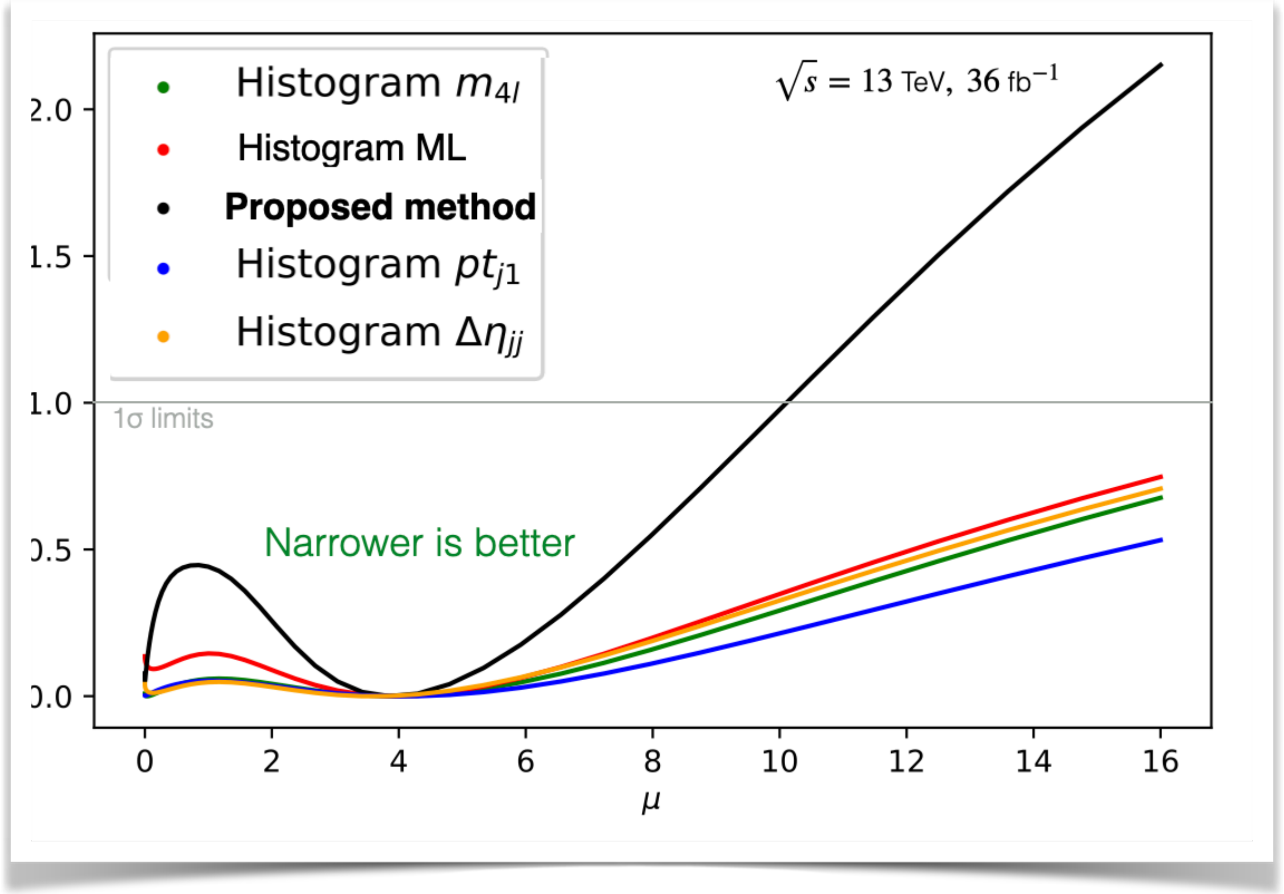
Neural Networks → Likelihood Ratio $\left(\dfrac{\mathscr{L}(\theta_1 | \mathscr{D})}{\mathscr{L}(ref | \mathscr{D})}\right)$



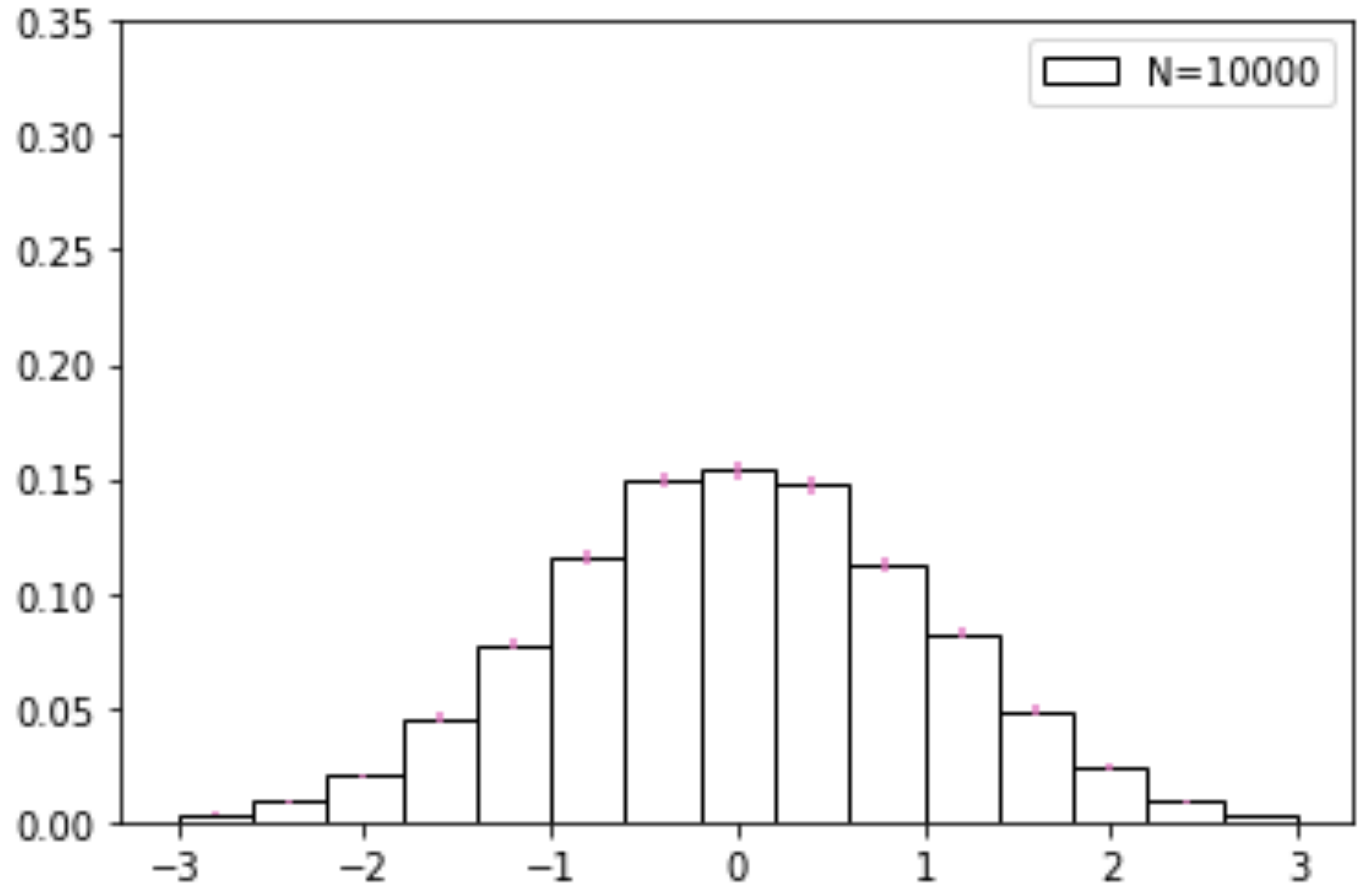
hal-02971995v3: **Ghosh**, et al

See more in 'Neural Simulation-Based Inference' talk by Andy & Aishik on Day 5

Question to the audience:

What is the danger here?

We loose the analytical form for likelihoods,
to get a high-dimensional and unbinned analysis



1-dim histogram

In each bin:

$$\ln P(N_{obs}) = N_{obs} \cdot N_{exp} - N_{exp} - ln(N_{obs}!)$$

Clear notion of per-bin MC statistical uncertainties

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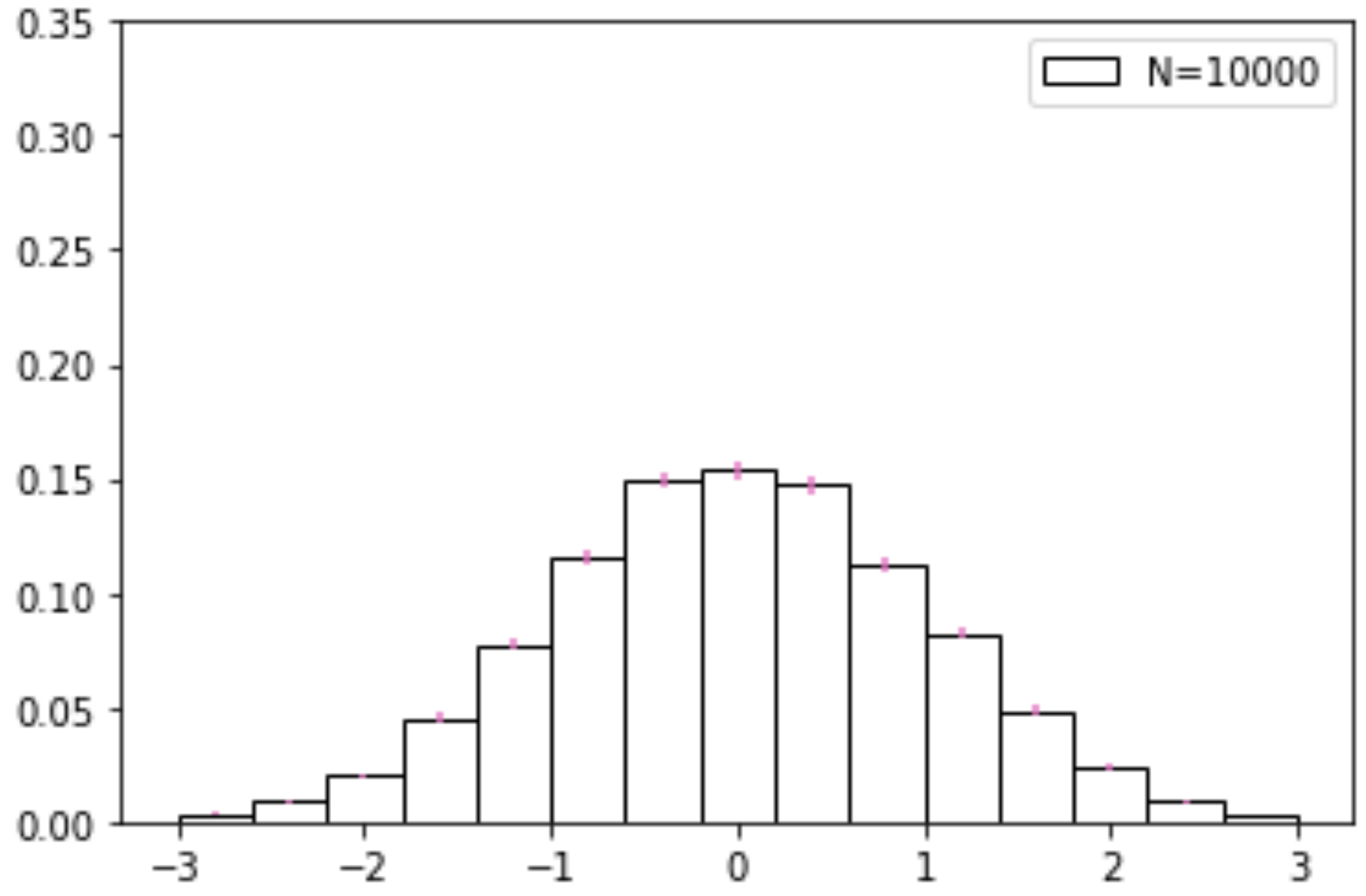

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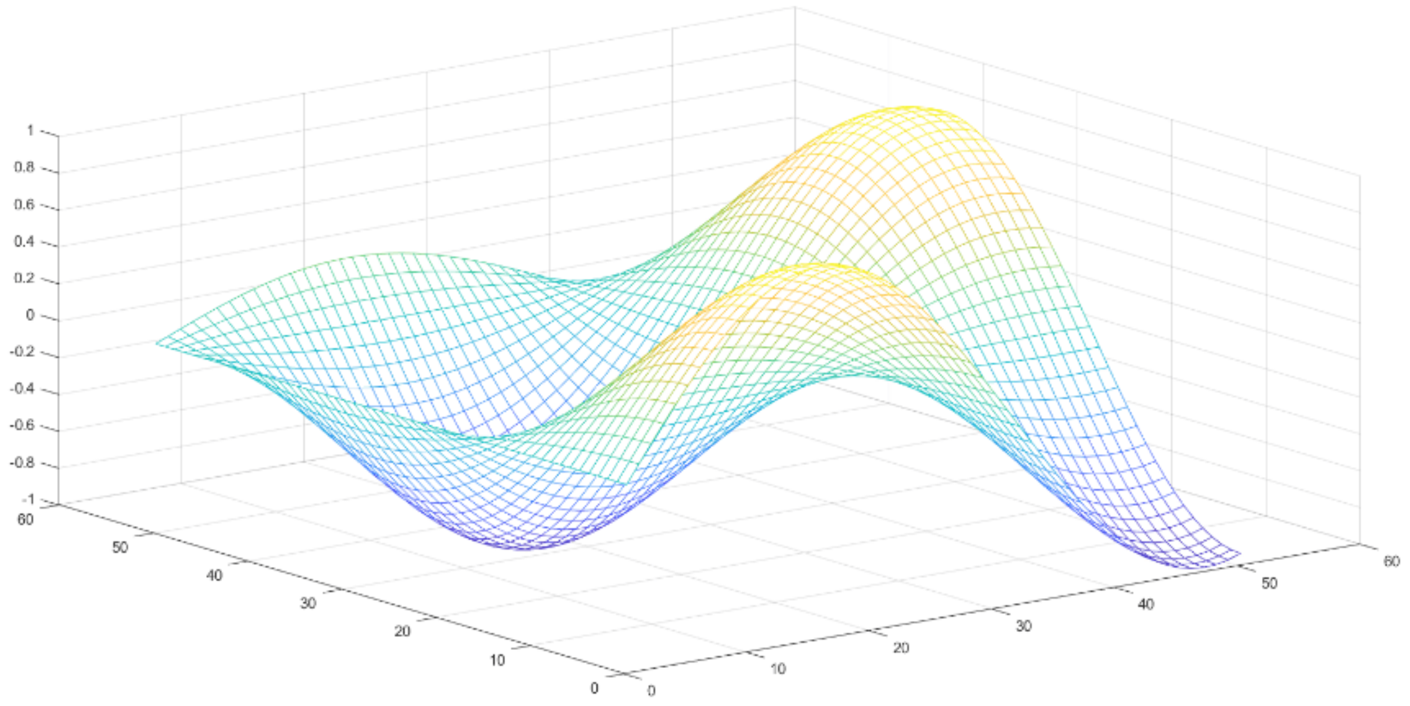

high-dim data

Likelihood (ratio) in high dimensions **estimated by a network**

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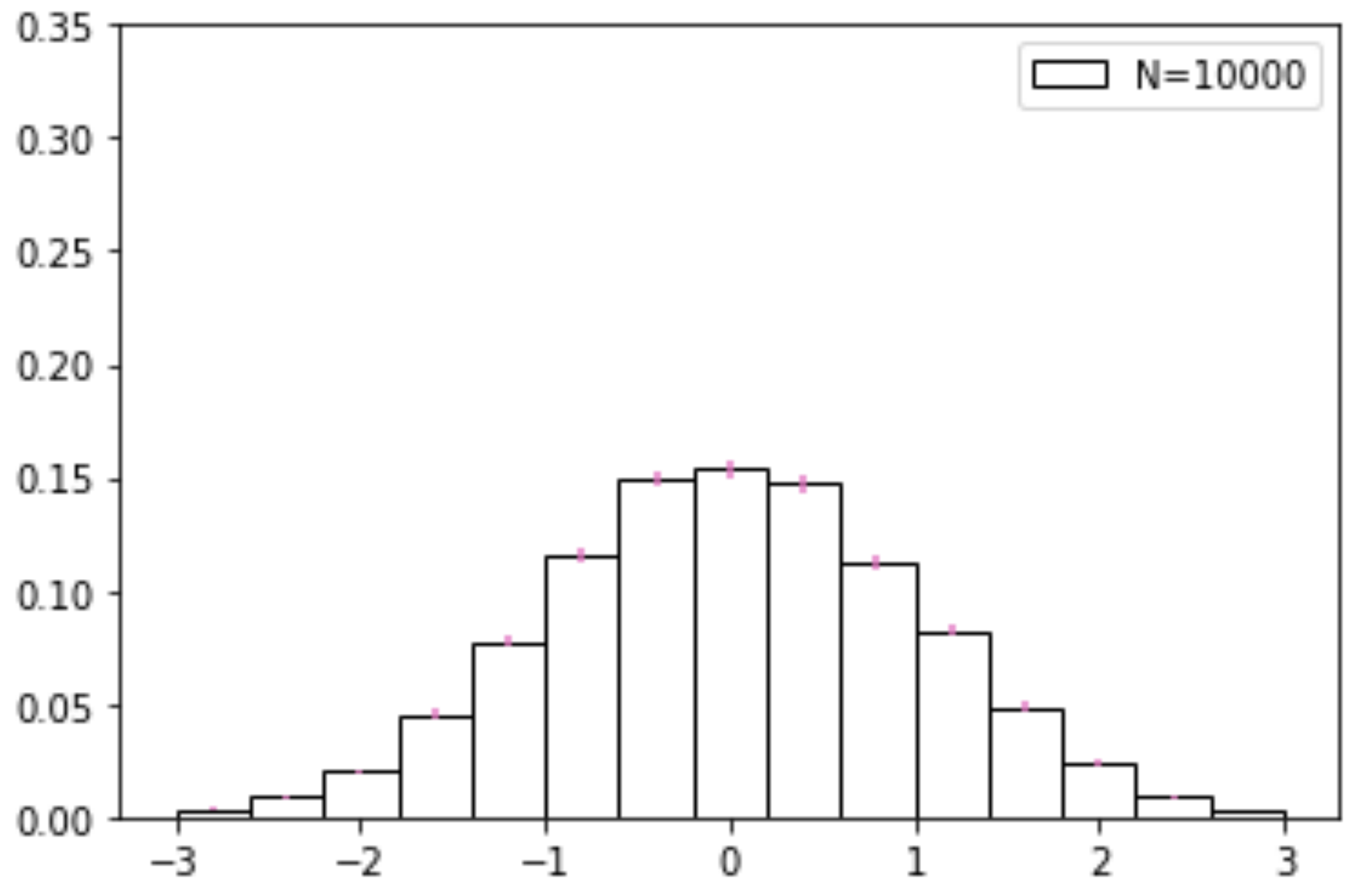

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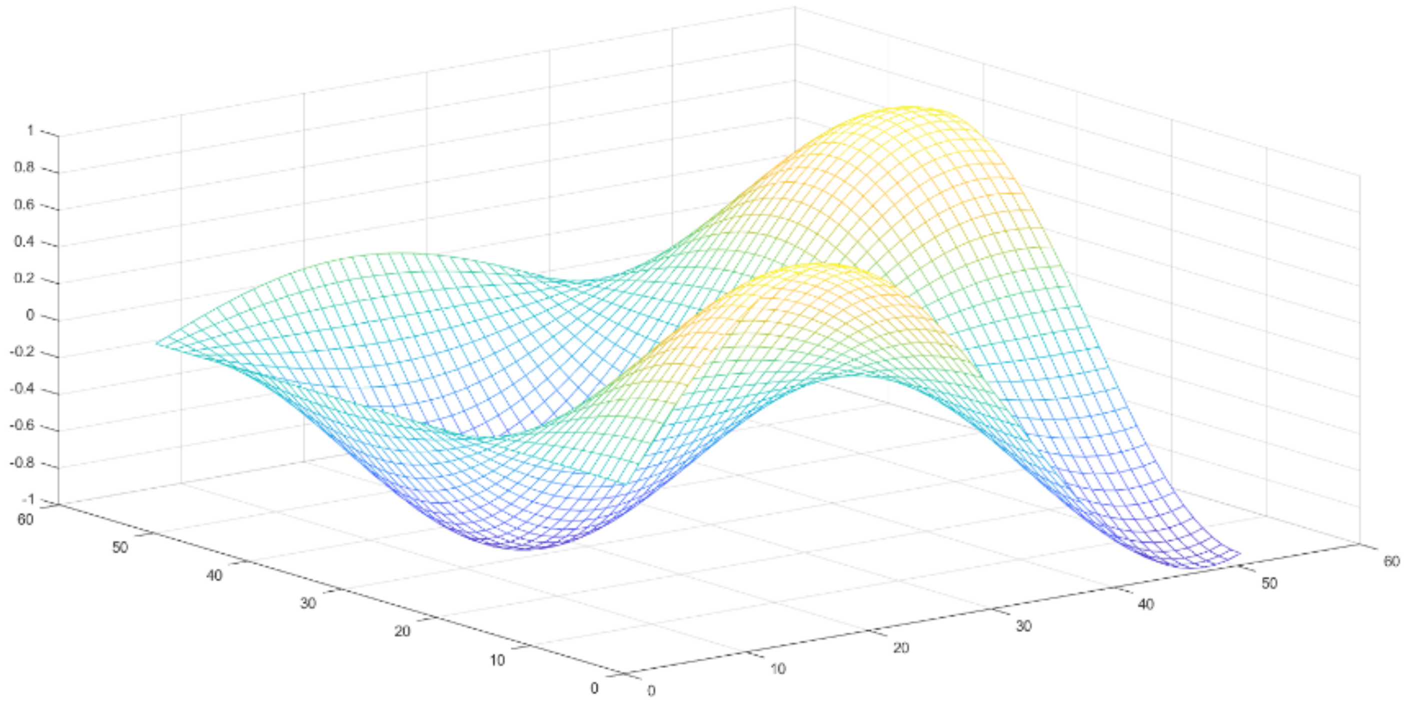


high-dim data

Likelihood (ratio) in high dimensions **estimated by a network**

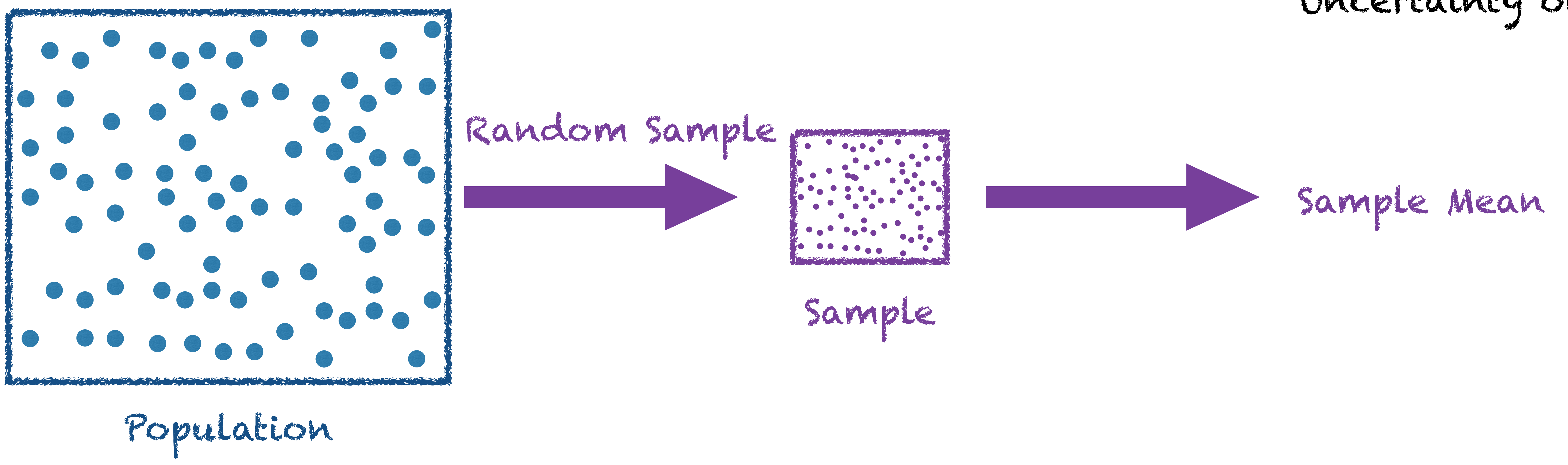
Image: [Source]

How much is your network limited my training statistics?

Estimating the variance on mean: Ideal Scenario

Want to estimate mean of population

Uncertainty on estimated mean?



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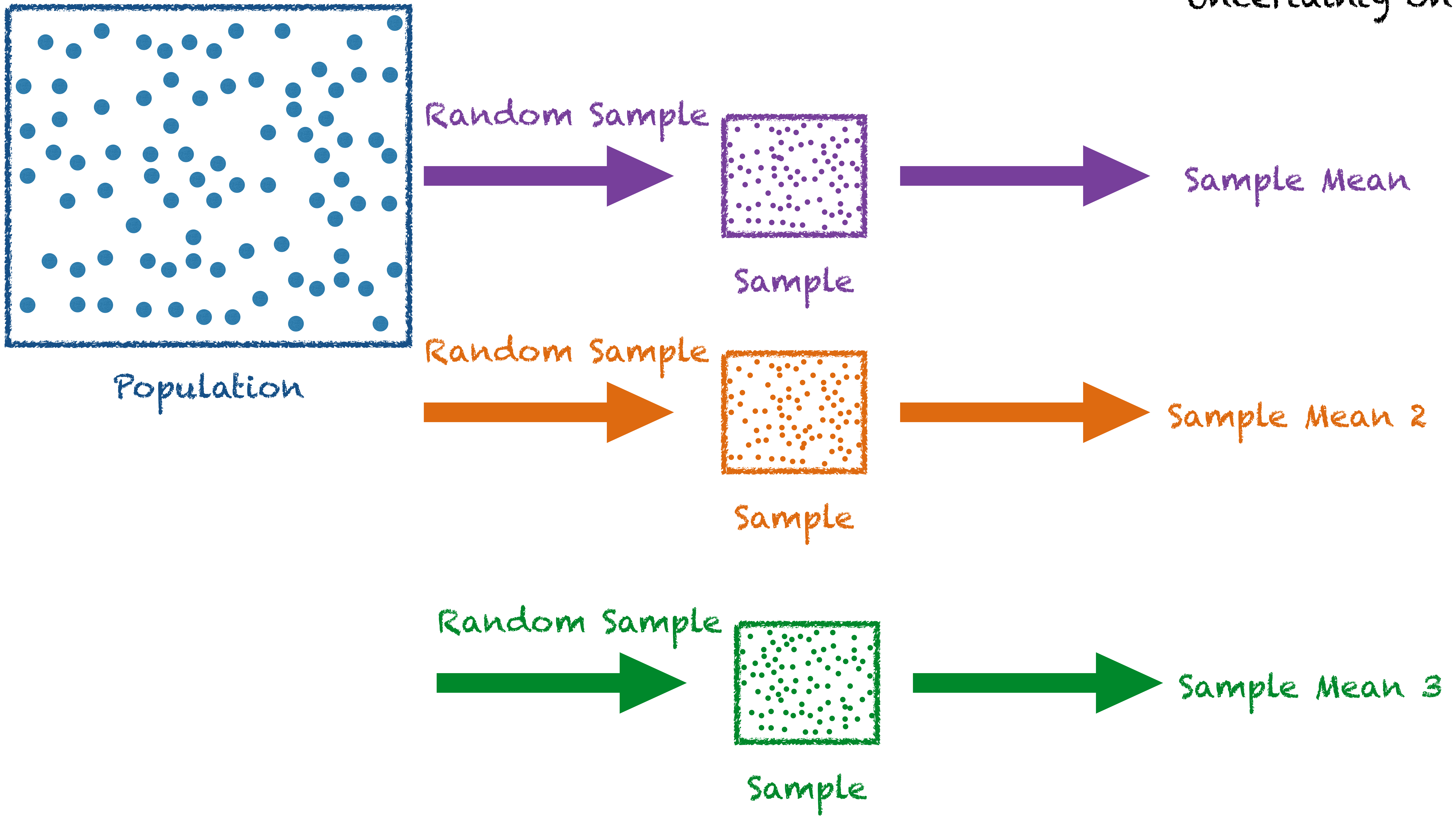

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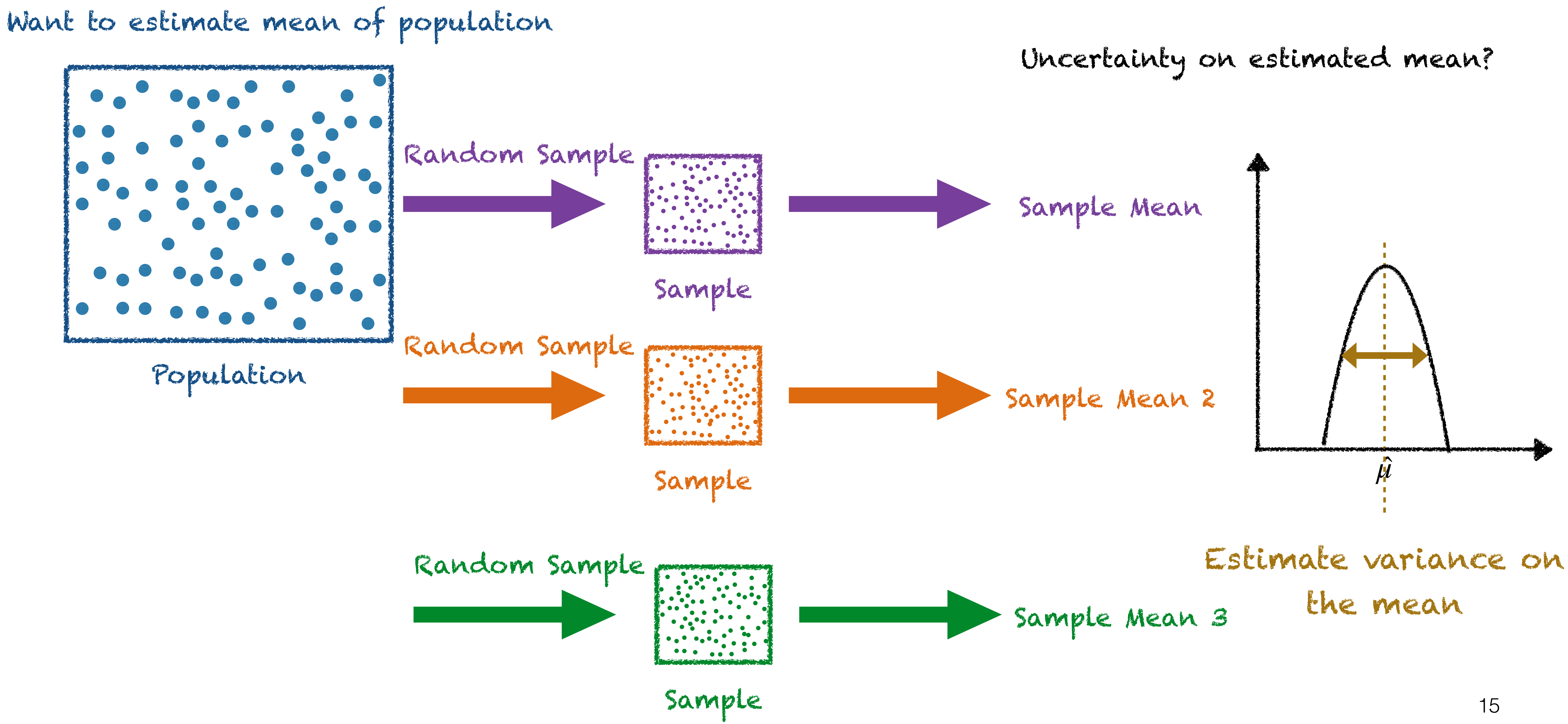
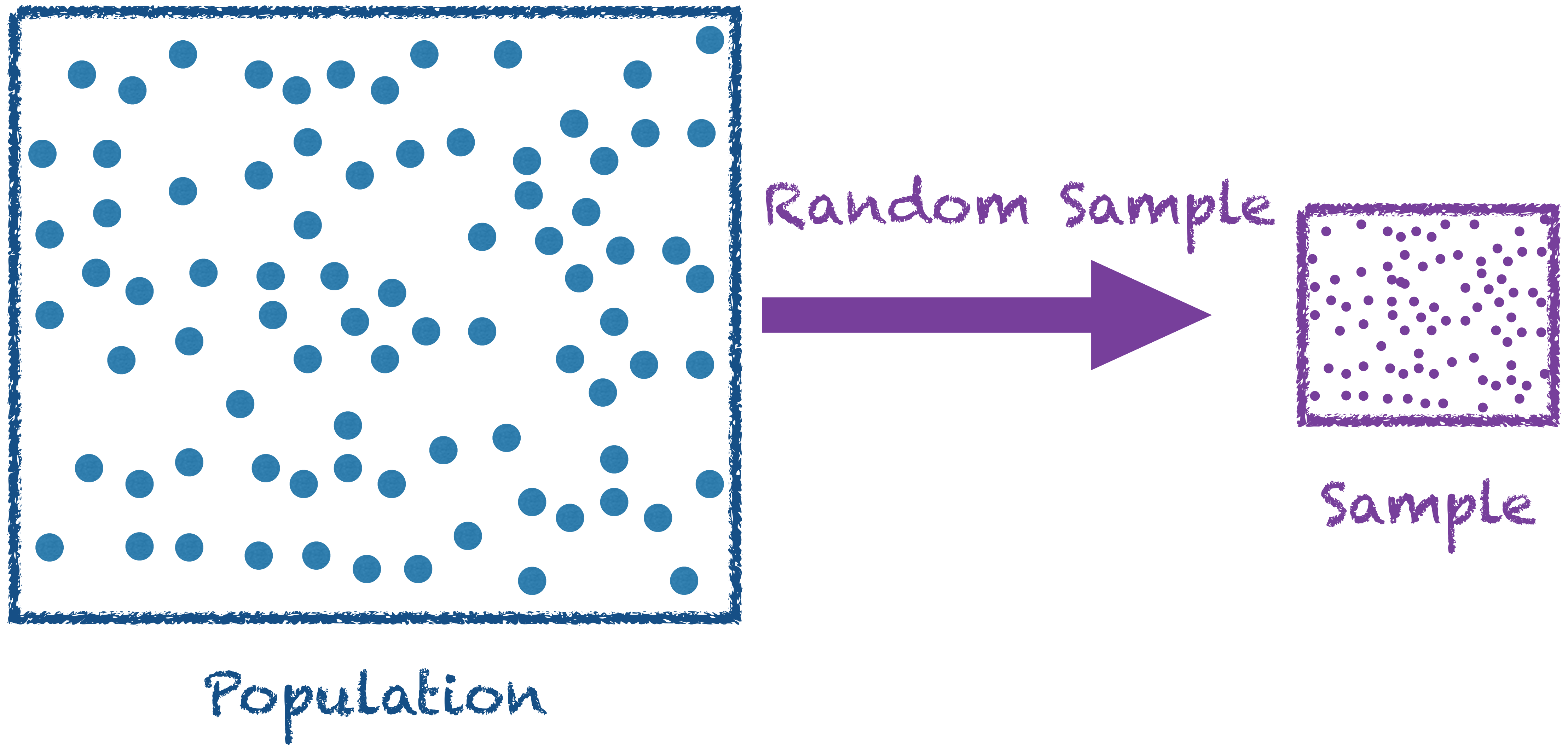


Estimating the variance on mean: Bootstrapping

Want to estimate mean of population



Re-Sample
with
replacement

Image: [Source]

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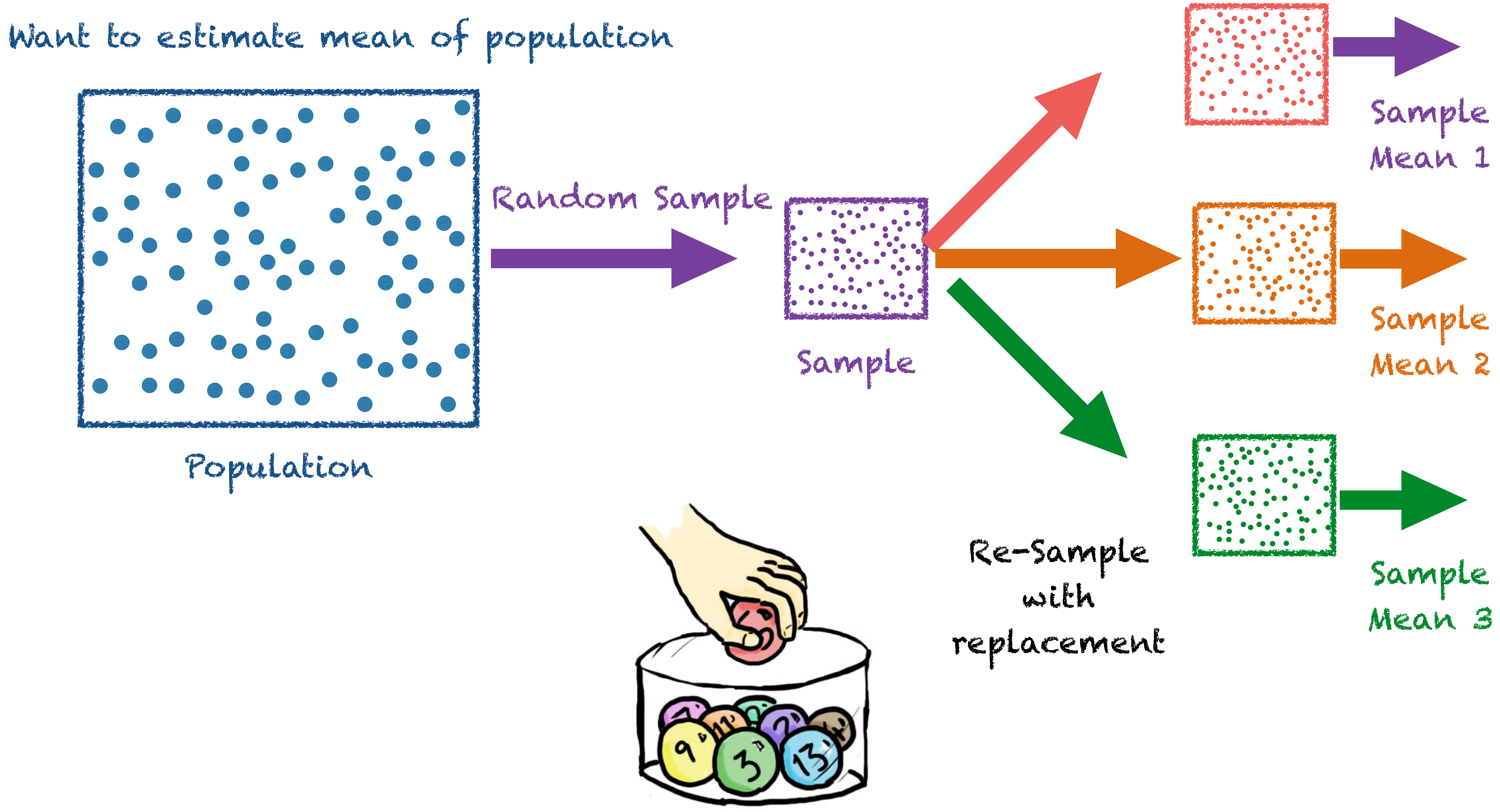

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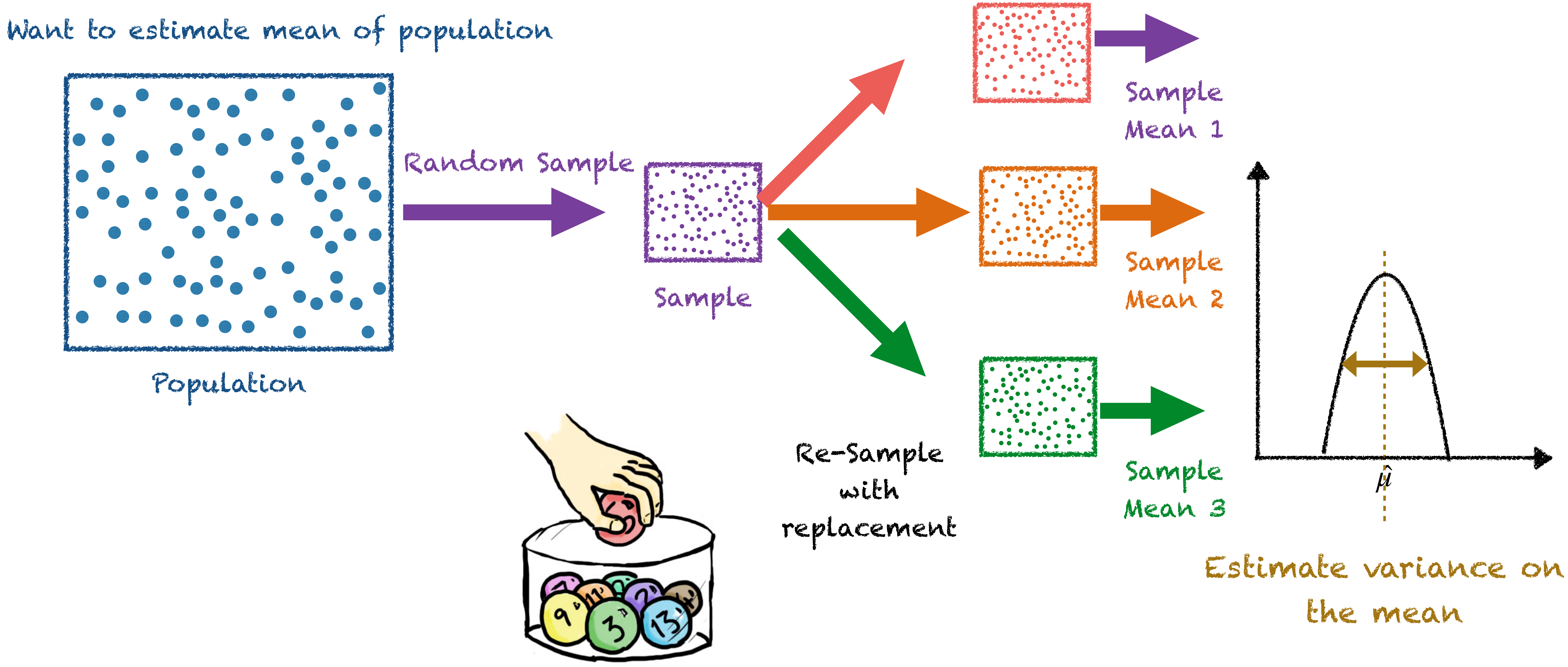


Image: Source

Propagating statistical uncertainty with bootstrapped samples

- Train an ensemble of networks, **each on a bootstrapped version of the training dataset**

- The spread in their prediction provides the uncertainty due to limited training statistics, and model uncertainty

- Variations of this core idea used in NSBI, unfolding, …

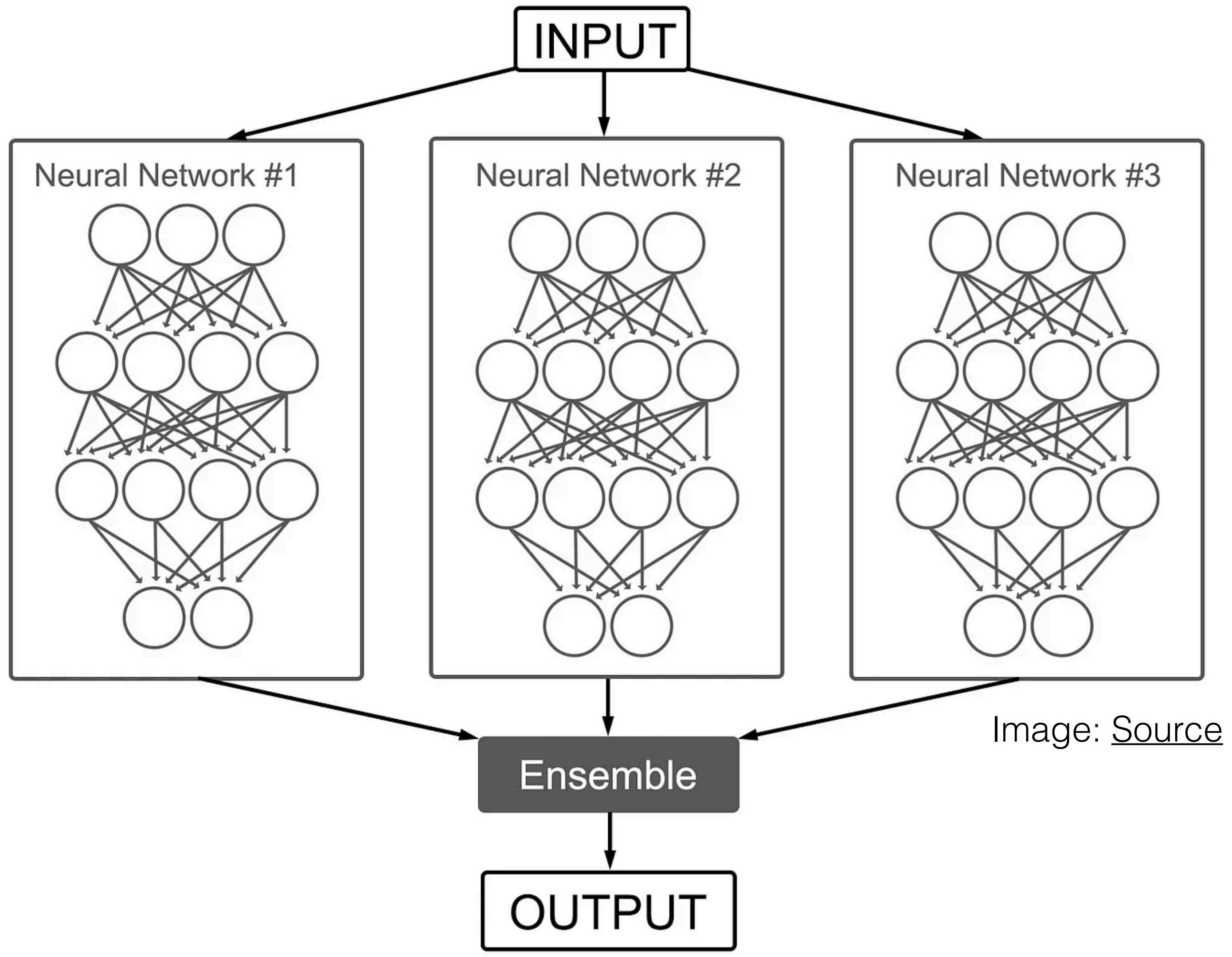
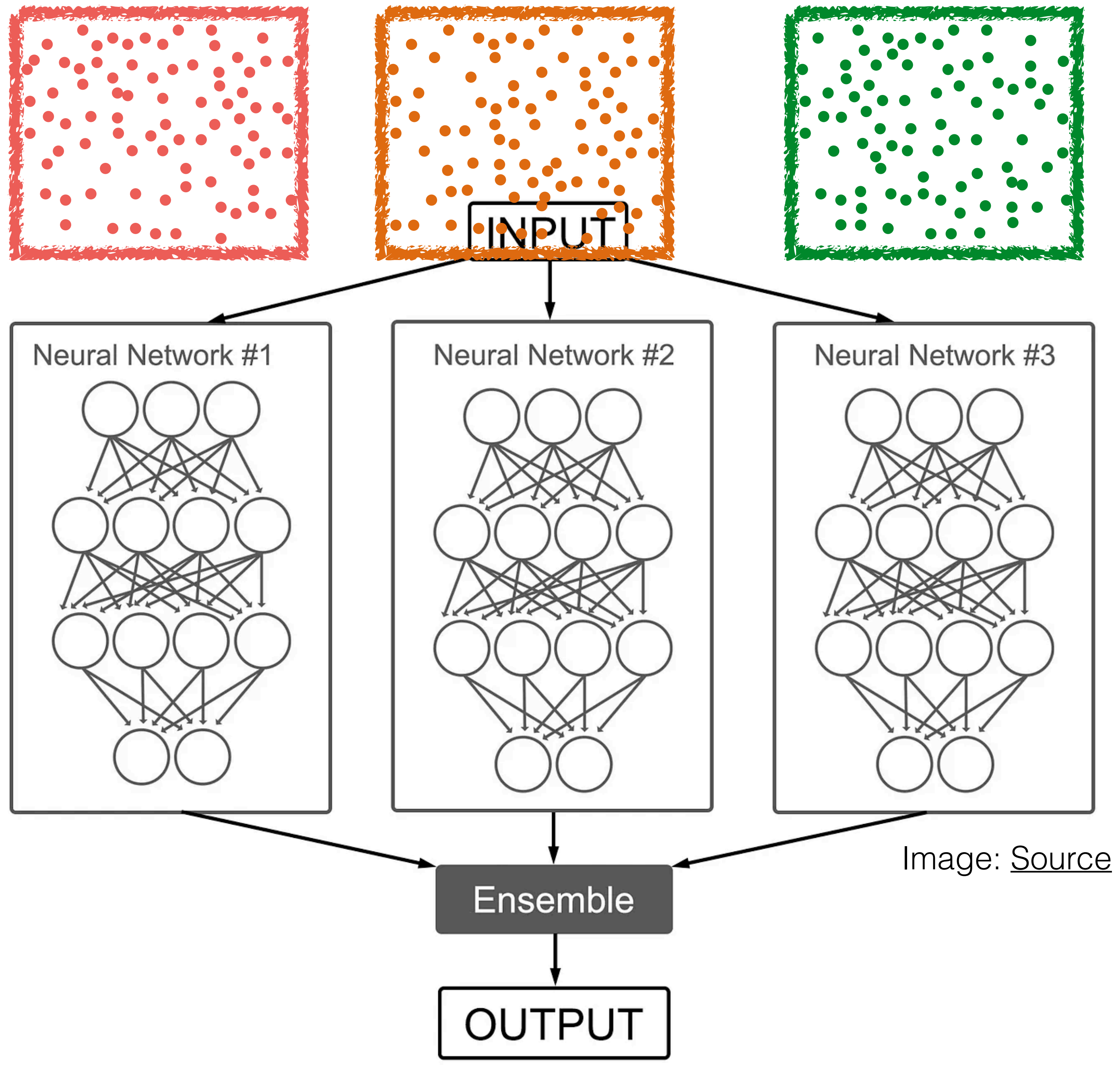


Image: Source

Propagating statistical uncertainty with bootstrapped samples

- Train an ensemble of networks, **each on a bootstrapped version of the training dataset**
- The spread in their prediction provides the uncertainty due to limited training statistics, and model uncertainty
- Variations of this core idea used in NSBI, unfolding, …



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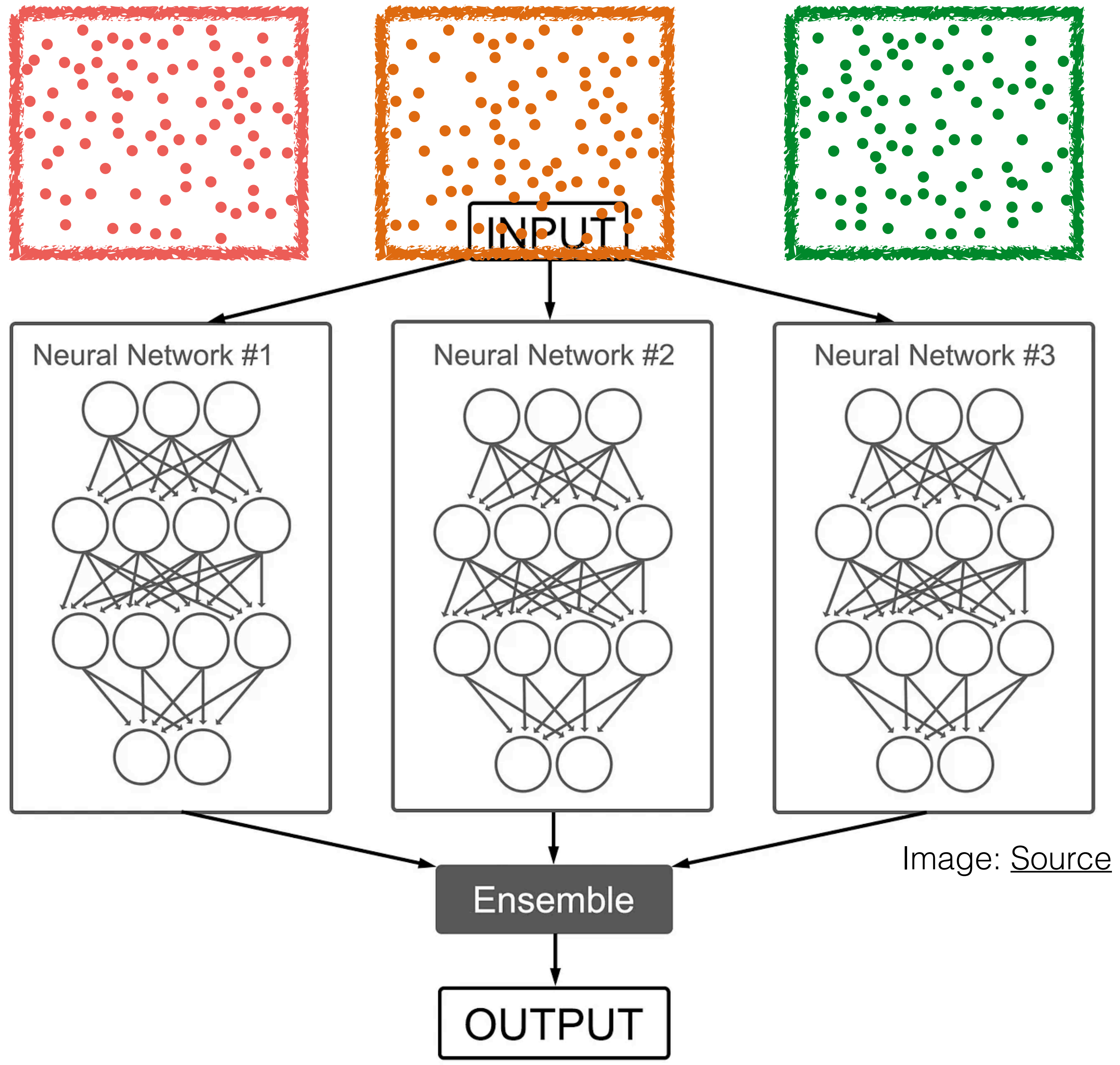

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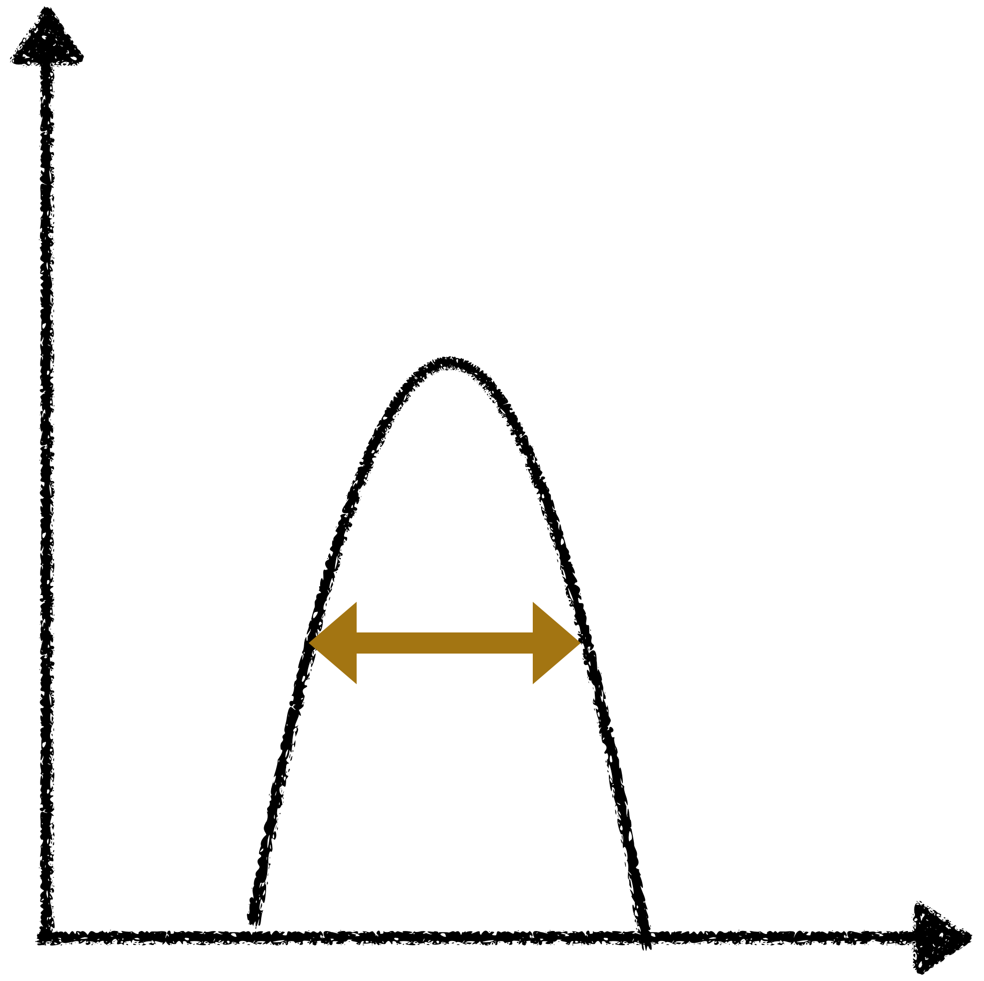
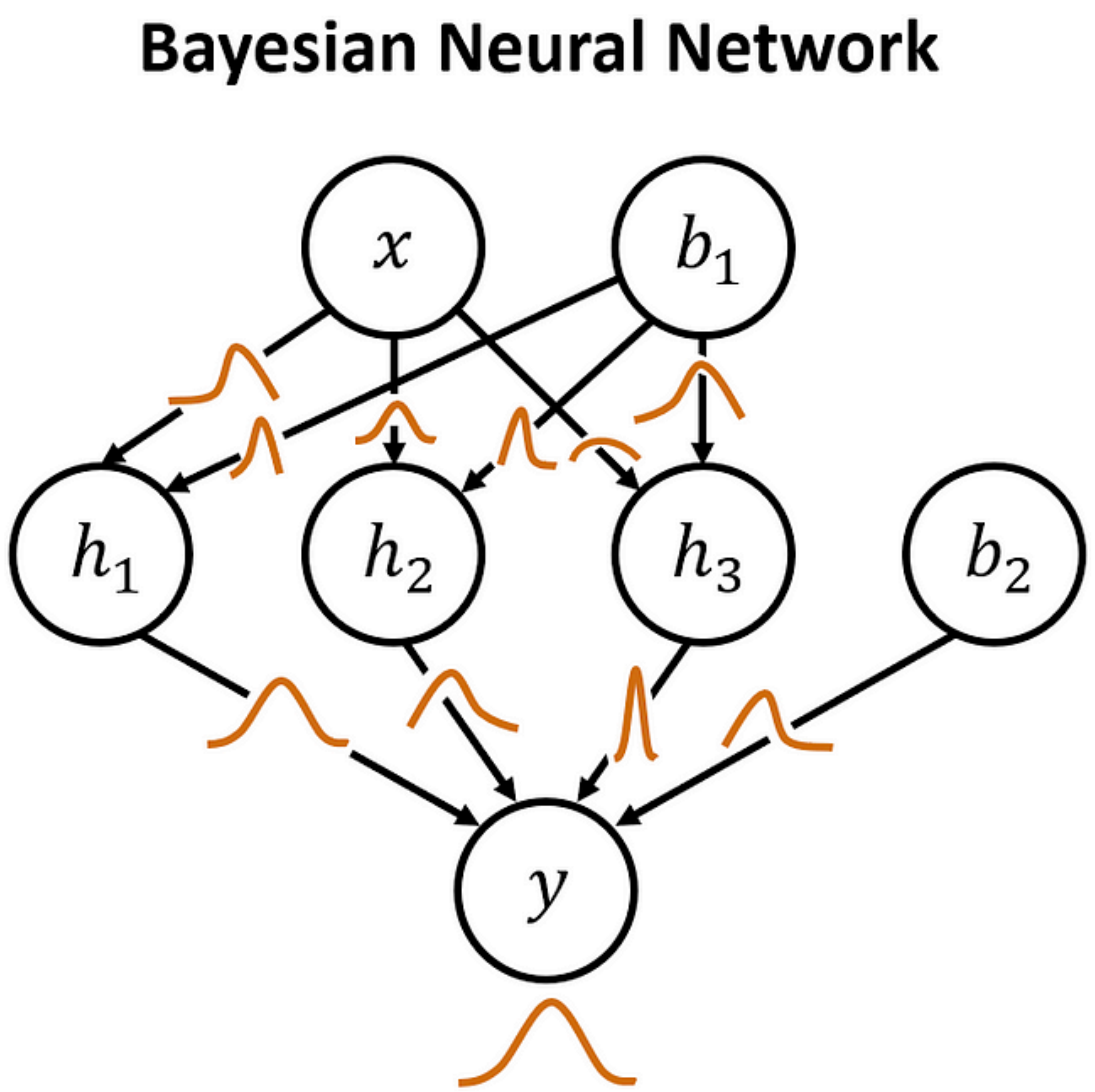


Bayesian Networks

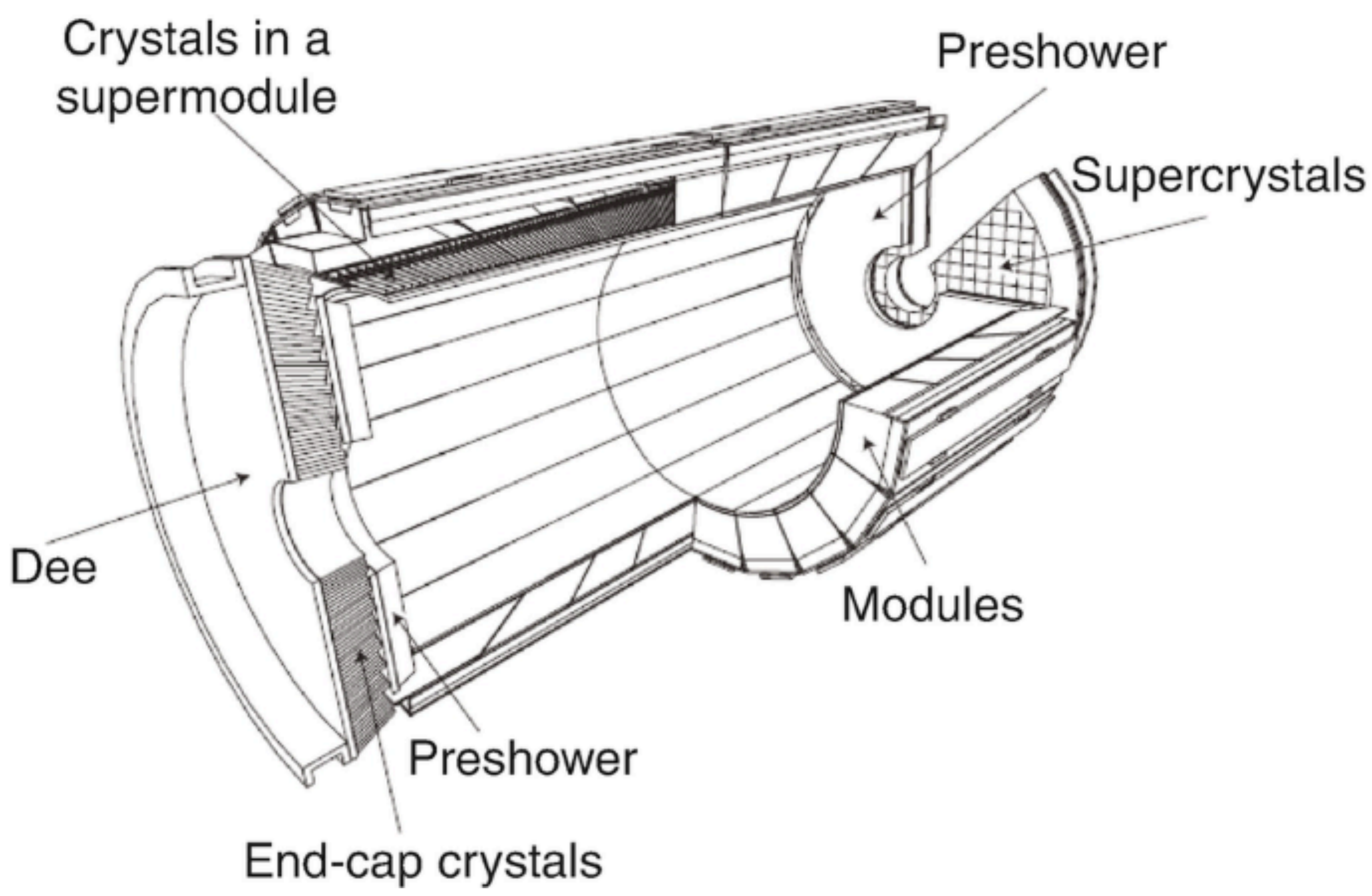
- Each weight replaced by a distribution of weights
  - Eg. Sampled from learnt {mean, std}

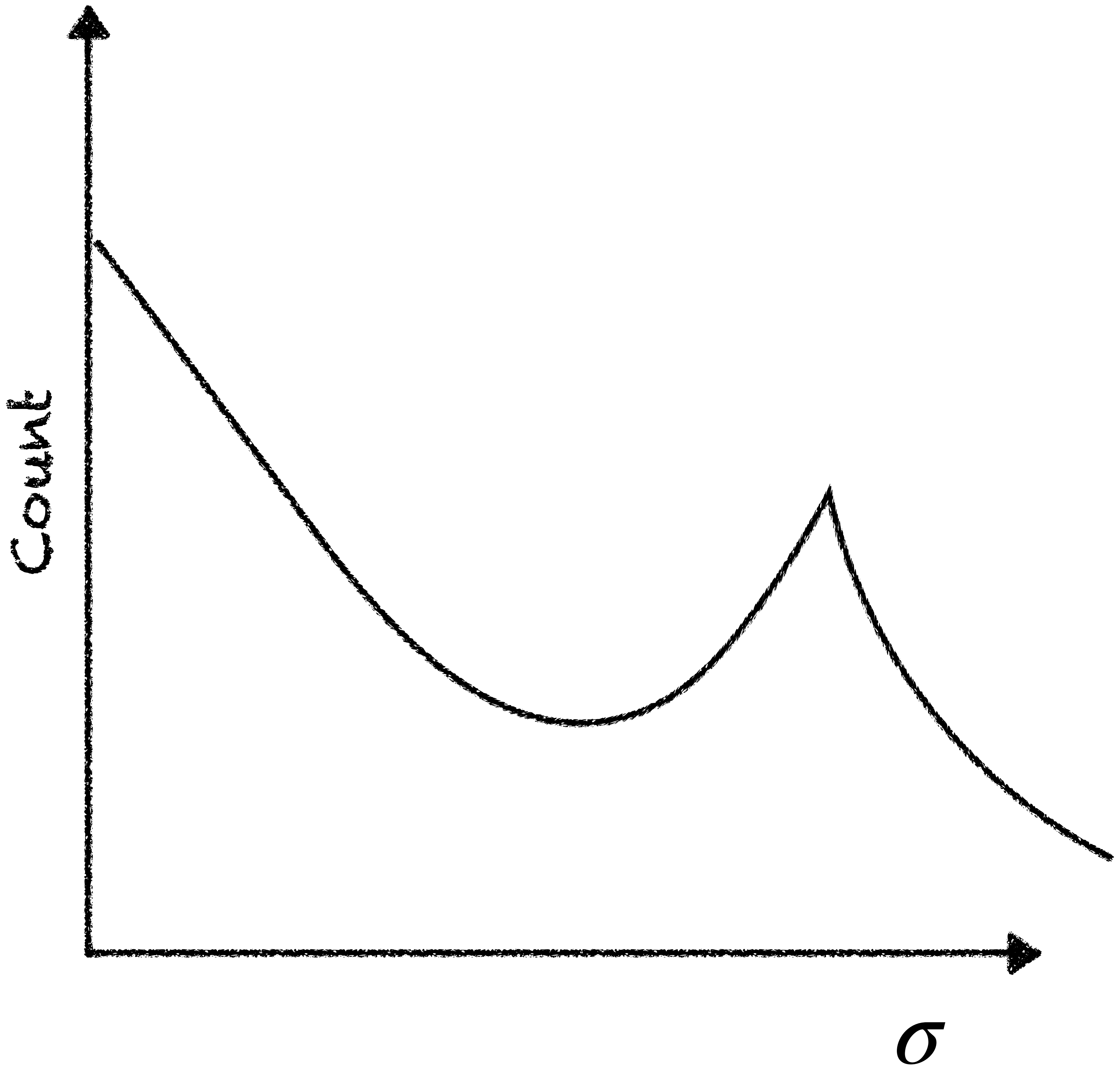
- The distribution in NN prediction for each event gives you an uncertainty estimate

- Open question: How to interpret this uncertainty? What is the coverage?
  - Calibrate the uncertainties [arXiv:2408.00838](https://arxiv.org/abs/2408.00838): Bringer et al (incl. Diefenbacher)
  - … more work needed here before if they are to become standard tools in frequentist frameworks



An exciting use case: Interpretability





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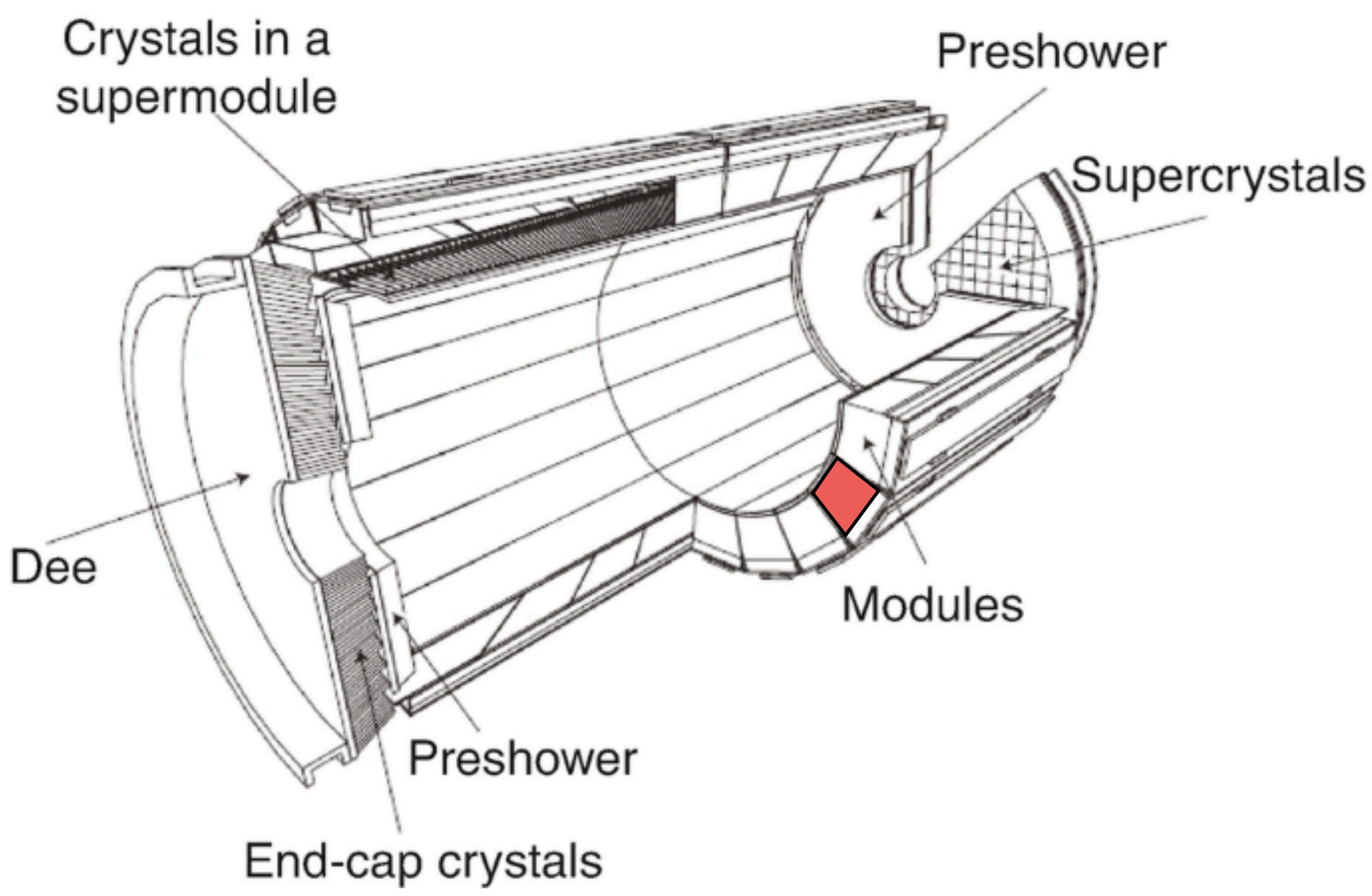
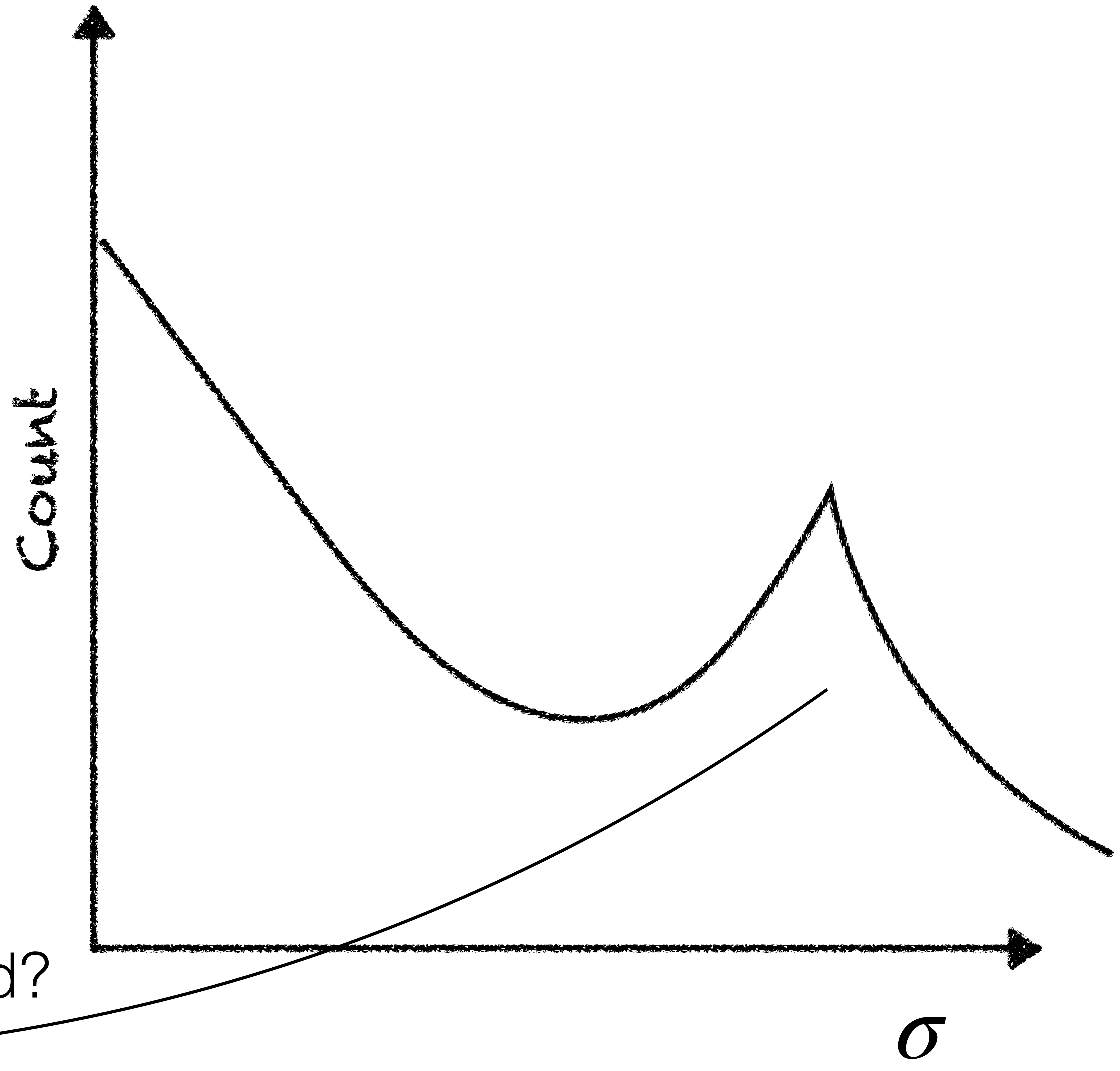


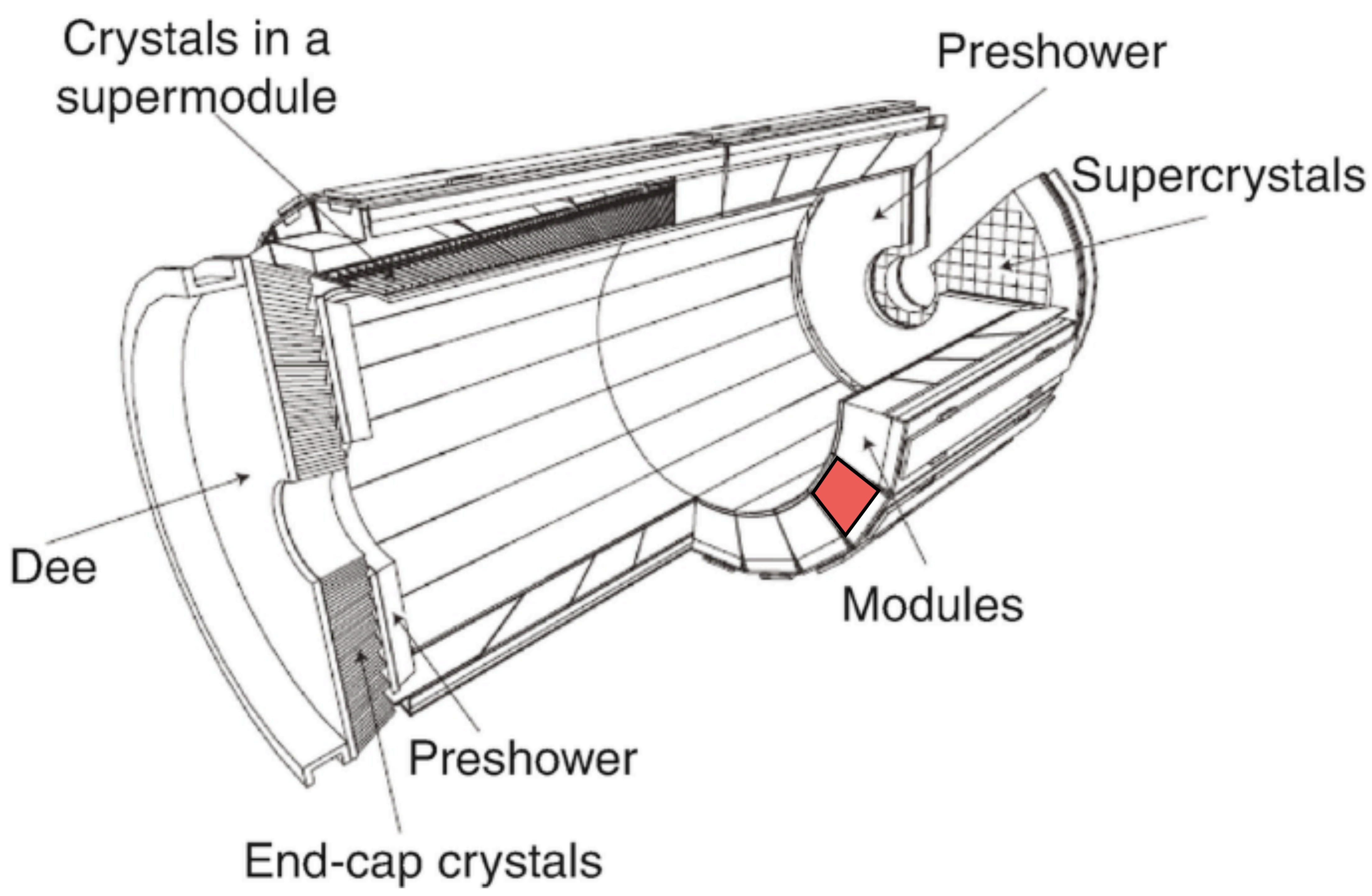


Is it events with missing jets?

