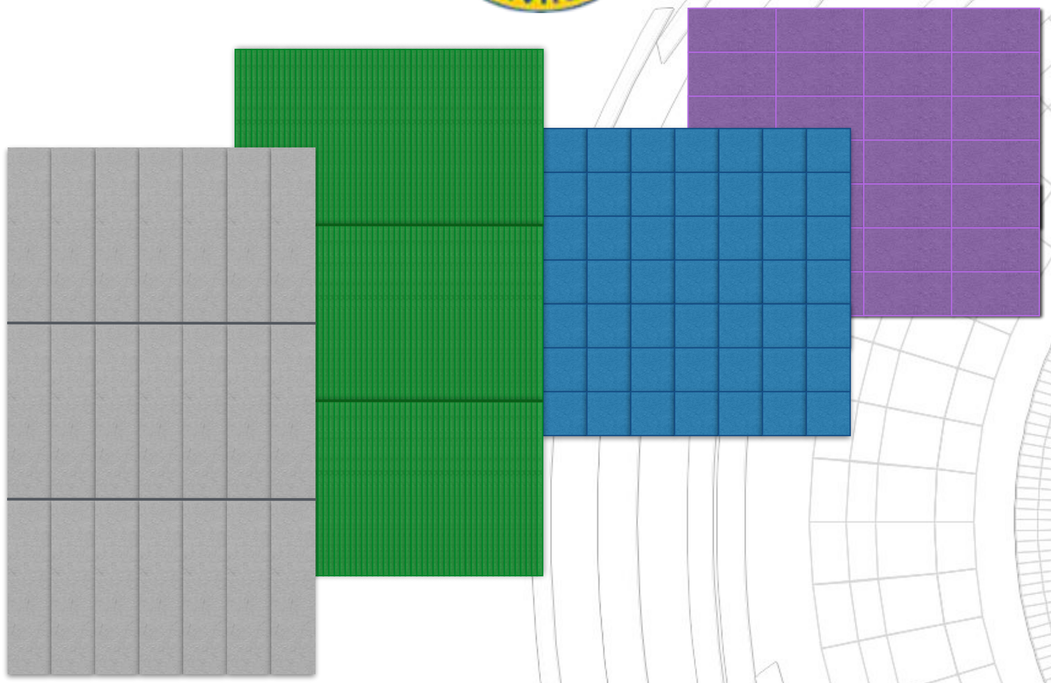
Uncertainties in the era of ML

Aishik Ghosh

Erice

14 April 2023



So much ML

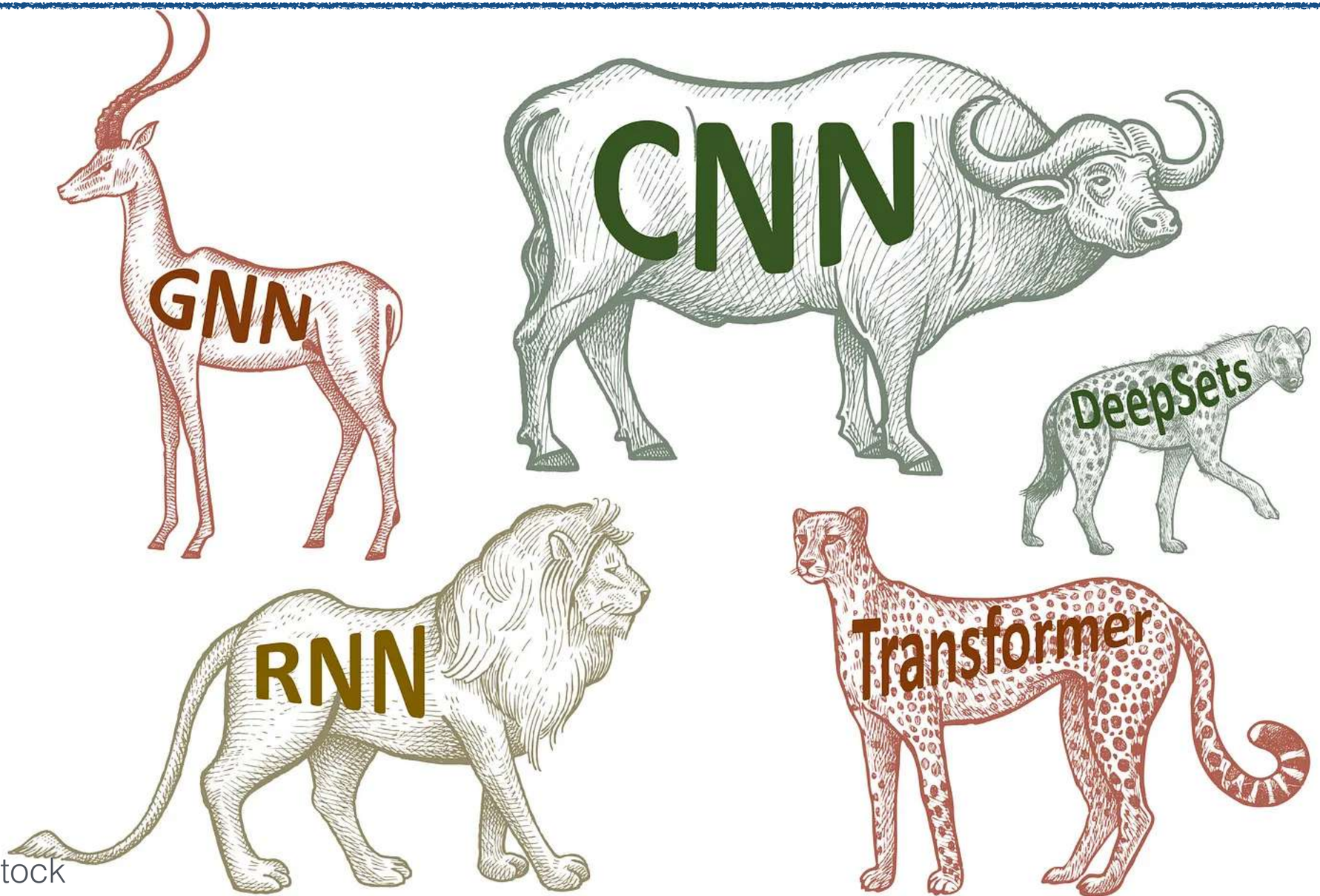


Image: ShutterStock

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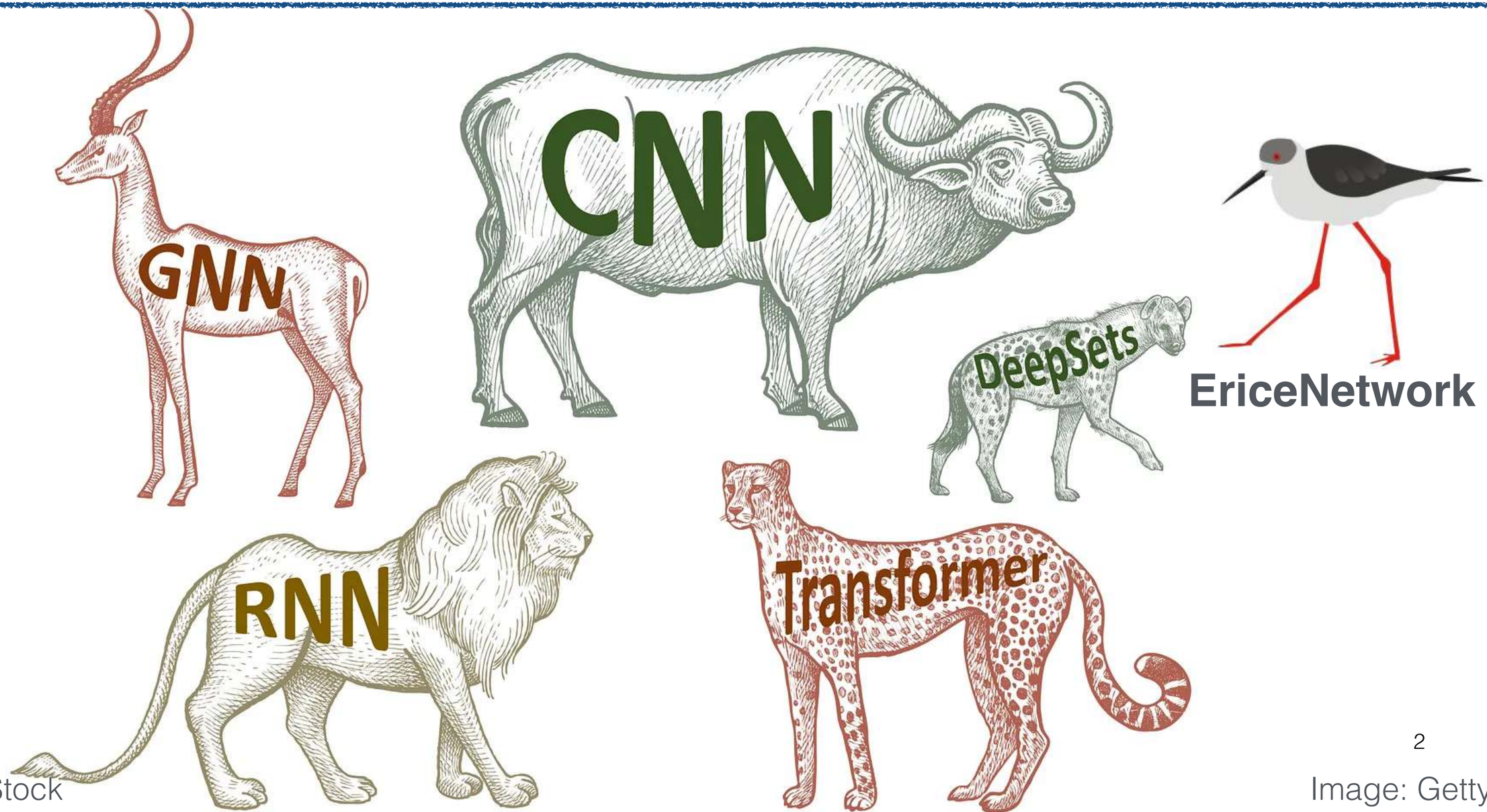
So much ML



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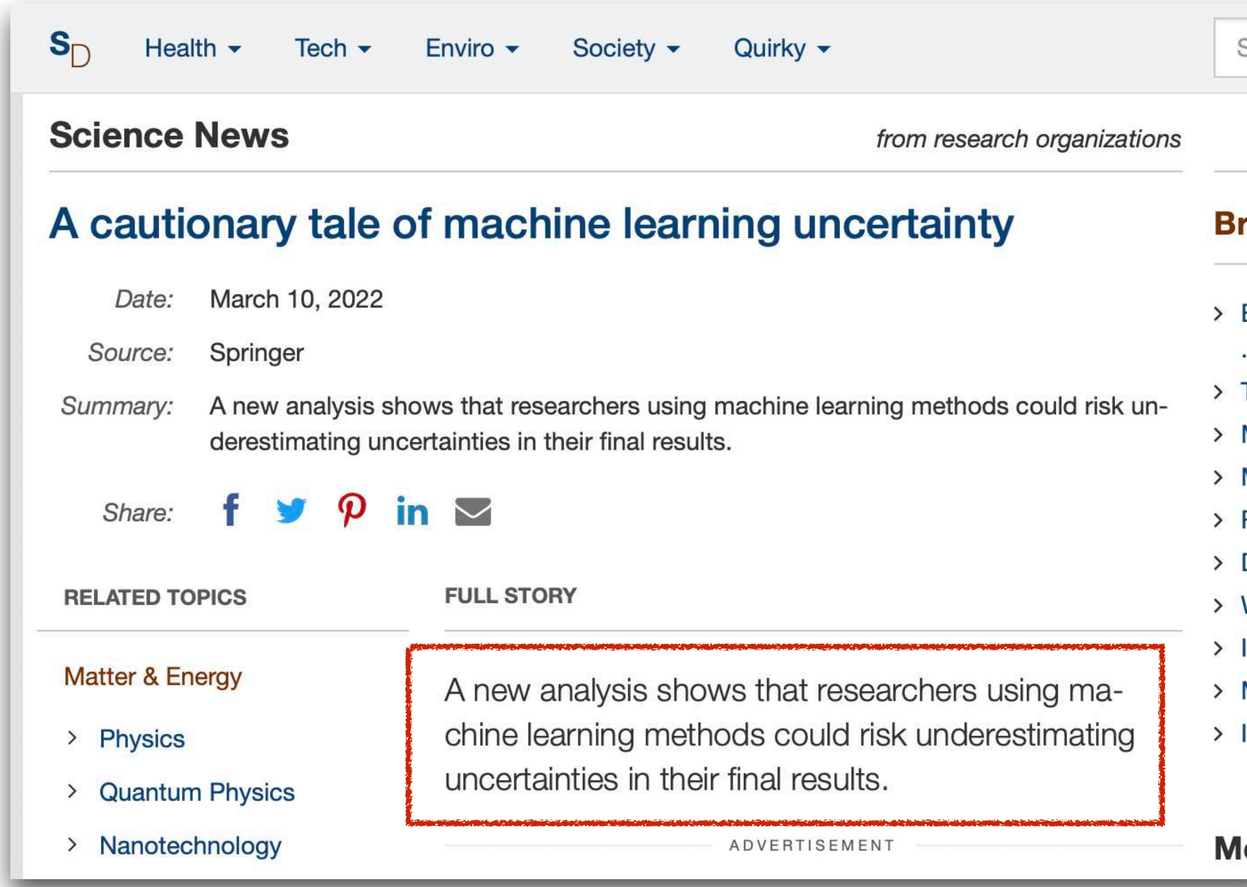
So much fear …


SD
Health
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Science News
from research organizations
A cautionary tale of machine learning uncertainty
Date: March 10, 2022
Source: Springer
Summary: A new analysis shows that researchers using machine learning methods could risk underestimating uncertainties in their final results.
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A new analysis shows that researchers using machine learning methods could risk underestimating uncertainties in their final results.
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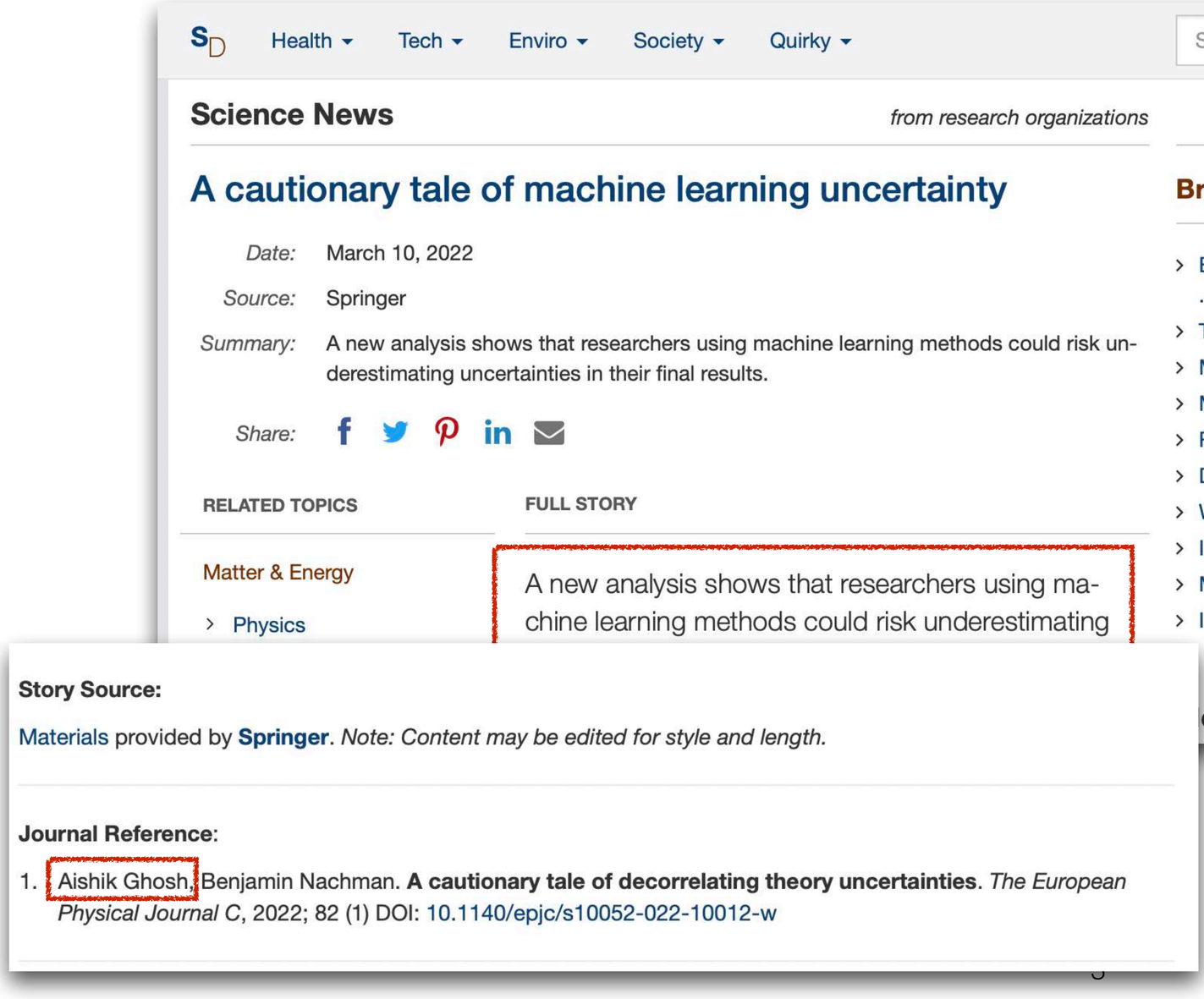
So much fear …



S_D Health Tech Enviro Society Quirky

Science News *from research organizations*

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FULL STORY

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Journal Reference:

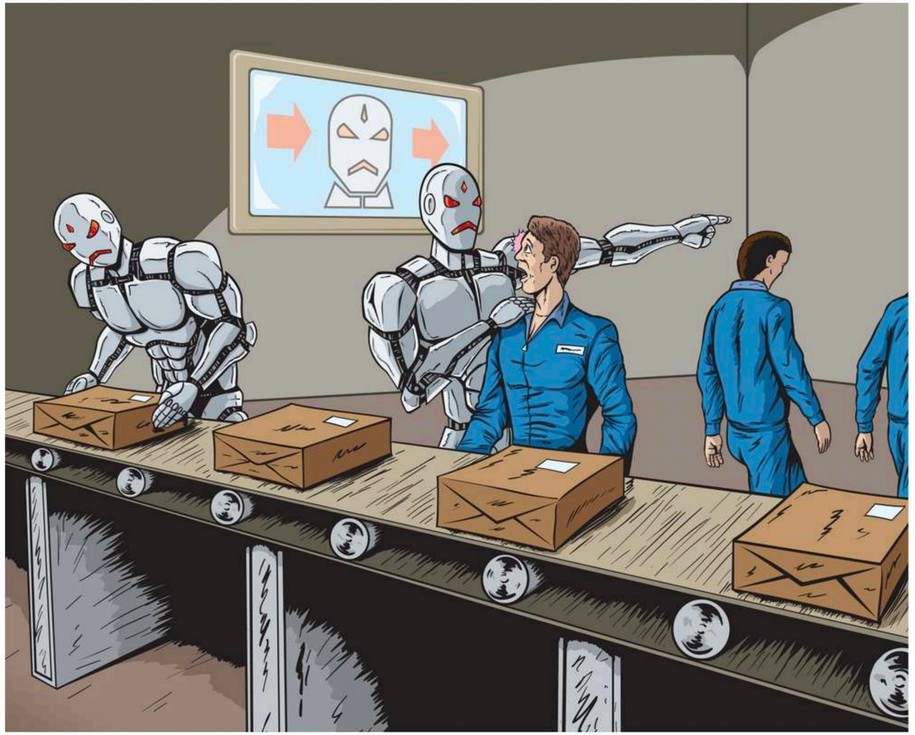
1. Aishik Ghosh, Benjamin Nachman. **A cautionary tale of decorrelating theory uncertainties**. *The European Physical Journal C*, 2022; 82 (1) DOI: 10.1140/epjc/s10052-022-10012-w

So much fear …

AI

Why you should fear artificial intelligence

Doc Huston 10:00 PM UTC • March 22, 2016 Comment



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Uncertainties, the bedrock of experimental science

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$$m_H = 125.25 \pm 0.17 \text{ GeV}$$

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Uncertainties, the bedrock of experimental science

$$m_H = 125.25 \pm 0.17 \text{ GeV}$$

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

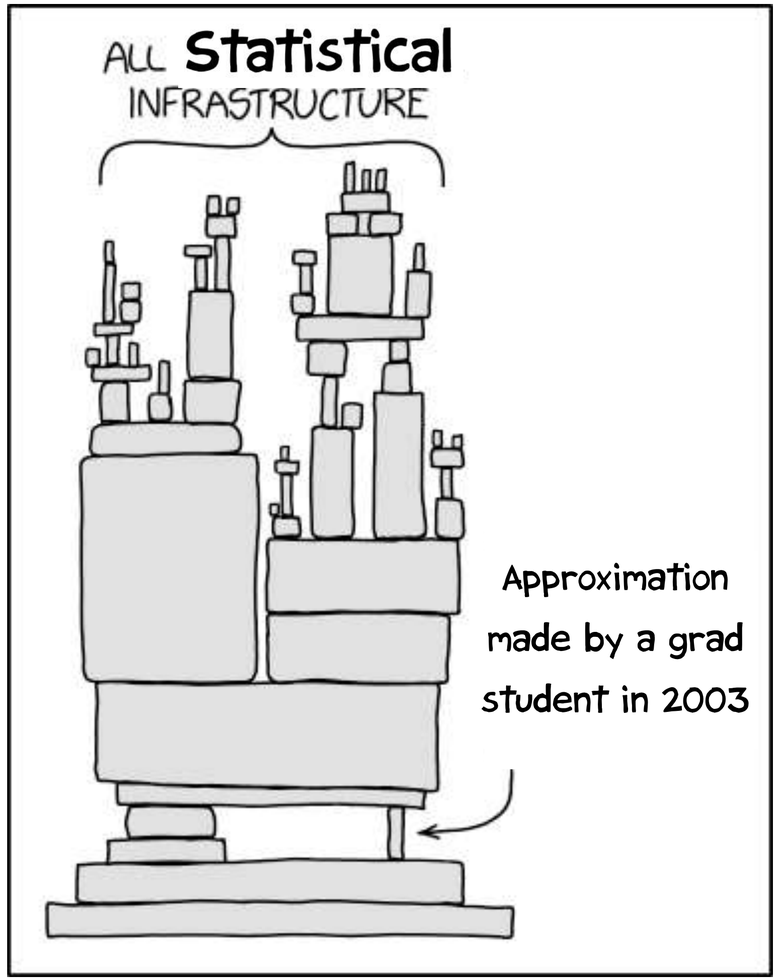
Uncertainties, the bedrock of experimental science

$$m_H = 125.25 \pm 0.17 \text{ GeV}$$

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

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

Nuisance Parameter Infrastructure



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?

A predictable evolution over ten years

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 methods to tackle uncertainties in a way classical methods couldn't

Revolution: Novel ML uncertainty quantification & mitigation methods have wider applications, also back-ported to traditional algorithms

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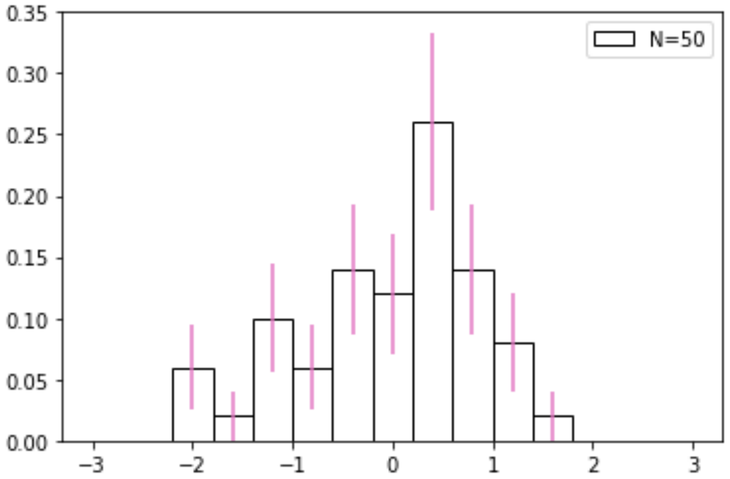
Revolution: Novel ML uncertainty quantification & mitigation methods have wider applications, also back-ported to traditional algorithms

STOP ME AND ASK ME QUESTIONS ! ! !

Typical Uncertainties in HEP

Statistical Uncertainty



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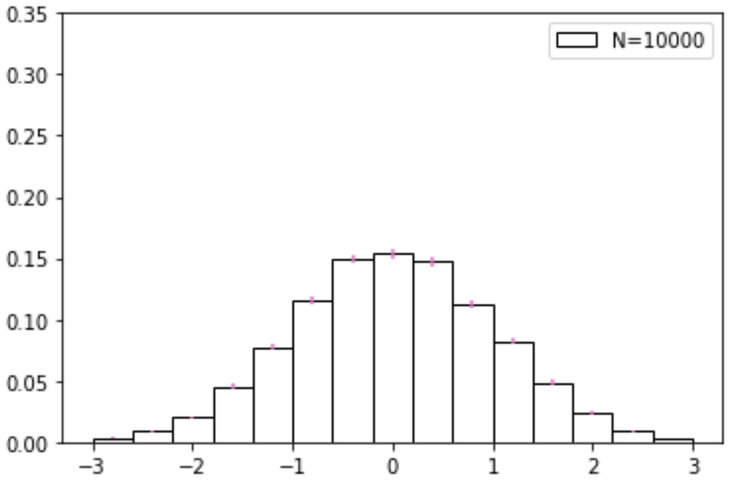
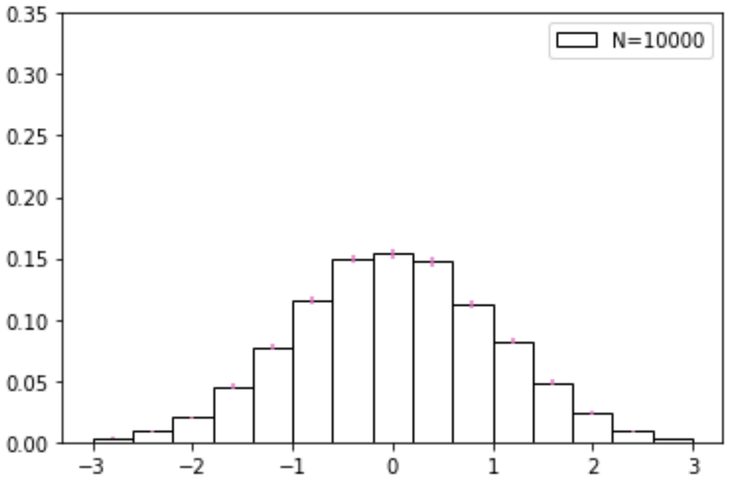
Statistical Uncertainty

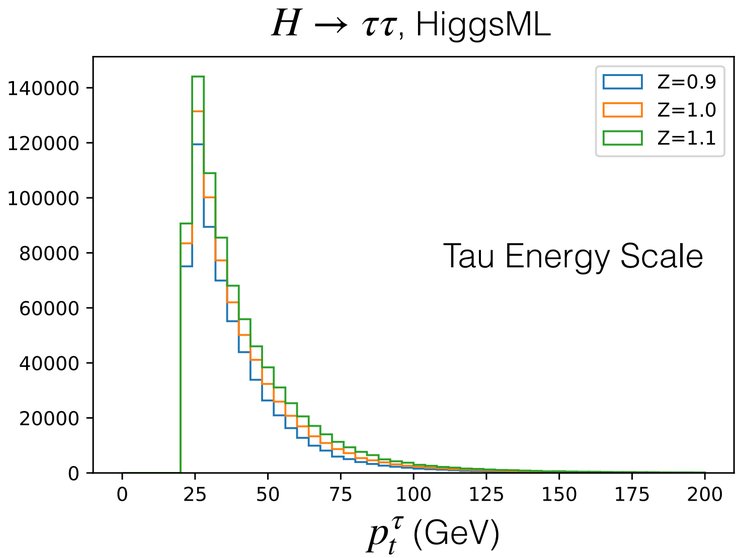


Typical Uncertainties in HEP

Statistical Uncertainty

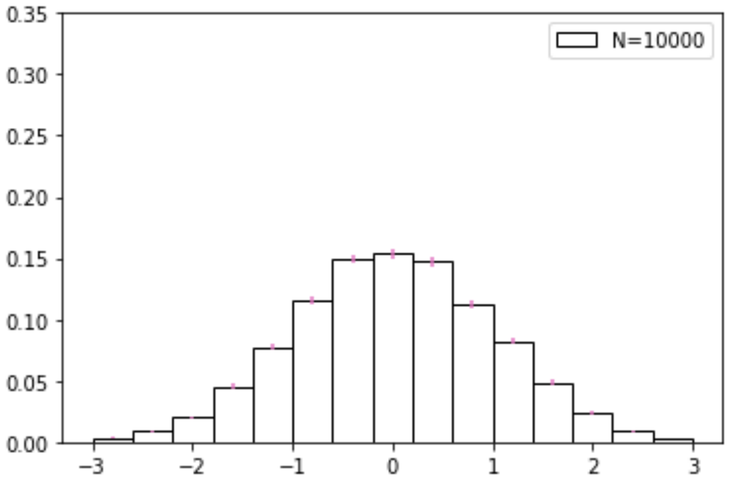


Systematic Experimental Uncertainty



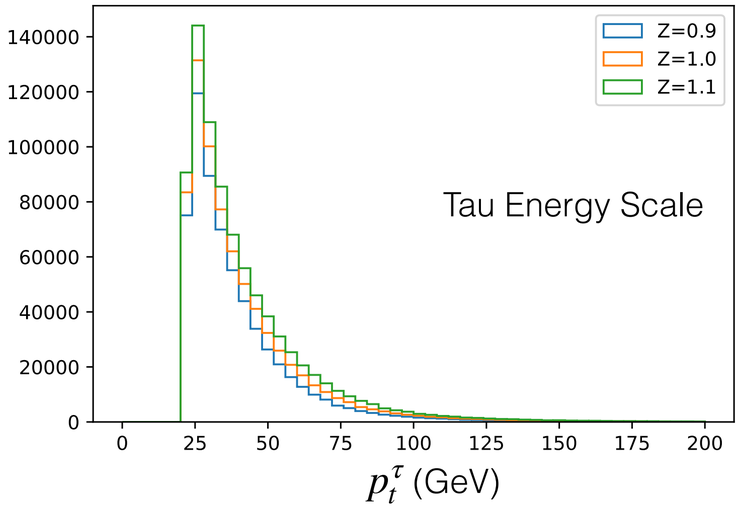
Typical Uncertainties in HEP

Statistical Uncertainty

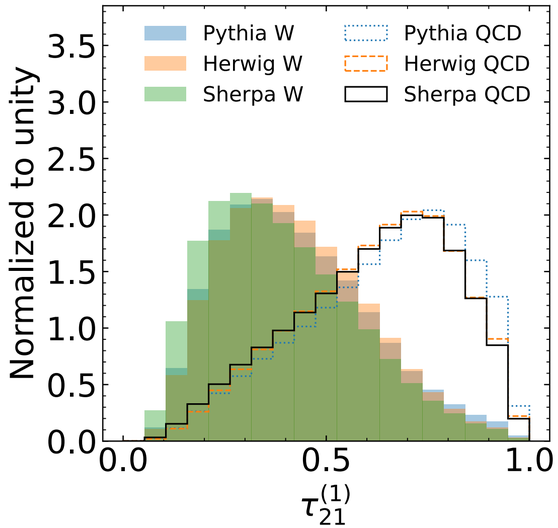


Systematic Experimental Uncertainty

$H \to \tau\tau$, HiggsML



Systematic Theory Uncertainty



SHERPA 2.2

Typical Uncertainties in ML

Typical Uncertainties in ML

Aleatoric Uncertainty

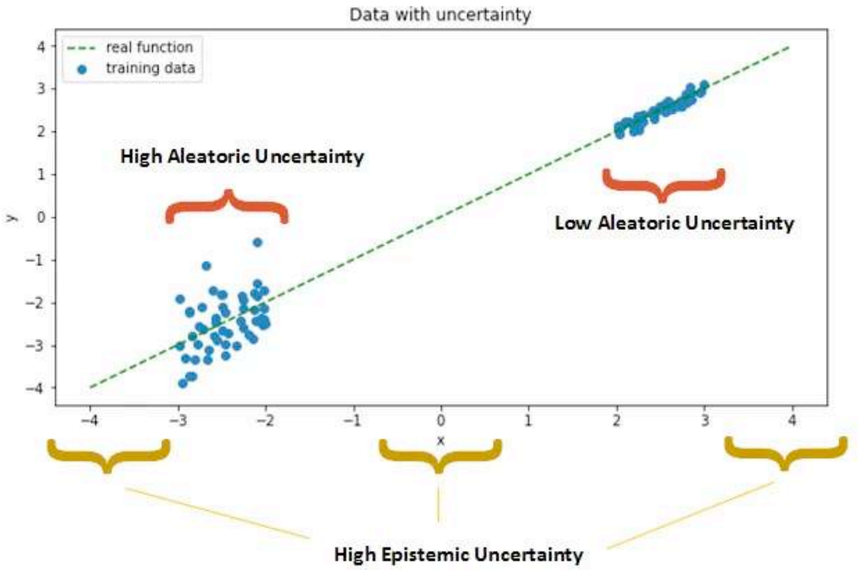
Inherent in data / experiment
Irreducible

Typical Uncertainties in ML

Aleatoric Uncertainty

Inherent in data / experiment
Irreducible

Epistemic Uncertainty



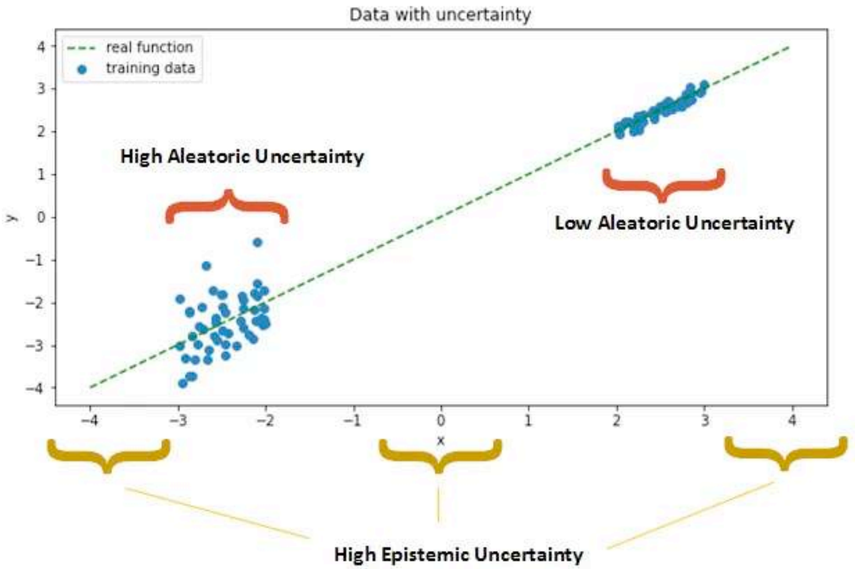
Could reduce by gathering more data

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

Epistemic Uncertainty



Inherent in data / experim
Irreducible

ng more data

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

arXiv > hep-ex > arXiv:2208.03284

High Energy Physics - Experiment

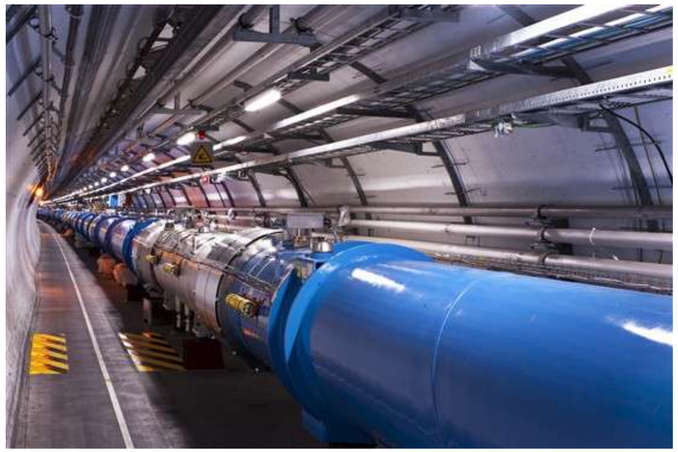
[Submitted on 5 Aug 2022 (v1), last revised 6 Sep 2022 (this version, v3)]

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

Simulation Based Inference at LHC



Unlabelled data from LHC

Compare to find New Physics

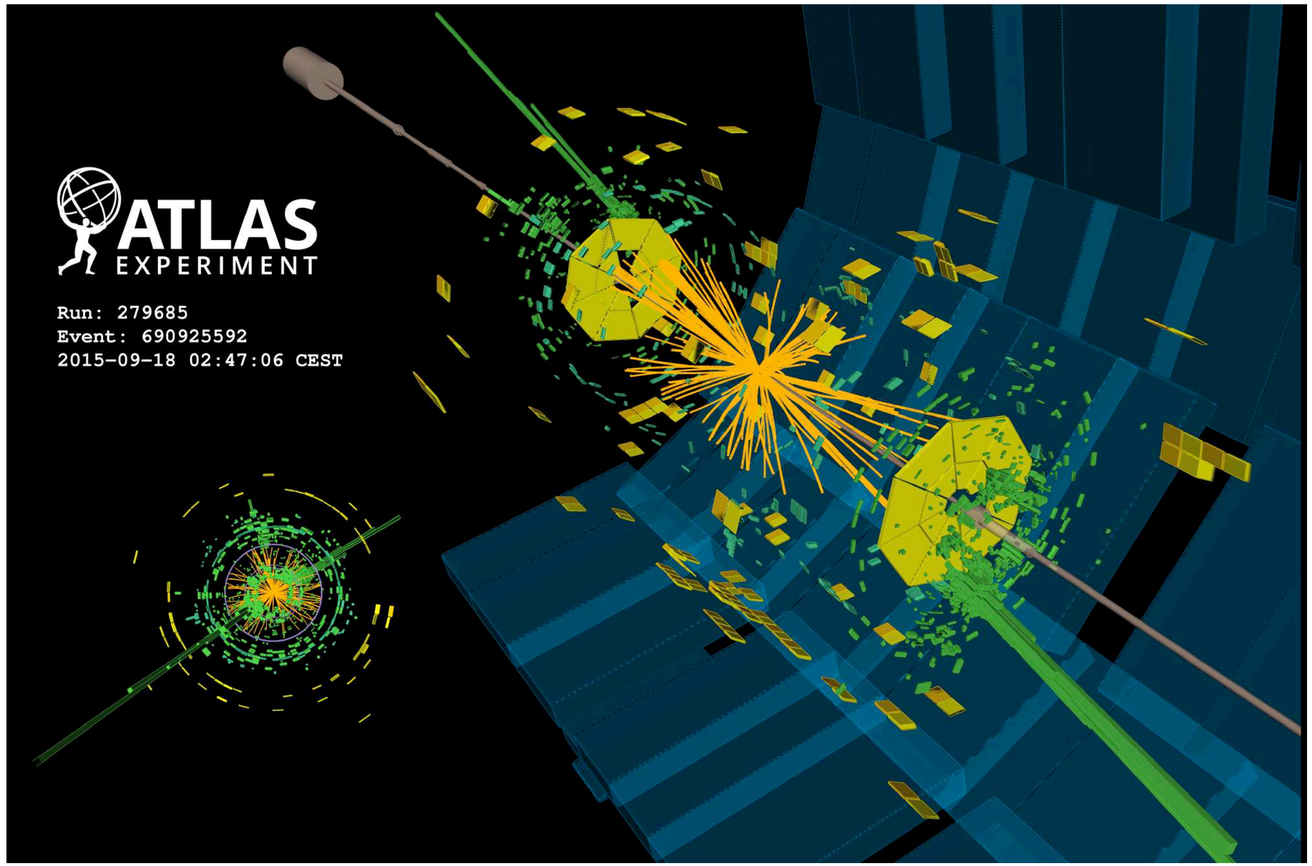
Simulation using Standard Model of particle physics

High dimensional data

Detector has ~100 million sensors

→ Combine information into 1 powerful variable

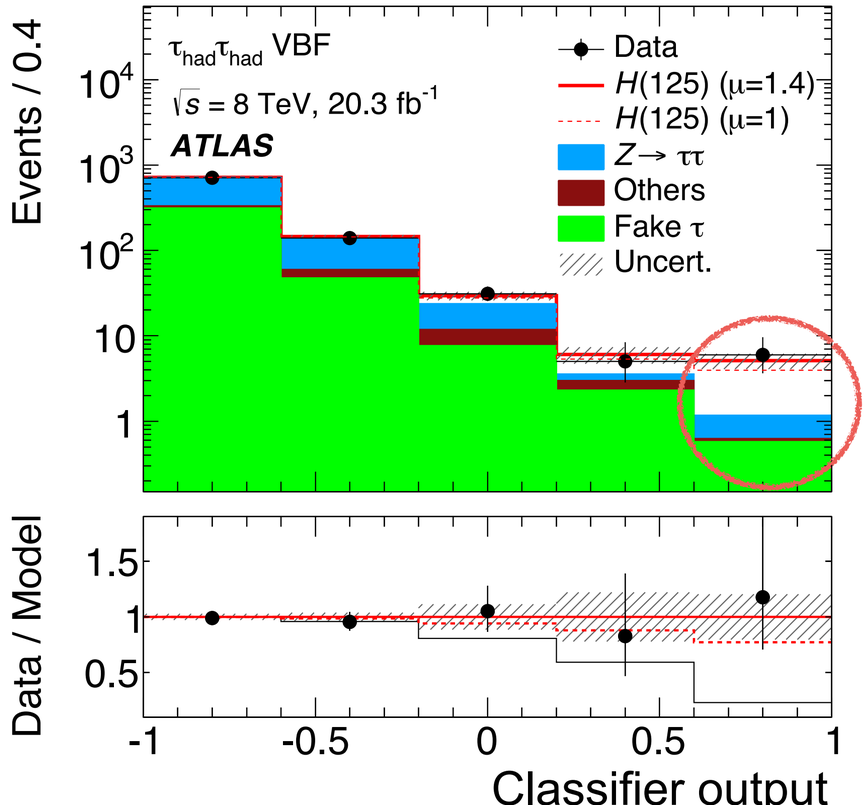
Look at histogram of this variable



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

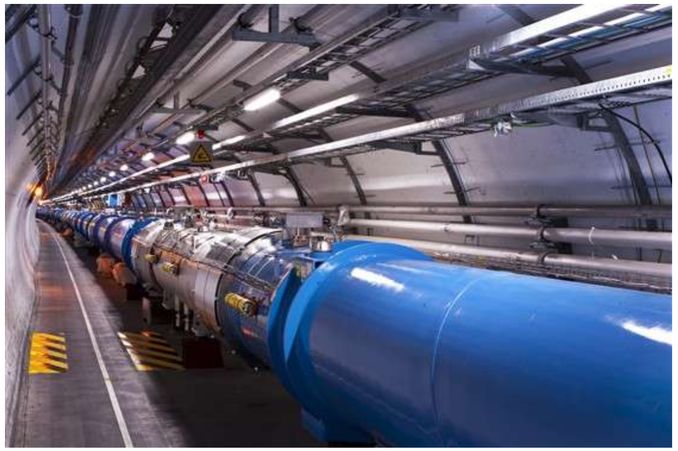
1501.04943

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

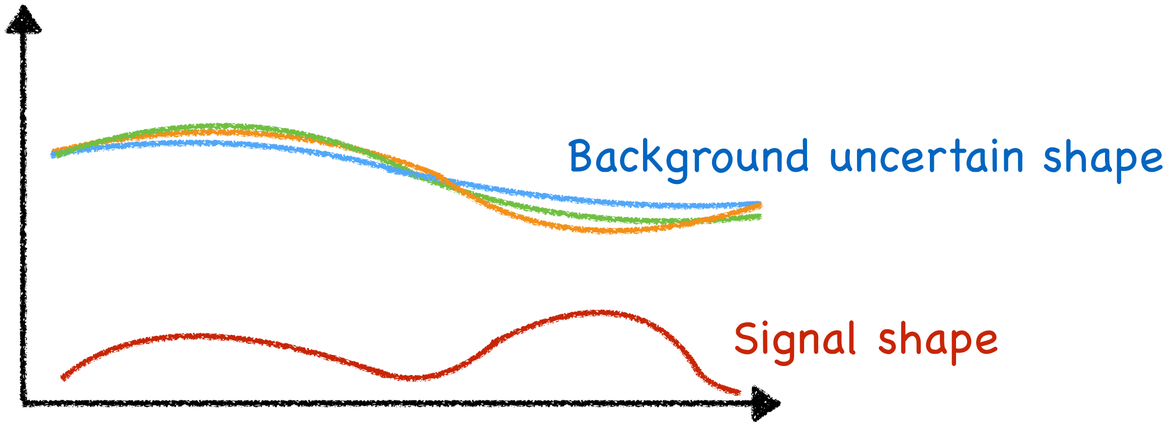
Known sources of differences between simulation and data… will systematically bias our measurements

Observable Sensitive to Nuisance Parameters

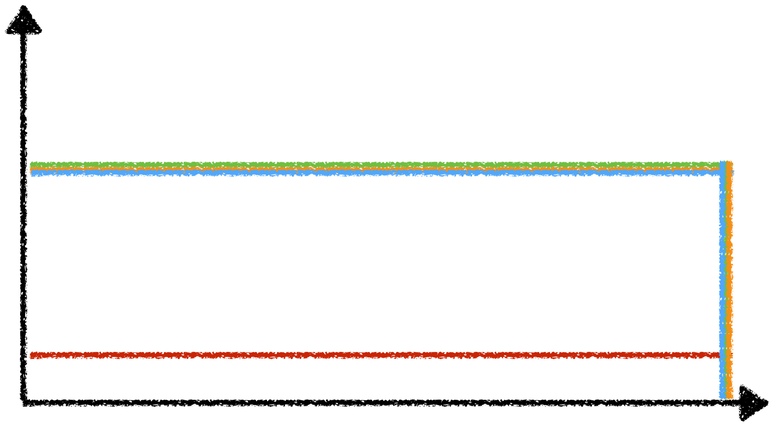
Traditionally, we reduce impact of NP by sacrificing something:

- 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

SOURCE

MNIST

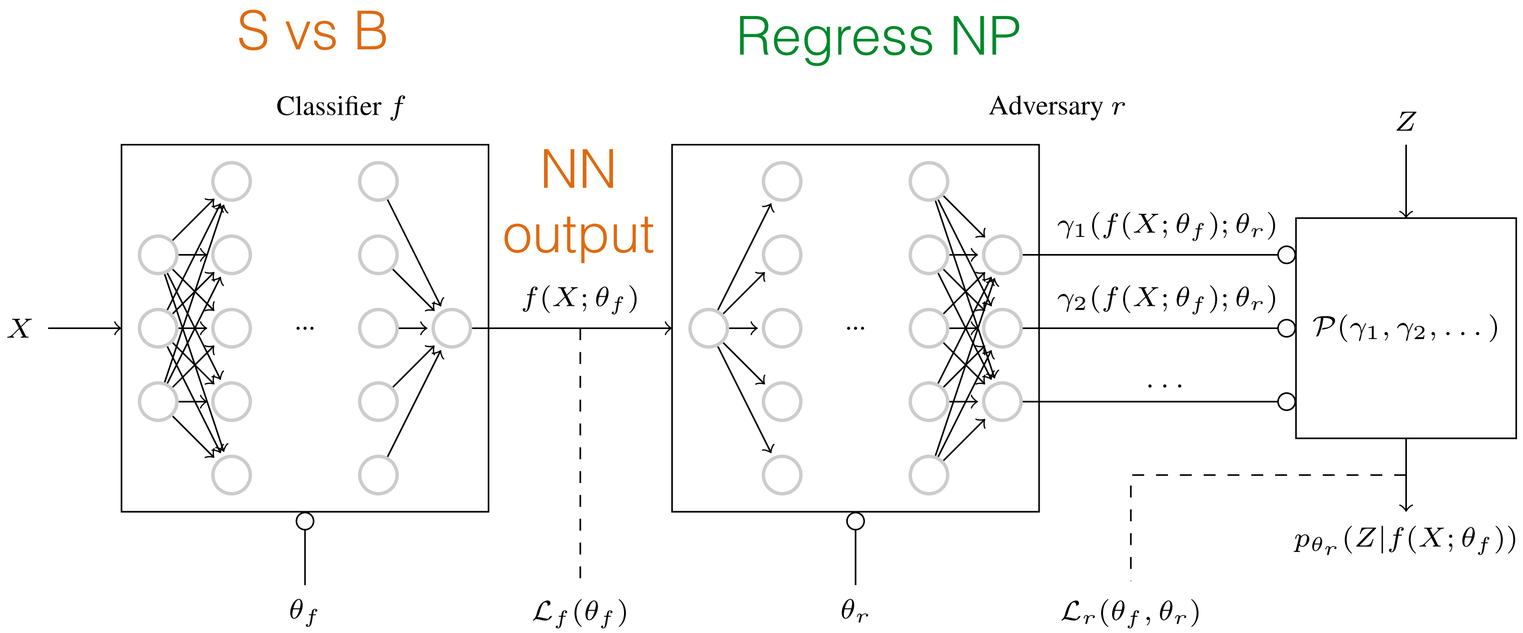
TARGET

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.

