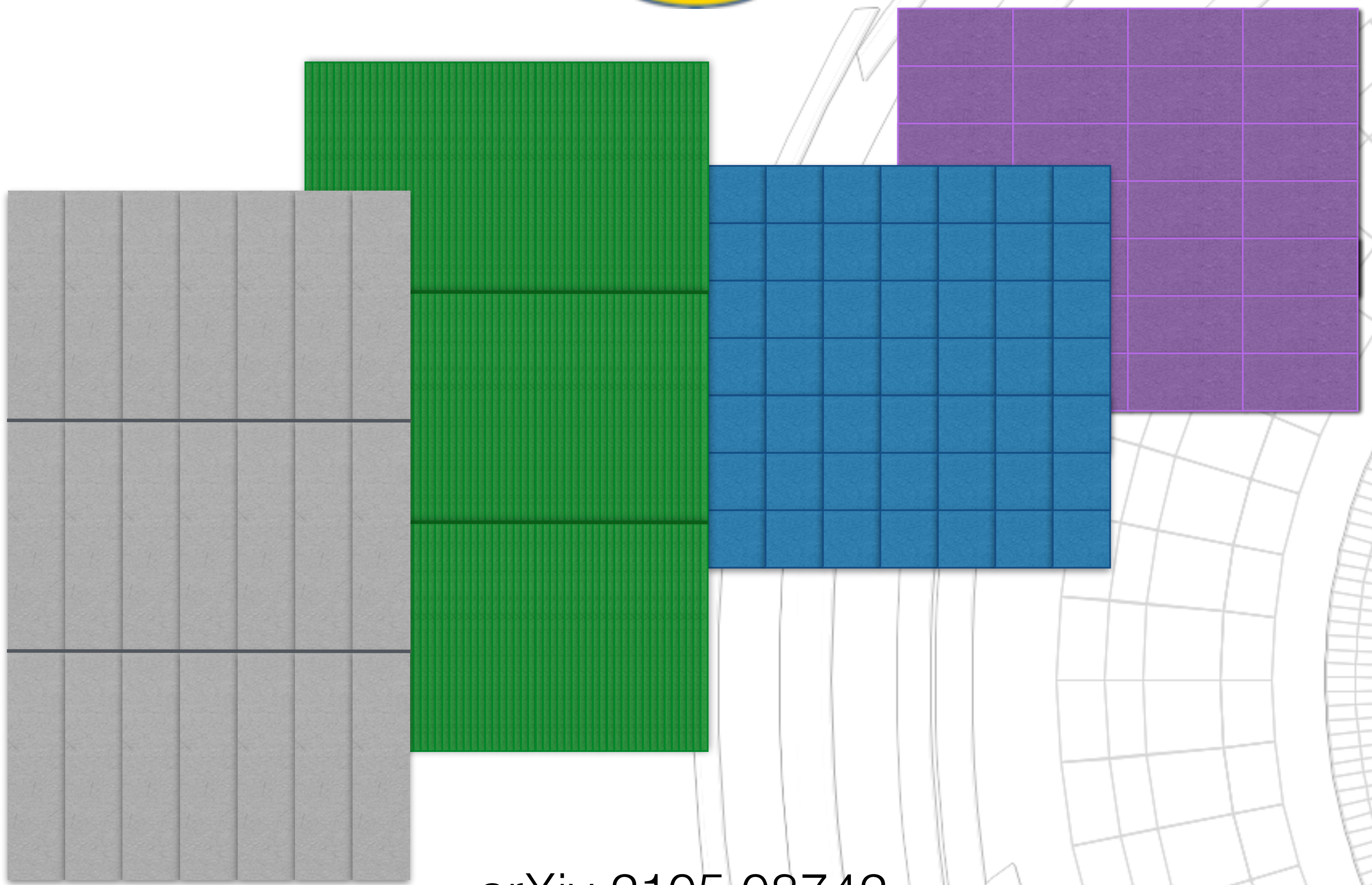
Uncertainty Aware Learning For High Energy Physics

Aishik Ghosh, Benjamin Nachman, Daniel Whiteson

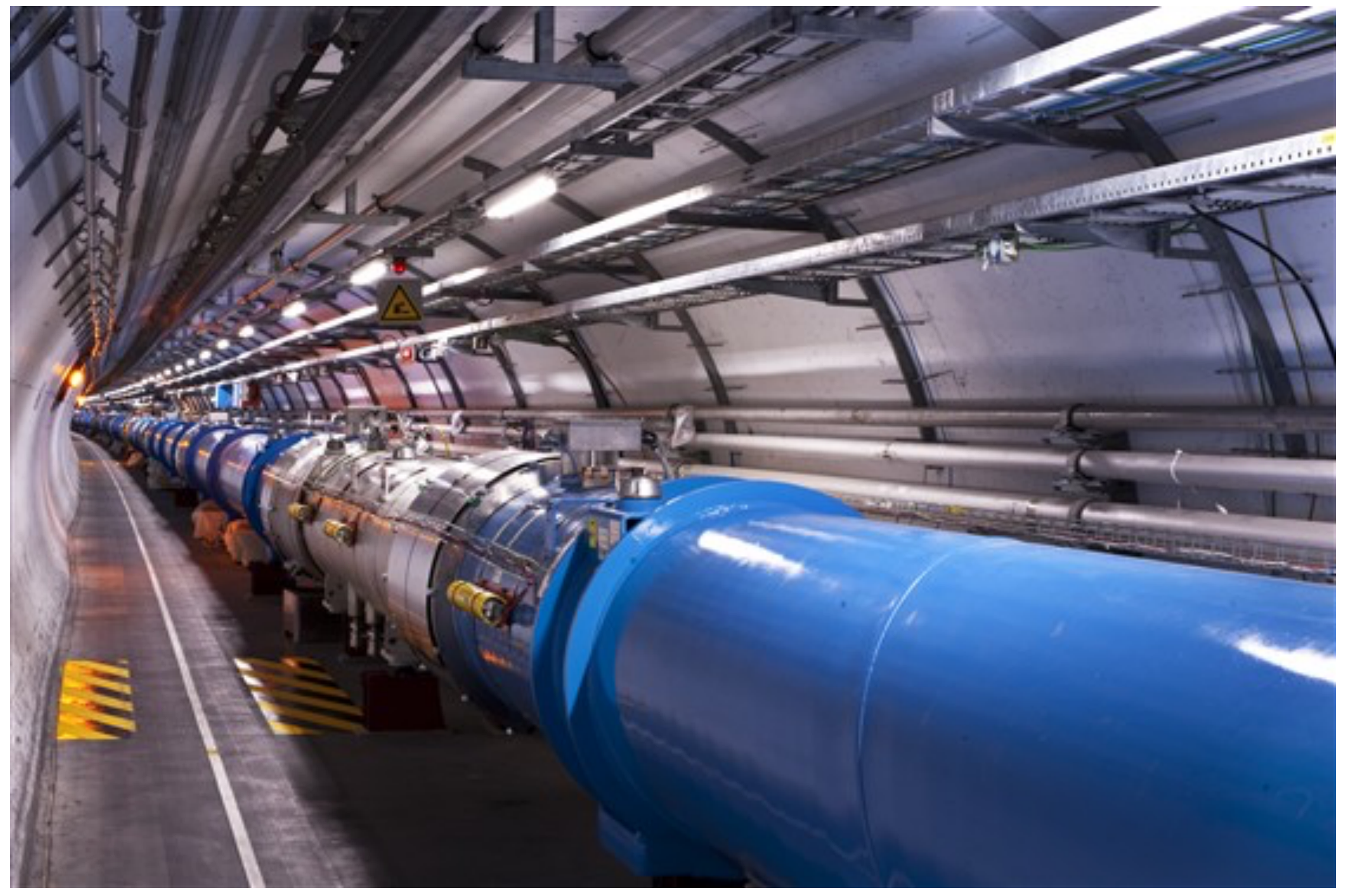
CMS ML Town Hall

26 July 2021



arXiv:2105.08742

Simulation-Based Inference



Real Data from LHC

Look for deviations to find New Physics

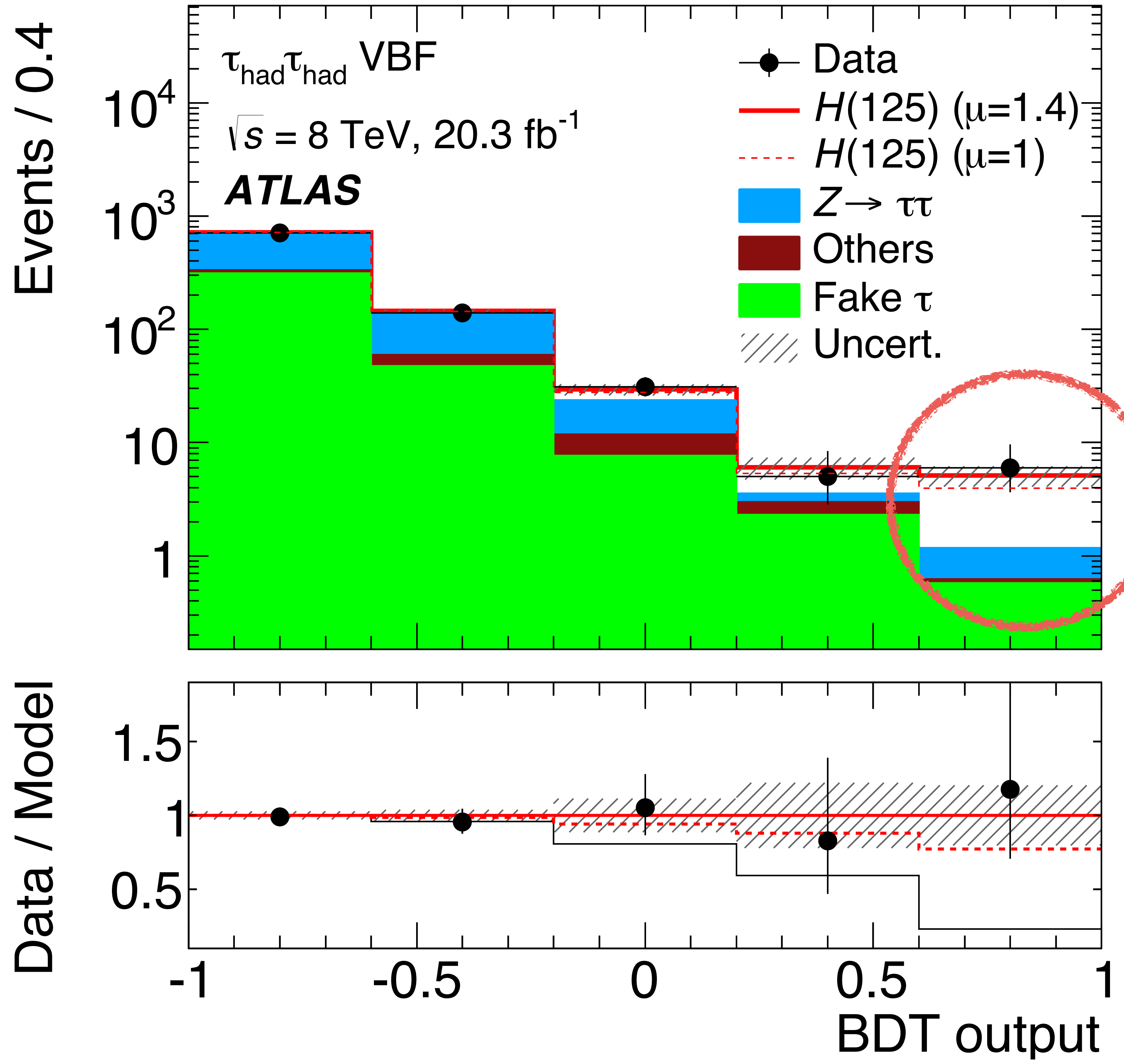
Simulation using Standard Model of Particle Physics

Typical use of ML

ML classifier trained for :

- Increase sensitivity to "signal" (example Higgs Bosons) events which give information about the theory parameters
- Reject "background" events

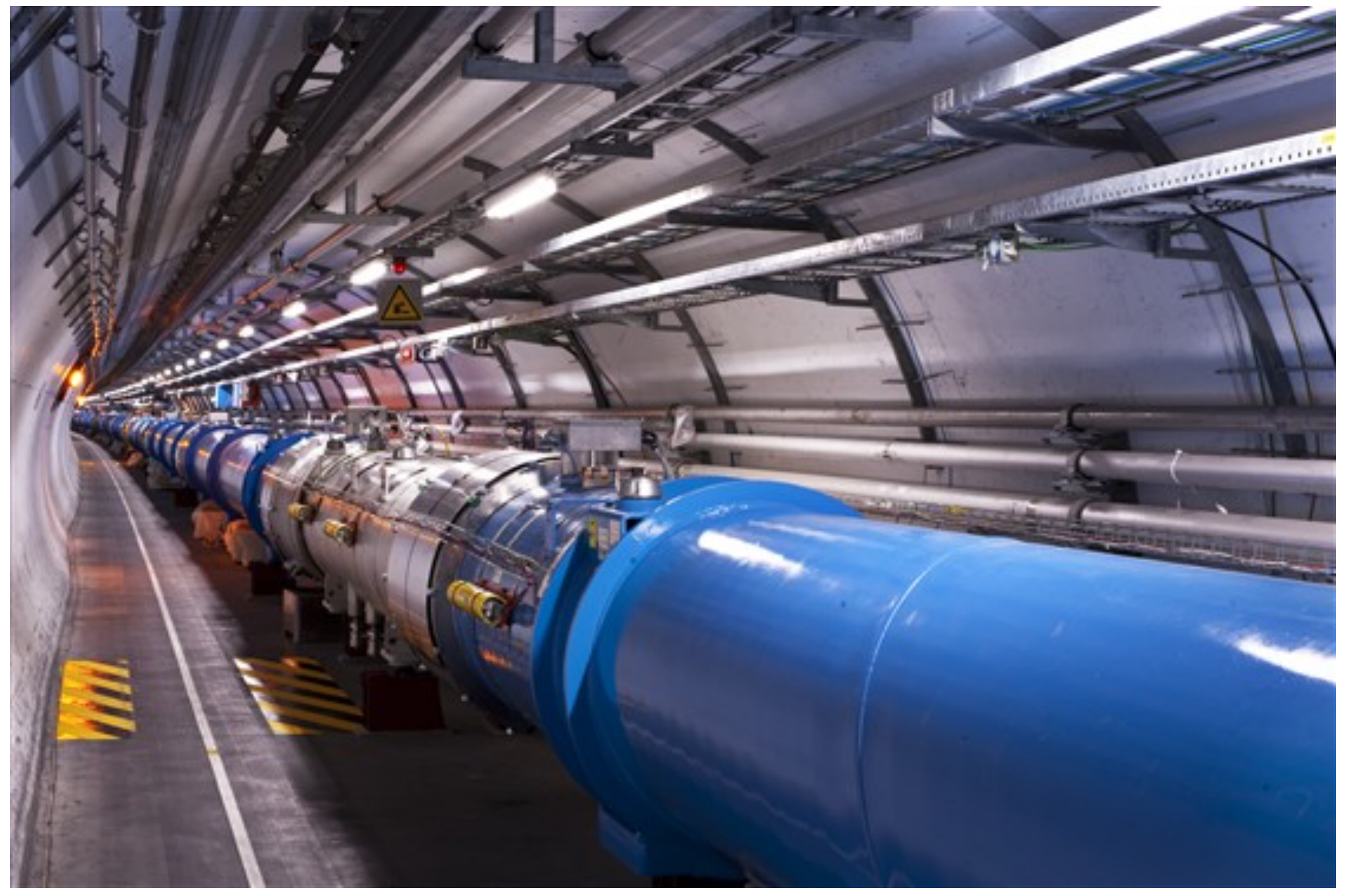
Output of classifier used as an "optimal" observable to measure theory parameters using a maximum likelihood fit over several bins of histogram



Compare various simulations to data to find best fit

[1501.04943](https://arxiv.org/abs/1501.04943)

Simulation-Based Inference - Systematic Uncertainties



Real Data from LHC

Look for deviations to find New Physics

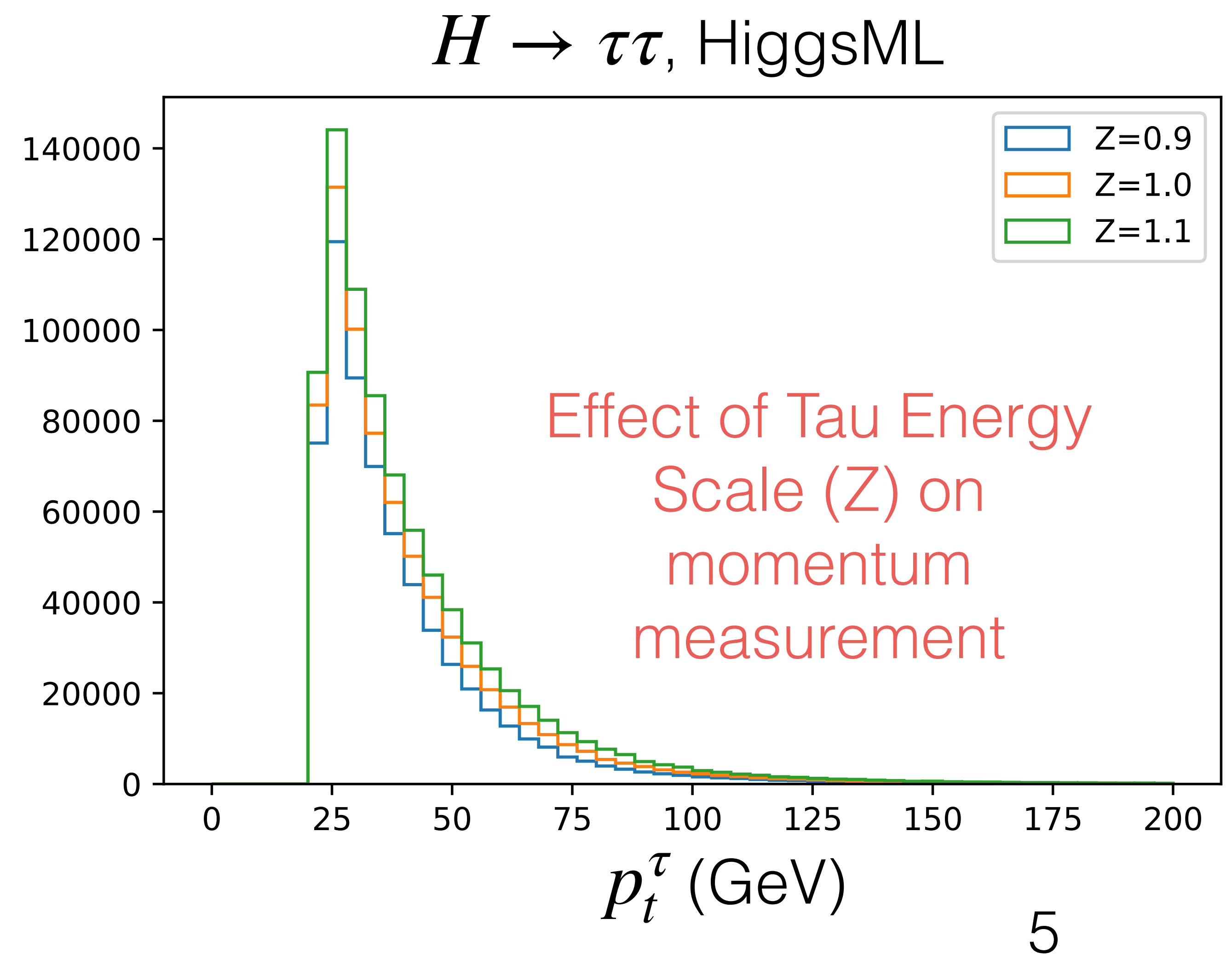
Simulation using Standard Model of Particle Physics

But simulation isn't perfect, known sources of differences between simulation and data…

Systematic Uncertainties

- Statistical uncertainties shrink as you take more data, systematic uncertainties usually don't
    - Imagine a metal ruler calibrated at room temperature but used at near 0 K
    - HEP example: Jet Energy Scale
    - Systematics may dominate over statistical uncertainties when a lot of data is available
- We can measure known unknown in the "control region"
    - Final measurement includes a fit on "parameters of interest" as well as these unknown "nuisance parameters"
    - The auxiliary measurement used as a prior on systematic (Z) or fit done simultaneously

Image: https://www.shutterstock.com/image-photo/measuring-stick-snow-ruler-shows-amount-1896983614



Nominal Classifier and Data Augmentation

- Baseline solution has been to train a classifier on nominal data (Z=1) and just account for uncertainties in measurement – which may be large. Full profile likelihood or shift Z and look at impact.

