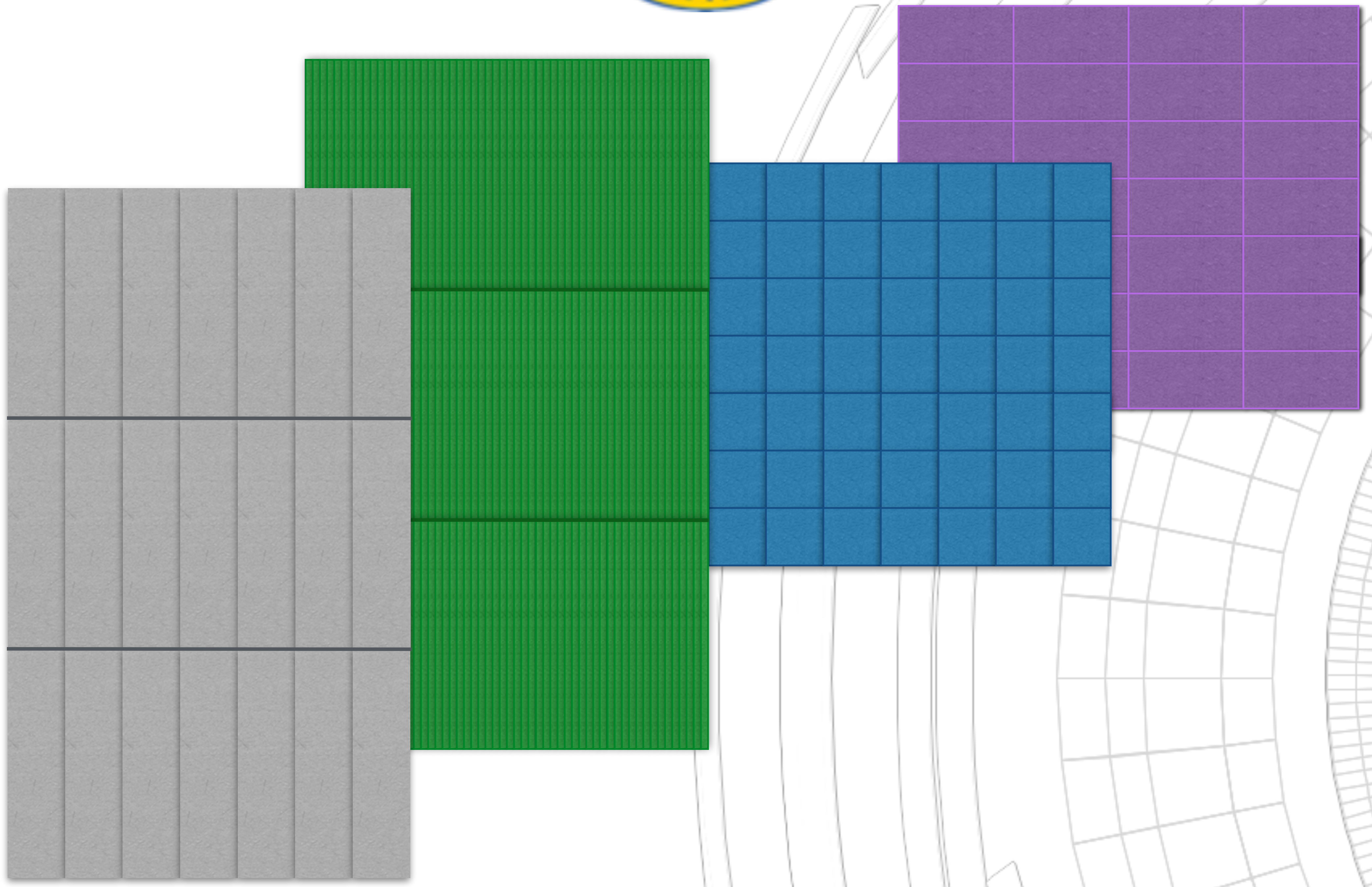
Uncertainties in the era of ML

Aishik Ghosh

KIAS Workshop at Konjiam Resort
13 Feb 2023



Polarising topic, expect spicy debate ..

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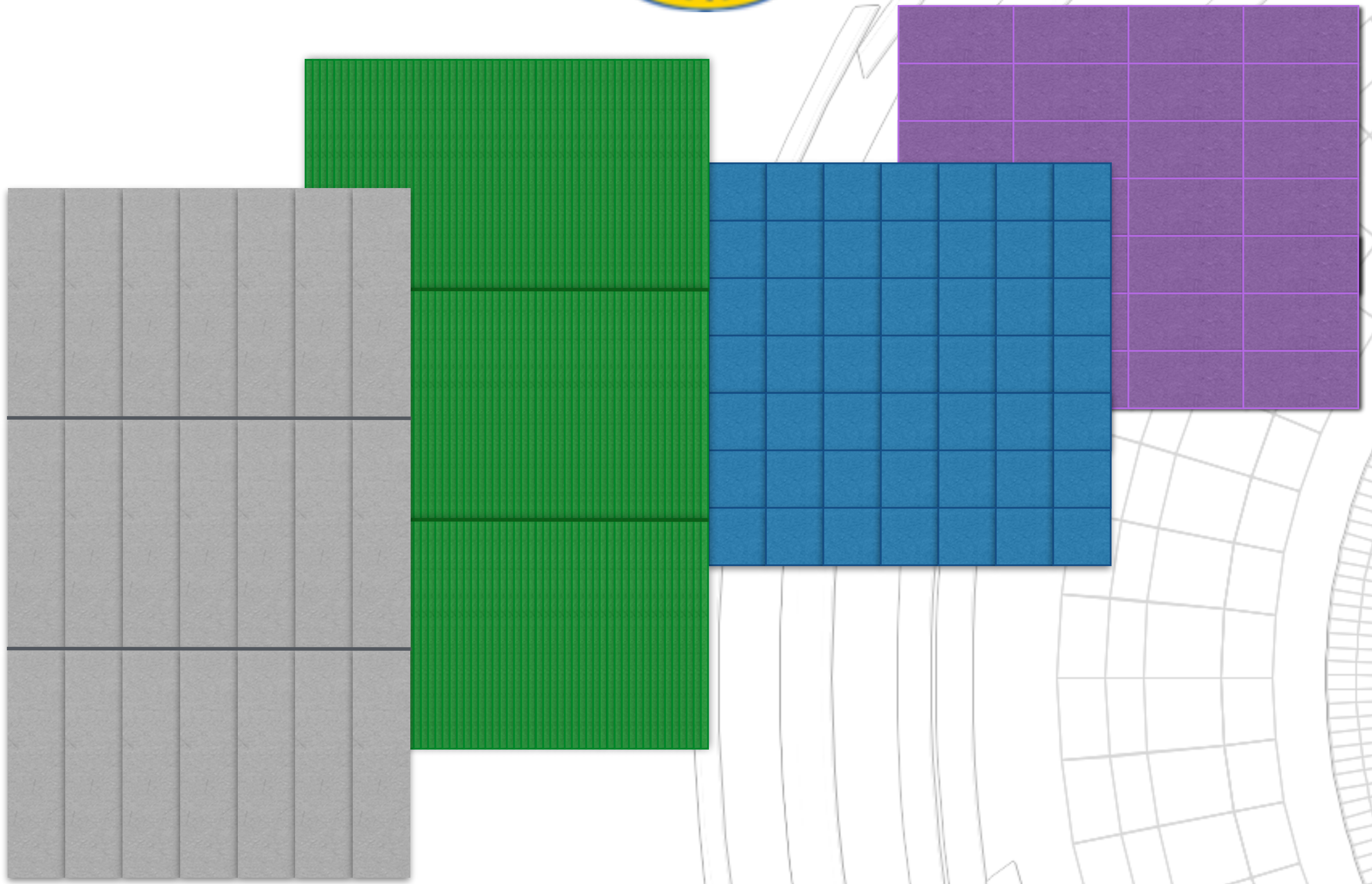

Uncertainties, the bedrock of experimental science

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$m_H = 125.25 \pm 0.17$ GeV

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Uncertainties, the bedrock of experimental science

mH = 125.25 ± 0.17 GeV

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

Uncertainties, the bedrock of experimental science

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

Systematic Uncertainties: What if all my measurements are biased in the same way !?

Uncertainties, the bedrock of experimental science

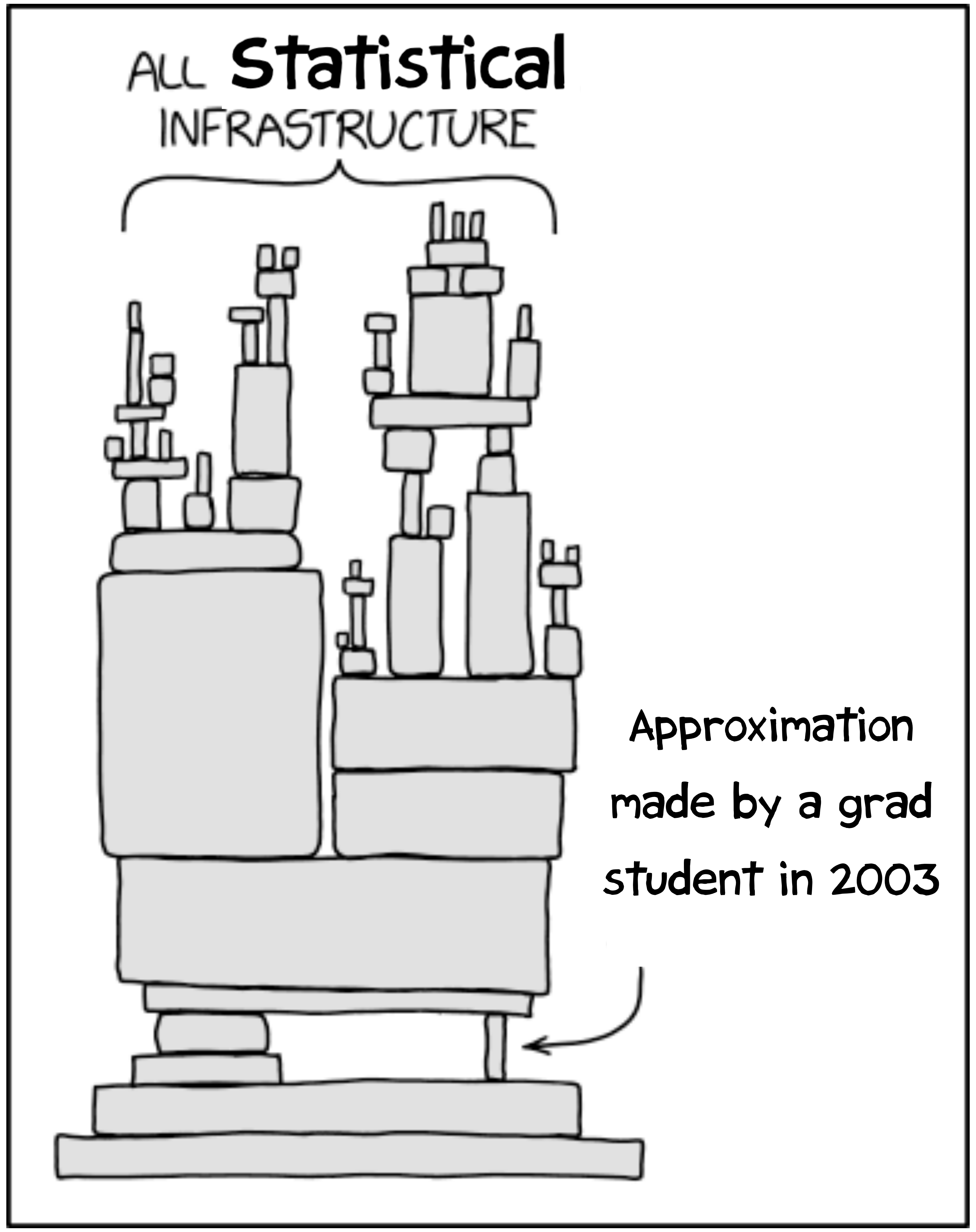
mH = 125.25 ± 0.17 GeV

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

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

Systematic Uncertainties: What if all my measurements are biased in the same way !?

Nuisance Parameter Infrastructure

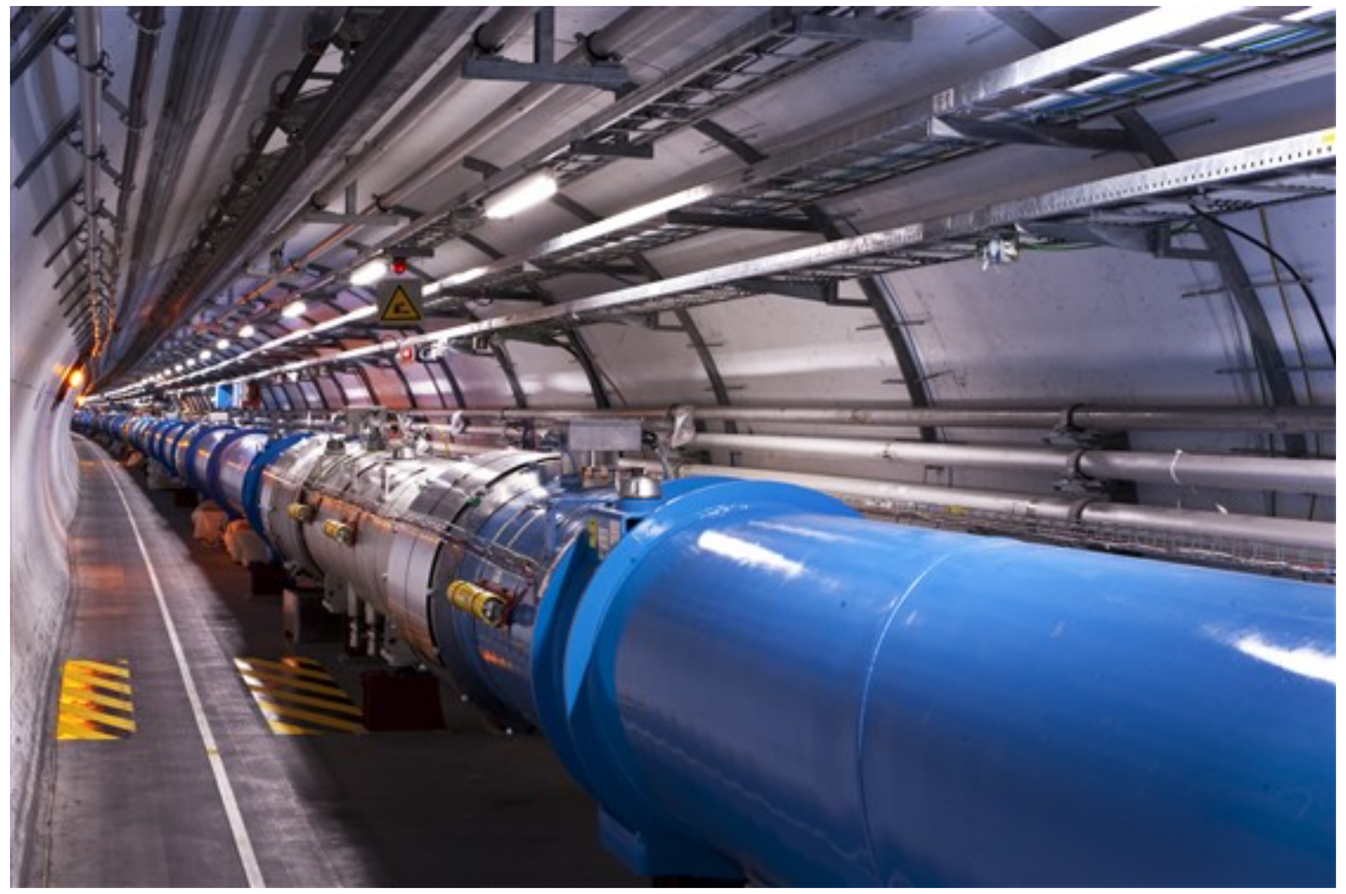


From Daniel Whiteson

Time to re-examine
some of the
underlying pieces

Are they up to the
task of the precision era?

Simulation Based Inference at LHC



Unlabelled data from LHC

Compare to find New Physics

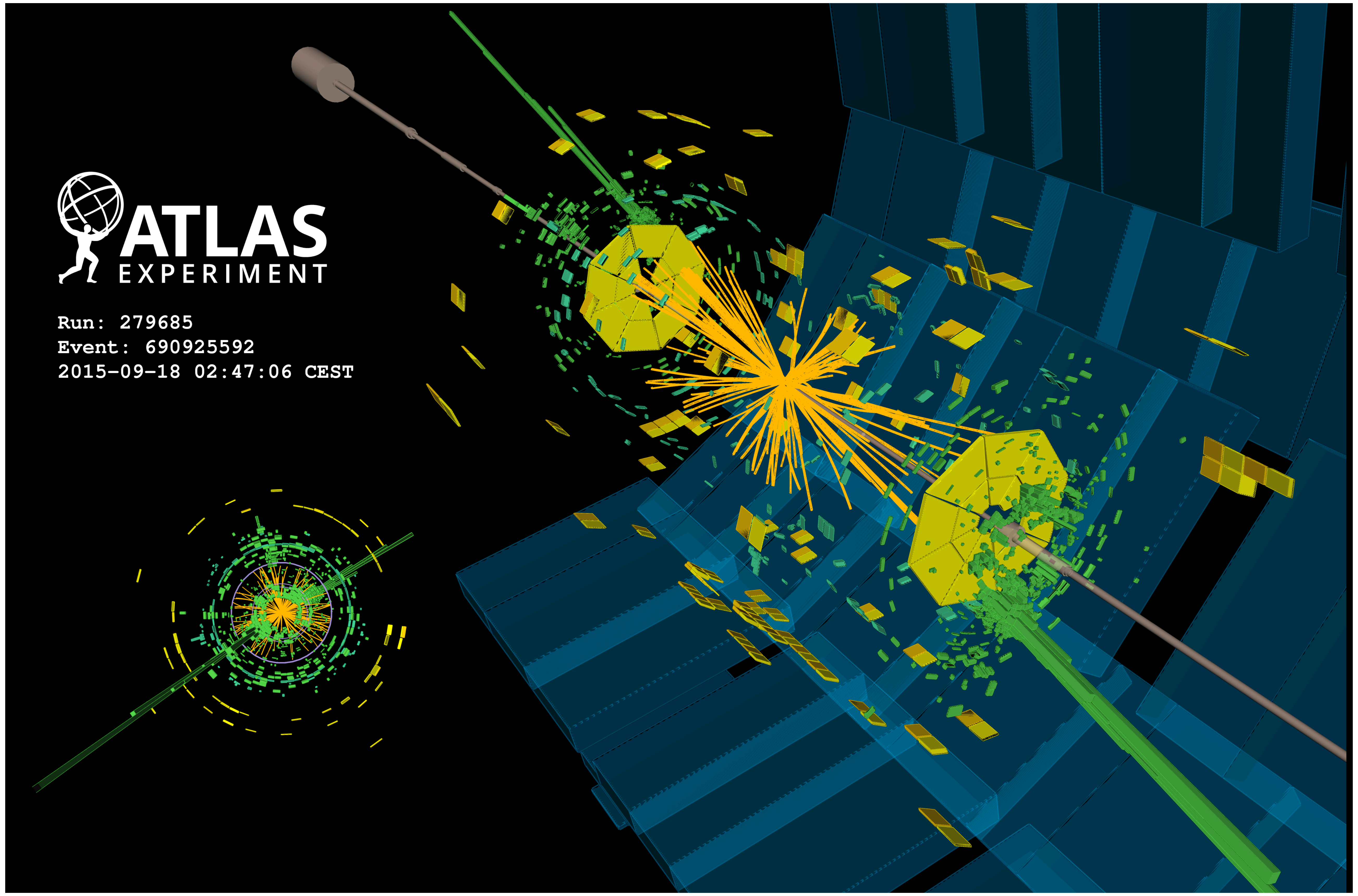
Simulation using Standard Model of particle physics

High dimensional data

Detector has ~100 million sensors

→ Combine information into 1 powerful variable

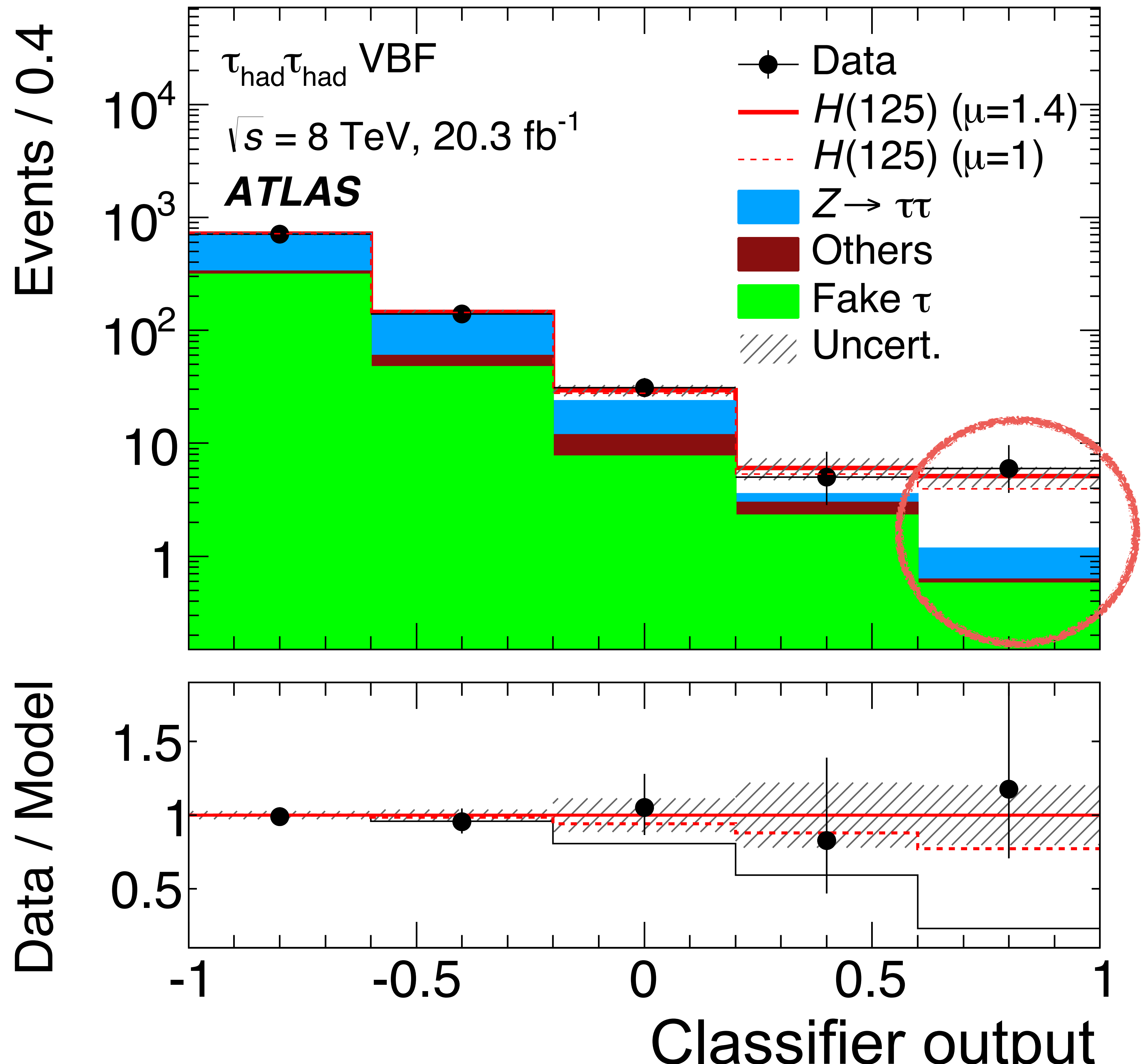
Look at histogram of this variable



Build this observable with ML

Bread & butter 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

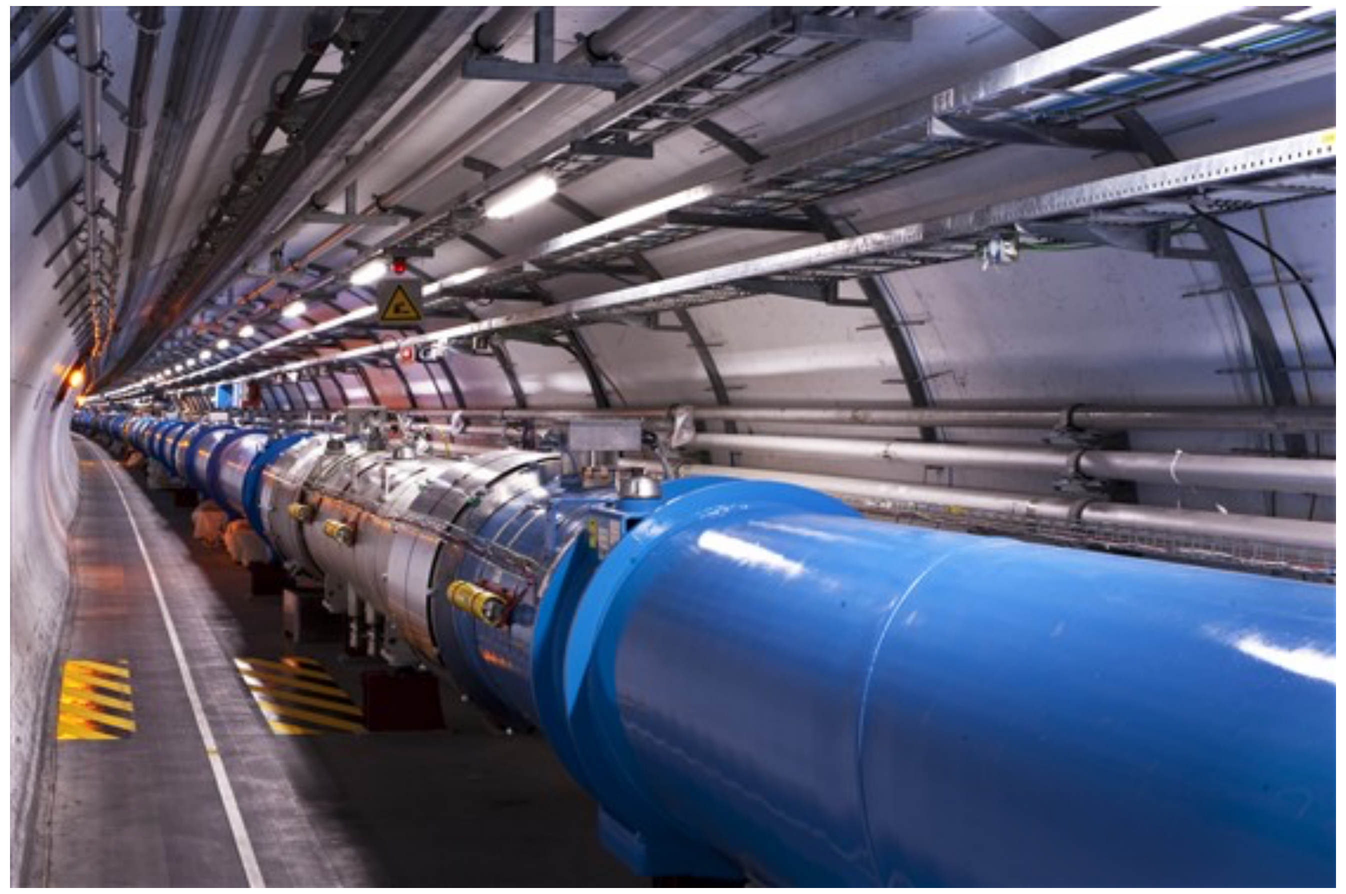
1501.04943

Known unknowns

Simulation using Standard Model of particle physics

Train ML models on simulation, apply on data

Unlabelled data from LHC



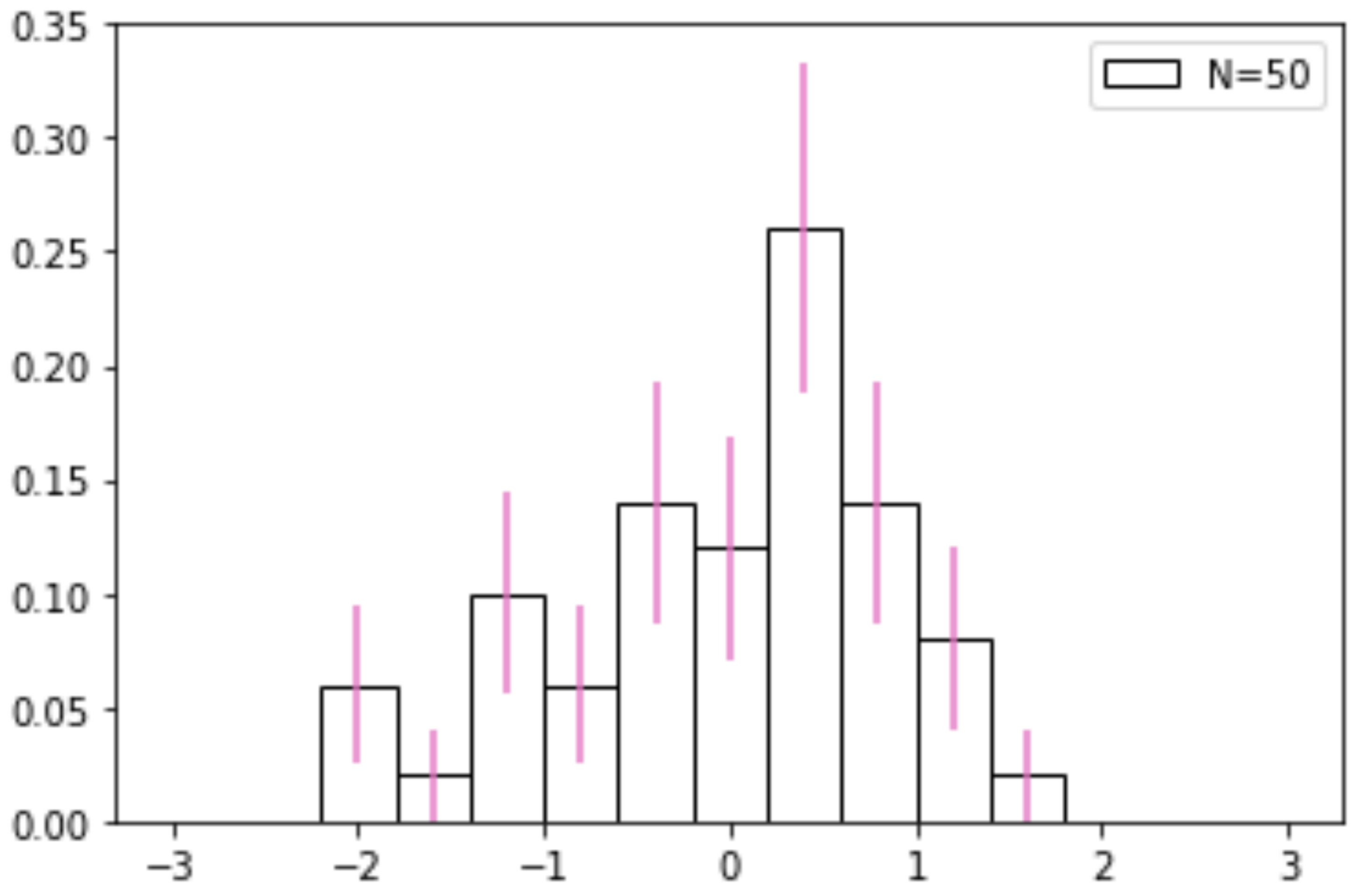
Simulate using best guess: Z=1

Detector state Z = ? in data

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

Typical Uncertainties in HEP

Statistical Uncertainty



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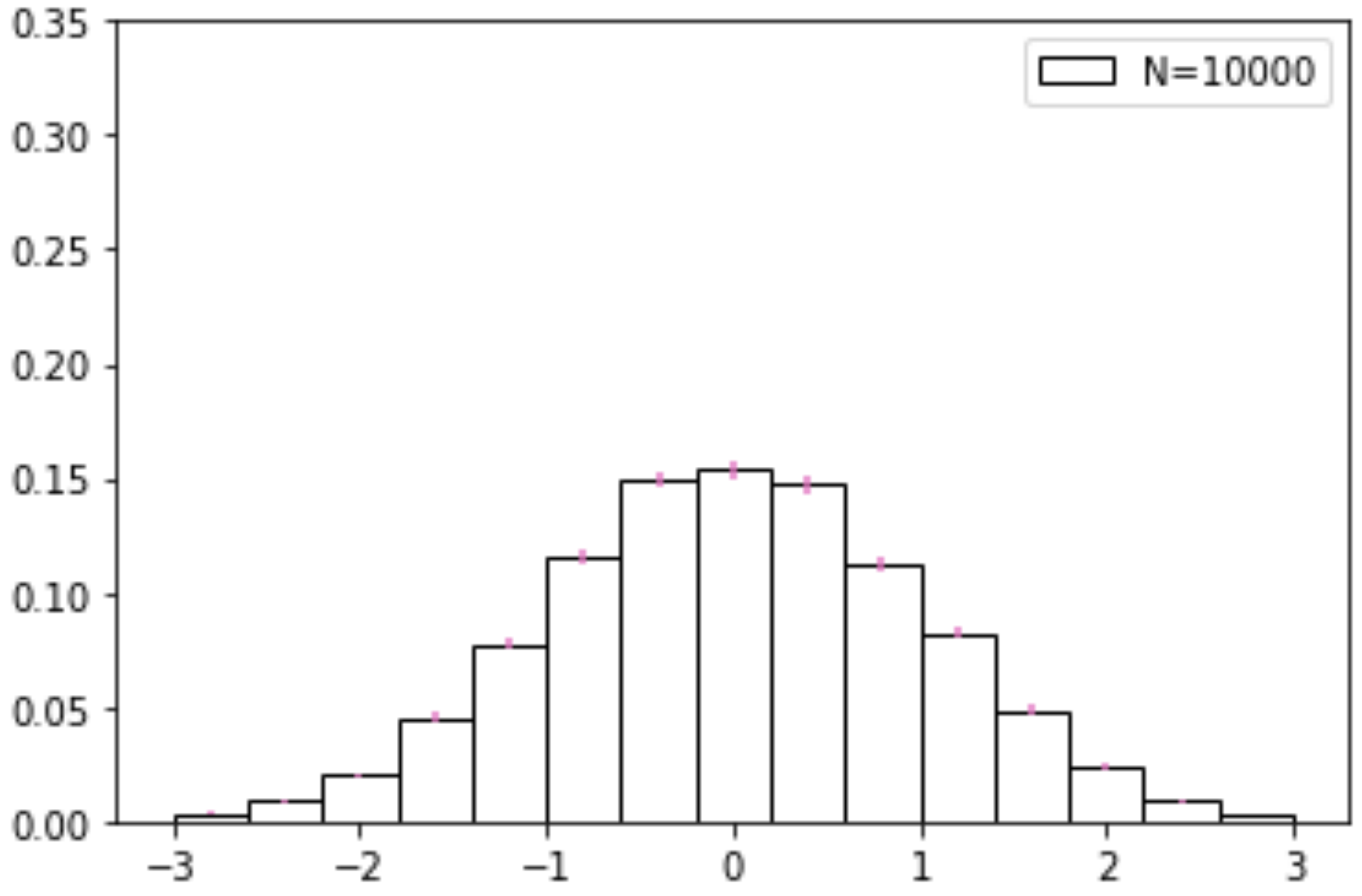

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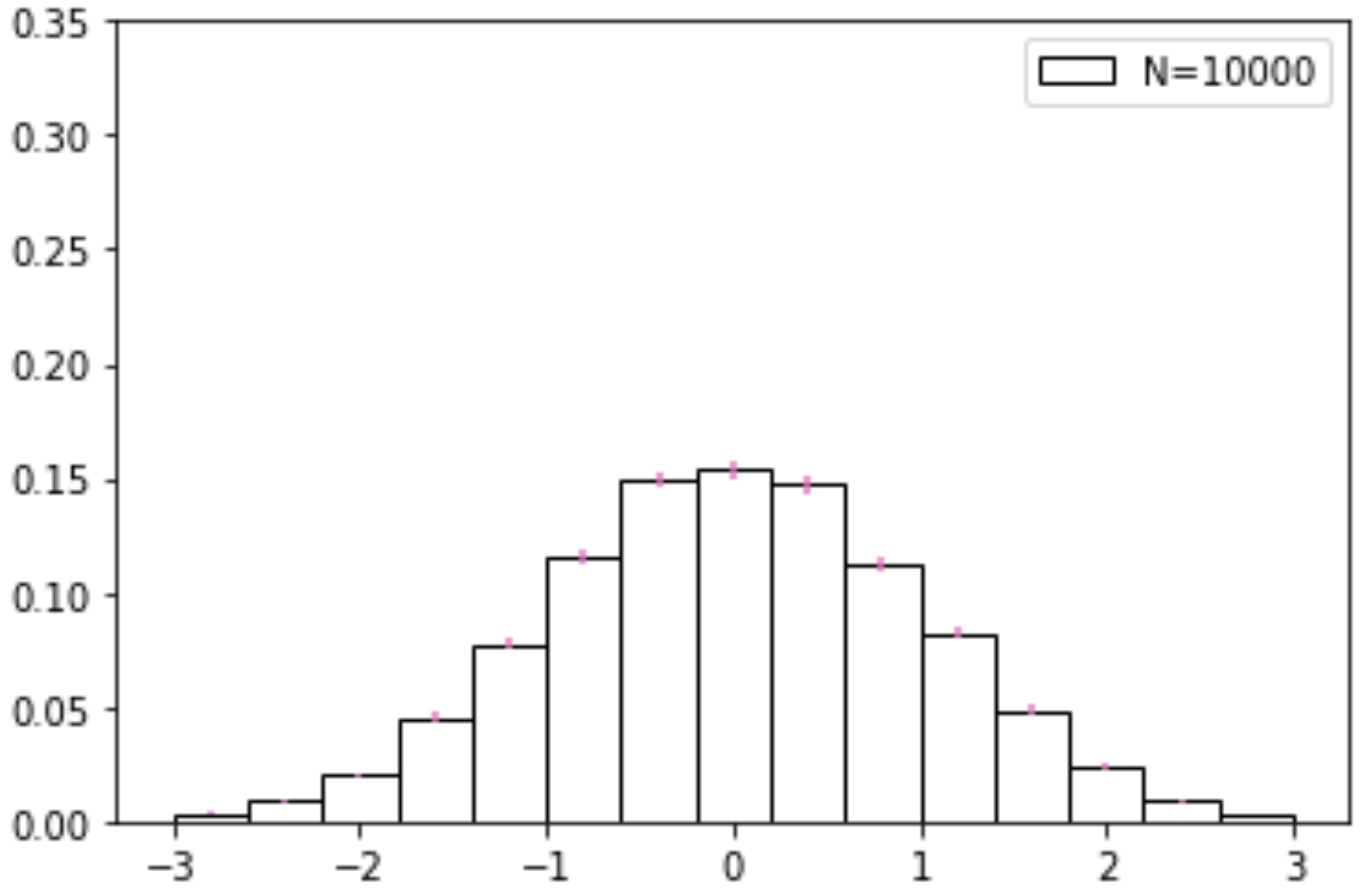
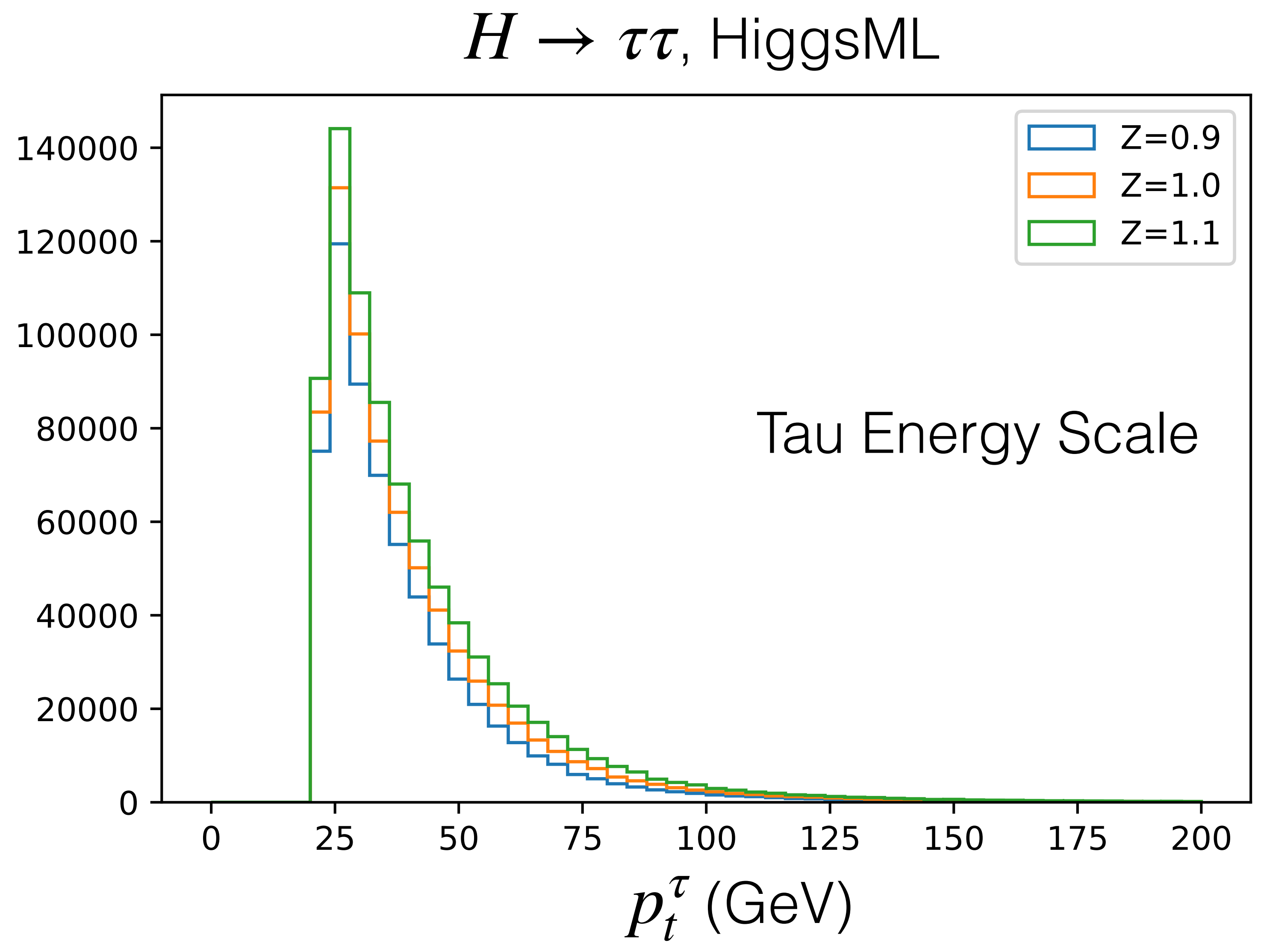
Statistical Uncertainty



Systematic Experimental Uncertainty



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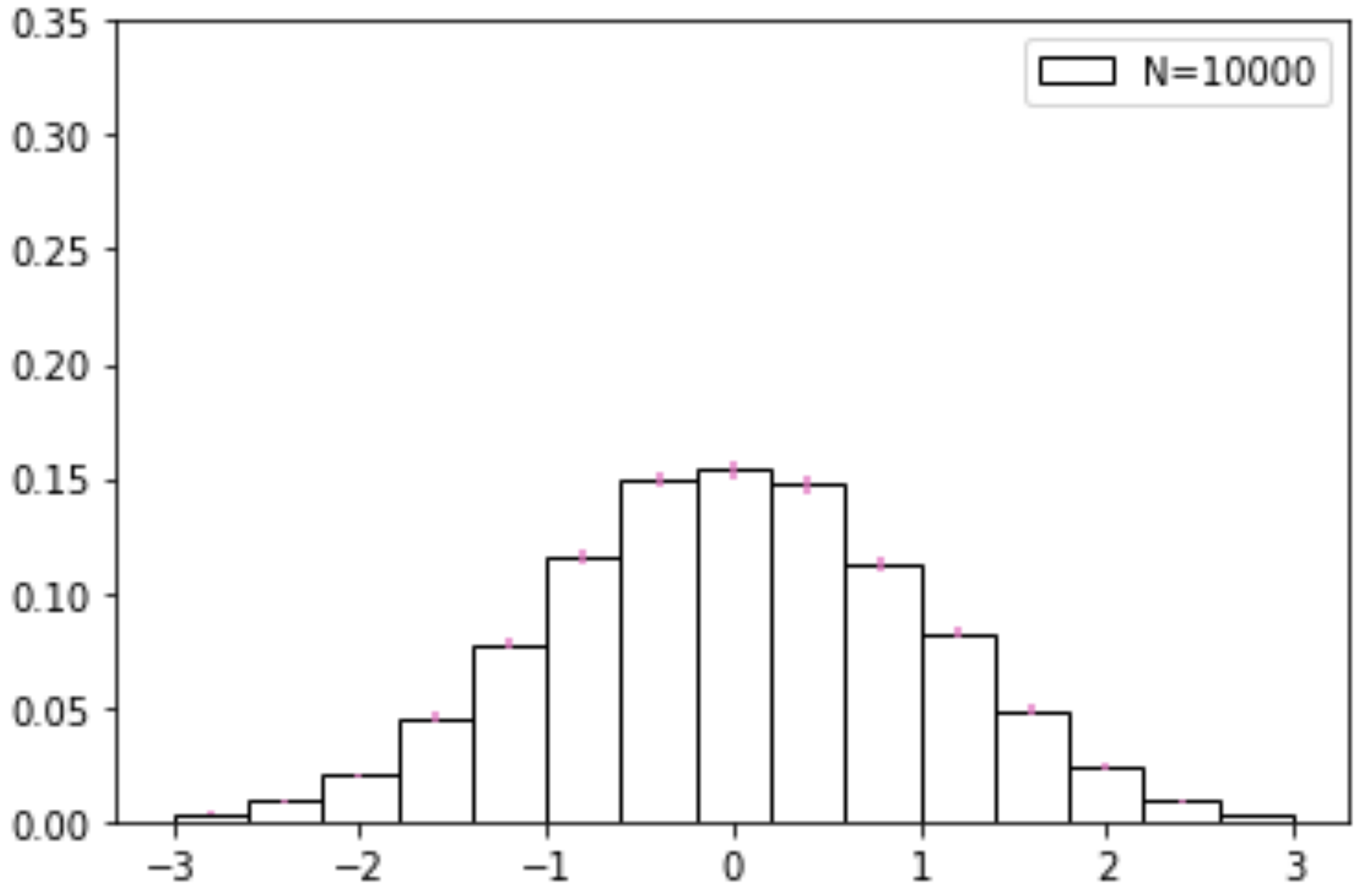

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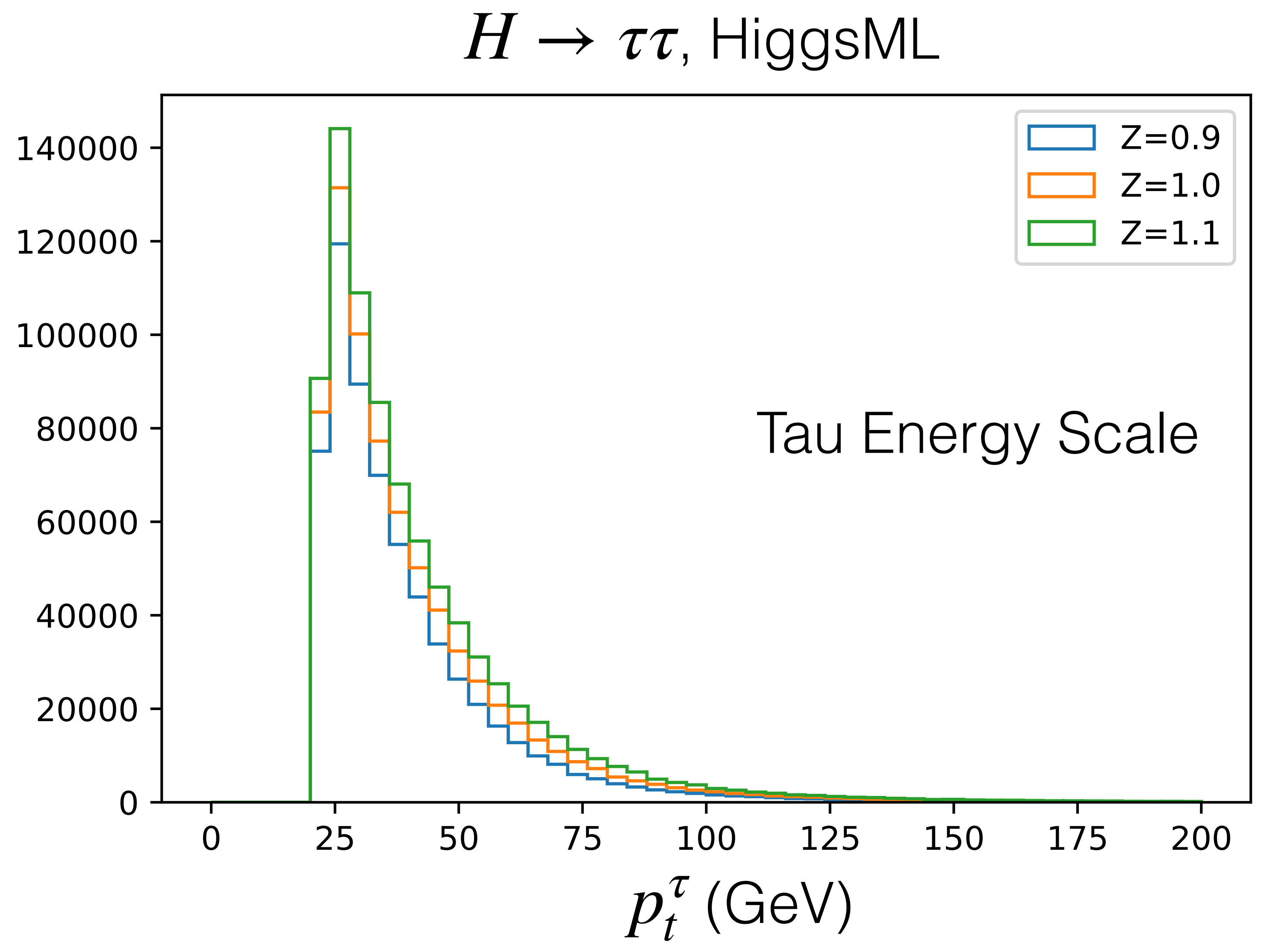
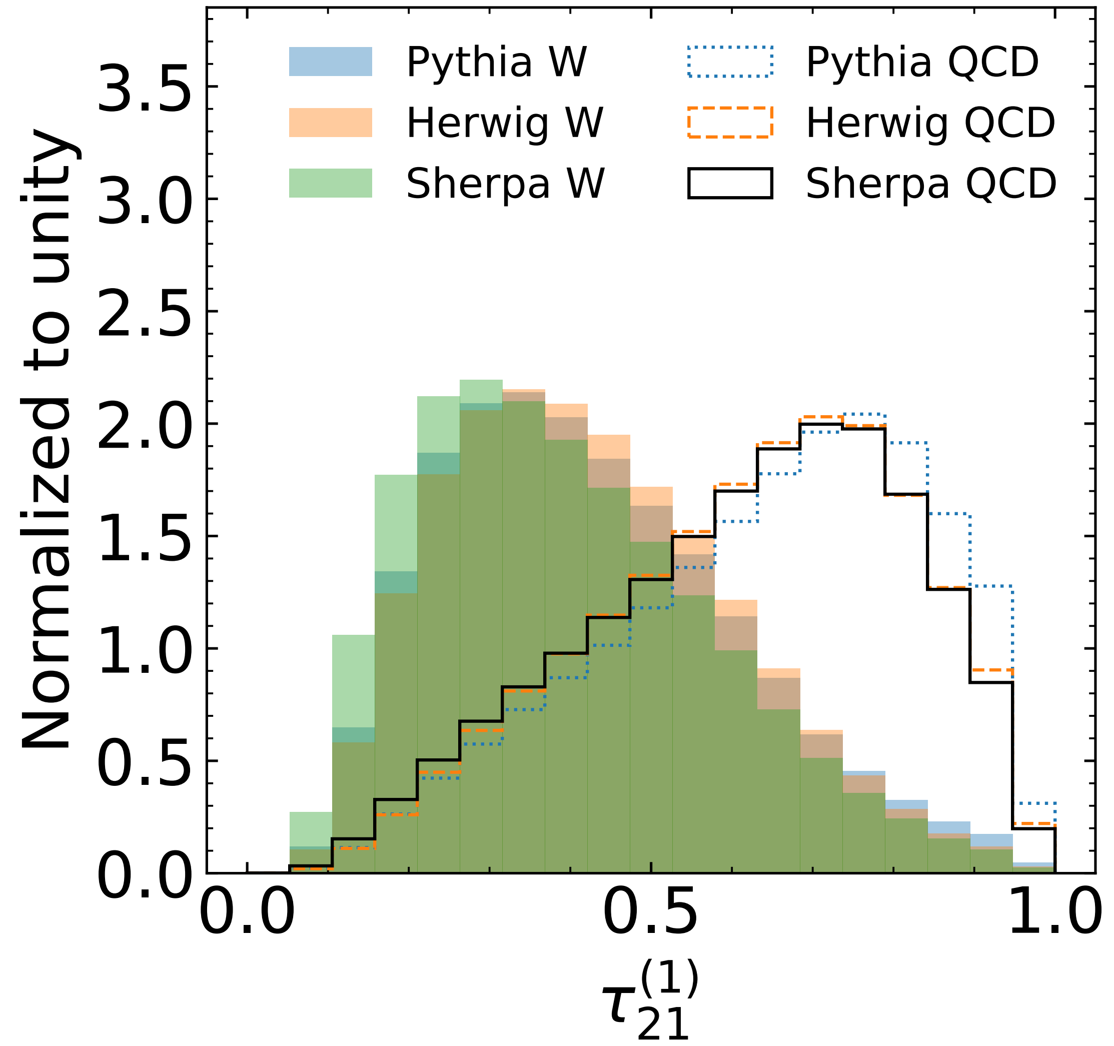


Systematic Theory Uncertainty



Typical Uncertainties in ML

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Aleatoric Uncertainty

Inherent in data / experiment
Irreducible

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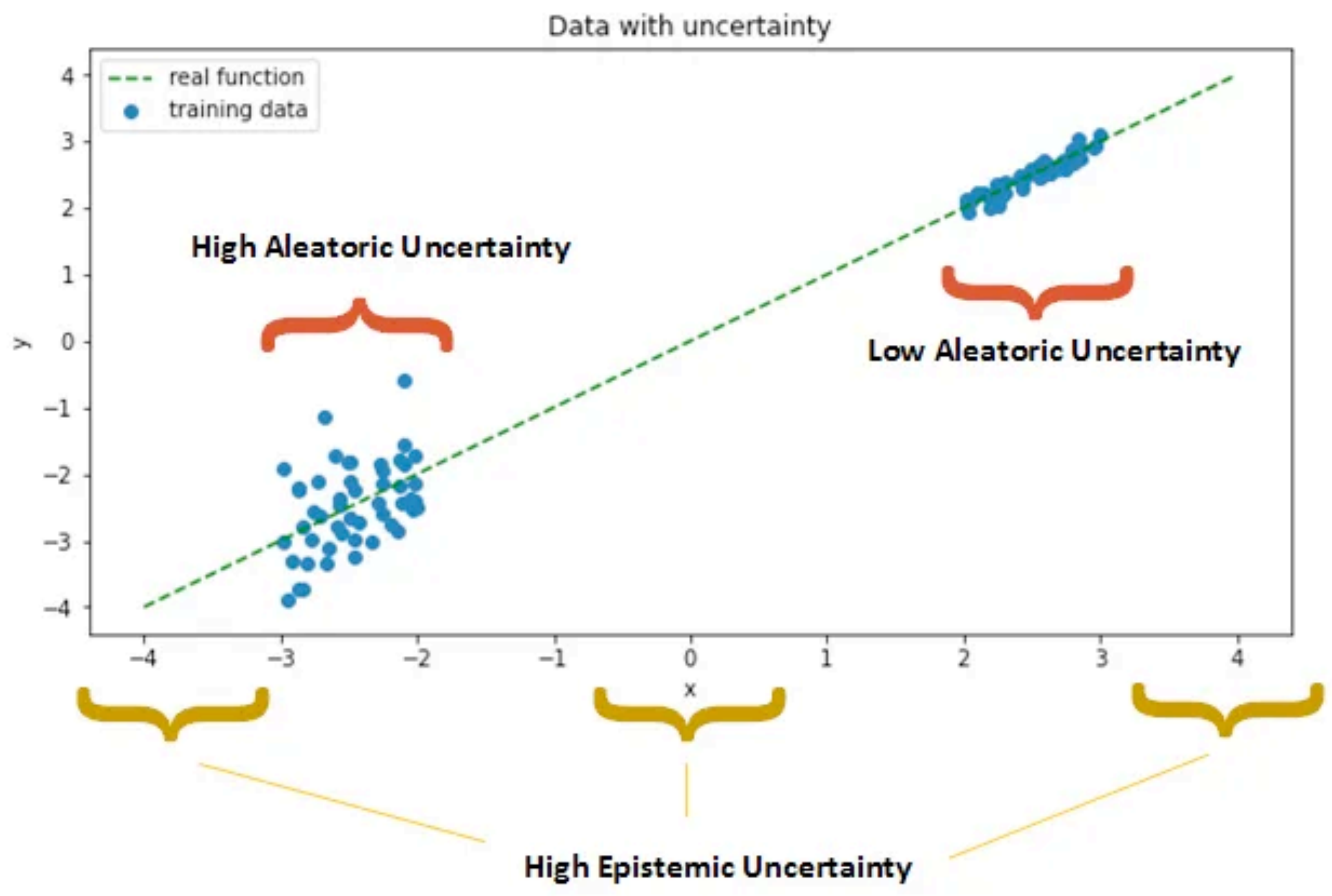
Epistemic Uncertainty