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

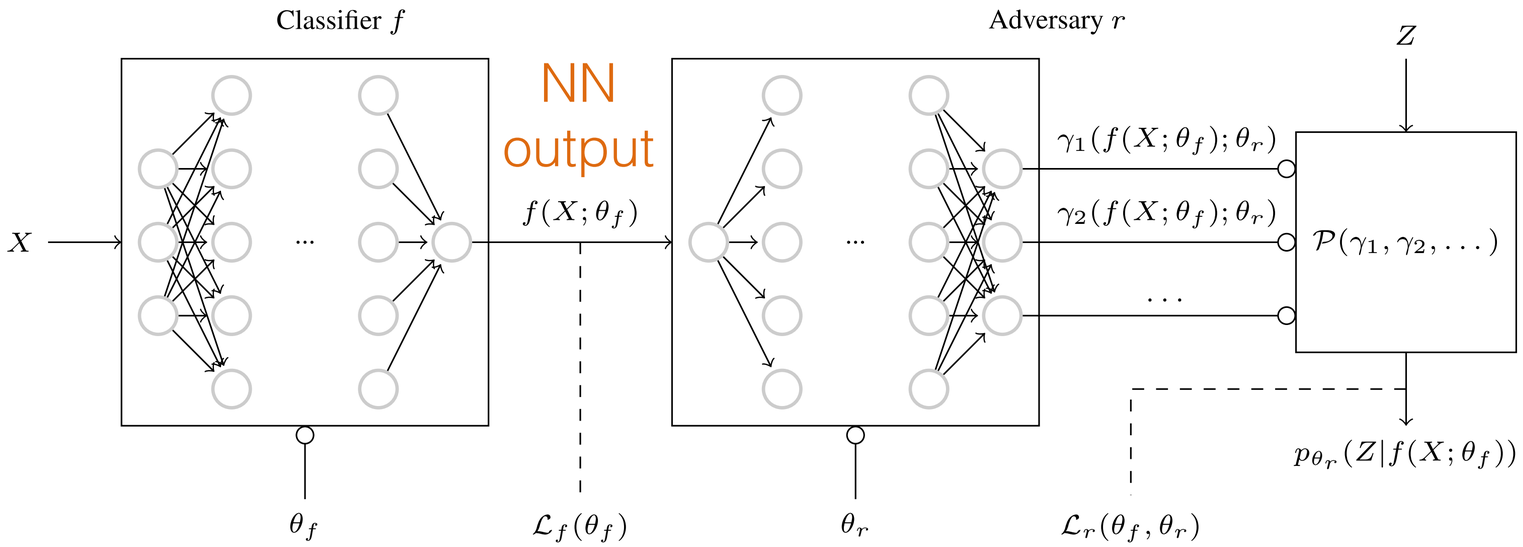
Learning to Pivot, Louppe et al.

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

Adversarial decorrelation

S vs B

Regress NP



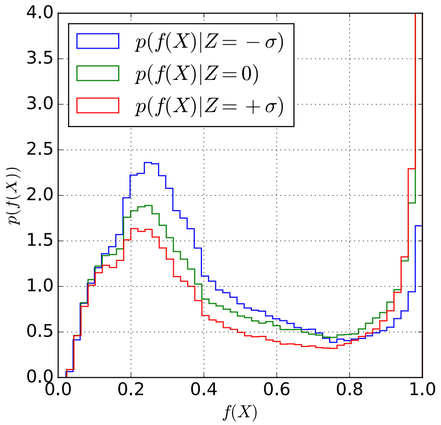
To fool the adversary, classifier output should be decorrelated to Z

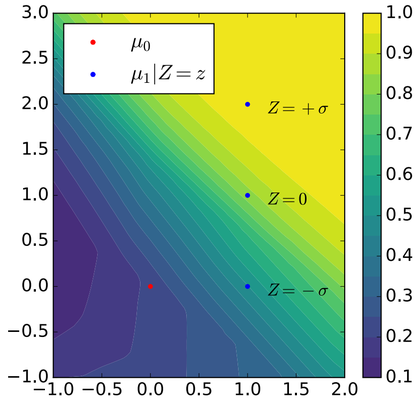
Learning to Pivot, Louppe et al.

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

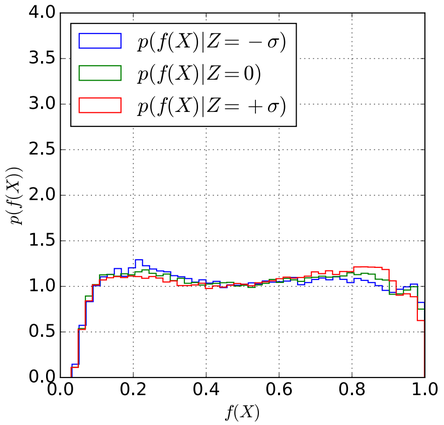
ML-Decorrelation Methods

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

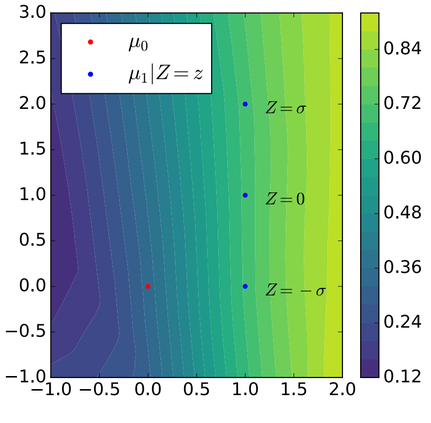




Adversarial Decorrelation



Classifier output for various values of Z



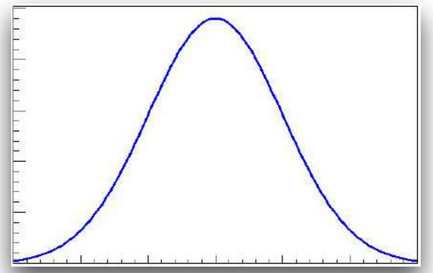
Learning to Pivot, Louppe et al.

Pause for questions

Eg:
- What is a nuisance parameter?
- Is it ethical to make two networks fight each other?
- ...

What if we could do better ?

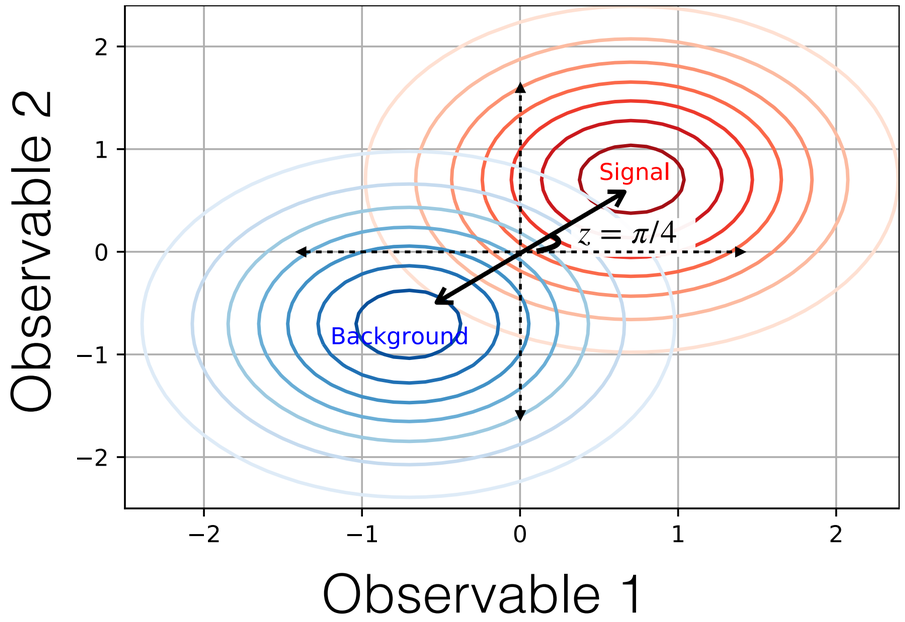
What if we could do better ?

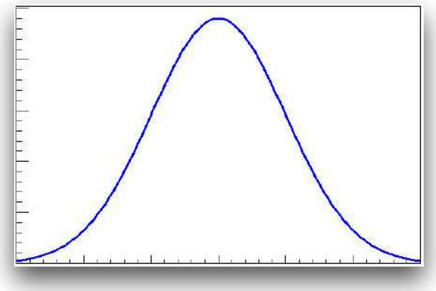


z = Nuisance Parameter

Prior

What if we could do better ?





z = Nuisance Parameter

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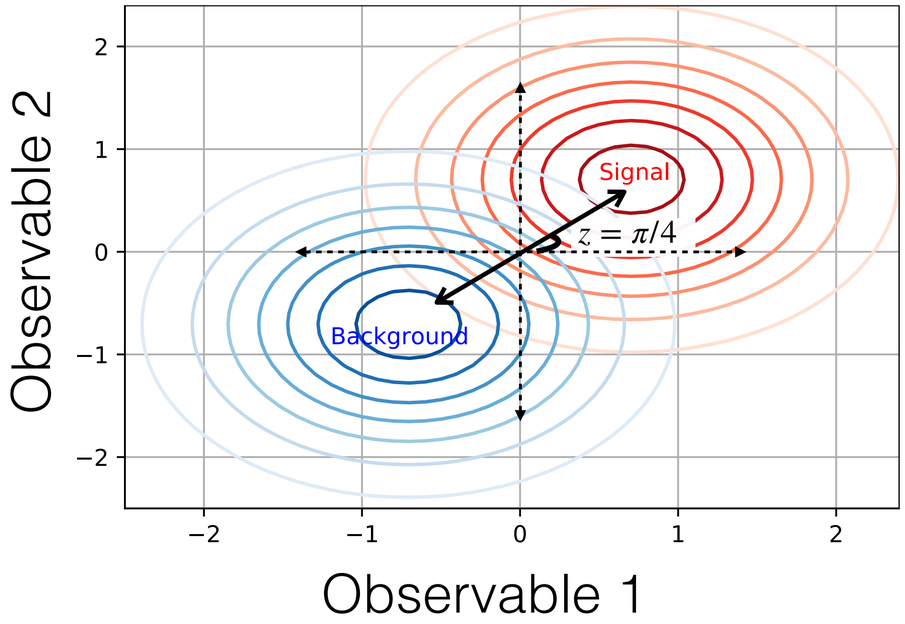

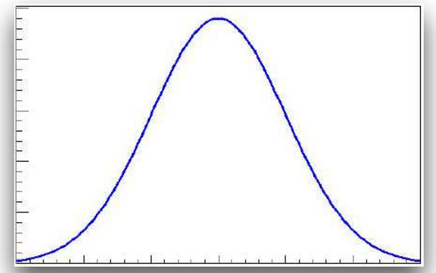

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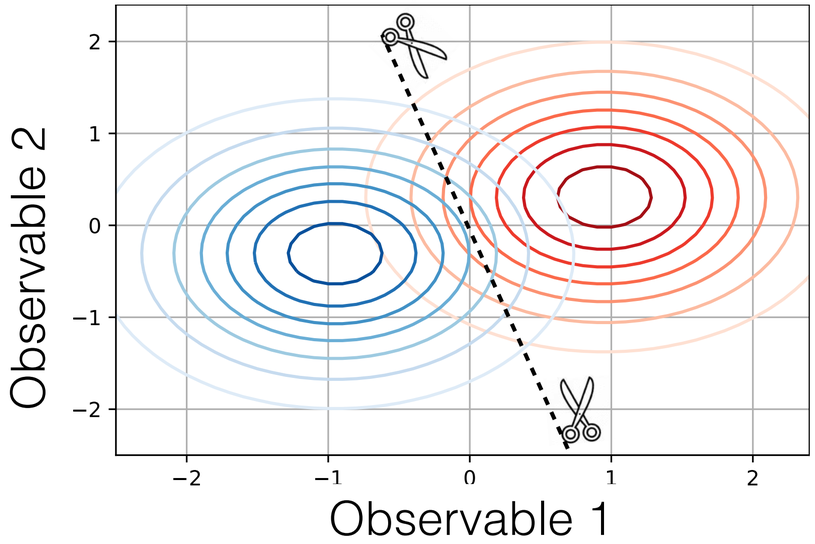

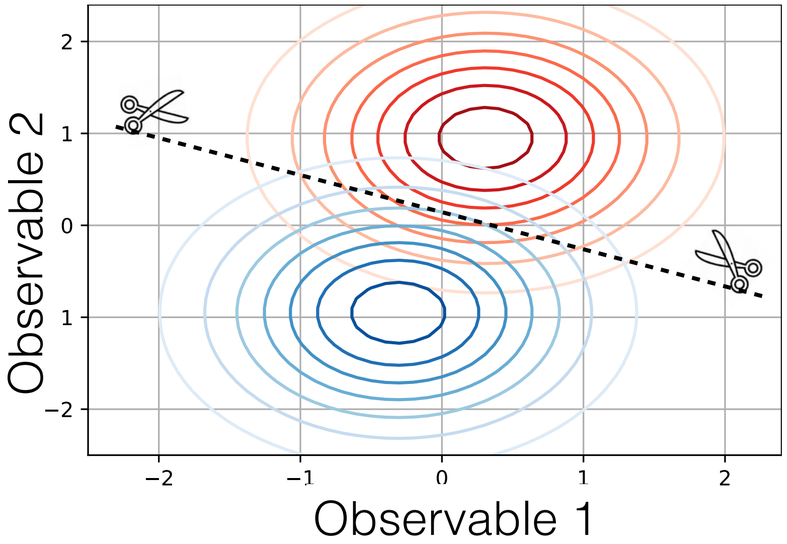

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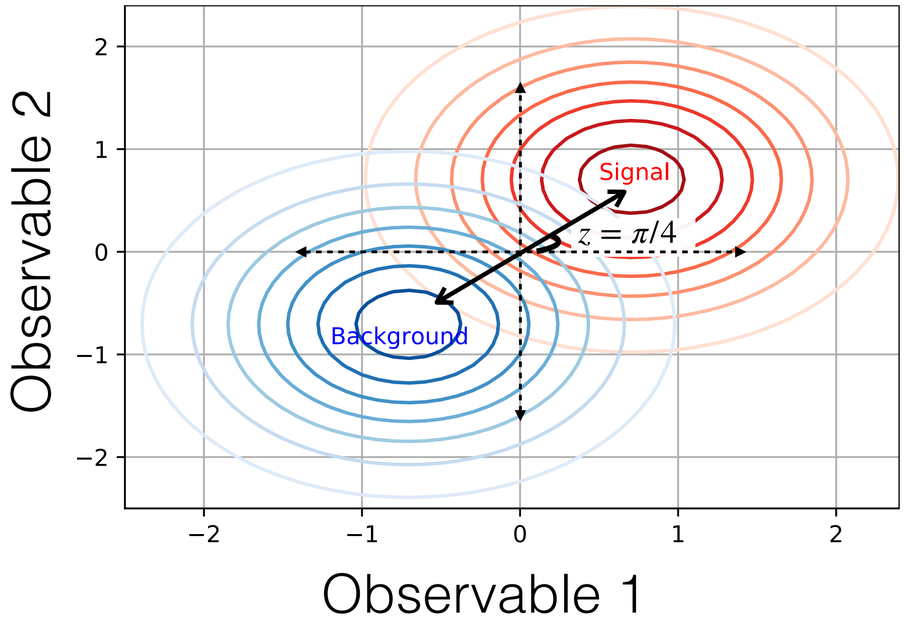

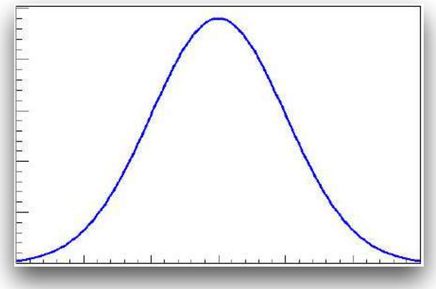

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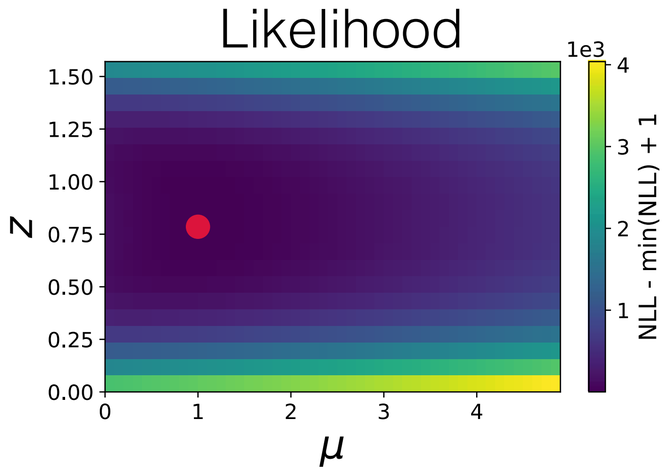
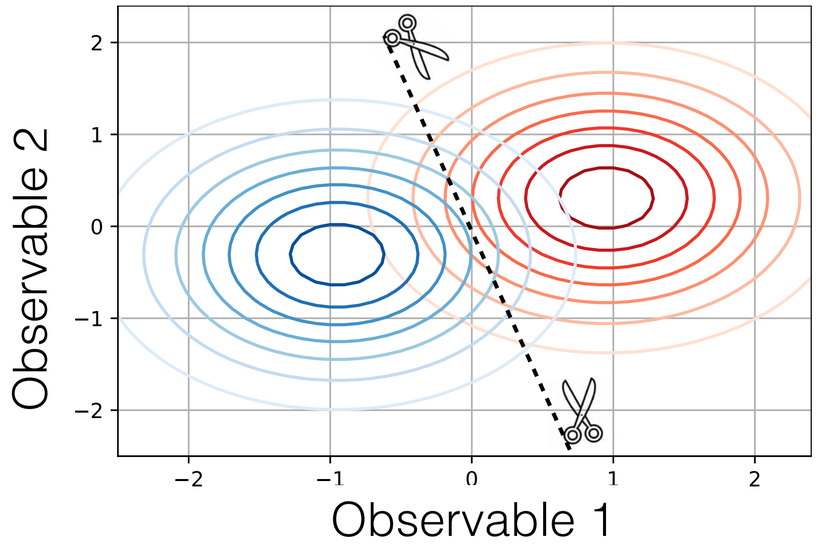
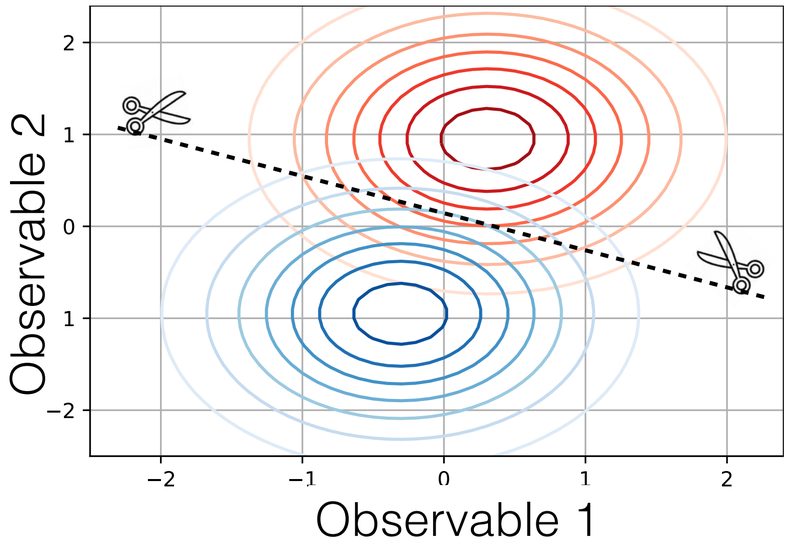
Prior

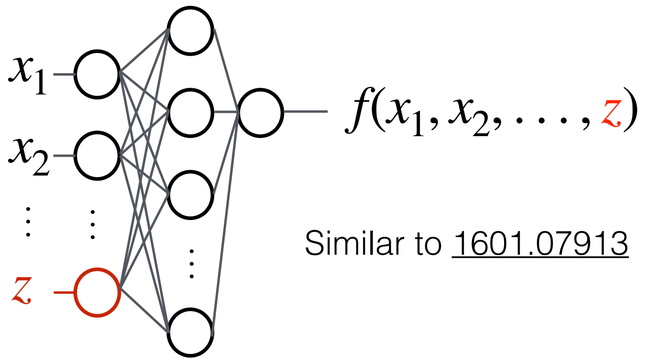




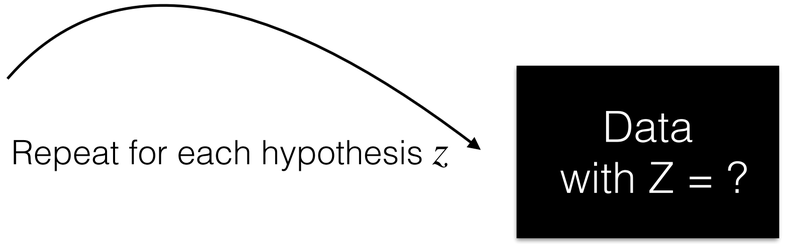


Opposite of decorrelation: Uncertainty-aware learning

- Propagate uncertainties through the classifier in an “uncertainty aware” way



Similar to 1601.07913



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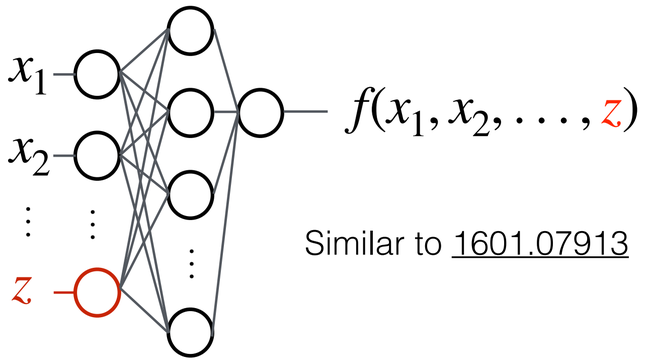

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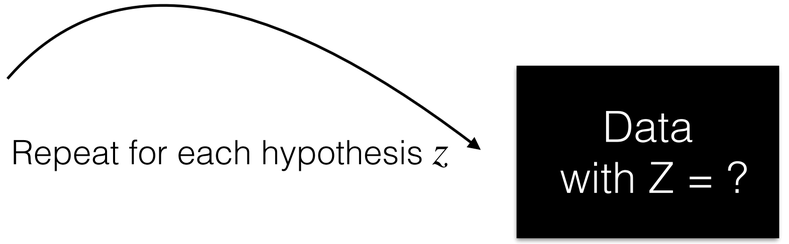
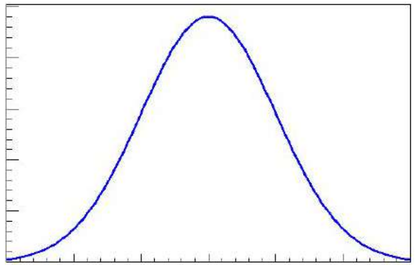


- Intuition: Allow the analysis technique to vary with Z
  You always get the best classifier for each value of Z

- Profile Z + incorporate prior

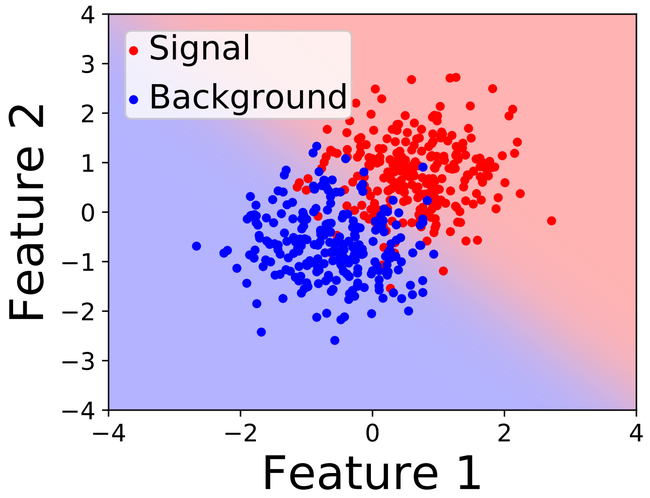


Nominal and Systematic Up Examples

Baseline Classifier

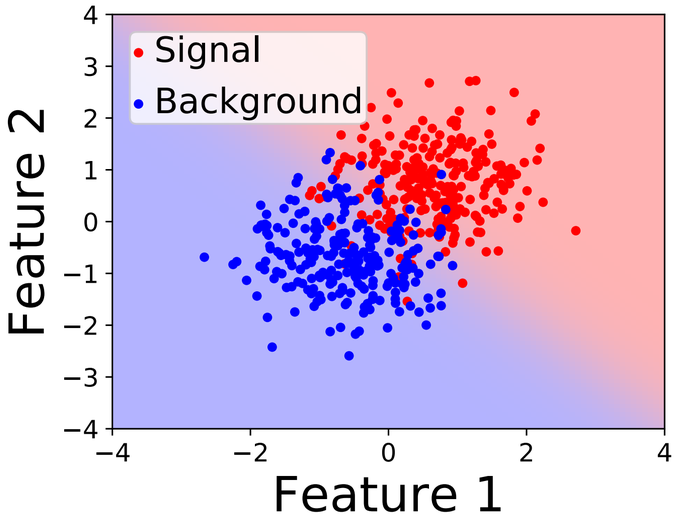
Uncertainty-Aware Classifier

Nominal "Data"



AUC=0.978

Optimal



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Optimal

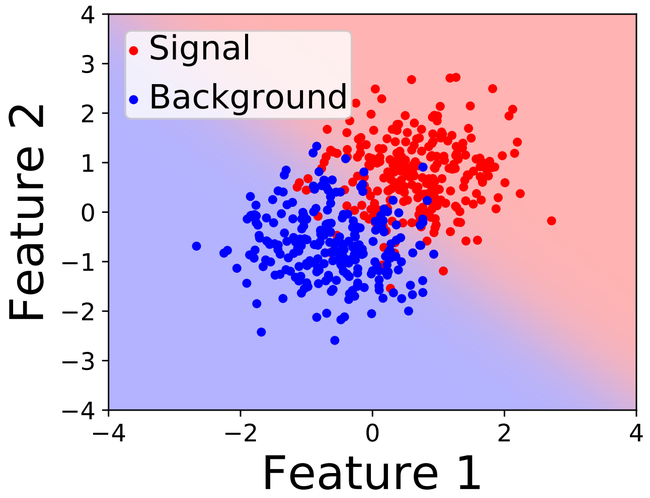
SystUp "Data"

Nominal and Systematic Up Examples

Baseline Classifier

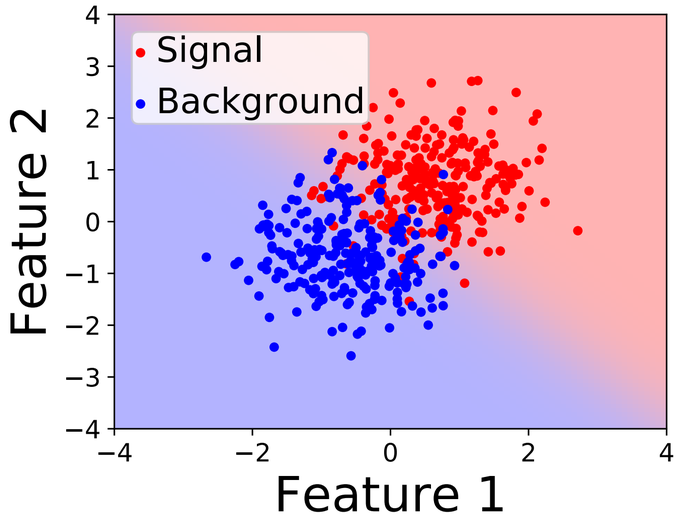
Uncertainty-Aware Classifier

Nominal "Data"



AUC=0.978

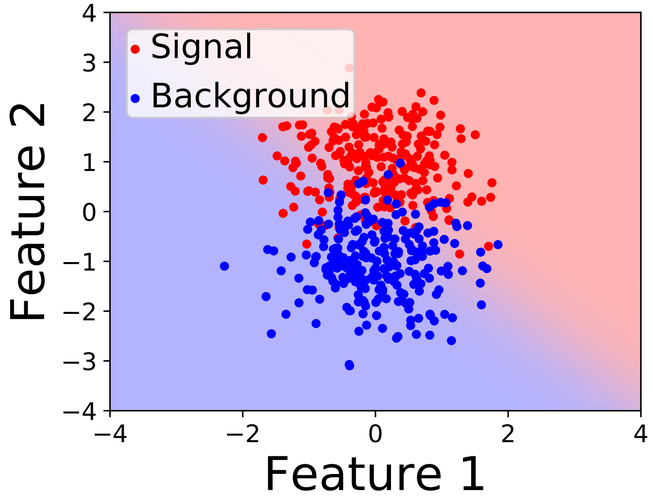
Optimal



AUC=0.978

Optimal

SystUp "Data"



AUC=0.924

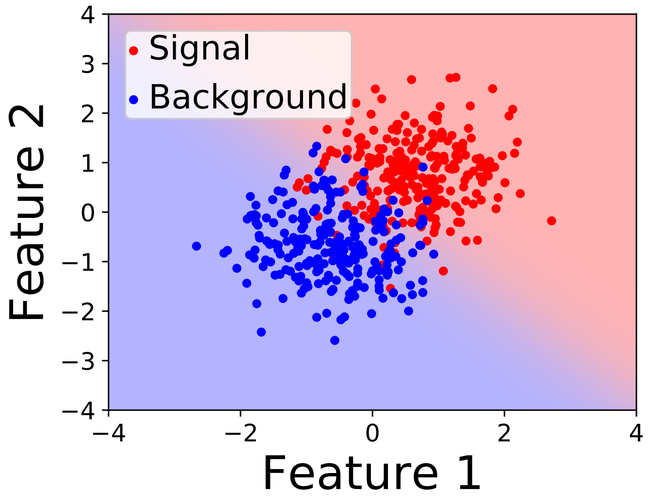
Sub-Optimal

Nominal and Systematic Up Examples

Baseline Classifier

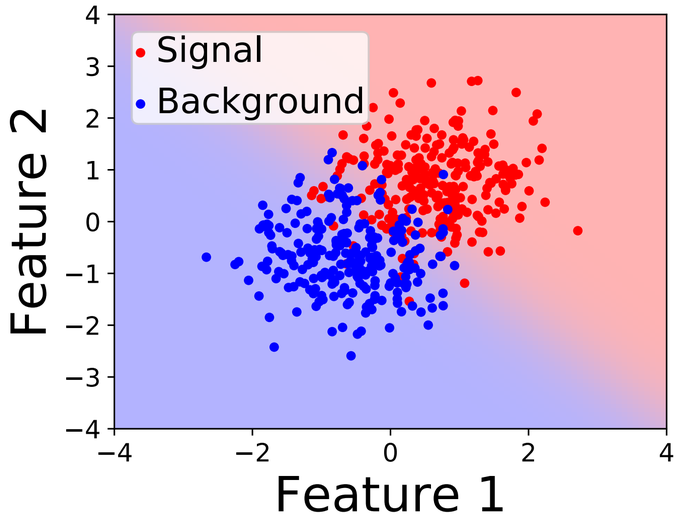
Uncertainty-Aware Classifier

Nominal "Data"



AUC=0.978

Optimal



AUC=0.978

Optimal

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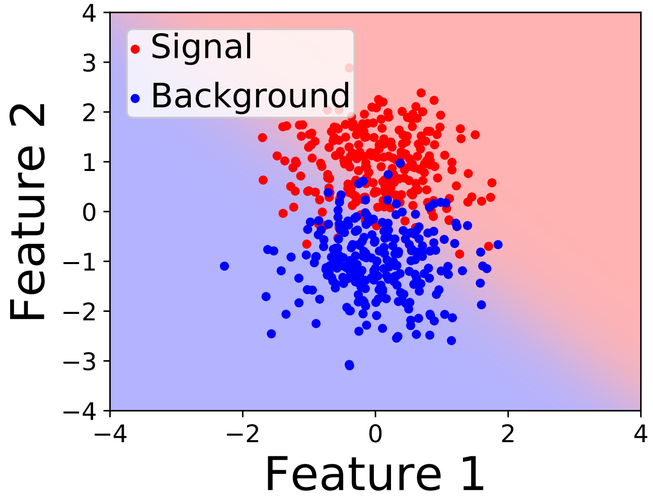
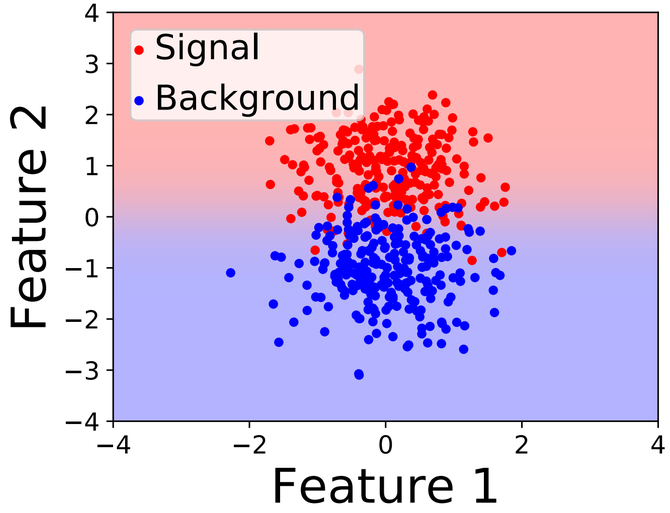


AUC=0.924

Sub-Optimal



AUC=0.978

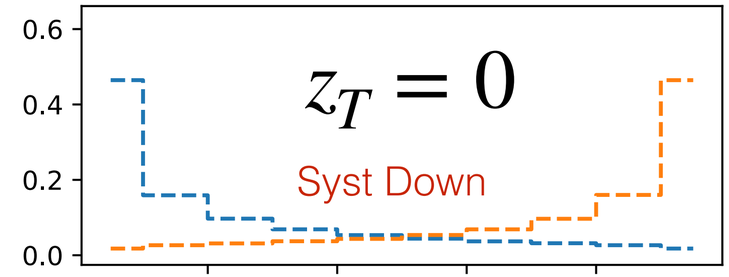
Optimal

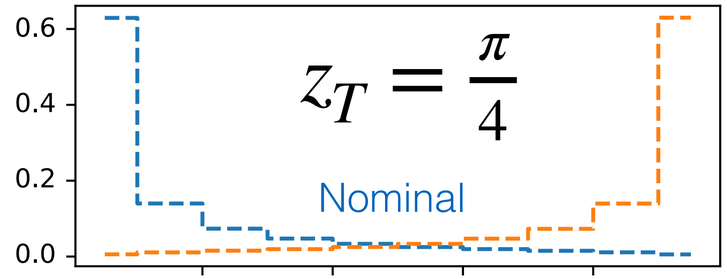
Syst-Aware Classifier is able to rotate its decision function based on Z while the Baseline Classifier decision function remains frozen

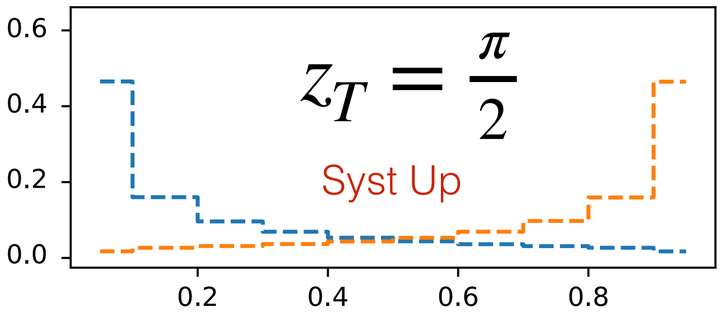
We don’t know Z in collision data, what value do we use ?

