Introduction to Machine Learning for Physics

BERKELEY LAB

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EFI Data Analytics Workshop
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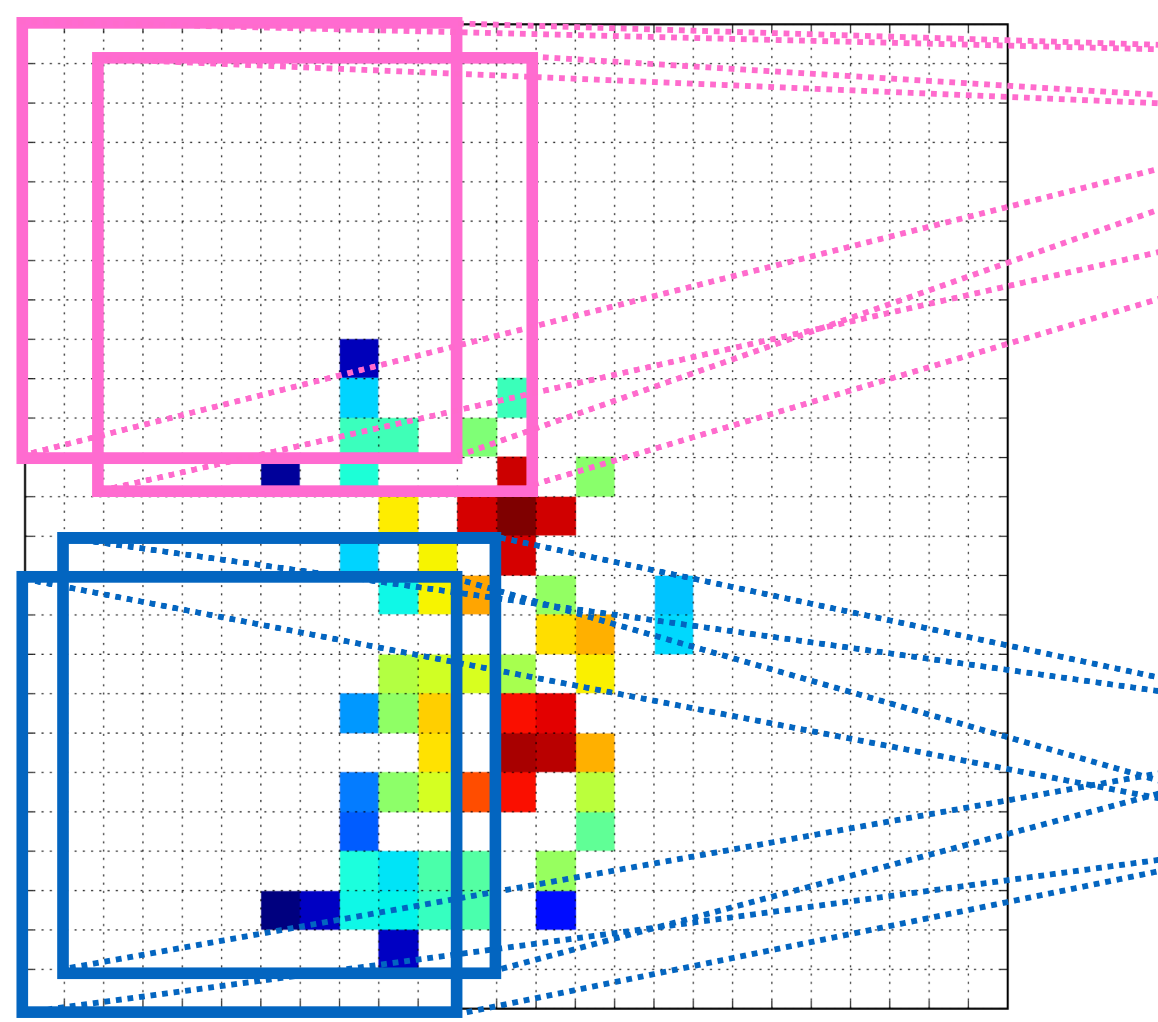

What this is not

What this is not

...the Higgs boson?

What this is not

A replacement for a great online tutorial or a UC course

(STAT 24400-24500)
CMSC 25025/STAT 37601
CMSC 25400/STAT 27725
TTIC 31020 (see Toyota Institute)
TTIC 31230/CMSC 35300
STAT 24610
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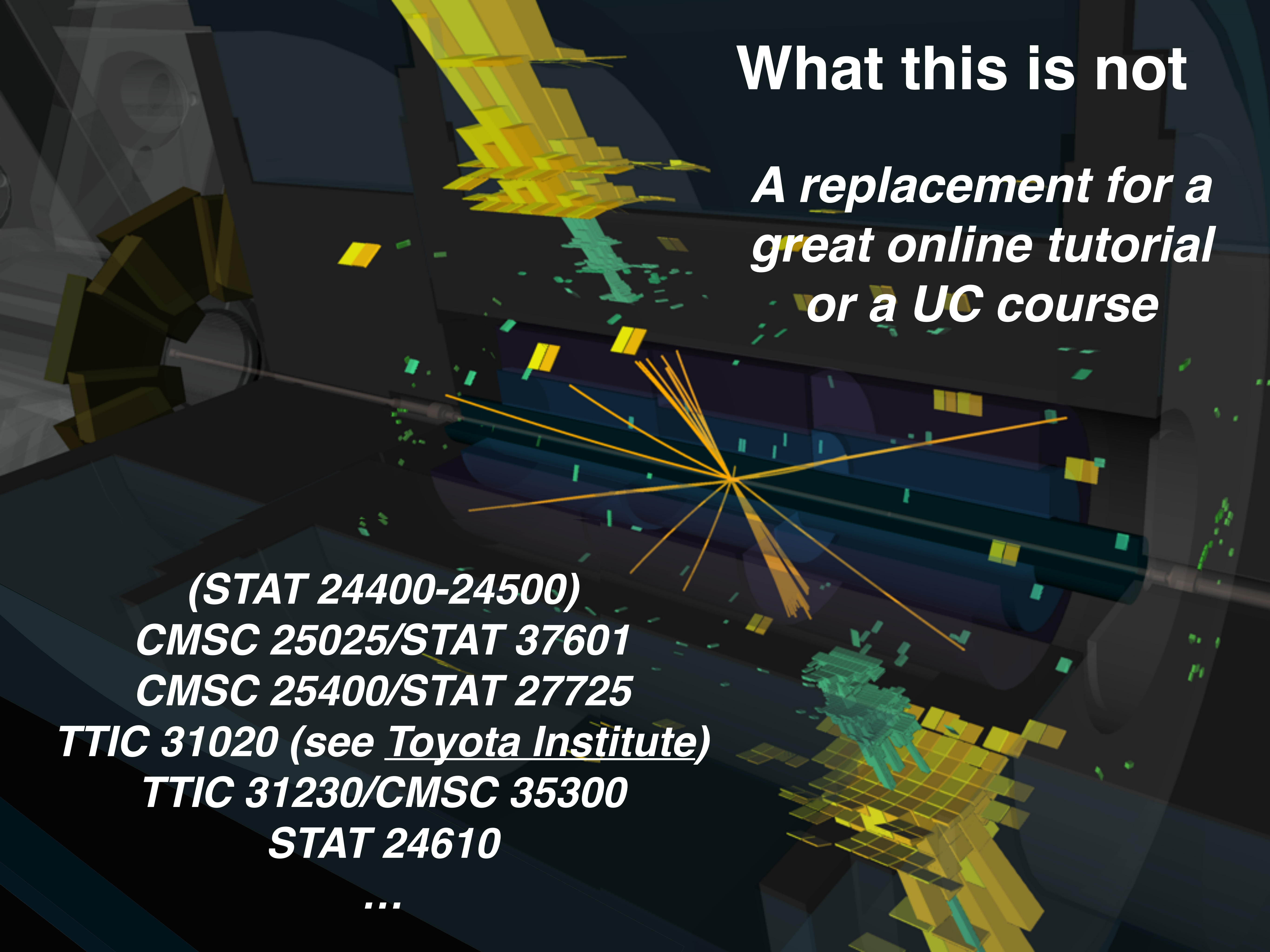
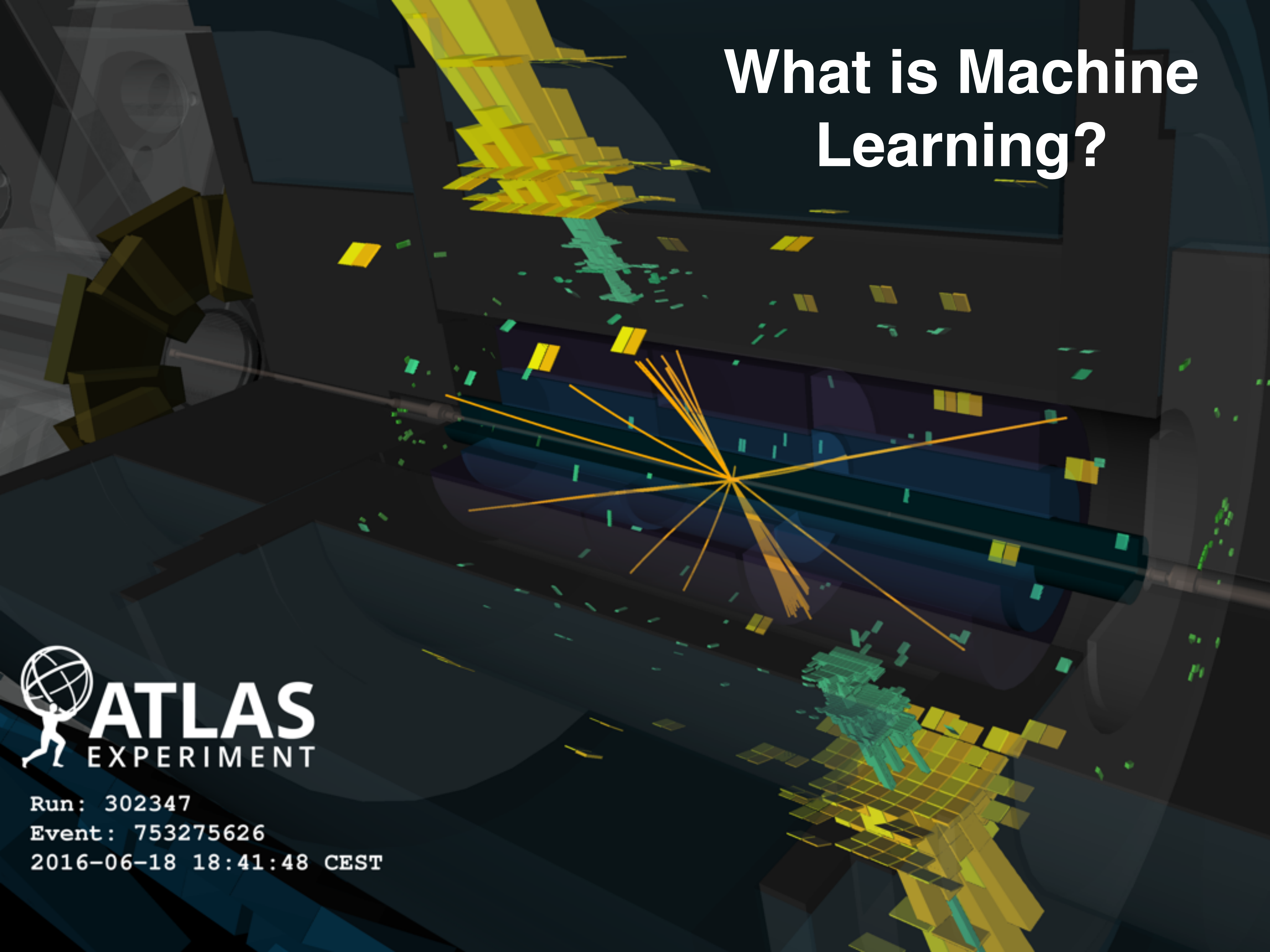
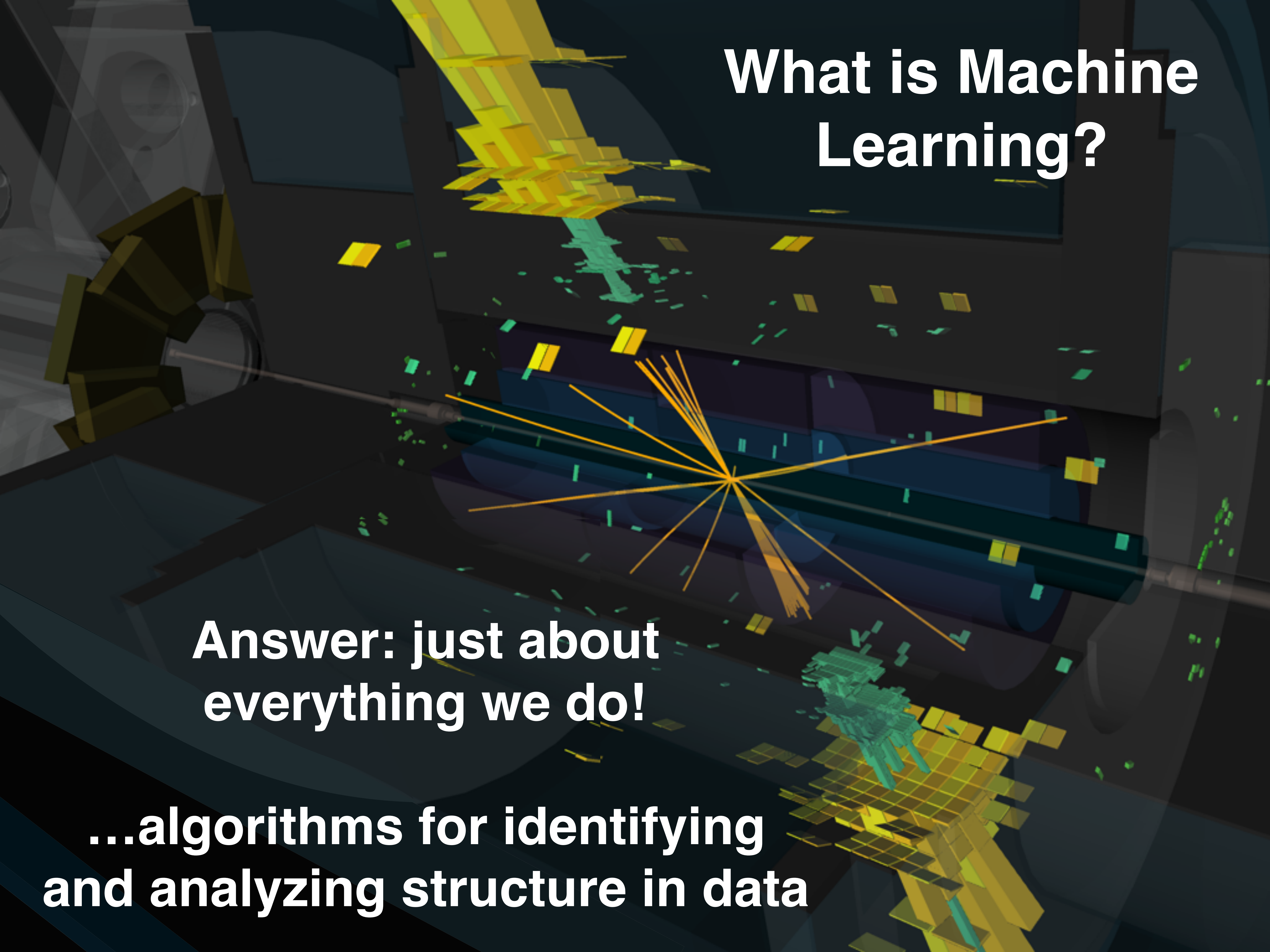


What is Machine Learning?





What is Machine Learning?

Answer: just about everything we do!

…algorithms for identifying and analyzing structure in data

What can we use machine learning for?

Supervised learning

Classification

Regression

Generation

the machine is presented examples of multiple classes and learns to differentiate

Unsupervised learning

Clustering

Anomaly detection

the machine is presented data and asked to give you multiple classes

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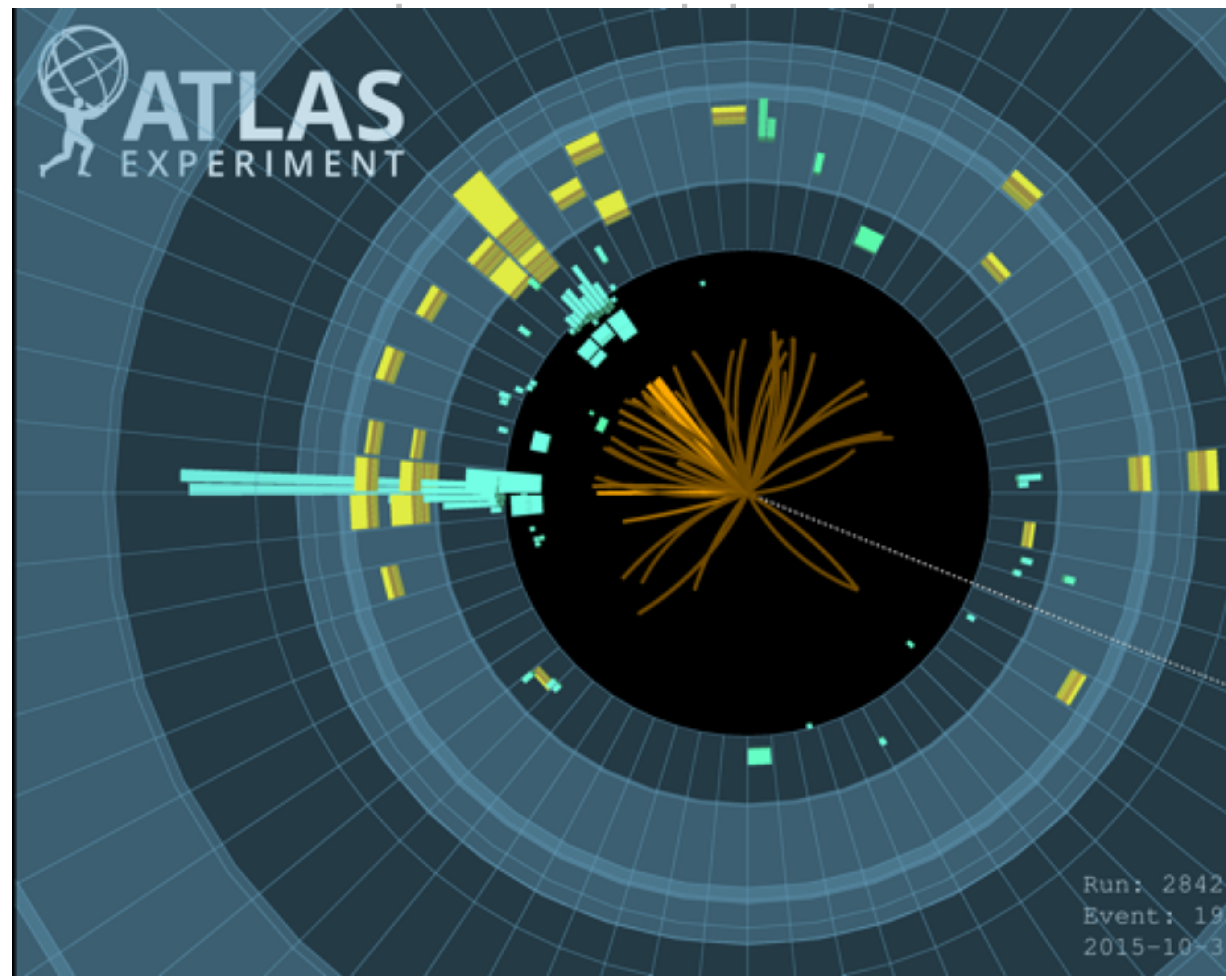
Higgs boson or gluon?