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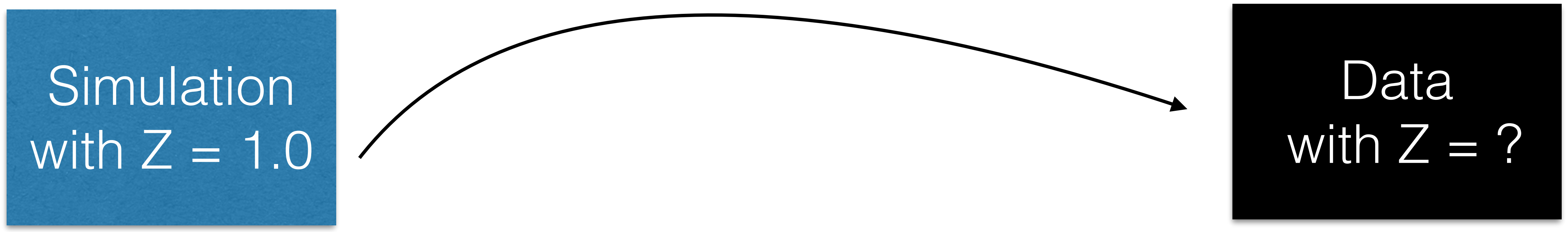

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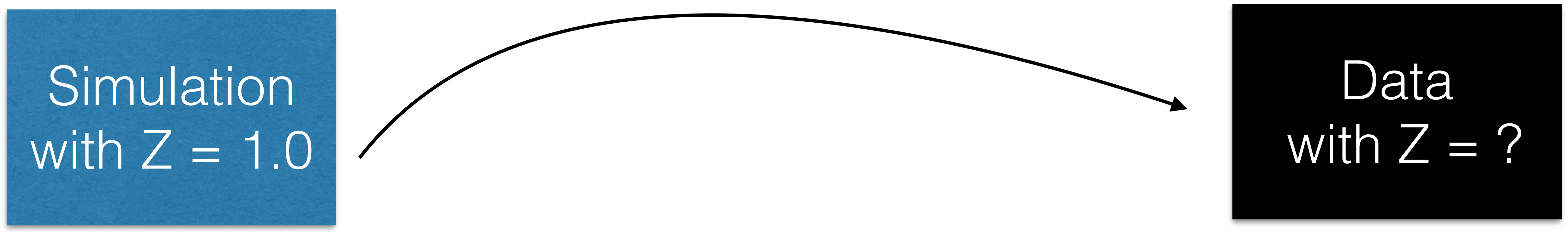
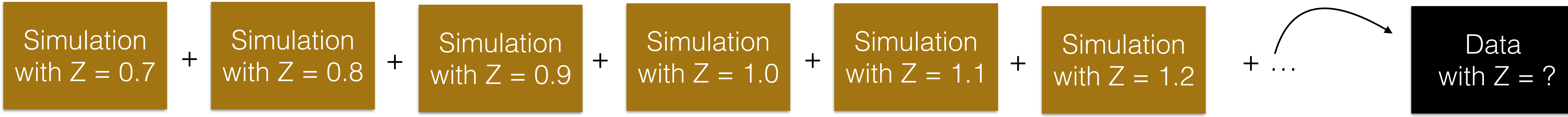


- One way to attack the problem is "Data Augmentation": Train classifier on simulated data generated with various values of Z, hope that it learns a robust decision function



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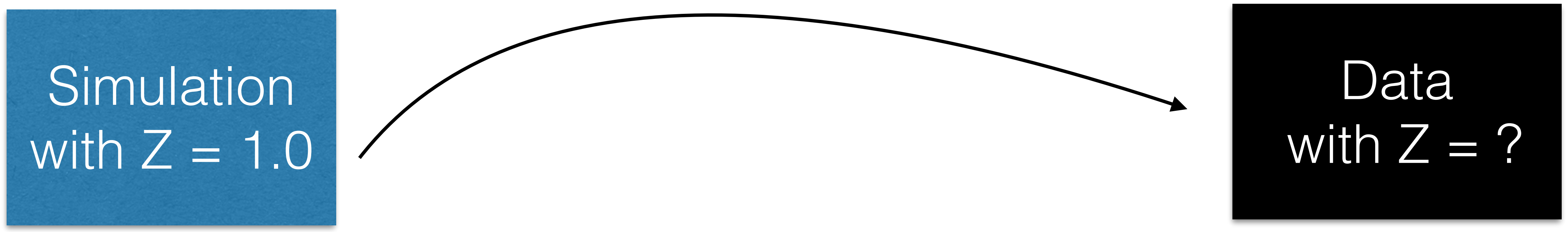

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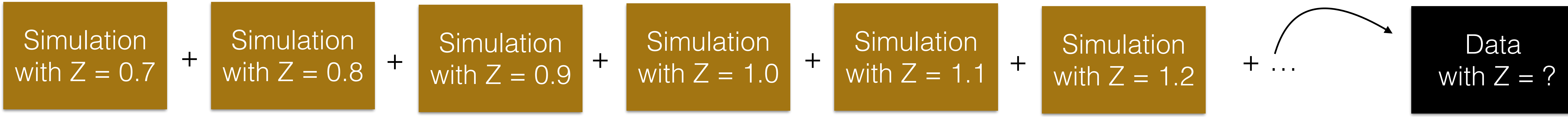


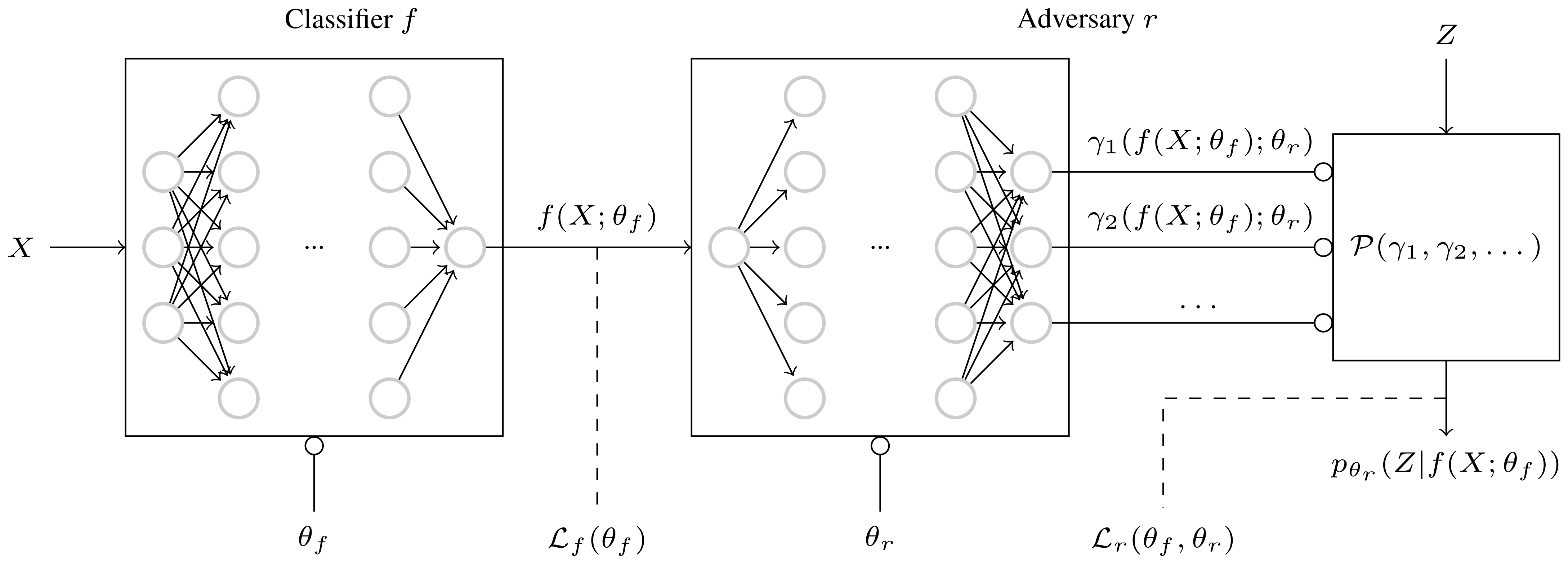
The classifier will learn some general characteristics, but will not be "optimal" for any particular value of Z

"Optimal": For us means classifier trained at the true value of Z

Invariance: Explicitly train for insensitivity to Z

1611.01046
Similar ideas: 1905.10384, 1305.7248, 1907.11674, epjconf_chep2018_06024

Domain adaptation strategies also used in the past: Eg. Pivot Adversarial Training to make classifier output invariant to systematic (Z)



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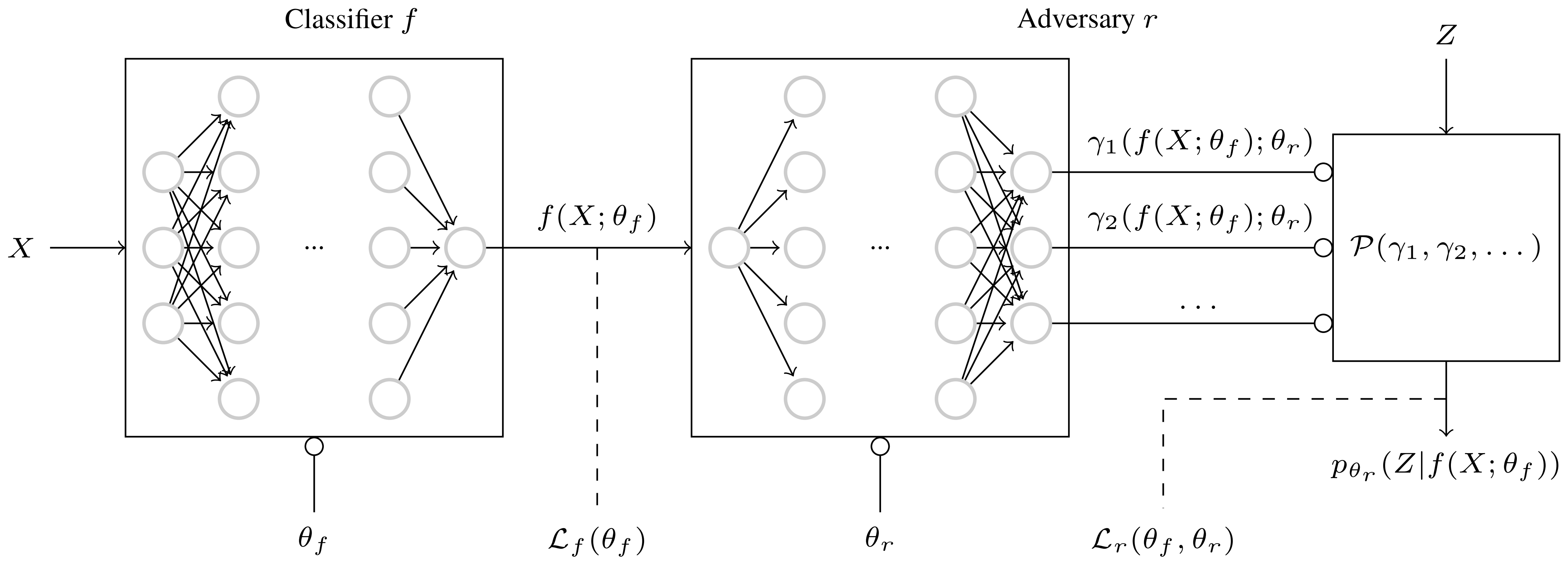
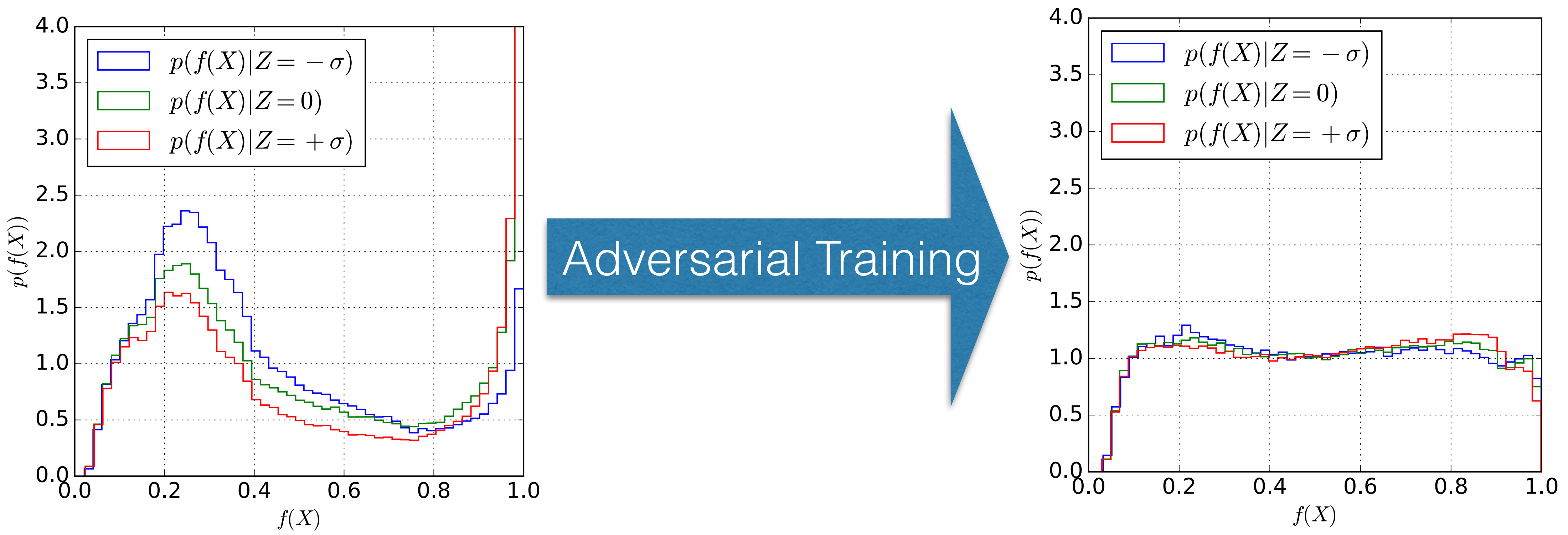


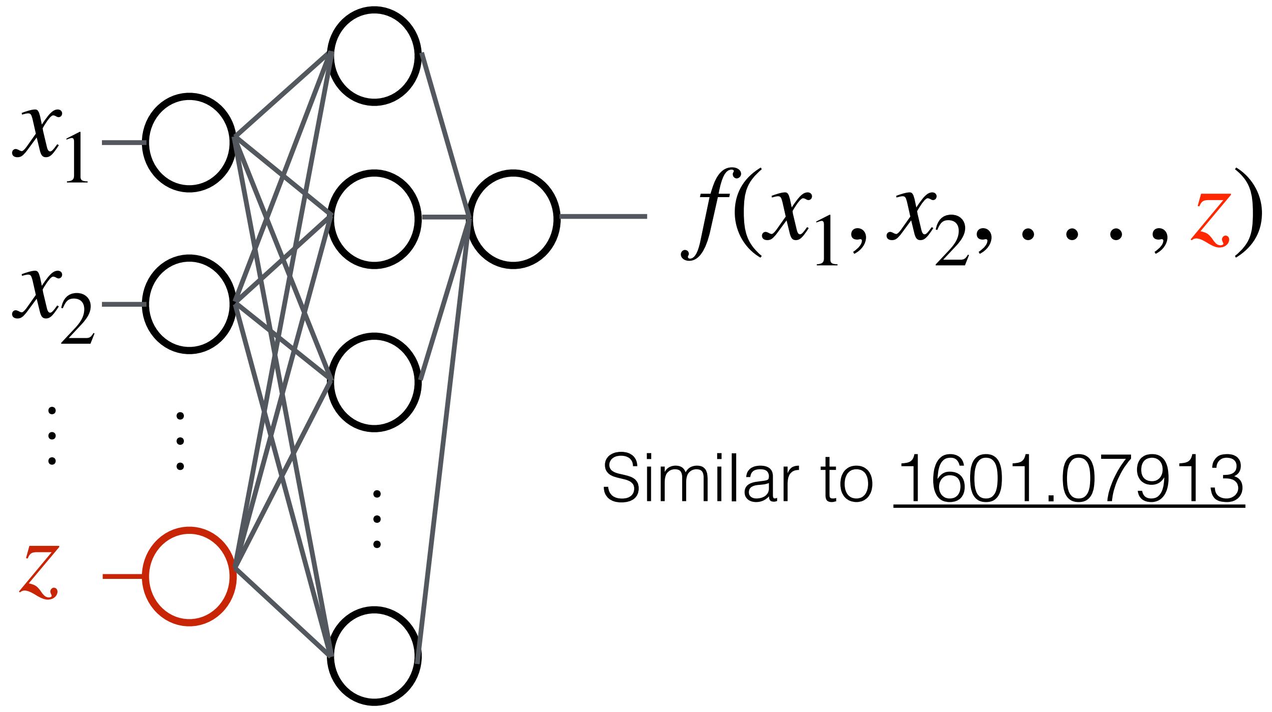


Classifier output for various values of Z

Classifier output becomes invariant to Z, but not necessarily optimal at any particular value of Z, also sometimes not even possible to be invariant

We advocate for the opposite

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



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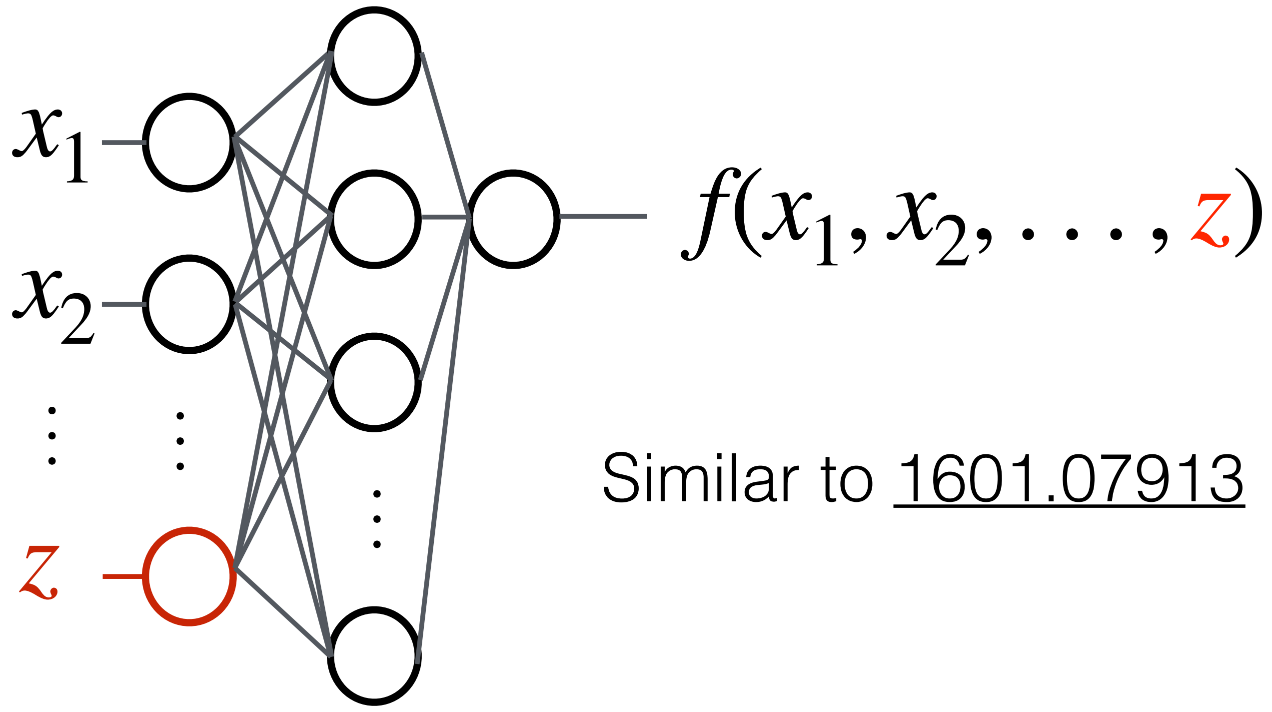

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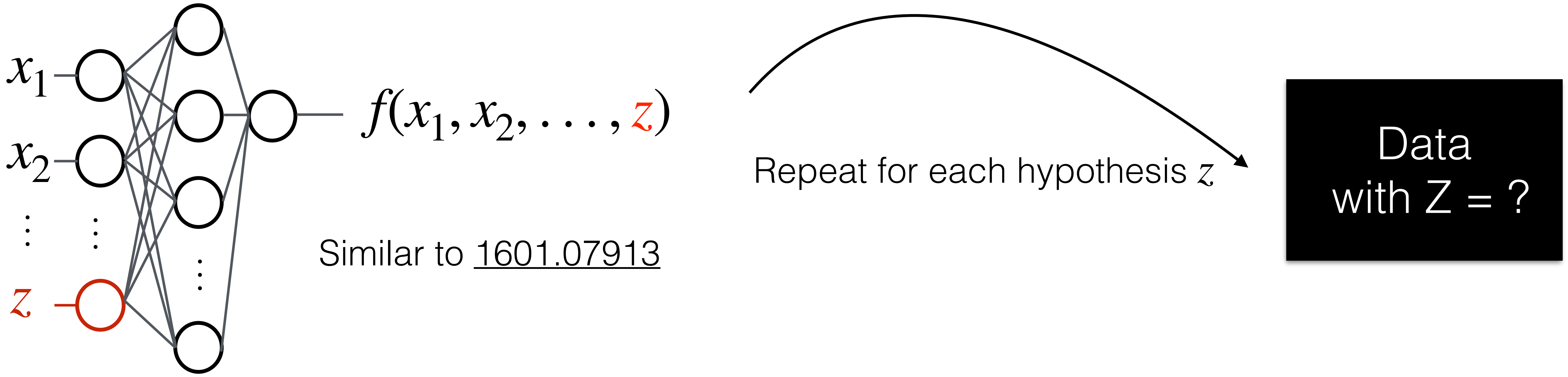

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- Use the parameterised classifier response for final likelihood fit to constrain parameters of interest (POI) and nuisance parameters (NP)

In following slides, POI will be the signal strength parameter 'μ' and the NP will be denoted 'Z'

Caveat: When not to use any of these models

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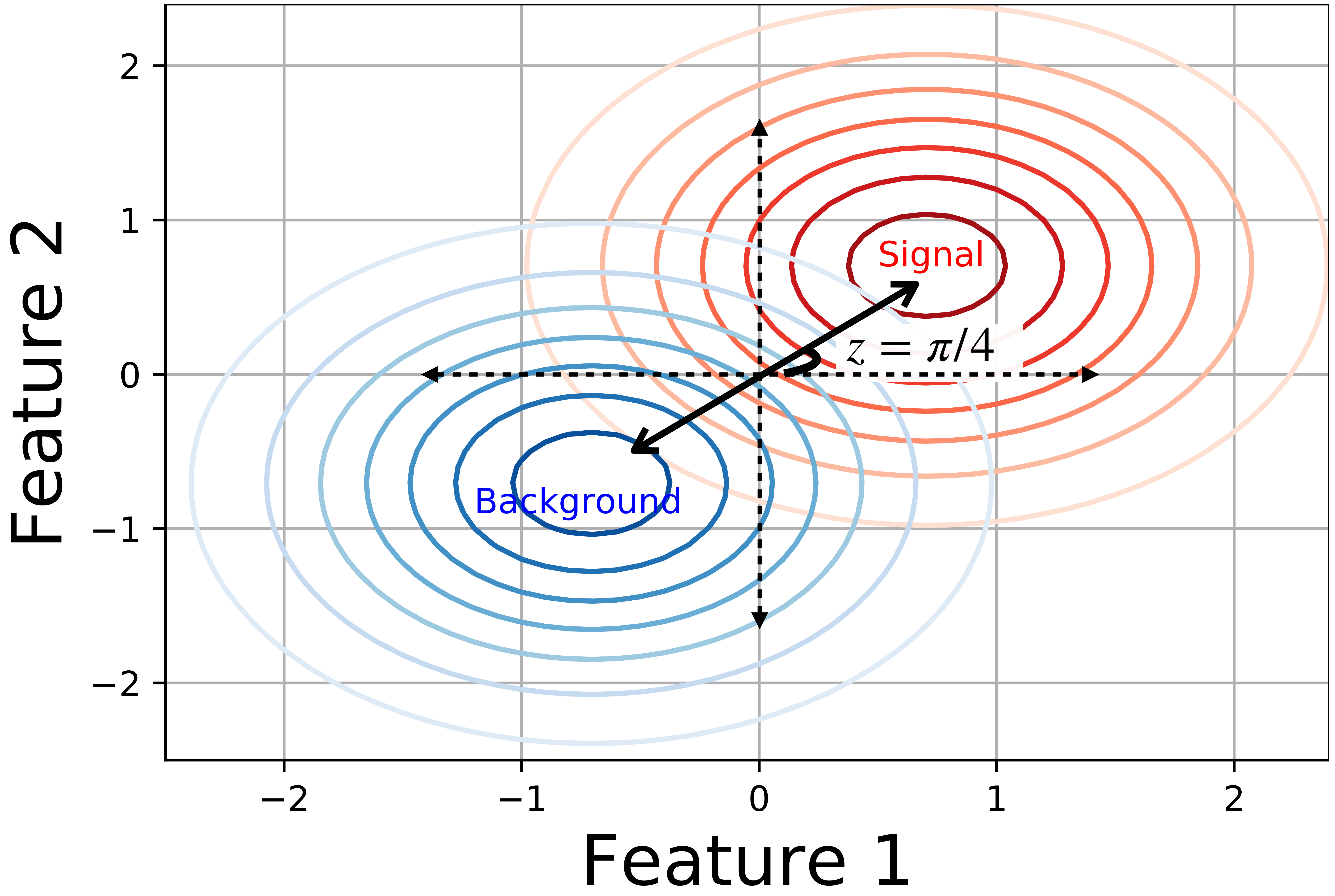
Two point systematics: Don't lose your only handle on these systematics!

Herwig vs Pythia - If you are invariant to this difference are you sure you are invariant to underlying physics reason for these differences?