Scan the 2D Likelihood space in Z vs μ

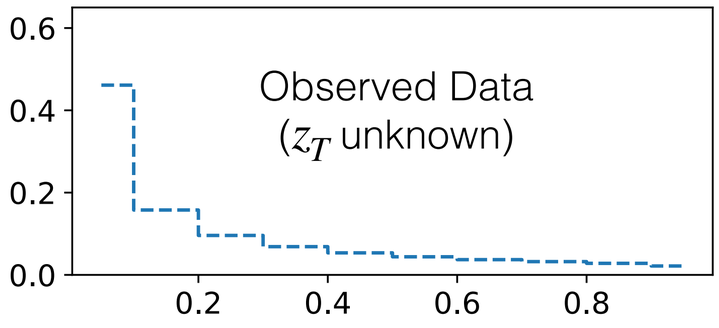
Template **Baseline Classifier** Score Histograms for various Z







$z_T \rightarrow$ True z



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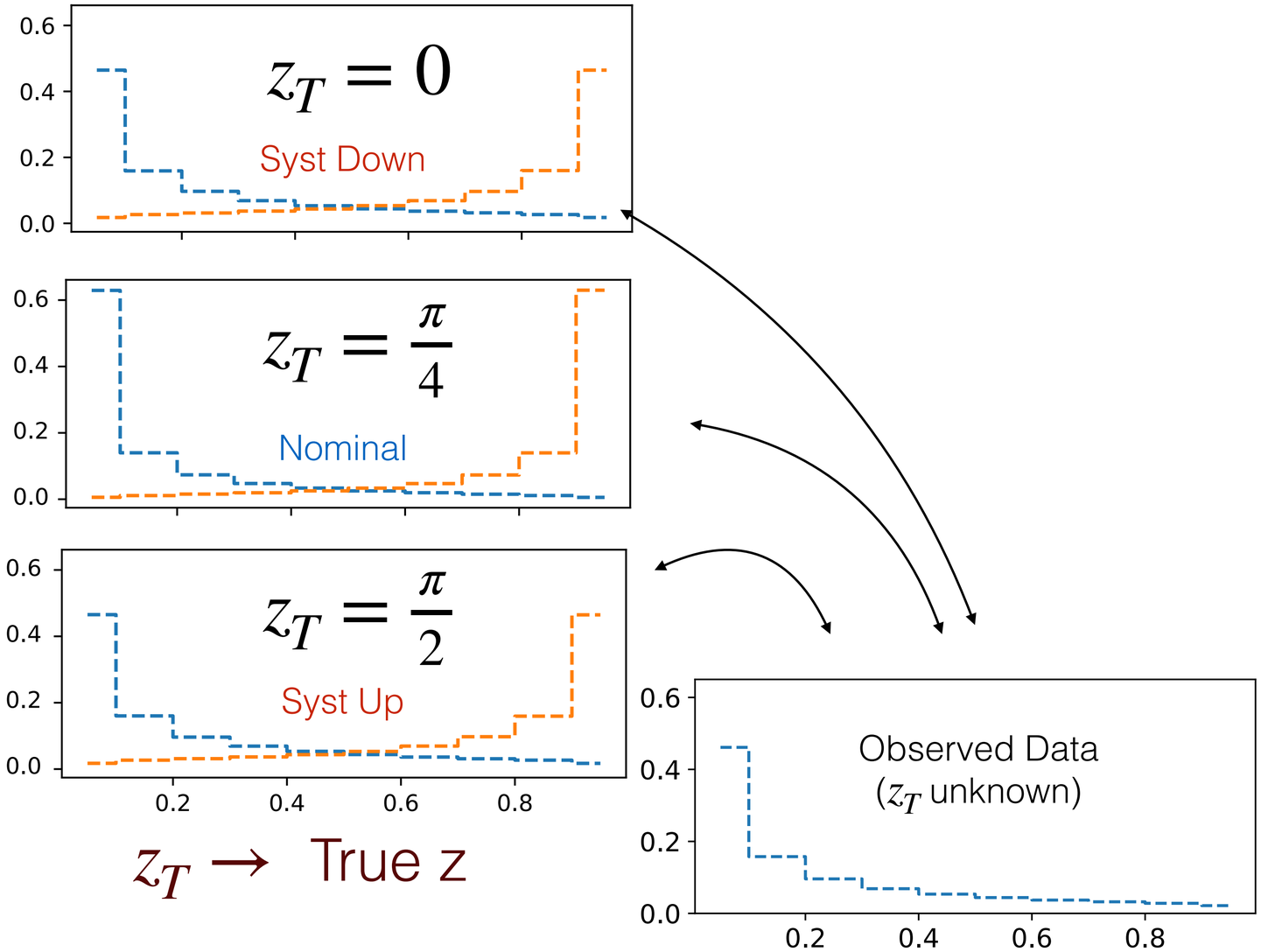

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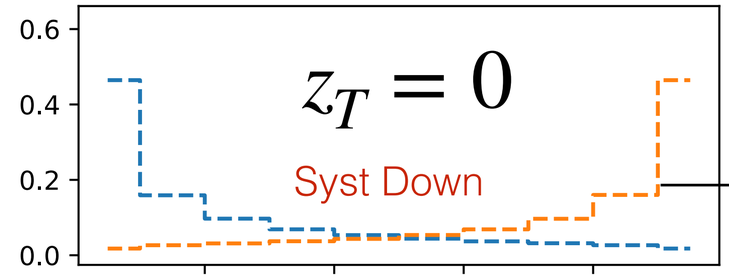

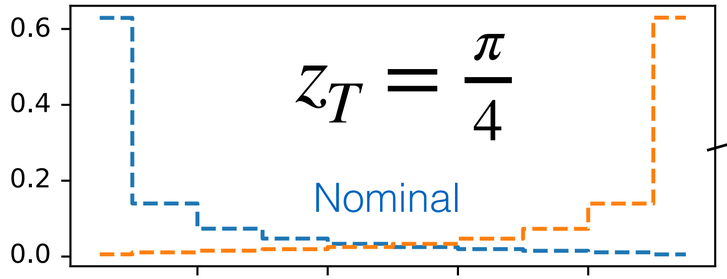

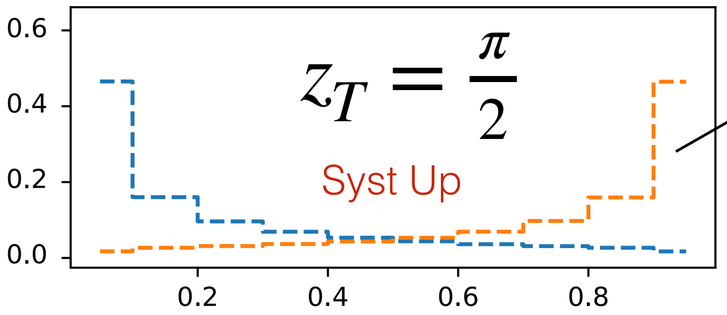

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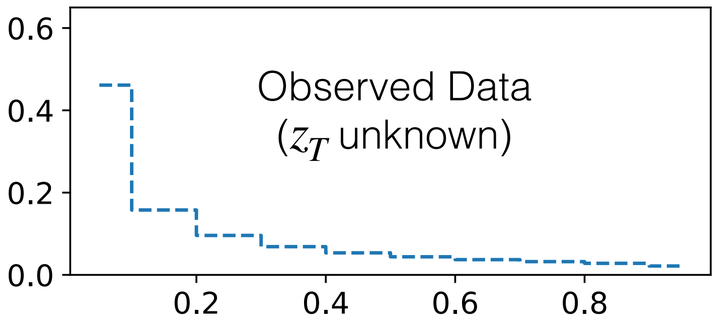

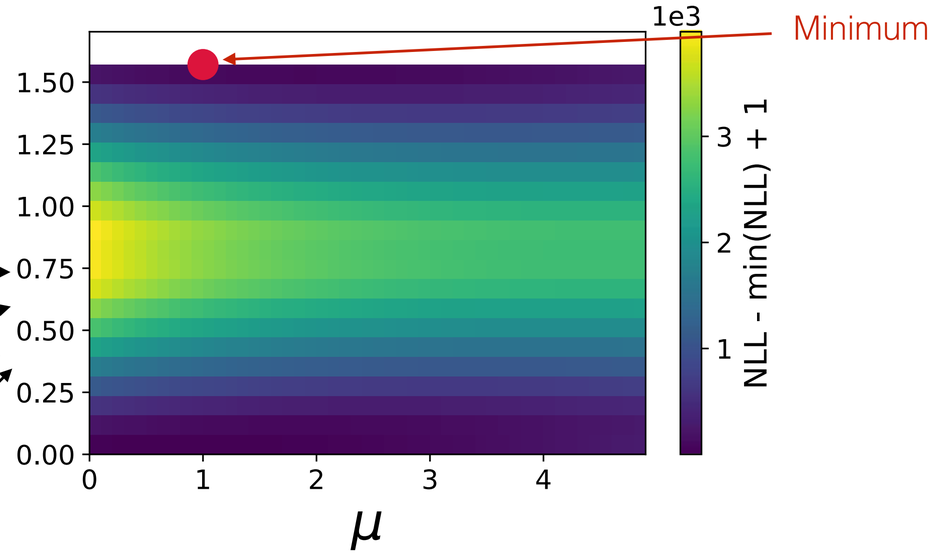

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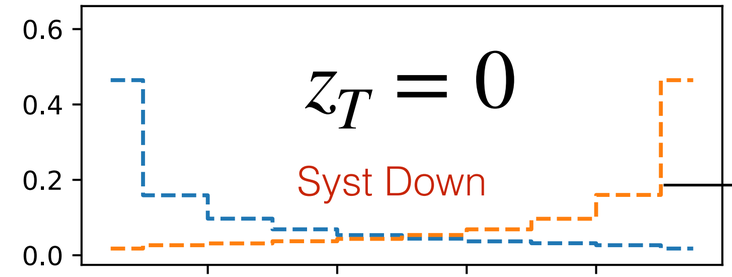

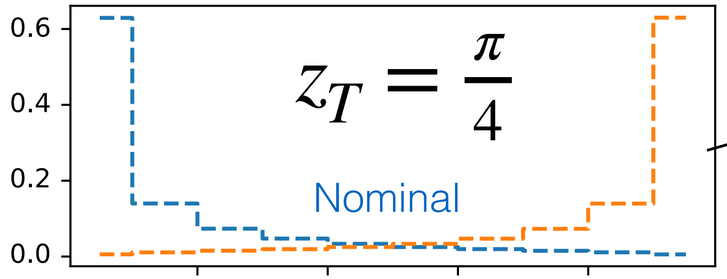

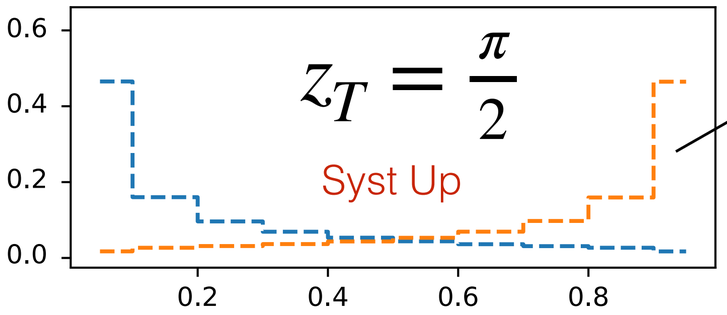

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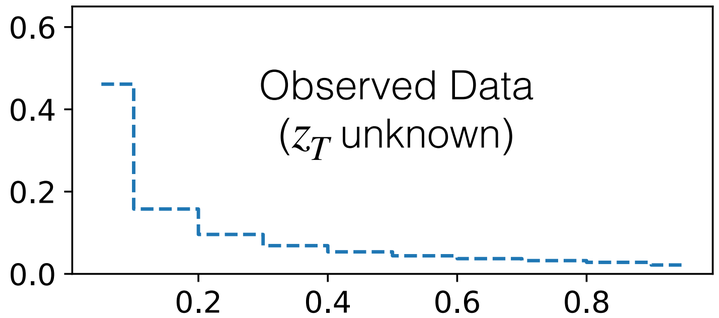

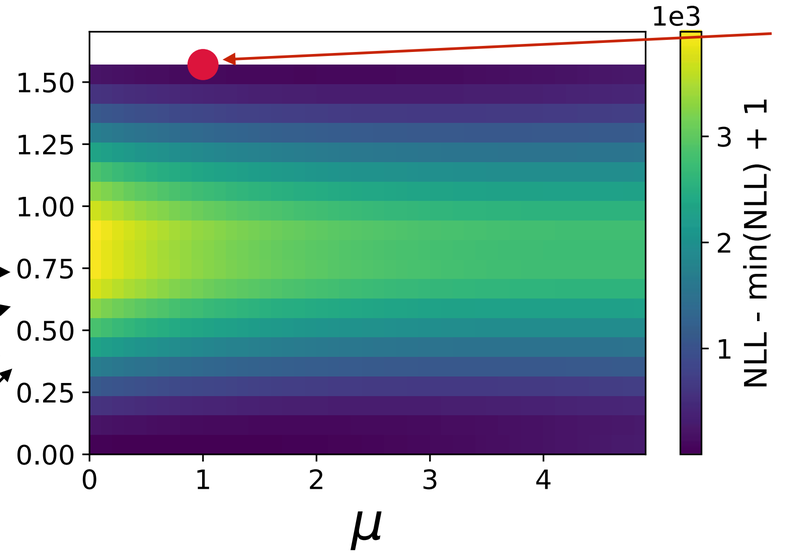

Likelihood statistical component = Poisson per histogram bin
Likelihood systematic component = Gaussian (1, 0.5) as prior on Z
Full Likelihood = statistical + systematic

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

But could be done unbinned/KDE too

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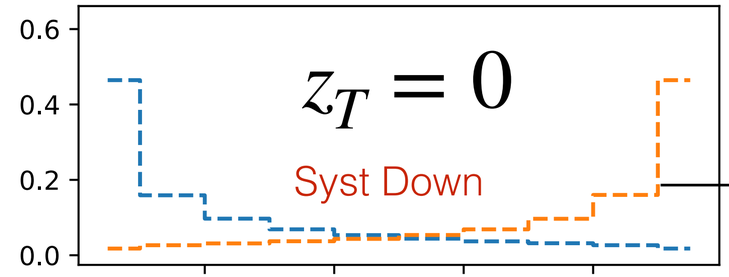

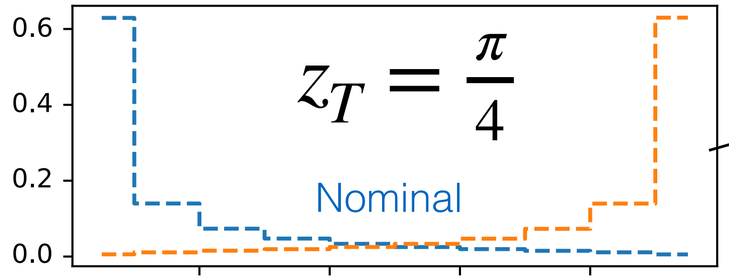

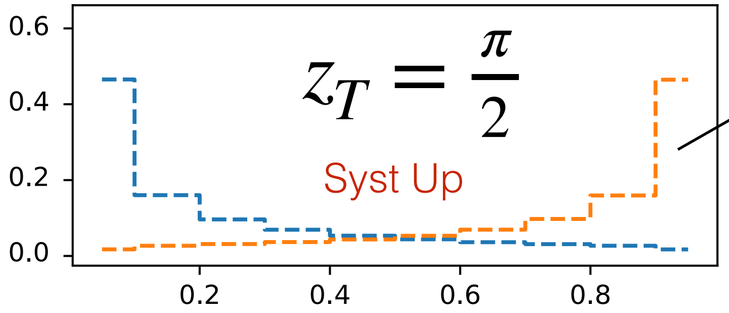

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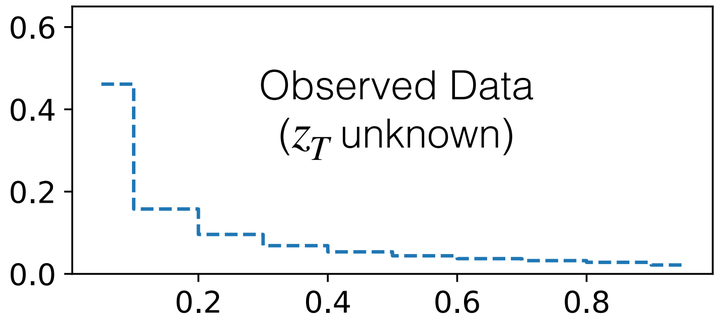

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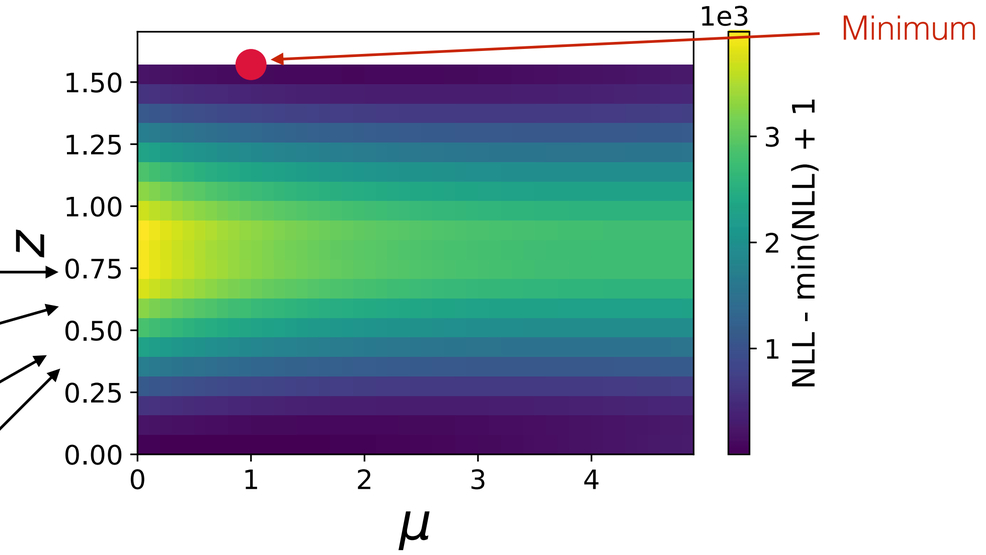

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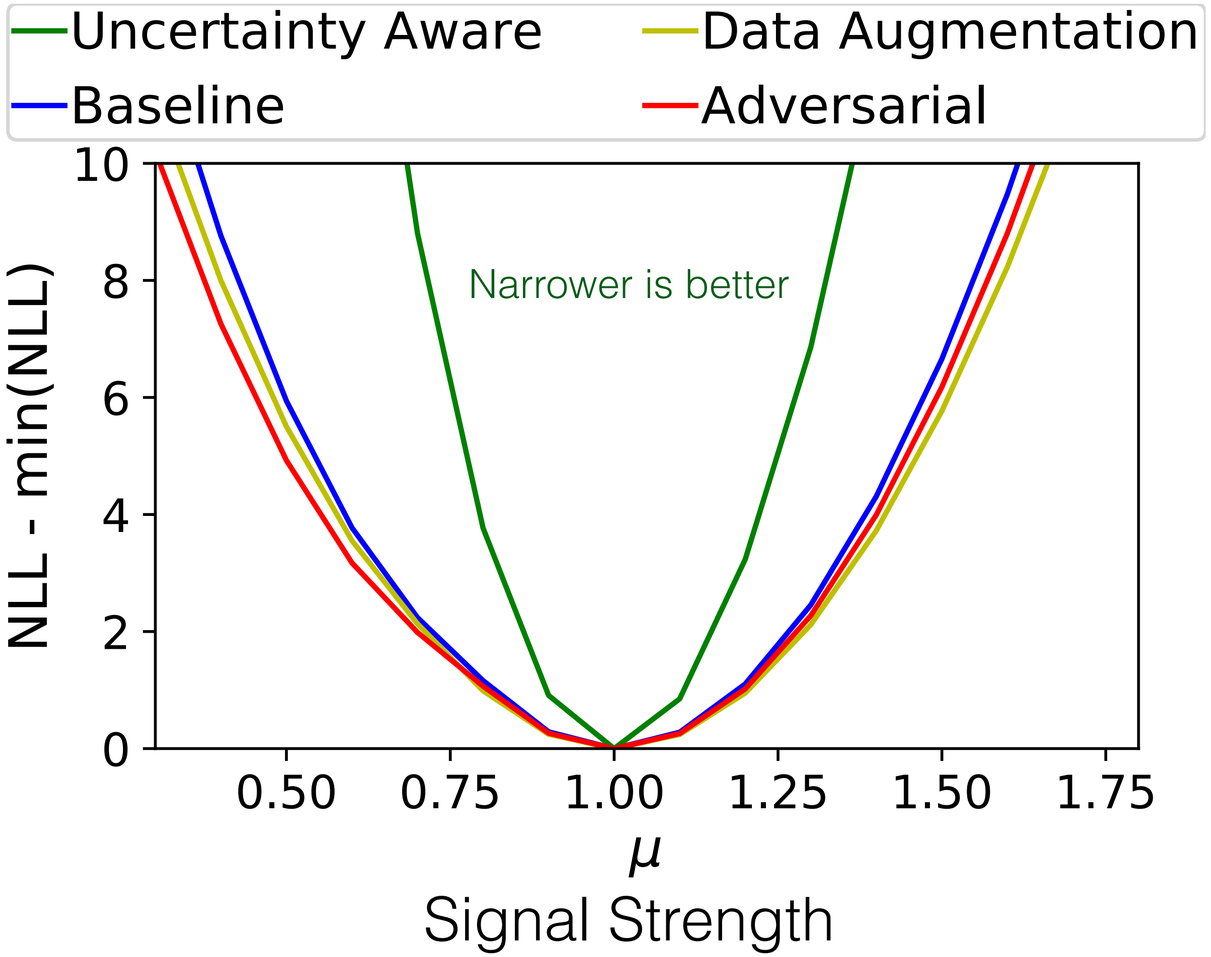
$$+ \left(\frac{z - z_0}{\sqrt{2}\sigma_z}\right)^2,$$

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

Better final measurements!



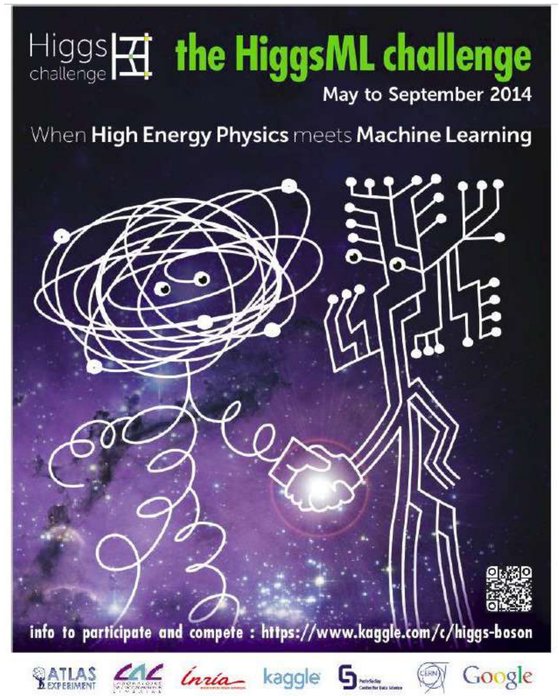
Narrower ⇒ Smaller [statistical + systematic] uncertainty on measurement

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

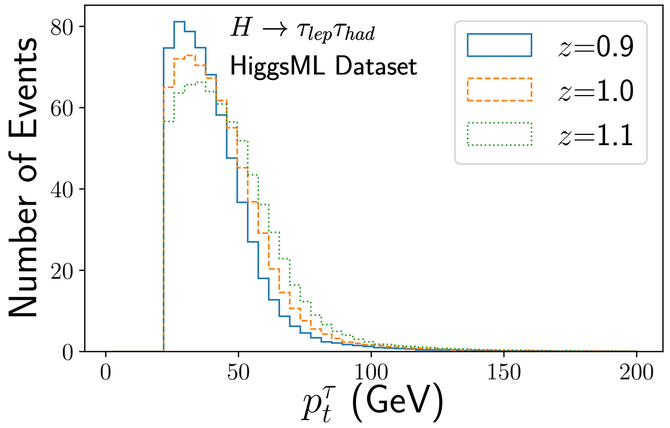
Pause for questions

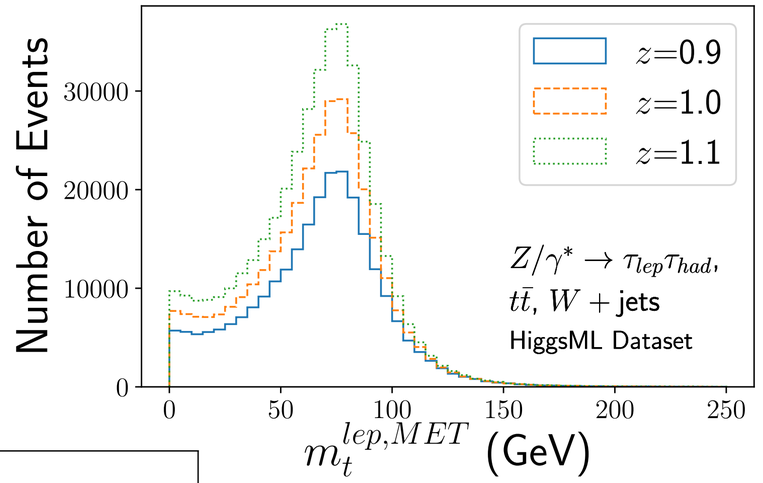
Eg:
- What is a prior?
- …

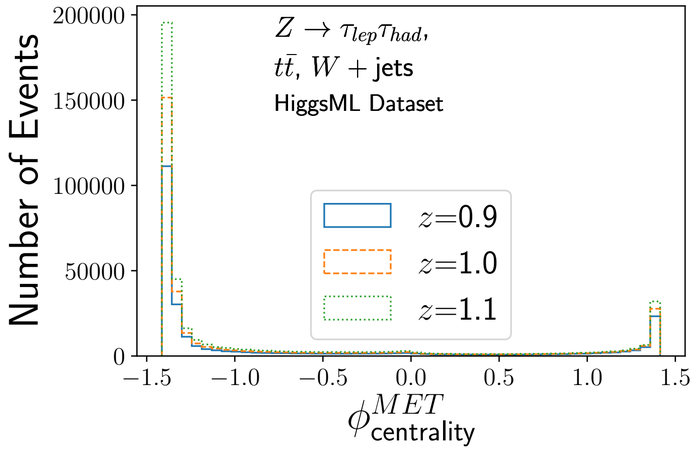
Real Physics Dataset with Tau Energy Scale (TES) as Z



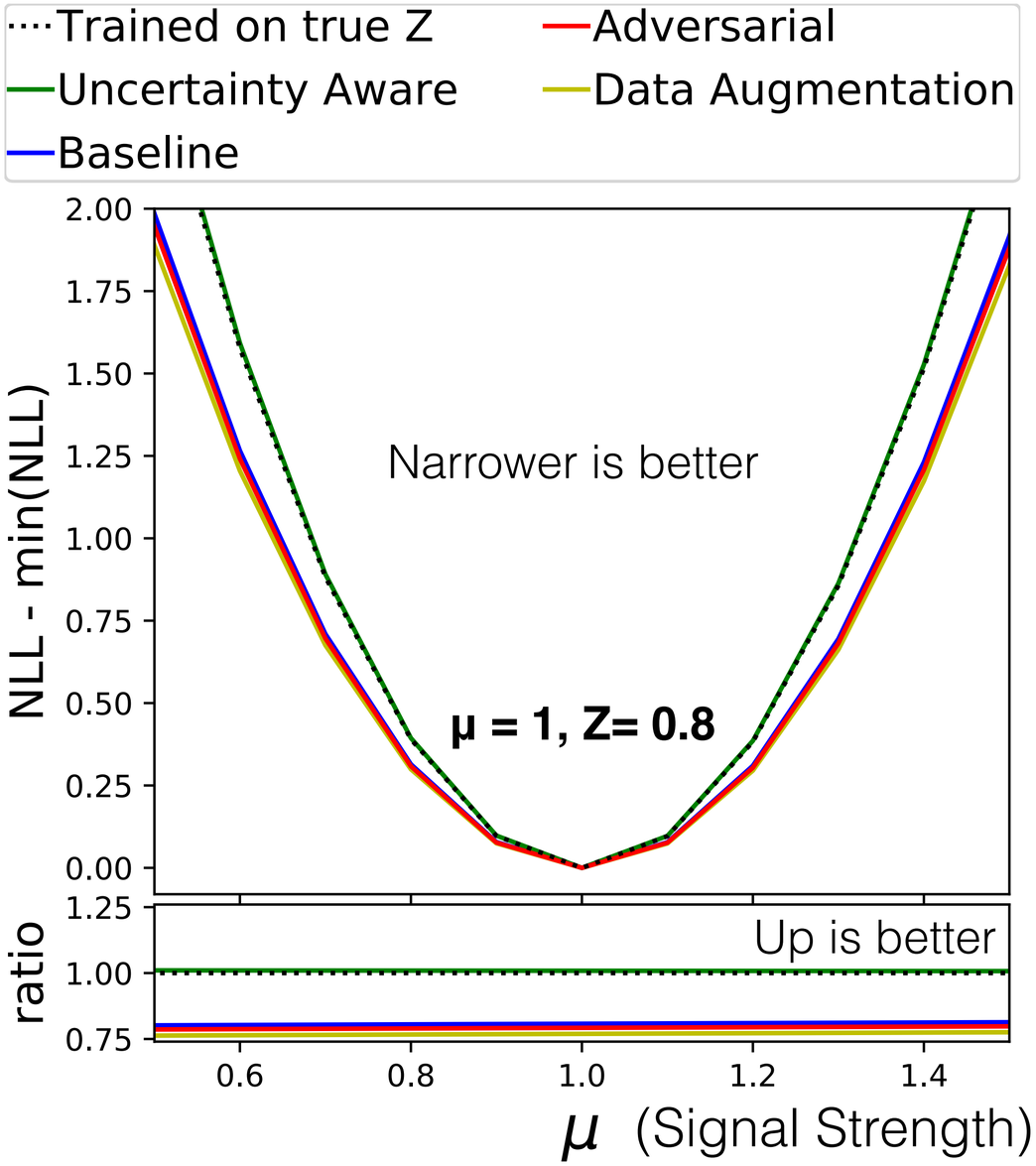
Parameter of Interest is Higgs signal strength μ, and TES is the nuisance parameter Z







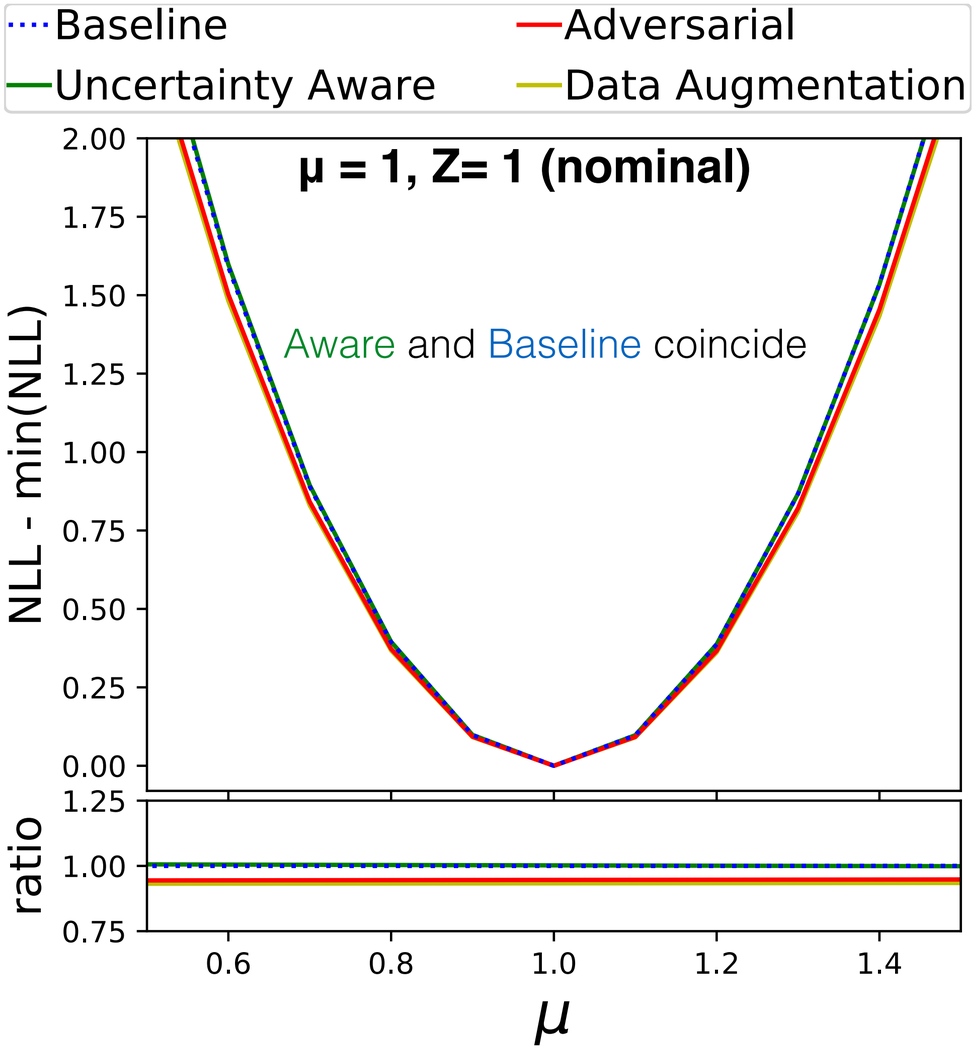
Test performance for “observed” data at Z below Nominal

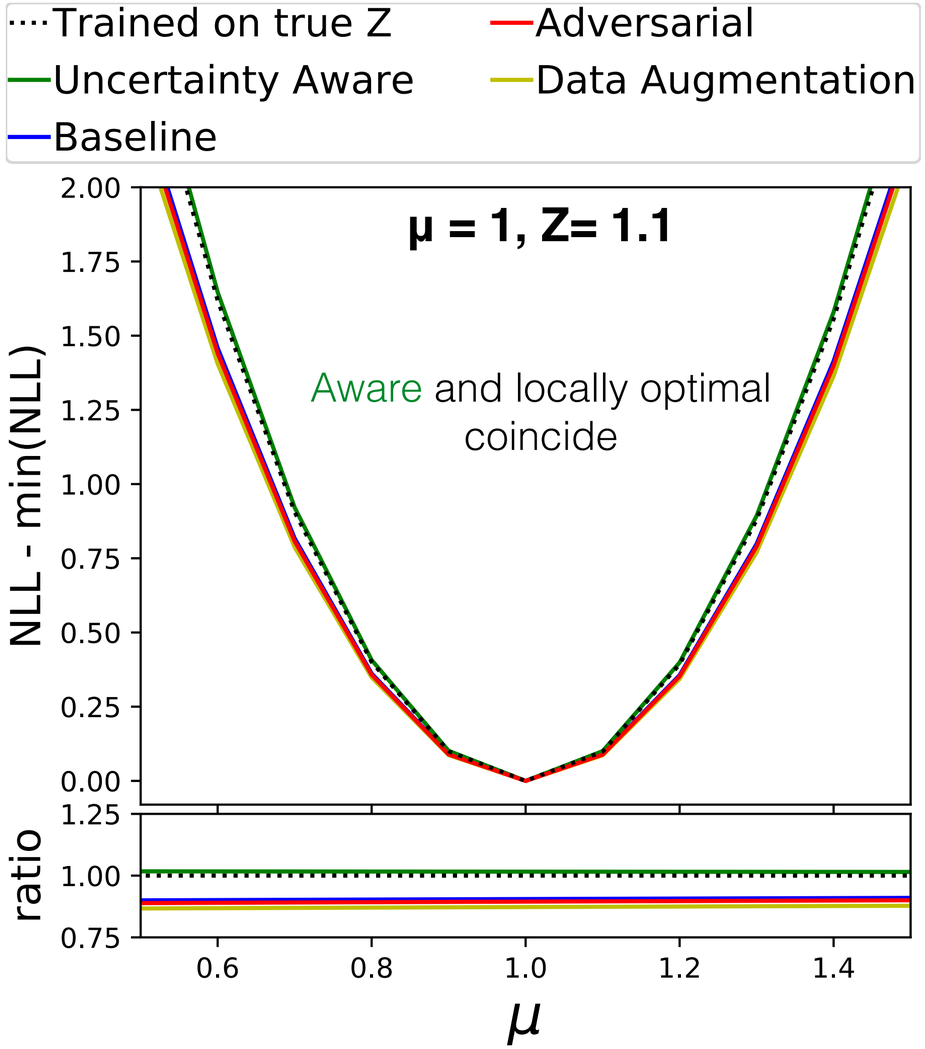


Uncertainty-Aware coincides with classifier trained on true Z

⇒ 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

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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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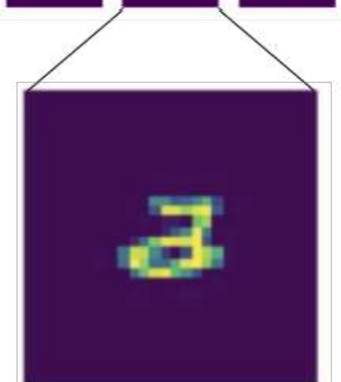


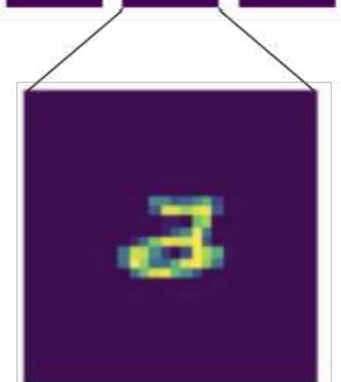
ERM → 2
ARM → a

arXiv:2007.02931

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

Idea fascinating also to ML researchers !

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



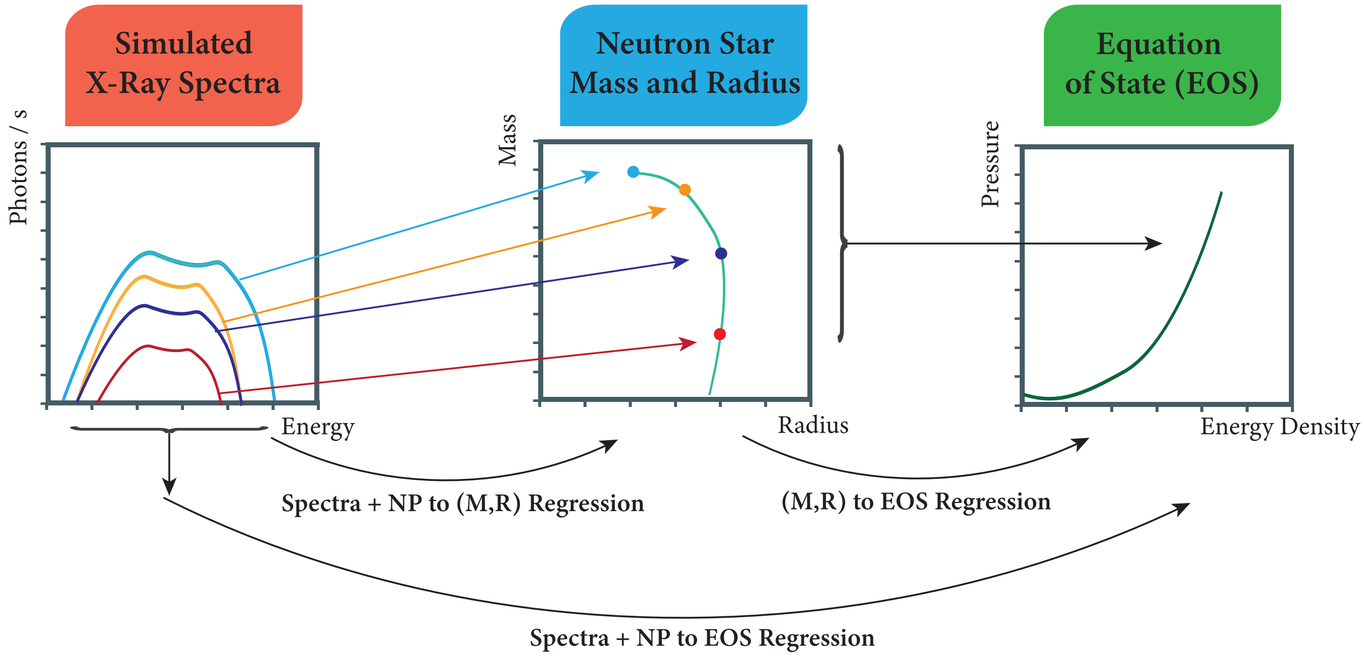
ERM → 2
ARM → a

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

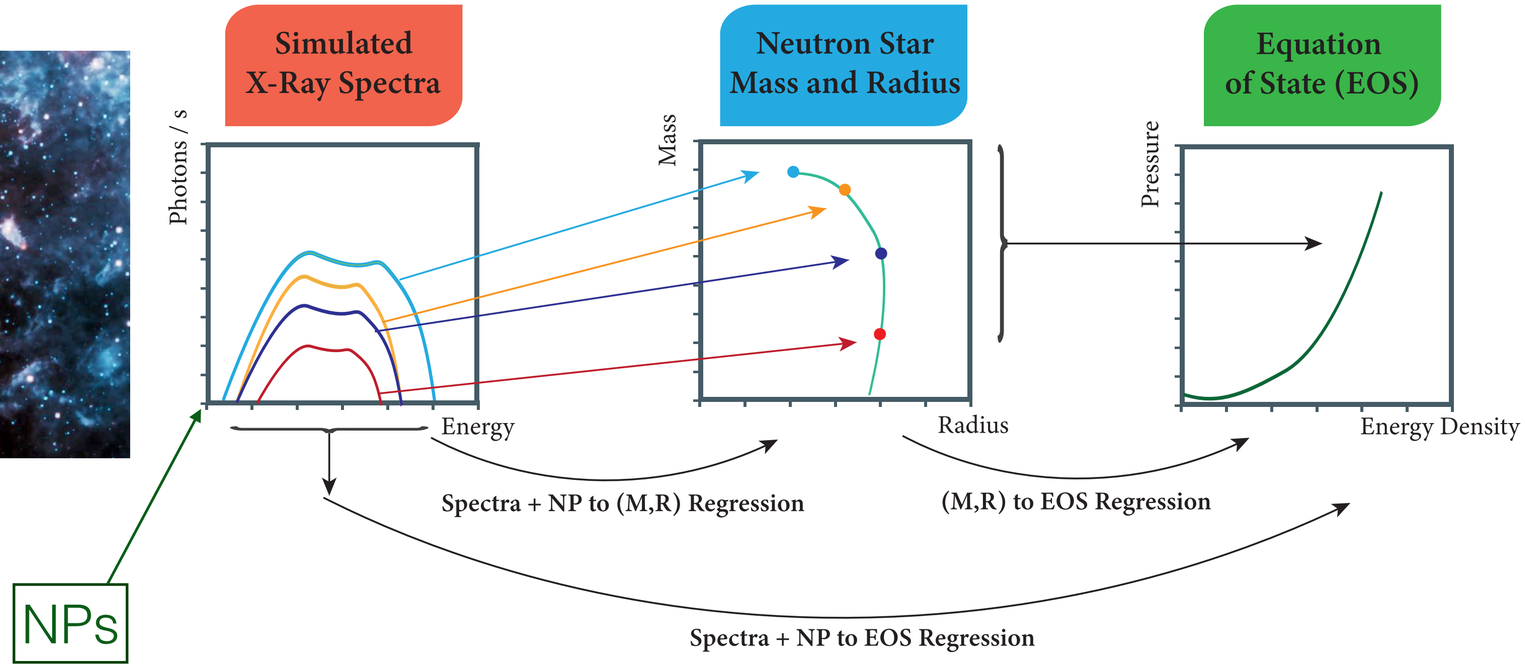
arXiv:2007.02931

An application in astrophysics

Application in Astrophysics: Full propagation of uncertainties



Application in Astrophysics: Full propagation of uncertainties

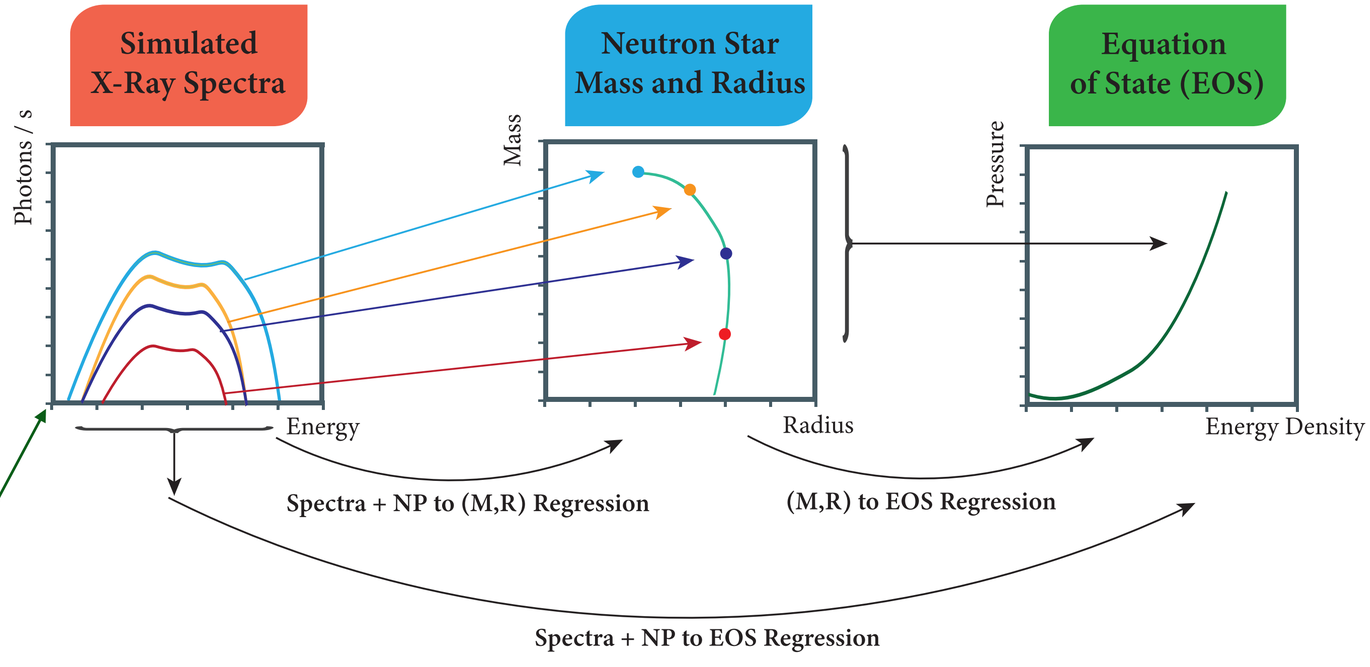


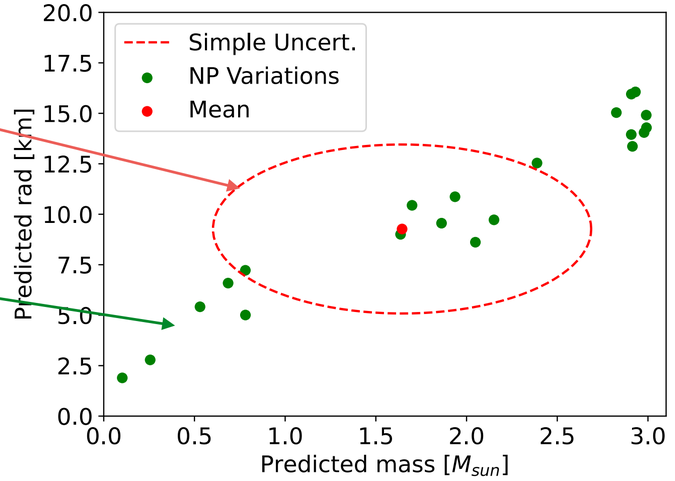
JCAP.020P.0922: Delaney Farrell, Pierre Baldi, Jordan Ott, Aishik Ghosh, Andrew W. Steiner, Atharva Kavitkar, Lee Lindblom, Daniel Whiteson, Fridolin Weber