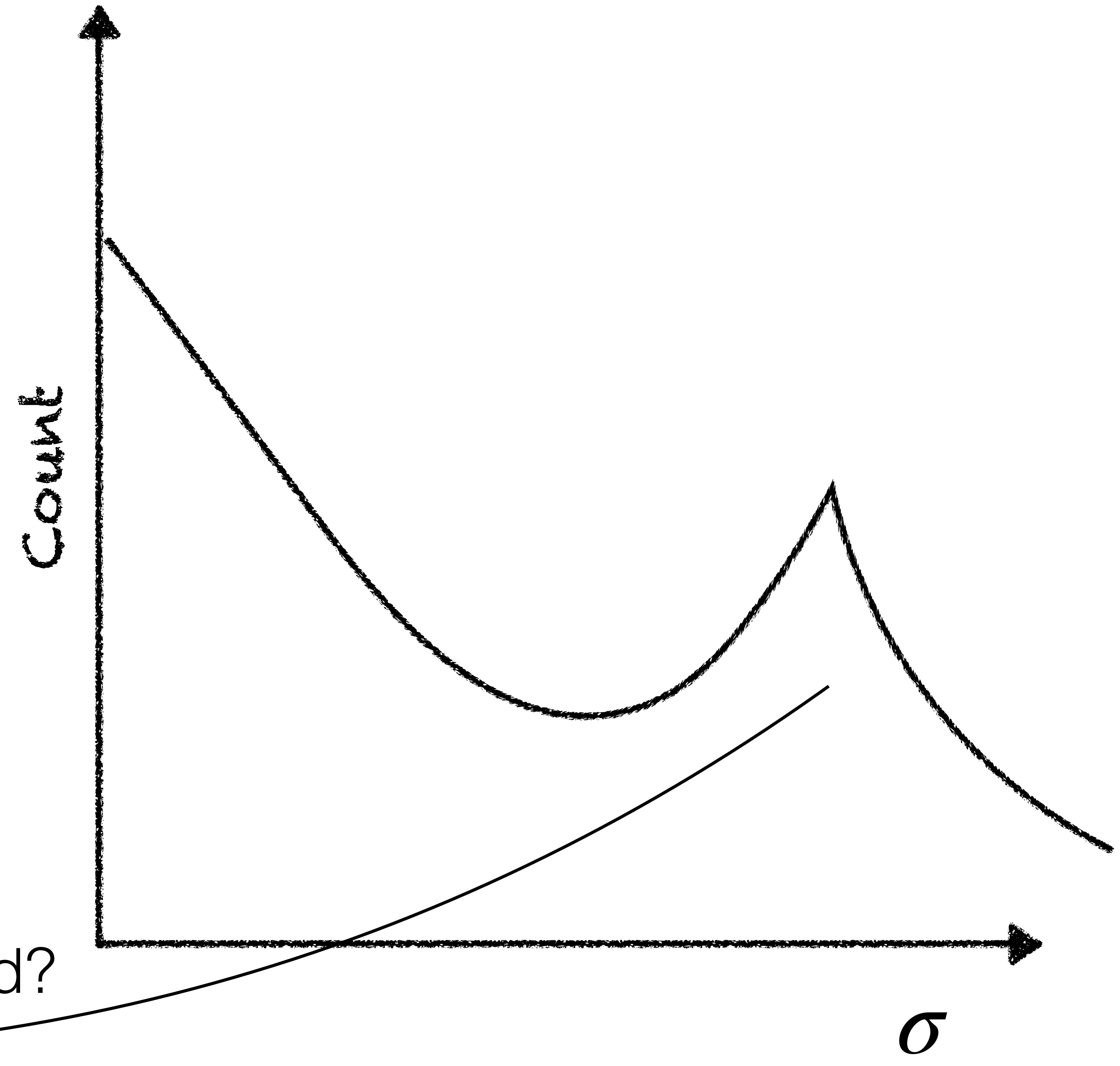
Low Pt events where simulation is poorly modelled?

Some sub-module of the detector?

An exciting use case: Interpretability



Gives you a new handle to understand your data !



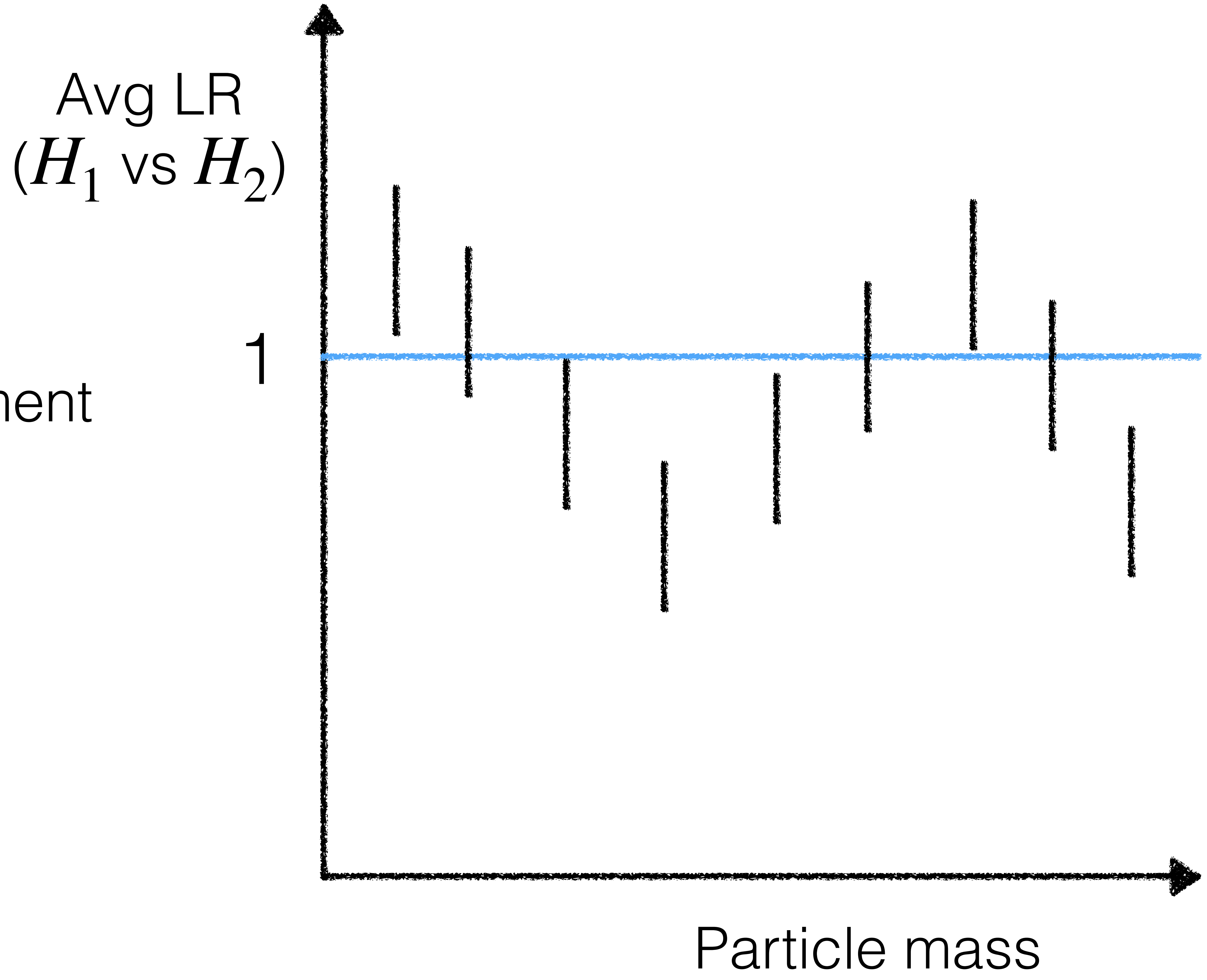
Is it events with missing jets?

Low Pt events where simulation is poorly modelled?

Some sub-module of the detector?

Similar story with neural likelihood ratio estimators

Which events favour my hypothesis ?

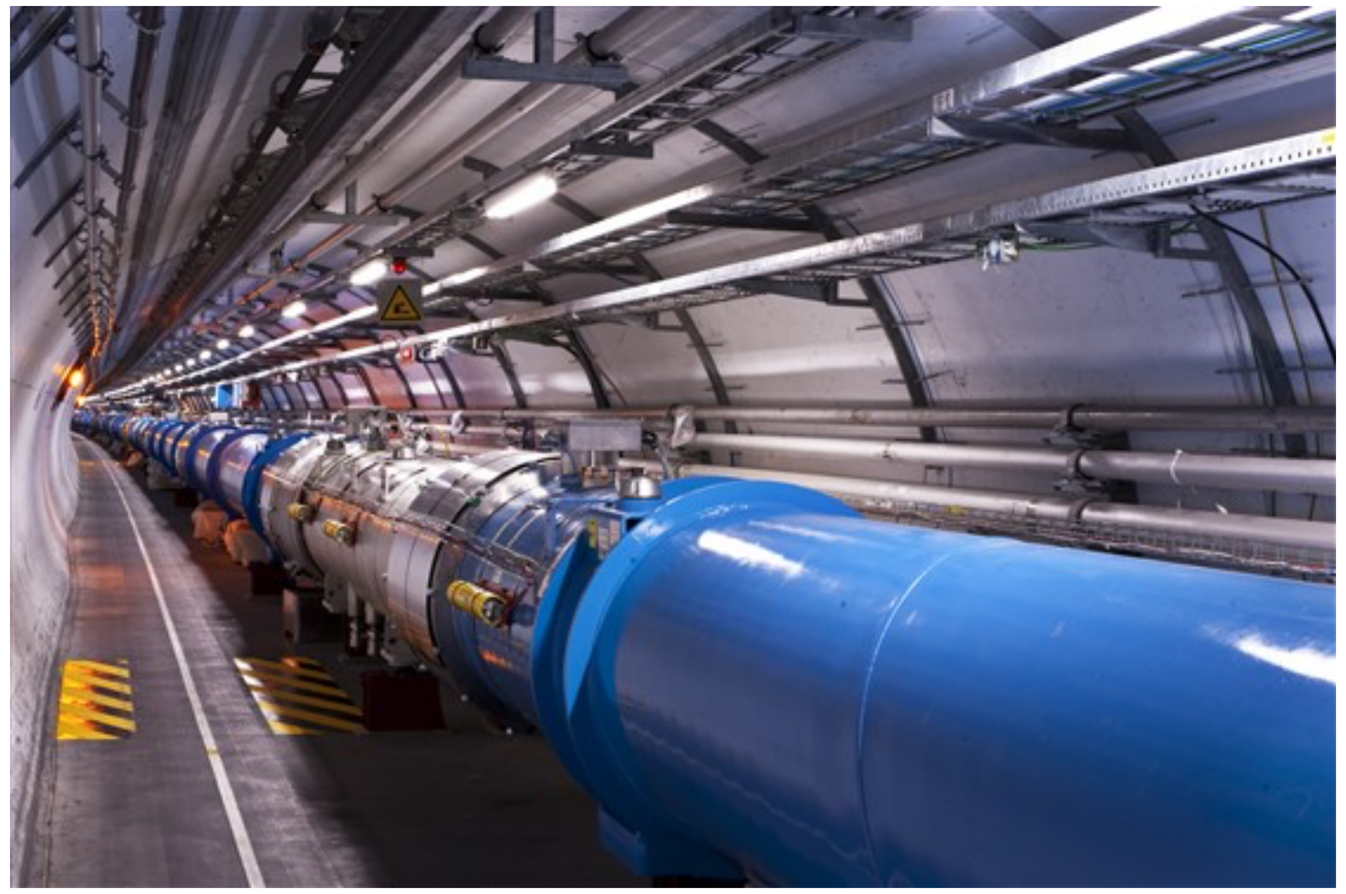


A new interpretability tool that let's you study the contribution of each event on your final measurement

A slew of new sanity checks become possible

Where ML model uncertainties are not essential…

Traditional analysis at LHC



Unlabelled data from LHC

Compare to find New Physics

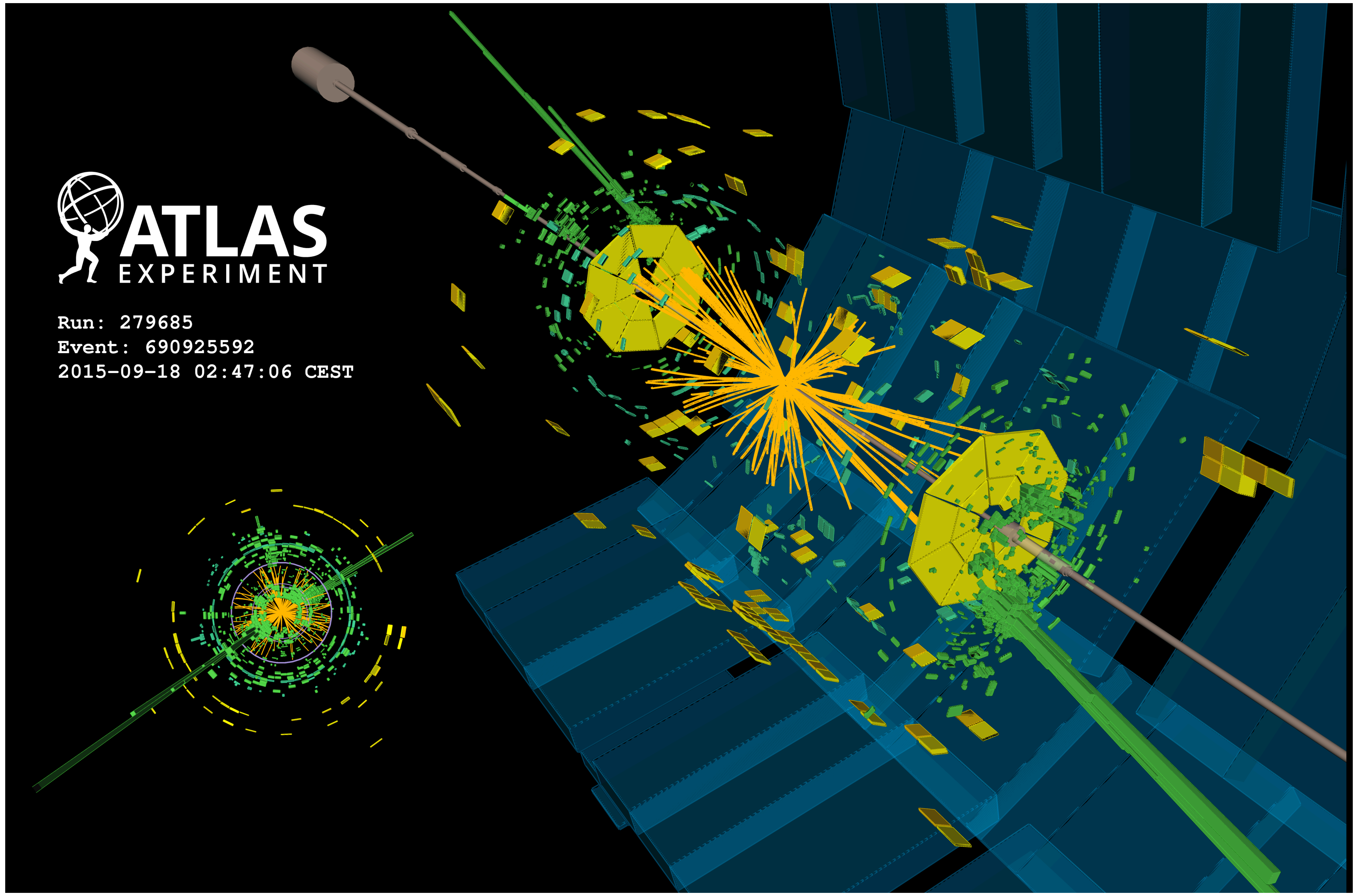
Simulation using Standard Model of particle physics

High dimensional data

Detector has ~100 million sensors

→ Combine information into 1 powerful summary variable

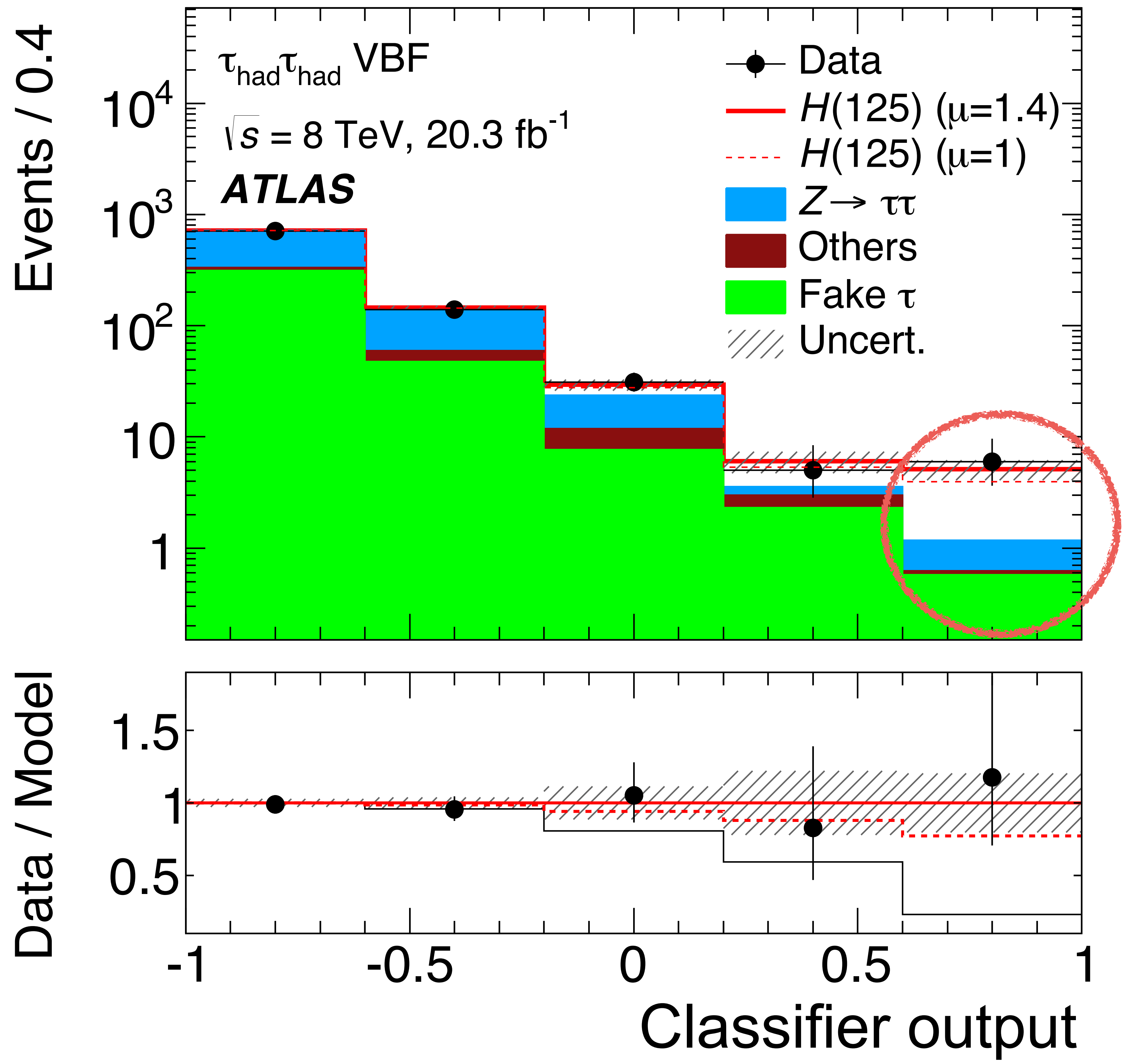
Look at histogram of this variable



Build this 'sensitive summary variable' with ML

Typical use of ML at LHC :

- Classifier for Signal vs Background
- Output observable is maximally sensitive to measure theory parameter → New Physics



Compare various simulations to data to find best fit

1501.04943

Build this ‘sensitive summary variable’ with ML

Typical use of ML at LHC :
- Classifier for Signal vs Background
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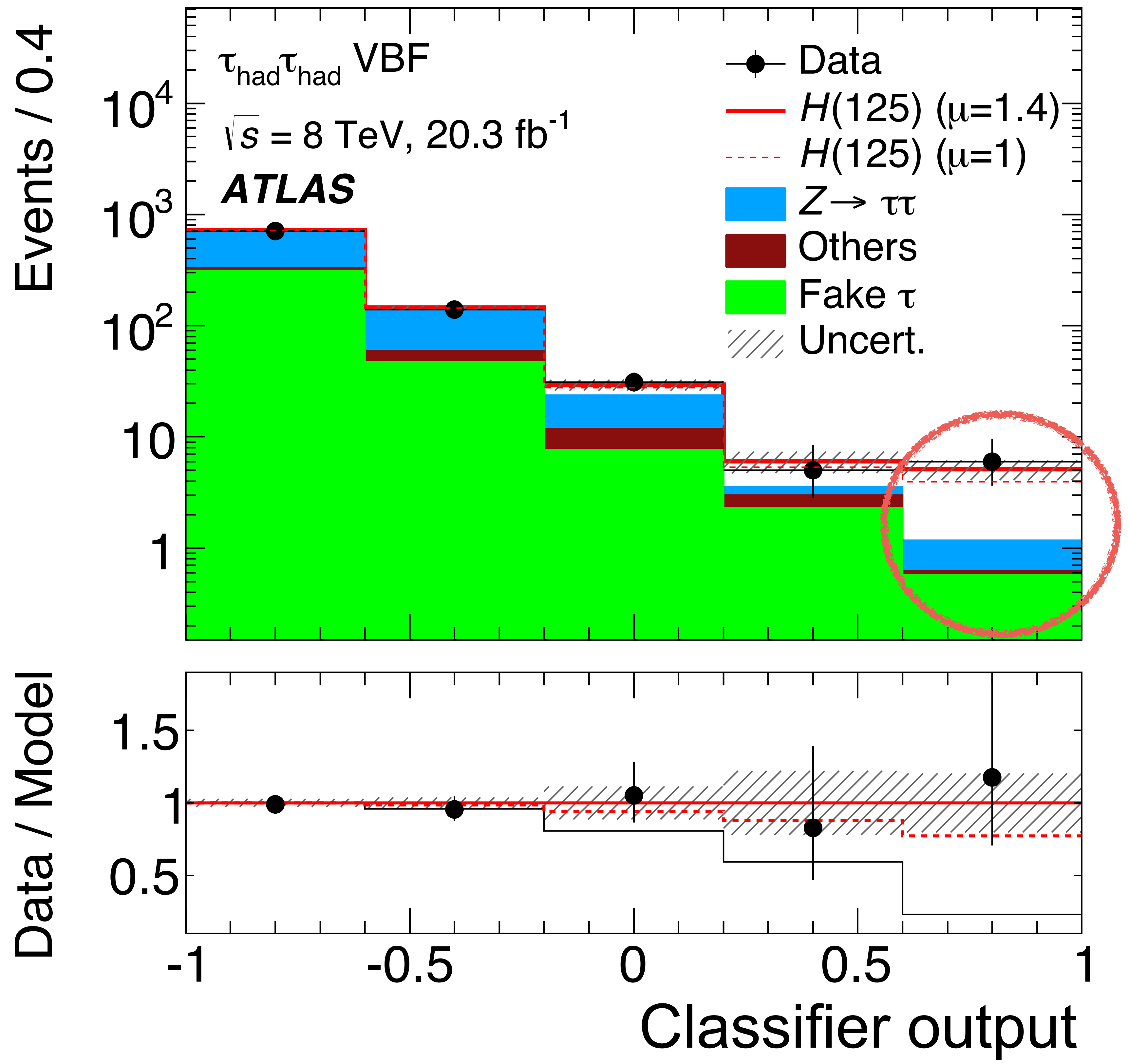
Don’t need uncertainty on ML model !
Treat the output like a regular observable

Worse classifier ⇒ Less sensitivity, but still

correct uncertainty estimates from histogram
(using Poisson probability model)



Compare various simulations to data to find best fit

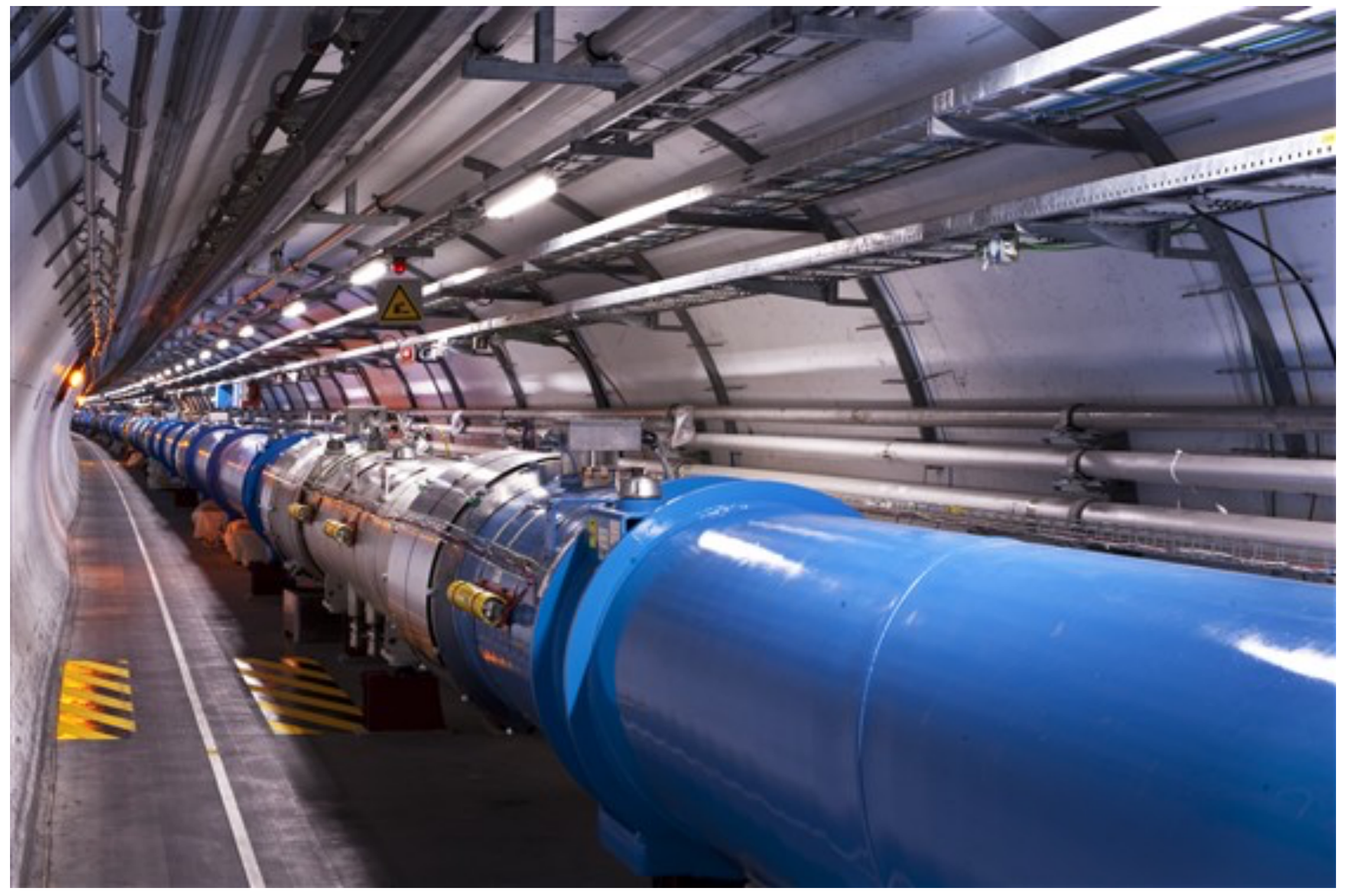
1501.04943

Known unknowns

Simulation using Standard Model of particle physics

Train ML models on simulation, apply on data

Unlabelled data from LHC



Simulate using best guess: Z=1

Detector state Z = ? in data

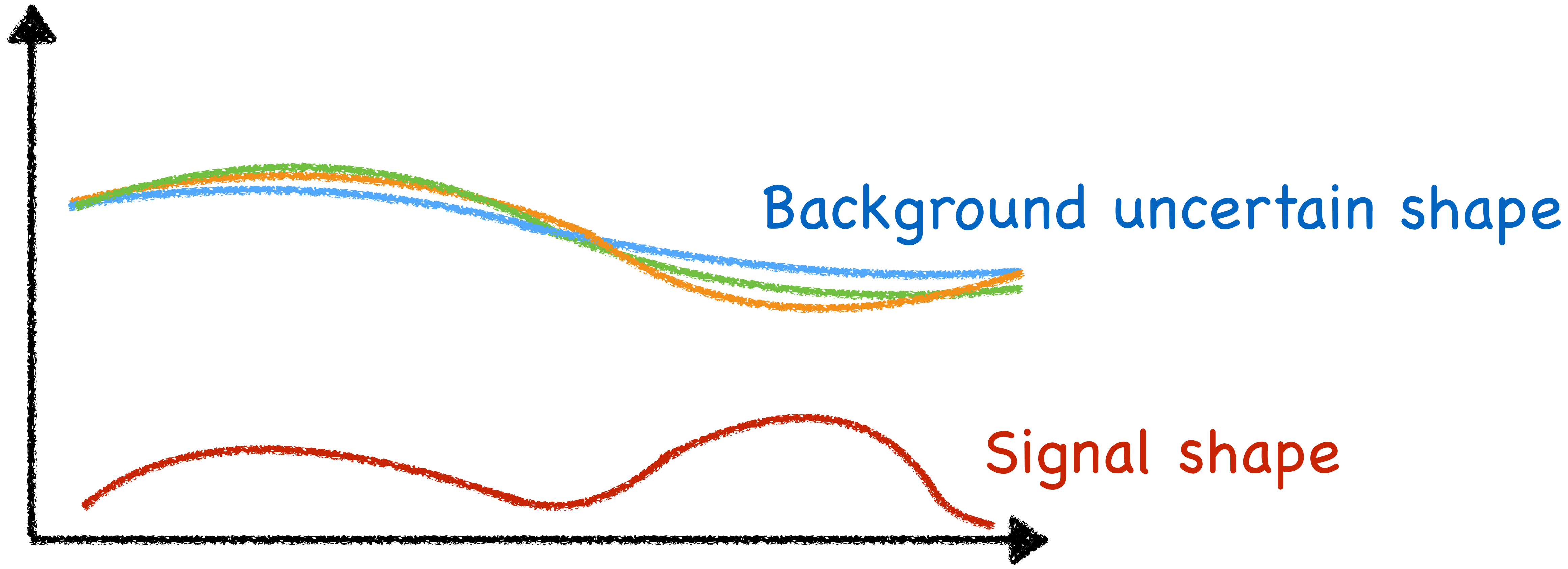
Known sources of differences between simulation and data… will systematically bias our measurements

Observable Sensitive to Nuisance Parameters

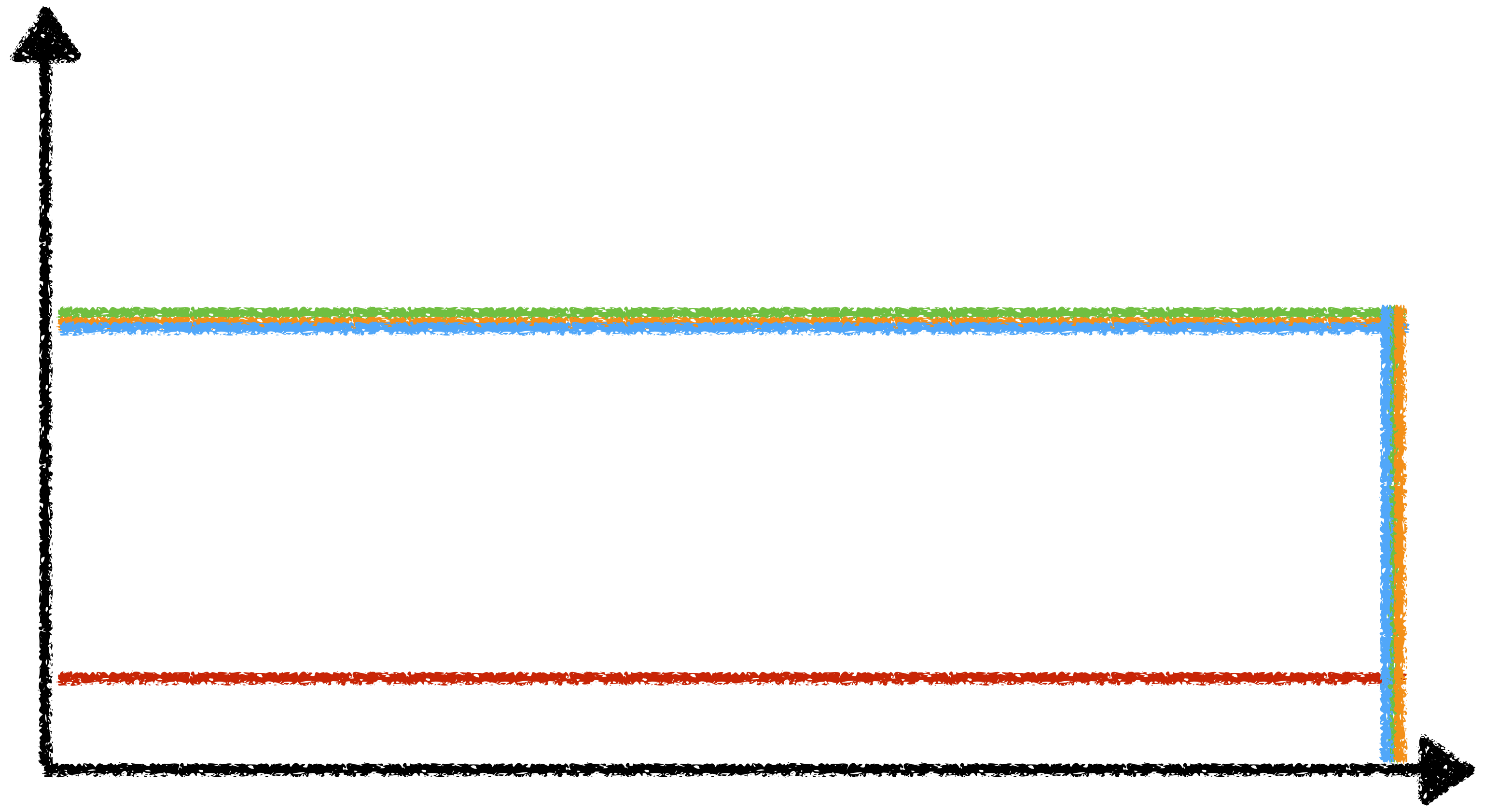
Traditionally, we reduce impact of NP by sacrificing something:

- Don't use observable
- Don't use phase space which is badly modelled by simulation
- Reduce sensitivity some other way

Infinite bin analysis, very sensitive to shape uncertainty



Single bin analysis, insensitive to shape uncertainty



ML equivalent problem: Domain Adaptation

arXiv:1505.07818

MNIST

SOURCE

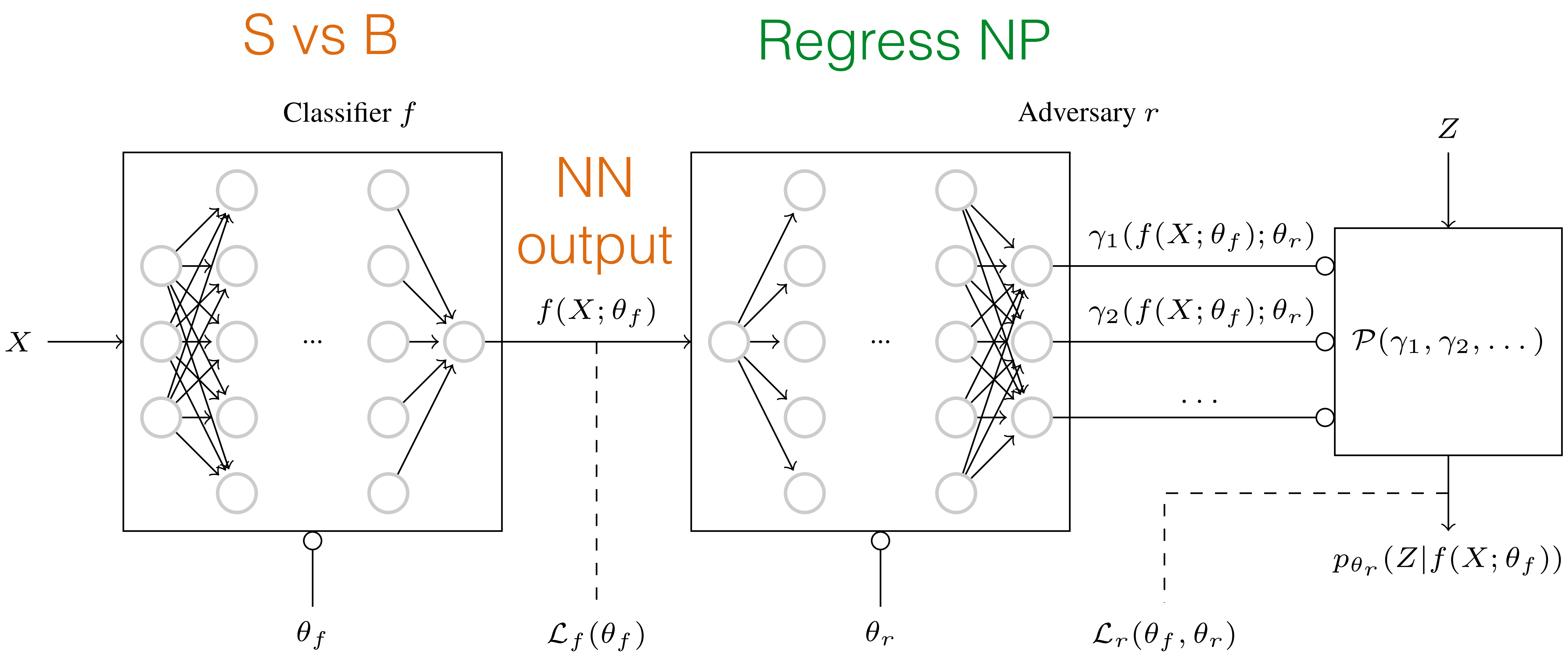
TARGET

MNIST-M

Learning to Pivot, Louppe et al.

Similar ideas: Blance et al., Stevens et al., Wunsch at al., Estrade at al. Kasieczka at al.

Adversarial decorrelation



Learning to Pivot, Louppe et al.

$$L_{Classifier} = L_{Classification} - \lambda \cdot L_{Adversary}$$

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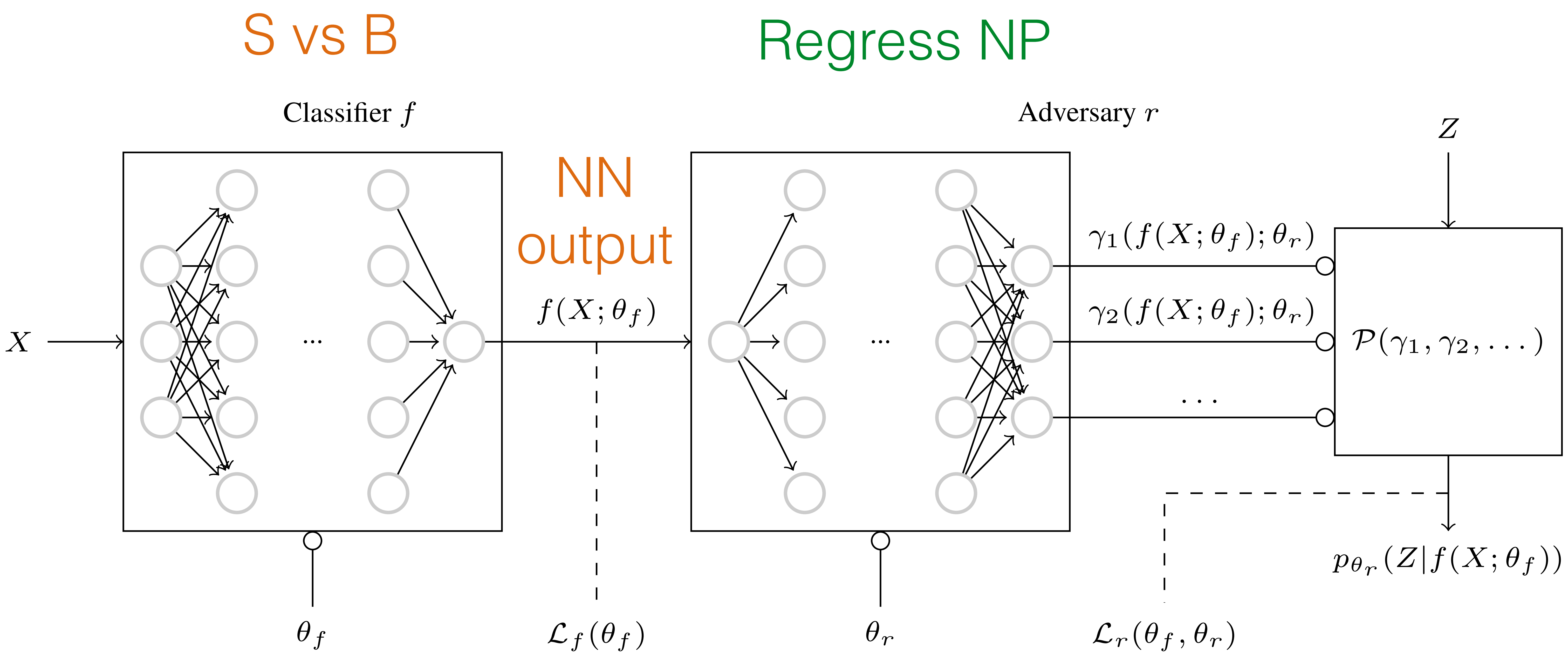
Adversarial decorrelation



To fool the adversary, classifier output should be decorrelated to Z

Learning to Pivot, Louppe et al.

$$L_{Classifier} = L_{Classification} - \lambda \cdot L_{Adversary}$$

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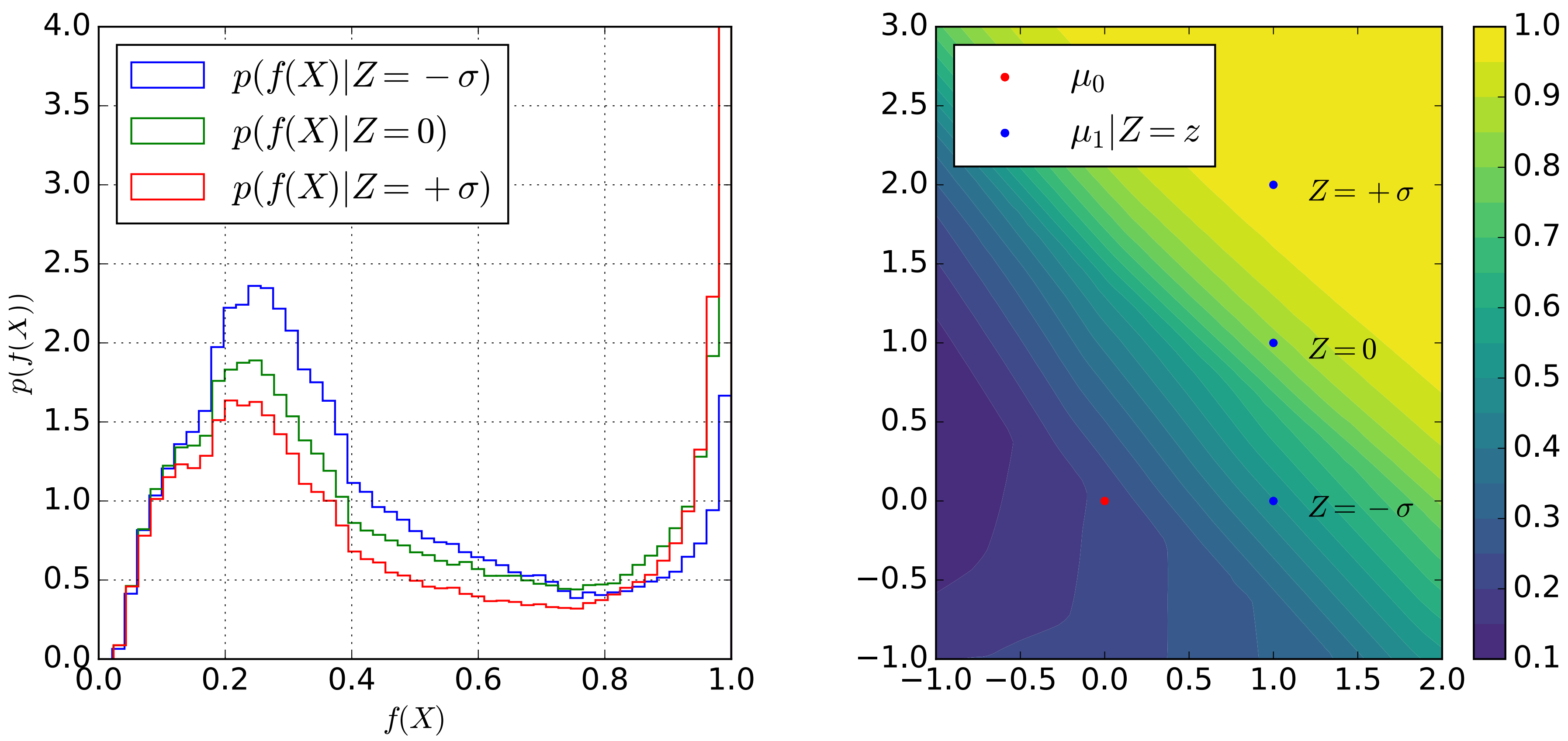
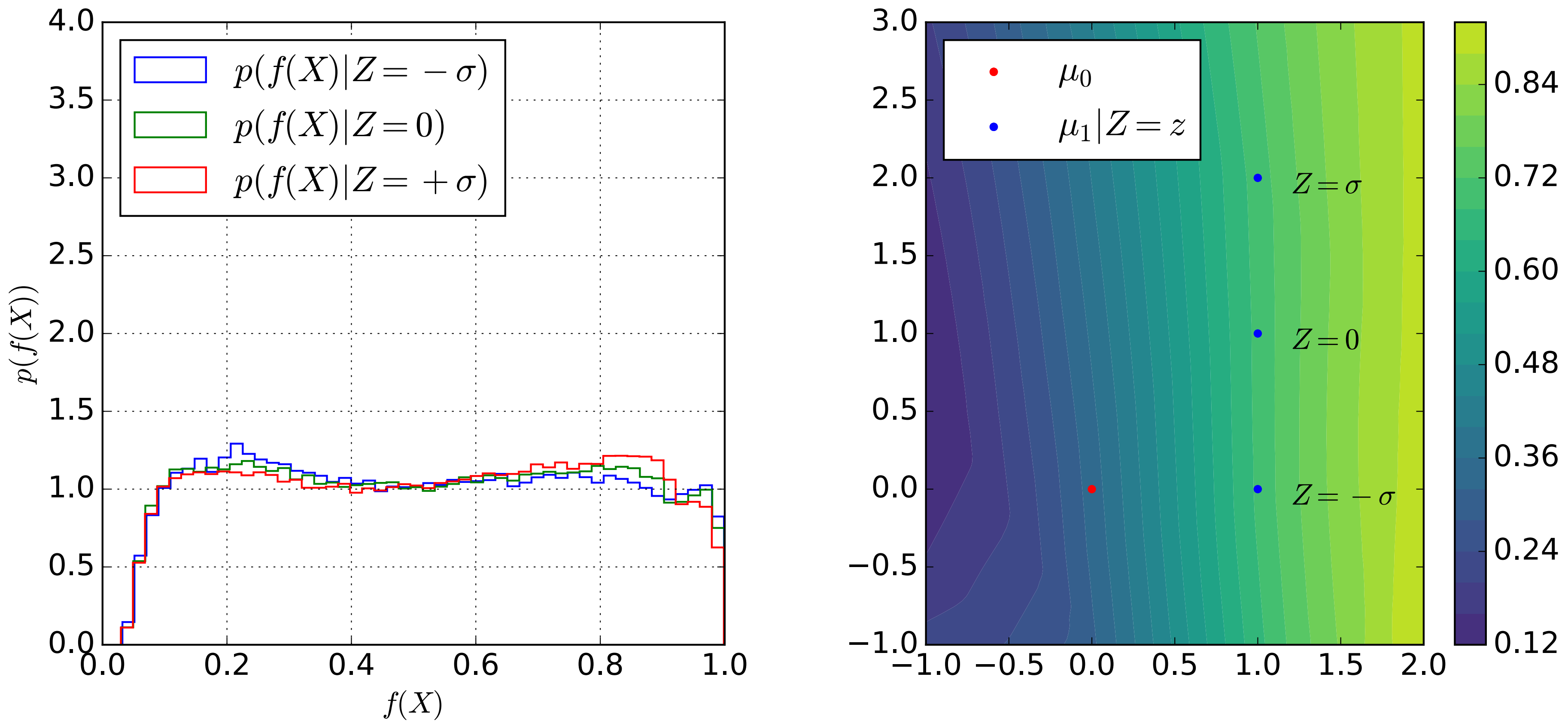
ML-Decorrelation Methods



Adversarial Decorrelation



Classifier output for various values of Z

Learning to Pivot: Louppe et al.

Again, we trade-off sensitivity to have a more robust analysis

Alternatively.. Can we exploit all the information we have ?

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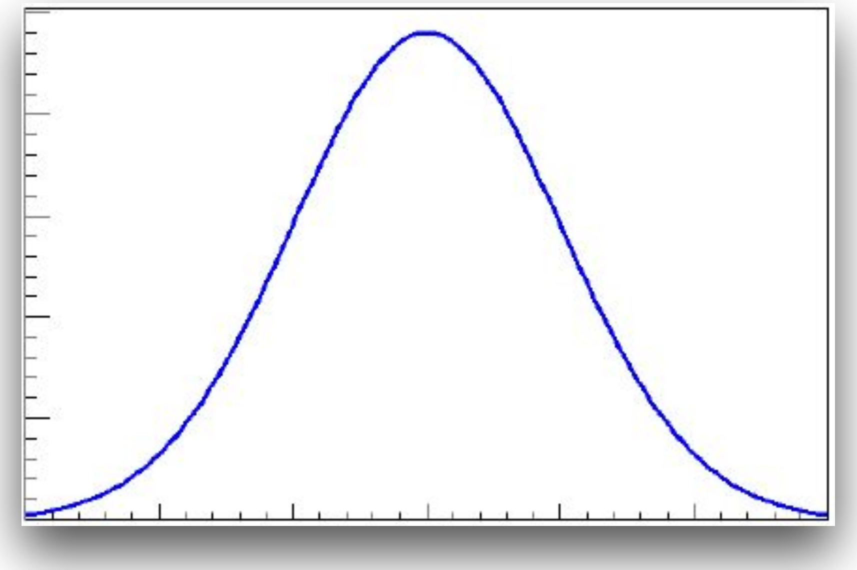

z = Nuisance Parameter

Prior

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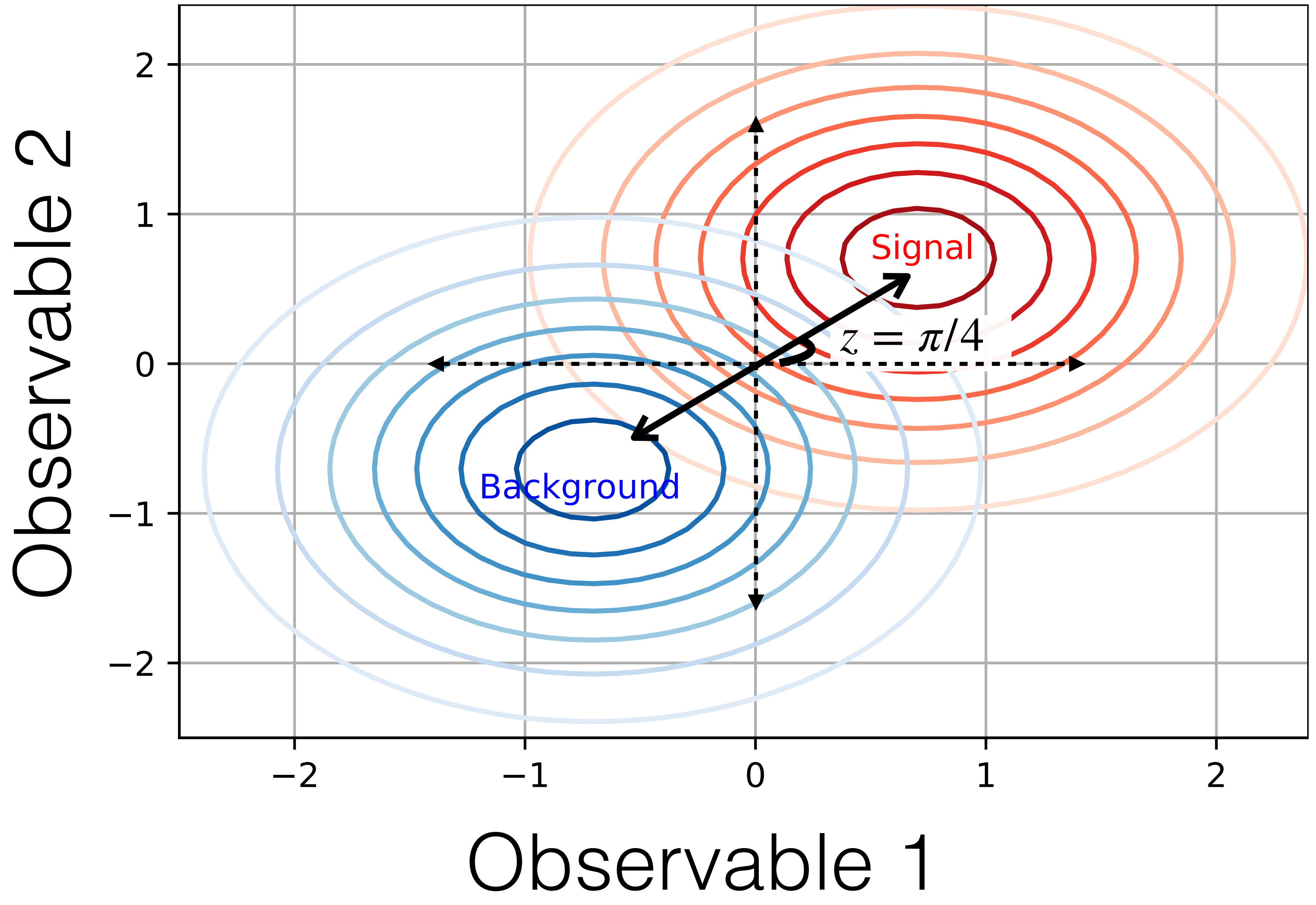

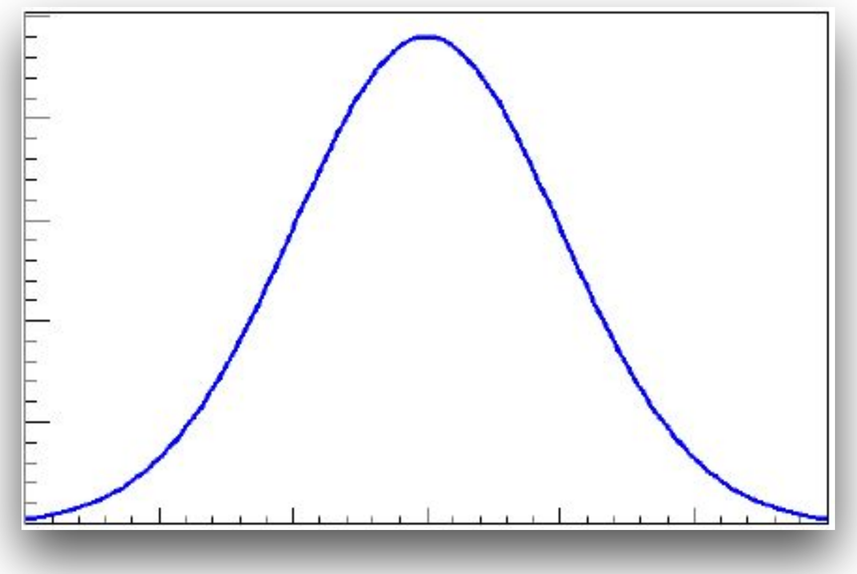

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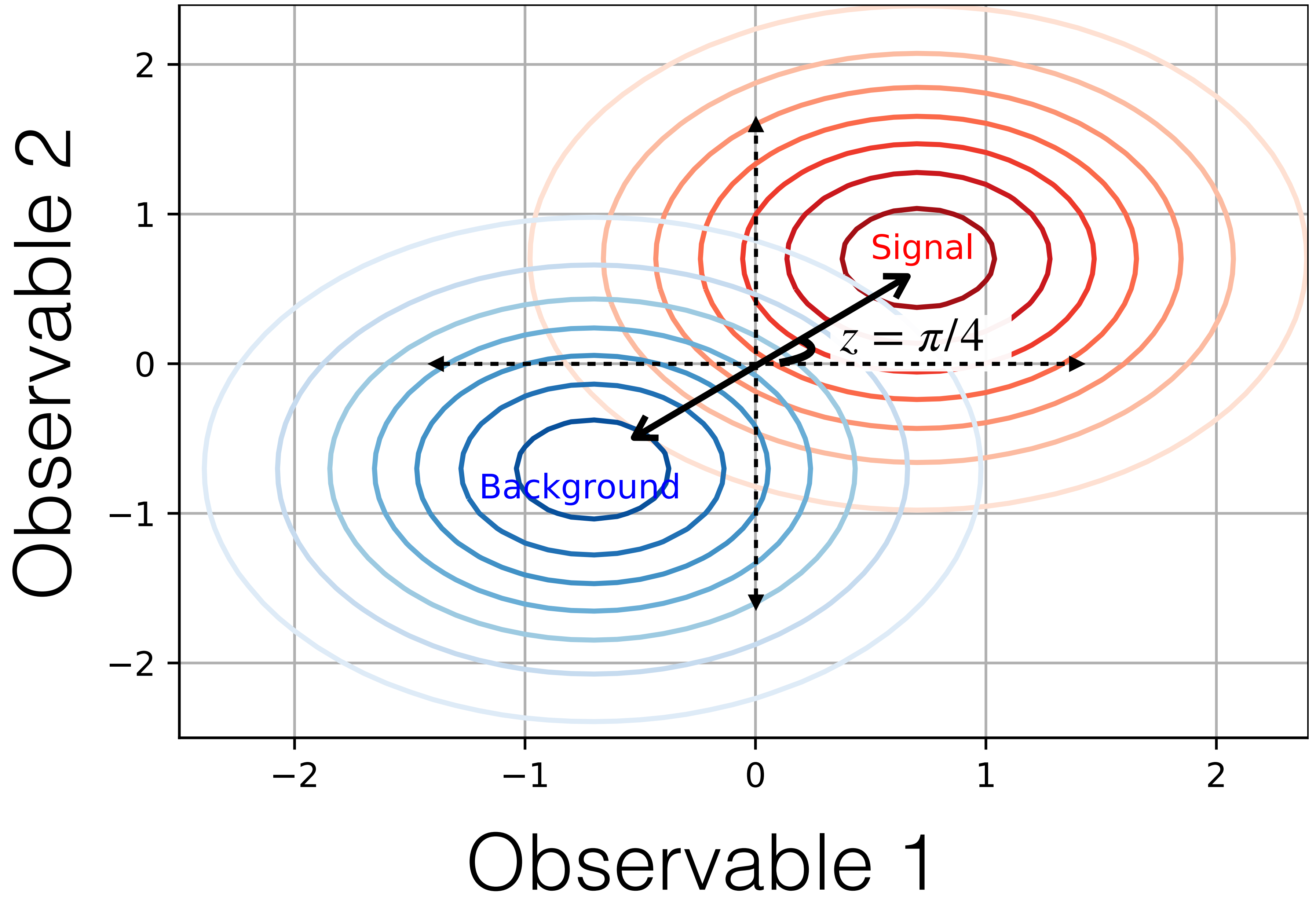

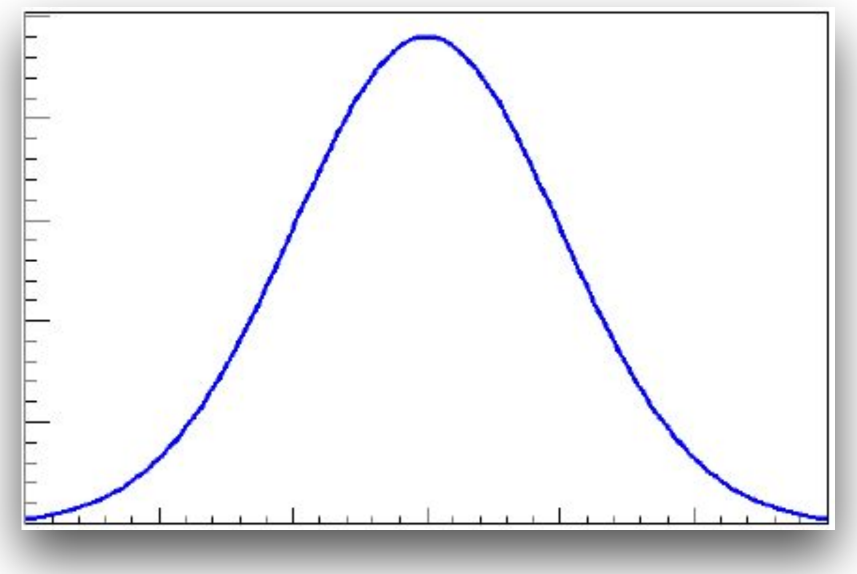

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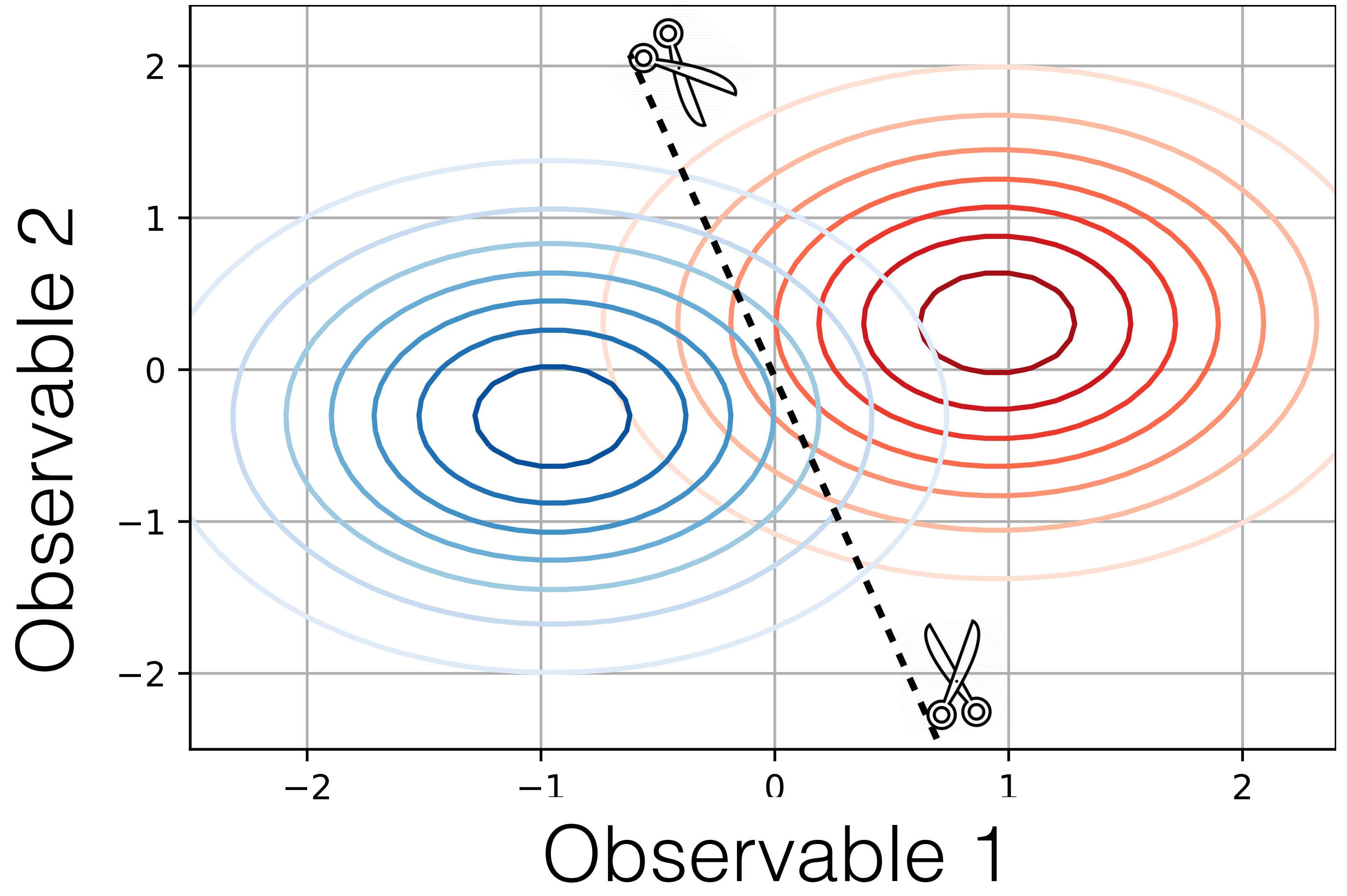

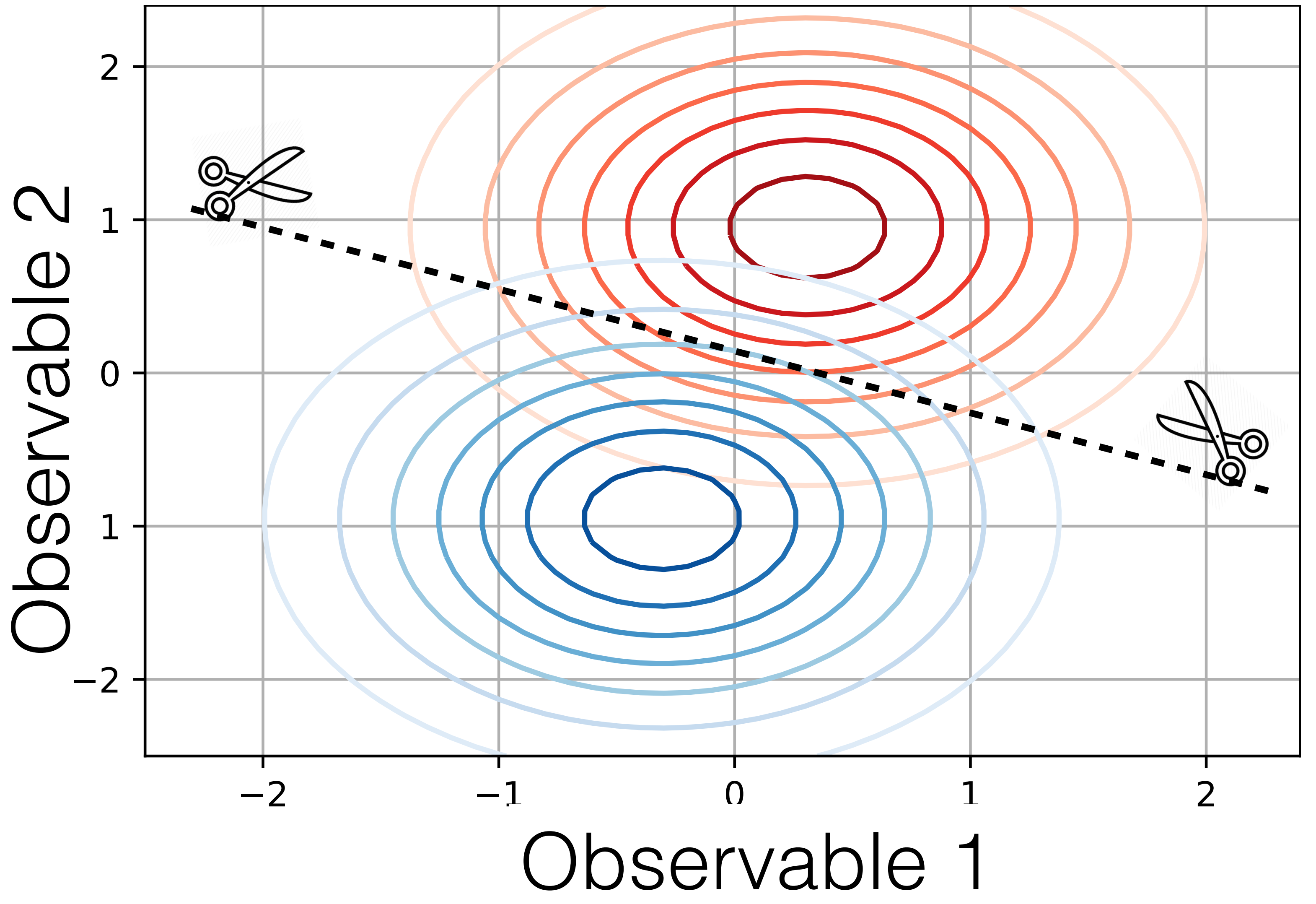

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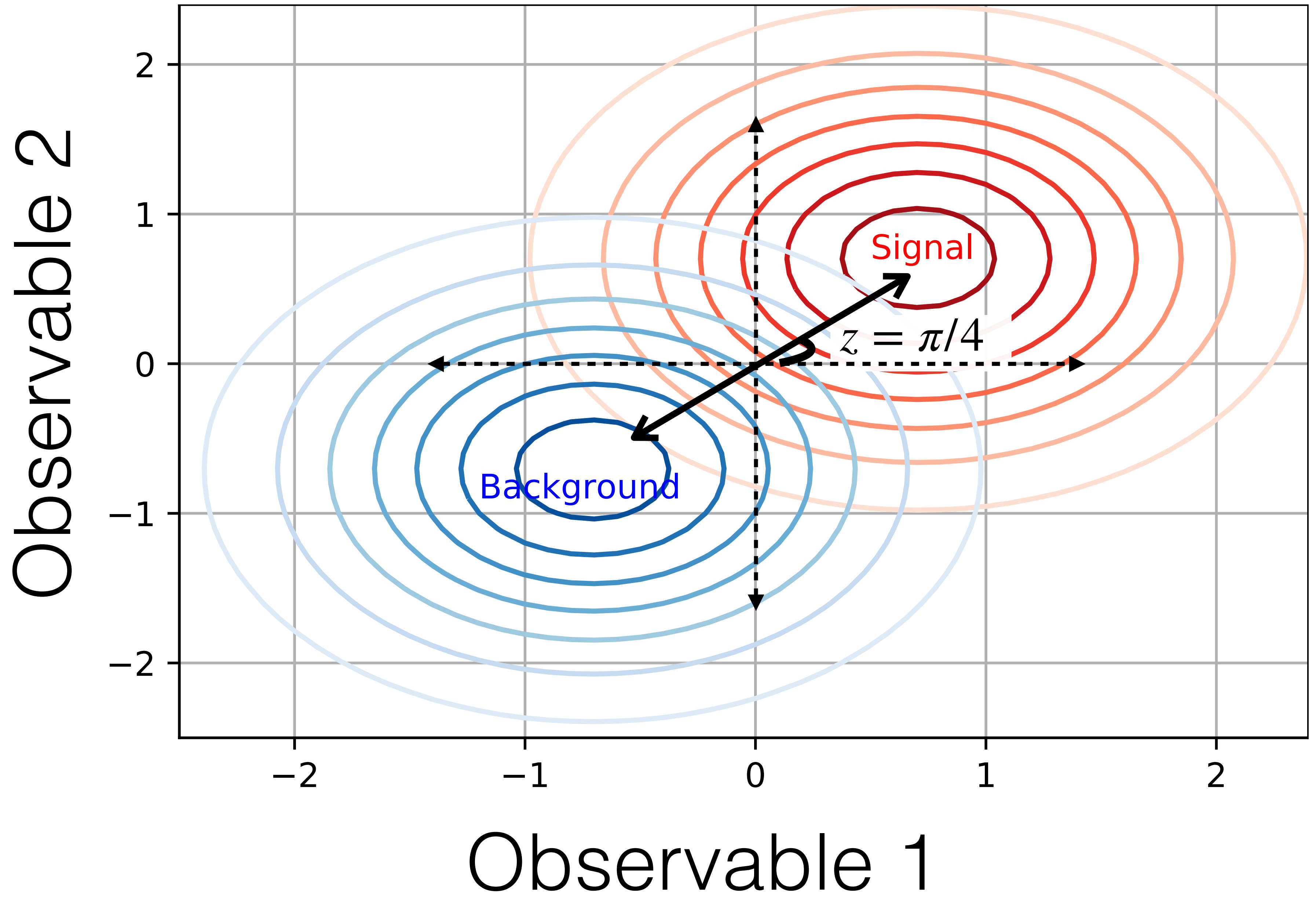

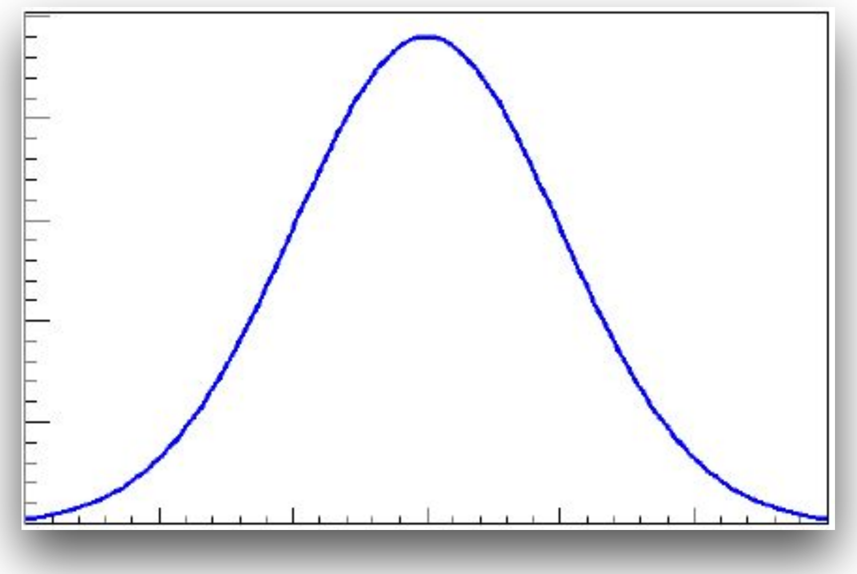

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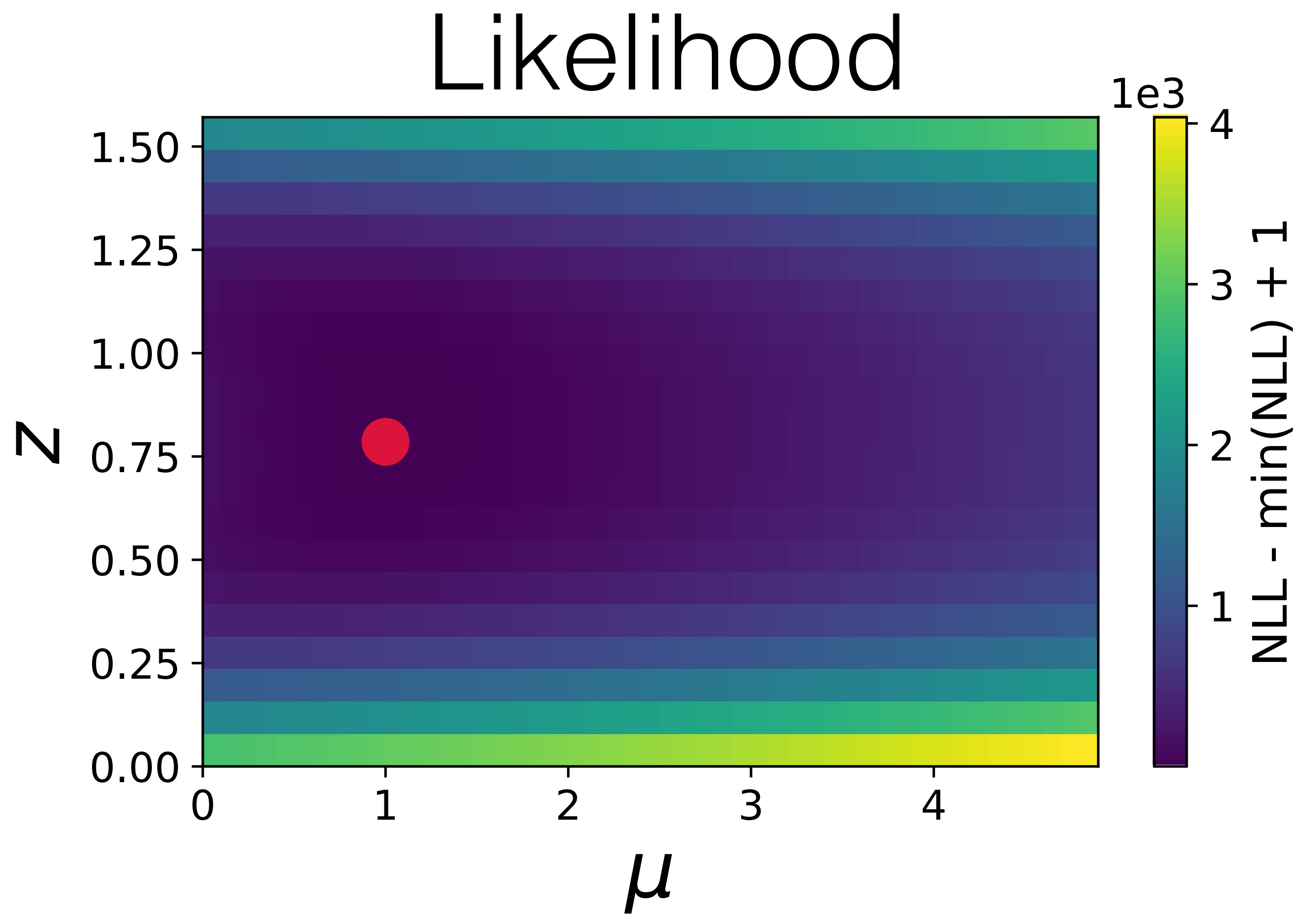
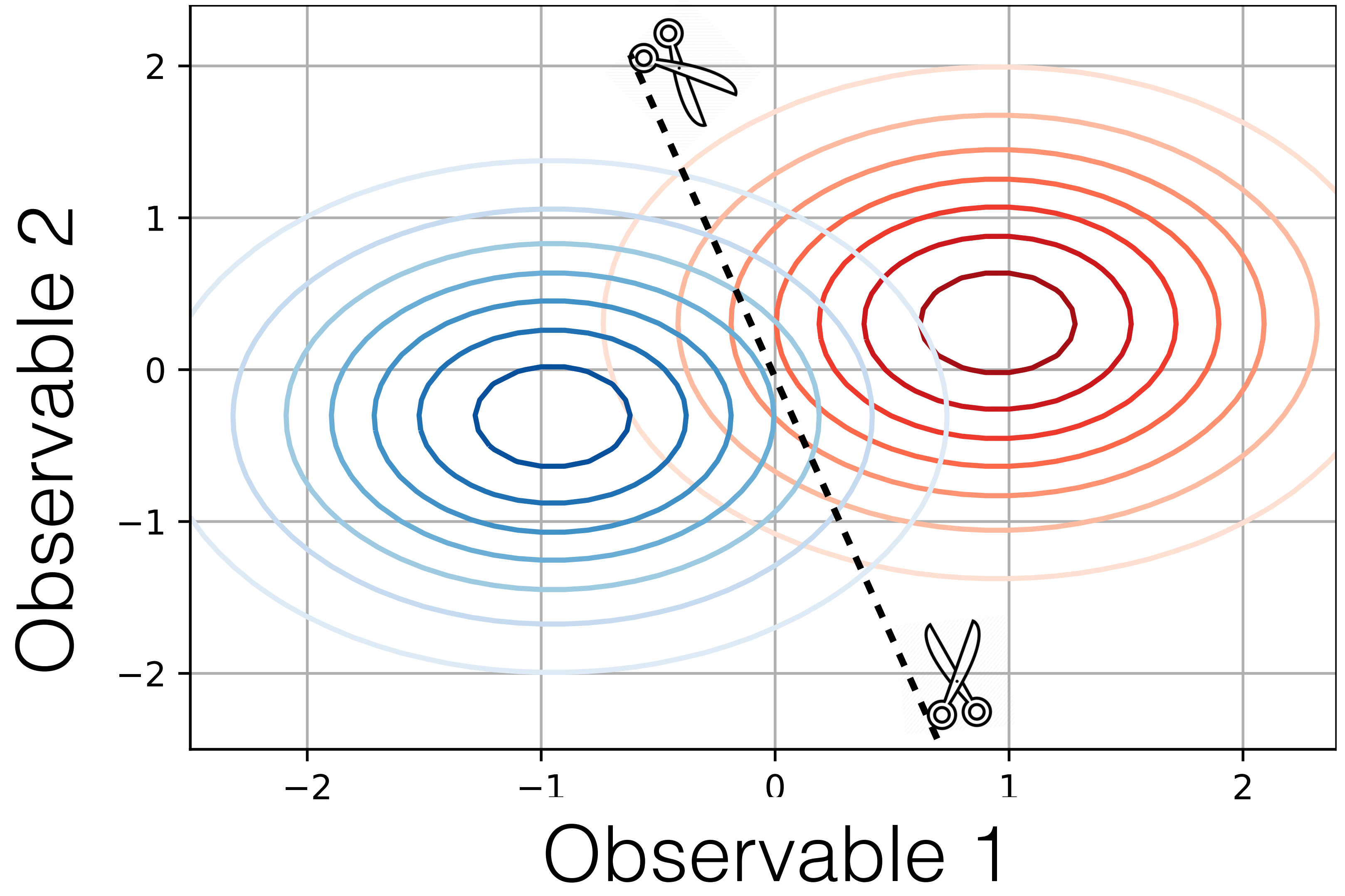
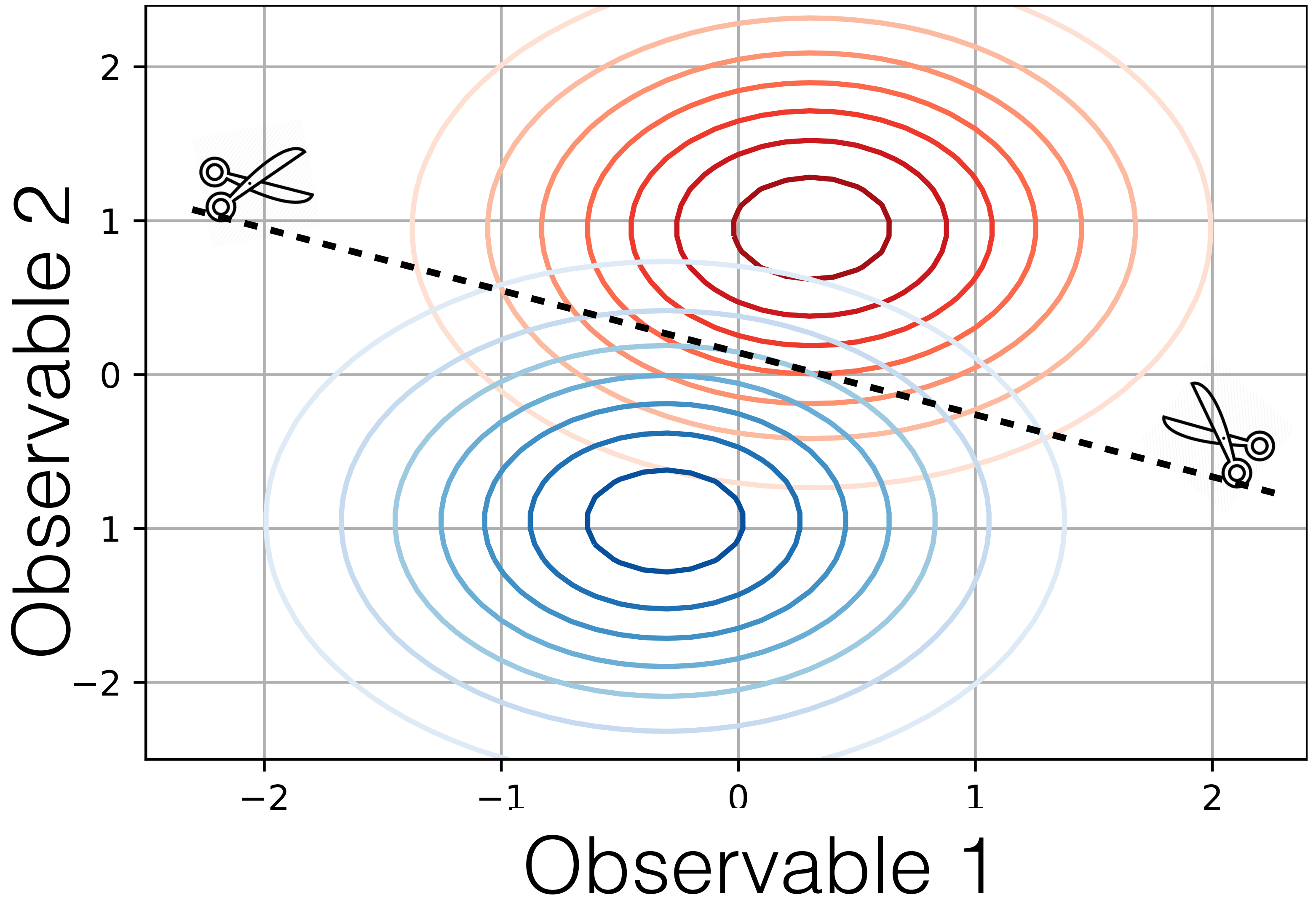
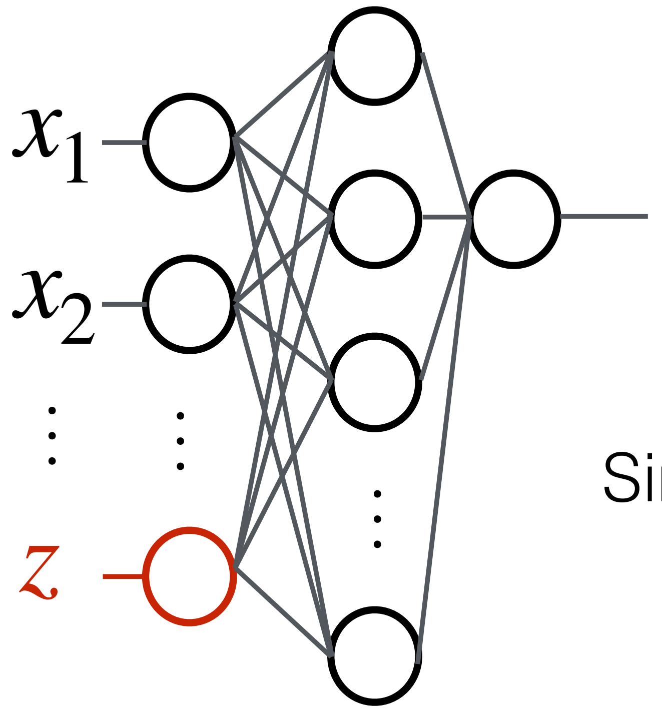






Opposite of decorrelation: Uncertainty-aware learning

- Propagate uncertainties through the classifier in an "uncertainty aware" way



$f(x_1, x_2, \ldots, z)$

Similar to 1601.07913

Repeat for each hypothesis z

Data
with Z = ?