multiple classes

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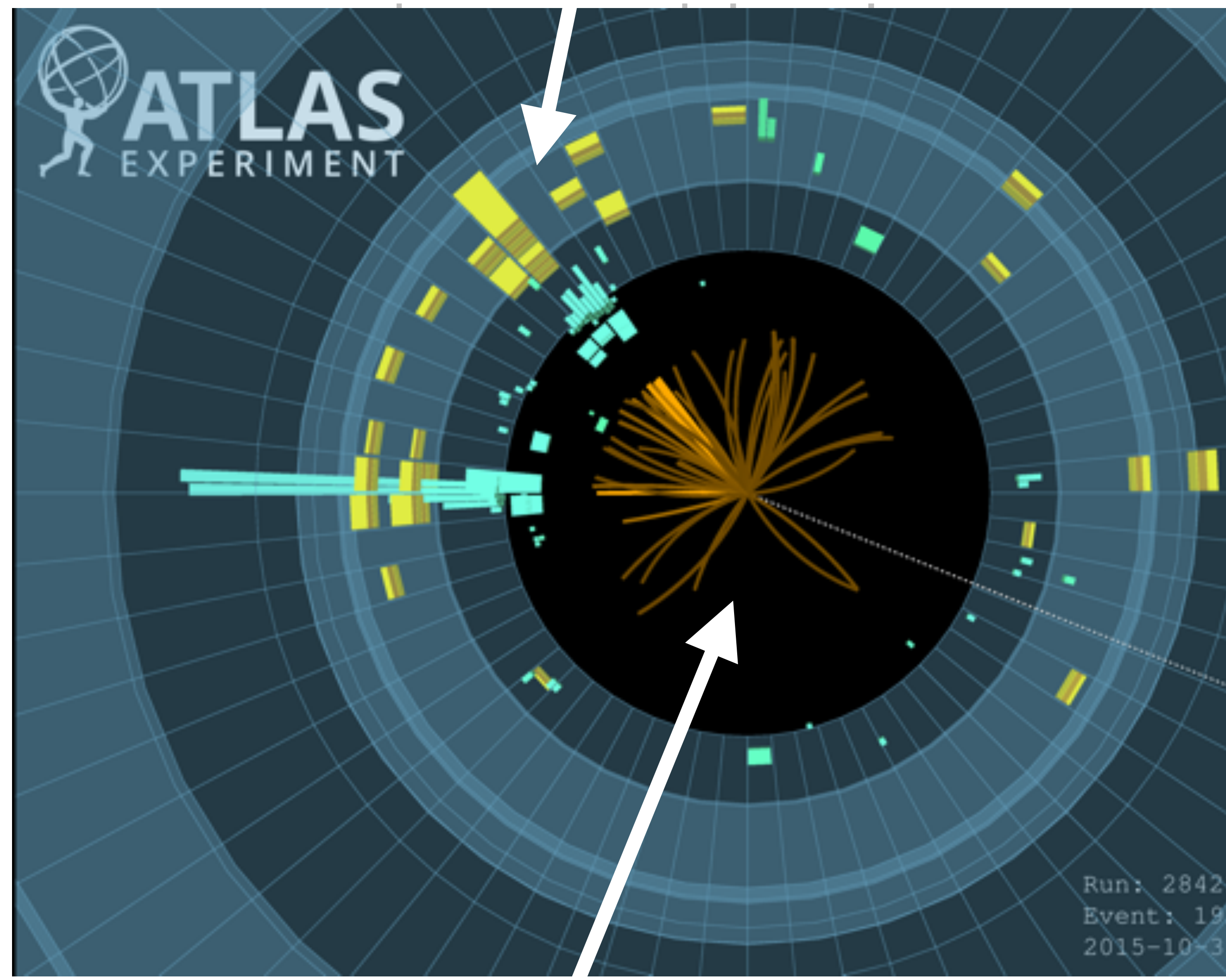
What is the energy of this spray of particles (jet)?



What are the momenta of these charged particles?

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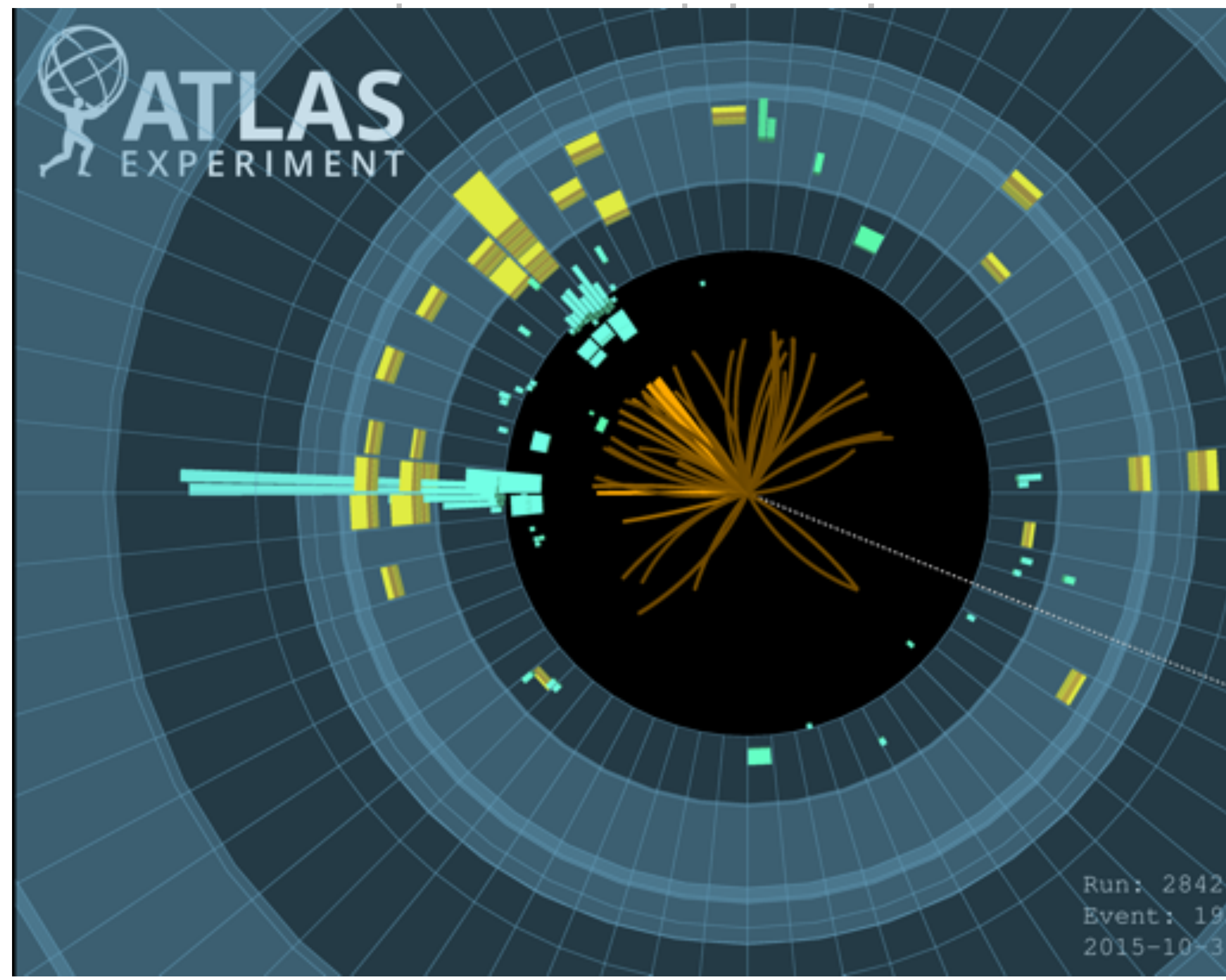

multiple classes

What would Higgs boson events look like with a different mass?

What can we use machine learning for?

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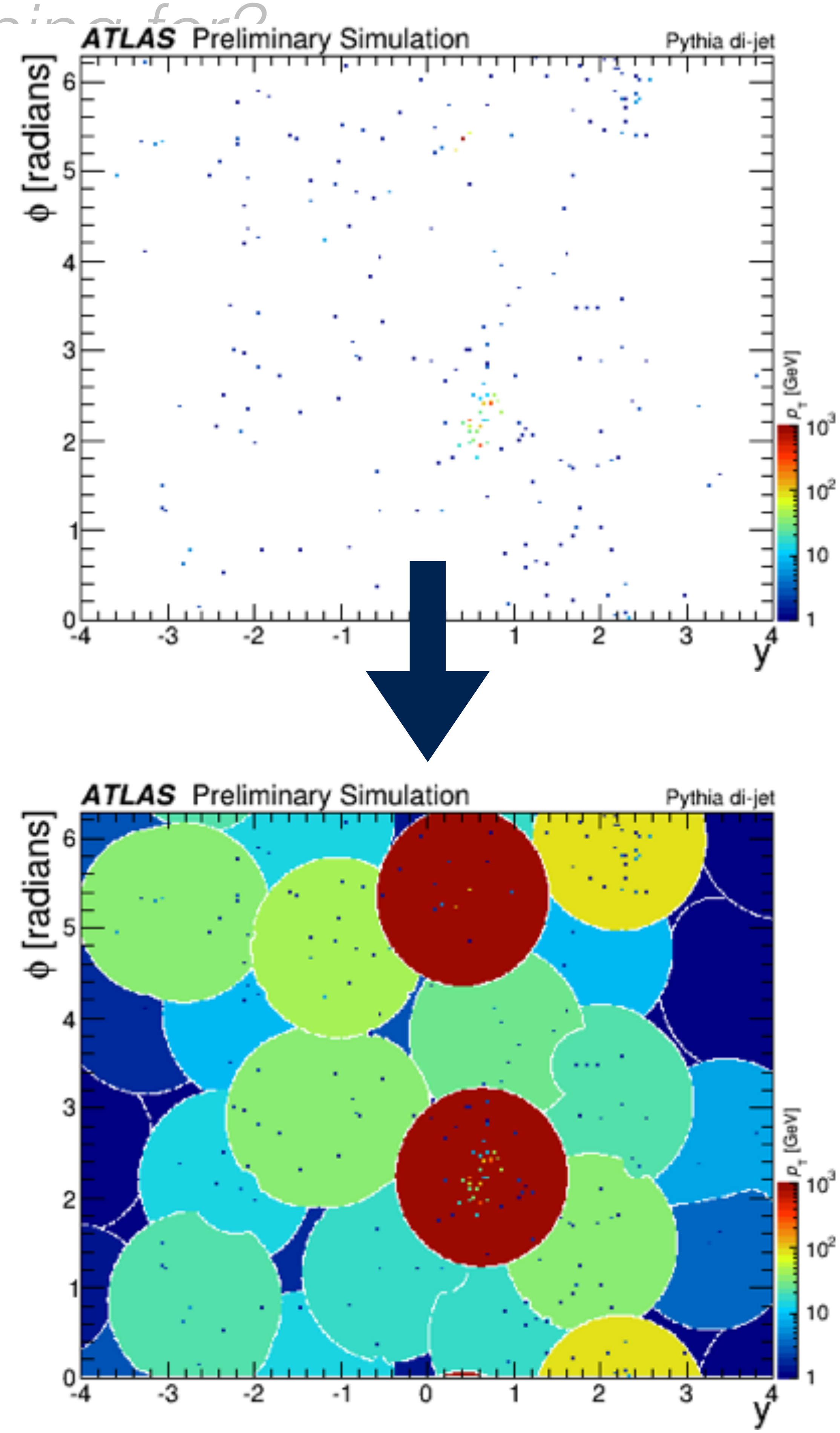

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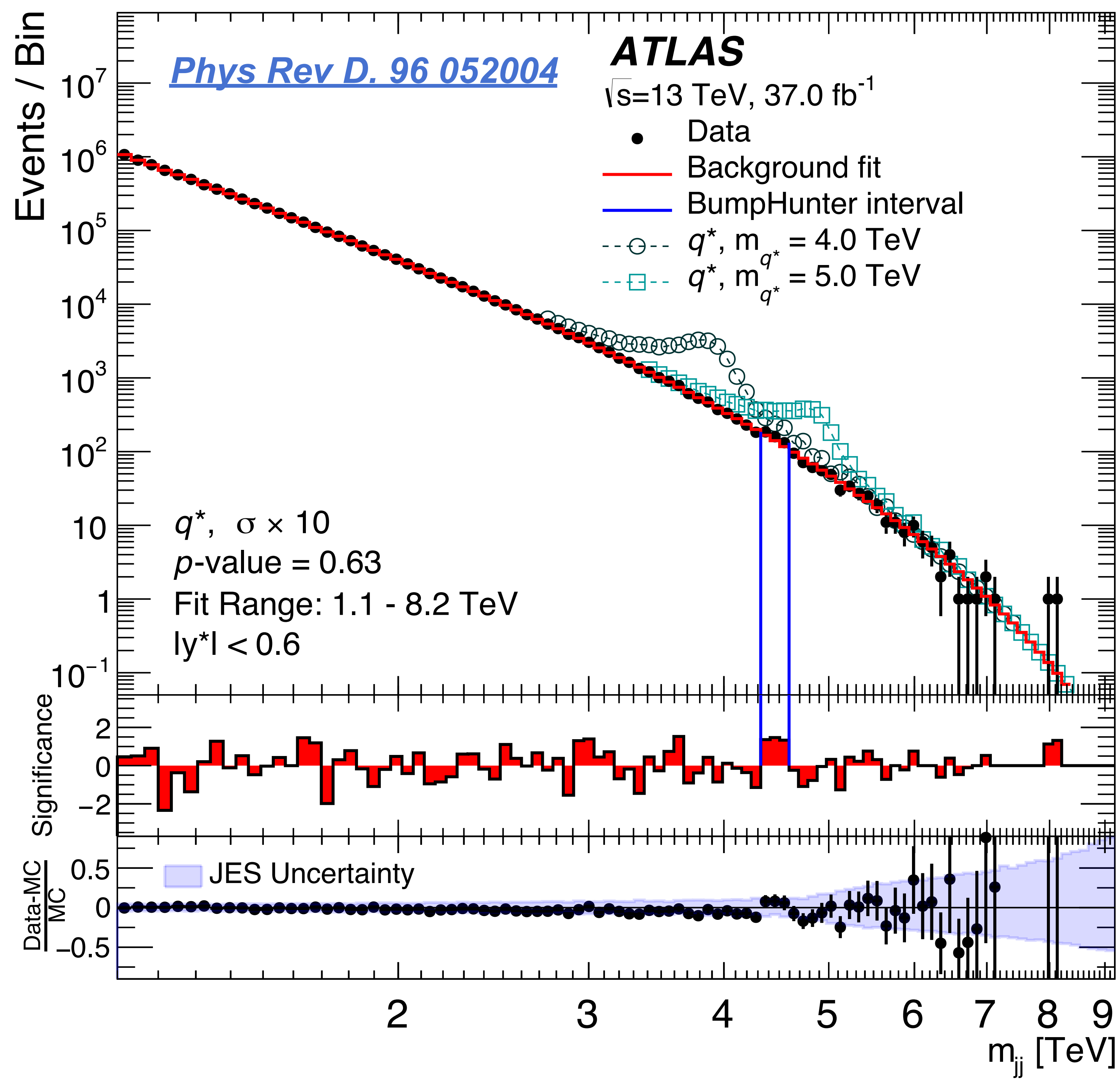


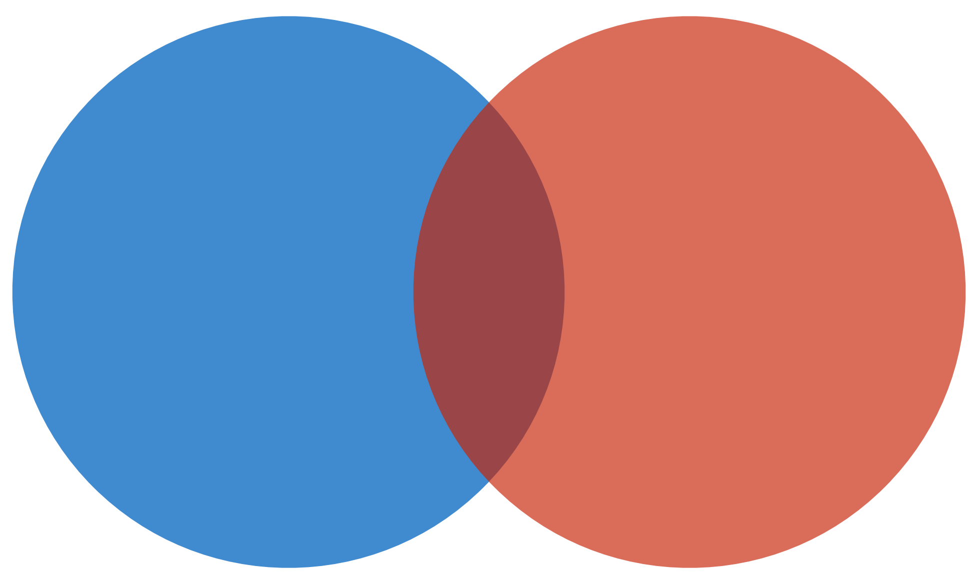
Classification

Goal: Given a *feature vector*, return an integer indexed by the set of possible *classes.*

In most cases, we care about *binary* classification in which there are only two classes (signal versus background)

There are some cases where we care about *multi-class classification*

Feature vector can be many-dimensional



Harder = more overlap between for **S** and **B**

Classification

Goal: Given a *feature vector*, return an integer indexed by the set of possible *classes.*

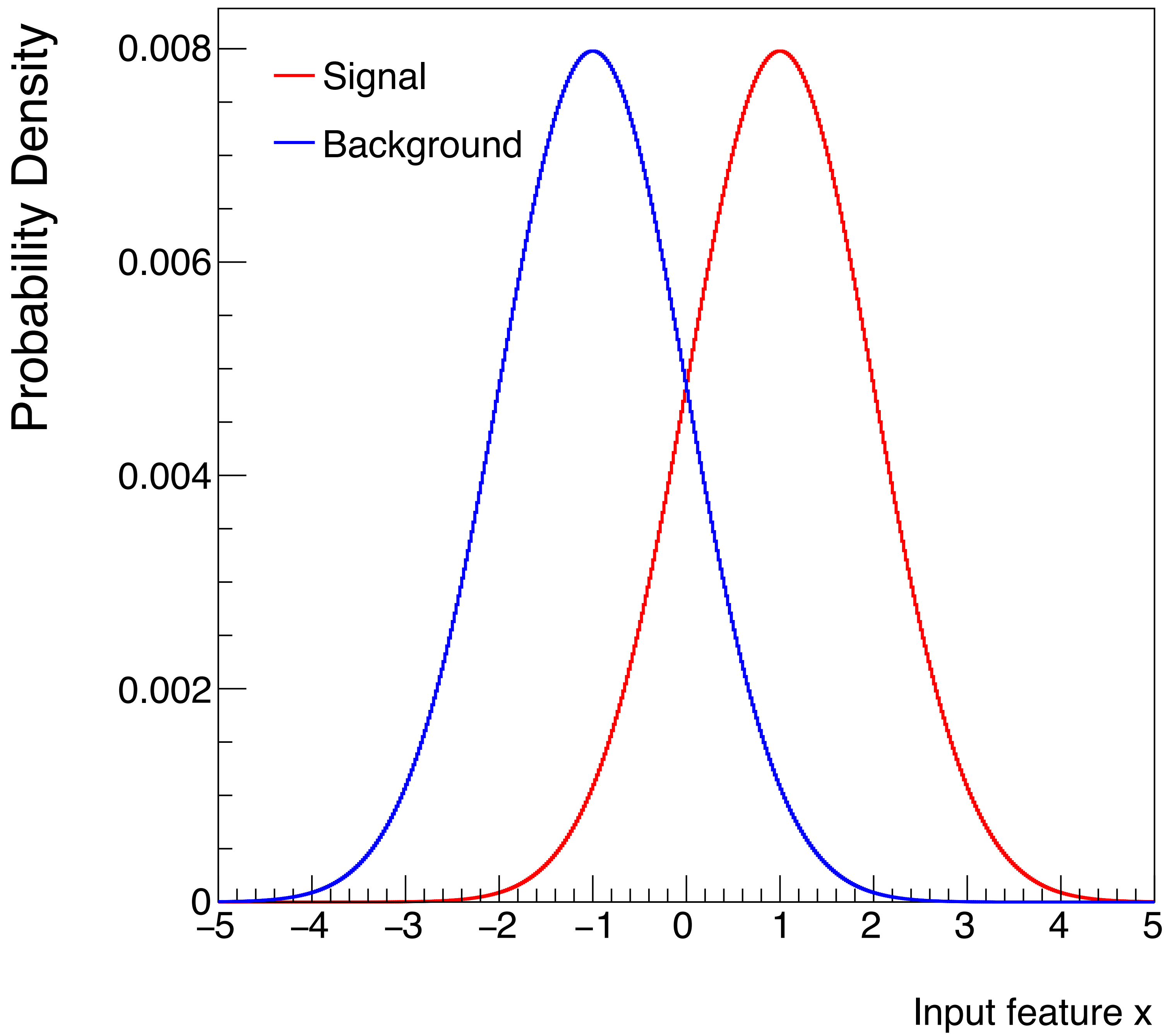
In practice, we don't just want one classifier, but an entire set of classifiers indexed by:

True Positive Rate = signal efficiency = Pr(label signal | signal) = sensitivity

True Negative Rate = 1 - background efficiency = rejection = Pr(label background | background) = specificity

For a given TPR, we want the lowest possible TNR!