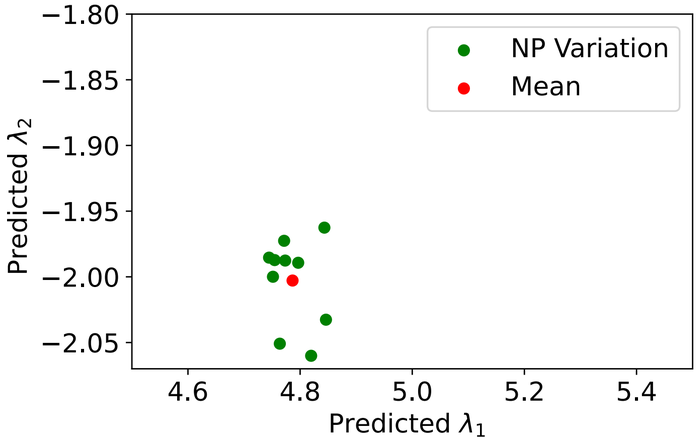
Application in Astrophysics: Full propagation of uncertainties

SOTA made a single point estimate + assumed uncorrelated Gaussian uncertainties

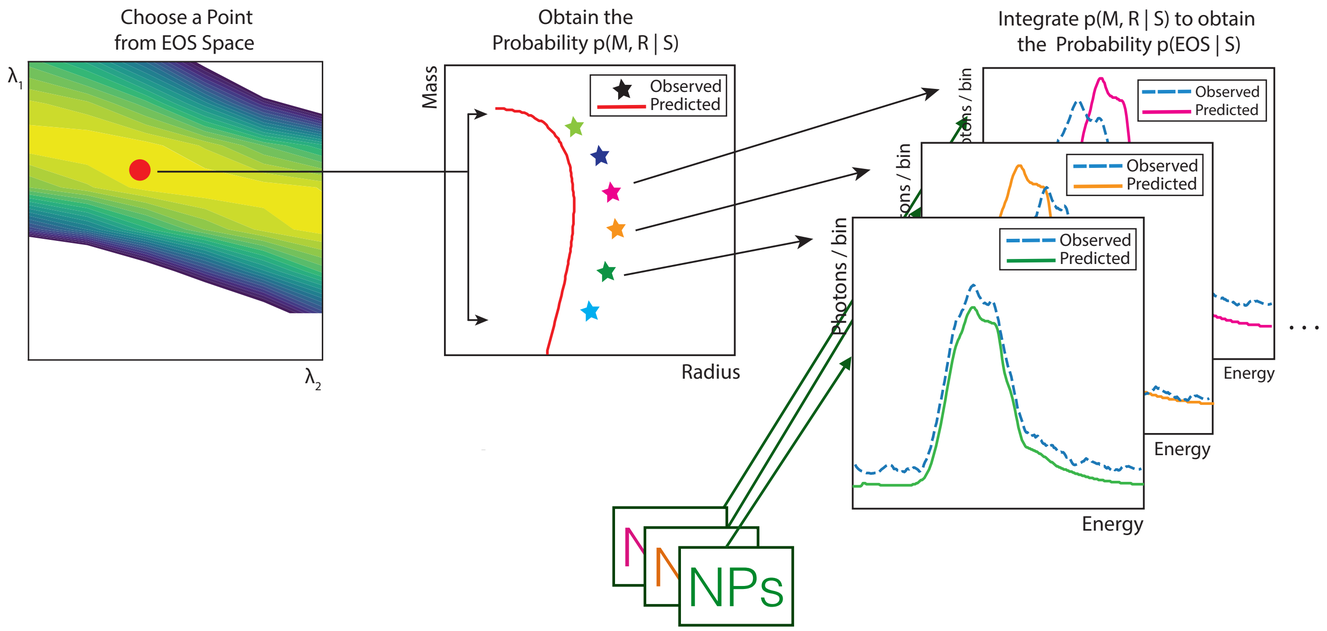
Real uncertainties look quite different







Learn forward process to access the likelihood



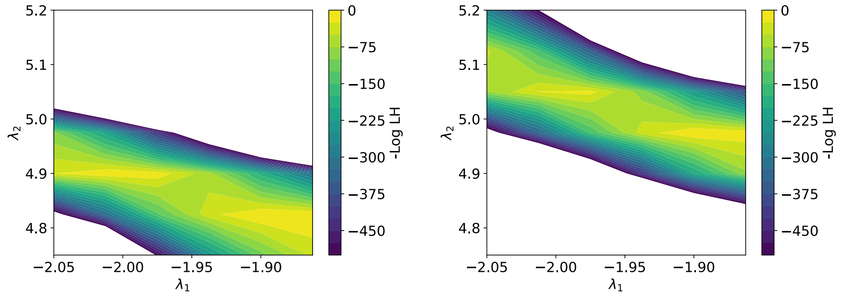
Deploy with ONNX Runtime to compute likelihoods on-the-fly

ONNX RUNTIME

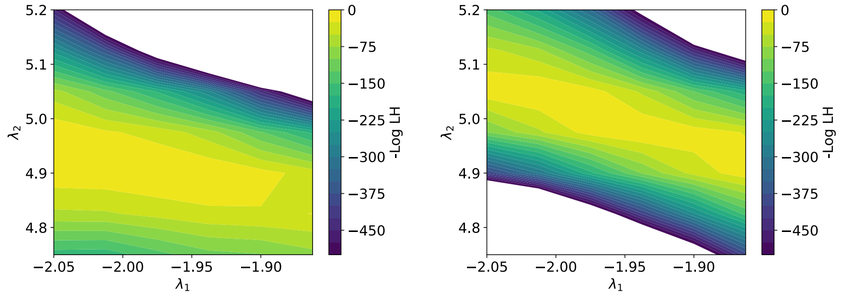
Nuisance Priors:

EOS parameter likelihoods:

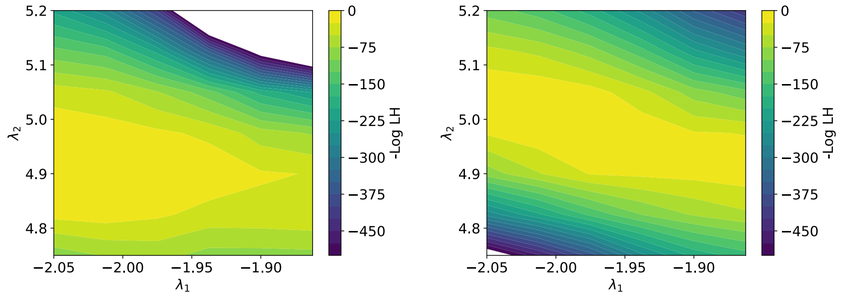
True:



Tight:



Loose:

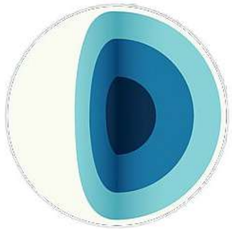


Paper in preparation

Forward process step-by-step

Intermediate steps remain interpretable physical quantities

Paper in preparation



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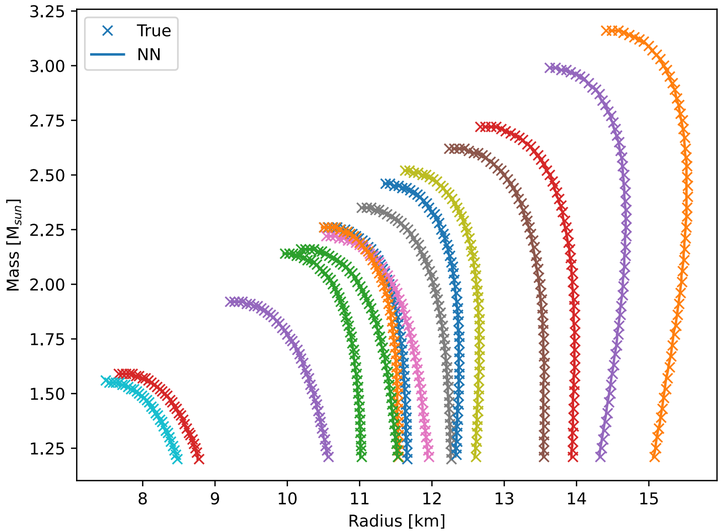
Intermediate steps remain interpretable physical quantities

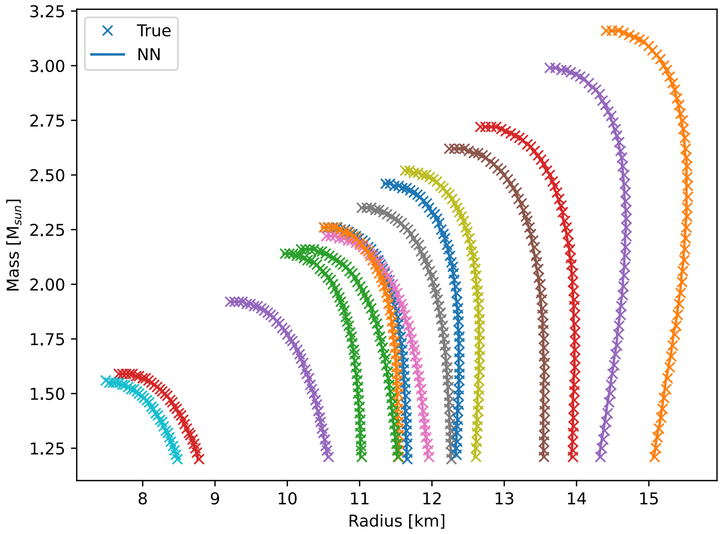


Learn EOS to M-R

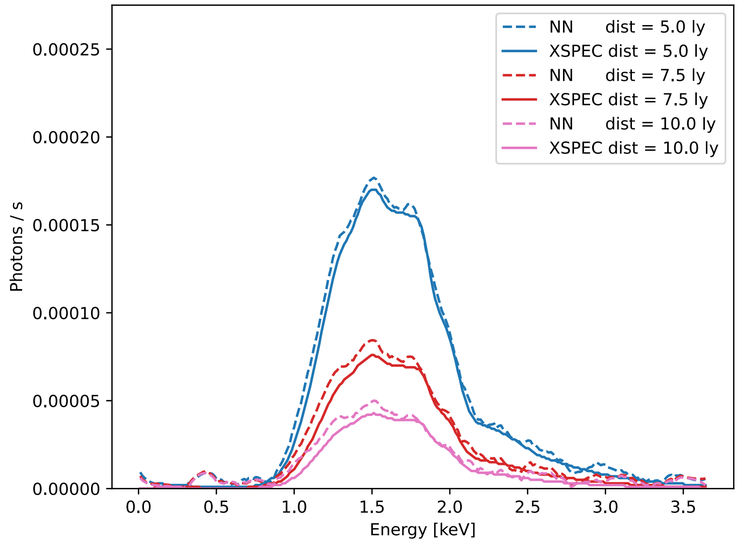
Paper in preparation

Forward process step-by-step

Intermediate steps remain interpretable physical quantities



Learn EOS to M-R

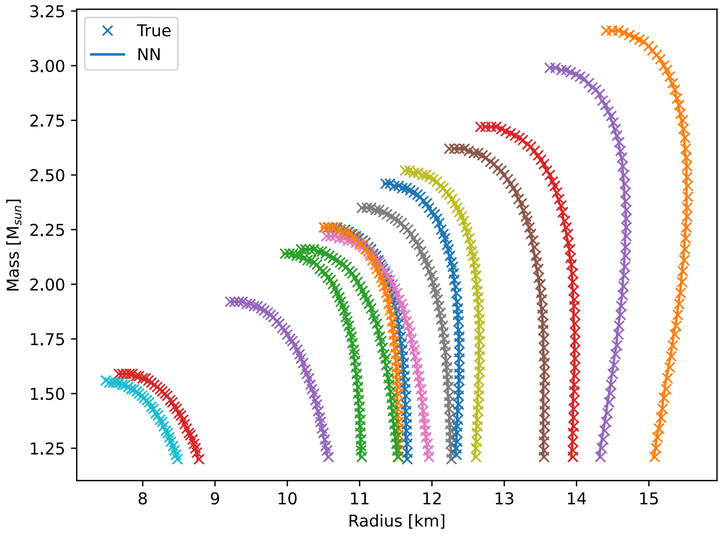


Learn {M,R,NPs} to Spectrum

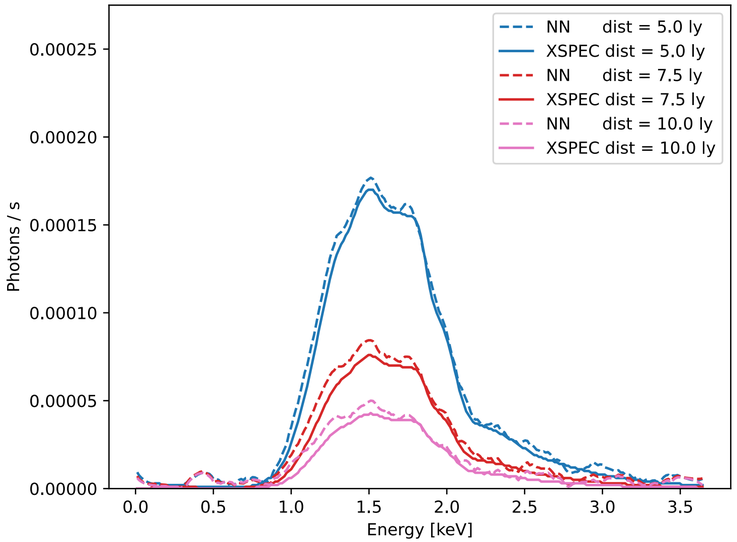
Paper in preparation

Forward process step-by-step

Intermediate steps remain interpretable physical quantities



Learn EOS to M-R



Learn {M,R,NPs} to Spectrum

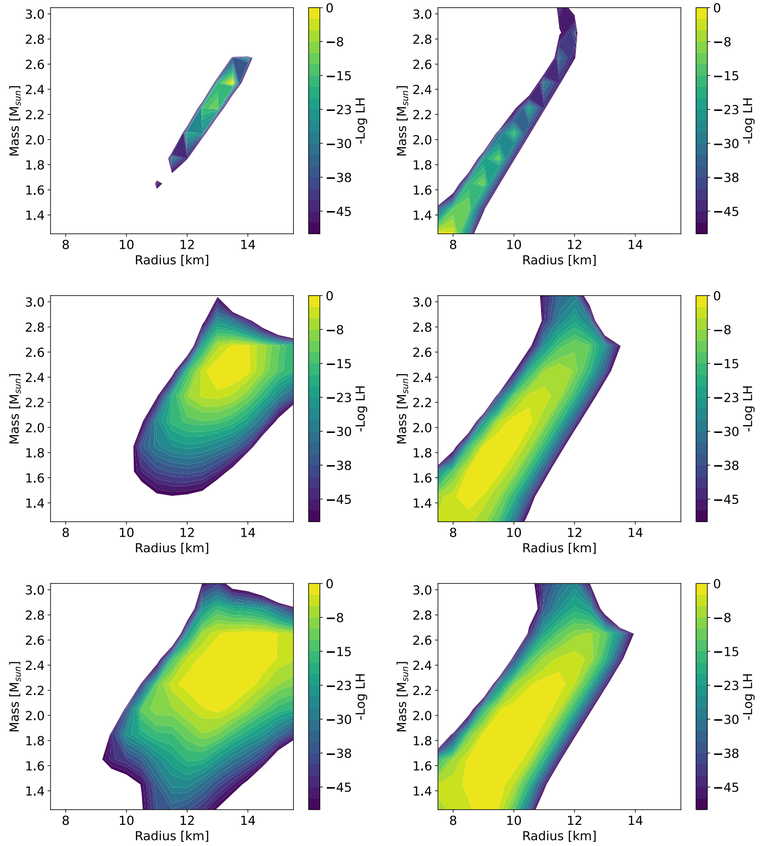
Nuisance Priors:

M-R likelihoods:

True:

Tight:

Loose:



Paper in preparation

Back to particle physics

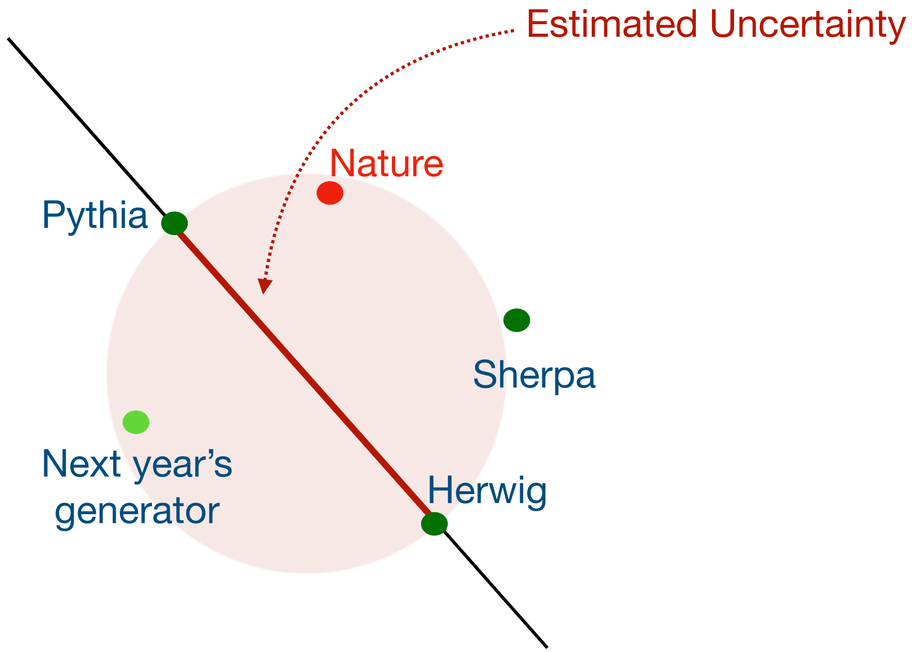
Back to particle physics

We also learnt what not to do …

What are theory uncertainties ?

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

No statistical origin for them (such as auxiliary measurement)



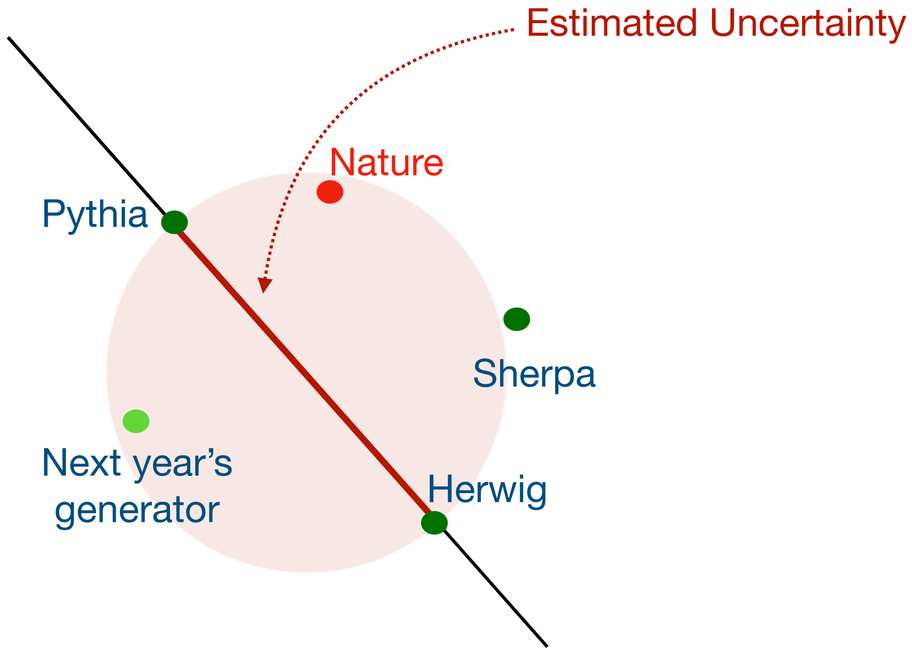
What are theory uncertainties ?

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 ?

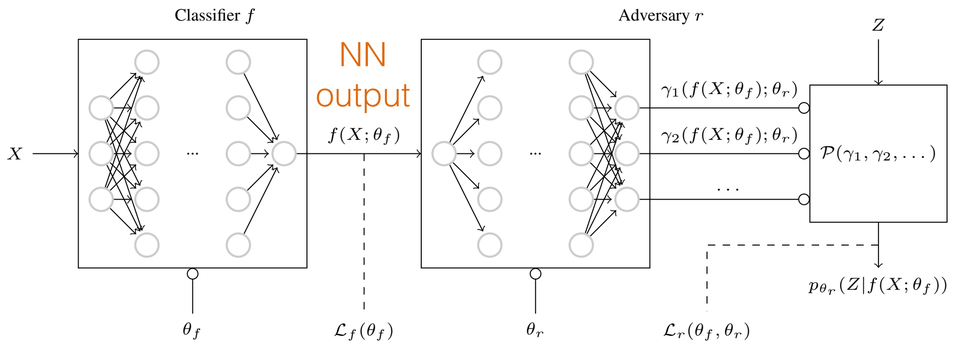
Adversarial decorrelation

Learning to Pivot, Louppe et al.

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

S vs B

Regress NP



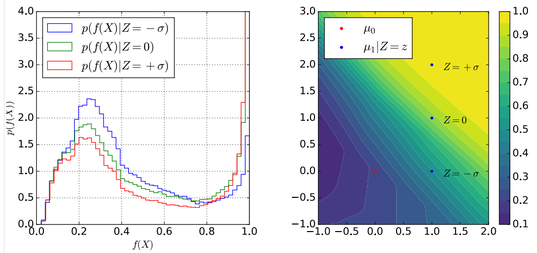
To fool the adversary, classifier output should be decorrelated to Z

Learning to Pivot, Louppe et al.

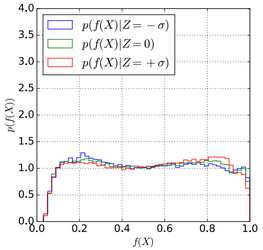
$$L_{Classifier} = L_{Classification} - \lambda \cdot L$$

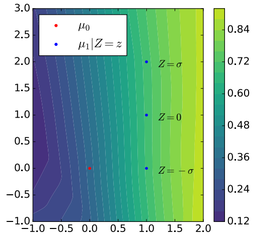
ML-Decorrelation Methods

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



Adversarial Decorrelation





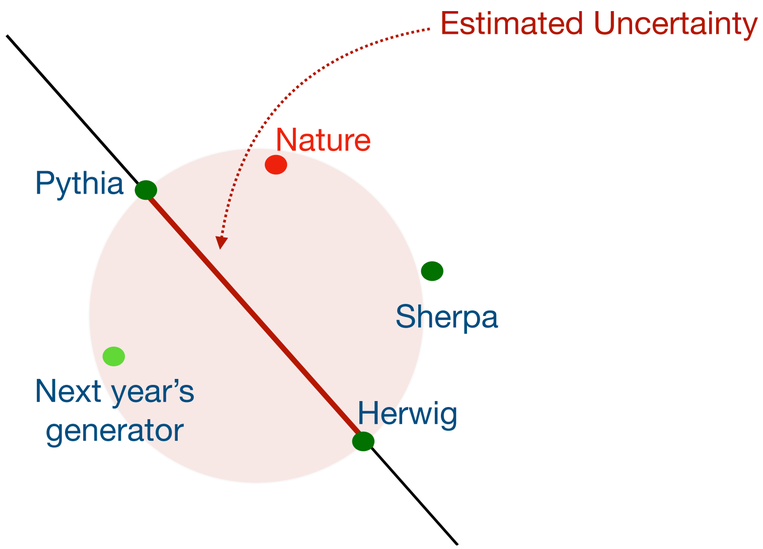
Classifier output for various values of Z

Learning to Pivot, Louppe et al.

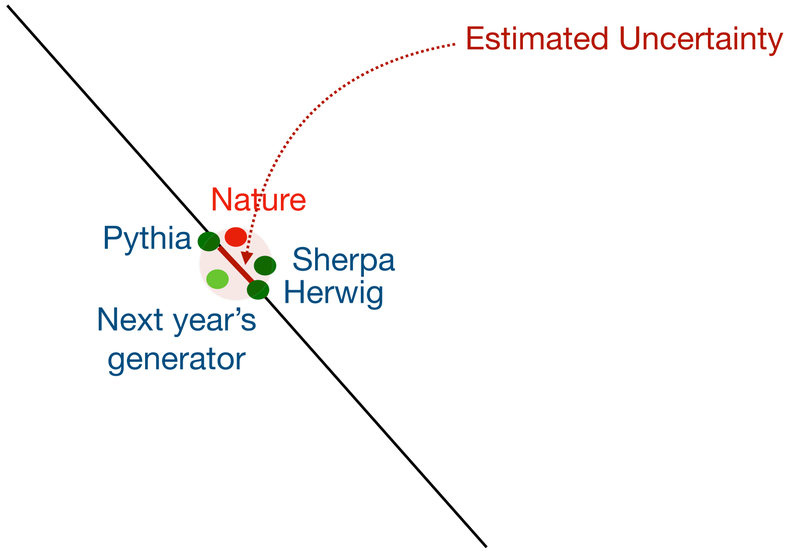
ML-decorrelating theory uncertainties

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

Default



What you want with decorrelation

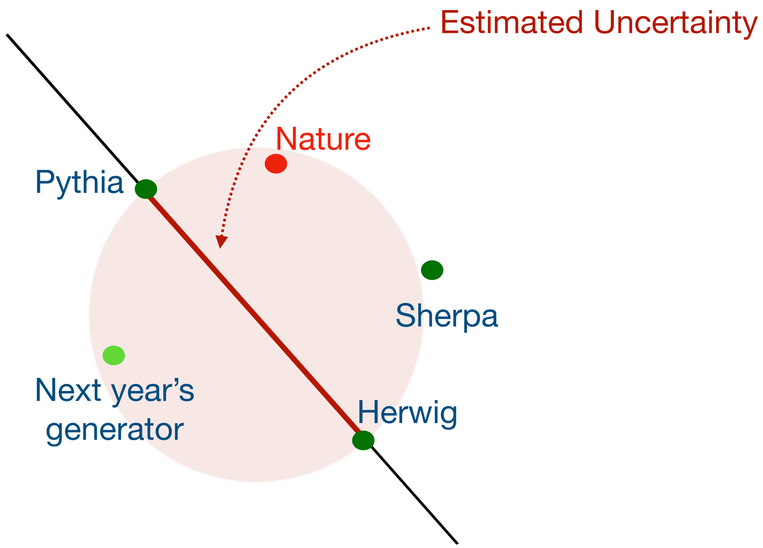


Instruction to ML: "Please shrink Pythia vs Herwig difference"

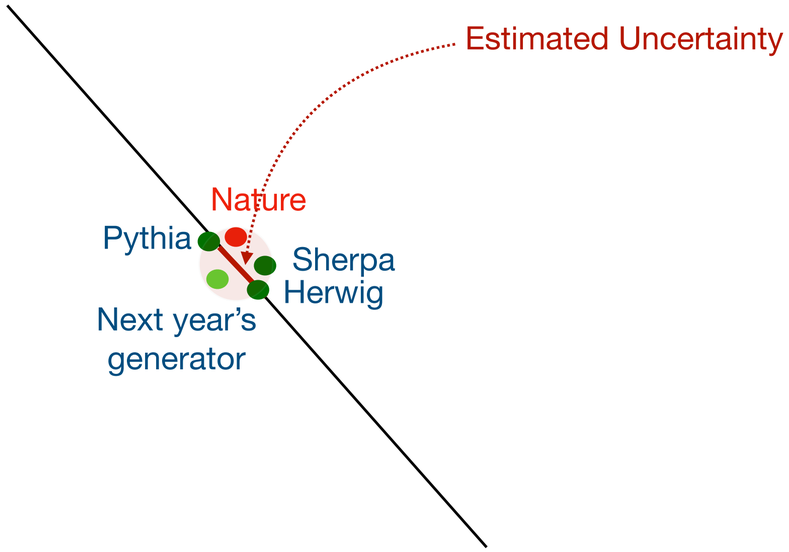
ML-decorrelating theory uncertainties

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

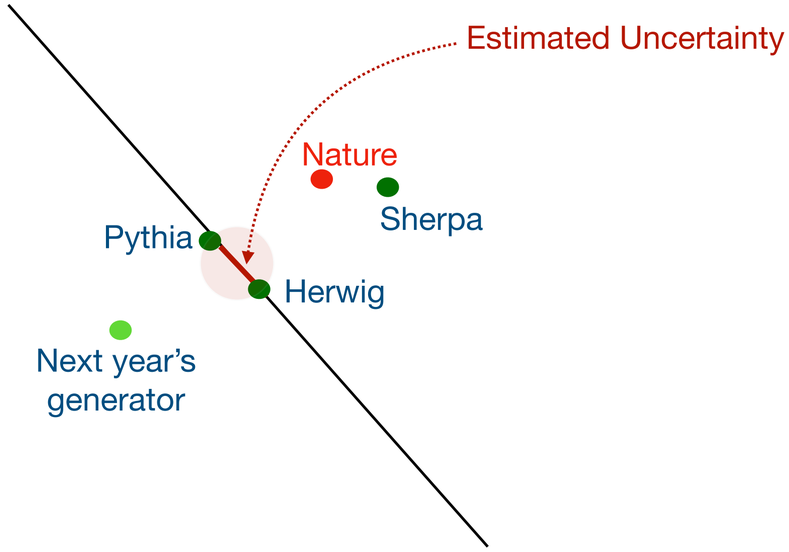
Default



What you want with decorrelation



What you get with decorrelation



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

Scale Uncertainties

Uncertainty of cross-section from truncating QFT series

Sensitivity to scale variation quantifies ‘uncertainty’

Scale Uncertainties

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

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

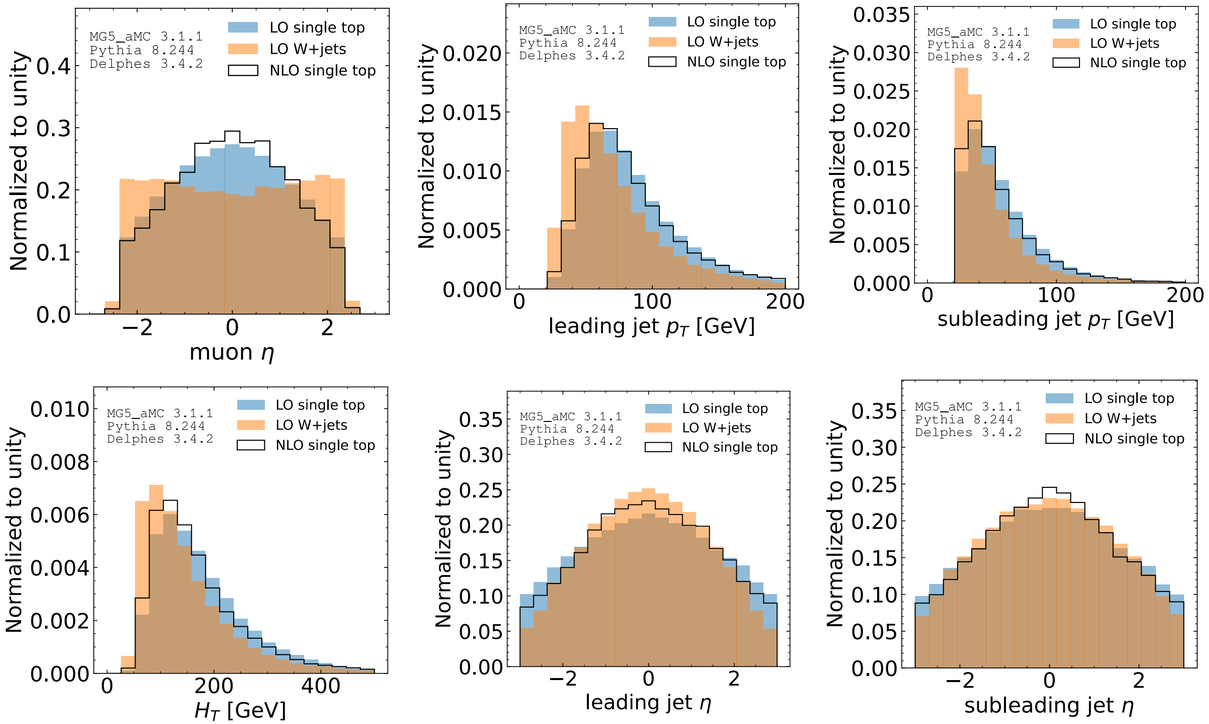
Uncertainty of cross-section from truncating QFT series

Sensitivity to scale variation quantifies ‘uncertainty’

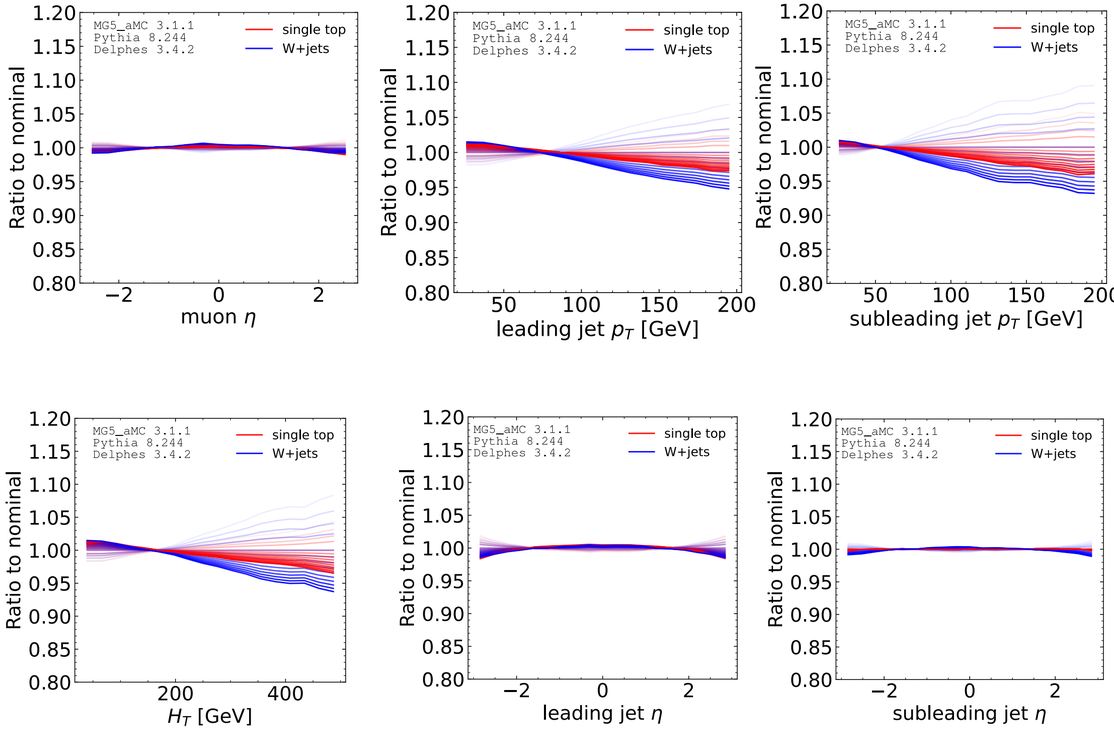
Down: $\mu_- = \frac{1}{2}\ \mu_0$

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

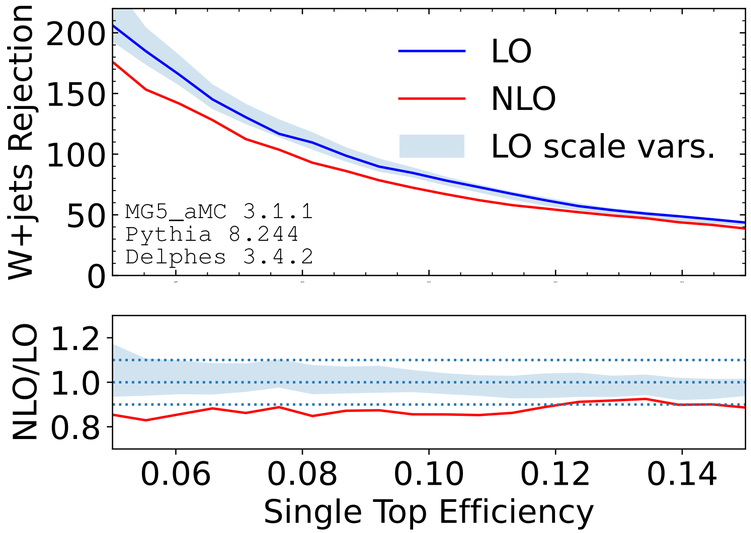


Factorisation scale variations going from 1/2 to 2

Case Study 2: Continuous uncertainty - Result

ROC curve (higher is better)

No adversary



Case Study 2: Continuous uncertainty - Result

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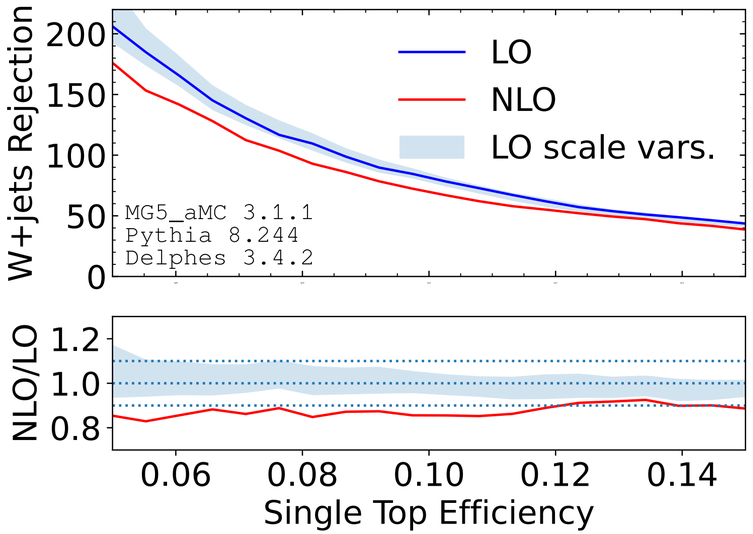
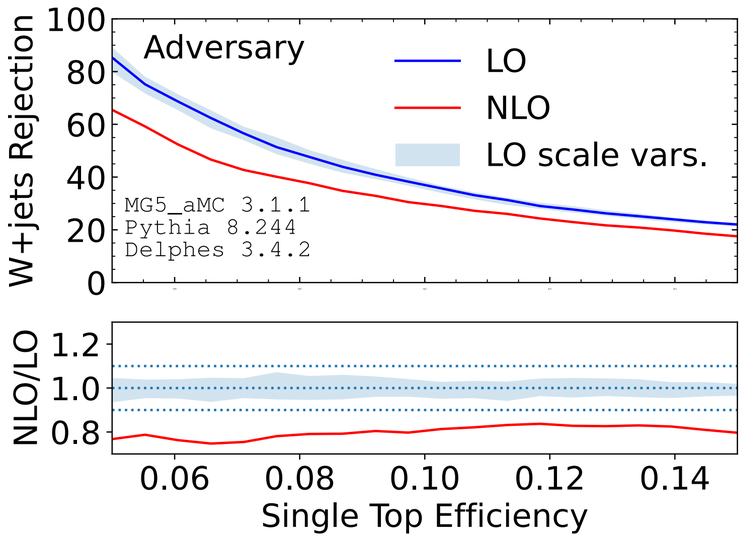


With adversary

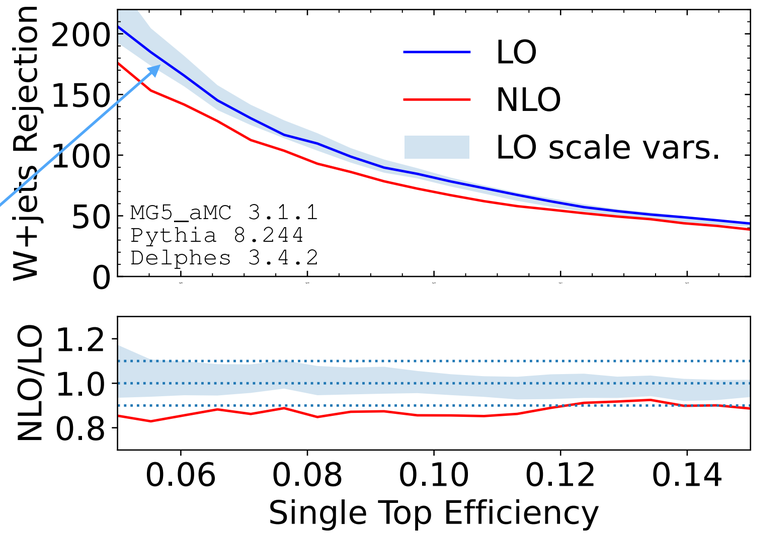


Case Study 2: Continuous uncertainty - Result

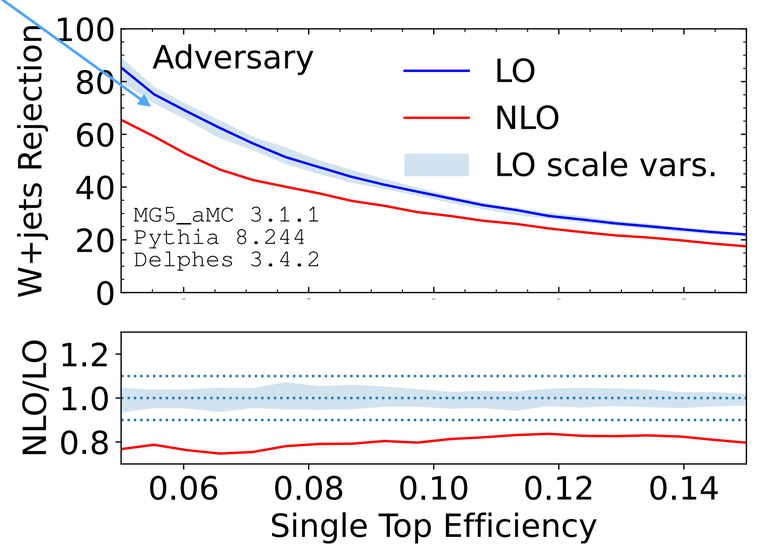
ROC curve (higher is better)

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

No adversary



With adversary



Case Study 2: Continuous uncertainty - Result

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

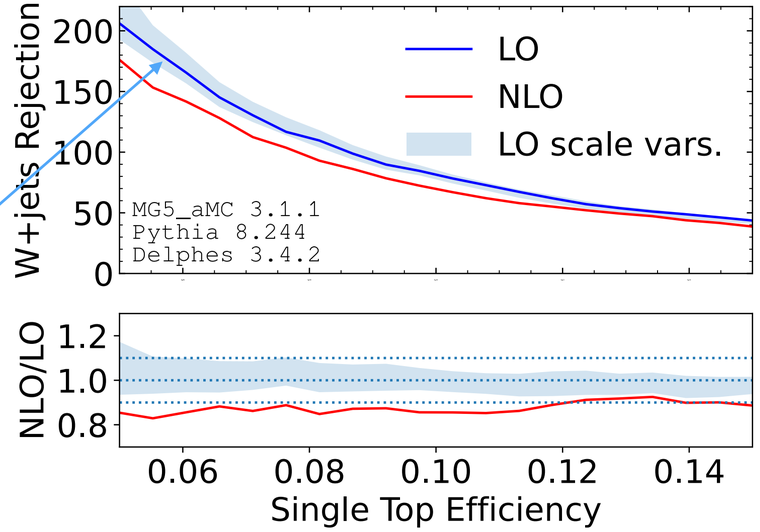
Cross-check with NLO reveals **uncertainty severely underestimated** by decorrelation approach

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

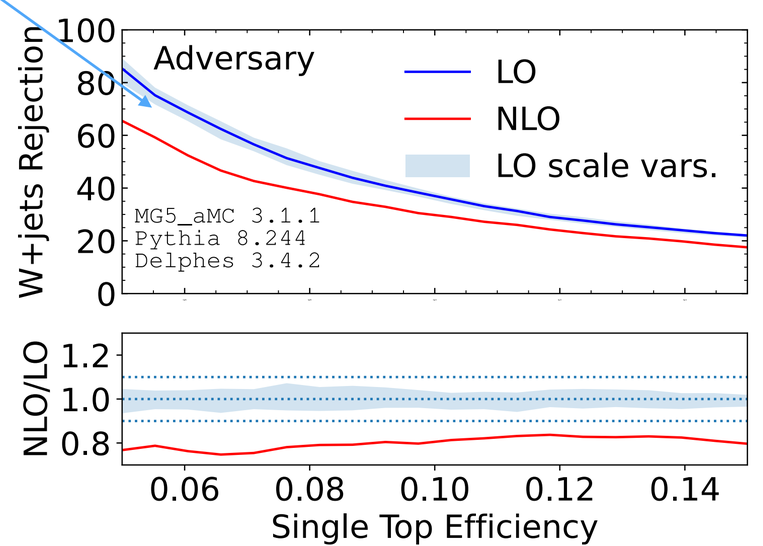
Decorrelation:
Only the error bars shrink, not the actual distance to NLO

ROC curve (higher is better)

No adversary



With adversary



Pause for questions

Eg:
- Why doesn't this happen for experimental uncertainties?
- Did you just tell us not to use ML at an ML school ?
- ...