Demonstration on Toy Problem



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

z = Angle

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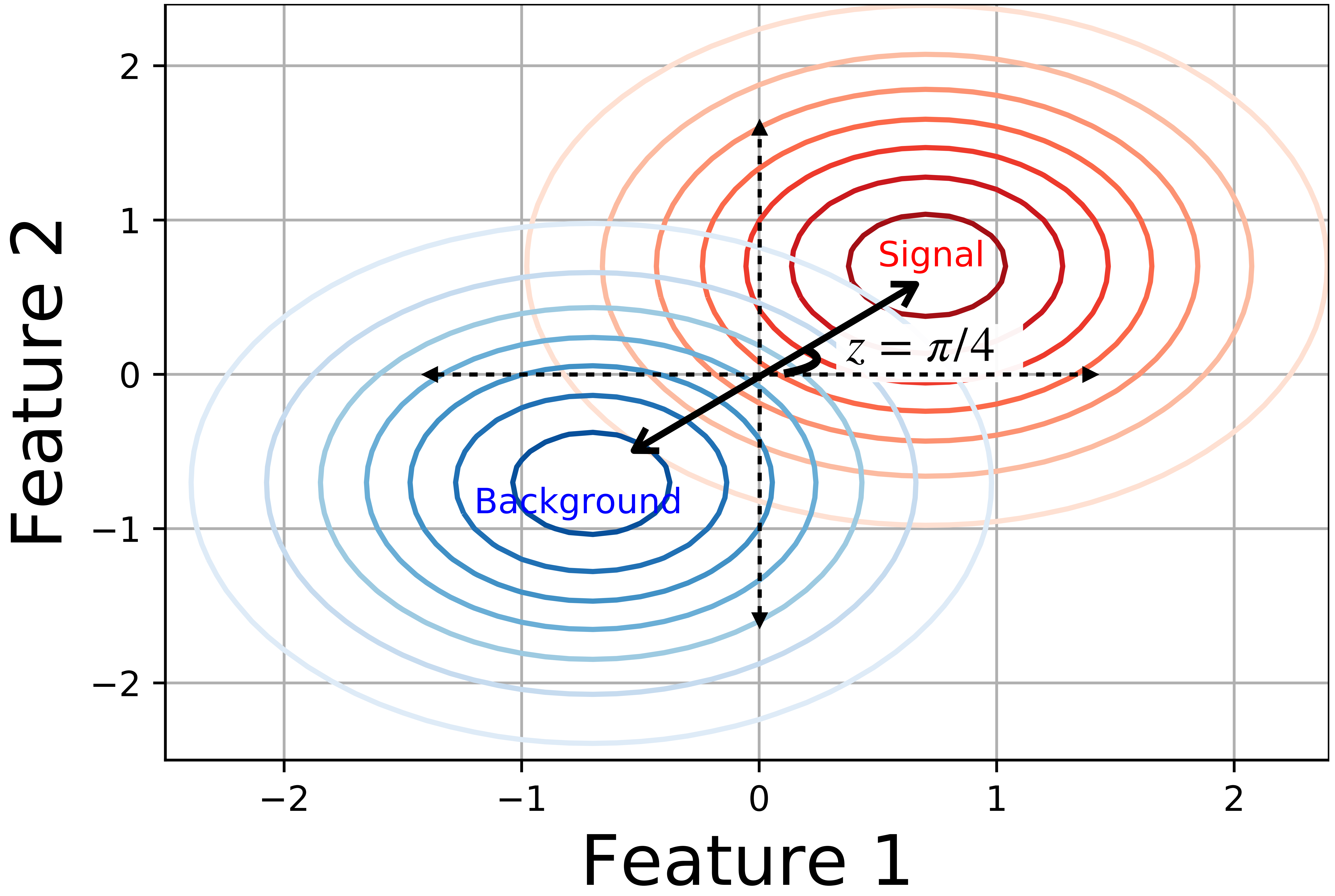

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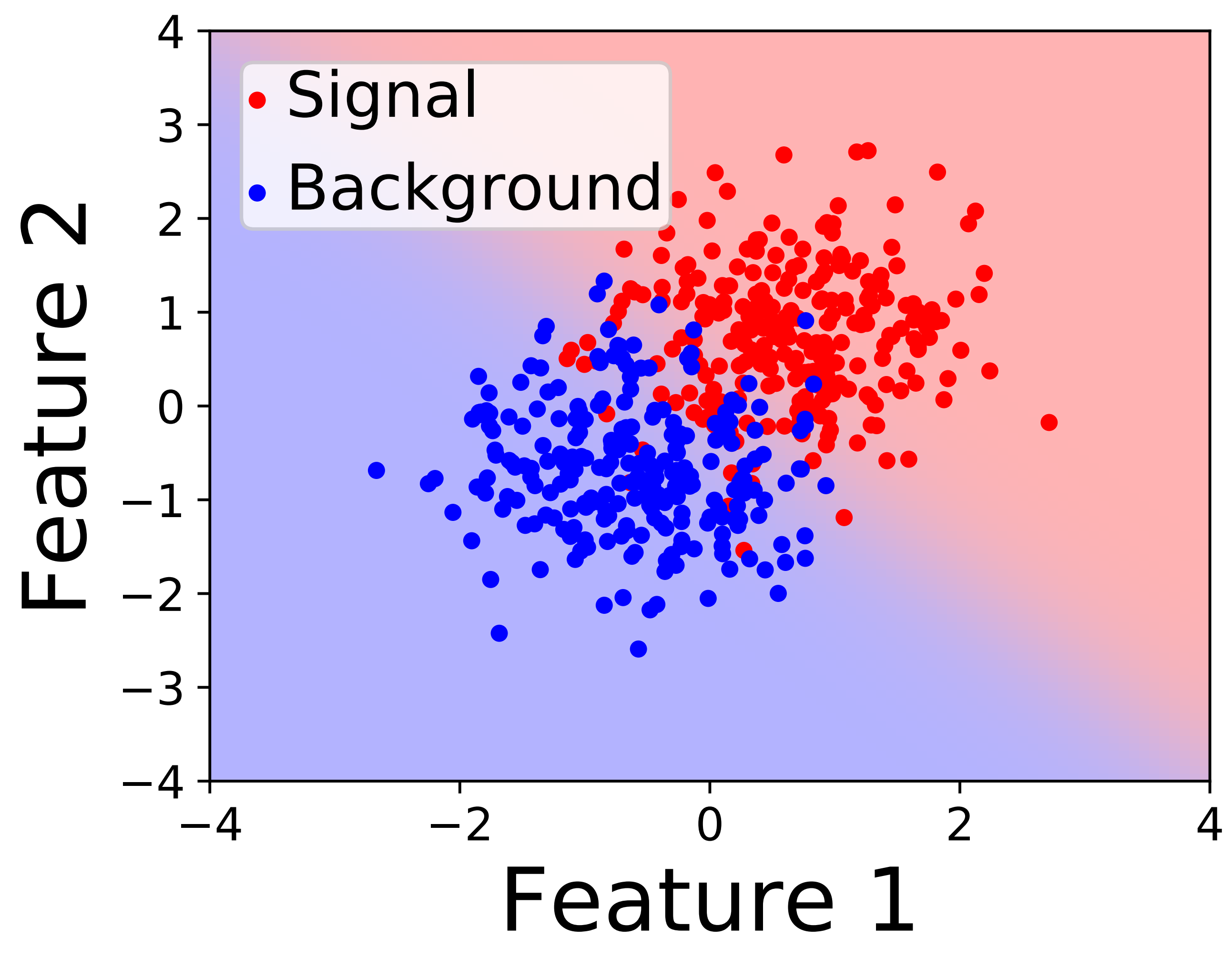
z = Angle

Being invariant to Z would result in a terrible classifier

Nominal and Systematic Up Examples

Nominal "Data"

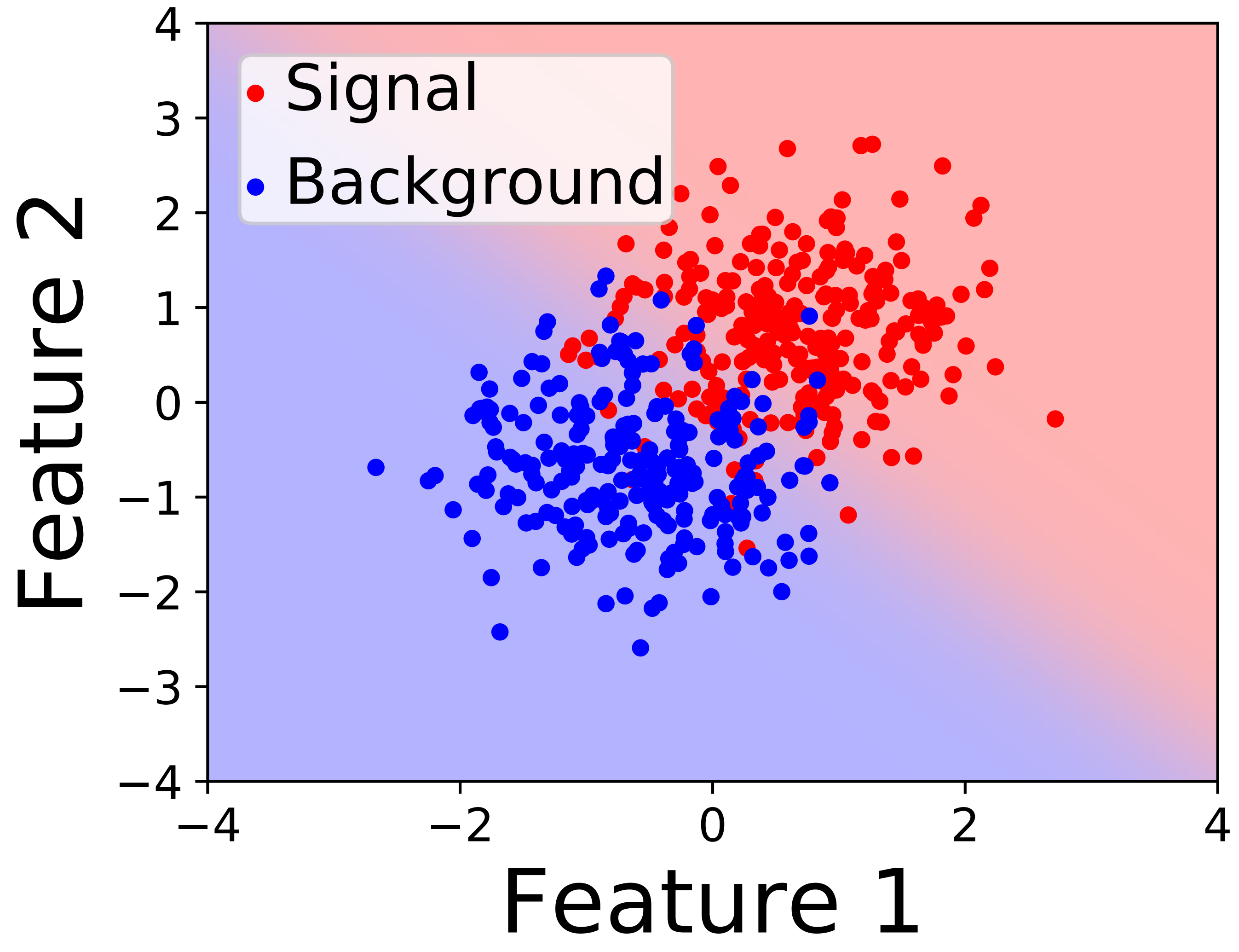
Baseline Classifier



AUC=0.978

Optimal

Uncertainty-Aware Classifier



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SystUp "Data"

Nominal and Systematic Up Examples

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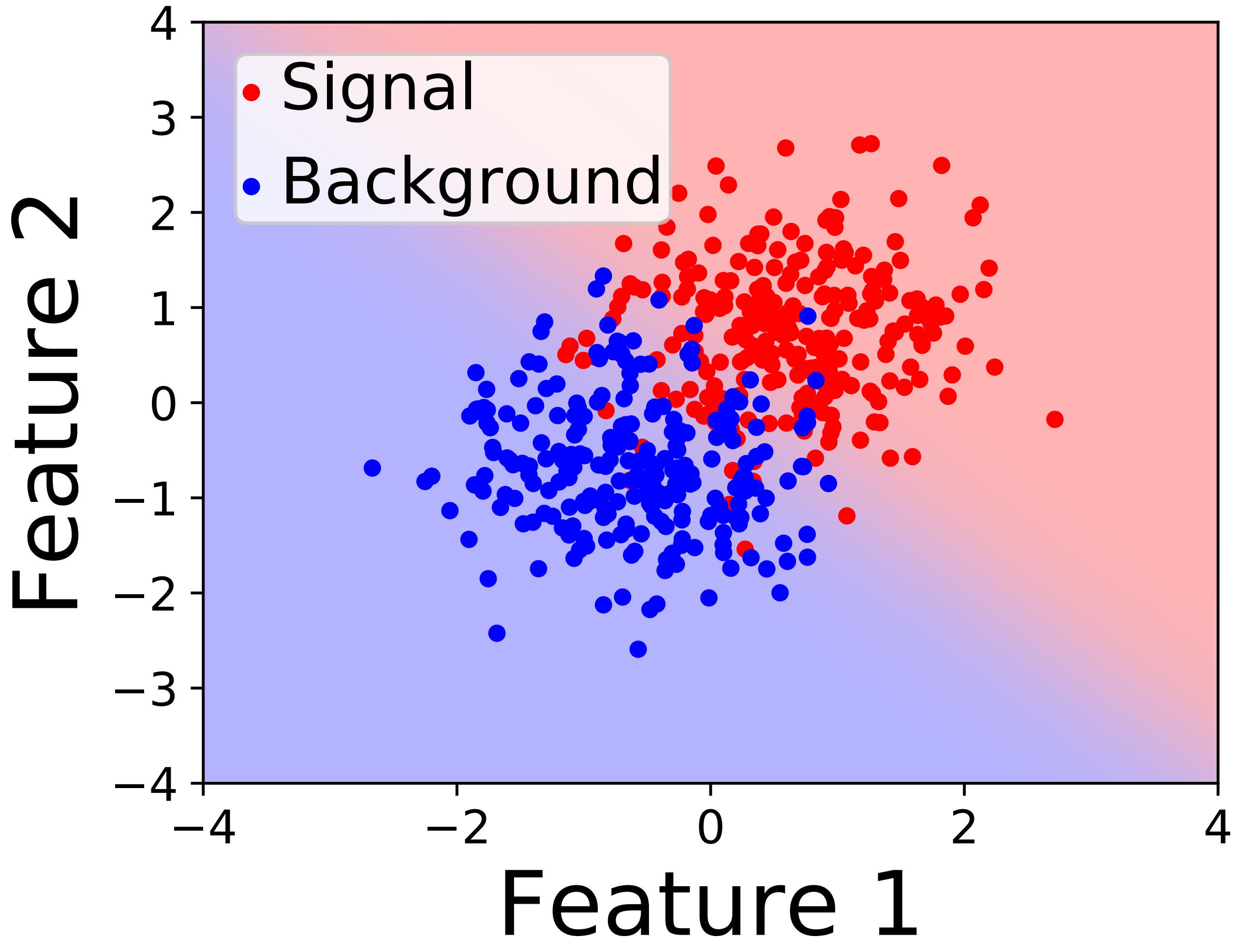
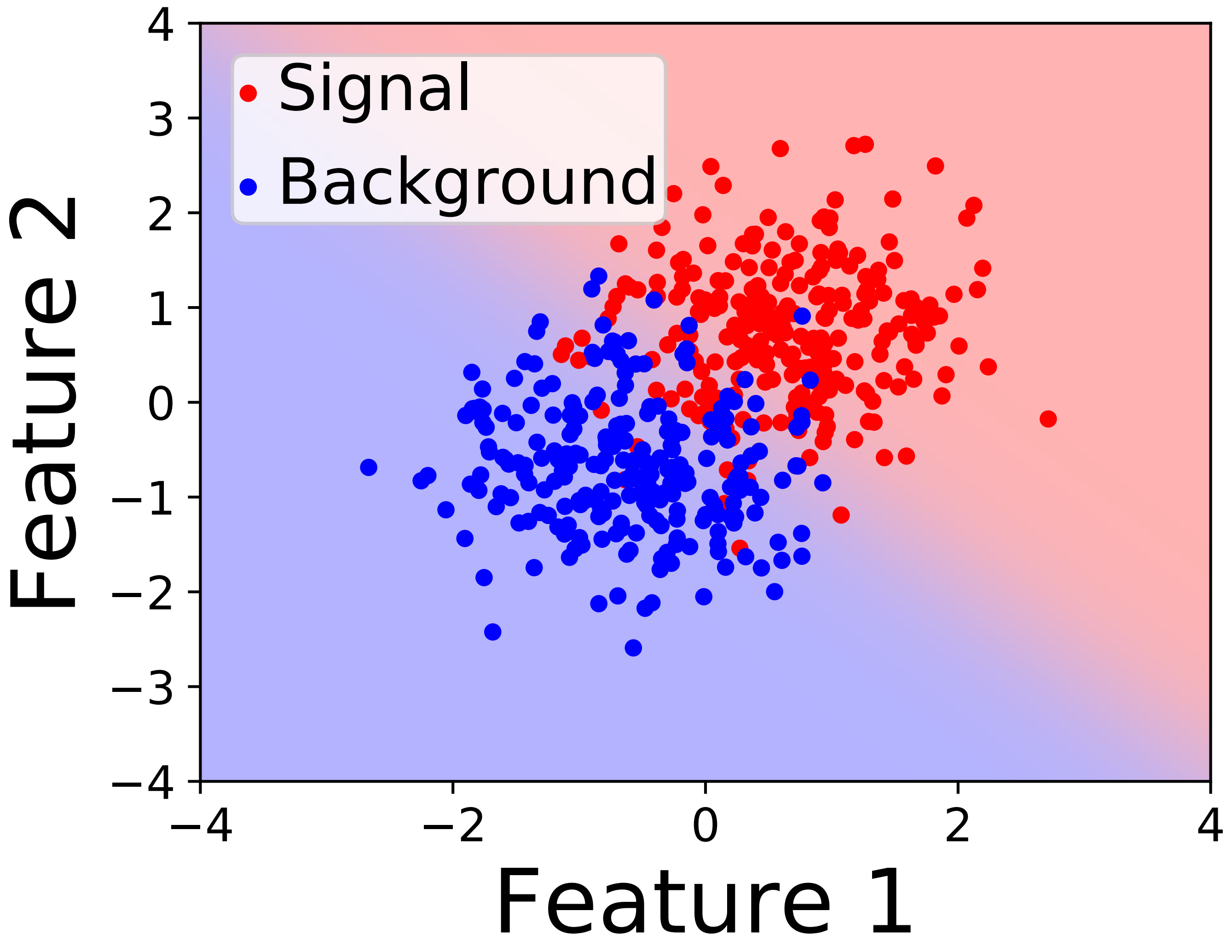
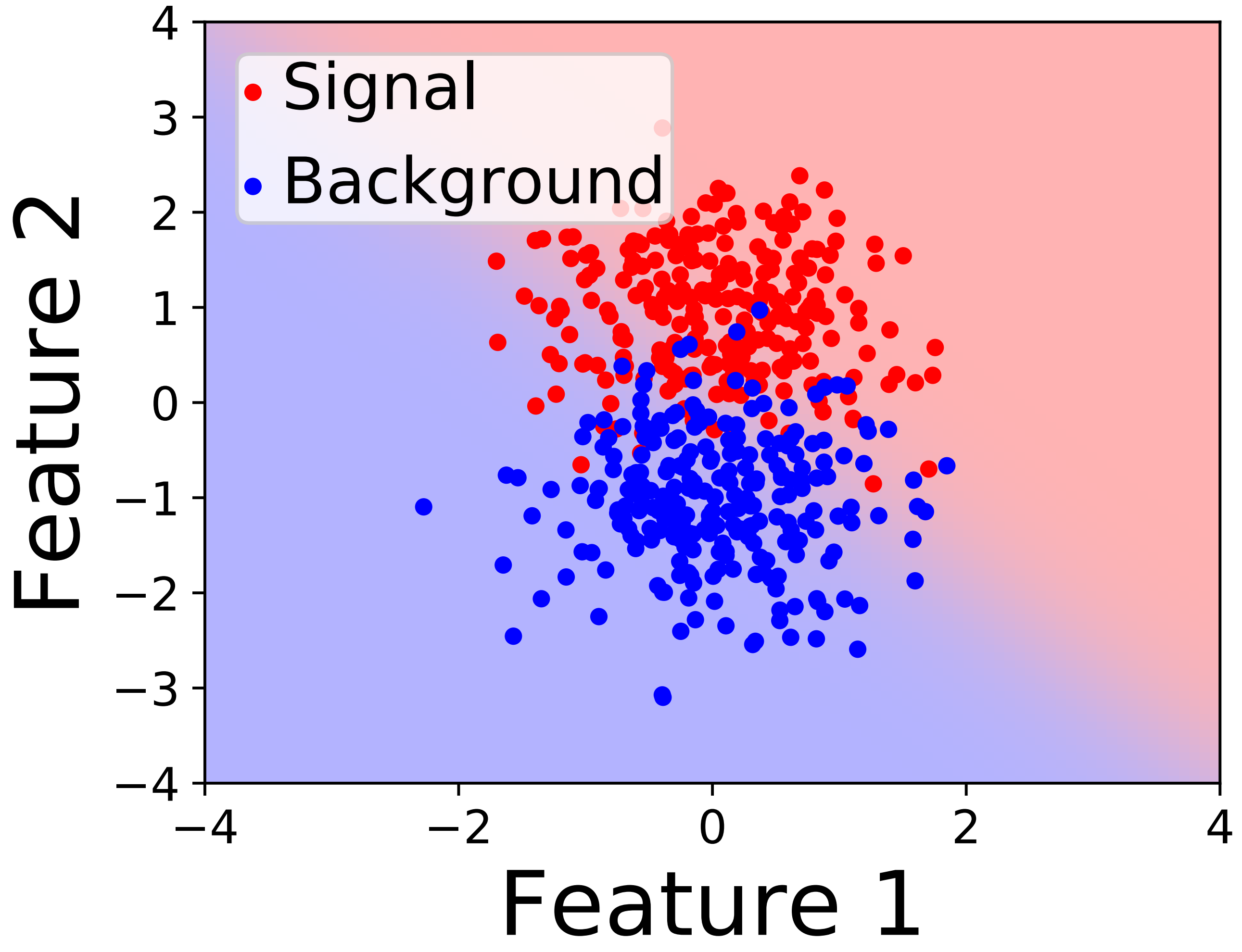
Nominal "Data"		AUC=0.978 Optimal		AUC=0.978 Optimal
SystUp "Data"		AUC=0.924 **Sub-Optimal**		