Let's consider an important special case: binary classification in 1D



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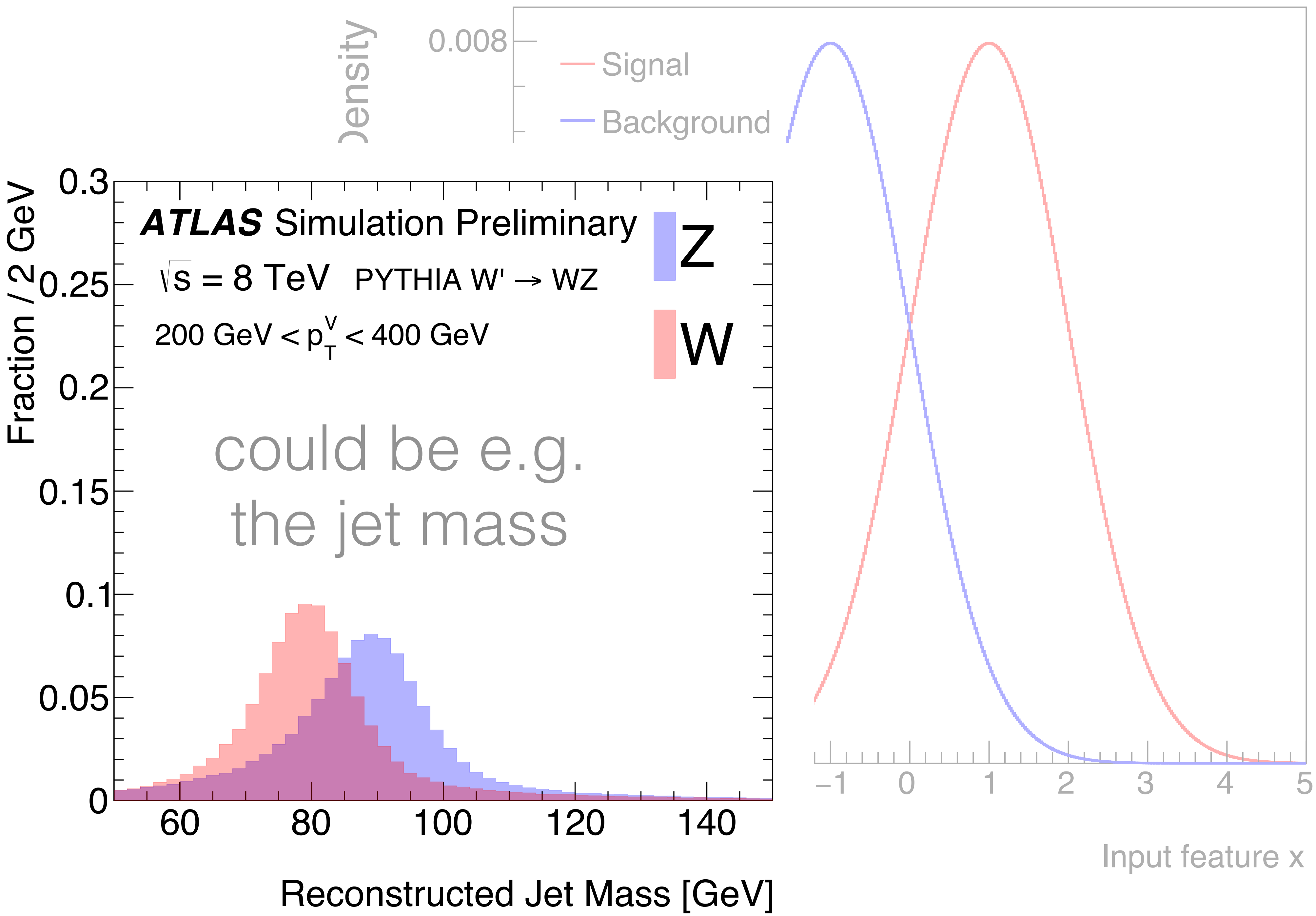

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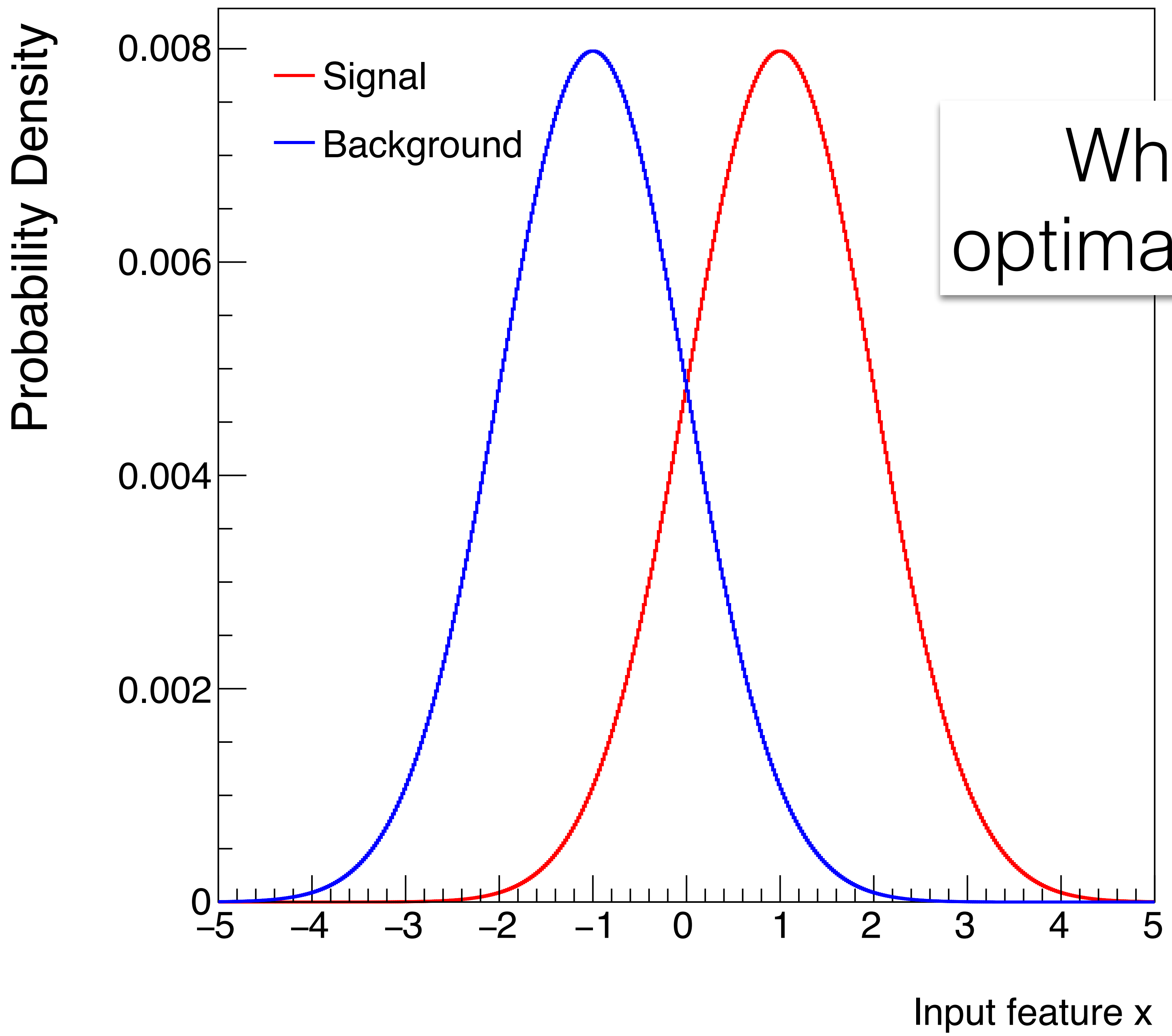
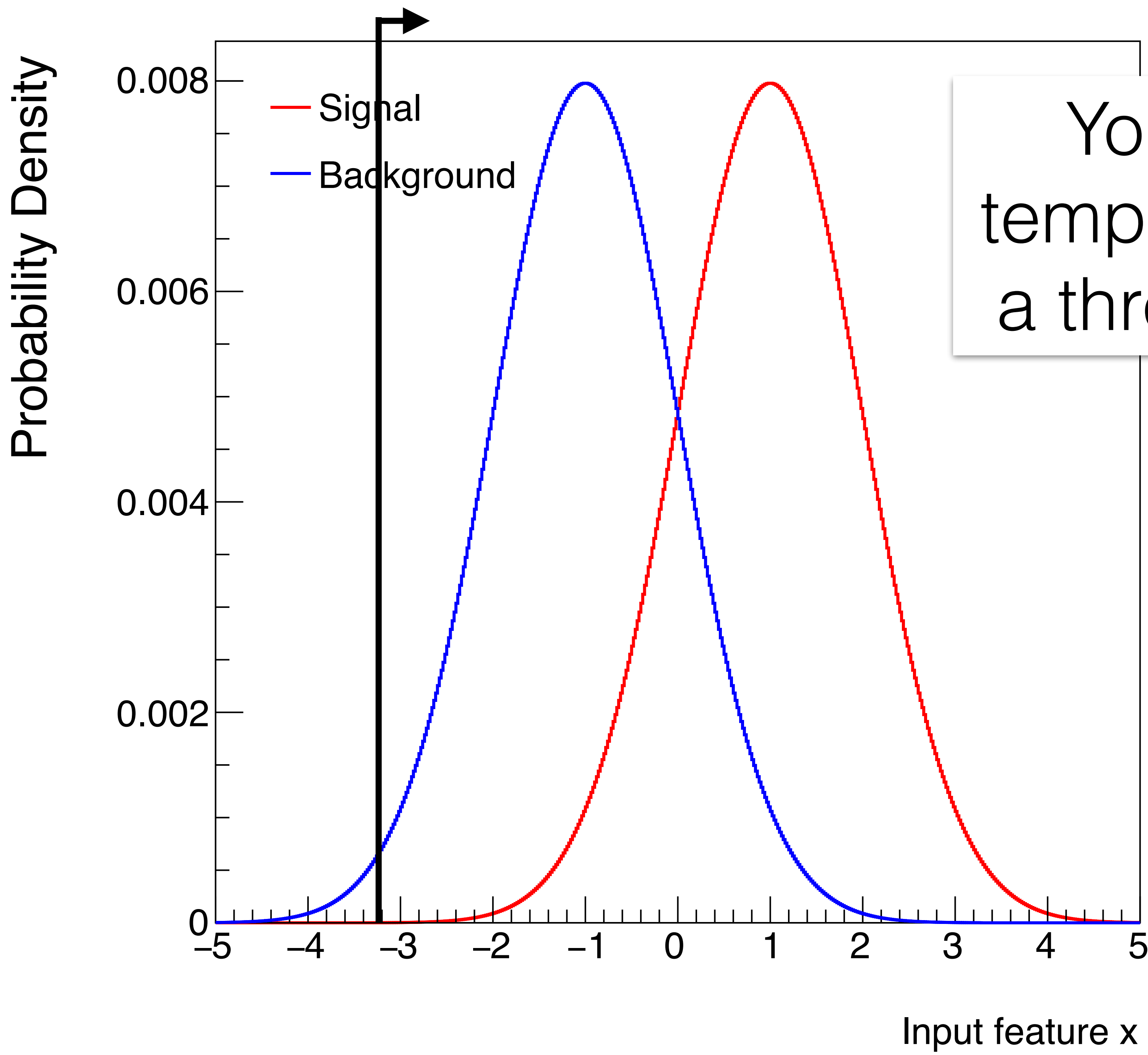


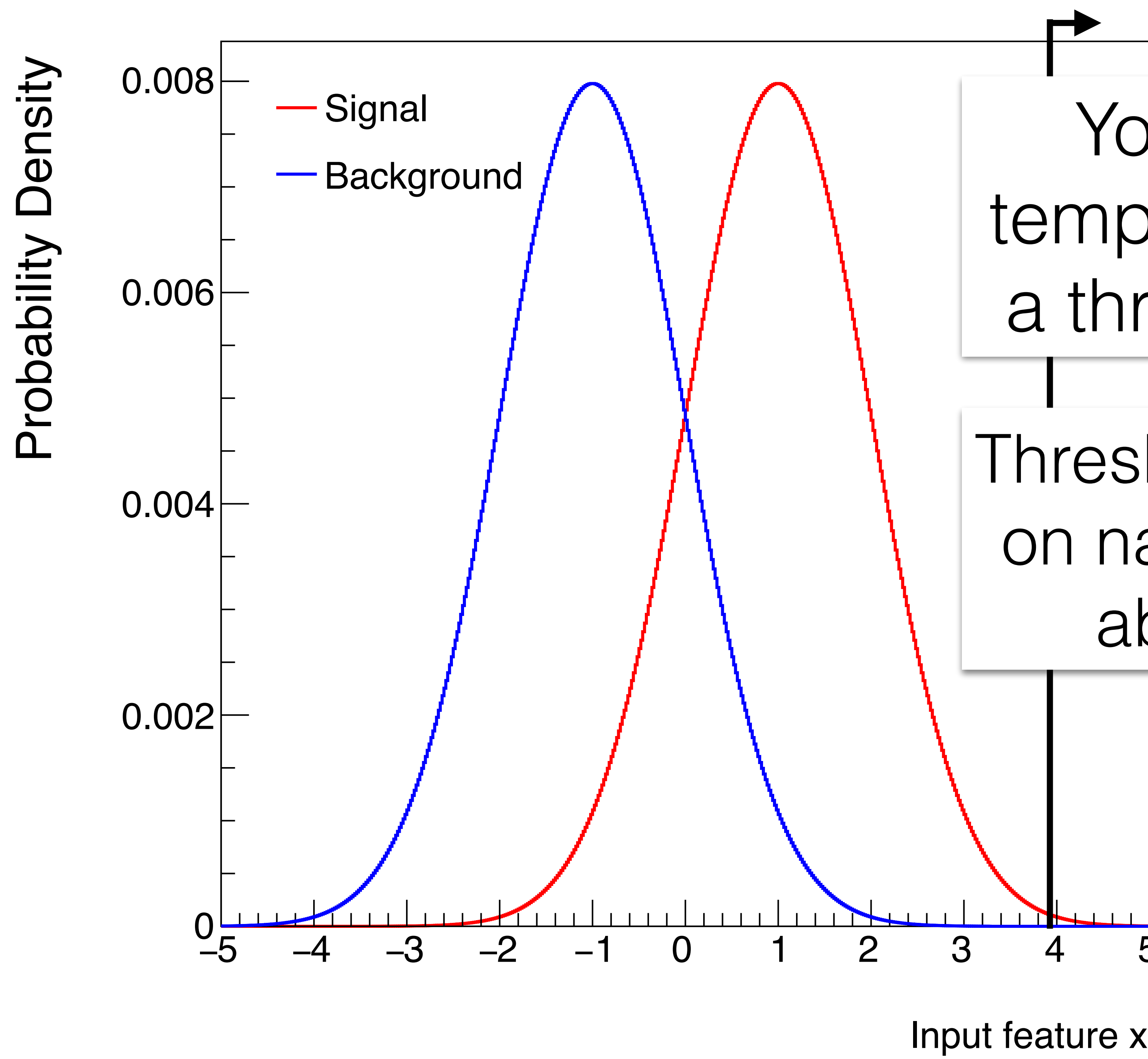
What is the optimal classifier?