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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Could we learn hadronization directly from Nature ?

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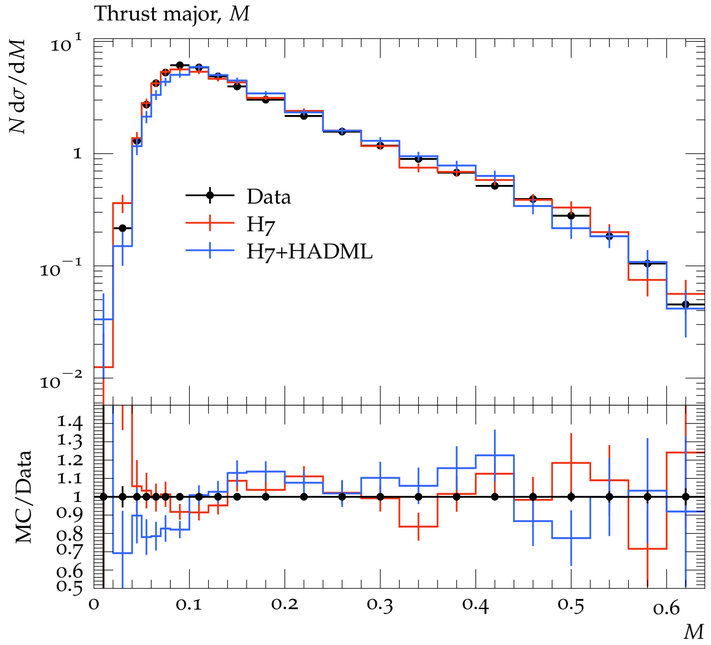
- Bypass theory, learn hadronization directly from data ?
- Proofs of concept on Herwig and Pythia simulations



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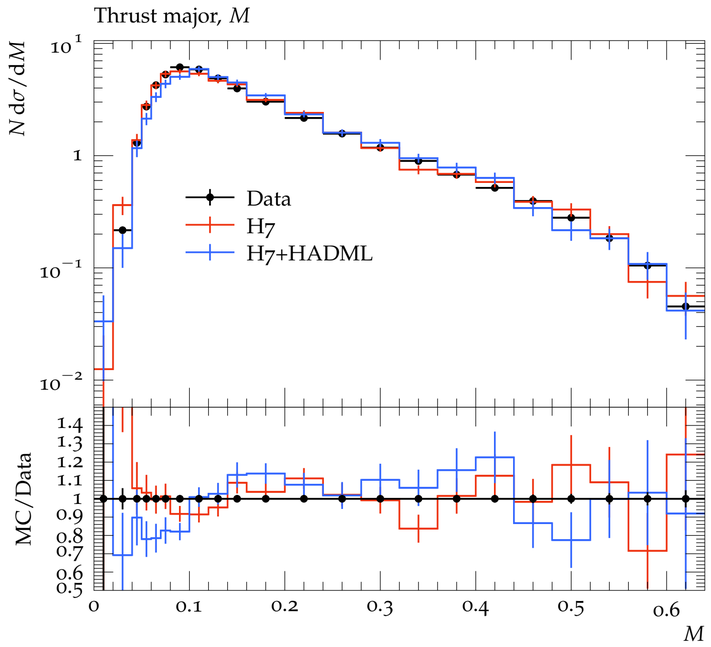
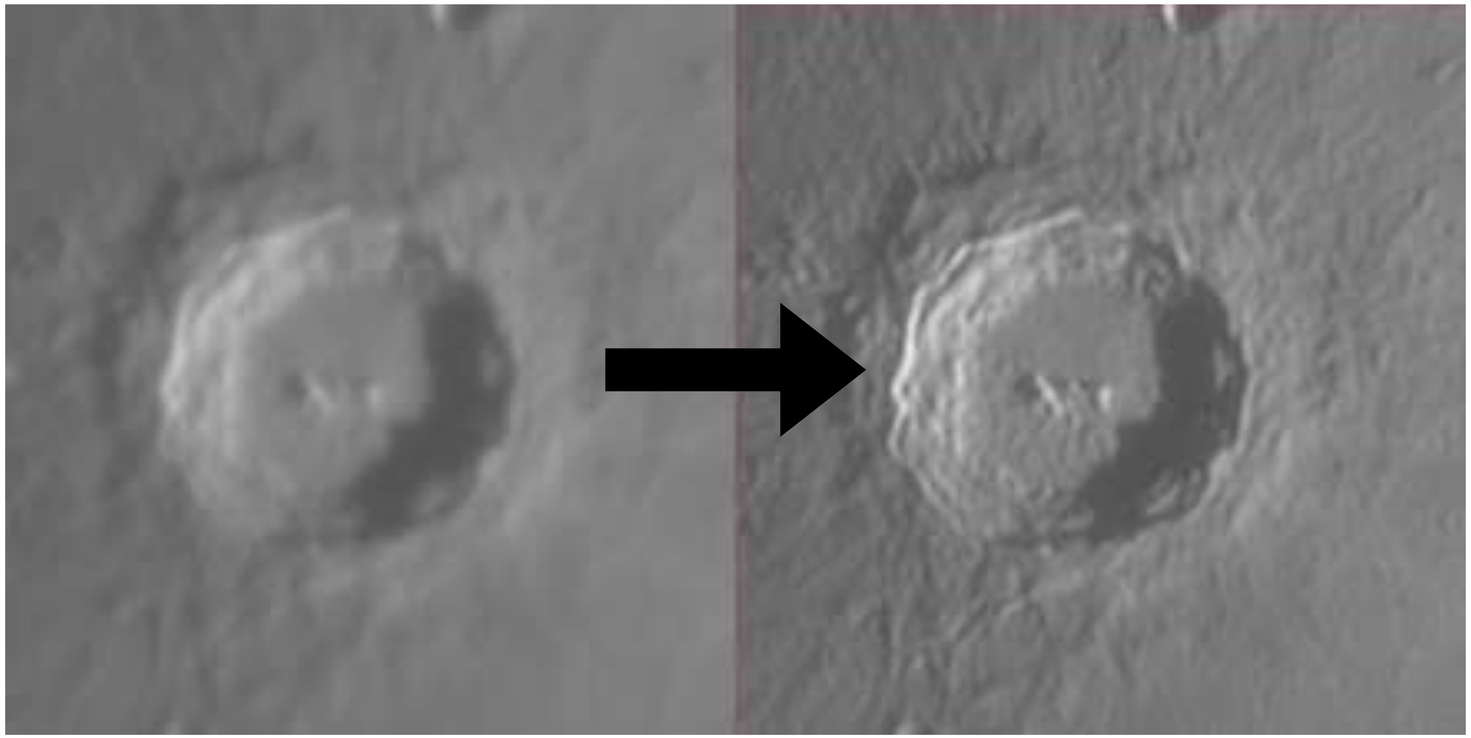


- To train on data, we need unfolded events <-—> data from experiments after removing detector effects
- Need **unbinned** unfolding of all observables simultaneously

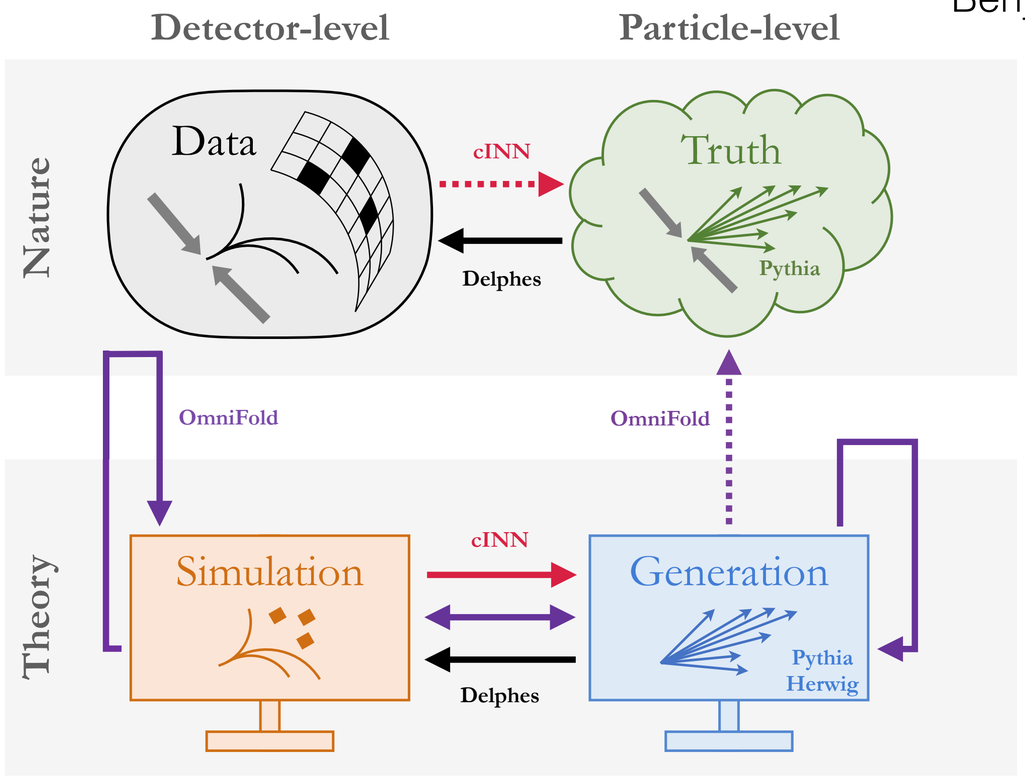
Unfolding = Deconvolution of Detector Effects

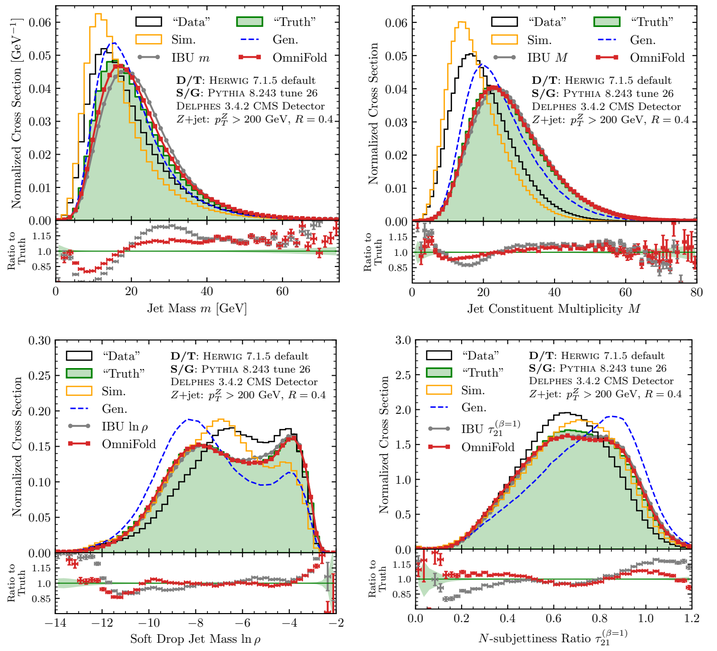
- Similar to de-noising
- Unfold distributions, not individual images
- Cannot use off-the-shelf ML methods because we care about biases
- Ill-posed problem - no deterministic mapping from detector level to particle level



ML for unfolding events

JINST.7.P01024: Miguel Arratia, Anja Butter, Mario Campanelli, Vincent Croft, Dag Gillberg, Aishik Ghosh, Kristin Lohwasser, Bogdan Malaescu, Vinicius Mikuni, Benjamin Nachman, Juan Rojo, Jesse Thaler, Ramon Winterhalder



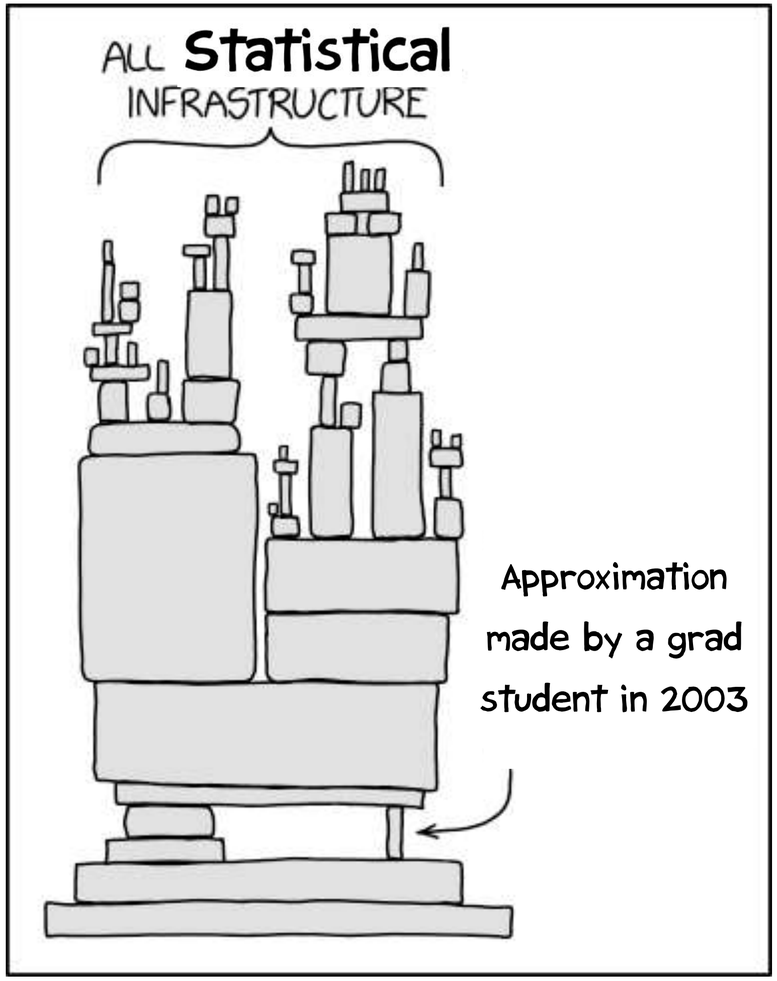


1. Re-weight MC generation to data (OmniFold)
2. Generative model (cINN) to map detector data to particle-level

OmniFold: Andreassen et al.

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!

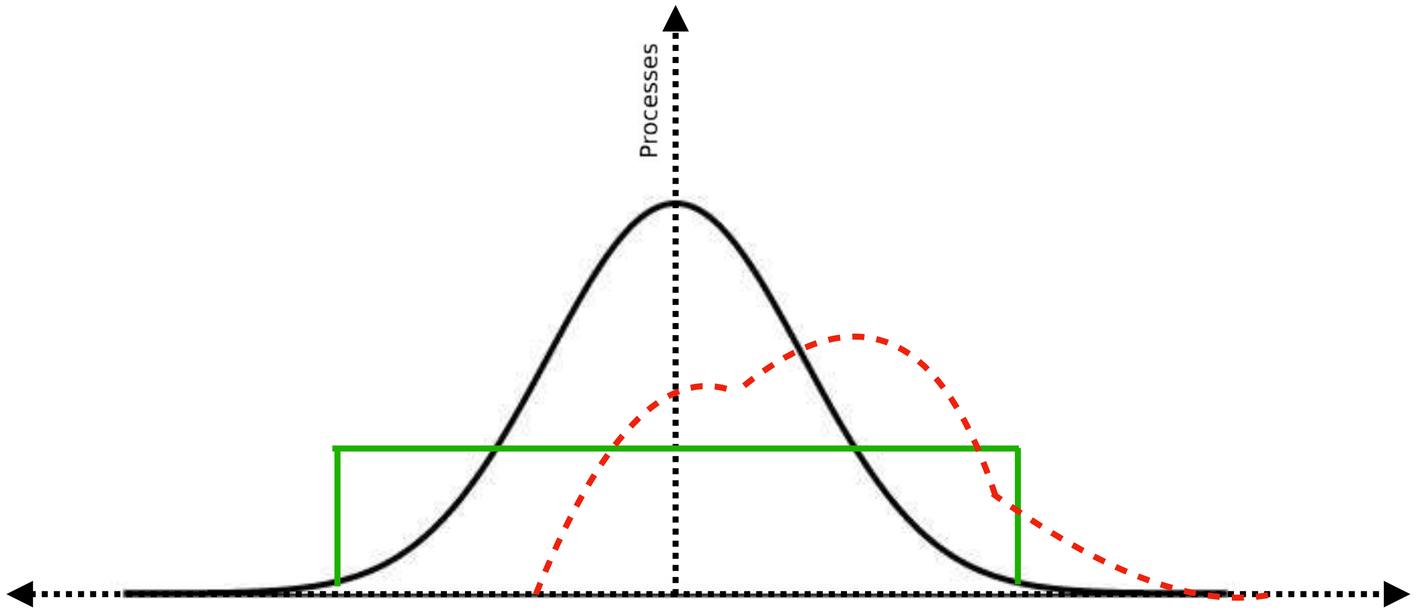
(Not a random sampling)

Alwall et al.

Plot the pulls

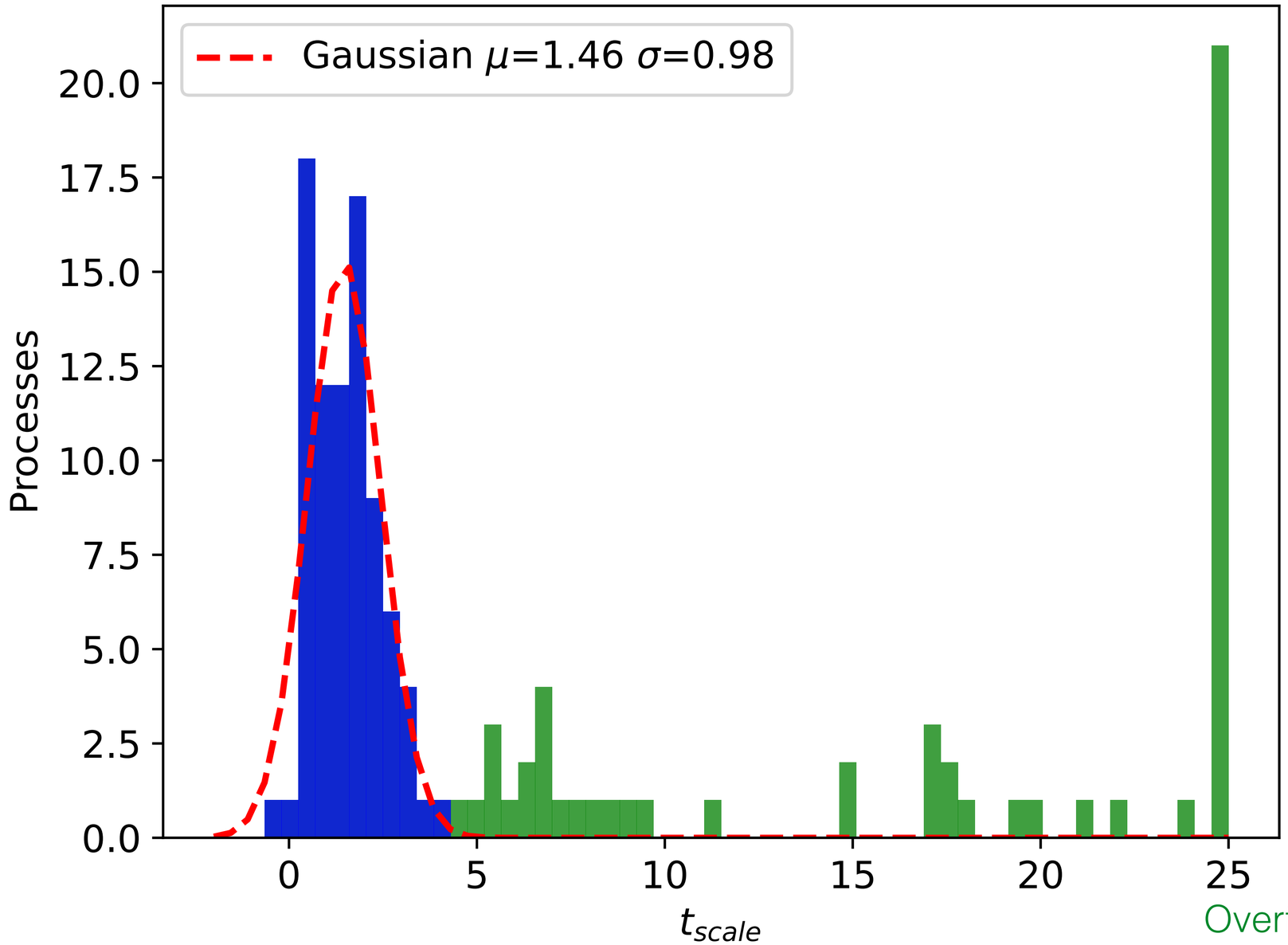
$$t_{scale} = \frac{\sigma_{NLO} - \sigma_{LO}}{\Delta\sigma_{LO\ scale}}$$

Which of these distributions do you expect?



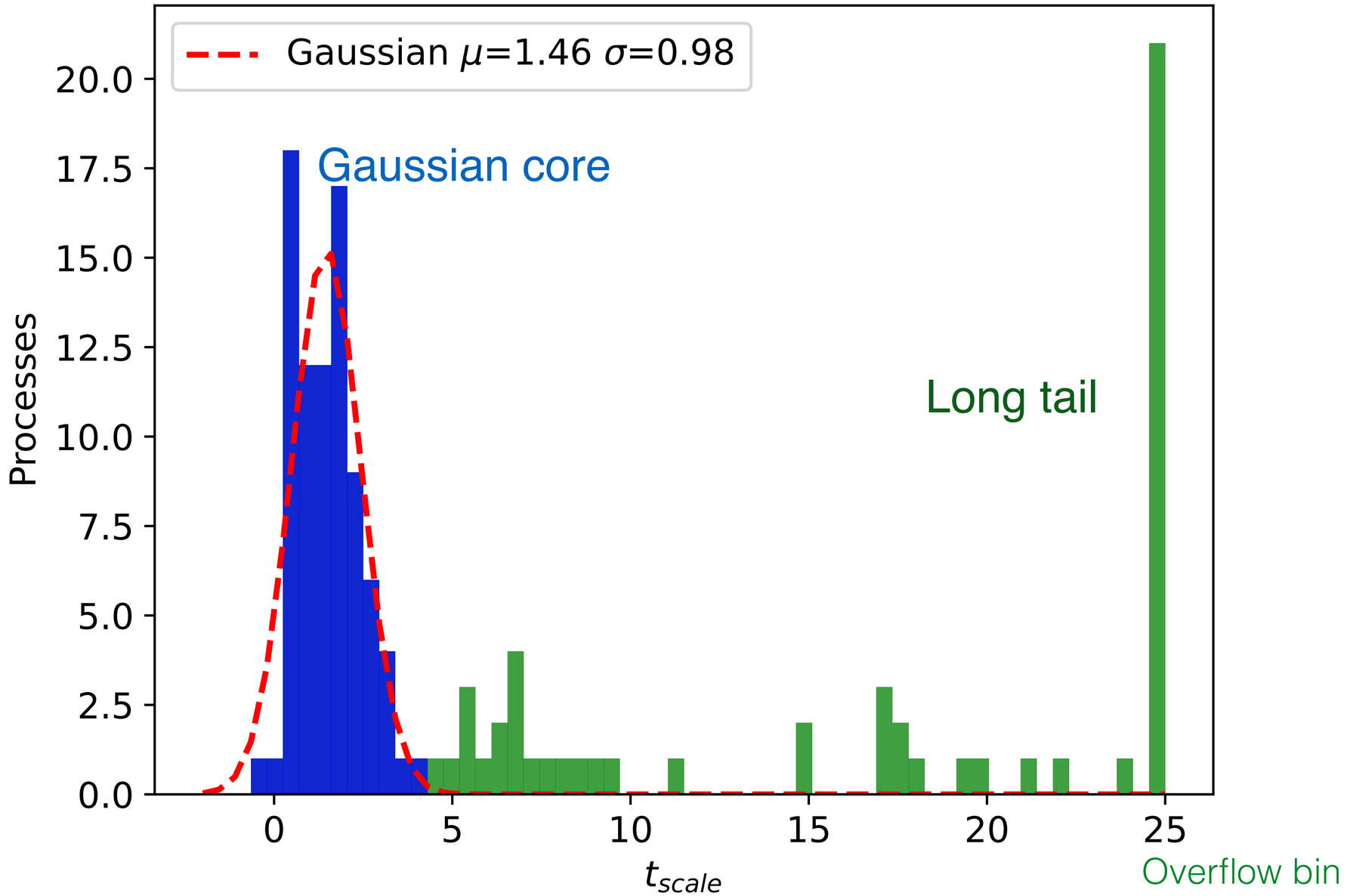
$$t_{scale} = \frac{\sigma_{NLO} - \sigma_{LO}}{\Delta\sigma_{LO\ scale}}$$

Pull distribution



Overflow bin

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

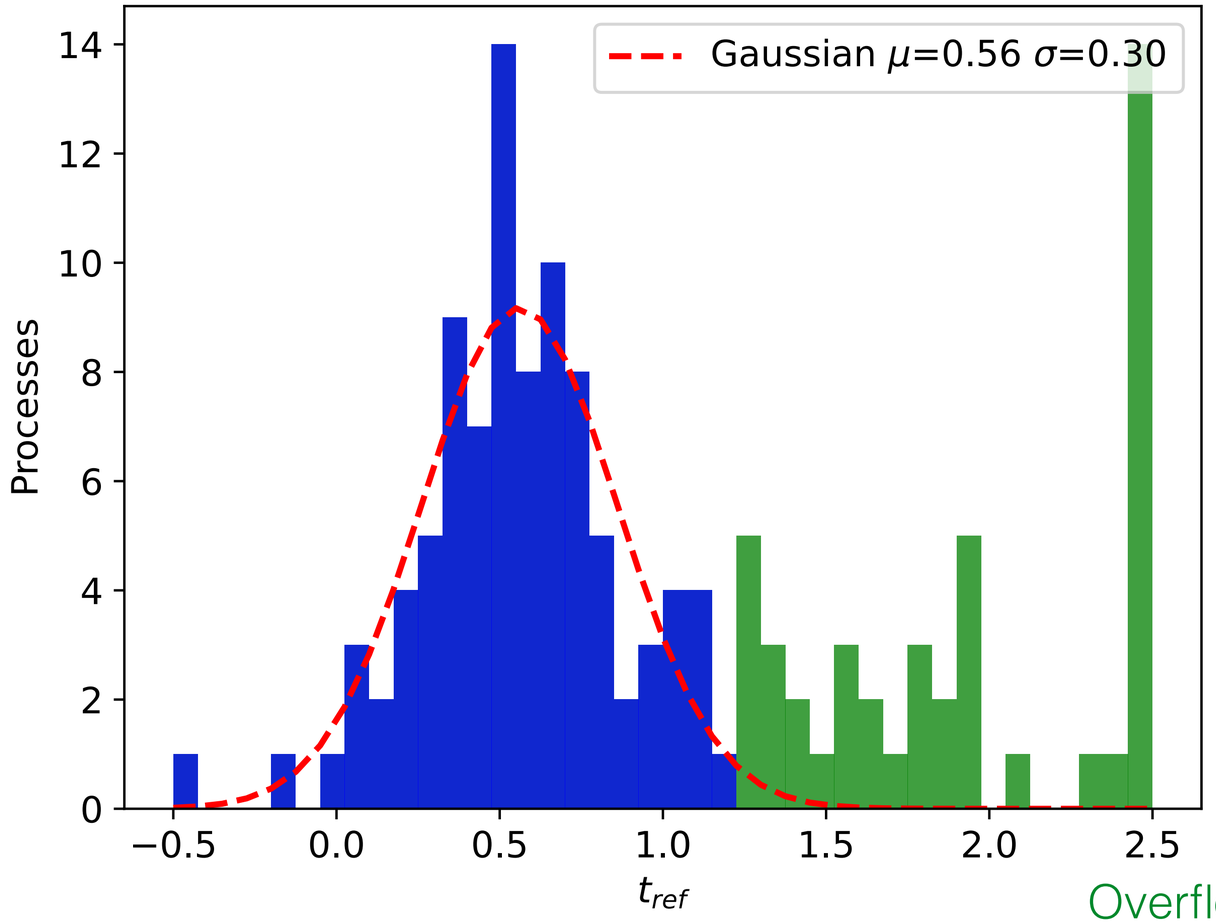
Process	$\frac{\Delta\sigma}{\sigma_0}$	n	$\frac{\Delta\sigma}{n\,\sigma_0}$
`p p > j j`	$+2.49\times10^{-1}\ -1.88\times10^{-1}$	2	$+1.24\times10^{-1}\ -9.40\times10^{-2}$
`p p > b b`	$+2.52\times10^{-1}\ -1.89\times10^{-1}$	2	$+1.26\times10^{-1}\ -9.45\times10^{-2}$
`p p > t t`	$+2.90\times10^{-1}\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

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

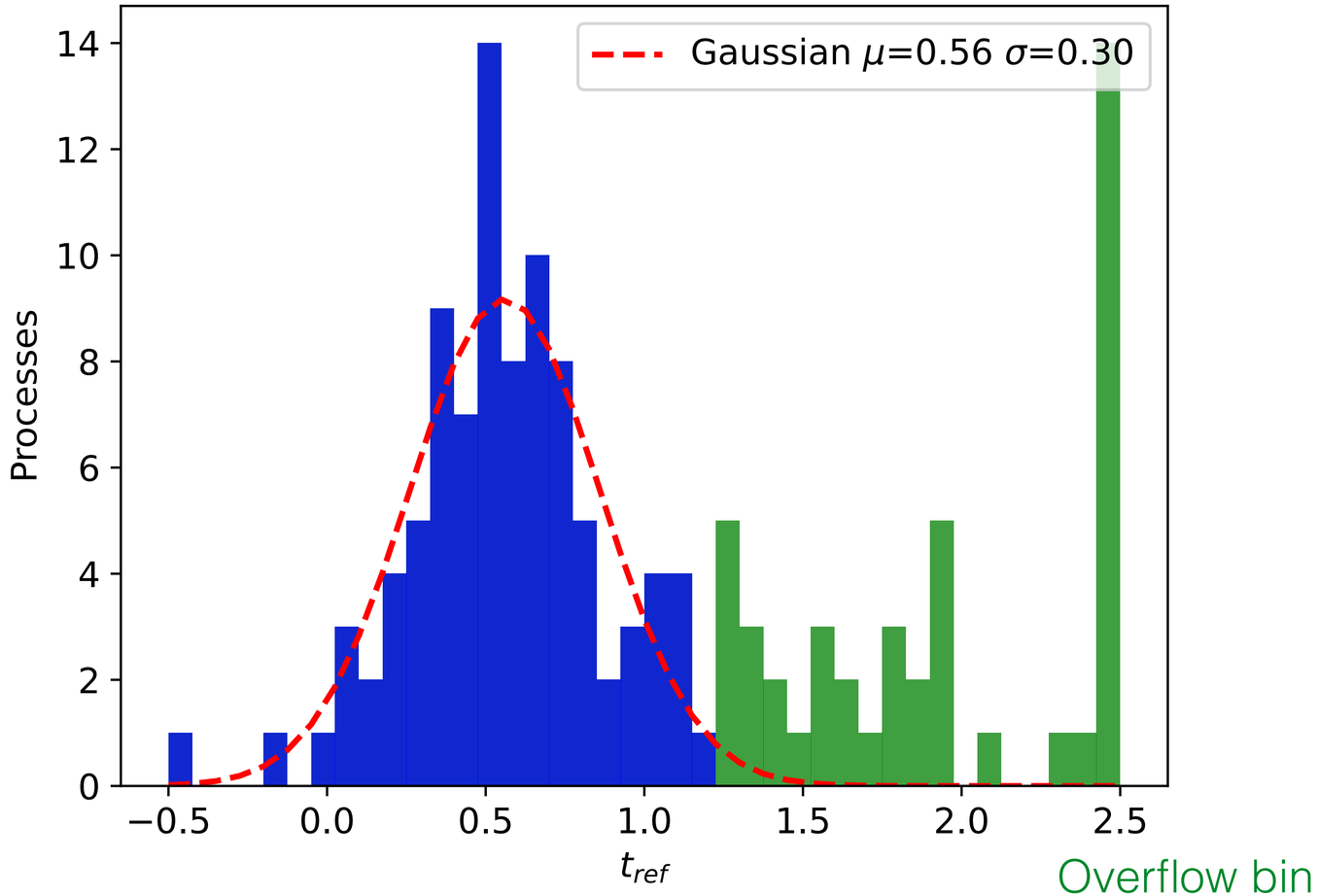


Much reduced tails

Overflow bin

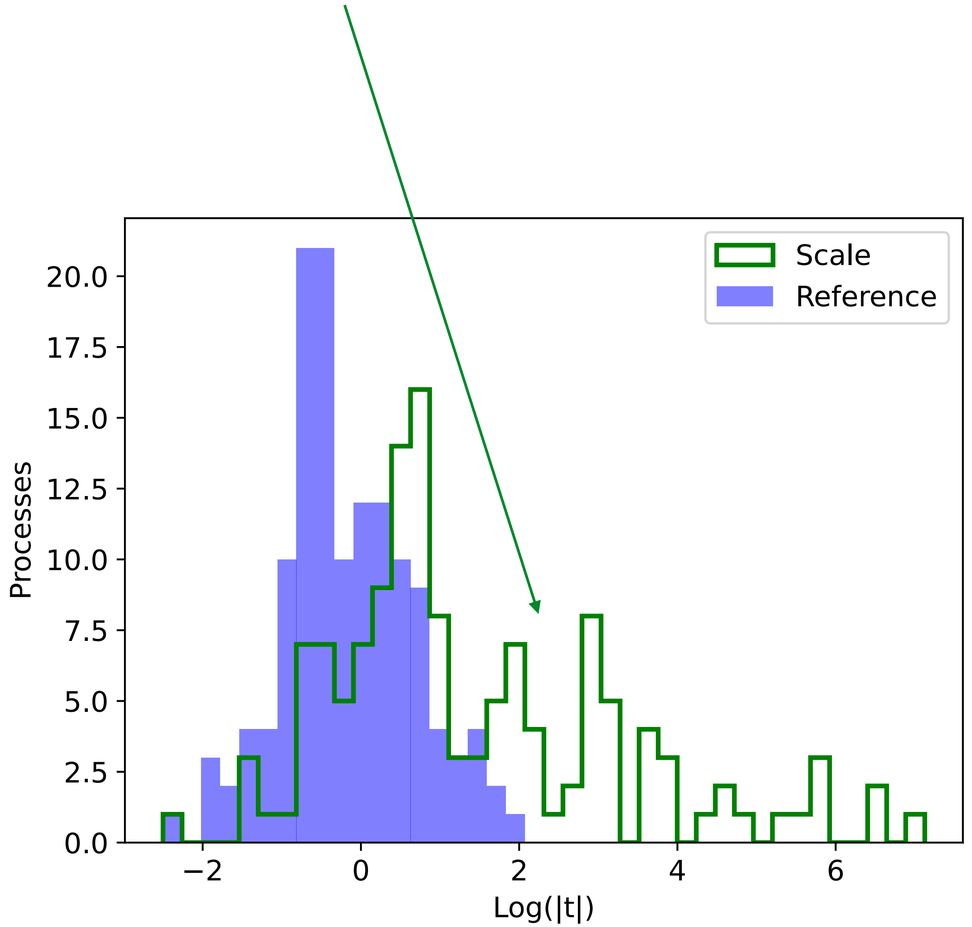
Tilman Plehn's 'reference process' method

Make correction in UQ for EW processes



Overflow bin

Much reduced tails



Tilman Plehn's 'reference process' method

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 ?

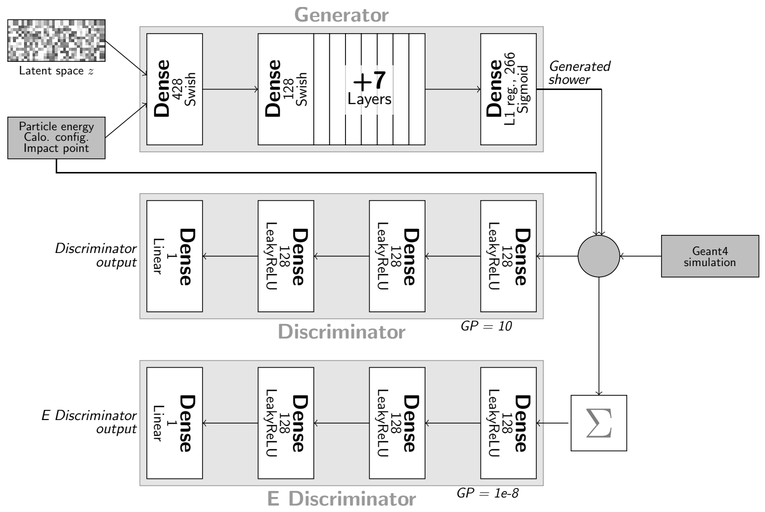
- Application in experiment: A new method for cross-checking sensitivity of advance ML methods to scale uncertainties

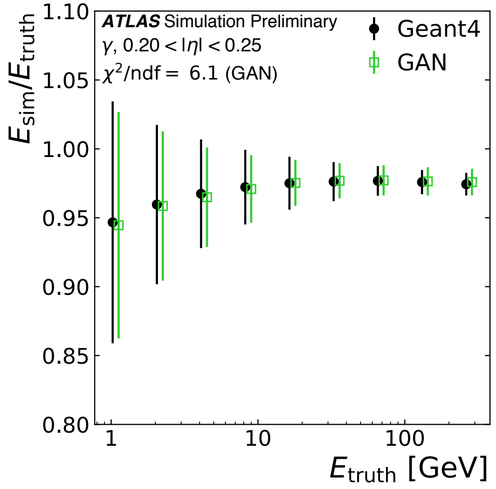
Pause for questions

Performance Metrics for Generative Models

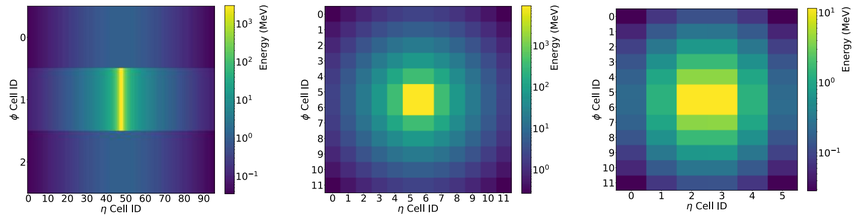
Generative Models for Simulation

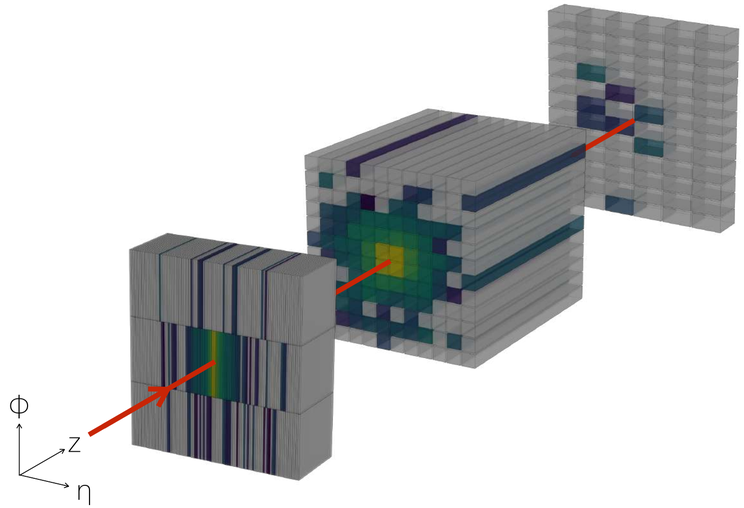
[ATLAS Collaboration [A. Ghosh], 2019]



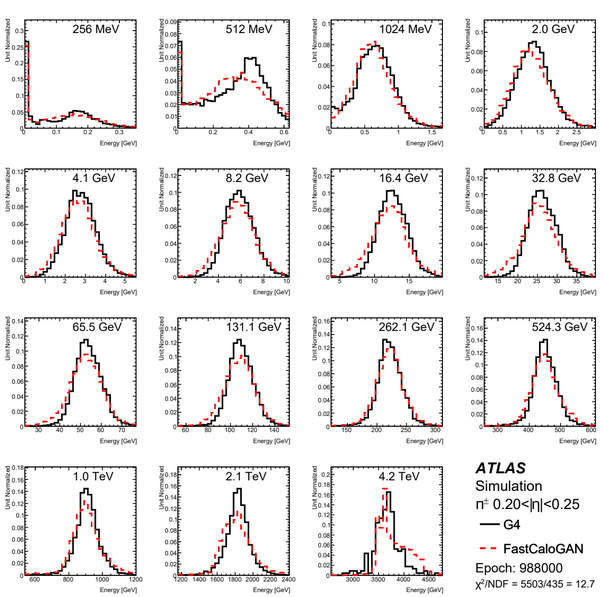


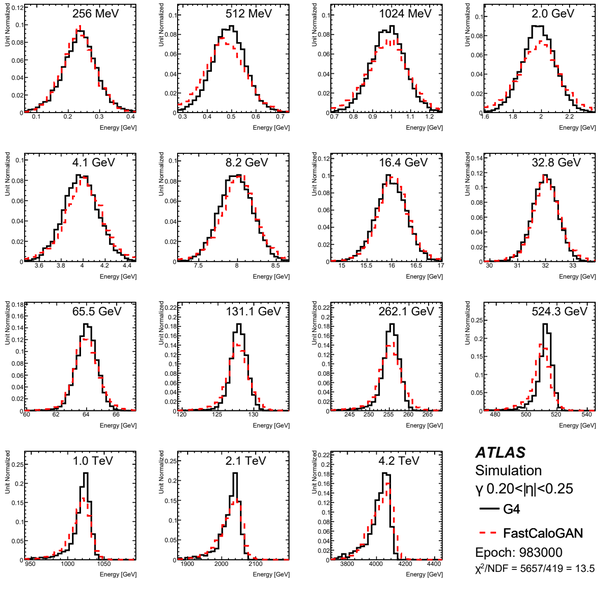
[Paganini et al.]