Opposite of decorrelation: Uncertainty-aware learning

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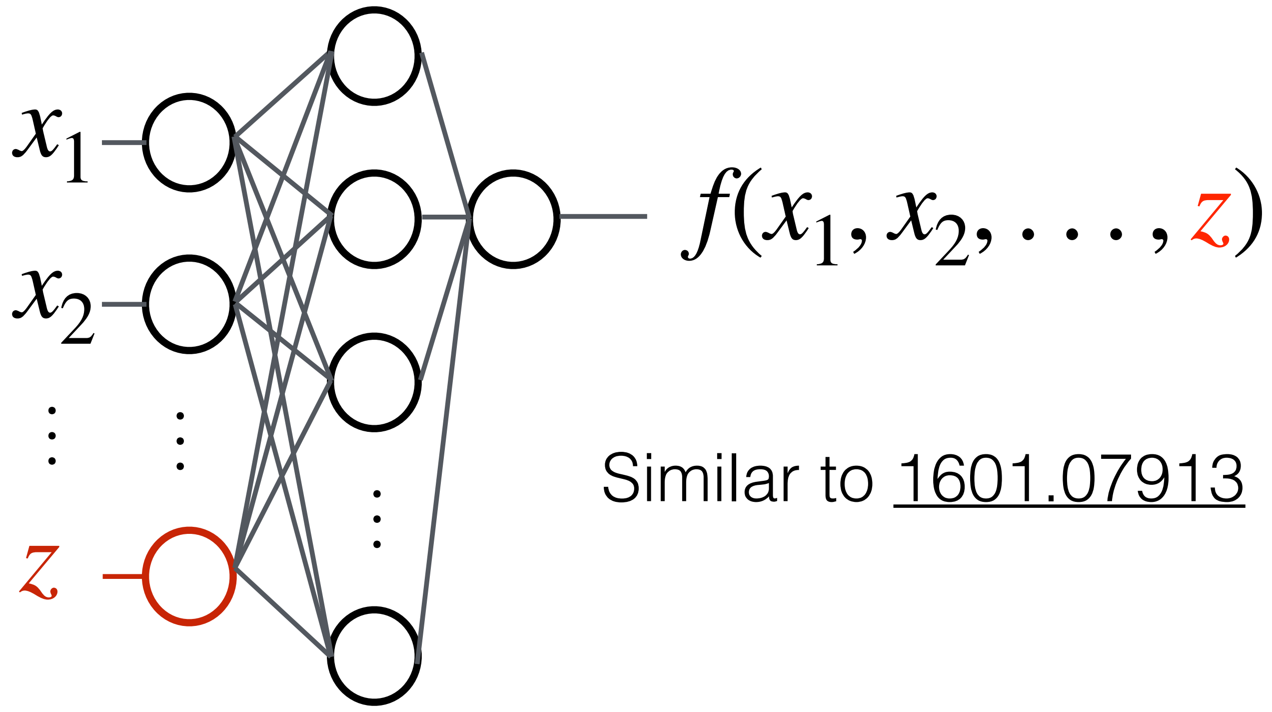

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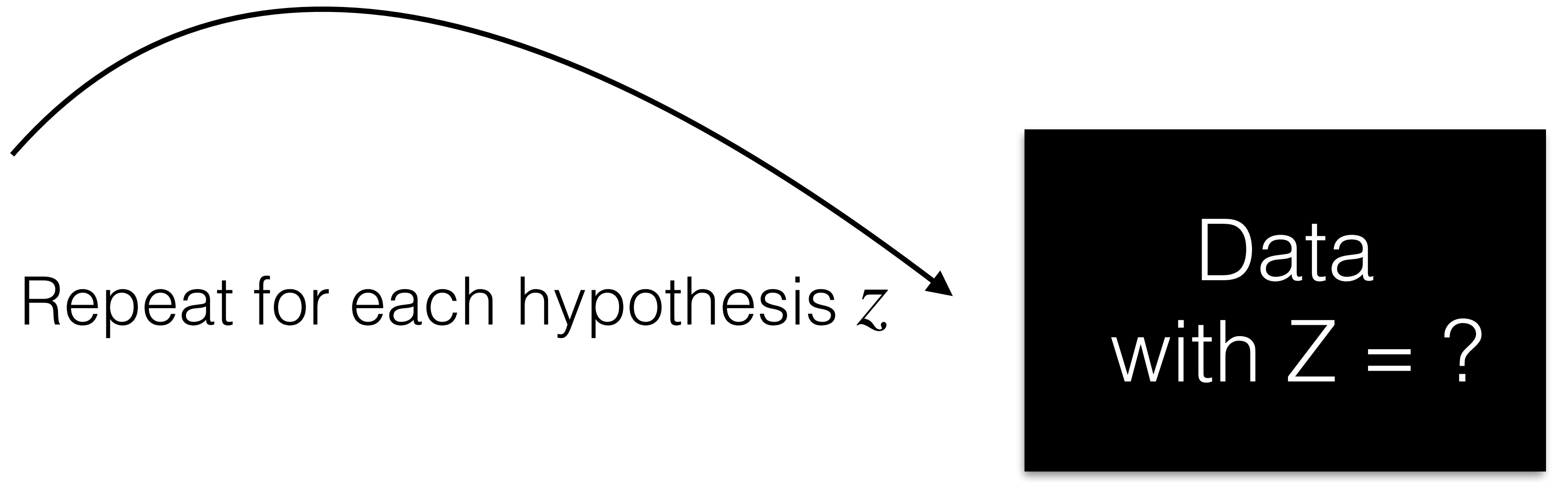
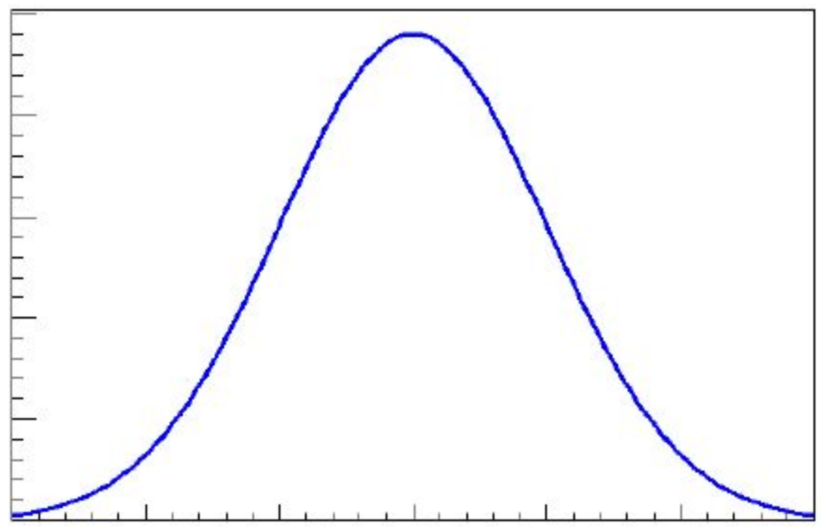


- Intuition: Allow the analysis technique to vary with Z
  You always get the best classifier for each value of Z

- Profile Z + incorporate prior

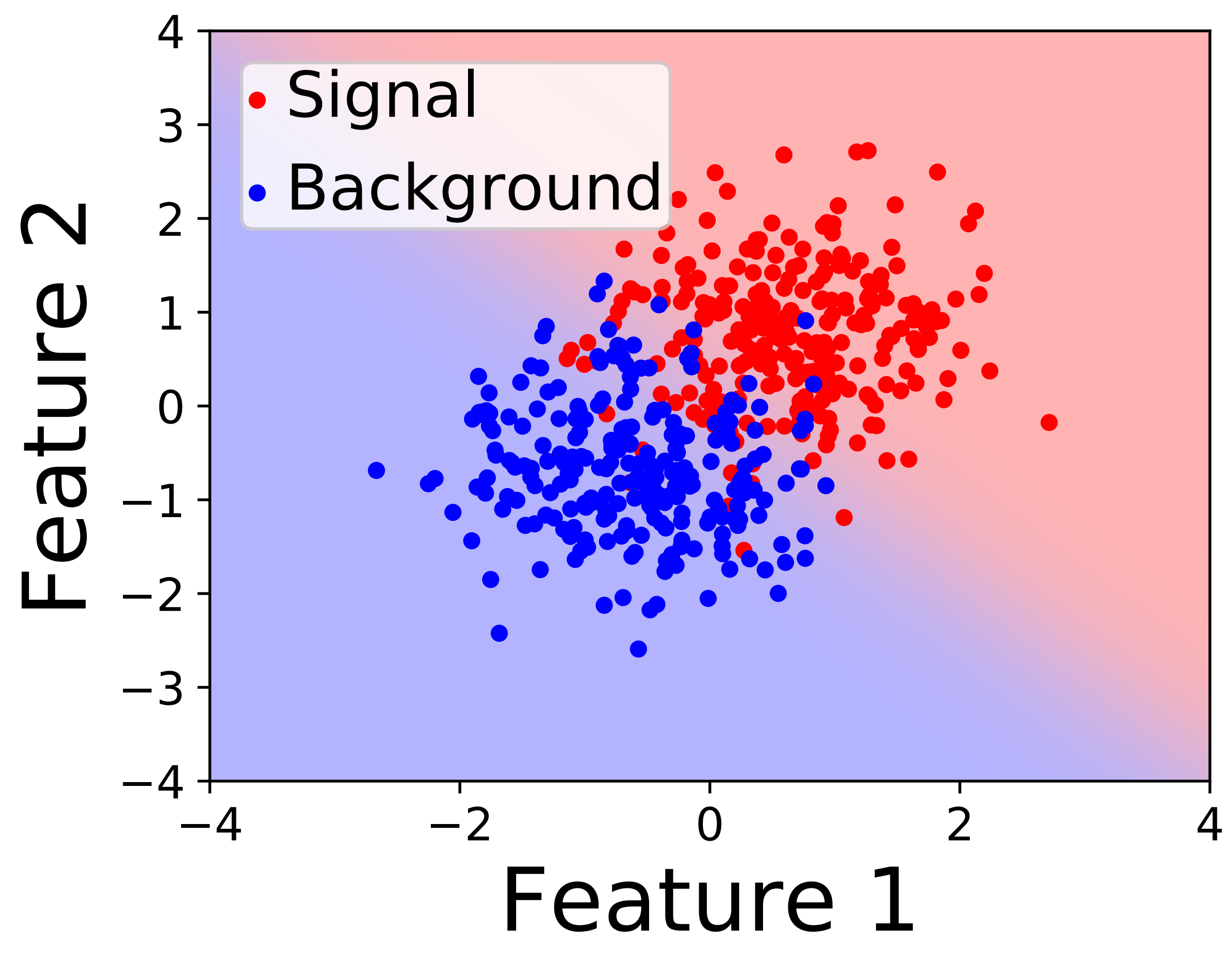


Nominal and Systematic Up Examples

Baseline Classifier

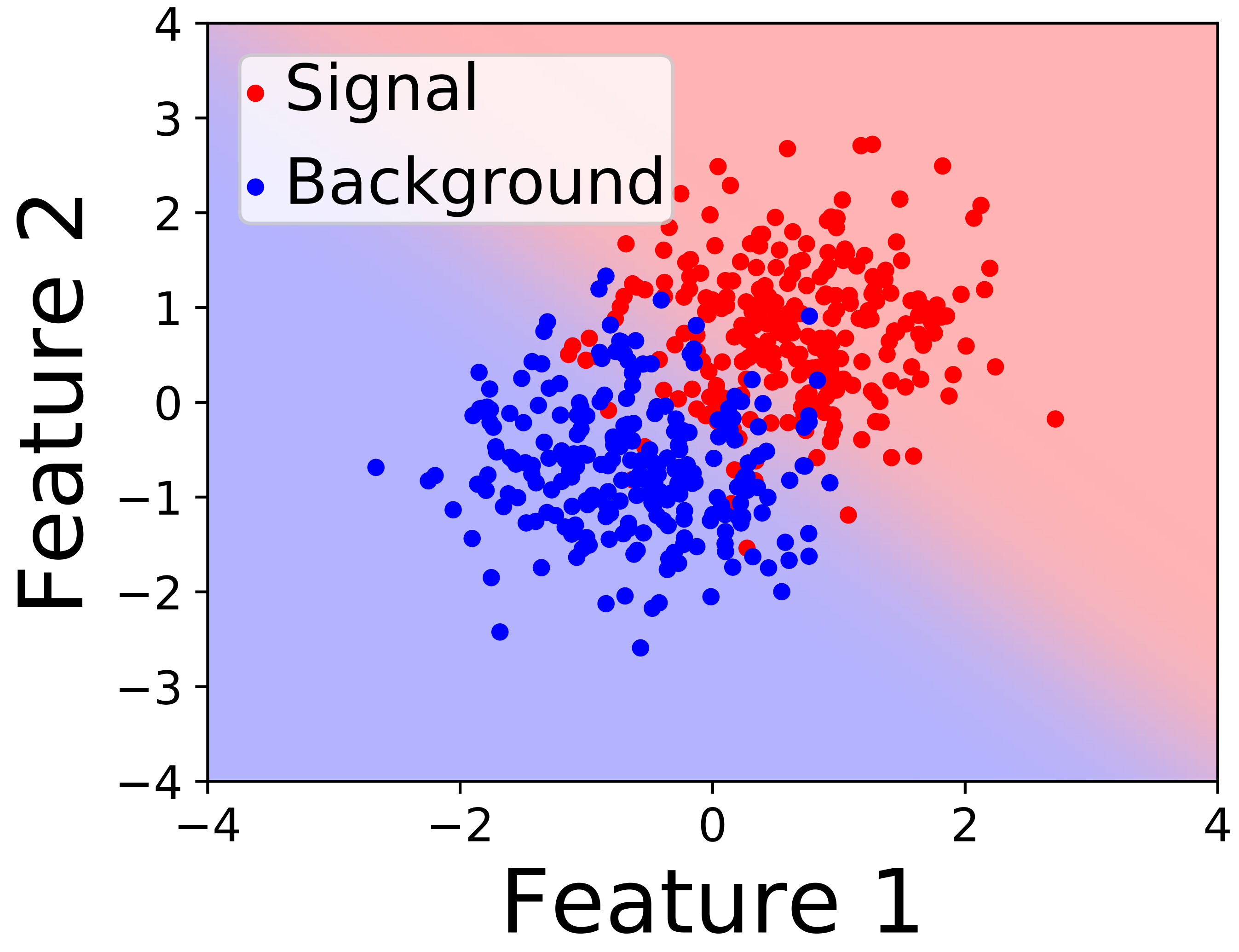
Uncertainty-Aware Classifier

Nominal "Data"



AUC=0.978

Optimal



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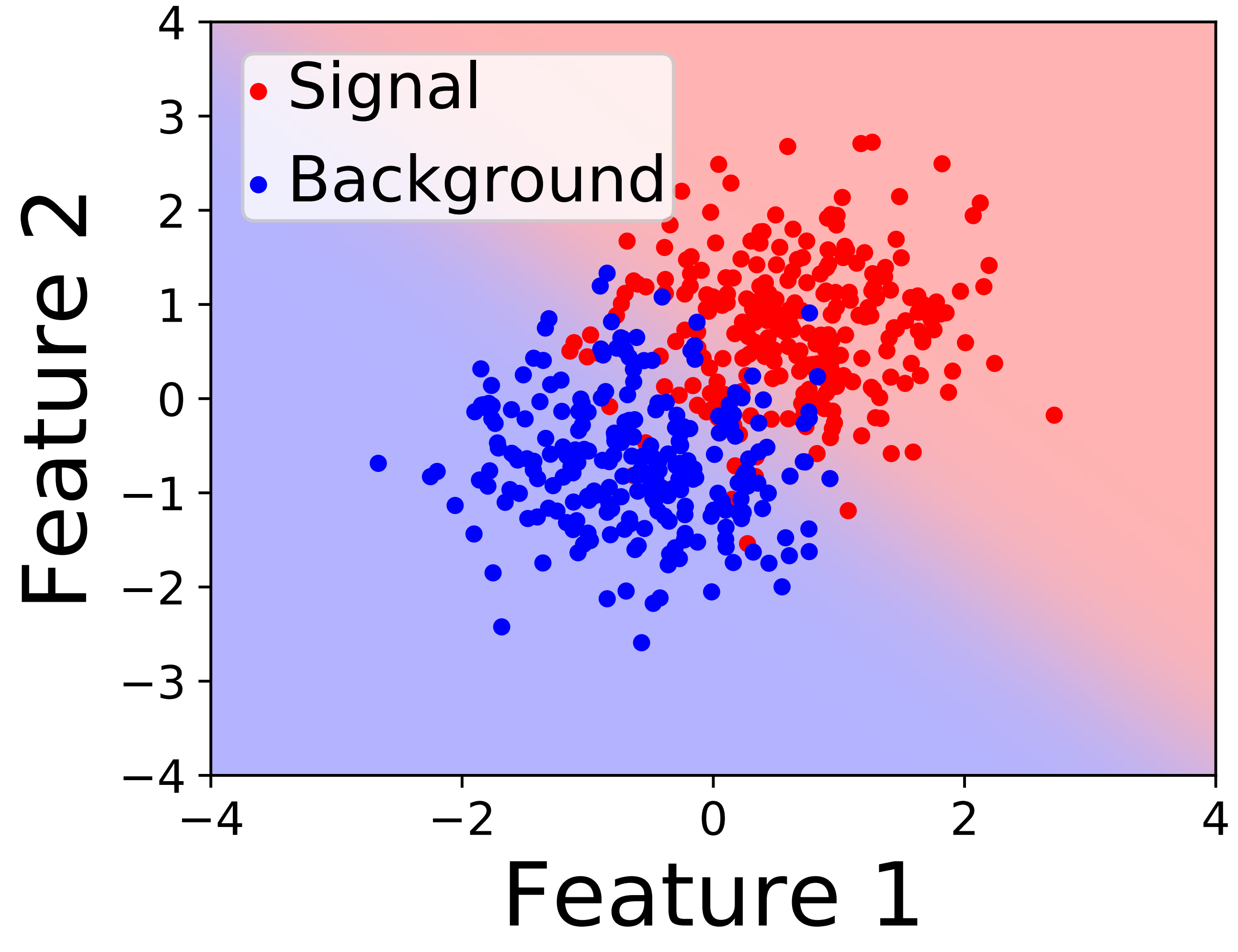
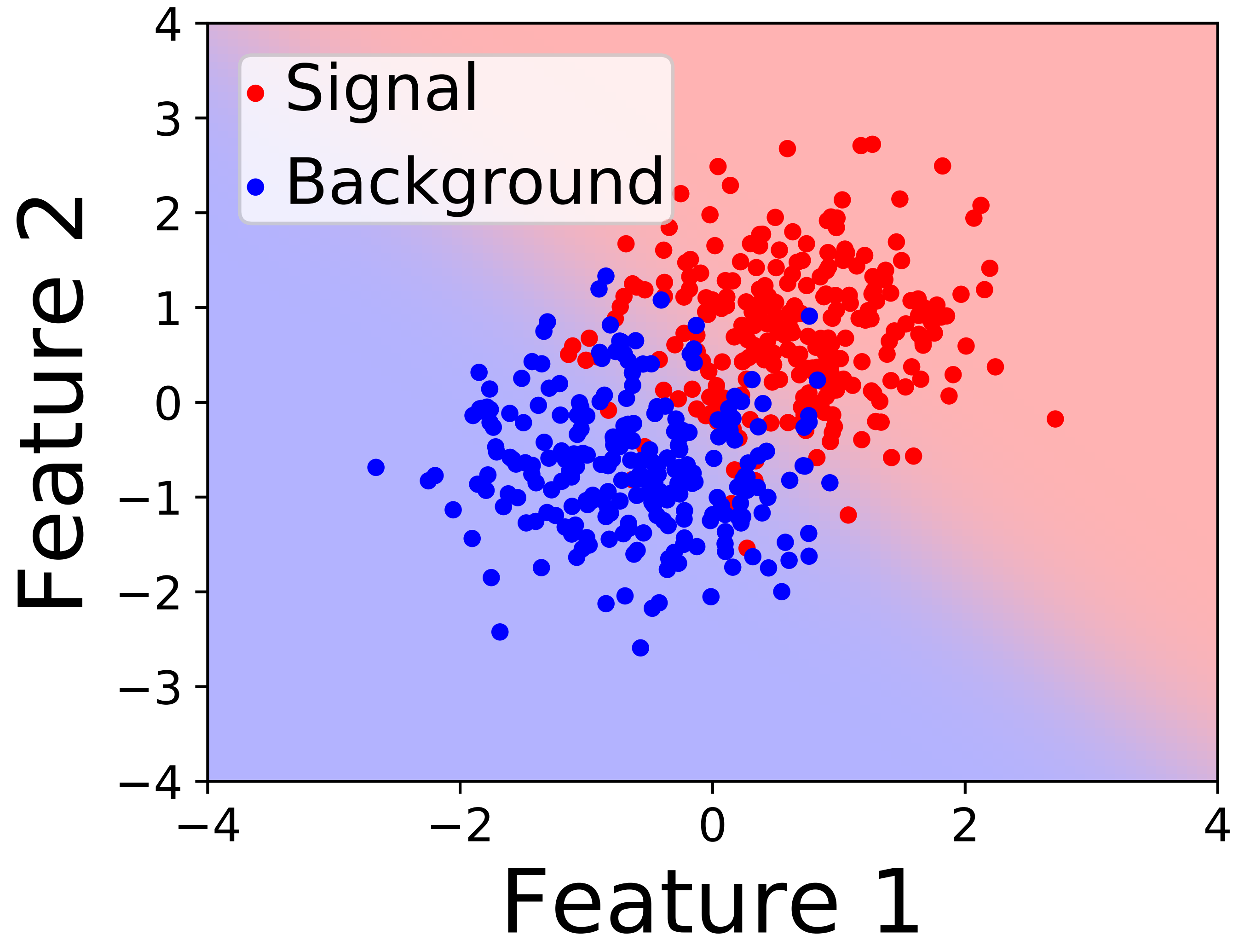
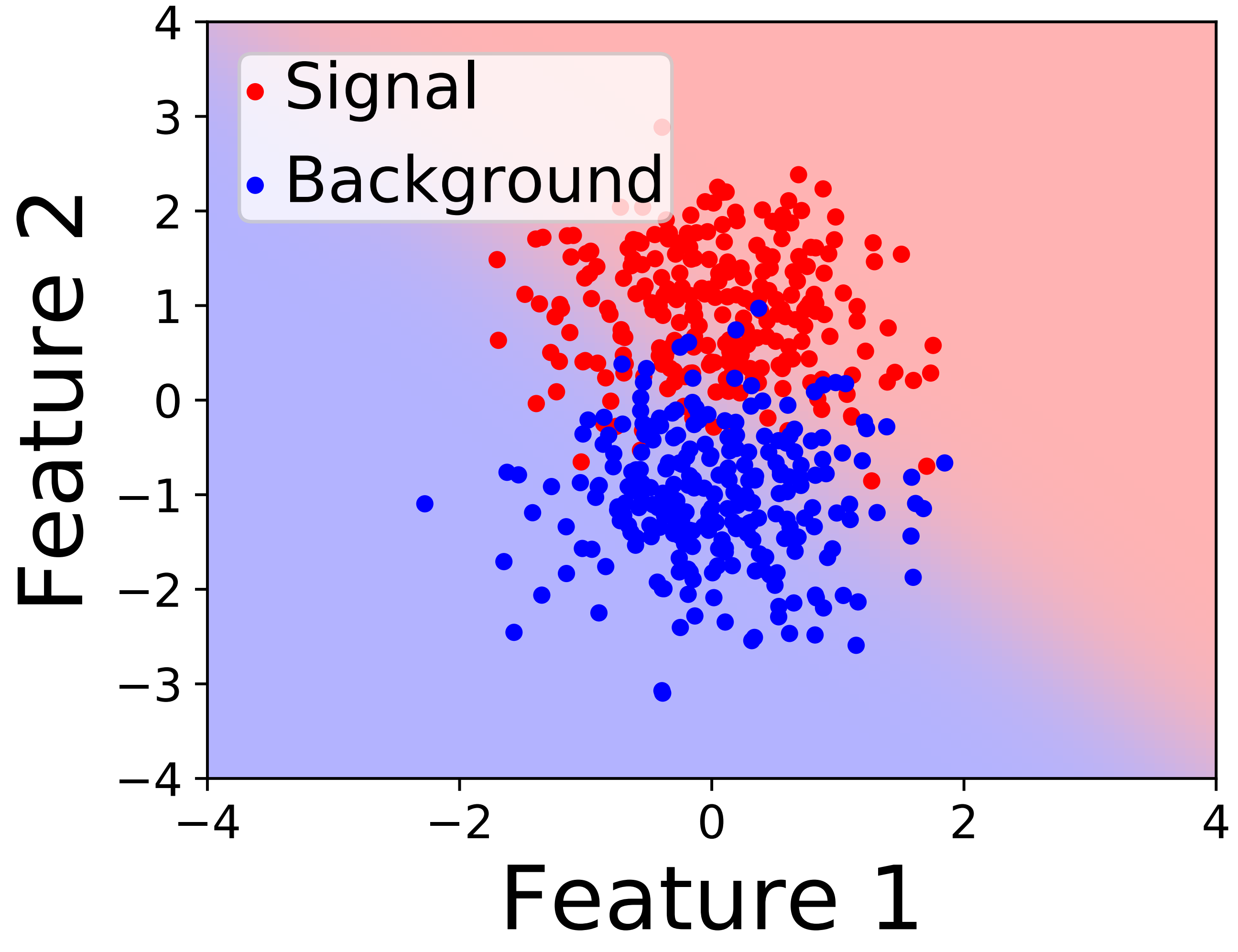
Optimal

SystUp "Data"

PRD.104.056026: Aishik Ghosh, Benjamin Nachman, and Daniel Whiteson

Nominal and Systematic Up Examples

	Baseline Classifier		Uncertainty-Aware Classifier	
Nominal "Data"		AUC=0.978 Optimal		AUC=0.978 Optimal
SystUp "Data"		AUC=0.924 **Sub-Optimal**		

Nominal and Systematic Up Examples

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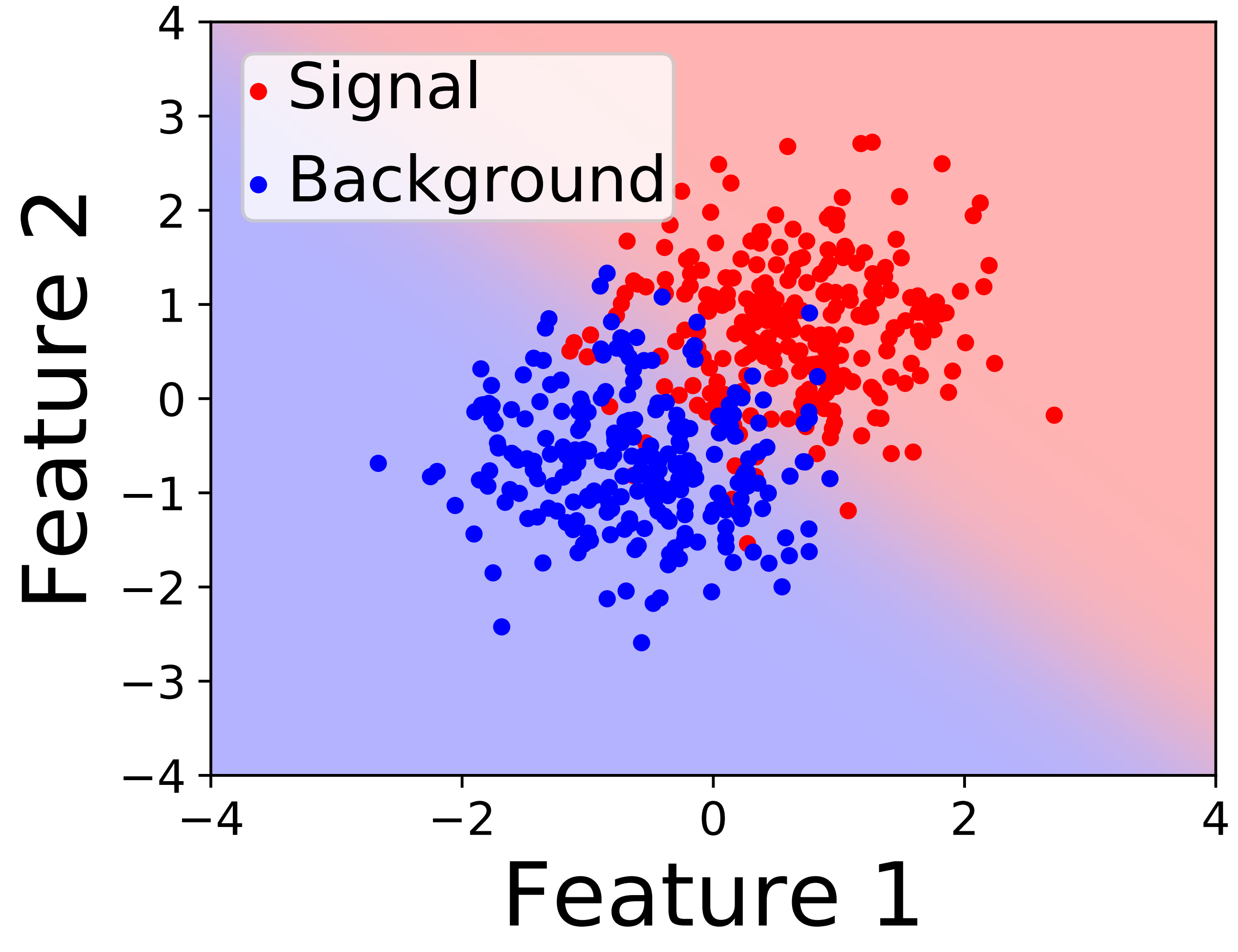
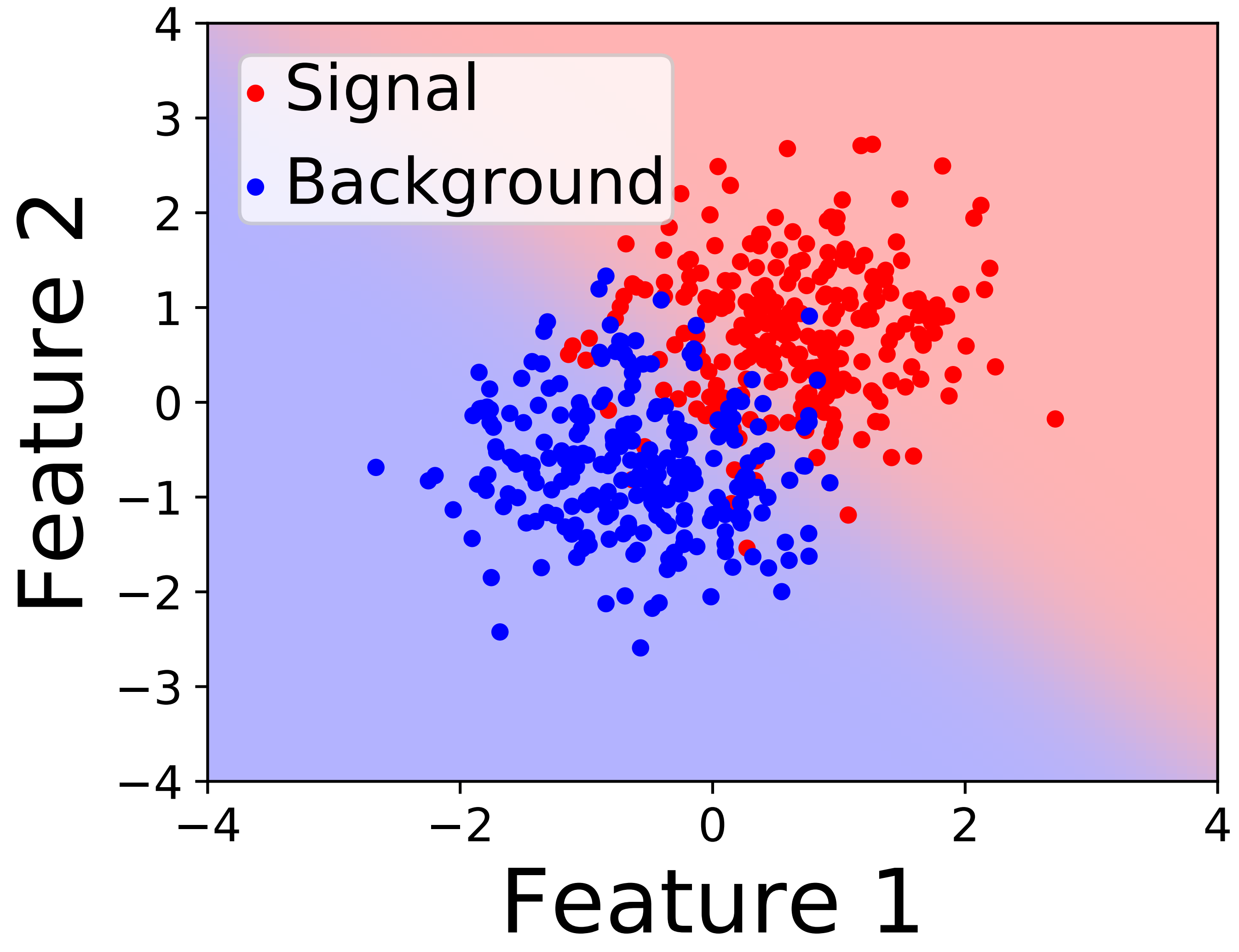
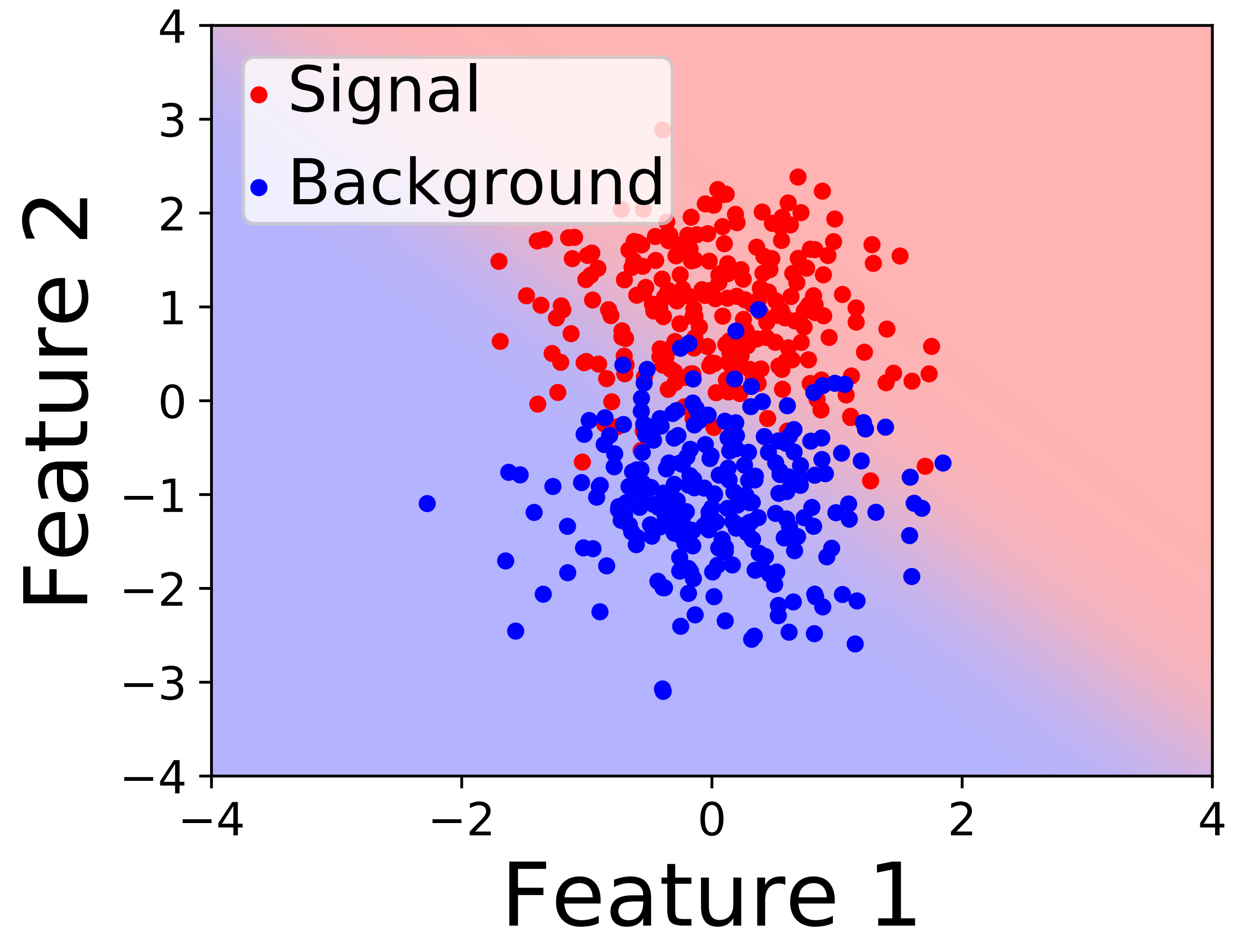
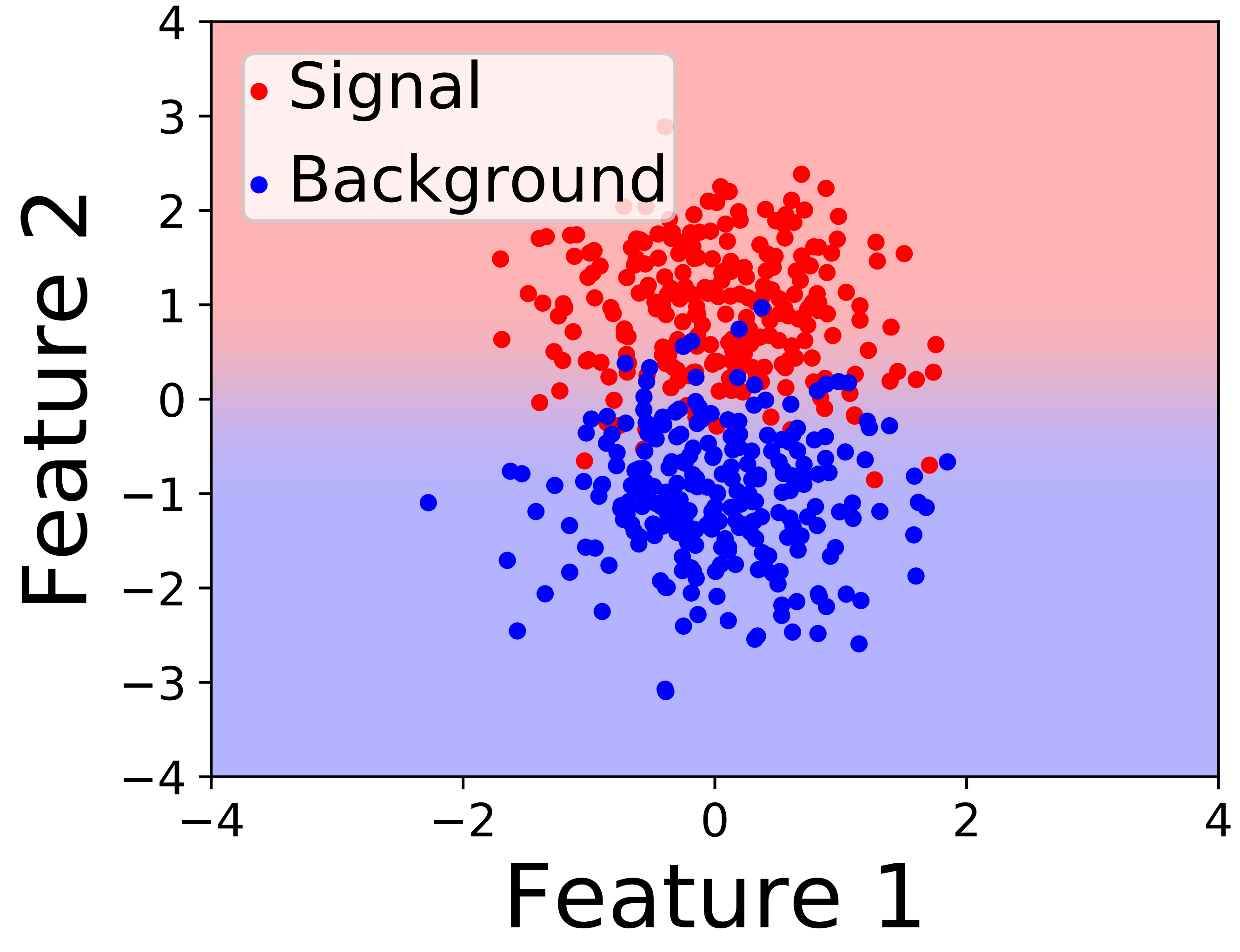
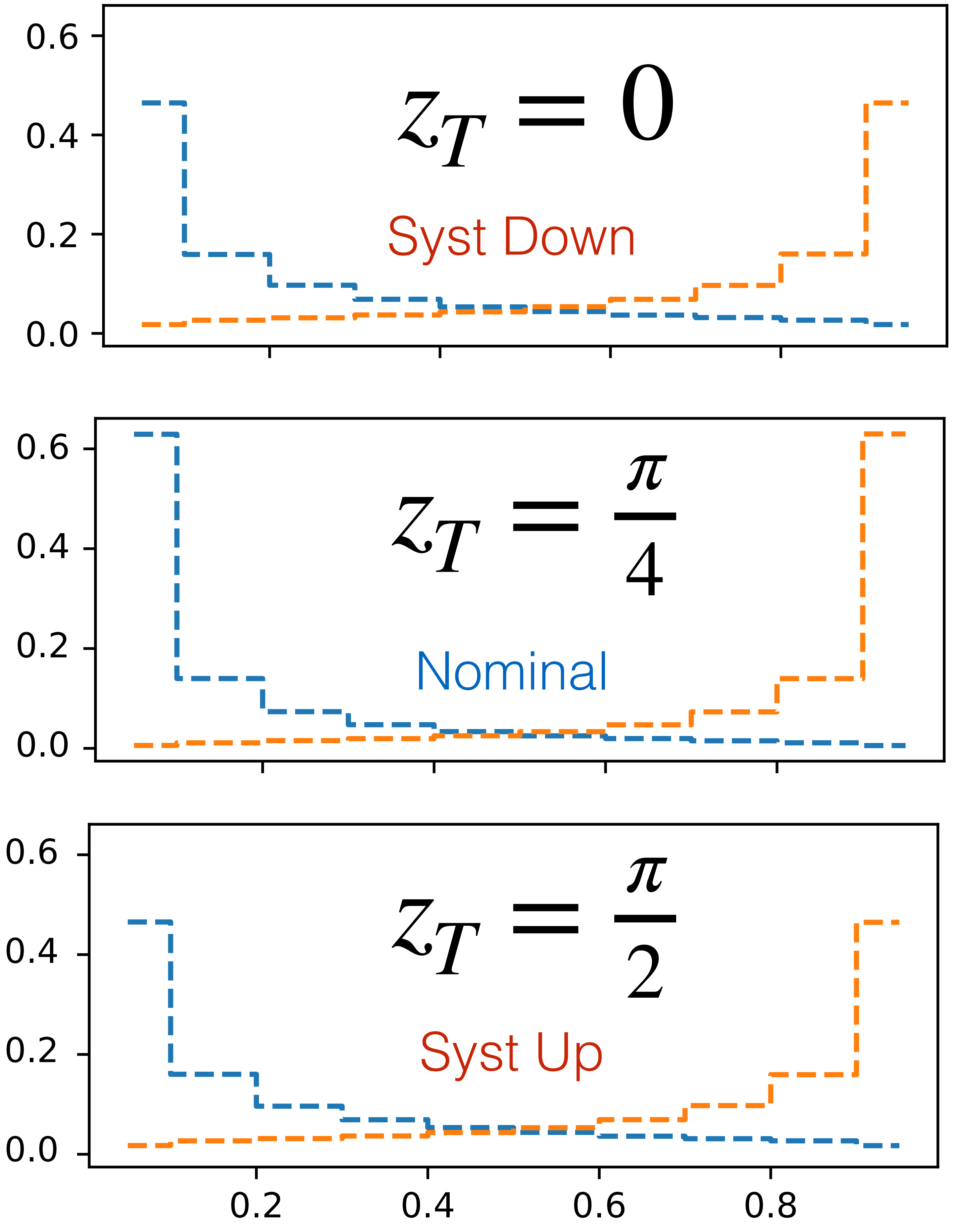
Nominal “Data”		AUC=0.978 Optimal		AUC=0.978 Optimal
SystUp “Data”		AUC=0.924 **Sub-Optimal**		AUC=0.978 **Optimal**

Syst-Aware Classifier is able to rotate its decision function based on Z while the Baseline Classifier decision function remains frozen

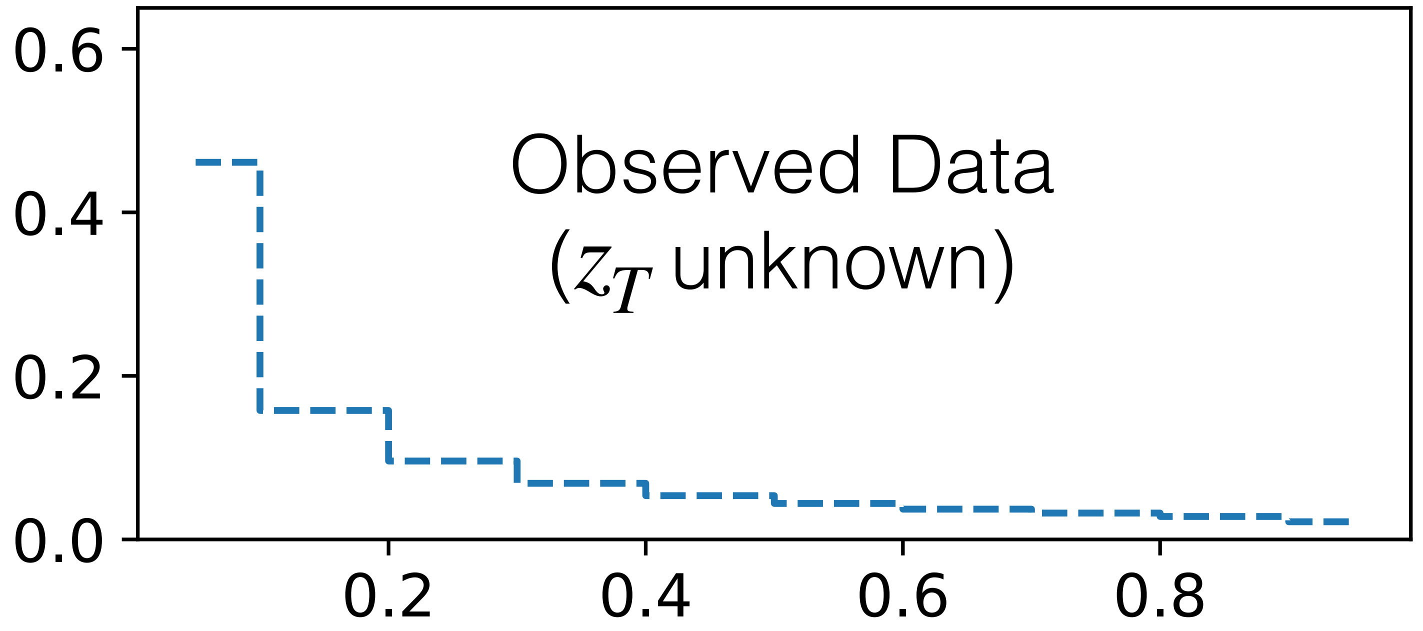
We don’t know Z in collision data, what value do we use ?

Scan the 2D Likelihood space in Z vs μ

Template **Baseline Classifier** Score Histograms for various Z



$z_T \rightarrow$ True z



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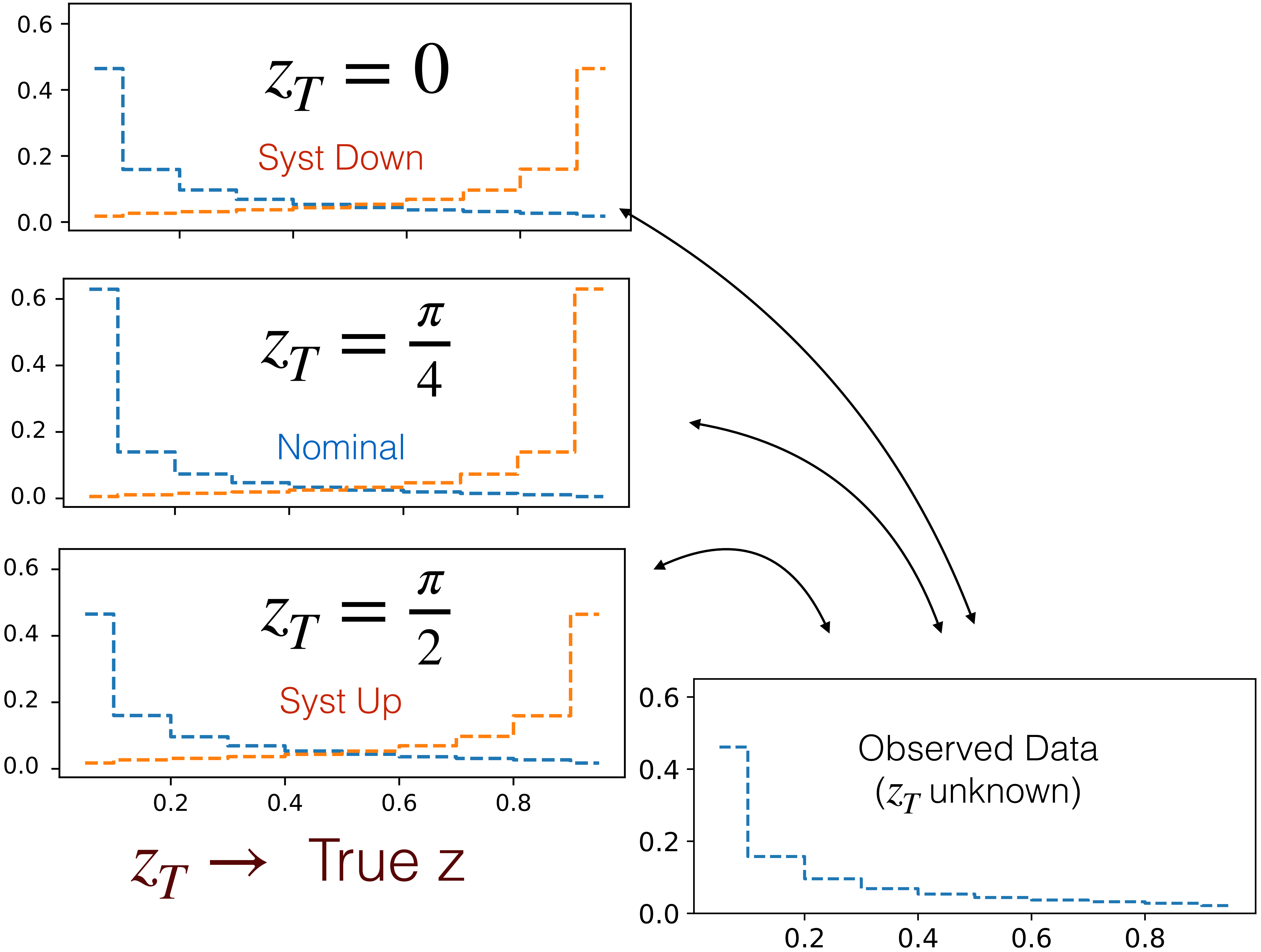

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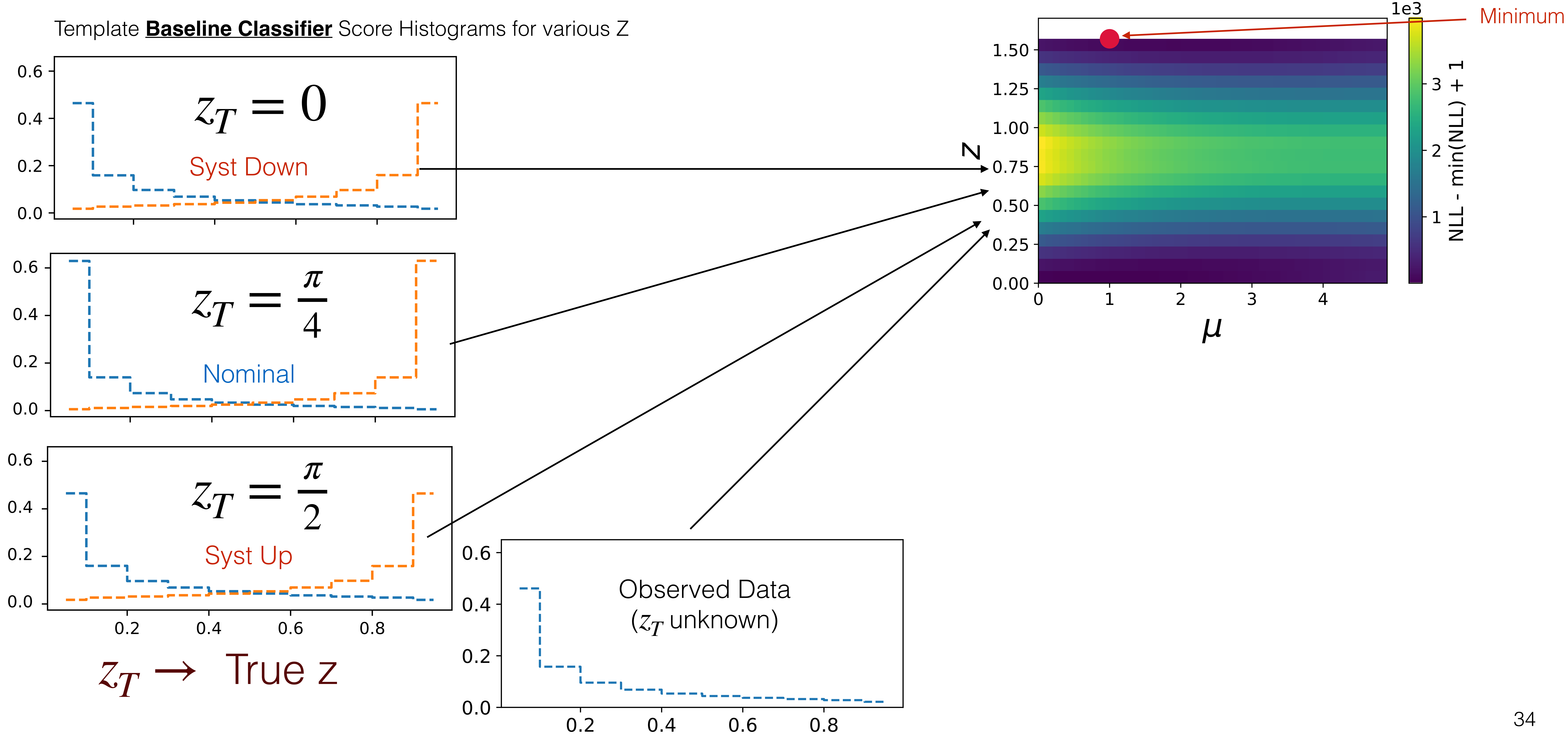

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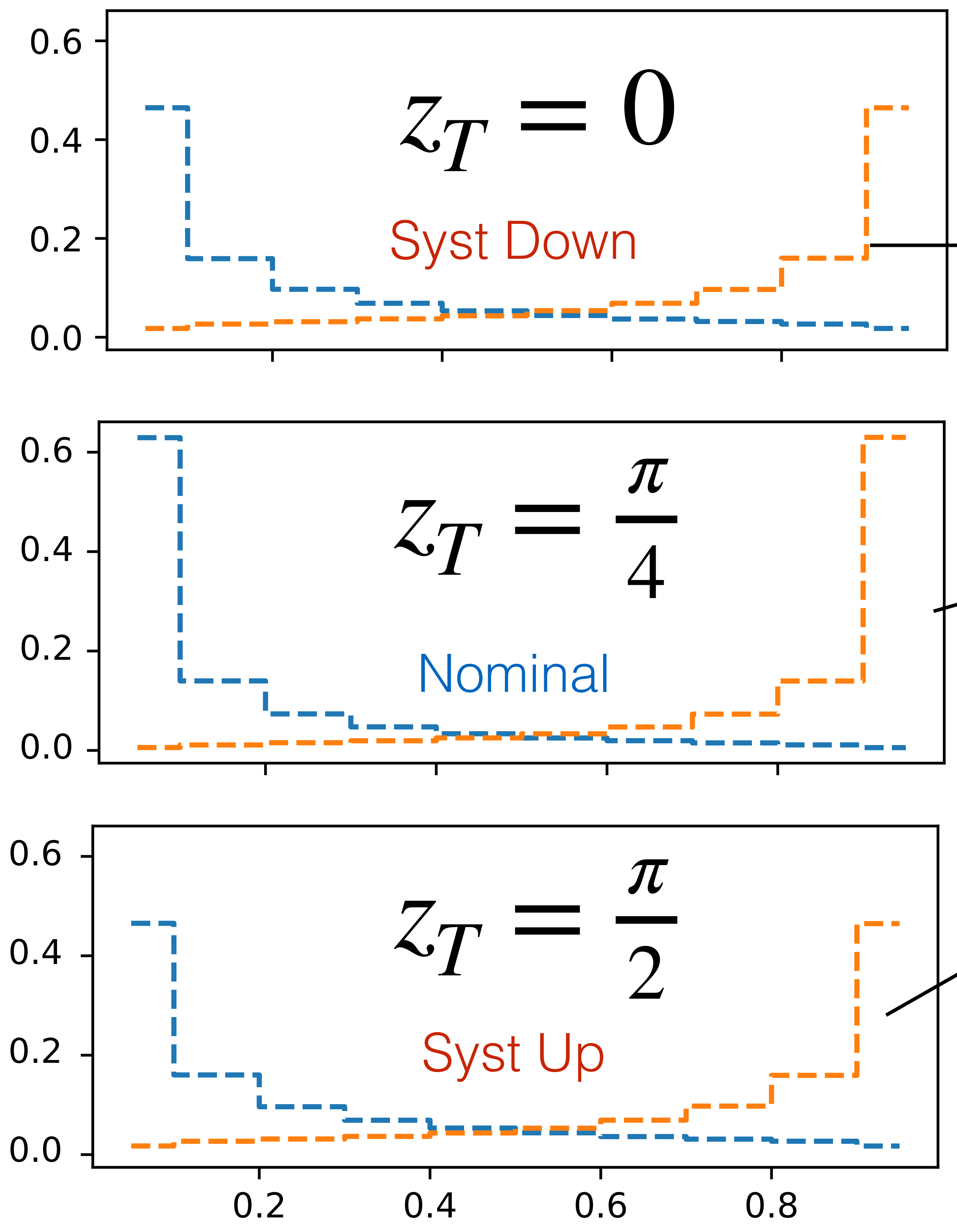
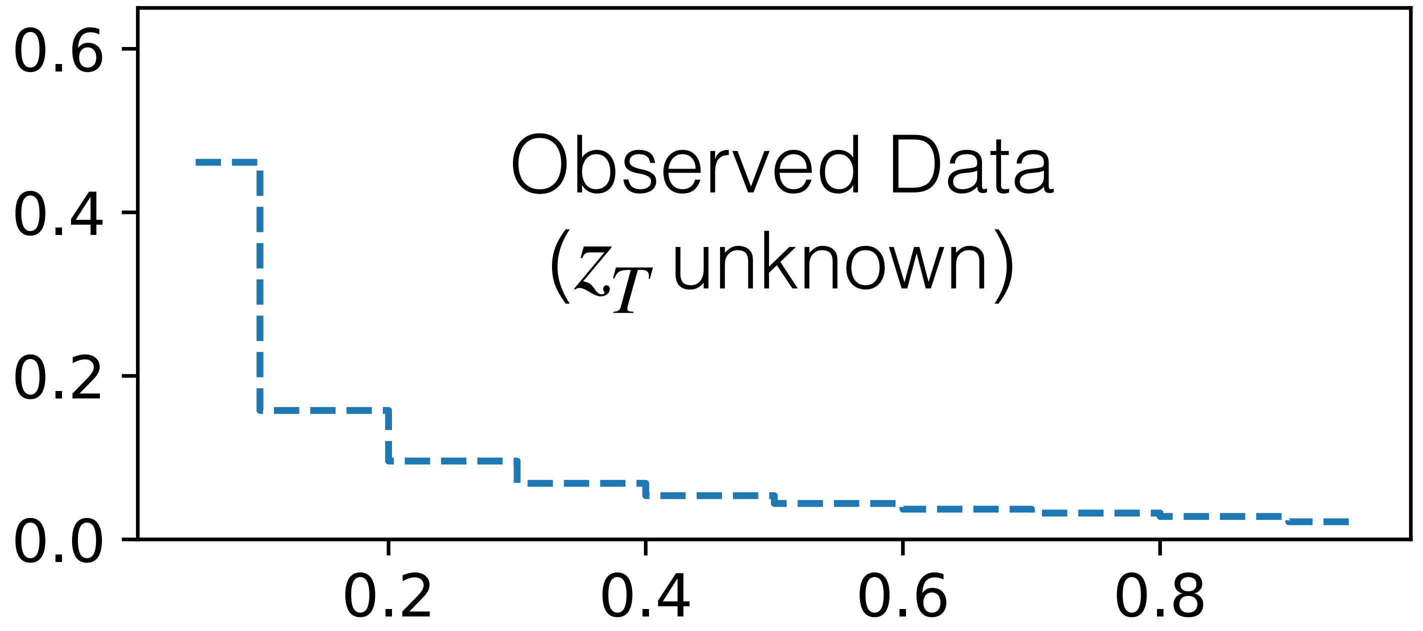
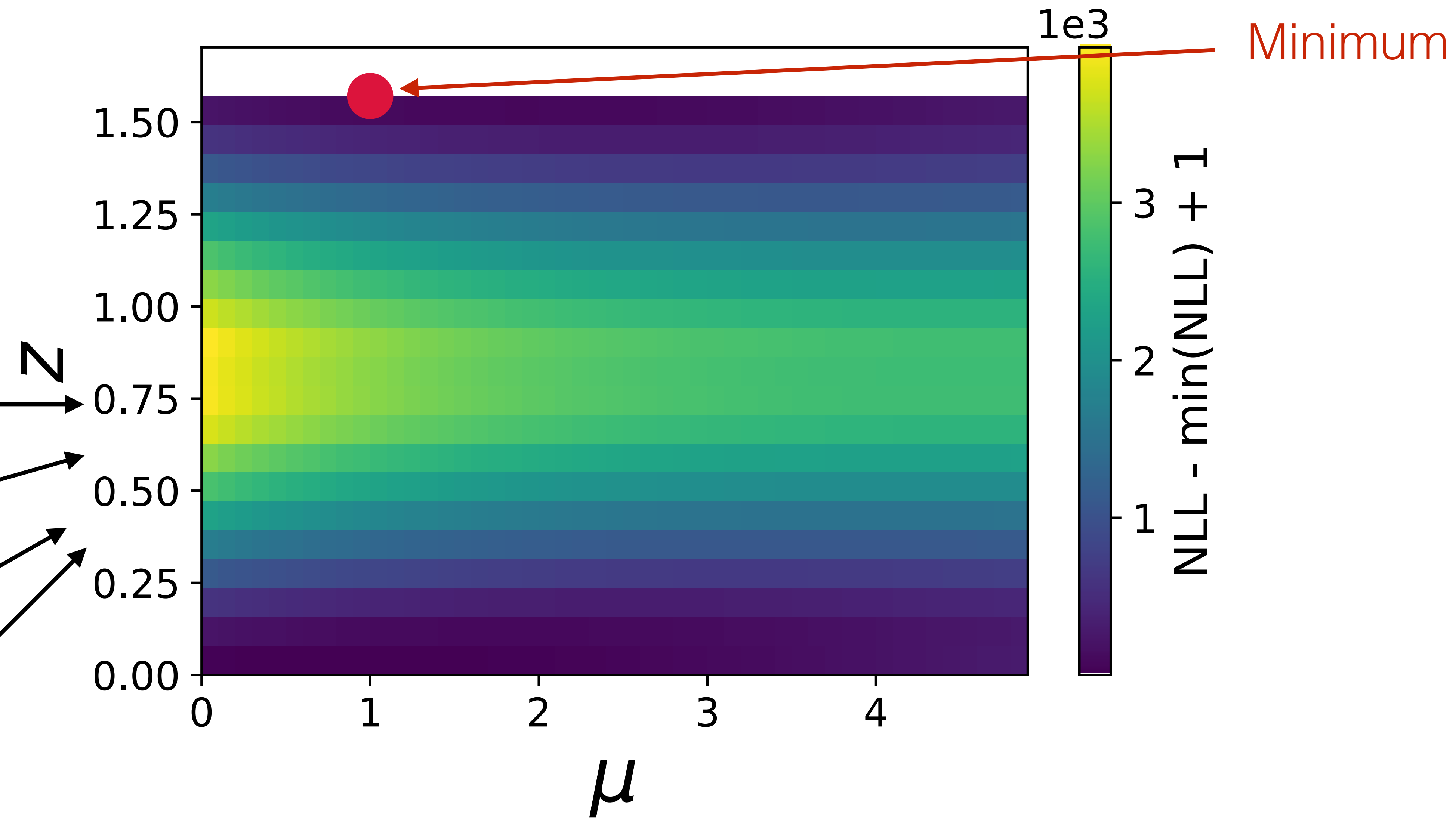


$z_T \rightarrow$ True z

But could be done unbinned/KDE too





Likelihood statistical component = Poisson per histogram bin
Likelihood systematic component = Gaussian (1, 0.5) as prior on Z
Full Likelihood = statistical + systematic

$$-\log \mathcal{L}(\mu, z|\{x_i\})$$
$$= -\sum_{j=1}^{n_{\mathrm{bins}}} \left[N_j \cdot \log\left(\mu s_j + b_j\right) - \mu s_j - b_j - \log(\Gamma(N_i)) \right]$$
$$+ \left(\frac{z - z_0}{\sqrt{2}\sigma_z} \right)^2 ,$$

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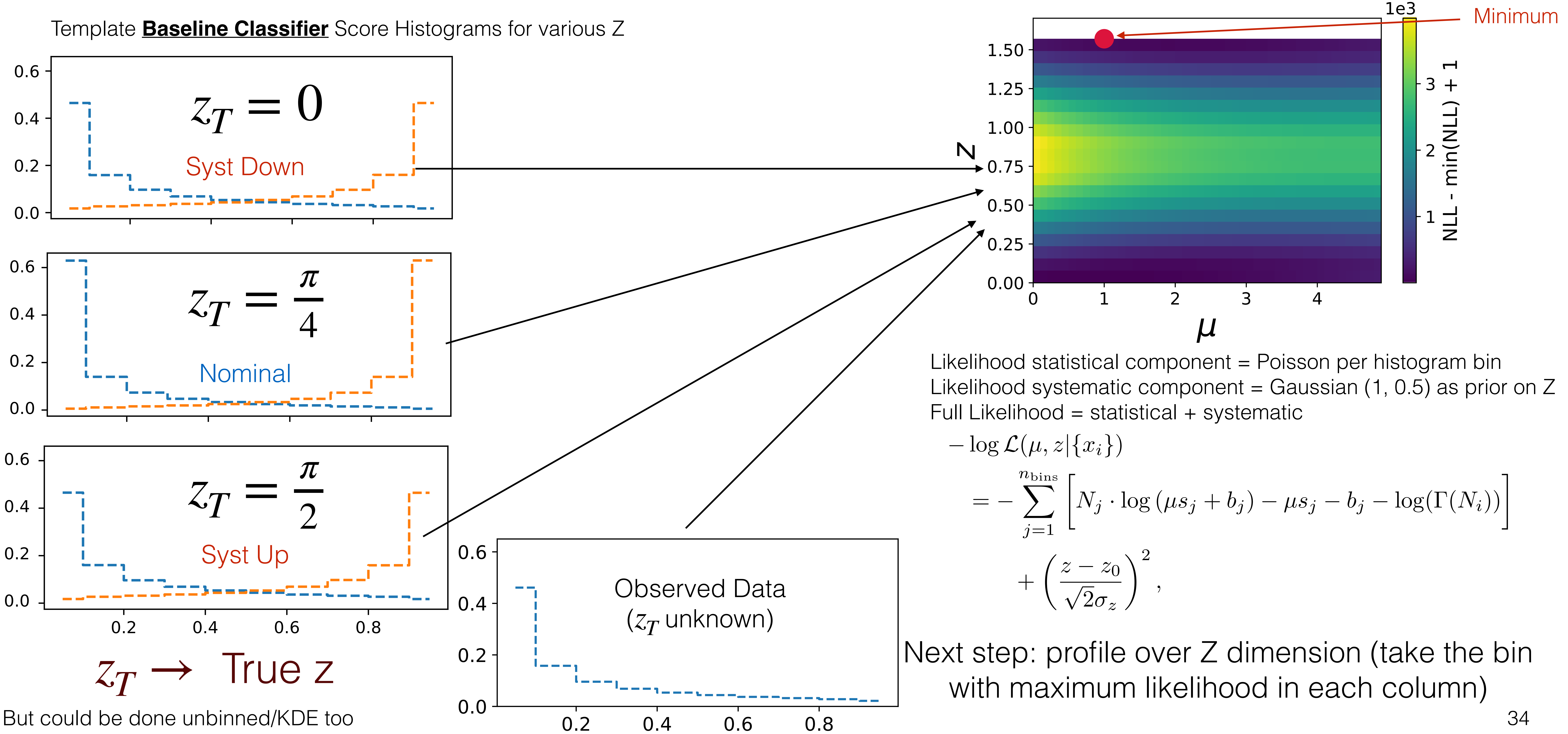

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Likelihood statistical component = Poisson per histogram bin
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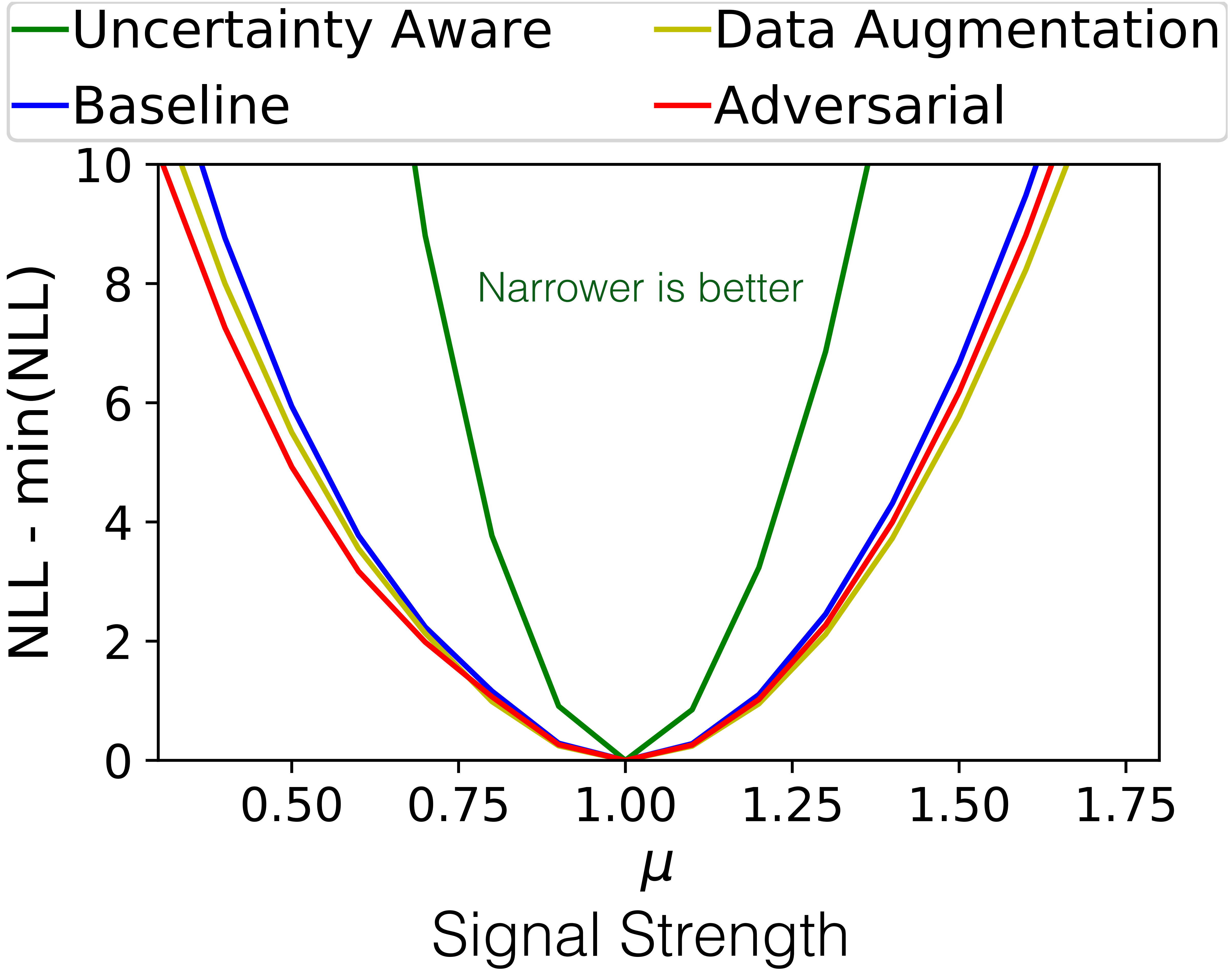
$$-\log \mathcal{L}(\mu, z|\{x_i\}) = -\sum_{j=1}^{n_{\text{bins}}} \left[N_j \cdot \log(\mu s_j + b_j) - \mu s_j - b_j - \log(\Gamma(N_i)) \right] + \left(\frac{z - z_0}{\sqrt{2}\sigma_z} \right)^2,$$

Next step: profile over Z dimension (take the bin with maximum likelihood in each column)

Better final measurements!