Could reduce by gathering more data

https://towardsdatascience.com/my-deep-learning-model-says-sorry-i-dont-know-the-answer-that-s-absolutely-ok-50ffa562cb0b

Typical Uncertainties in ML

Aleatoric Uncertainty

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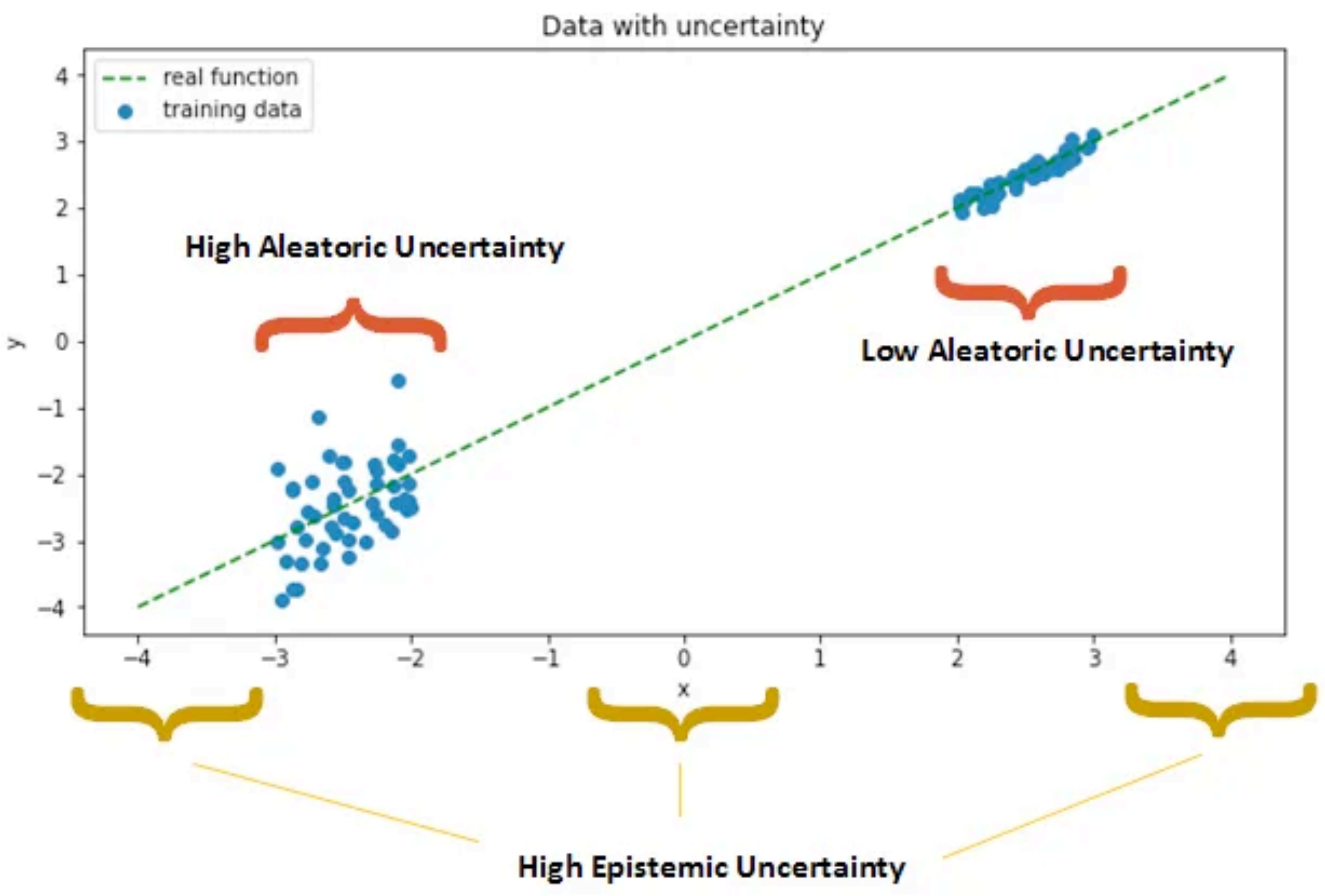


ng more data

om/my-deep-learning-model-says-sorry-i-
-absolutely-ok-50ffa562cb0b


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

Outline

- Experimental Uncertainties
- Theory Uncertainties
- Performance Quantification Metrics for Generative Models

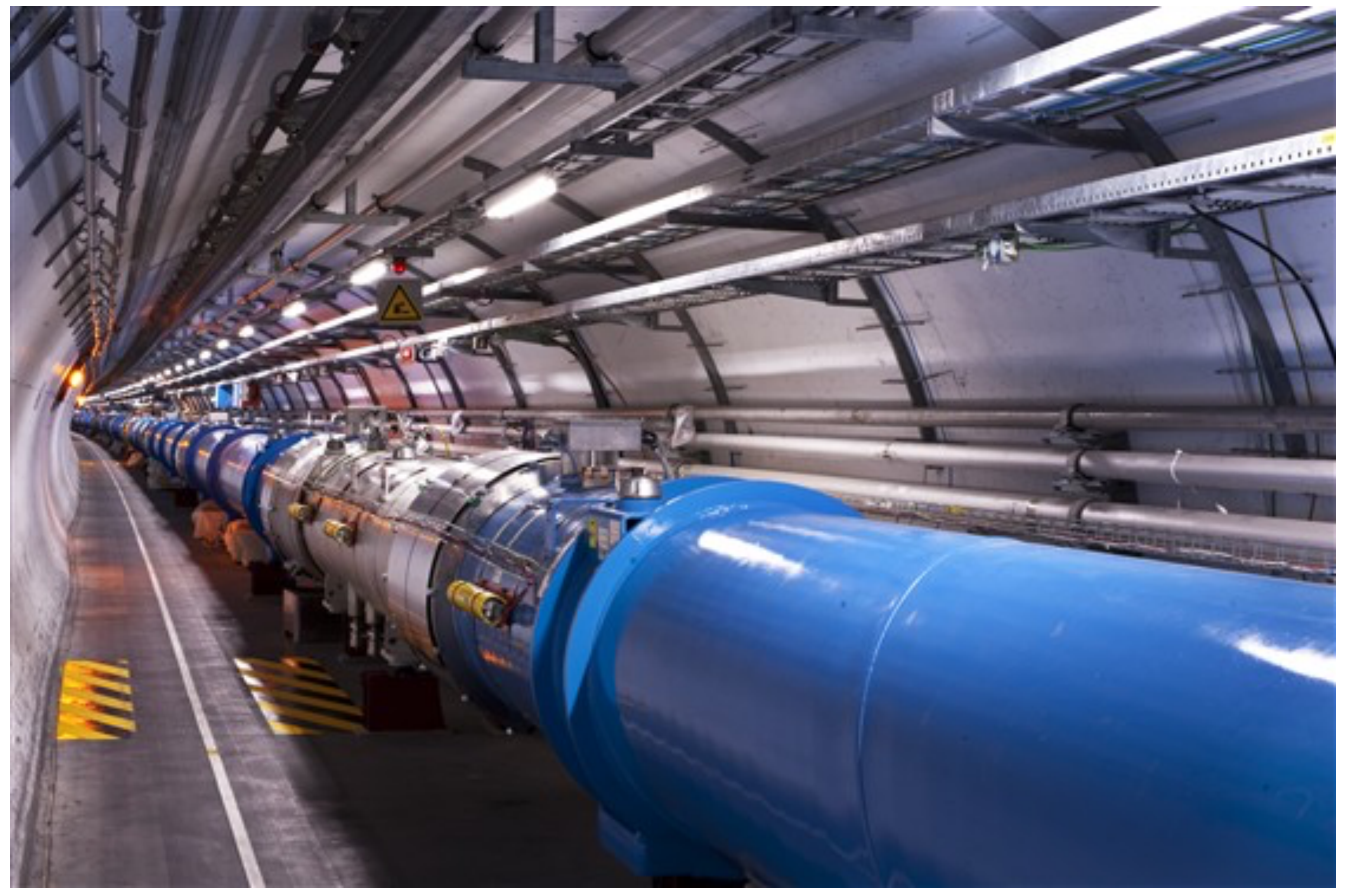
Experimental Uncertainties

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

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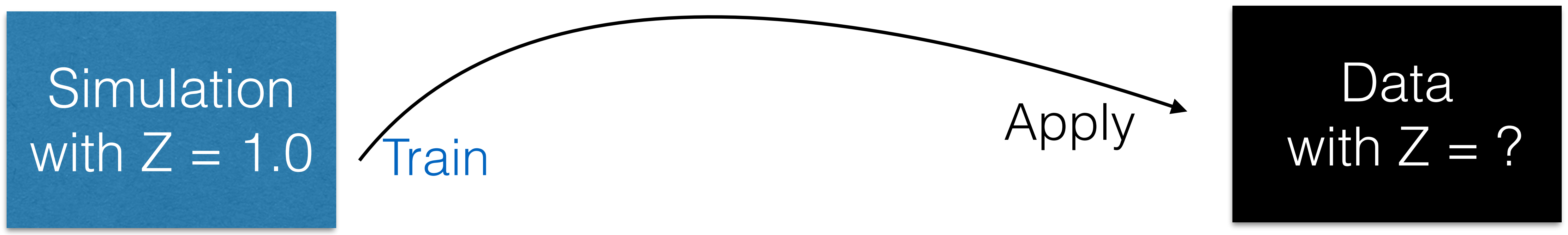
Baseline Approach to Uncertainty Quantification

Train AI classifier on nominal data (assume detector state Z=1) and estimate uncertainties using alternate simulations



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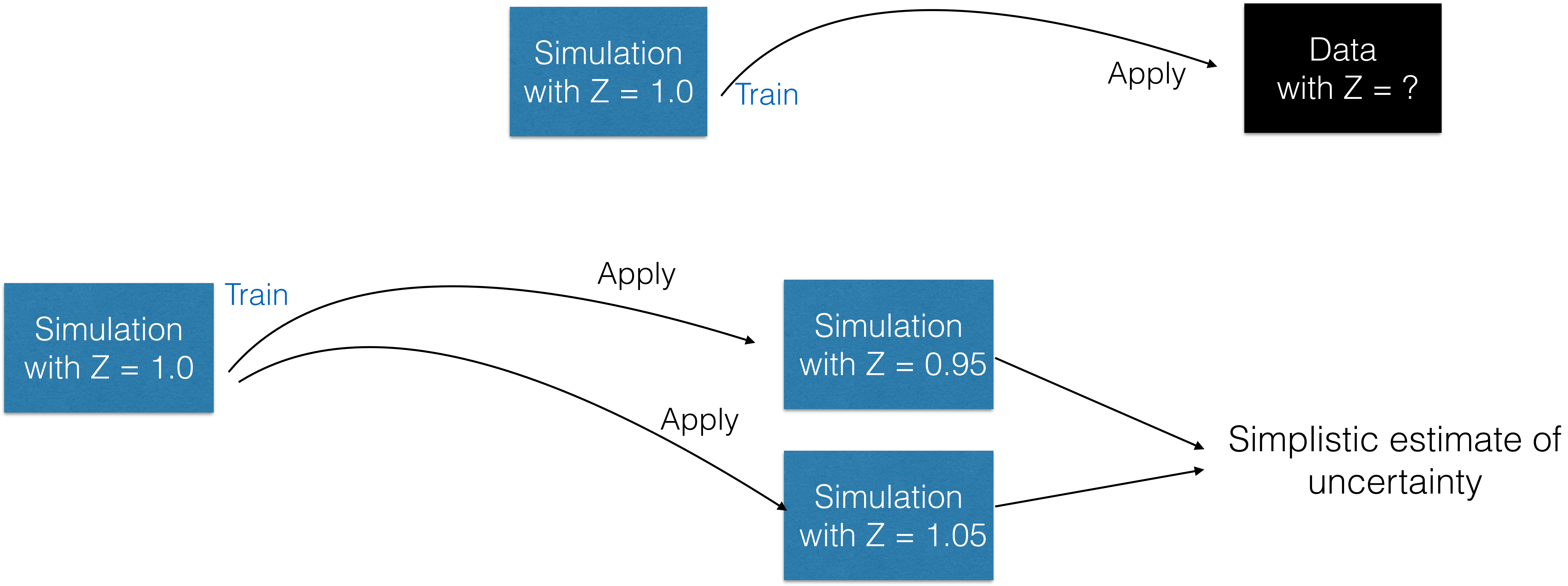


Full statistical treatment → Expensive 'Profile Likelihood'

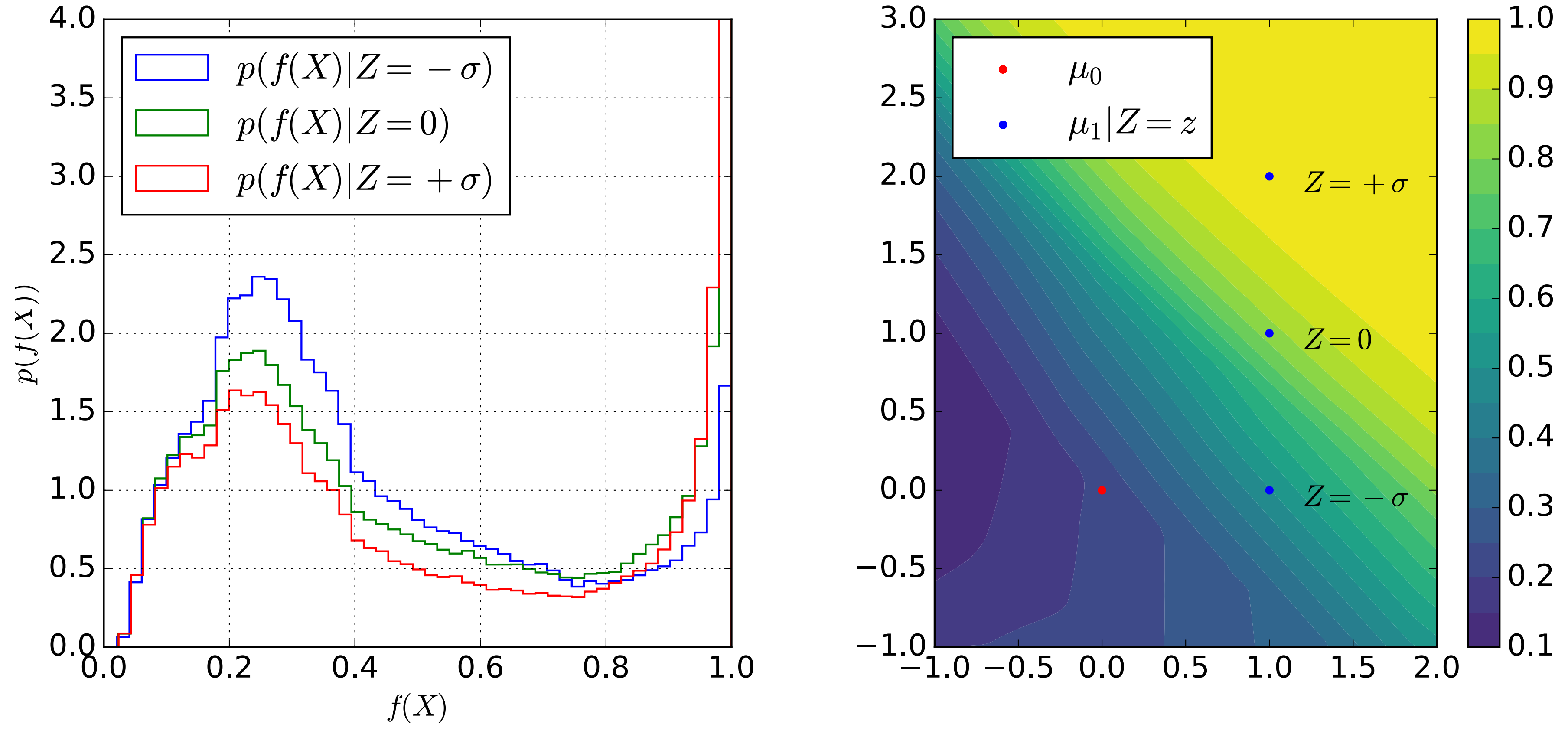
Learning to Pivot [1611.01046]

Similar ideas: 1905.10384, 1305.7248, 1907.11674, epjconf_chep2018_06024

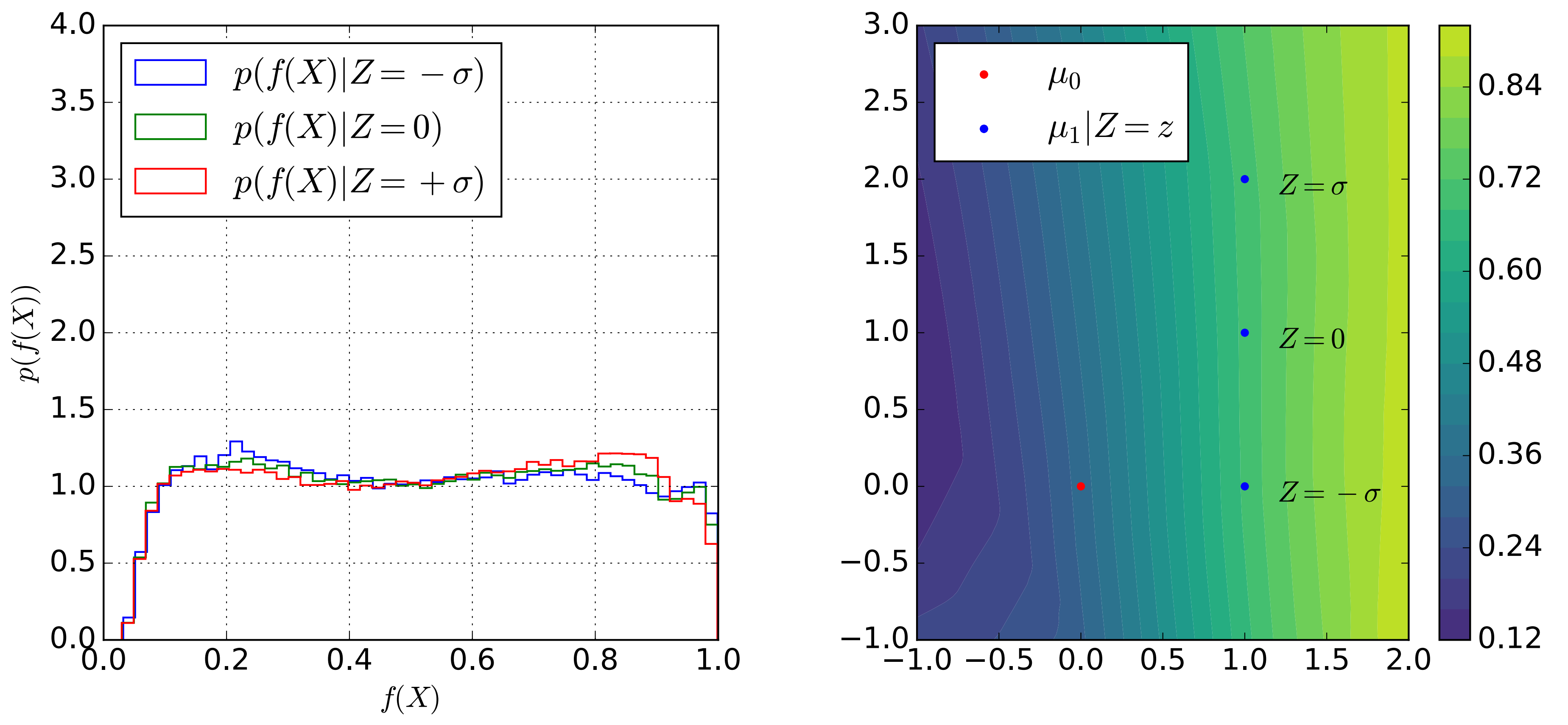
Lots of innovation towards decorrelated classifiers

Ideas from AI fairness: Make the classifier make the same response regardless of race / gender

Imported to physics: Make classifier robust to changes in Z (invariant to impact of nuisance parameters)

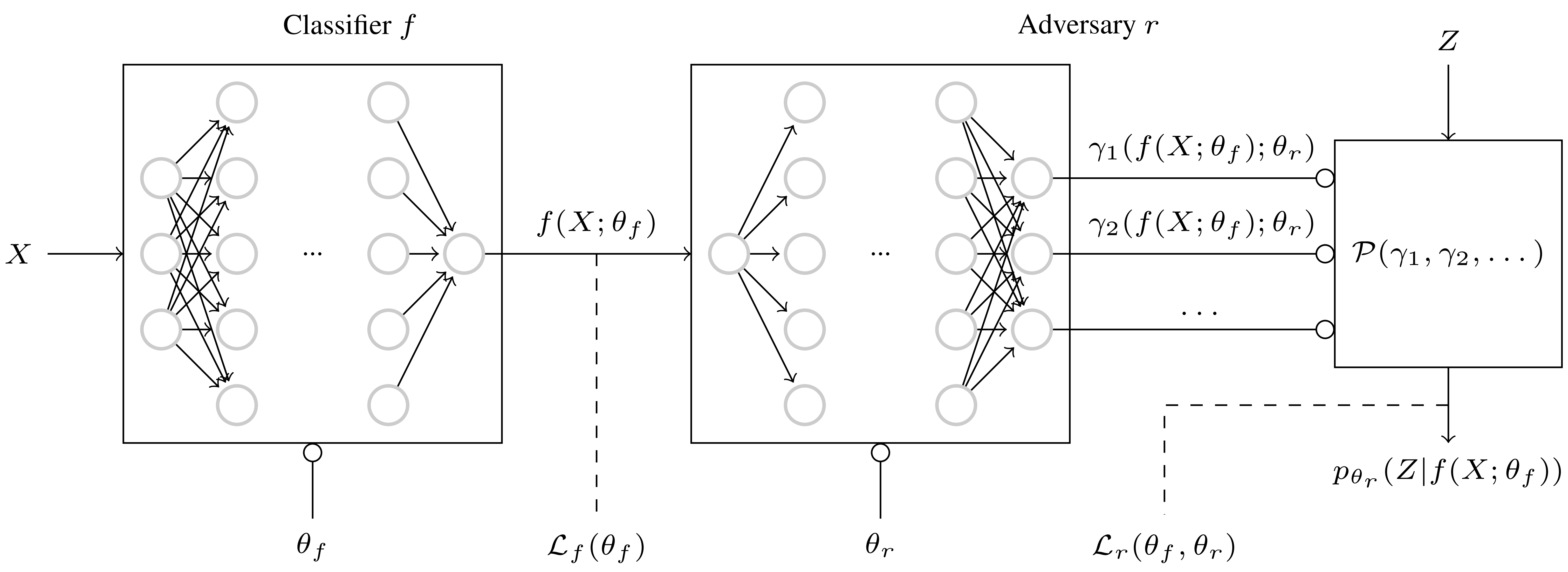


DL Decorrelation



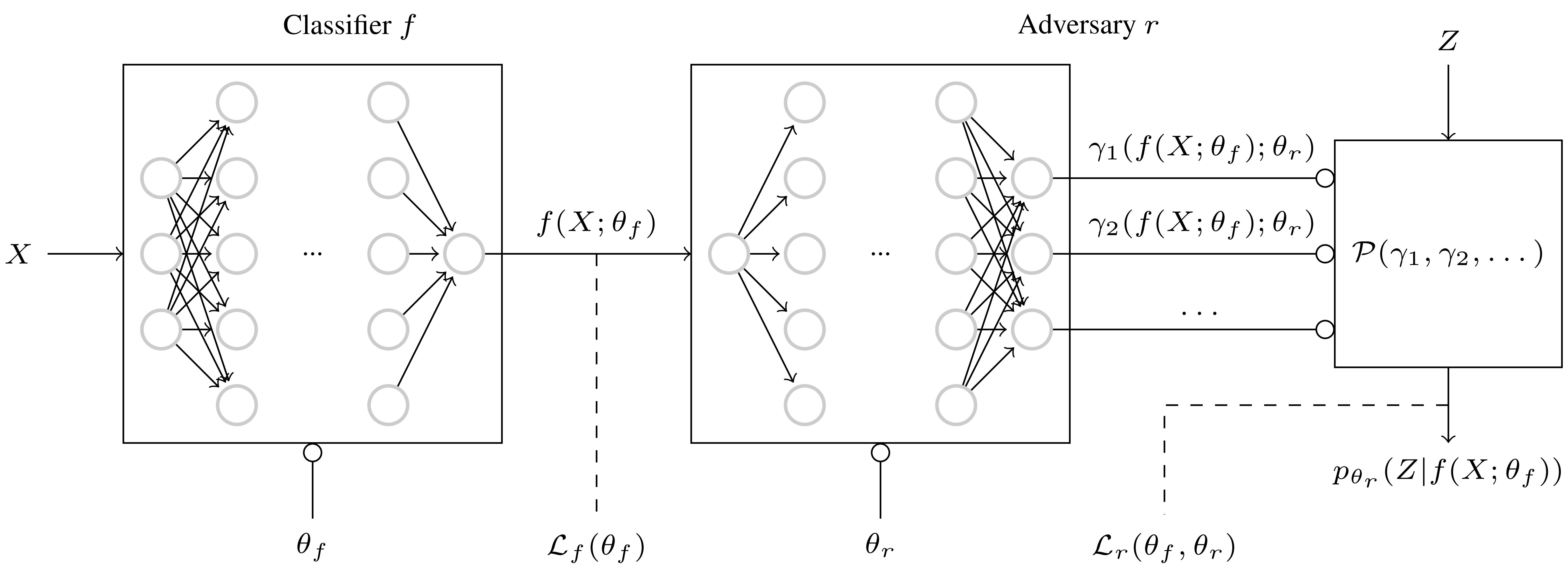
Classifier output for various values of Z

Adversarial decorrelation



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

Adversarial decorrelation

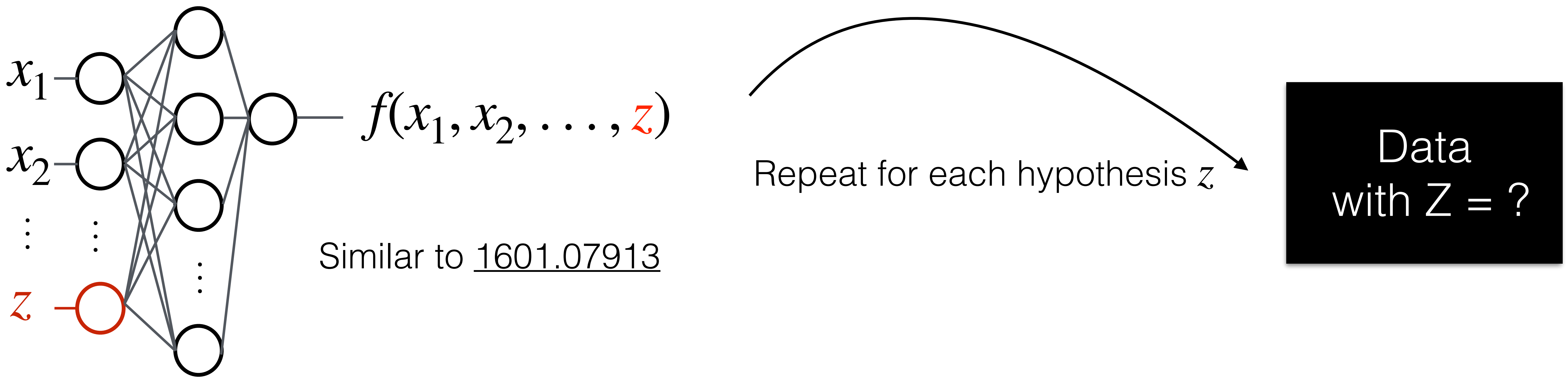


To fool the adversary, classifier output should be decorrelated to Z

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

Advocated for the opposite of decorrelation

- Fully parameterise the classifier on Z in a “uncertainty aware” way



Similar to 1601.07913

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

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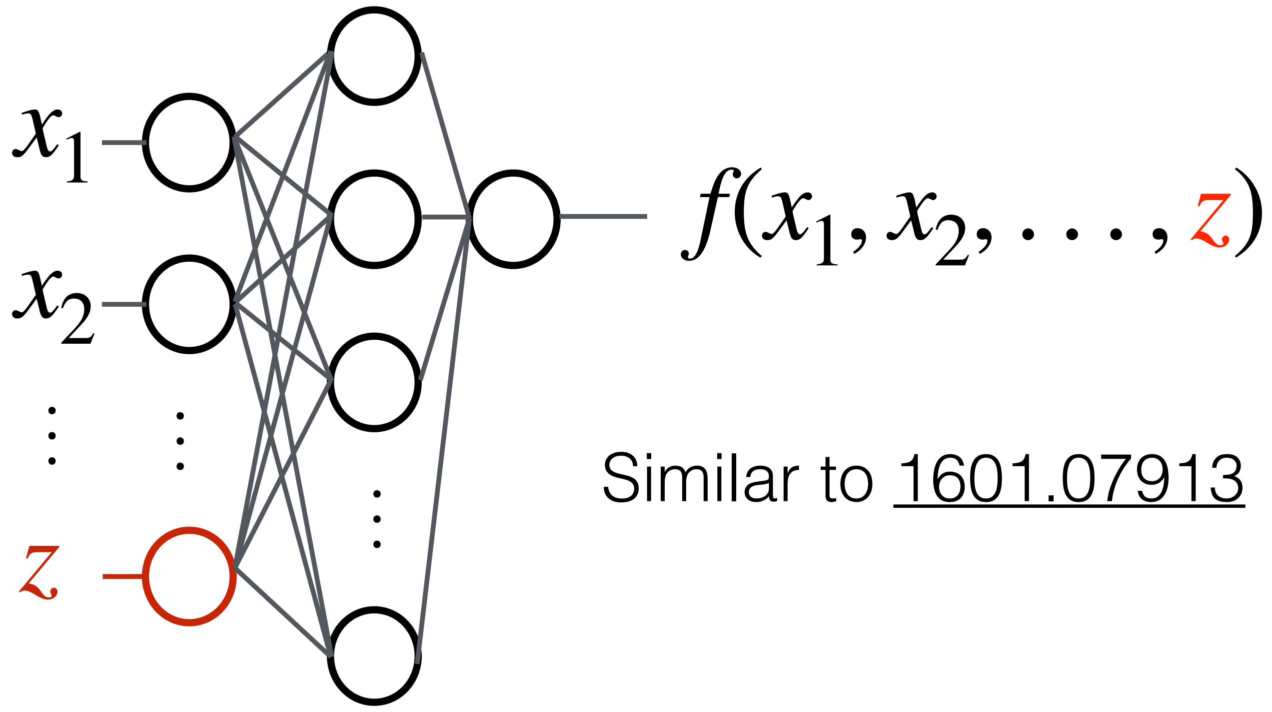
- Fully parameterise the classifier on Z in a "uncertainty aware" way



Similar to 1601.07913

Repeat for each hypothesis z

Data
with Z = ?

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

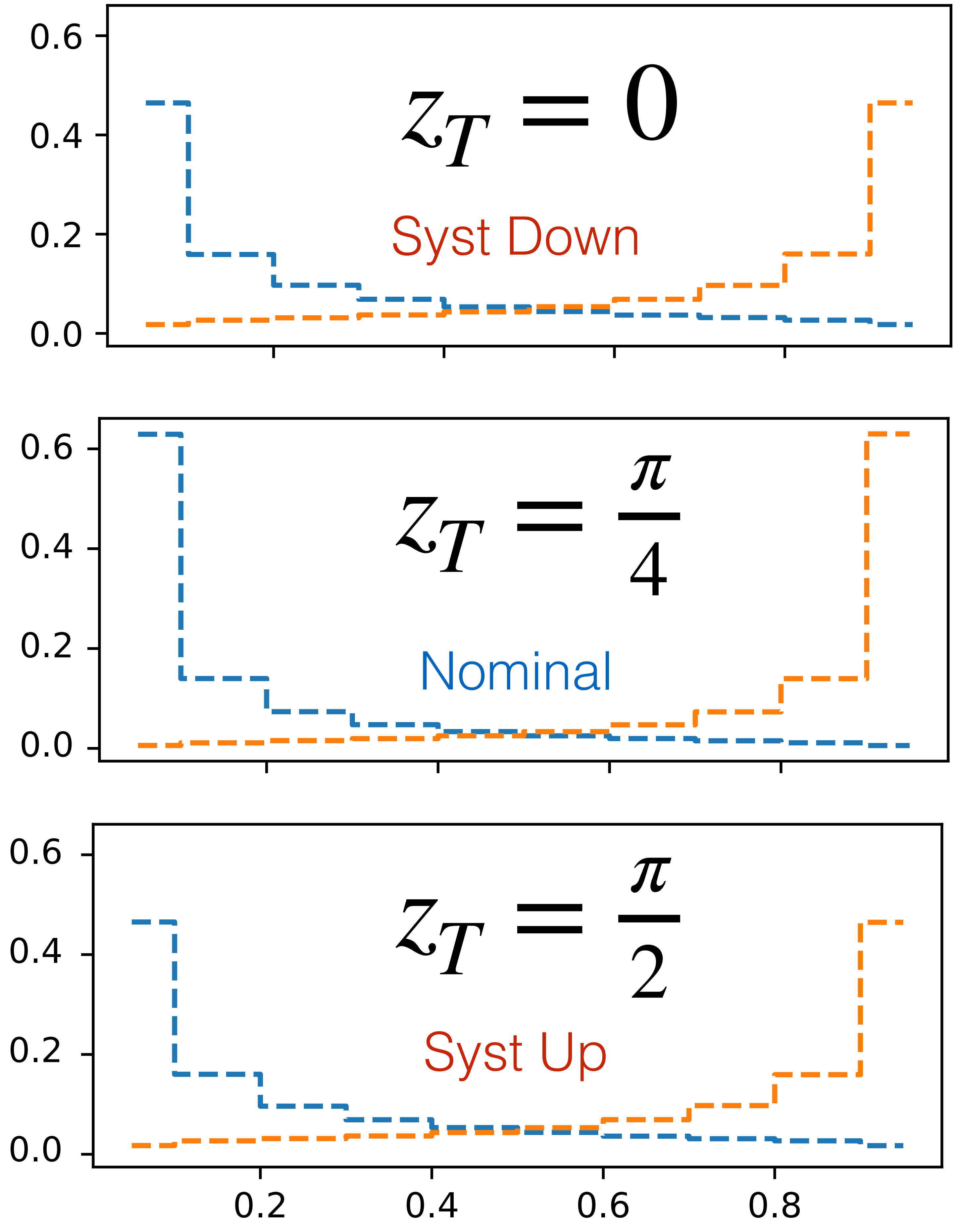
- Constrain nuisance parameters (NP) from data + incorporate prior

- **Evaluation: The actual profile likelihood**

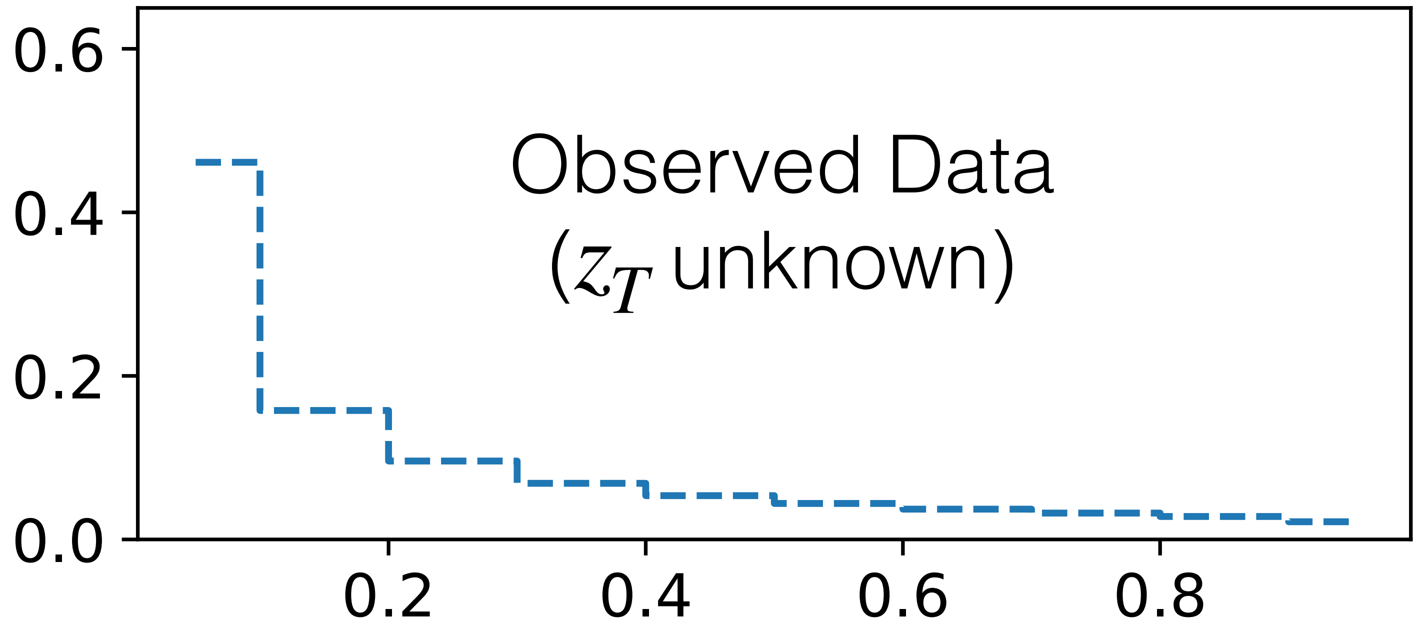
We don’t know Z in collision data, what value do we use ?

Scan the 2D Likelihood space in Z vs μ

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



$z_T \rightarrow$ True z



Scan the 2D Likelihood space in Z vs μ

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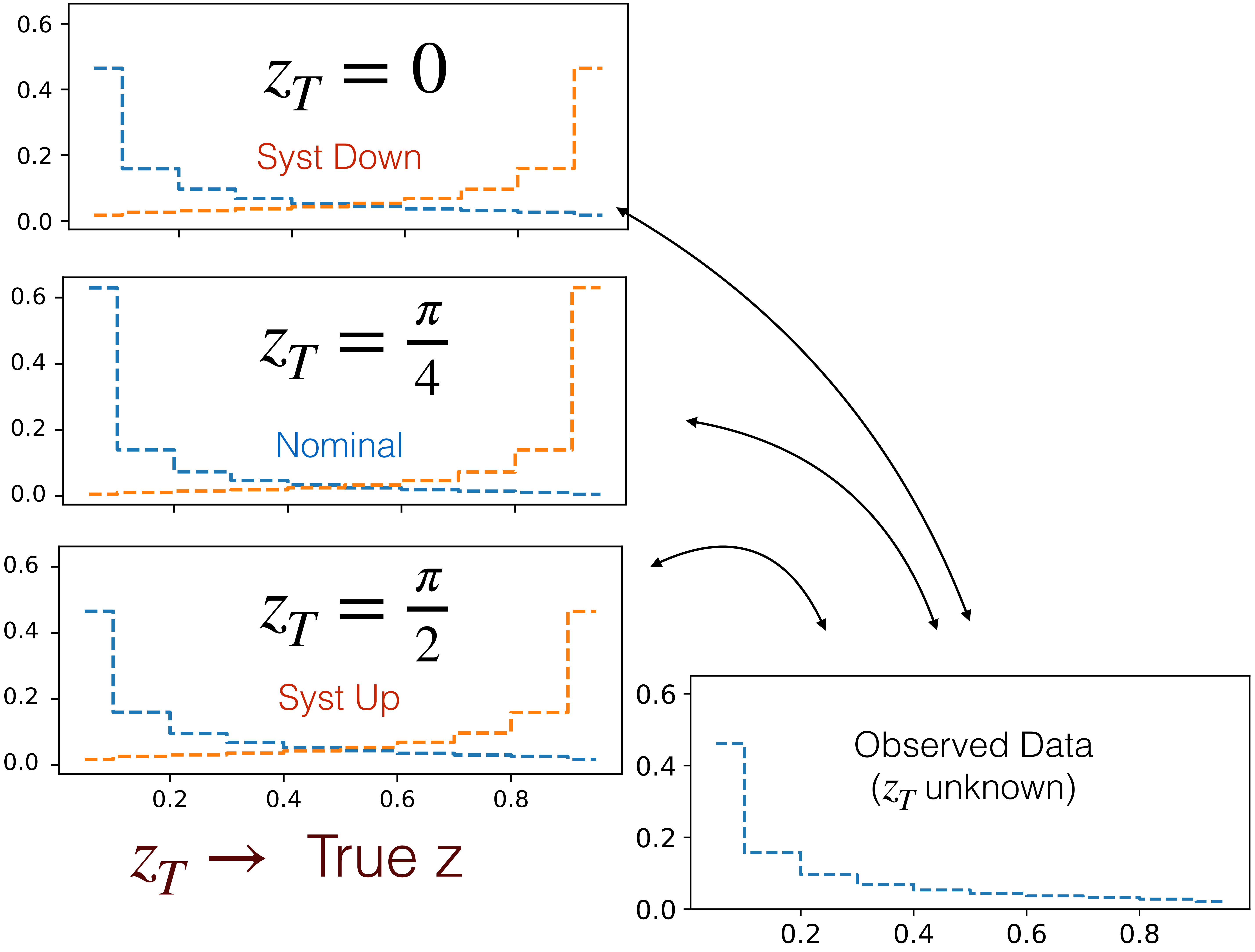

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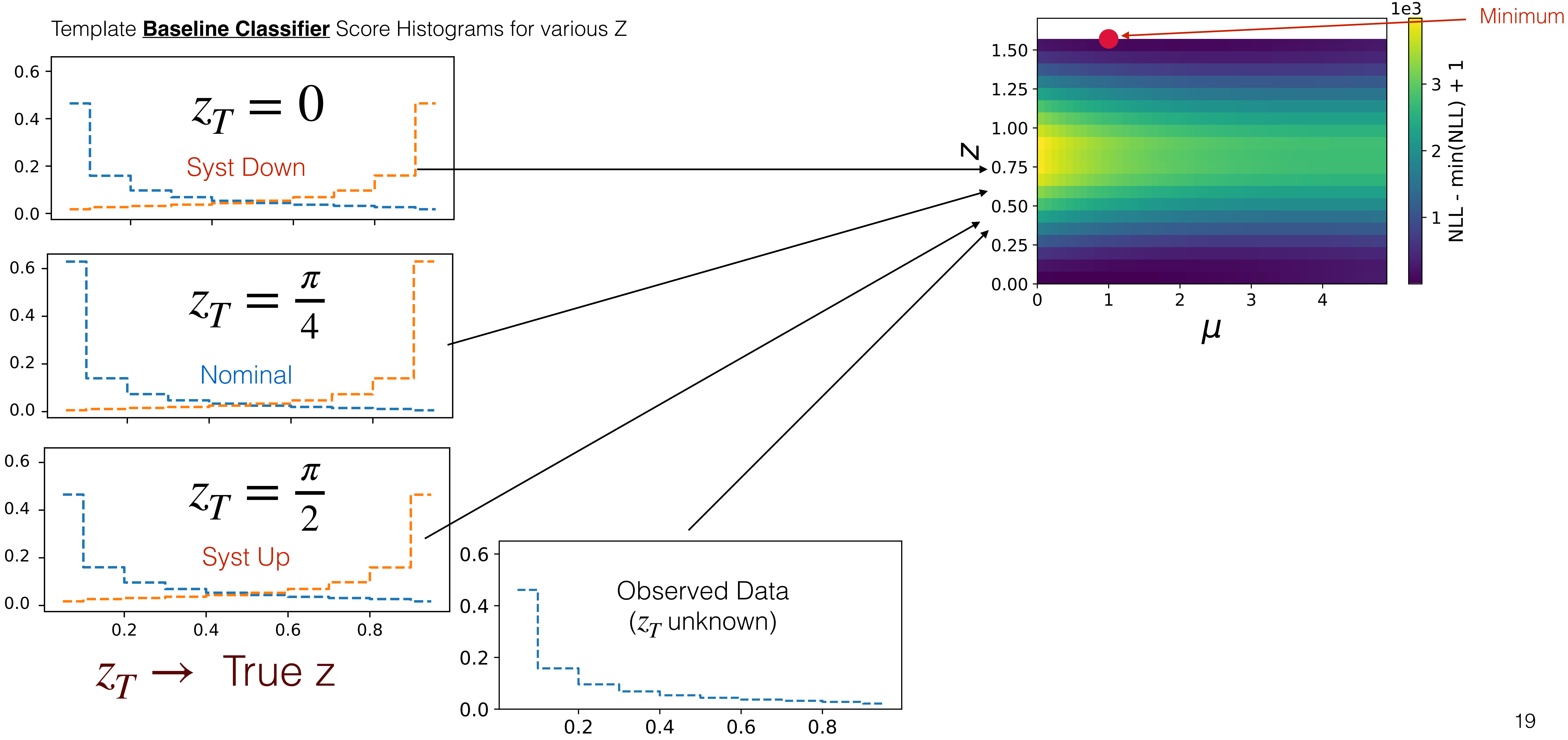
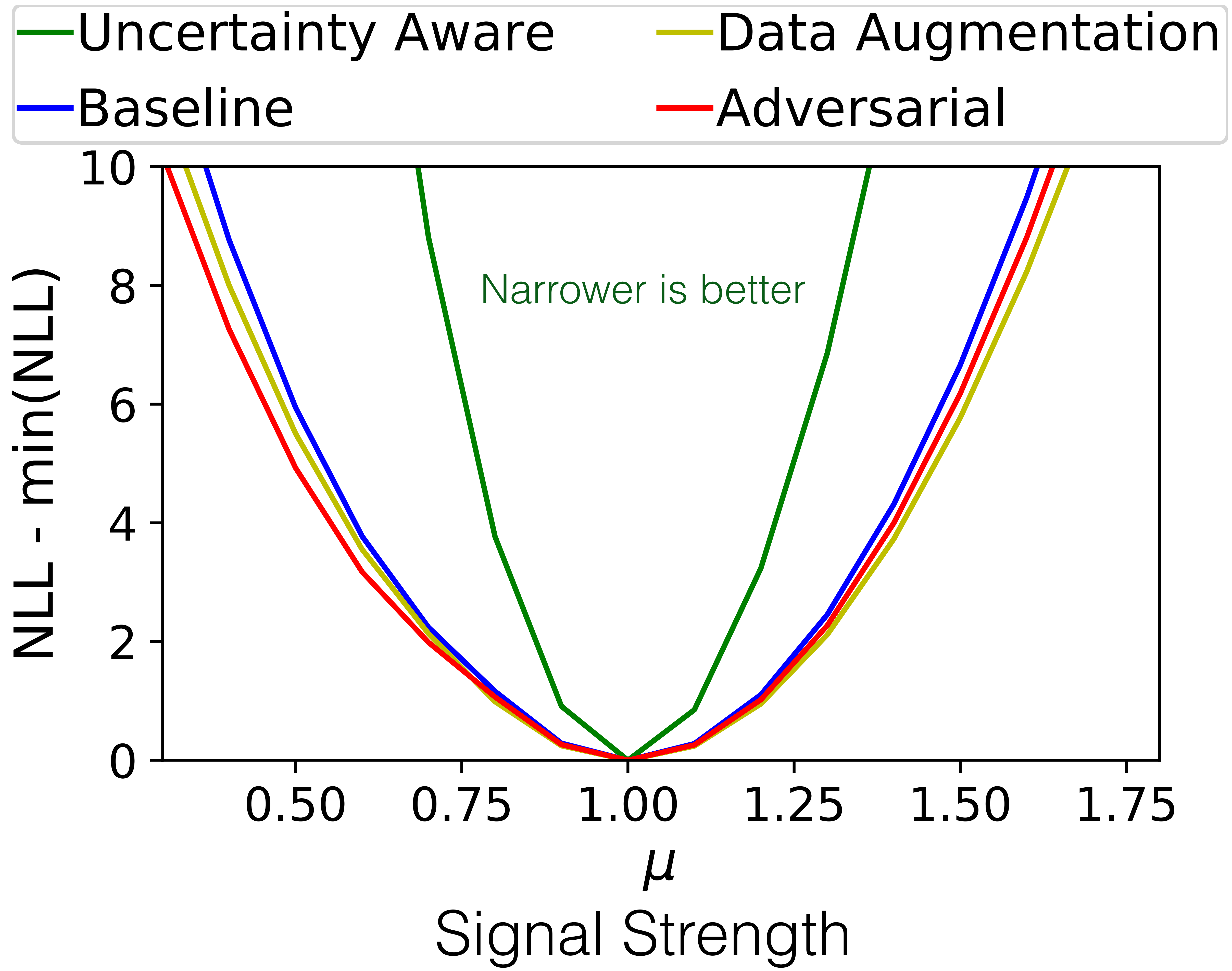


Profile away Z - Example at $(\mu, Z)_{True} = (1, 1.57)$



Narrower ⇒ Smaller [statistical + systematic] uncertainty on measurement

Narrower ⇒ We can exclude wrong values of μ with greater confidence

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

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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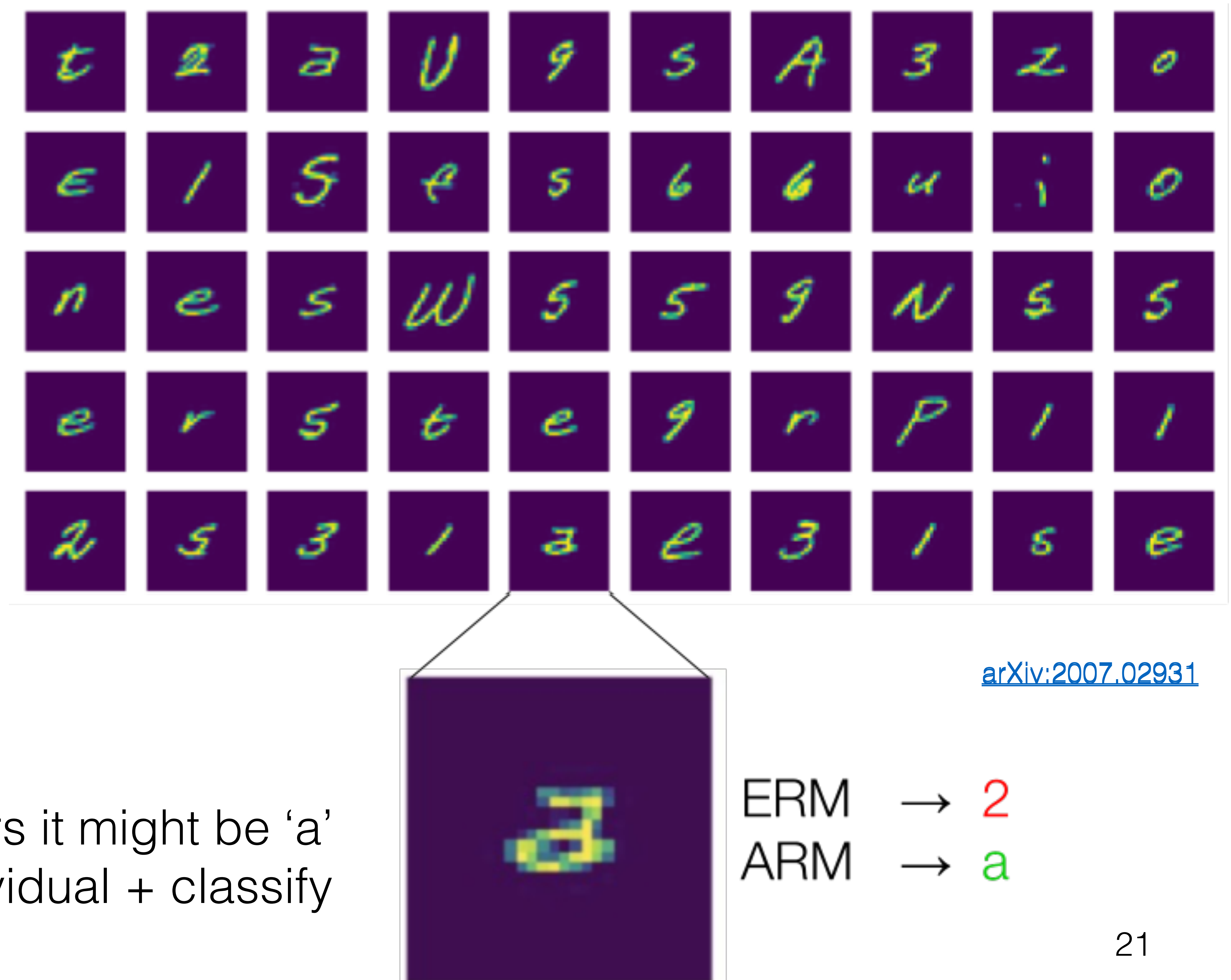
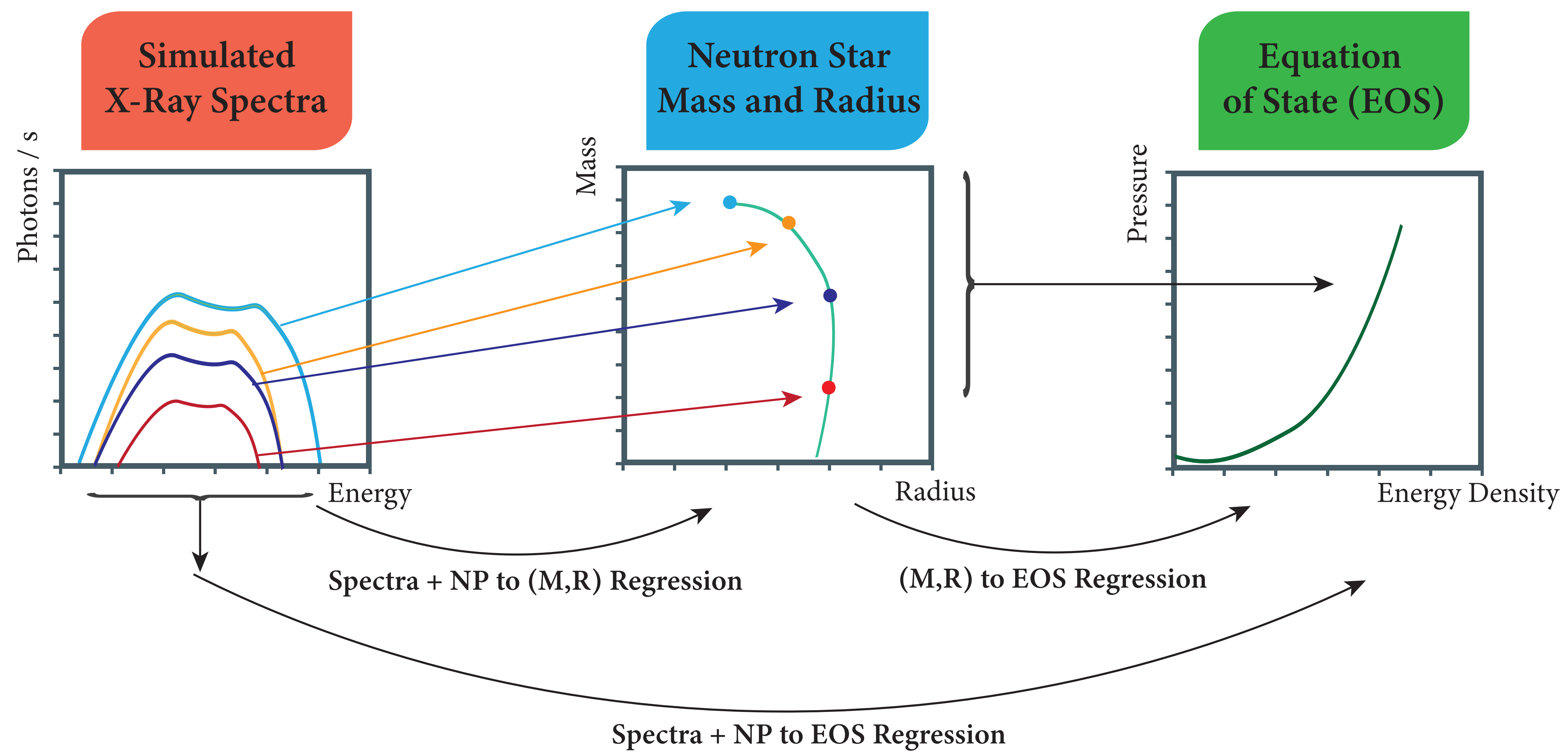


arXiv:2007.02931

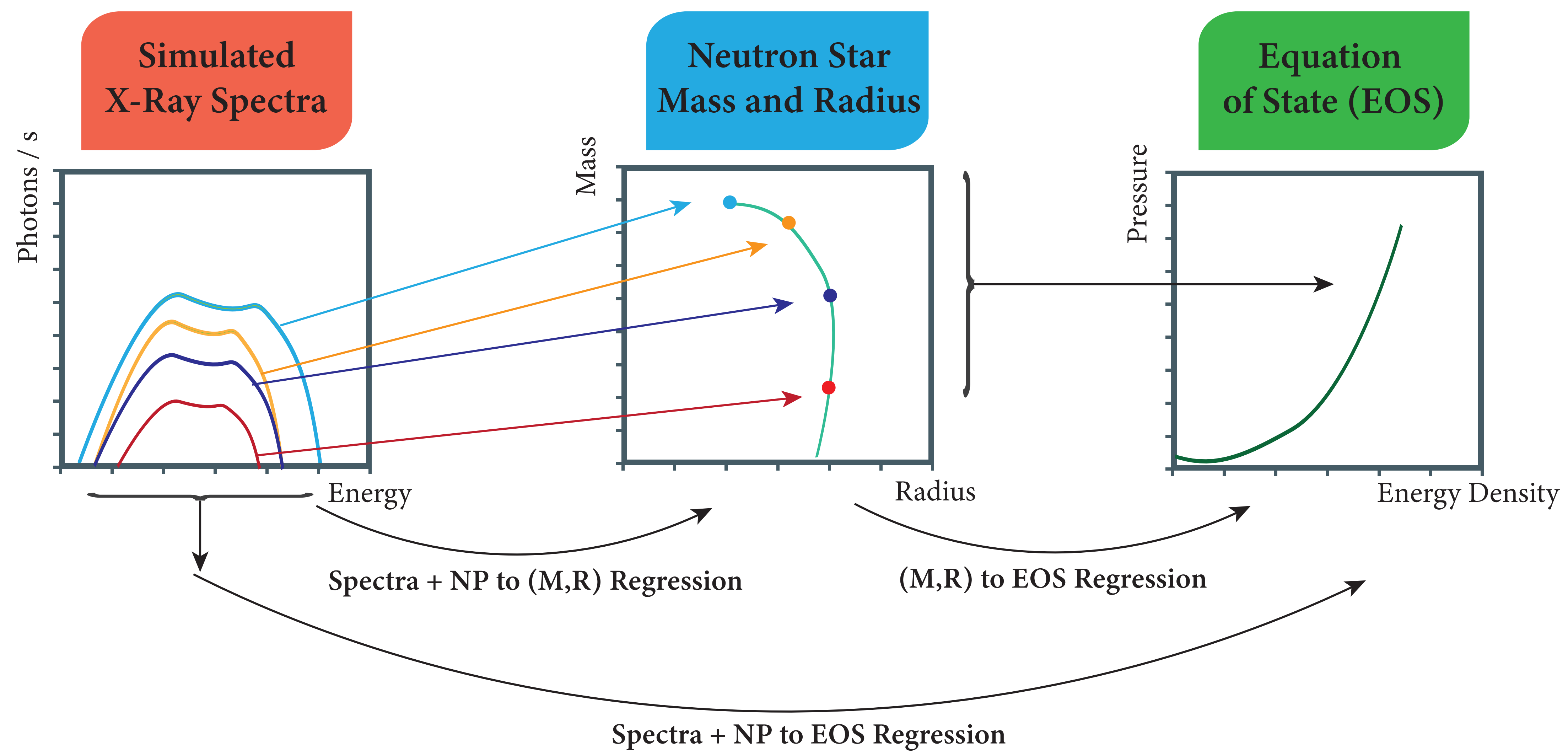
For my handwriting this is ‘2’, for yours it might be ‘a’
ARM: Adapt to the individual + classify