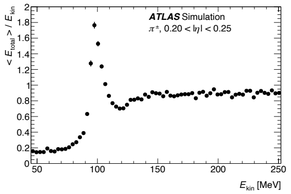


Evaluating Fast Calo Simulators





Evaluating Fast Calo Simulators



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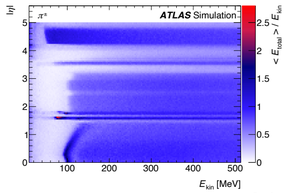

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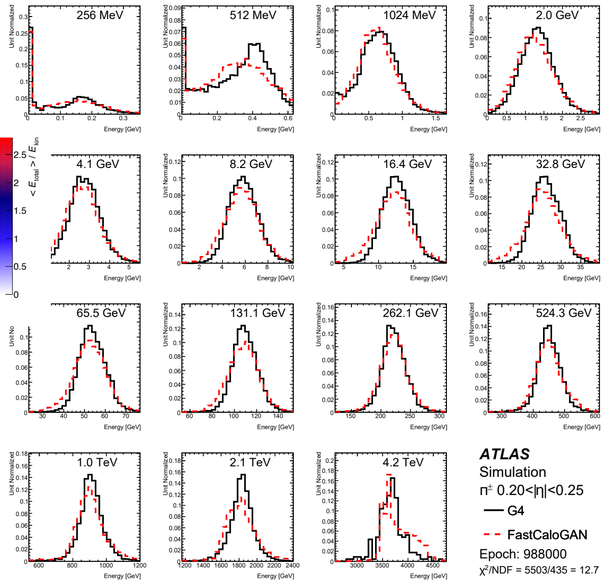

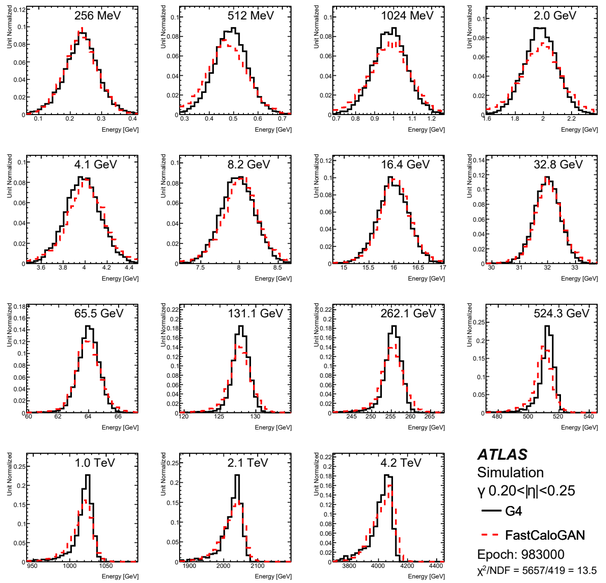

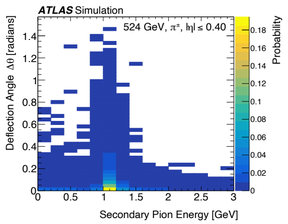

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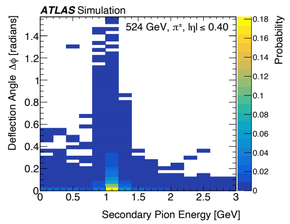

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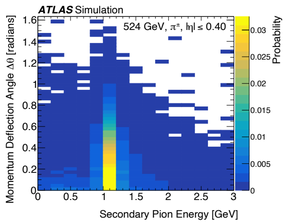

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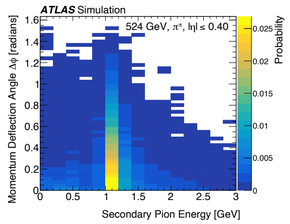

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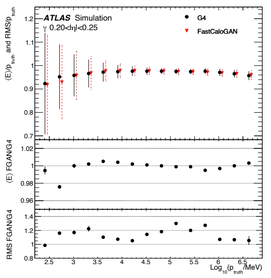
Evaluating Fast Calo Simulators



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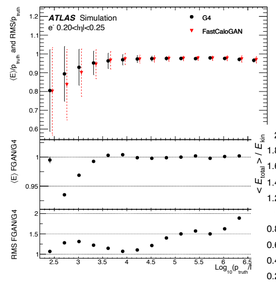

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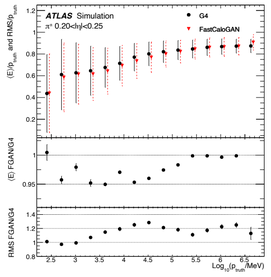

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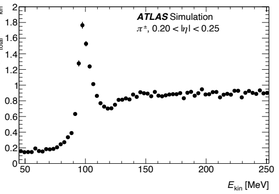

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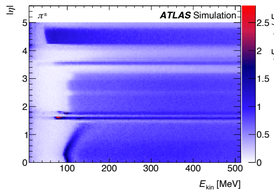

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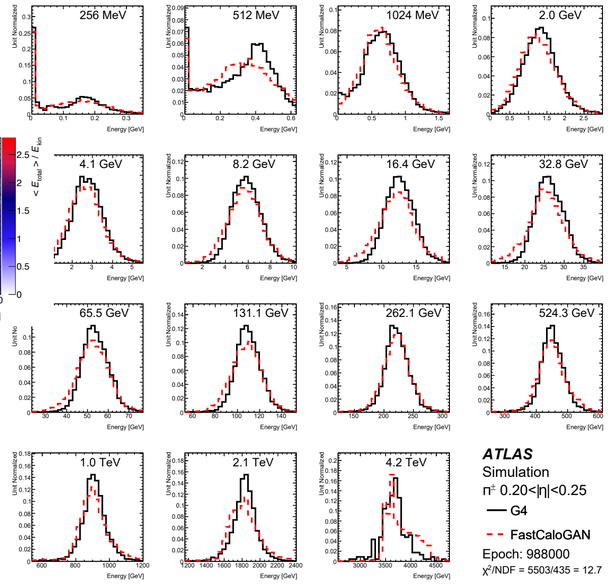

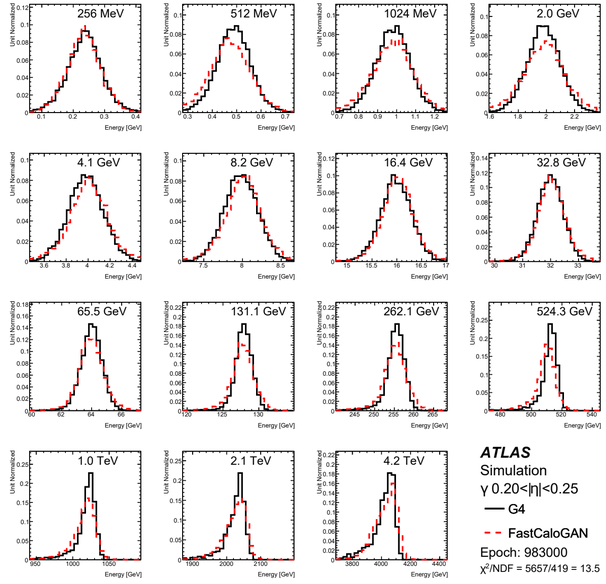

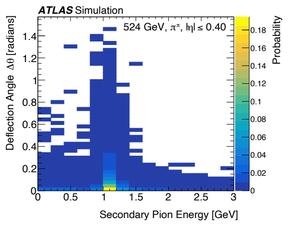

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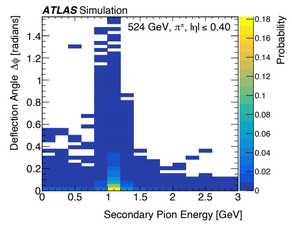

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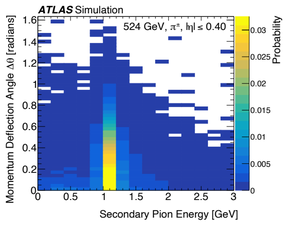

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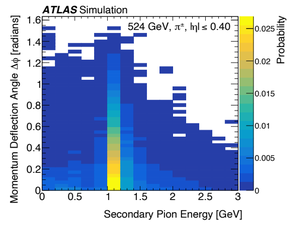

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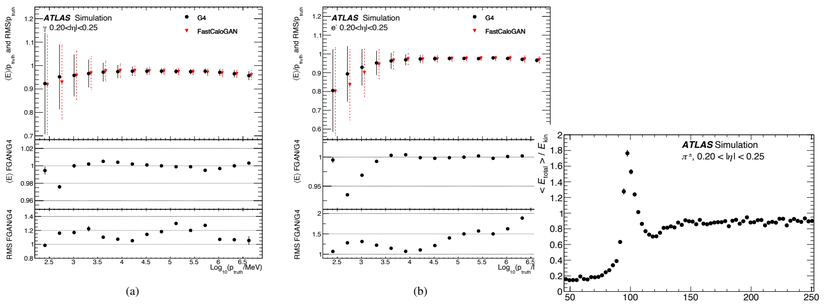
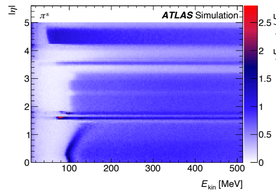
Evaluating Fast Calo Simulators



(a)

(b)

(a)



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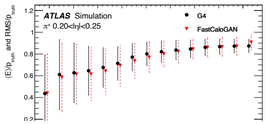

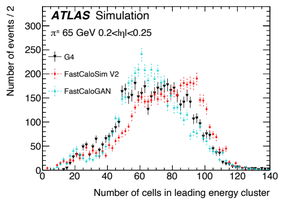

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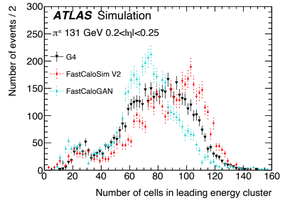

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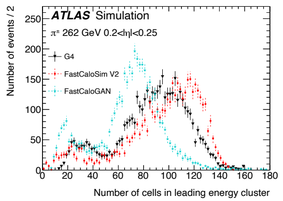

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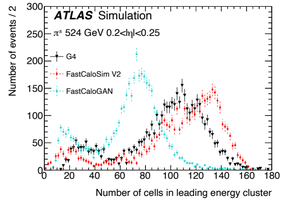

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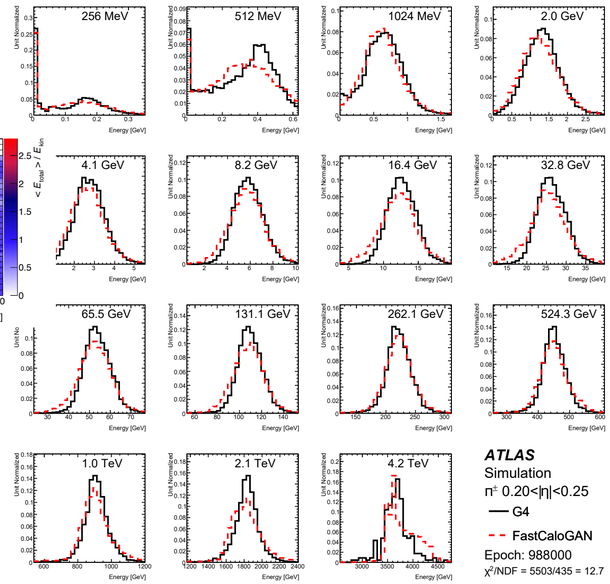

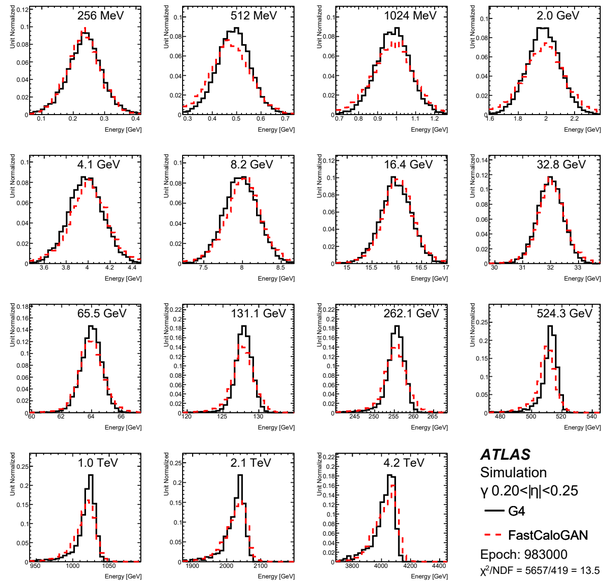

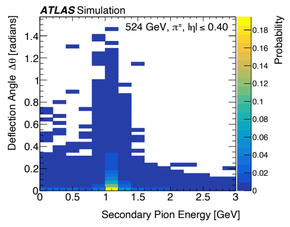

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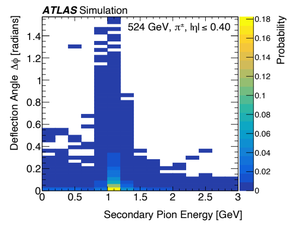

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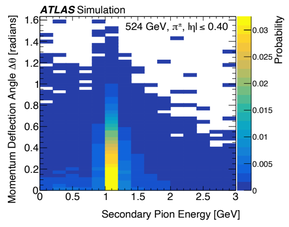

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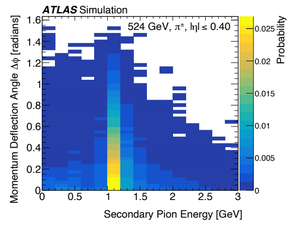

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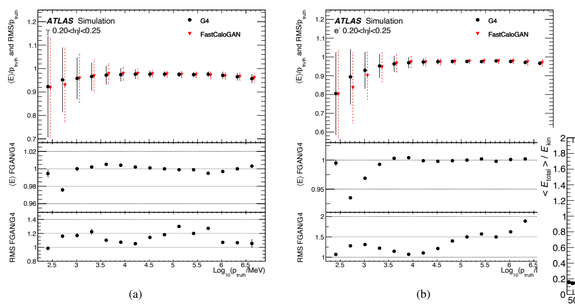
Evaluating Fast Calo Simulators



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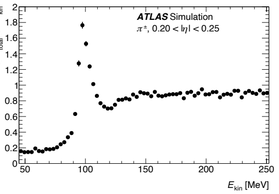

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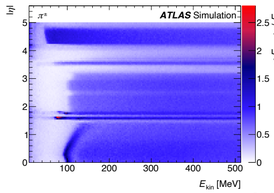

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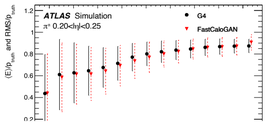

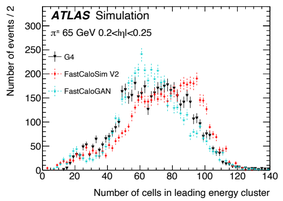

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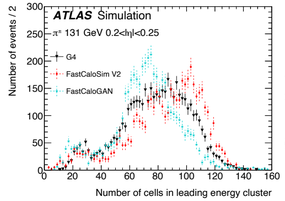

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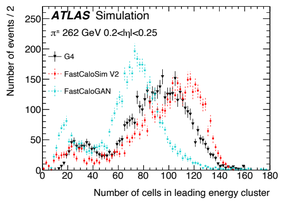

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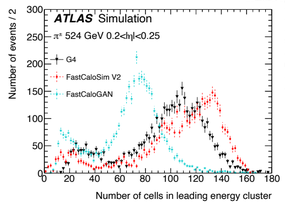

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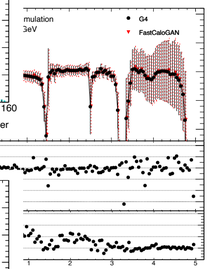

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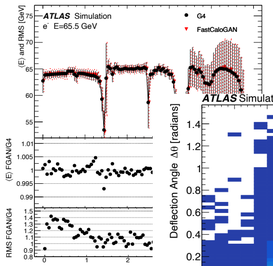

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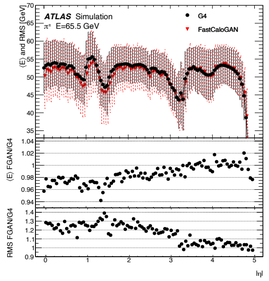

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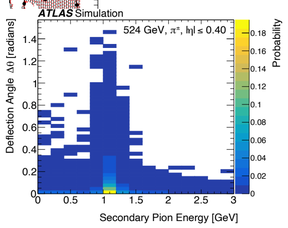

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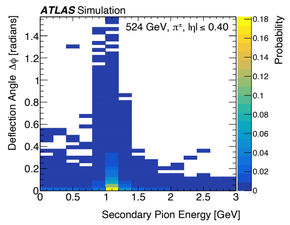

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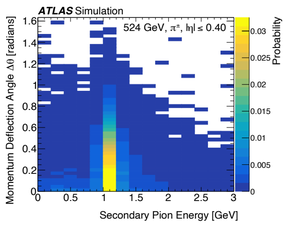

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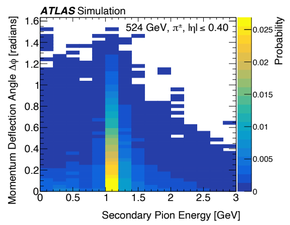

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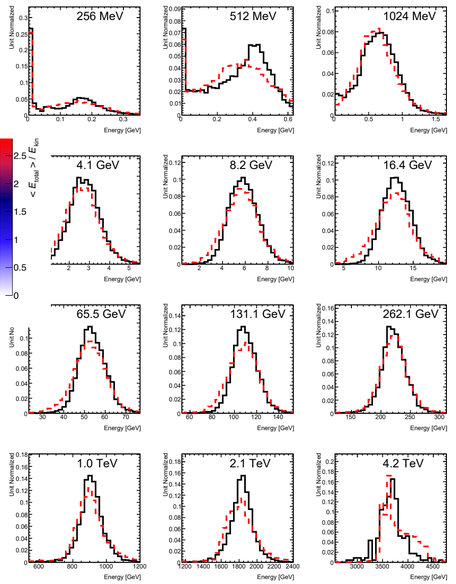
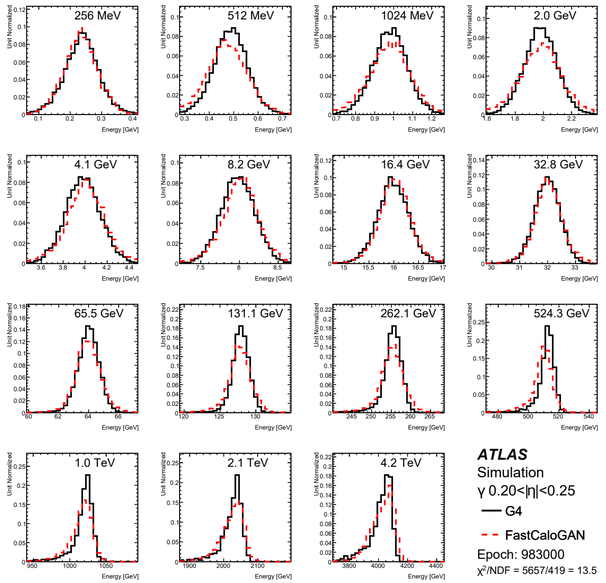
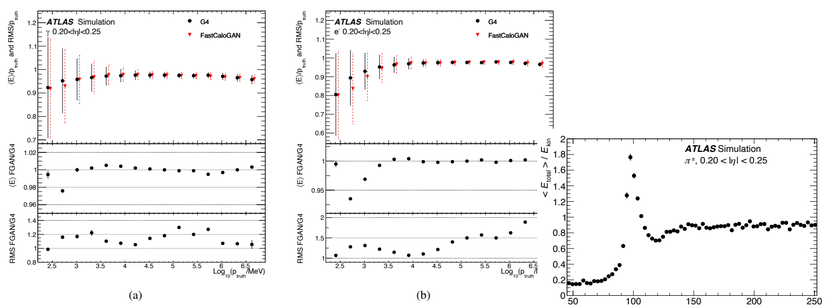




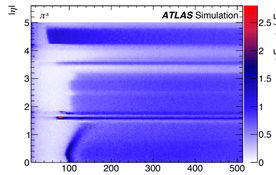
Evaluating Fast Calo Simulators



(a)

(b)

(a)



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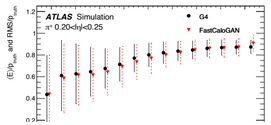

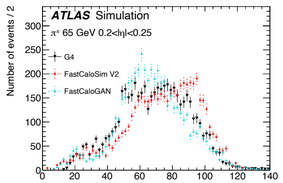

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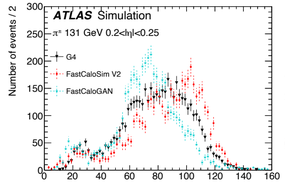

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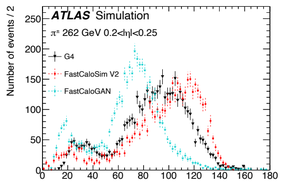

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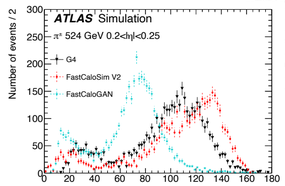

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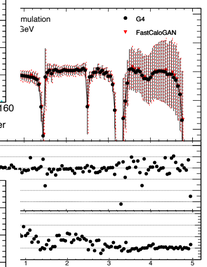

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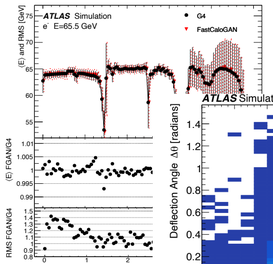

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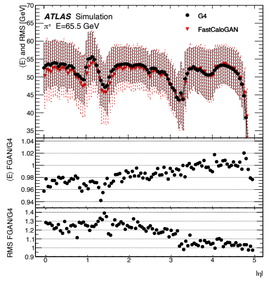

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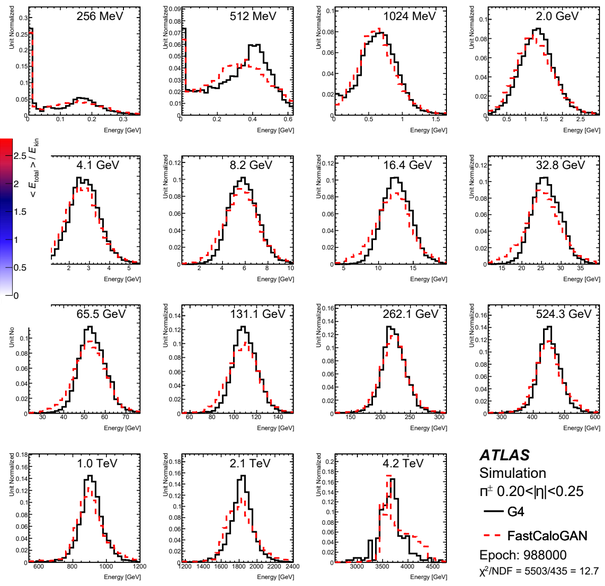

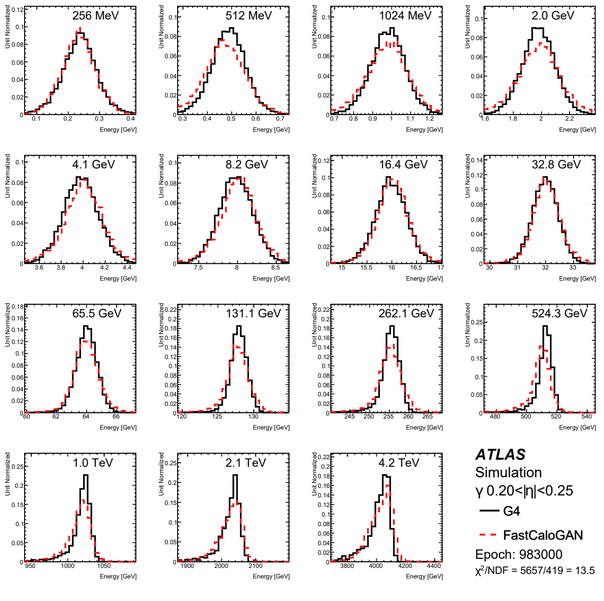

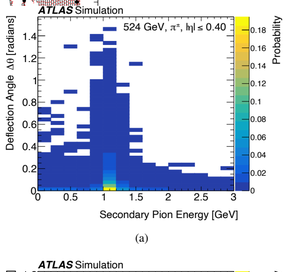

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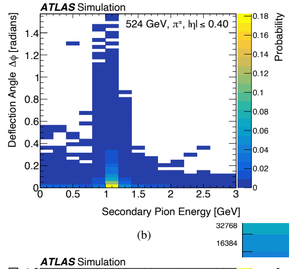

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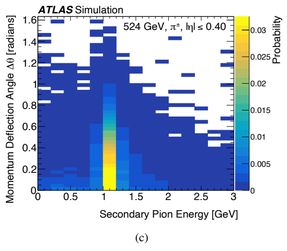

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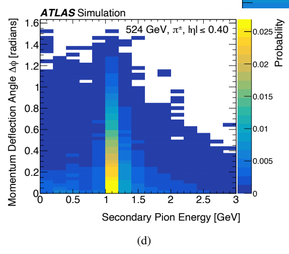

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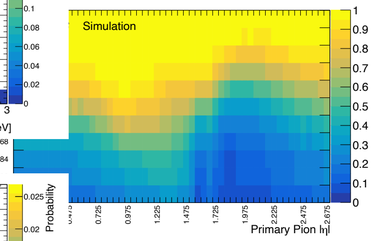

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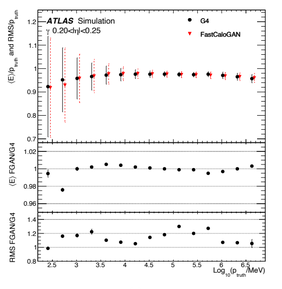

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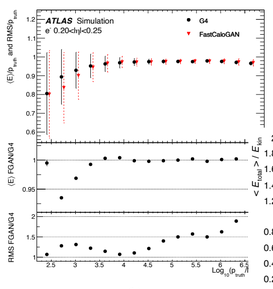

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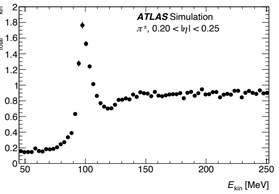

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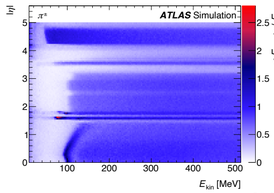

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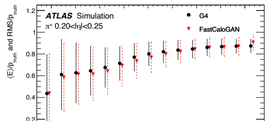

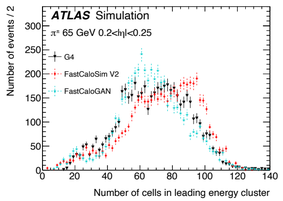

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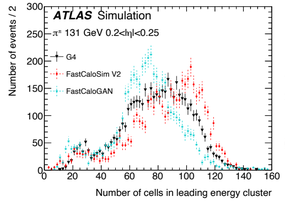

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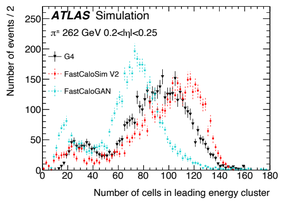

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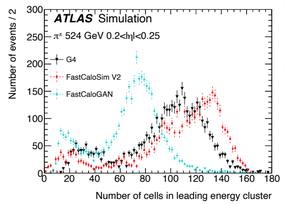

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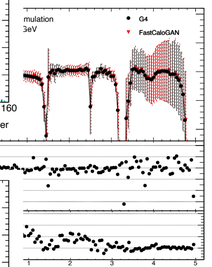

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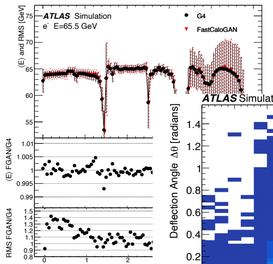

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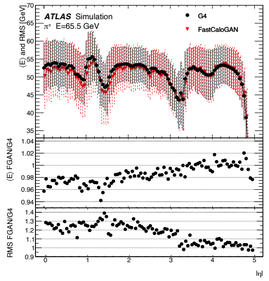

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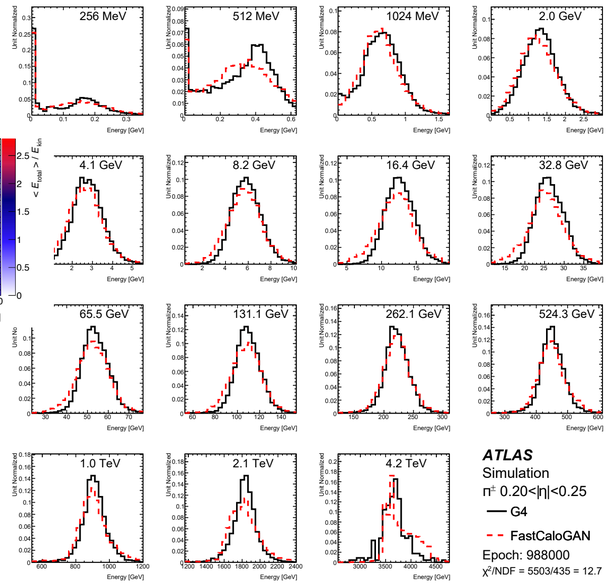

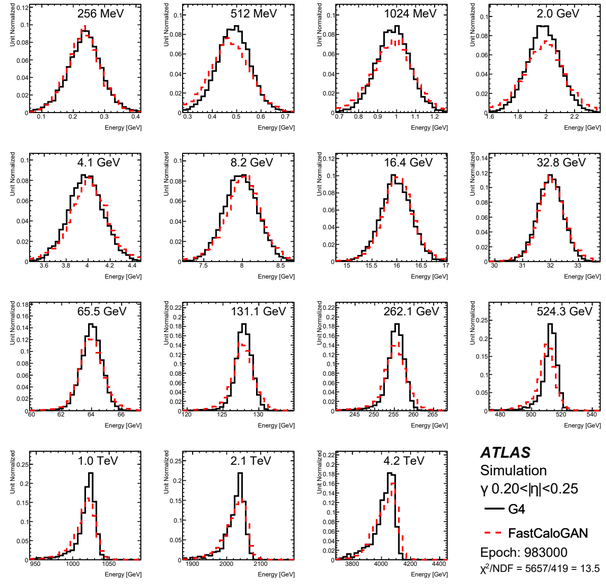

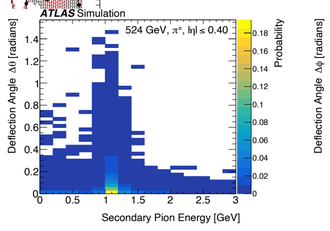

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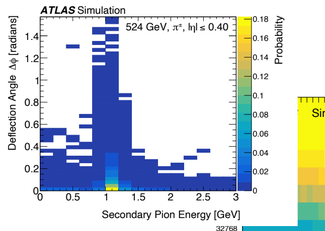

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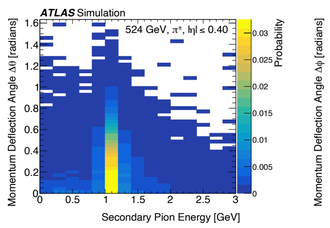

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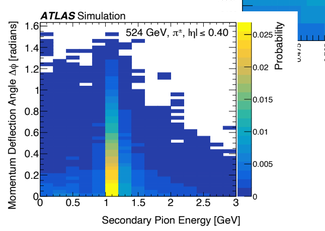

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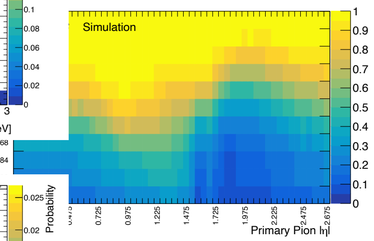

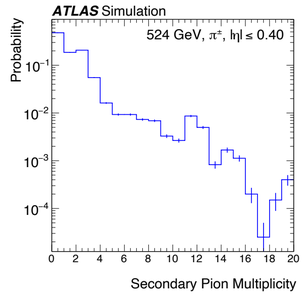

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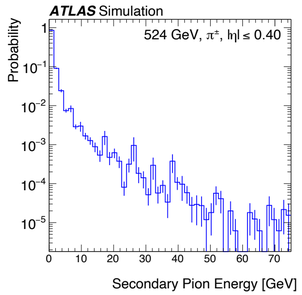
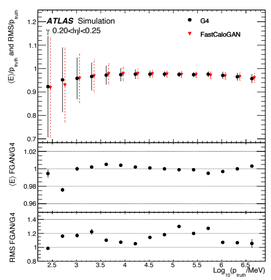


(b)

Evaluating Fast Calo Simulators



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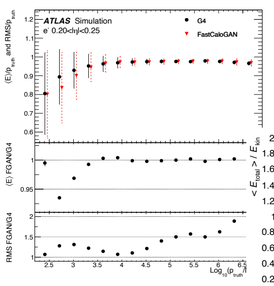

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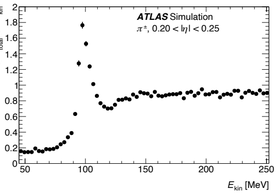

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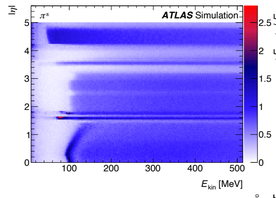

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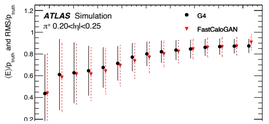

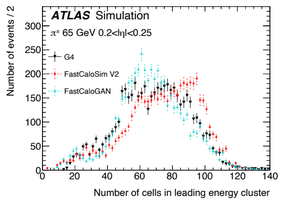

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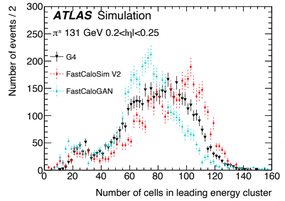

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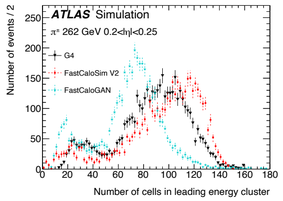

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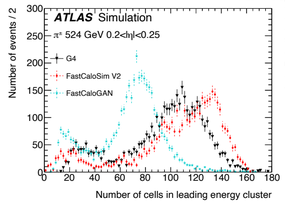

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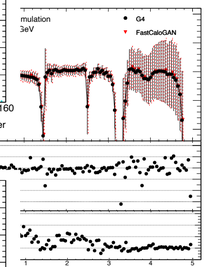

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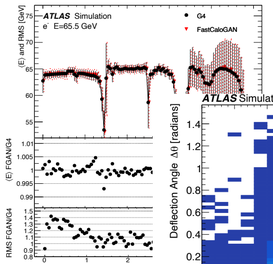

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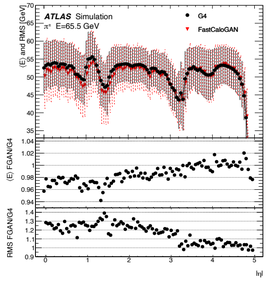

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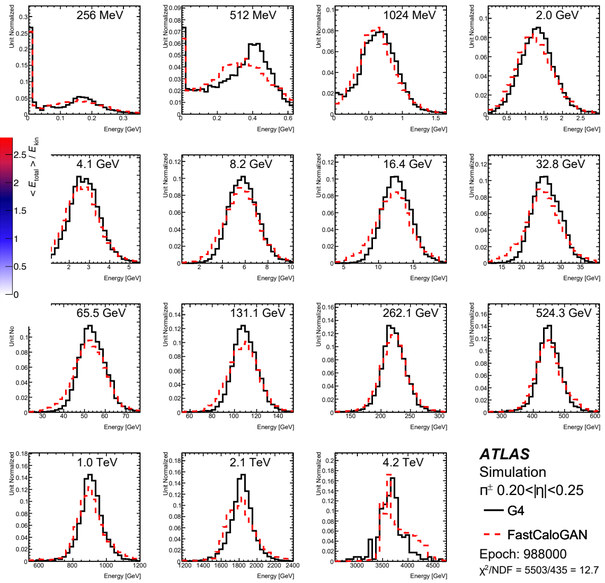

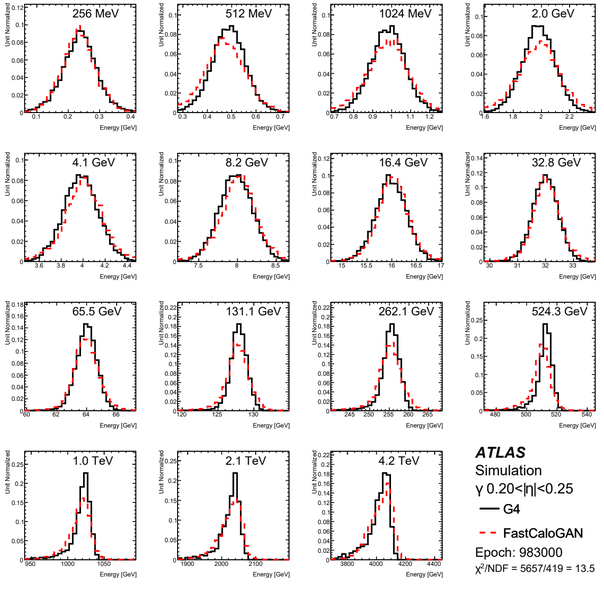

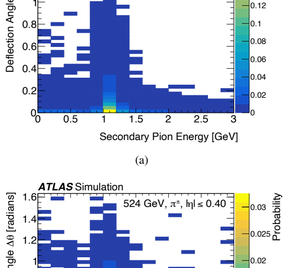

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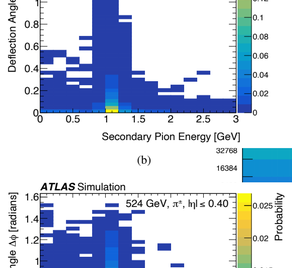

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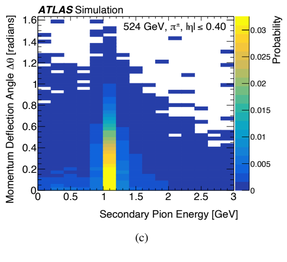

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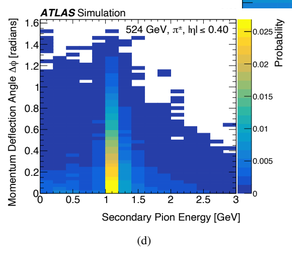

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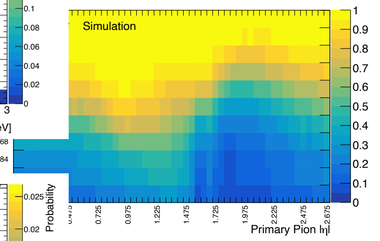

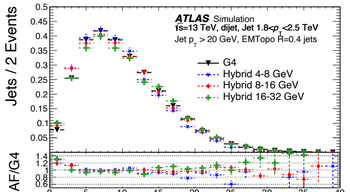

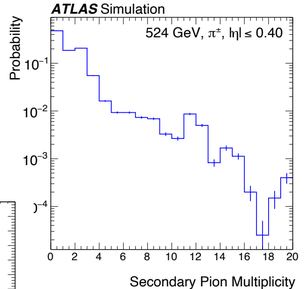

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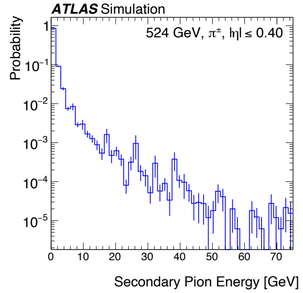

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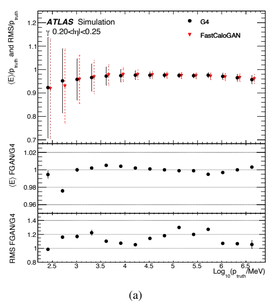
Evaluating Fast Calo Simulators



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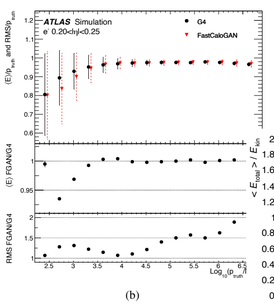

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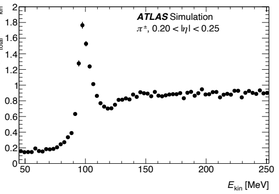

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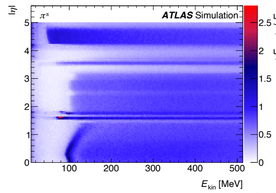