Let's consider an important special case: binary classification in 1D



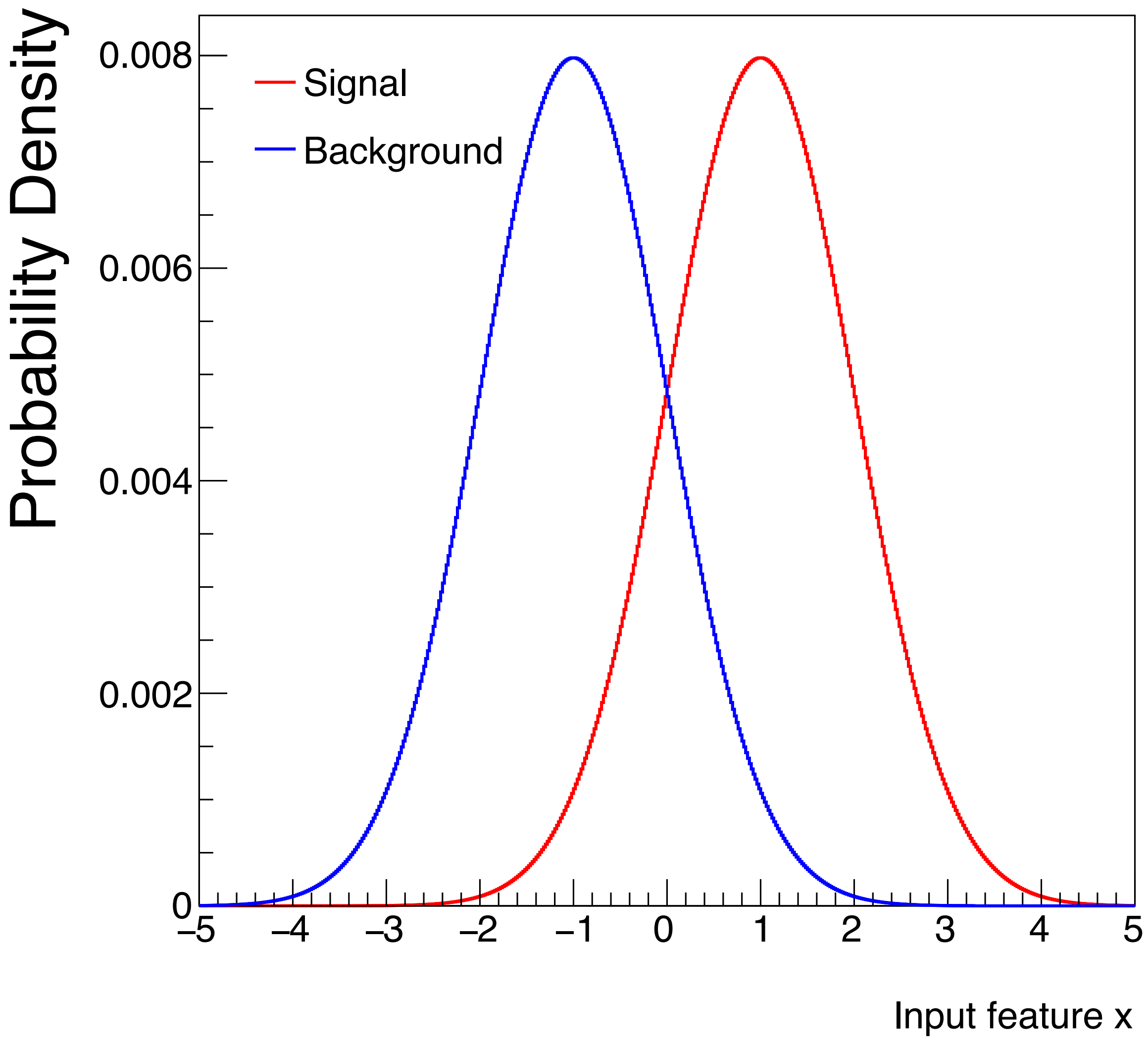
You may be tempted to place a threshold on x

Let's consider an important special case: binary classification in 1D

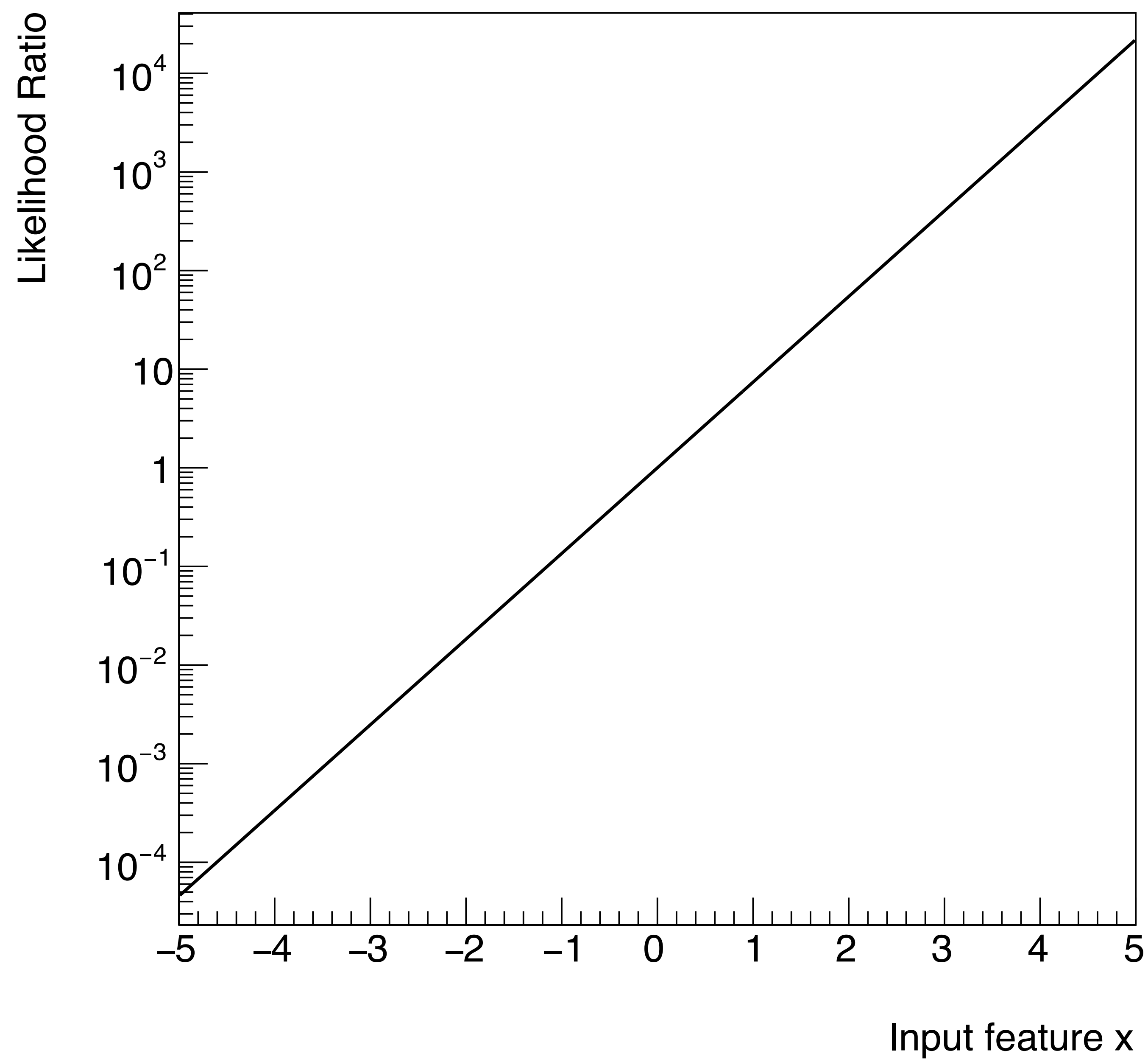


You may be tempted to place a threshold on x

Threshold depends on natural relative abundance

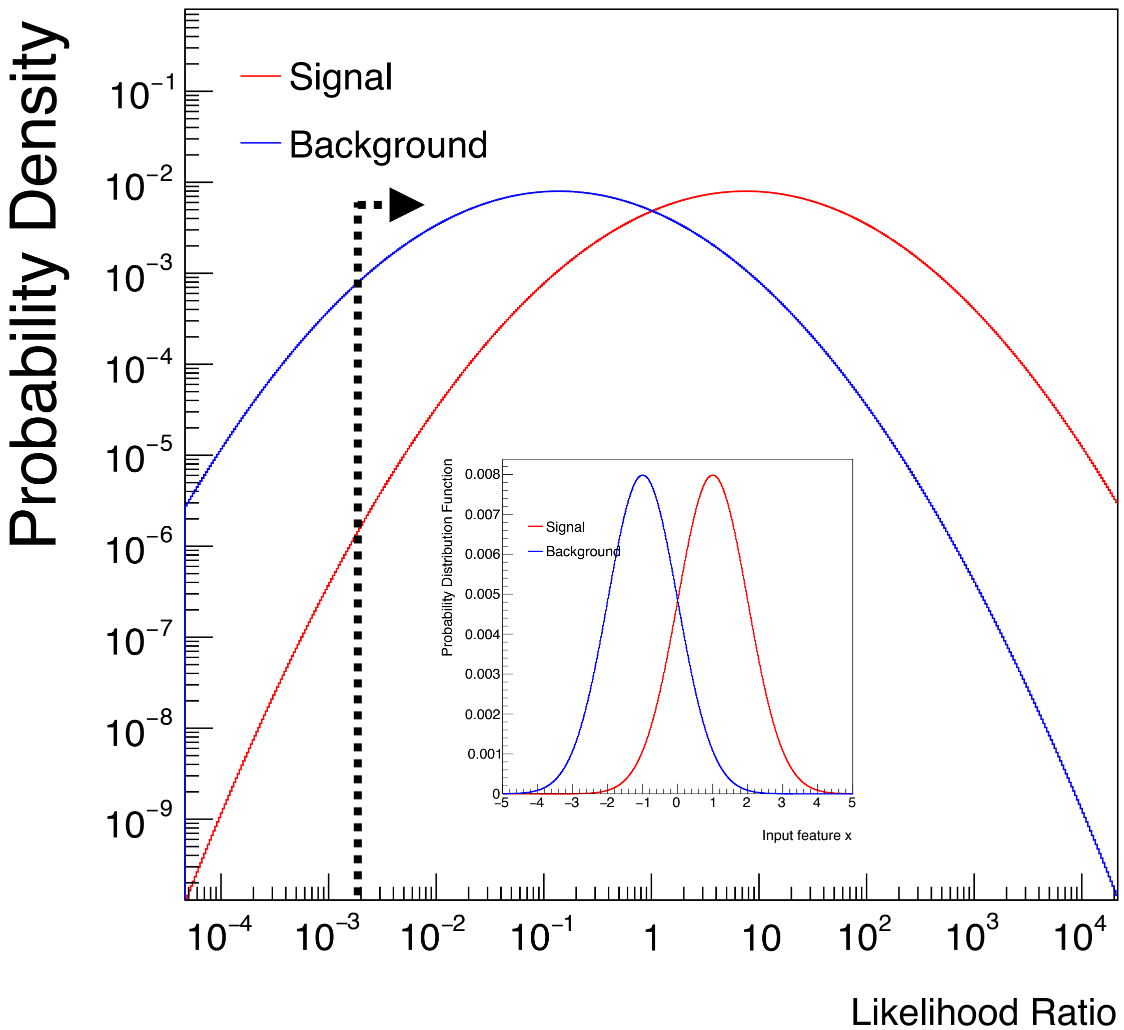


Is the simple threshold cut optimal?

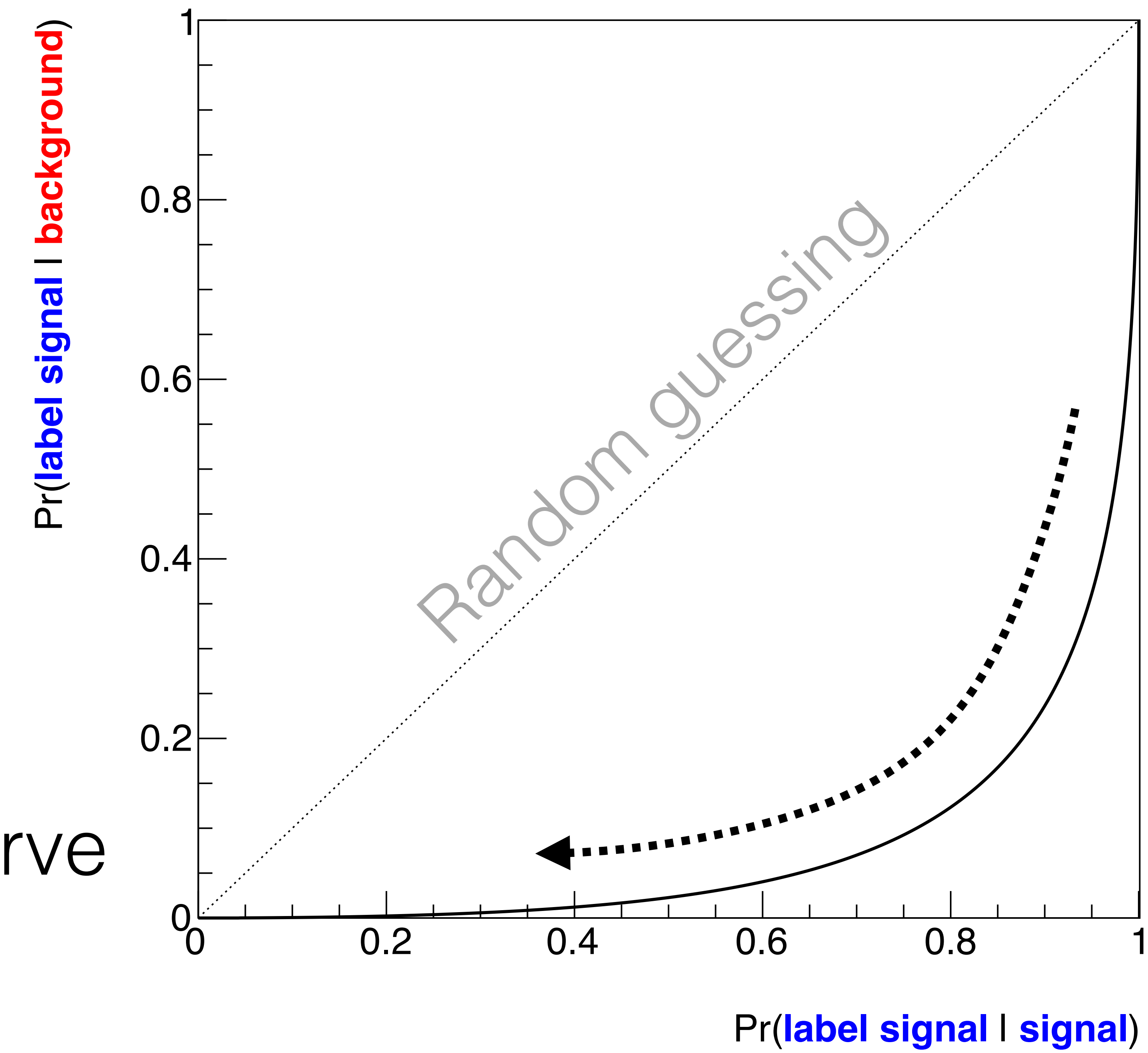


In this simple case, the log LL is proportional to x:
no need for non-linearities!

Threshold cut is optimal



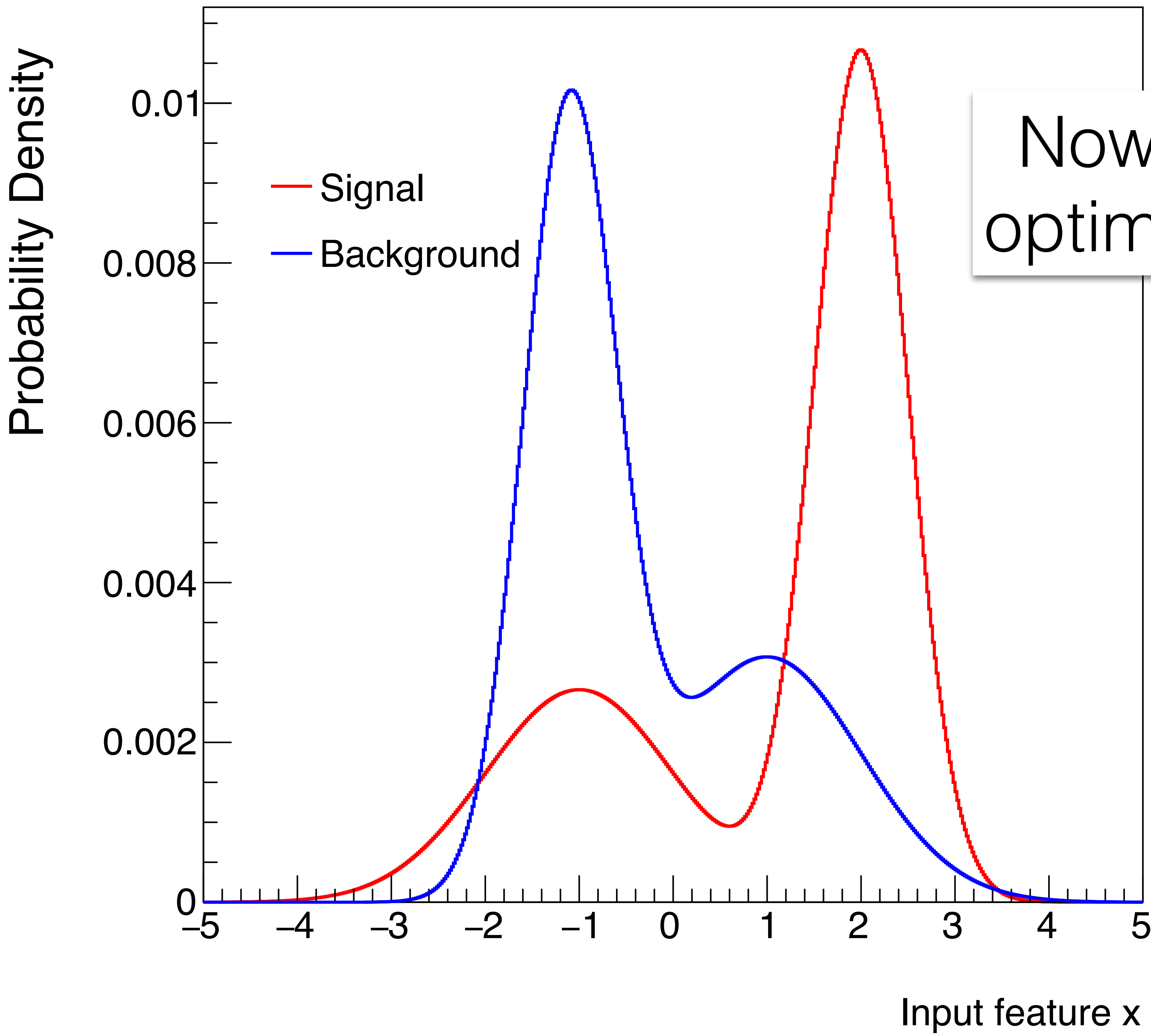
The optimal procedure is a threshold on the LL



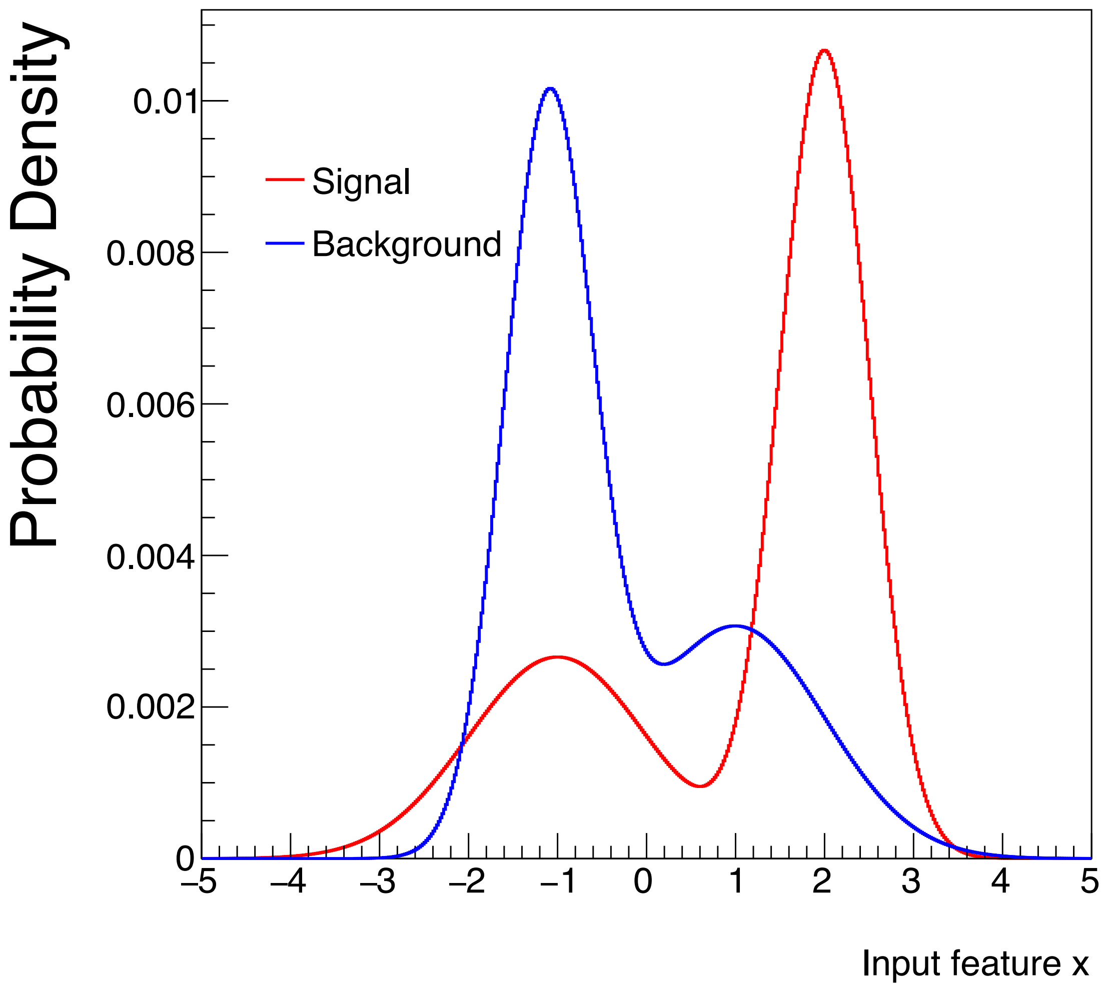
"Receiver Operating Characteristic" (**ROC**) Curve

What if the distribution of x is complicated?