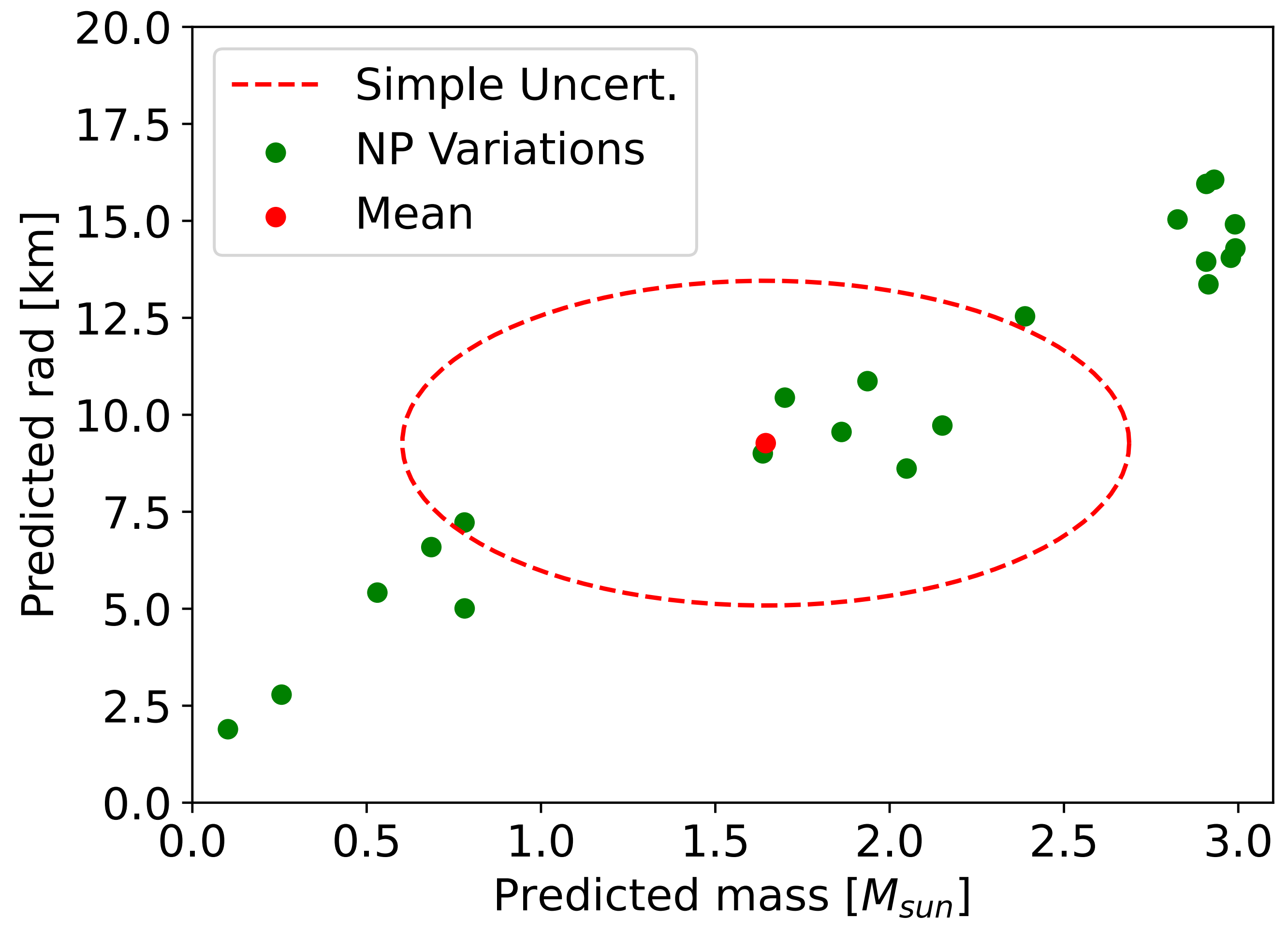
Application in Astrophysics: Propagate Uncertainties

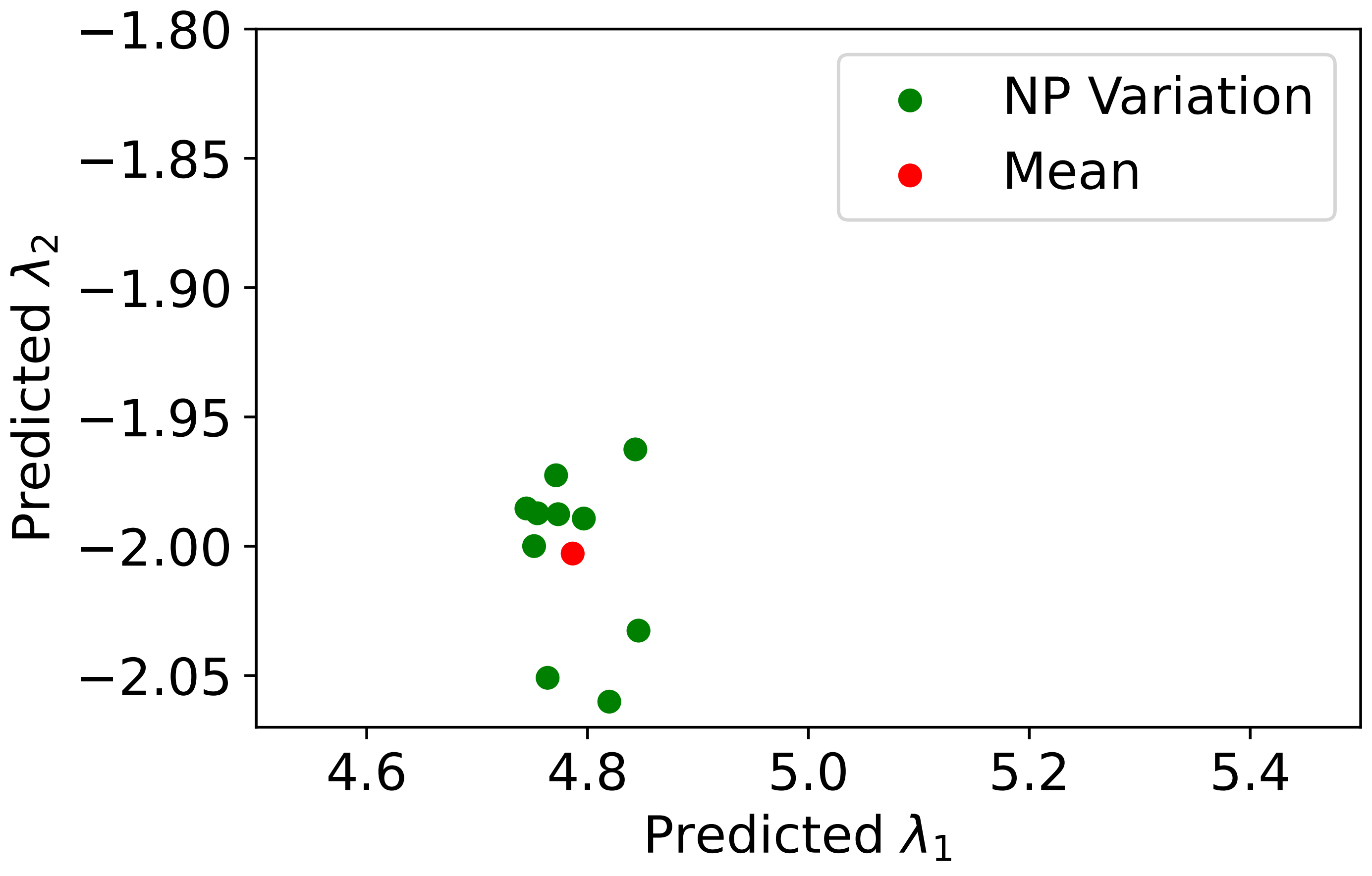


SOTA assumed uncorrelated Gaussian uncertainties

Application in Astrophysics: Propagate Uncertainties







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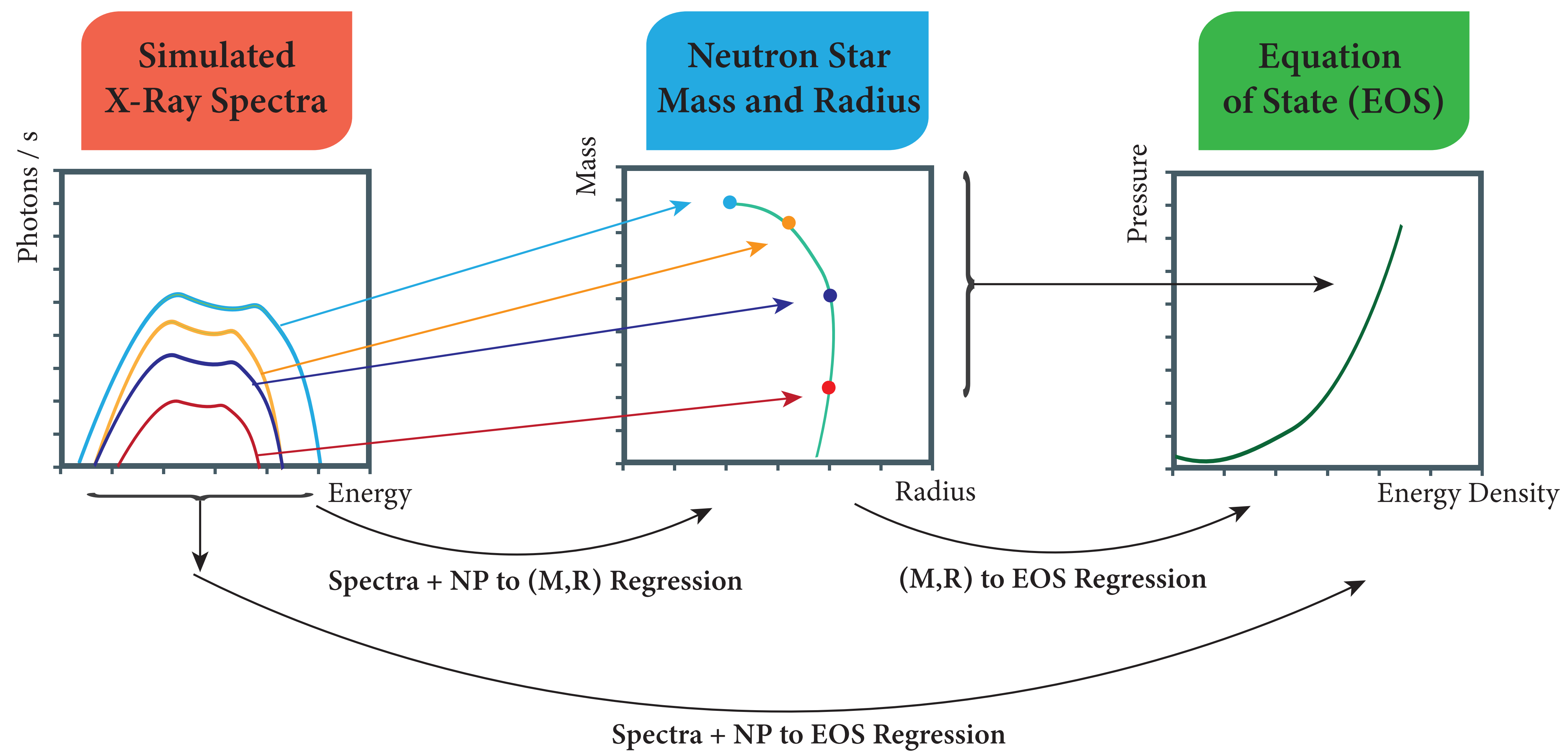

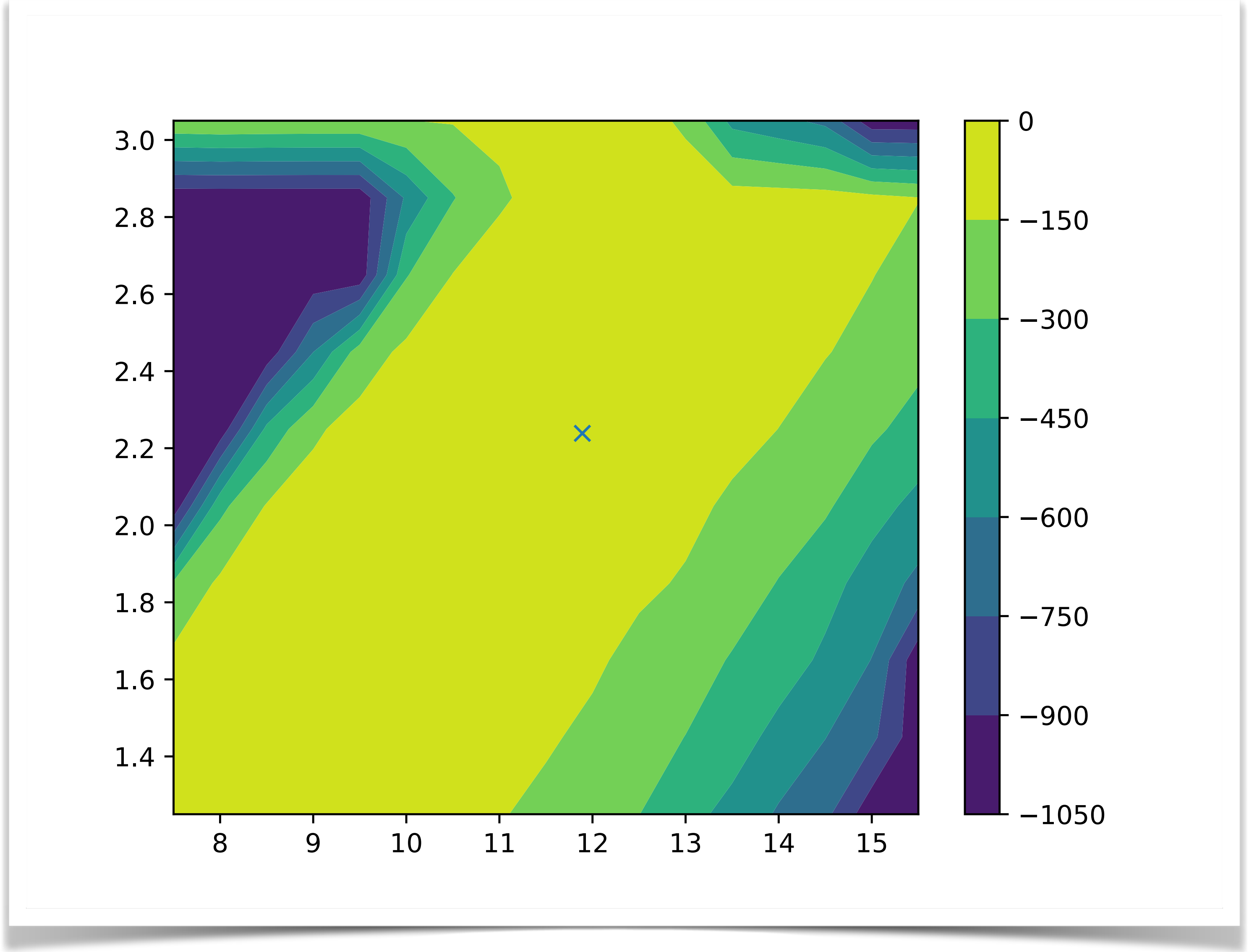

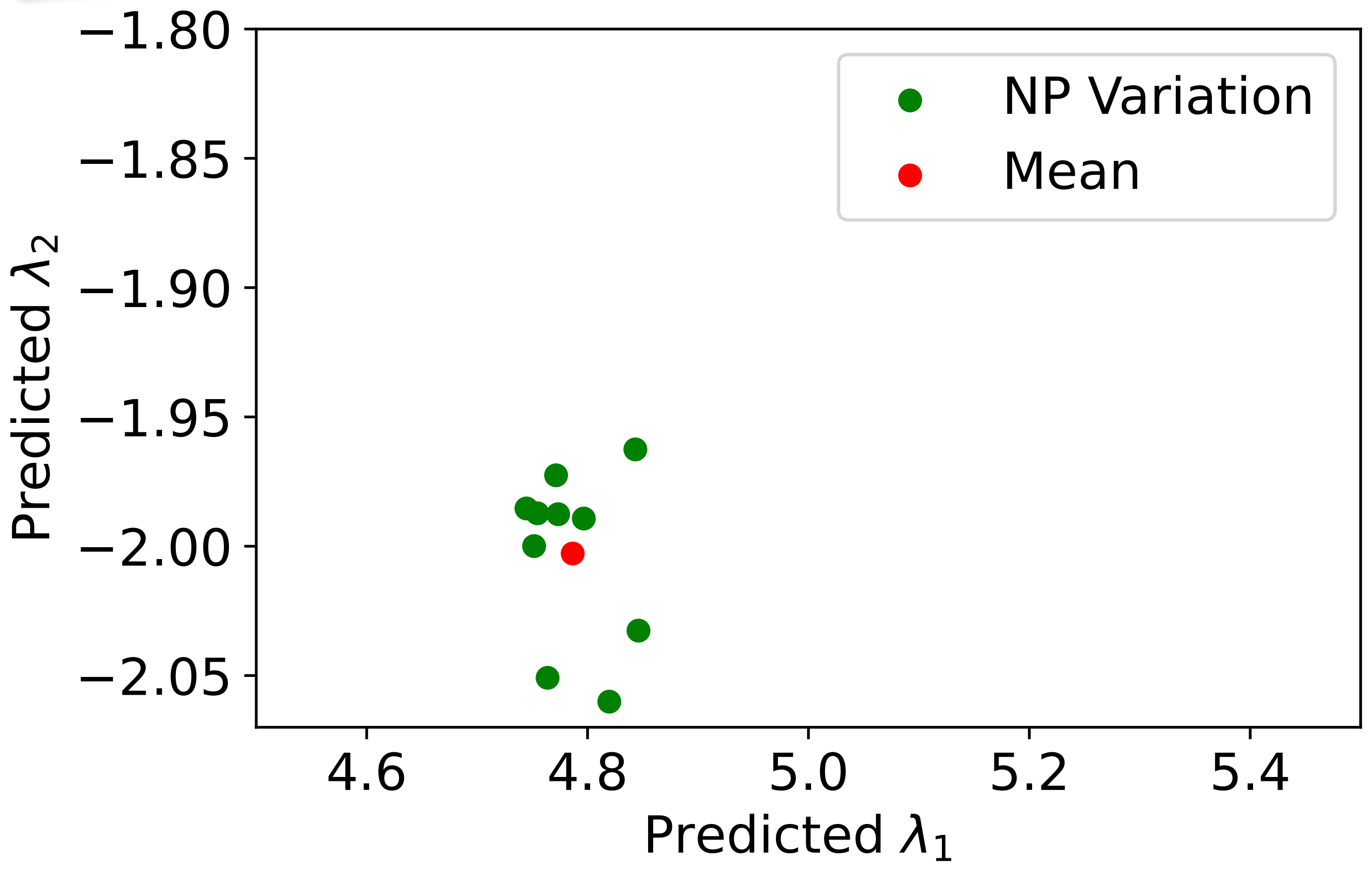

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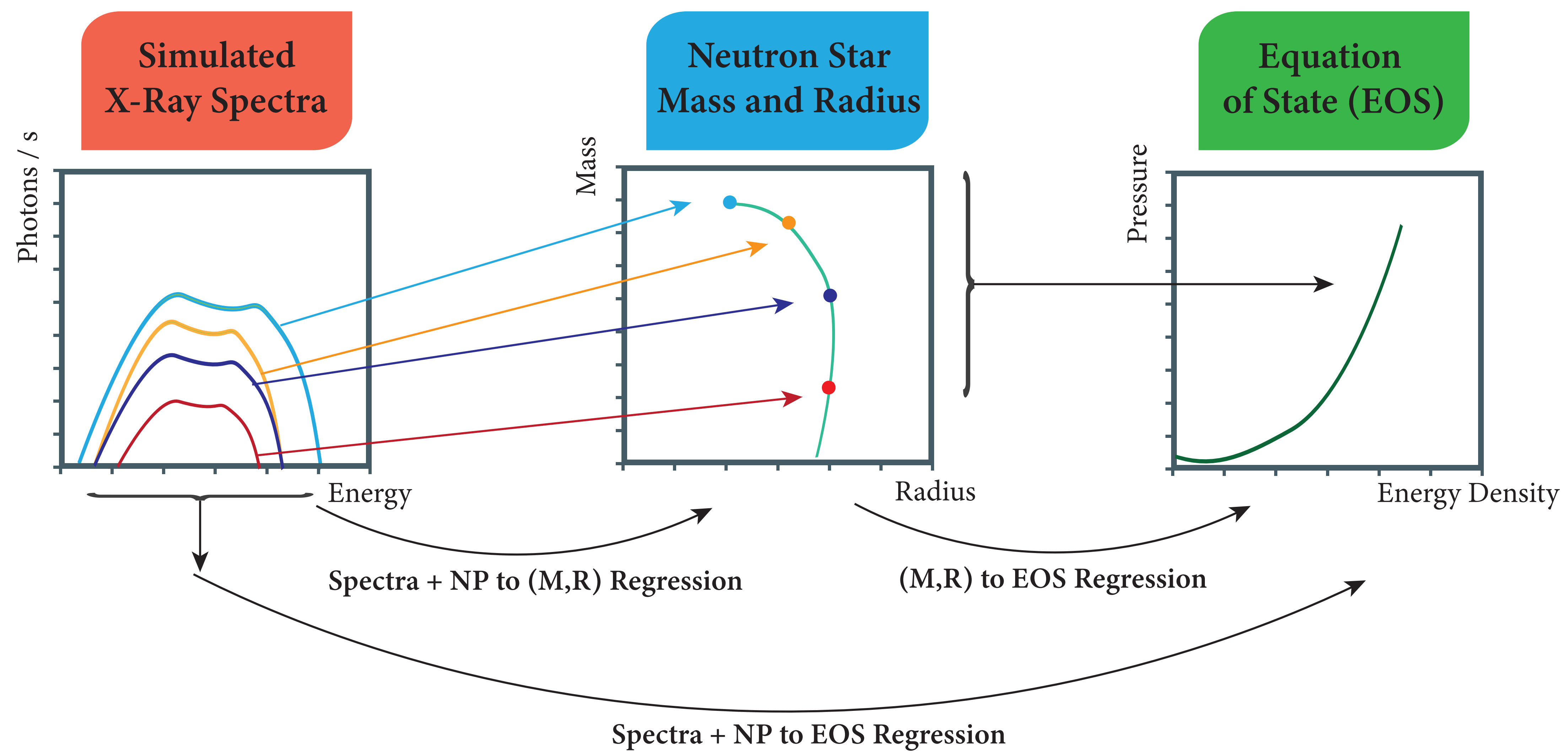
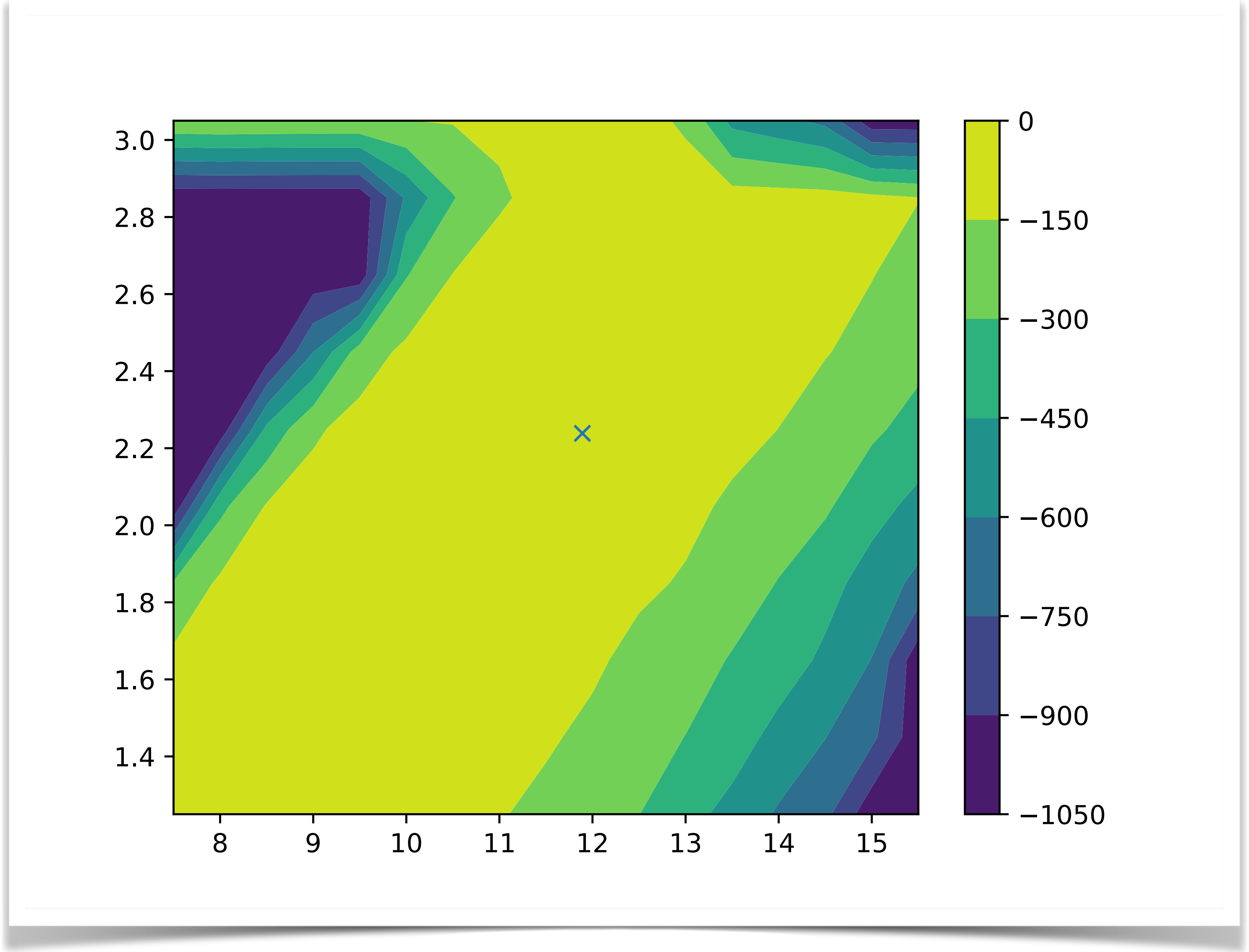
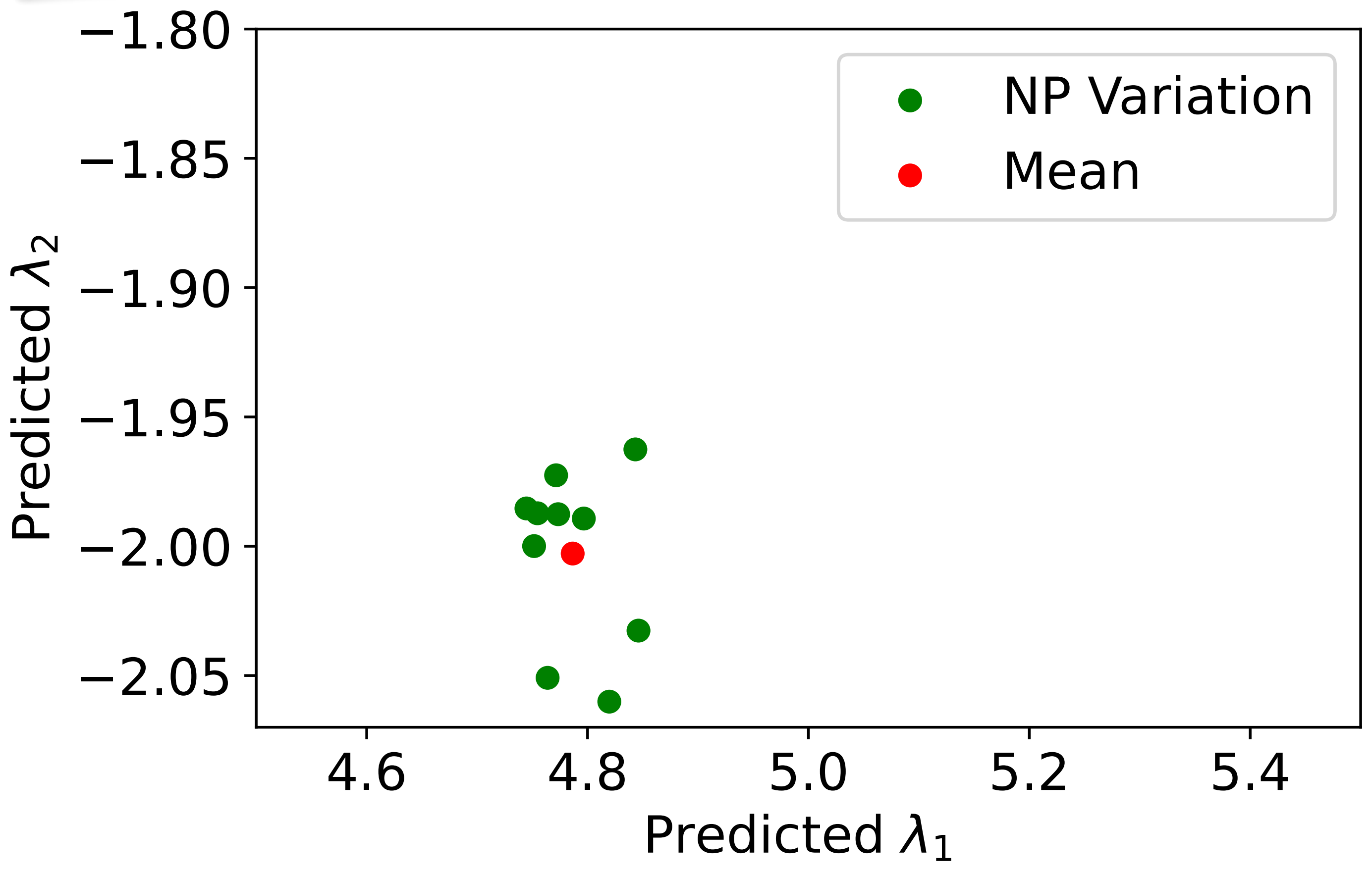


SOTA assumed uncorrelated Gaussian uncertainties

Challenge: Scan & profile over likelihood too expensive for 5×10 NPs



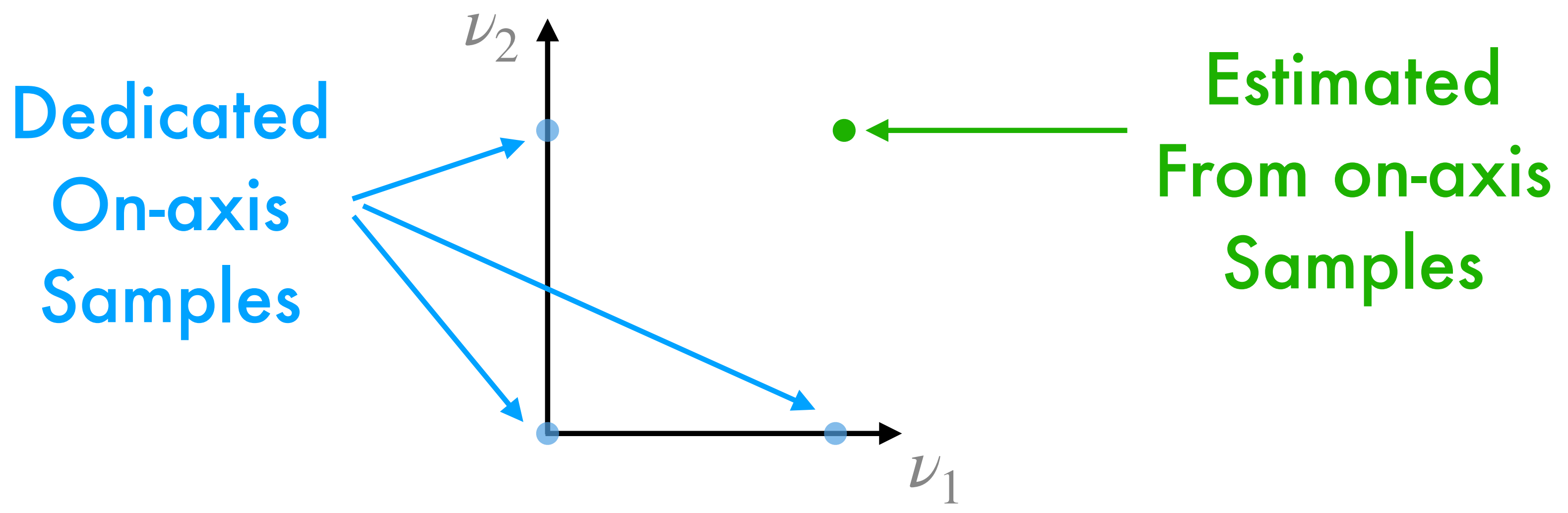


Challenges & Opportunities

- Train parameterised models on many NPs difficult: Need training data for full NP phase space

- Make it computationally feasible to scan & profile likelihood

- NP profiling for detector unfolding



Challenges & Opportunities

Related ideas:
arxiv:2110.00449
arxiv:1506.02169

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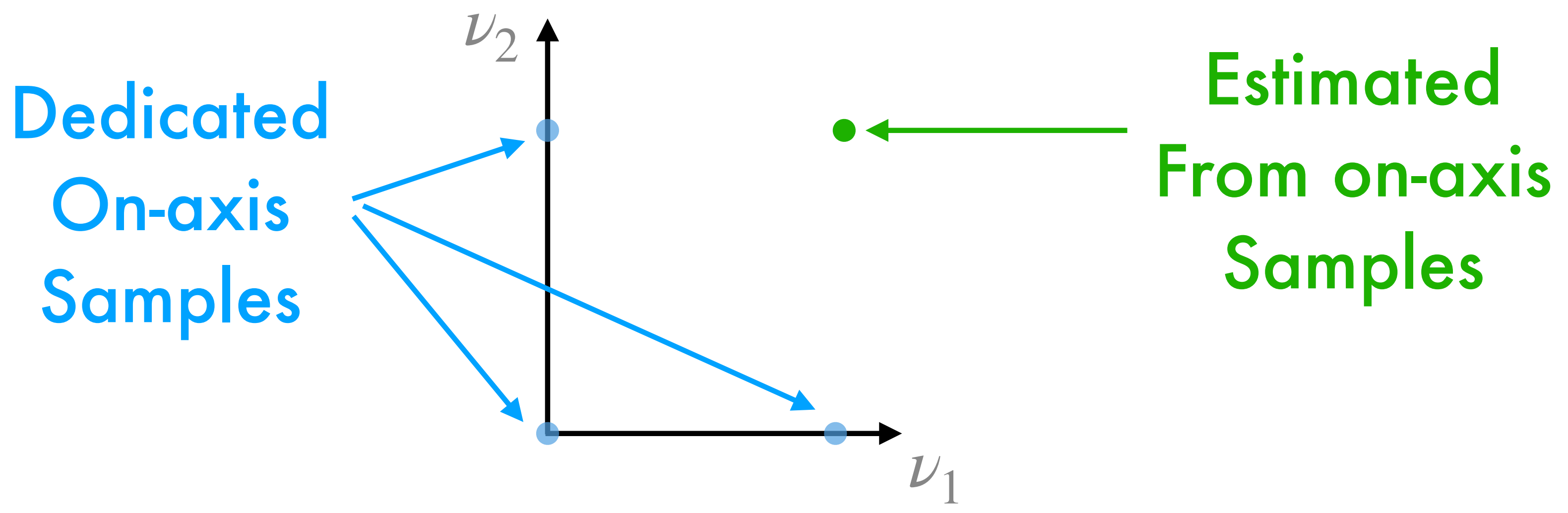
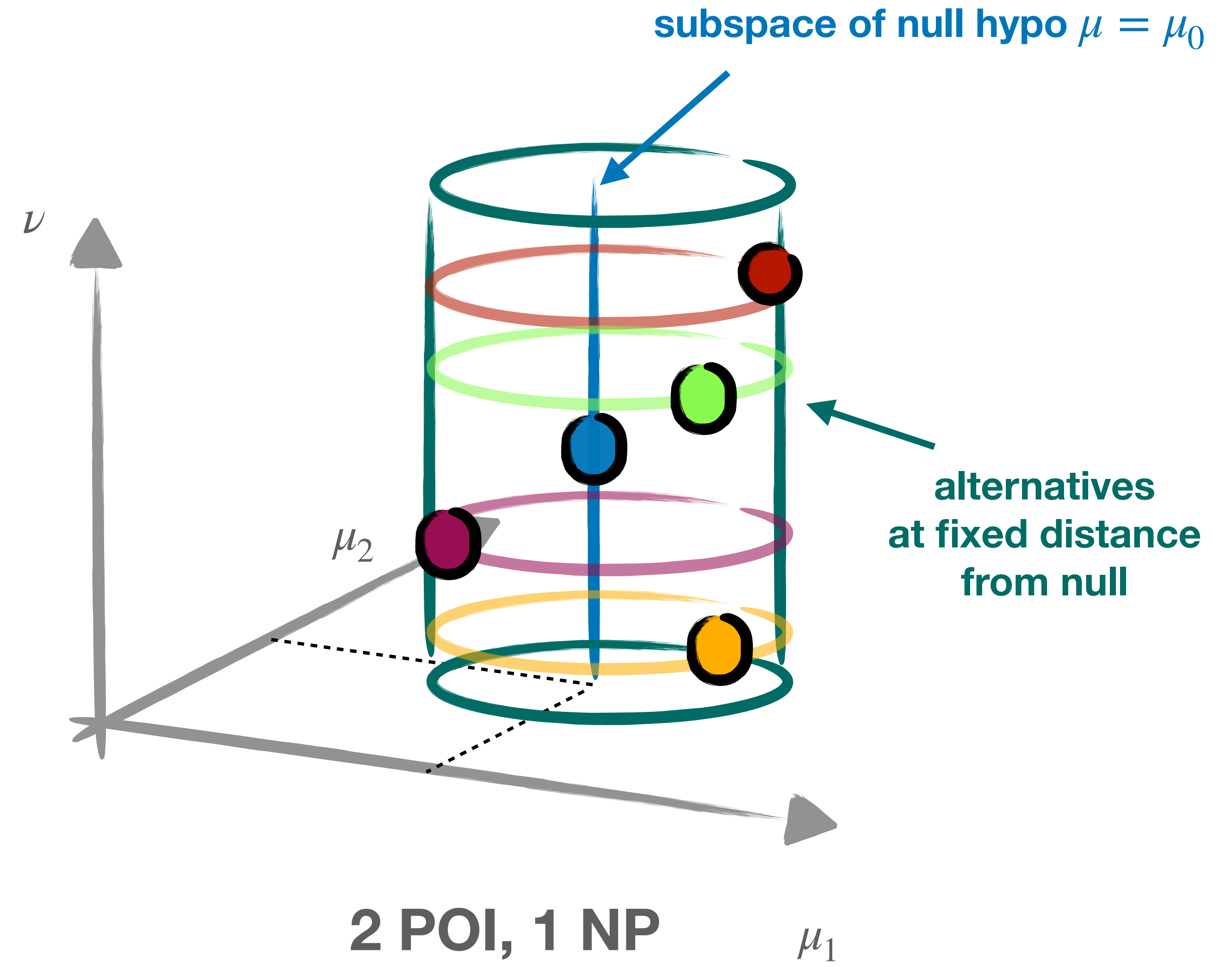
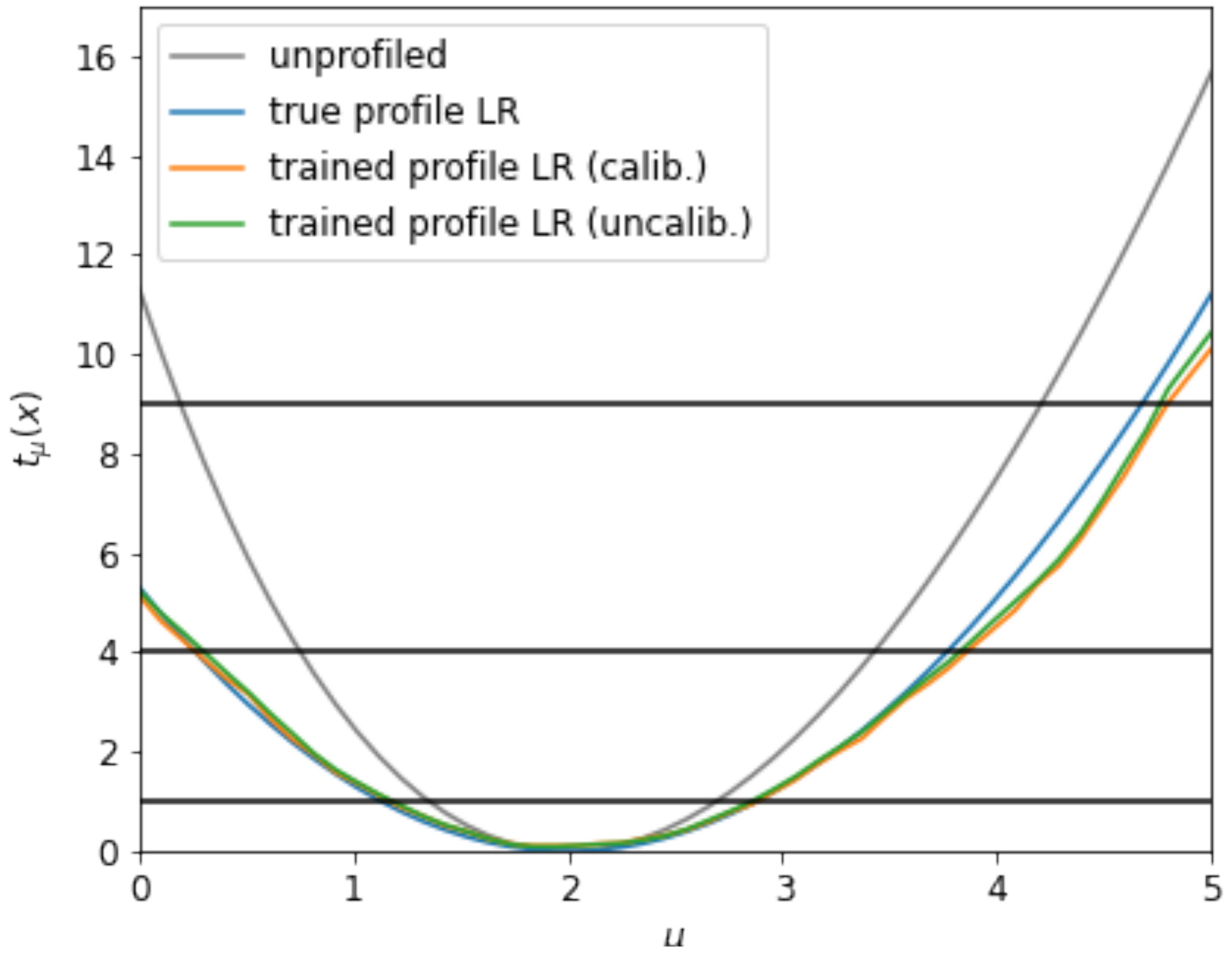
- NP profiling for detector unfolding





alternatives at fixed
“radius” from the **null space**



NN gives you profile likelihood directly ?

Challenges & Opportunities

- Train parameterised models on many NPs difficult: Need training data for full NP phase space
- Make it computationally feasible to scan & profile likelihood
- ~~NP profiling for detector Unfolding~~

Fresh off the press! : [Chan and Nachman arXiv:2302.05390]()

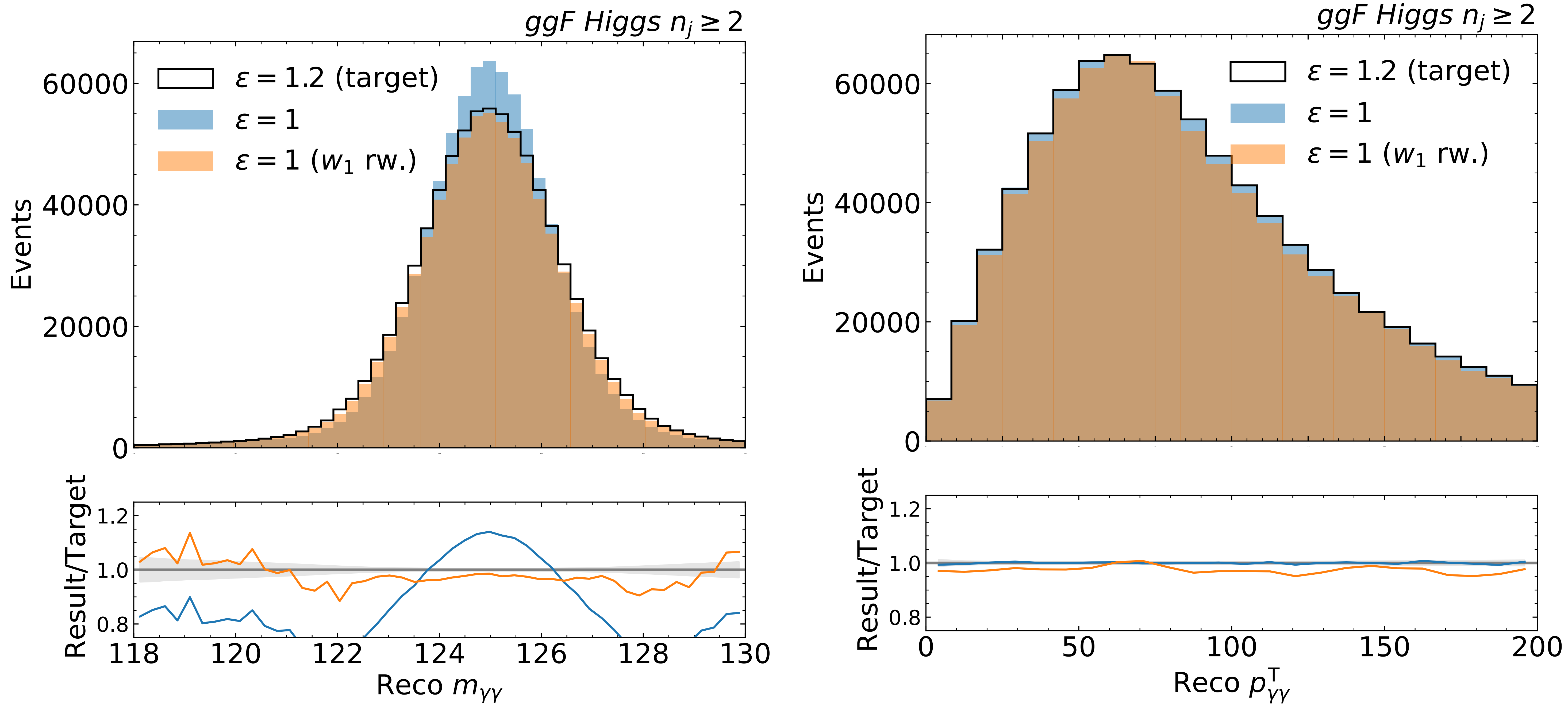


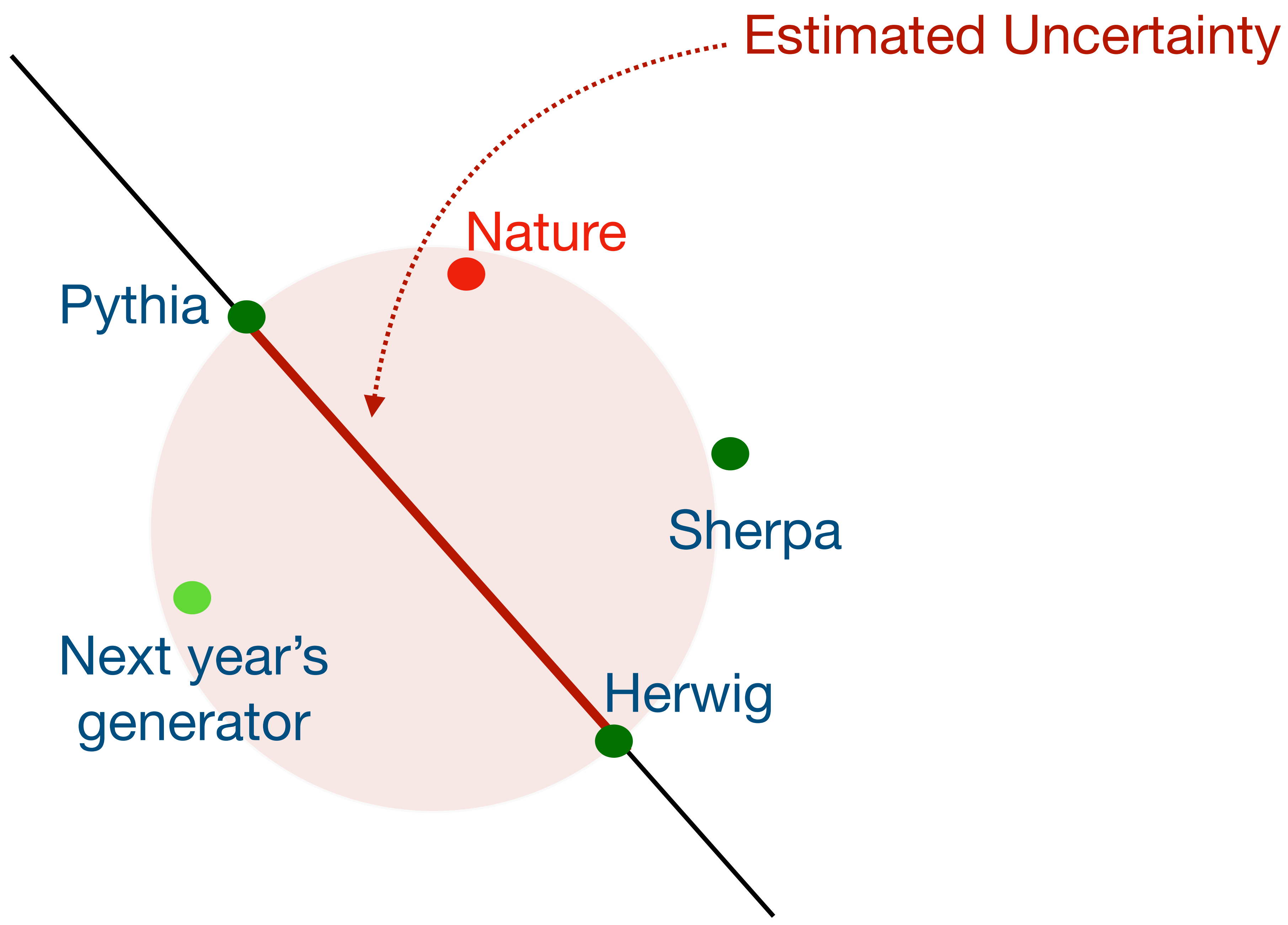
FIG. 6. Higgs boson cross section: the nominal detector-level spectra $m_{\gamma\gamma}$ (left) and $p^{T}_{\gamma\gamma}$ (right) with $\epsilon_\gamma = 1$ reweighted by the trained w_1 conditioned at $\epsilon_\gamma = 1.2$ and compared to the spectra with $\epsilon_\gamma = 1.2$.

Theory Uncertainties

What are they ?

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

No statistical origin for them (such as auxiliary measurement)



What are they ?