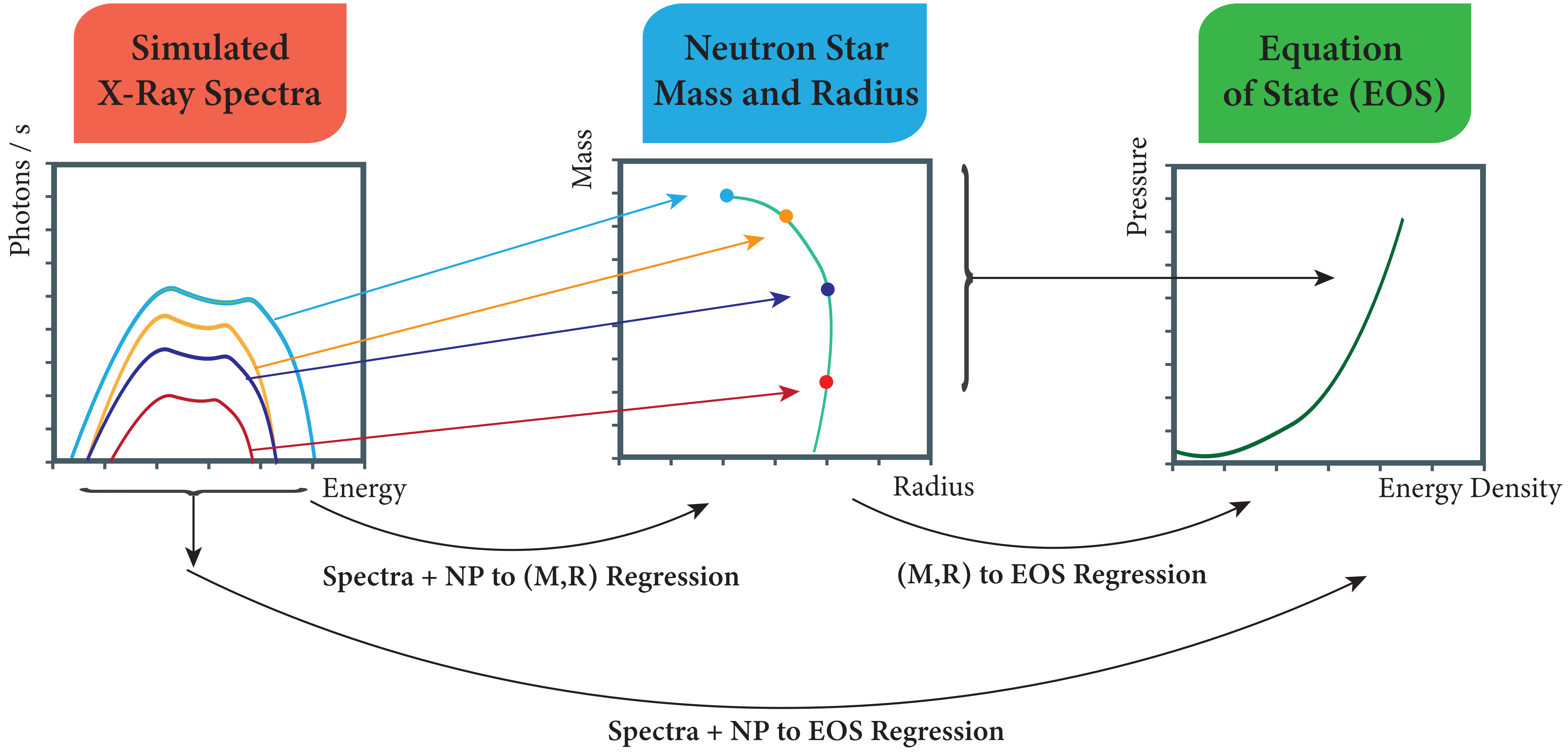


Narrower ⇒ Smaller [statistical + systematic] uncertainty on measurement

Practical for LHC analysis: Parameterise your main nuisance parameter but no need to train on all 100 NPs

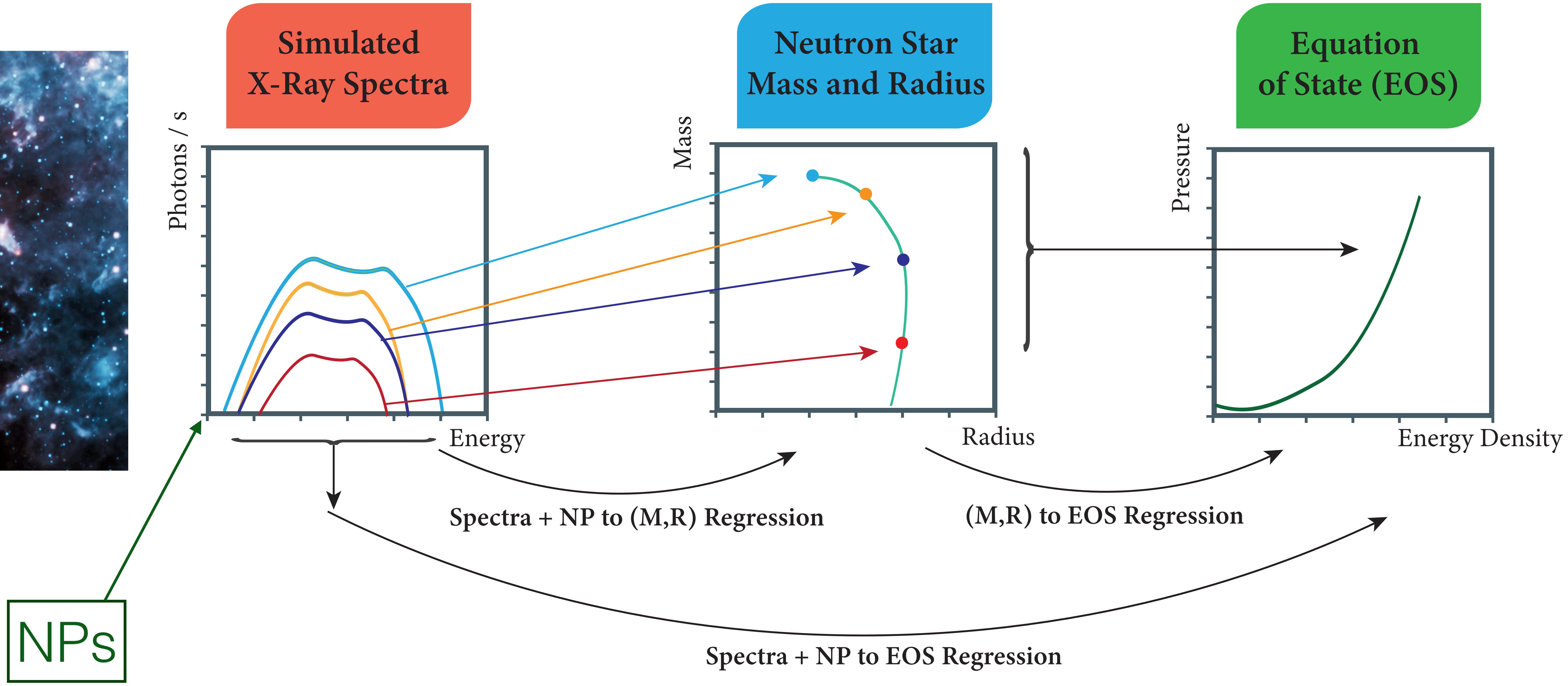
A simple idea, that we exported to astrophysics !

Application in Astrophysics: Full propagation of uncertainties



JCAP.020P.0922: Delaney Farrell, Pierre Baldi, Jordan Ott, **Aishik Ghosh**, Andrew W. Steiner, Atharva Kavitkar, Lee Lindblom, Daniel Whiteson, Fridolin Weber

Application in Astrophysics: Full propagation of uncertainties

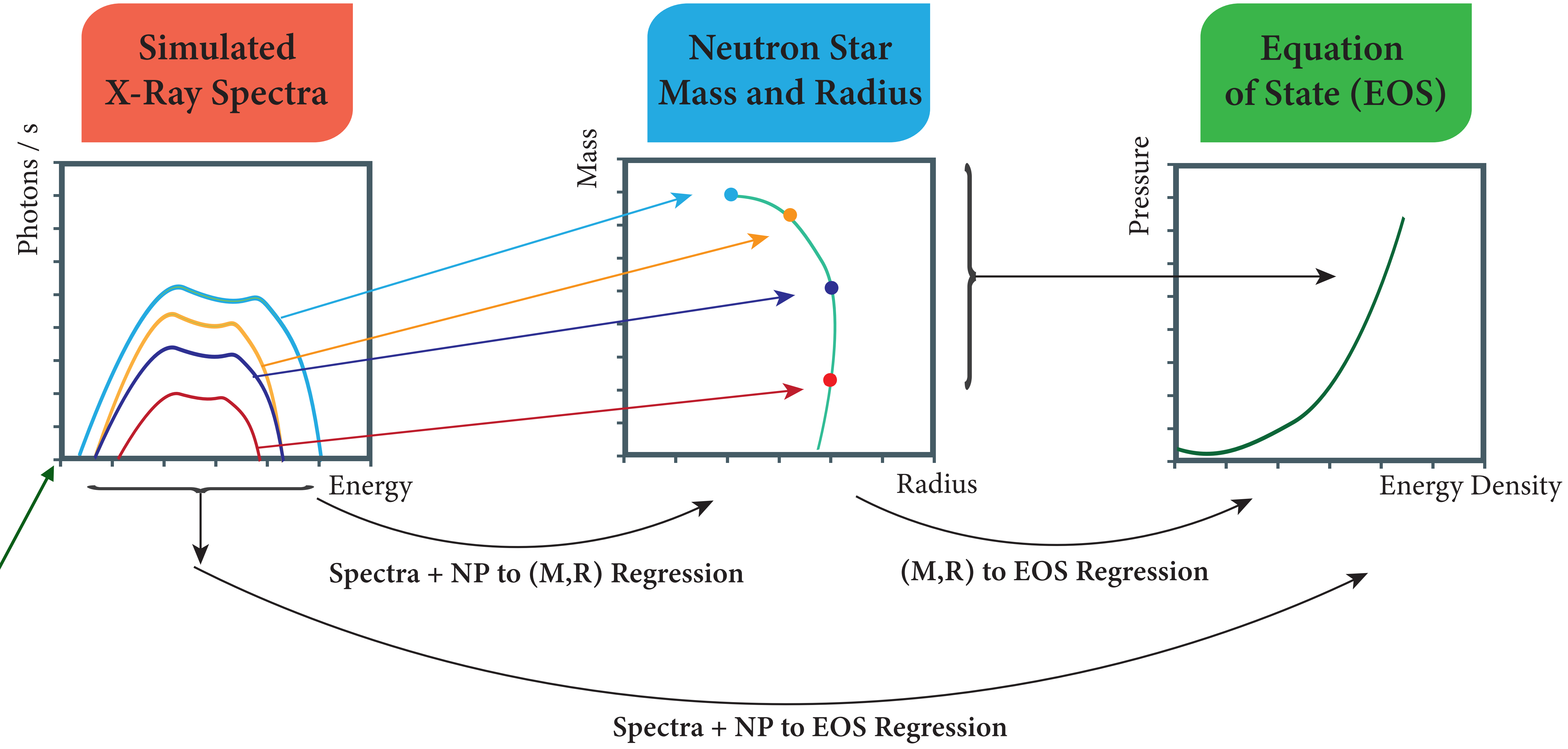


JCAP.020P.0922: Delaney Farrell, Pierre Baldi, Jordan Ott, **Aishik Ghosh**, Andrew W. Steiner, Atharva Kavitkar, Lee Lindblom, Daniel Whiteson, Fridolin Weber

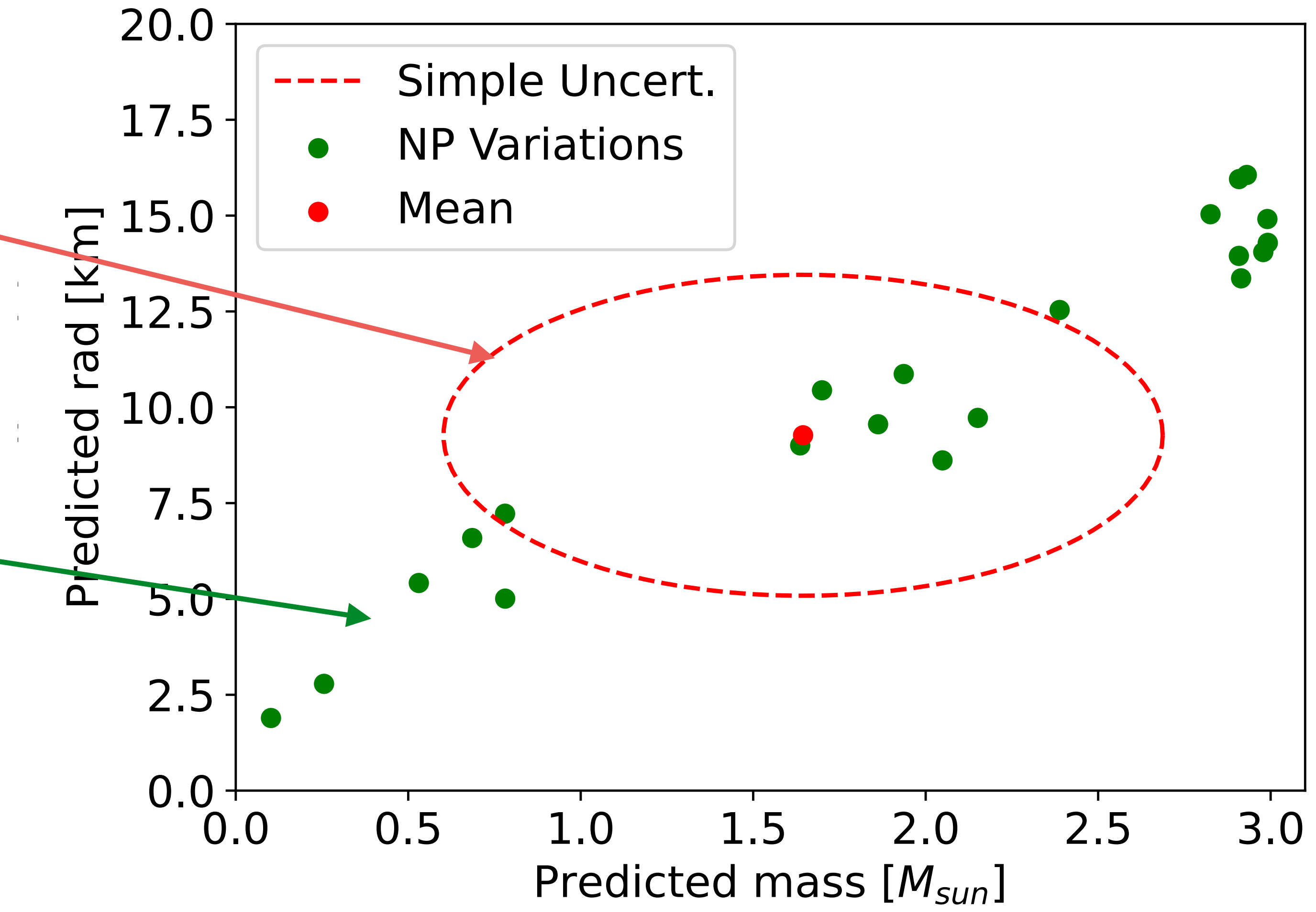
Application in Astrophysics: Full propagation of uncertainties

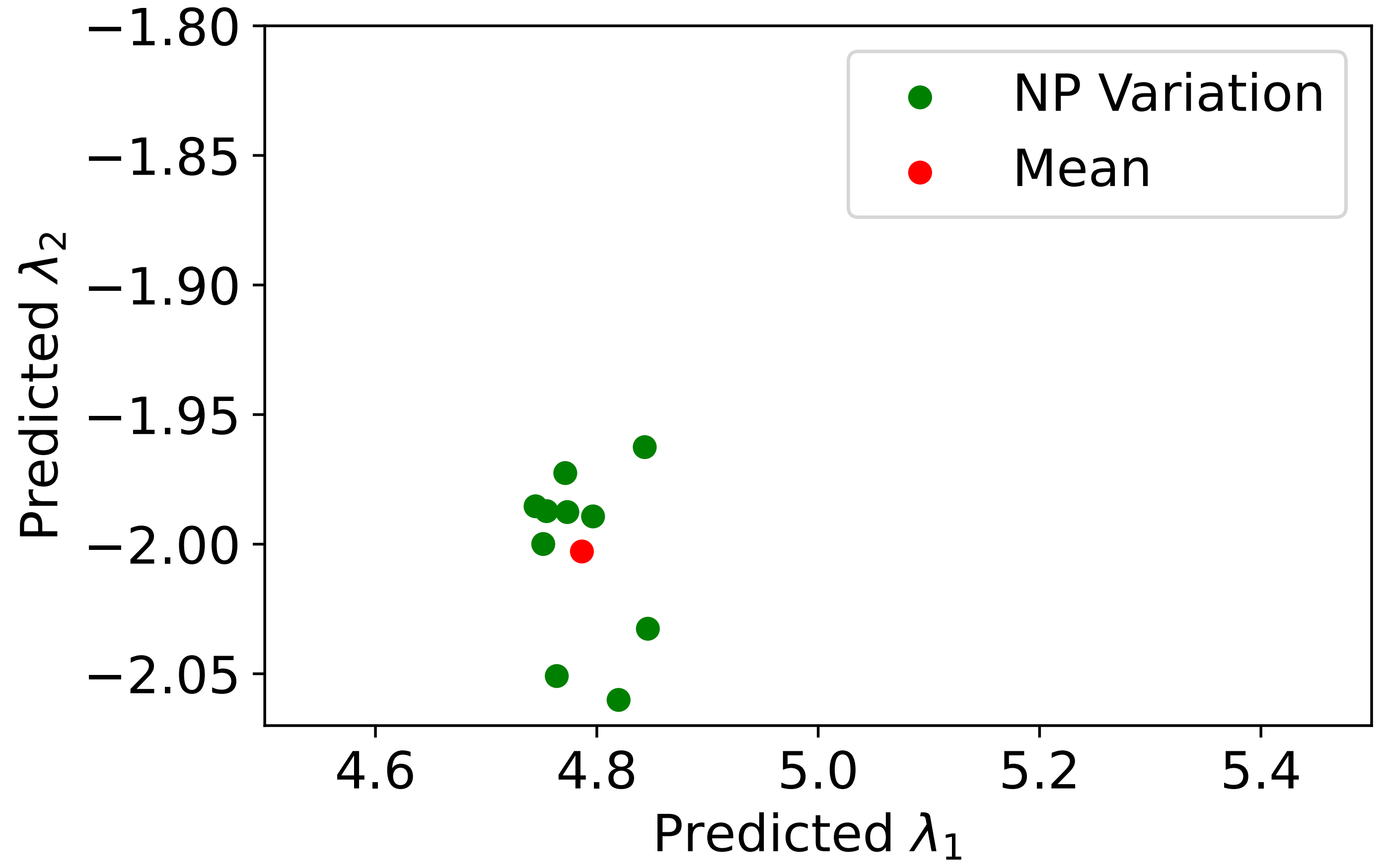
SOTA made a single point estimate + assumed uncorrelated Gaussian uncertainties

Real uncertainties look quite different



NPs





Unnamed participant at ML4FP:

"Okay all these ML solutions are cool but ...

have you tried the obvious?"

Inference-aware methods

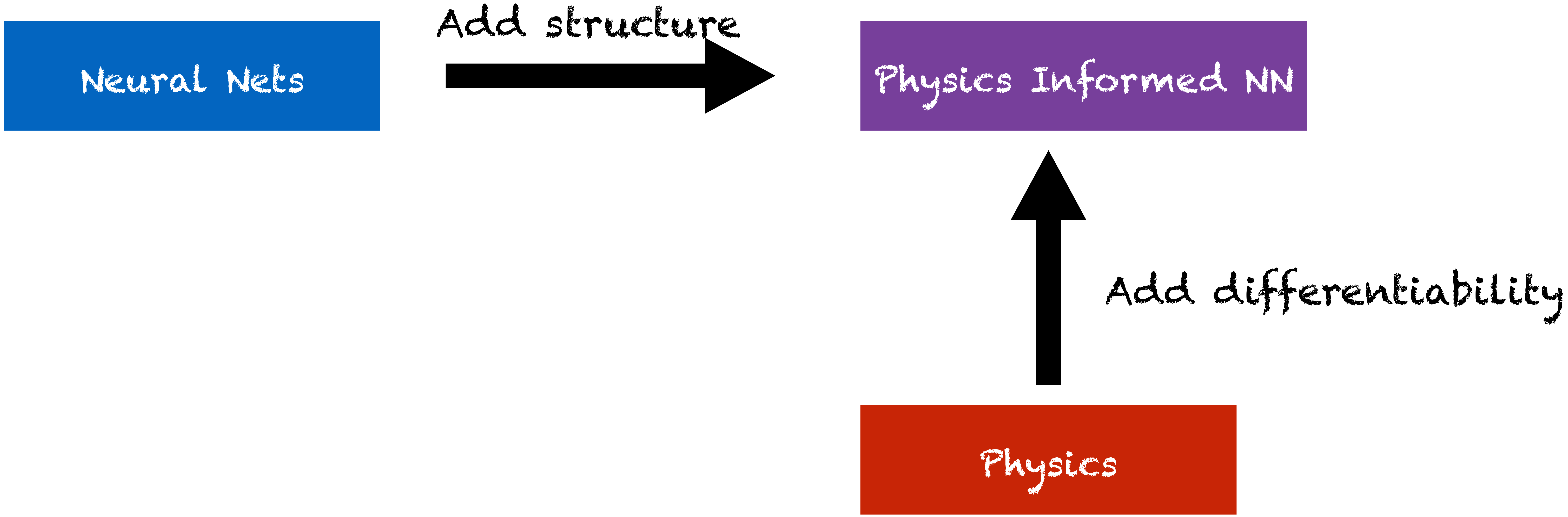


Figure inspiration: Lukas Heinrich

Inference-aware methods

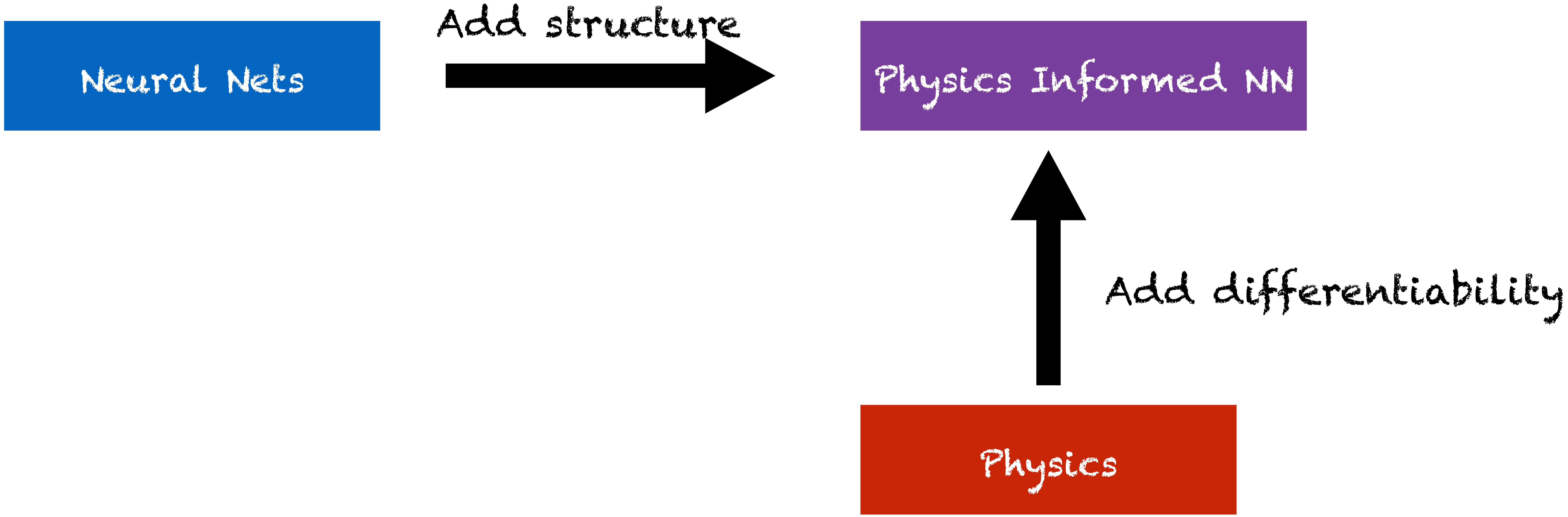


Figure inspiration: Lukas Heinrich

See more in ‘Differentiable Programming’ talk later today by Sean Gasiorowski

Inference-aware methods

[Simpson et al.](#) Following Inferno [[de Castro et al.](#)]

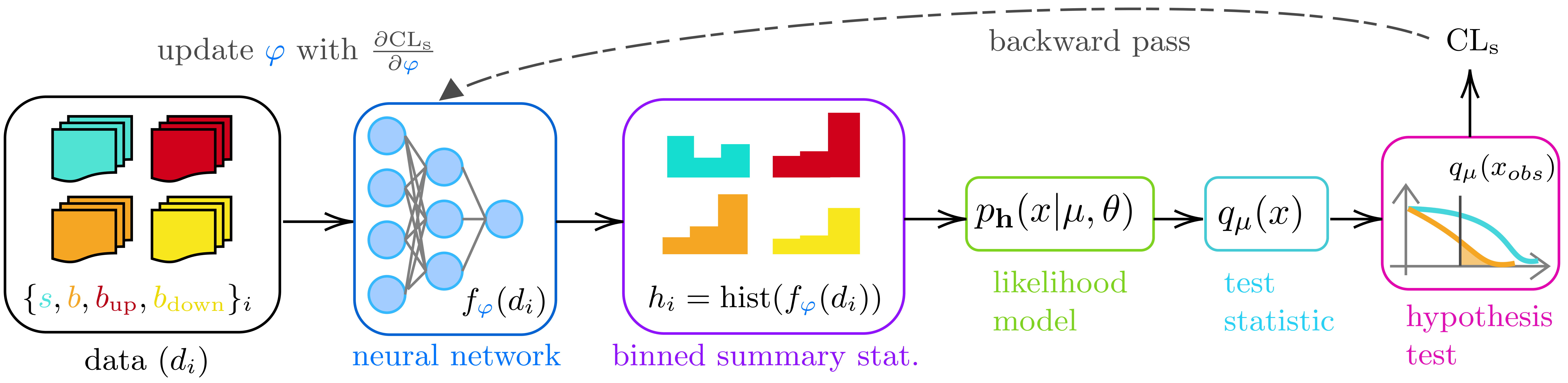


Figure 1. The pipeline for `neos`. The dashed line indicating the backward pass involves updating the weights φ of the neural network via gradient descent.

Inference-aware methods

[Simpson et al.](#)

Following Inferno [[de Castro et al.](#)]

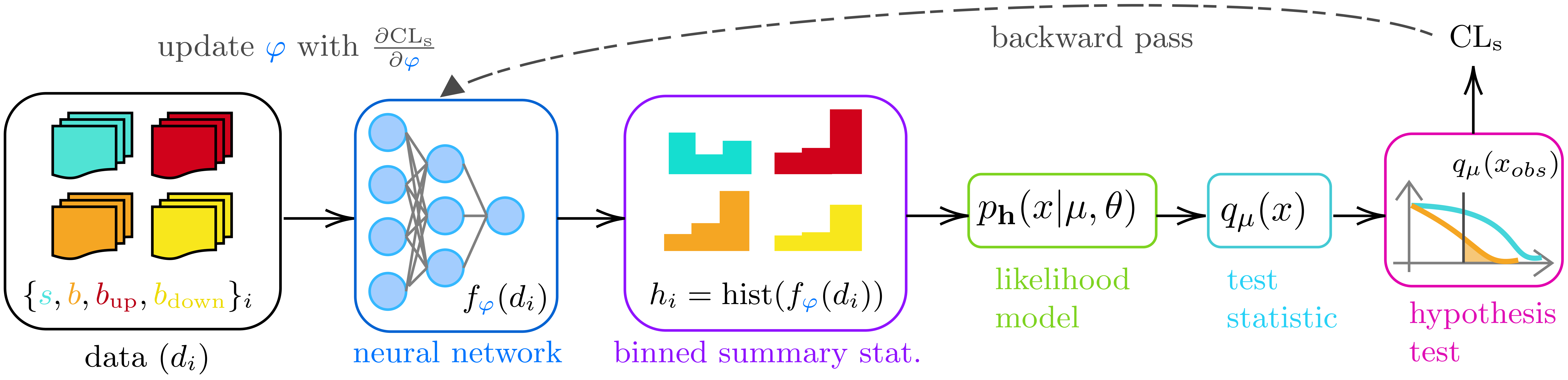
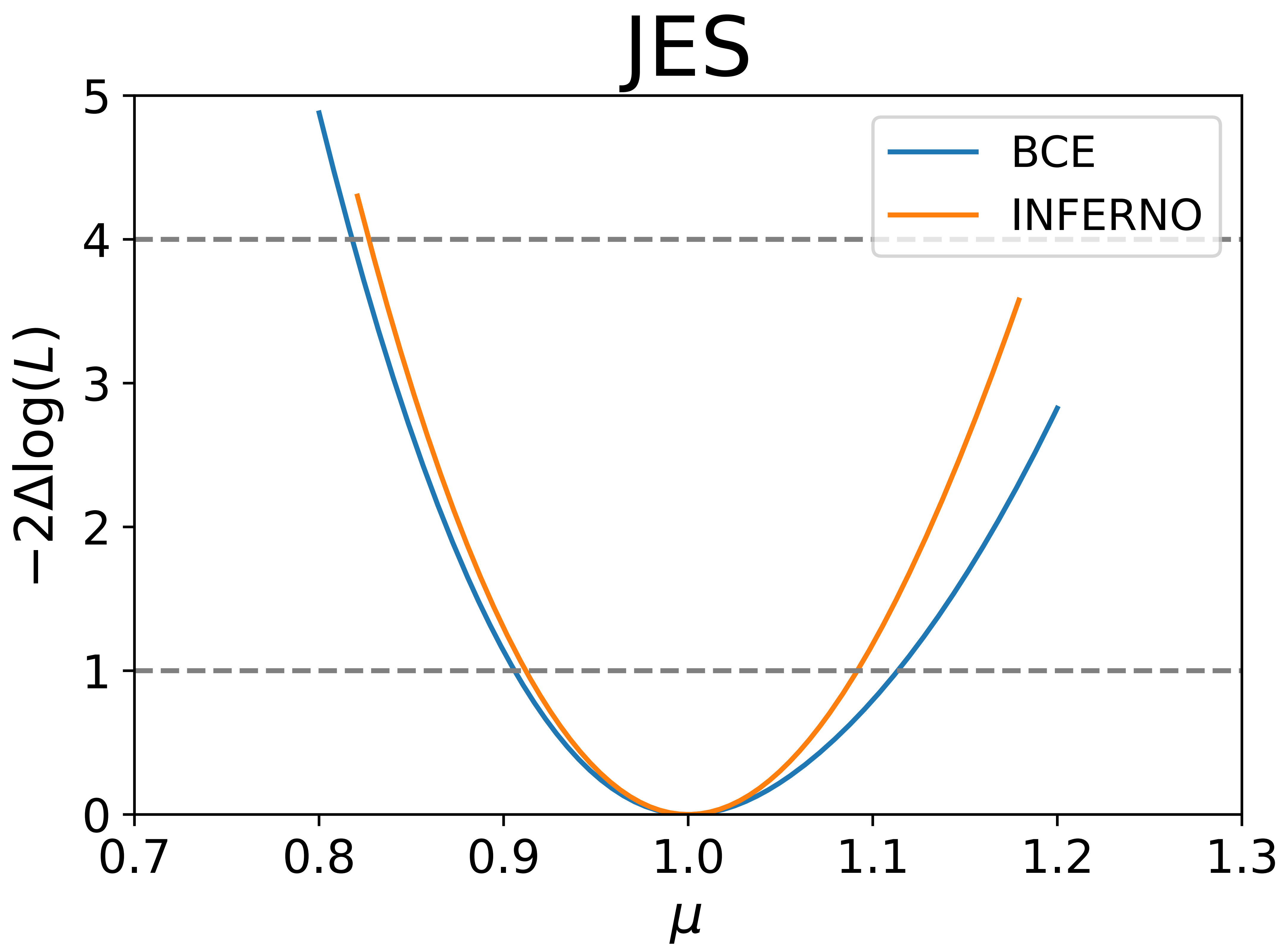


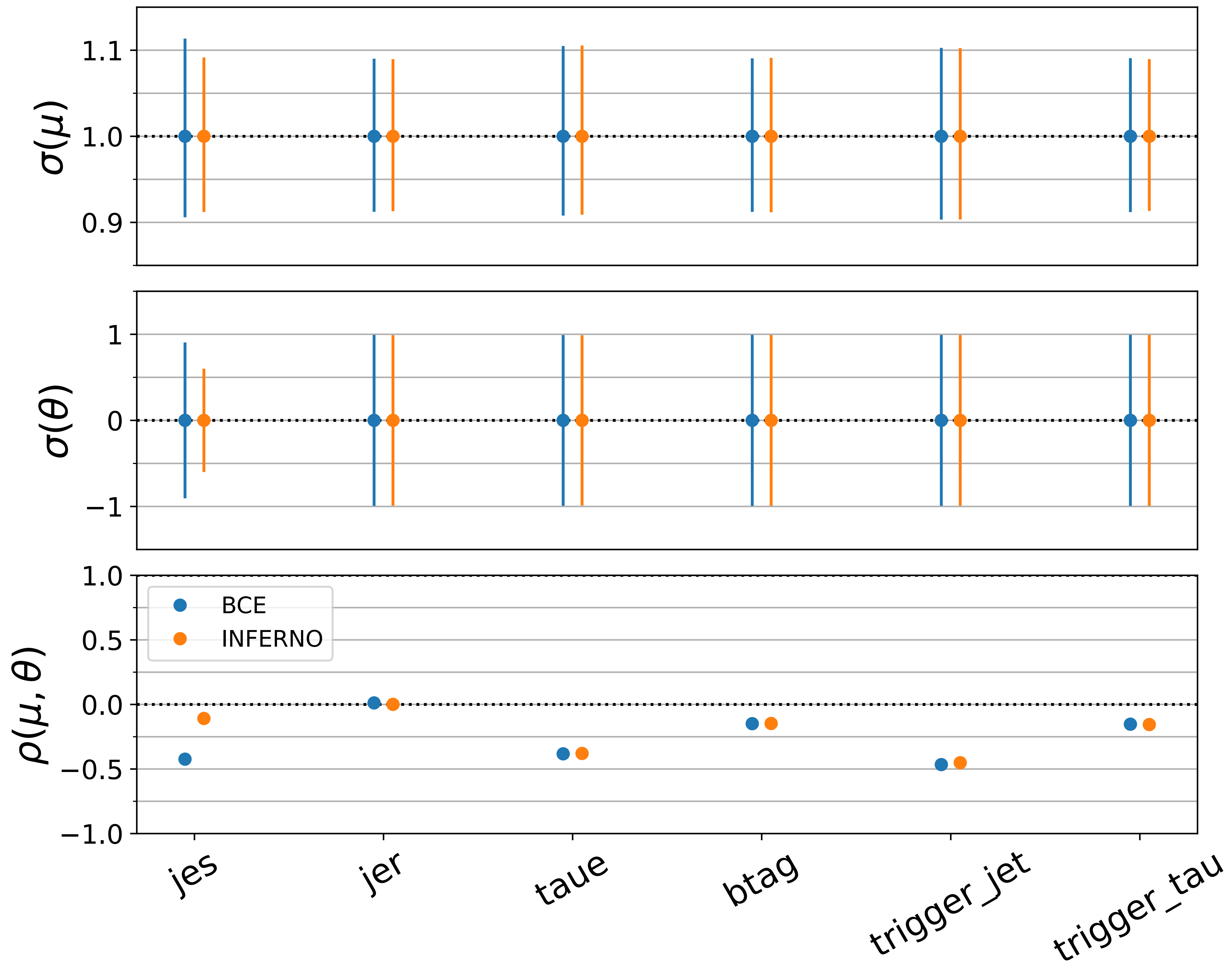
Figure 1. The pipeline for **neos**. The dashed line indicating the backward pass involves updating the weights φ of the neural network via gradient descent.

Requires 'relaxation tricks' to pass gradients through non-differentiable operations

Applied to CMS open data

arXiv:2301.10358: Layer et al





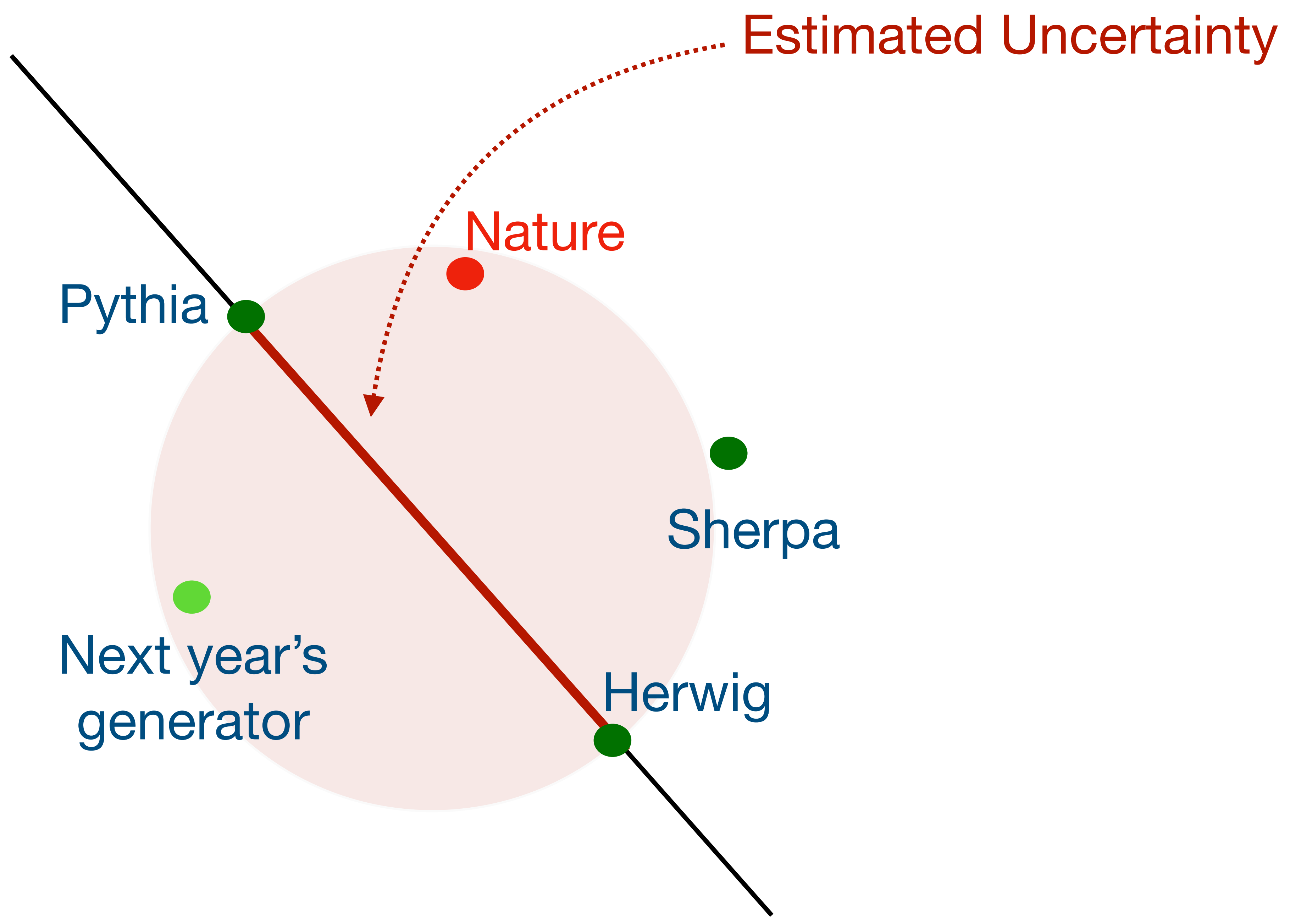
Improvement over traditional analysis in mitigating effects of systematics

But be careful about theory ‘nuisance parameters’ ..

What are theory uncertainties ?

Theory uncertainties often describe our **lack of understanding / ability to calculate**

No statistical origin for them (such as auxiliary measurement)



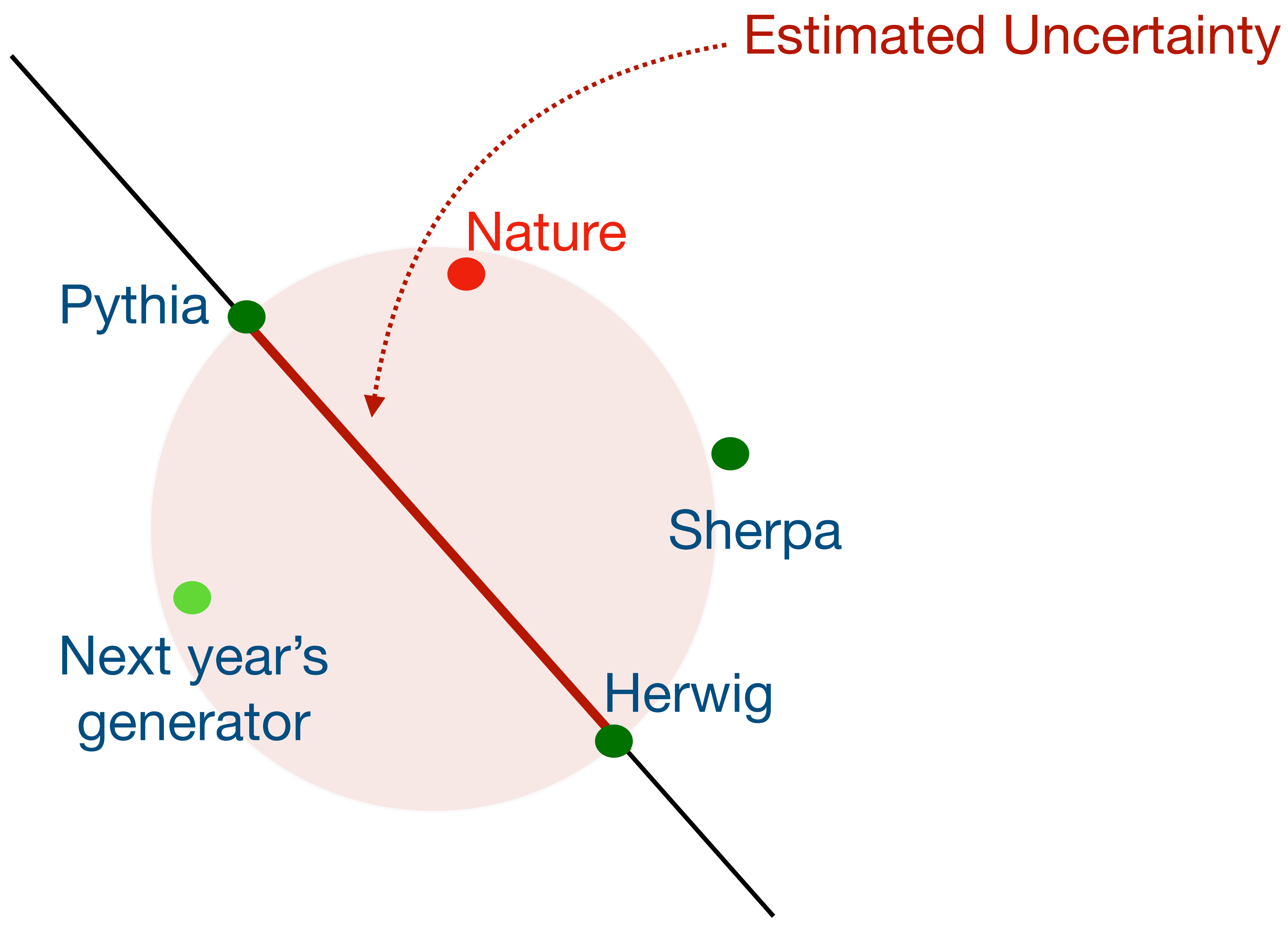
What are theory uncertainties ?

Theory uncertainties often describe our **lack of understanding / ability to calculate**

No statistical origin for them (such as auxiliary measurement)

Eg. **Hadronisation**:

- Few different packages to simulate it
- None are correct!
- Use difference in performance of your data analysis algorithm on **Pythia simulator** vs **Herwig simulator** ad-hoc estimate of uncertainty



Remember ML decorrelation ?

[Learning to Pivot, Louppe et al.](#)

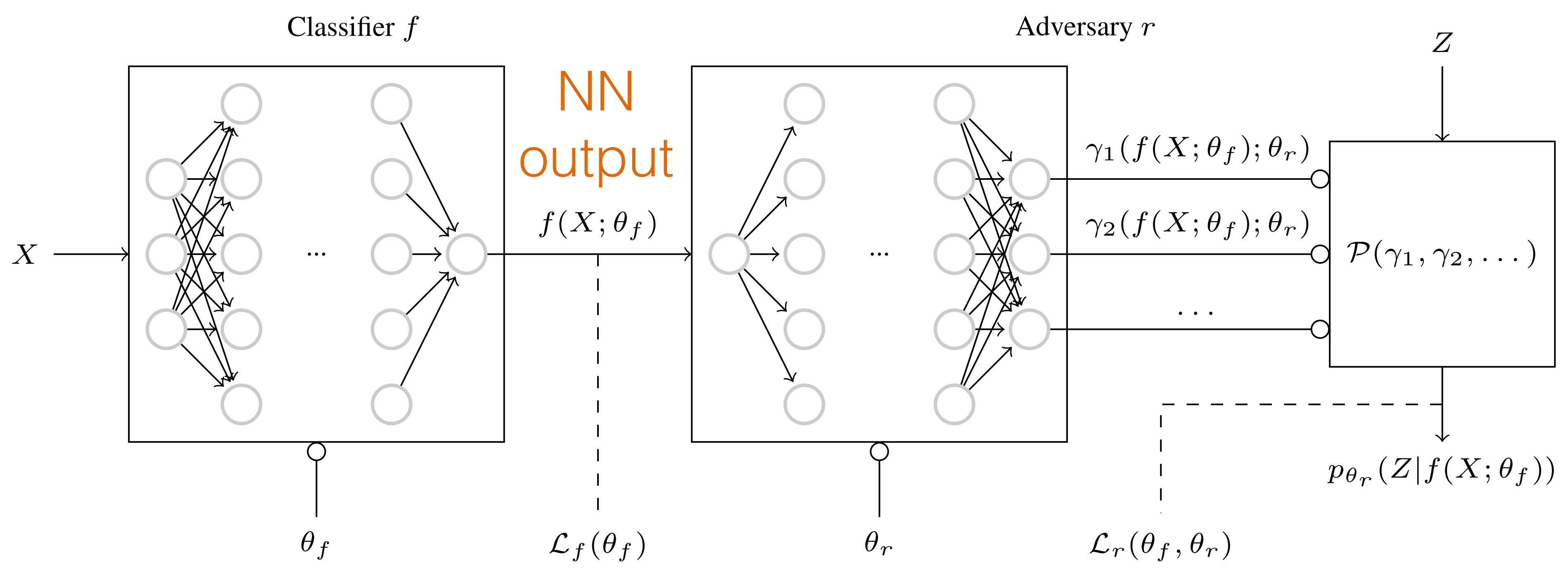
Similar ideas: Blance et al., Stevens et al., Wunsch at al., Estrade at al., Kasieczka at al.

Adversarial decorrelation

S vs B

Regress NP

NN output



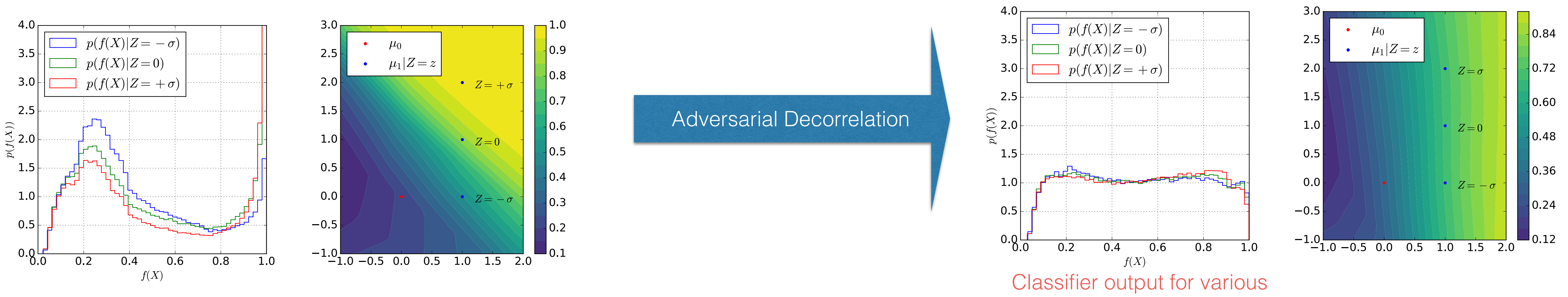
To fool the adversary, classifier output should be decorrelated to Z

[Learning to Pivot, Louppe et al.](#)

$$L_{Classifier} = L_{Classification} - \lambda \cdot L$$

Similar ideas: Blance et al., Stevens et al., Wunsch at al., Estrade at al., Kasieczka at al.

ML-Decorrelation Methods

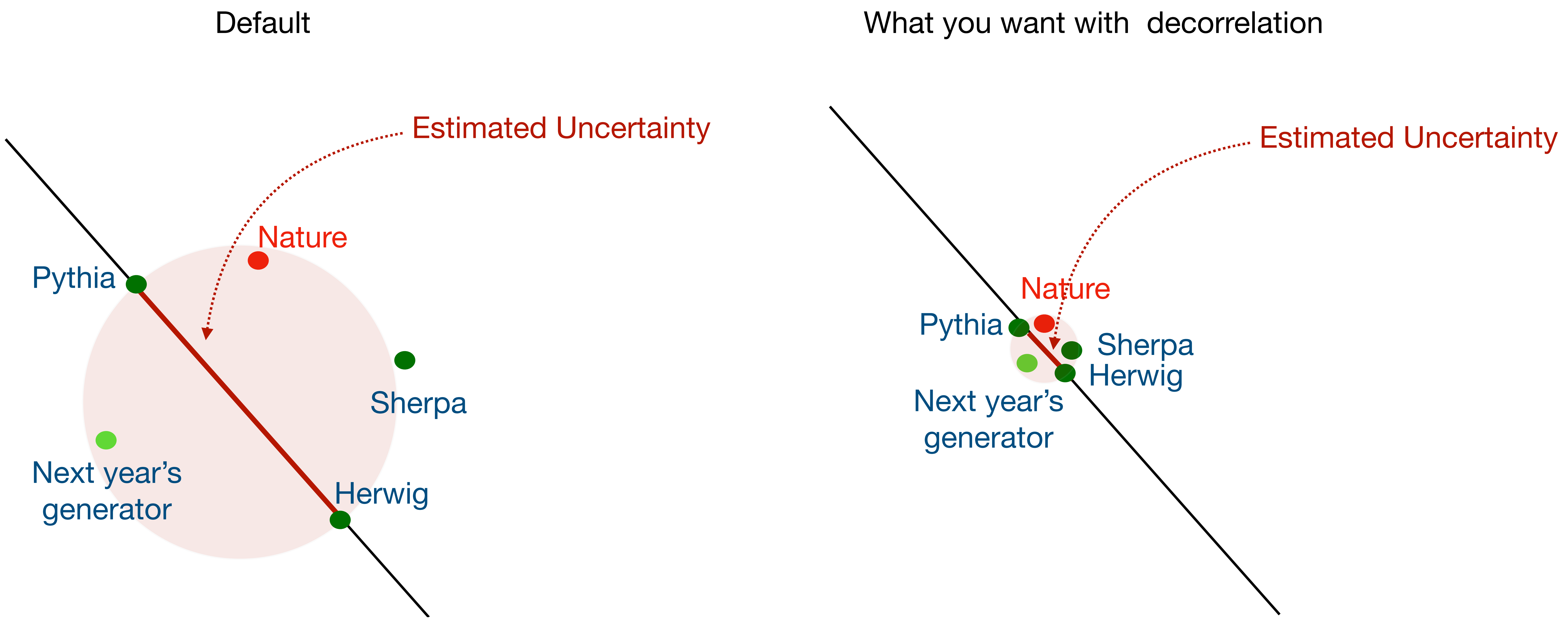


Classifier output for various values of Z

[Learning to Pivot, Louppe et al.](#)

ML-decorrelating theory uncertainties

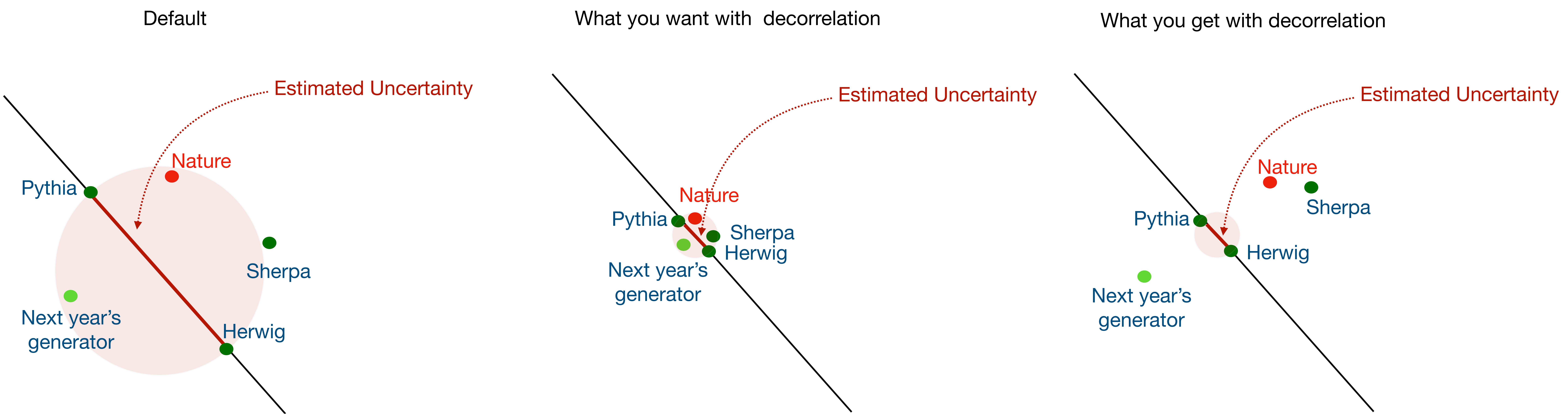
EPJC:s10052.022.10012.w: Aishik Ghosh, Benjamin Nachman



Instruction to ML: “Please shrink Pythia vs Herwig difference”

ML-decorrelating theory uncertainties

EPJC:s10052.022.10012.w: Aishik Ghosh, Benjamin Nachman



Instruction to ML: "Please shrink Pythia vs Herwig difference"

Model will learn to fool you !

ML methods don't often generalise the way you would hope

Goodhart's Law

When a measure becomes a target, it ceases to be a good measure

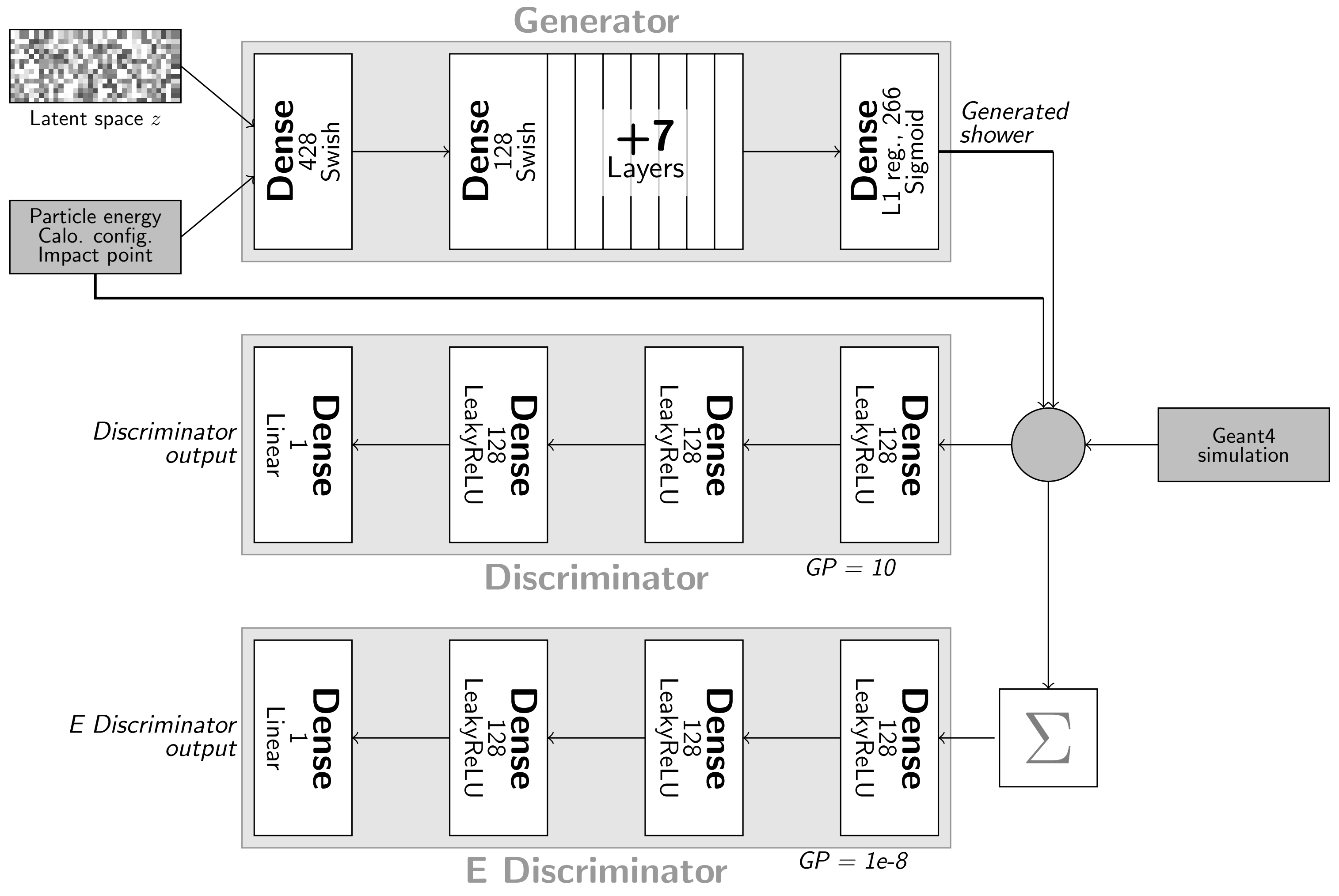
=> Dangerous to optimise proxy metrics of uncertainty

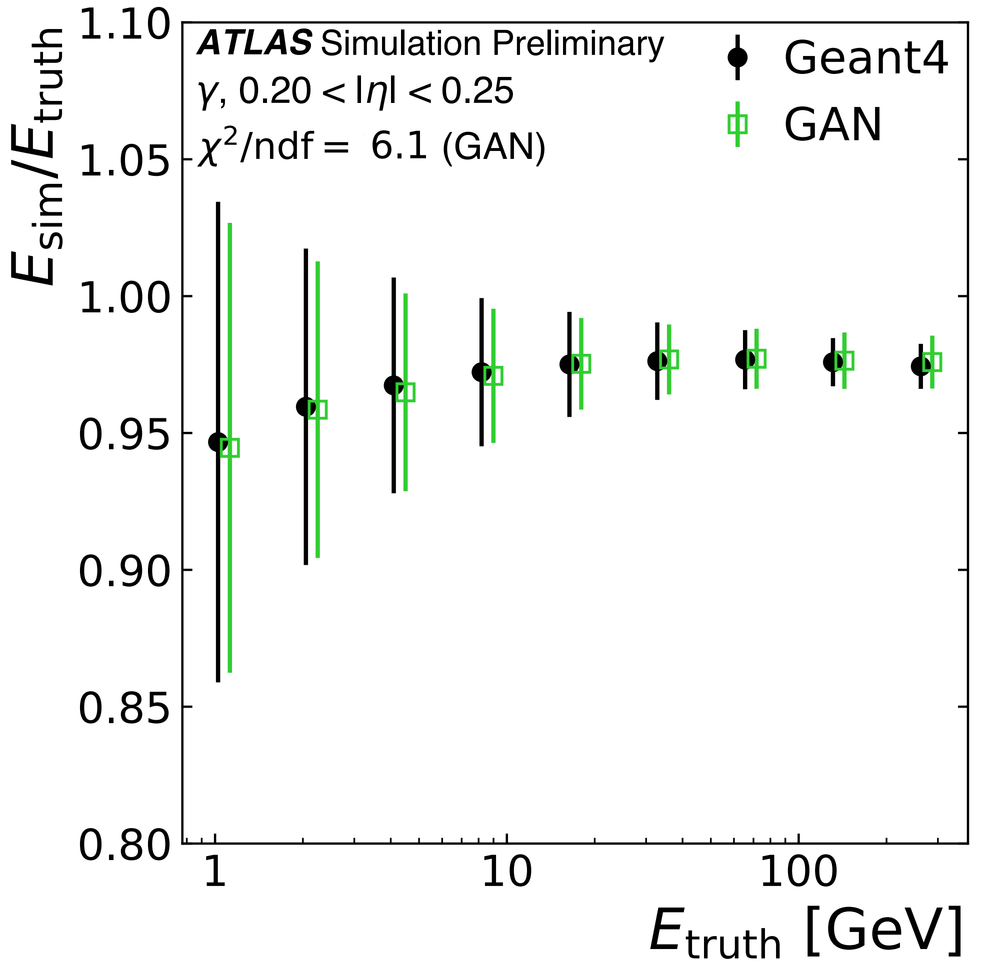
Performance Metrics for Generative Models

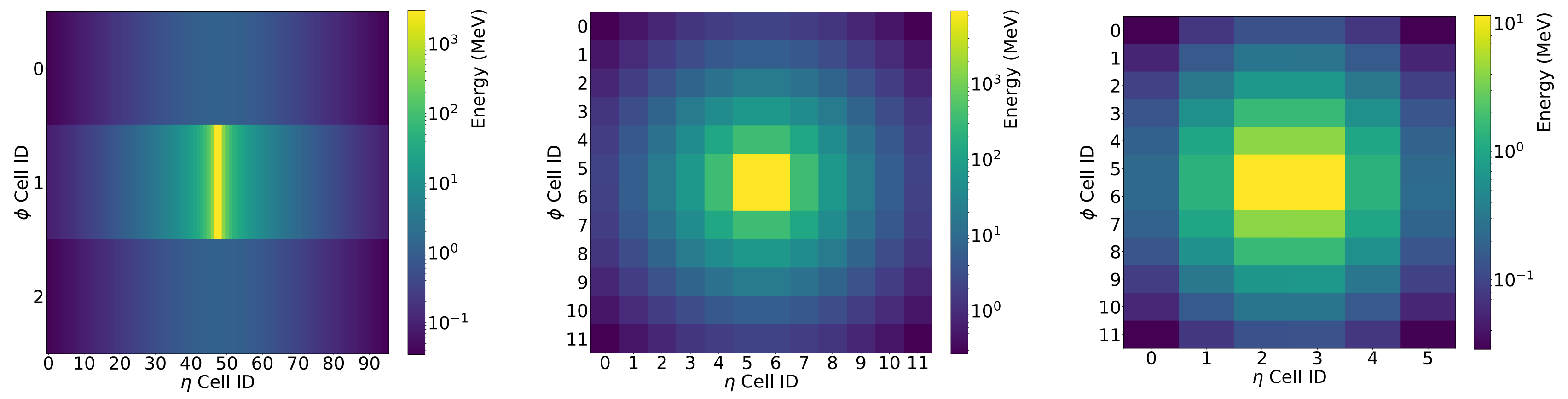
Generative Models for Simulation

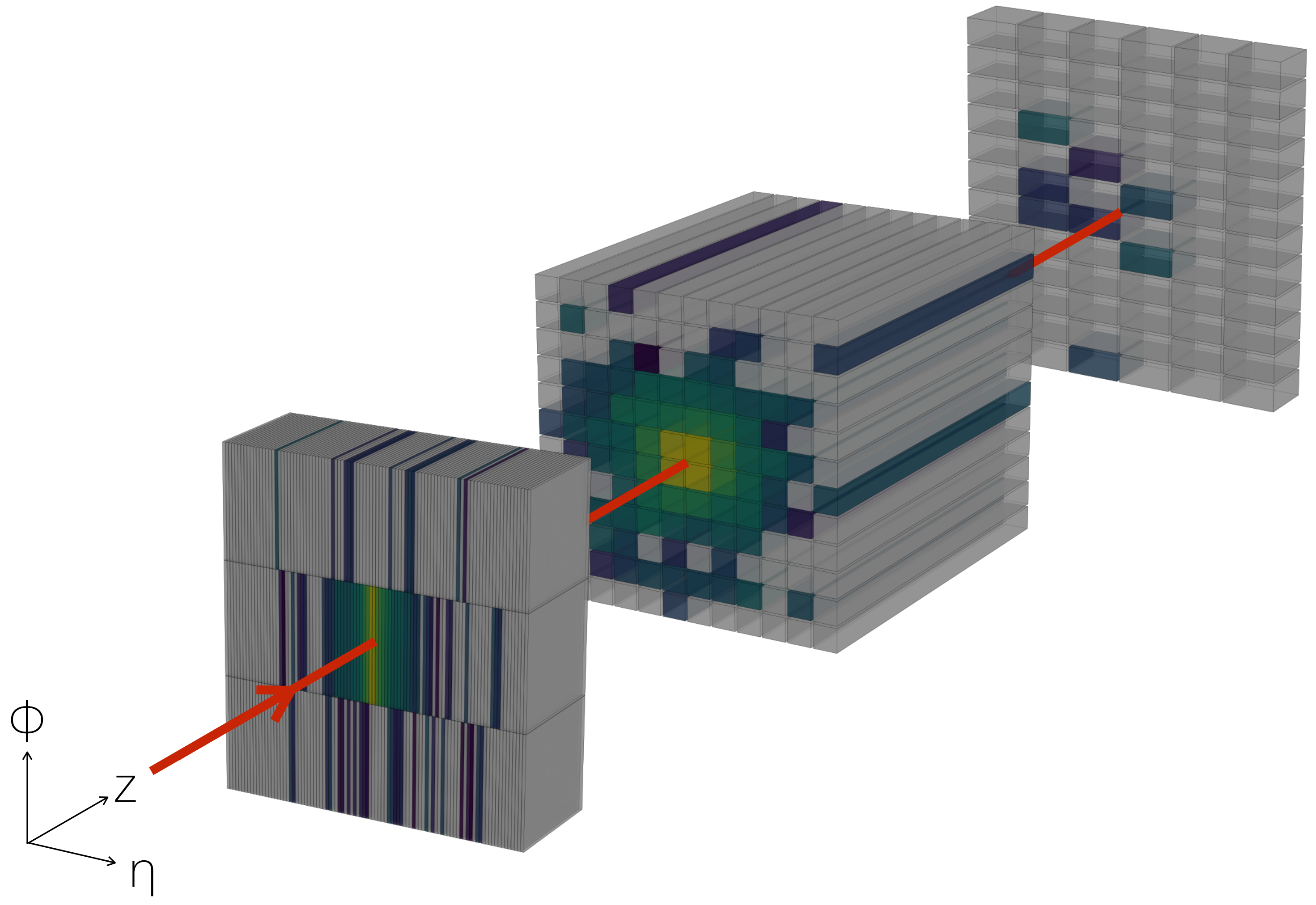
ATLAS Collaboration [A. Ghosh], 2019

Paganini et al.

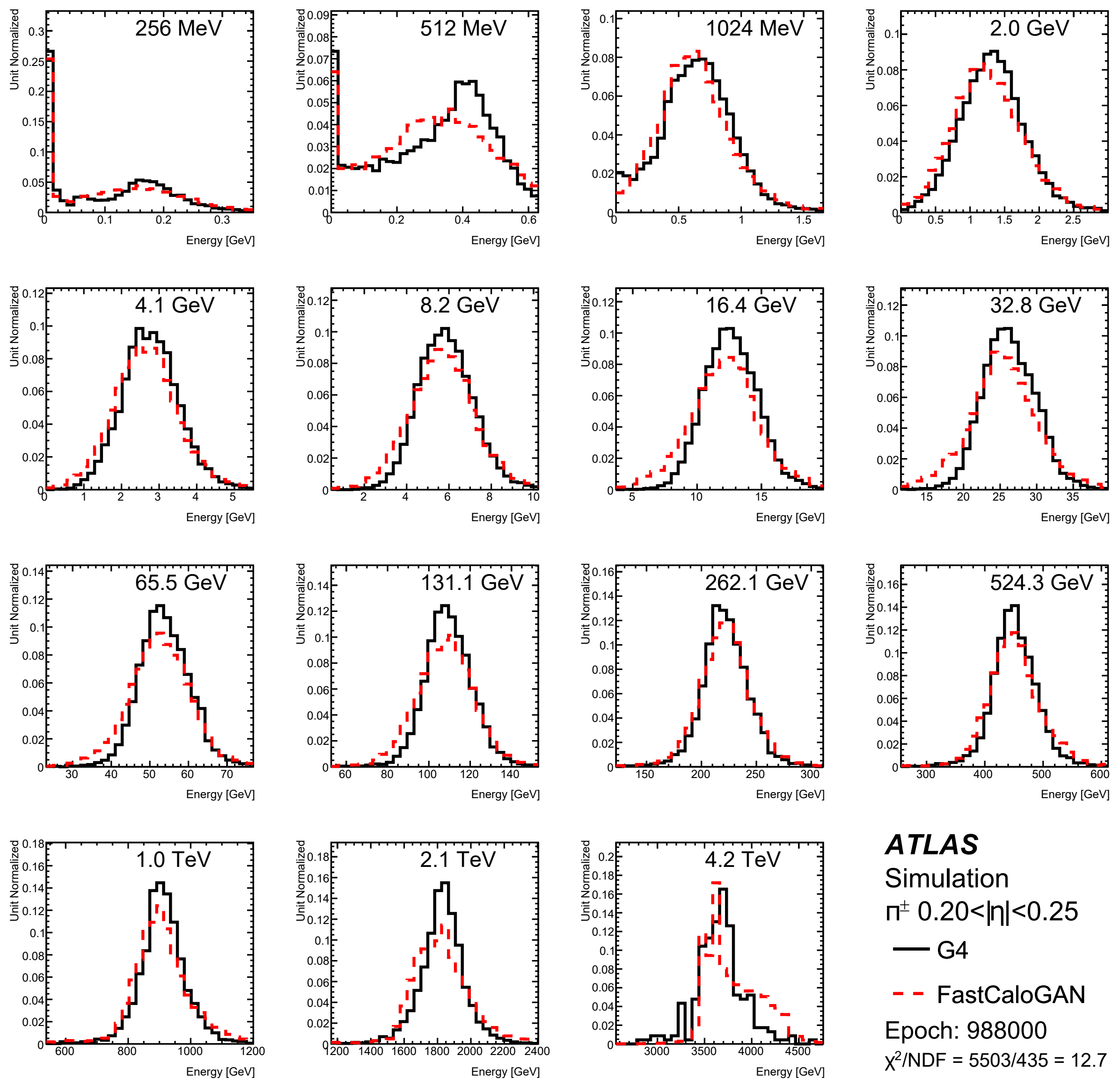


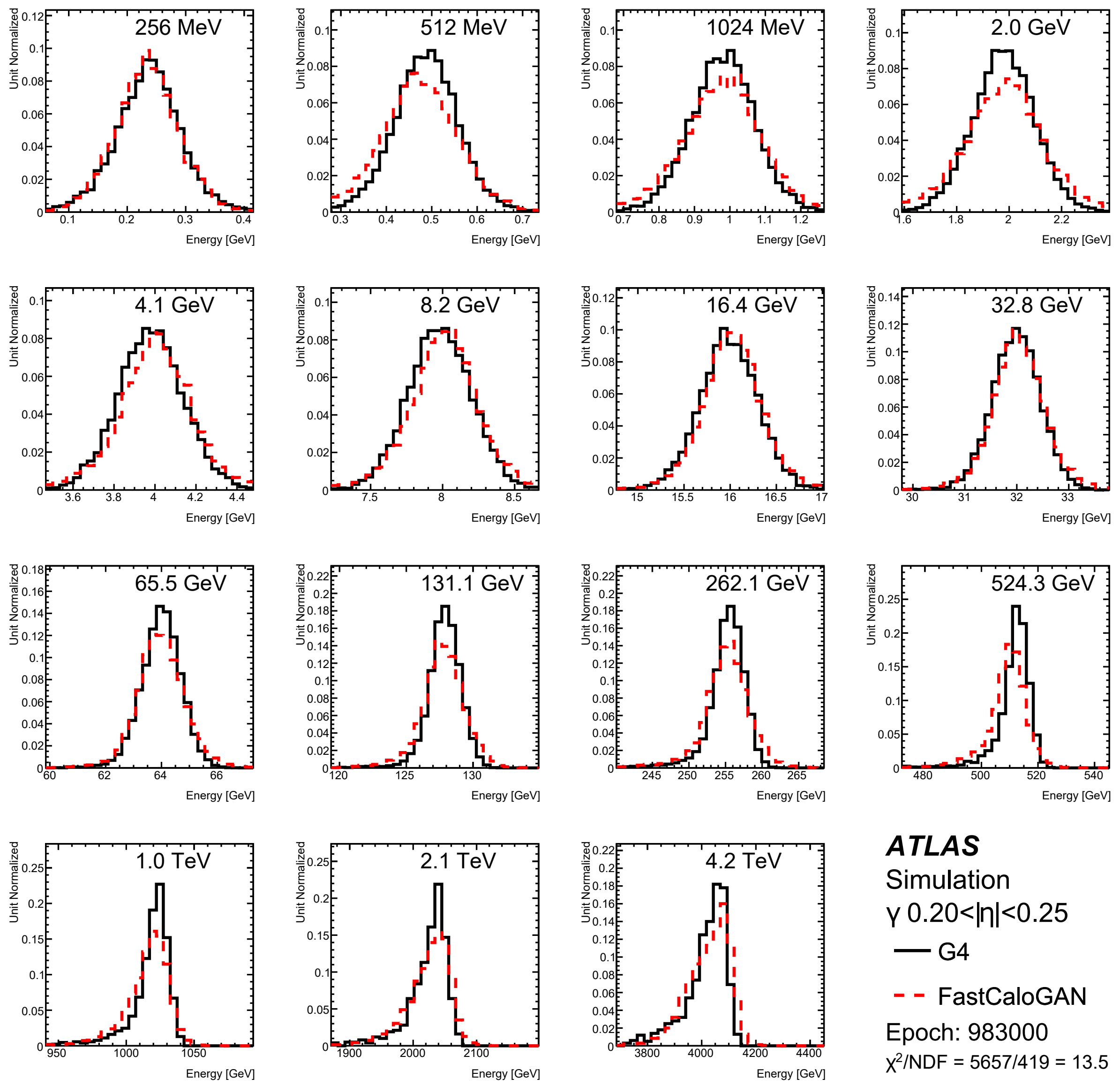






Evaluating Fast Calo Simulators





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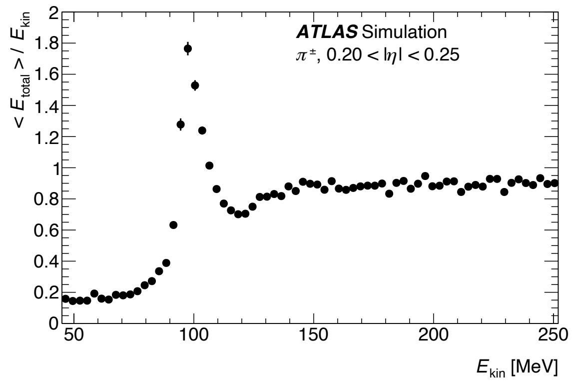

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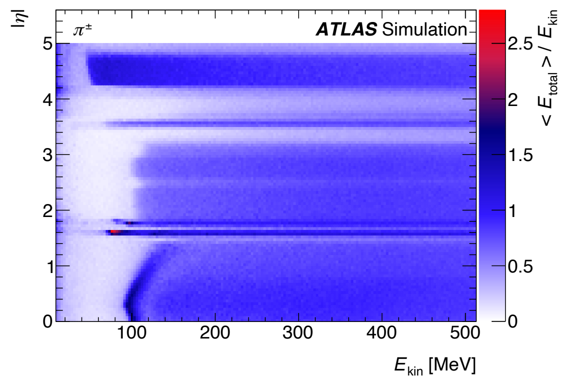

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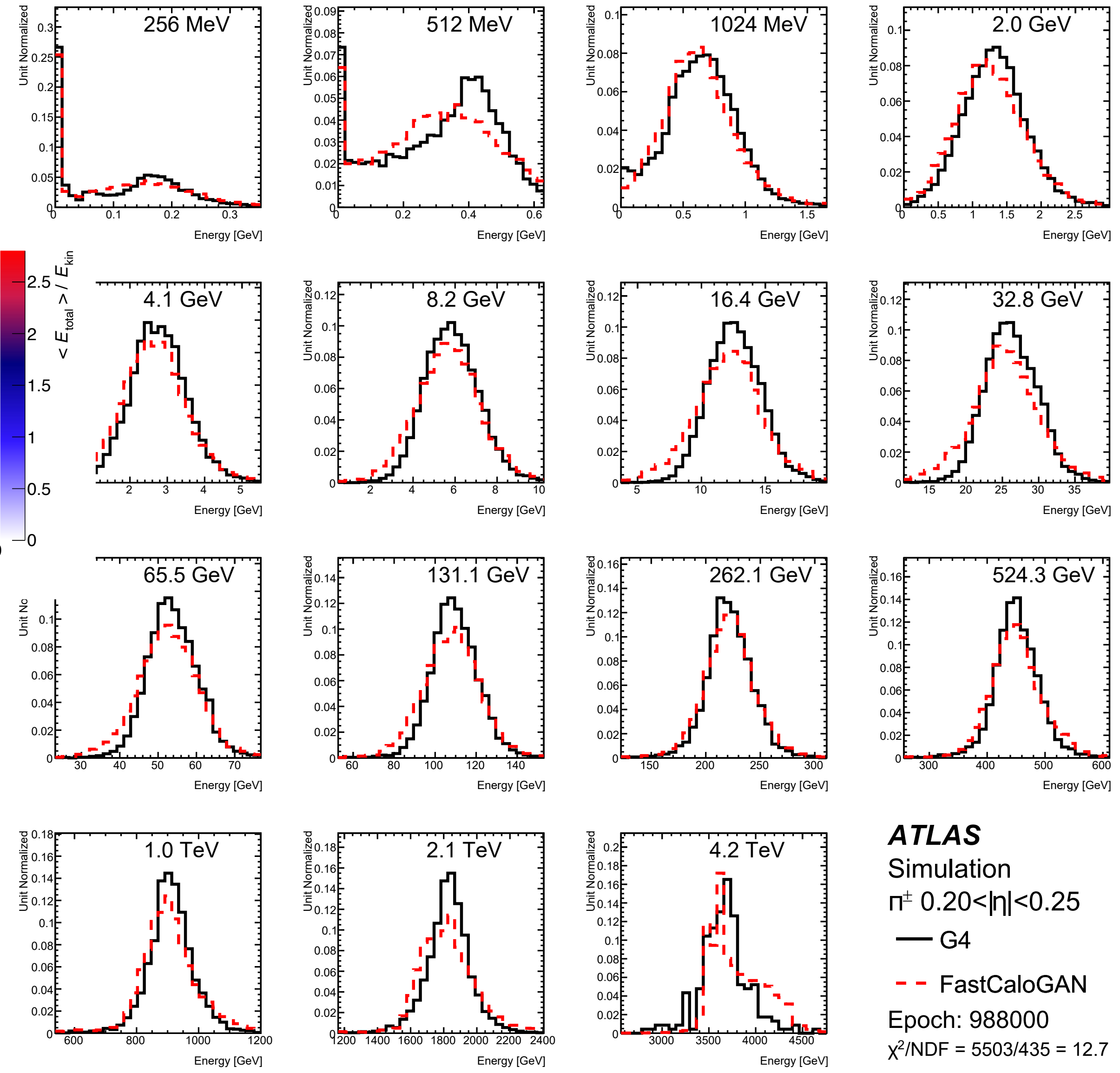