Nominal and Systematic Up Examples

Baseline Classifier | Uncertainty-Aware Classifier

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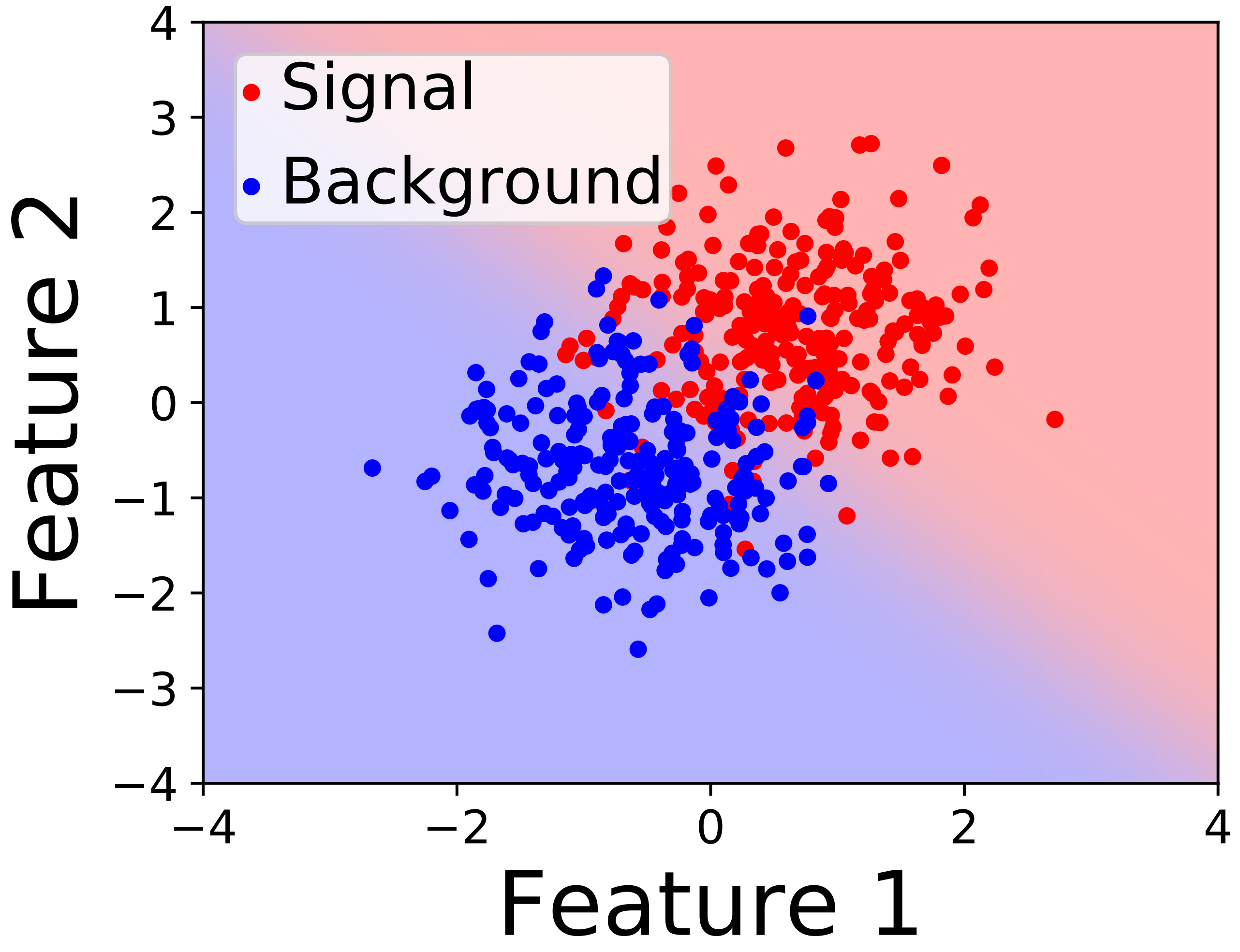

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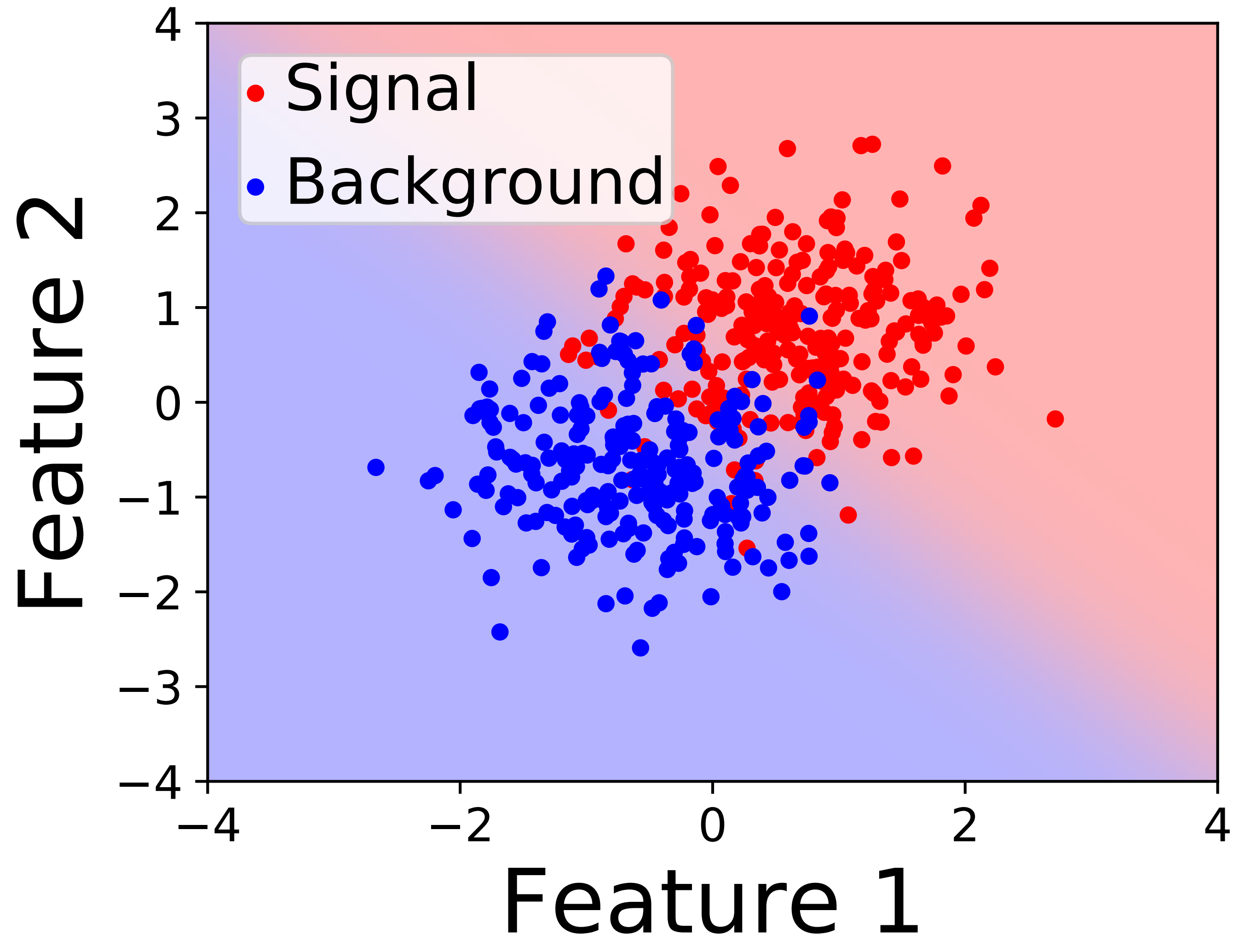

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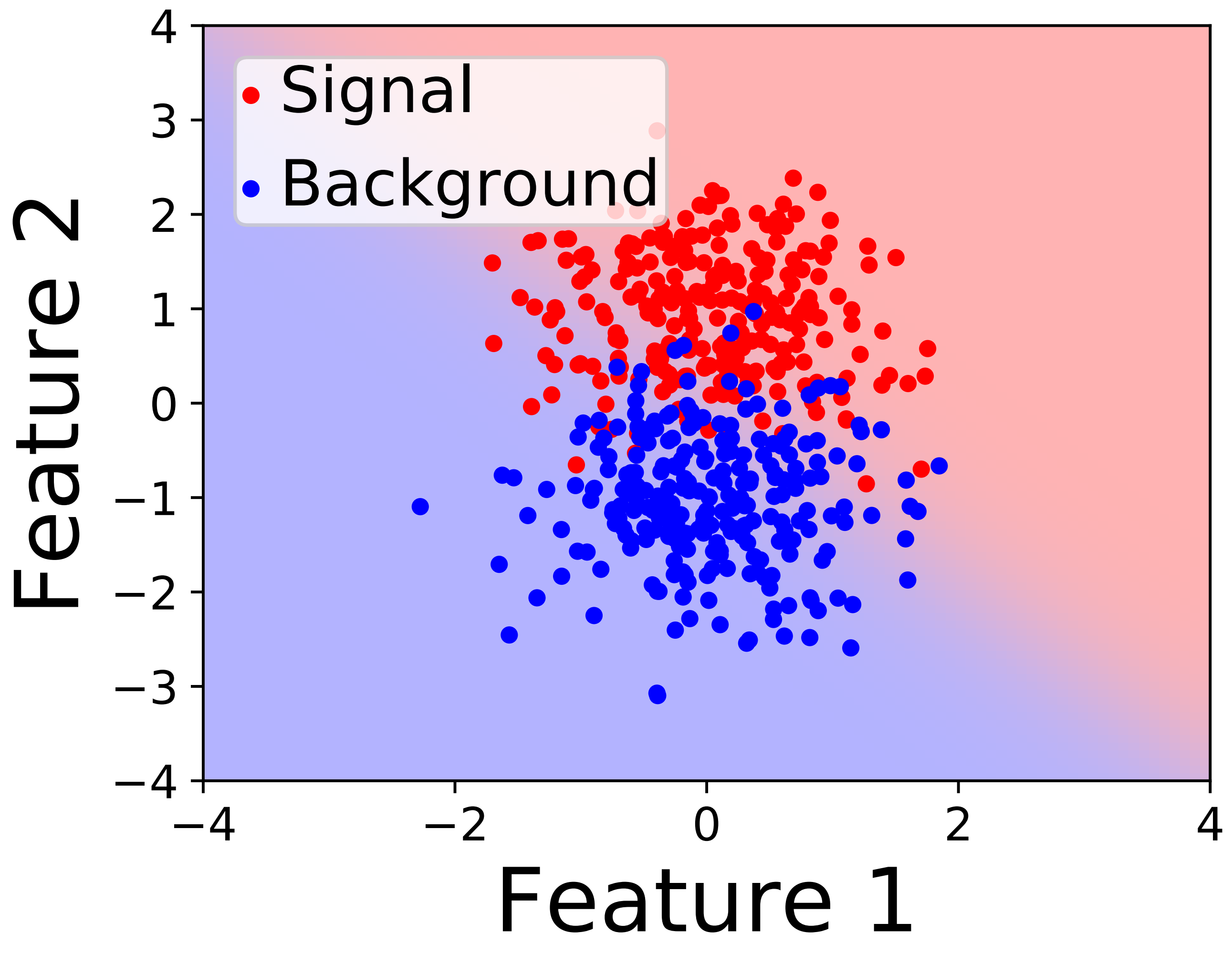

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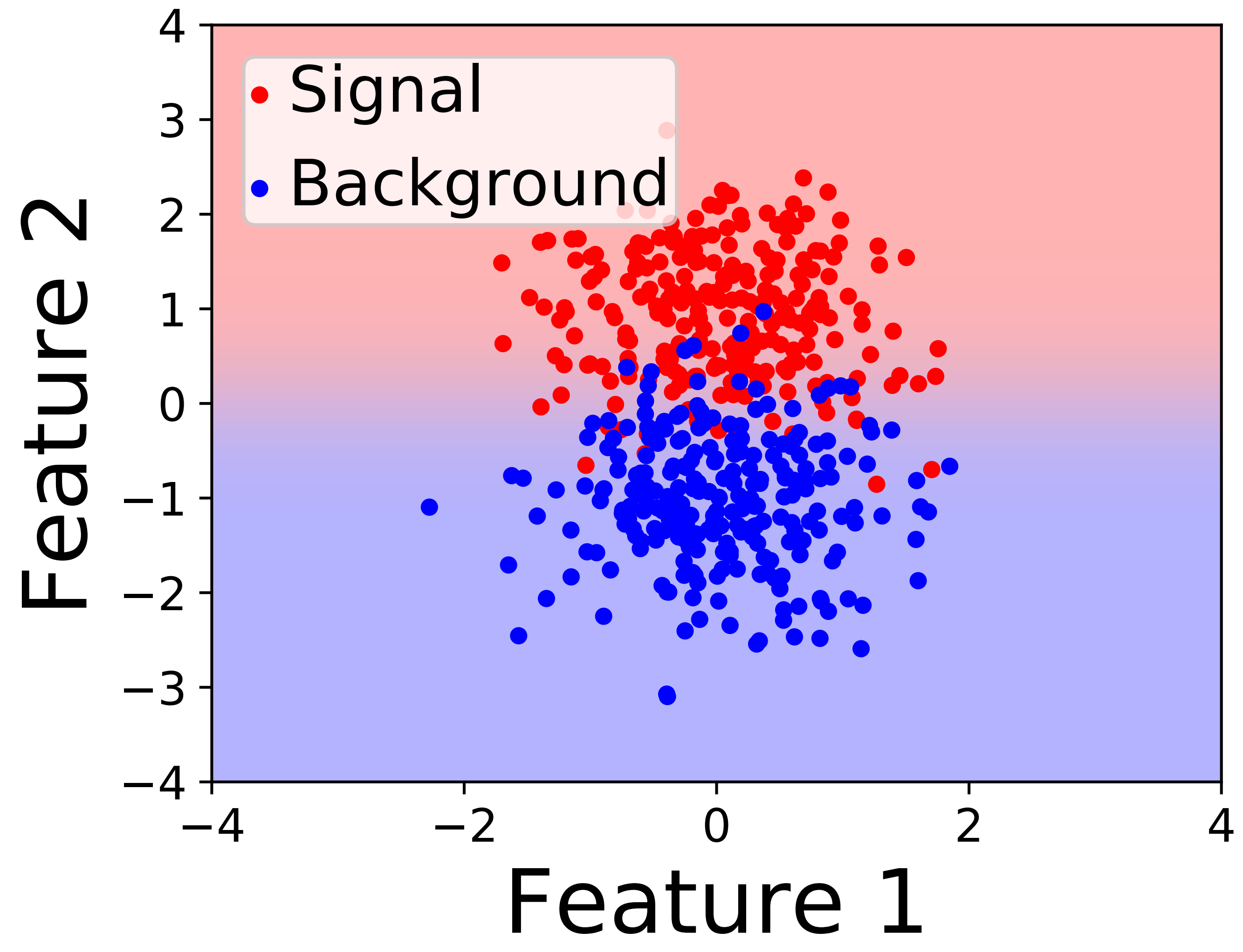

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Optimal

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

Nominal and Systematic Up Examples

Baseline Classifier

Uncertainty-Aware Classifier

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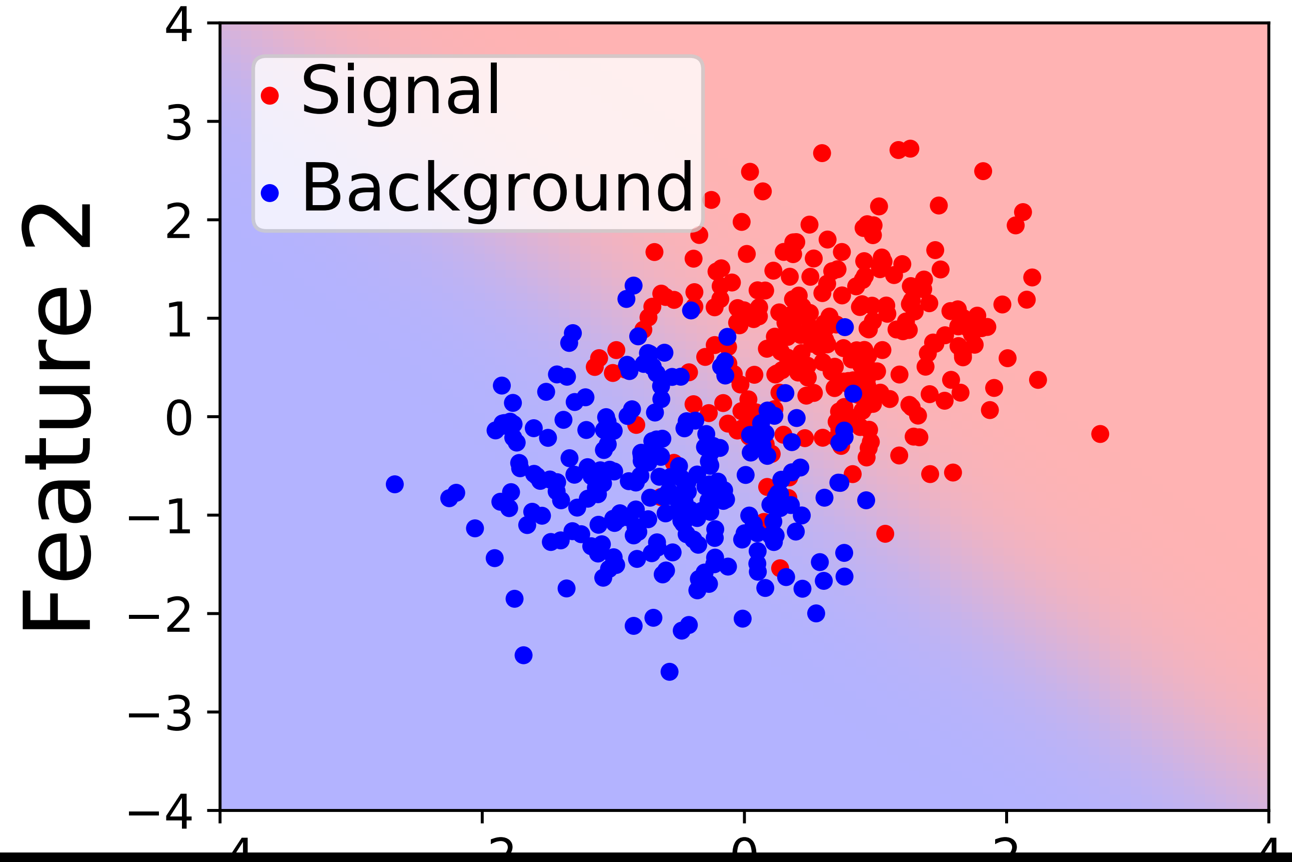

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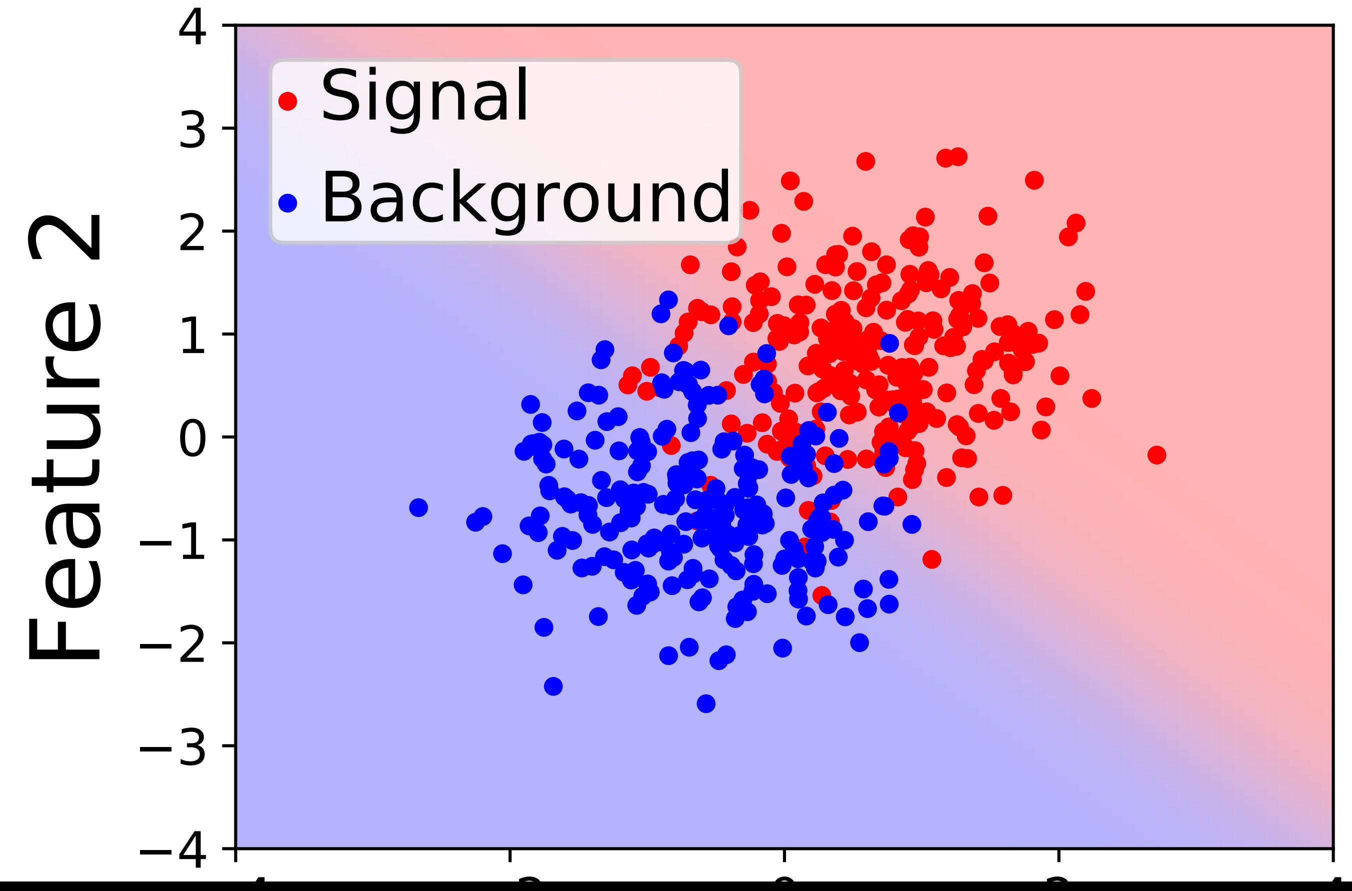

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In fact for the toy problem we used analytical classifiers instead of training networks