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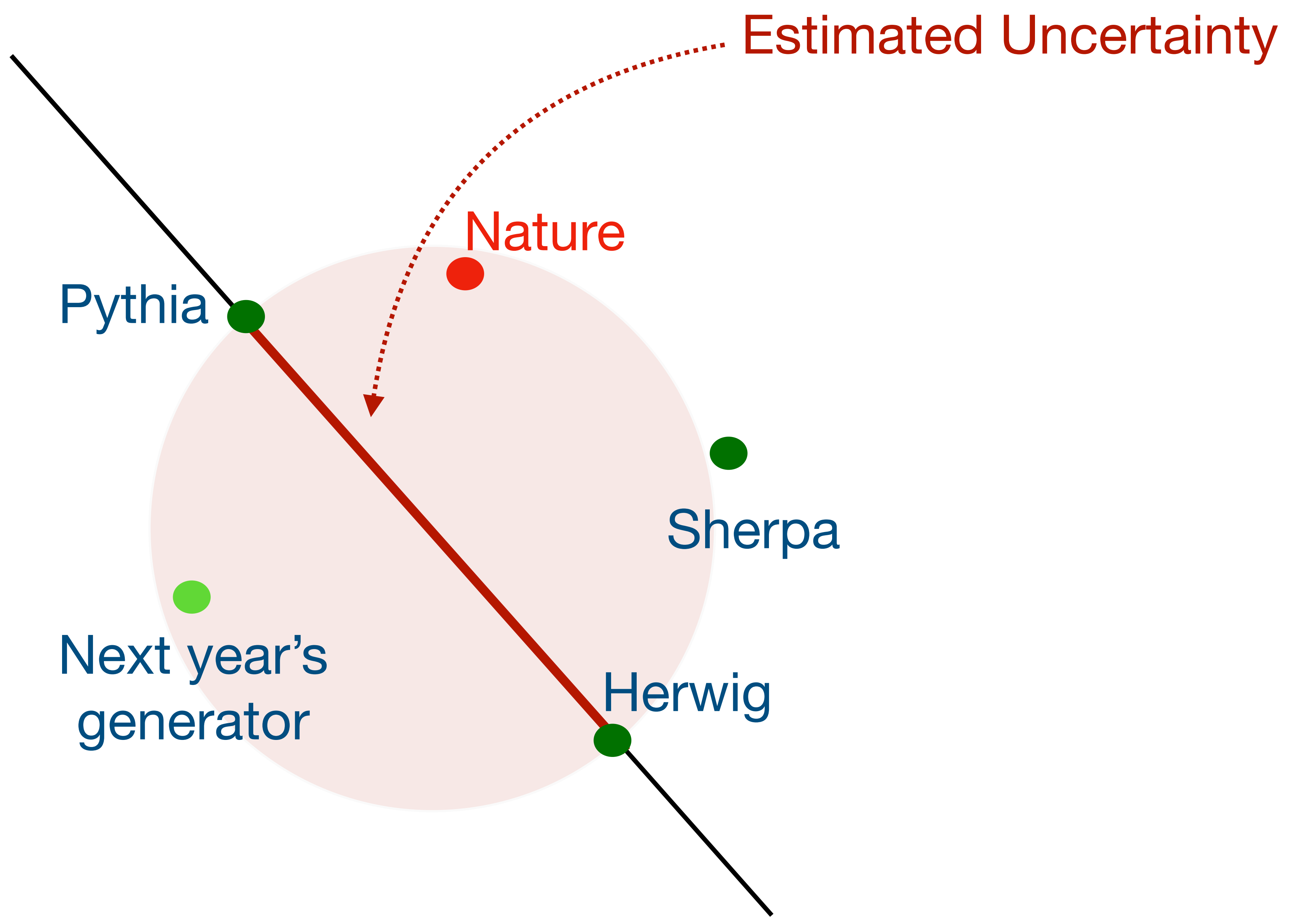
No statistical origin for them (such as auxiliary measurement)

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



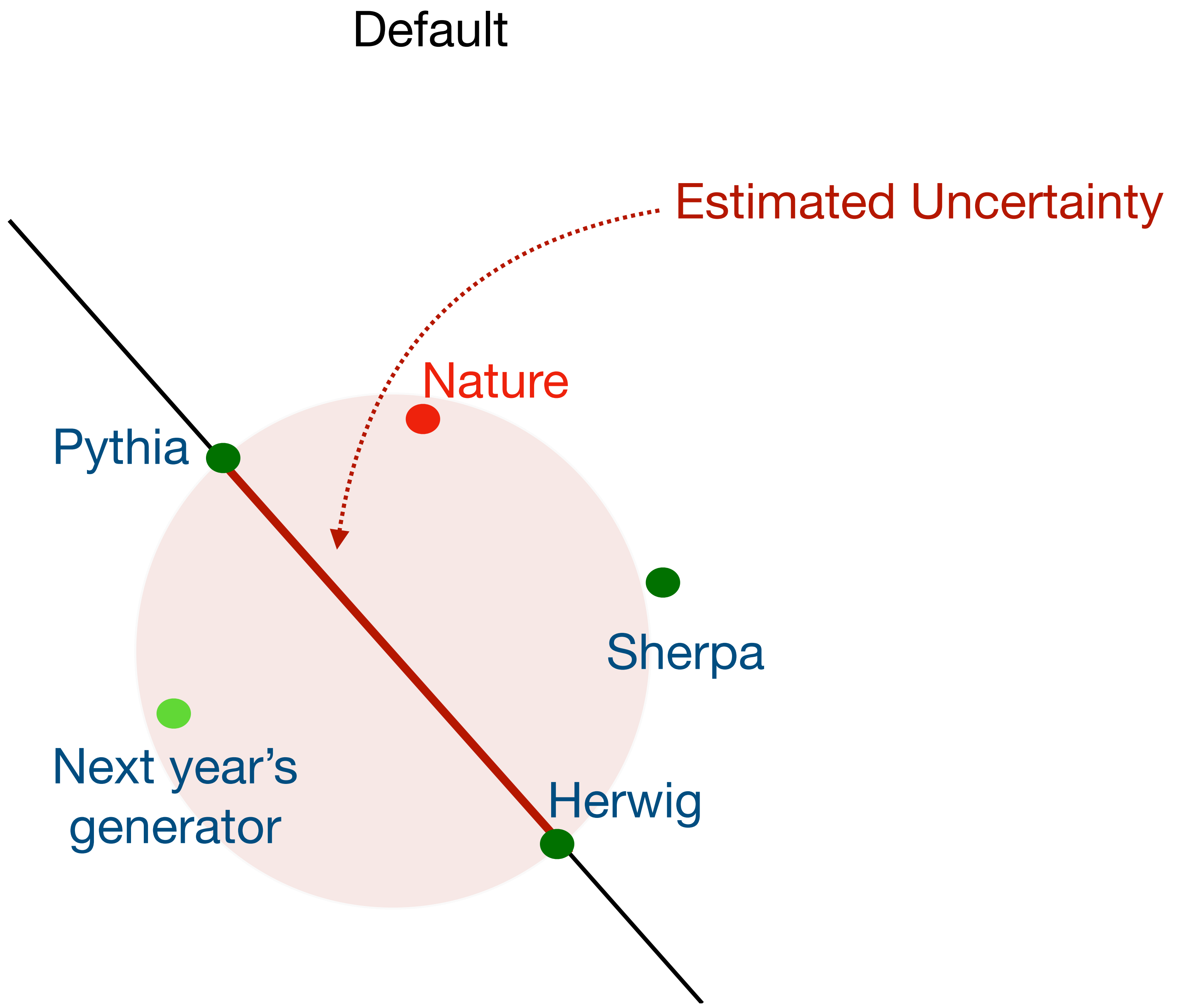
Open problems!

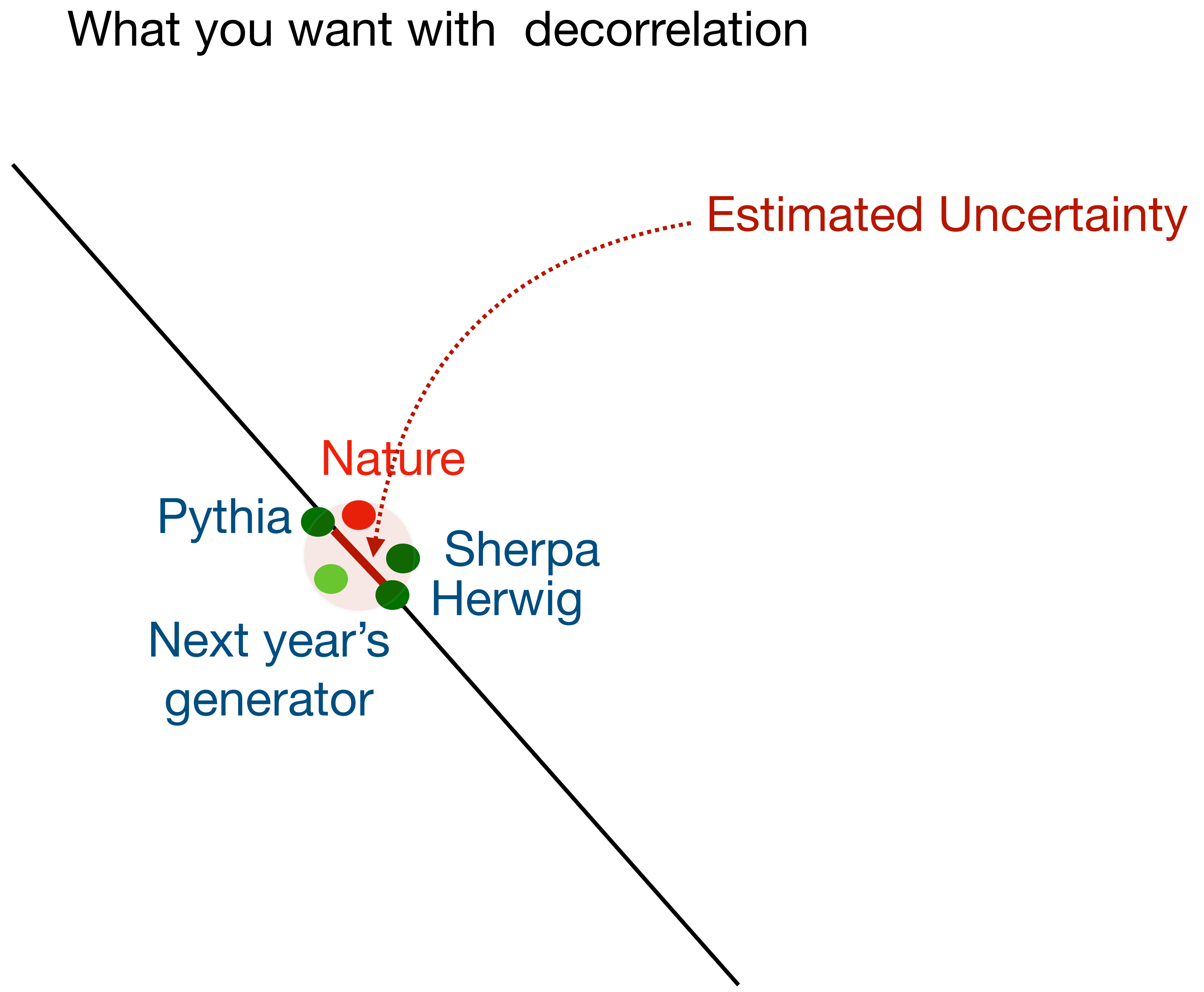
Not many new ideas on how to handle theory uncertainties

Besides suggestions for ML decorrelation …

Danger of ML Decorrelation of Uncertainty

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



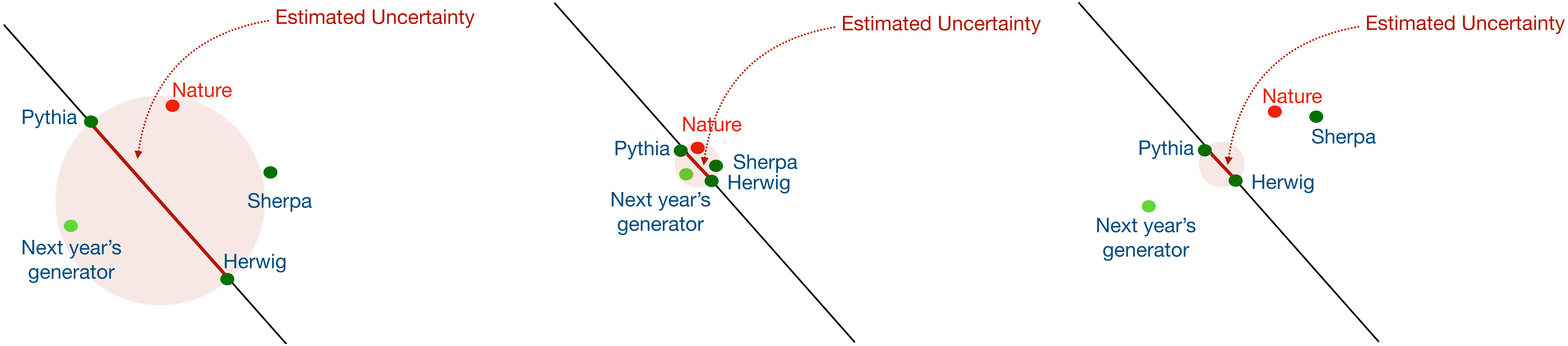


Instruction to AI: "Please shrink Pythia vs Herwig difference"

Danger of ML Decorrelation of Uncertainty

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

Default | What you want with decorrelation | What you get with decorrelation



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

Model will learn to fool you !

(To really shrink these uncertainties, ask a different question)

Goodhart's Law

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

=> Dangerous to optimise proxy metrics of uncertainty

Case Study 2: Higher-order corrections

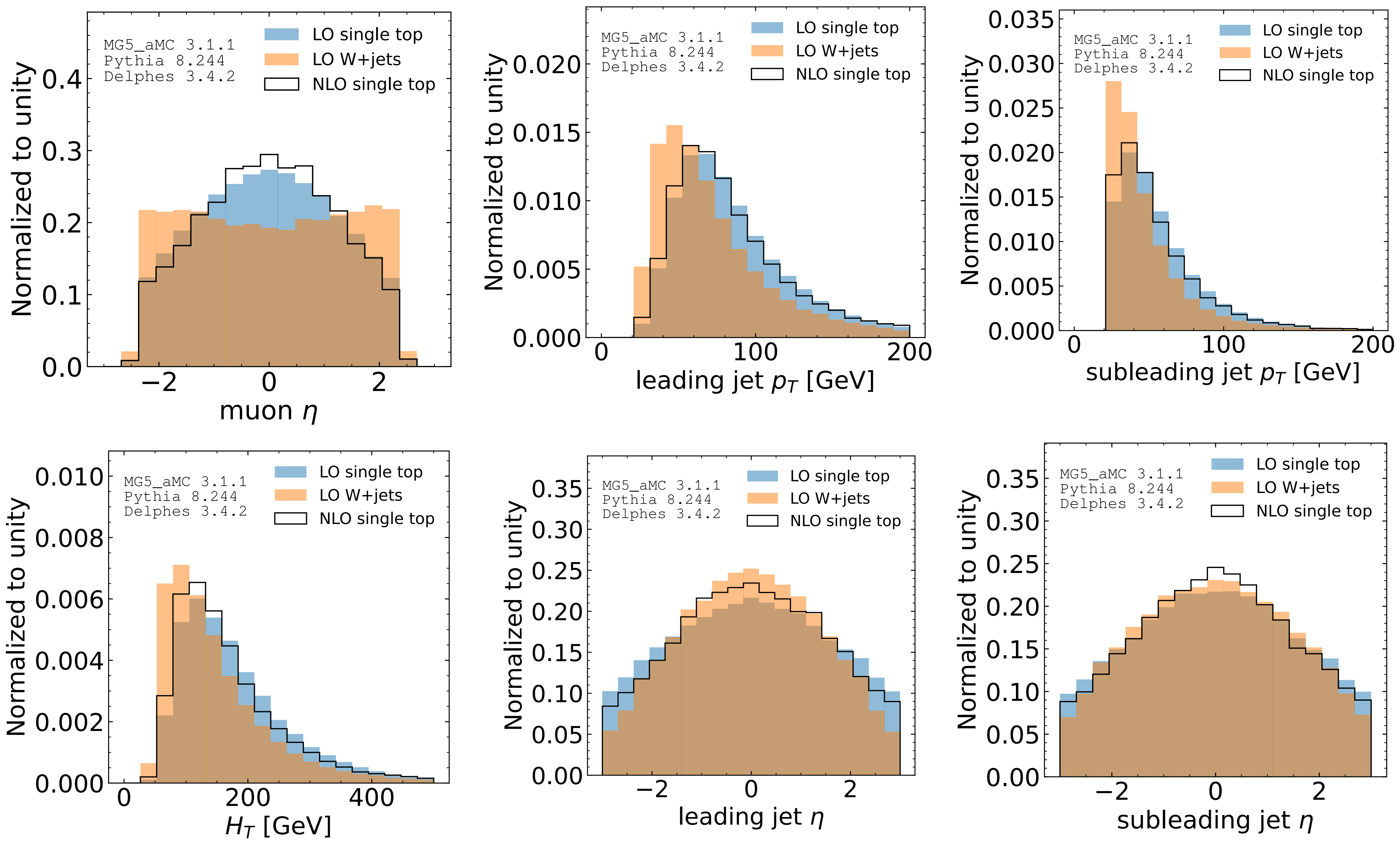
- We can’t calculate QFT to infinite order
- Artefact of truncation of series: Varying certain unphysical scales changes predictions
- Uncertainty quantification: Vary scales (renormalization scale, factorisation scale) between 1/2 to 2 in MC, see change in prediction

Scale uncertainty – Problem Setup

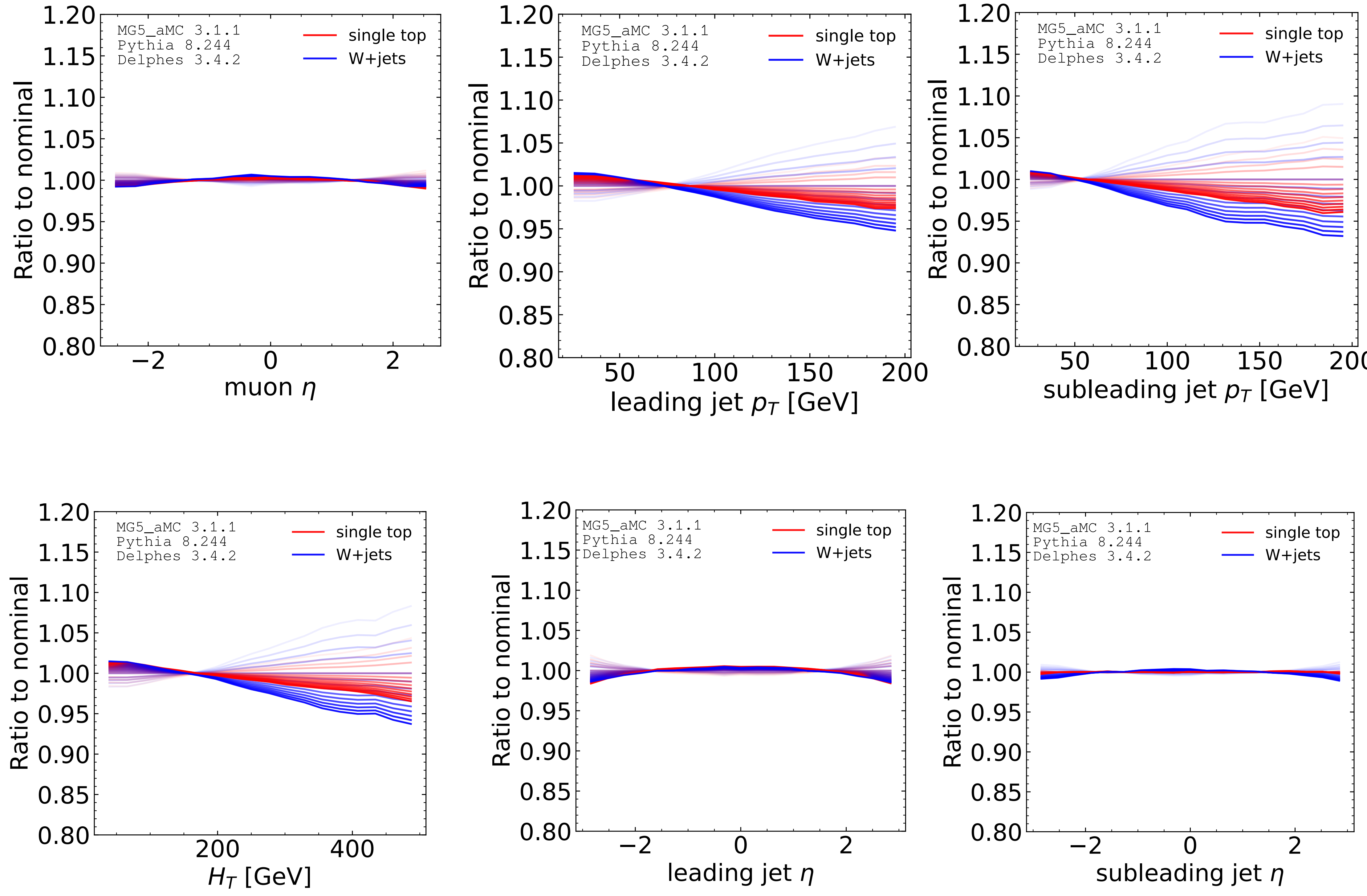
Goal: Single top vs W+Jets

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

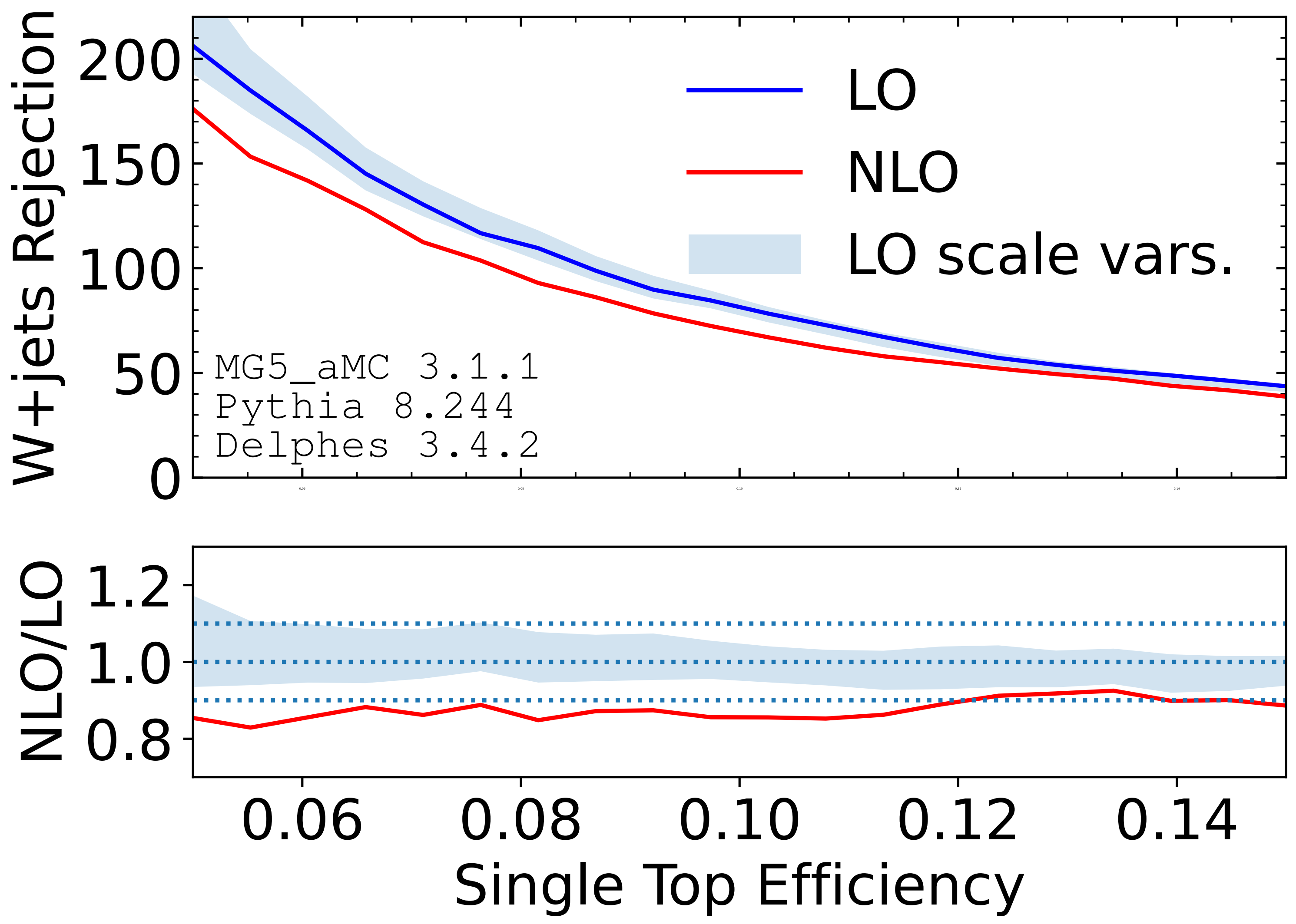


Factorisation scale variations going from 1/2 to 2

Case Study 2: Continuous uncertainty - Result

ROC curve (higher is better)

No adversary



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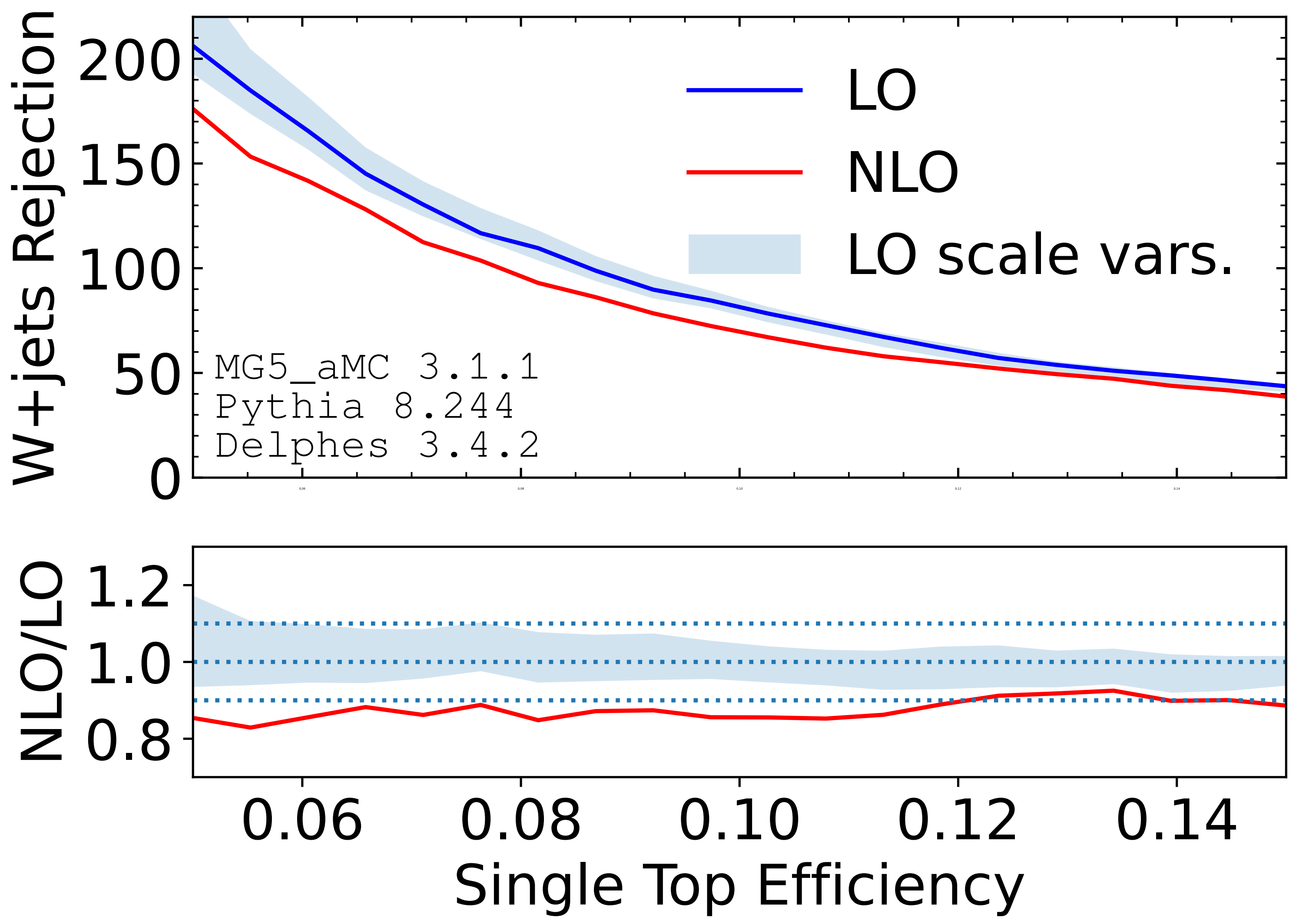
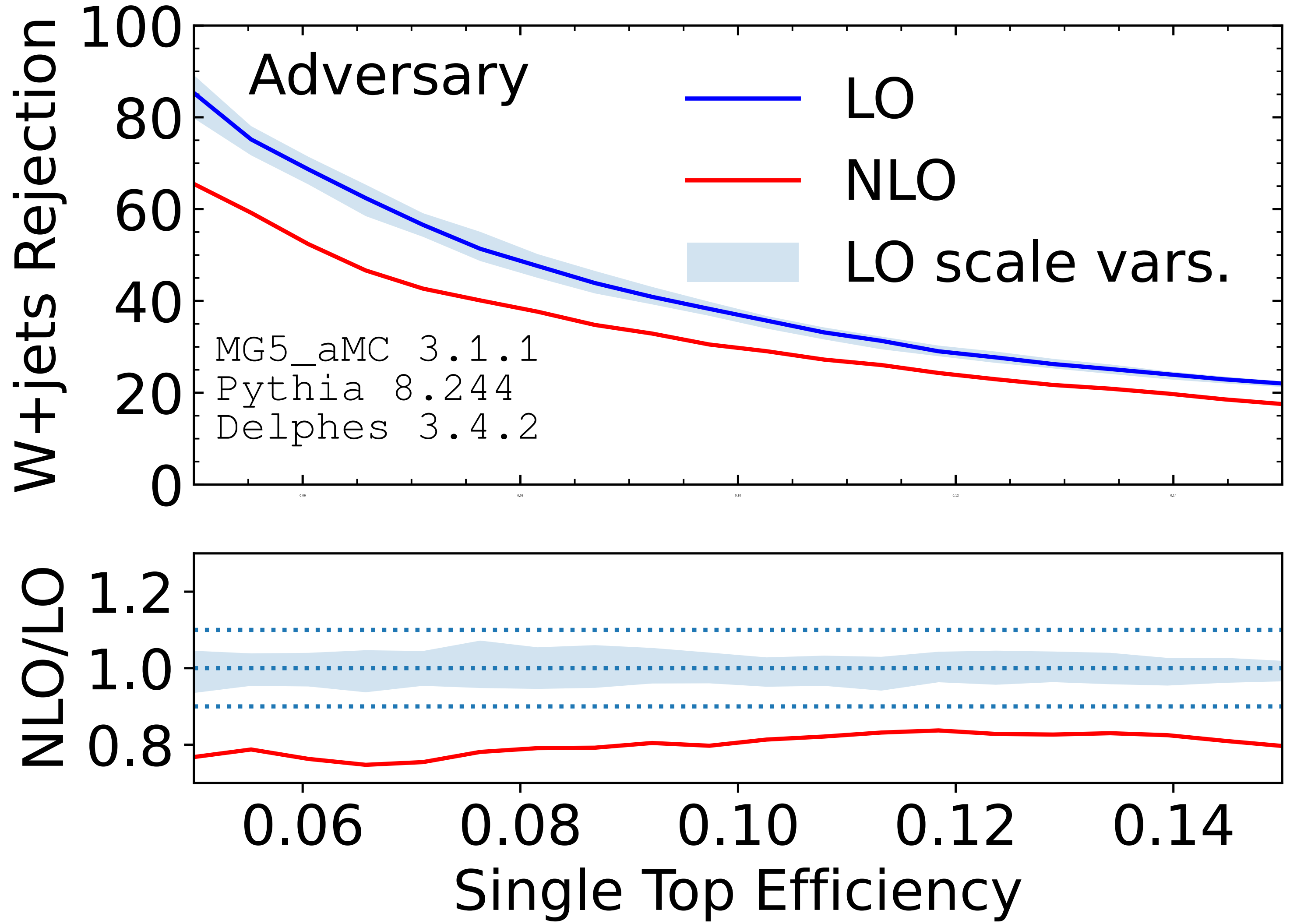


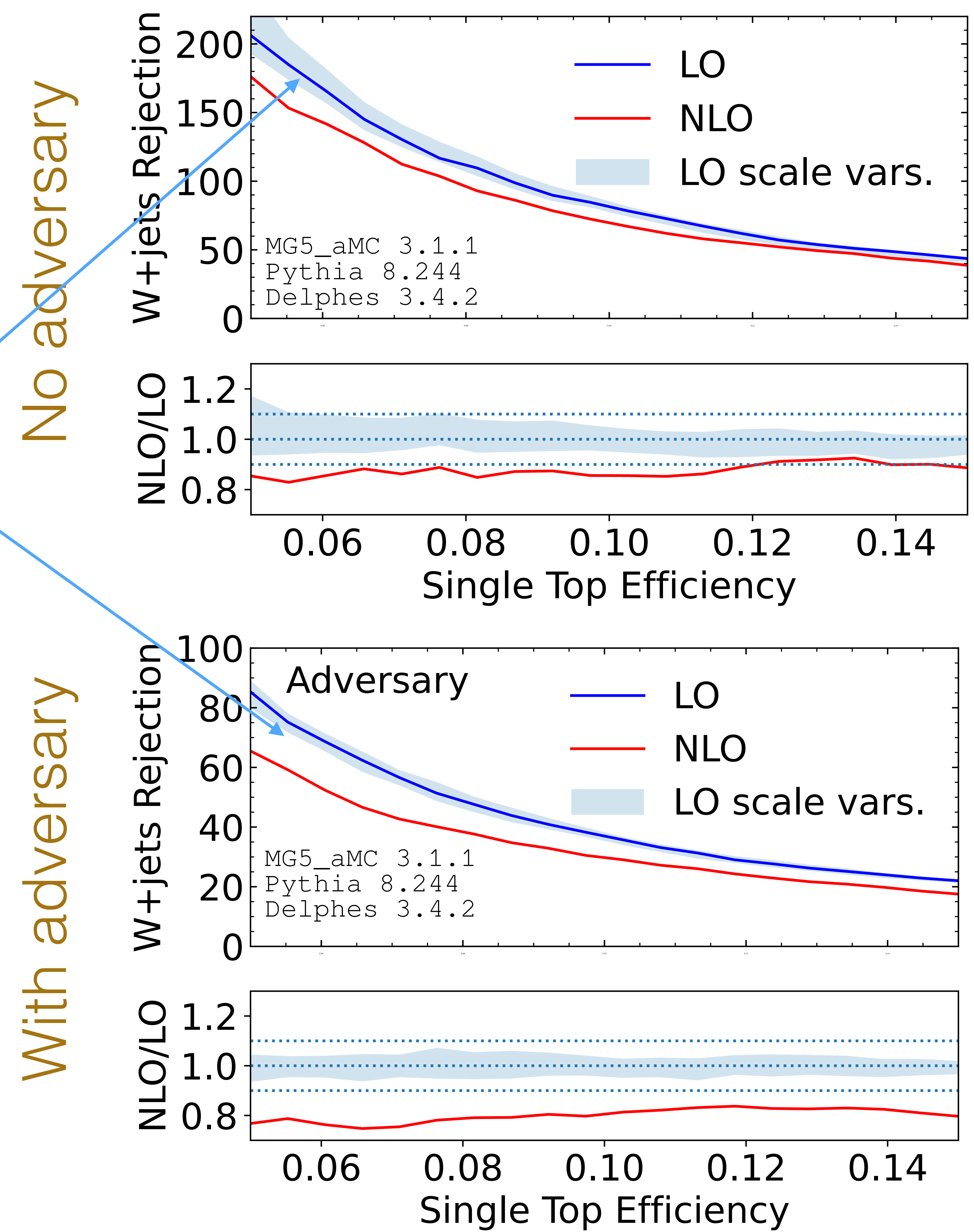
With adversary



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

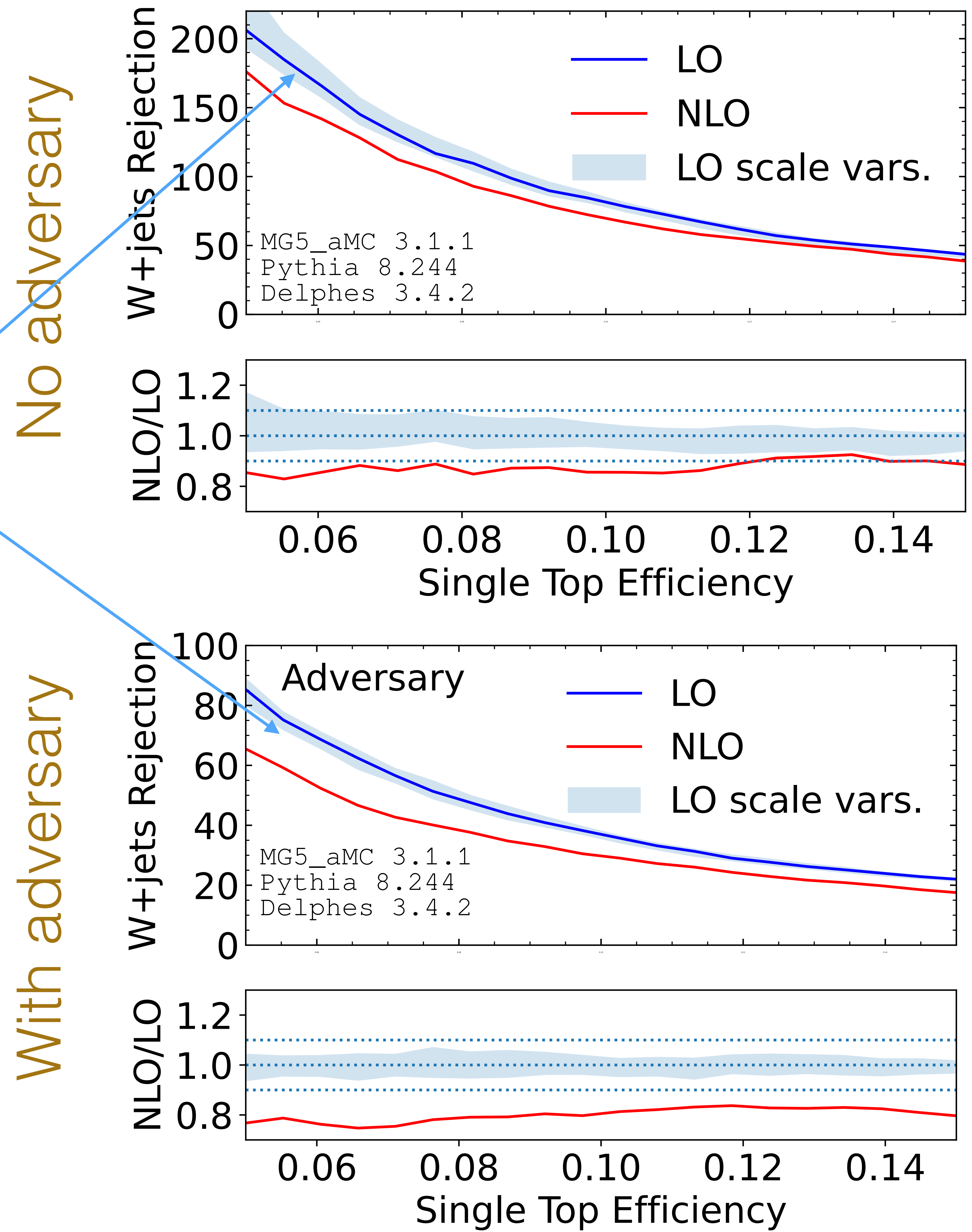
Adversary successfully **sacrifices separation power** in order to reduce difference in performance between scale variations

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)



If we can’t decorrelate, what can we do ?

If we can’t decorrelate, what can we do ?

Deep dive into scale uncertainties !

Scales

What is the error in cross-section due to truncation?

$$\sigma \in [\sigma_-, \sigma_+] \equiv \left[\sigma(\mu_{R,+}), \sigma(\mu_{R,-})\right] ,$$

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

$$\mu_{R,+} = 2 \quad \mu_0$$

$$\mu_{R,-} = 1/2 \quad \mu_0$$

Use dependence on scale to
estimate uncertainty

Questions

- How accurate are these scale uncertainties ?
- Is 1/2 to 2 a good range ?
- Can we feed them into your stats package just like an experimental uncertainty ?

https://link.springer.com/article/10.1007/JHEP07(2014)079

Questions

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Use pull to examine

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

Critical issue:

need a large (>>10)
set of processes calculated
under identical conditions

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<u>**Critical issue:**</u>

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under identical conditions

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!

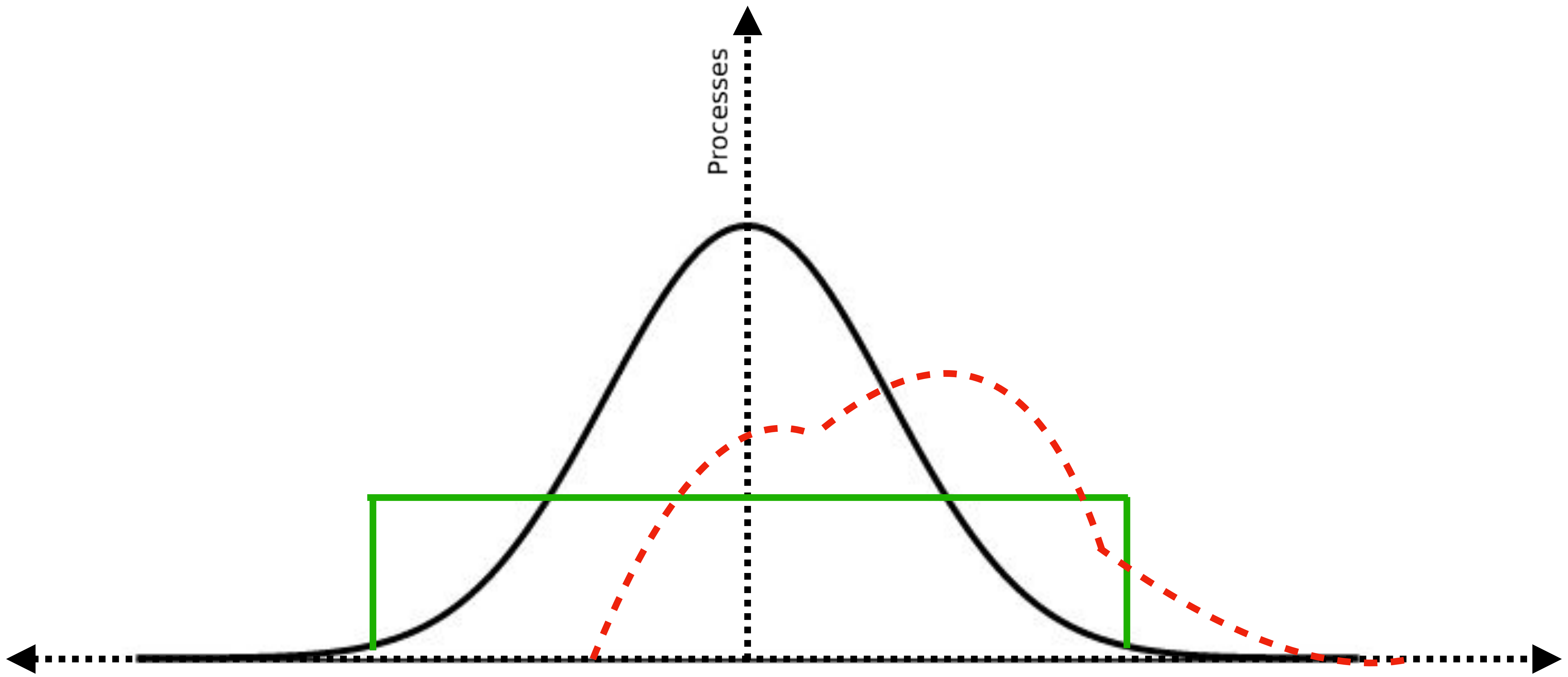
(Not a random sampling)

https://link.springer.com/article/10.1007/JHEP07(2014)079

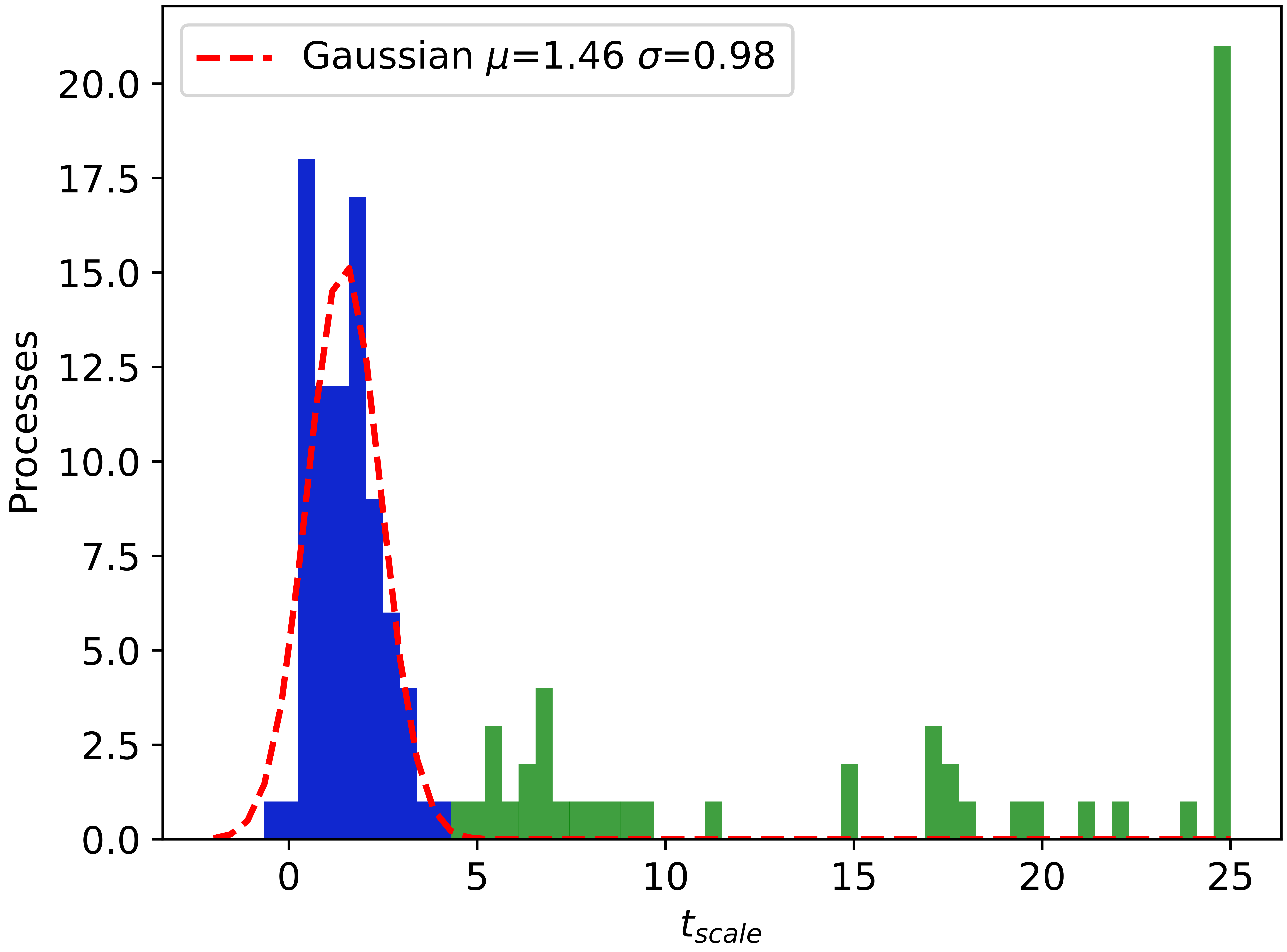
Plot the pulls

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

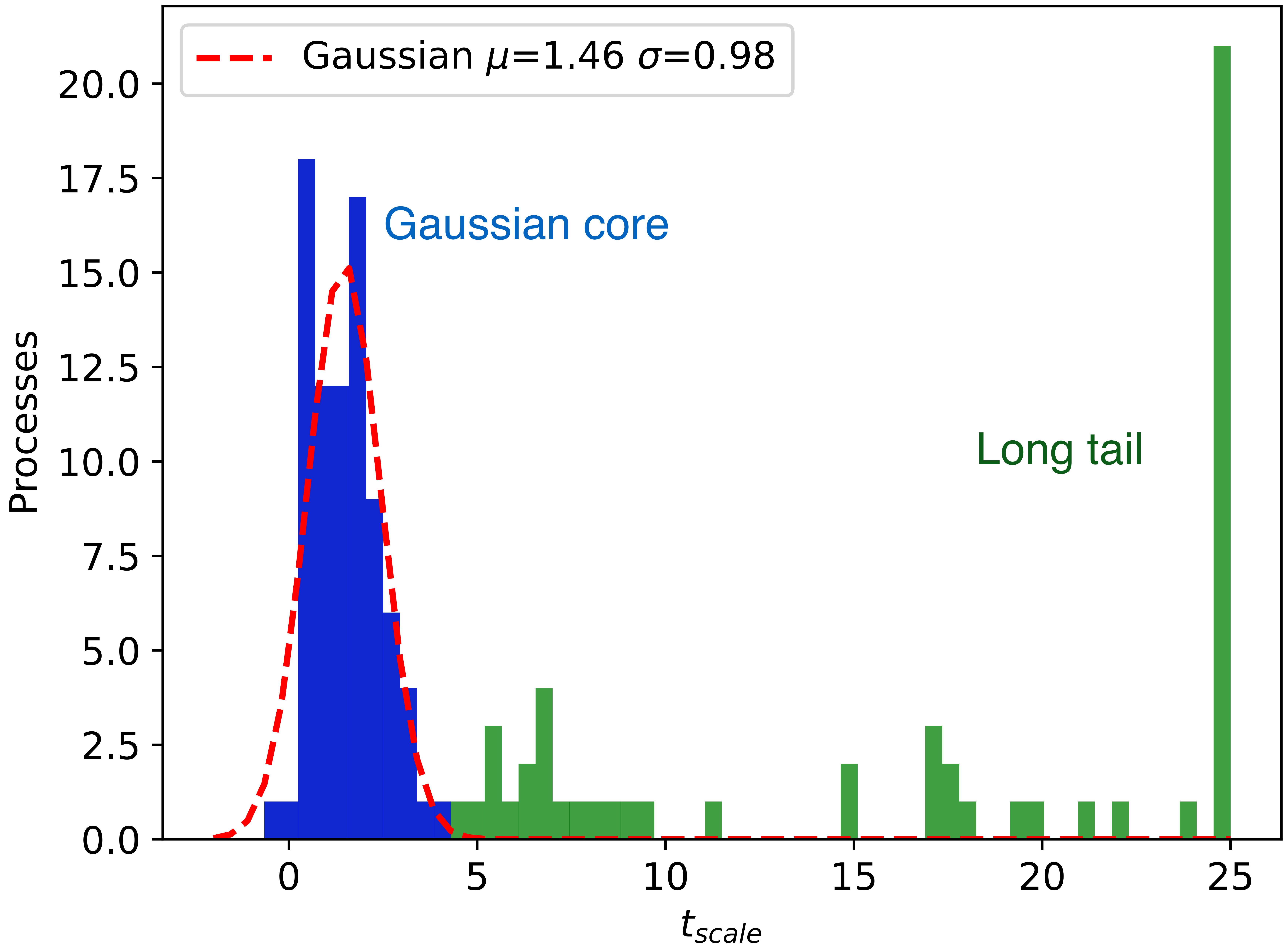
Which of these distributions do you expect?



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



Gaussian μ=1.46 σ=0.98
Processes
t_{scale}
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
0
5
10
15
20
25



Gaussian μ=1.46 σ=0.98
Gaussian core
Long tail
Processes
t_{scale}
20.0
17.5
15.0
12.5
10.0
7.5
5.0
2.5
0.0
0
5
10
15
20
25

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

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Process	$\frac{\Delta\sigma}{\sigma_0}$		n	$\frac{\Delta\sigma}{n\,\sigma_0}$	
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`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}
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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

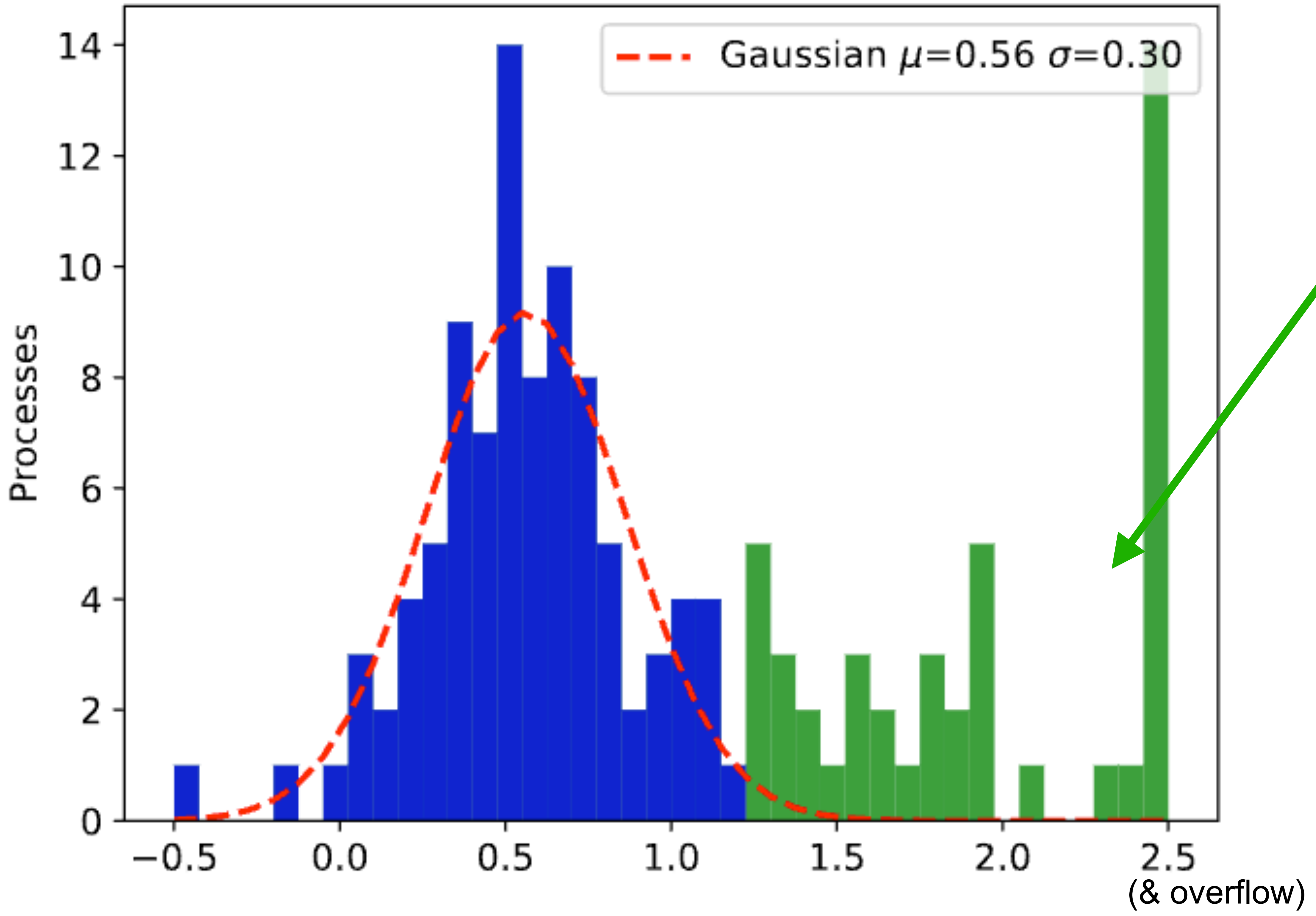
$$\frac{\Delta\sigma_{\text{ref}}}{\sigma_0} = n \times \left\langle \frac{\Delta\sigma}{n\sigma_0} \right\rangle_{\text{QCD}} .$$

https://arxiv.org/abs/2210.15167

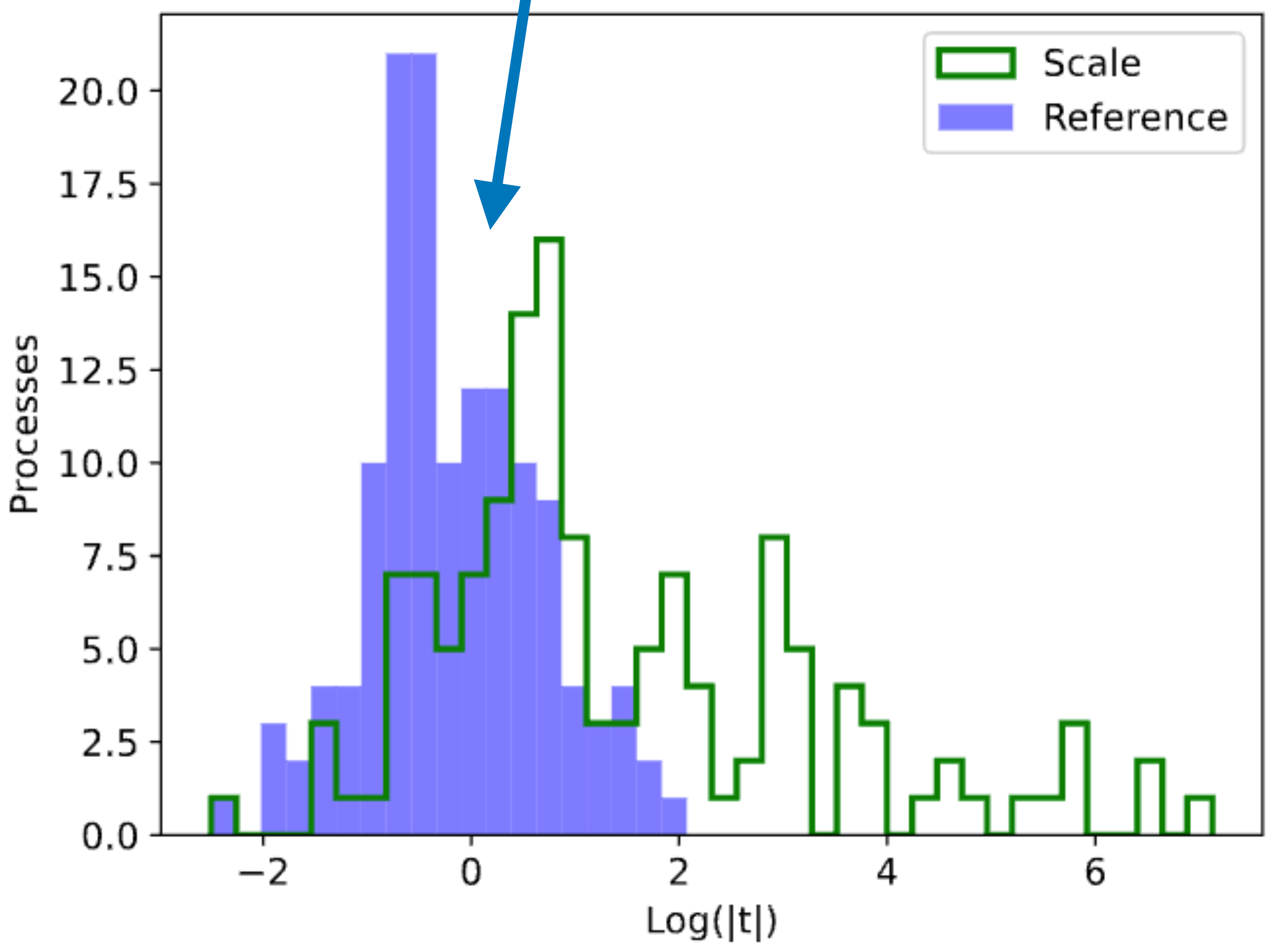
Make correction in UQ for EW processes

Still tails

Much reduced



$$t_{\text{ref}} = \frac{\sigma_{\text{NLO}} - \sigma_0}{\Delta\sigma_{\text{ref}}}$$



Tilman Plehn's 'reference process' method

Follow up, open questions

- Would be even more interesting to repeat study for NLO → NNLO

- Can we use ML to automatically find patterns of failure ?