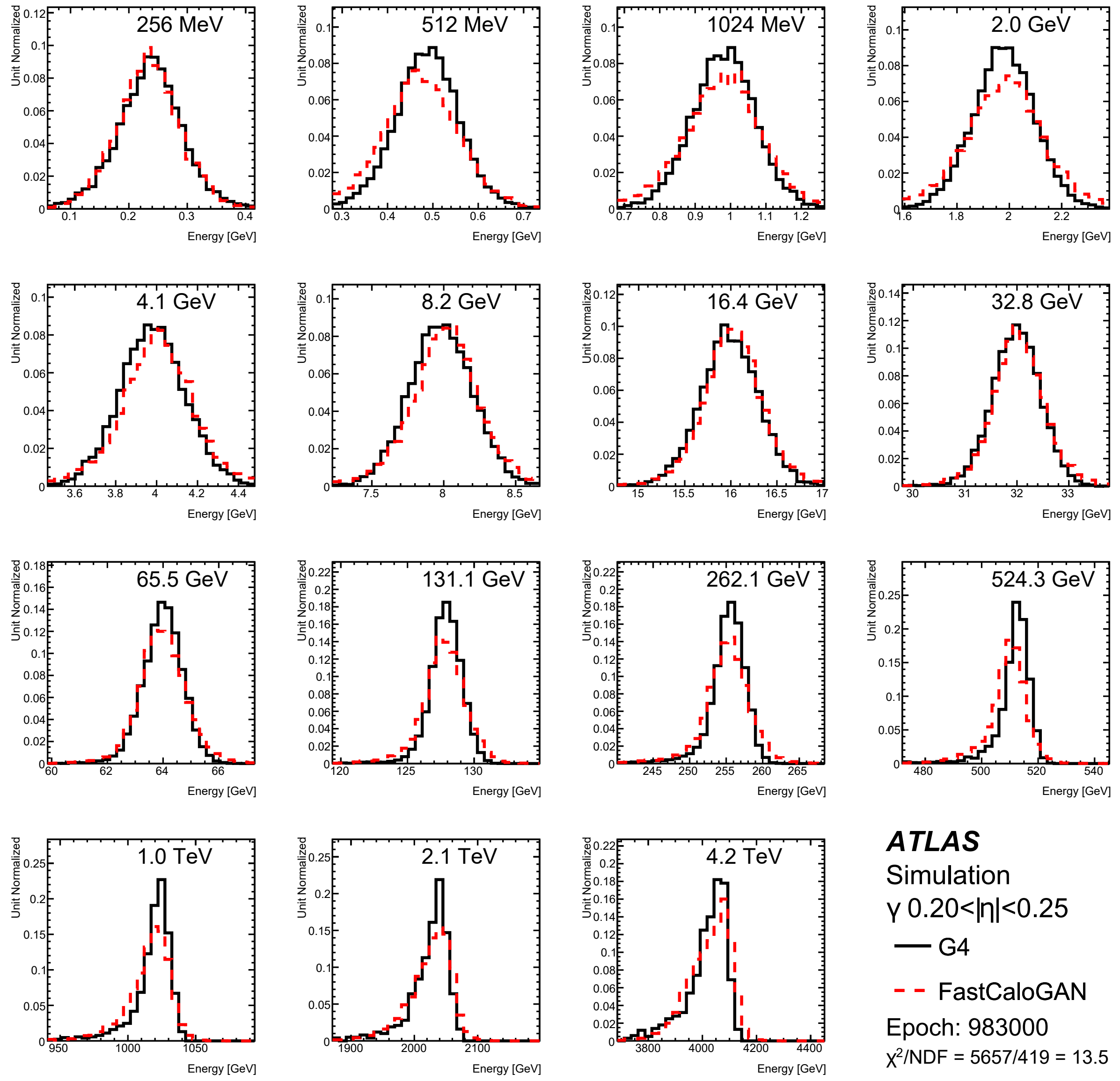

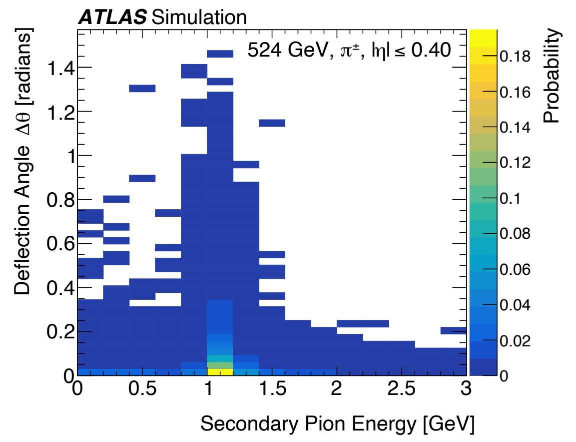

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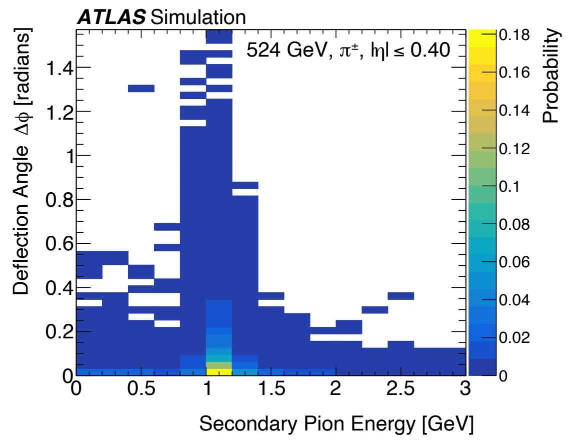

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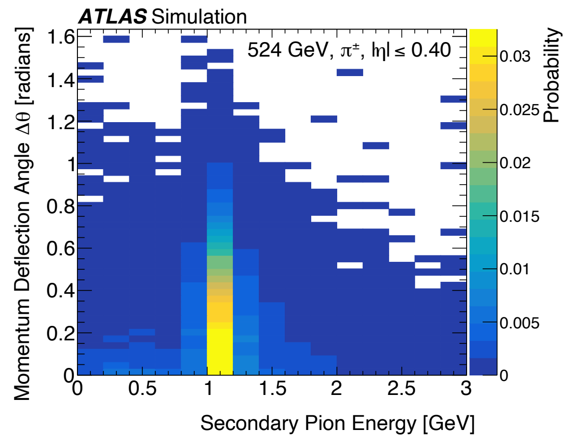

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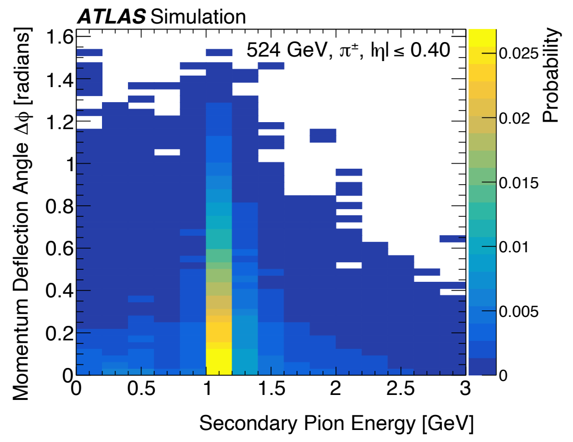

(d)

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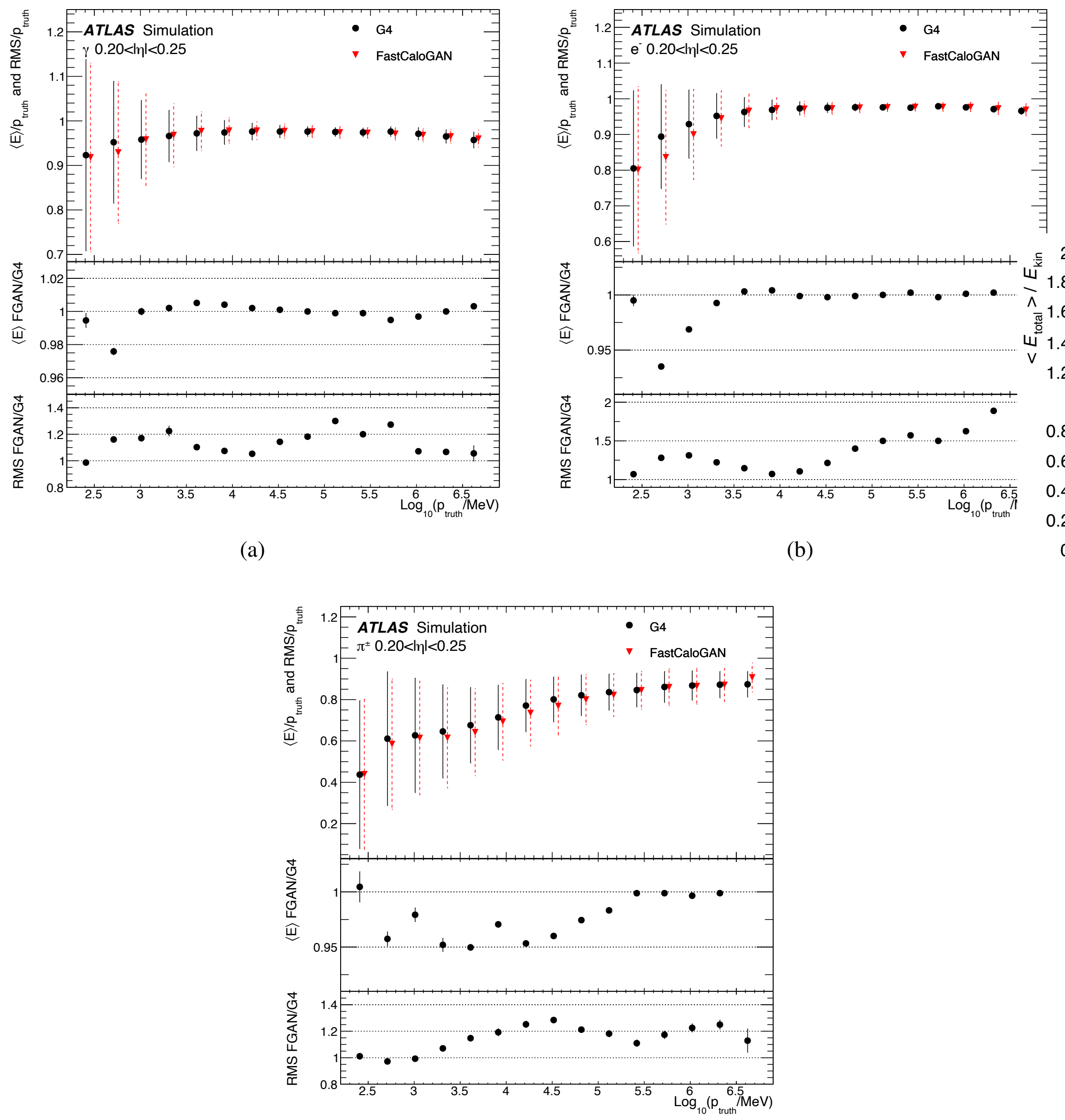

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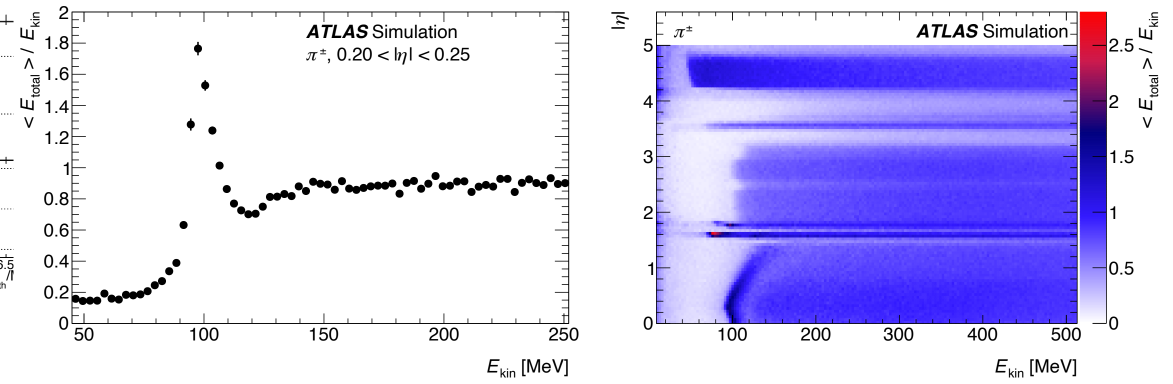

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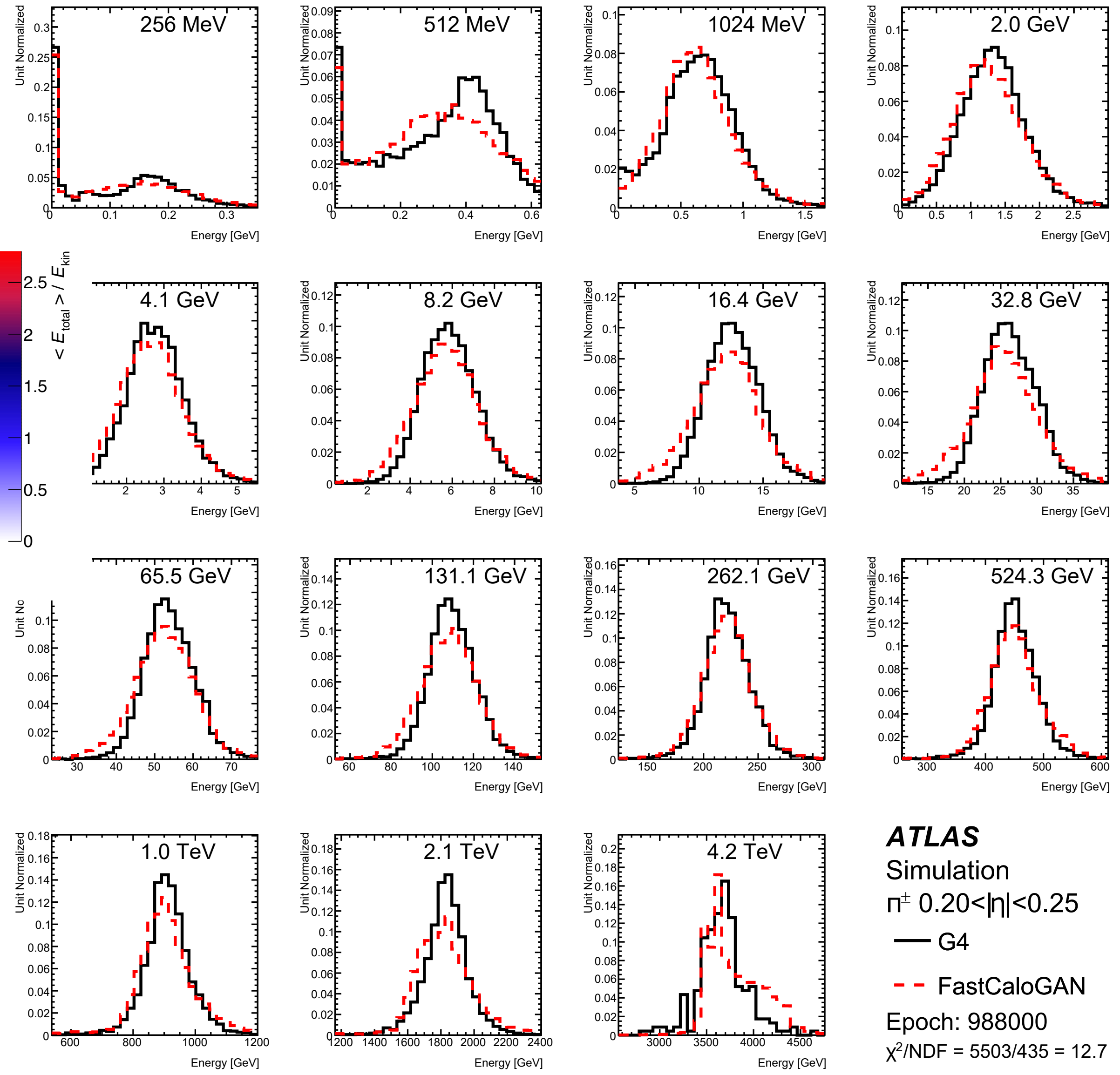

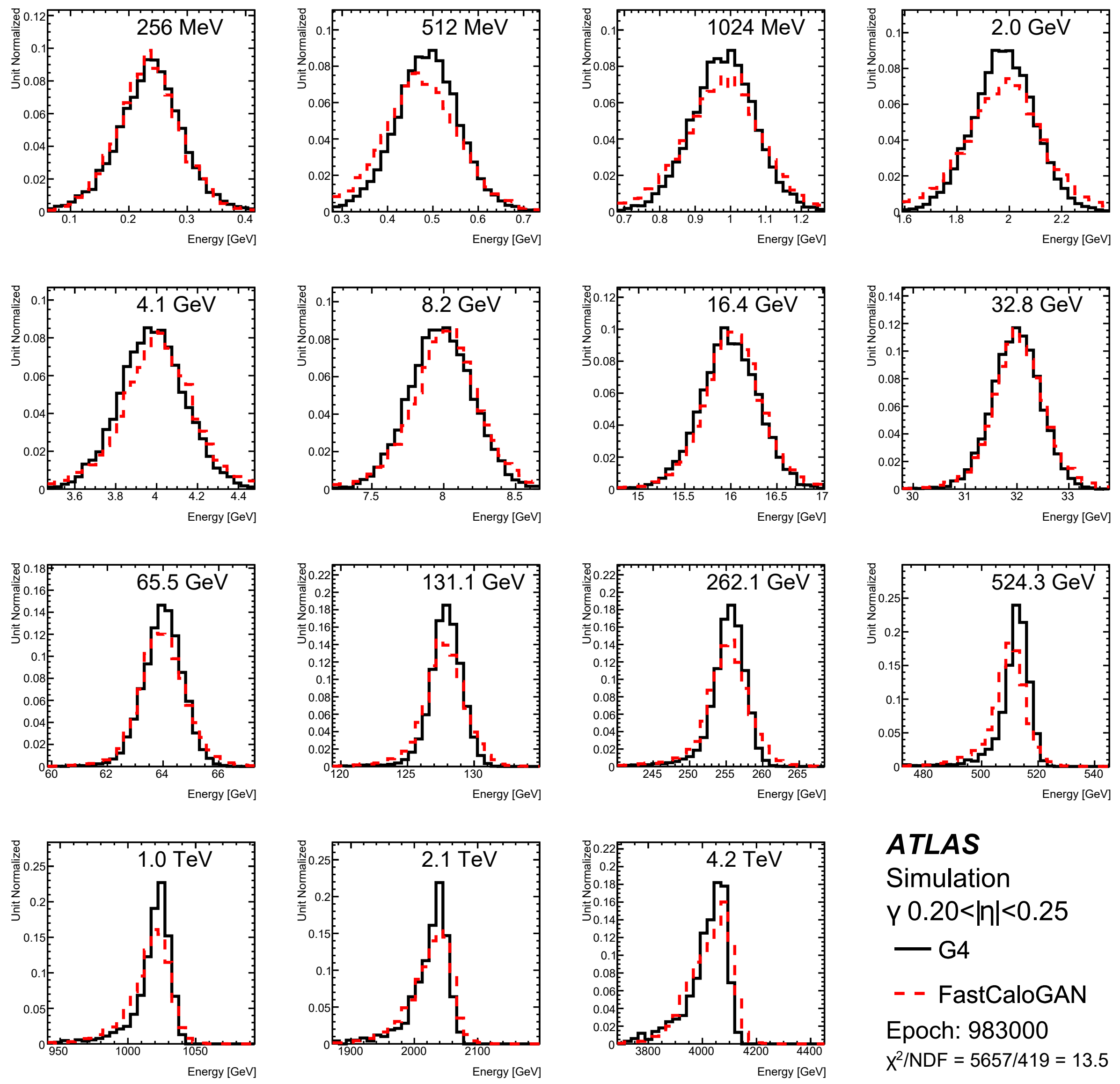

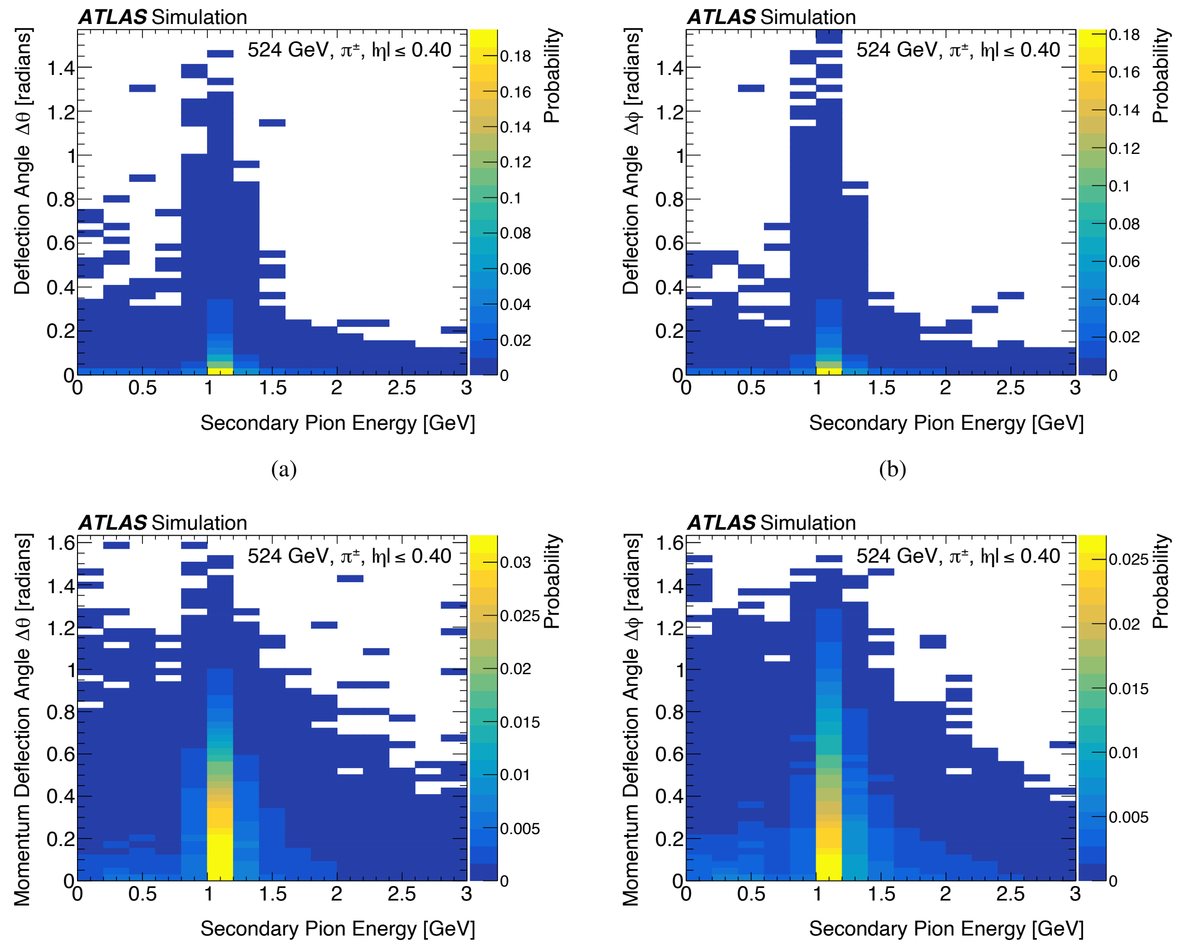

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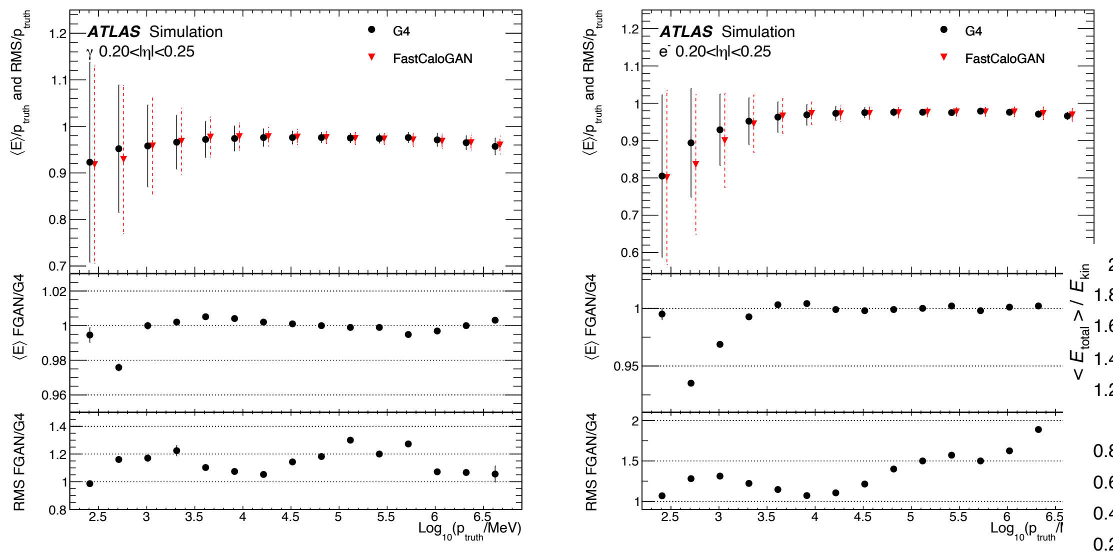

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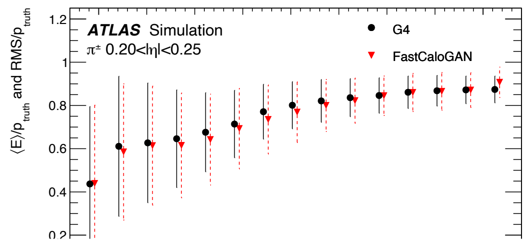

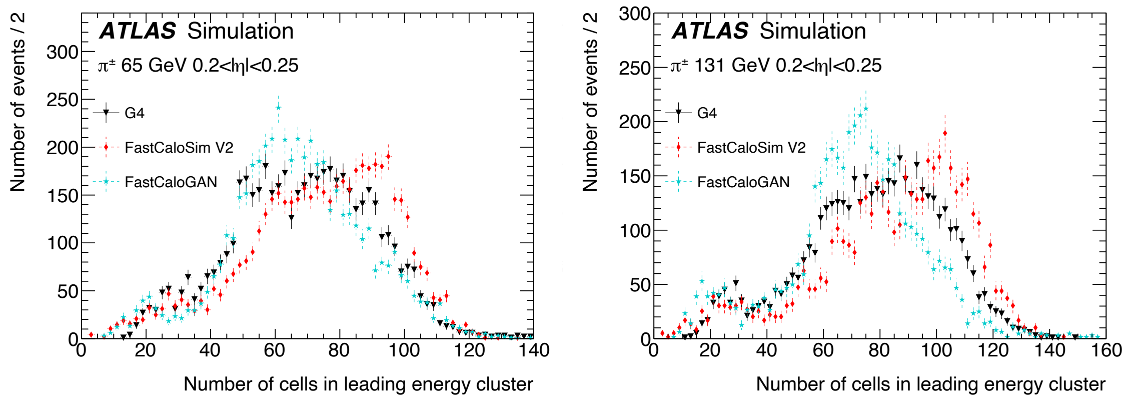

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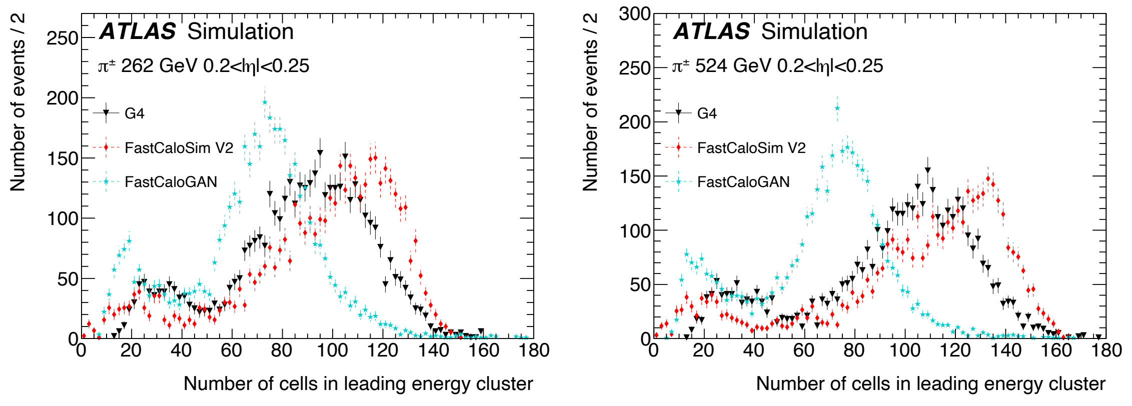

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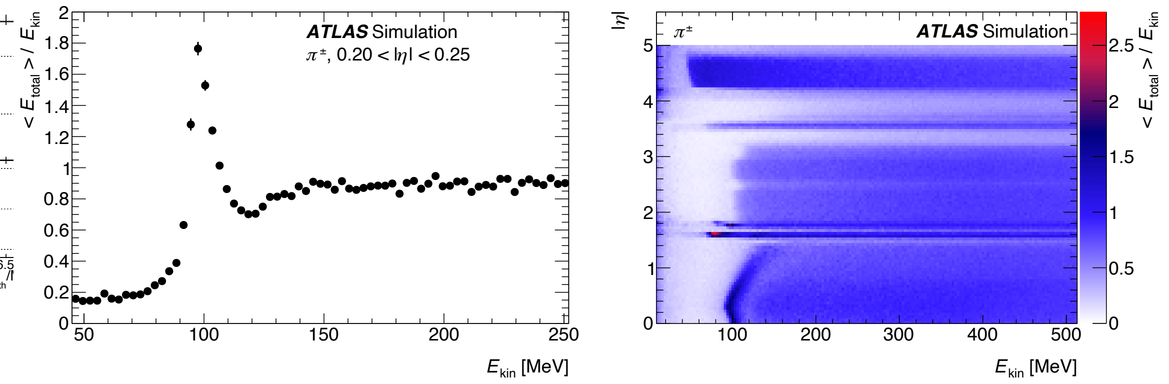

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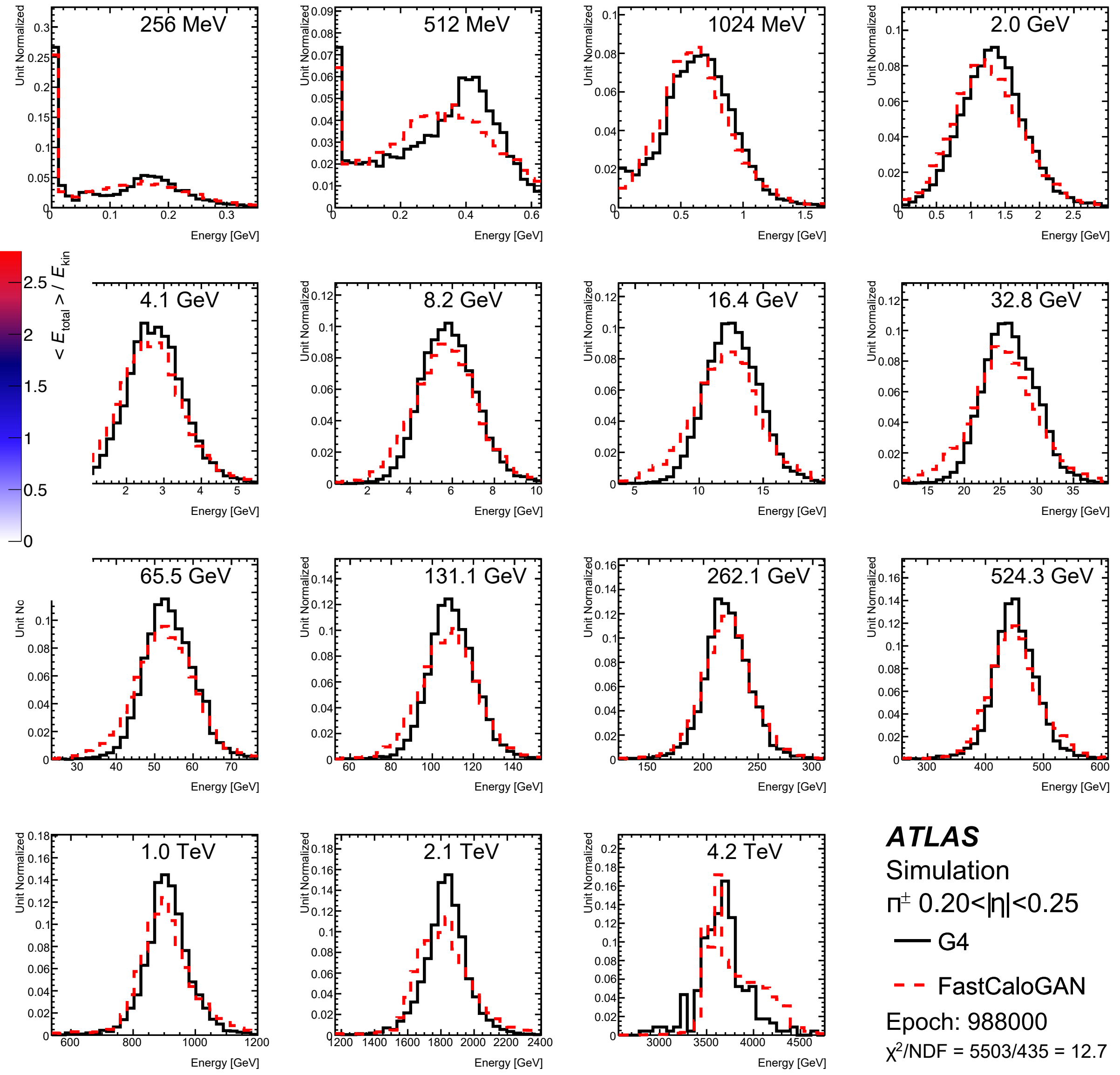

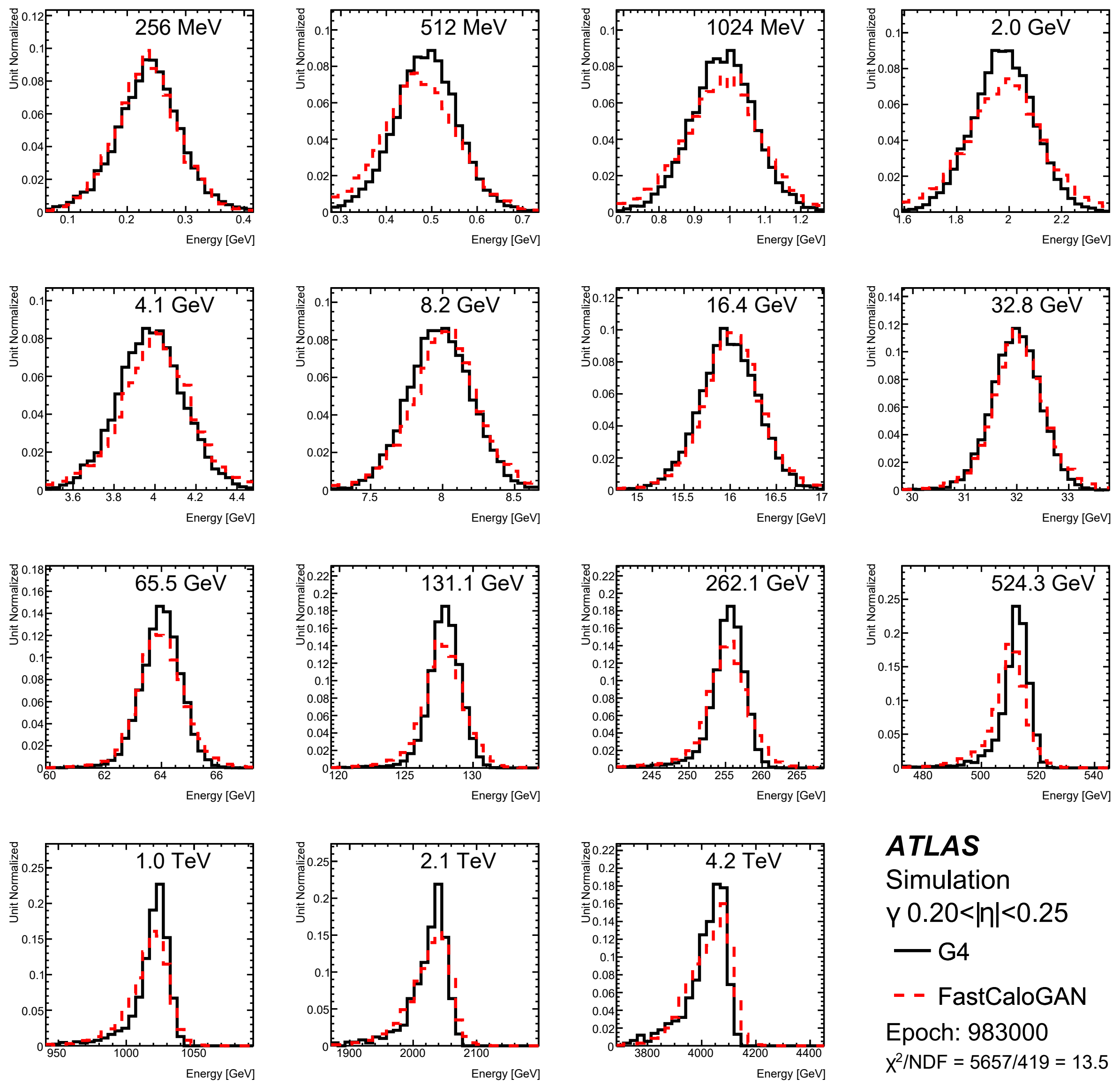

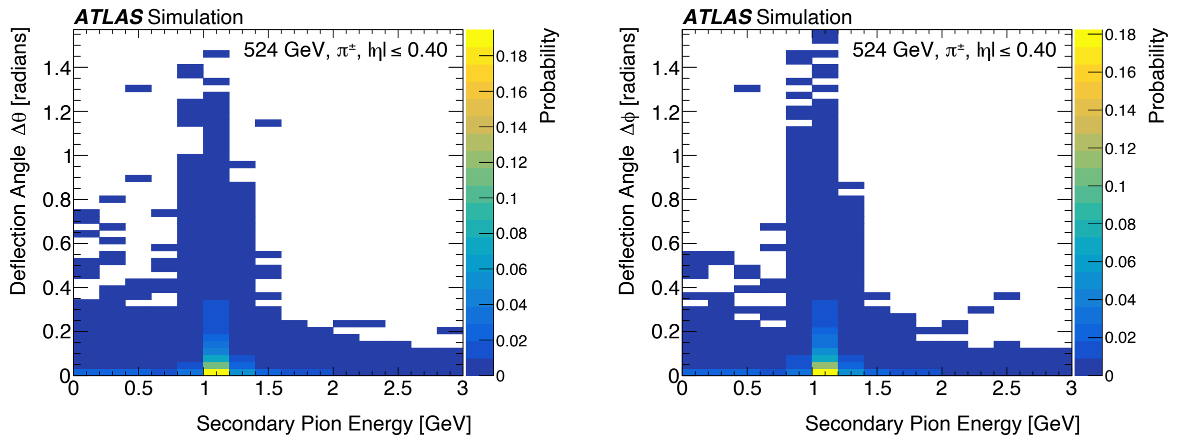

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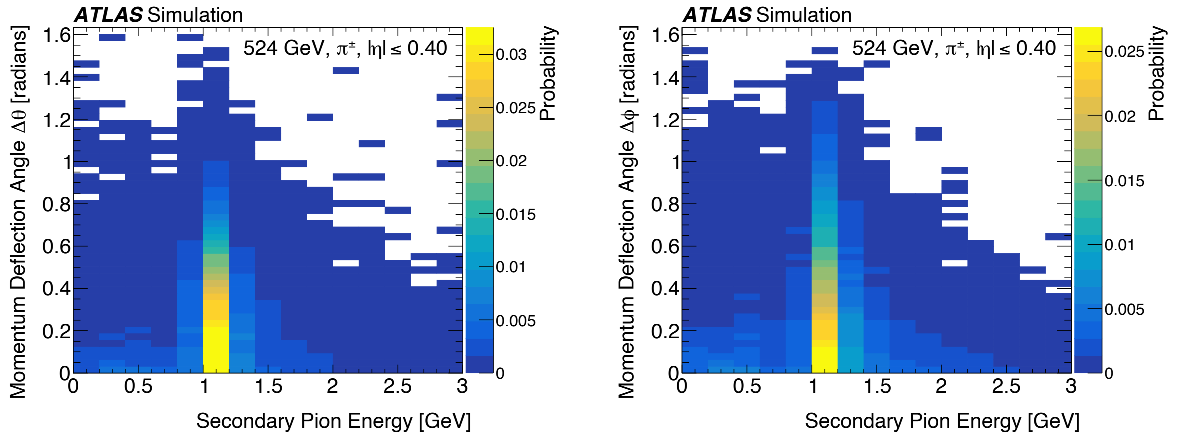

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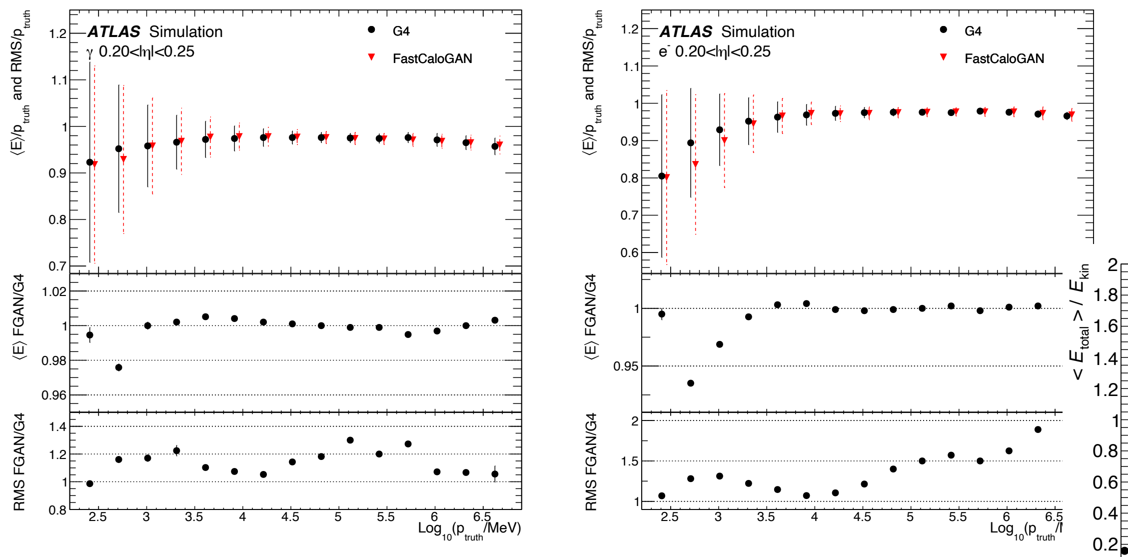

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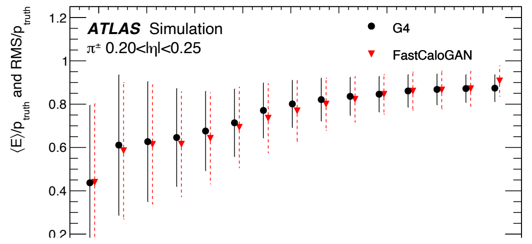

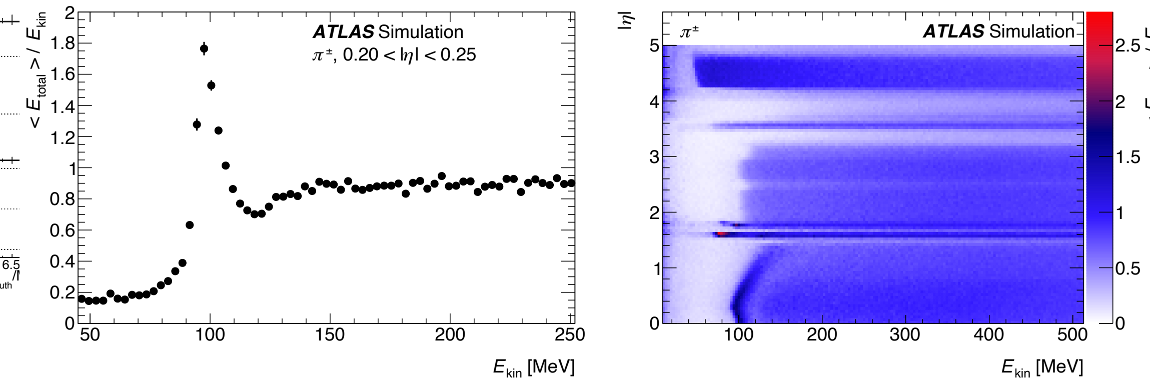

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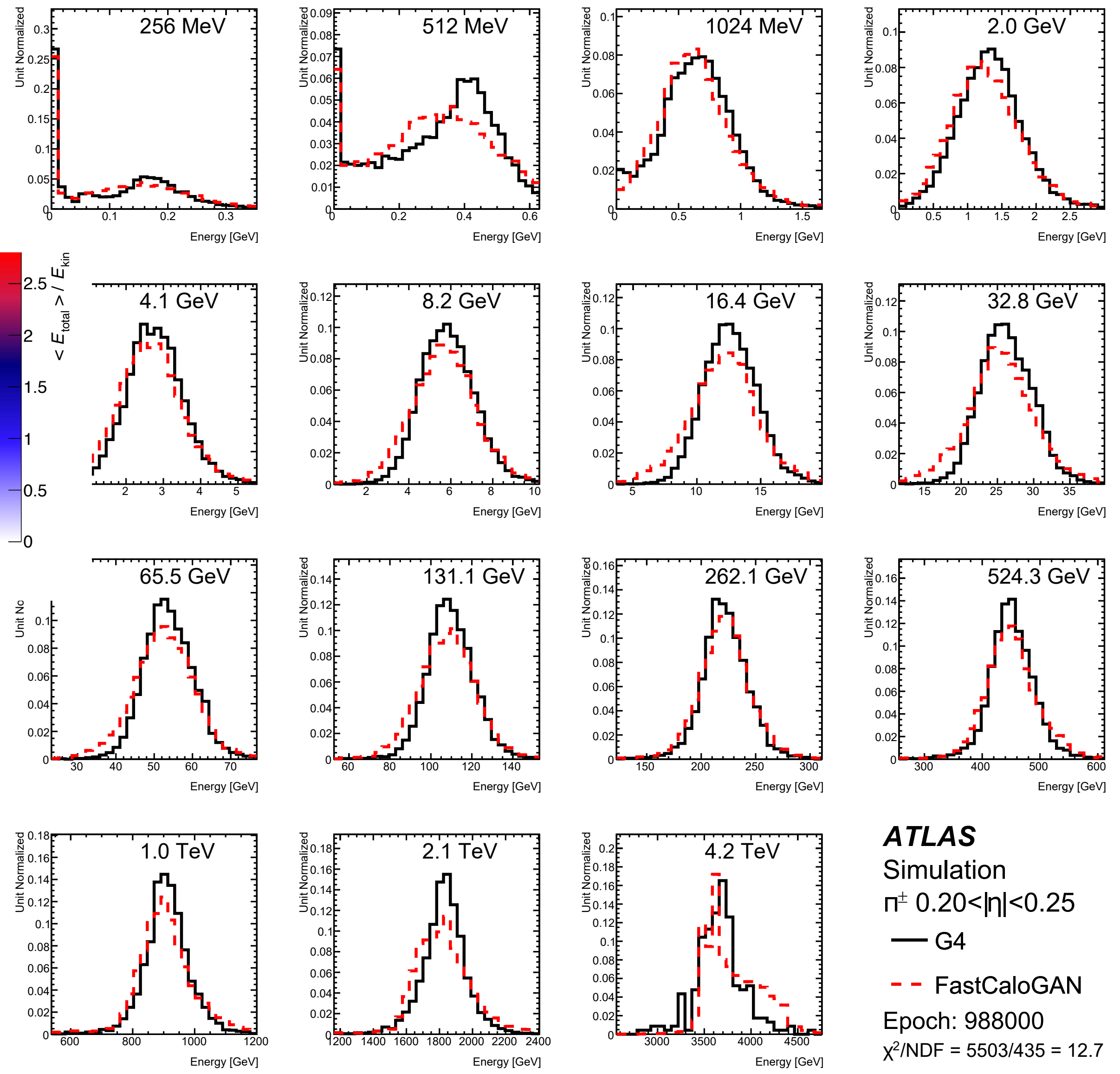

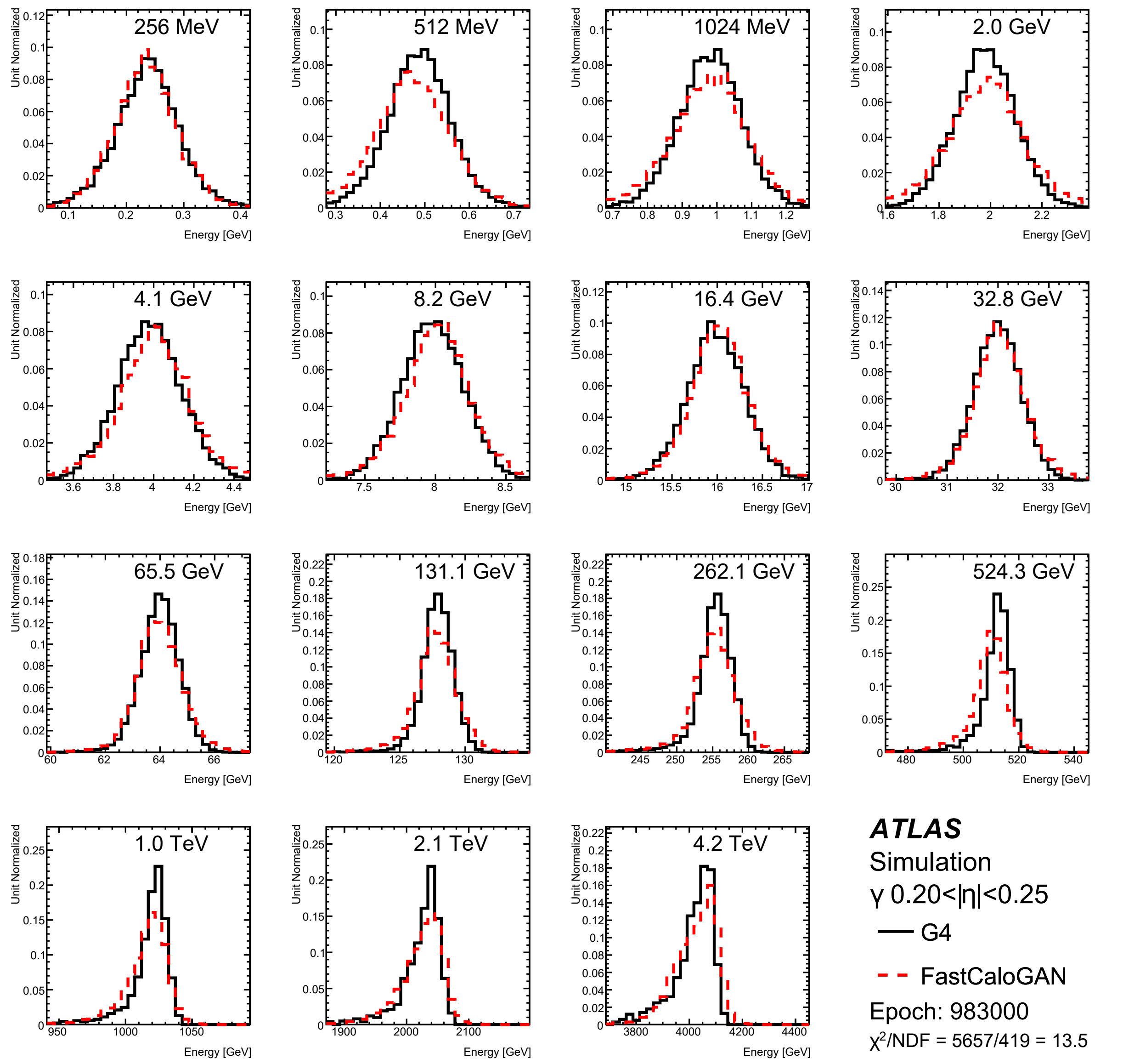

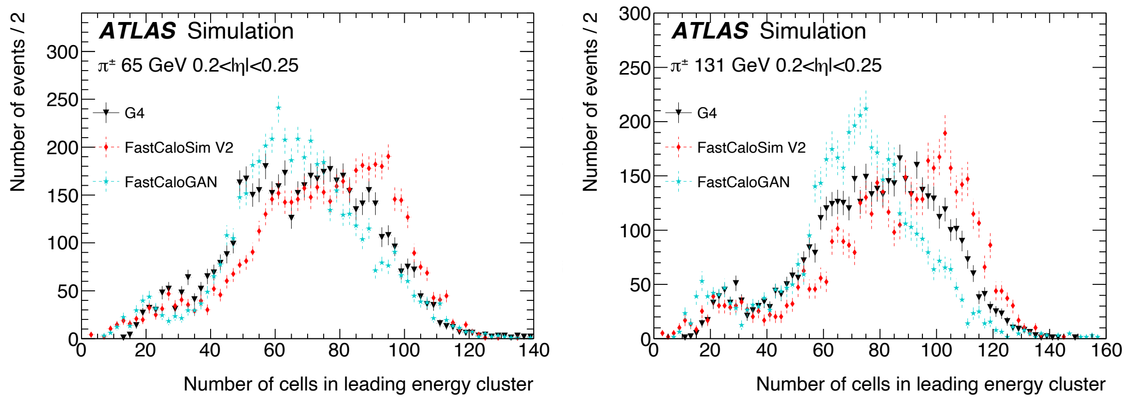

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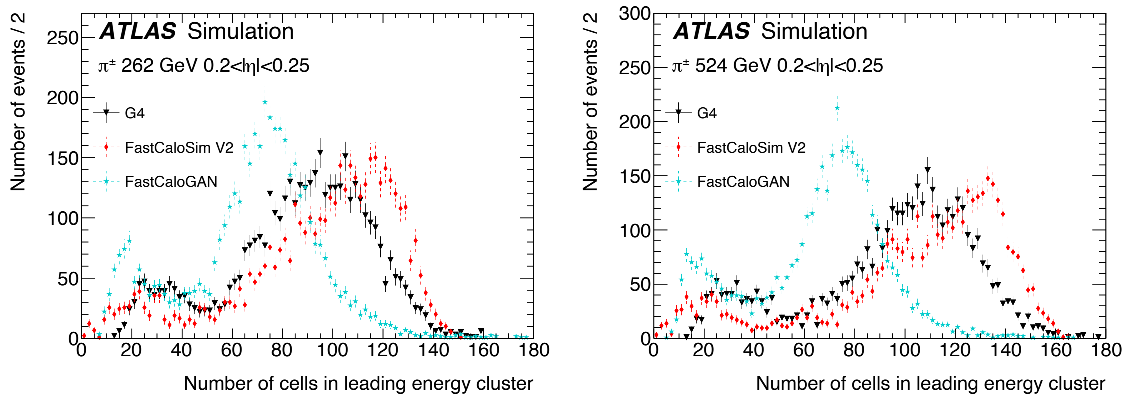

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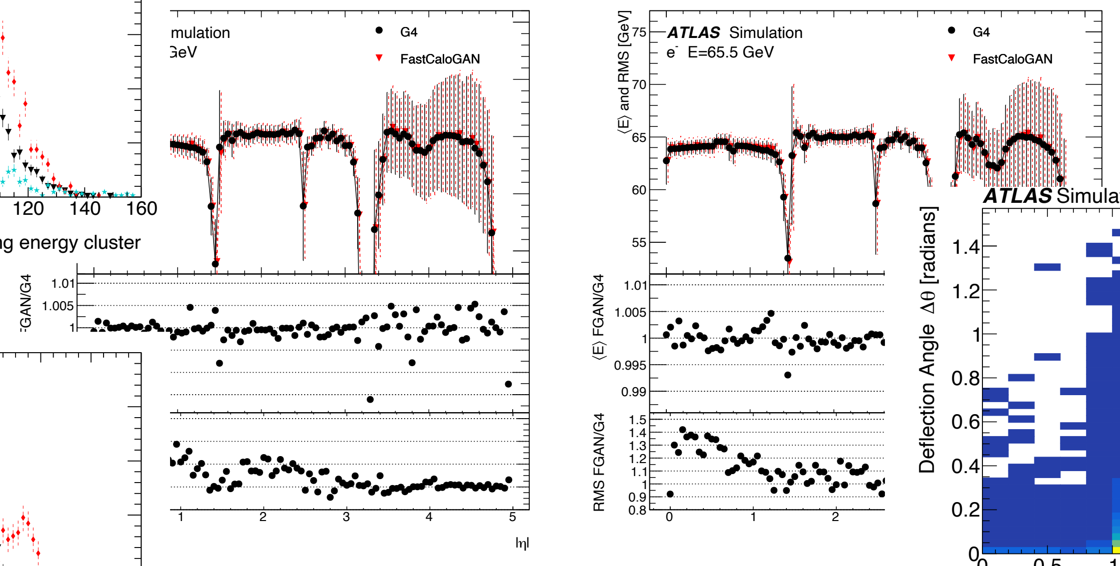

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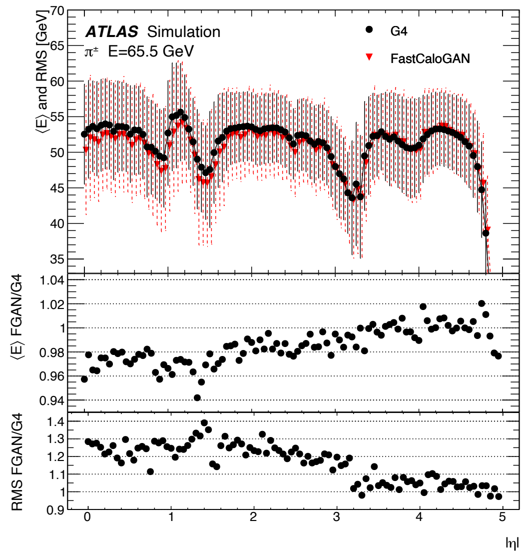

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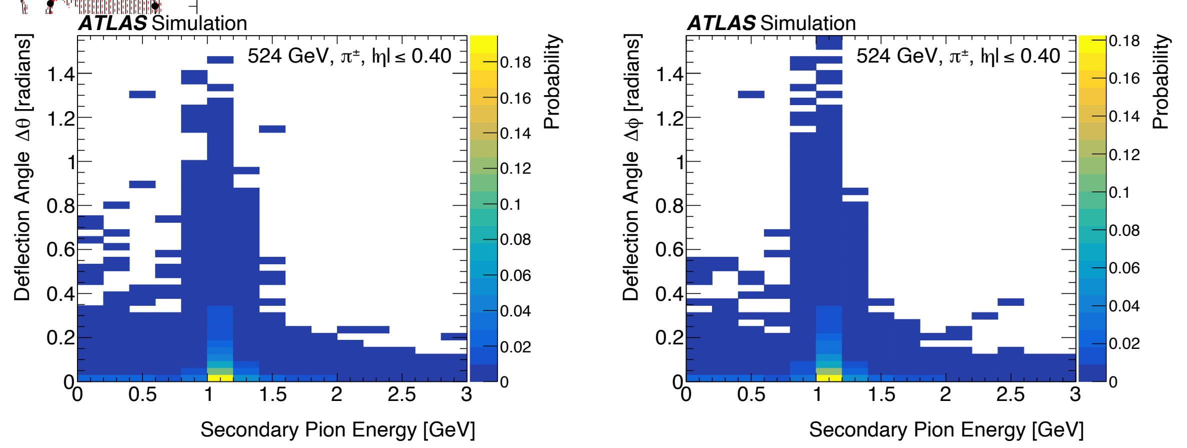

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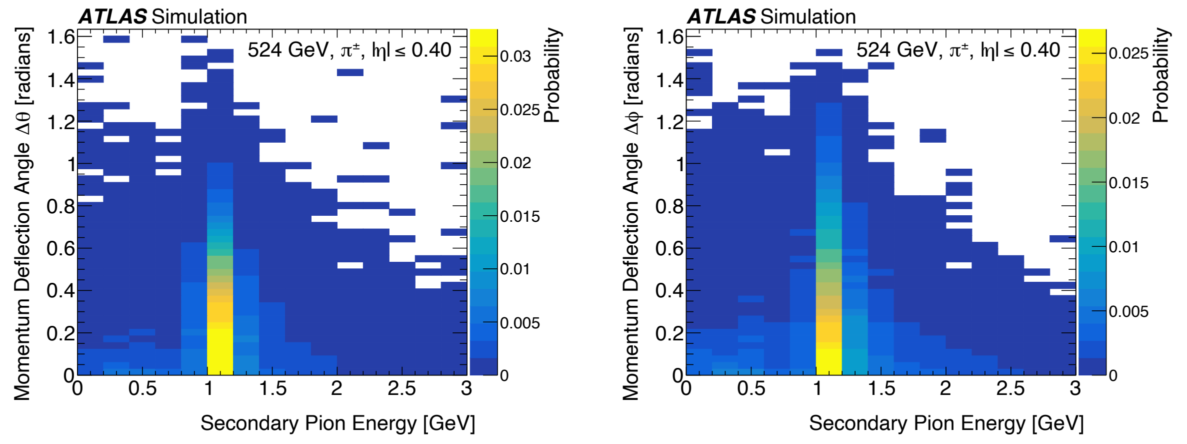

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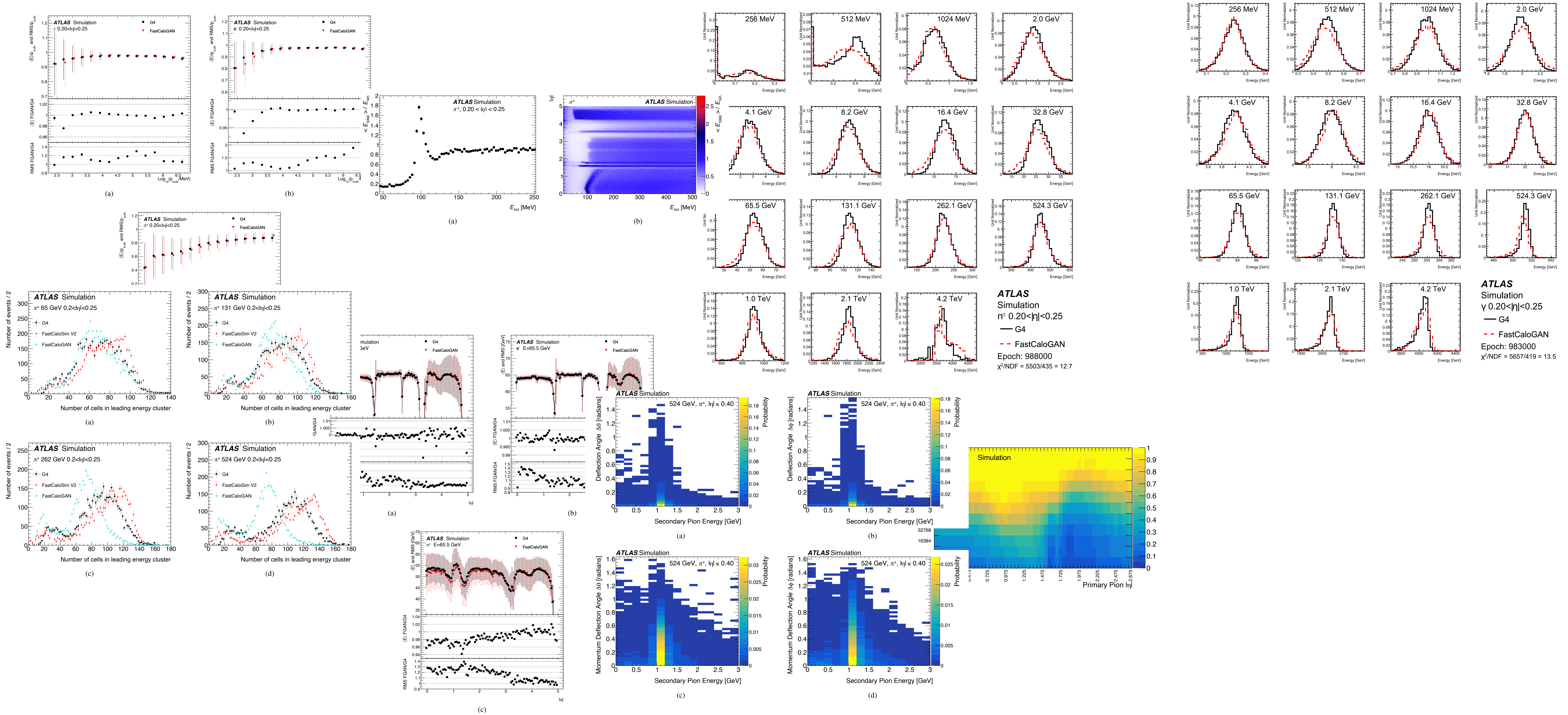

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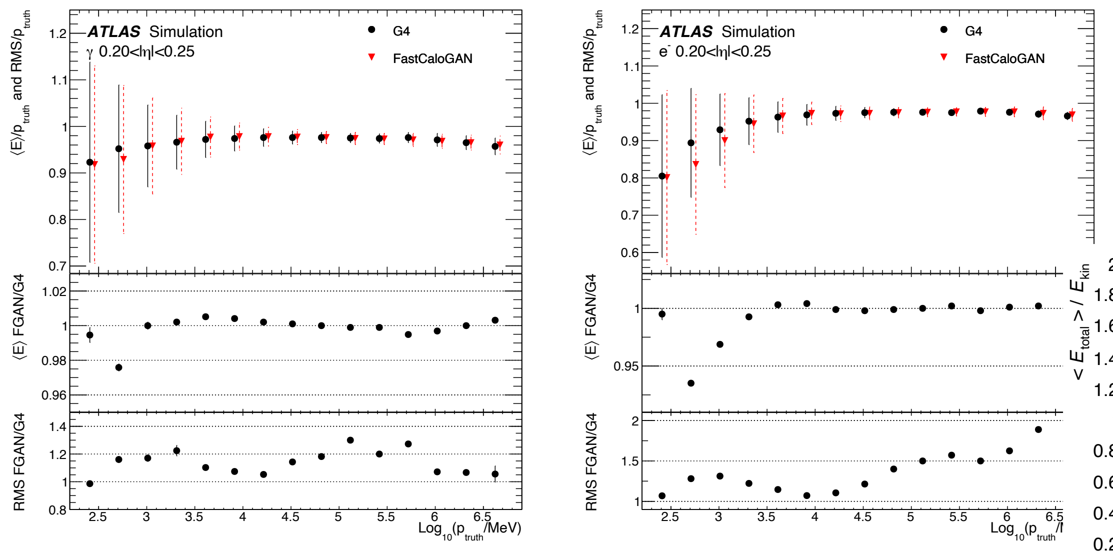

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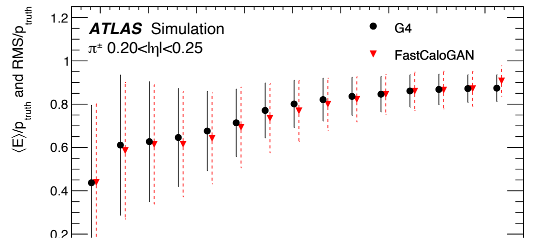

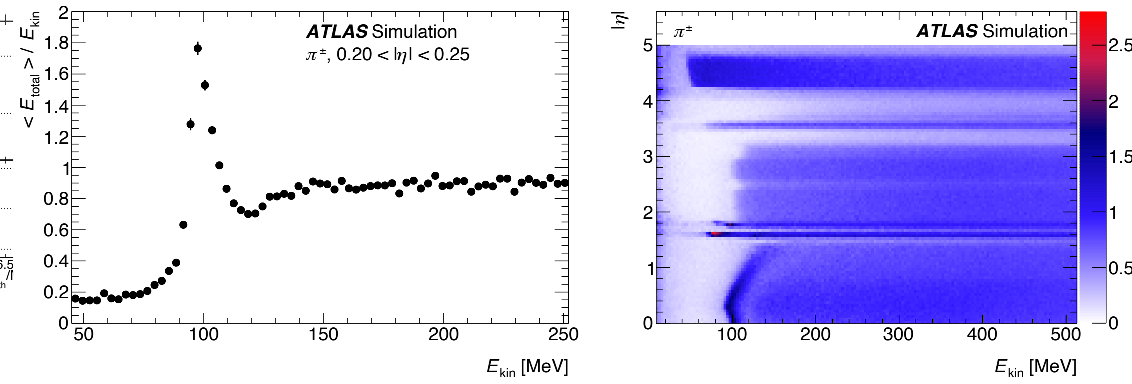

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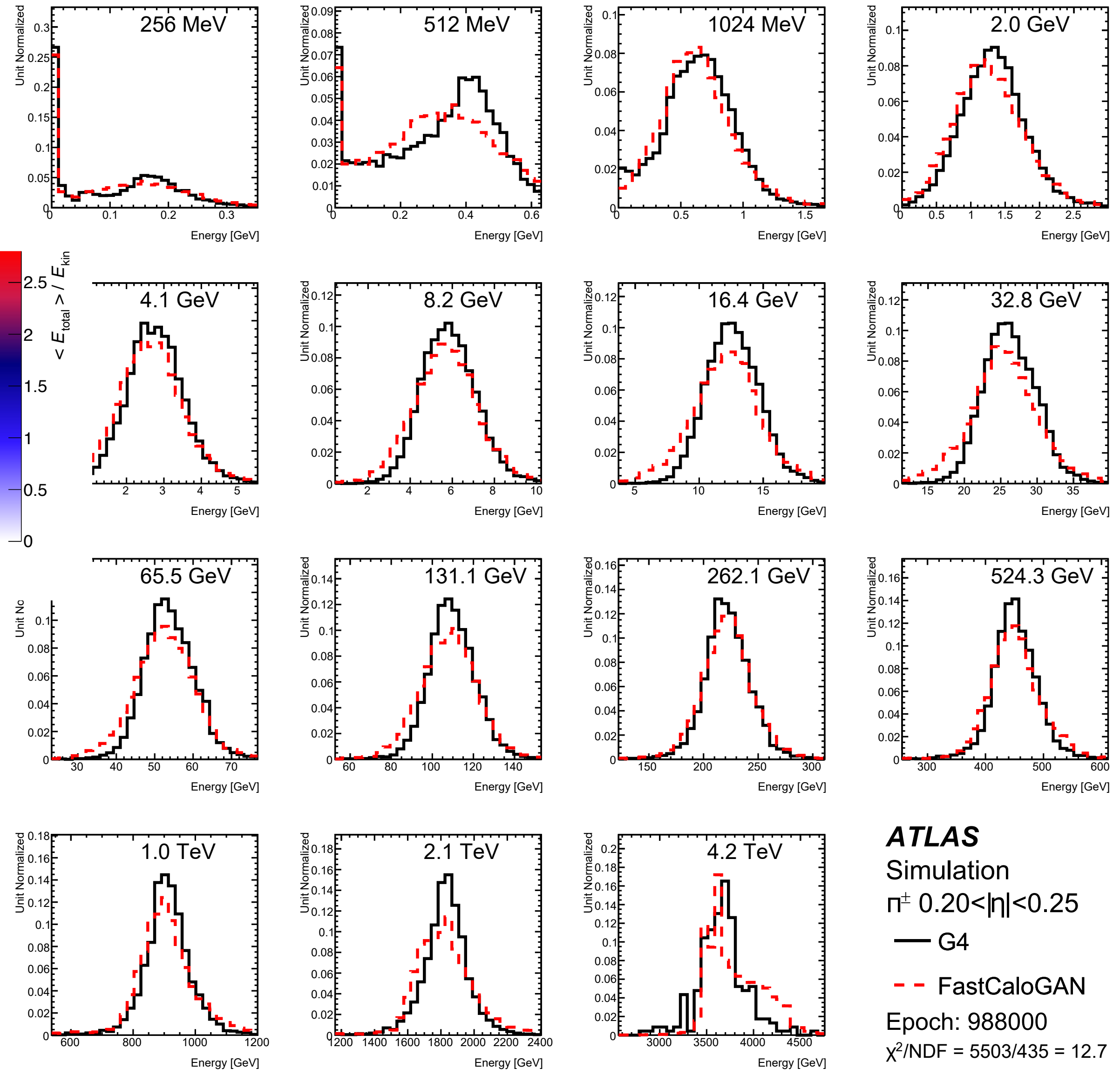

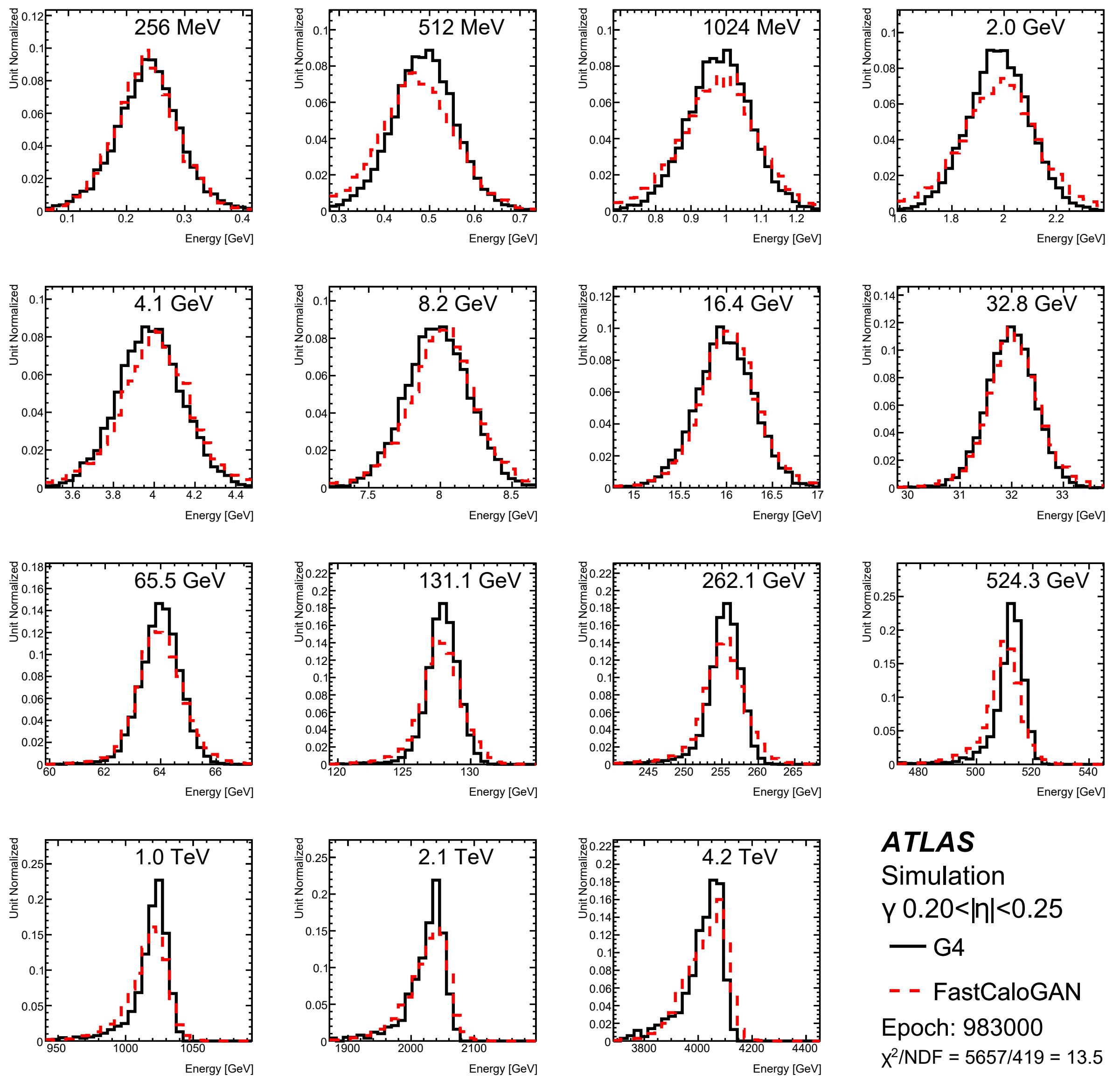

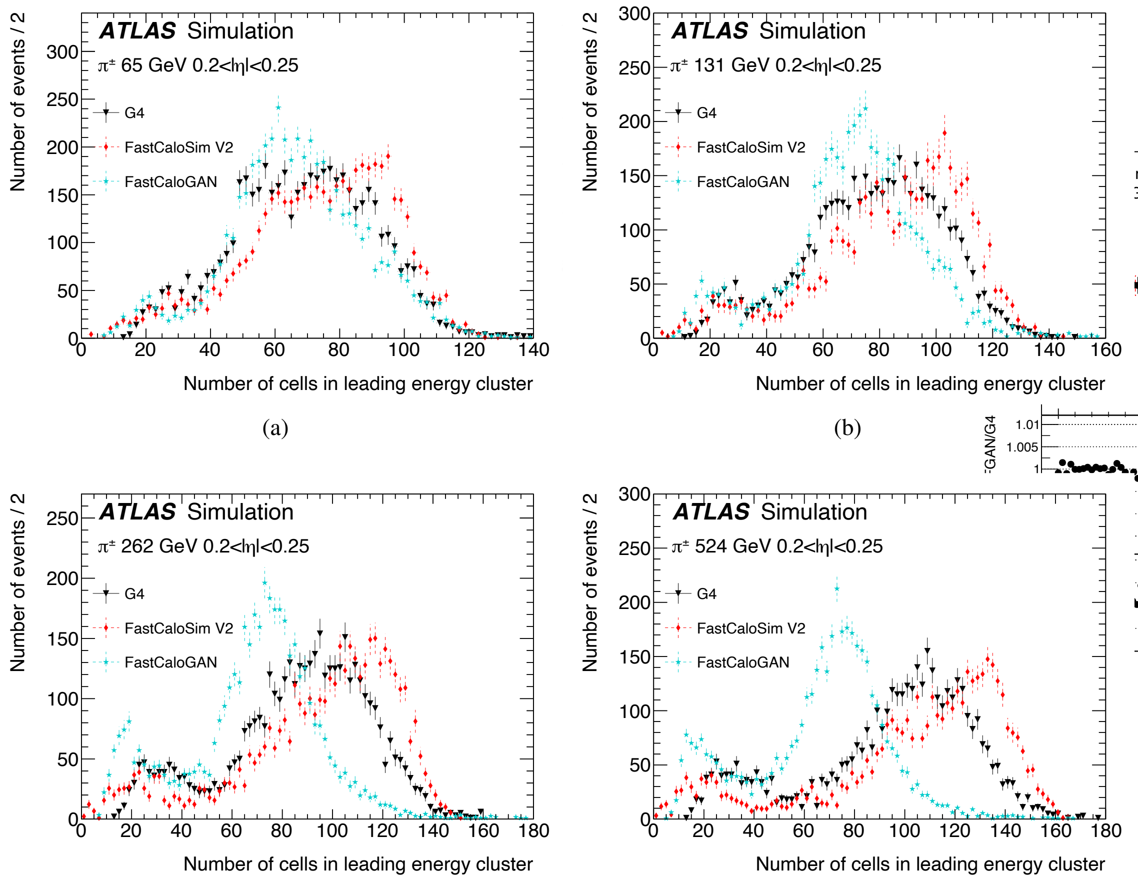

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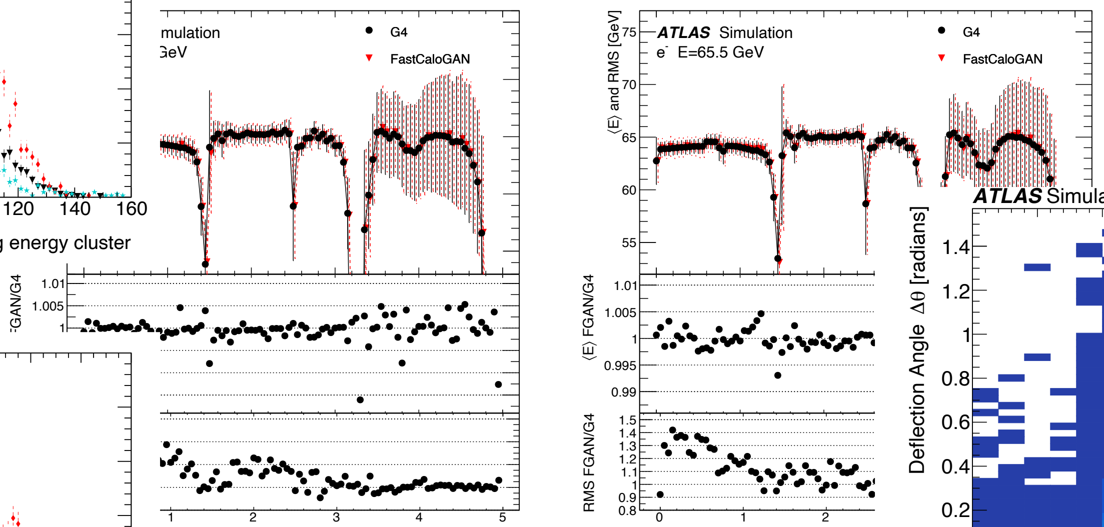