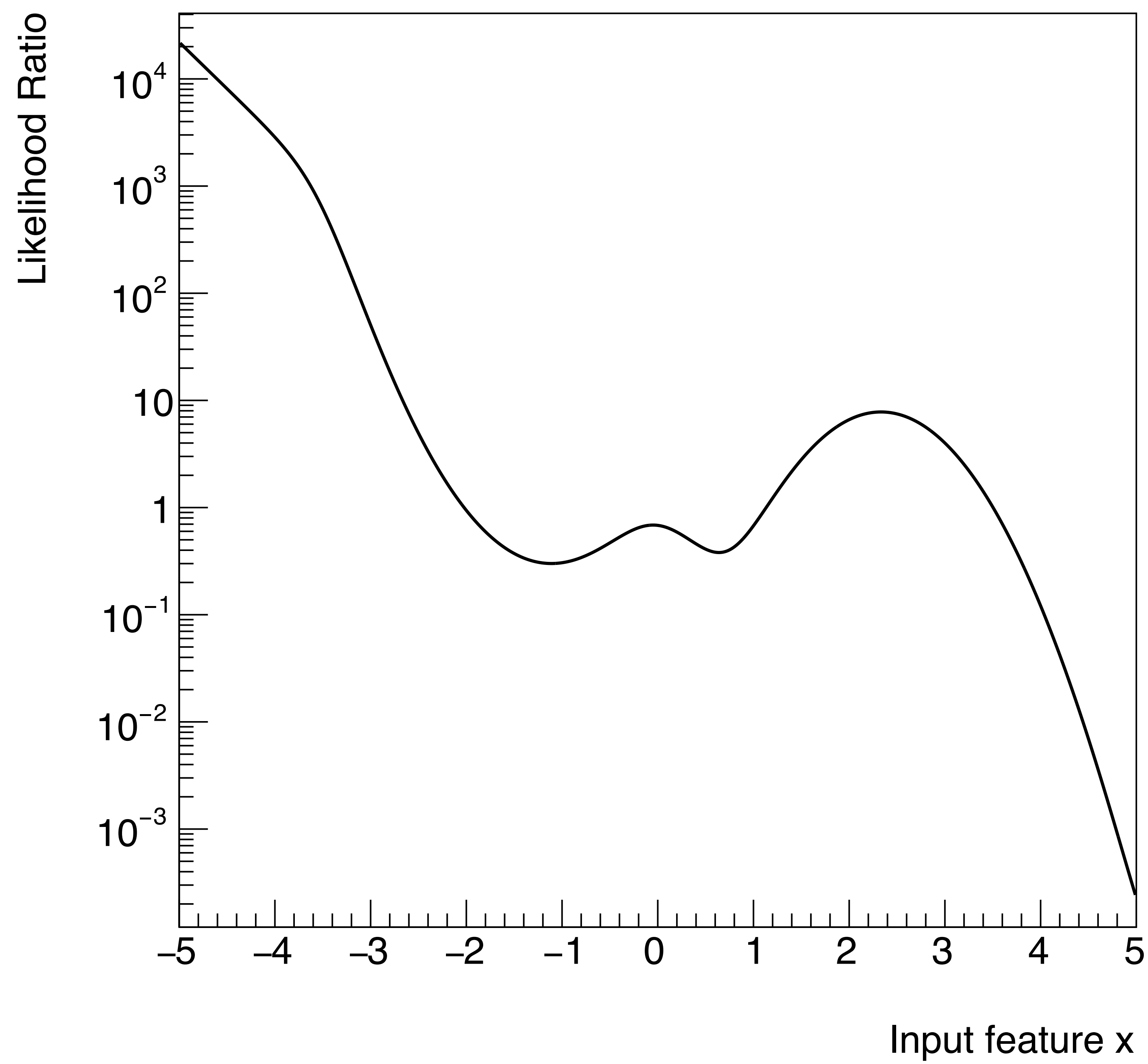
Real life is complicated!



Now what is the optimal classifier?

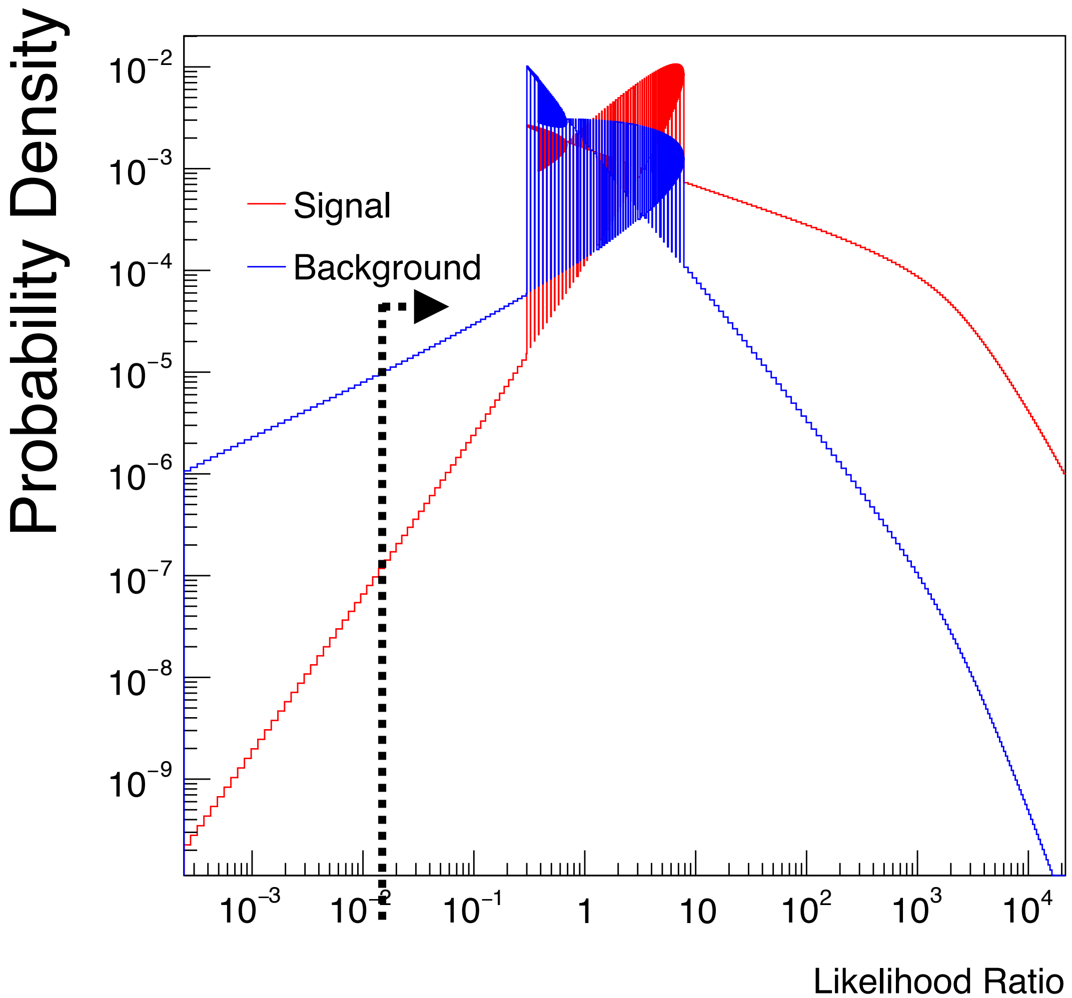


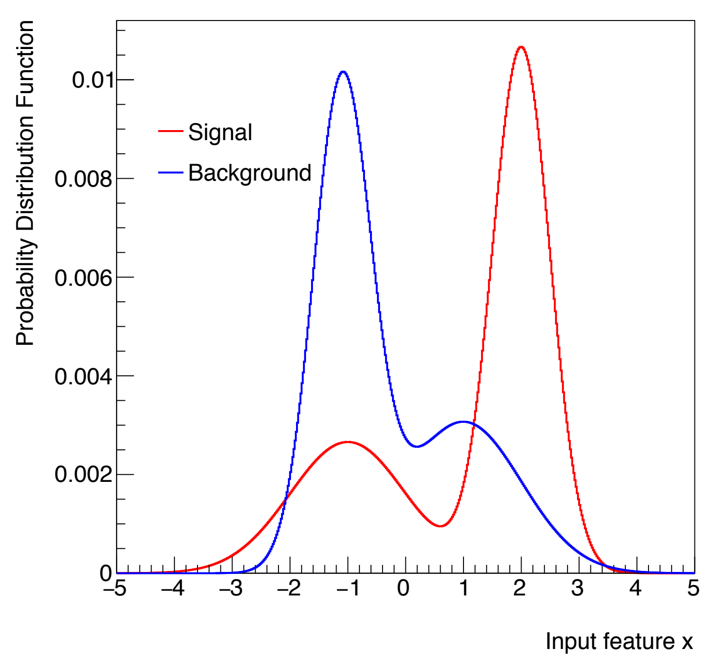
In this case, LL is highly non-linear (**non-monotonic**) function of x

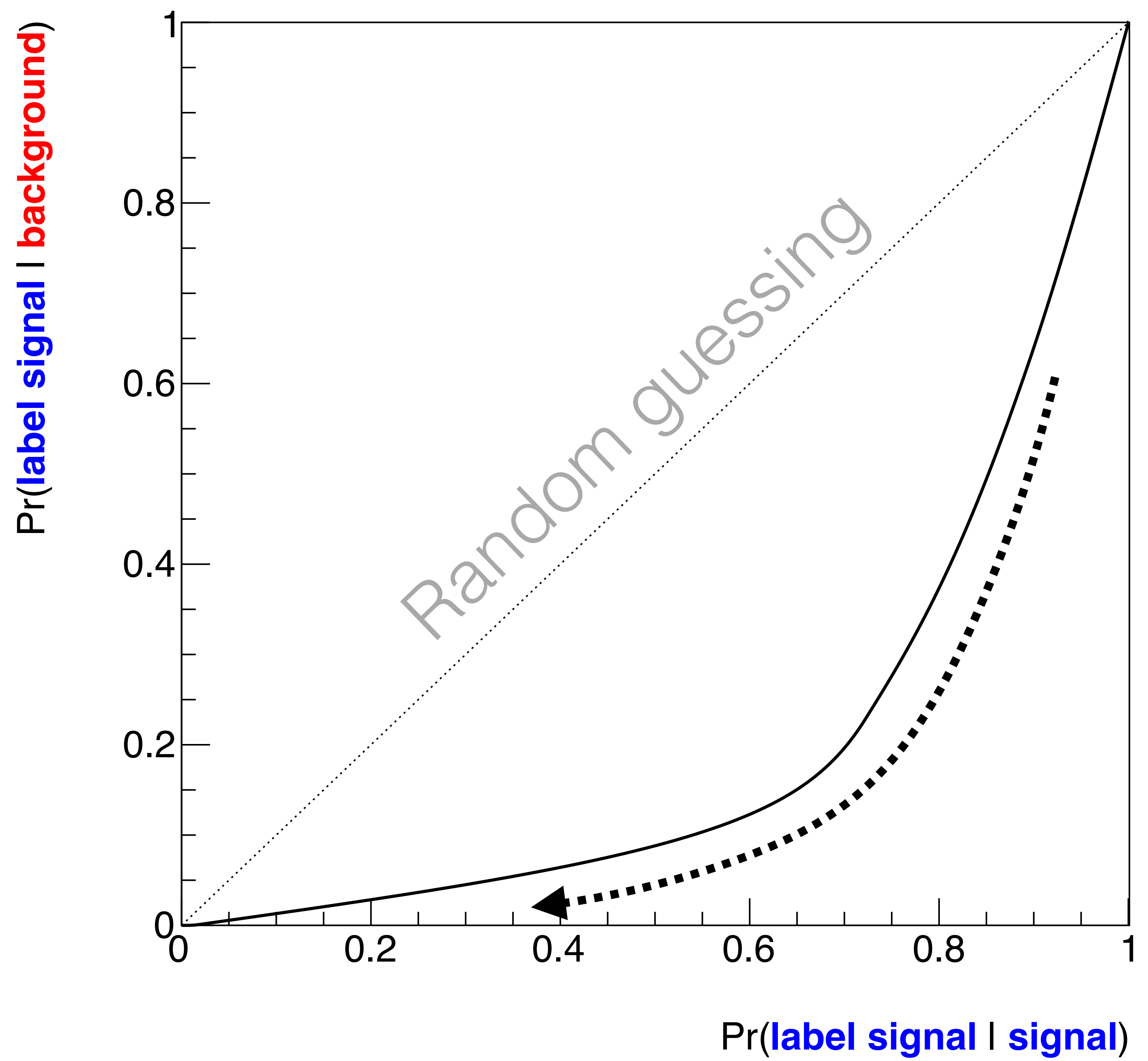


A threshold on x would be sub-optimal

ROC is worse than the Gaussians, but that is expected since the overlap in their PDFs is higher.







Why don’t we always just compute the optimal classifier?

In the last slides, we had to estimate the likelihood ratio - this required binning the PDF

binning works very well in 1D, but becomes quickly intractable as the feature vector dimension >> 1 (“curse of dimensionality”)

machine learning for classification is simply **the art of estimating the likelihood ratio with limited training examples**

Tools for Classification

=tools for likelihood ratio estimation

- "Histograming"
- Nearest Neighbors
- Support Vector Machines (SVM)
- (Boosted) Decision Trees
- (Deep) Neural Networks
- …

Not widely used; only useful if decision boundary is 'simple'

has most things and ROOT-compatible but the community base is **much** smaller than the other ones

Software: TMVA, scikit-learn, keras, …

does "everything" exempt DNNs

python interface to DNN tools TensorFlow, Theano, CNTK

Data formats: .root, .npy, .hdf5

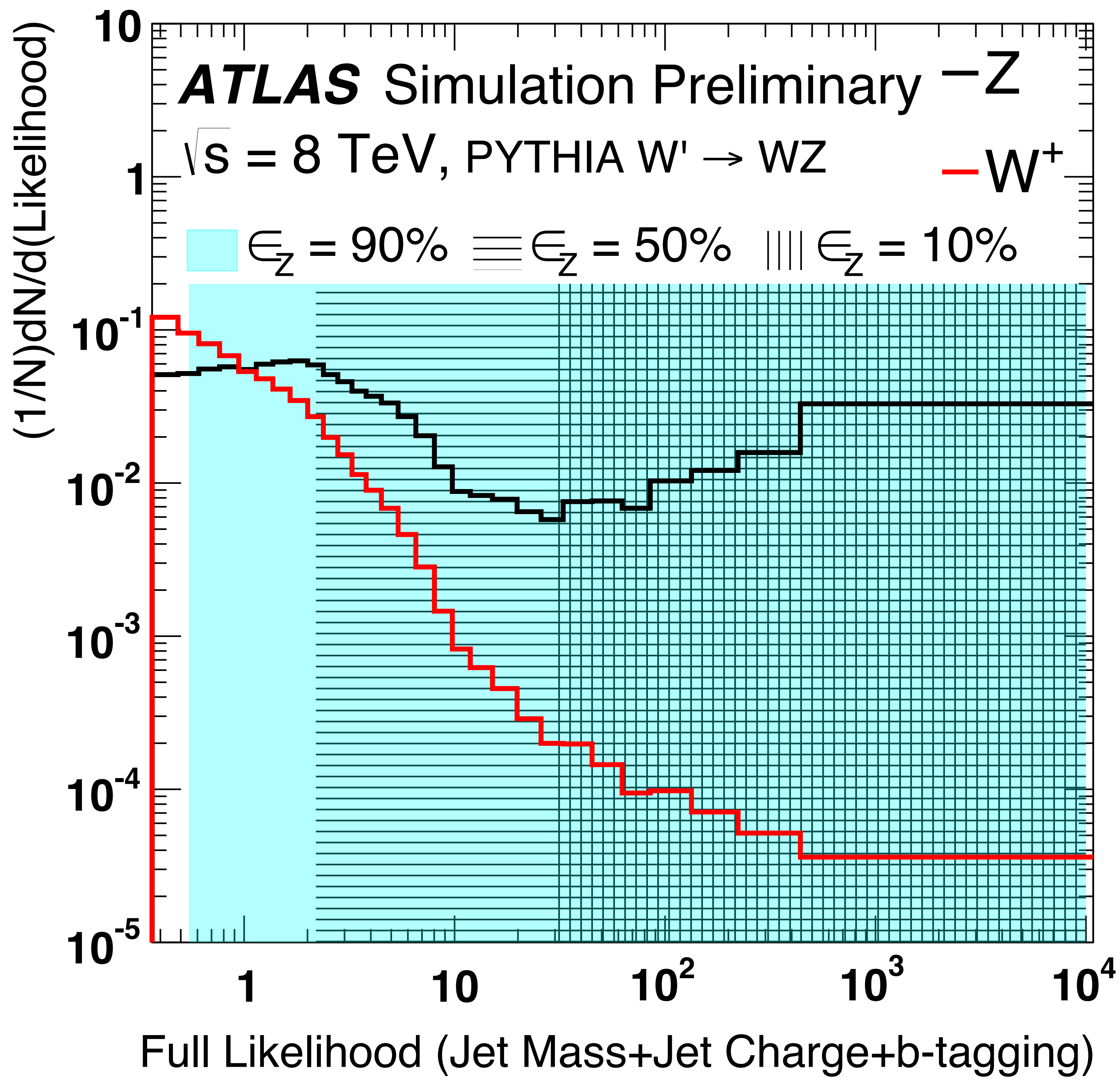
Histograming

If you have a 1D problem, look no further!

If your problem can be decomposed into a product/sum of 1D problems…look no further!

If these do not apply… look elsewhere.

Eur. Phys. J. C76 (2016) 238



$$p(M, Q, B|V) = \sum_{\mathcal{F}} \Pr(\mathcal{F}|V)p(M|\mathcal{F}, V)p(Q|\mathcal{F}, V)\Pr(B|\mathcal{F}, V),$$

Nearest Neighbors

In 2D, a nice extension of histogramming is to estimate the likelihood ratio based on the number of S and B points nearby.