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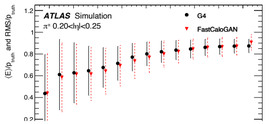

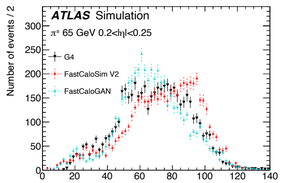

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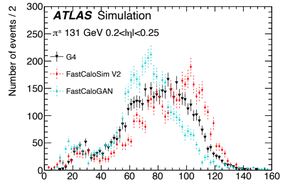

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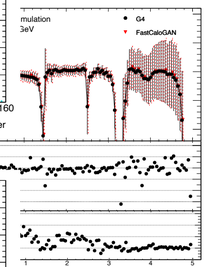

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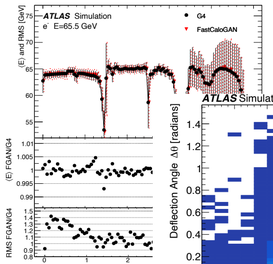

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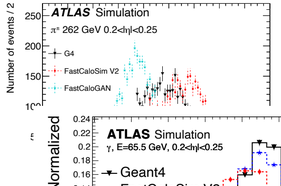

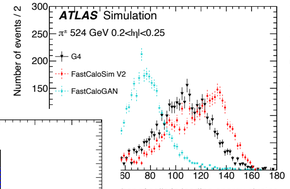

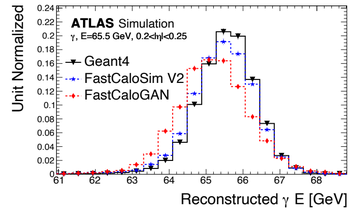

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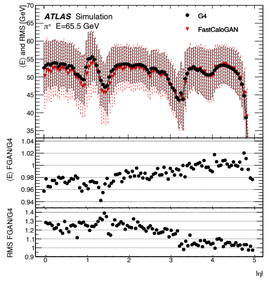
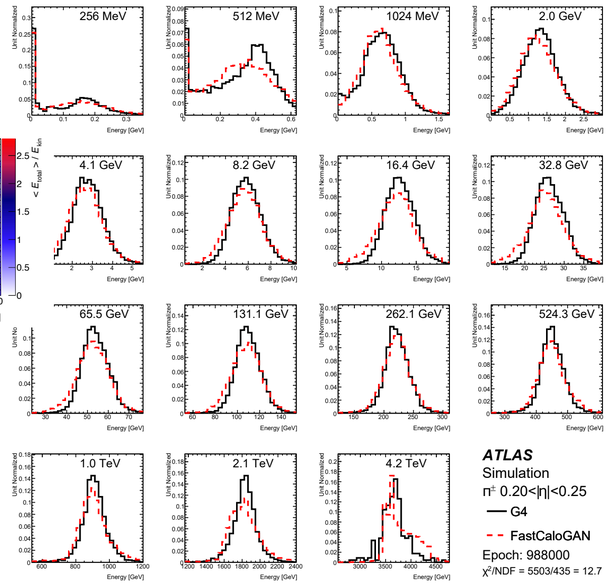
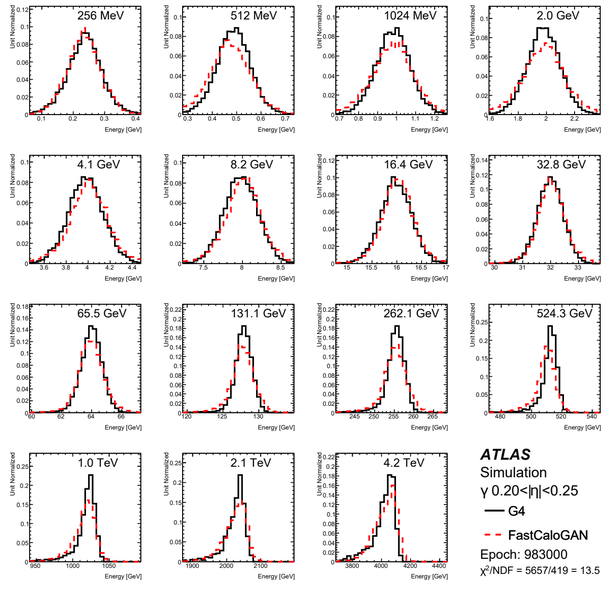
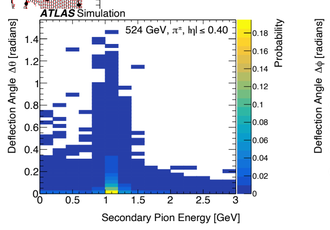


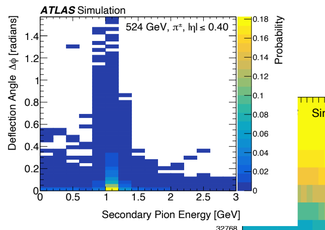
(c)



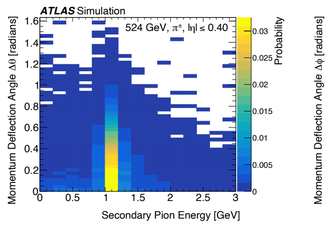




(a)



(b)



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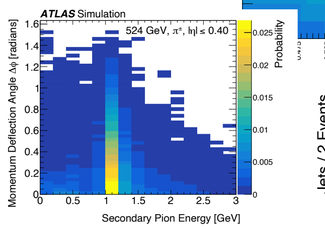

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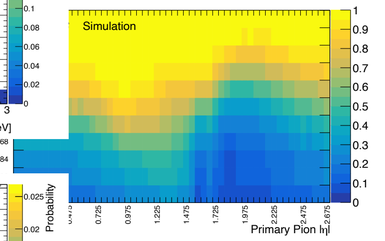

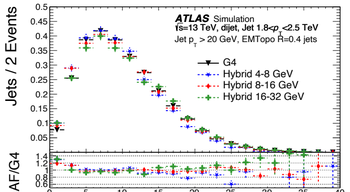

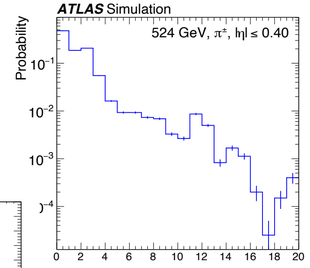

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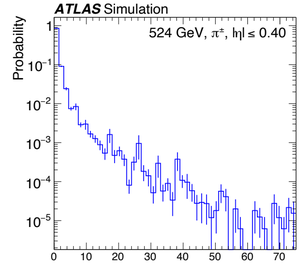
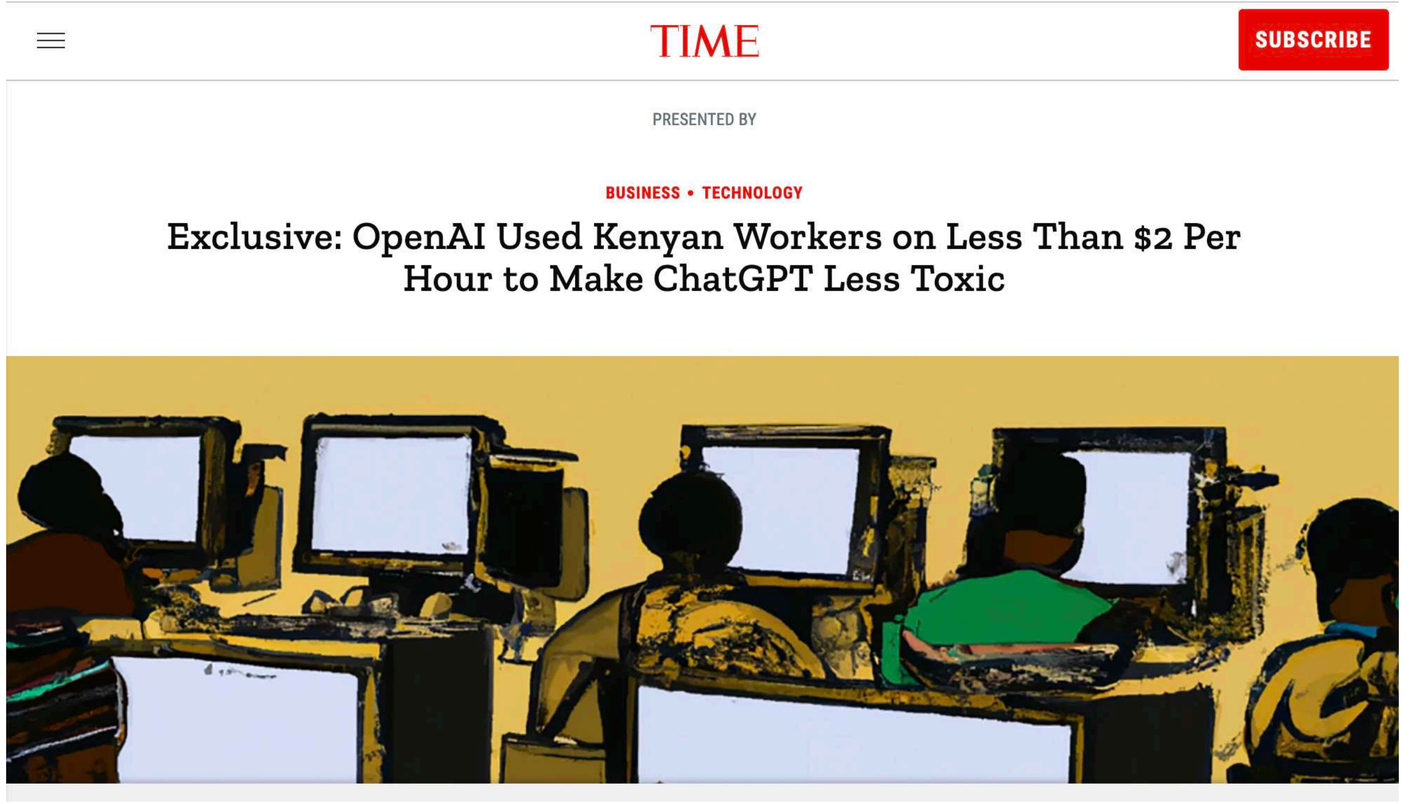


(b)

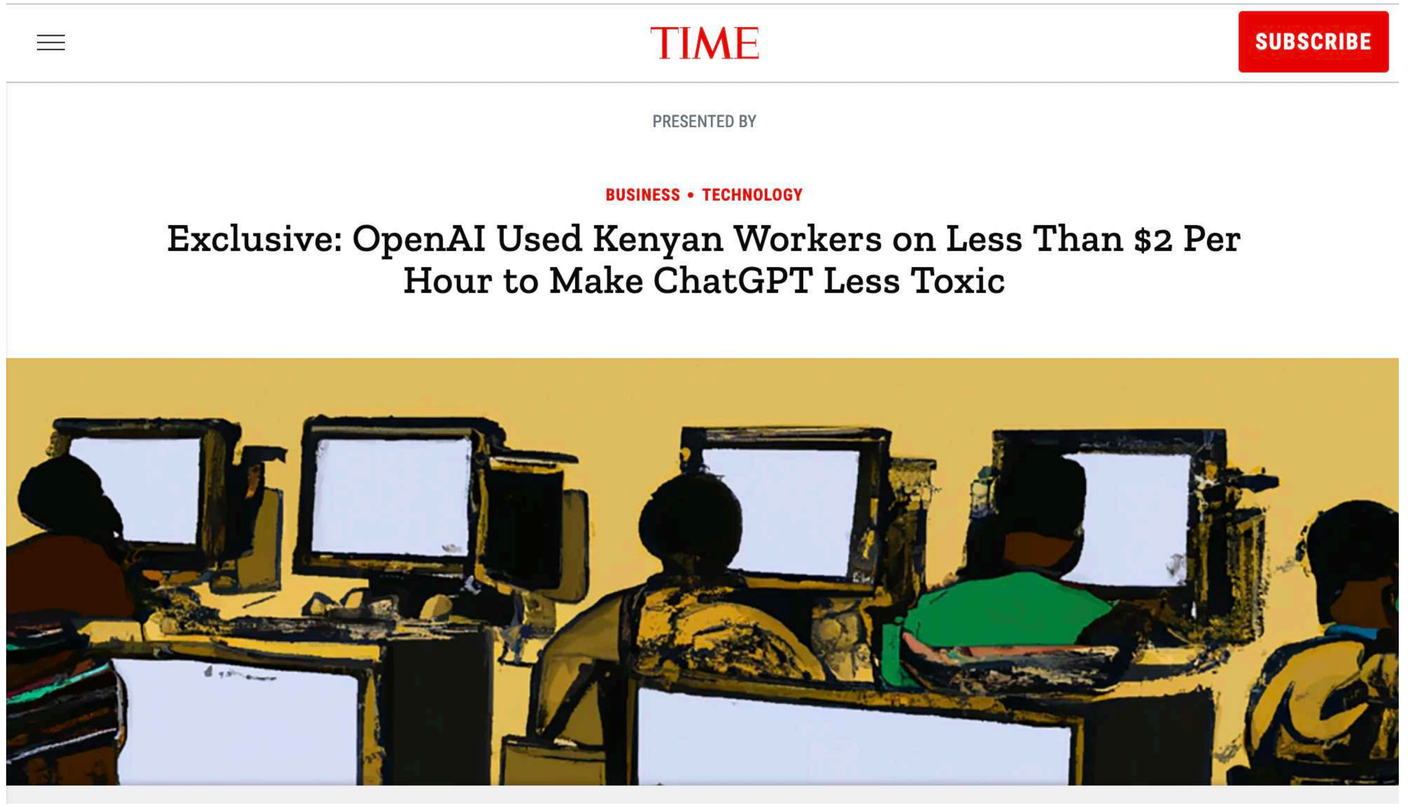
The evaluation bottleneck



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 !



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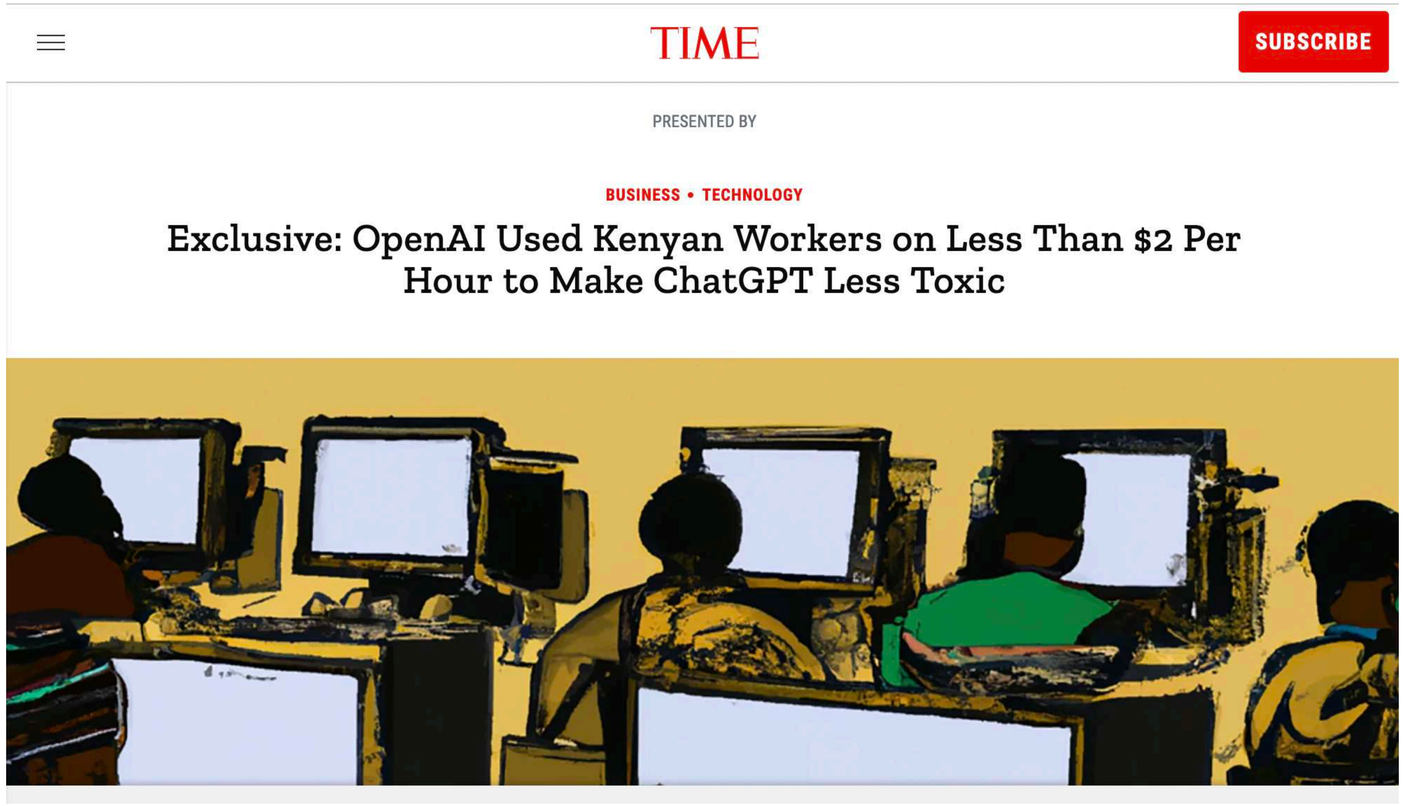

PhD in Plot Evaluation

Can we automise the evaluation ?

Need measures of distance → Active field of research in ML / statistics / mathematics

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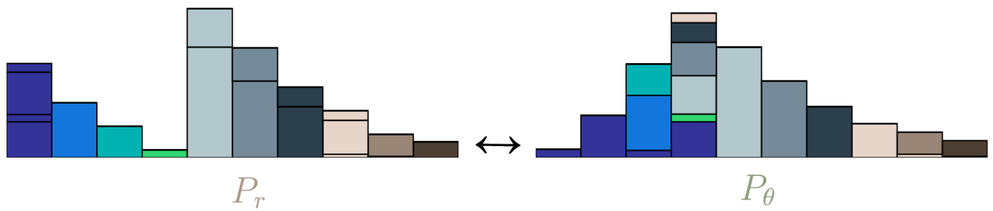

Wasserstein Distance

Can we automise the evaluation ?

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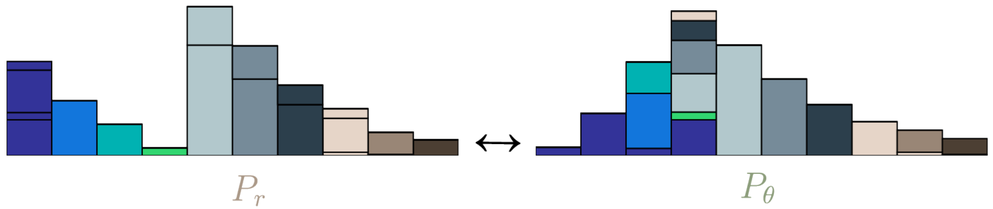
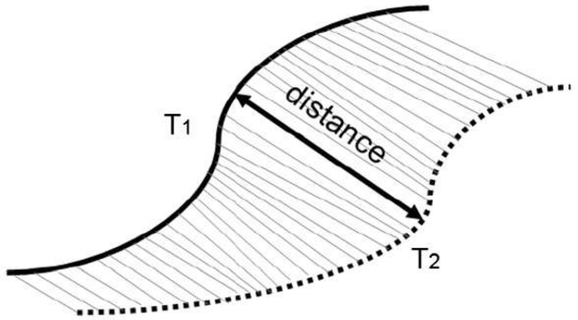


Wasserstein Distance



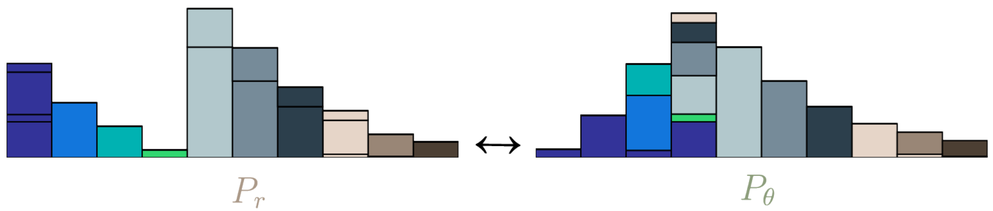
Fréchet Distance

Can we automise the evaluation ?

Need measures of distance → Active field of research in ML / statistics / mathematics

$$\frac{P(x \mid Geant)}{P(x \mid Gen)}$$

Likelihood Ratio



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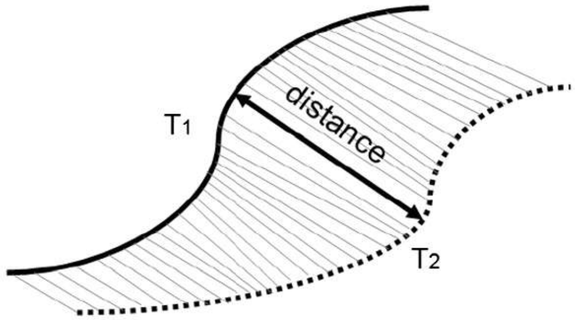


Fréchet Distance

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

Classify Geant4 vs generated and use AUC as single metric

Classifiers secretly learn the likelihood ratio

A Bayes optimal classifier learns function c:

$$c^*(x) = \frac{P(x\,|\,Geant)}{P(x\,|\,Geant) + P(x\,|\,Gen)}$$

(Neyman-Pearson lemma: Likelihood ratio is most powerful test statistic)

$$\frac{P(x\,|\,Geant)}{P(x\,|\,Gen)} = \frac{c(x)}{1 - c(x)}$$

Classifier output has all the same information as LR, the most powerful test statistic

*If perfectly trained

A large comparison of metrics

Kansal et al, 2022

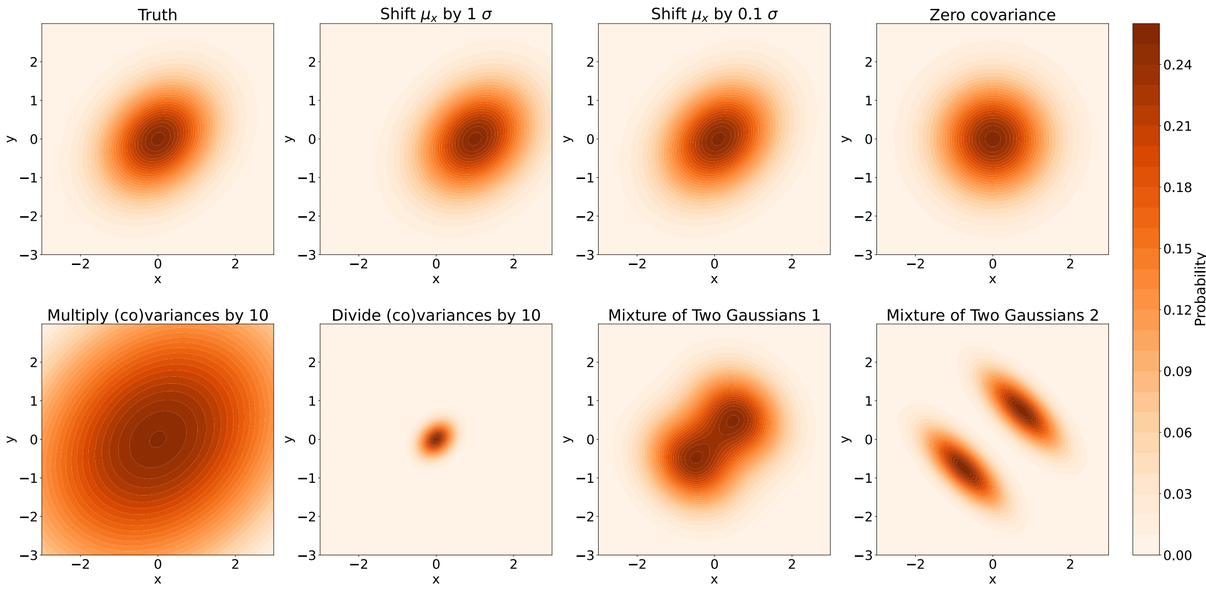
On the Evaluation of Generative Models in High Energy Physics

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

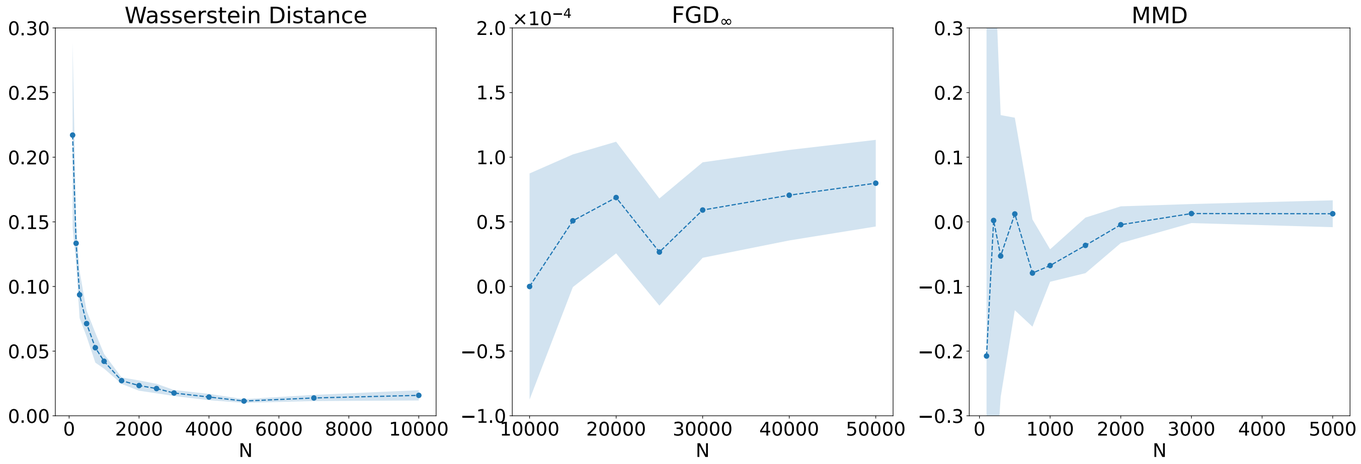
(Dated: November 21, 2022)



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	$\mathbf{0.036 \pm 0.003}$	$\mathbf{0.191 \pm 0.005}$
FGD_∞ $\times 10^3$	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	$\mathbf{19}\text{k} \pm \mathbf{1}\text{k}$	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 $p_{\text{T}}^{\text{rel}}$ smeared	Particle $p_{\text{T}}^{\text{rel}}$ 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 !

Future

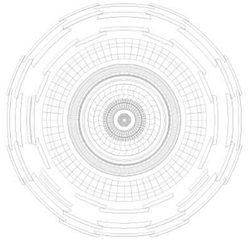
- Move away from black-box metrics ——> O(5) metrics that provide meaningful, orthogonal information about different aspects
  - Stats based: Metrics focused on tails, bulk, higher moments, lower moments, overfitting, interpolation
  - Physics info: Energy modelling, pointing, substructure, shape, interpolation

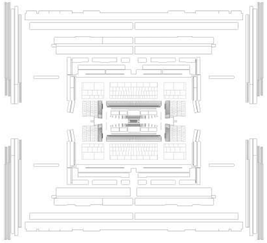
- Back-port these ideas for uncertainty quantification of traditional simulators

Conclusion

- ML more sensitive to simulation artefacts → building better uncertainty quantification tools
- ML lets us better propagate experimental uncertainties and build analyses optimised for all possibilities: HEP, Astro
- Solutions have wider use cases
    - Tractable likelihoods
    - Uncertainty quantification of ML-simulators [Performance metrics, Bayesian networks]
    - Optimise true objective with differentiable programming [Inferno, NEOS]
    - Learn physics from machine: Mapping ML into a human-readable space [CNN to EFPs]

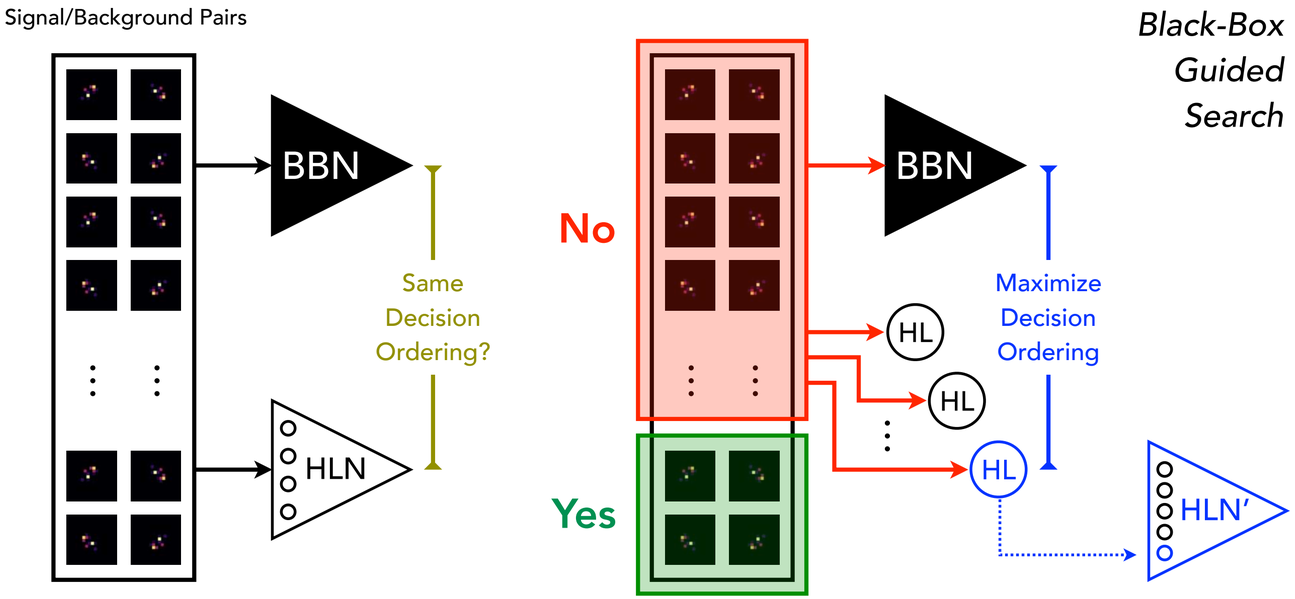
And more cool solutions to come !





Thank you!

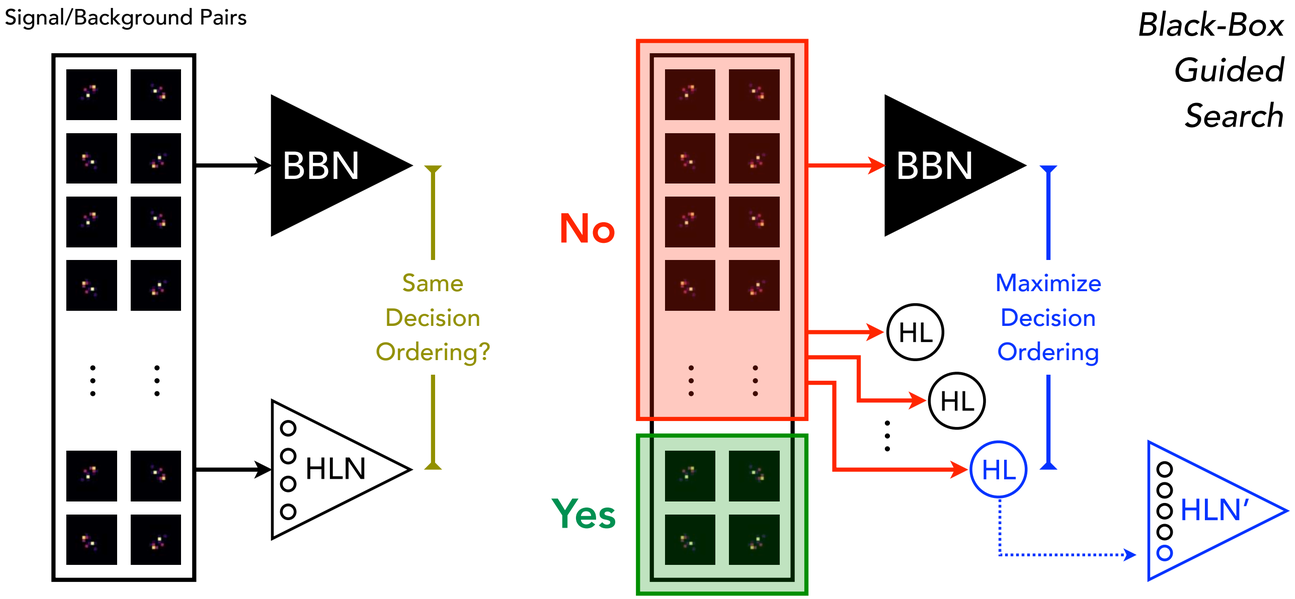
Mapping machine-learned physics into a human-readable space

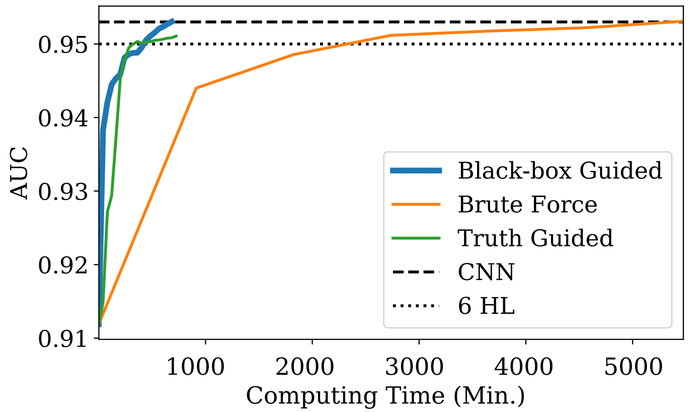


Rank	EFP	κ	β	Chrom #	ADO[EFP, CNN]$_{X_6}$	AUC[EFP]	ADO[6HL + EFP, CNN]$_{X_{\text{all}}}$	AUC[6HL + EFP]
1		2	$\frac{1}{2}$	3	0.6207	0.8031	0.9714	0.9528 ± 0.0003
2		2	$\frac{1}{2}$	3	0.6205	0.8203	0.9714	0.9524
3		0	–	1	0.6205	0.6737	0.9715	0.9525
4		2	$\frac{1}{2}$	3	0.6199	0.8301	0.9715	0.9527
5		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

Faucett et al.

Mapping machine-learned physics into a human-readable space





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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

Faucett et al.

Snowmass Whitepaper: Recommendations for the future

- Common language for uncertainty between ML and Physics communities
- Funding to test ML UQ methods for physics
- Create benchmark datasets for uncertainty tests
- Develop and study interpretability methods

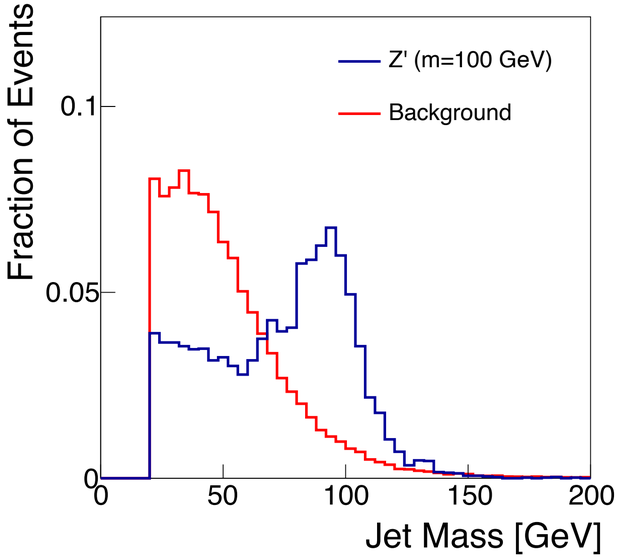
Snowmass Whitepaper: Recommendations for the future

Snowmass 2021: Summary of past work and future roadmap

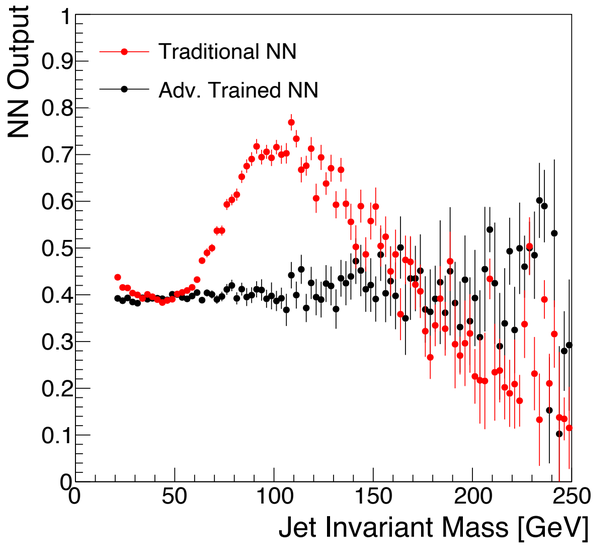
- Common language for uncertainty between ML and Physics communities
- Funding to test ML UQ methods for physics
- Create benchmark datasets for uncertainty tests
- Develop and study interpretability methods

Decorrelation to remove background sculpting

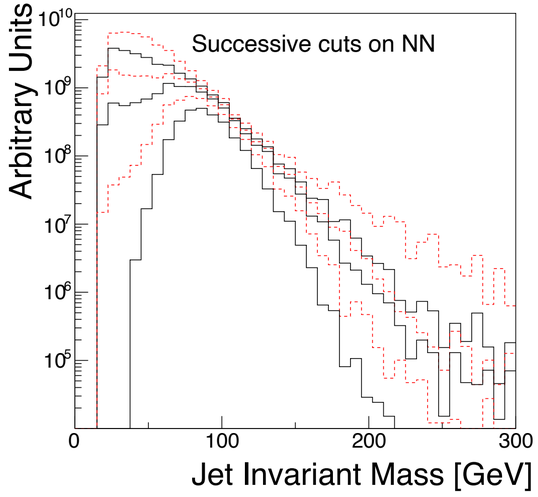
1703.03507



Signal peak at 100 GeV



Traditional NN learns to select 100 GeV events



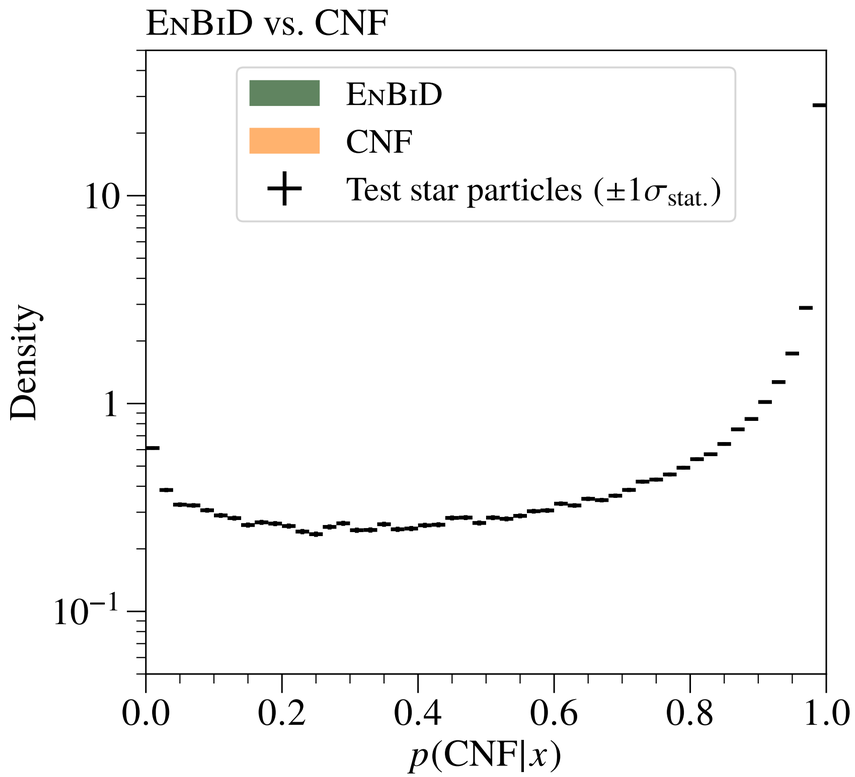
Event selection sculpts background distribution

Another classifier test

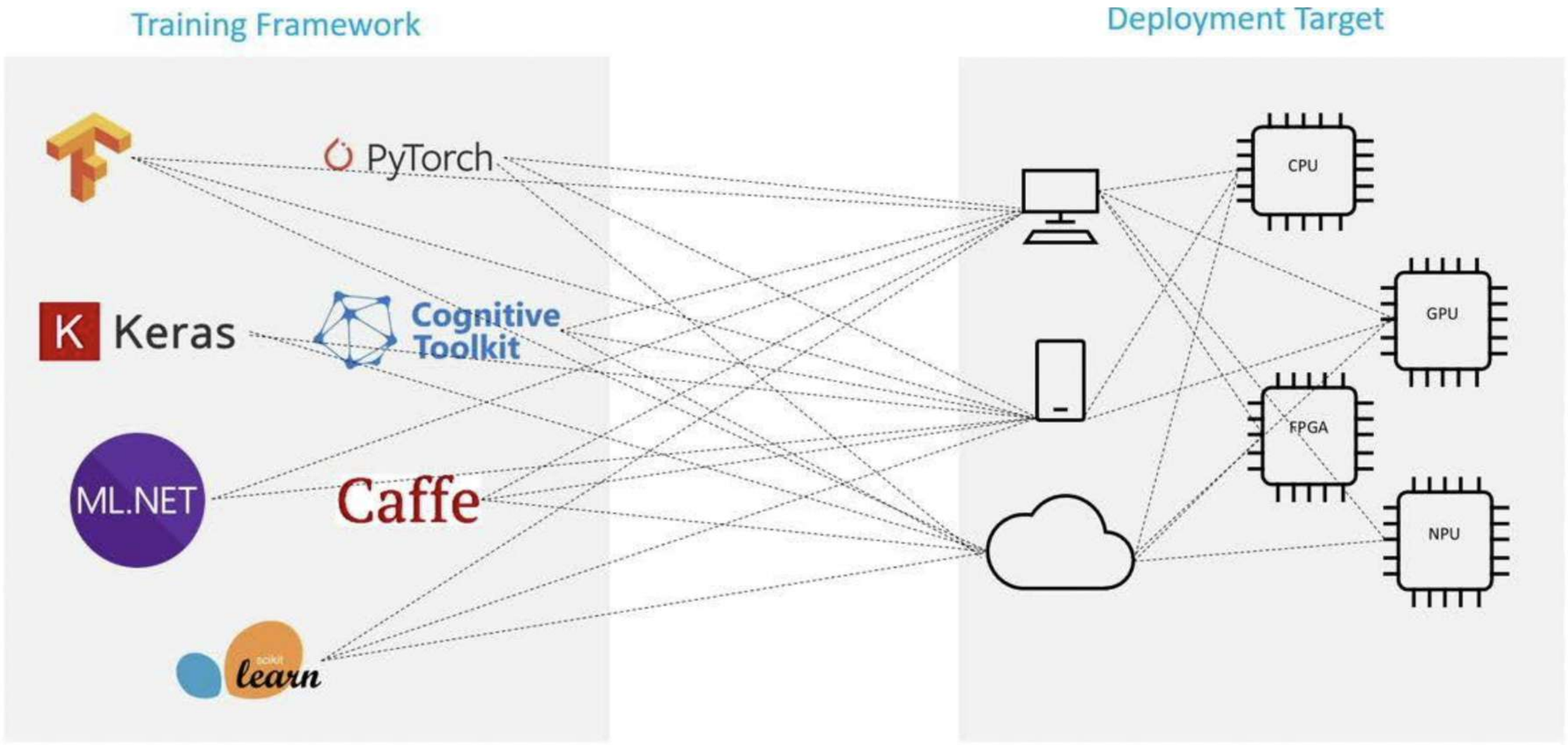
Lim et al, 2022

Compare two generative models:

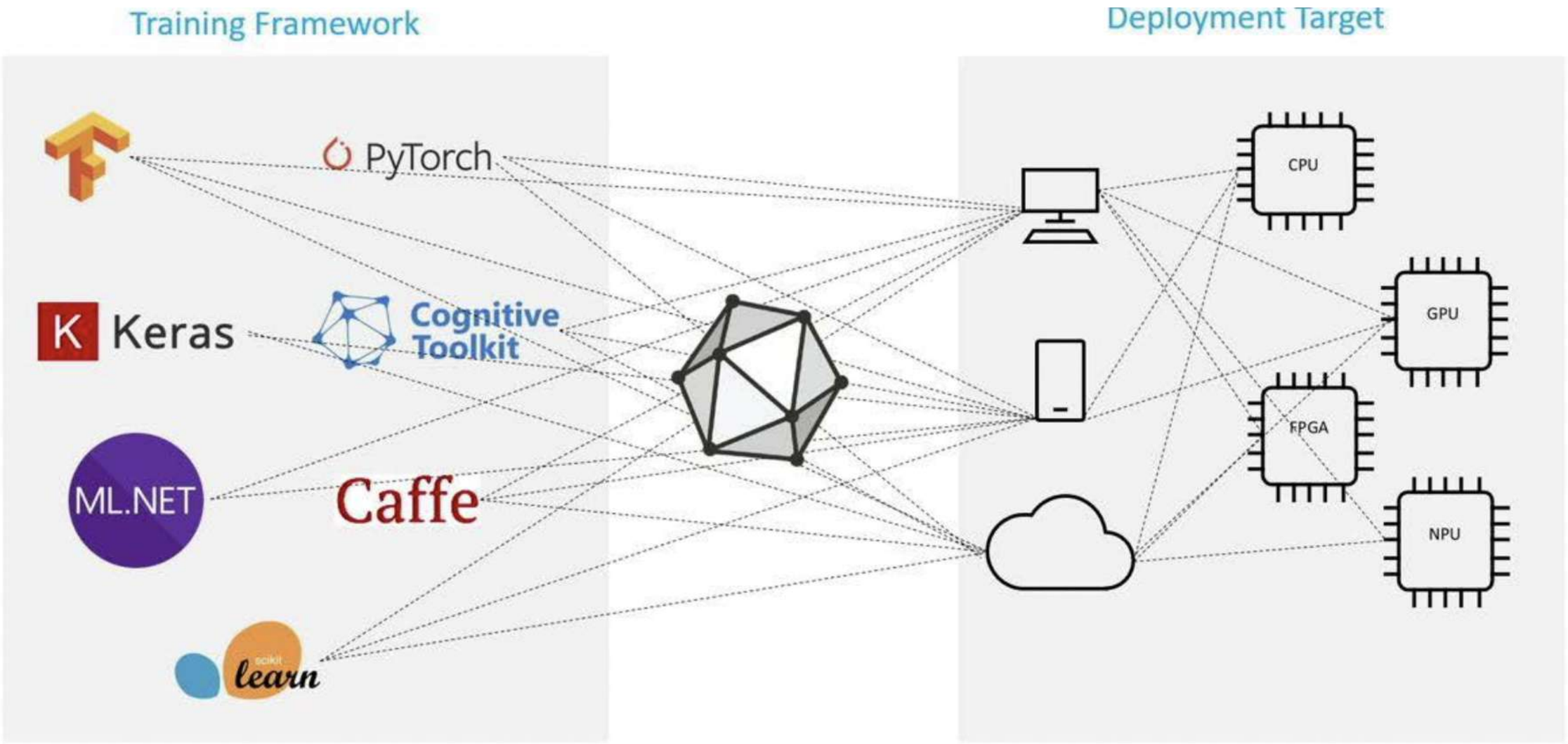
Classify generative model1 vs model2, check if test dataset agrees better with one or the other



Reality: Many ML platforms

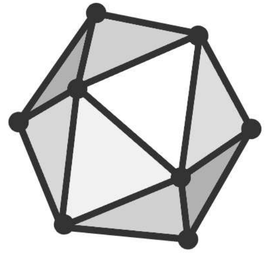


Reality: Many ML platforms



ML community effort to converge to Open Neural Network Exchange (ONNX) format

Why ONNX?