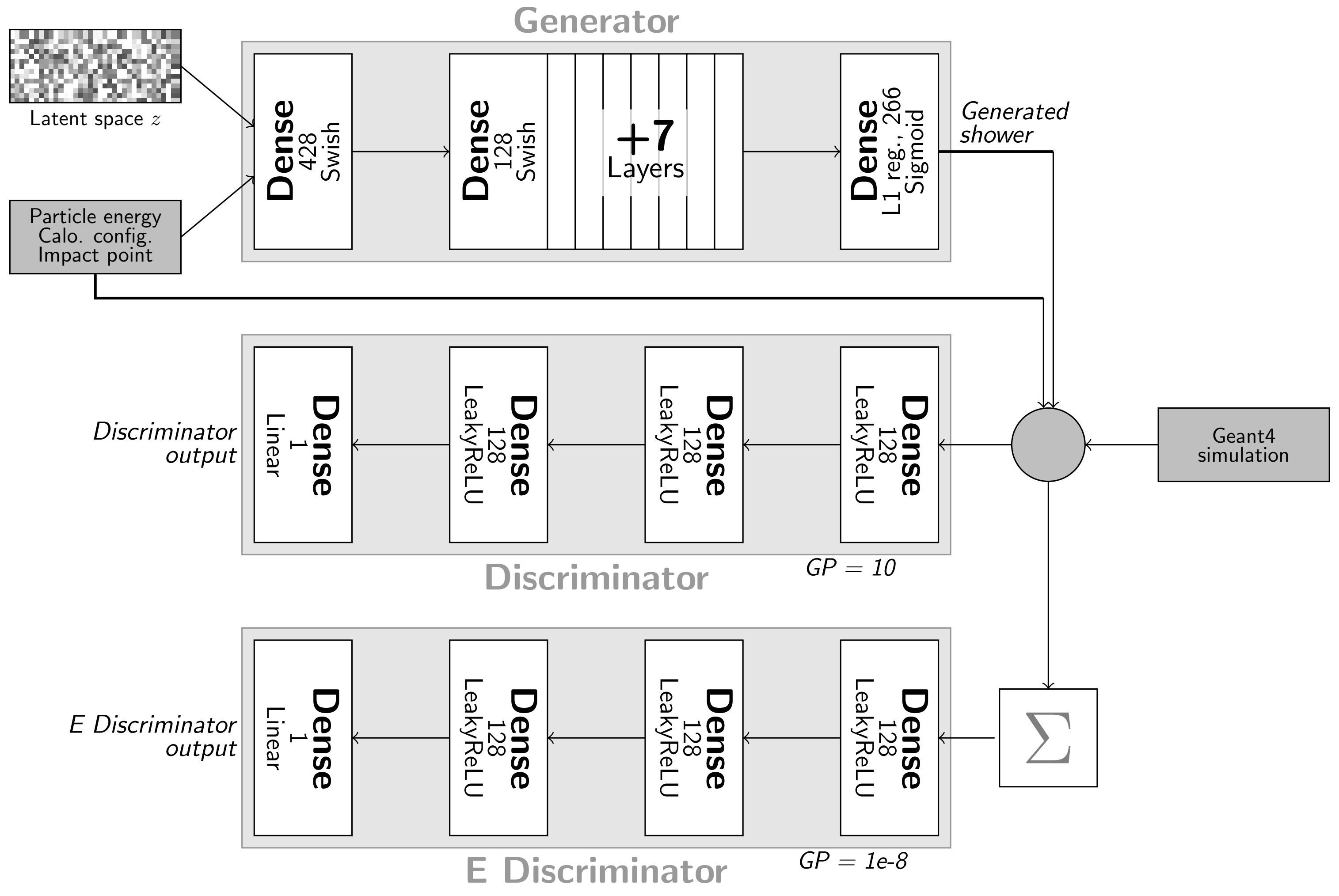
- Why did we find a Gaussian-ish core ?

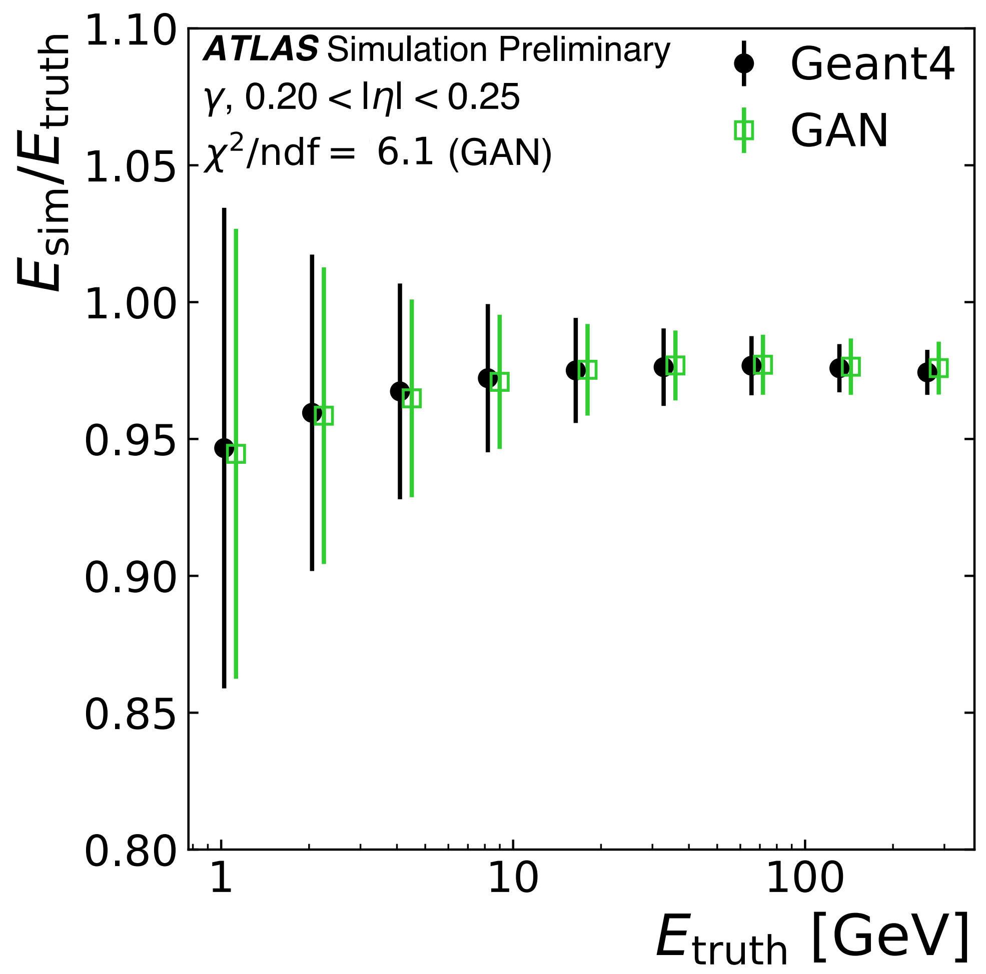
Quantifying Metrics for Generative Models

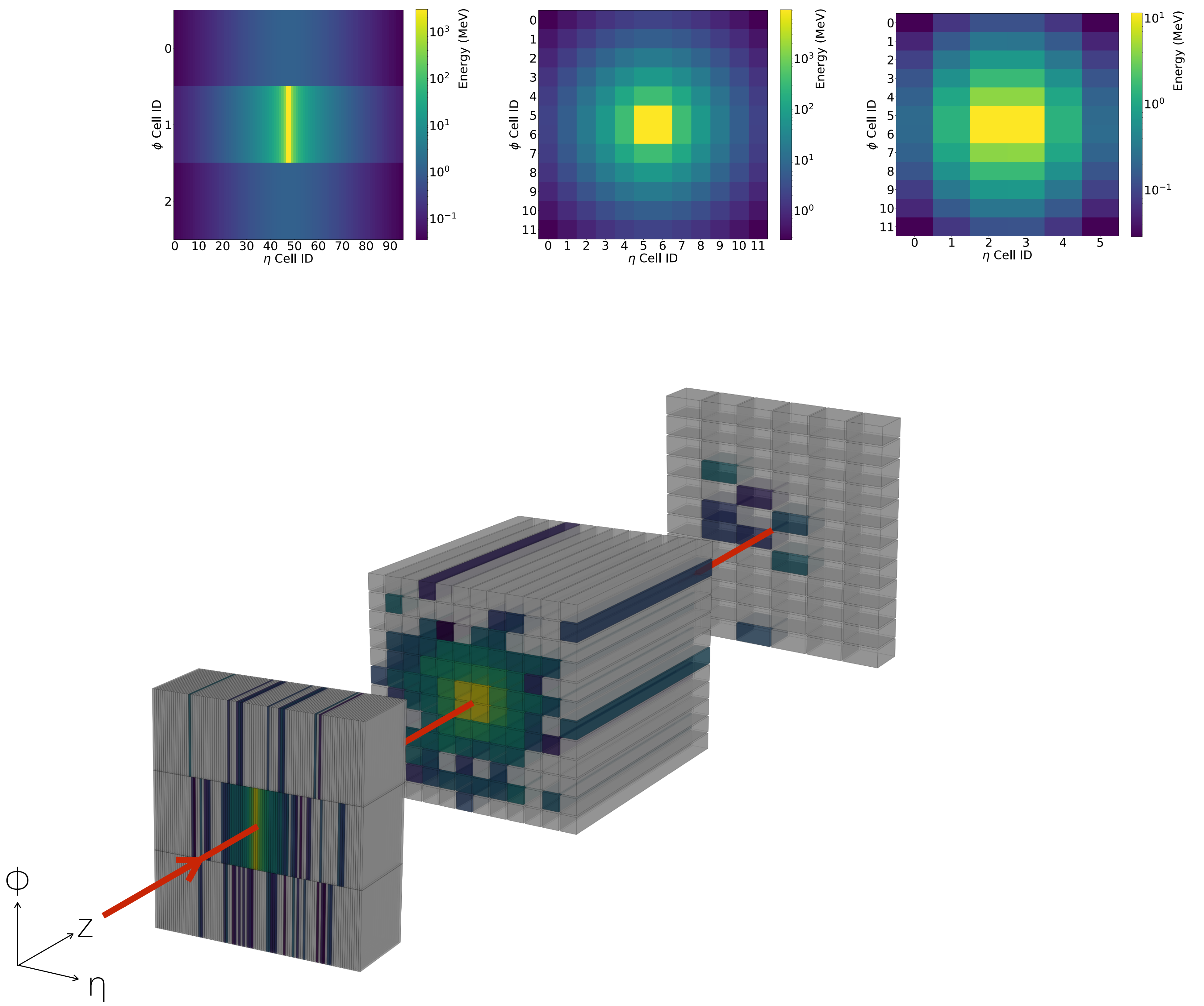
Generative Models for Simulation

Ghosh, ATLAS Collaboration, 2019

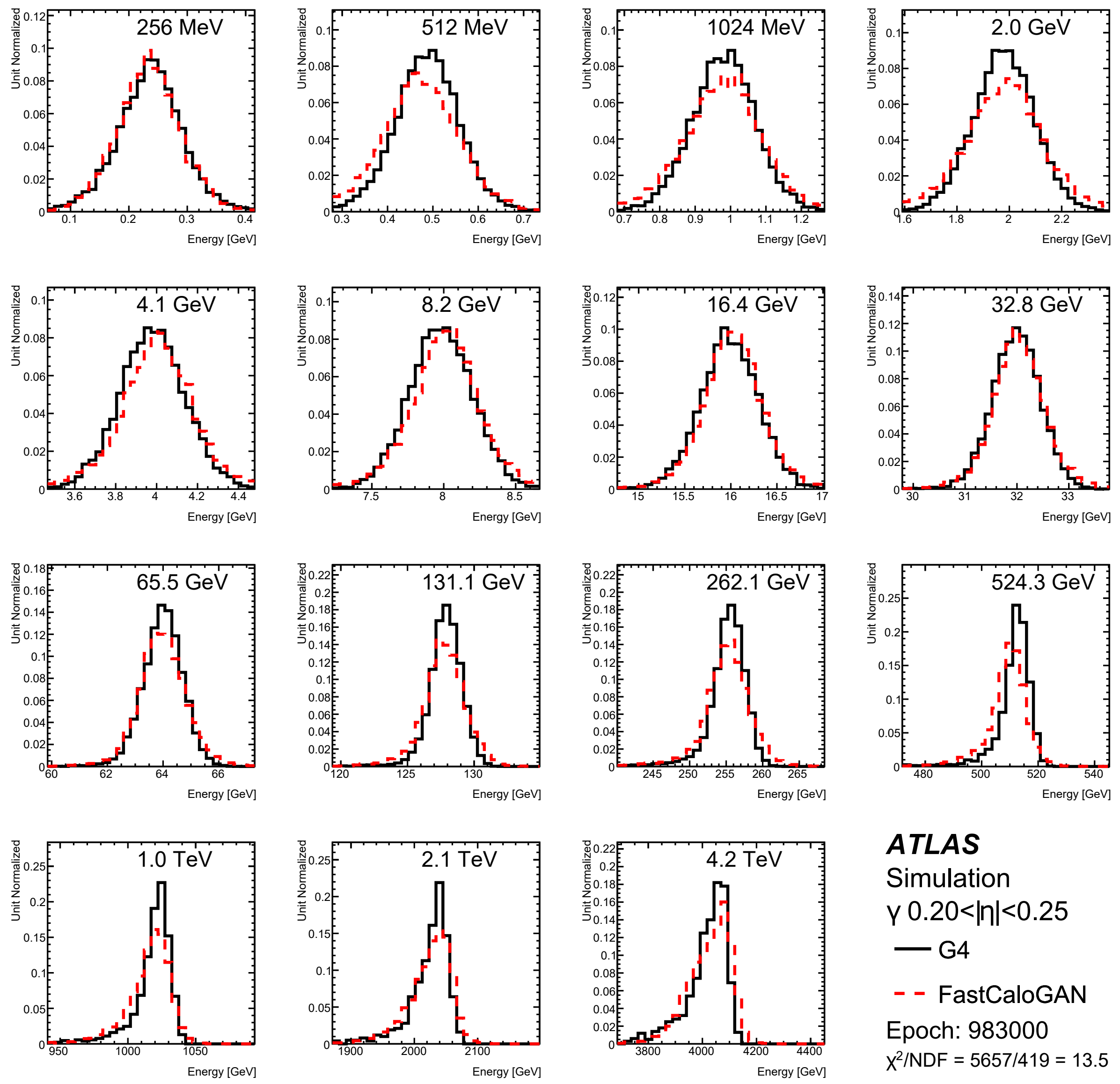
Paganini et al.







Evaluating Fast Calo Simulators



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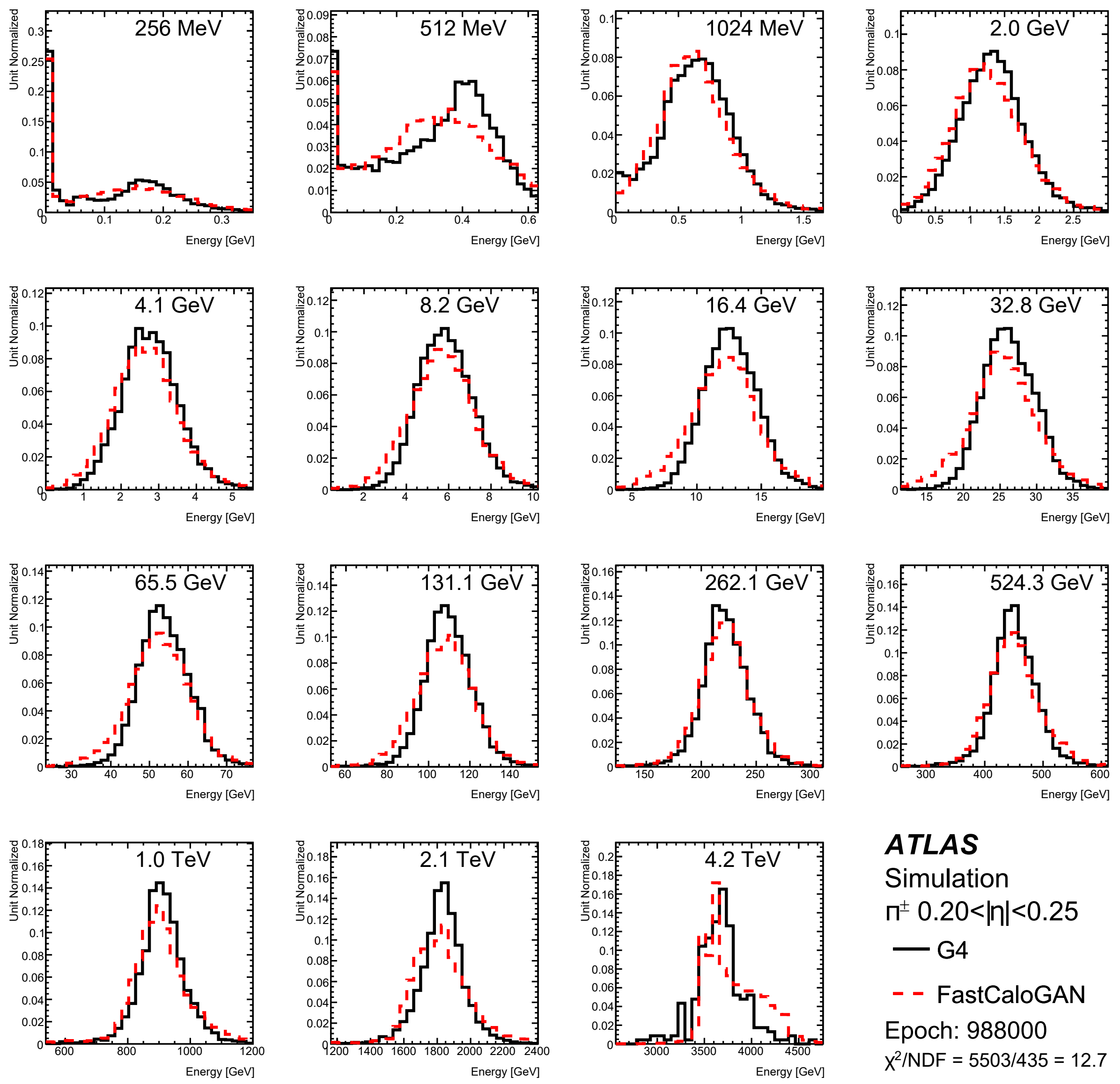

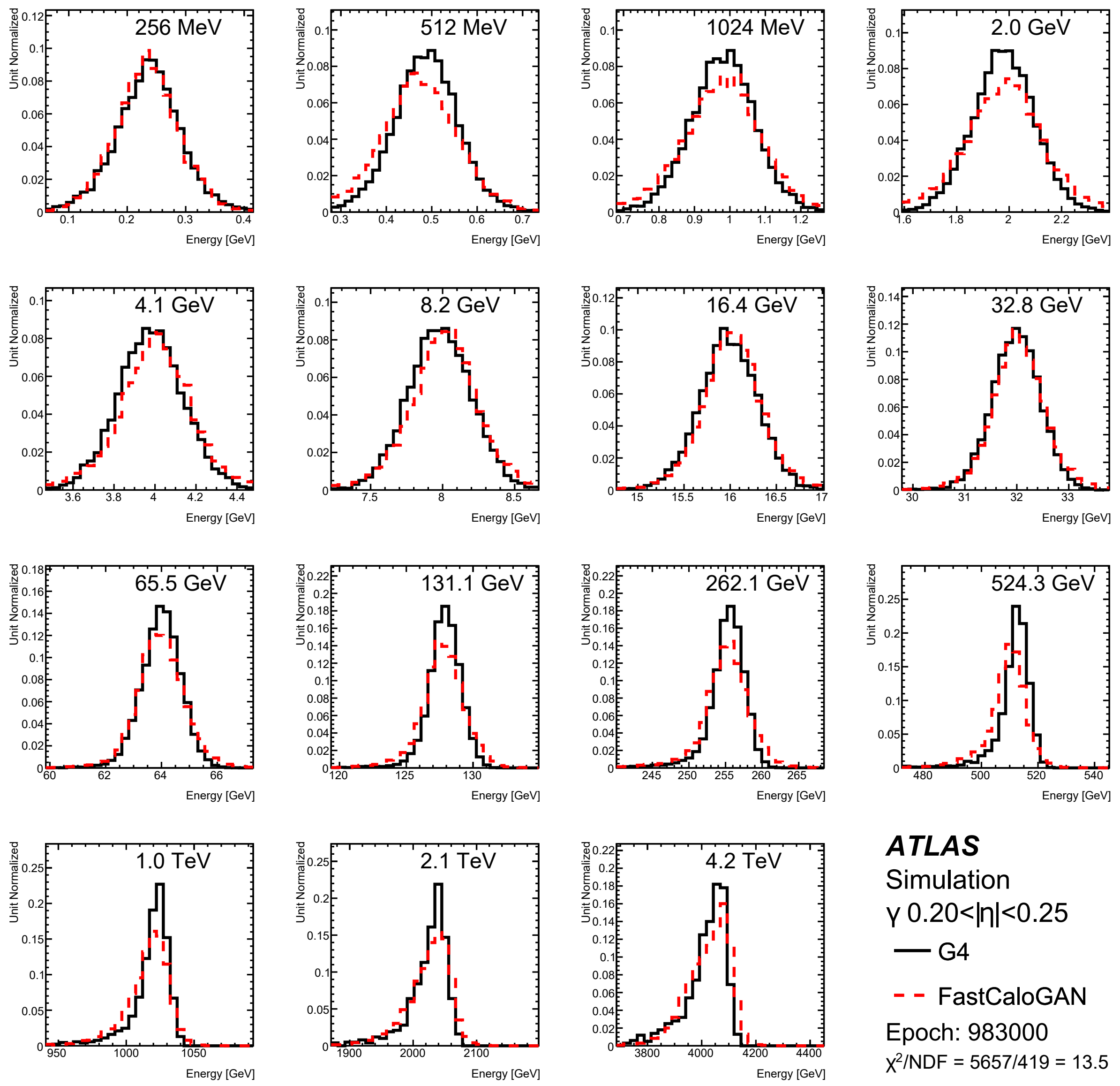

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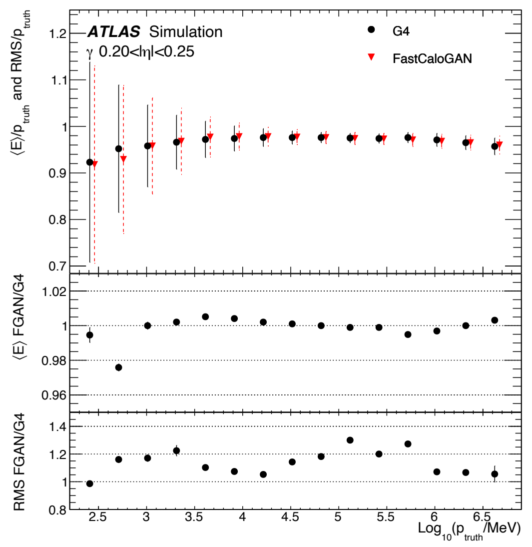
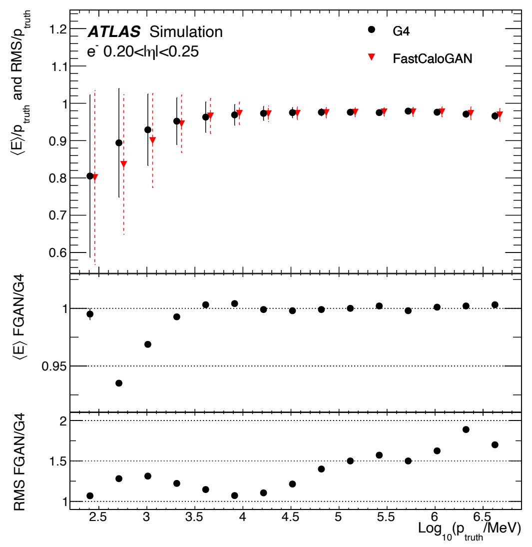


(a)



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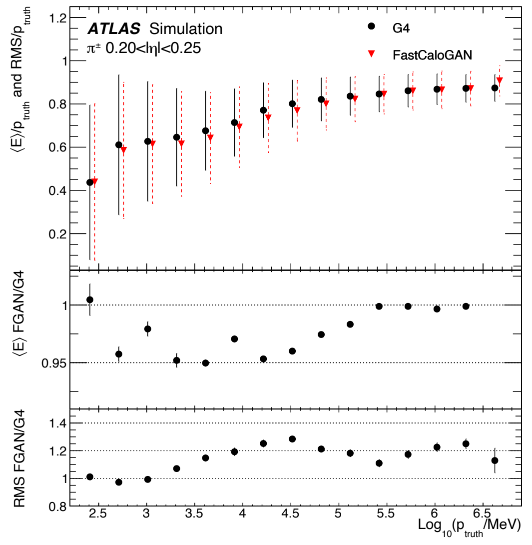
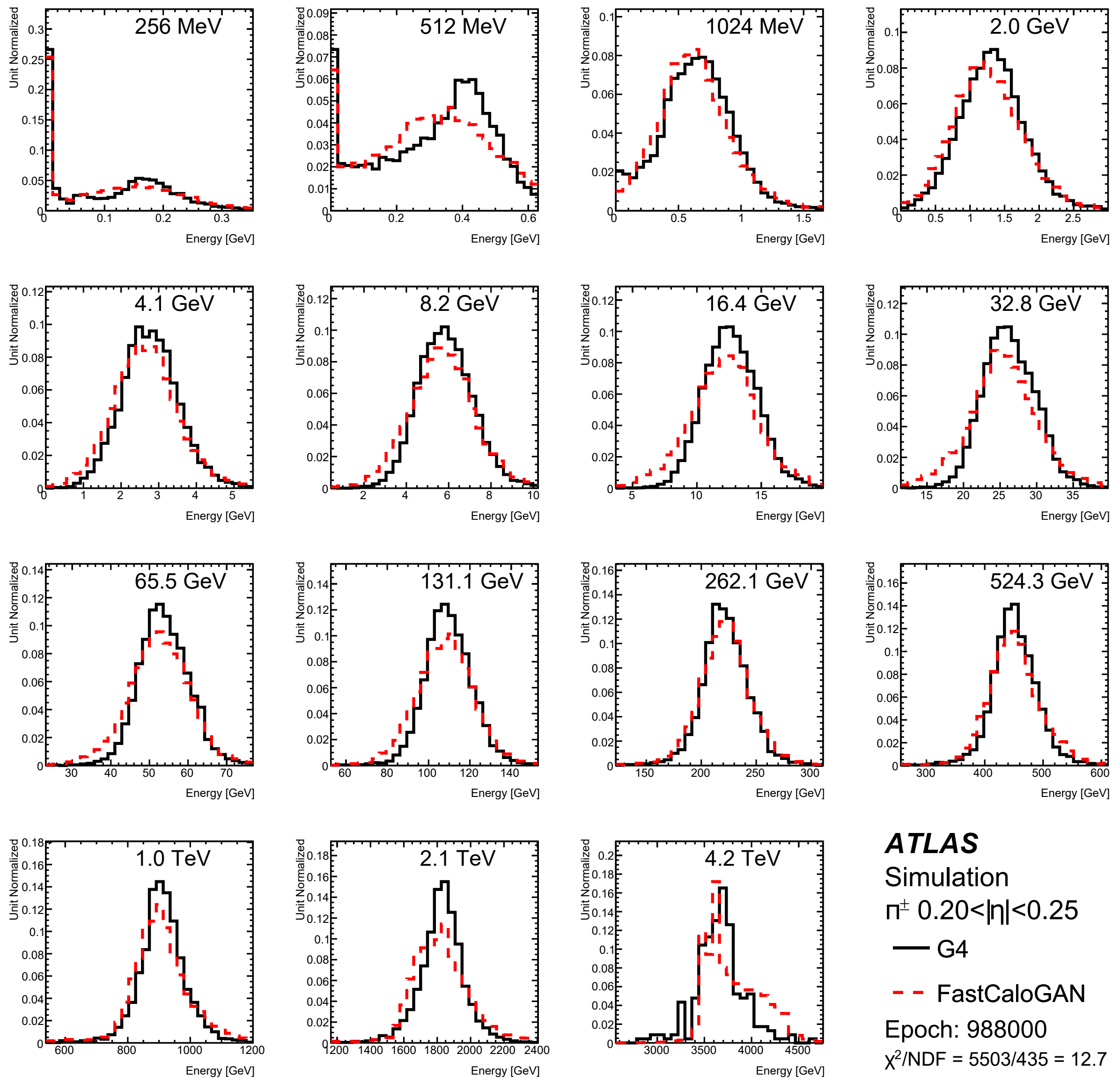
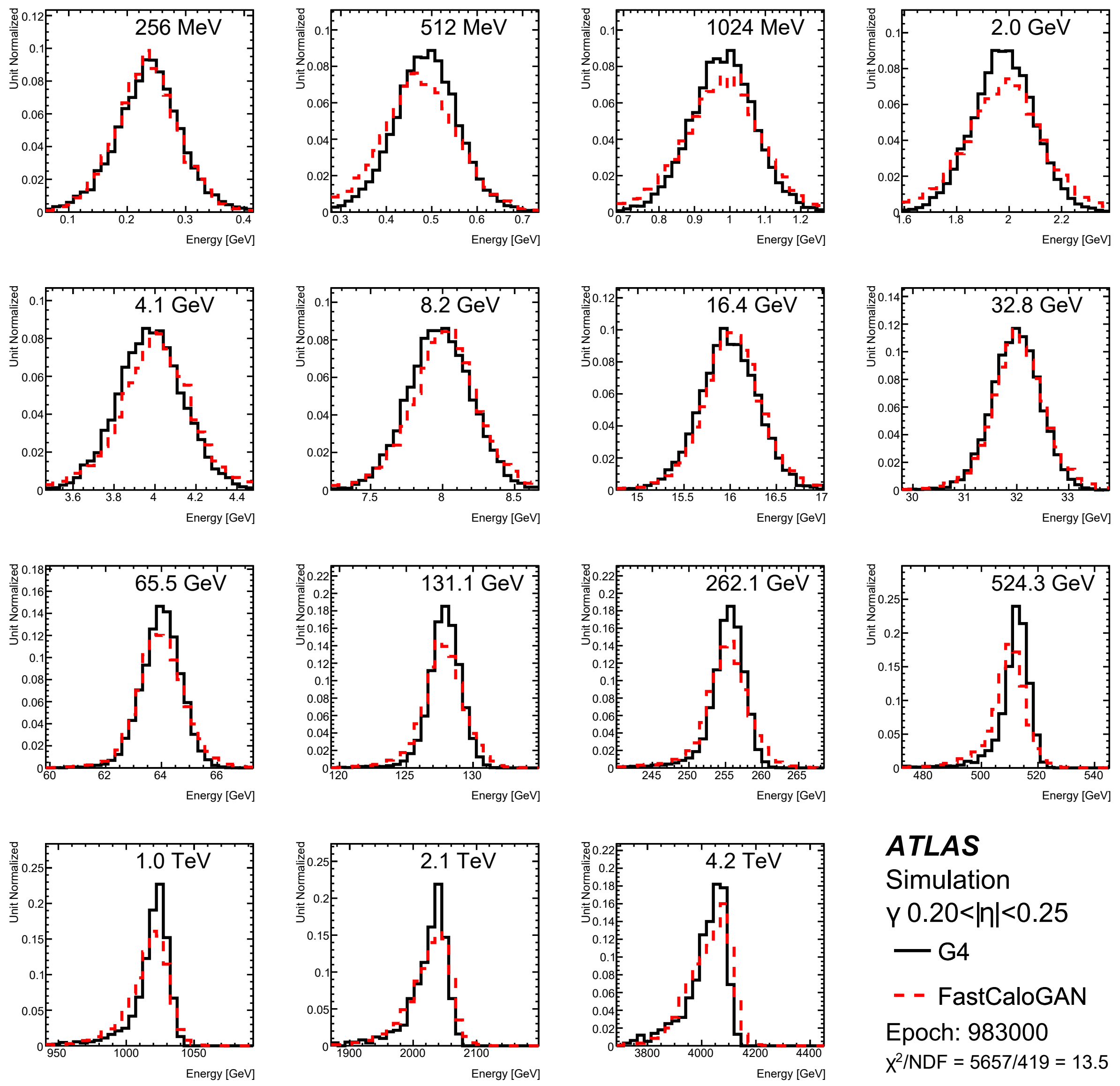


(c)





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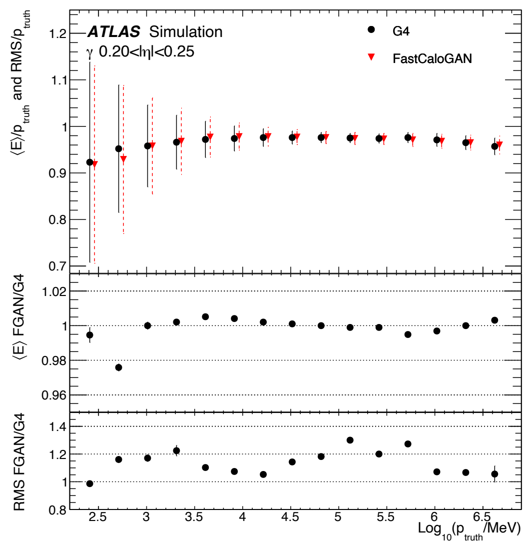

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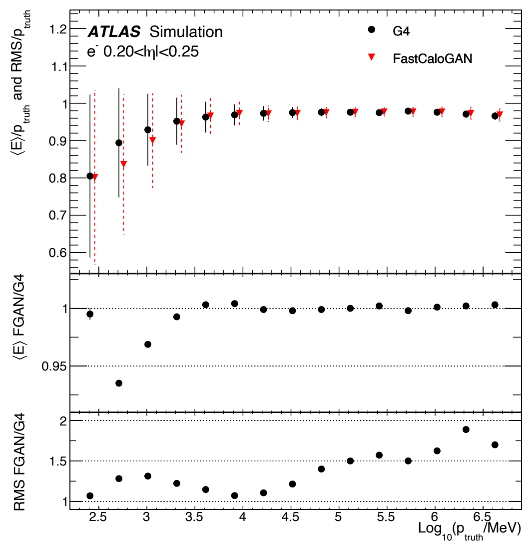

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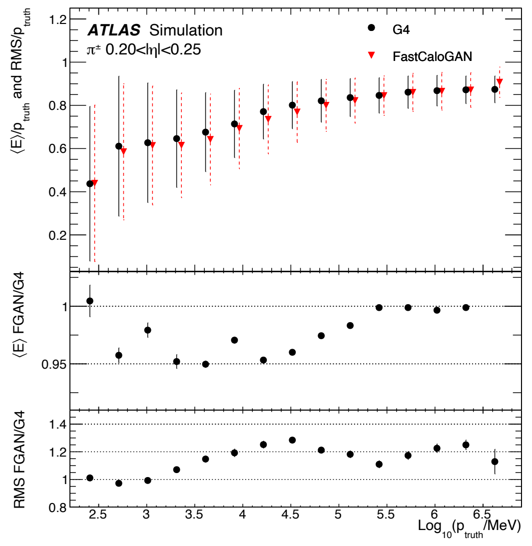

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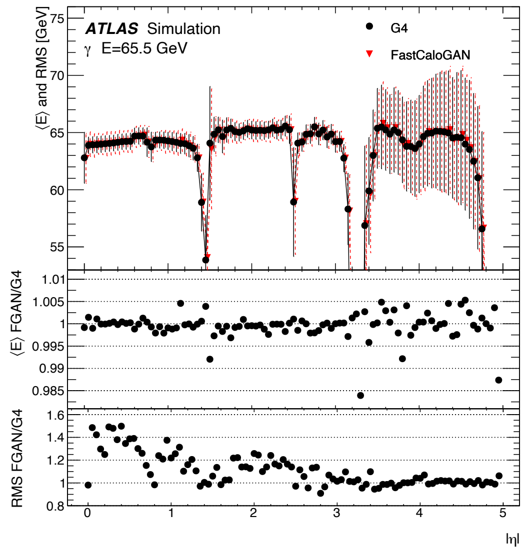

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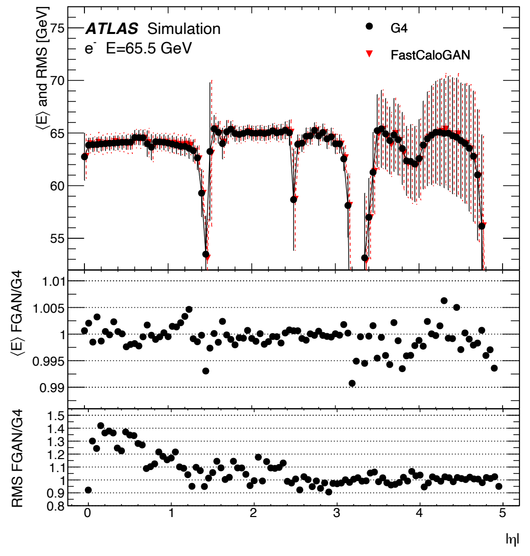

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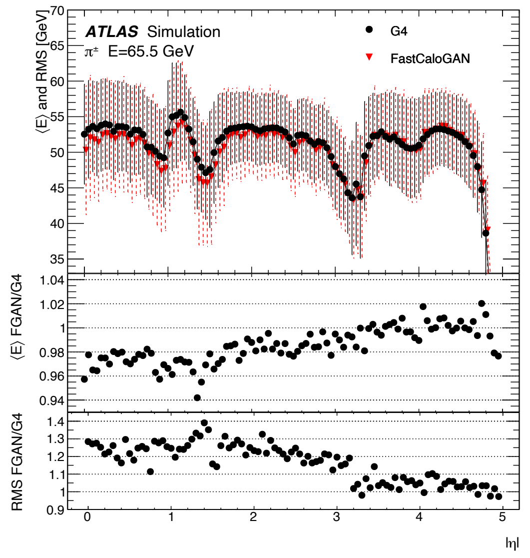
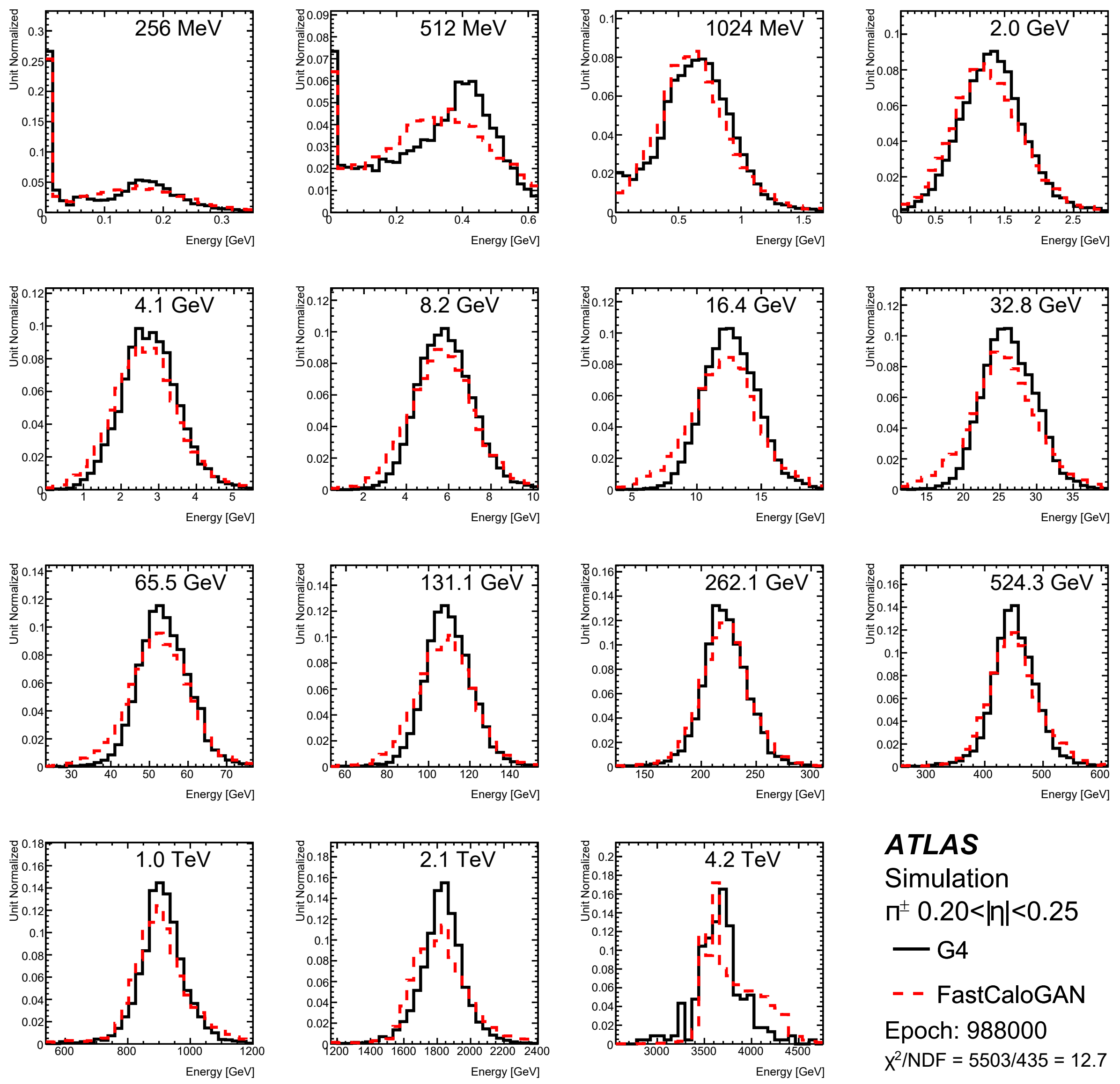
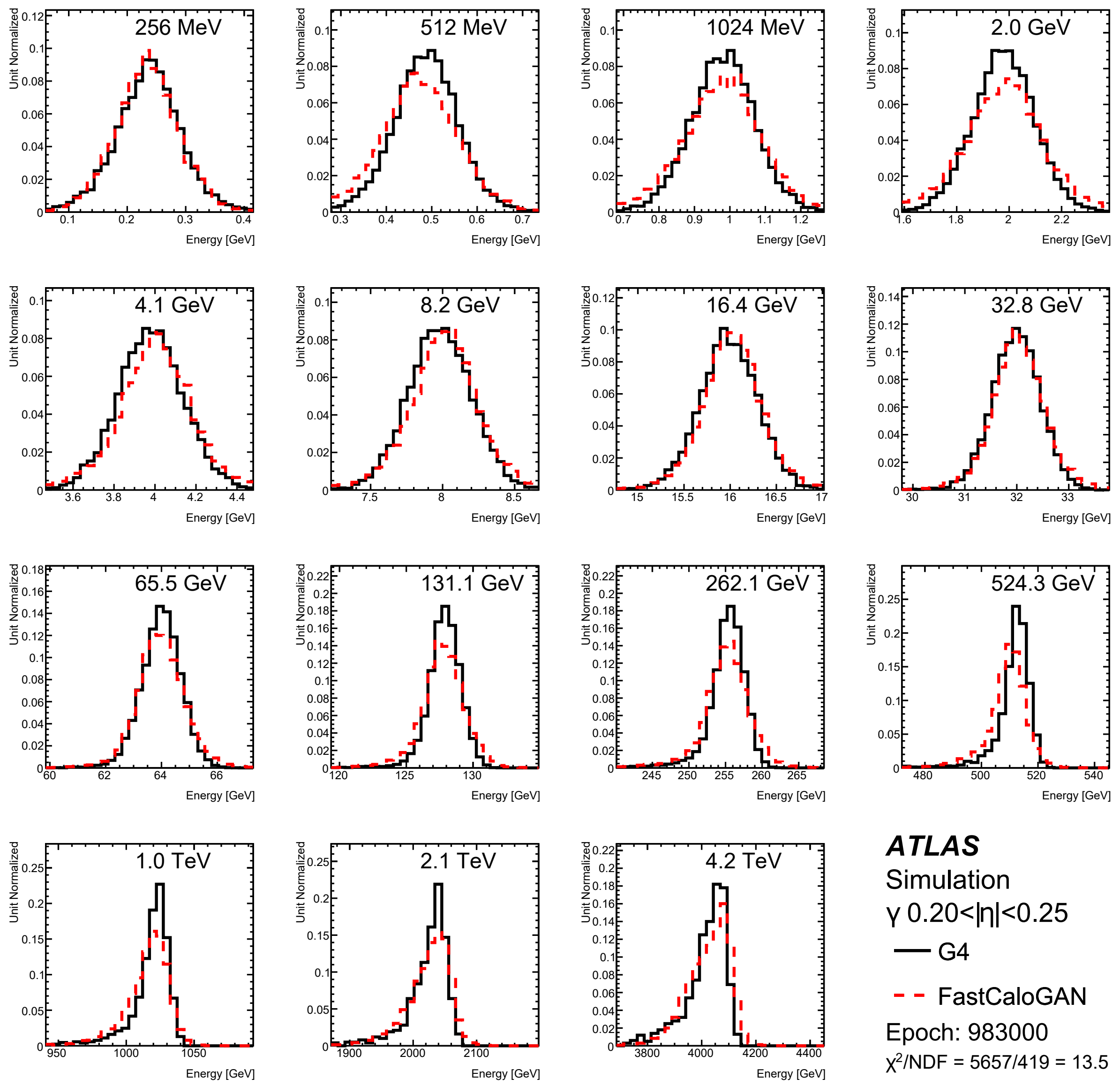


(c)





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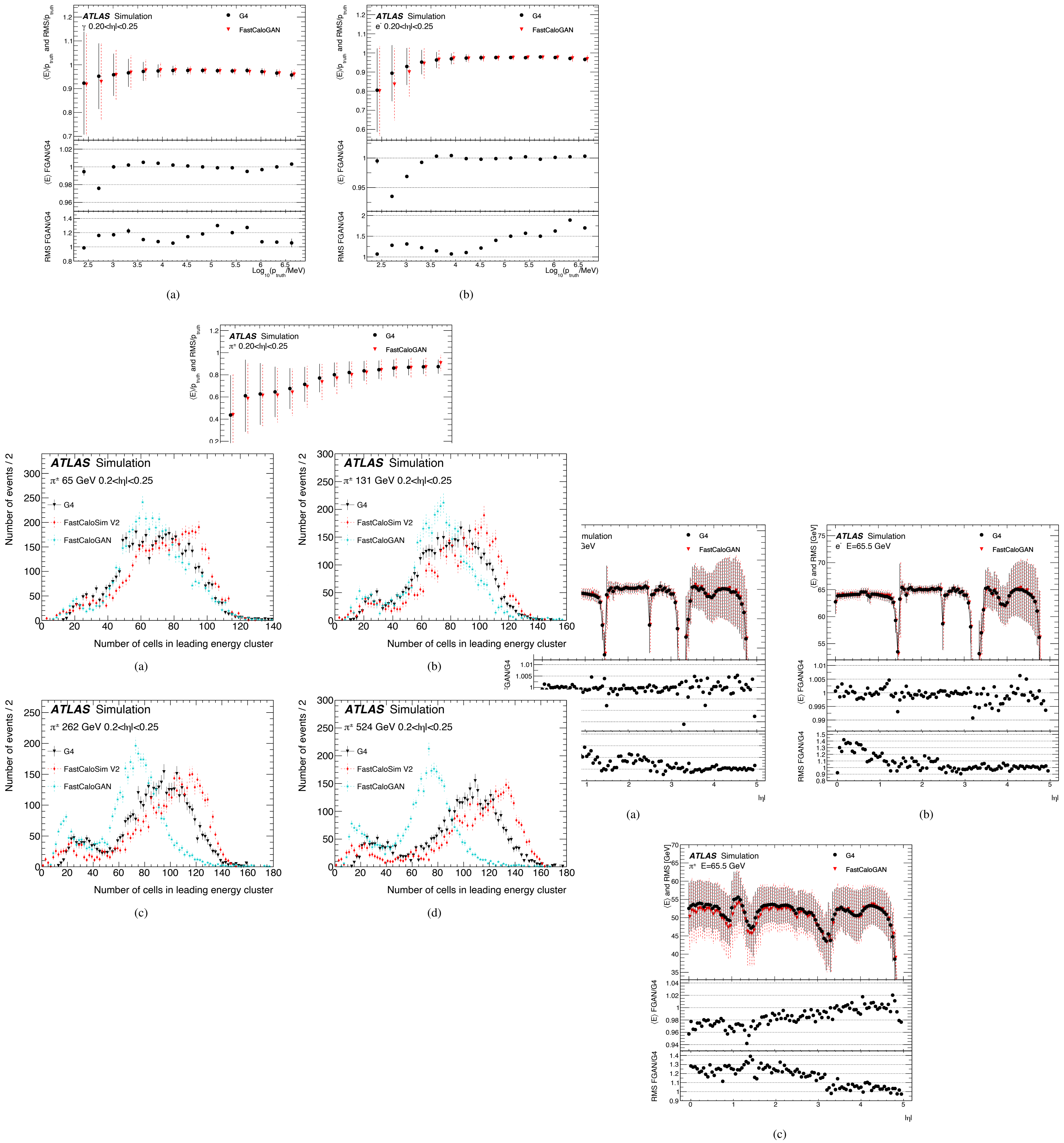
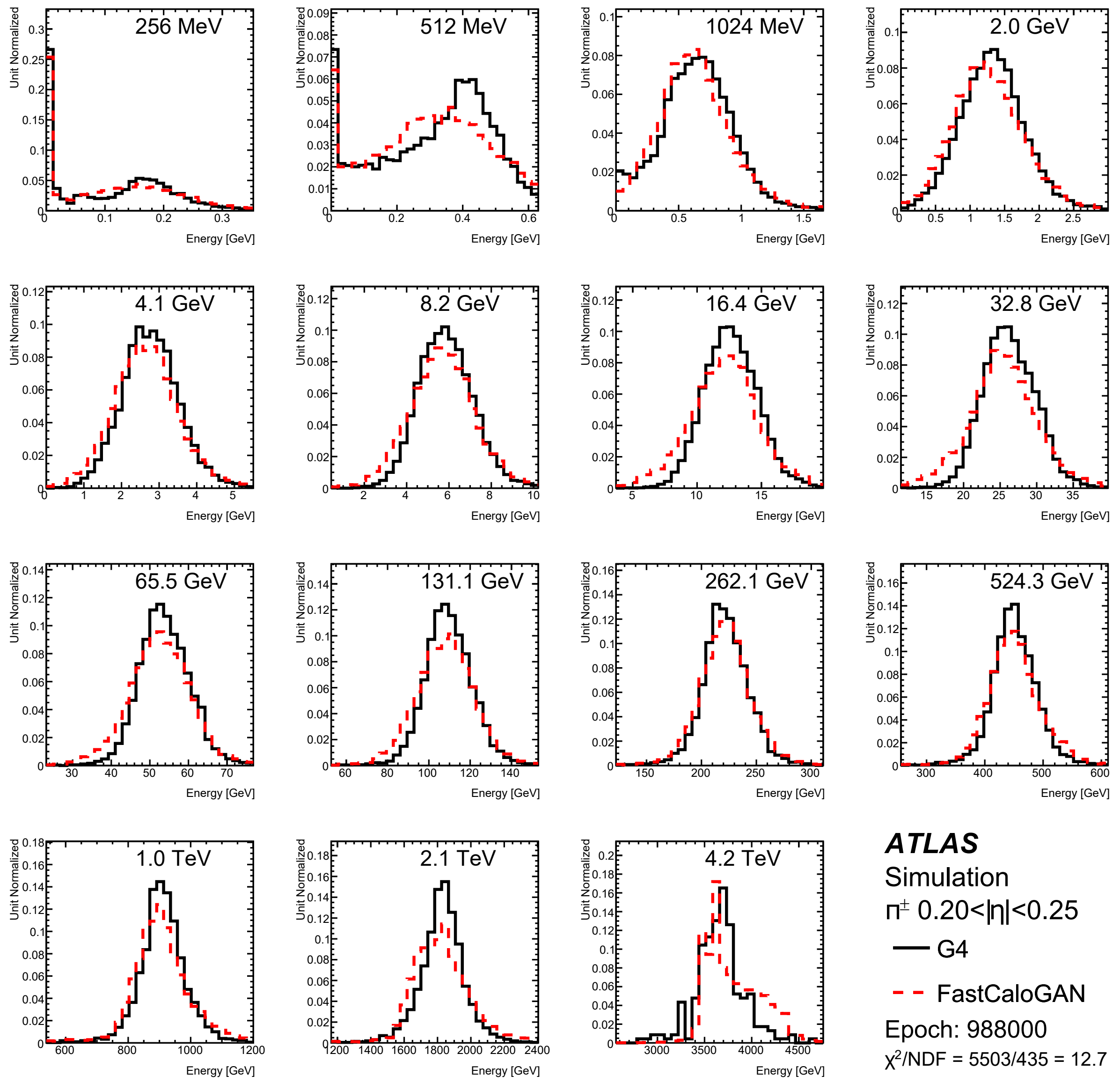
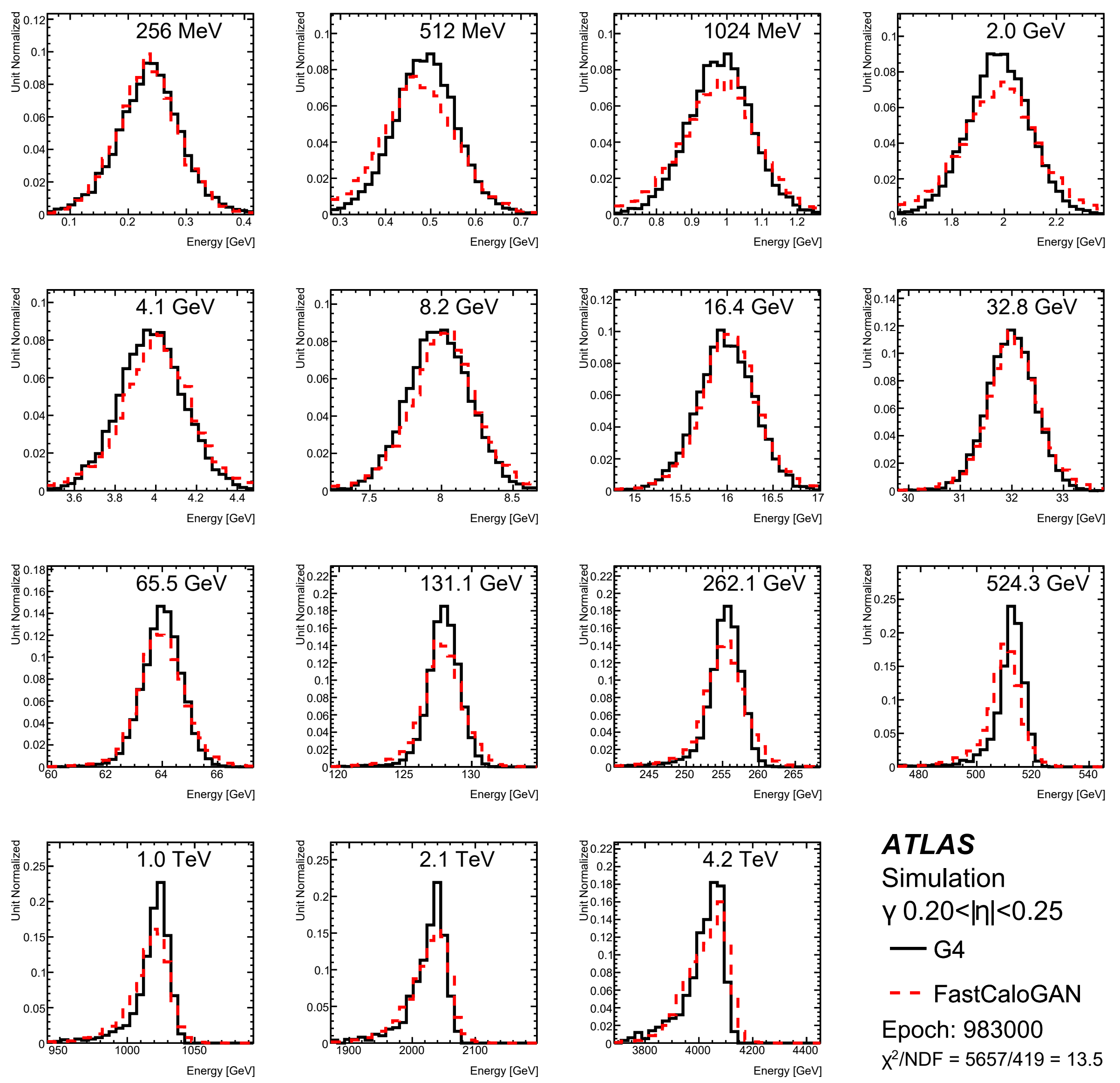
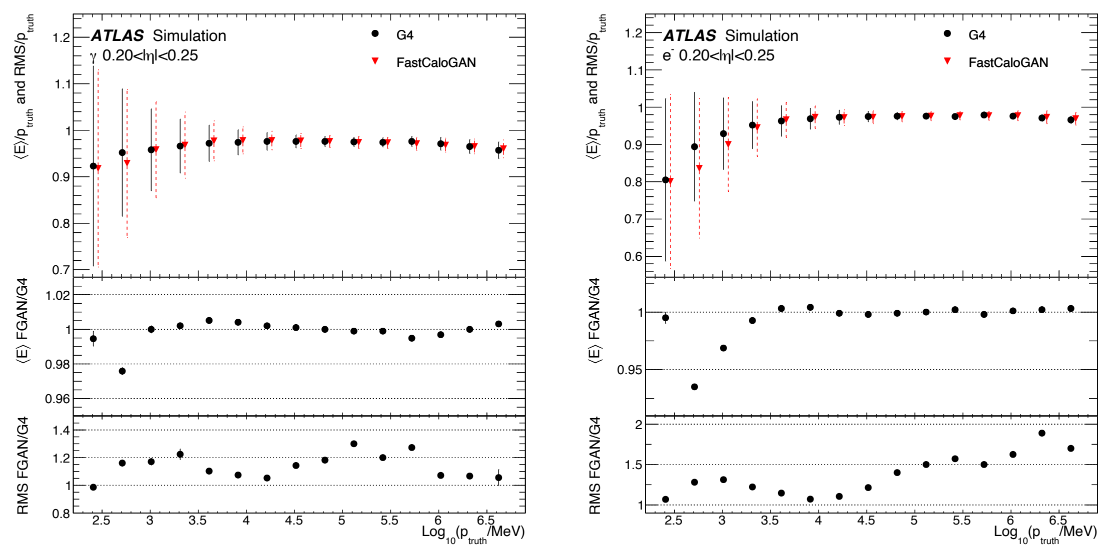