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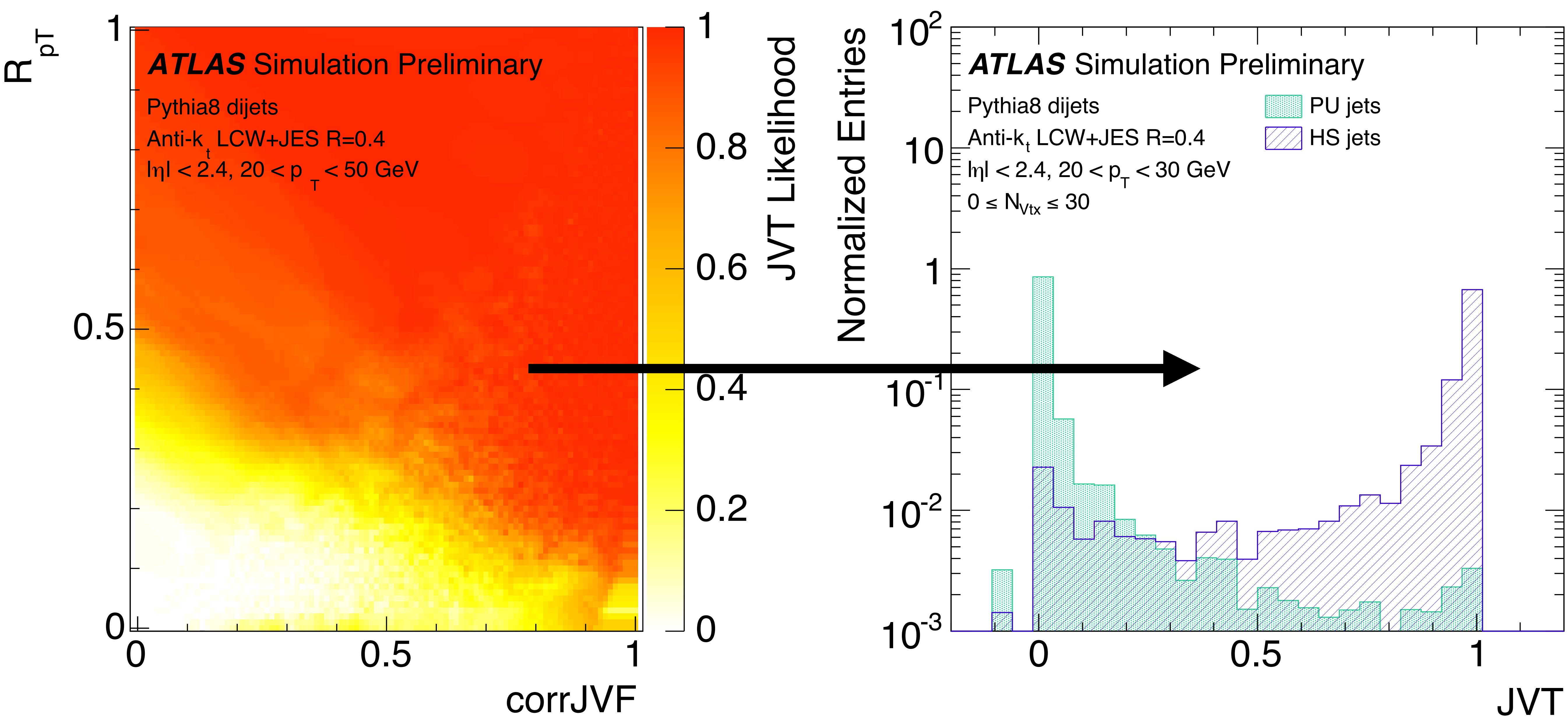
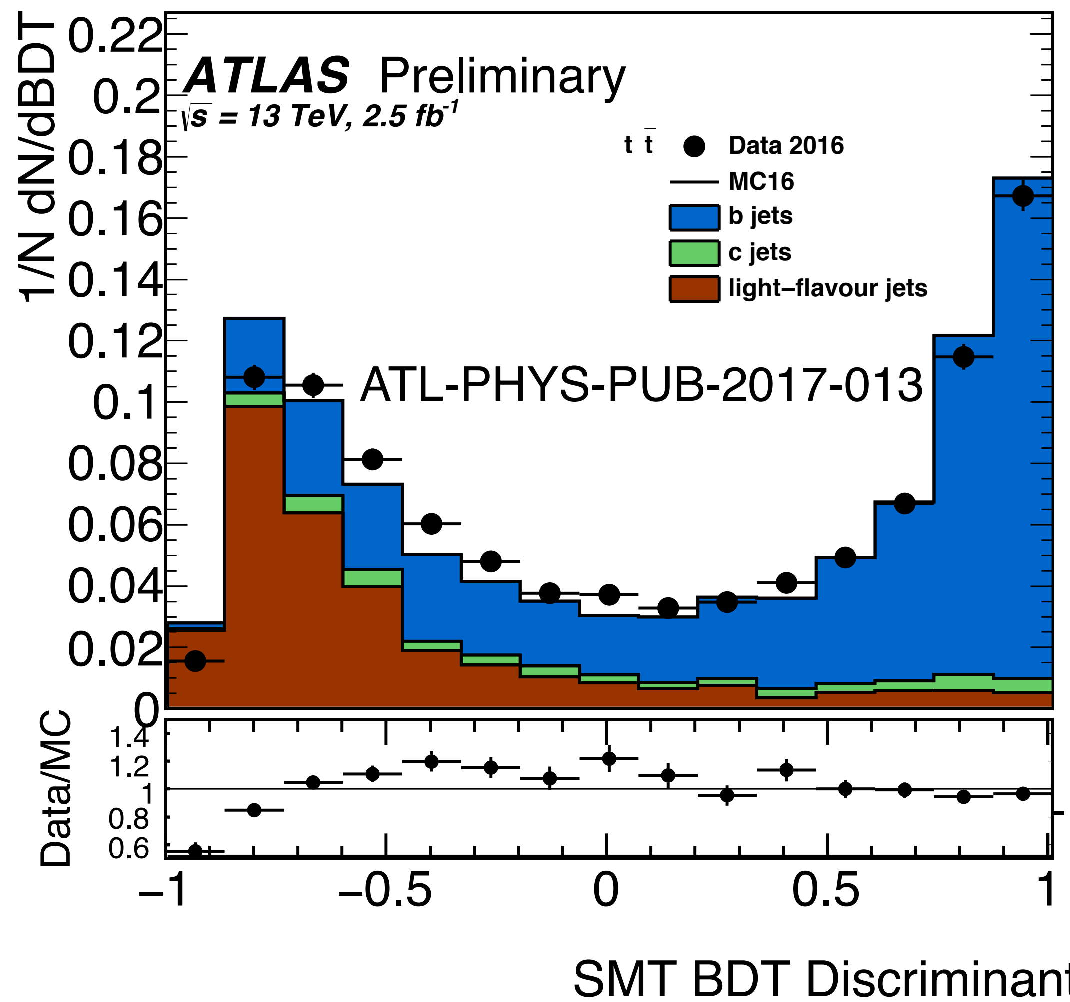


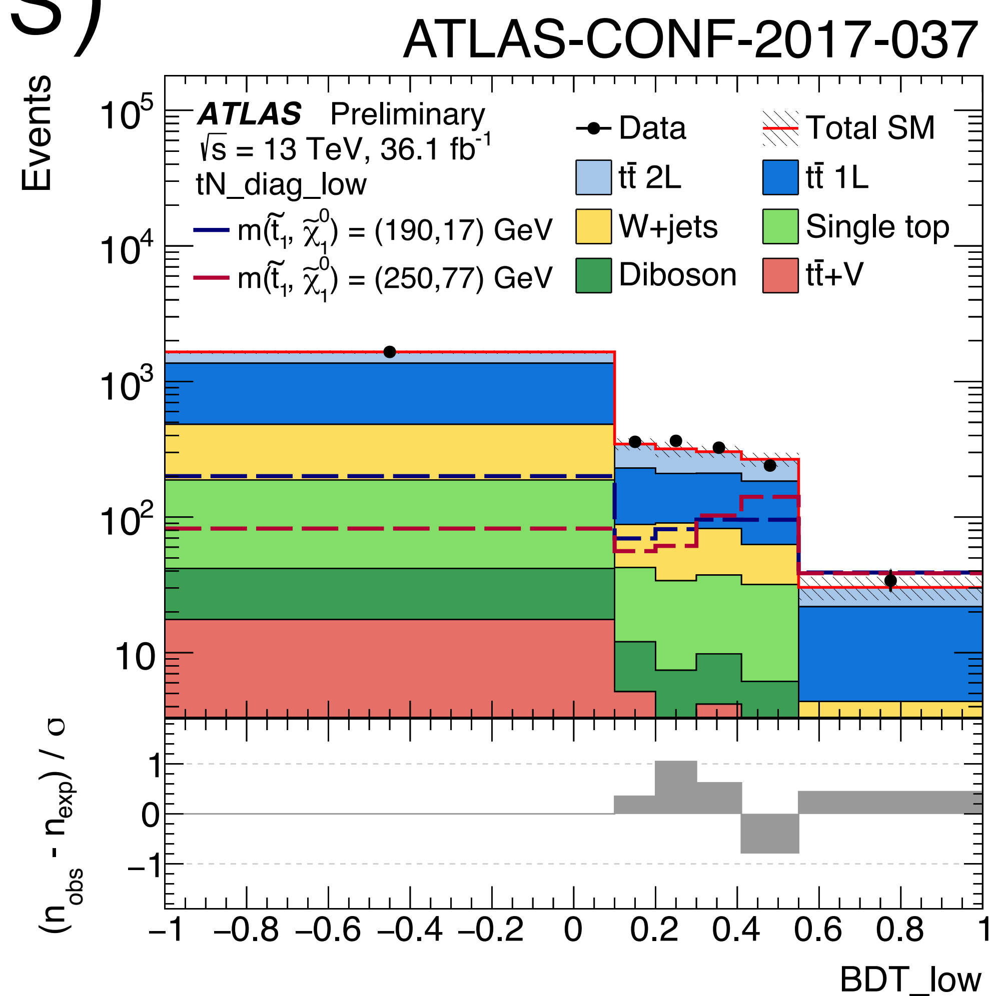
Boosted Decision Trees (BDTs)

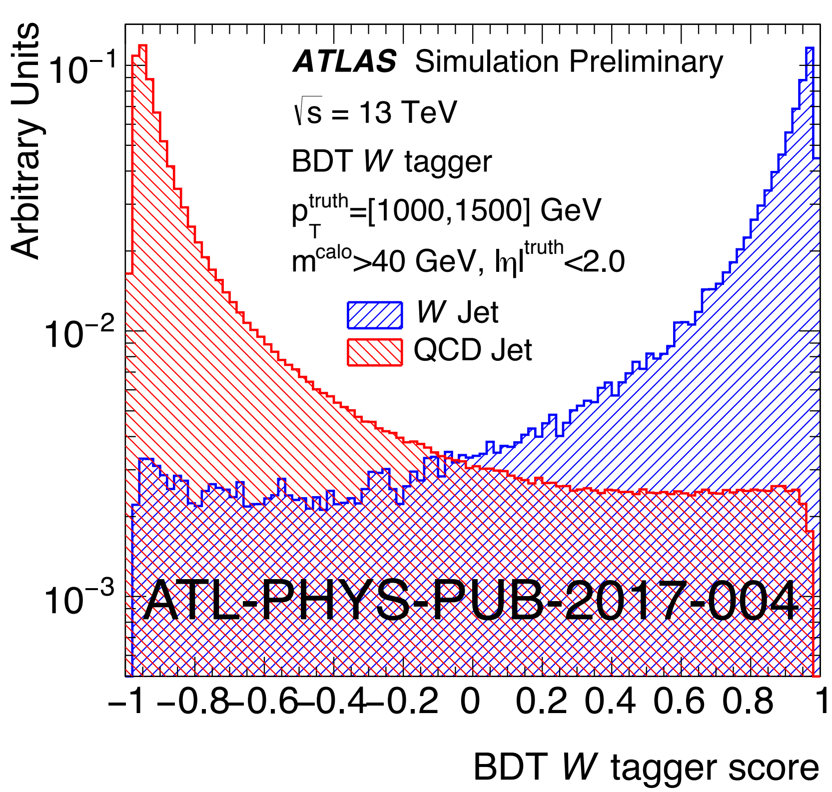


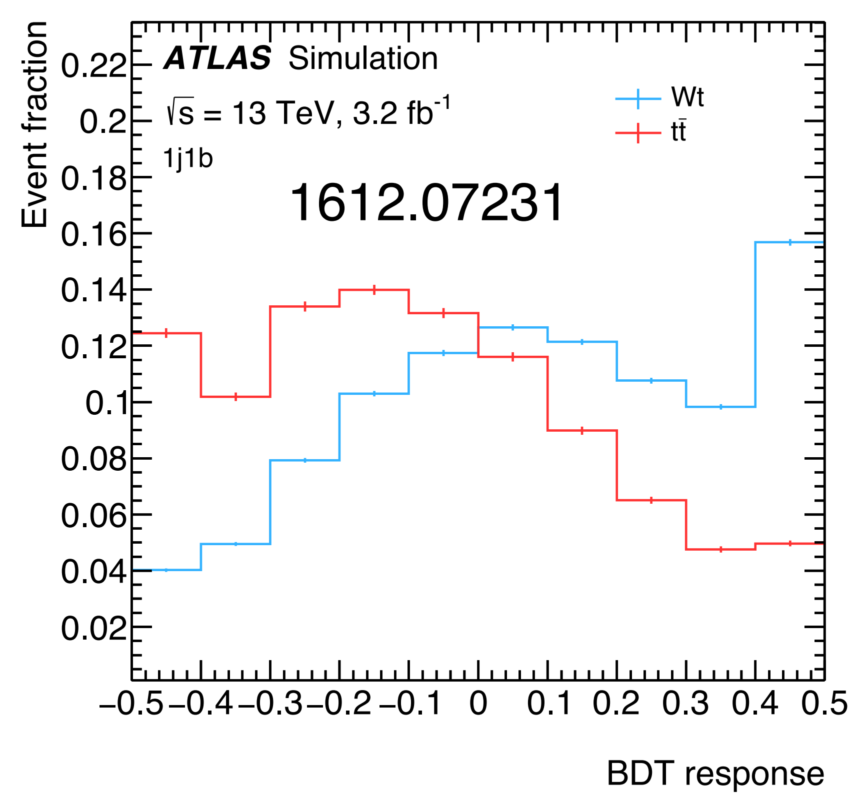
We love BDTs.

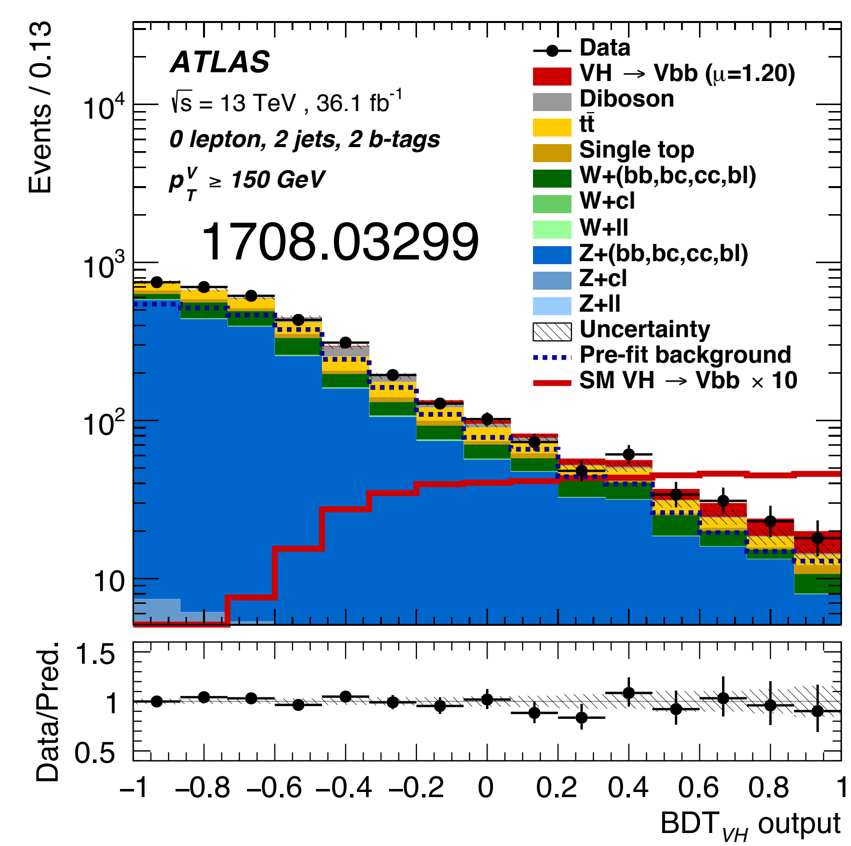
If 3 < dim(feature vector) < O(100)

this is probably right for you!