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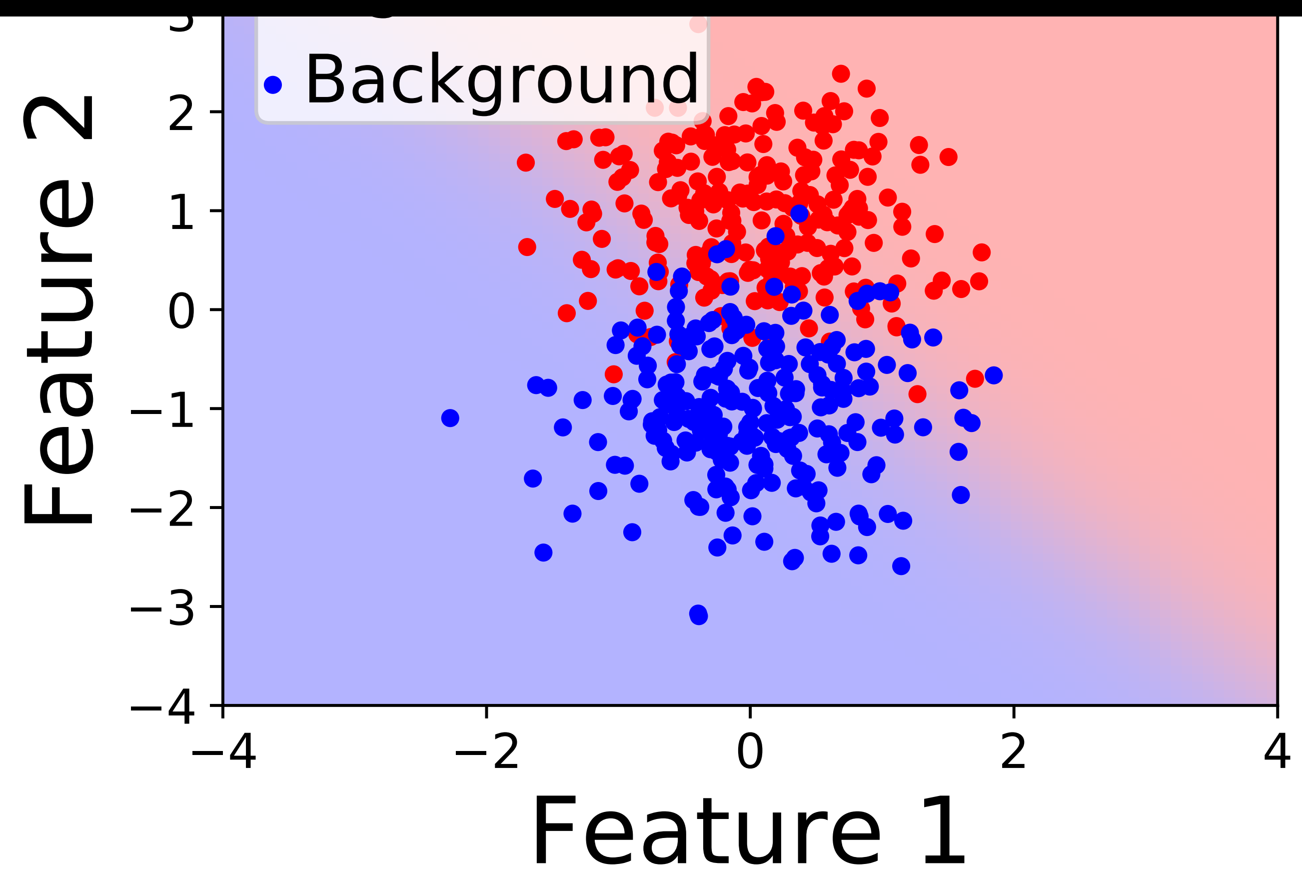

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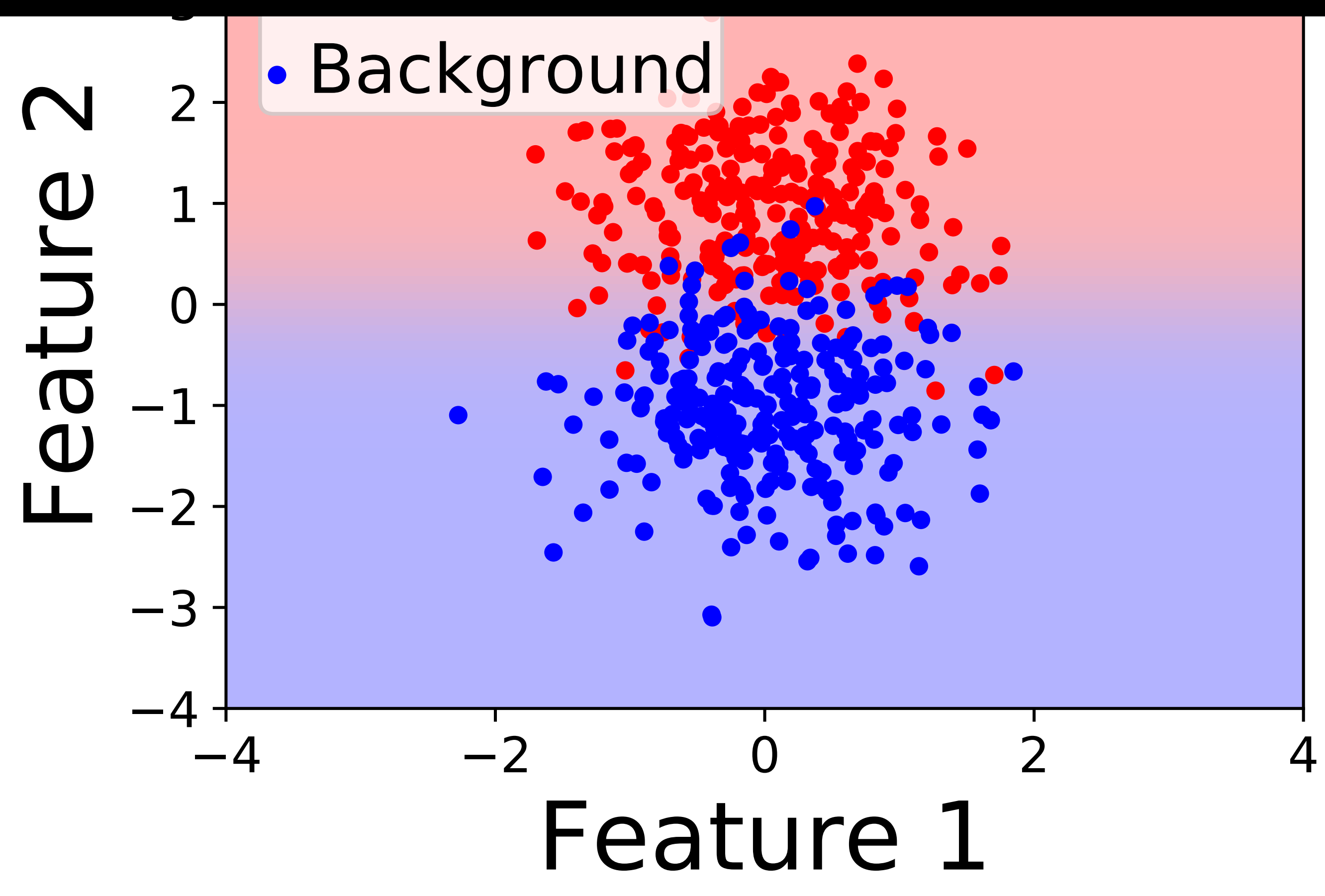

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Syst-Aware Classifier is able to rotate its decision function based on Z while the Baseline Classifier decision function remains frozen

But in a real measurement we don’t know true Z a priori, would this still help?

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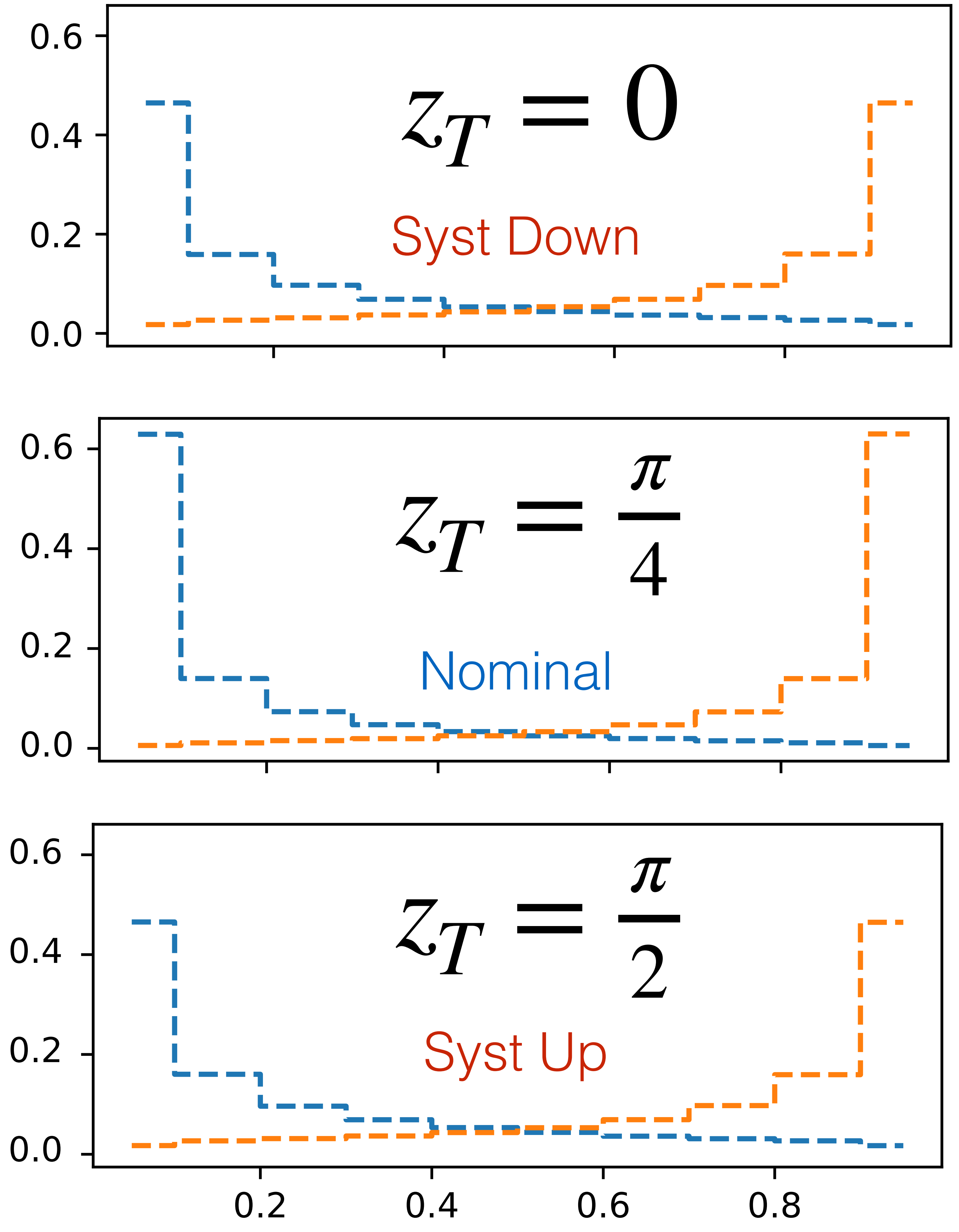
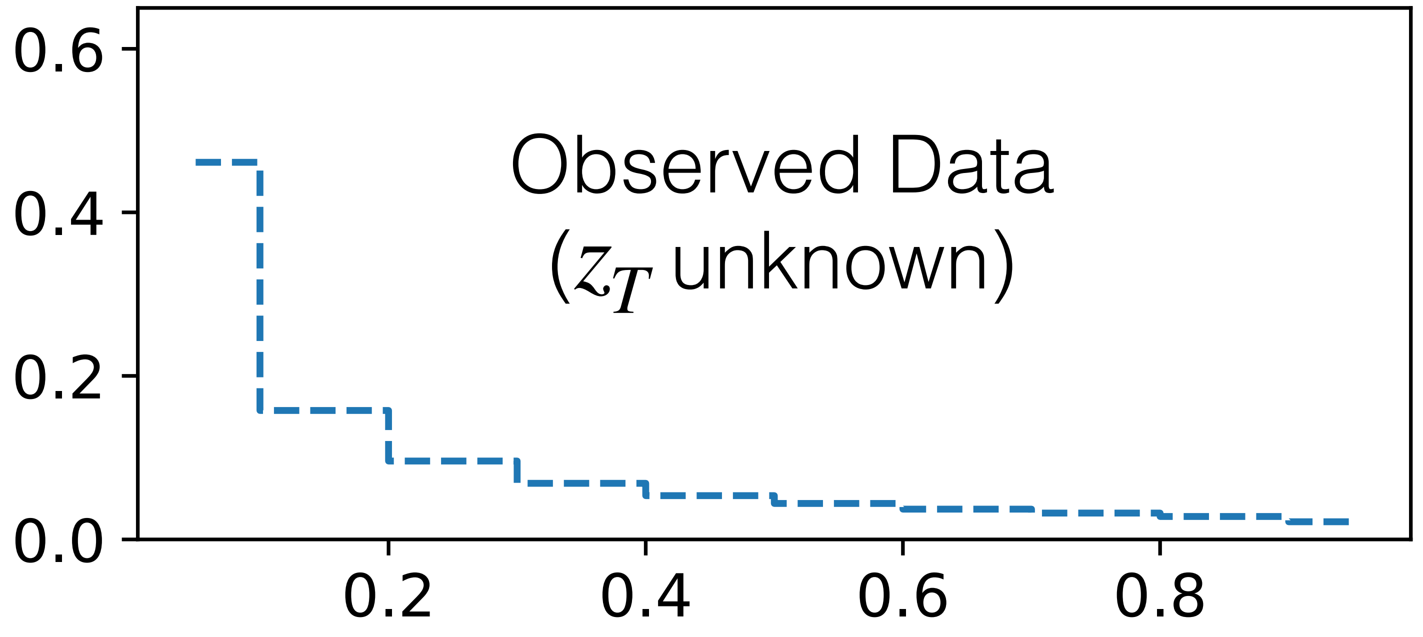
Let’s see what we’ll need to do..

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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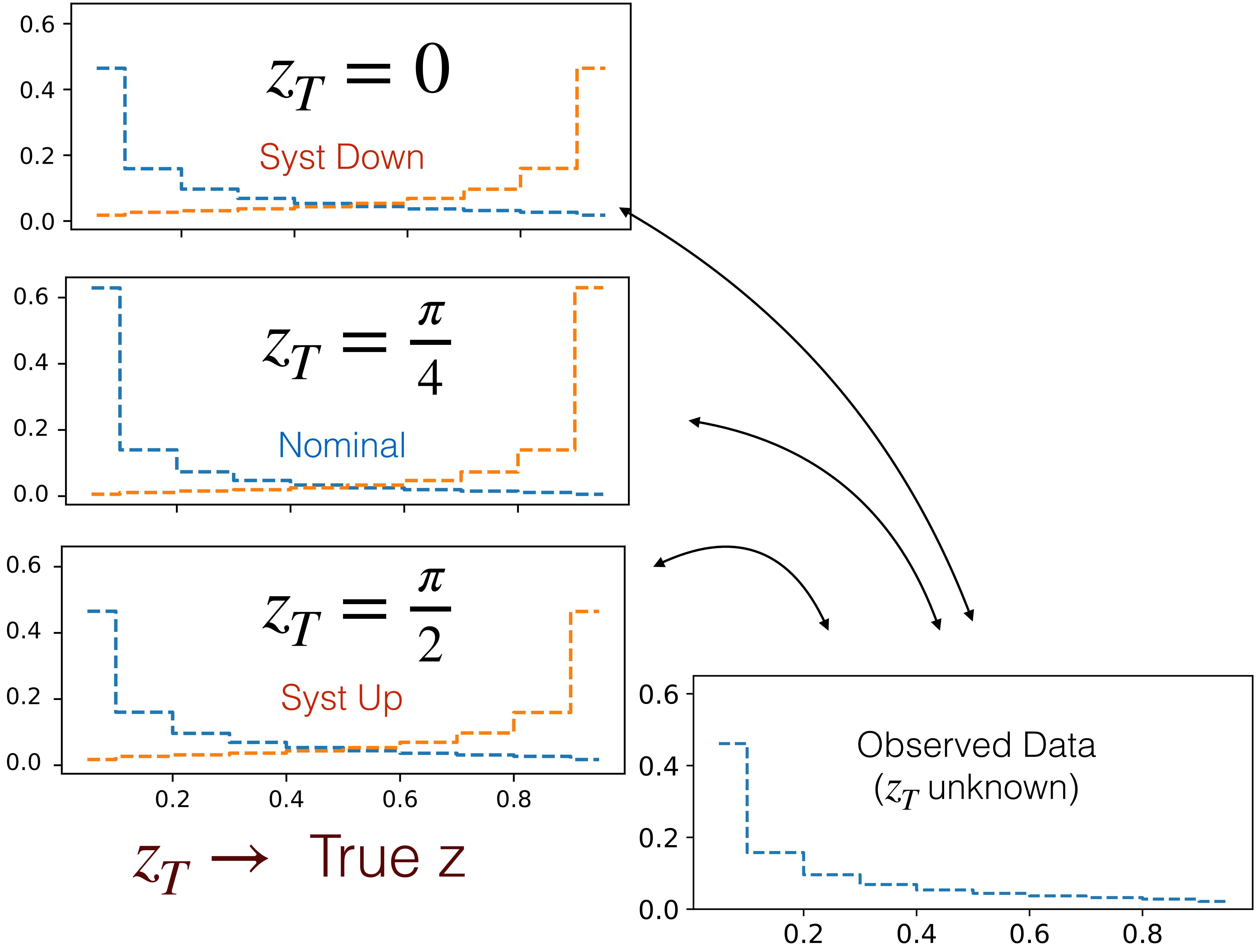

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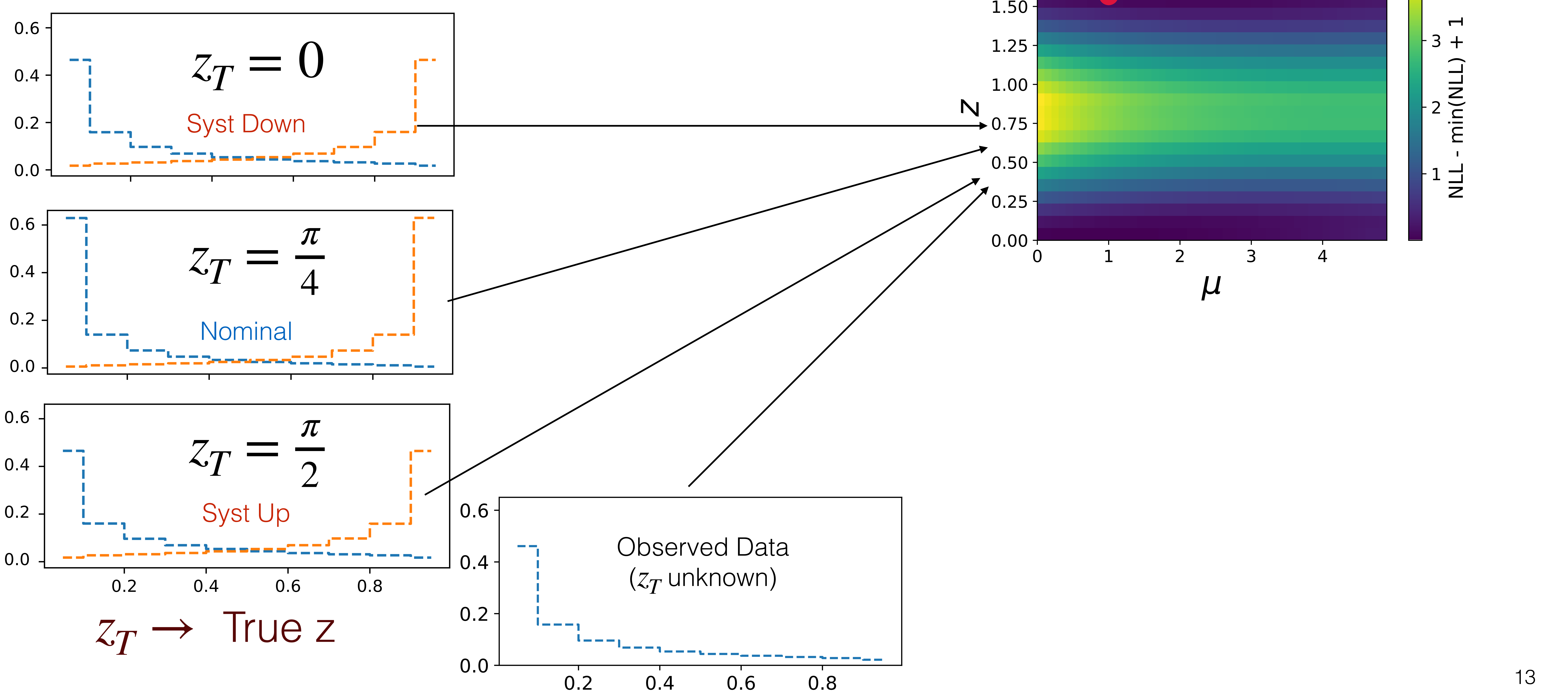

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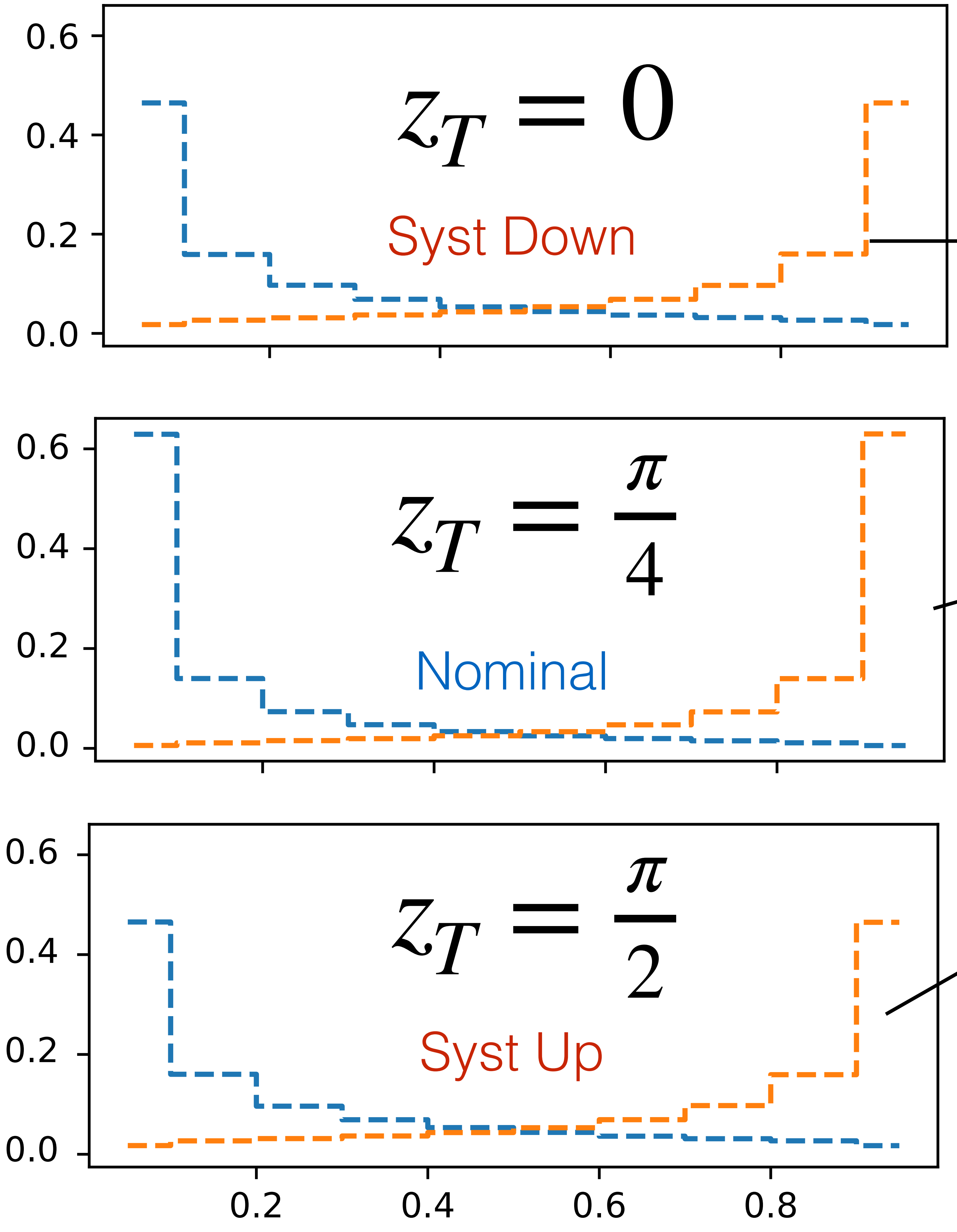