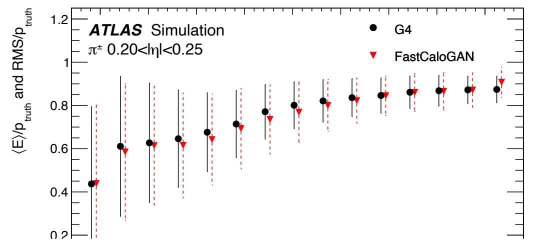


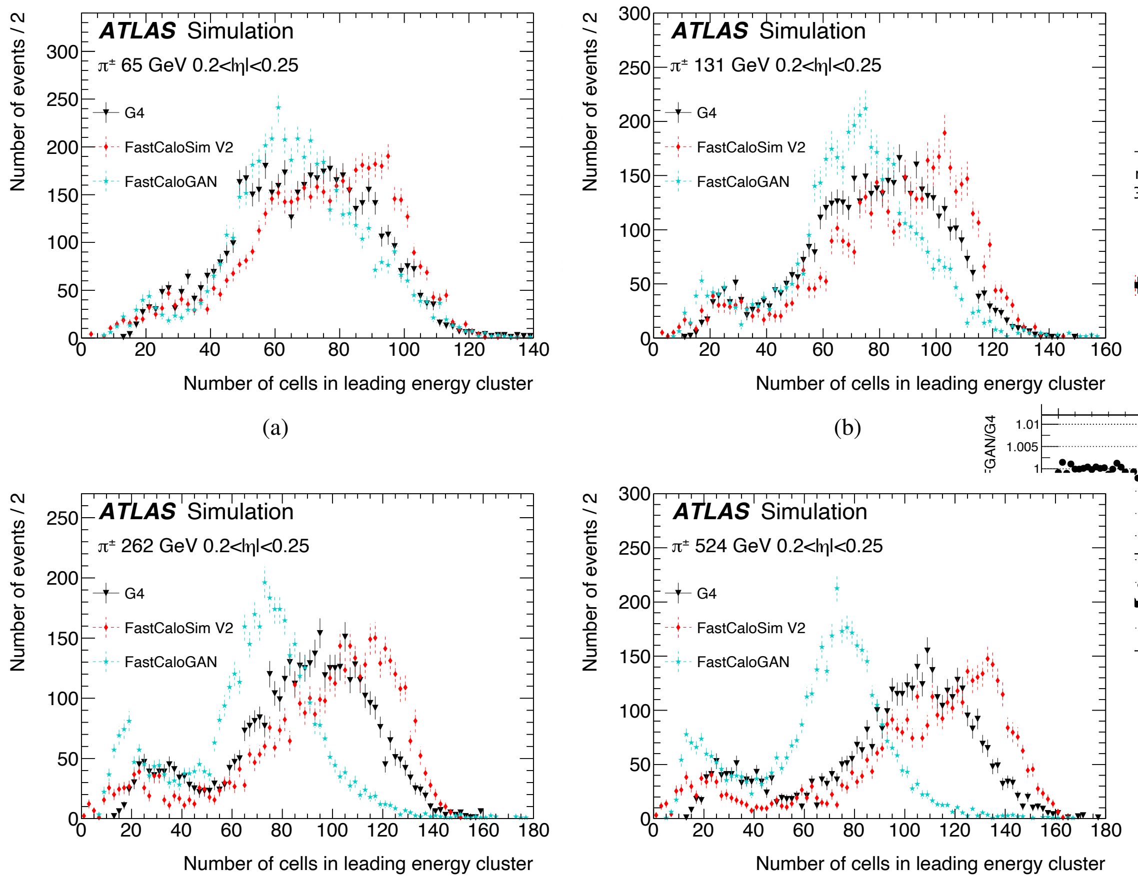


Evaluating Fast Calo Simulators



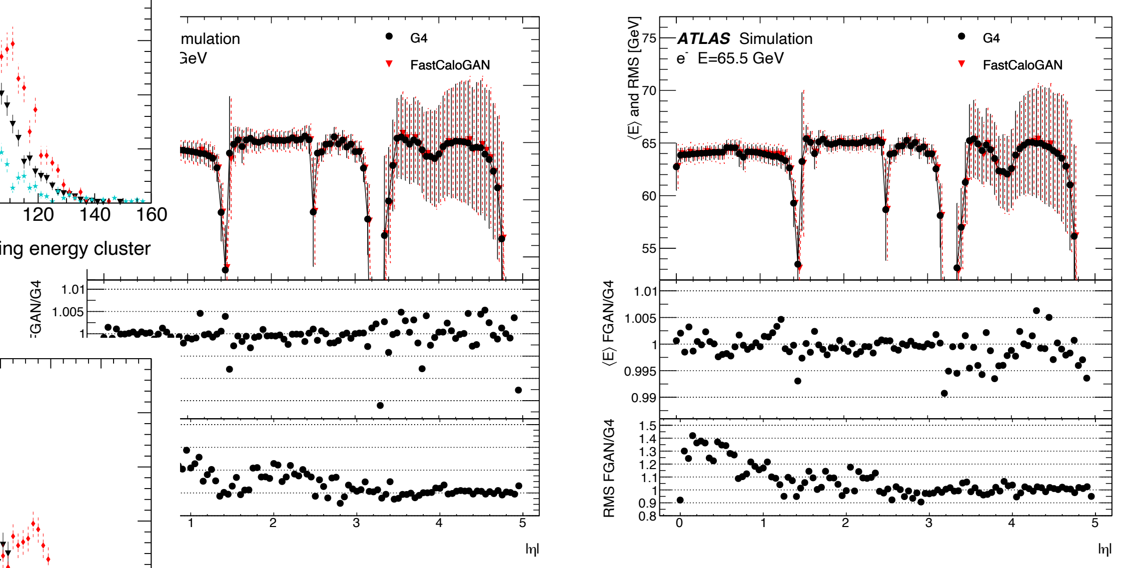
(a) (b)





(a) (b)

(c) (d)



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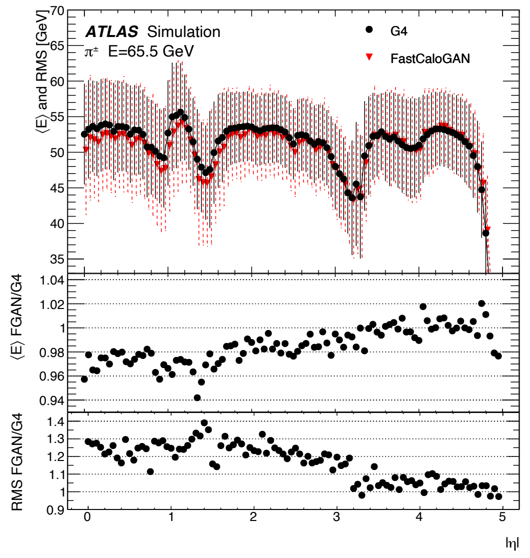
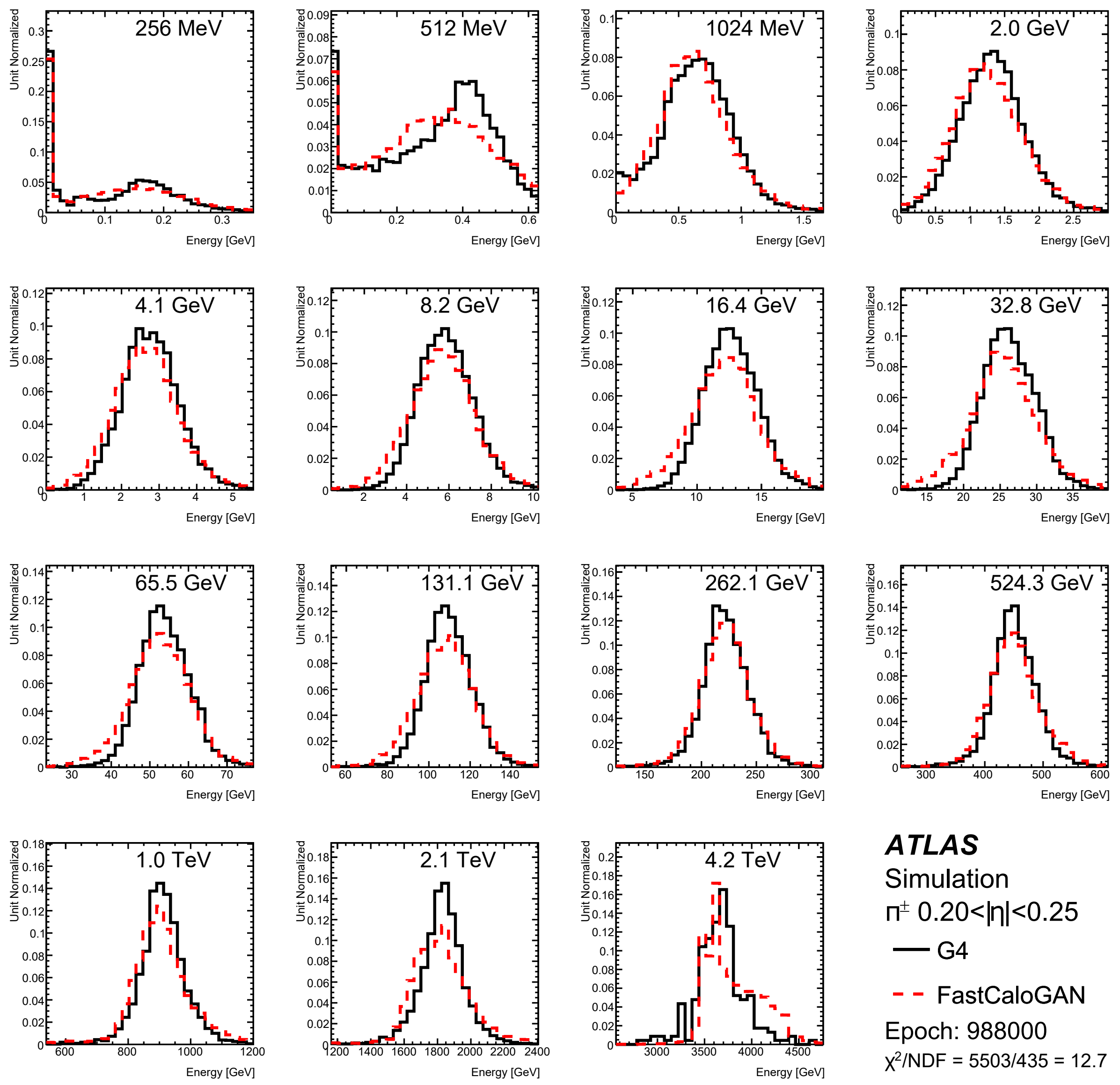
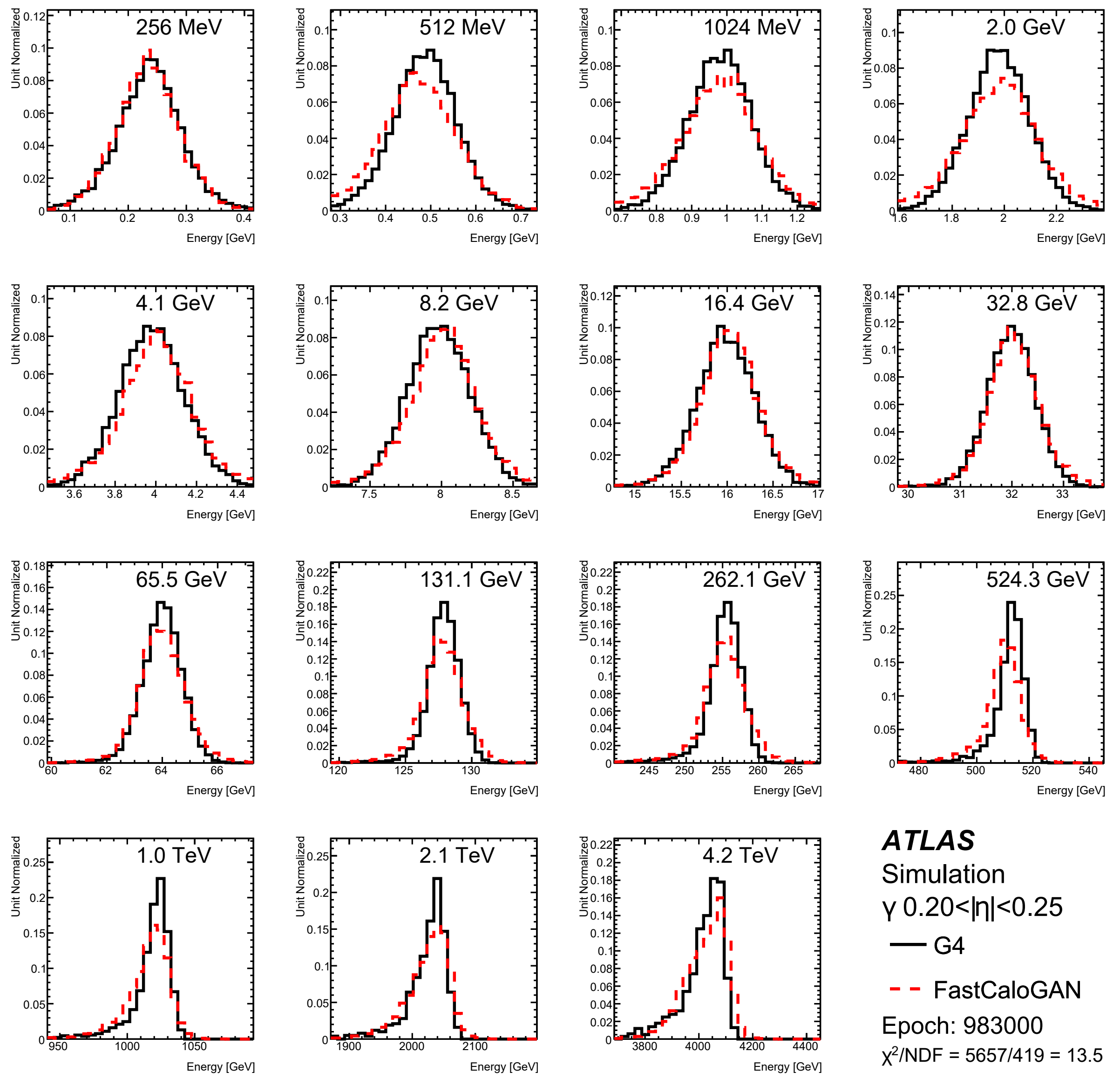
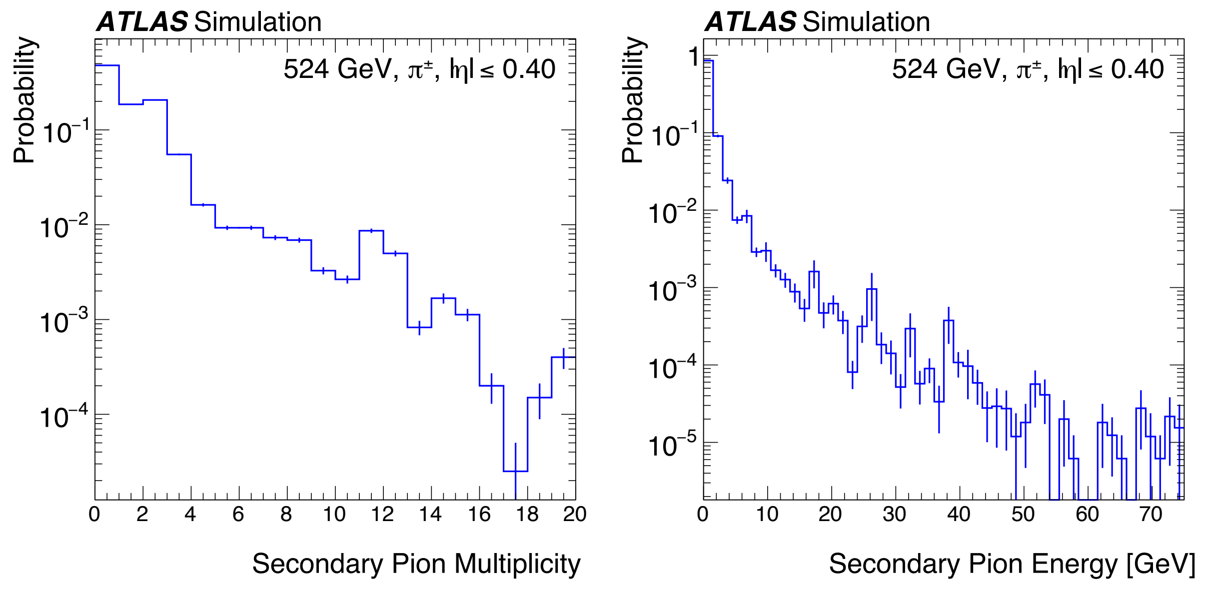


(c)







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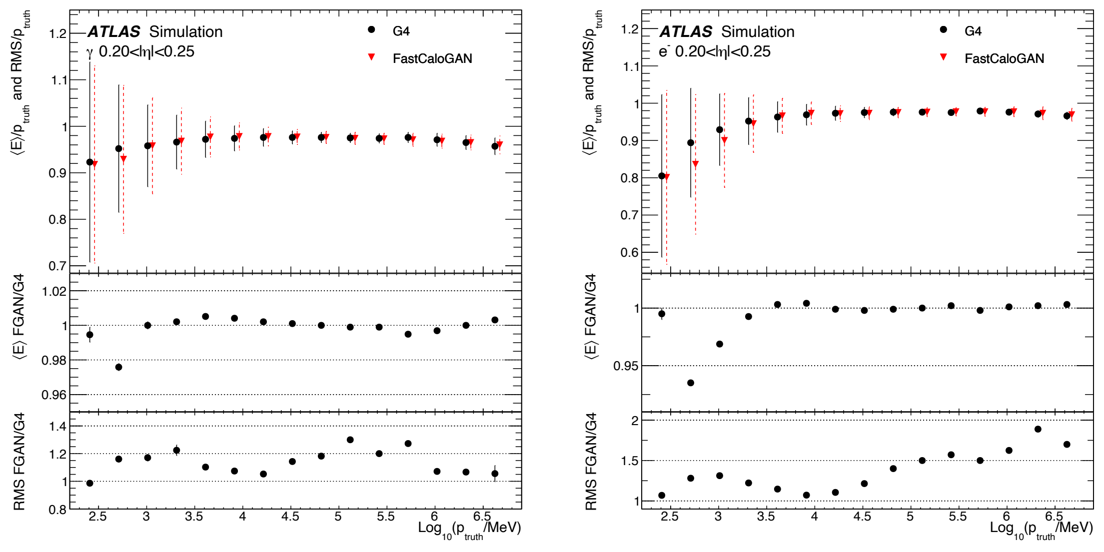

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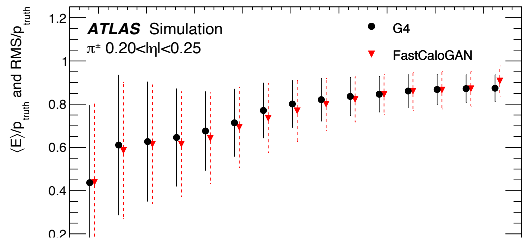

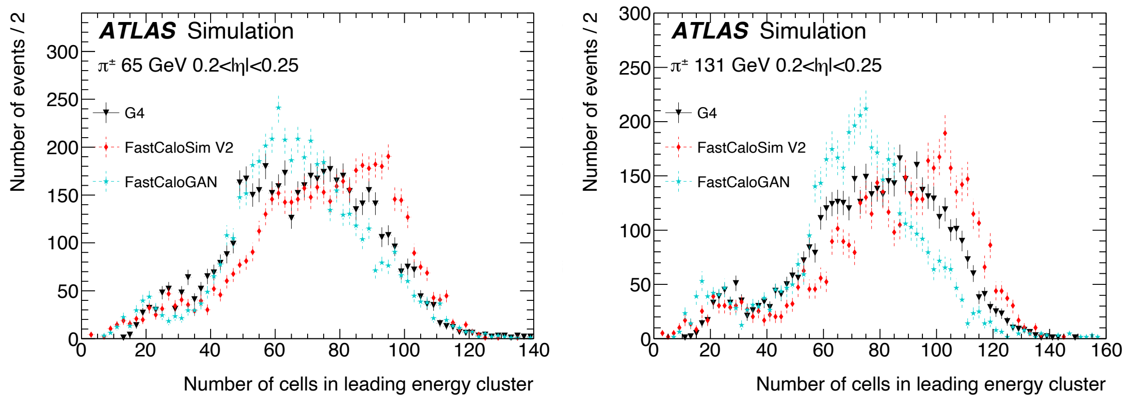

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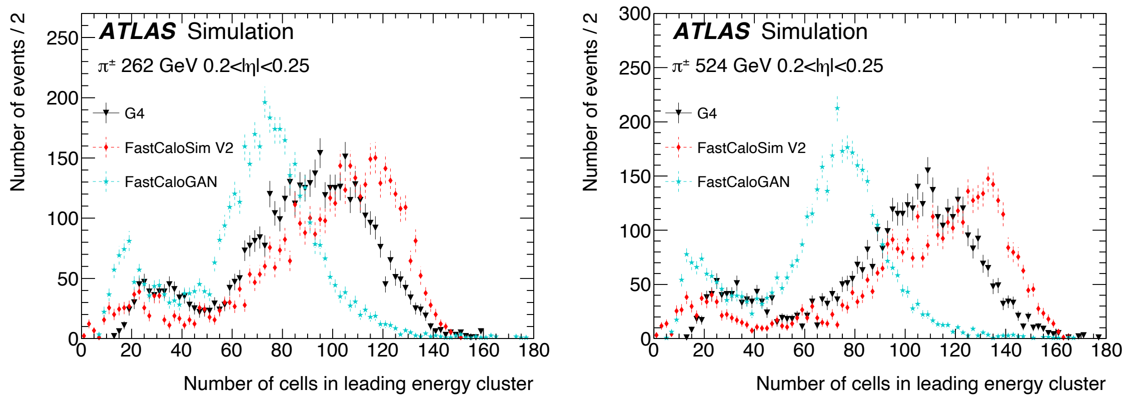

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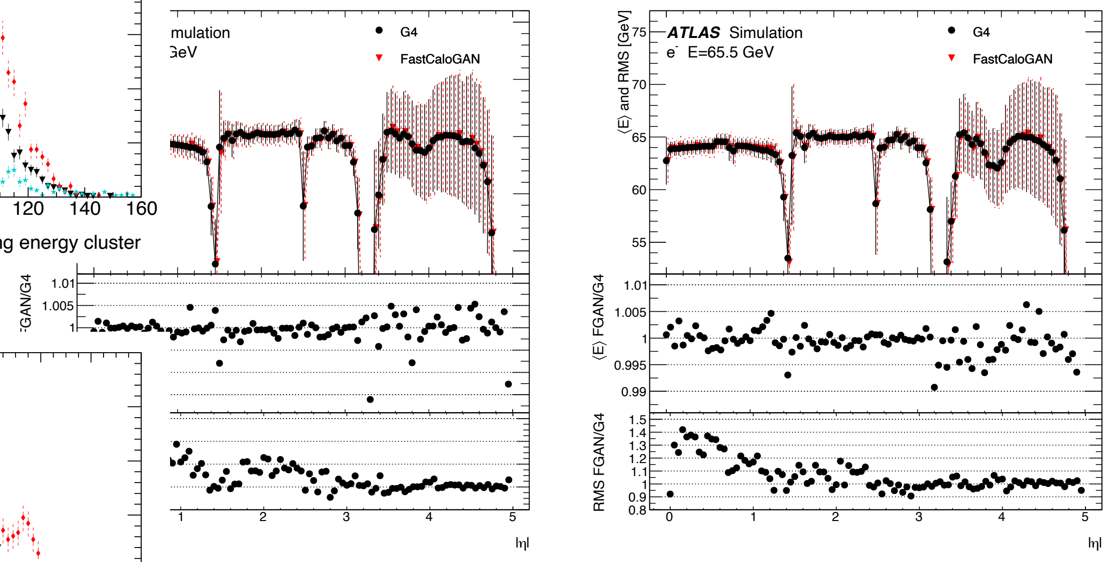

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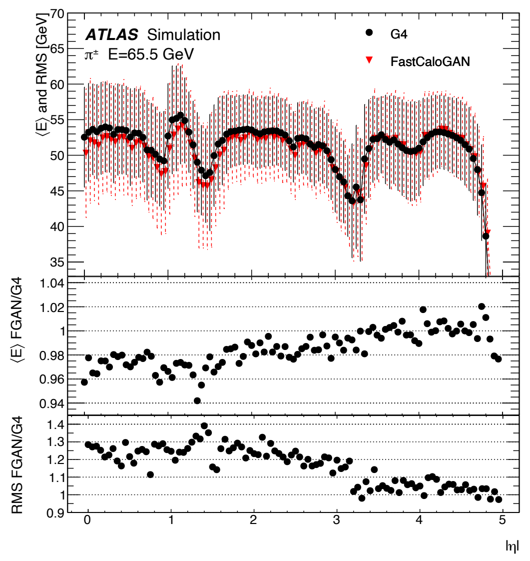
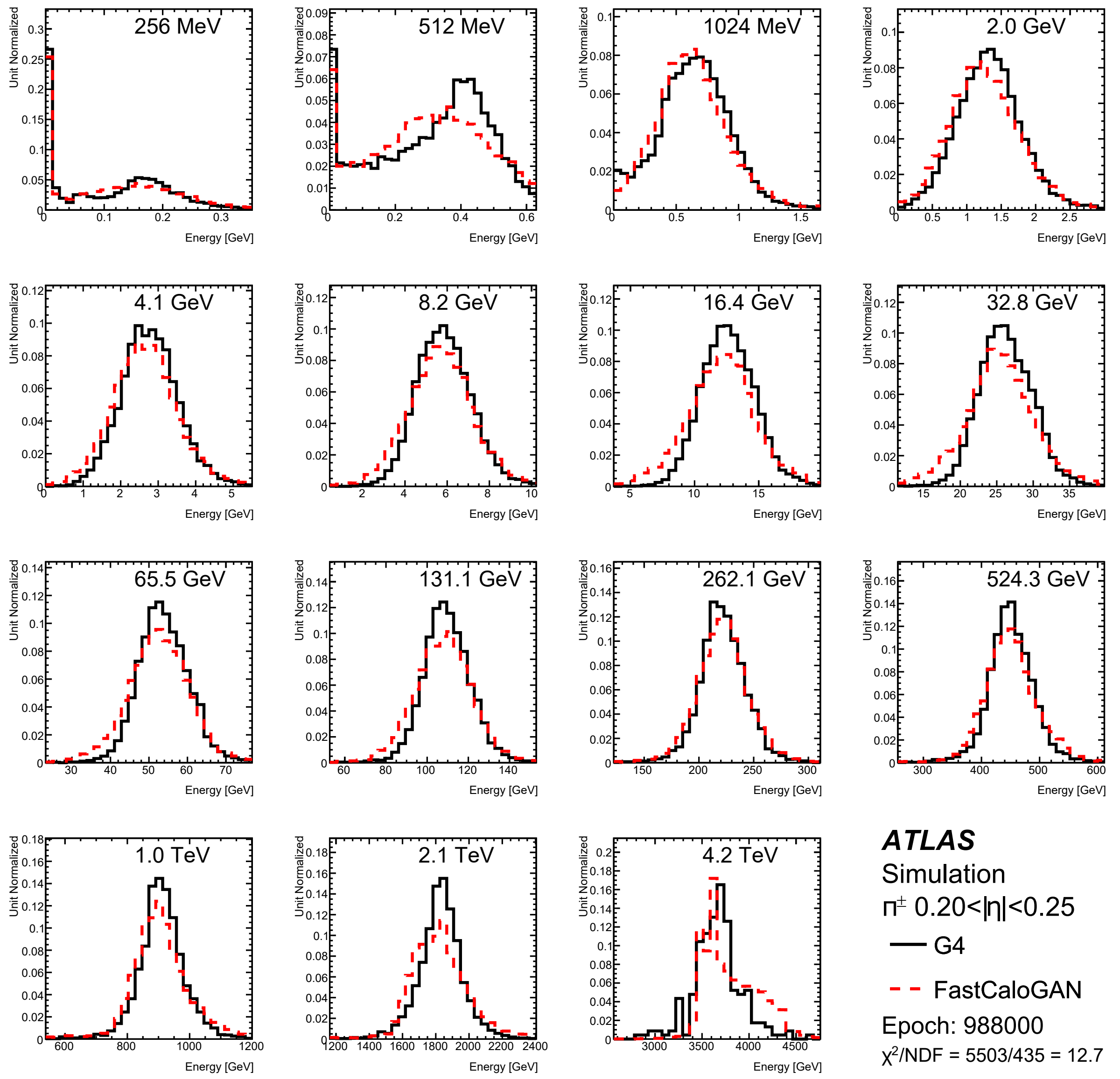
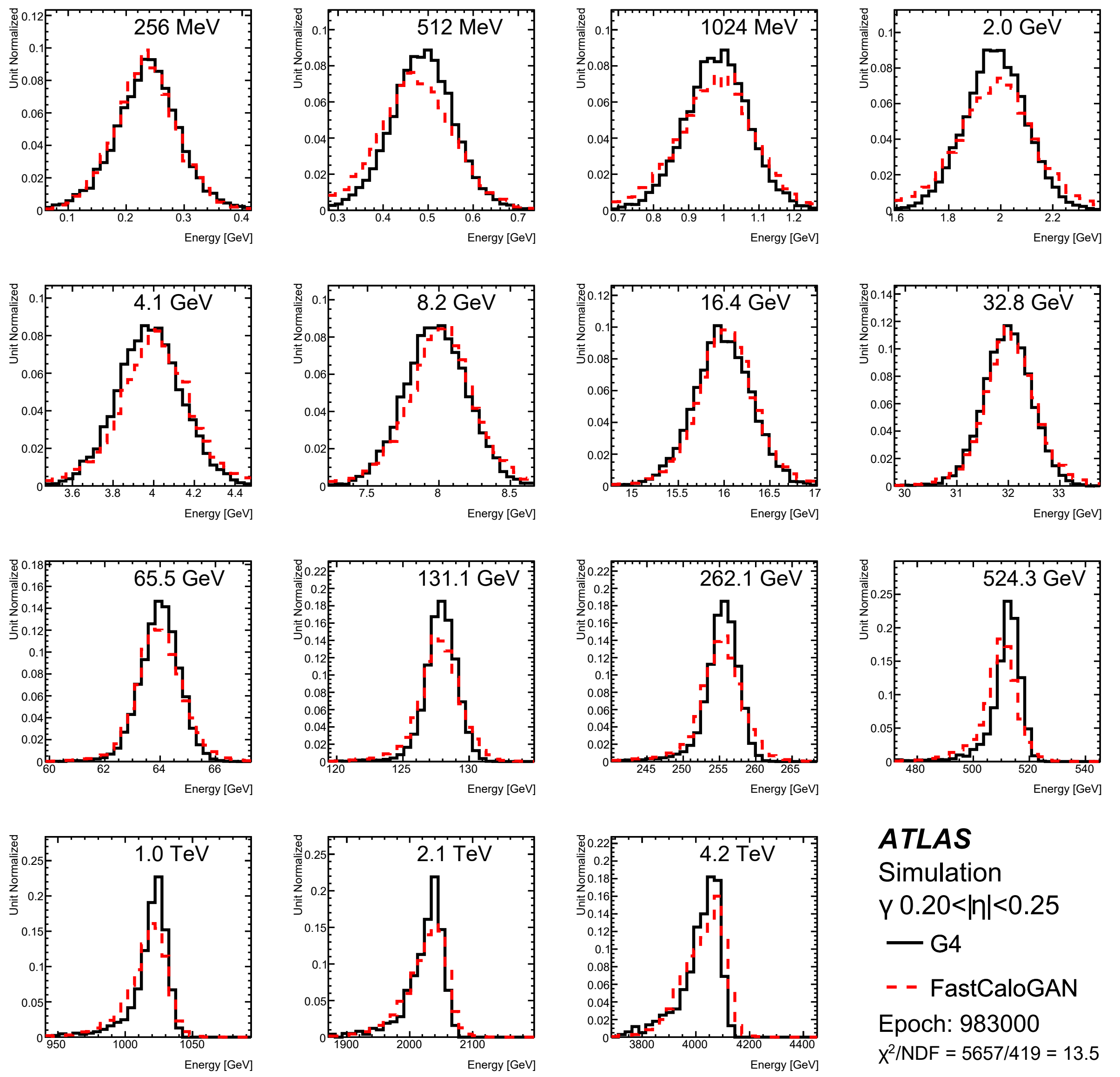
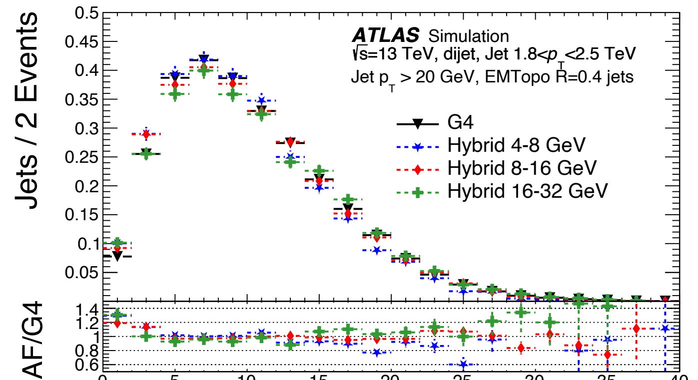
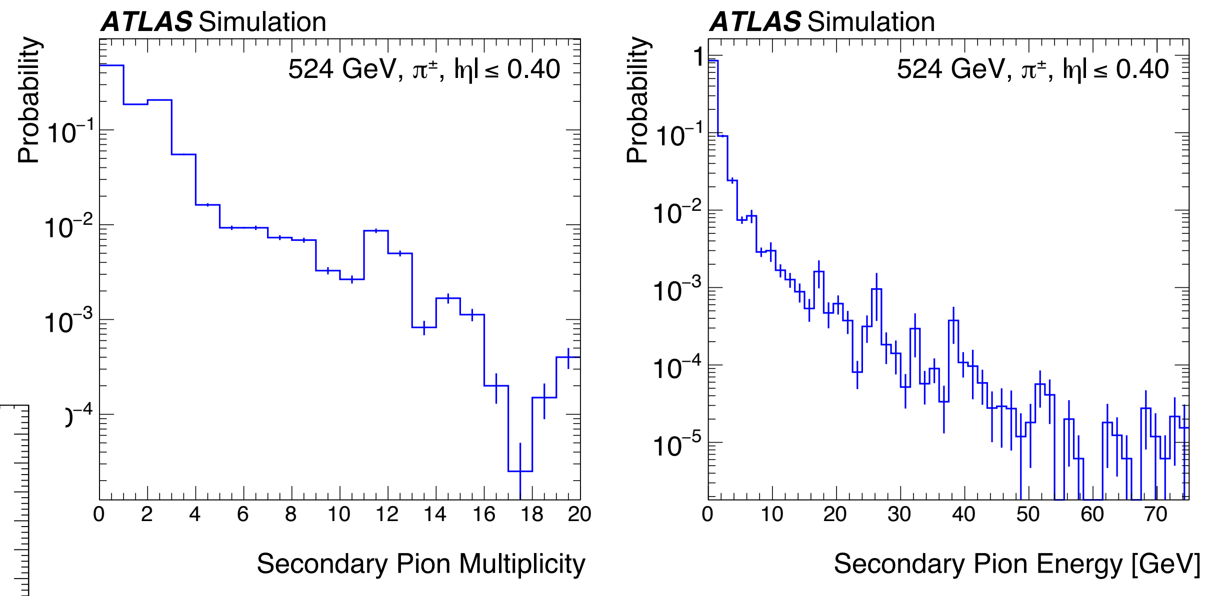


(c)









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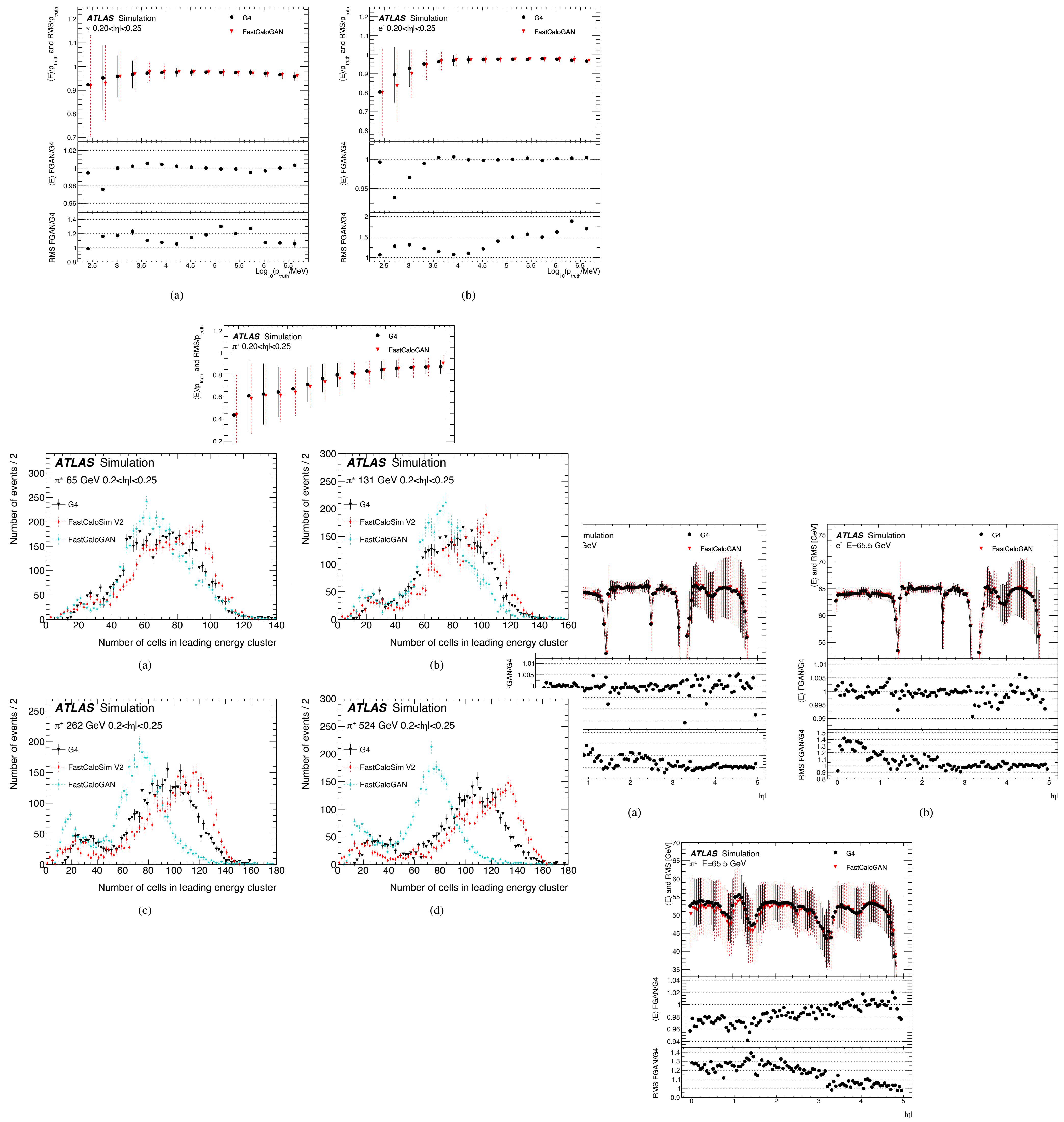

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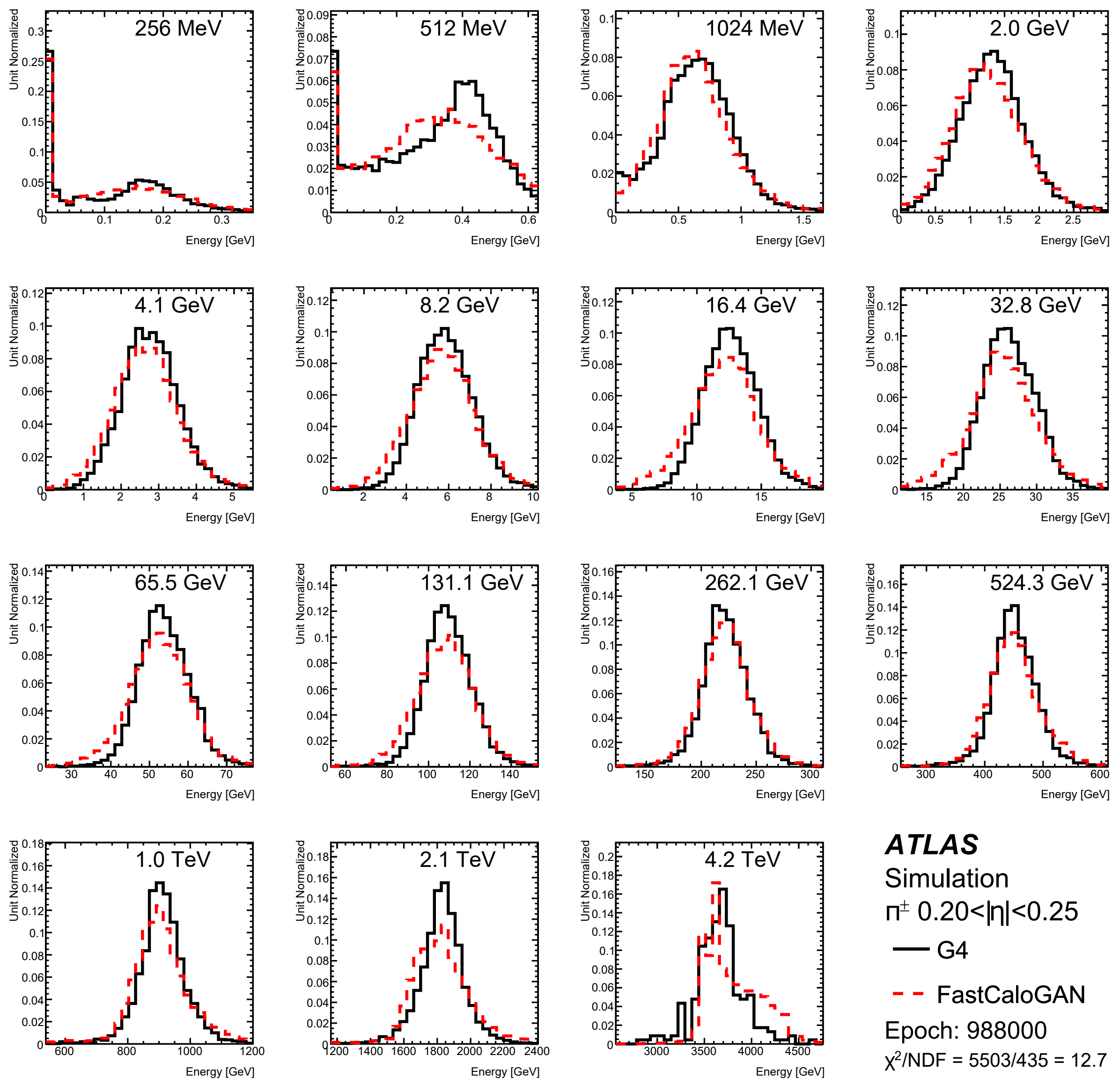

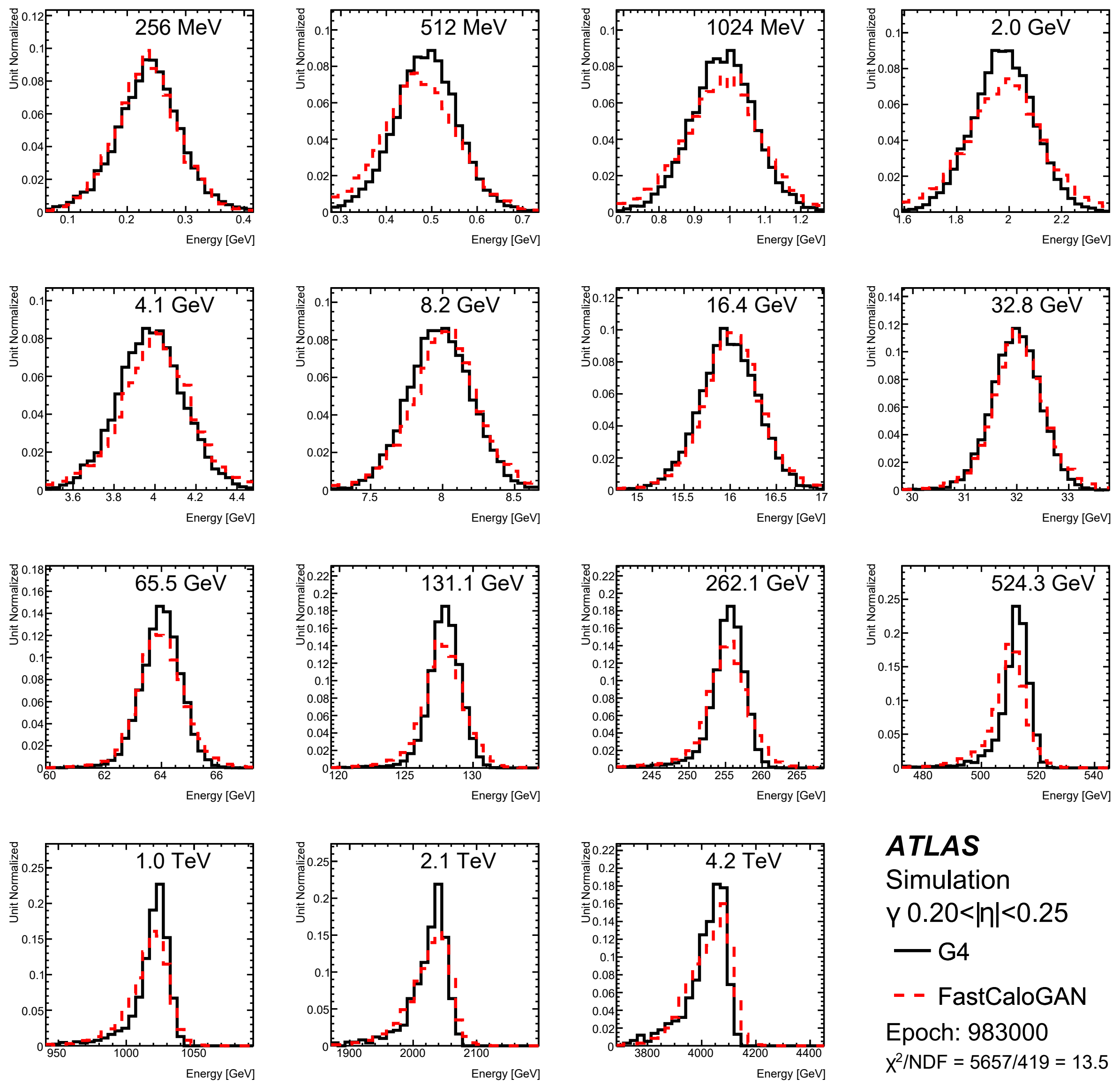

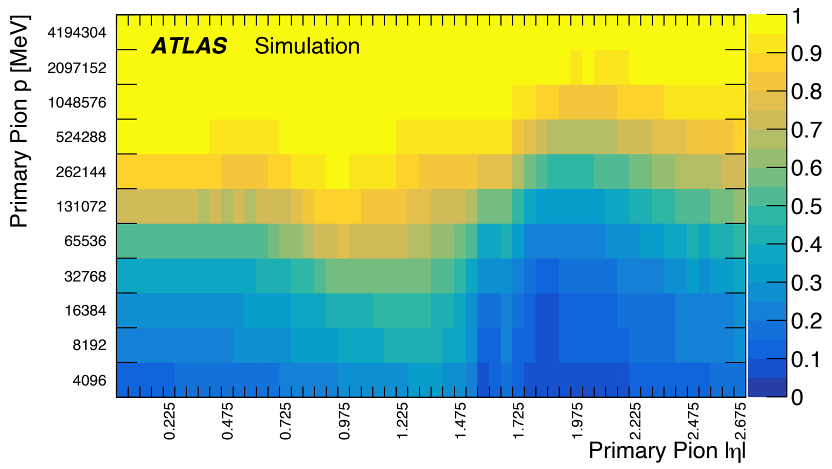

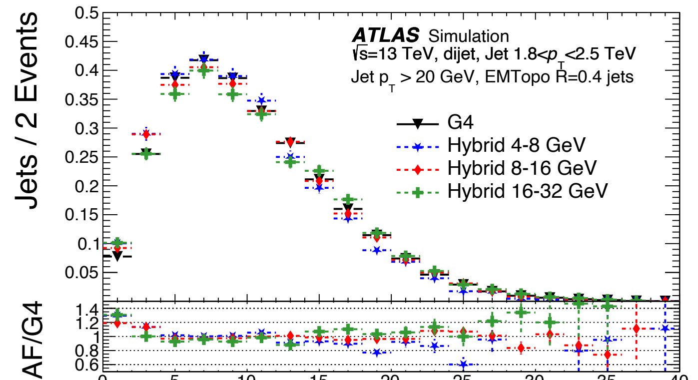

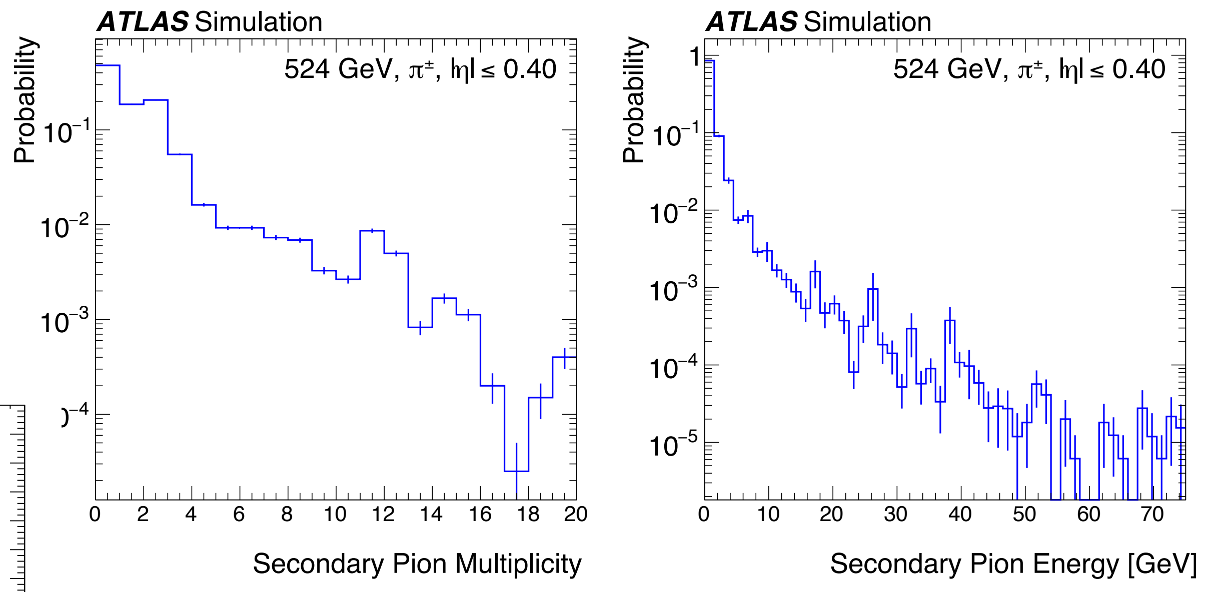

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Evaluating Fast Calo Simulators

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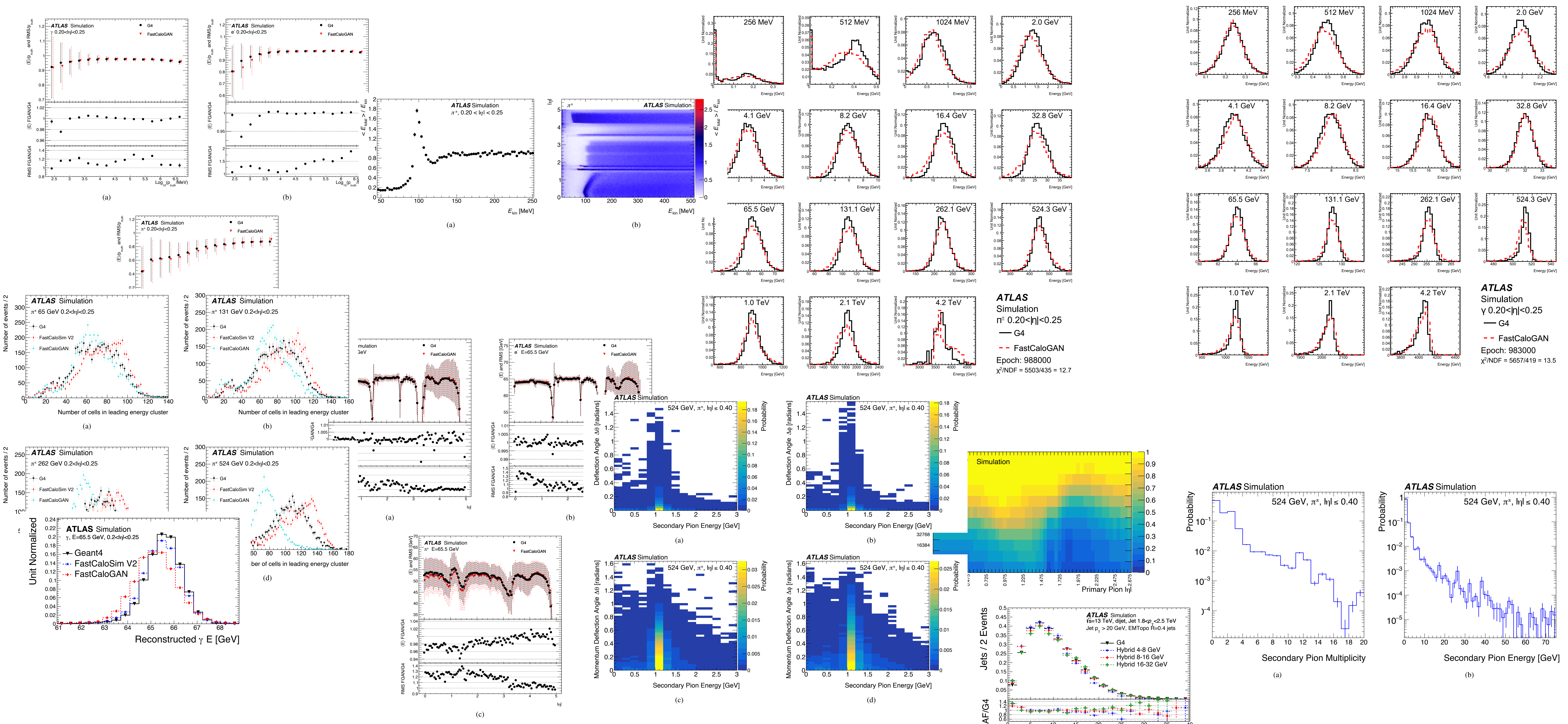

Can we automise the evaluation ?