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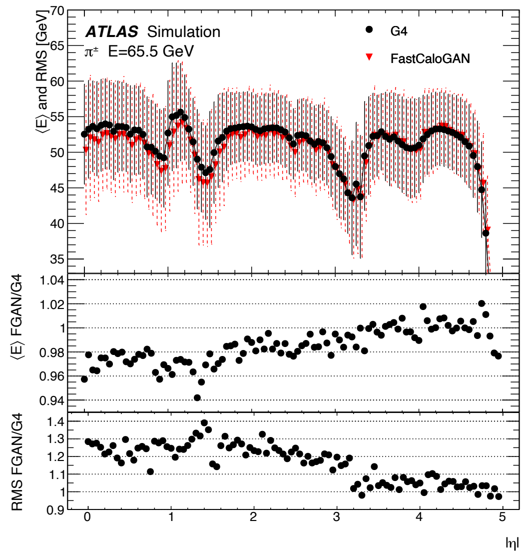

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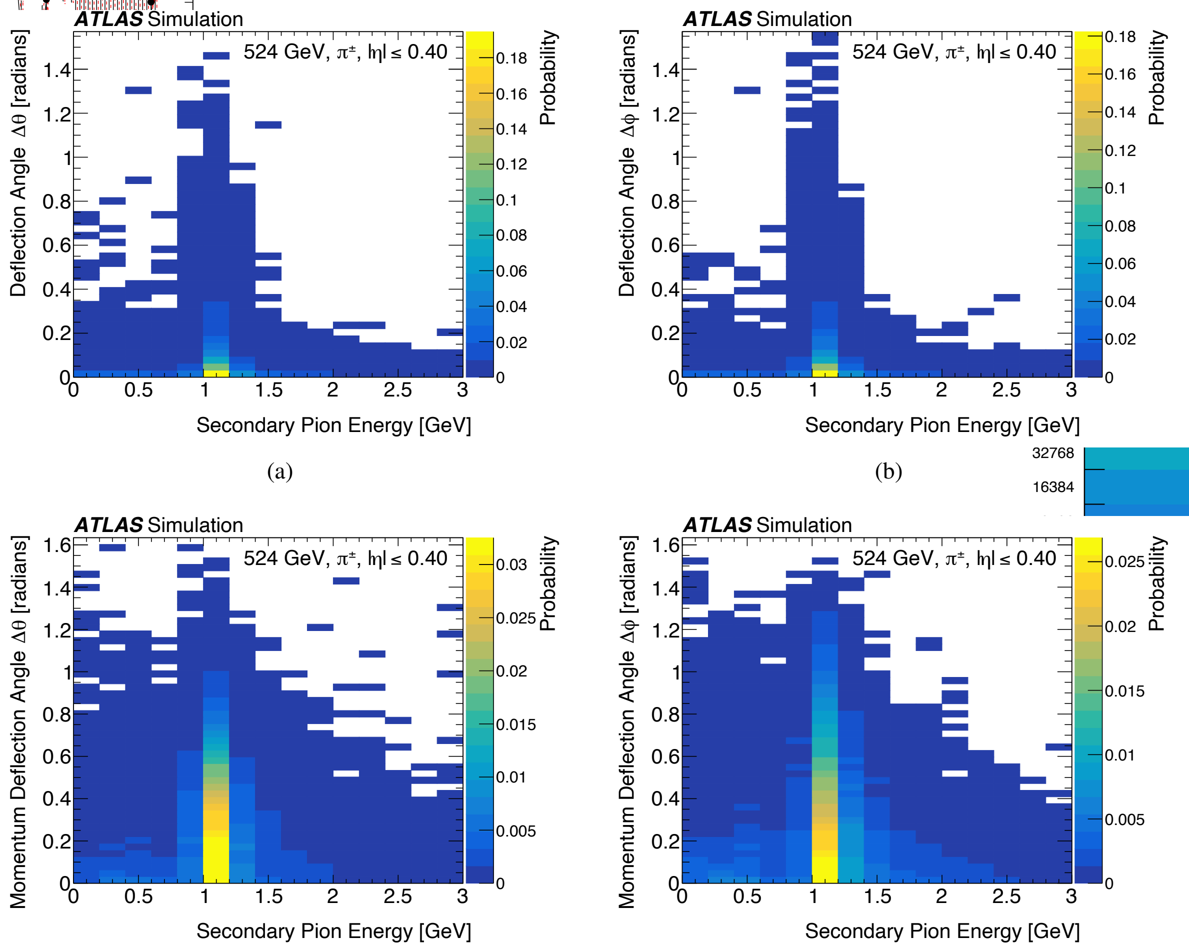
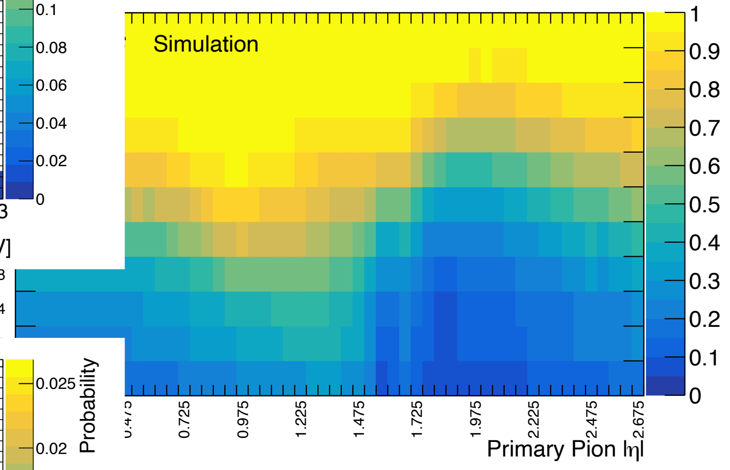
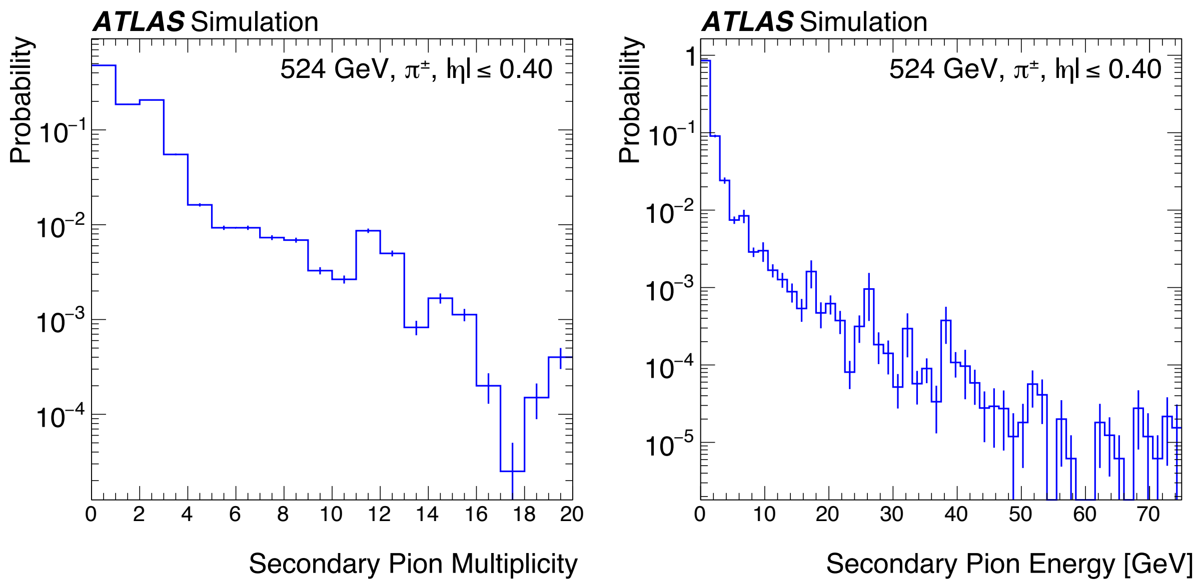


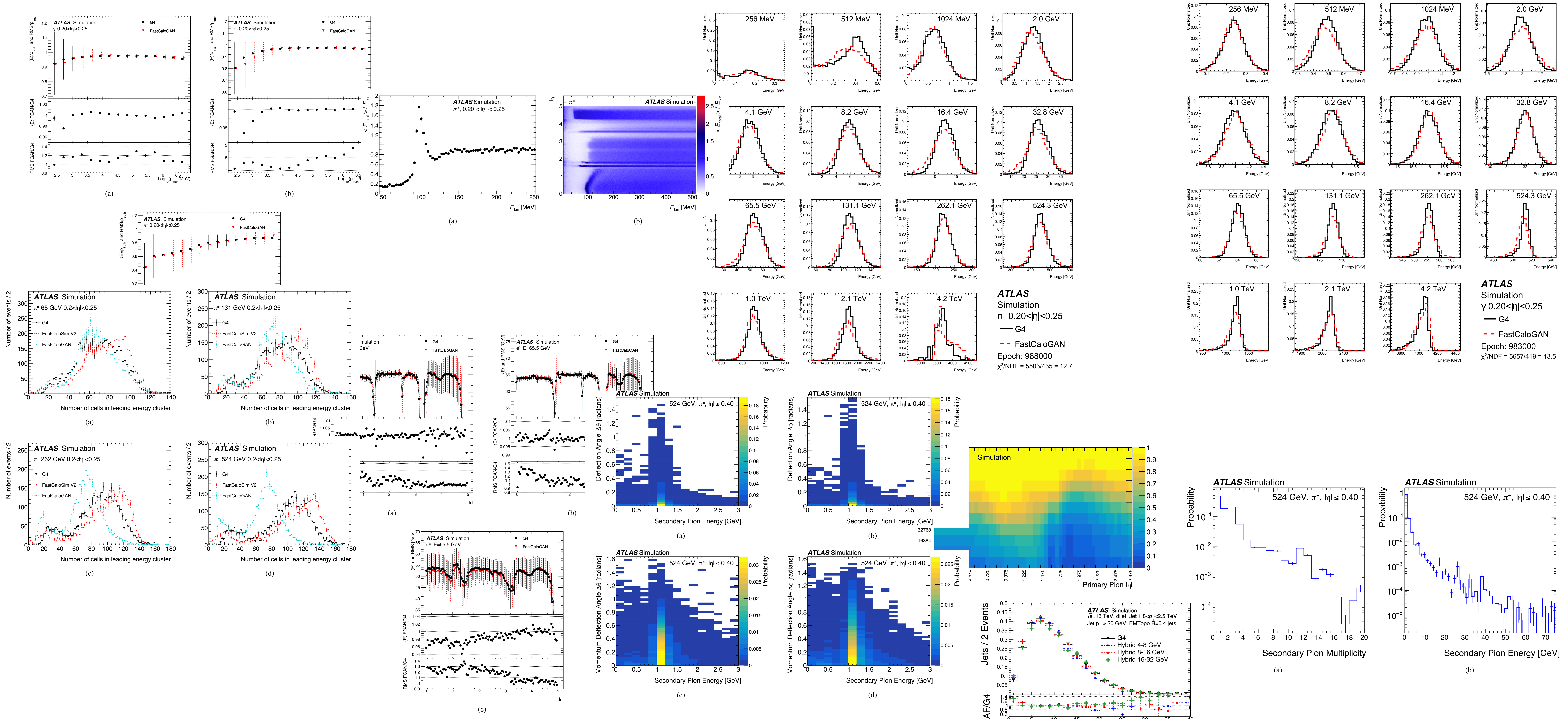
(a) (b) (c) (d)





(a) (b)

Evaluating Fast Calo Simulators



Evaluating Fast Calo Simulators

The evaluation bottleneck

TIME

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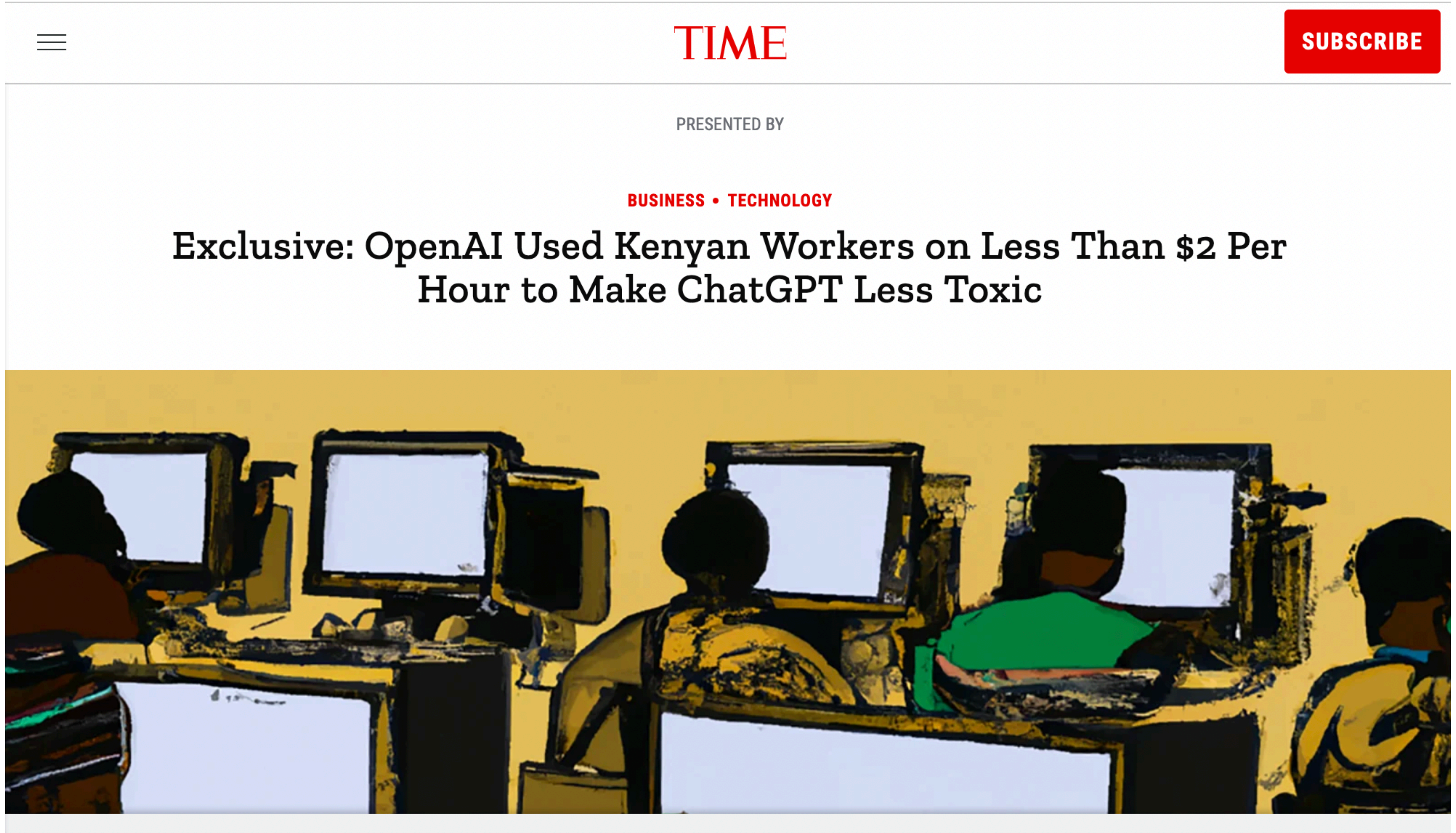
Exclusive: OpenAI Used Kenyan Workers on Less Than $2 Per Hour to Make ChatGPT Less Toxic

The evaluation bottleneck

- Old simulation tools: Took weeks to optimise and update
- ML → Faster turn around time

⇒ Large fraction of human time spent on evaluating models !


TIME

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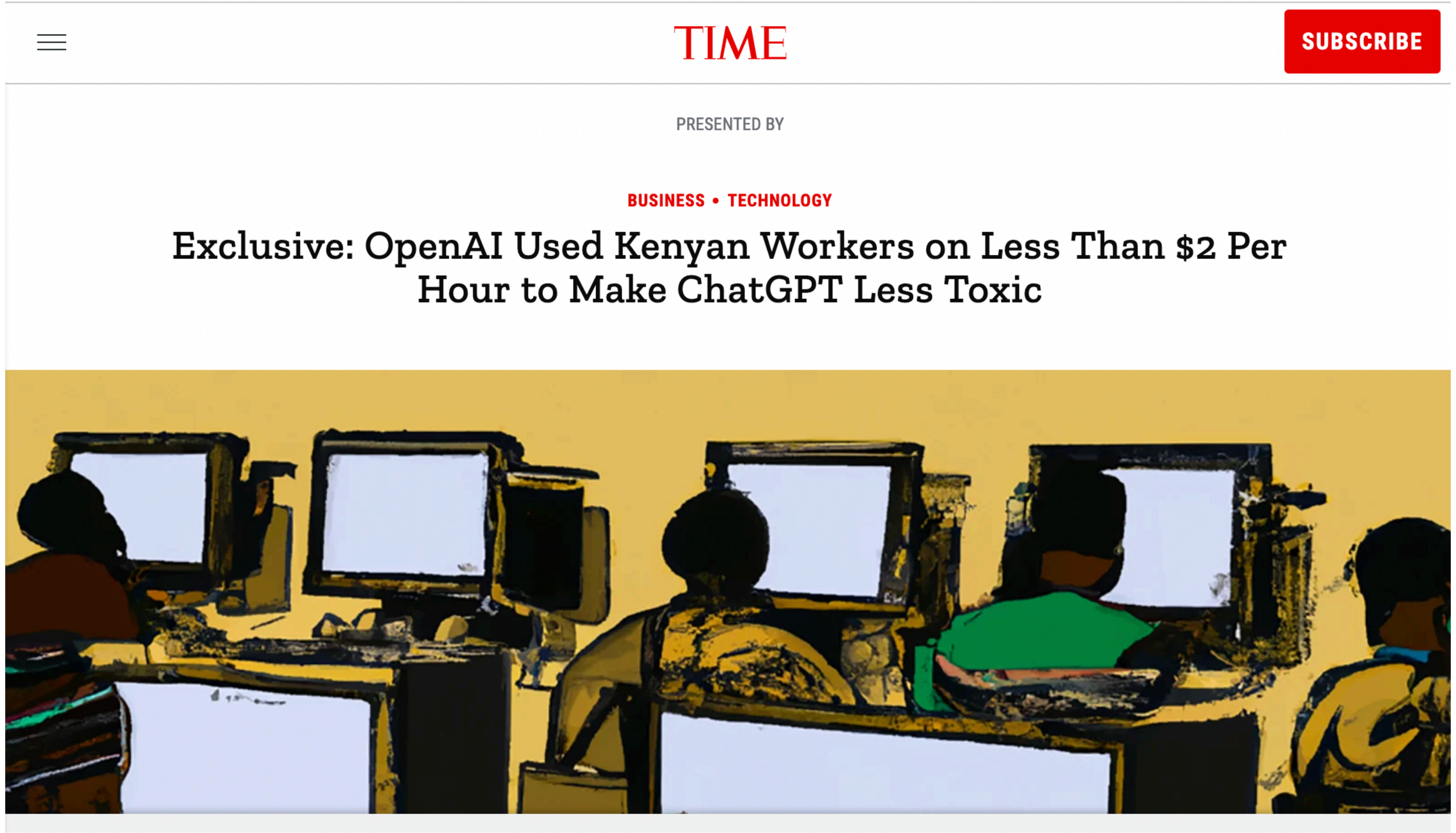


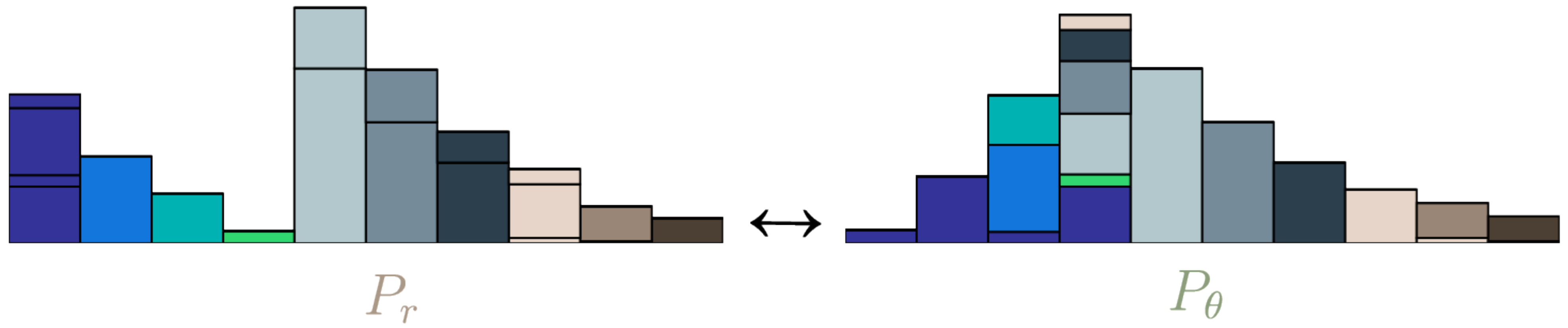
PhD in Plot Evaluation

How can we automise the evaluation ?

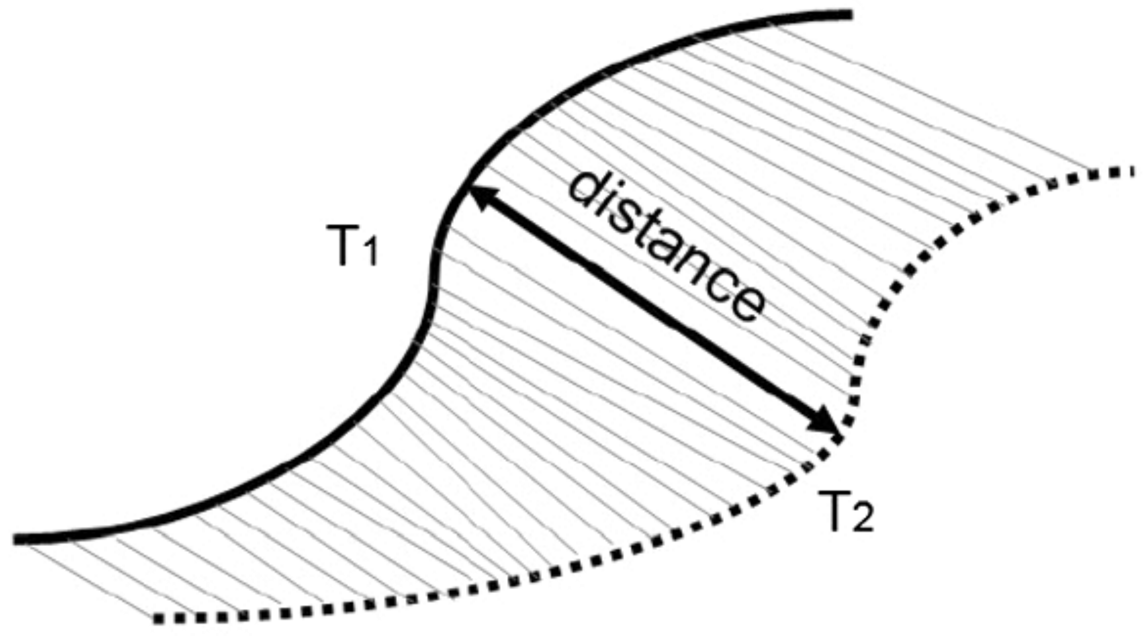
Need measures of distance → Several options thrown around in recent years

$$\frac{P(x \,|\, Geant)}{P(x \,|\, Gen)}$$

Likelihood Ratio



Wasserstein Distance



Fréchet Distance

A large comparison of metrics

[Kansal et al, 2022](#)

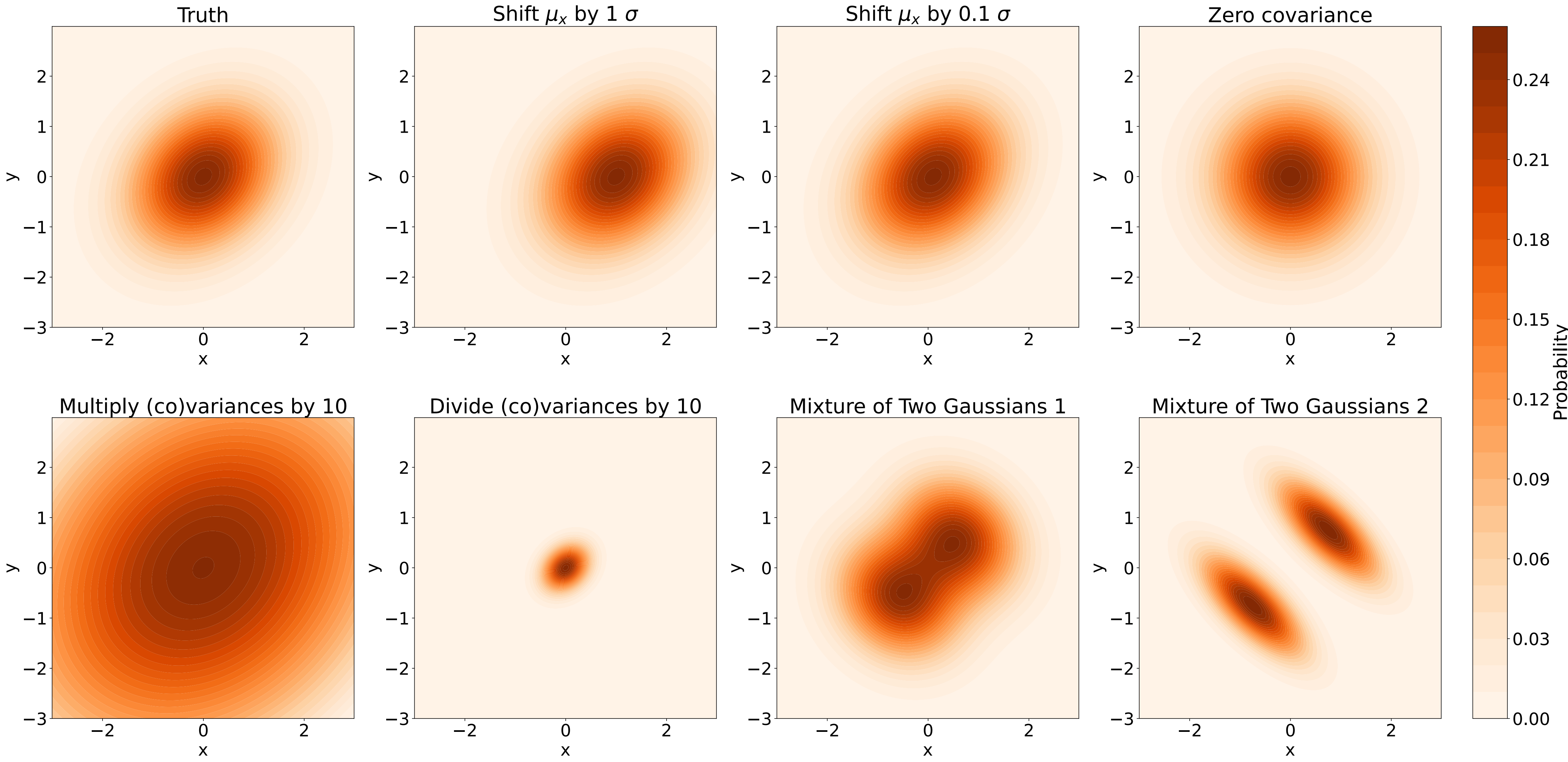
On the Evaluation of Generative Models in High Energy Physics

Raghav Kansal,* Anni Li, and Javier Duarte
University of California San Diego, La Jolla, CA 92093, USA

Nadezda Chernyavskaya, Maurizio Pierini
European Center for Nuclear Research (CERN), 1211 Geneva 23, Switzerland

Breno Orzari, Thiago Tomei
Universidade Estadual Paulista, São Paulo/SP, CEP 01049-010, Brazil

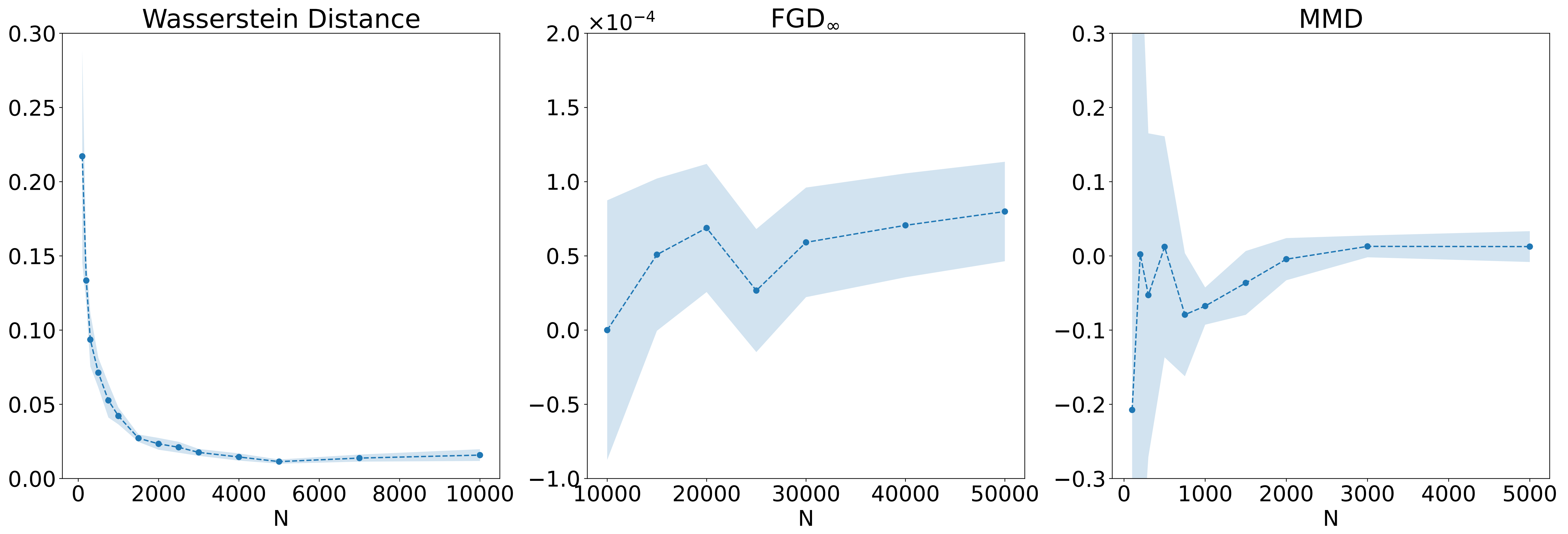
(Dated: November 21, 2022)



Detailed comparison on Gaussian toys where you have full control

Application on jet dataset with hand designed distortions

Gaussian Study



- FGD_∞, MMD unbiased
- W too expensive for large N

Metric	Truth	Shift μ_x by 1σ	Shift μ_x by 0.1σ	Zero covariance	Multiply (co)variances by 10	Divide (co)variances by 10	Mixture of Two Gaussians 1	Mixture of Two Gaussians 2
Wasserstein	0.016 ± 0.004	1.14 ± 0.02	0.043 ± 0.008	0.077 ± 0.006	9.8 ± 0.1	0.97 ± 0.01	$\mathbf{0.036 \pm 0.003}$	$\mathbf{0.191 \pm 0.005}$
$\mathrm{FGD}_\infty \times 10^3$	0.08 ± 0.03	$\mathbf{1011 \pm 1}$	$\mathbf{11.0 \pm 0.1}$	$\mathbf{32.3 \pm 0.2}$	9400 ± 8	$\mathbf{935.1 \pm 0.7}$	0.07 ± 0.03	0.03 ± 0.03
MMD	0.01 ± 0.02	16.4 ± 0.9	0.07 ± 0.04	0.40 ± 0.08	$\mathbf{19k \pm 1k}$	4.3 ± 0.1	0.06 ± 0.02	0.35 ± 0.03
Precision	0.972 ± 0.005	0.91 ± 0.01	0.976 ± 0.004	0.969 ± 0.006	0.34 ± 0.01	1.0 ± 0.0	0.975 ± 0.003	0.9976 ± 0.0007
Recall	0.997 ± 0.001	0.992 ± 0.003	0.997 ± 0.001	0.9976 ± 0.0006	0.998 ± 0.001	0.58 ± 0.02	0.996 ± 0.001	0.9970 ± 0.0009
Density	3.23 ± 0.06	2.48 ± 0.08	3.19 ± 0.07	3.1 ± 0.1	0.60 ± 0.02	5.7 ± 0.3	2.99 ± 0.09	0.989 ± 0.009
Coverage	0.876 ± 0.002	0.780 ± 0.006	0.872 ± 0.005	0.872 ± 0.004	0.60 ± 0.01	0.406 ± 0.008	0.871 ± 0.002	0.956 ± 0.006

FGD_∞ most promising
(with caveats)

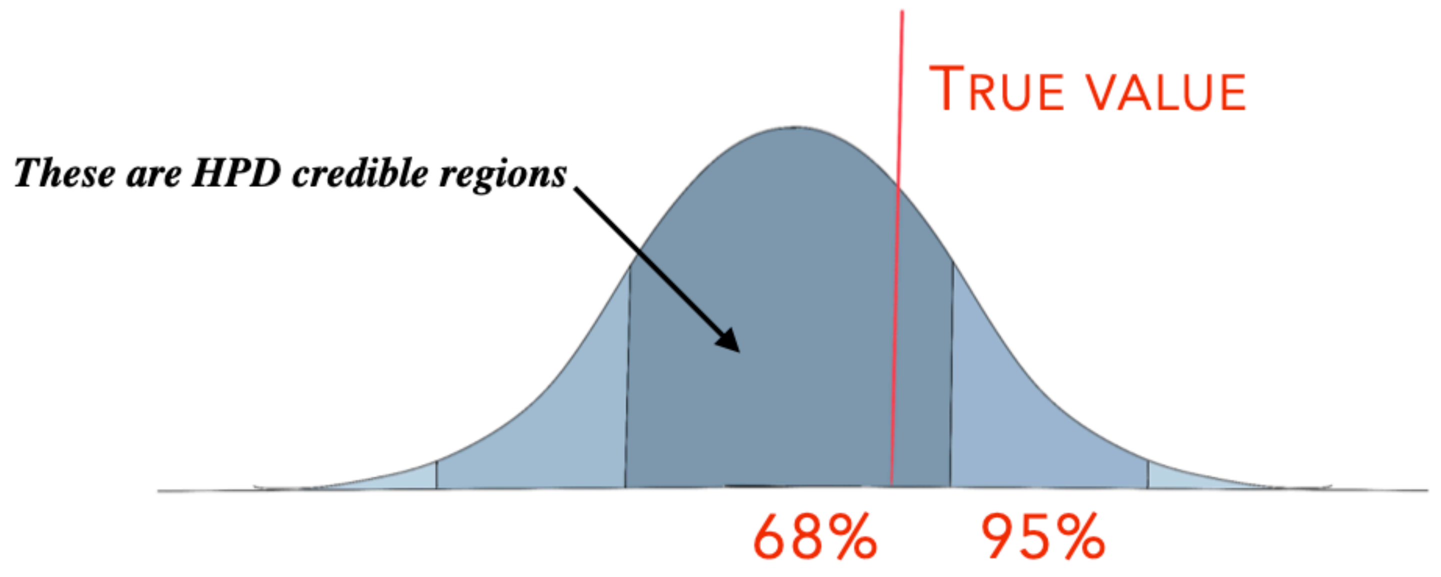
Physics study with jets

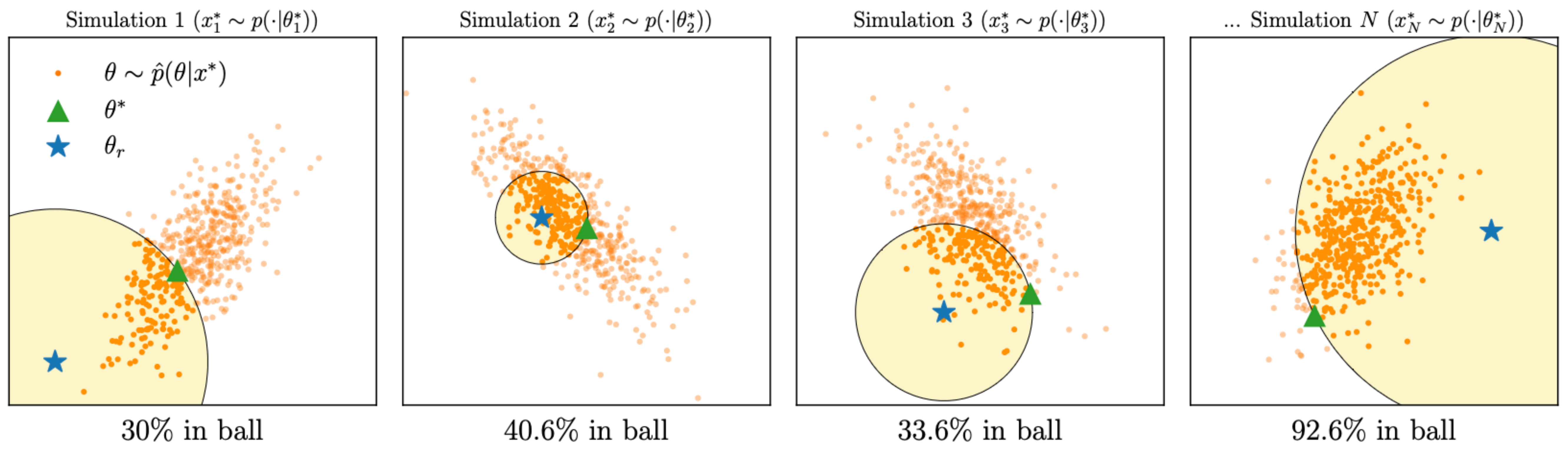
[Kansal et al, 2022](#)

Metric	Truth	Smeared	Shifted	Removing tail	Particle features smeared	Particle η^{rel} smeared	Particle p_T^{rel} smeared	Particle p_T^{rel} shifted
$W_1^M \times 10^3$	0.28 ± 0.05	2.1 ± 0.2	6.0 ± 0.3	0.6 ± 0.2	1.7 ± 0.2	0.9 ± 0.3	0.5 ± 0.2	5.8 ± 0.2
Wasserstein EFP	0.02 ± 0.01	0.09 ± 0.05	0.10 ± 0.02	0.016 ± 0.007	0.19 ± 0.08	0.03 ± 0.01	0.03 ± 0.02	0.06 ± 0.02
FGD_∞ EFP $\times 10^3$	0.01 ± 0.02	$\mathbf{21.5 \pm 0.3}$	$\mathbf{26.8 \pm 0.3}$	$\mathbf{2.31 \pm 0.07}$	23.4 ± 0.3	$\mathbf{3.59 \pm 0.09}$	2.29 ± 0.05	28.9 ± 0.2
MMD EFP $\times 10^3$	-0.006 ± 0.005	0.17 ± 0.06	0.9 ± 0.1	0.03 ± 0.02	0.35 ± 0.09	0.08 ± 0.05	0.01 ± 0.02	1.8 ± 0.1
Precision EFP	0.9 ± 0.1	0.94 ± 0.04	0.978 ± 0.005	0.88 ± 0.08	0.7 ± 0.1	0.94 ± 0.06	0.7 ± 0.1	0.79 ± 0.09
Recall EFP	0.9 ± 0.1	0.88 ± 0.07	0.97 ± 0.01	0.92 ± 0.06	0.83 ± 0.05	0.92 ± 0.07	0.8 ± 0.1	0.8 ± 0.1
Wasserstein PN	1.65 ± 0.06	1.7 ± 0.1	2.4 ± 0.4	1.71 ± 0.08	4.5 ± 0.1	1.79 ± 0.05	4.0 ± 0.4	7.6 ± 0.2
FGD_∞ PN $\times 10^3$	0.8 ± 0.7	40 ± 2	193 ± 9	5.0 ± 0.9	$\mathbf{1250 \pm 10}$	20 ± 1	$\mathbf{1230 \pm 10}$	$\mathbf{3640 \pm 10}$
MMD PN $\times 10^3$	-2 ± 2	4 ± 8	80 ± 10	-1 ± 4	500 ± 100	3 ± 2	560 ± 60	1100 ± 40
Precision PN	0.68 ± 0.07	0.64 ± 0.04	0.71 ± 0.06	0.73 ± 0.03	0.09 ± 0.04	0.75 ± 0.08	0.08 ± 0.04	0.39 ± 0.08
Recall PN	0.70 ± 0.05	0.61 ± 0.04	0.61 ± 0.08	0.73 ± 0.06	0.014 ± 0.009	0.7 ± 0.1	0.01 ± 0.01	0.57 ± 0.09
Classifier LLF AUC	0.50	0.52	0.54	0.50	0.97	0.81	0.93	0.99
Classifier HLF AUC	0.50	0.53	0.55	0.50	0.84	0.64	0.74	0.92

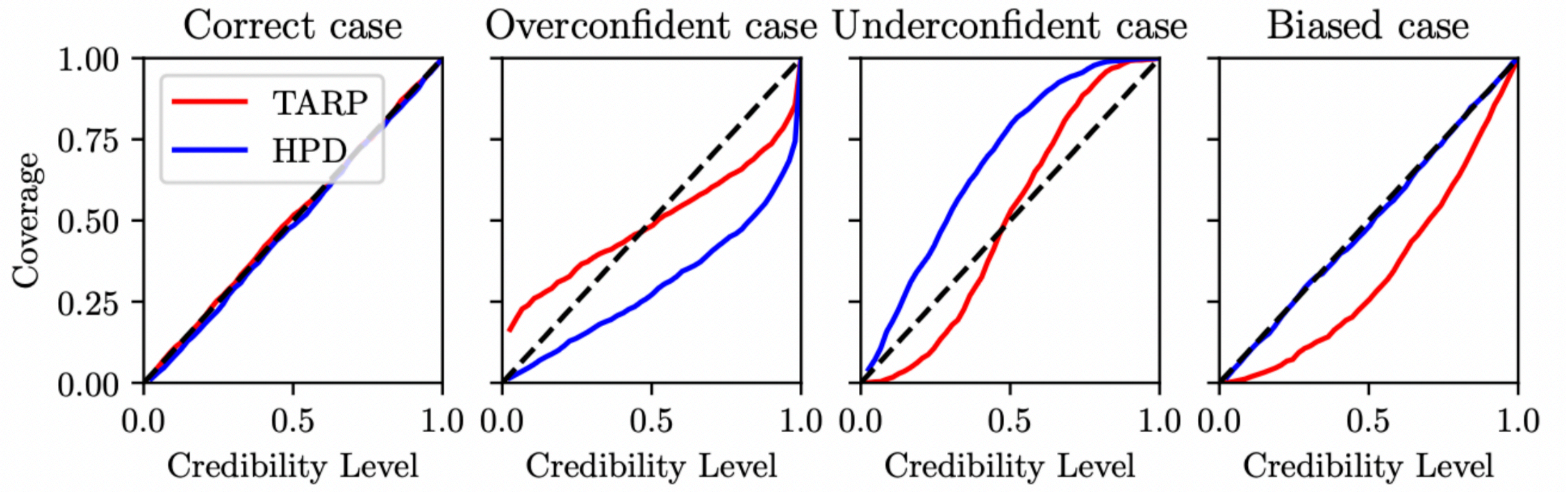
- FGD_∞ on EFPs does quite well in these tests
- Would be interesting to see it used and stress tested !

Coverage tests for generative models in cosmology



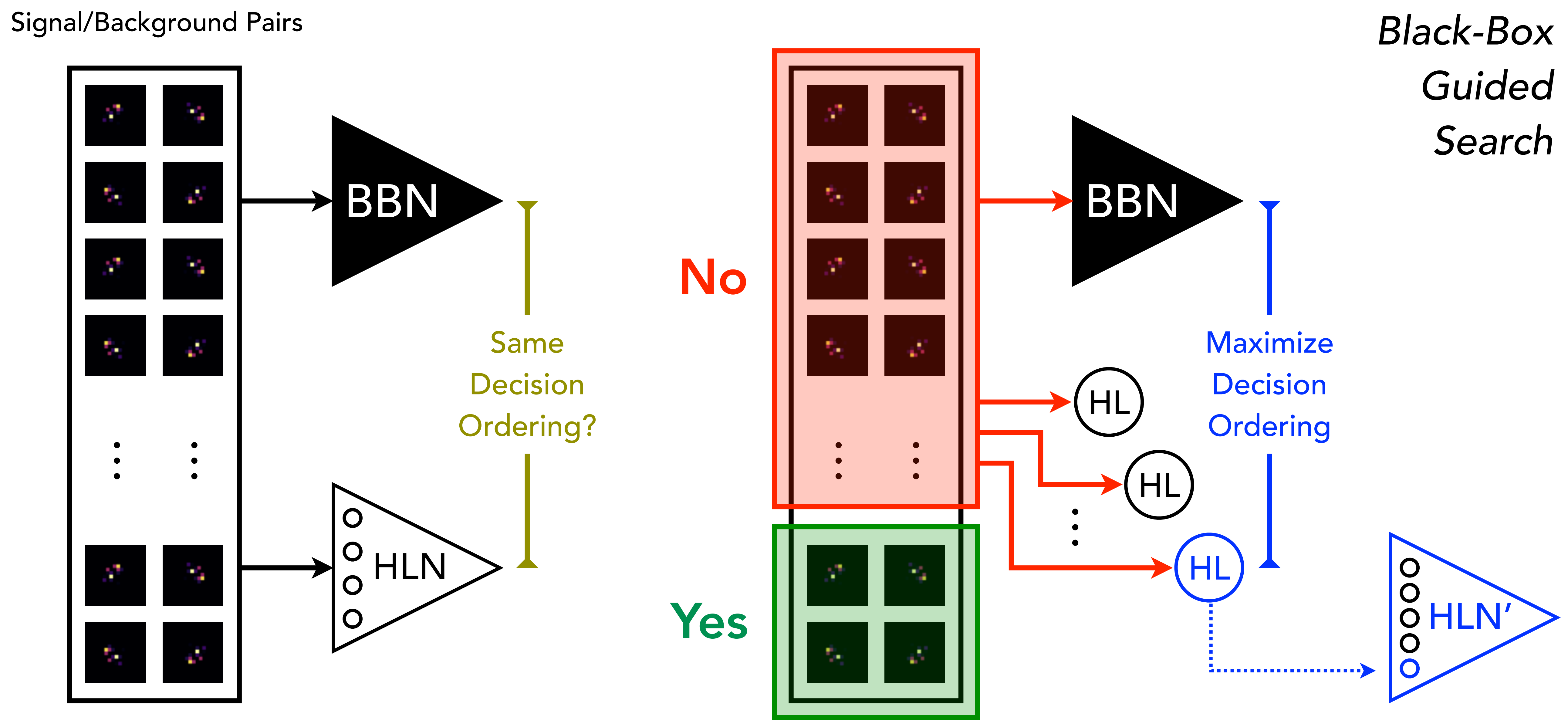


TARP: General purpose diagnostic!



Interpretability

Mapping machine-learned physics into a human-readable space



Rank	EFP	κ	β	Chrom #	ADO[EFP, CNN]$_{X_6}$	AUC[EFP]	ADO[6HL + EFP, CNN]$_{X_{\mathrm{all}}}$	AUC[6HL + EFP]
1		2	$\frac{1}{2}$	3	0.6207	0.8031	0.9714	0.9528 ± 0.0003
2		2	$\frac{1}{2}$	3	0.6205	0.8203	0.9714	0.9524
3		0	–	1	0.6205	0.6737	0.9715	0.9525
4		2	$\frac{1}{2}$	3	0.6199	0.8301	0.9715	0.9527
5		2	$\frac{1}{2}$	3	0.6197	0.8290	0.9714	0.9527
6		2	$\frac{1}{2}$	3	0.6196	0.8251	0.9715	0.9522
7		0	$\frac{1}{2}$	2	0.6187	0.7511	0.9715	0.9526
8		2	$\frac{1}{2}$	3	0.6184	0.8257	0.9712	0.9527
9		2	$\frac{1}{2}$	3	0.6182	0.8090	0.9714	0.9527
10		2	$\frac{1}{2}$	3	0.6180	0.8314	0.9714	0.9526
60		0	1	2	0.6163	0.7194	0.9715	0.9525
341		-1	$\frac{1}{2}$	4	0.6142	0.6286	0.9714	0.9509
589		0	2	2	0.6109	0.7579	0.9714	0.9523
3106		-1	–	1	0.5891	0.5882	0.9714	0.9510
3519		$\frac{1}{2}$	$\frac{1}{2}$	2	0.5664	0.7698	0.9715	0.9524
3521		$\frac{1}{2}$	–	1	0.5663	0.7093	0.9714	0.9522
5531		1	2	1	0.5290	0.7454	0.9714	0.9507
5554		1	$\frac{1}{2}$	2	0.5279	0.8210	0.9713	0.9505
5610		2	–	1	0.5245	0.7117	0.9714	0.9507
5657		1	1	3	0.5224	0.8257	0.9712	0.9506
5793		1	1	2	0.5191	0.8640	0.9714	0.9505
6052		1	2	3	0.5153	0.8500	0.9716	0.9504
7438		1	2	2	0.5011	0.8835	0.9716	0.9506

Energy flow polynomials:
A complete basis to describe jet substructure
arXiv:1712.07124: Komiske et al

Faucett et al.

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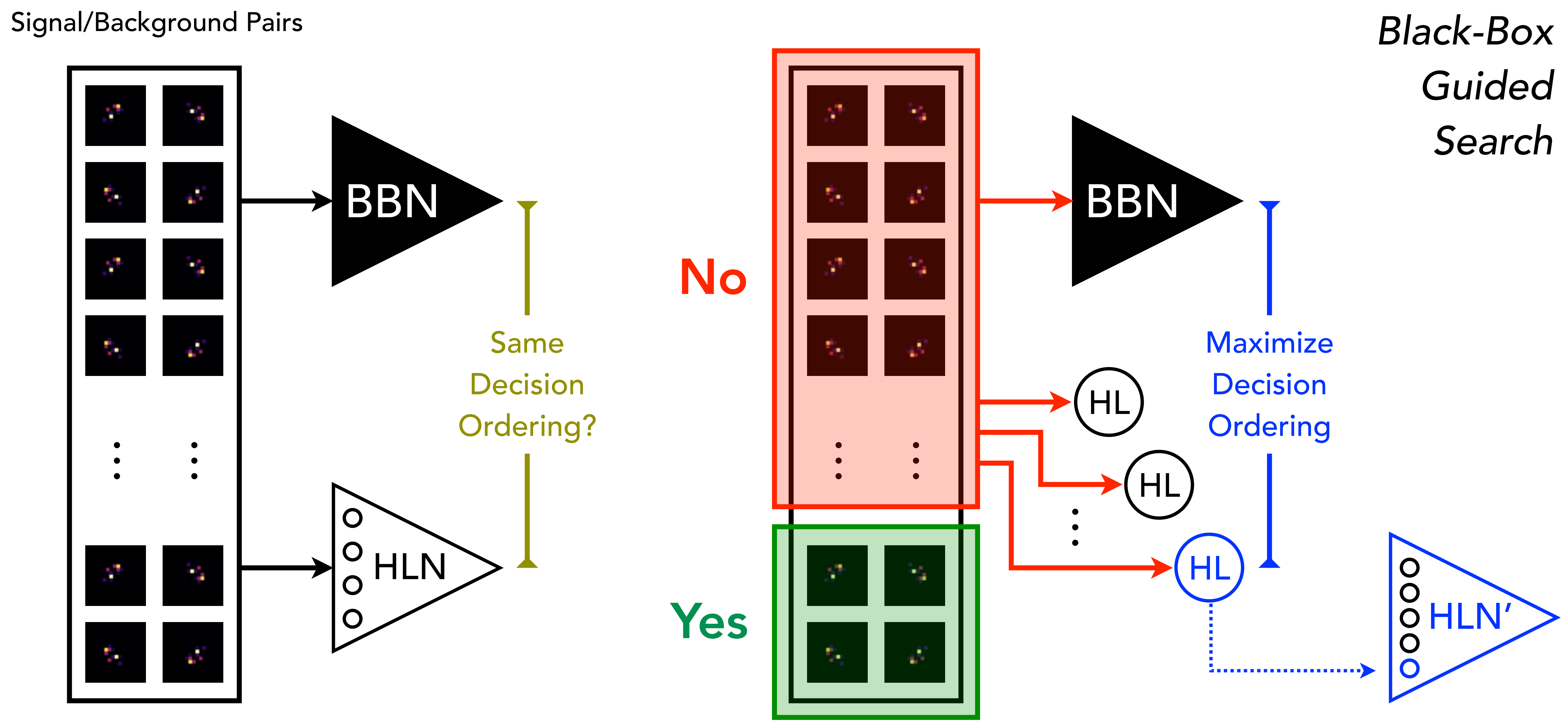

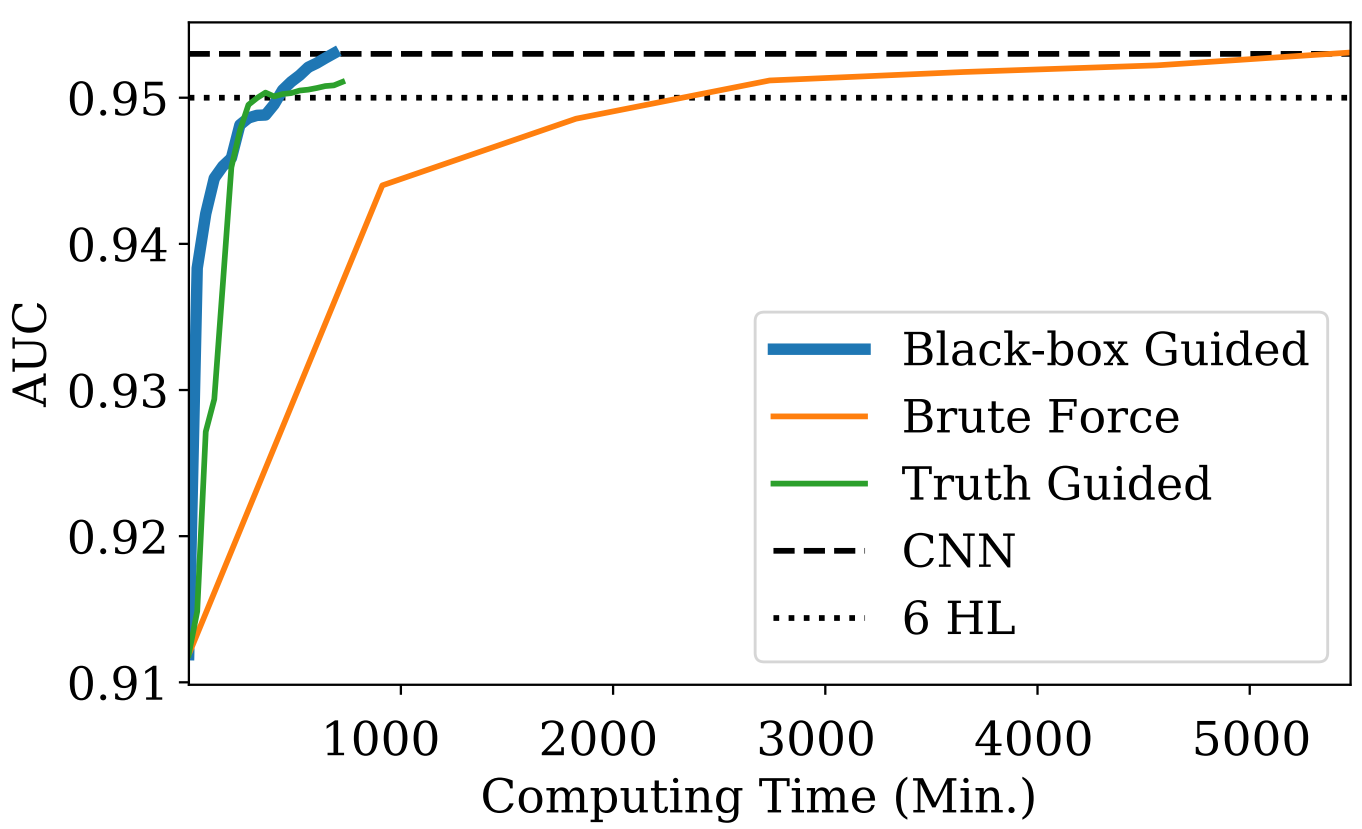

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Faucett et al.

Conclusion

- Significant progress in uncertainty quantification, propagation, mitigation in recent years
    - Expect to see methods adopted in the bigger experiments in coming years

- Research in UQ often motivated my needs in science

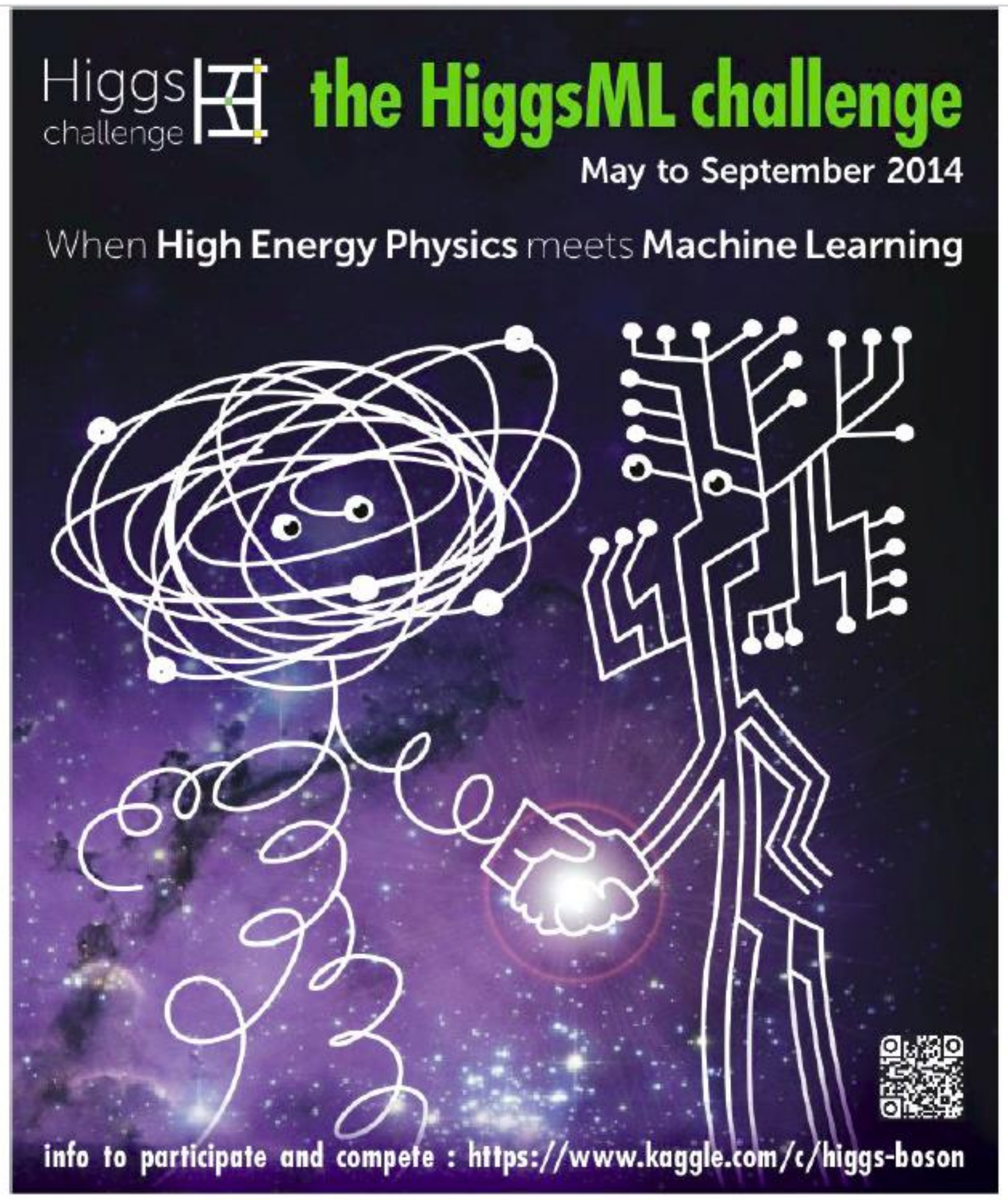
- We talked about:
    - Propagating statistical uncertainties
    - Experimental systematic uncertainties
    - Caution to be taken for theory uncertainties
    - Interpretability
    - Coverage tests and performance evaluation of generative models

- If these questions matter to you, come chat with me!

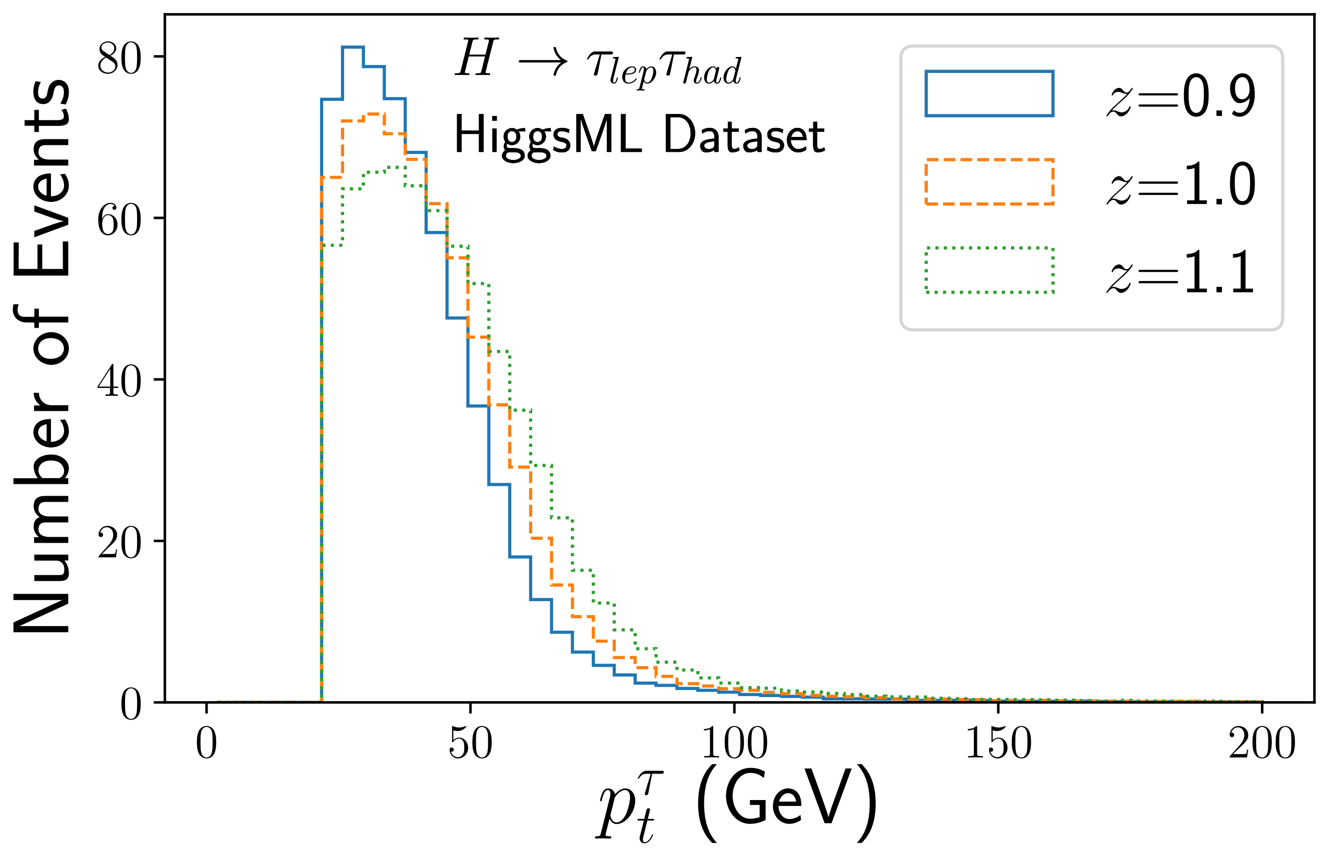
Thank you !

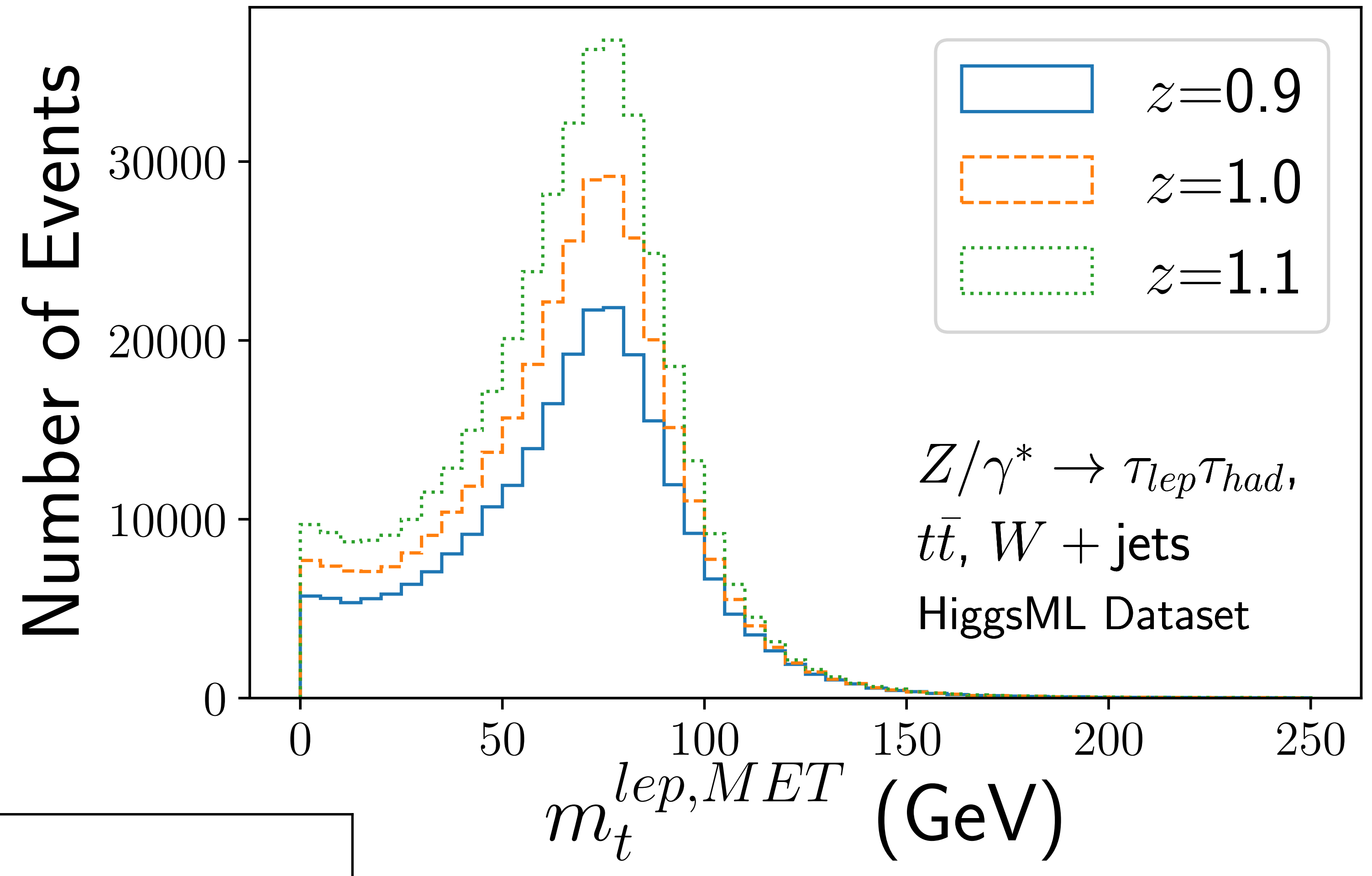
@Aishik_Ghosh_

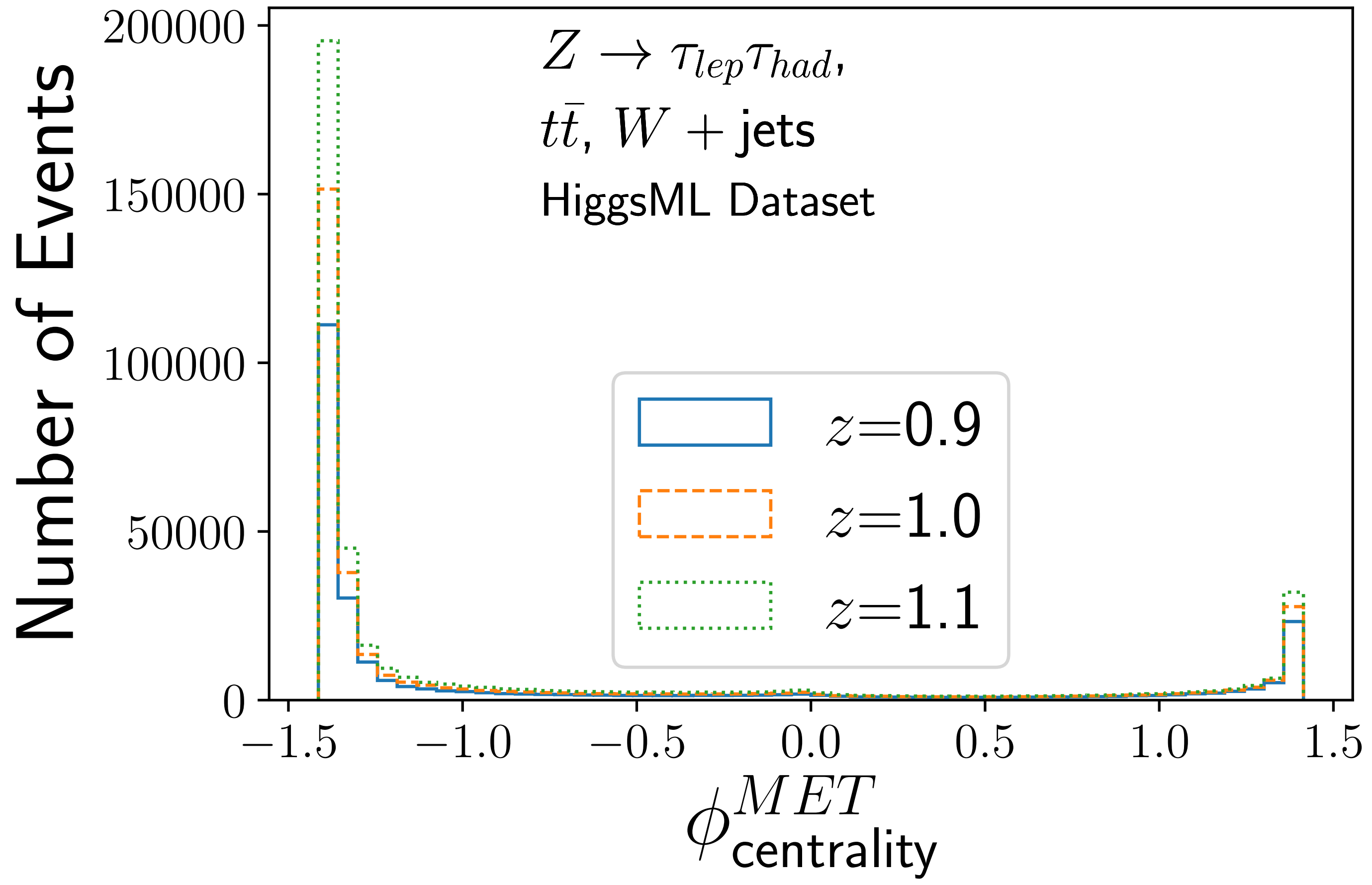
Real Physics Dataset with Tau Energy Scale (TES) as Z



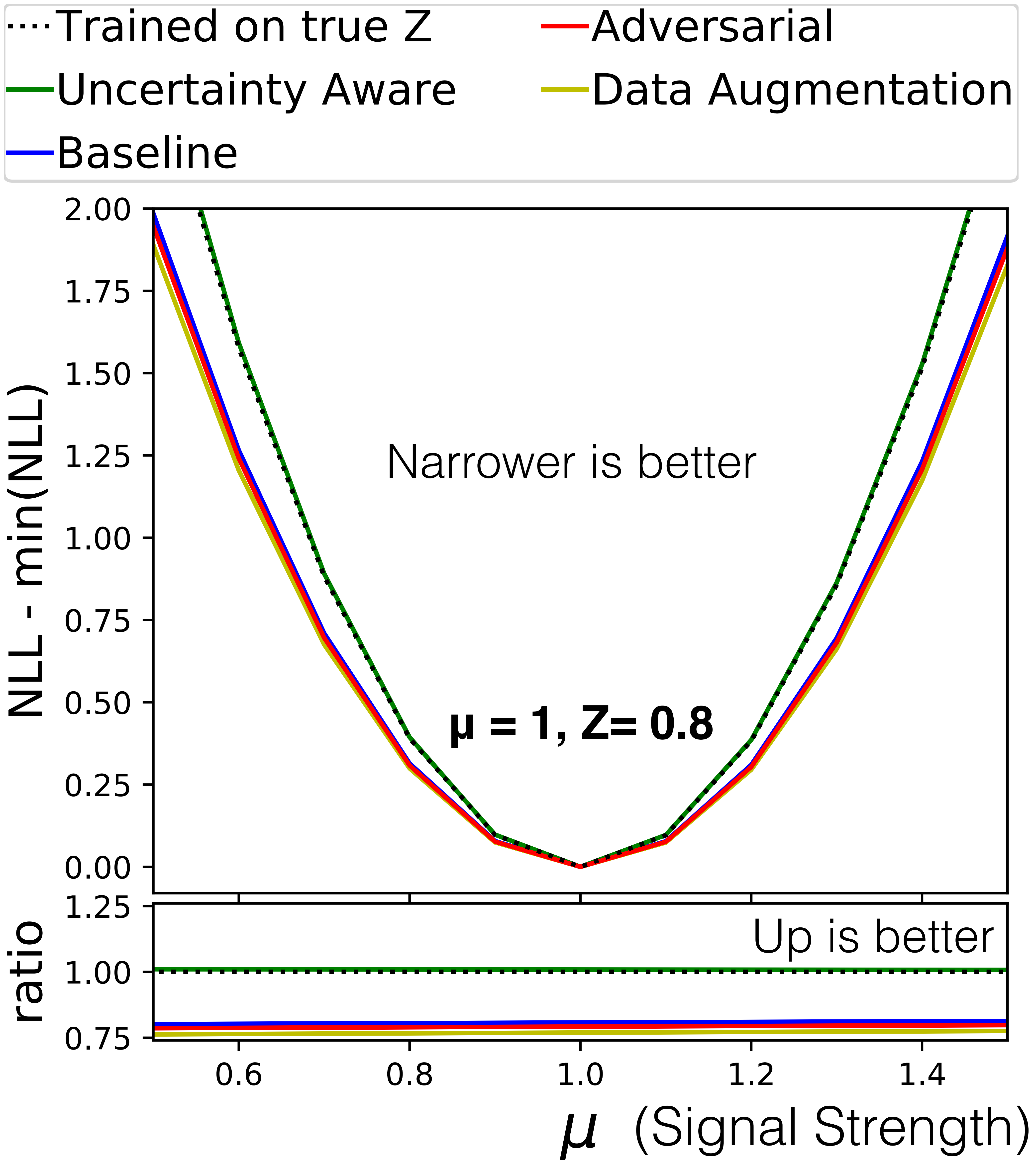
Parameter of Interest is Higgs signal strength μ, and TES is the nuisance parameter Z







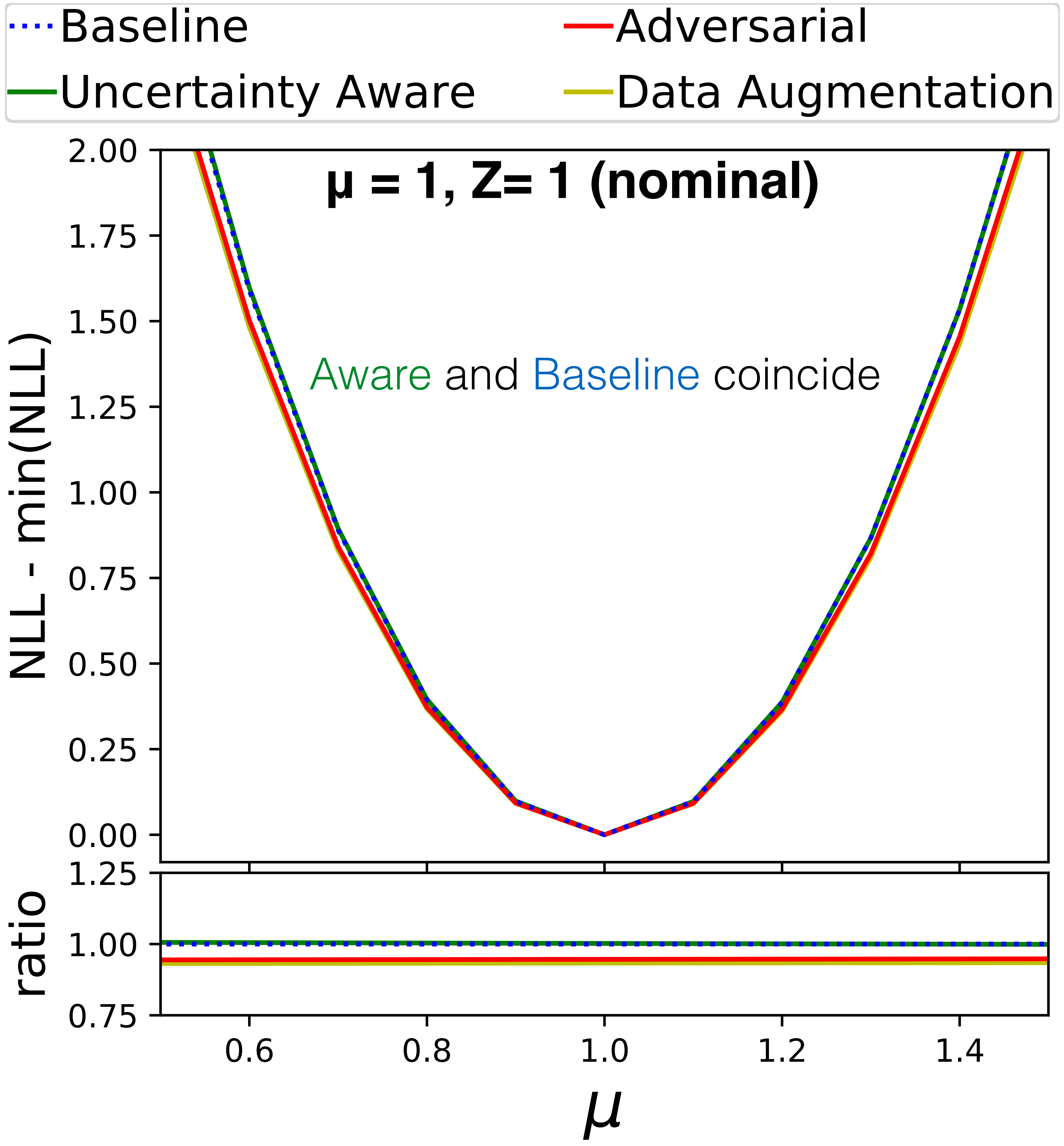
Test performance for “observed” data at Z below Nominal

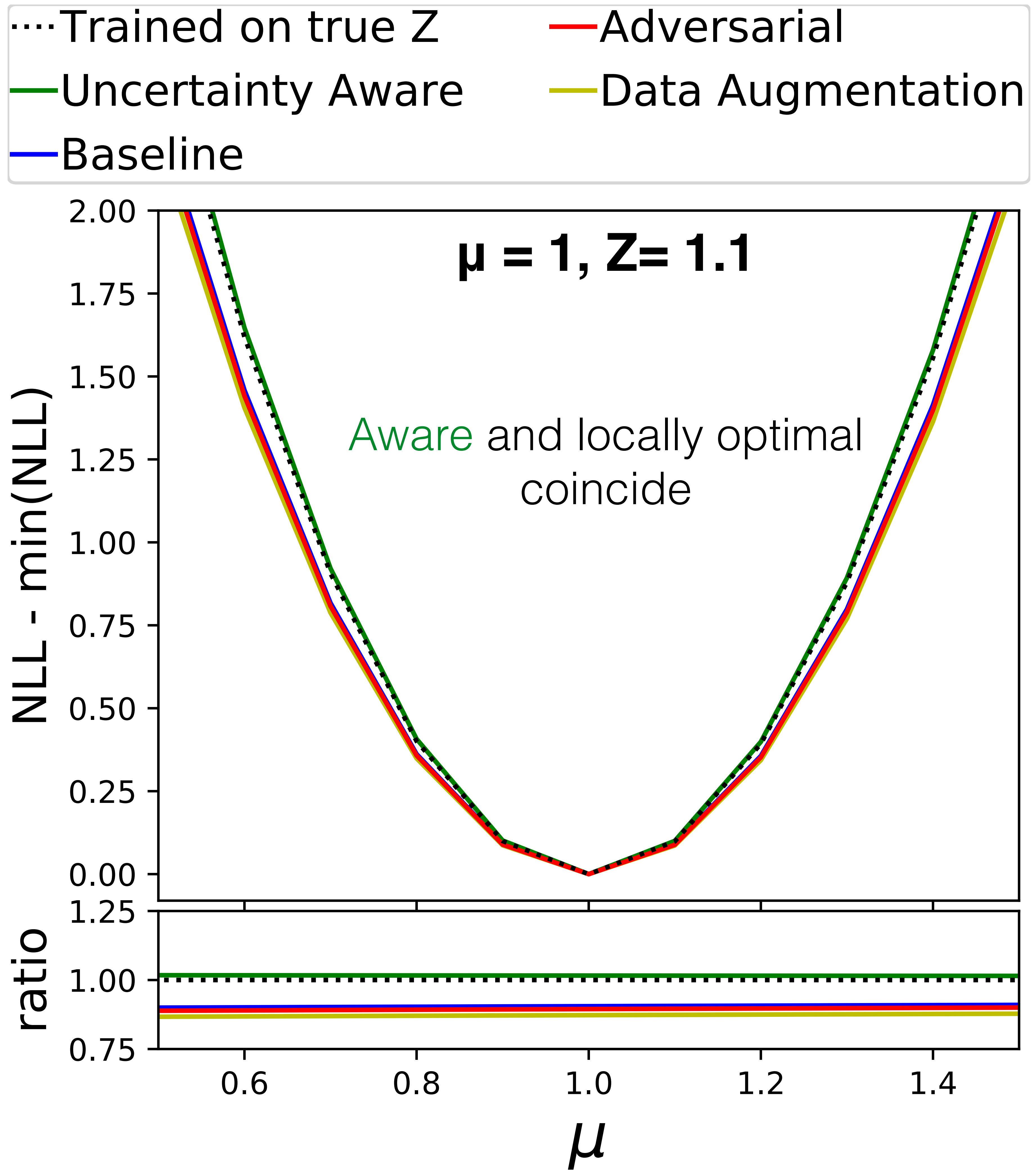


Uncertainty-Aware coincides with classifier trained on true Z

⇒ It is optimal!