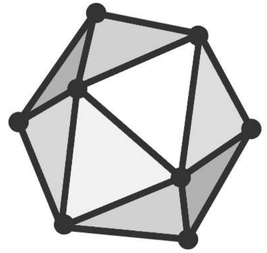
Open **N**eural **N**etwork E**x**change (ONNX)

Open-source artificial intelligence ecosystem that allows us to exchange deep learning models

https://onnx.ai/

- **Interoperability**
- **Hardware Access:** Optimize differently for training vs inference environment
- **Preservation:** ML packages evolve quickly (remember theano?), common format will be supported by all

Life before ONNX



Lightweight Trained Neural Network

CI passing | coverity passed | DOI 10.5281/zenodo.597221

Led by Dan Guest

What is this?

The code comes in two parts:

1. A set of scripts to convert saved neural networks to a standard JSON format
2. A set of classes which reconstruct the neural network for application in a C++ production environment

The main design principles are:

- **Minimal dependencies:** The C++ code depends on C++11, Eigen, and boost PropertyTree. The converters have additional requirements (Python3 and h5py) but these can be run outside the C++ production environment.
- **Easy to extend:** Should cover 95% of deep network architectures we would realistically consider.
- **Hard to break:** The NN constructor checks the input NN for consistency and fails loudly if anything goes wrong.

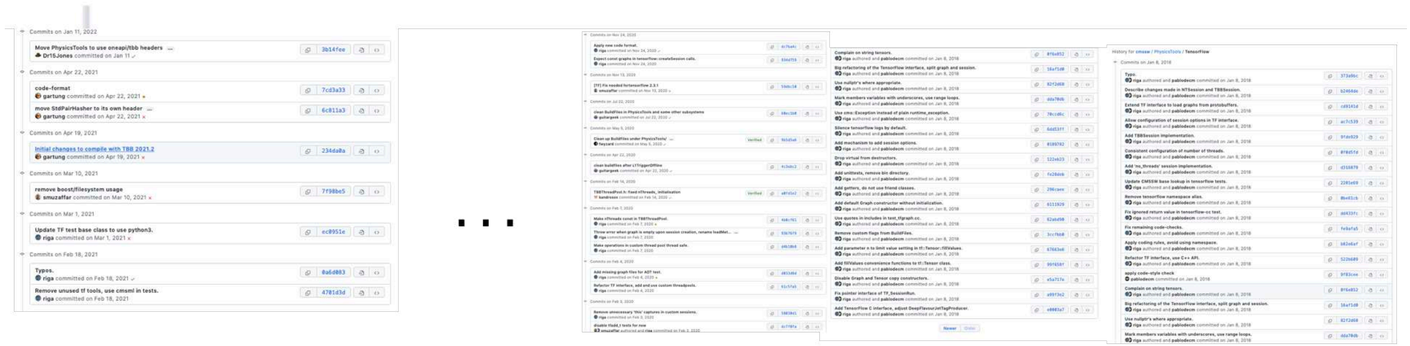
Cannot bring your own layer / new architecture without re-implementing it in C++

We still use **LWTNN** everywhere in Athena

https://github.com/lwtnn/lwtnn

ATLAS EXPERIMENT

Life before ONNX



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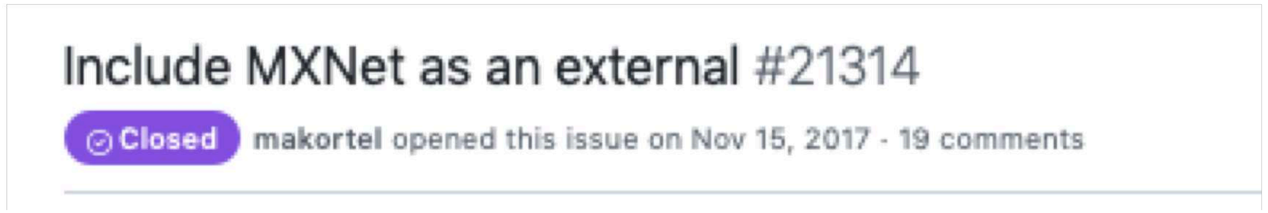
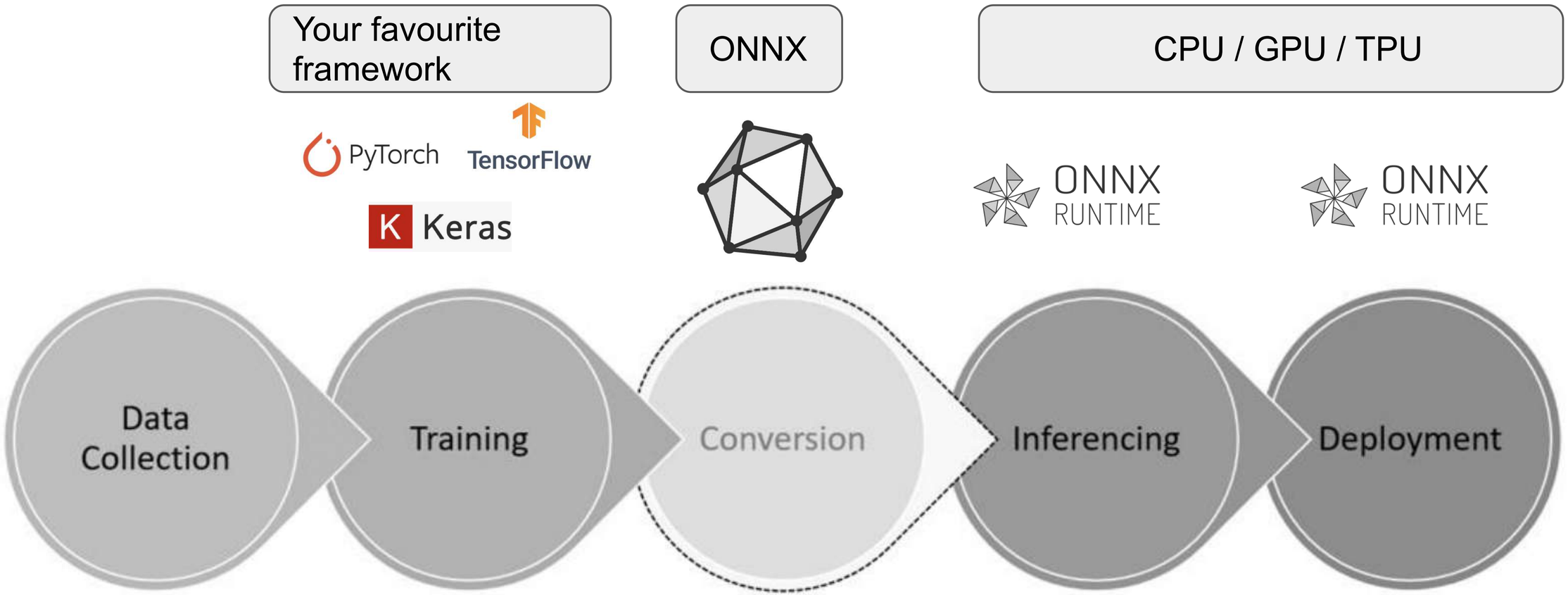


CMS took another path.

Added TensorFlow, MXNet etc to CMS software

- A lot of work to merge
- Some work to maintain them all simultaneously

ML production pipeline



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

Bayesian Generative Models

Bayesian Generative Models

Butter et al.

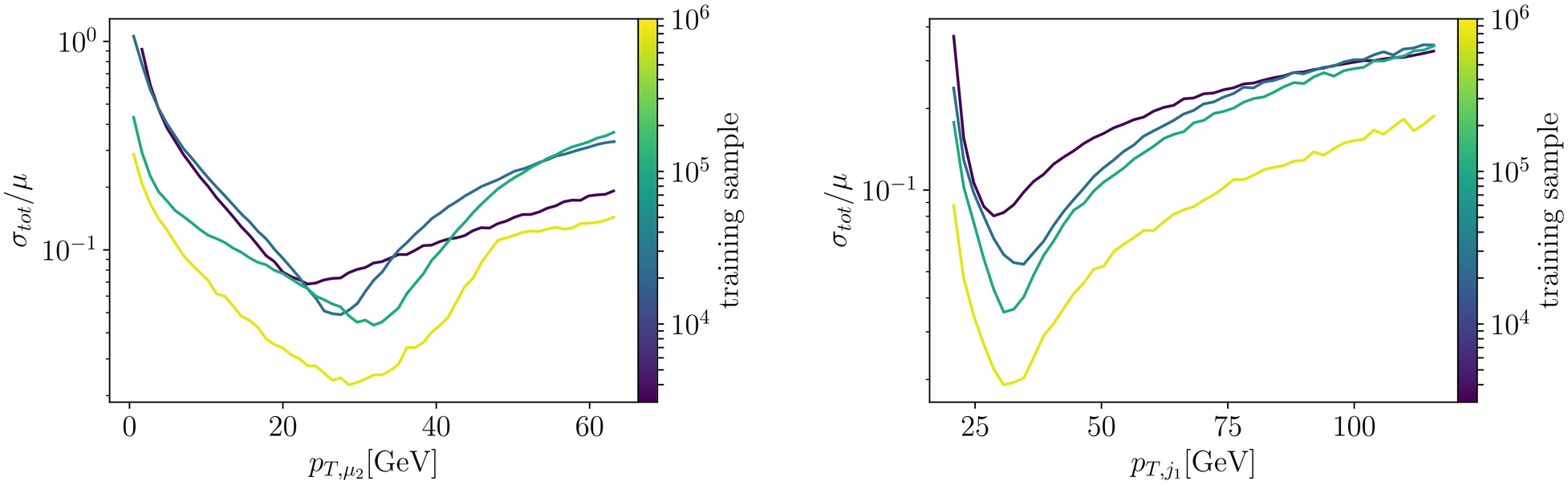


Figure 12: Relative uncertainty from the BINN for the $Z + 1$ jet sample, as a function of the size of the training sample.

Other uncertainty methods

Differentiable Programming: Optimise your final objective directly

Simpson et al.

Following Inferno [de Castro et al.]

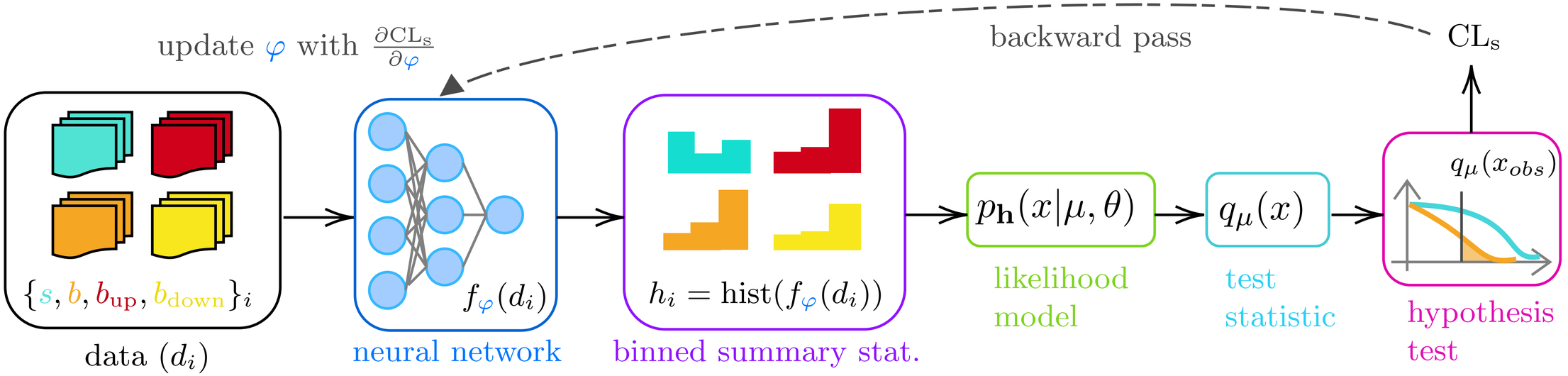


Figure 1. The pipeline for `neos`. The dashed line indicating the backward pass involves updating the weights φ of the neural network via gradient descent.

Unfolding with nuisance parameters

Chan and Nachman arXiv:2302.05390

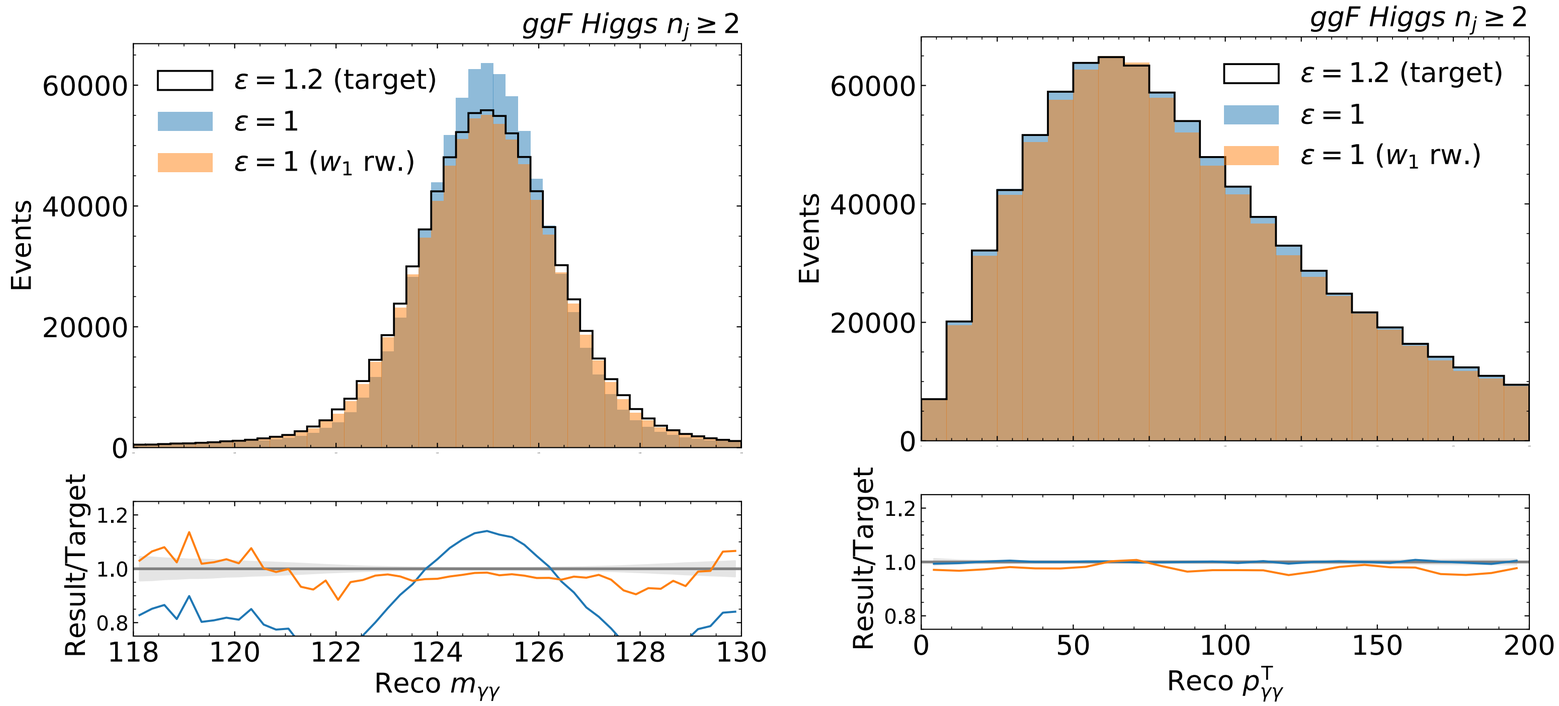
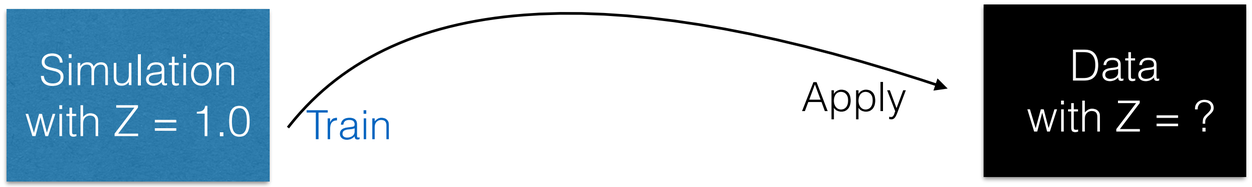


FIG. 6. Higgs boson cross section: the nominal detector-level spectra $m_{\gamma\gamma}$ (left) and $p_{\gamma\gamma}^{\mathrm{T}}$ (right) with $\epsilon_\gamma = 1$ reweighted by the trained w_1 conditioned at $\epsilon_\gamma = 1.2$ and compared to the spectra with $\epsilon_\gamma = 1.2$.

More on uncertainty-aware networks

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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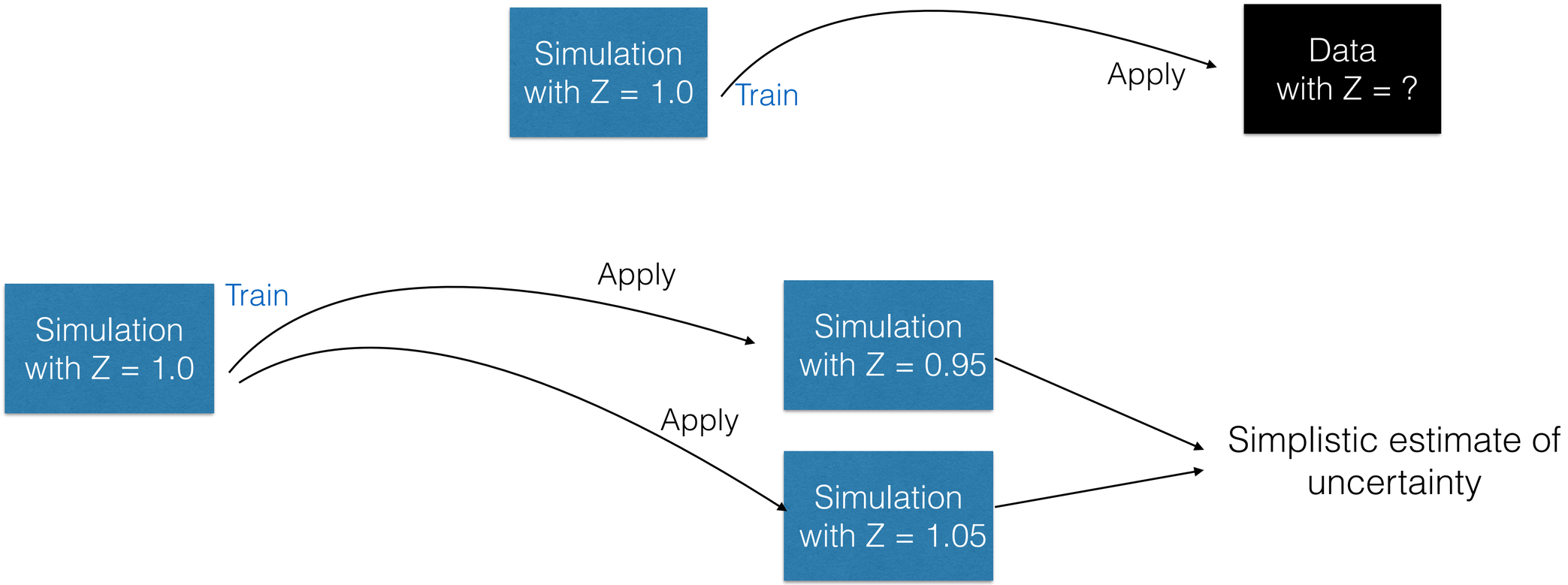
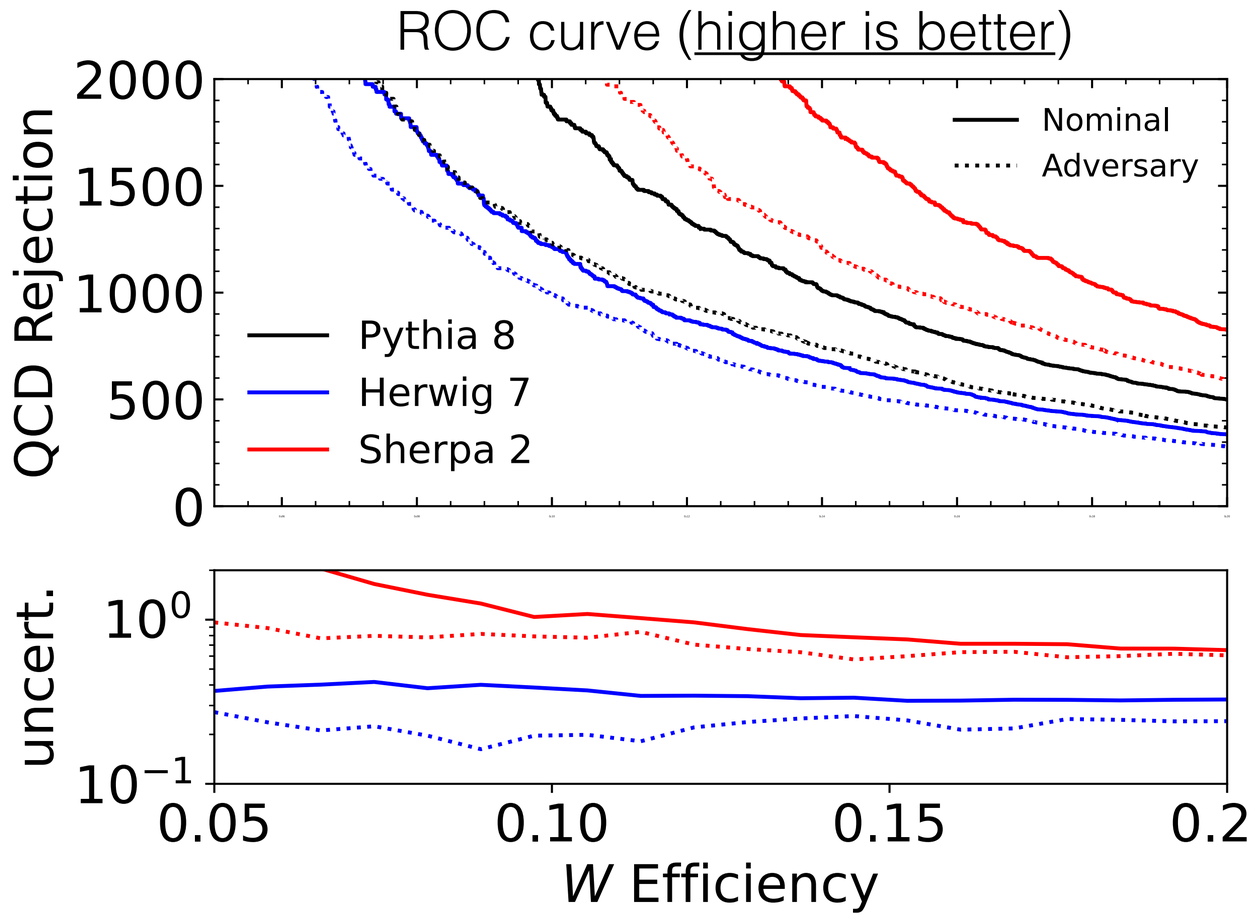


Full statistical treatment → Expensive ‘Profile Likelihood’

Case Study 1: Two-point uncertainty - Result

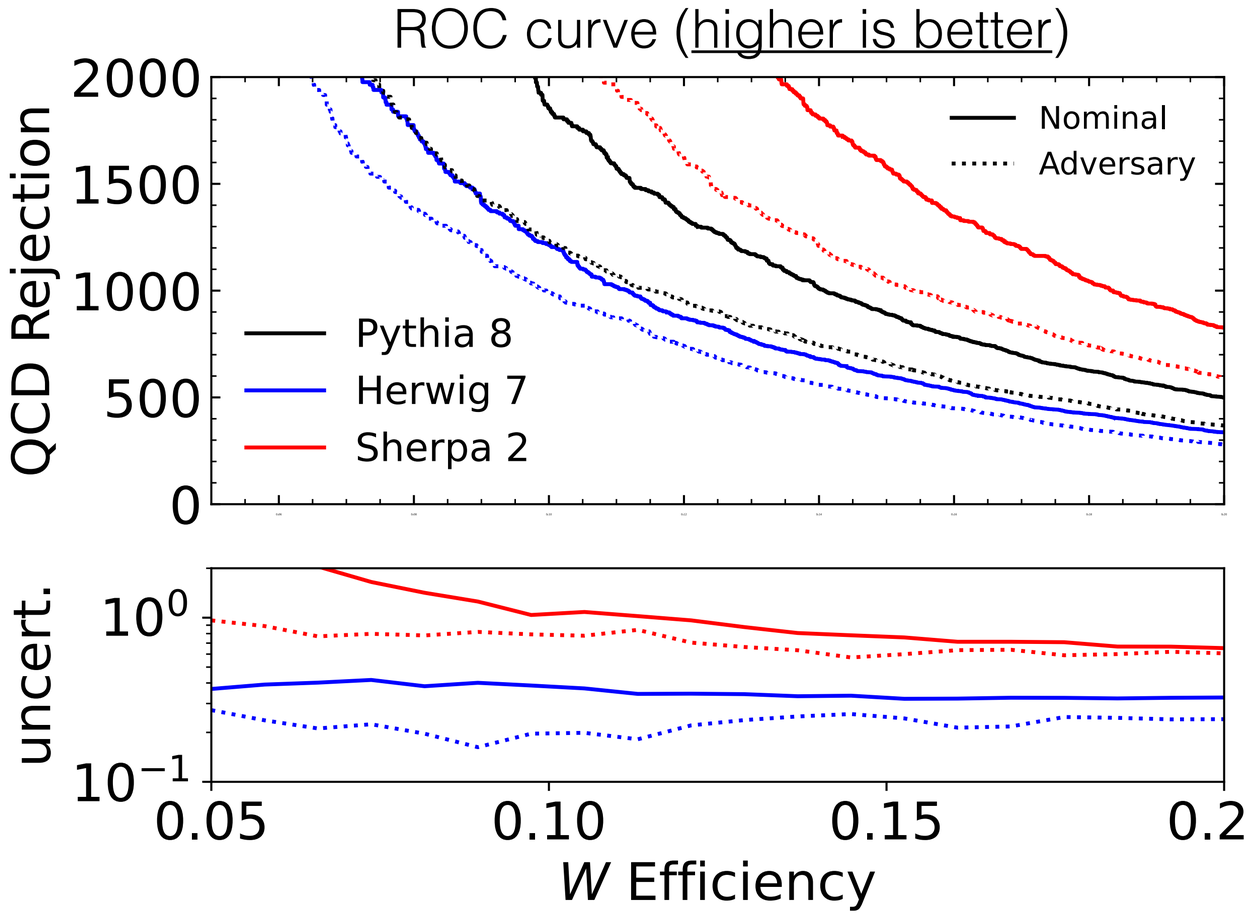


Case Study 1: Two-point uncertainty - Result

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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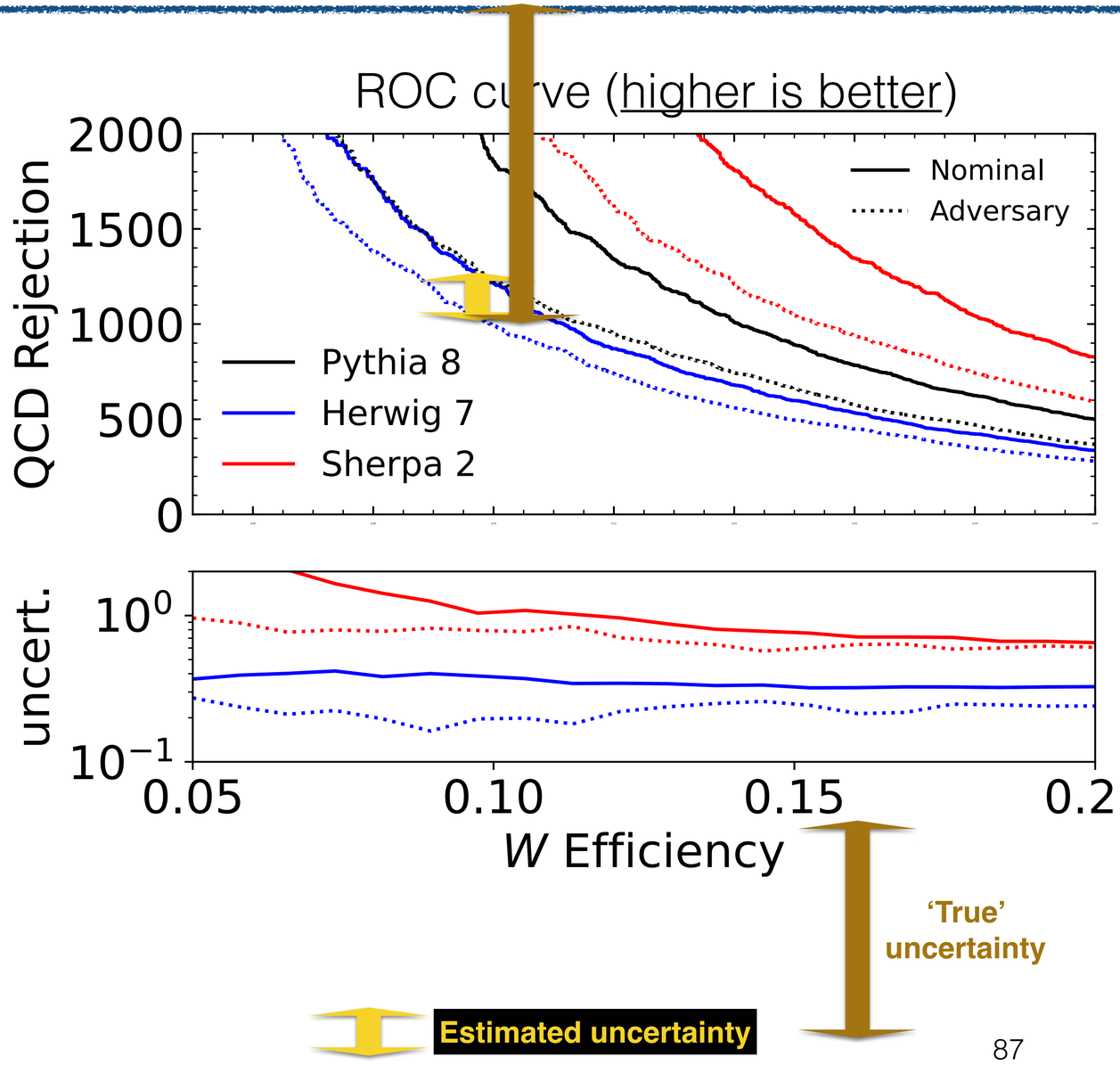
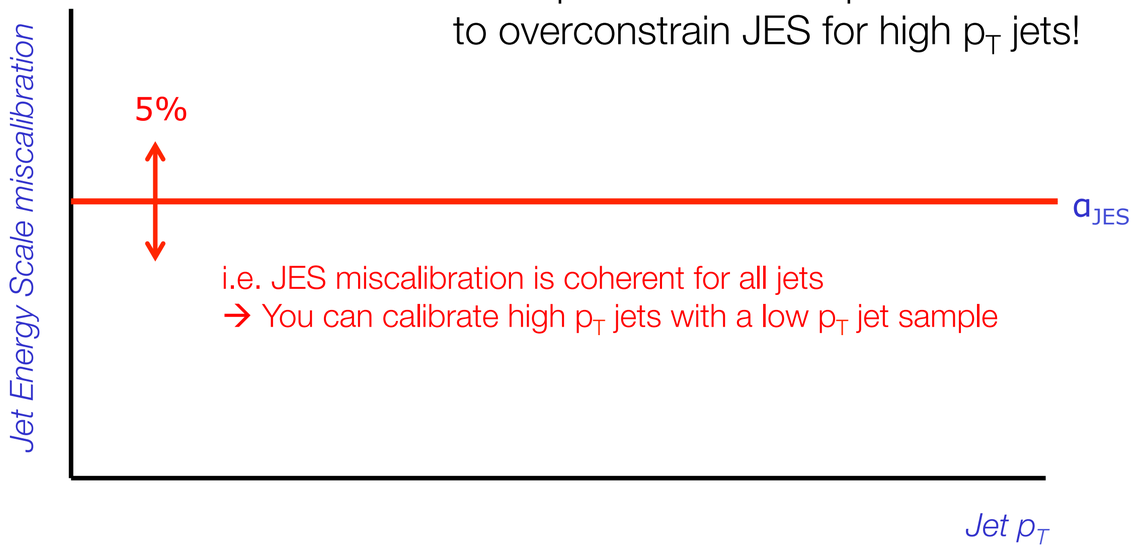


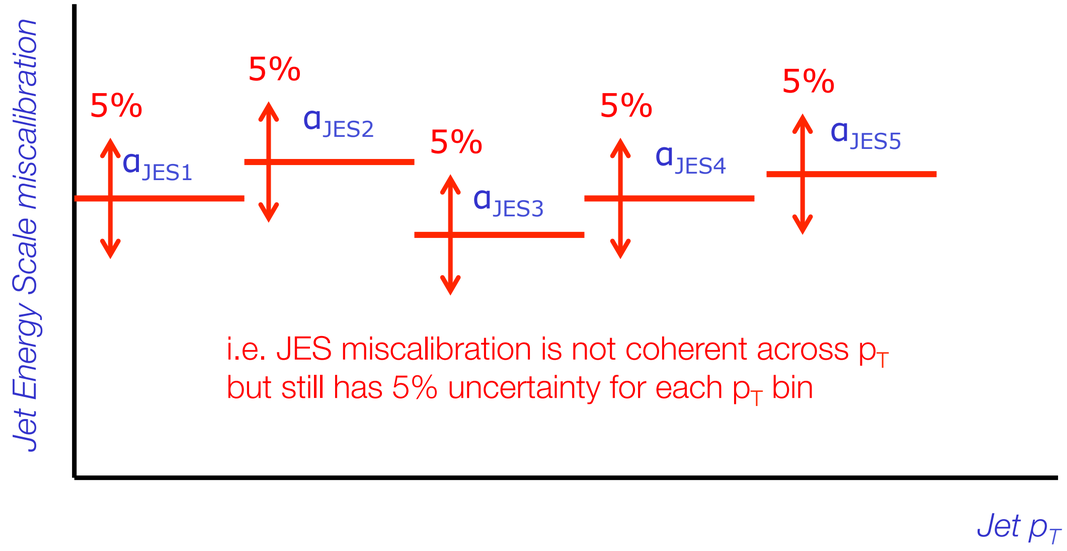
Overconstraining NP

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!





The secret sauce: Likelihood Ratio Trick

Neyman-Pearson lemma: Likelihood ratio is most powerful test statistic

A Bayes optimal classifier learns function c: $c^*(x) = \frac{p(x \mid S)}{p(x \mid B) + p(x \mid S)},$

which gives you the likelihood-ratio:

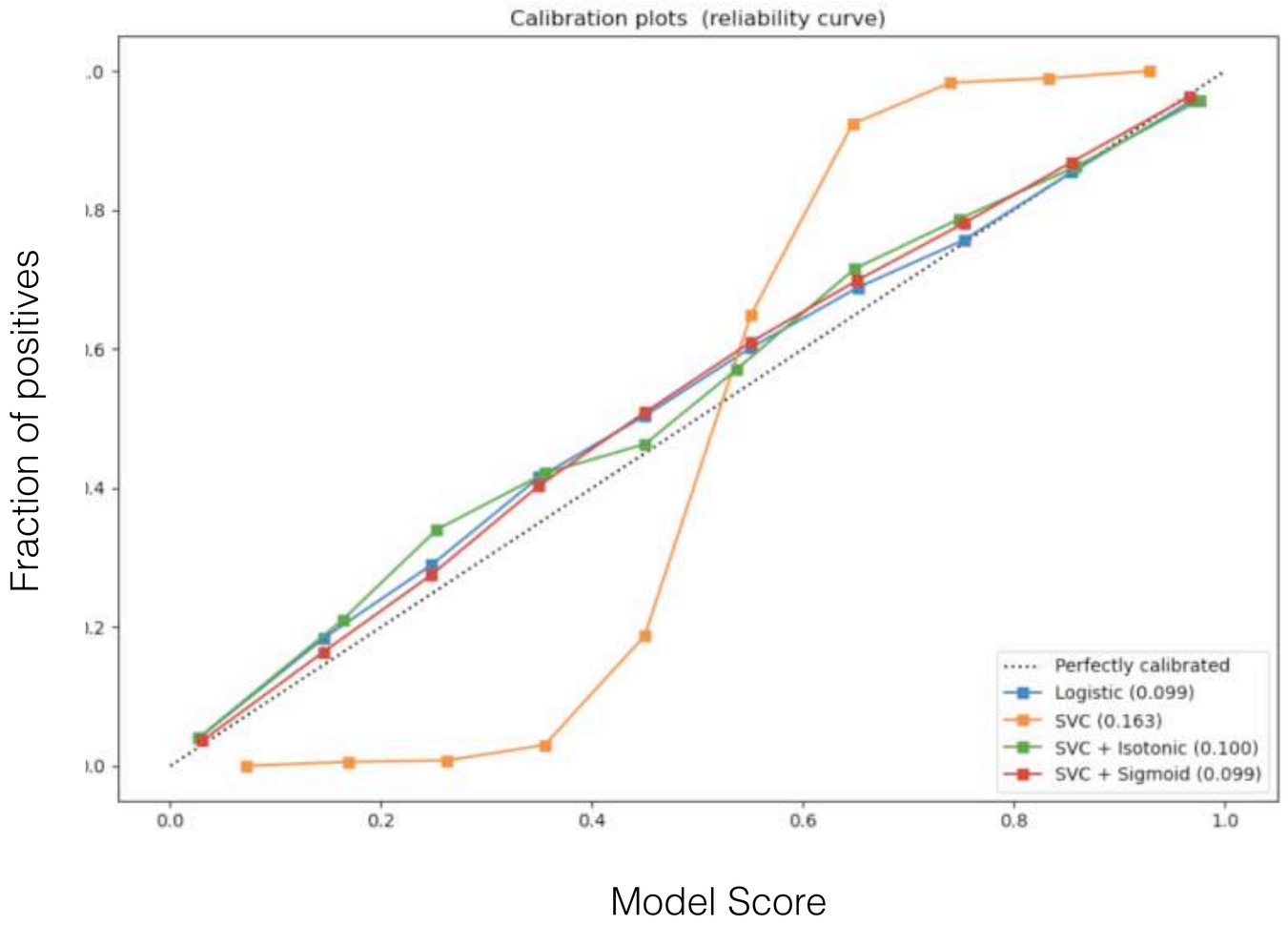
$$\frac{p(x_i \mid \mu = 1)}{p(x_i \mid \mu = 0)} = \frac{p(x_i \mid S) + p(x_i \mid B)}{p(x_i \mid B)} = \frac{c(x)}{(1 - c(x))} + 1,$$

This is why we can use classifiers to improve sensitivity for signal strength measurements

Calibration Curves

NNs tend to be overconfident

Can calibrate them (eg. With SKLearn)



Plot: https://neptune.ai/blog/brier-score-and-model-calibration