Krause and Shih, 2021

5.4 Classifier metrics

In much of the GAN literature (see e.g. [8]), a common metric is to train classifiers to distinguish between different categories of data (e.g. e^+ vs. π^+), and to see if there is any difference in classifier performance when real data and generated data are interchanged. For example, one might train a classifier on e^+ vs. π^+ GEANT4 images, and compare this to a classifier trained on e^+ vs. π^+ GAN images. If the classifier trained on real images performs similarly to the classifier trained on generated images, then this is evidence that the generated images are approximating the real images well. One can repeat this test for different combinations of real and generated data.

The ultimate test of whether $p_{\text{generated}}(x) = p_{\text{data}}(x)$ would be a direct binary classifier between real and generated images of the *same* type. If the generated and true probability

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Classify Geant4 vs generated and use AUC as single metric

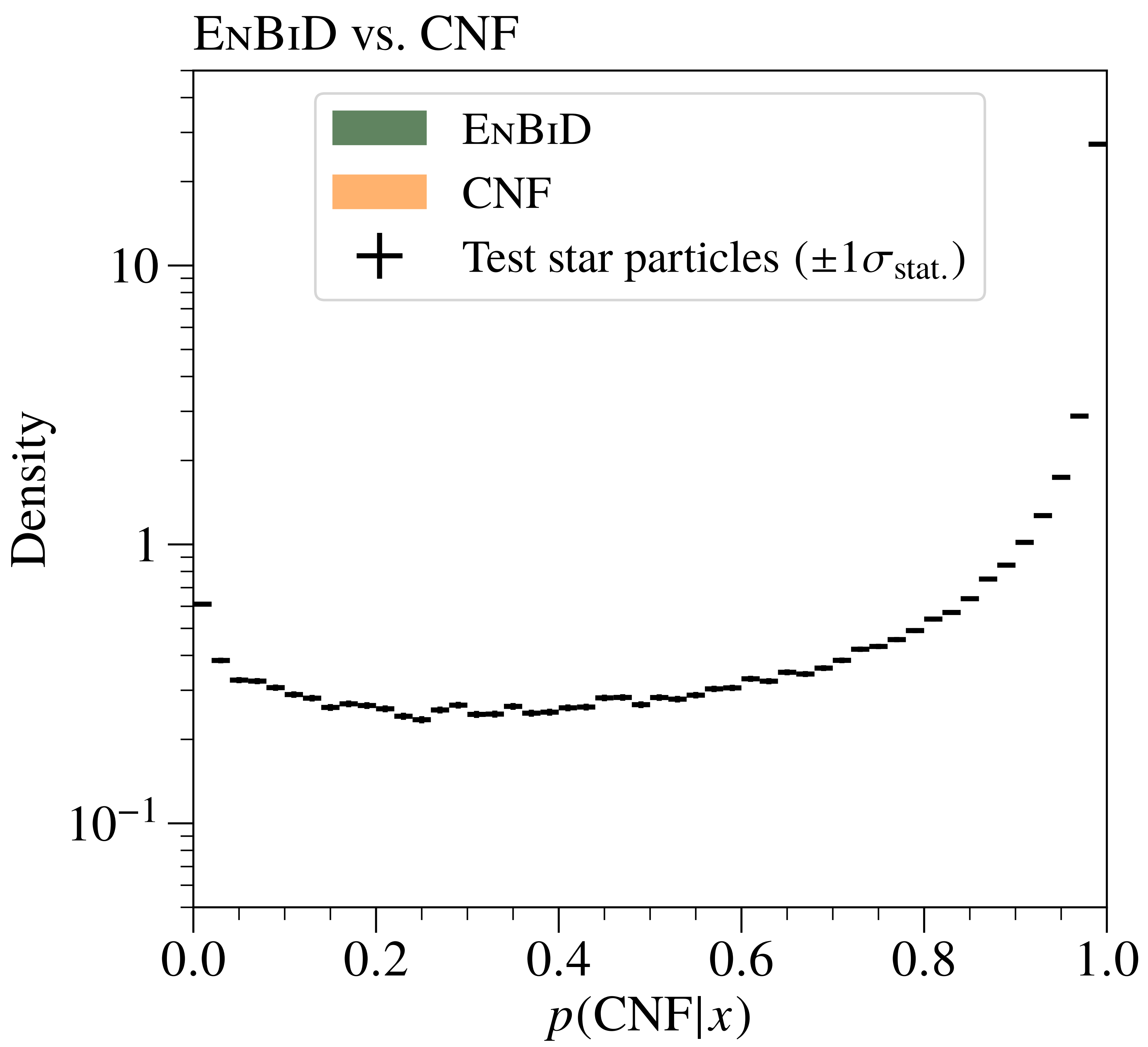
But not the end of the story..

Another classifier test

Lim et al, 2022

Compare two generative models:

Classify generative model1 vs model2, check if test dataset agrees better with one or the other



A comparison of metrics

Kansal et al, 2022

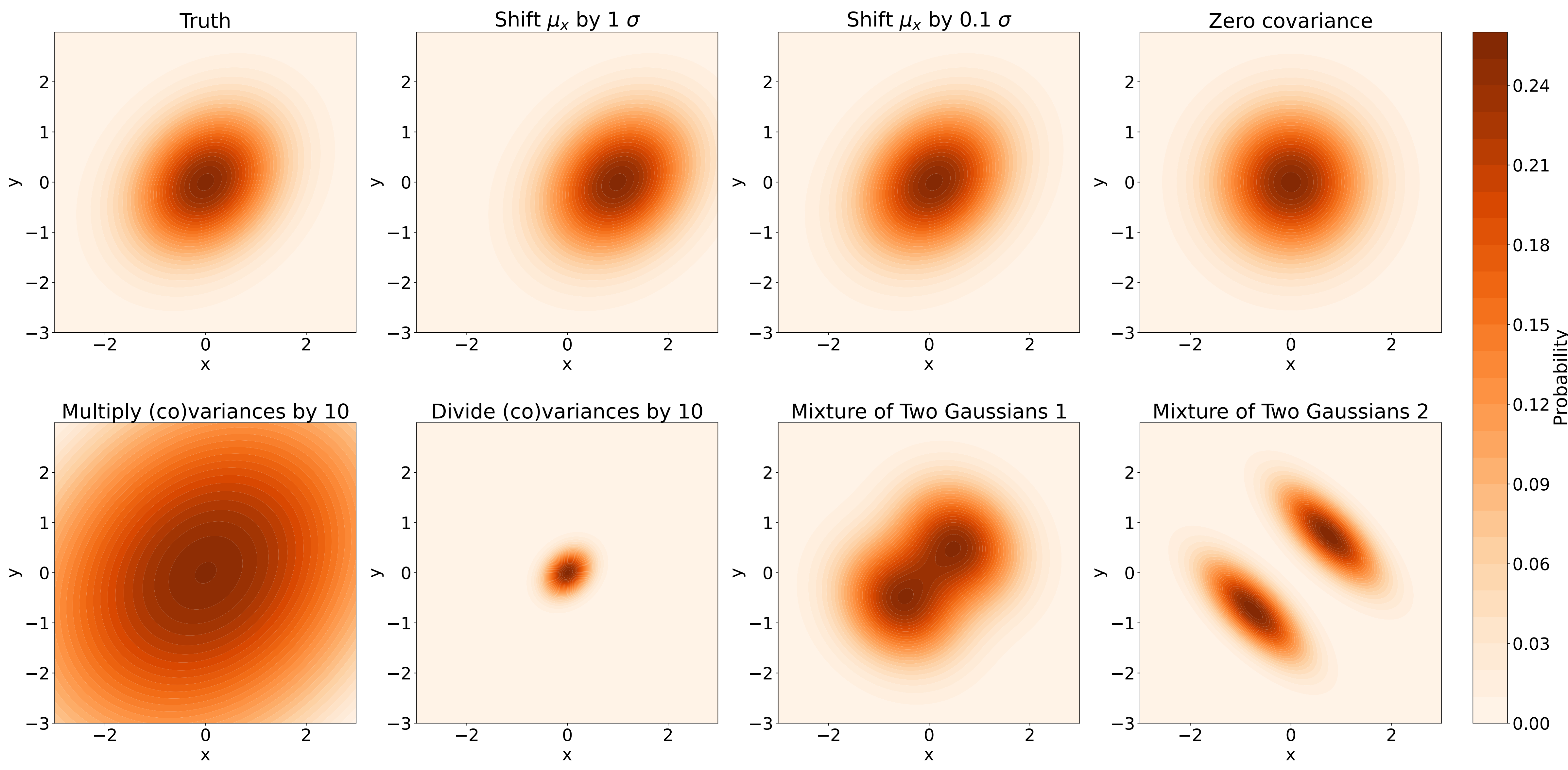
On the Evaluation of Generative Models in High Energy Physics

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

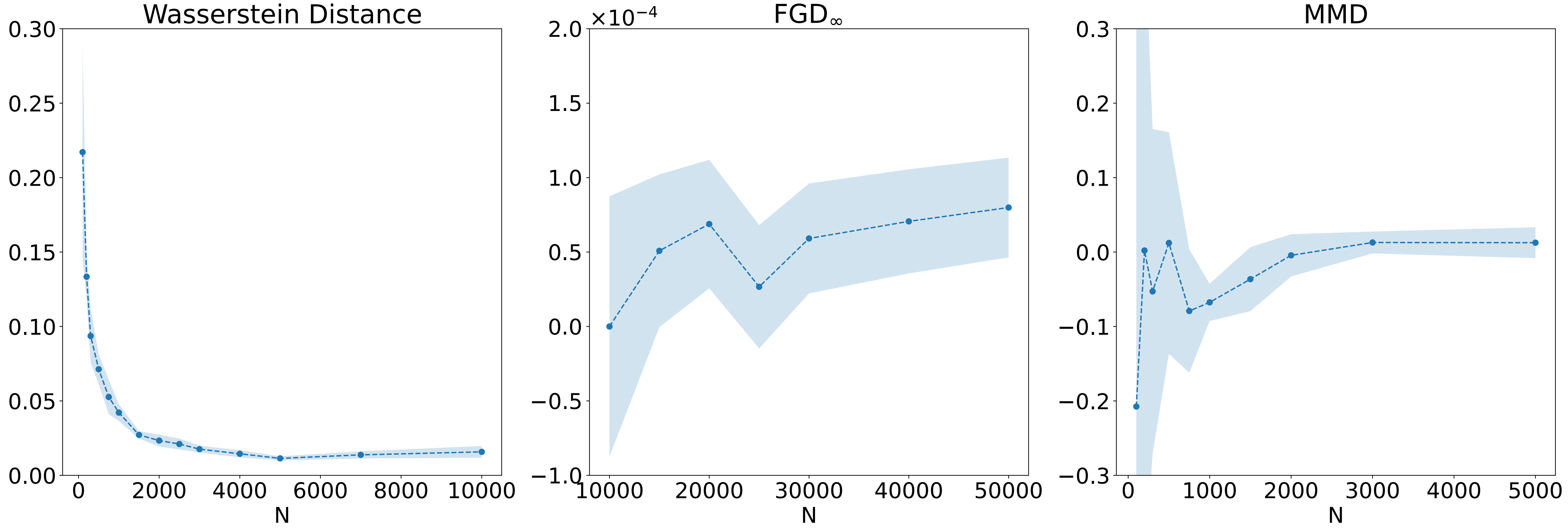
Breno Orzari, Thiago Tomei
Universidade Estadual Paulista, São Paulo/SP, CEP 01049-010, Brazil

(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	$\mathbf{0.036 \pm 0.003}$	$\mathbf{0.191 \pm 0.005}$
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_∞ promising but no sensitivity to higher moments, requires extrapolation

Jet Study

Kansal et al, 2022

Metric	Truth	Smeared	Shifted	Removing tail	Particle features smeared	Particle η^{rel} smeared	Particle $p_{\mathrm{T}}^{\mathrm{rel}}$ smeared	Particle $p_{\mathrm{T}}^{\mathrm{rel}}$ 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 !

Jet Study

Does this convince us to stop looking at plots ?

1D Histograms, 2D correlations, … *oh but did you look at that plot ?*

What would we ideally want ?
(Open Problem)

- Metric that let’s us quickly compare generative models, meaningful numbers (does not saturate quickly)
- Reproducible and stable, comparable between different studies
- Insensitive to irrelevant numerical differences eg. Discrete output models
- Robust to simple transformation of input ? Expect it to be sensitive to eg. log transformations
- If we truly had a “single ultimate metric”, could we use it as a loss function / automated HPO ? Would metric still be meaningful ?

---

oh but did you look at that plot ? → oh but did you look at that metric for this E/η/ϕ ?

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<u>Realistic Target</u>

- Have O(5) metrics, that provide meaningful, orthogonal information about different aspects
  - Stats based: Metrics focused on tails, bulk, higher moments, lower moments, overfitting, interpolation
  - Physics info: energy modelling, pointing, substructure, shape, interpolation

oh but did you look at that plot ? → oh but did you look at that metric for this E/η/ϕ ?

- Back-port these ideas for **uncertainty quantification** of traditional simulators

Conclusion

- Uncertainties a central problem in experimental science, ML can help (but use mindfully!)
- Lots of room for novel ideas and innovative work
    - Multiple NPs, fast profiling
    - ML to improve quantification & mitigation of theory uncertainties
- Generative models: Metrics that capture specific range of properties worth exploring
    - What we develop could be back-ported to traditional simulation!

Thank you!

Data analysis strategy optimisation

- We want to select an analysis strategy with best final measurement performance
- Full statistical quantification of performance → Computationally expensive 'Profile Likelihood'
- But there's an old trick! If you've collapsed your high-dimensional data into a single observable, you can estimate your sensitivity with cheaper performance metrics:

http://proceedings.mlr.press/v42/cowa14.pdf

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Median Significance of Discovery
(Including uncertainties)

$$\mathrm{AMS}_1 = \sqrt{2\left((s+b)\ln\frac{s+b}{b_0} - s - b + b_0\right) + \frac{(b-b_0)^2}{{\sigma_\mathrm{b}}^2}},$$

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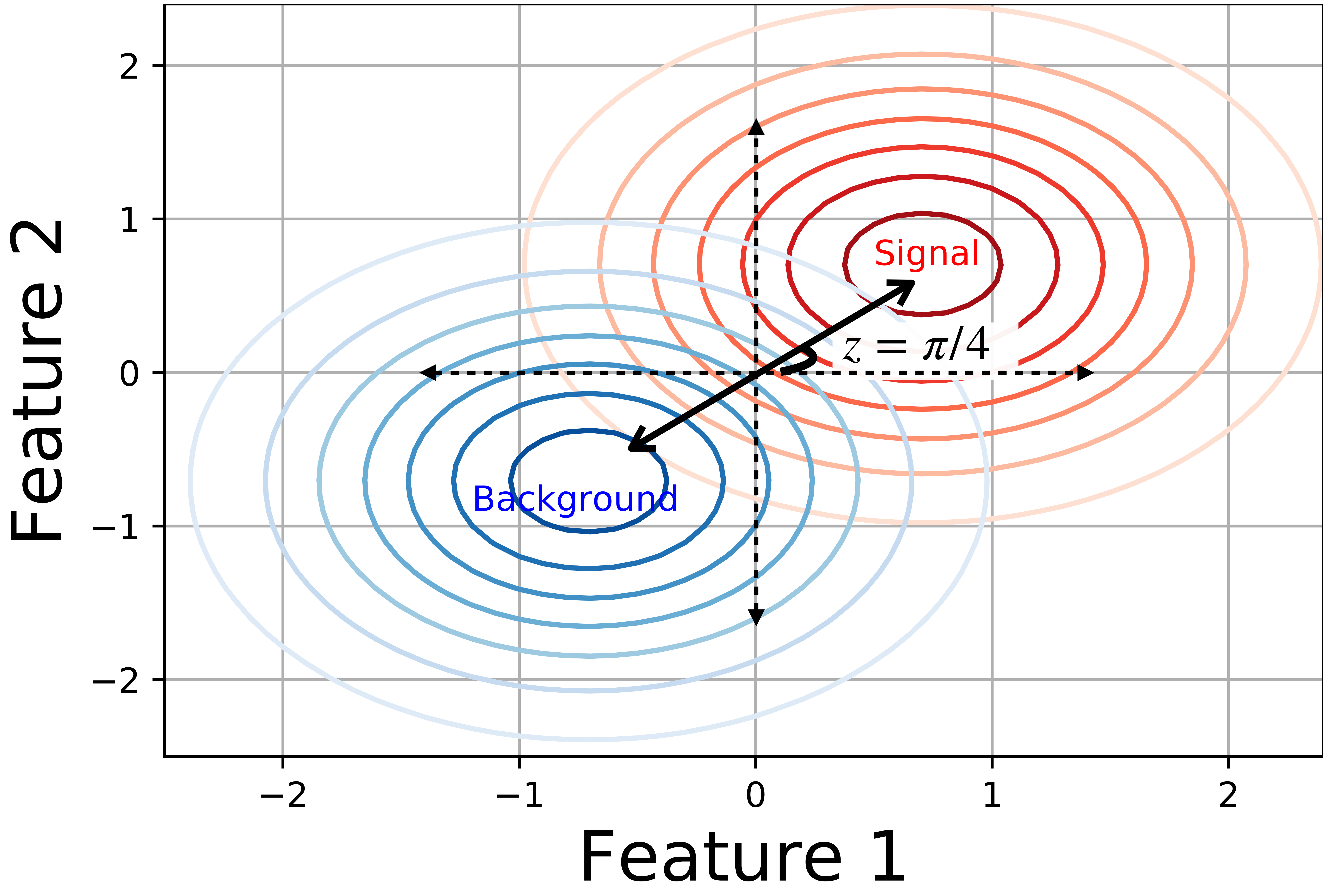
Toy Problem Definition



$$\mu = \frac{N_{s,obs}}{N_{s,exp}}$$

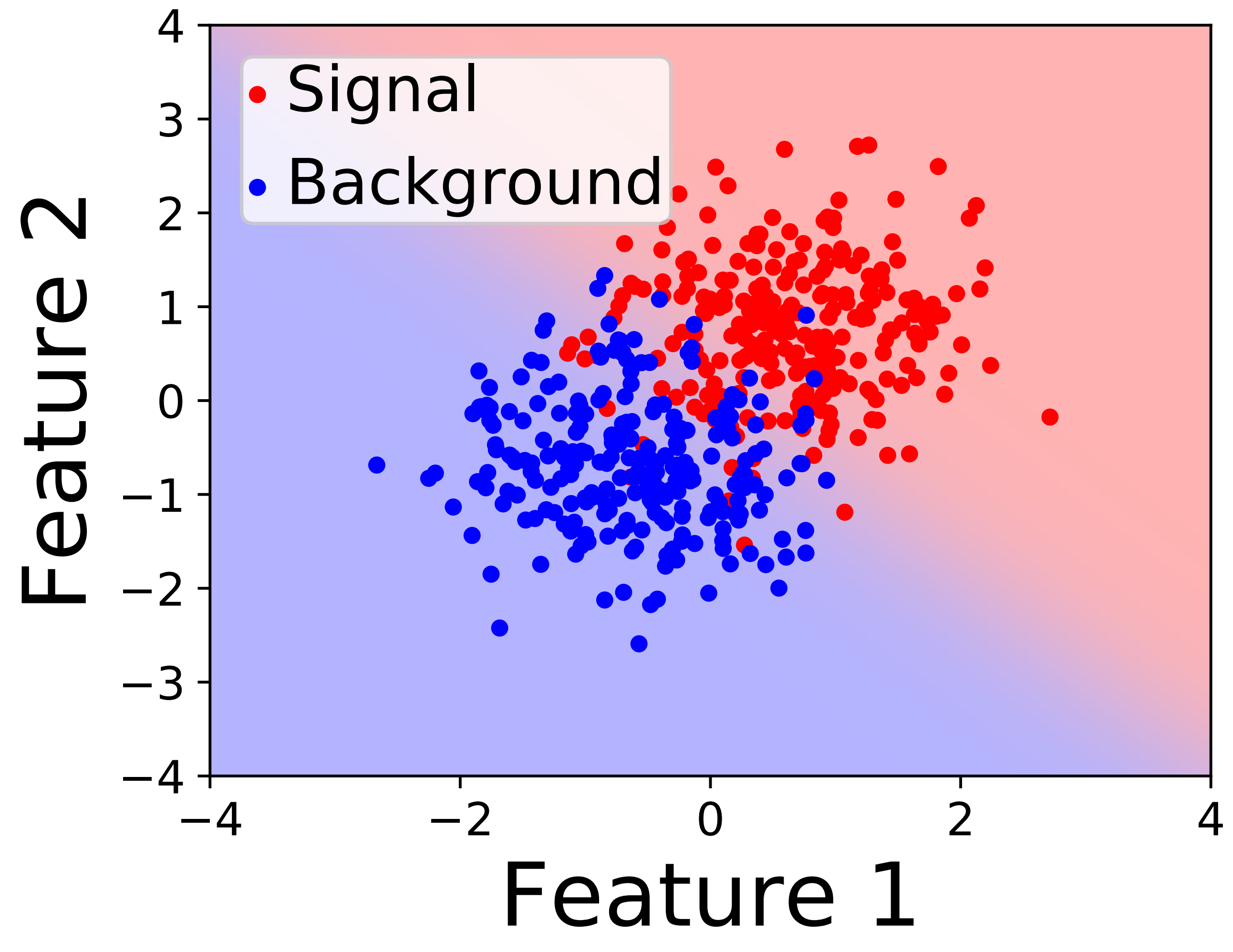
z = Angle

Nominal and Systematic Up Examples

Baseline Classifier

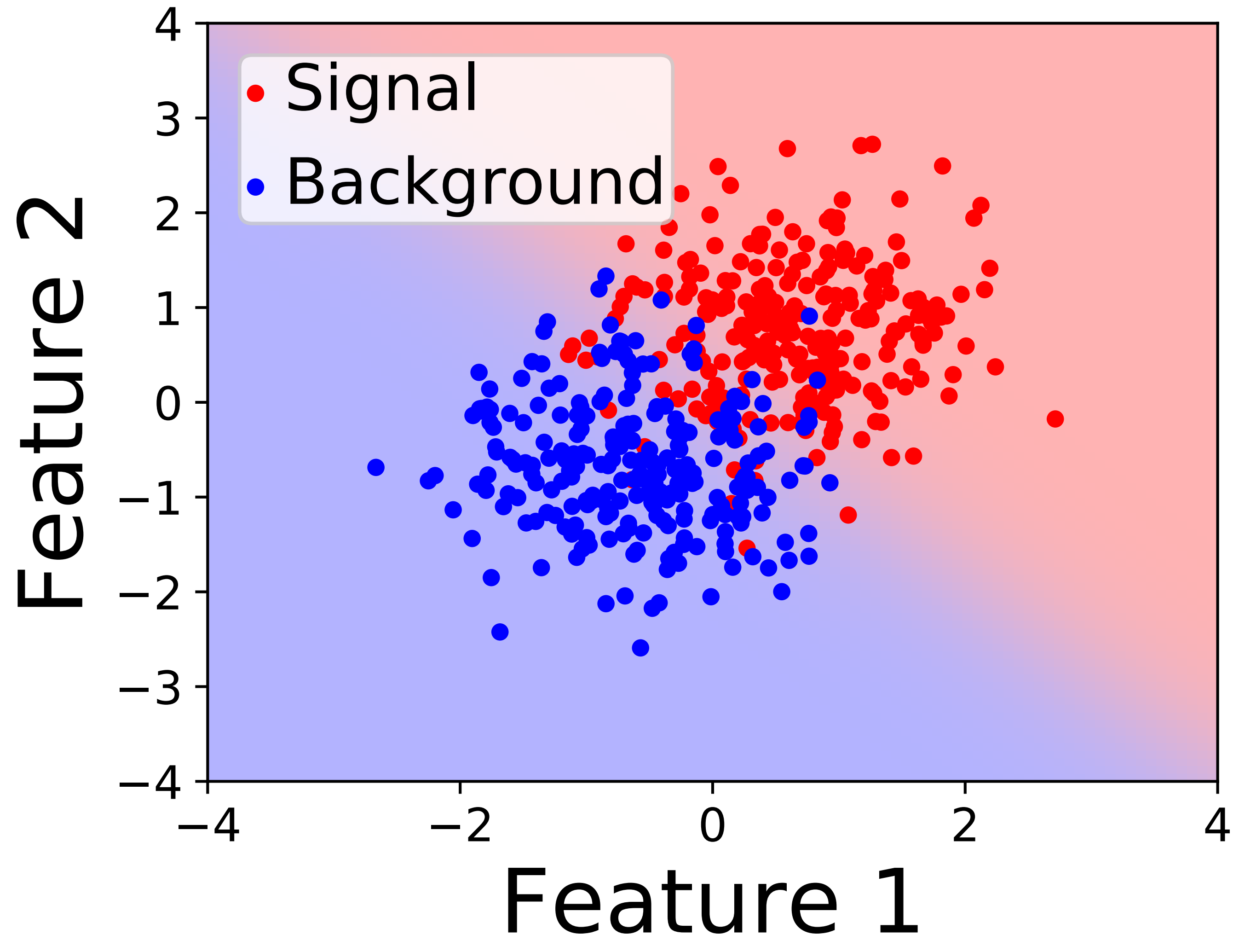
Uncertainty-Aware Classifier

Nominal "Data"



AUC=0.978

Optimal



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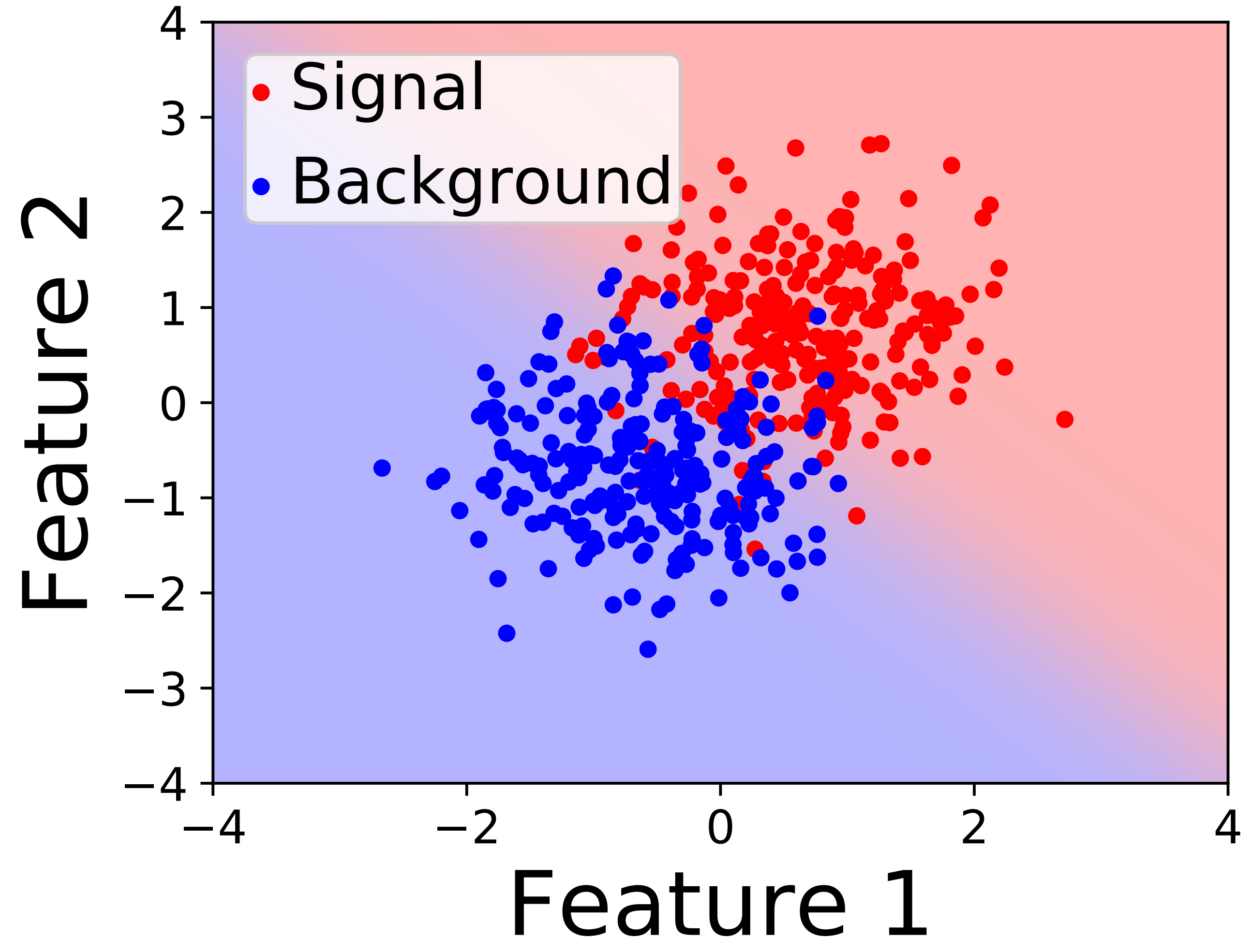
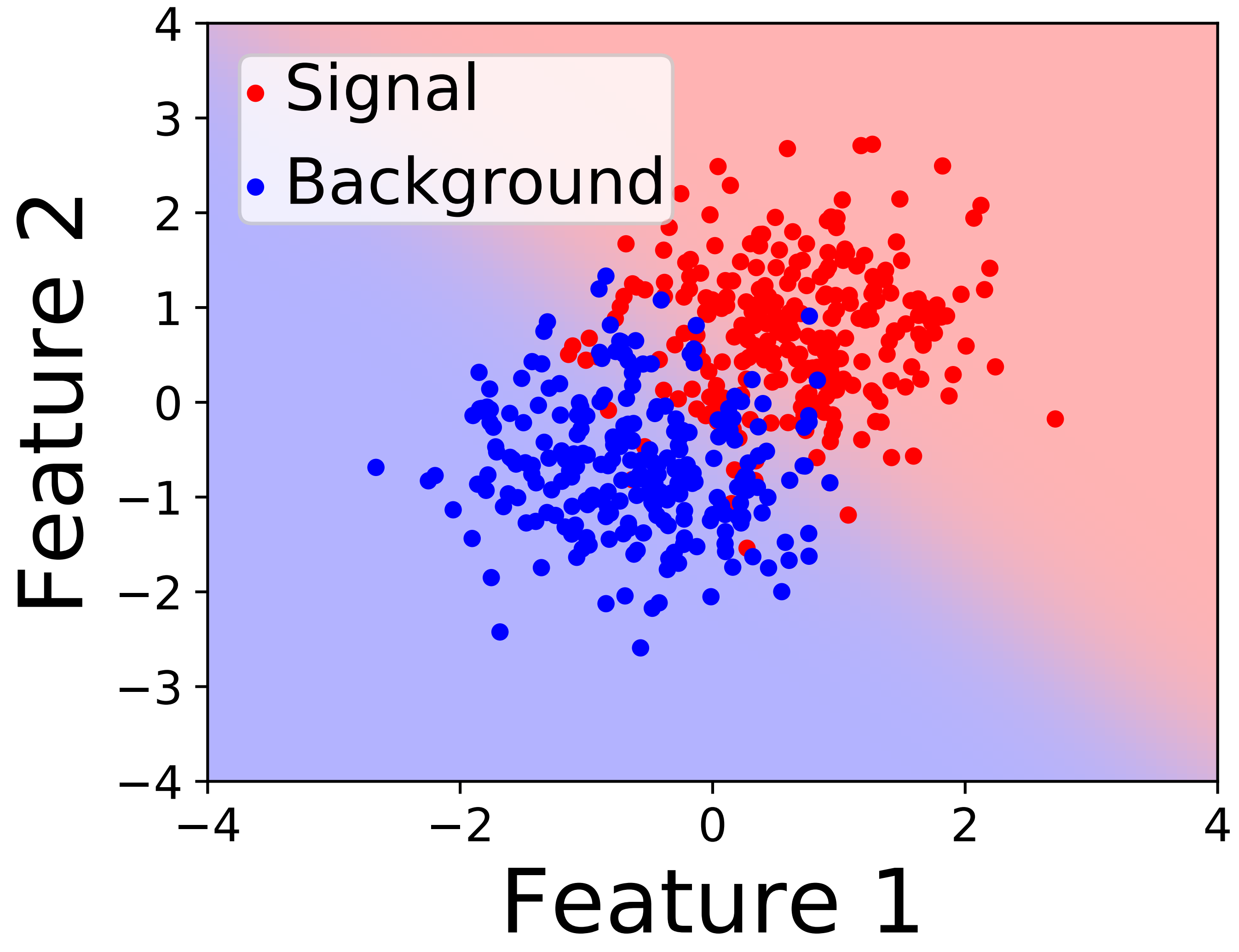
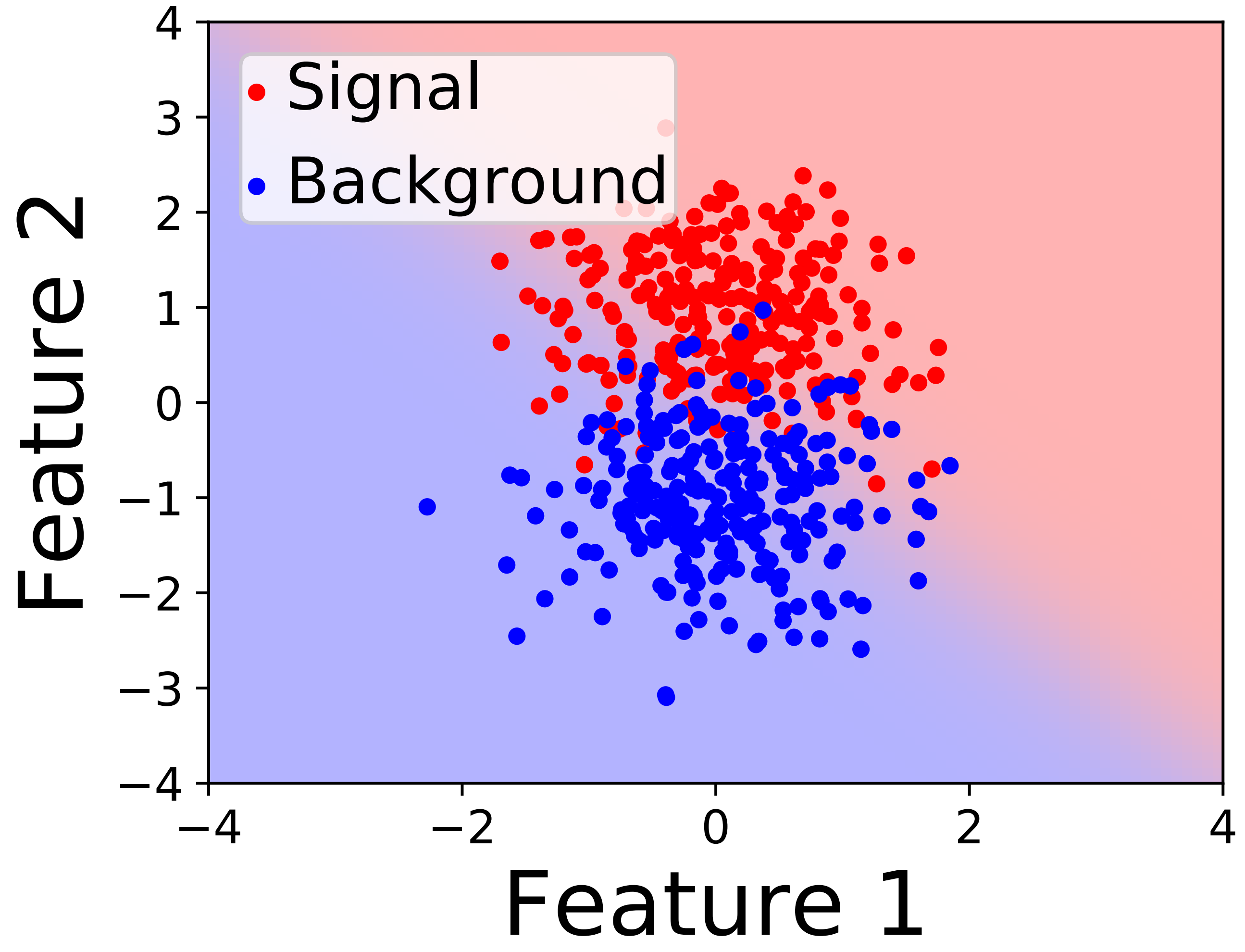
Optimal

SystUp "Data"

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**		

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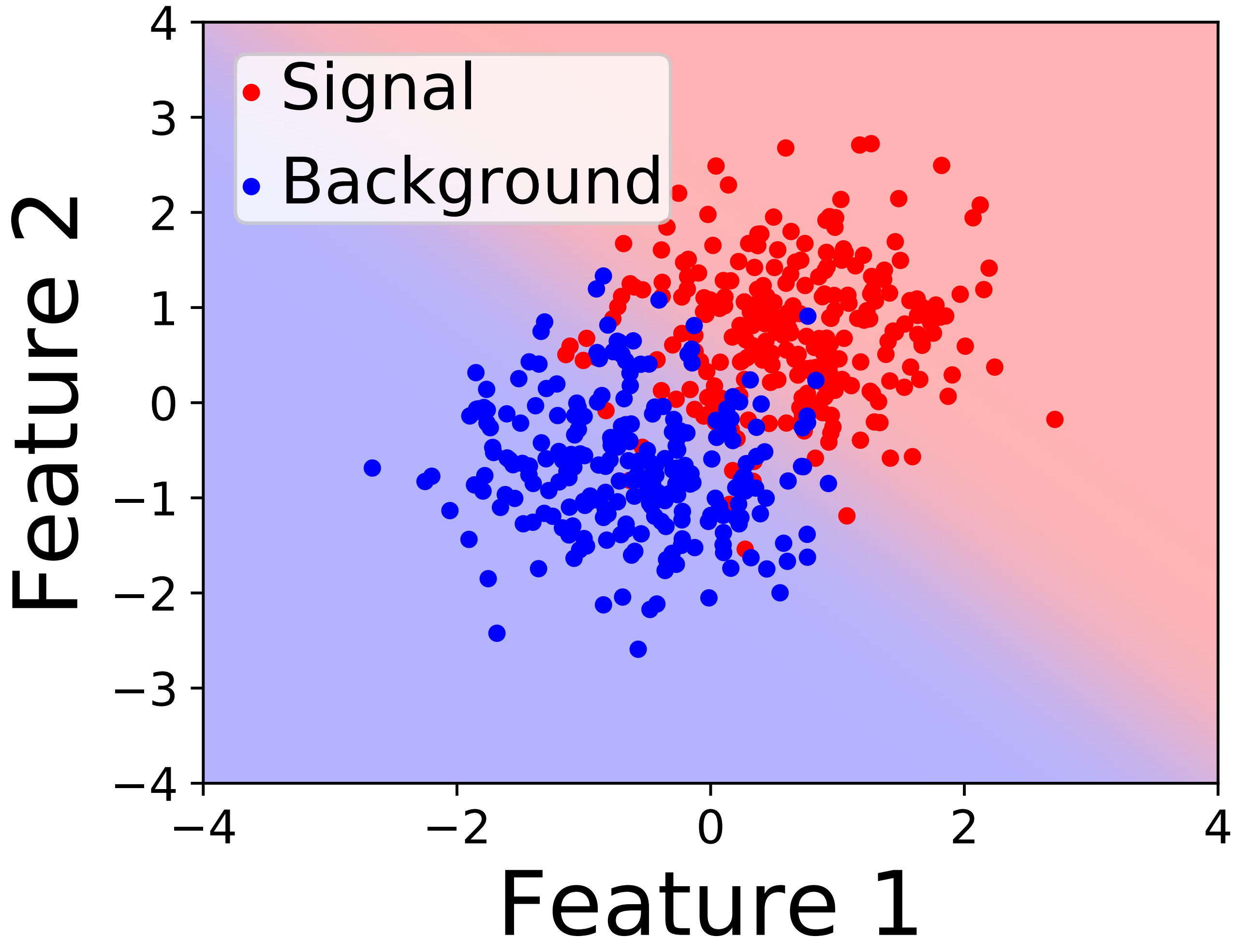

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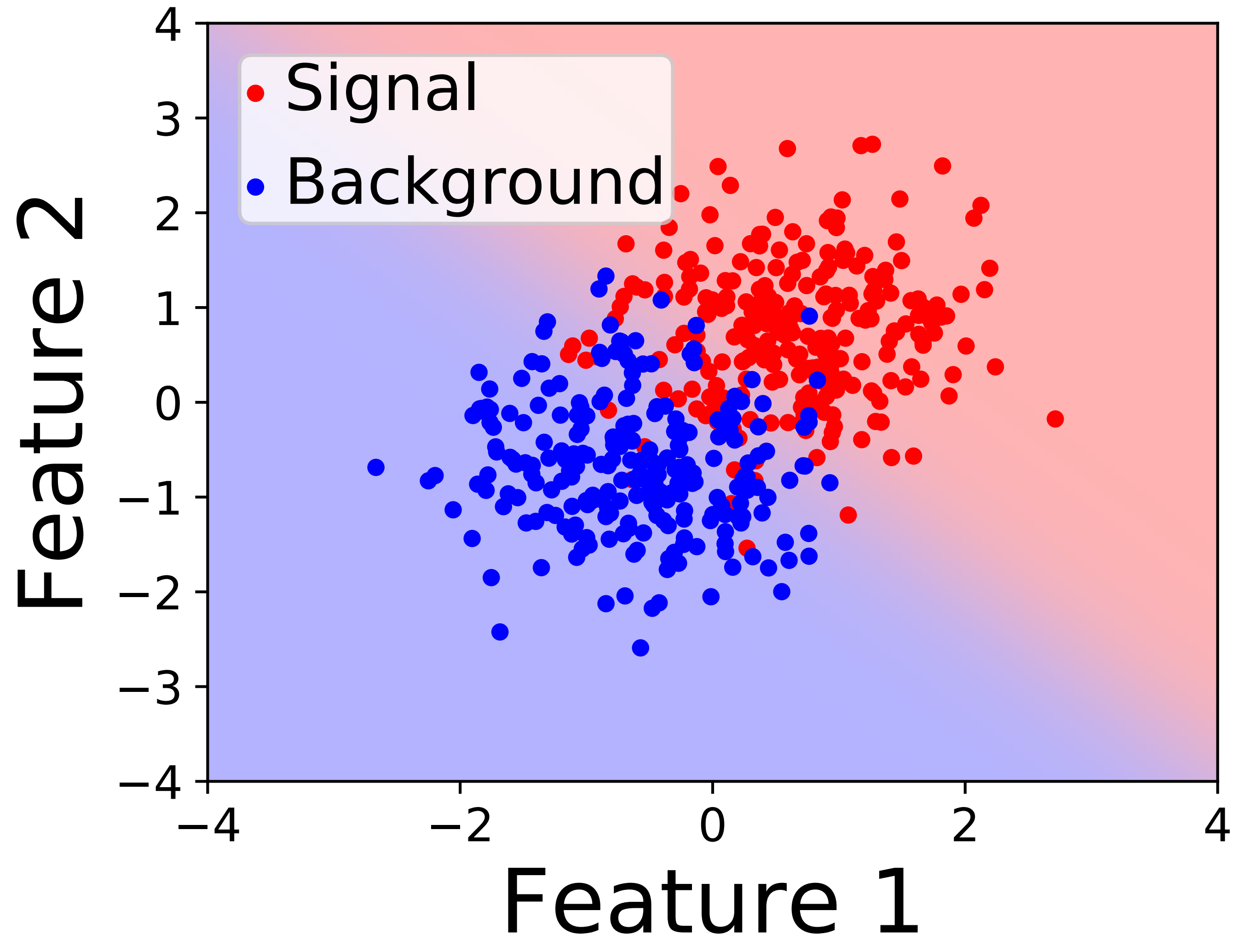

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Optimal

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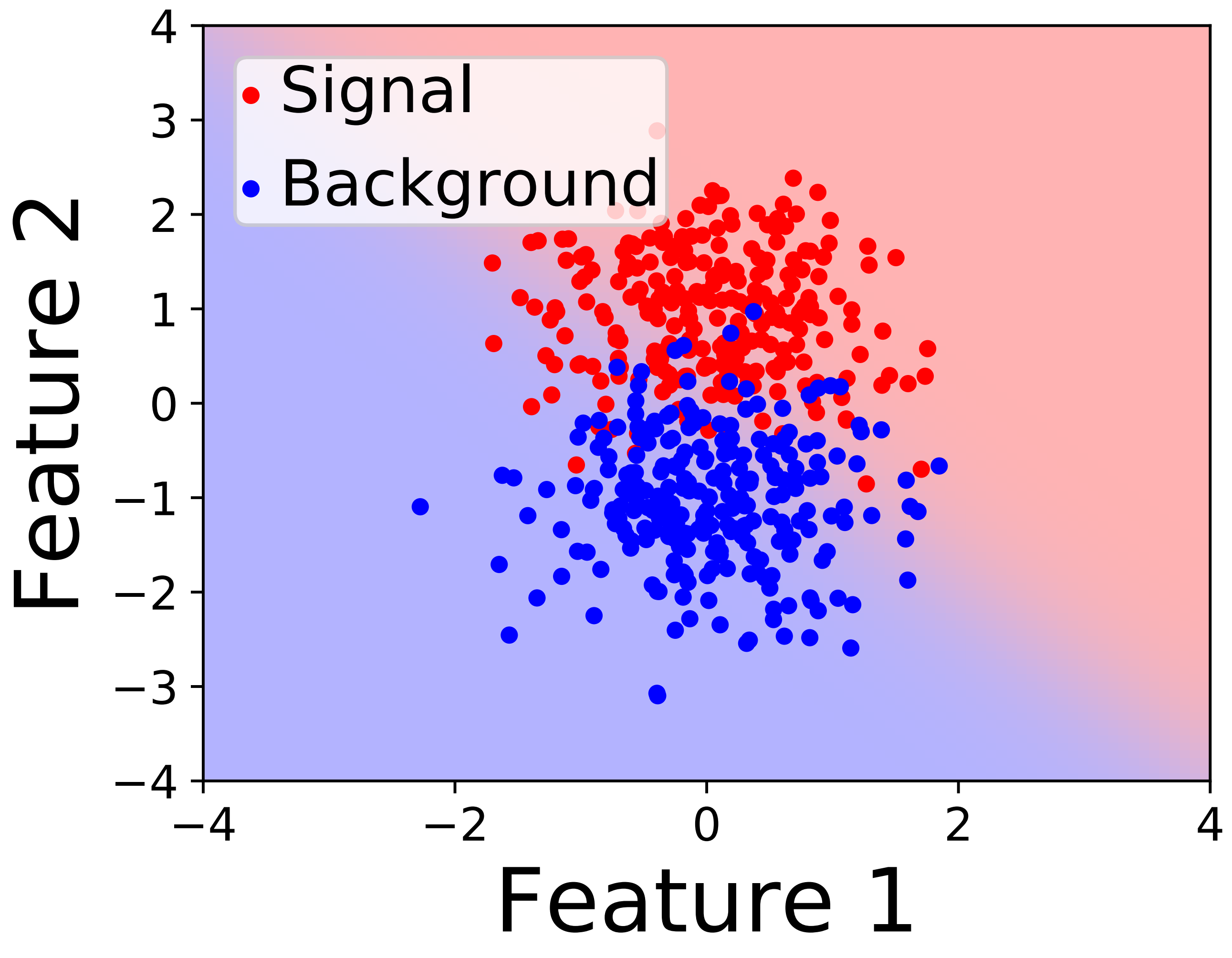
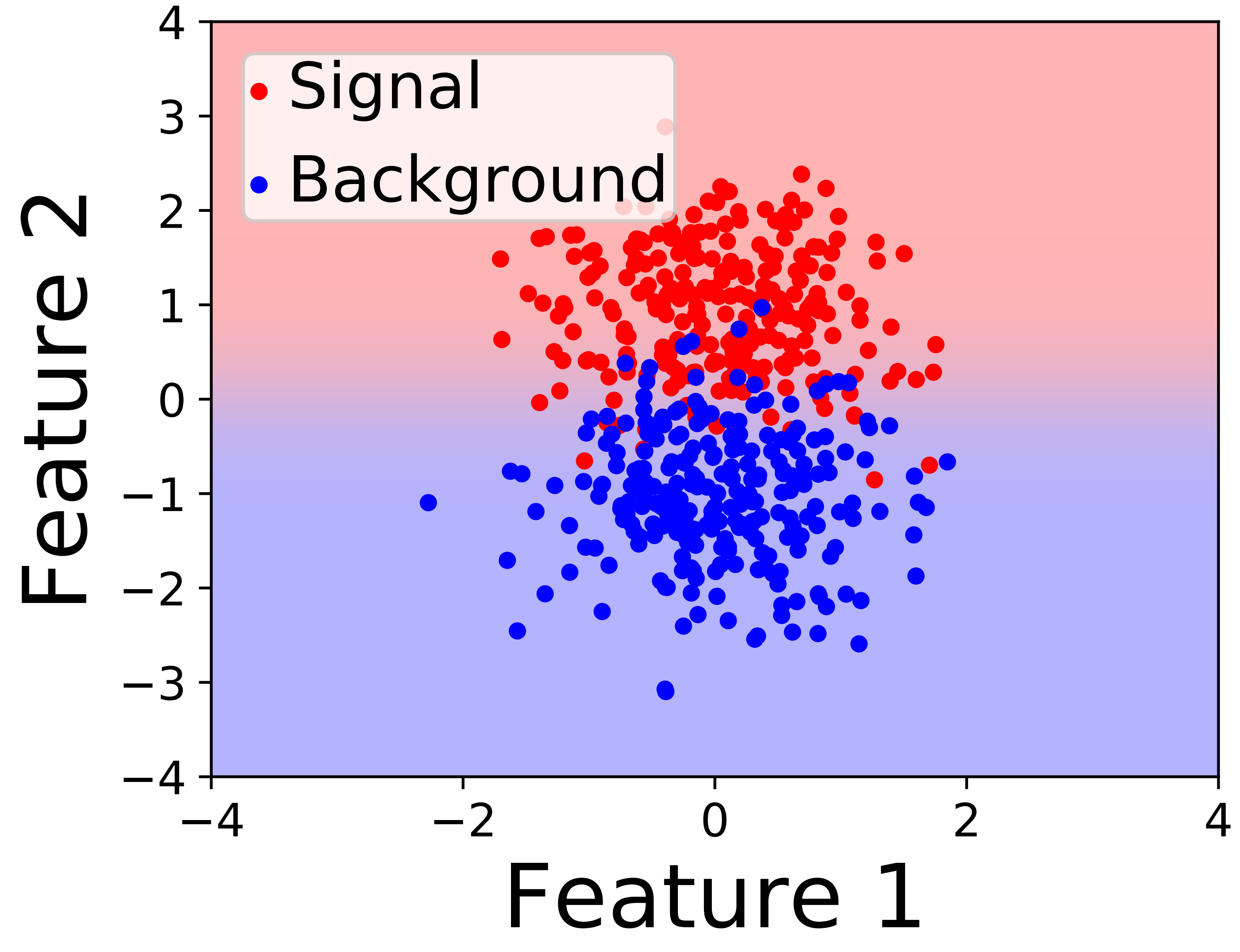


AUC=0.924

Sub-Optimal



AUC=0.978

Optimal

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

Profile Likelihood

Standard method of including the systematic uncertainty into the likelihood computation

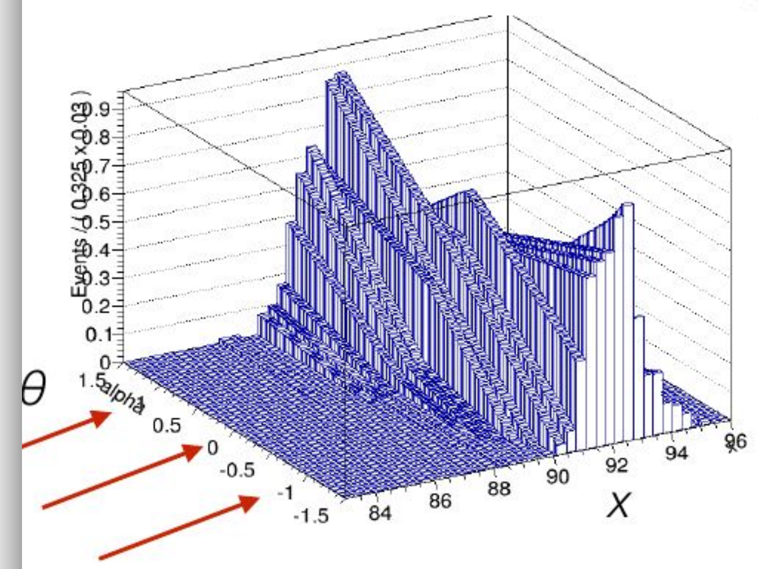
We simply make the selection/observable a function of z

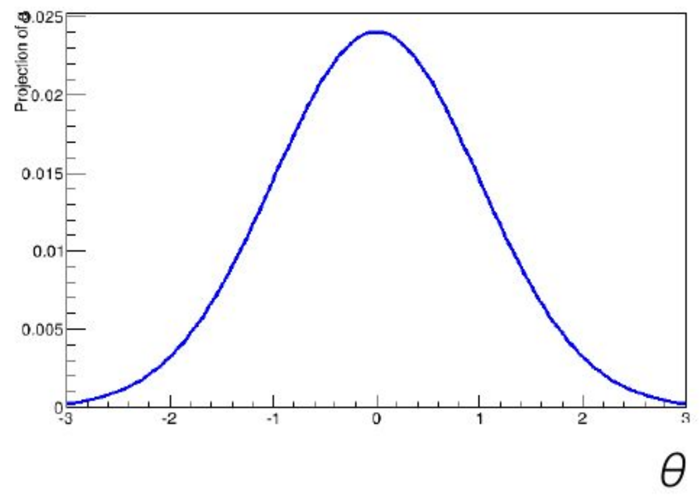
In principle could also be done in cut-based analysis: make cut a continuous function of z

The Profile Likelihood approach

- The profile likelihood is a way to include **systematic uncertainties in the likelihood**
  - systematics included as "***constrained***" **nuisance parameters**
  - the idea behind is that systematic uncertainties on the measurement of μ come from ***imperfect knowledge*** of parameters of the model (S and B prediction)
    - still *some knowledge* is implied: "$\theta = \theta_0 \pm \Delta\theta$"

$$\mathcal{L}(\boldsymbol{n}, \boldsymbol{\theta}^0 | \mu, \boldsymbol{\theta}) = \prod_{i \in bins} \mathcal{P}(n_i | \mu \cdot S_i(\boldsymbol{\theta}) + B_i(\boldsymbol{\theta})) \times \prod_{j \in syst} \mathcal{G}(\theta_j^0 | \theta_j, \Delta\theta_j)$$





- usually θ^0=0 and $\Delta\theta$=1 (convention)
- define **effect of systematic** *j* on prediction *x* in bin *i* at "+1" and "-1",
- then interpolate & extrapolate for any value of θ

  - external / *a priori* knowledge interpreted as "**auxiliary/subsidiary measurement**", implemented as **constraint/penalty term**, i.e. probability density function (*usually Gaussian, interpreting "±Δθ" as Gaussian standard deviation*)