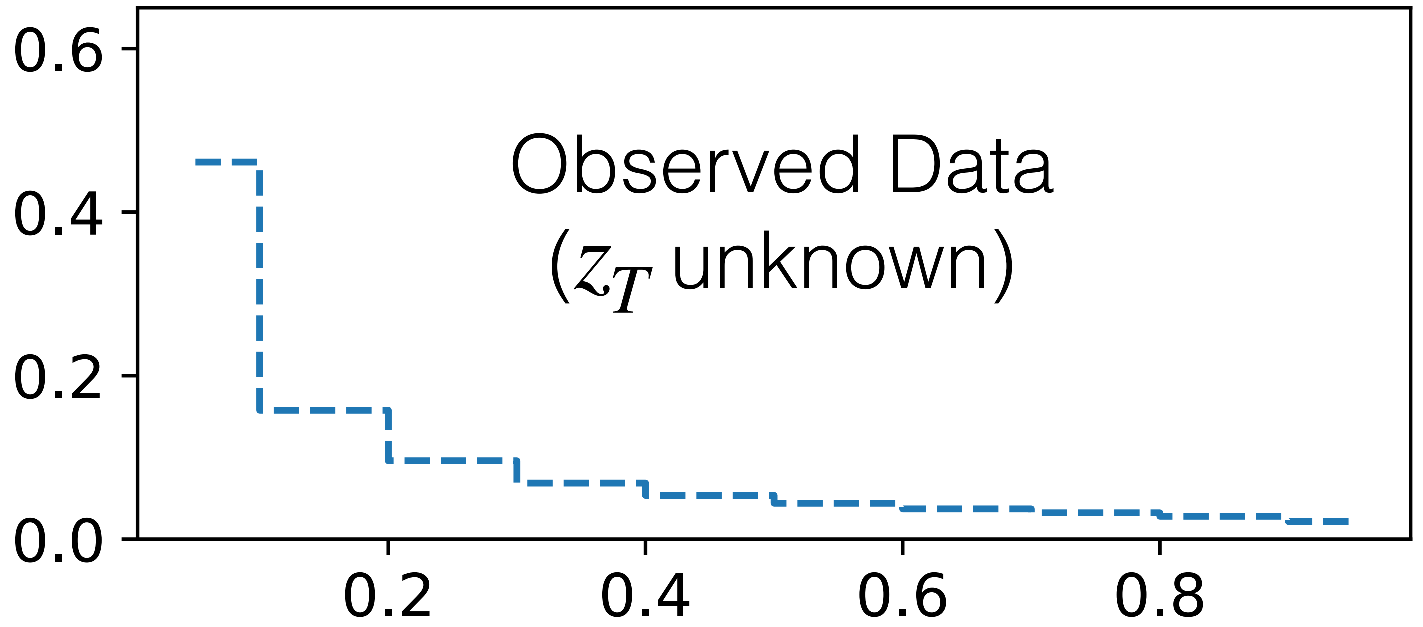

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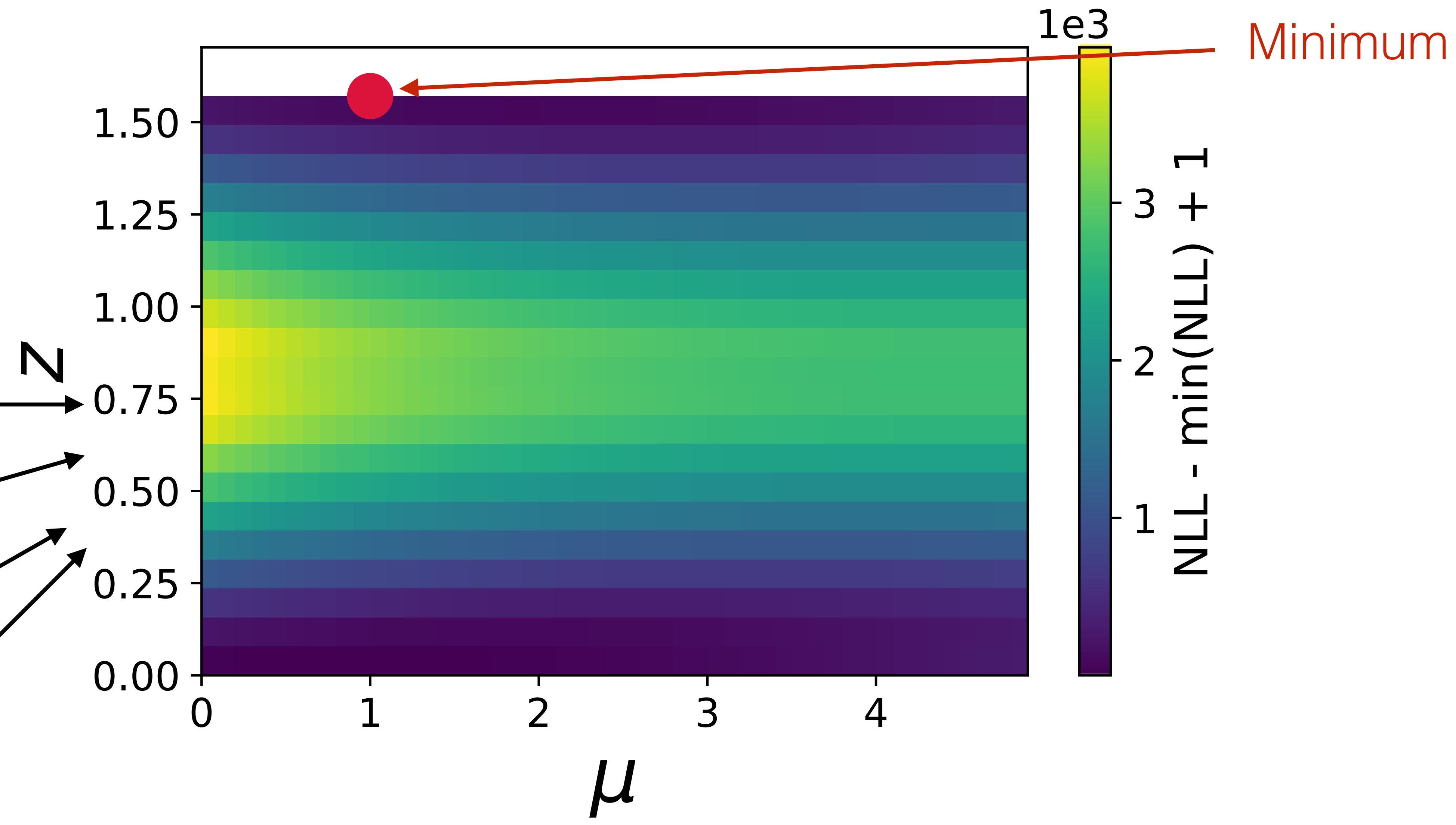
But could be done unbinned/KDE too



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

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

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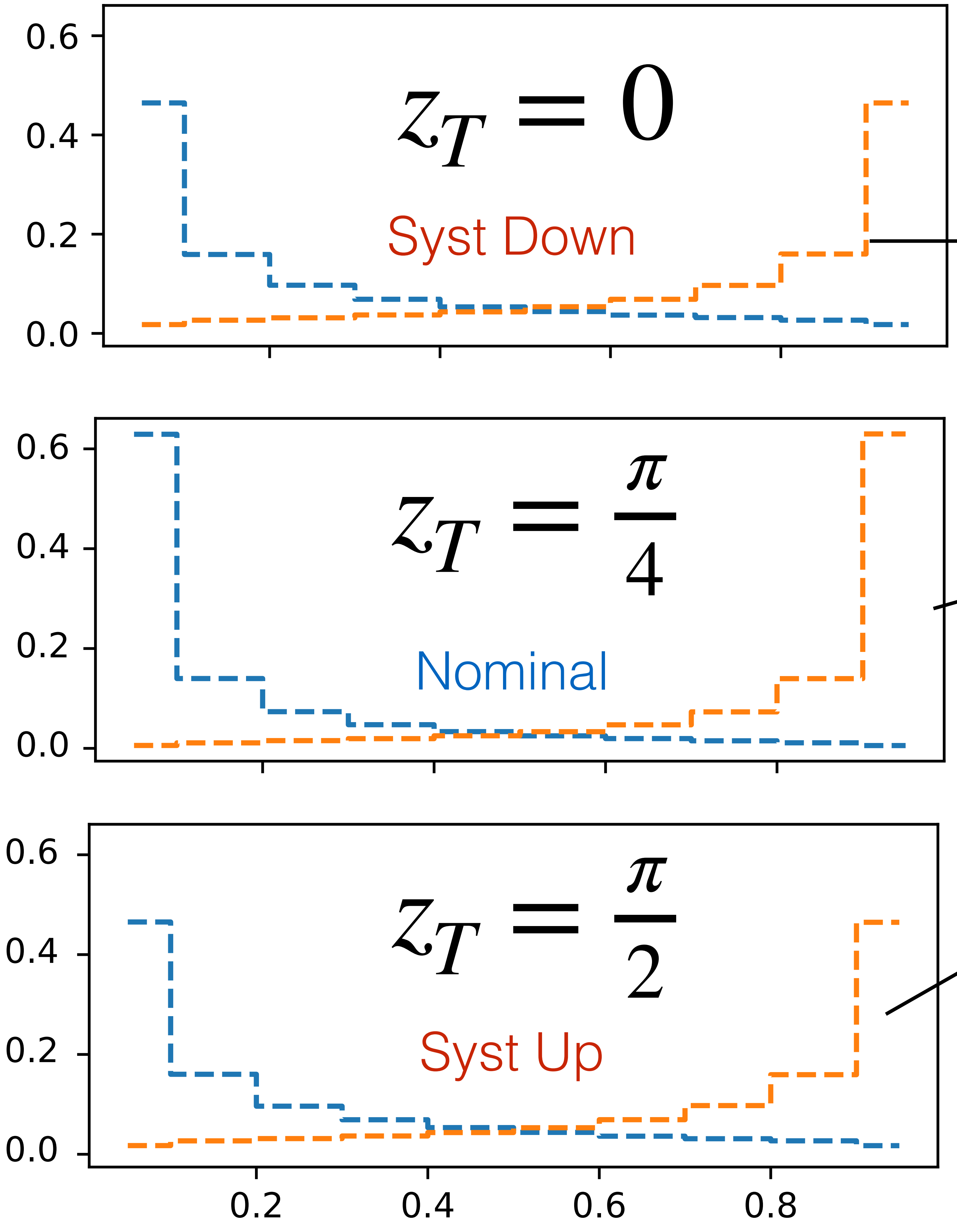

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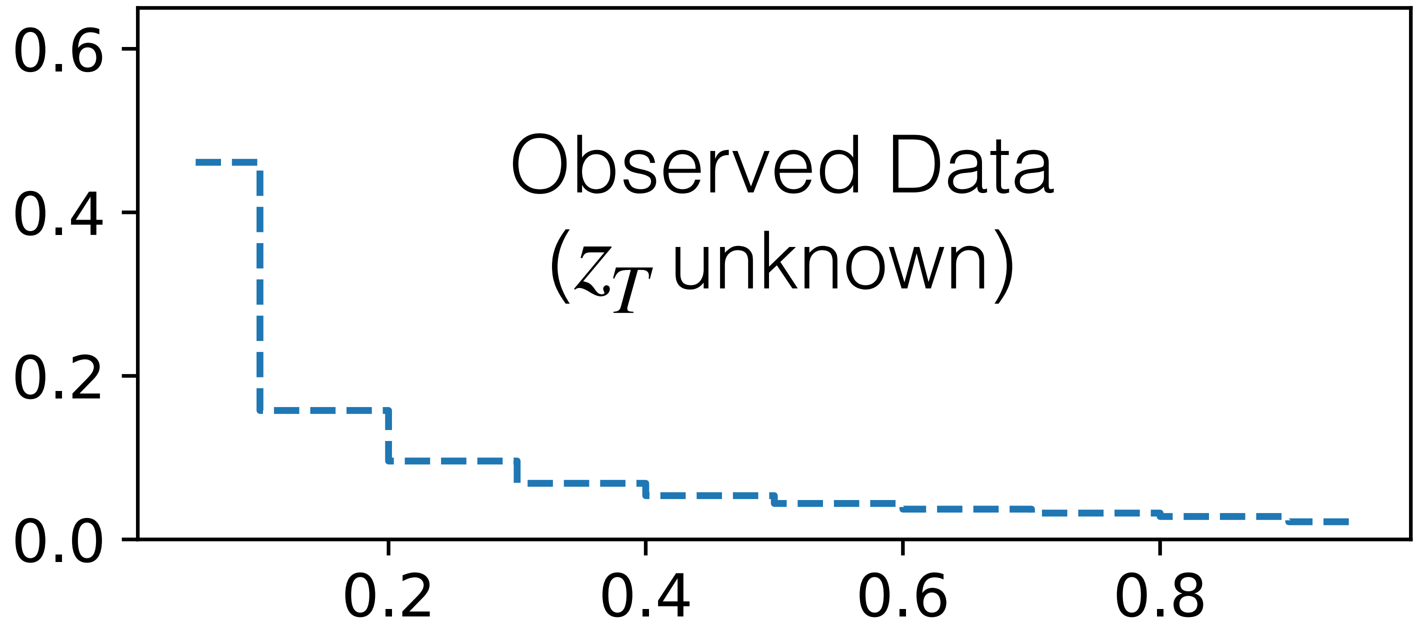

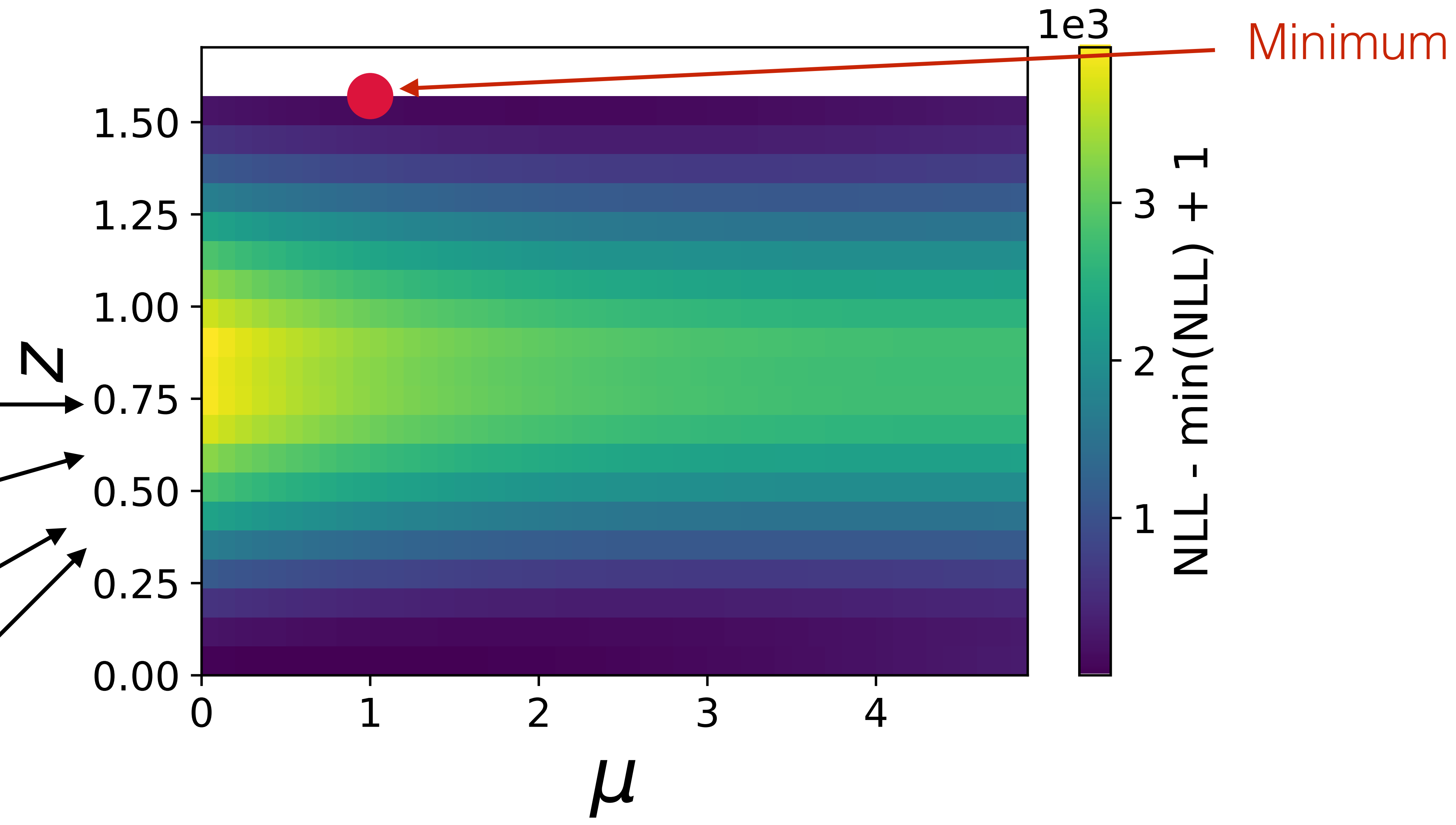

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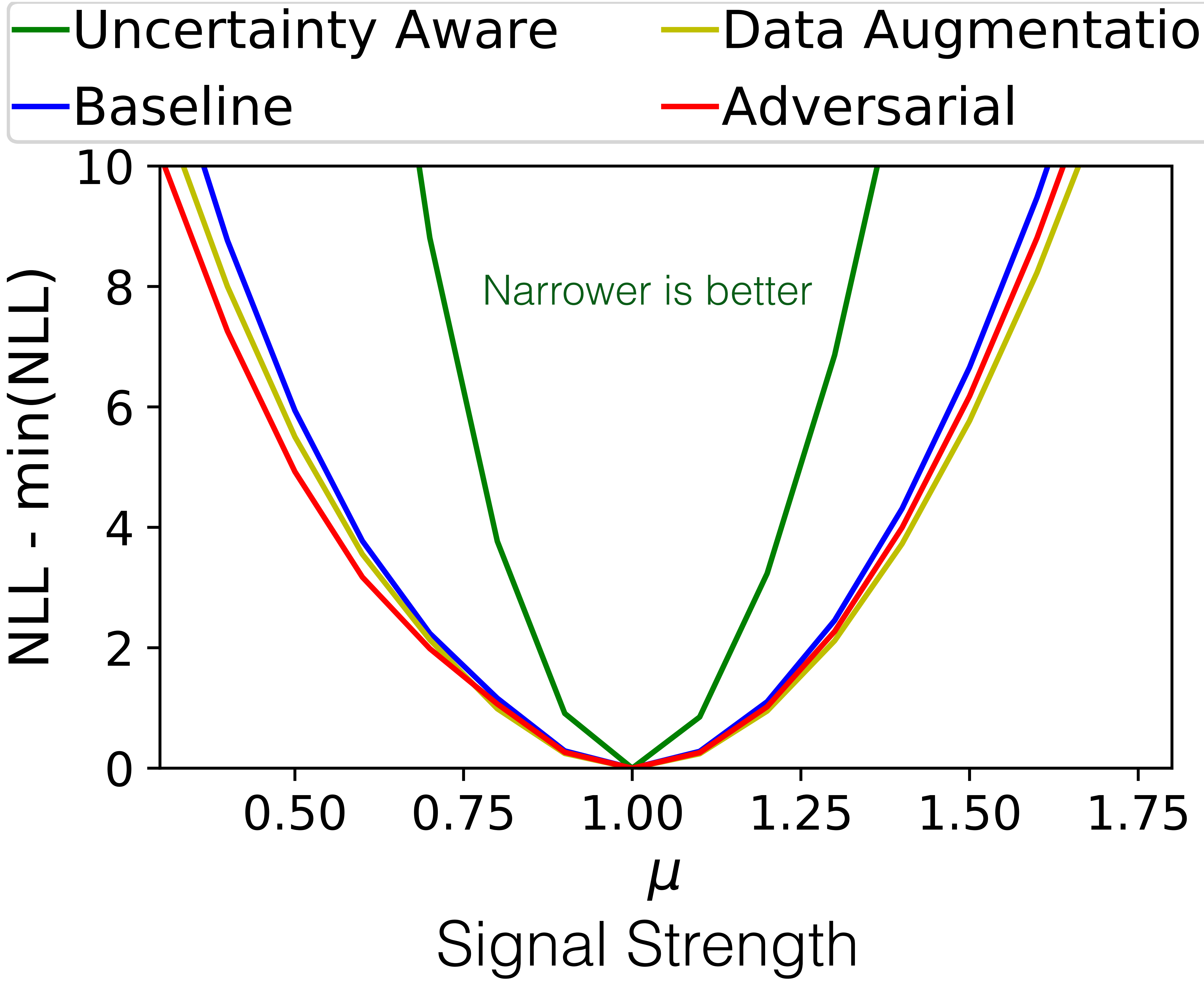
Next step: profile over Z dimension (take the bin with maximum likelihood in each column)

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



Narrower is better: We can exclude wrong values of μ with greater confidence.