Test performance for “observed” data at nominal and above nominal Z





In every case the Aware Classifier is as good as the optimal one, no other technique matches its performance everywhere

Idea fascinating also to ML researchers !

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- ML researchers assume i.i.d
- This technique exploits correlations between samples – a different paradigm
- Interesting applications outside of physics

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arXiv:2007.02931

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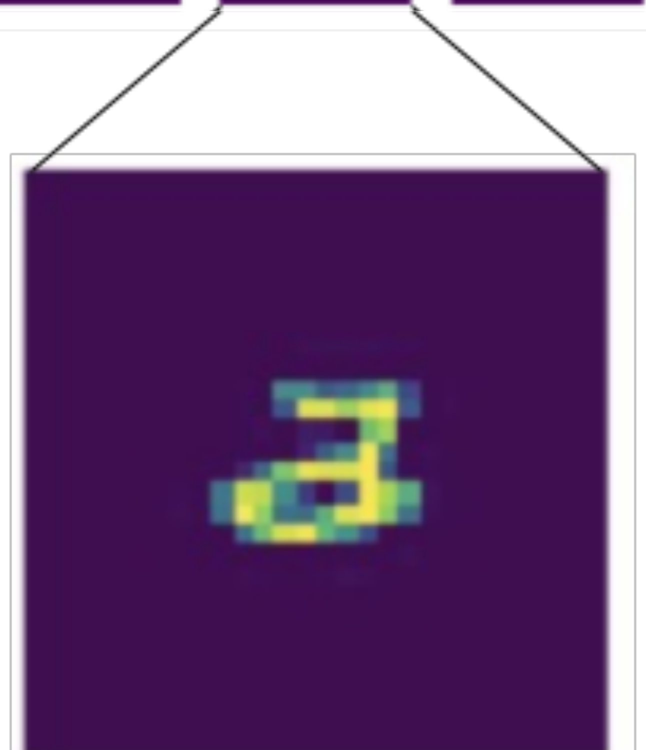

ERM → 2
ARM → a

For my handwriting this is ‘2’, for yours it might be ‘a’
ARM: Adapt to the individual + classify

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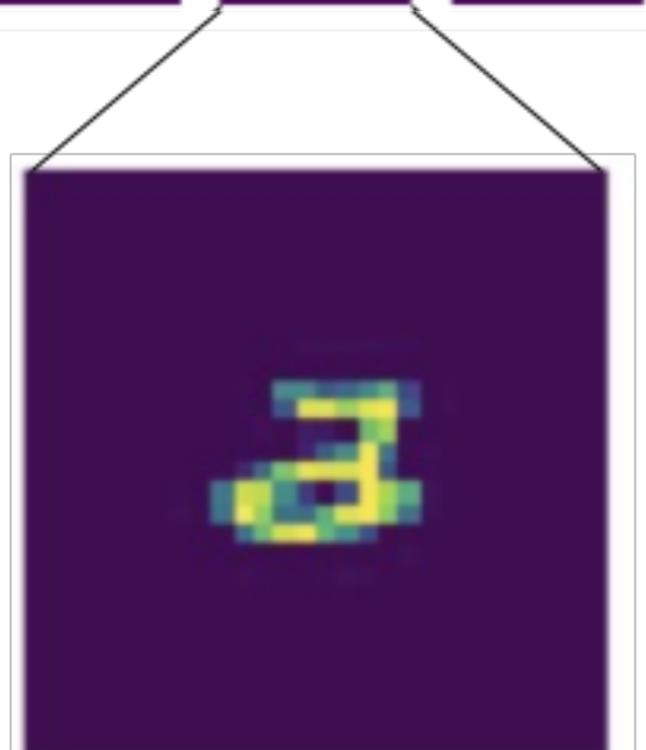

ERM → 2
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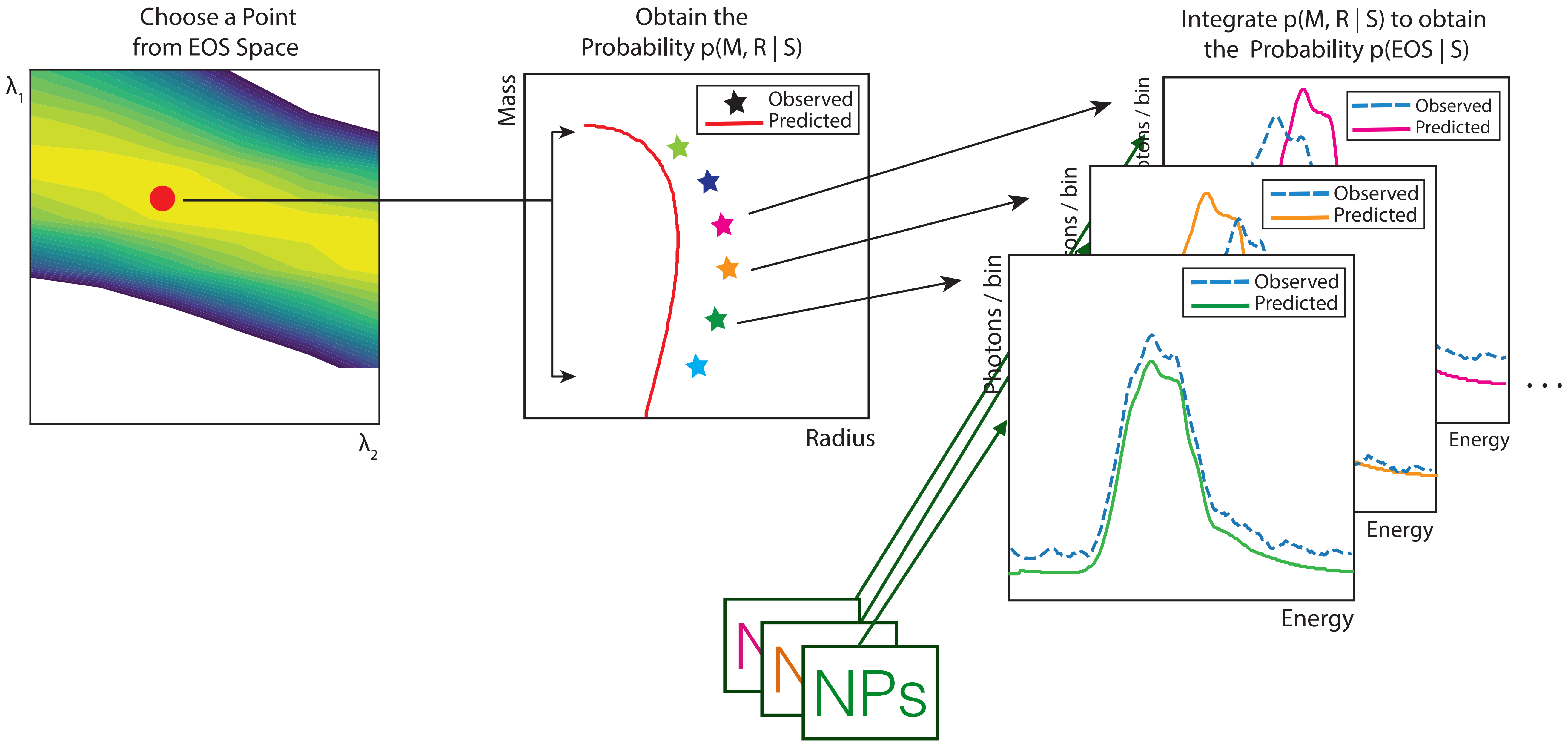
Learn forward process to access the likelihood

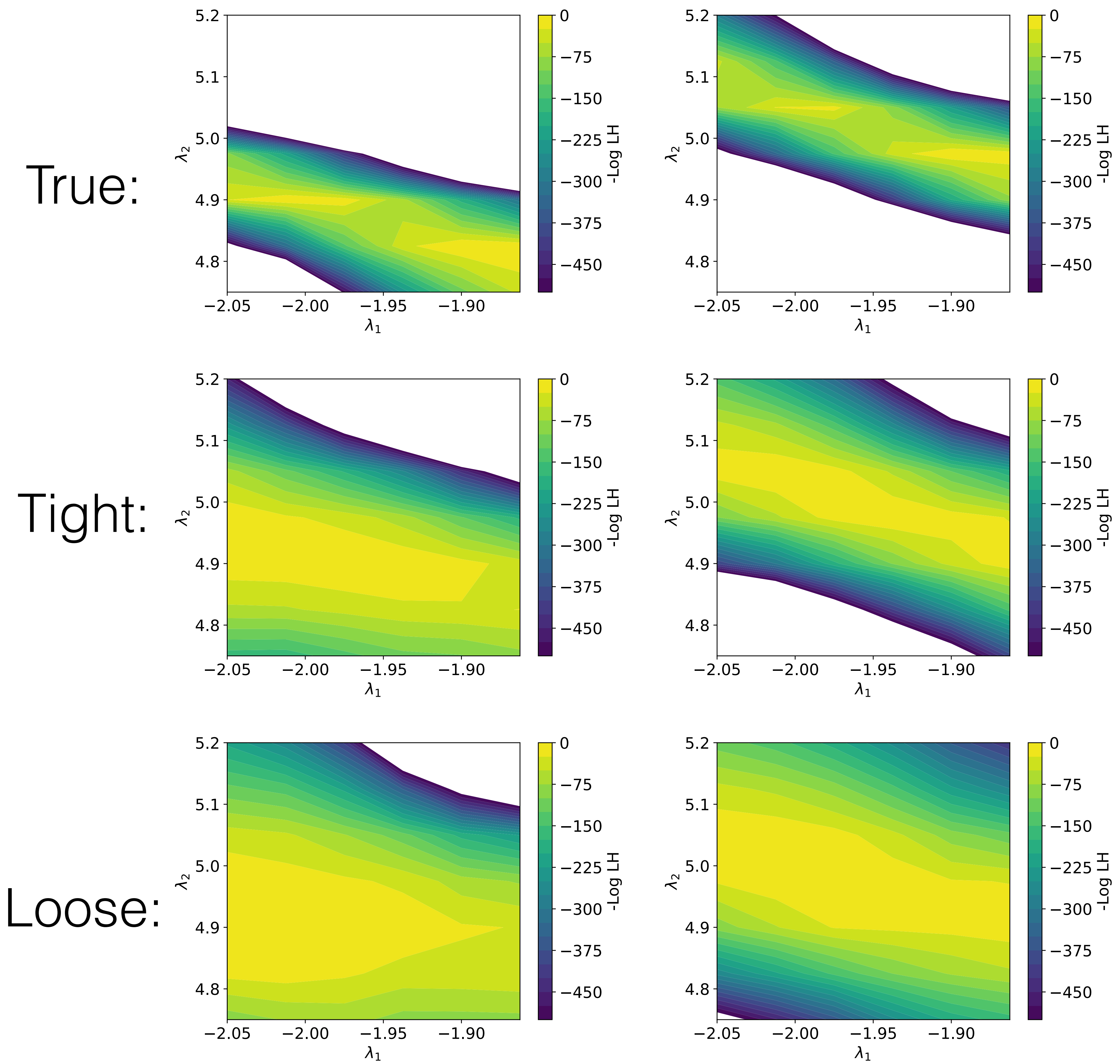


Deploy with ONNX Runtime to compute likelihoods on-the-fly

ONNX RUNTIME

Nuisance Priors:

EOS parameter likelihoods:



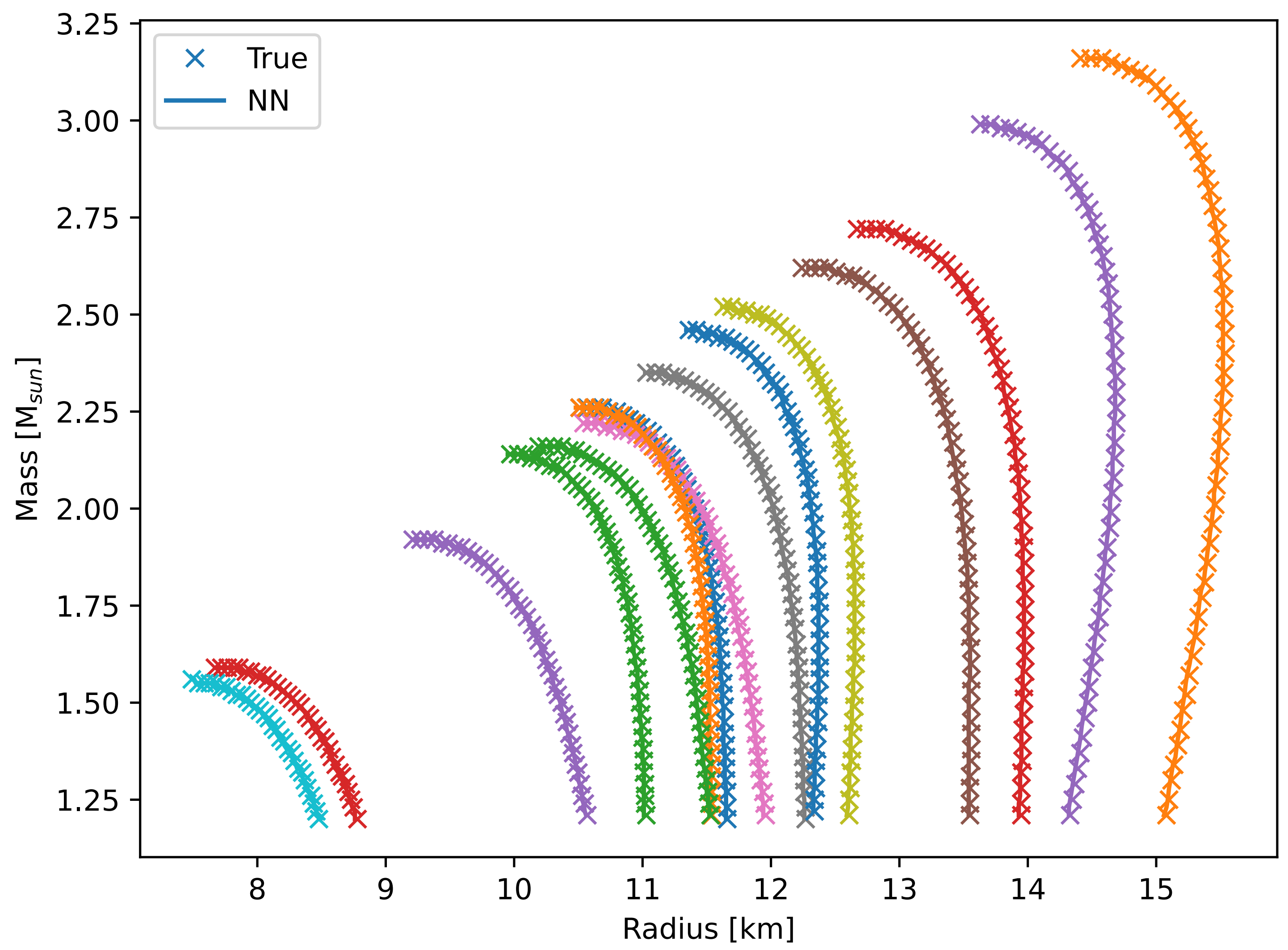
Paper in preparation

Forward process step-by-step

Intermediate steps remain interpretable physical quantities

Forward process step-by-step

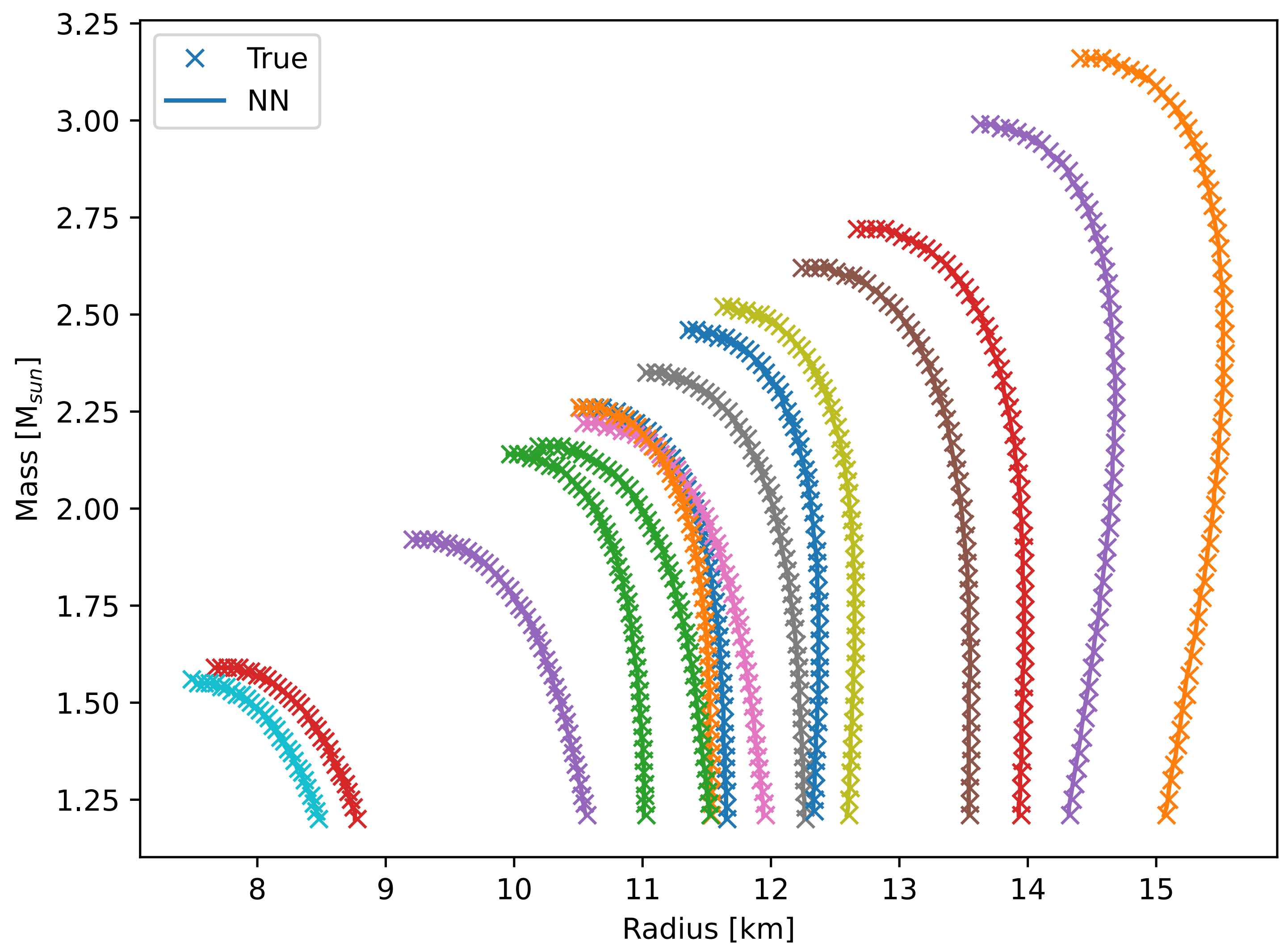
Intermediate steps remain interpretable physical quantities

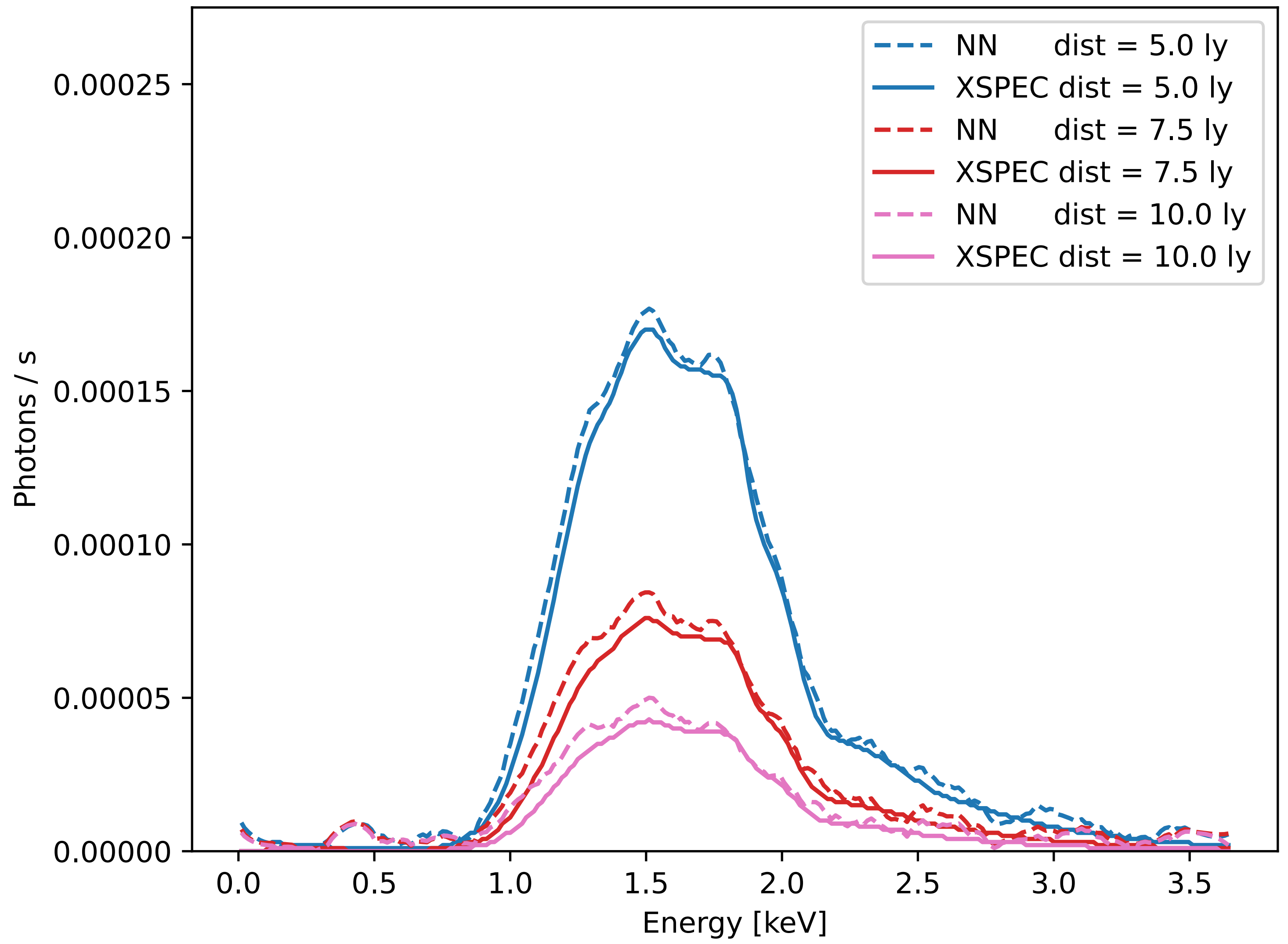


Learn EOS to M-R

Forward process step-by-step

Intermediate steps remain interpretable physical quantities





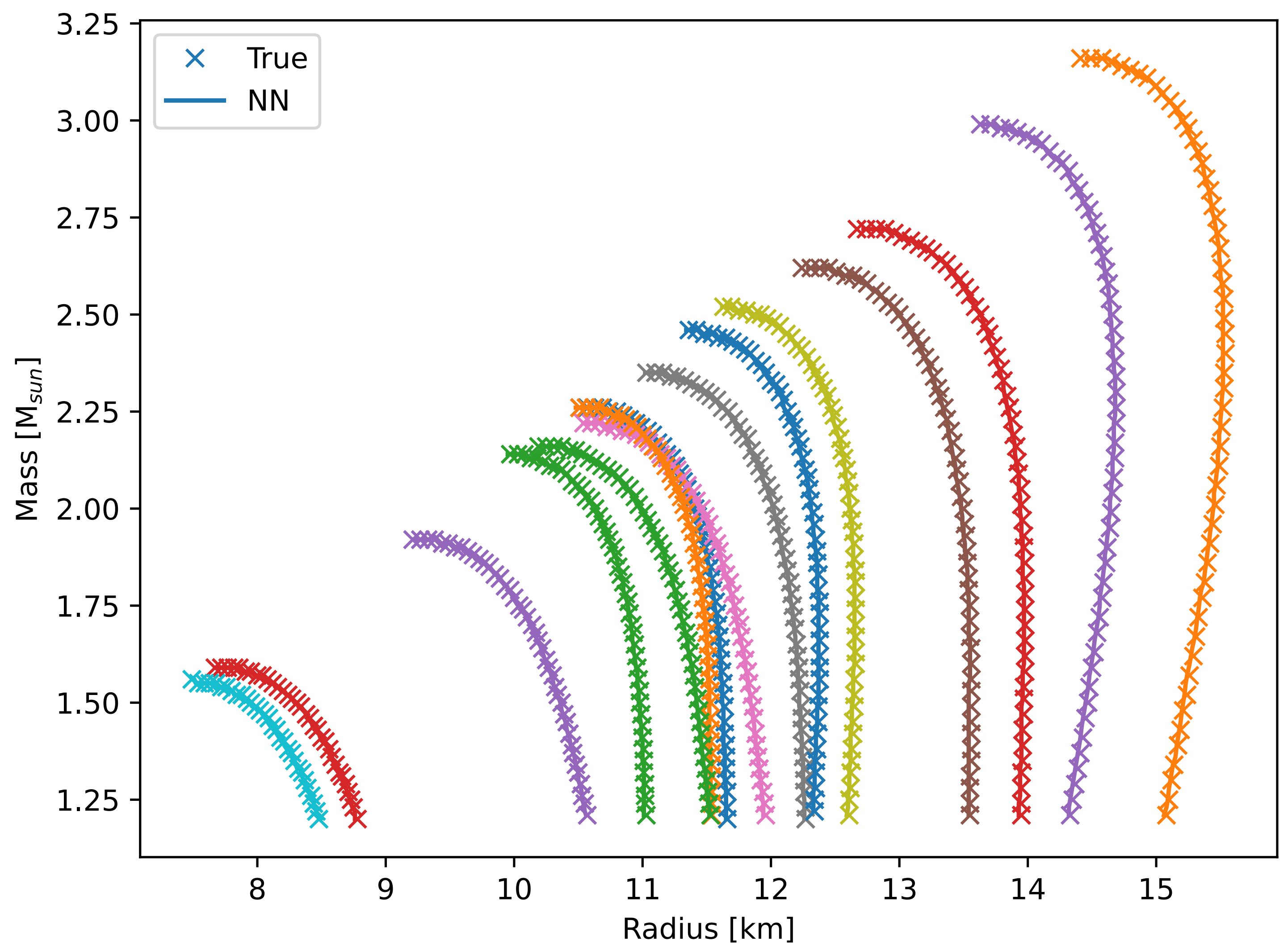
Learn EOS to M-R

Learn {M,R,NPs} to Spectrum

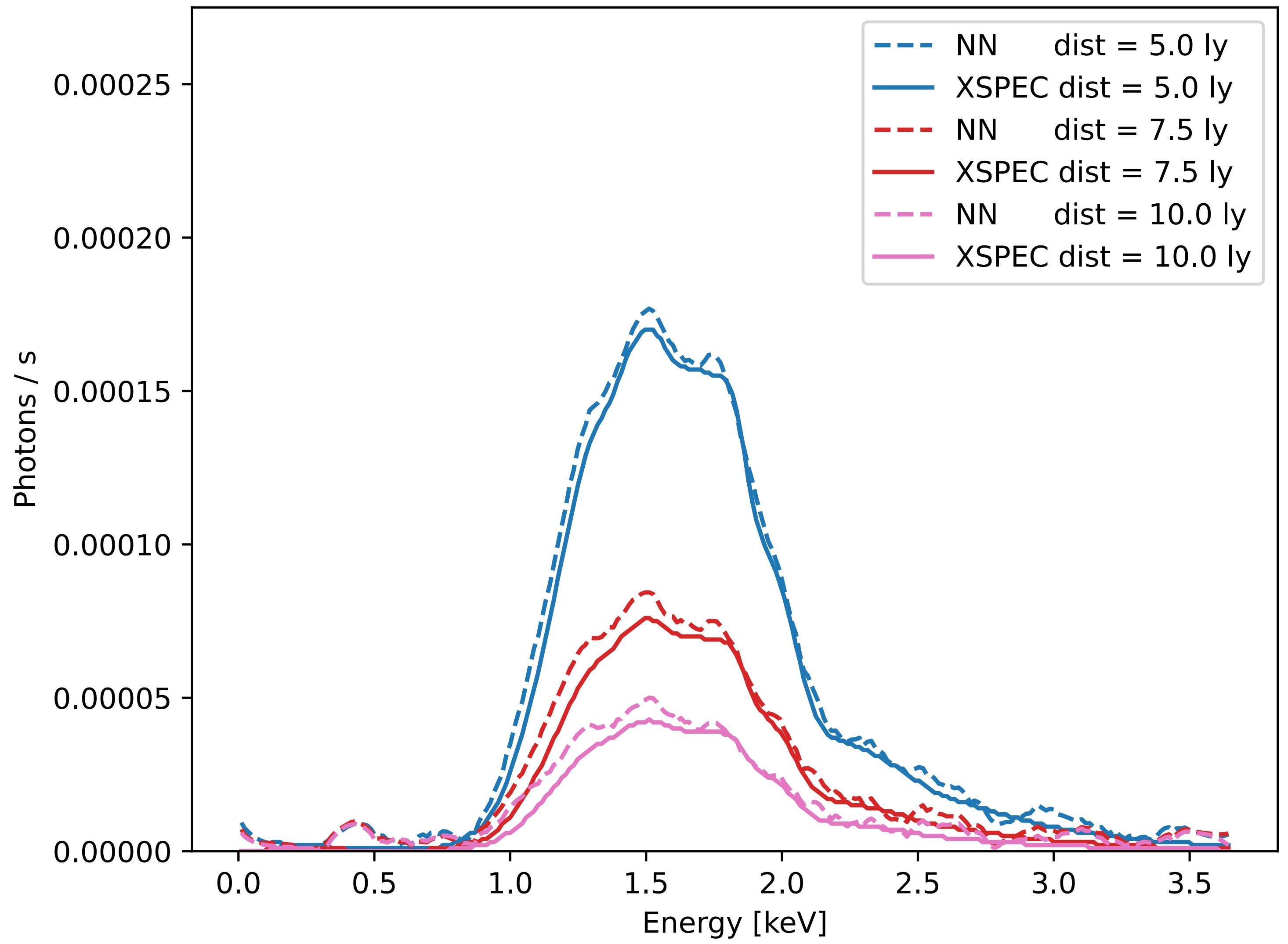
Paper in preparation

Forward process step-by-step

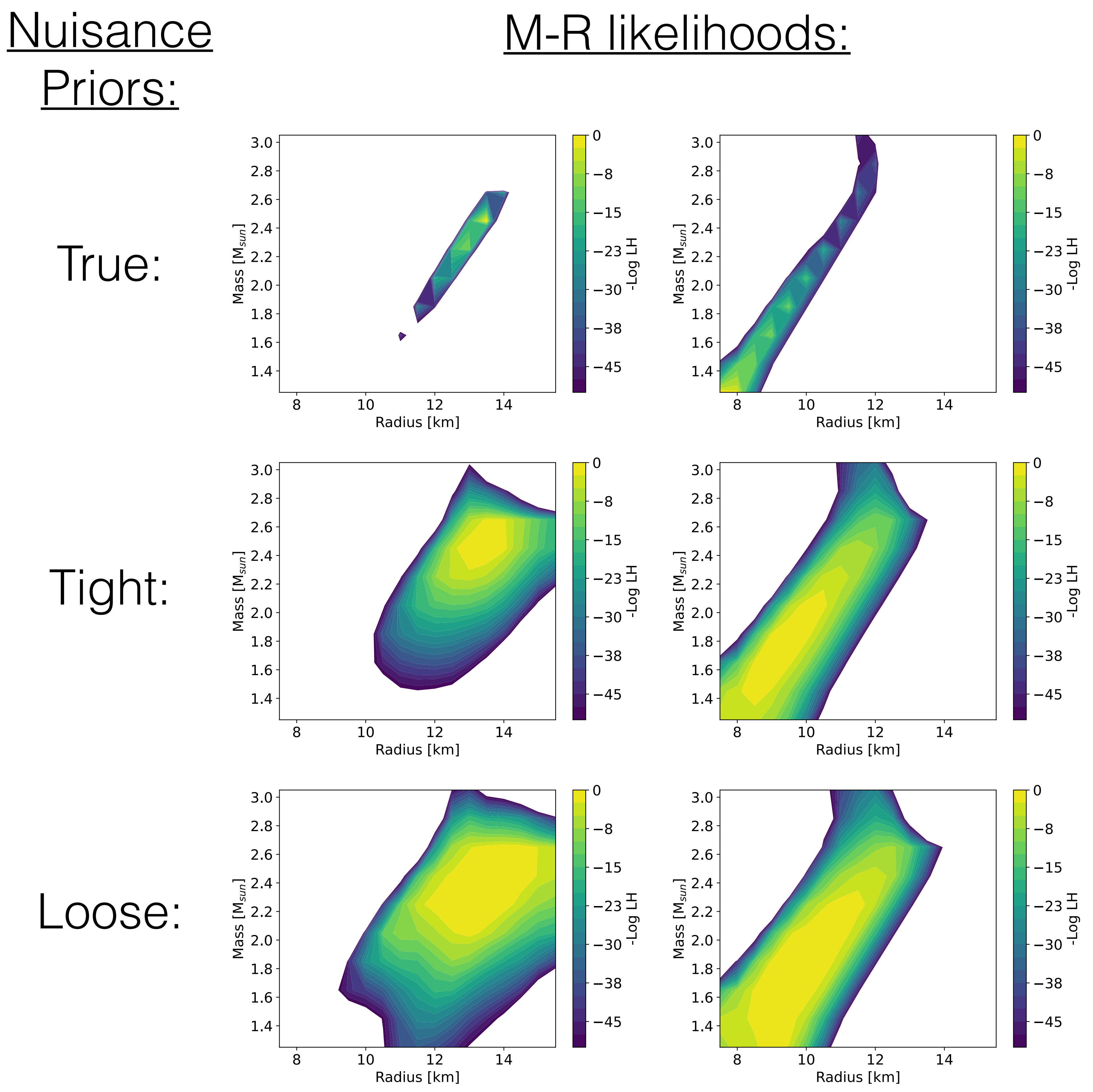
Intermediate steps remain interpretable physical quantities



Learn EOS to M-R



Learn {M,R,NPs} to Spectrum



Paper in preparation

Uncertainties for active learning

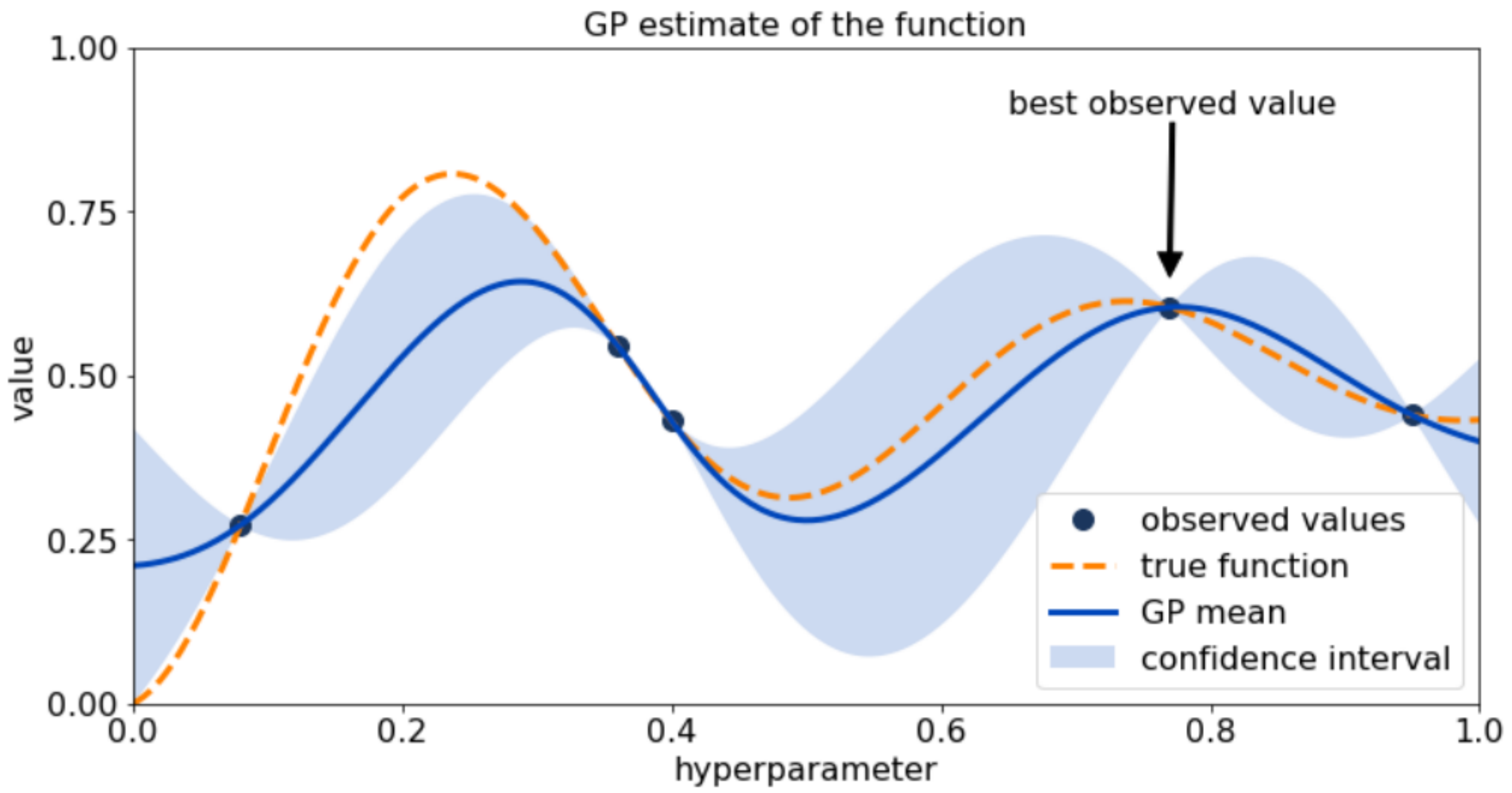


Image: [Source]

Scale Uncertainties

Uncertainty of cross-section from truncating QFT series

Sensitivity to scale variation quantifies ‘uncertainty’

Scale Uncertainties

Up: $\mu_+ = 2\ \mu_0$

$$\mu_0 = \frac{H_T}{2} = \frac{1}{2} \sum_{final\ state} \sqrt{m^2 + p_T^2}$$

Uncertainty of cross-section from truncating QFT series

Sensitivity to scale variation quantifies ‘uncertainty’

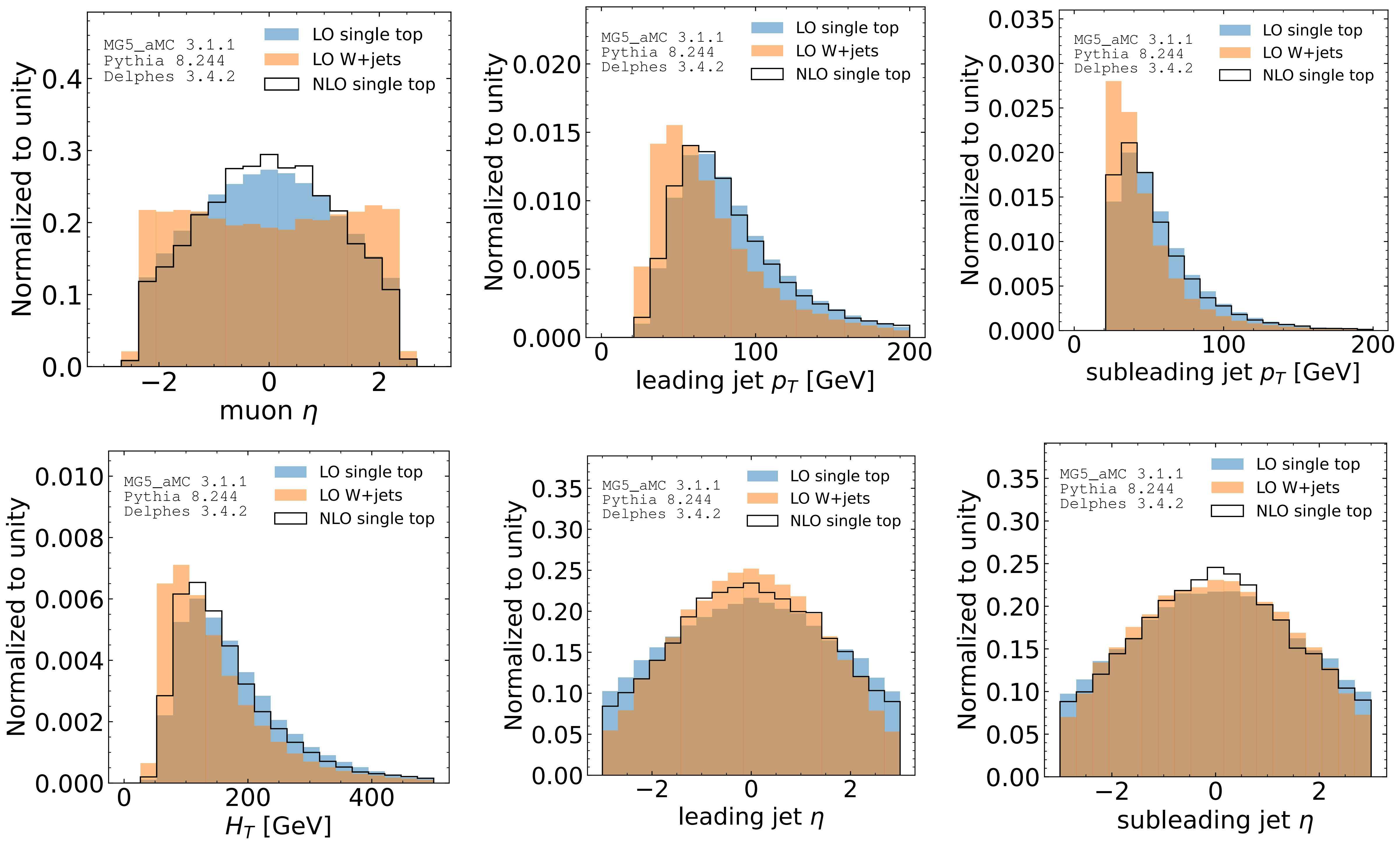
Down: $\mu_- = \frac{1}{2}\ \mu_0$

Scale uncertainty – Problem Setup

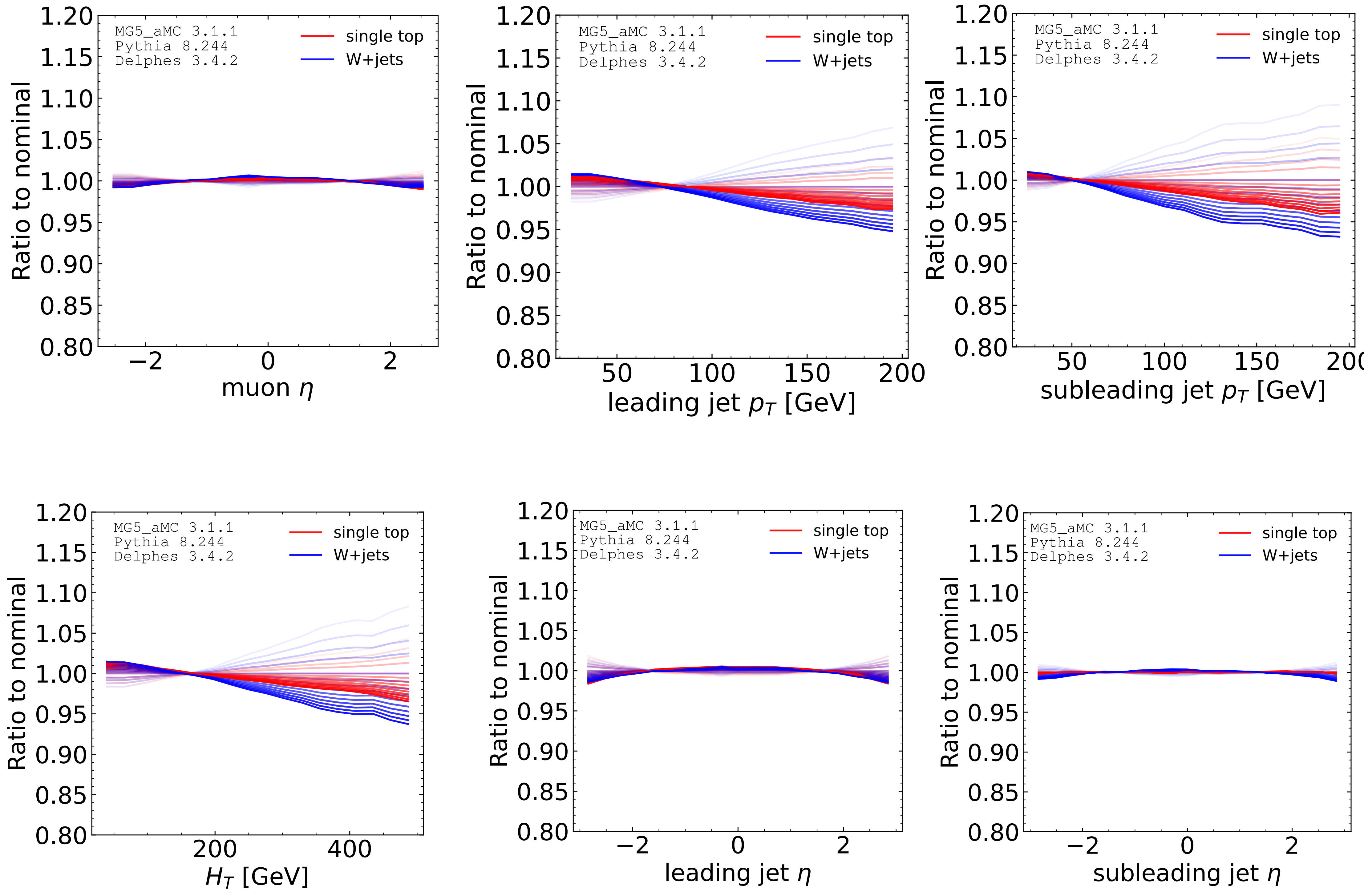
Goal: Single top vs W+Jets

Decorrelation: Reduce difference in performance on scale variations at LO

Cross-check: Test uncertainty estimate from {scale variations at LO} using NLO



NLO vs LO

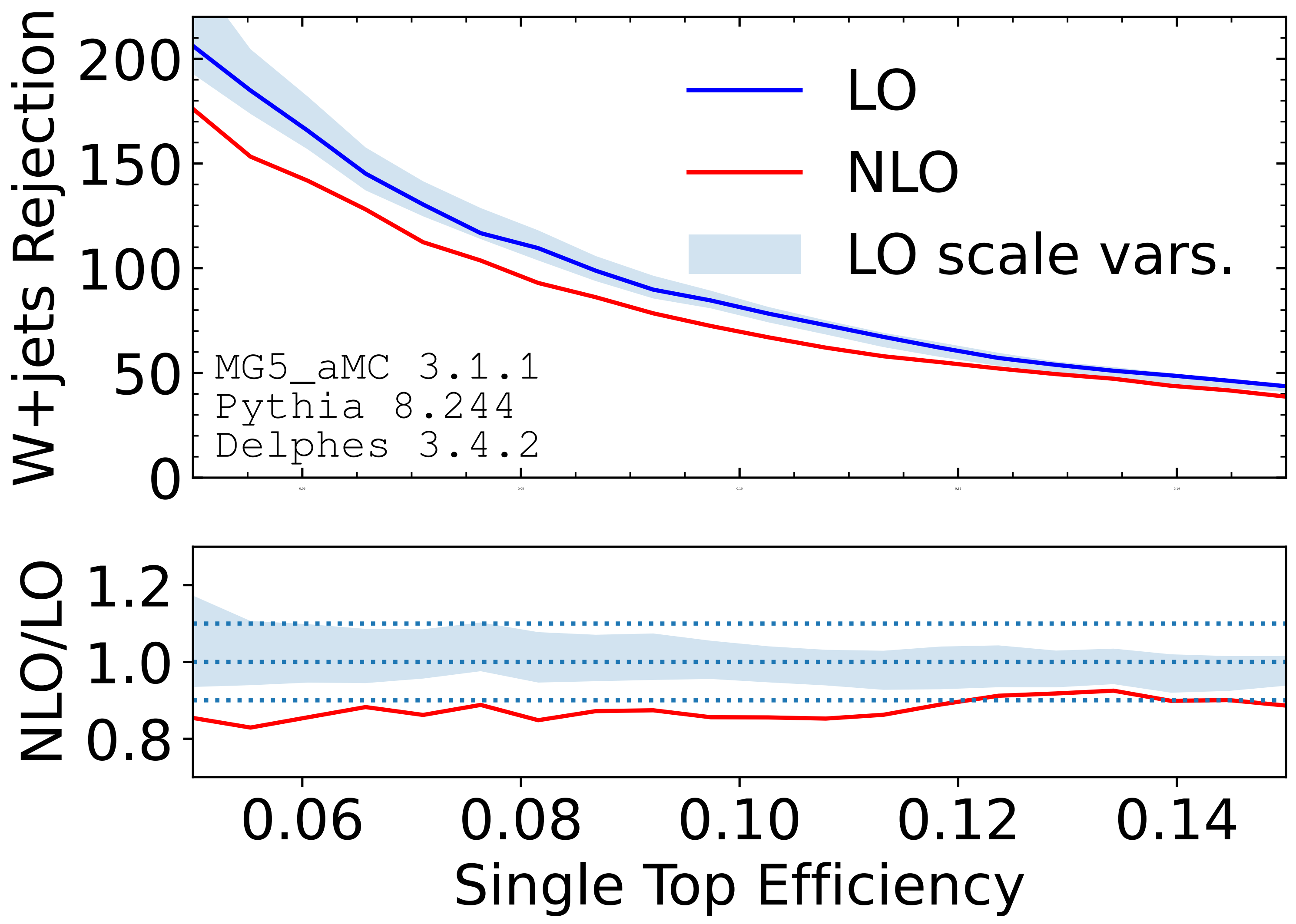


Factorisation scale variations going from 1/2 to 2

Case Study 2: Continuous uncertainty - Result

ROC curve (<u>higher is better</u>)

No adversary



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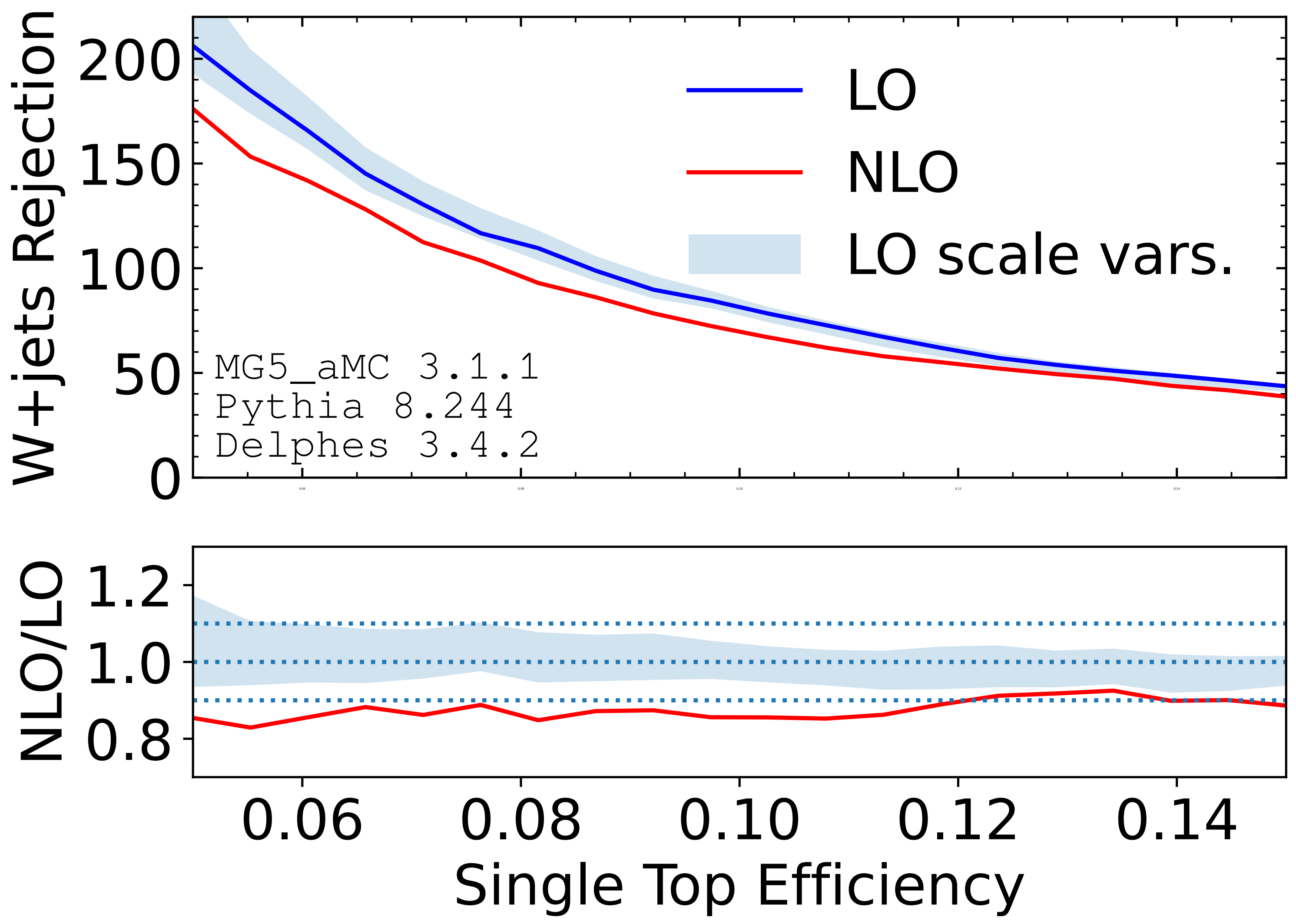
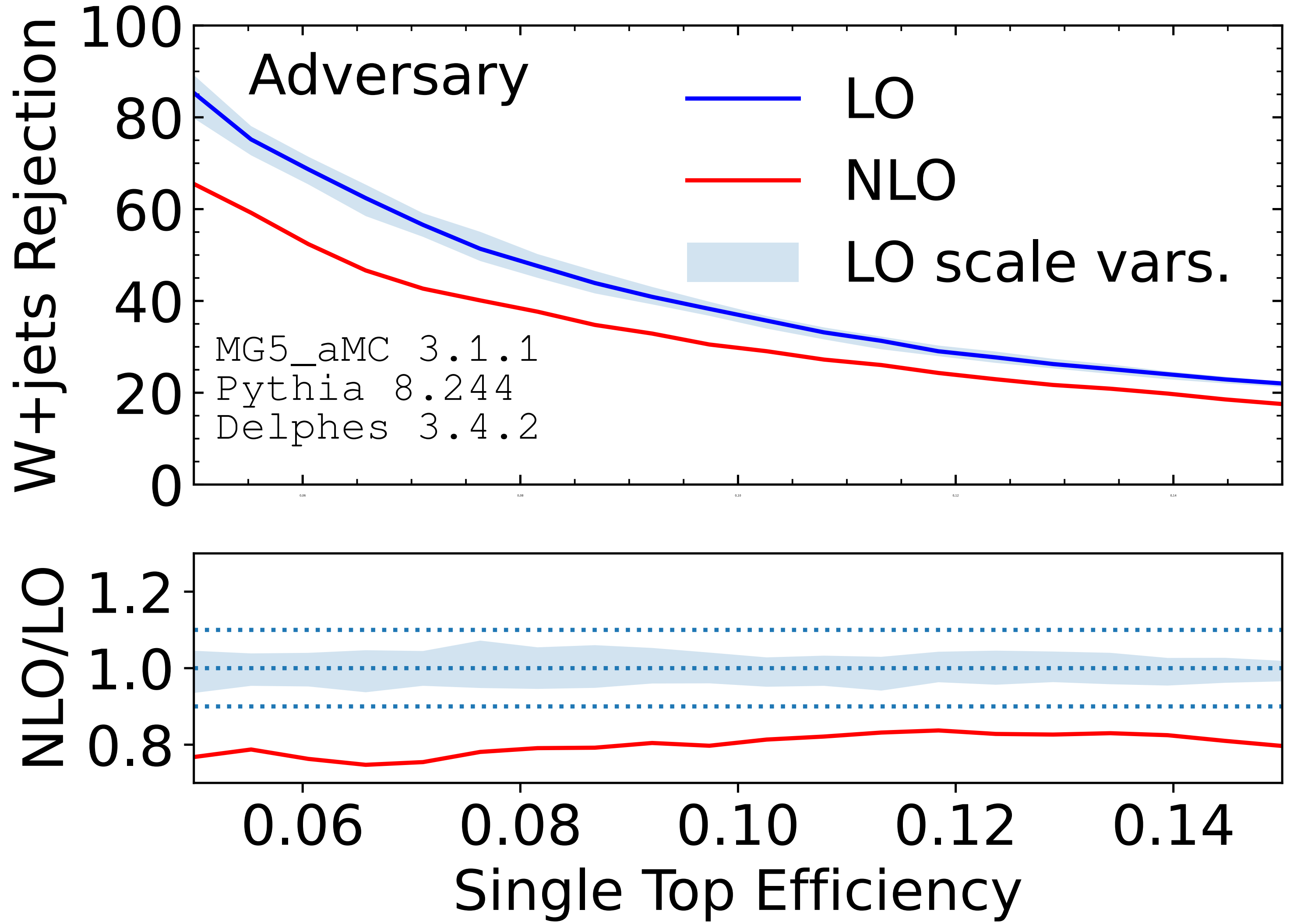


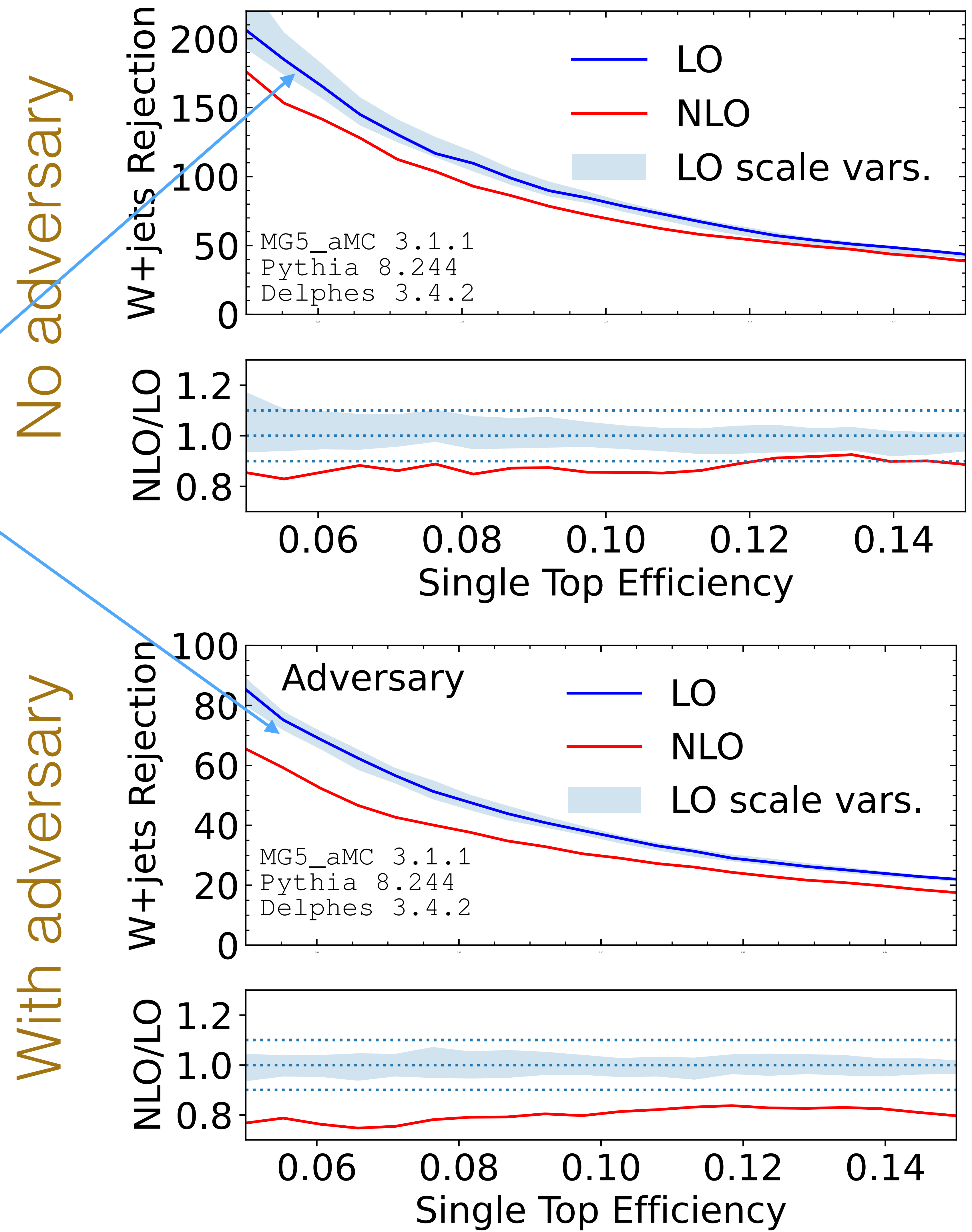
With adversary



Case Study 2: Continuous uncertainty - Result

ROC curve (higher is better)

Decorrelation:
Only the error bars shrink, not the actual distance to NLO



Case Study 2: Continuous uncertainty - Result

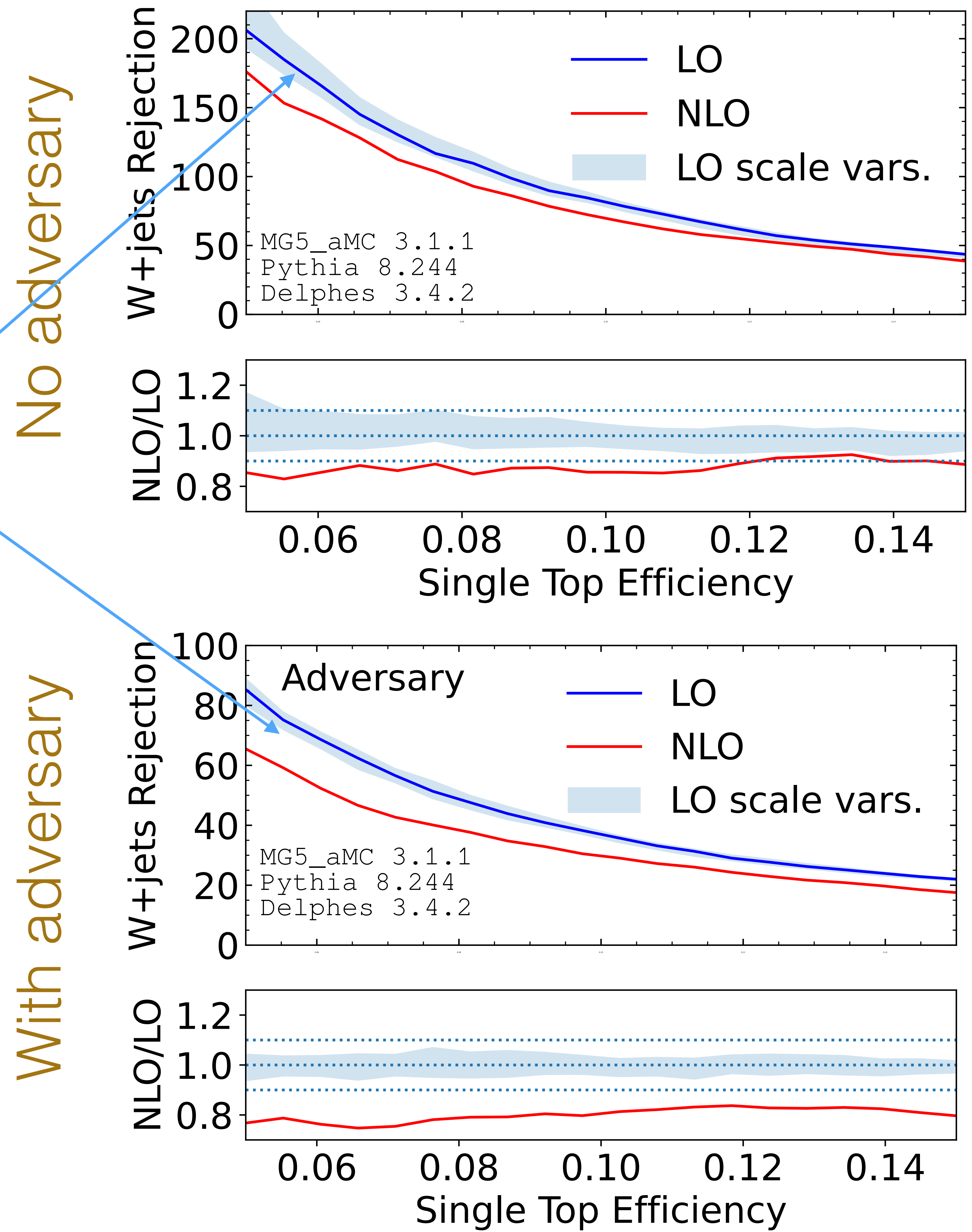
Adversary successfully **sacrifices separation power** in order to reduce difference in performance between scale variations

Cross-check with NLO reveals **uncertainty severely underestimated** by decorrelation approach

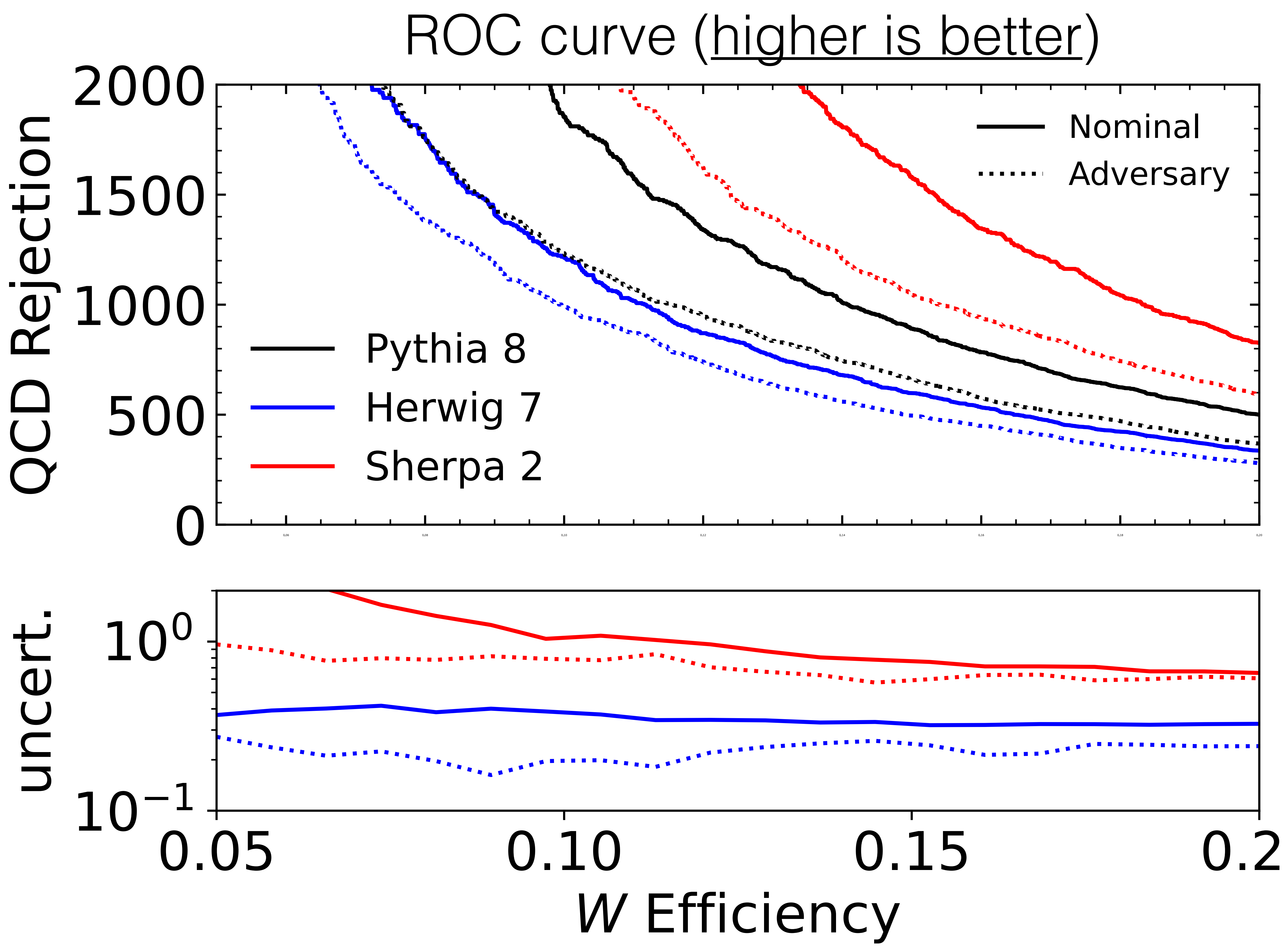
In an typical LHC analysis, a cross-check with higher-order usually unavailable

Decorrelation:
Only the error bars shrink, not the actual distance to NLO

ROC curve (higher is better)



Case Study 1: Two-point uncertainty - Result



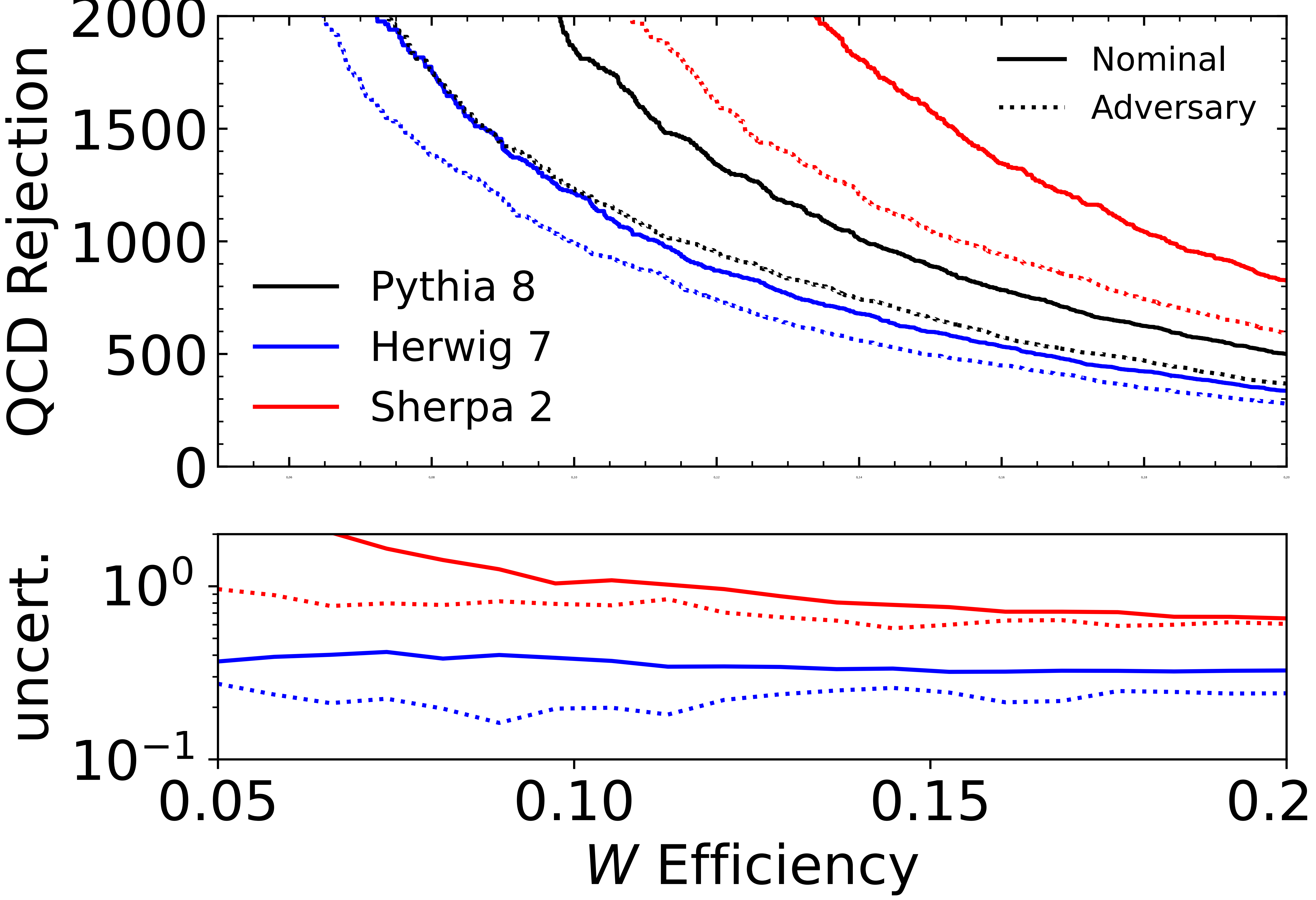
Case Study 1: Two-point uncertainty - Result

Adversary successfully sacrifices separation power in order to reduce difference in performance between Herwig and **Pythia**

Cross-check with Sherpa reveals uncertainty severely underestimated by usual Herwig vs **Pythia** comparison

In an typical LHC analysis, a cross-check with third generator rarely performed, similar to prior work suggesting decorrelation for theory uncertainties

ROC curve (higher is better)



Case Study 1: Two-point uncertainty - Result

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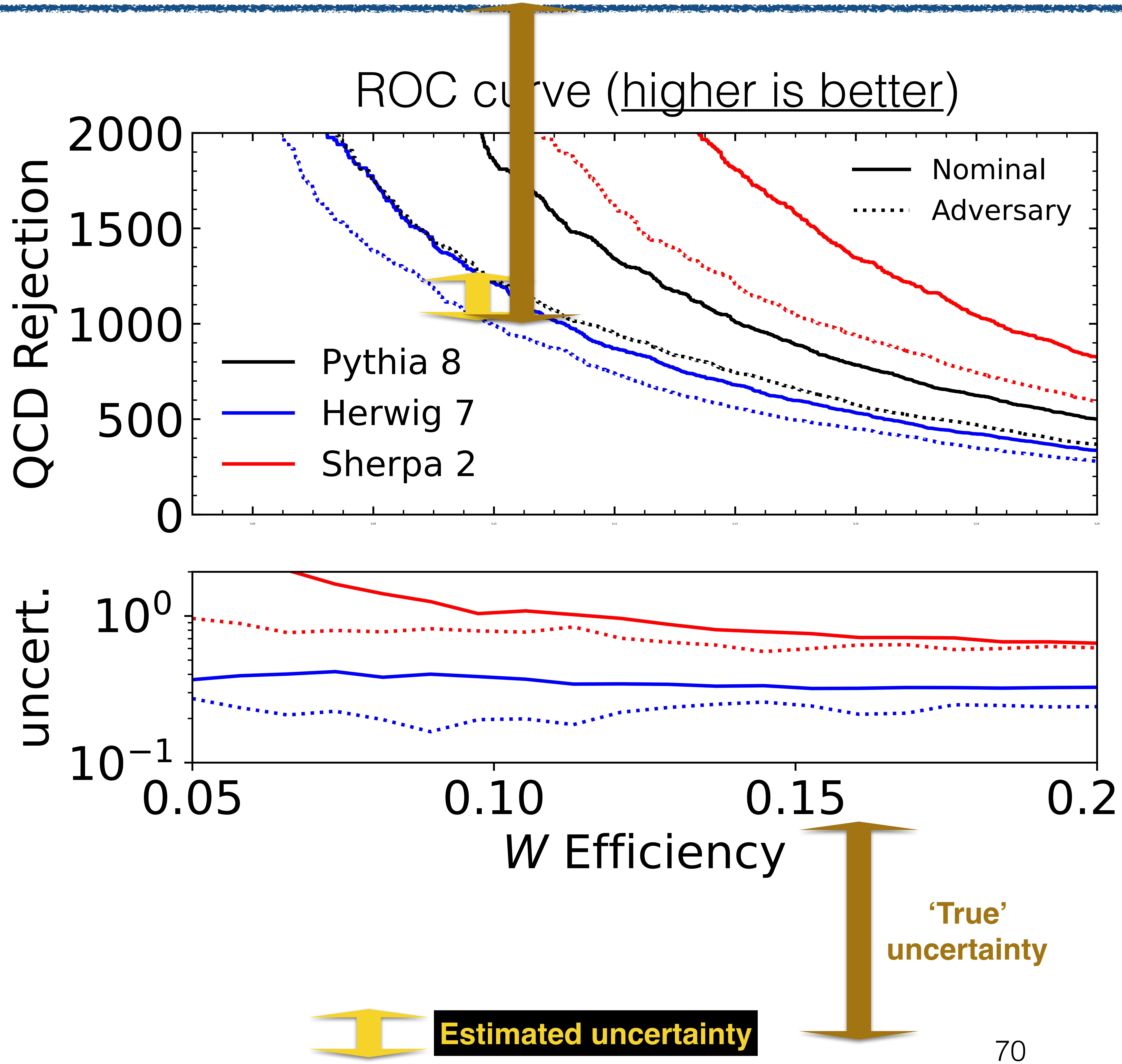
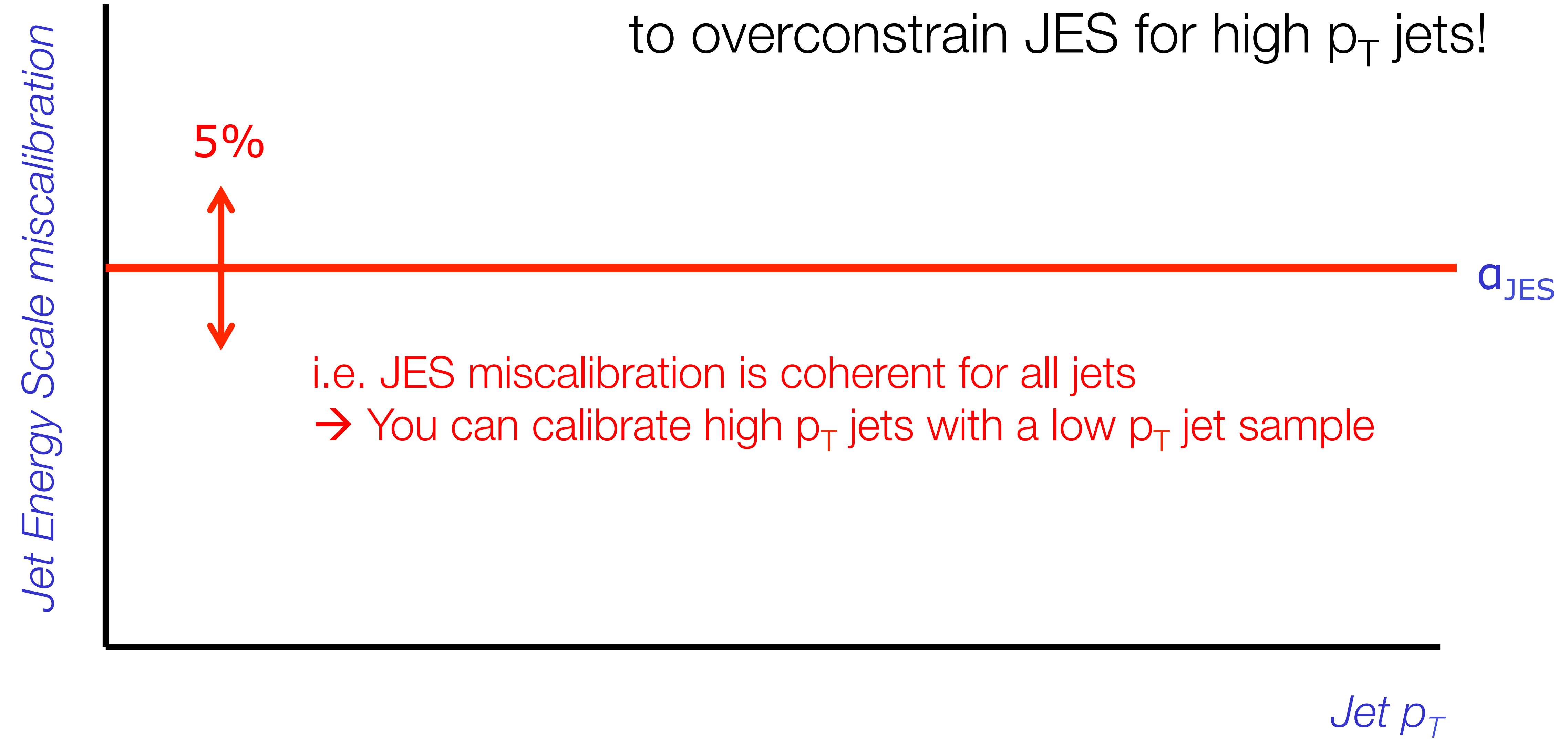


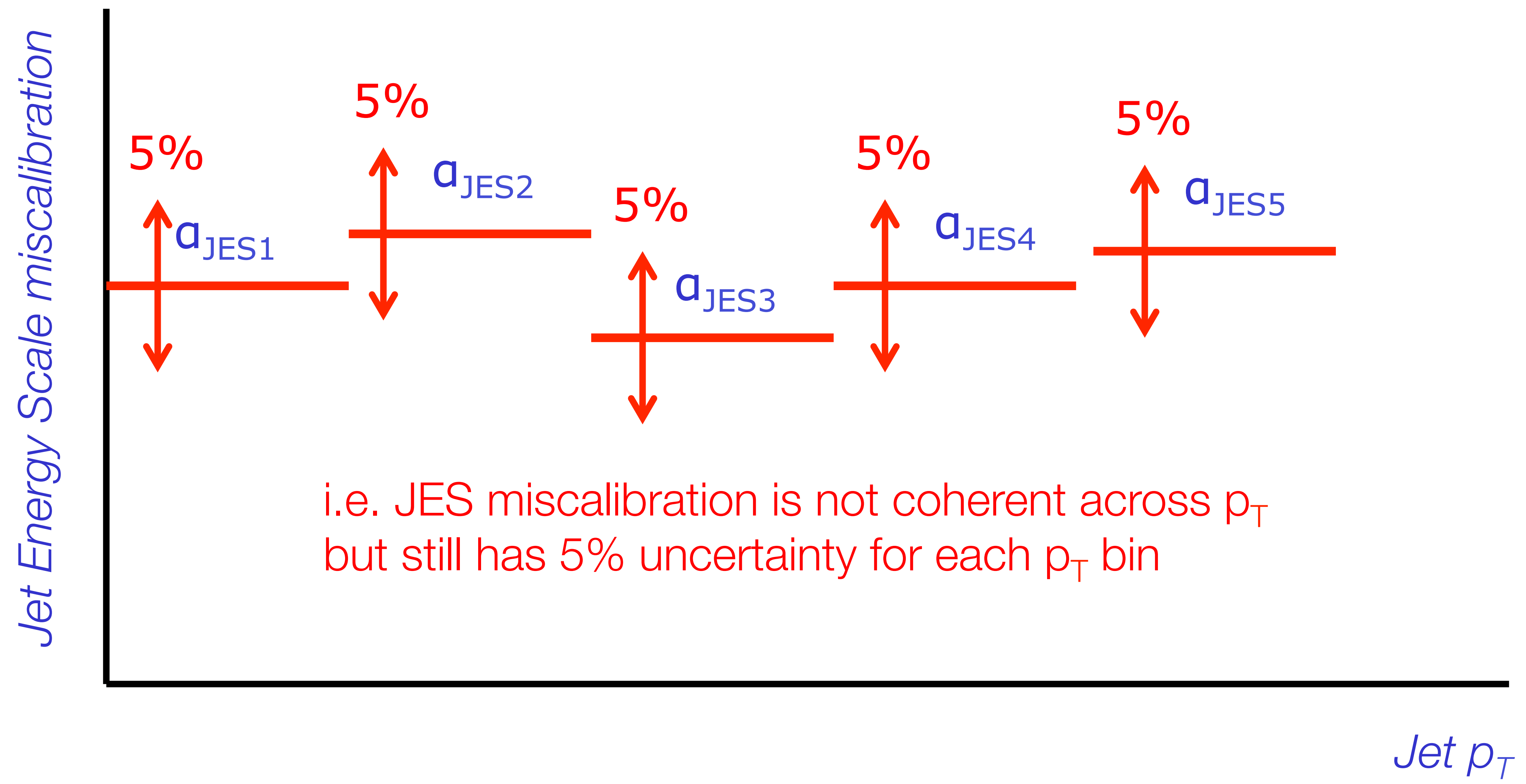
Overconstraining NP

From W. Verkerke:

Our modelling of NPs might be over-simplified

- If you assume one NP – chances are that your physics Likelihood will exploit this oversimplified JES model to overconstrain JES for high p_T jets!