3

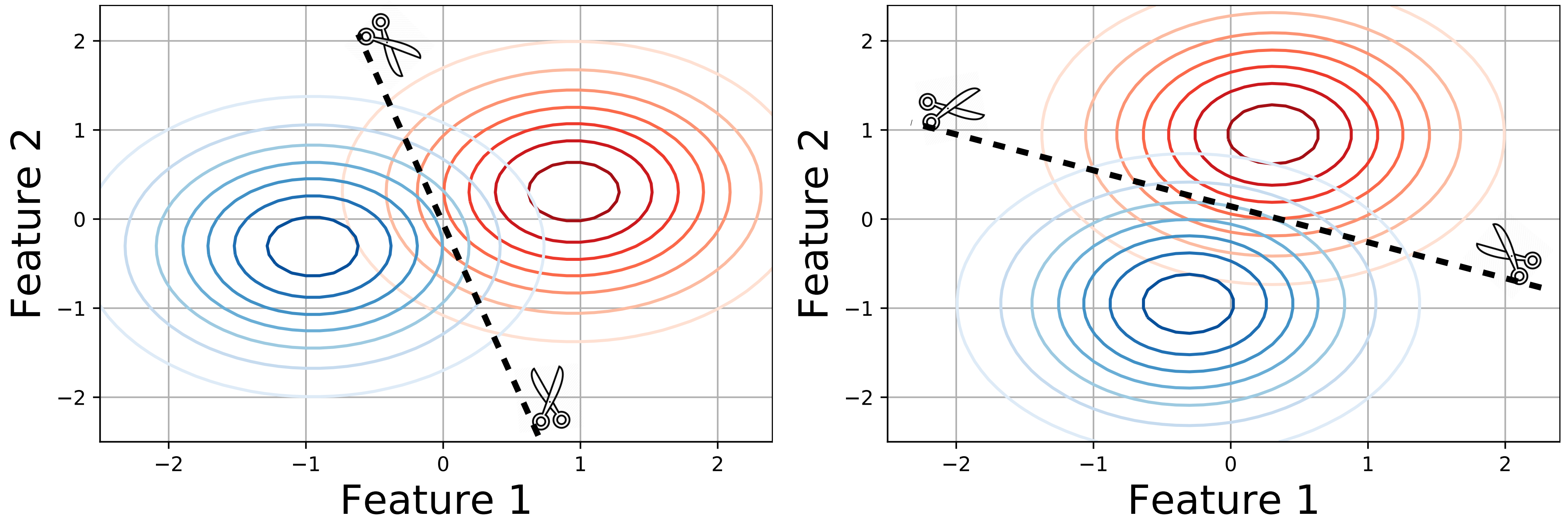
From Michele Pinamonti's talk:
https://indico.cern.ch/event/727396/contributions/3021899/attachments/1657532/2654085/Statistical_methods_at_ATLAS_and_CMS_2.pdf

Profile Likelihood

Standard method of including the systematic uncertainty into the likelihood computation

We simply make the selection/observable a function of z

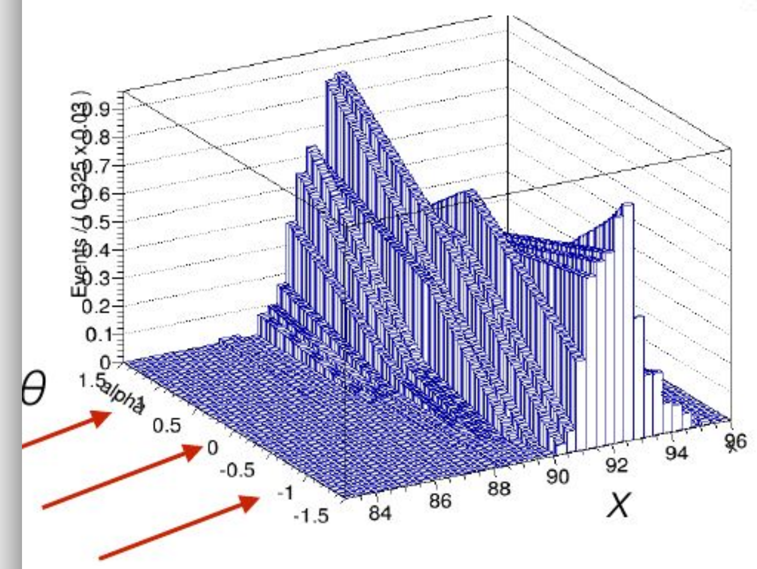
In principle could also be done in cut-based analysis: make cut a continuous function of z

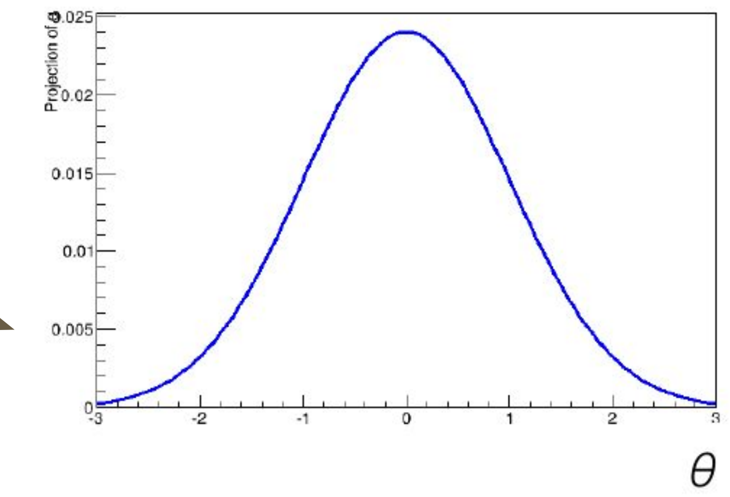


The Profile Likelihood approach

- The profile likelihood is a way to include **systematic uncertainties in the likelihood**
  - systematics included as "***constrained***" **nuisance parameters**
  - the idea behind is that systematic uncertainties on the measurement of μ come from ***imperfect knowledge*** of parameters of the model (S and B prediction)
    - still *some knowledge* is implied: "$\theta = \theta_0 \pm \Delta\theta$"

$$\mathcal{L}(\boldsymbol{n}, \boldsymbol{\theta}^0|\mu, \boldsymbol{\theta}) = \prod_{i \in bins} \mathcal{P}(n_i|\mu \cdot S_i(\boldsymbol{\theta}) + B_i(\boldsymbol{\theta})) \times \prod_{j \in syst} \mathcal{G}(\theta_j^0|\theta_j, \Delta\theta_j)$$





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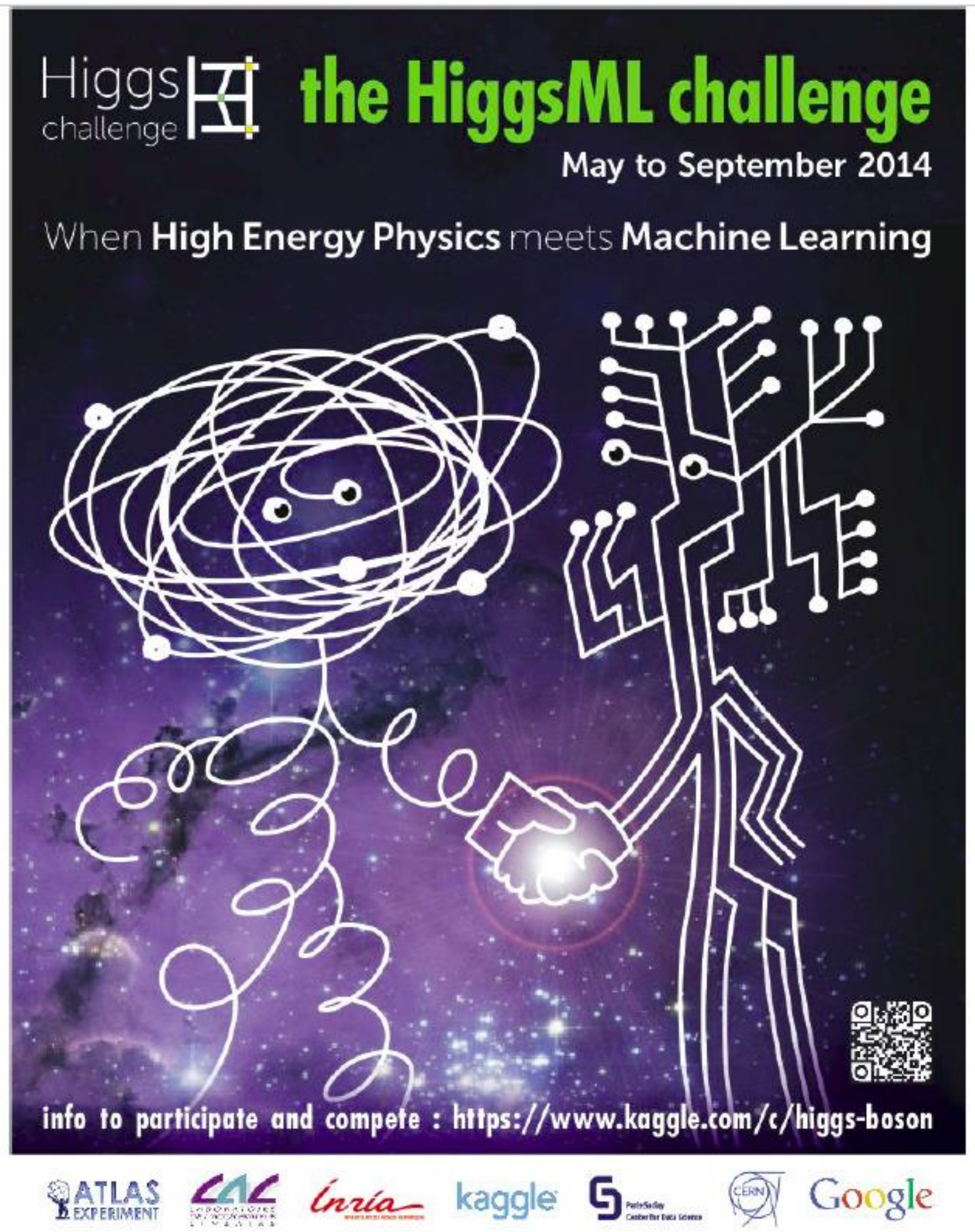
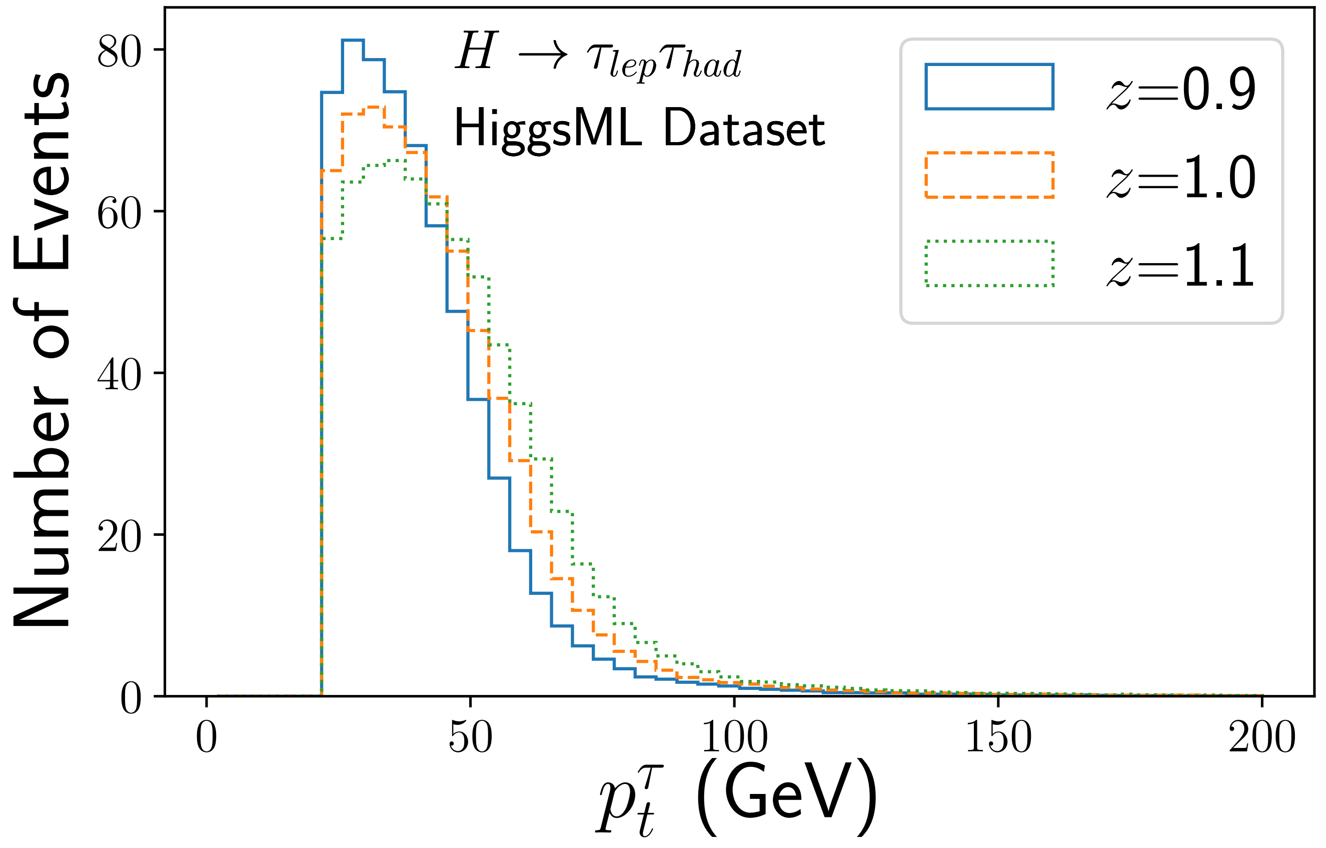
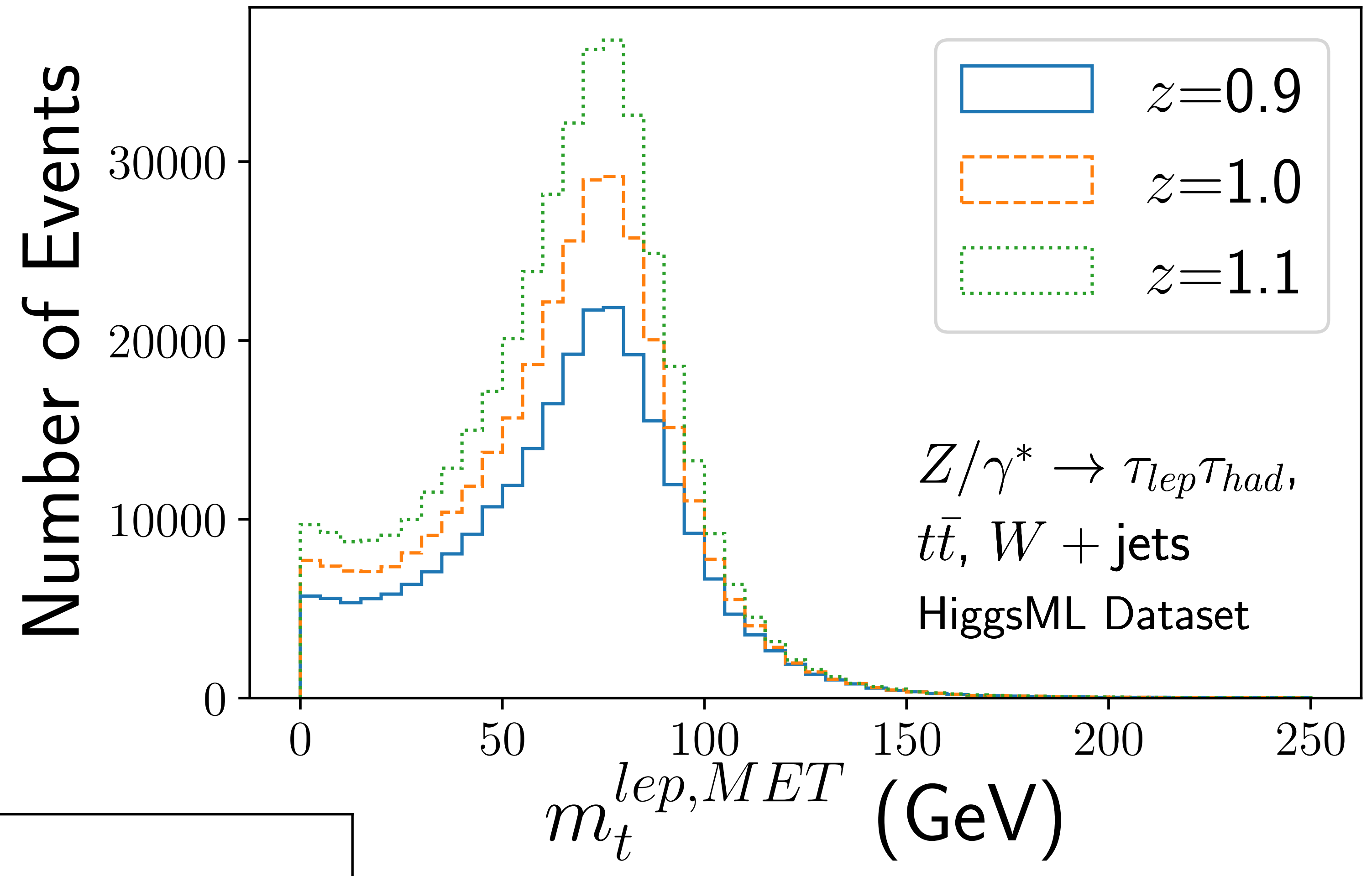
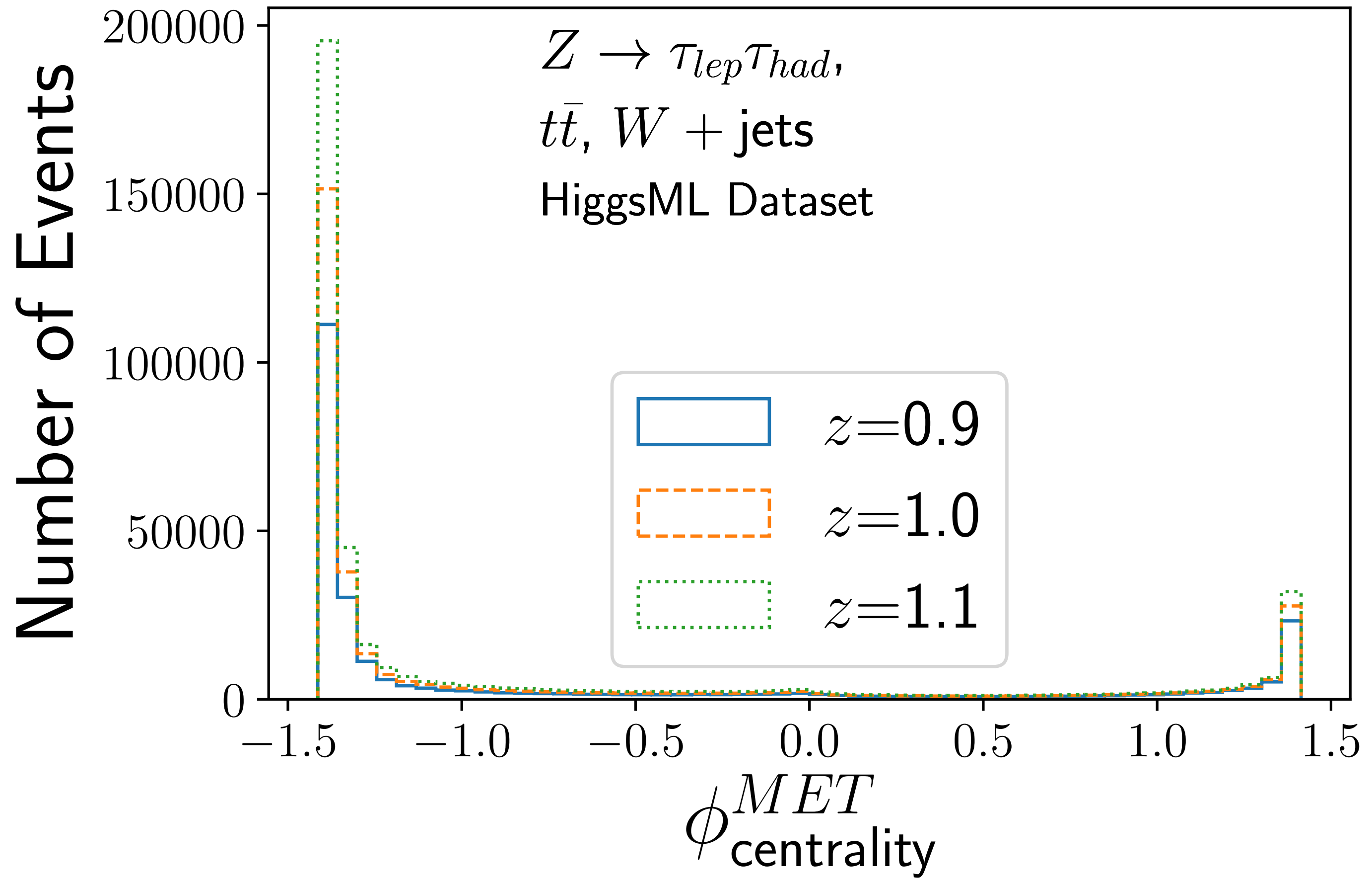
Physics Data: HiggsML + Tau Energy Scale (TES) Uncertainty



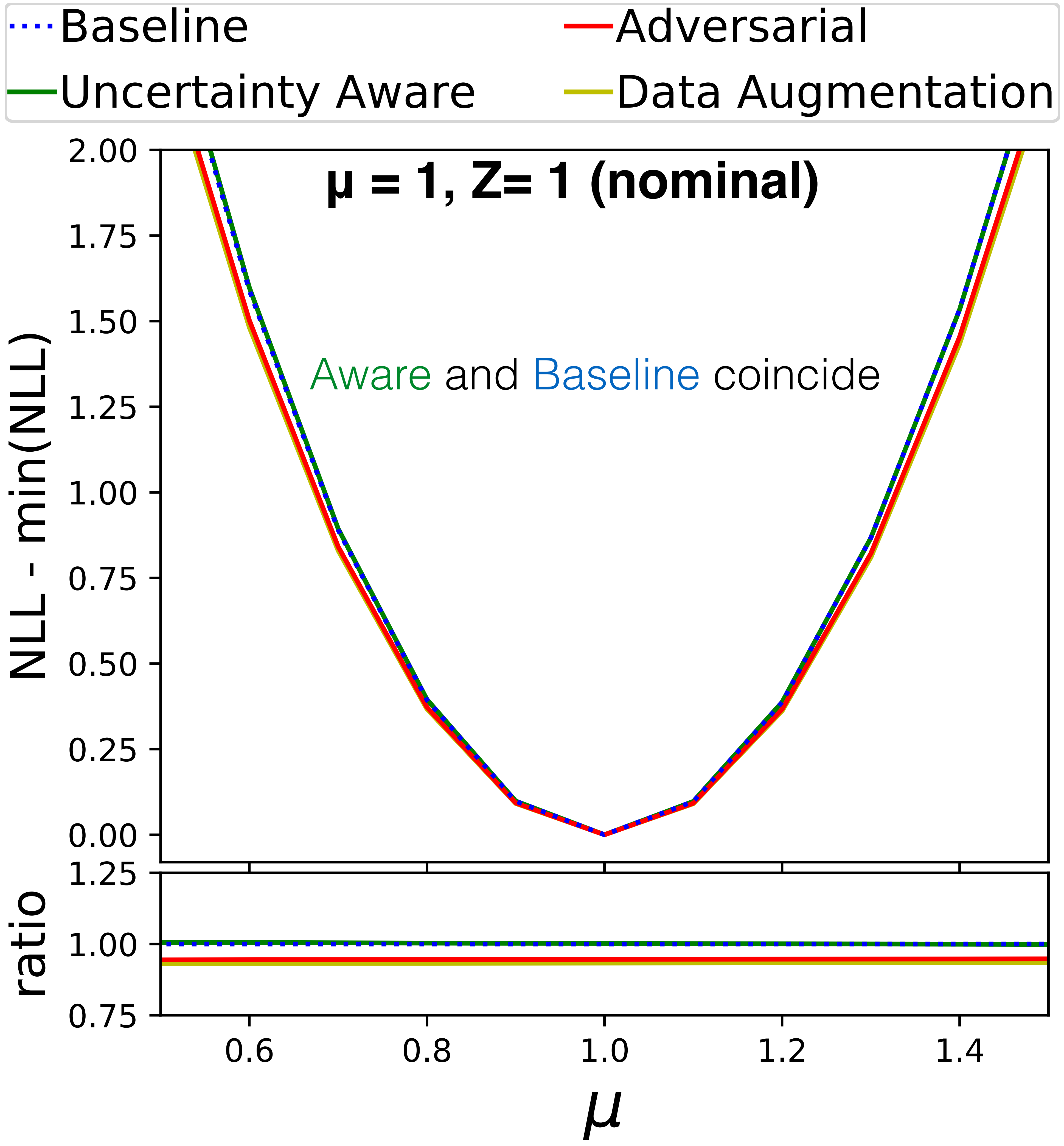
Parameter of Interest is Higgs signal strength μ, and TES is the nuisance parameter Z

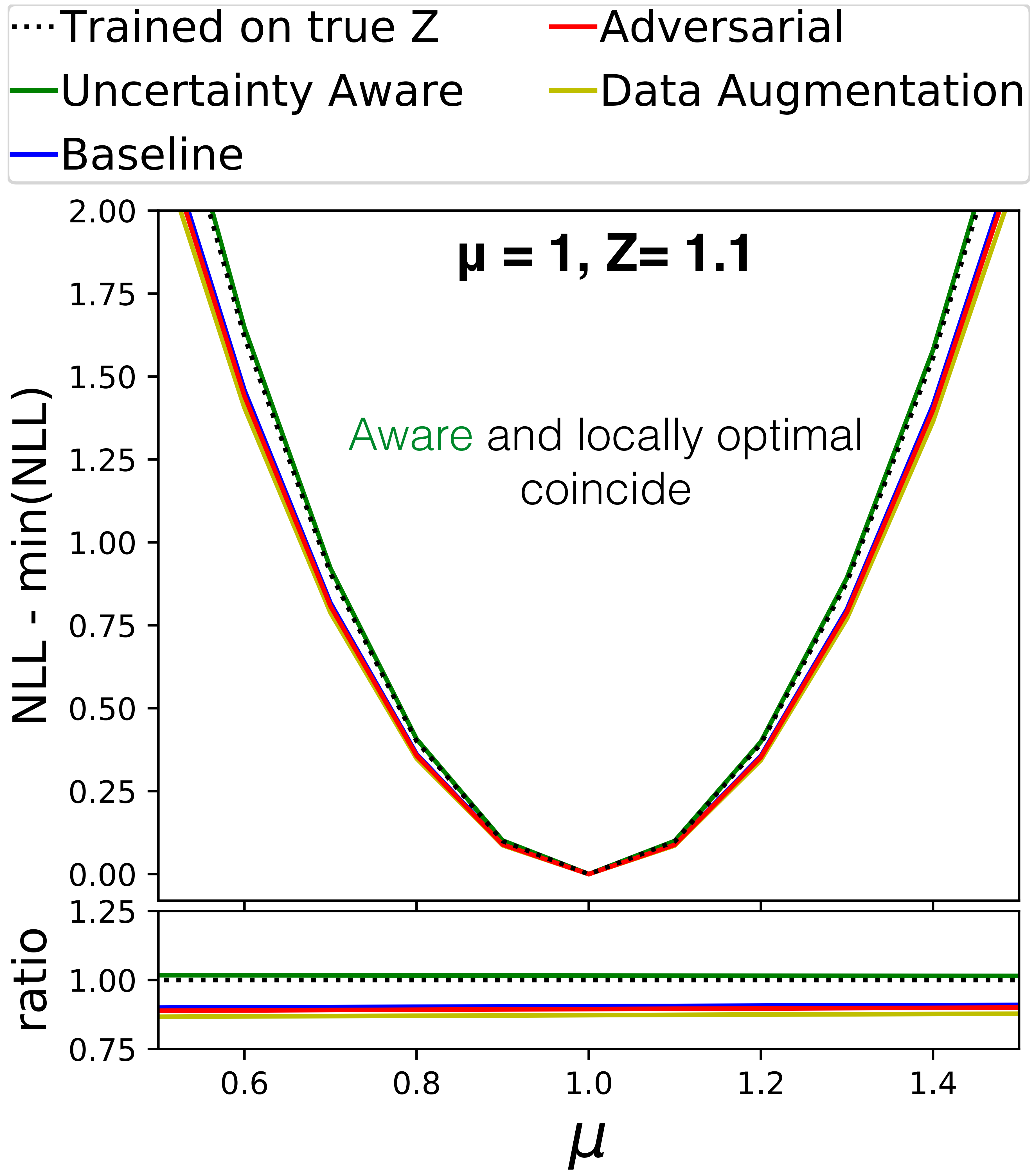






Test performance for “observed” data at nominal and above nominal Z



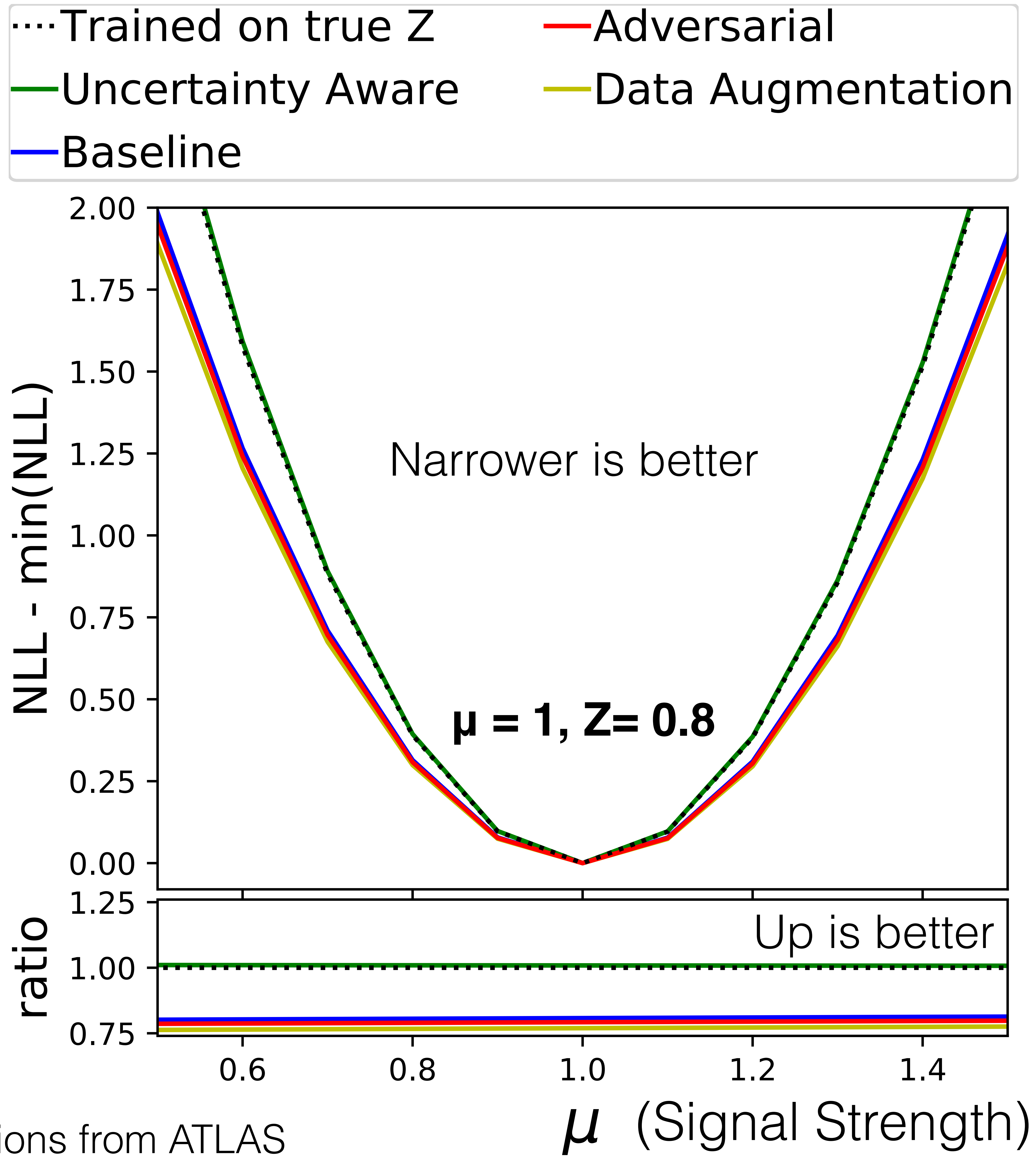


In every case the Aware Classifier is as good as the optimal one, no other technique matches its performance everywhere

Test performance for “observed” datasets at $\mu = 2$

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

Physics Data: HiggsML + Tau Energy Scale (TES) Uncertainty



Uncertainty-Aware coincides with classifier trained on true Z

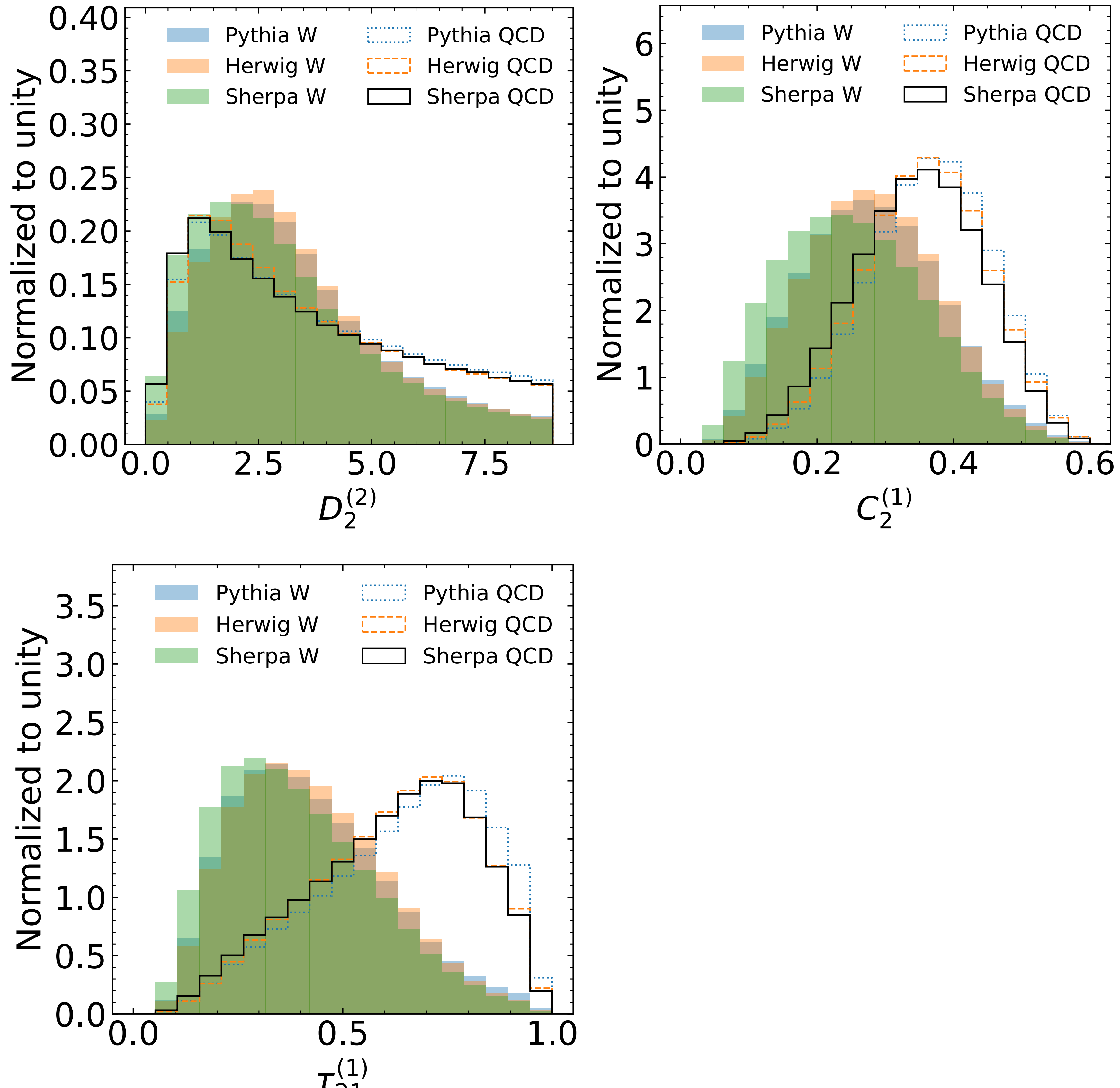
⇒ Can't get much better than that!

Case Study 1: Two-point uncertainty (fragmentation modelling)

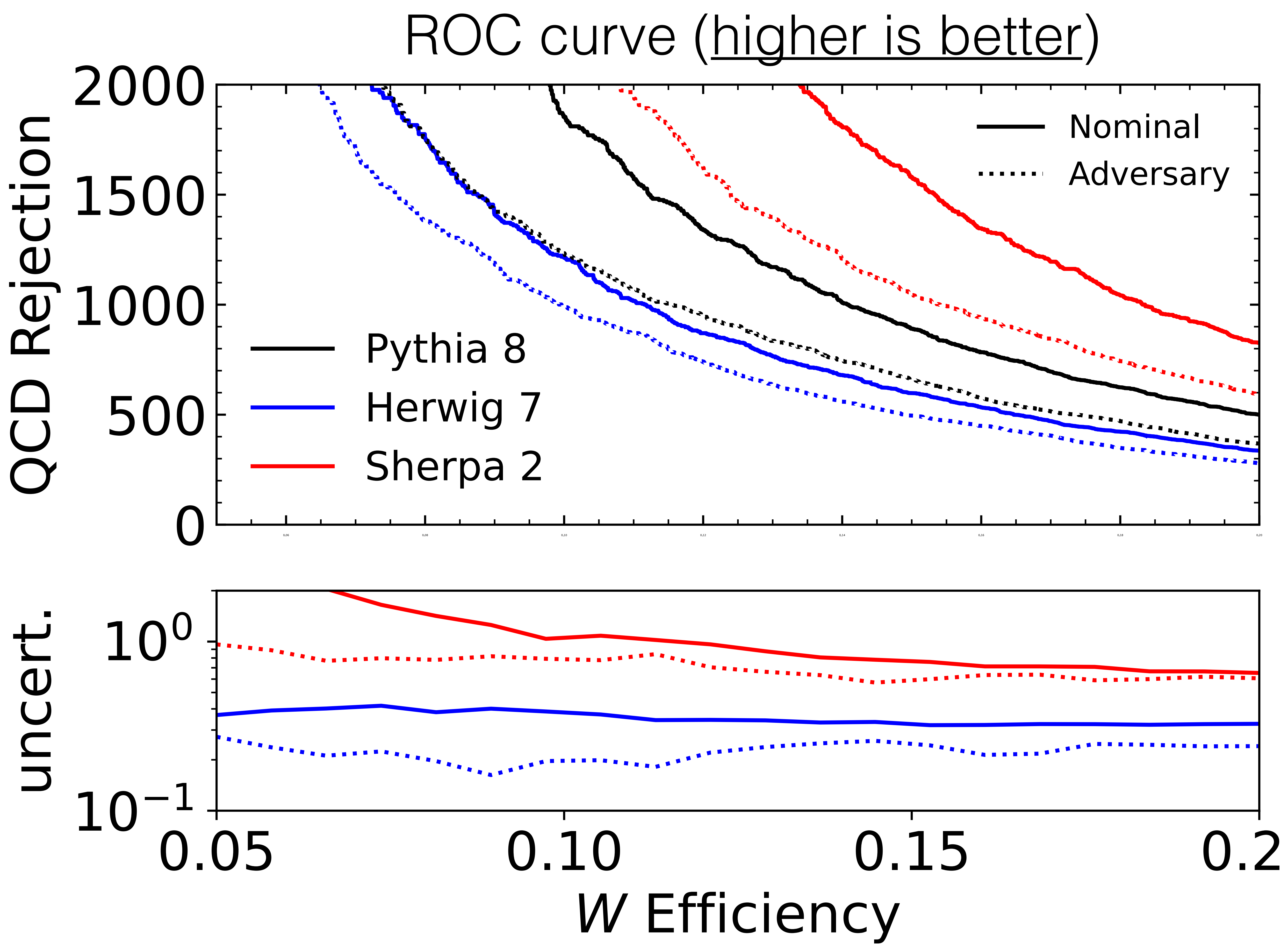
Goal: W jets vs QCD jets

Decorrelation: Reduce difference in performance on Herwig vs Pythia

Cross-check: Test uncertainty estimate from {Herwig vs Pythia} using Sherpa



Case Study 1: Two-point uncertainty - Result

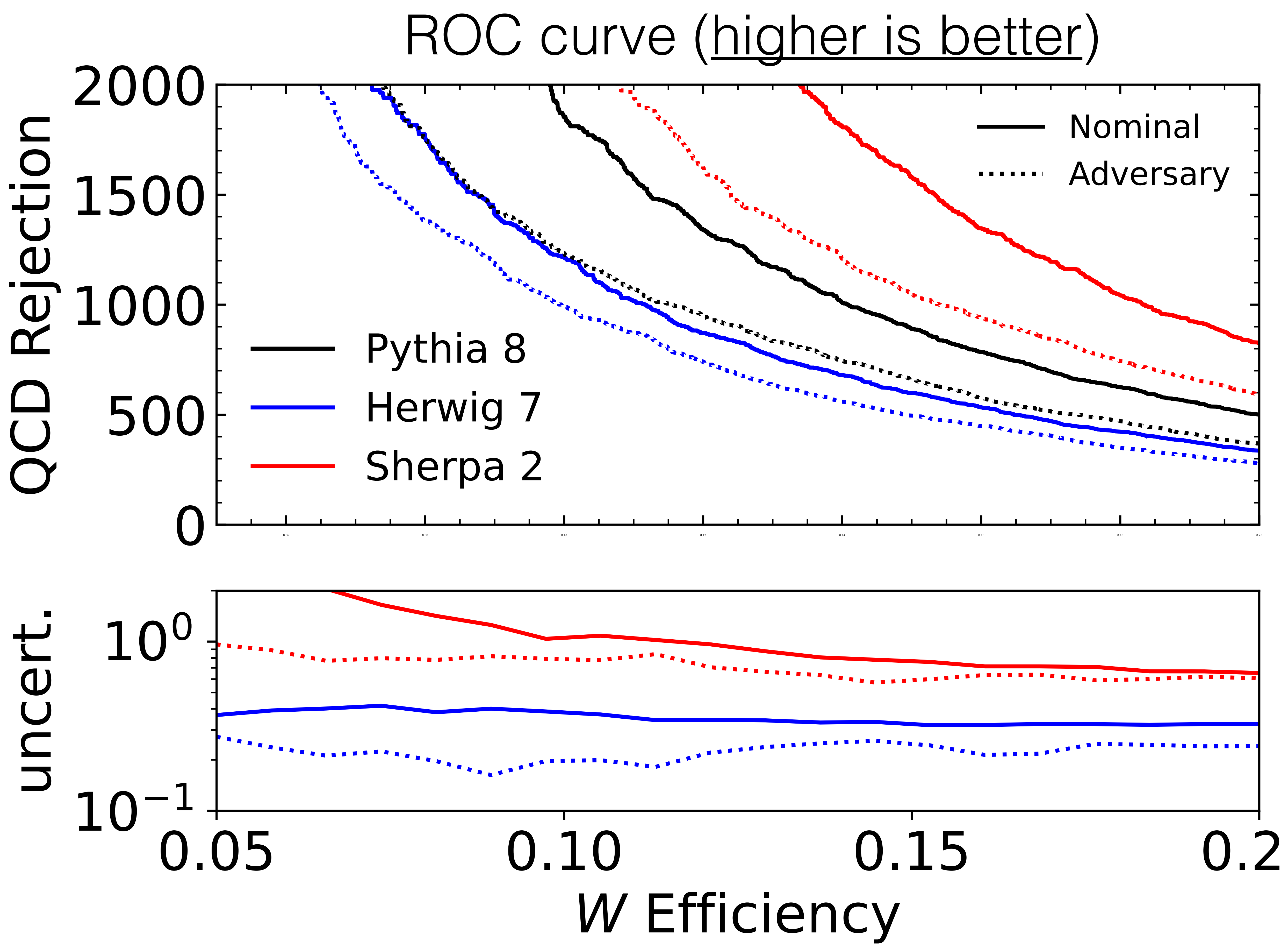


Case Study 1: Two-point uncertainty - Result

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



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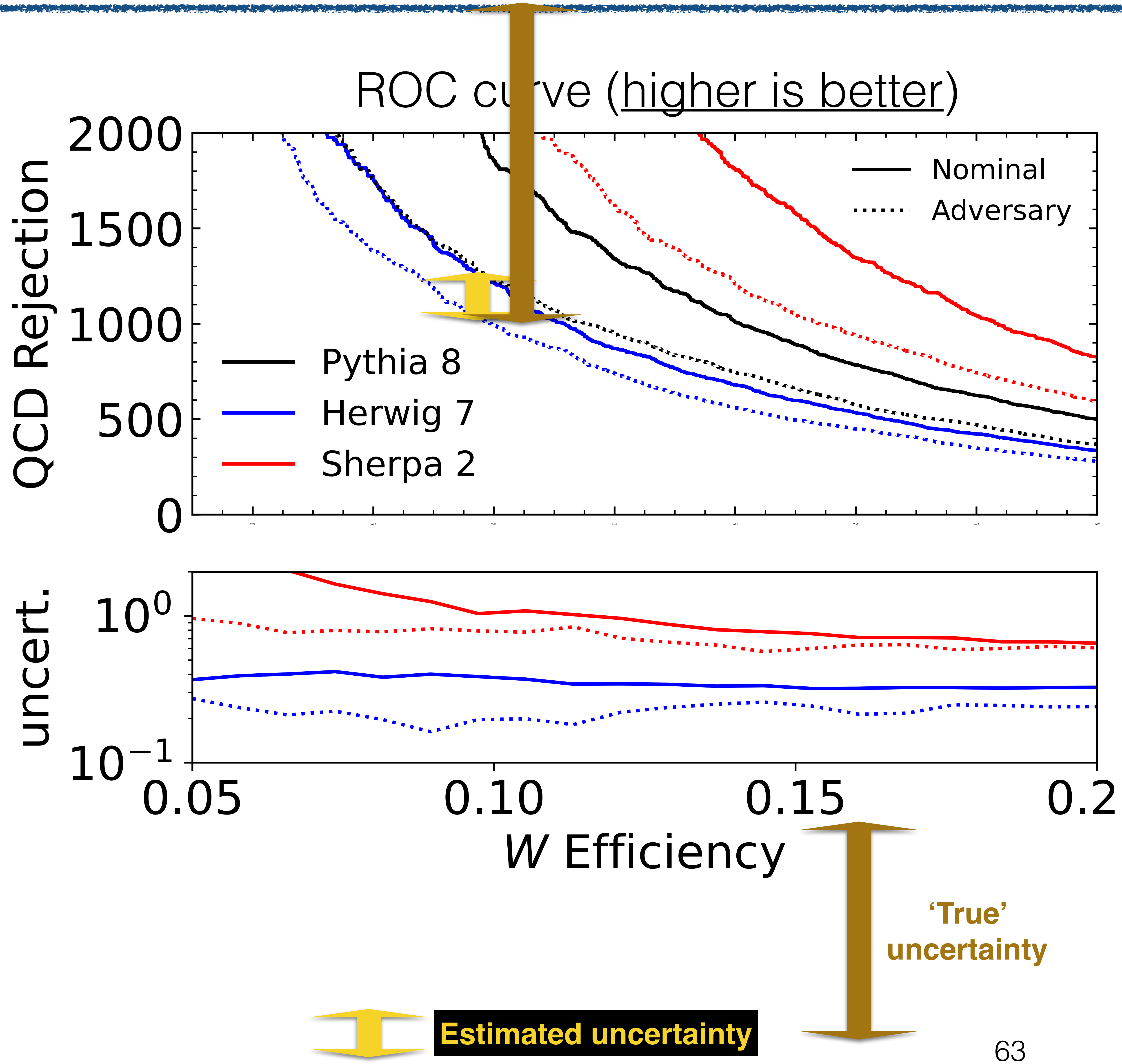


https://arxiv.org/abs/2210.15167

Make correction in UQ for EW processes

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 > wpm`	1	1.54×10^{-1}	1.84	1.47×10^{-1}	1.92
`p p > wpm j`	2	1.97×10^{-1}	1.96	2.94×10^{-1}	1.31
`p p > wpm j j`	3	2.45×10^{-1}	0.59	4.41×10^{-1}	0.33
`p p > wpm j j j`	4	4.10×10^{-1}	0.25	5.88×10^{-1}	0.18
`p p > z`	1	1.46×10^{-1}	1.87	1.47×10^{-1}	1.86
`p p > z j`	2	1.93×10^{-1}	1.82	2.94×10^{-1}	1.19
`p p > z j j`	3	2.43×10^{-1}	0.56	4.41×10^{-1}	0.31
`p p > z j j j`	4	4.08×10^{-1}	0.27	5.88×10^{-1}	0.19
`p p > a j`	2	3.12×10^{-1}	5.33	2.94×10^{-1}	5.66
`p p > a j j`	3	3.28×10^{-1}	0.85	4.41×10^{-1}	0.63
`p p > w+ w- wpm`	3	1.00×10^{-3}	610.69	4.41×10^{-1}	1.39
`p p > z w+ w-`	3	8.00×10^{-3}	92.39	4.41×10^{-1}	1.68
`p p > z z wpm`	3	1.00×10^{-2}	85.00	4.41×10^{-1}	1.93
`p p > z z z`	3	1.00×10^{-3}	302.75	4.41×10^{-1}	0.69
`p p > a w+ w-`	3	1.90×10^{-2}	42.33	4.41×10^{-1}	1.82
`p p > a a wpm`	3	4.40×10^{-2}	47.24	4.41×10^{-1}	4.72
`p p > a z wpm`	3	1.00×10^{-3}	1244.49	4.41×10^{-1}	2.82
`p p > a z z`	3	2.00×10^{-2}	17.24	4.41×10^{-1}	0.78

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

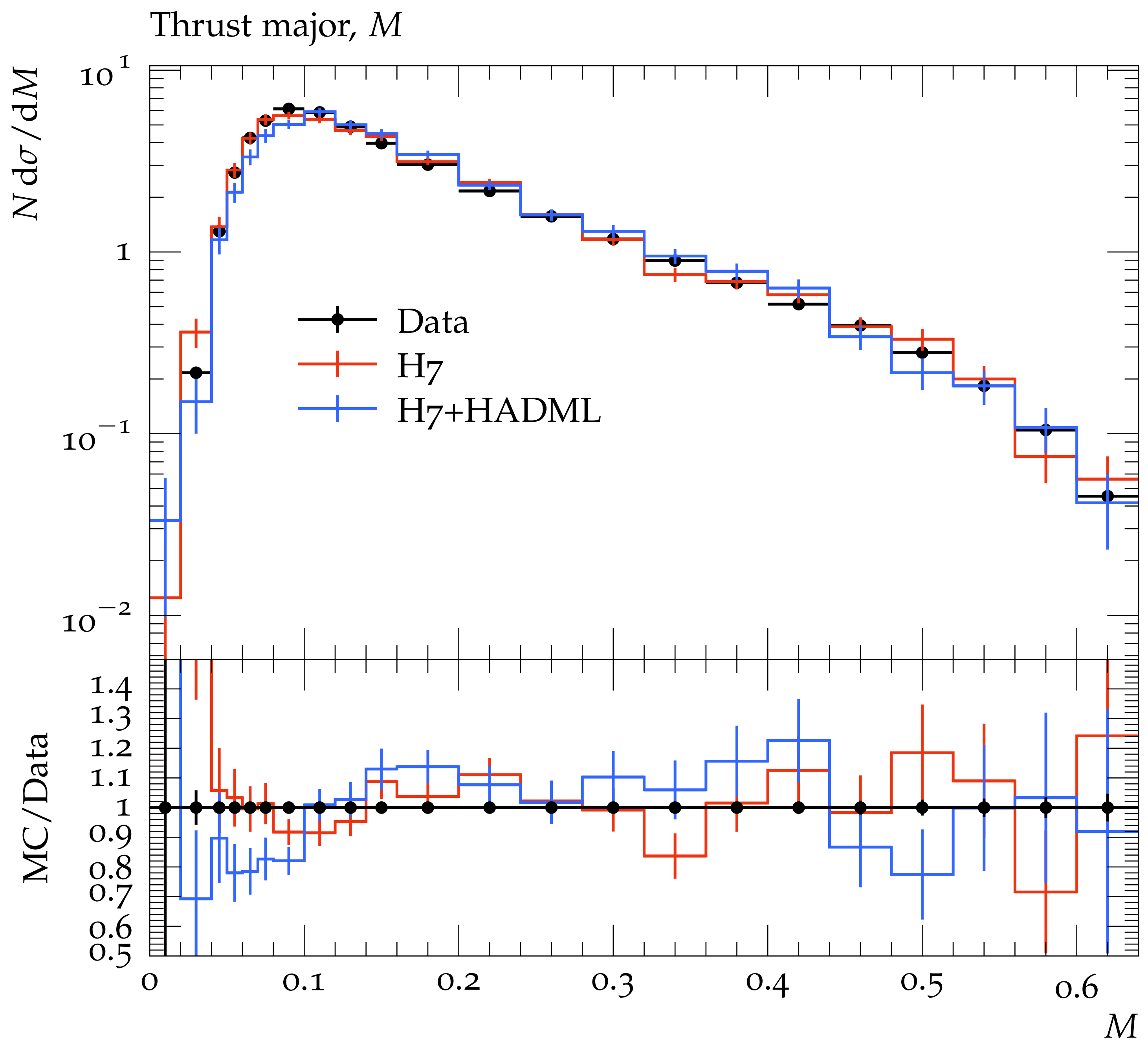
Universe is a perfect simulator

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

Universe is a perfect simulator

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

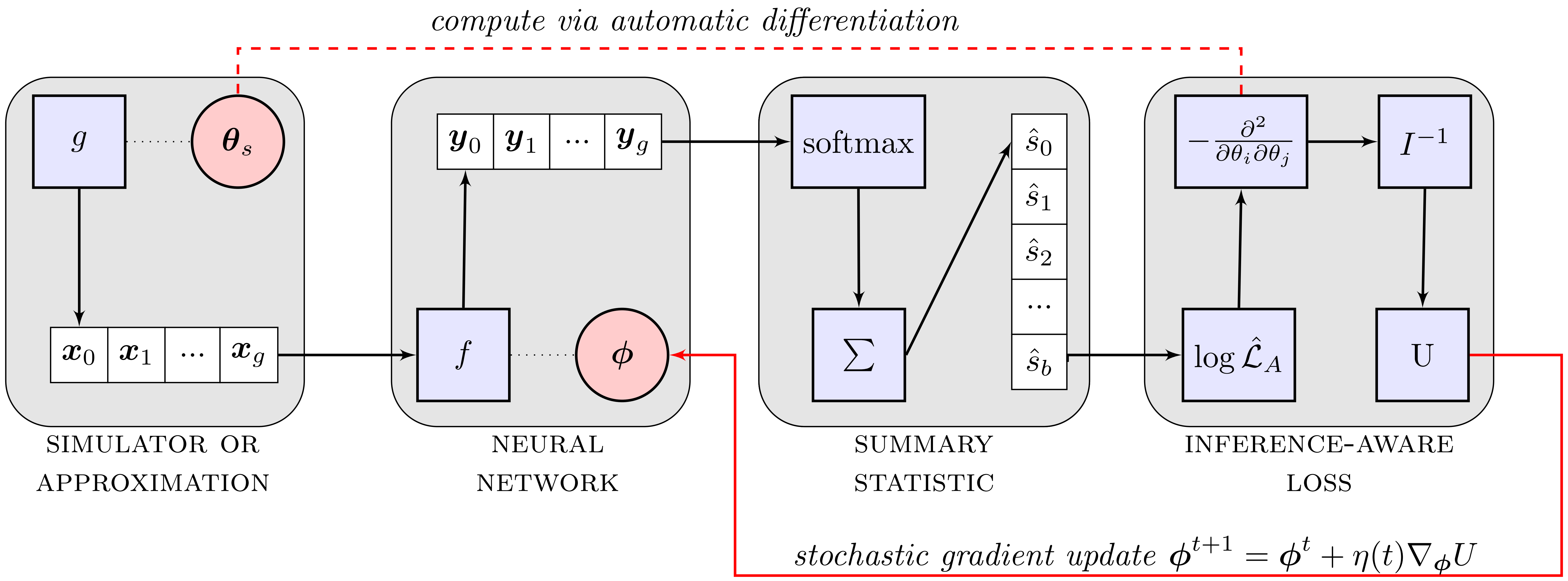
- Bypass theory, can we learn hadronization directly from data ?
- We show a proof of concept



https://arxiv.org/abs/1806.04743

Example 1: INFERNO

- Write your analysis code differentiably, use uncertainty on final measurement as loss function
- Model is like a multi-class classifier, but classes have no meaning —> **no concept of AUC**
- **Evaluation: Poisson fit of simulation vs data in each category**, similar to histograms



In modern implementation (NEOS arxiv:2203.05570), classes are KDE bins

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!