The profiled (Negative-Log-) Likelihood curve for Uncertainty-Aware classifier is much narrower ⇒ smallest

[statistical + systematic] uncertainty on measurement

Profile Likelihood

Standard method of including the systematic uncertainty into the likelihood computation

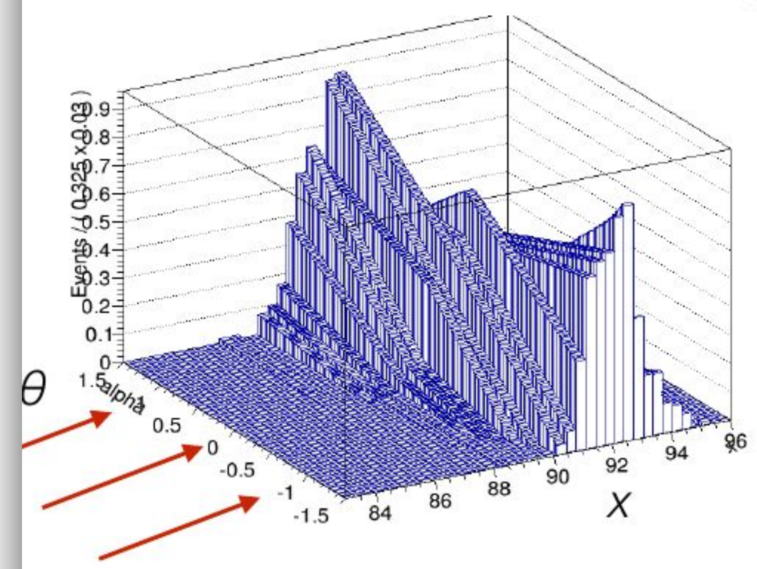
We simply make the selection/observable a function of z

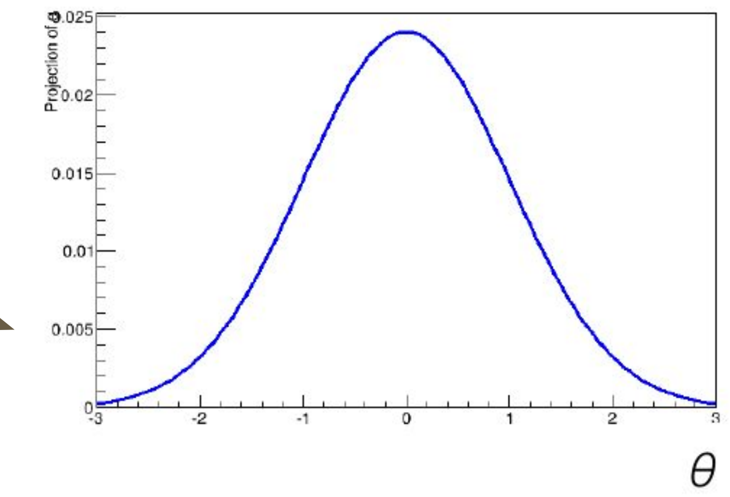
In principle could also be done in cut-based analysis: make cut a continuous function of z

The Profile Likelihood approach

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

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





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

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

3

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

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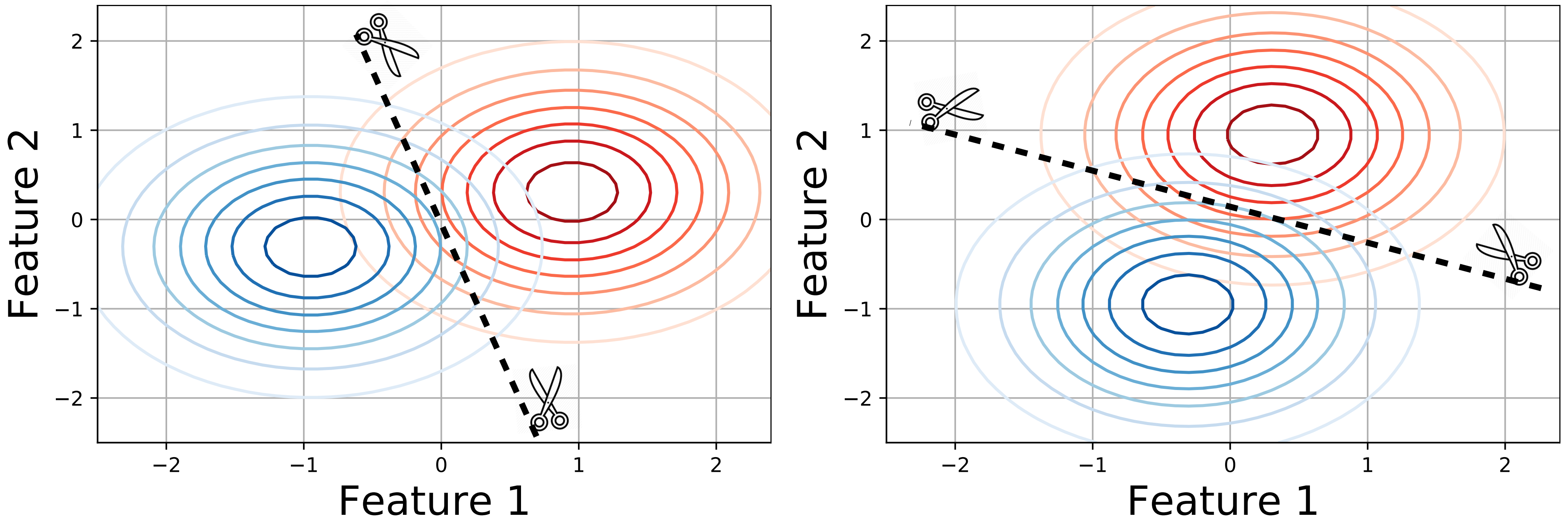

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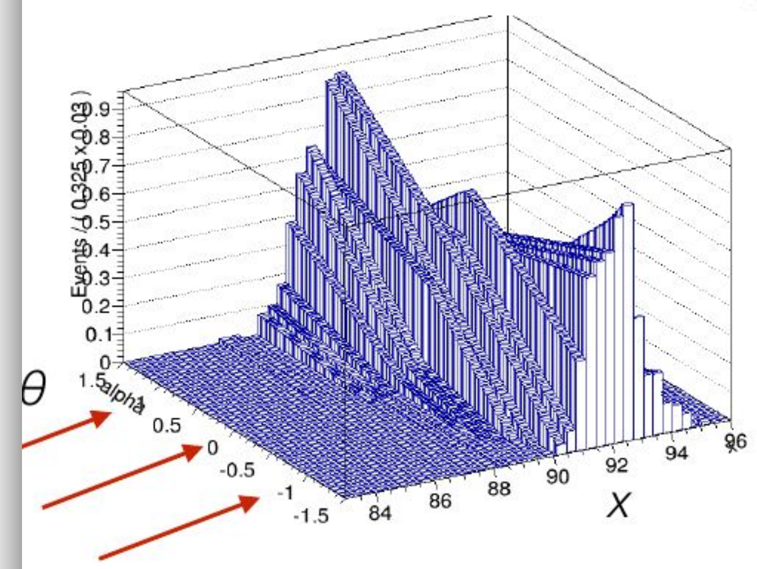

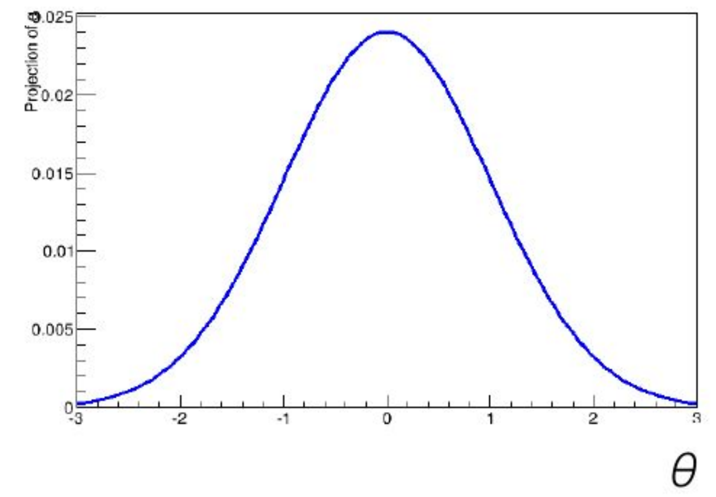

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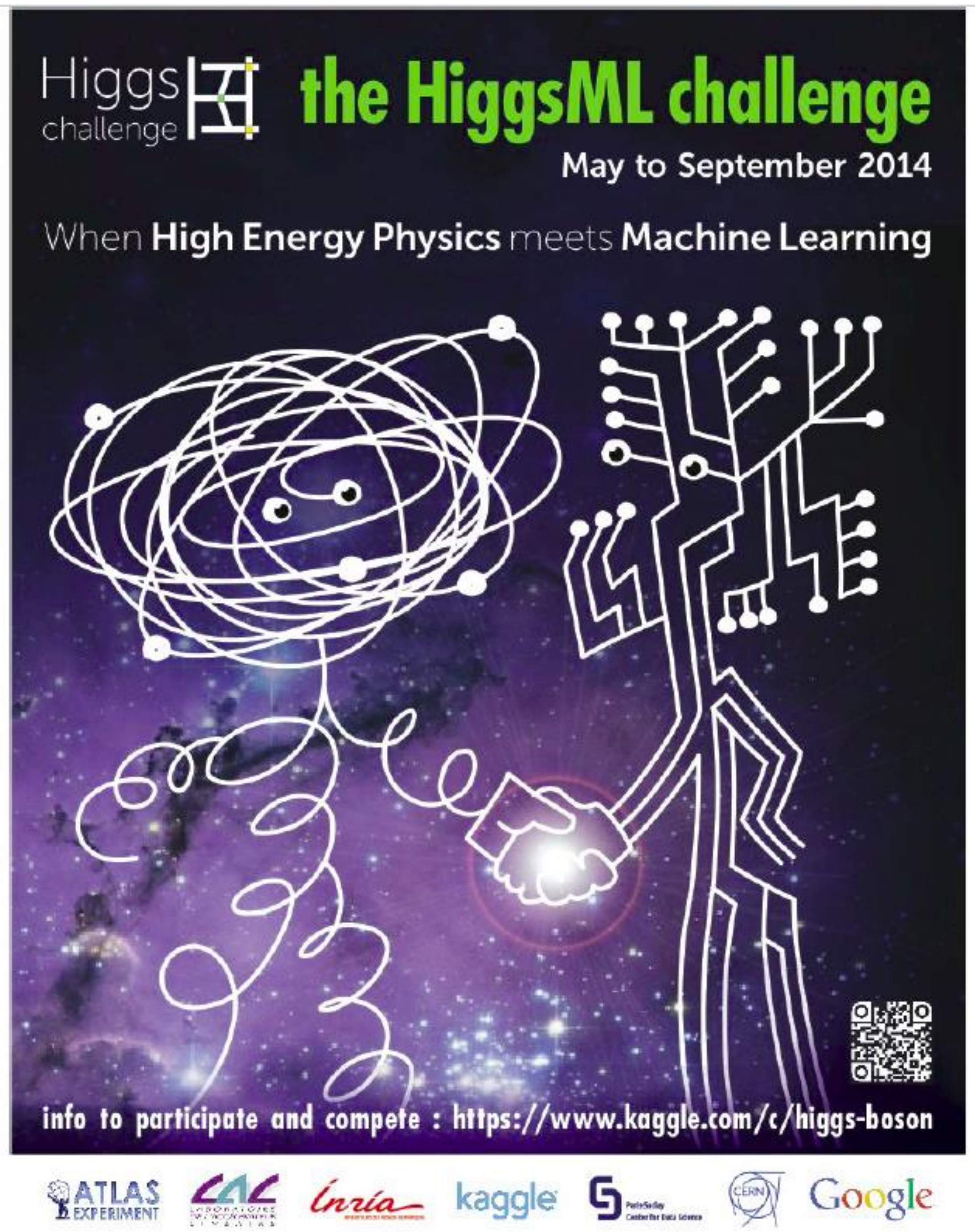
Yes!

But in a real measurement we don’t know true Z a priori, would this still help?

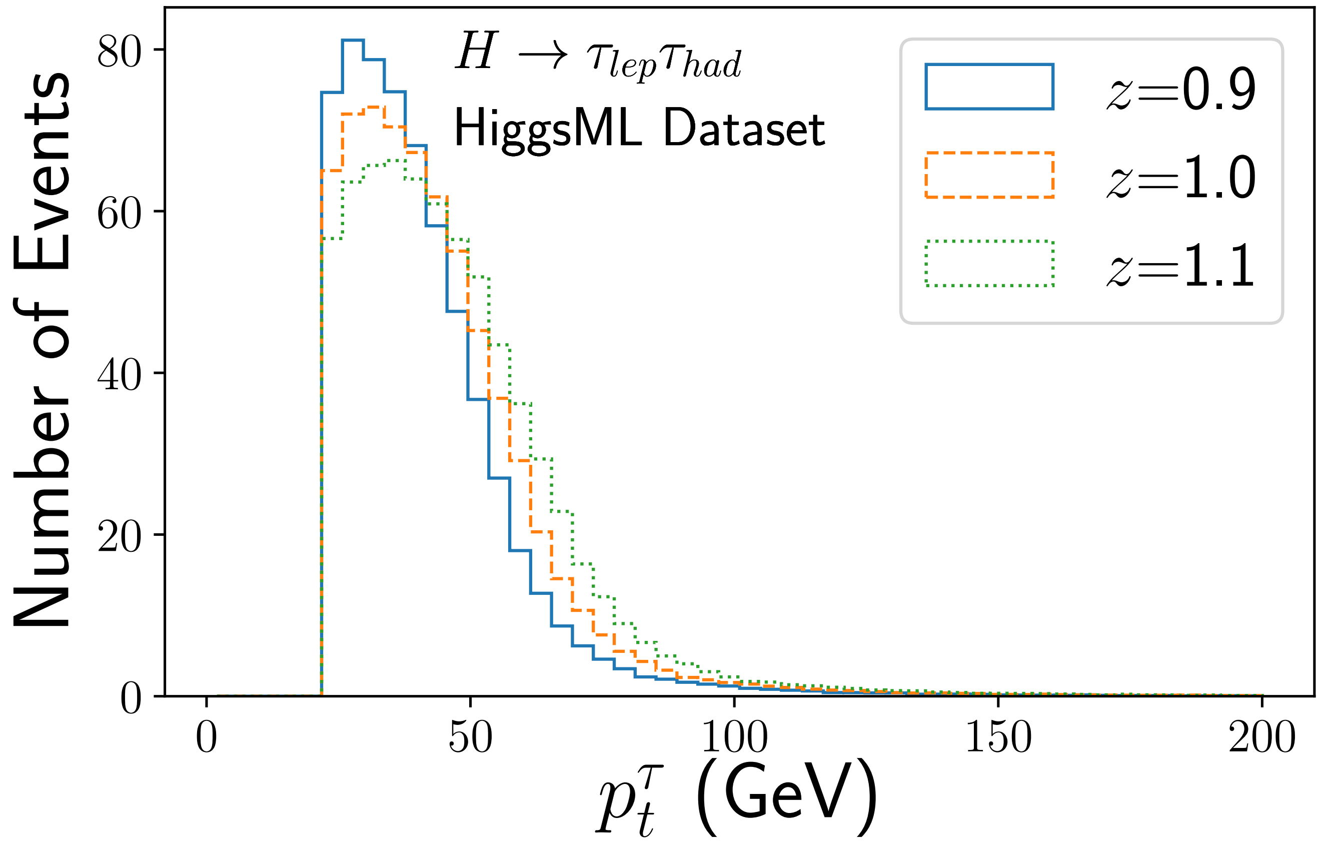
Yes!

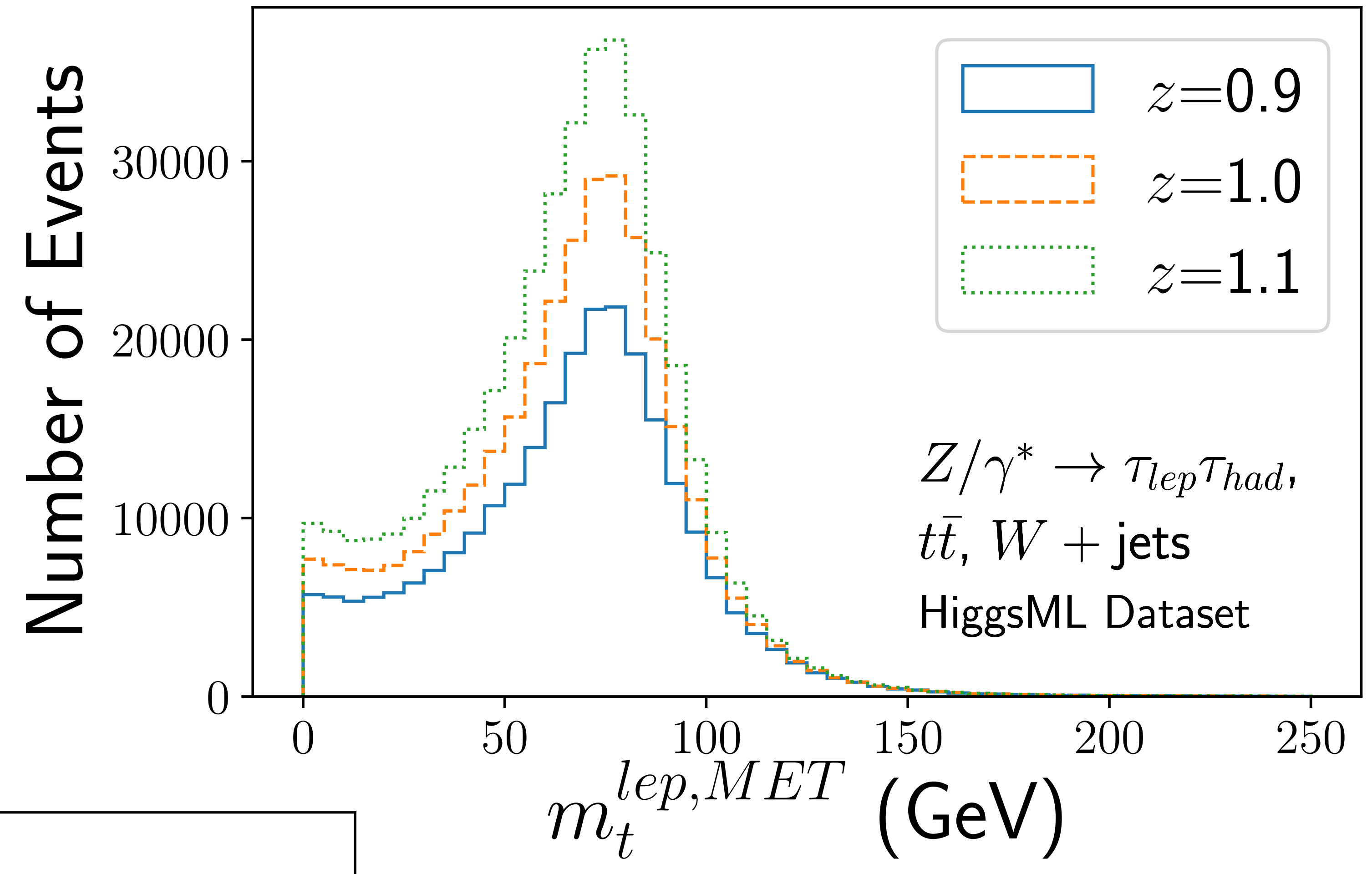
Okay, it works on your handcrafted toy problem. What about a real physics dataset?

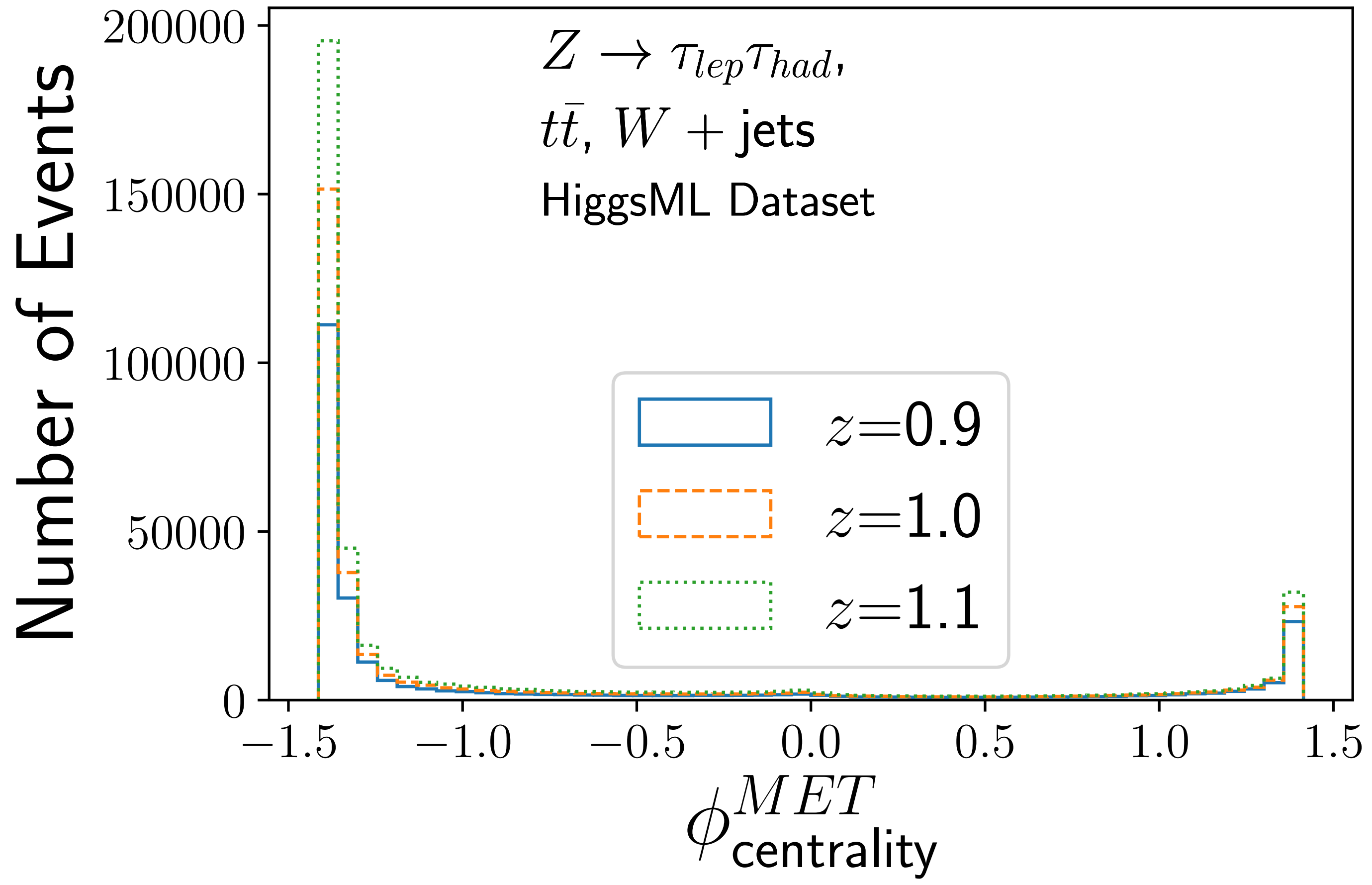
HiggsML Public Dataset with Tau Energy Scale (TES) as Z



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







We later realised dataset isn’t ideal, stats limited..