So.. we can’t use ML to reduce theory uncertainties in our measurements ?

So.. we can’t use ML to reduce theory uncertainties in our measurements ?

Attack the source of the problem !

Similar effort: arXiv:2203.04983: Ilten et al.

Could we learn hadronization directly from Nature ?

PRD.106.096020: Aishik Ghosh, Xiangyang Ju, Benjamin Nachman, and Andrzej Siodmok

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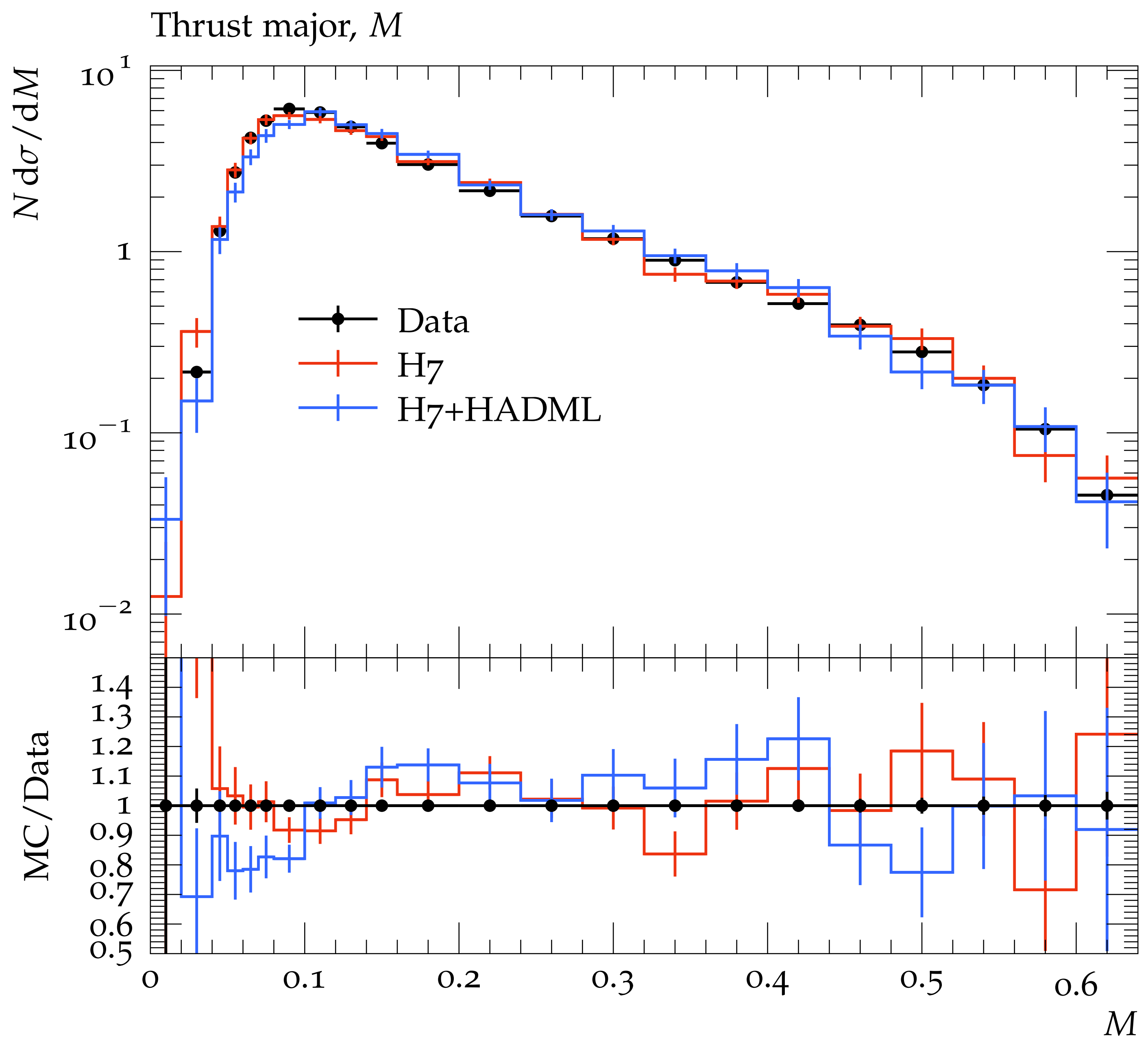
- Bypass theory, learn hadronization directly from data ?
- Proofs of concept on Herwig and Pythia simulations



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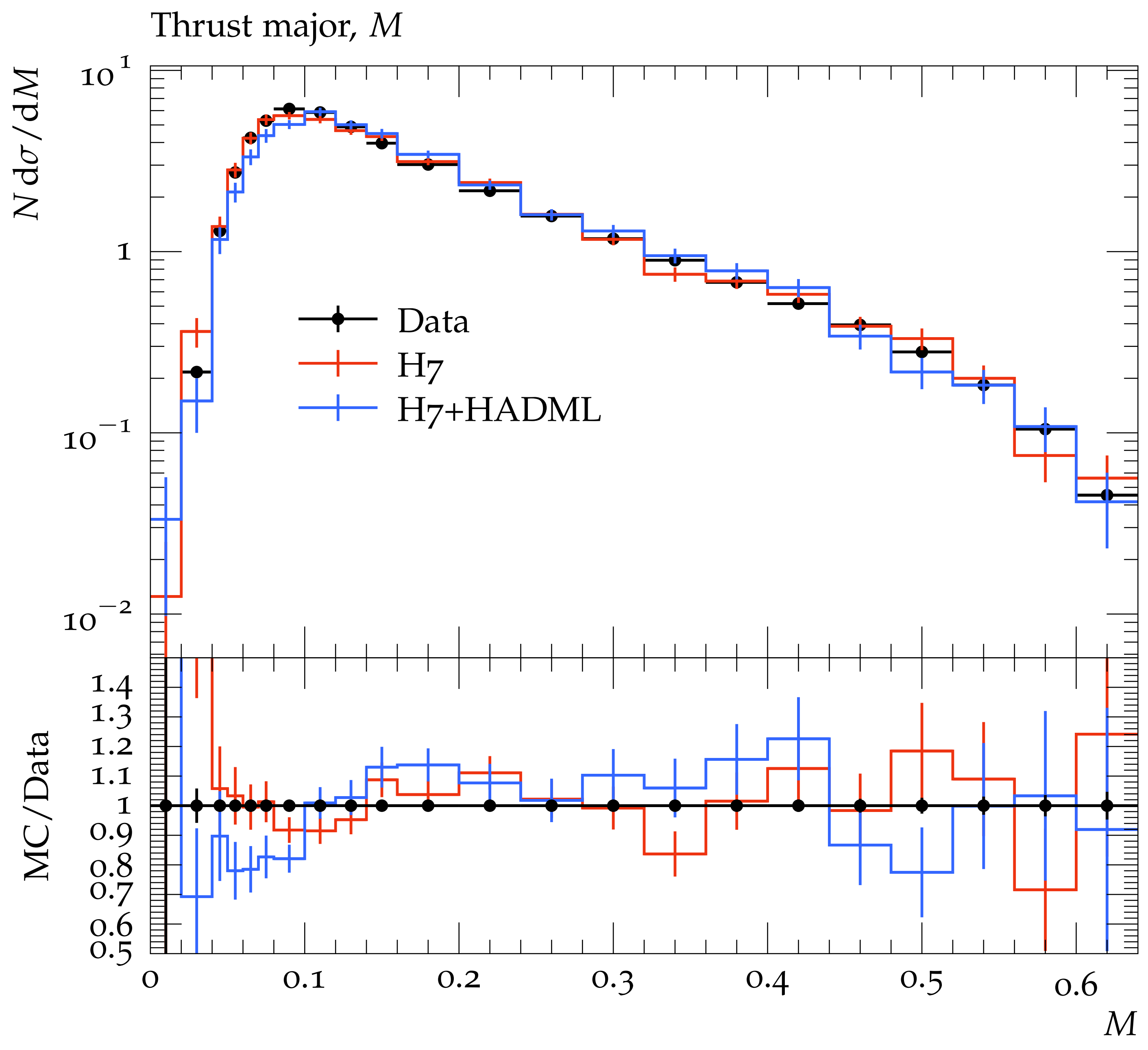
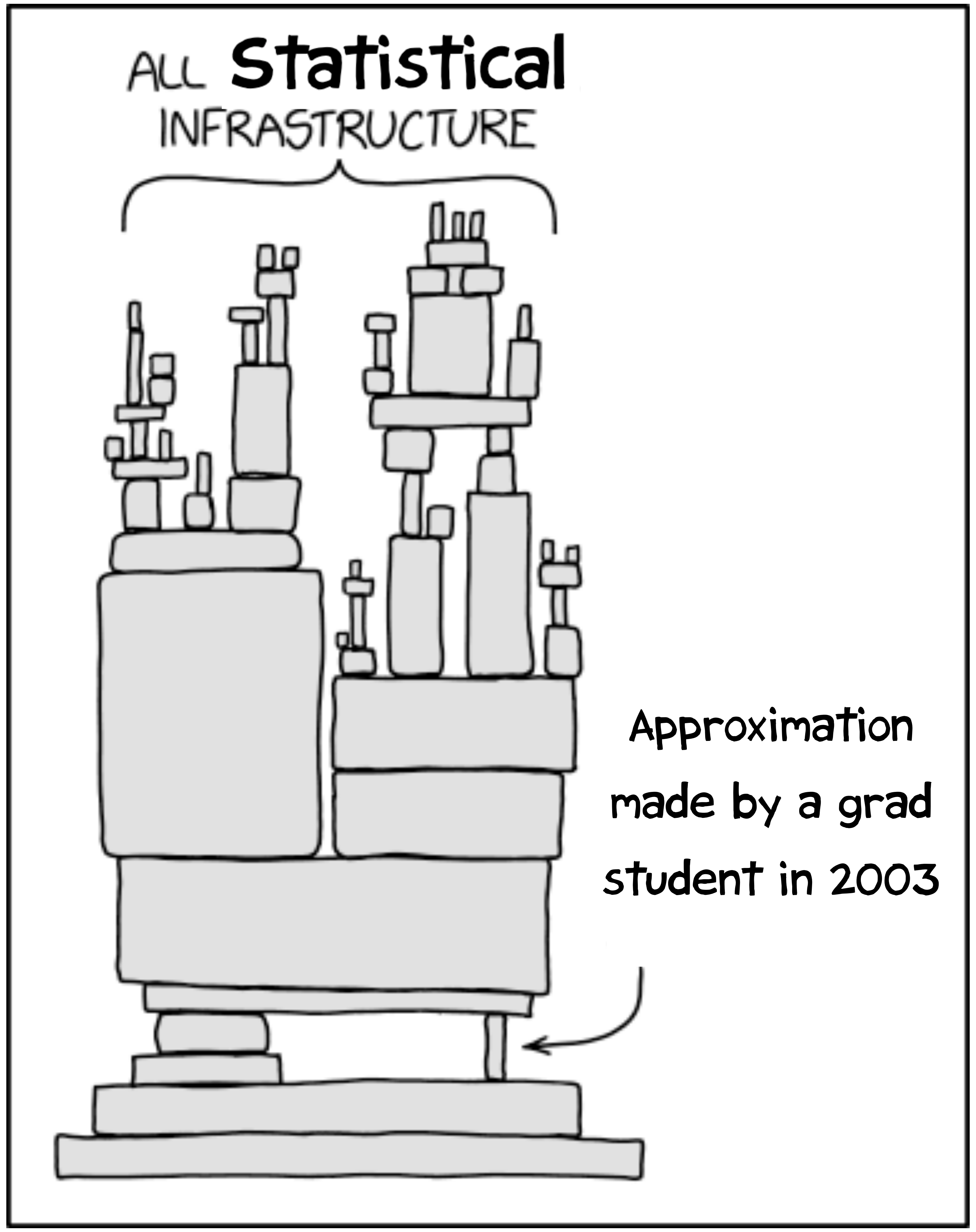


- To train on data, we need unfolded events <-—> data from experiments after removing detector effects
- Need **unbinned** unfolding of all observables simultaneously

What about scale variation uncertainties ?

Let's try to understand scale variation uncertainties



From Daniel Whiteson

It's dangerous to use ML methods to mitigate theory uncertainties

But we continue to treat Δ_{theory} and Δ_{exp} on same footing in statistical fits

What even is their statistical behaviour?

Questions

- How accurate are these scale uncertainties ?
- Is 1/2 to 2 a good range ?

Study pull distribution

$$t_{scale} = \frac{\sigma_{NLO} - \sigma_{LO}}{\Delta\sigma_{LO\ scale}}$$

Questions

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Madgraph paper

The automated computation of tree-level and next-to-leading order differential cross sections, and their matching to parton shower simulations

J. Alwall[a], R. Frederix[b], S. Frixione[b], V. Hirschi[c], F. Maltoni[d], O. Mattelaer[d], H.-S. Shao[e], T. Stelzer[f], P. Torrielli[g], M. Zaro[hi]

Process		Syntax	Cross section (pb)			
Vector boson +jets			LO 13 TeV		NLO 13 TeV	
a.1	$pp \to W^{\pm}$	`p p > wpm`	$1.375 \pm 0.002 \cdot 10^5$	$^{+15.4\%}_{-16.6\%}$ $^{+2.0\%}_{-1.6\%}$	$1.773 \pm 0.007 \cdot 10^5$	$^{+5.2\%}_{-9.4\%}$ $^{+1.9\%}_{-1.6\%}$
a.2	$pp \to W^{\pm}j$	`p p > wpm j`	$2.045 \pm 0.001 \cdot 10^4$	$^{+19.7\%}_{-17.2\%}$ $^{+1.4\%}_{-1.1\%}$	$2.843 \pm 0.010 \cdot 10^4$	$^{+5.9\%}_{-8.0\%}$ $^{+1.3\%}_{-1.1\%}$
a.3	$pp \to W^{\pm}jj$	`p p > wpm j j`	$6.805 \pm 0.015 \cdot 10^3$	$^{+24.5\%}_{-18.6\%}$ $^{+0.8\%}_{-0.7\%}$	$7.786 \pm 0.030 \cdot 10^3$	$^{+2.4\%}_{-6.0\%}$ $^{+0.9\%}_{-0.8\%}$
a.4	$pp \to W^{\pm}jjj$	`p p > wpm j j j`	$1.821 \pm 0.002 \cdot 10^3$	$^{+41.0\%}_{-27.1\%}$ $^{+0.5\%}_{-0.5\%}$	$2.005 \pm 0.008 \cdot 10^3$	$^{+0.9\%}_{-6.7\%}$ $^{+0.6\%}_{-0.5\%}$
a.5	$pp \to Z$	`p p > z`	$4.248 \pm 0.005 \cdot 10^4$	$^{+14.6\%}_{-15.8\%}$ $^{+2.0\%}_{-1.6\%}$	$5.410 \pm 0.022 \cdot 10^4$	$^{+4.6\%}_{-8.6\%}$ $^{+1.9\%}_{-1.5\%}$
a.6	$pp \to Zj$	`p p > z j`	$7.209 \pm 0.005 \cdot 10^3$	$^{+19.3\%}_{-17.0\%}$ $^{+1.2\%}_{-1.0\%}$	$9.742 \pm 0.035 \cdot 10^3$	$^{+5.8\%}_{-7.8\%}$ $^{+1.2\%}_{-1.0\%}$
a.7	$pp \to Zjj$	`p p > z j j`	$2.348 \pm 0.006 \cdot 10^3$	$^{+24.3\%}_{-18.5\%}$ $^{+0.6\%}_{-0.6\%}$	$2.665 \pm 0.010 \cdot 10^3$	$^{+2.5\%}_{-6.0\%}$ $^{+0.7\%}_{-0.7\%}$
a.8	$pp \to Zjjj$	`p p > z j j j`	$6.314 \pm 0.008 \cdot 10^2$	$^{+40.8\%}_{-27.0\%}$ $^{+0.5\%}_{-0.5\%}$	$6.996 \pm 0.028 \cdot 10^2$	$^{+1.1\%}_{-6.8\%}$ $^{+0.5\%}_{-0.5\%}$
a.9	$pp \to \gamma j$	`p p > a j`	$1.964 \pm 0.001 \cdot 10^4$	$^{+31.2\%}_{-26.0\%}$ $^{+1.7\%}_{-1.8\%}$	$5.218 \pm 0.025 \cdot 10^4$	$^{+24.5\%}_{-21.4\%}$ $^{+1.4\%}_{-1.6\%}$
a.10	$pp \to \gamma jj$	`p p > a j j`	$7.815 \pm 0.008 \cdot 10^3$	$^{+32.8\%}_{-24.2\%}$ $^{+0.9\%}_{-1.2\%}$	$1.004 \pm 0.004 \cdot 10^4$	$^{+5.9\%}_{-10.9\%}$ $^{+0.8\%}_{-1.2\%}$

+127 more pp processes from 1405.0301!

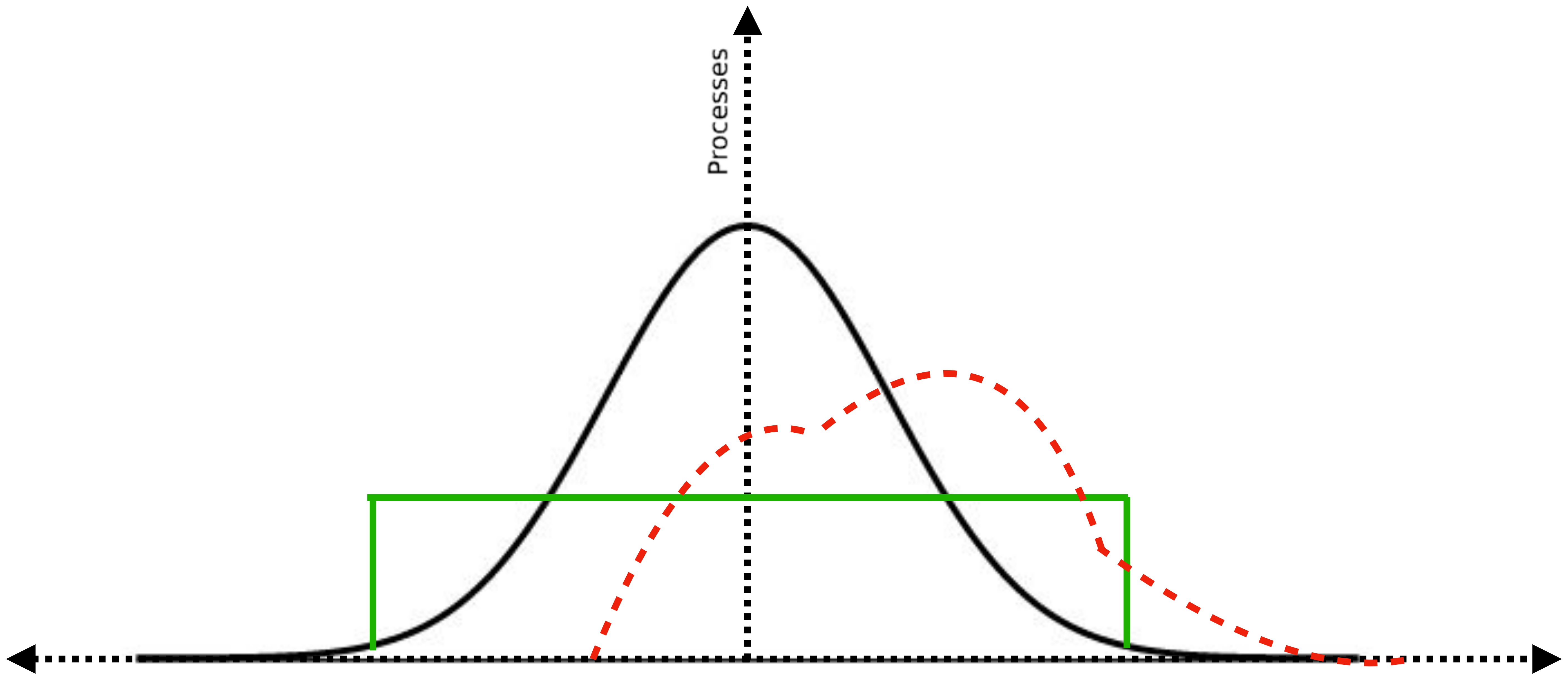
(Not a random sampling)

Alwall et al.

Plot the pulls

$$t_{scale} = \frac{\sigma_{NLO} - \sigma_{LO}}{\Delta\sigma_{LO\ scale}}$$

Which of these distributions do you expect?



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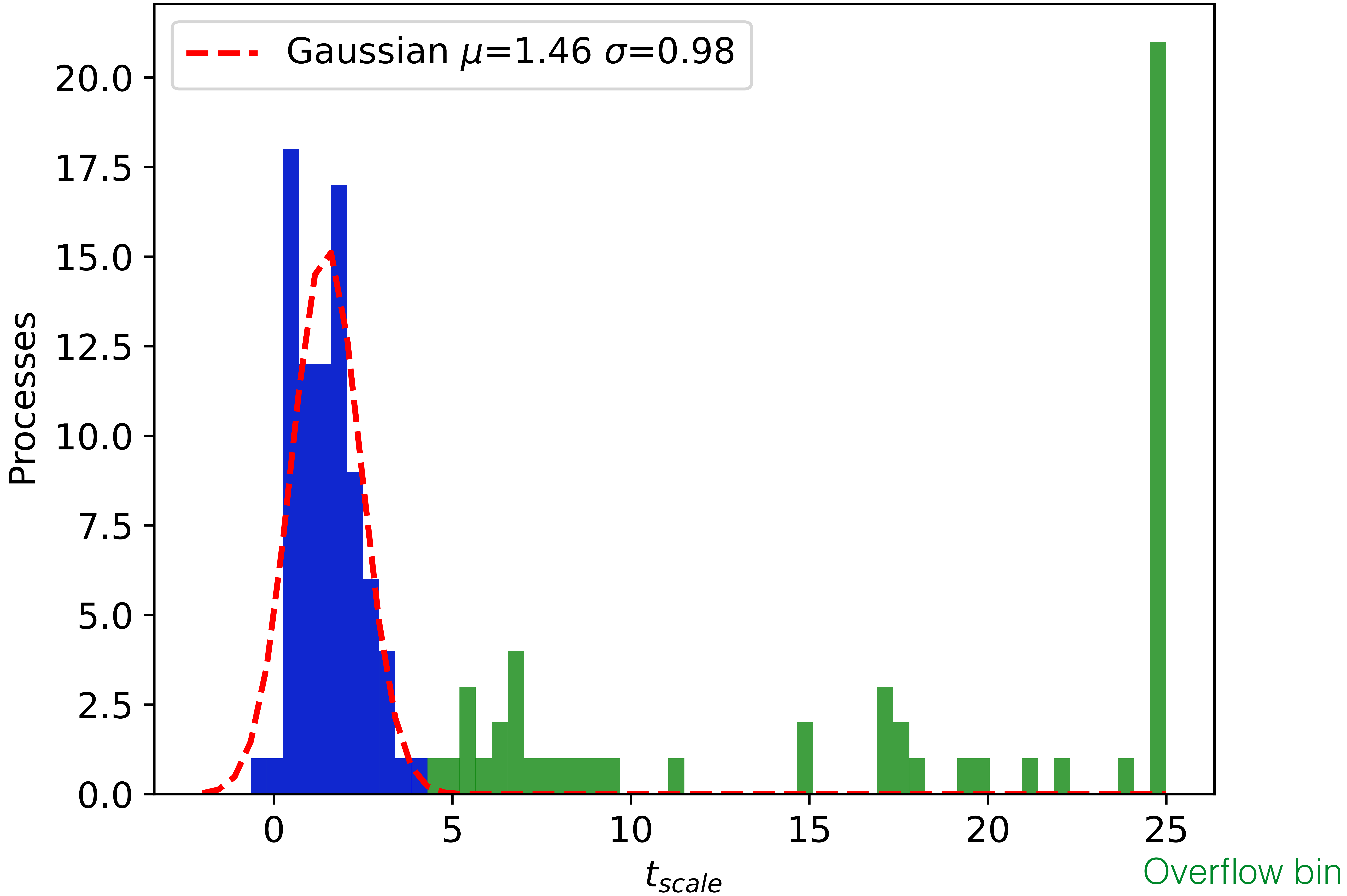
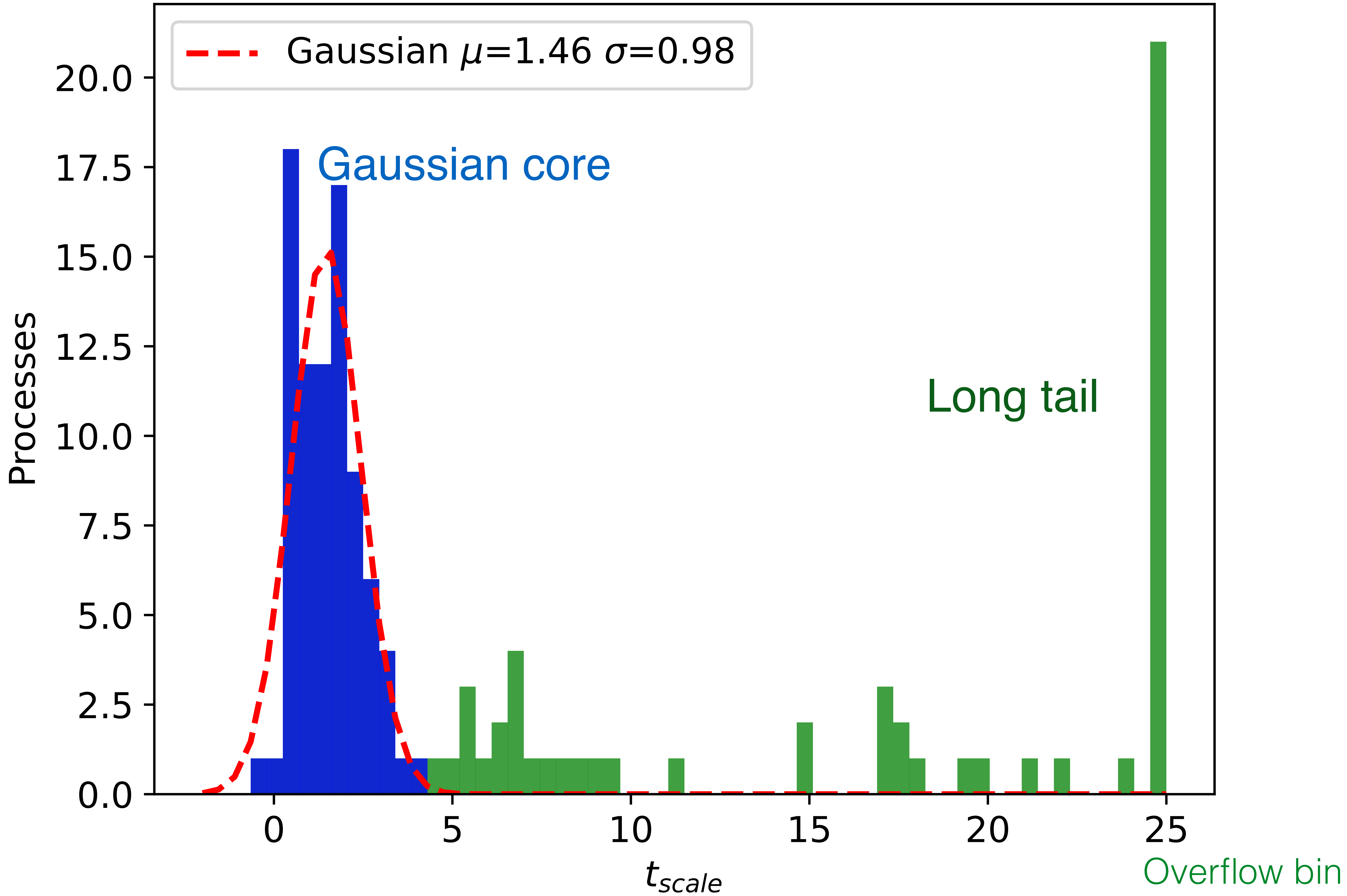
Pull distribution



Pull distribution



What processes populate the tail ?

Process	n_{part}	$\Delta\sigma/\sigma_0$	$\frac{\sigma_{\text{NLO}}-\sigma_0}{\Delta\sigma}$
`p p > wpm`	1	1.54×10^{-1}	1.84
`p p > wpm j`	2	1.97×10^{-1}	1.96
`p p > wpm j j`	3	2.45×10^{-1}	0.59
`p p > wpm j j j`	4	4.10×10^{-1}	0.25
`p p > z`	1	1.46×10^{-1}	1.87
`p p > z j`	2	1.93×10^{-1}	1.82
`p p > z j j`	3	2.43×10^{-1}	0.56
`p p > z j j j`	4	4.08×10^{-1}	0.27
`p p > a j`	2	3.12×10^{-1}	5.33
`p p > a j j`	3	3.28×10^{-1}	0.85
`p p > w+ w- wpm`	3	1.00×10^{-3}	610.69
`p p > z w+ w-`	3	8.00×10^{-3}	92.39
`p p > z z wpm`	3	1.00×10^{-2}	85.00
`p p > z z z`	3	1.00×10^{-3}	302.75
`p p > a w+ w-`	3	1.90×10^{-2}	42.33
`p p > a a wpm`	3	4.40×10^{-2}	47.24
`p p > a z wpm`	3	1.00×10^{-3}	1244.49
`p p > a z z`	3	2.00×10^{-2}	17.24

QCD processes follow (an expected) pattern

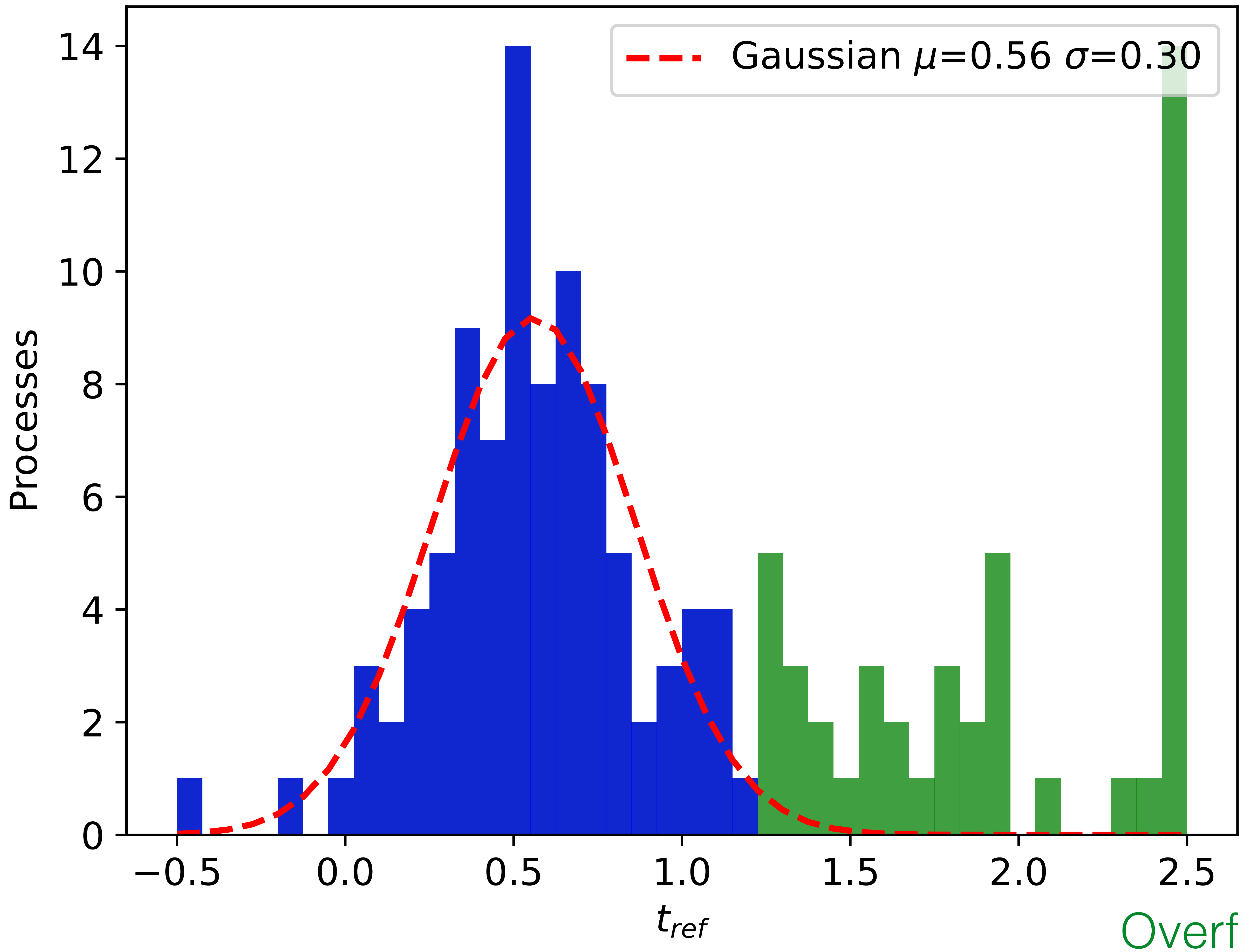
Process	$\frac{\Delta\sigma}{\sigma_0}$		n	$\frac{\Delta\sigma}{n\,\sigma_0}$	
`p p > j j`	$+2.49\times10^{-1}$	-1.88×10^{-1}	2	$+1.24\times10^{-1}$	-9.40×10^{-2}
`p p > b b`	$+2.52\times10^{-1}$	-1.89×10^{-1}	2	$+1.26\times10^{-1}$	-9.45×10^{-2}
`p p > t t`	$+2.90\times10^{-1}$	-2.11×10^{-1}	2	$+1.45\times10^{-1}$	-1.06×10^{-1}
`p p > j j j`	$+4.38\times10^{-1}$	-2.84×10^{-1}	3	$+1.46\times10^{-1}$	-9.47×10^{-2}
`p p > b b j`	$+4.41\times10^{-1}$	-2.85×10^{-1}	3	$+1.47\times10^{-1}$	-9.50×10^{-2}
`p p > t t j`	$+4.51\times10^{-1}$	-2.90×10^{-1}	3	$+1.50\times10^{-1}$	-9.67×10^{-2}
`p p > b b j j`	$+6.18\times10^{-1}$	-3.56×10^{-1}	4	$+1.54\times10^{-1}$	-8.90×10^{-2}
`p p > b b b b`	$+6.17\times10^{-1}$	-3.56×10^{-1}	4	$+1.54\times10^{-1}$	-8.90×10^{-2}
`p p > t t j j`	$+6.14\times10^{-1}$	-3.56×10^{-1}	4	$+1.53\times10^{-1}$	-8.90×10^{-2}
`p p > t t t t`	$+6.38\times10^{-1}$	-3.65×10^{-1}	4	$+1.60\times10^{-1}$	-9.12×10^{-2}
`p p > t t b b`	$+6.21\times10^{-1}$	-3.57×10^{-1}	4	$+1.55\times10^{-1}$	-8.93×10^{-2}
average				$+1.47\times10^{-1}$	-9.34×10^{-2}

Table 1: Scale dependence for LHC processes with only QCD particles in the final state. For each process, we report the relative scale uncertainty, the number of final state particles, and the per-particle relative scale uncertainty.

→Tilman Plehn's 'reference process' method

$$\frac{\Delta\sigma_{\text{ref}}}{\sigma_0} = n \times \left\langle \frac{\Delta\sigma}{n\sigma_0} \right\rangle_{\text{QCD}} .$$

Make correction in UQ for EW processes



Overflow bin

Much reduced tails

Tilman Plehn's 'reference process' method

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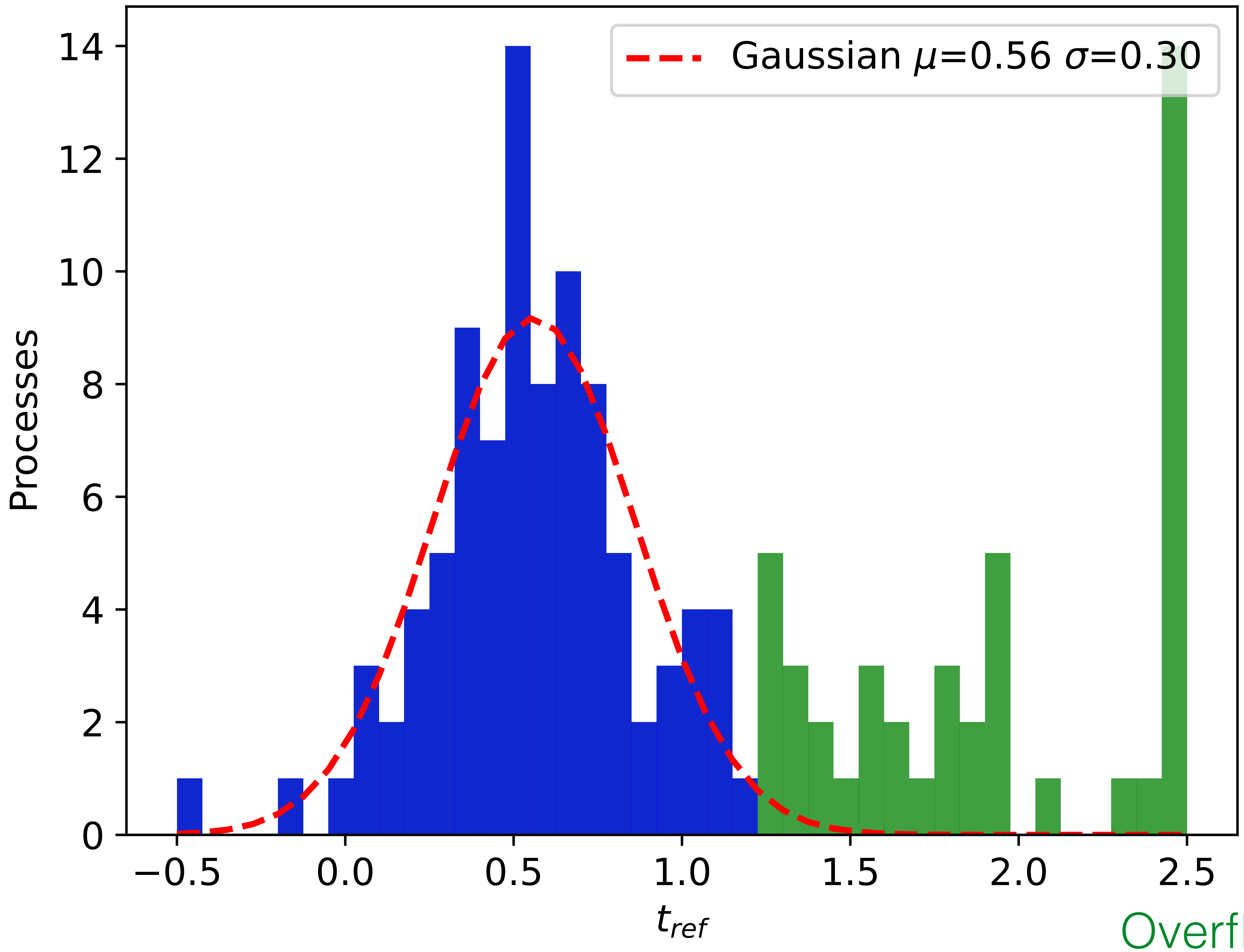

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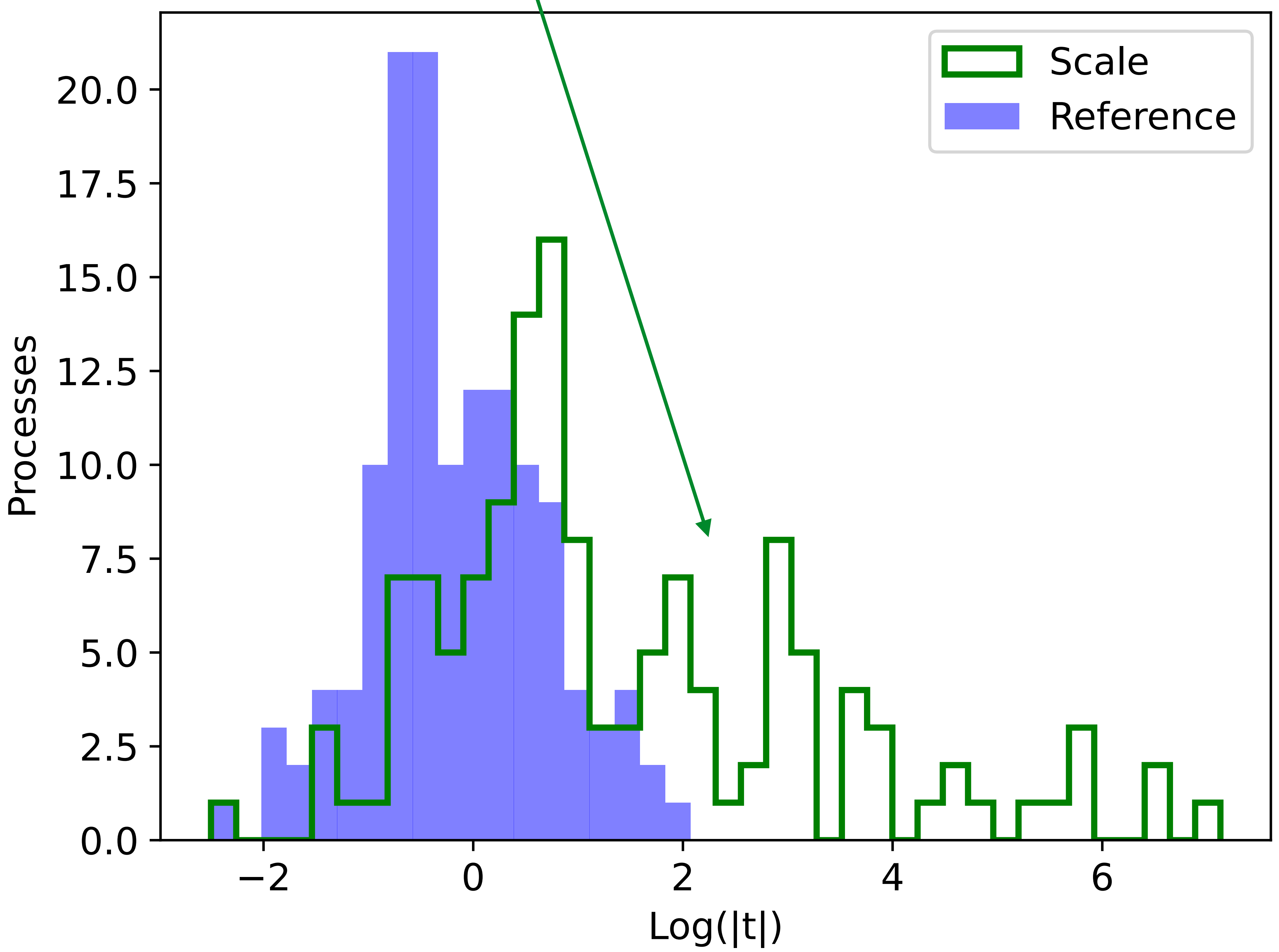


Tilman Plehn's 'reference process' method

Surviving tails

Process	n_{part}	$\Delta\sigma/\sigma_0$	$\frac{\sigma_{\text{NLO}}-\sigma_0}{\Delta\sigma}$	$\Delta\sigma_{\text{ref}}/\sigma_0$	$\frac{\sigma_{\text{NLO}}-\sigma_0}{\Delta\sigma_{\text{ref}}}$
`p p > h`	1	3.48×10^{-1}	3.02	1.47×10^{-1}	7.15

Large corrections loop-induced 2->1 process

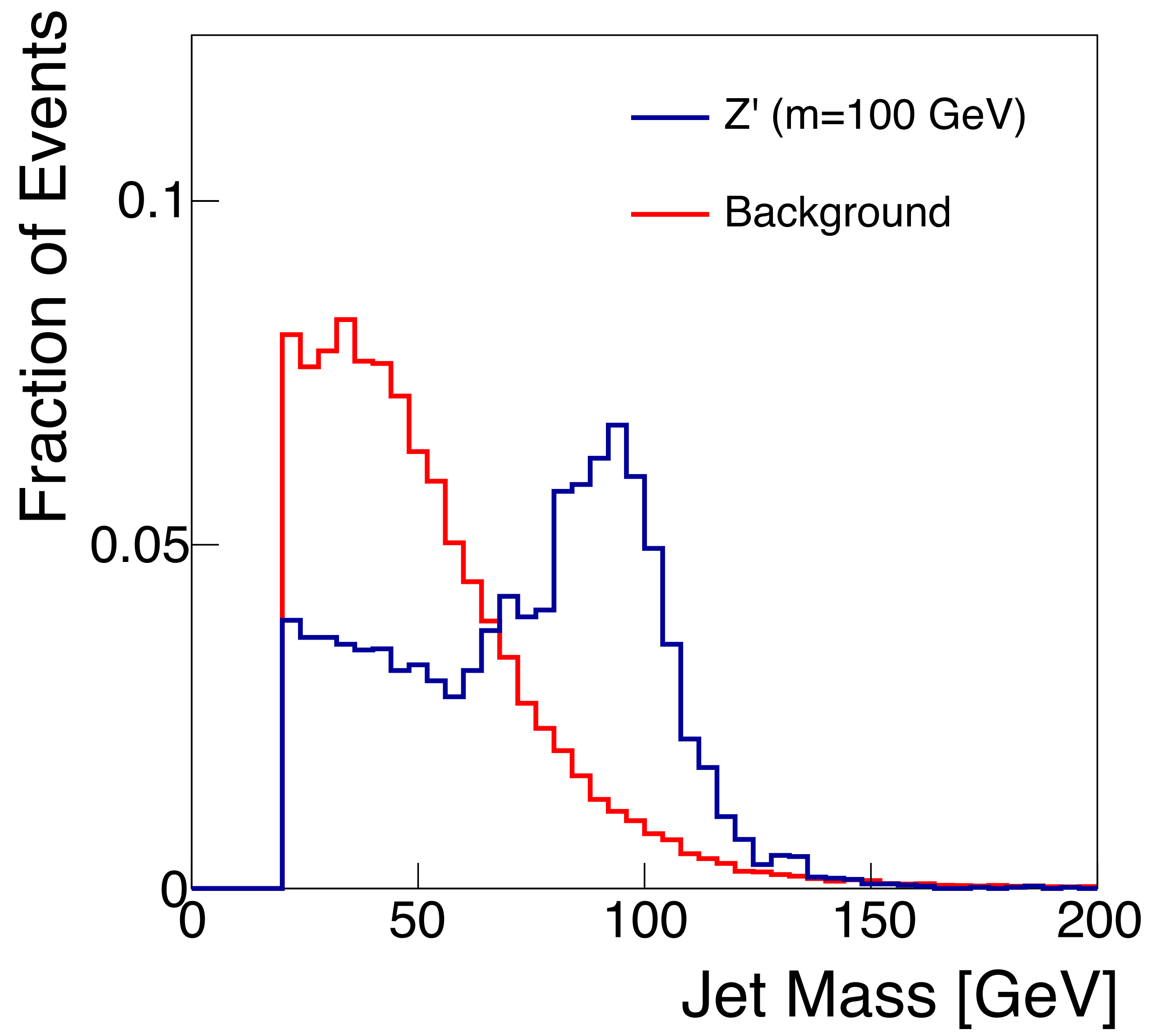
Leaves us wanting more …

- Would be even more interesting to repeat study for NLO → NNLO, differential distributions
    - Can we use ML to automatically find patterns of failure ?

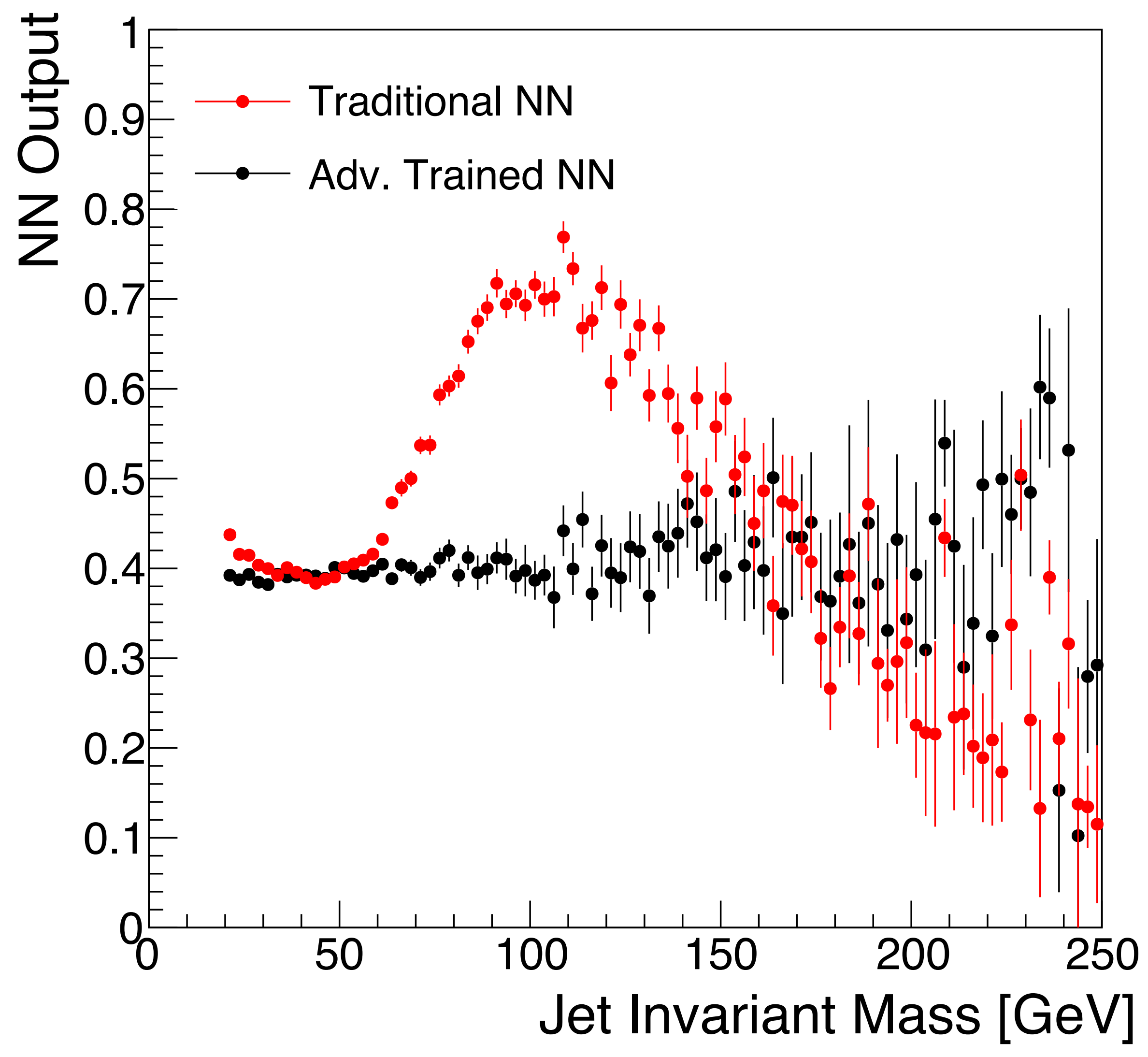
- Application in experiment: A new method for cross-checking sensitivity of advance ML methods to scale uncertainties

Decorrelation to remove background sculpting

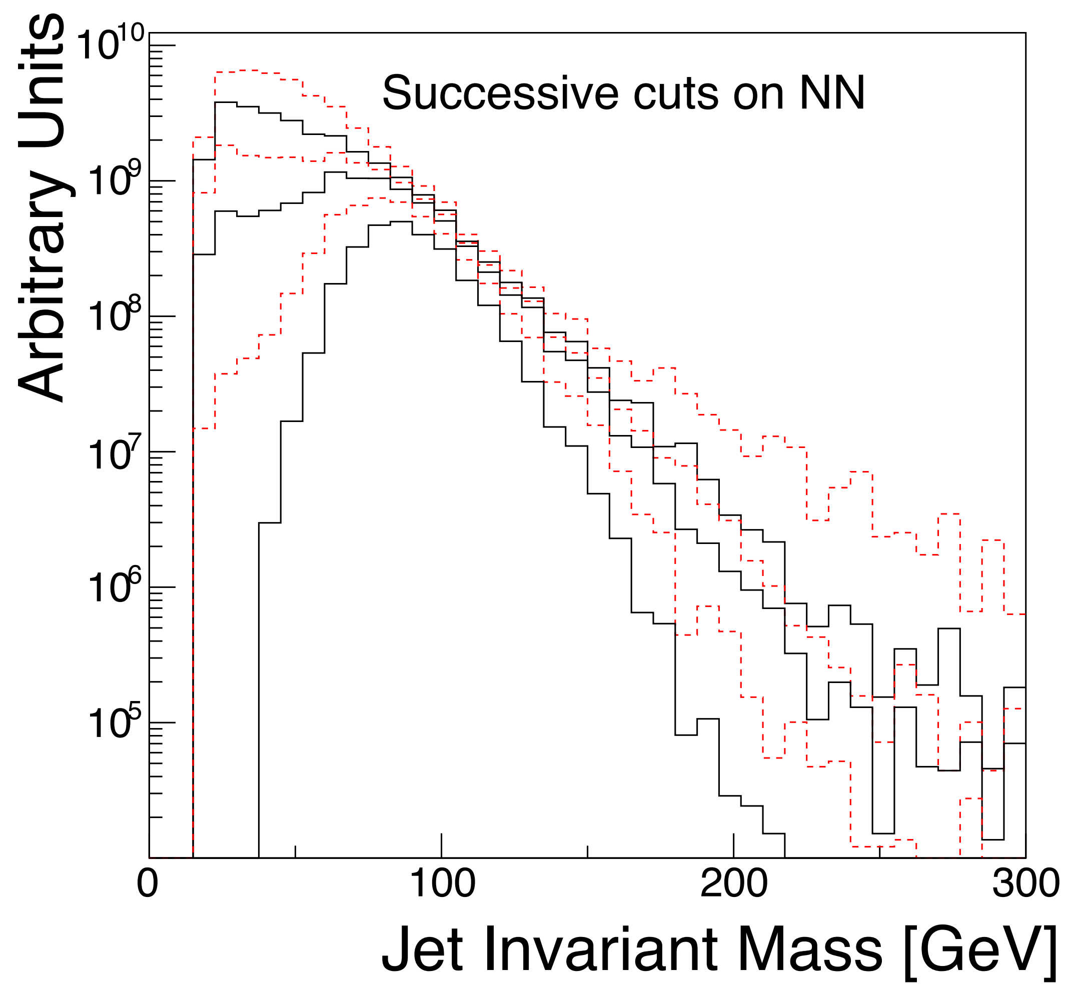
1703.03507



Signal peak at 100 GeV



Traditional NN learns to select 100 GeV events



Event selection sculpts background distribution

Unfolding with nuisance parameters

Chan and Nachman arXiv:2302.05390

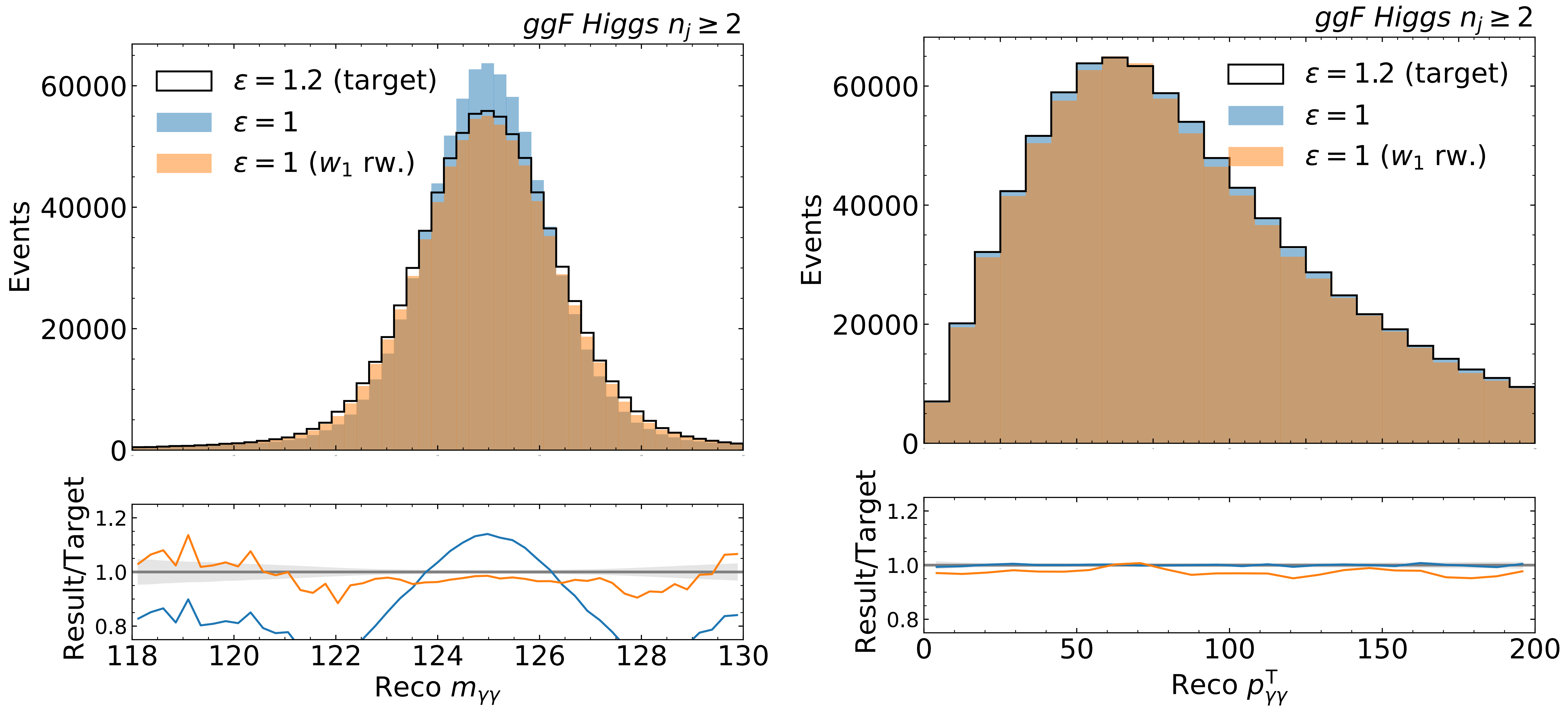


FIG. 6. Higgs boson cross section: the nominal detector-level spectra $m_{\gamma\gamma}$ (left) and $p^{\mathrm{T}}_{\gamma\gamma}$ (right) with $\epsilon_\gamma = 1$ reweighted by the trained w_1 conditioned at $\epsilon_\gamma = 1.2$ and compared to the spectra with $\epsilon_\gamma = 1.2$.

Inference-aware methods

Auto-differentiation builds shadow functions

```
y = x1*x2 + sin(x1)

def exp(x1,x2):
    a = x1*x2
    b = sin(x1)
    y = a+b
    return y

def shadow_exp(point,diff):
    x1,x2 = point
    dx1, dx2 = diff
    da = x1 * dx2 + x2 * dx1
    db = cos(x1) * dx1
    dy = da + db
    return dy

print ("Value for (x1,x2)=(1,2): ", exp(1,2))
print ("Differentiation w.r.t. x1 at (x1,x2)=(1,2): ", shadow_exp((1,2),(1,0)))
print ("Differentiation w.r.t. x2 at (x1,x2)=(1,2): ",shadow_exp((1,2),(0,1)))
```

```
Value for (x1,x2)=(1,2):  2.8414709848078967
Differentiation w.r.t. x1 at (x1,x2)=(1,2):  2.5403023058681398
Differentiation w.r.t. x2 at (x1,x2)=(1,2):  1.0
```

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```

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Value for (x1,x2)=(1,2):  2.8414709848078967
Differentiation w.r.t. x1 at (x1,x2)=(1,2):  2.5403023058681398
Differentiation w.r.t. x2 at (x1,x2)=(1,2):  1.0
```

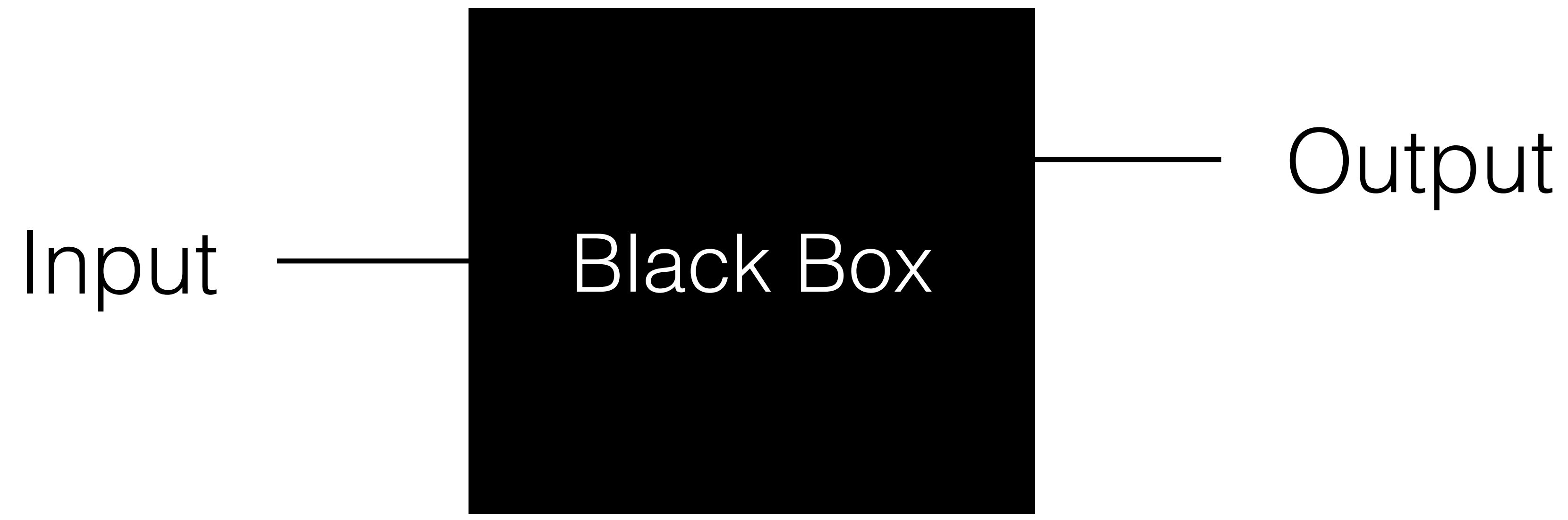
```
import jax.numpy as jnp
from jax import grad, jit, vmap
from jax import random
```

```
def sum_logistic(x):
  return jnp.sum(1.0 / (1.0 + jnp.exp(-x)))

x_small = jnp.arange(3.)
derivative_fn = grad(sum_logistic)
print(derivative_fn(x_small))
```

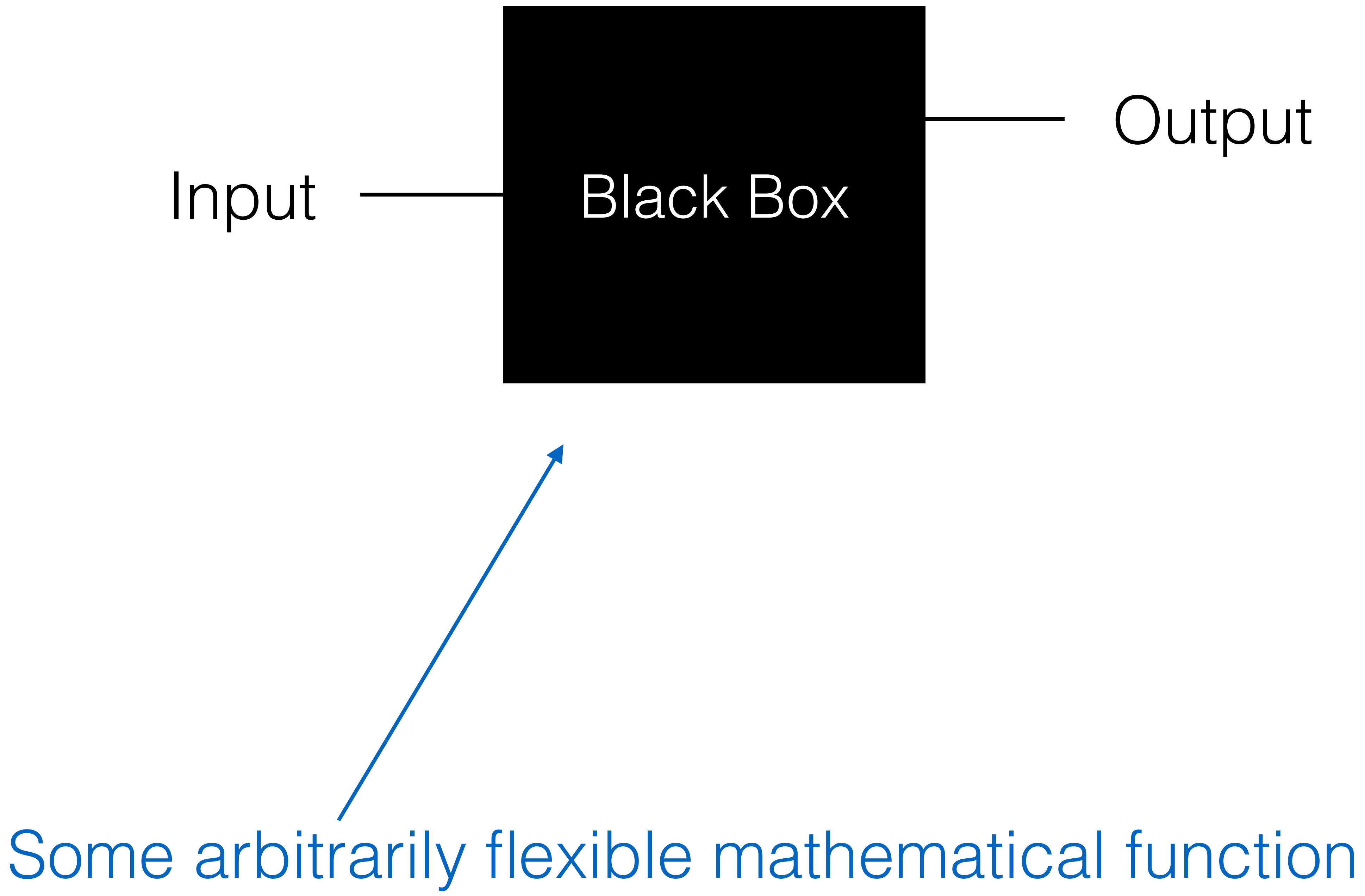
```
[0.25       0.19661194 0.10499357]
```

Black-box => maximally physics informed



- Cannot expect extrapolation
- Interpretability
- Loss function is some ML objective rather than your physics objective

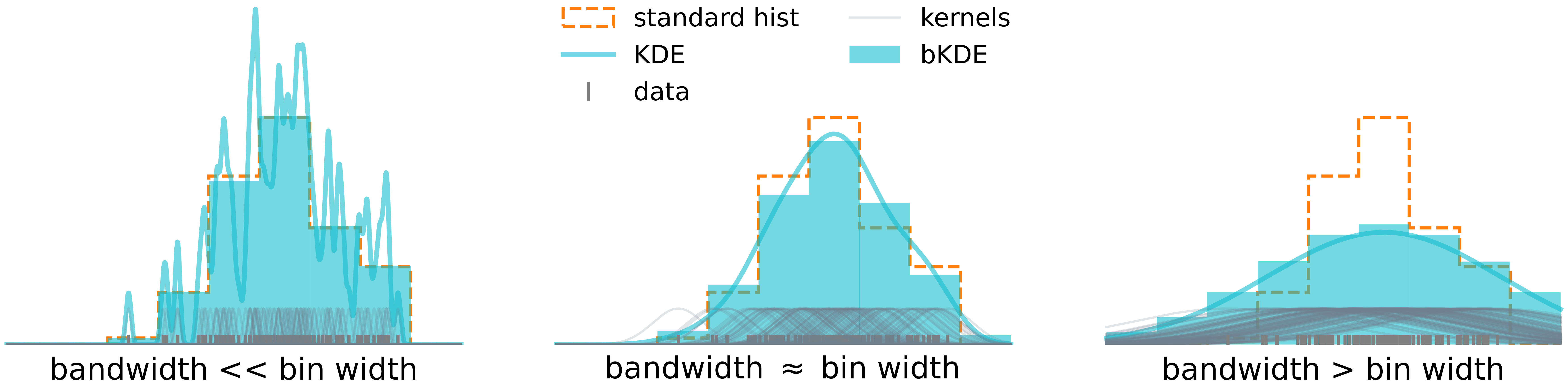
Black-box => maximally physics informed



- Cannot expect extrapolation
- Interpretability
- Loss function is some ML objective rather than your physics objective

Tricks to make everything easily differentiable

- Histogram -> Kernel Density Estimation
- Straight-through gradients
- NN surrogates
- Implicit differentiation to avoid unnecessary gradient propagation
- …



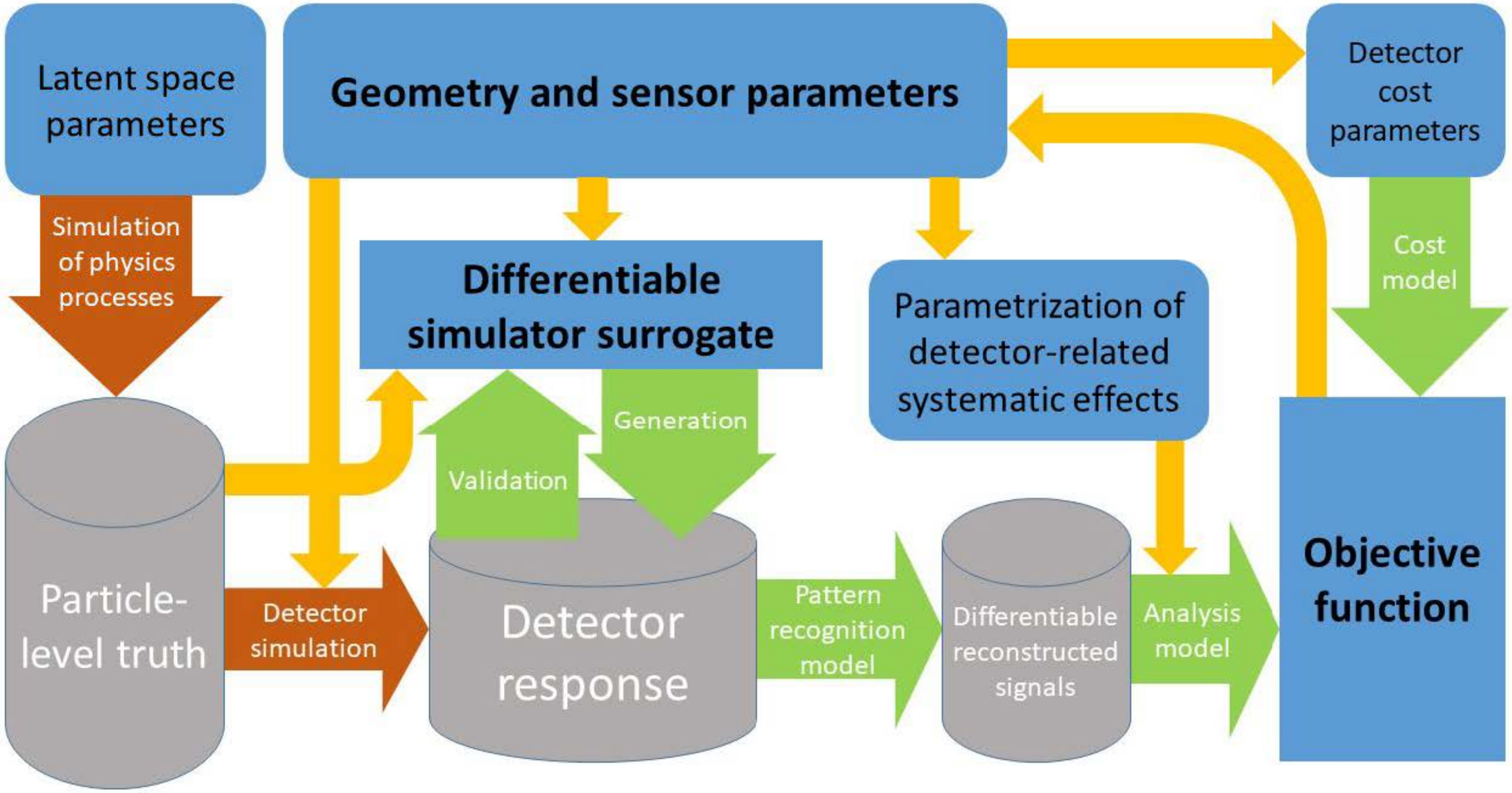
[Simpson et al.](#)

Next generation of detector design …

Toward the End-to-End Optimization
of Particle Physics Instruments
with Differentiable Programming:
a White Paper

White Paper

Next generation of detector design …



Toward the End-to-End Optimization of Particle Physics Instruments with Differentiable Programming: a White Paper

[White Paper]

ML tools powering new generation of histfactory

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