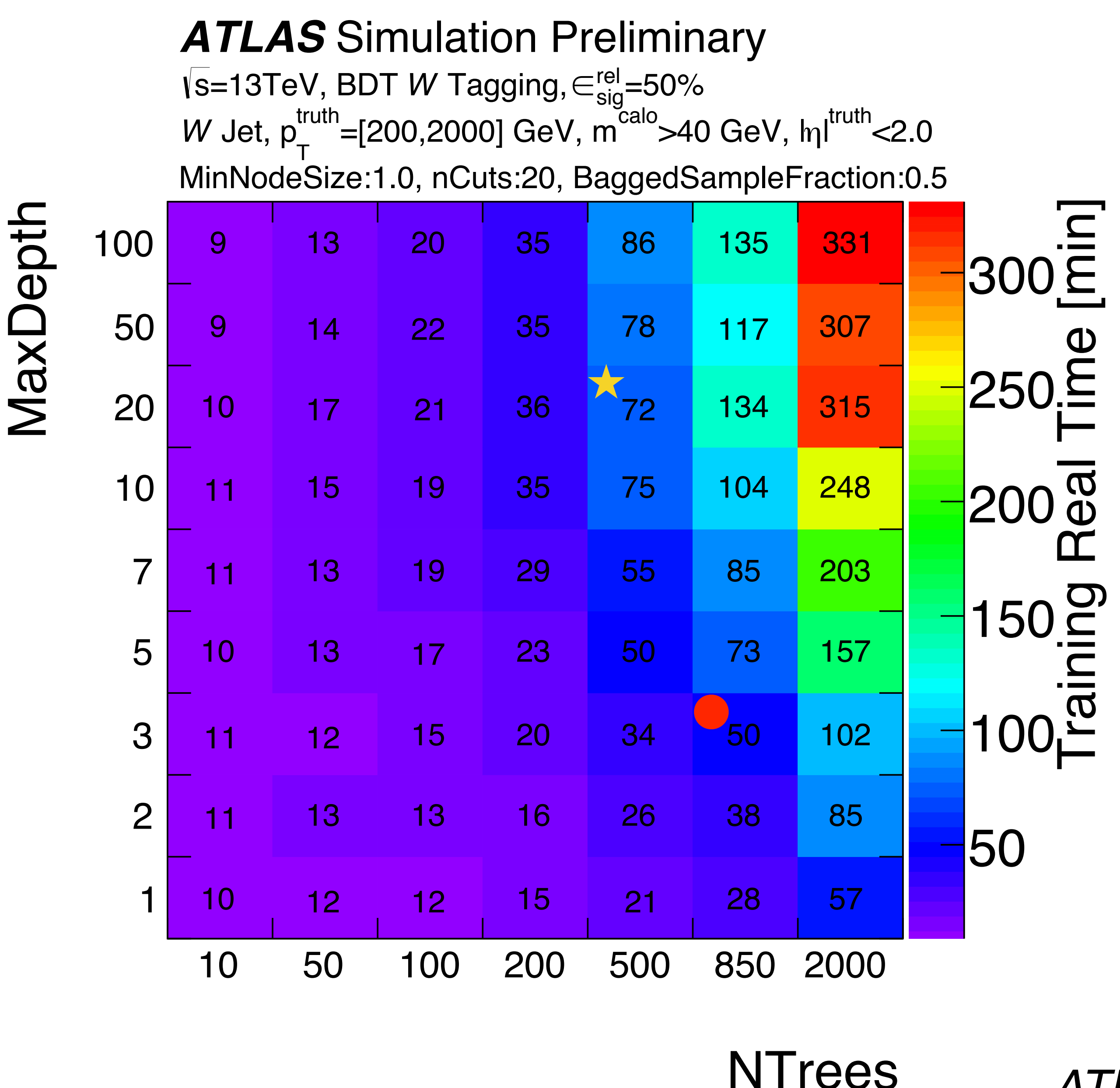


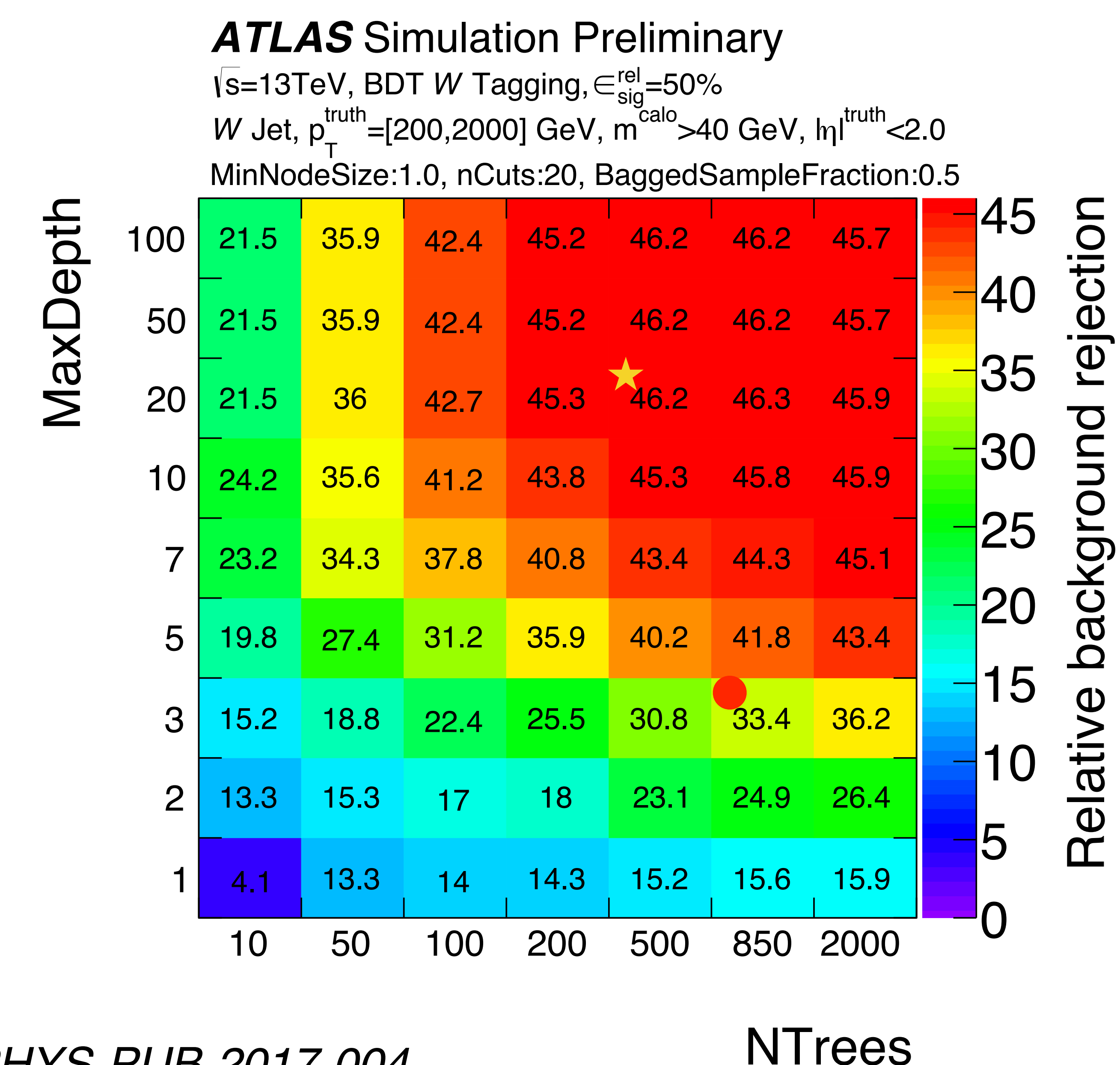




Boosted Decision Trees (BDTs)

We love BDTs because they are fast to train
and do not have very many parameters.
They are also rather robust to *overtraining*.





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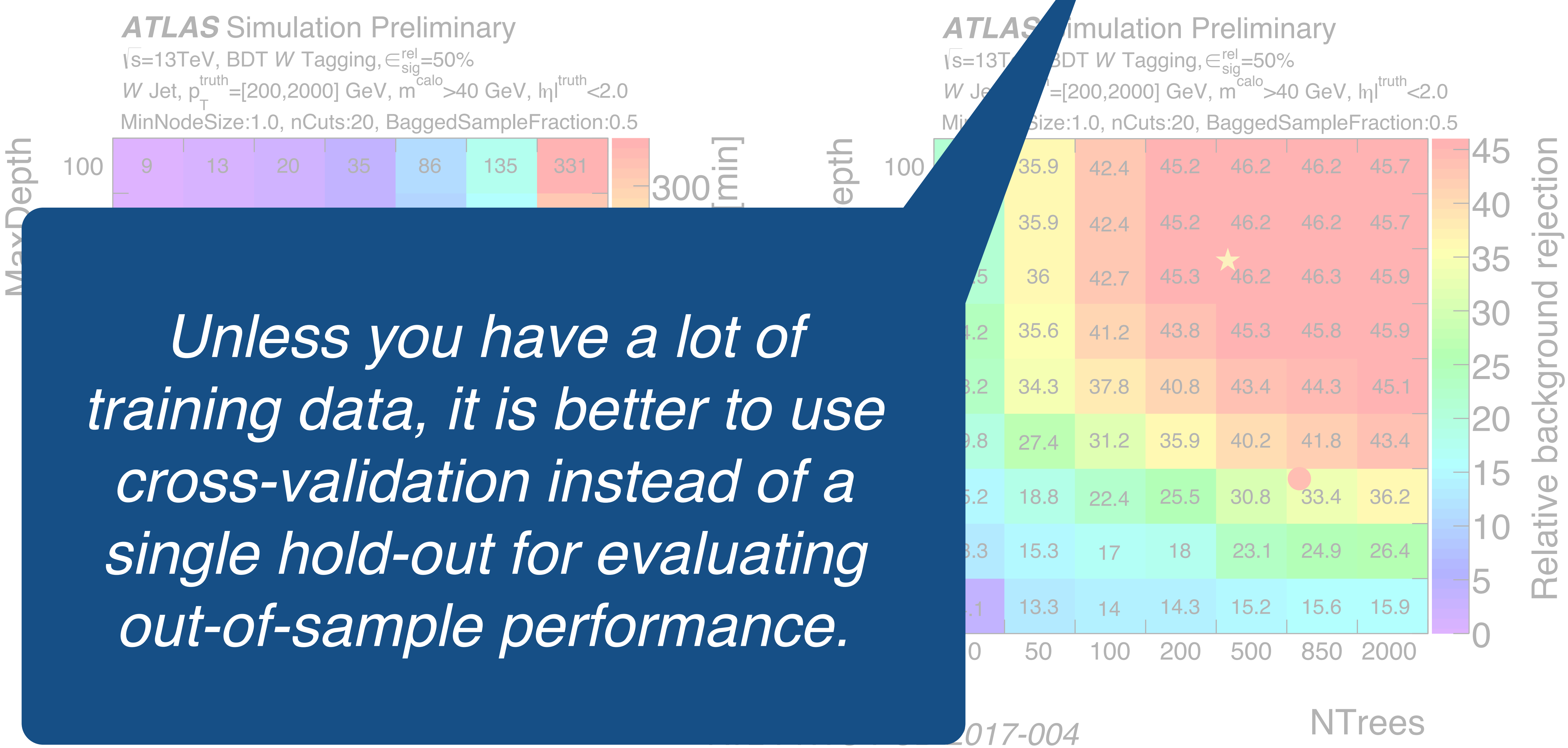
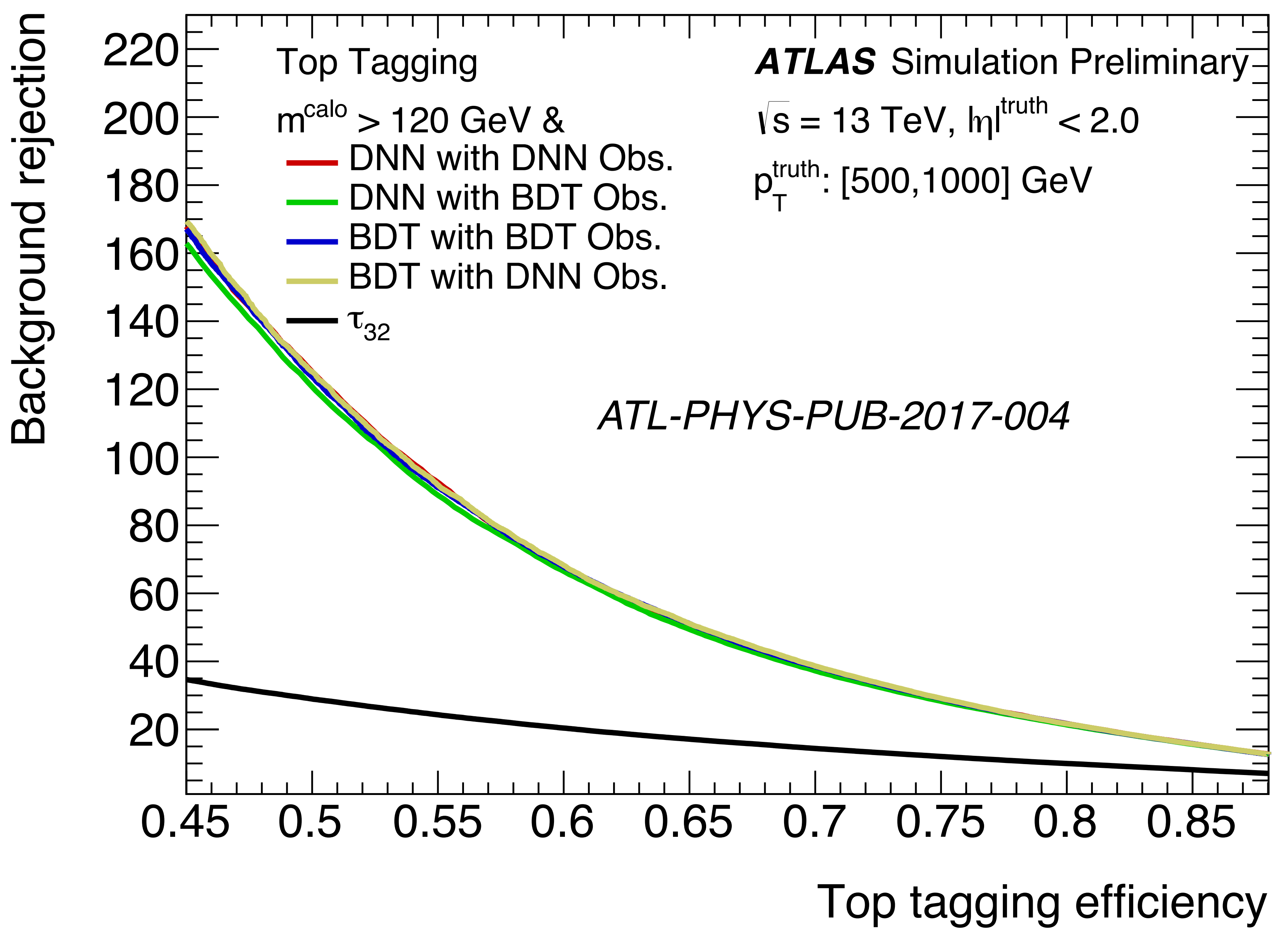


Unless you have a lot of training data, it is better to use cross-validation instead of a single hold-out for evaluating out-of-sample performance.

Boosted Decision Trees (BDTs)

There is really not a good reason to use a DNN with << O(100) dimensions.

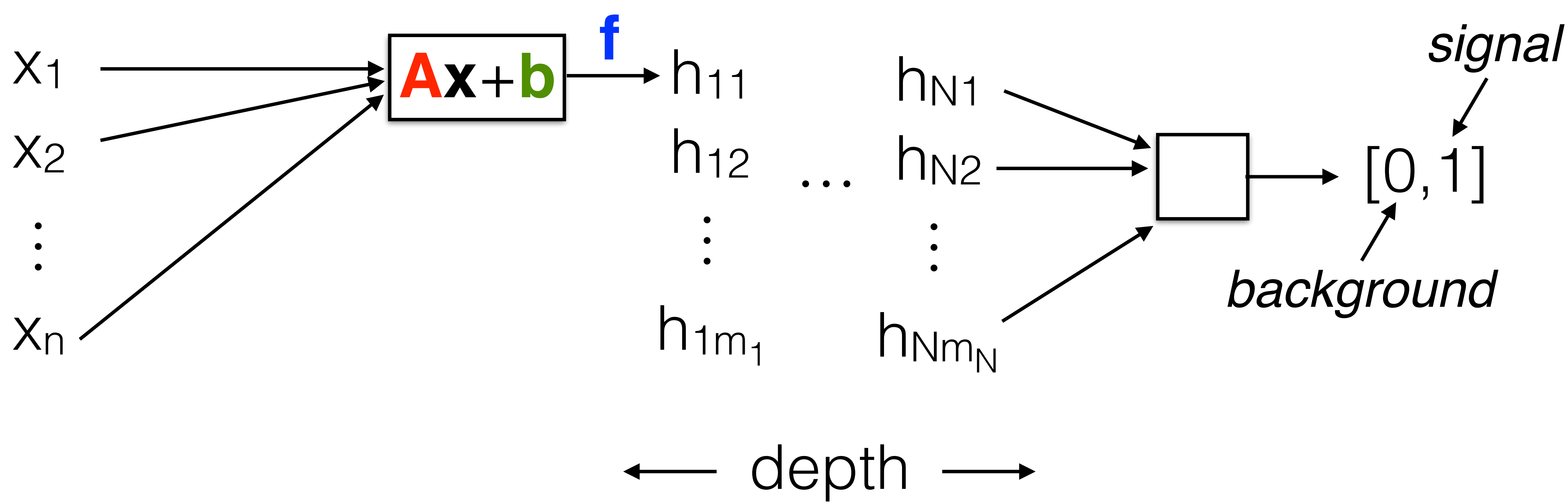


However, they are becoming increasingly easy to train …

Modern Deep NN's for Classification

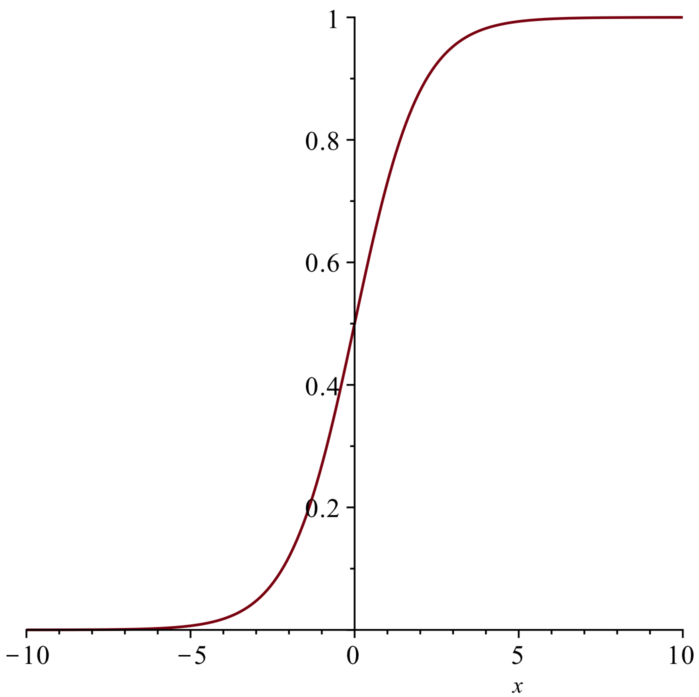
Neural Network: composition of functions $\mathbf{f}(\mathbf{A}\mathbf{x}+\mathbf{b})$ for inputs $\mathbf{x}$ (features) matrix $\mathbf{A}$ (weights), bias $\mathbf{b}$, non-linearity $\mathbf{f}$.

N.B. I'm not mentioning biology - there may be a vague resemblance to parts of the brain, but that is not what modern NN's are about.



Fact: NN's can approximate "any" function.

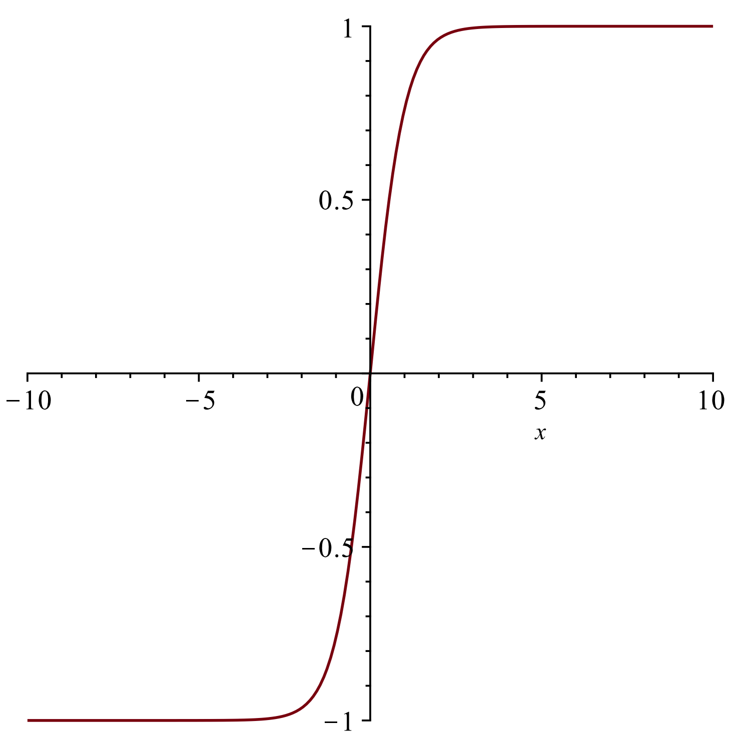
Choosing the non-linearity (activation function) f



Logistic (aka Sigmoid): one of the most widely-used functions in the past, no basically only used for the last layer.

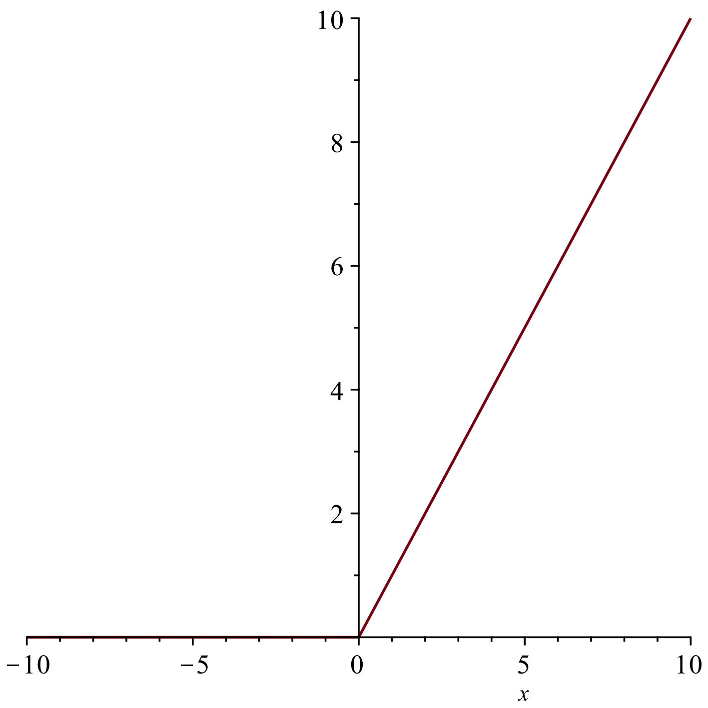
generalization to multi-dimensional input: softmax

$$\mathbf{f}(\vec{x}) = e^{x_i} / \sum_i e^{x_i}$$



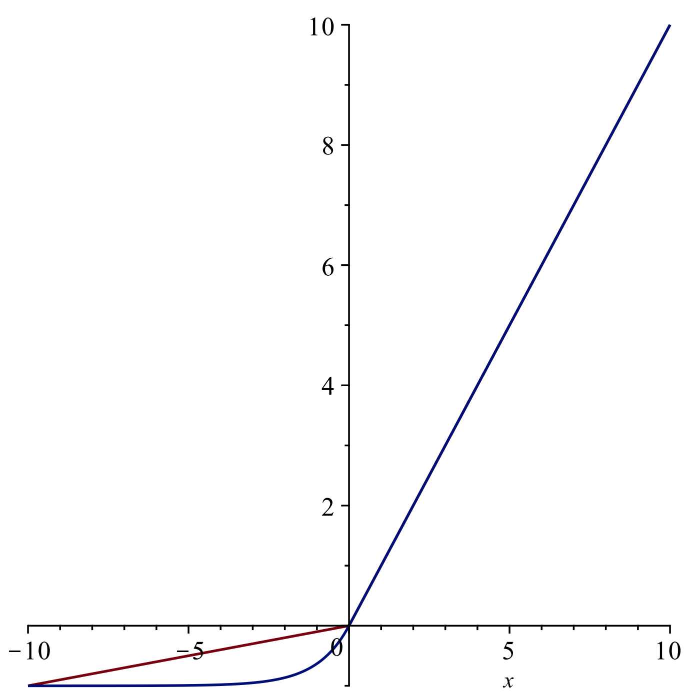
tanh: similar story to sigmoid.