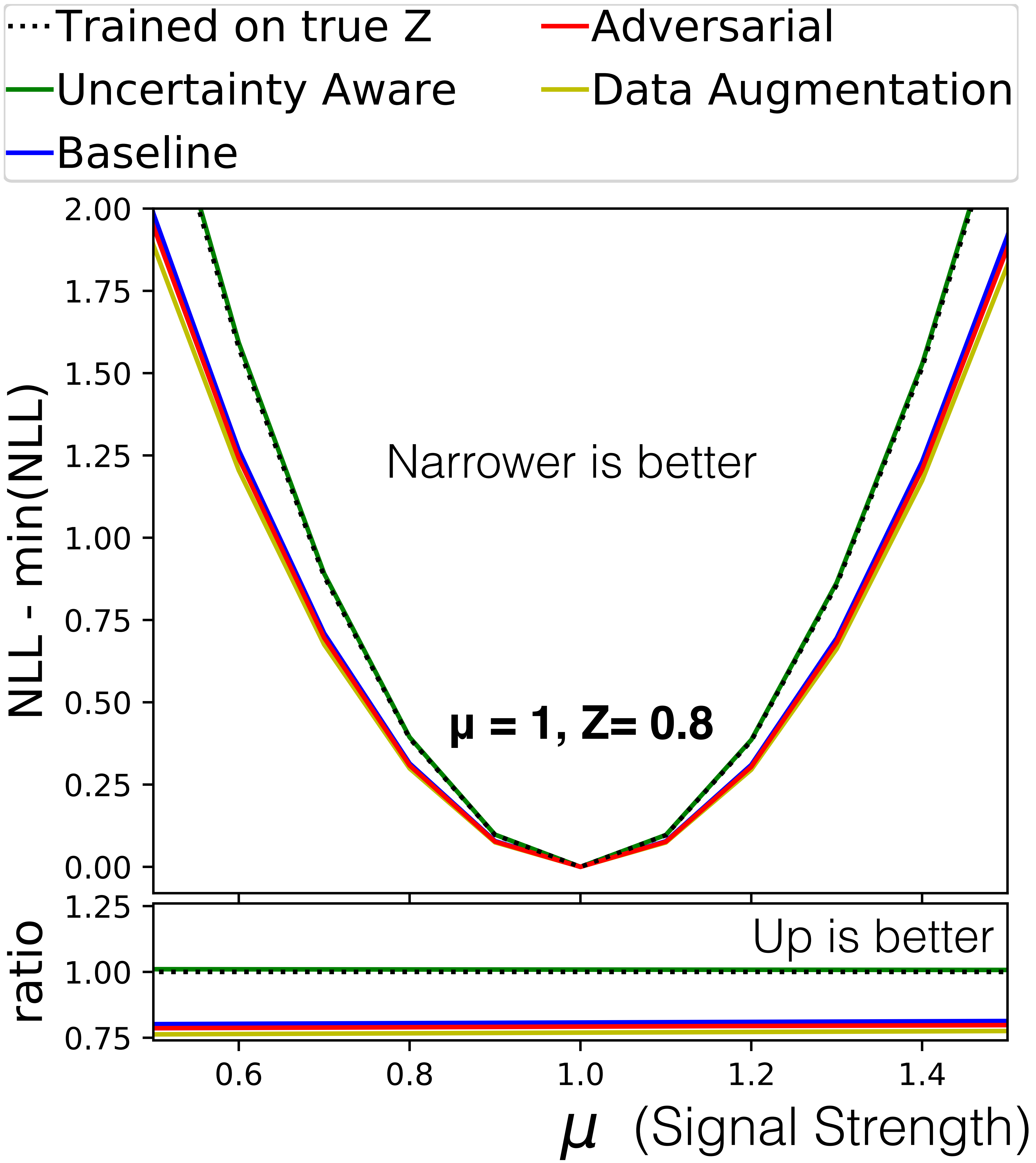
Test performance for “observed” at Systematic below Nominal

Train actual networks this time

μ = 1, Z= 0.8

(Signal Strength)

Test performance for “observed” at Systematic below Nominal

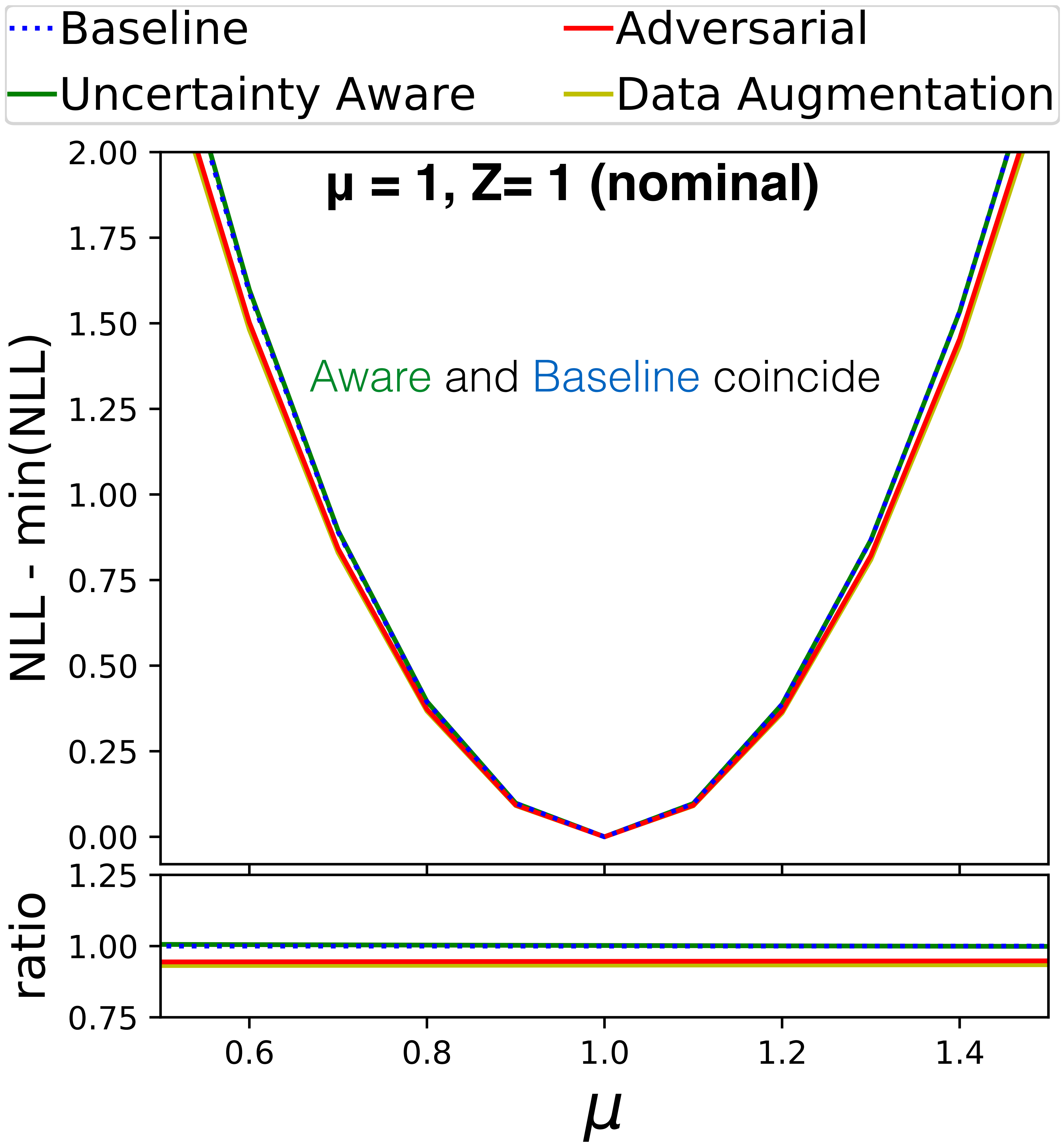


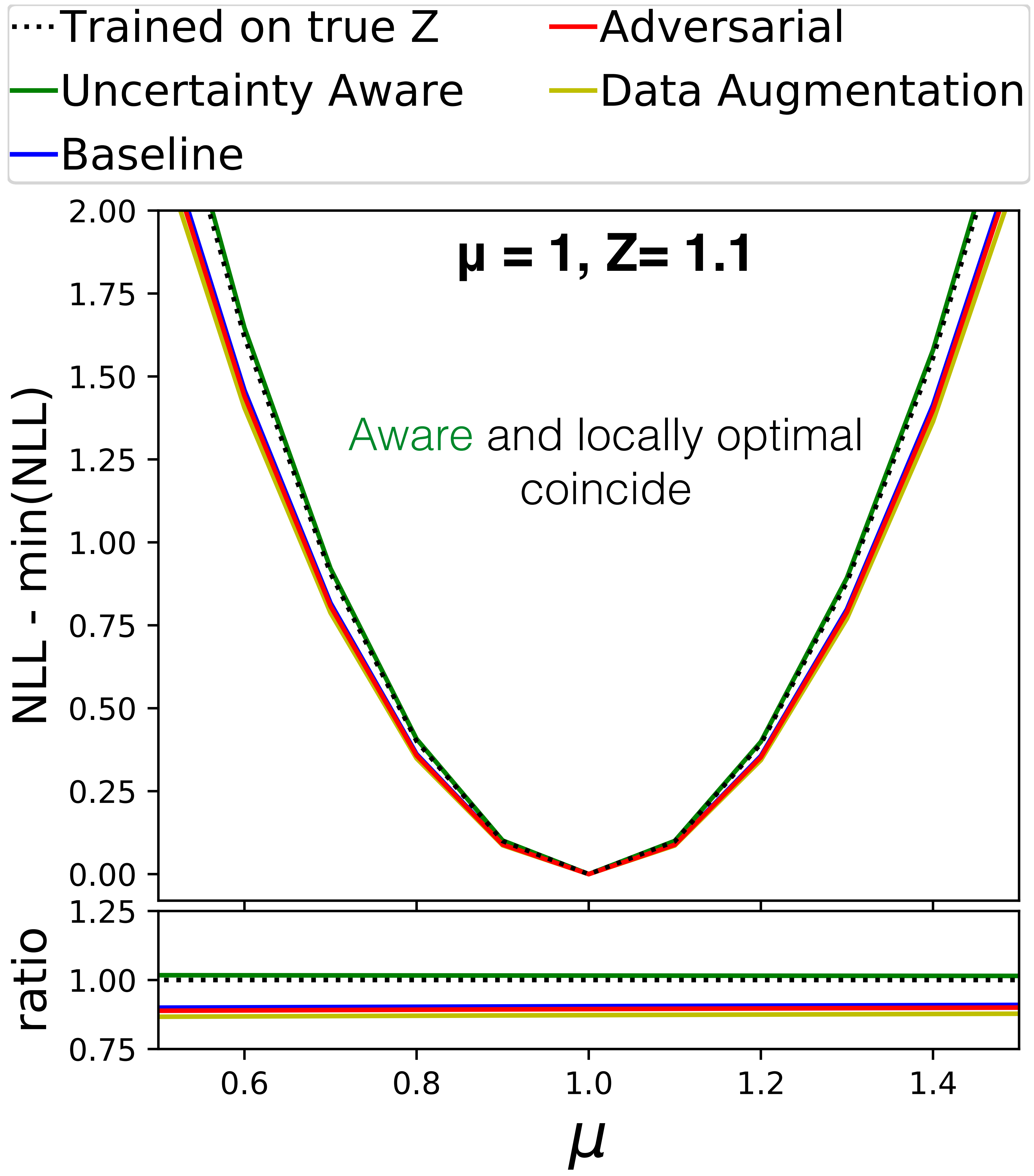
Train actual networks this time

Uncertainty-Aware coincides with classifier trained on true Z

⇒ It is optimal!

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



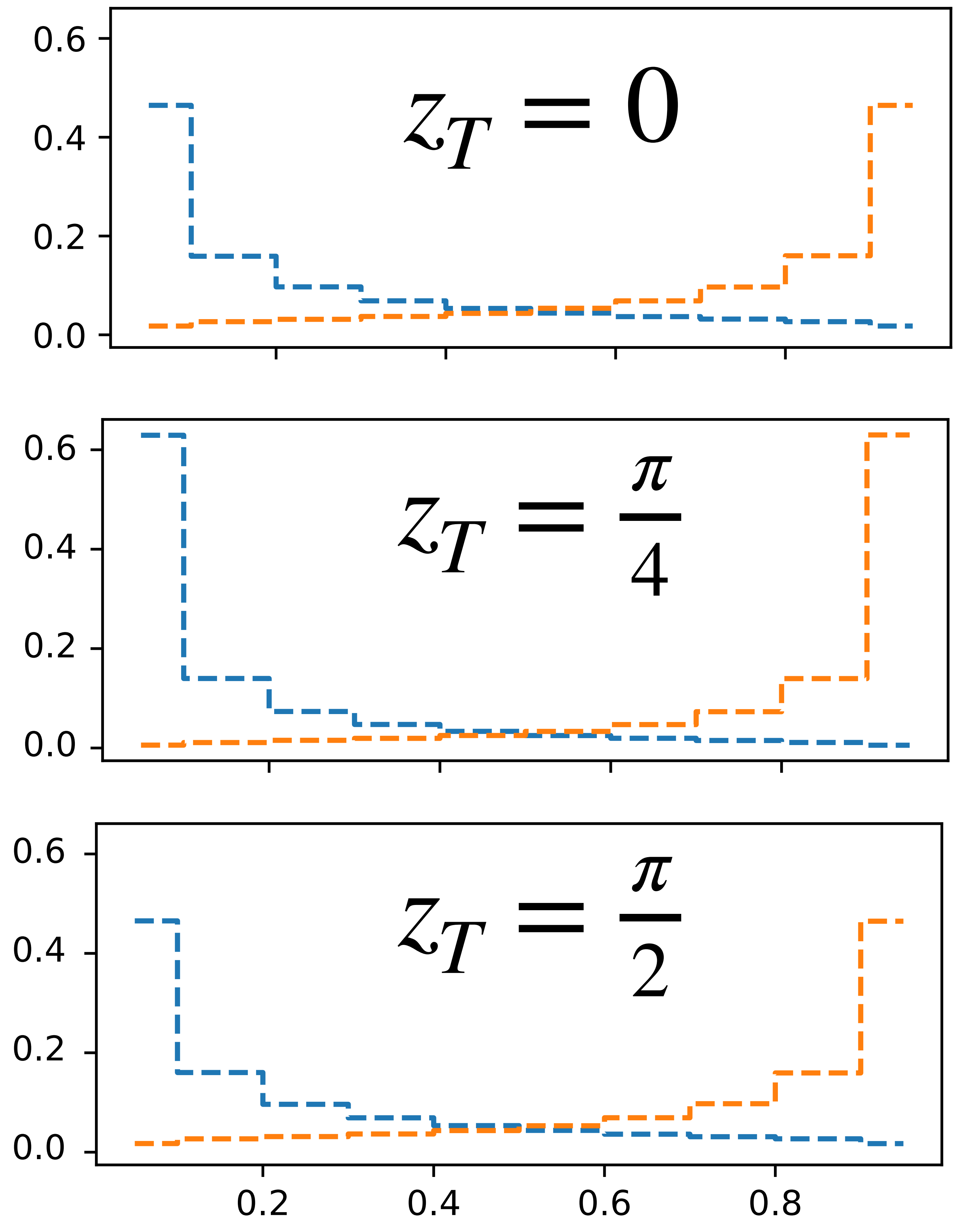


In every case the Aware Classifier is as good as the optimal one, no other technique matches its performance everywhere

Practical advantages of factorising inference

While using histogram (or KDE) templates seems clunky, it has practical advantages:

- More diagnostic tools: look at histograms, test for over-constraining of z
- Study impact of/profile over untrained nuisance parameters
- No worries about calibration of NN



Possible Extensions

- Uncertainty aware Baysean Networks?
- Combine uncertainty awareness with inference awareness?
- How to deal with uncertainties when training directly on calo images / raw data ?
- …

Conclusion

- Systematic uncertainties are a nuisance in HEP, even more relevant as we collect more data
- Training a systematic aware classifier and profiling over the nuisance parameter provides performance similar to a locally optimal classifier
- This prescription can also handle auxiliary measurements of the nuisance parameter straightforwardly by combining the likelihoods
- Not a black-box procedure: Can also study impact of untrained systematics on sensitivity
- Solution scales to real physics dataset, easy to integrate into ATLAS/CMS chain

arXiv:2105.08742

Backup

Auxiliary measurement of Z instead of prior

Simplistic auxiliary measurement of z_T

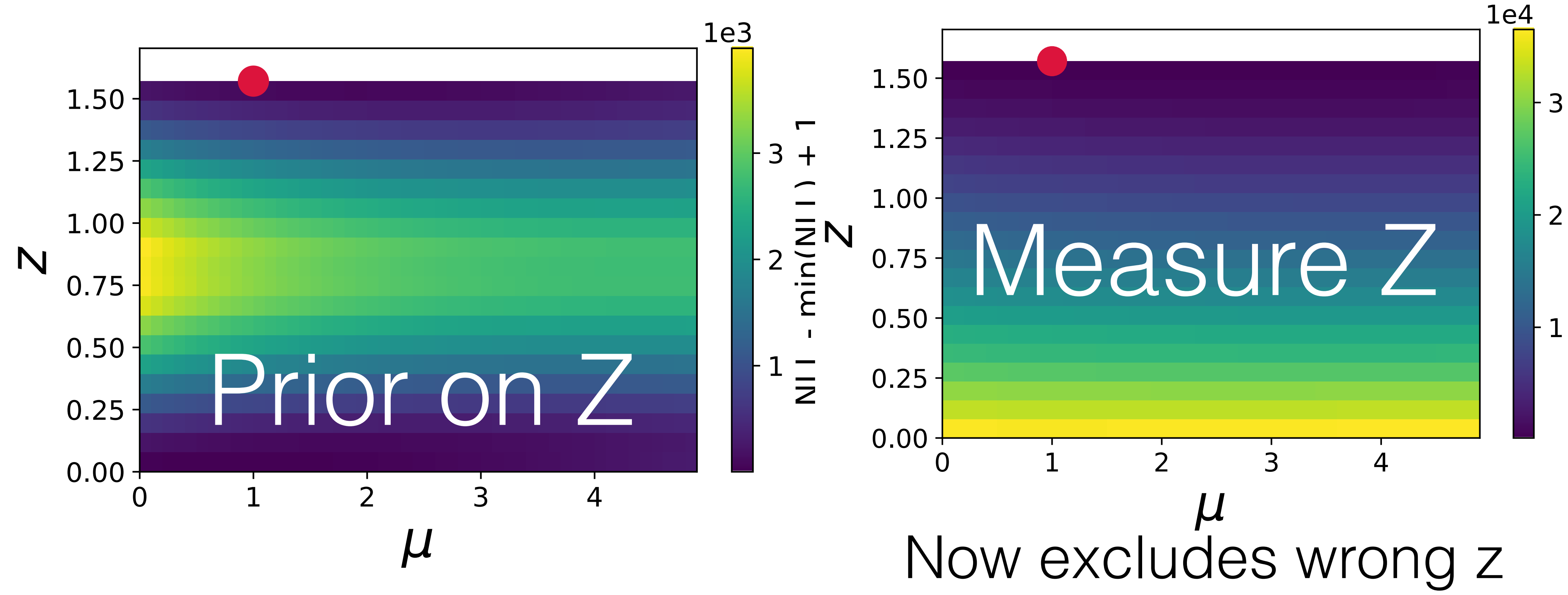
No need to re-train any network, change only in likelihood computation step

All methods provide improved limits on μ if Z is tightly constrained

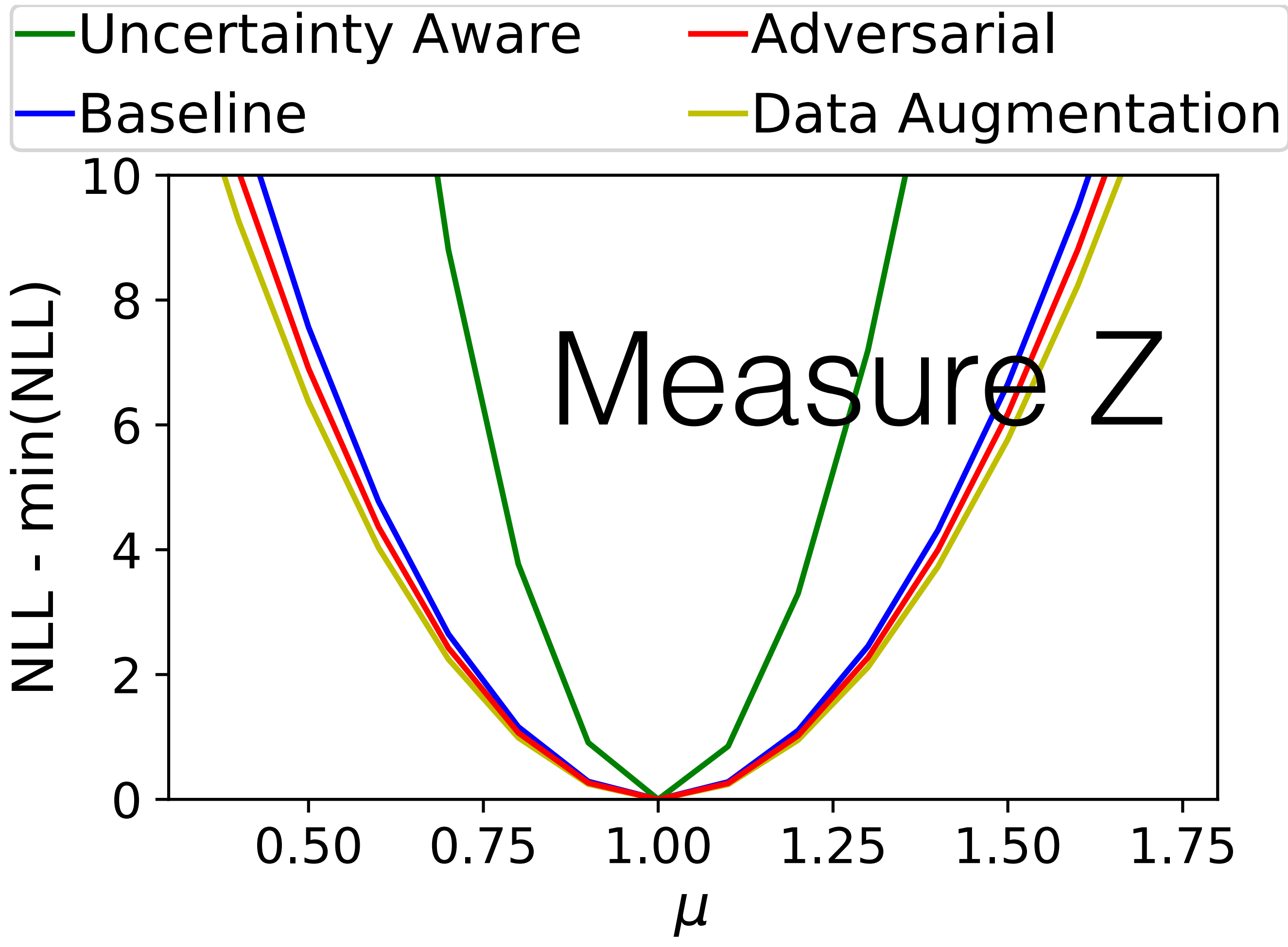
Aware classifier still best one to use

$$
\begin{aligned}
-\log \mathcal{L}(\mu, z|\{x_i\}) \\
&= -\sum_{j=1}^{n_{\text{bins}}} \left[N_j \cdot \log\left(\mu s_j + b_j\right) - \mu s_j - b_j - \log(\Gamma(N_i)) \right] \\
&\quad - \sum_{k=1}^{m_{\text{bins}}} \left[N_k^{aux} \cdot \log\left(a_{\mathrm{k}}^z\right) - a_{\mathrm{k}}^z - \log(\Gamma(N_k^{aux})) \right],
\end{aligned}
$$

Baseline classifier trained on nominal



Now excludes wrong z confidently



(b) Data generated with $z = \frac{\pi}{2}$.

Test performance for "observed" datasets at $\mu = 2$

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

Training Sub-Networks Individually

- Systematic effects are very subtle and often difficult to learn (effect of random noise much larger than systematic)
- A simple dense network parameterised on Z tends to overtrain before learning the full dependence on Z

- Solution: Train two subnetworks independently for Z<1 and Z≥1 and combine with a if-else

```
def combineModels(ModelUp, ModelDown):
    input1 = Input(shape=(X_syst_train.shape[1],))
    input2       = Input(shape=(1,))

    selectModel1 = Lambda(lambda x: K.greater_equal(x, K.constant(1.)))(input2)
    selectModel2 = Lambda(lambda x: K.less(x, K.constant(1.)))(input2)

    selectModel1 = Lambda(lambda x: K.cast(x, dtype='float32'))(selectModel1)
    selectModel2 = Lambda(lambda x: K.cast(x, dtype='float32'))(selectModel2)

    out1 = Multiply()([ModelUp([input1,input2]), selectModel1])
    out2 = Multiply()([ModelDown([input1,input2]), selectModel2])

    out  = Add()([out1, out2])
    model = Model(inputs=[input1,input2], outputs=out)
    return model

aware_model = combineModels(netAweUp_model, netAweDown_model)
aware_model.compile(optimizer='RMSProp',
              loss='binary_crossentropy',
              metrics=['accuracy'])
```