Choosing the non-linearity (activation function) **f**



Rectified Linear Unit **ReLU**: one of the most widely-used functions now.

do not suffer from the vanishing gradient problem



Leaky ReLU / Exponential LU (ELU): variations on the ReLU that are popular.

Functions that act on multiple nodes in one layer

MaxOut: Take the maximum of multiple inputs

reduces the dimensionality of a hidden layer

DropOut: Randomly remove (for one forward/backward pass) nodes from a layer.

helps with over-training

(D)NN Training

Training proceeds by minimizing a loss function.

Typical loss functions

Squared error: $$(y_i - \hat{y}_i)^2$$

Cross-entropy: $$\underbrace{-y_i}_{\text{True label (0 or 1)}} \log(\underbrace{\hat{y}_i}_{\text{NN output}}) - (1 - y_i)\log(1 - \hat{y}_i)$$

(D)NN Training

Objective function is minimized using stochastic gradient decent (almost exclusively with the Adam algorithm)

Stochastic gradient decent: Using single (or multiple "mini-batches") examples, weights are updated:

$$A_{ij} \mapsto A_{ij} - \eta \nabla_{ij} \mathcal{L}$$

learning rate

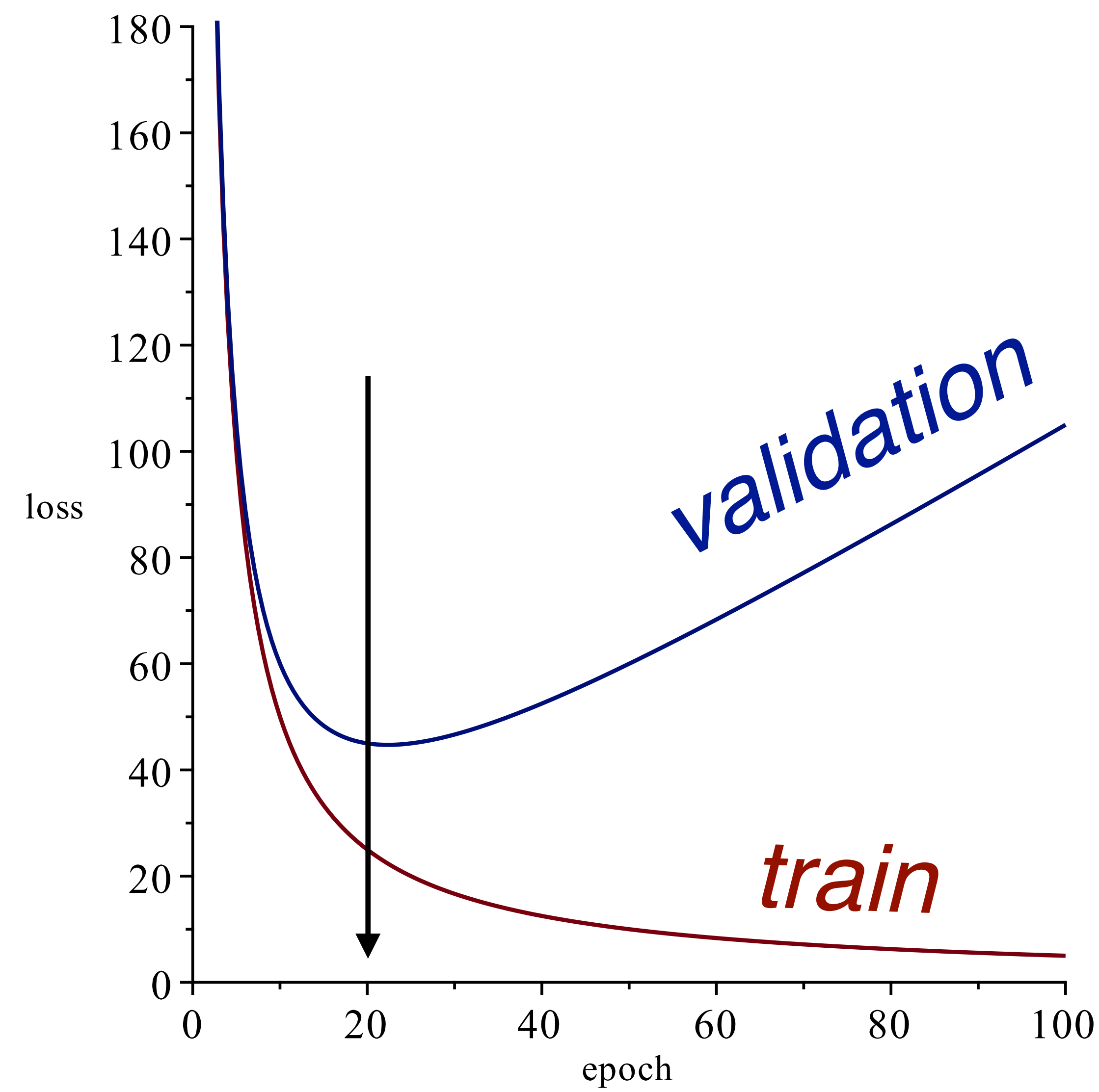
back-propagation: weights updated backwards and gradients are recycled.

N.B. a NN can do better than random **before any training**! For instance, if you initialize all the weights to 1 and the signal has generally higher values then the NN will beat random.

(D)NN Training

Training proceeds multiple times (epochs), reshuffling the data.

Early stopping: stop at the epoch where the validation error starts to increase



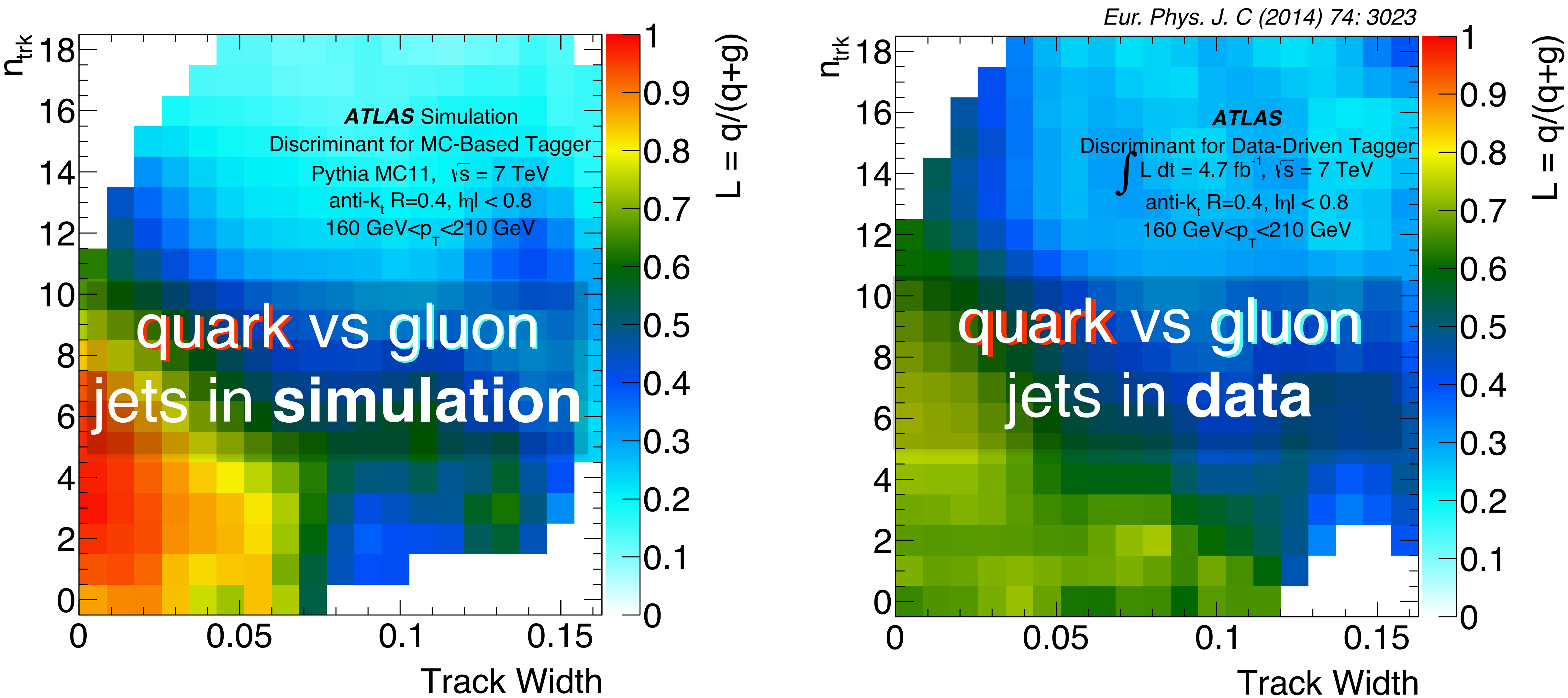
In the tutorials today, you will get a chance to apply these concepts in practice.

Before closing, I'll leave you with one last concept: semi-supervised learning.

unsupervised	semi-supervised	supervised
nothing	e.g. class proportions	everything

how much you know about per-example labels

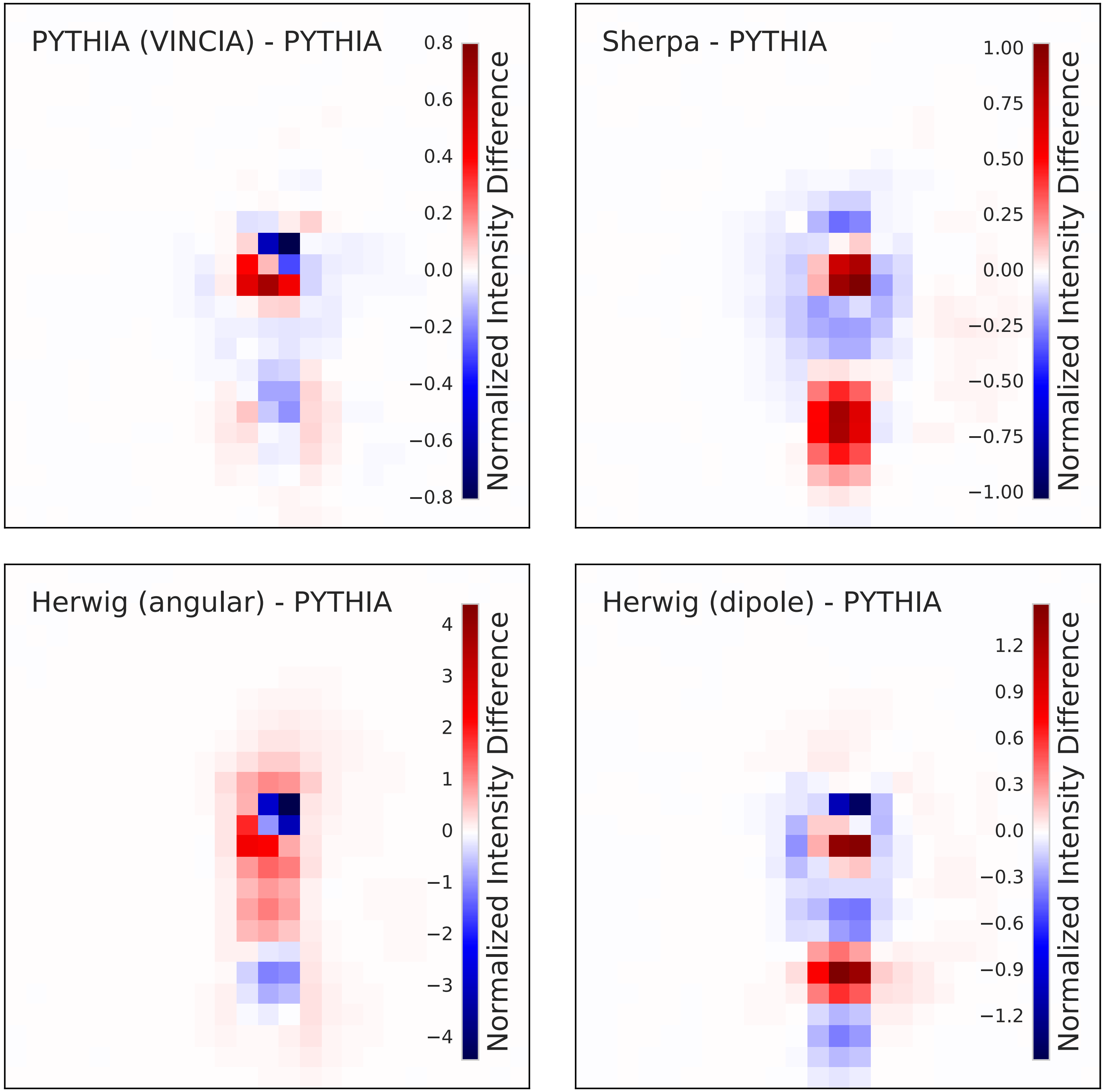
For supervised learning, we depend on labels
labels usually come from simulation



What if data and simulation are very different?

…your classifier will be sub-optimal

Boosted *W* boson jets



N.B. not all of these have been tuned to the same data

J. Barnard et al.
Phys. Rev. D 95, 014018 (2017)

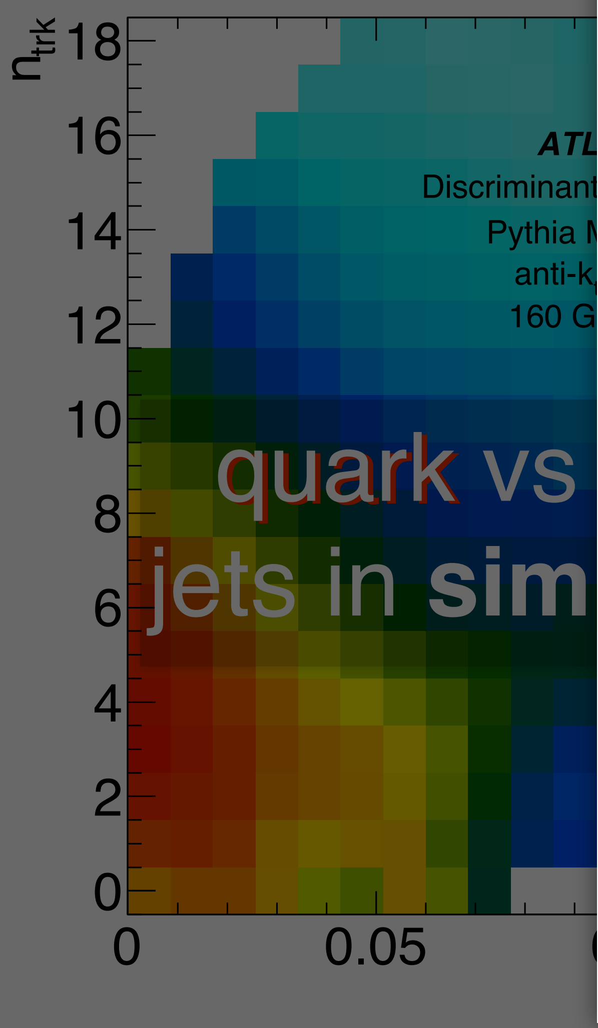
DNN classifiers can **exploit** subtle features

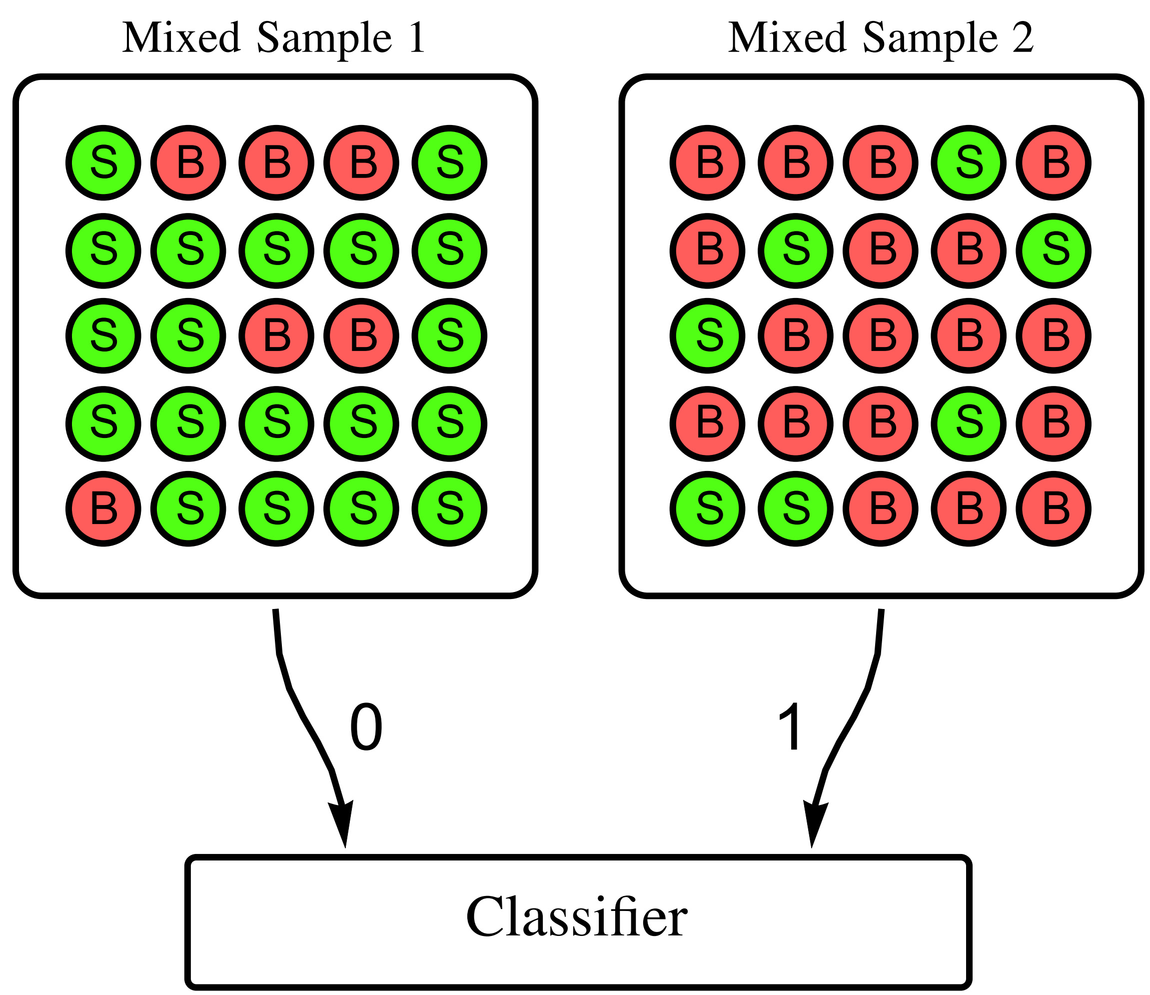
subtle features are **hard to model** !

we need to be careful about which models we use - **only data is correct**

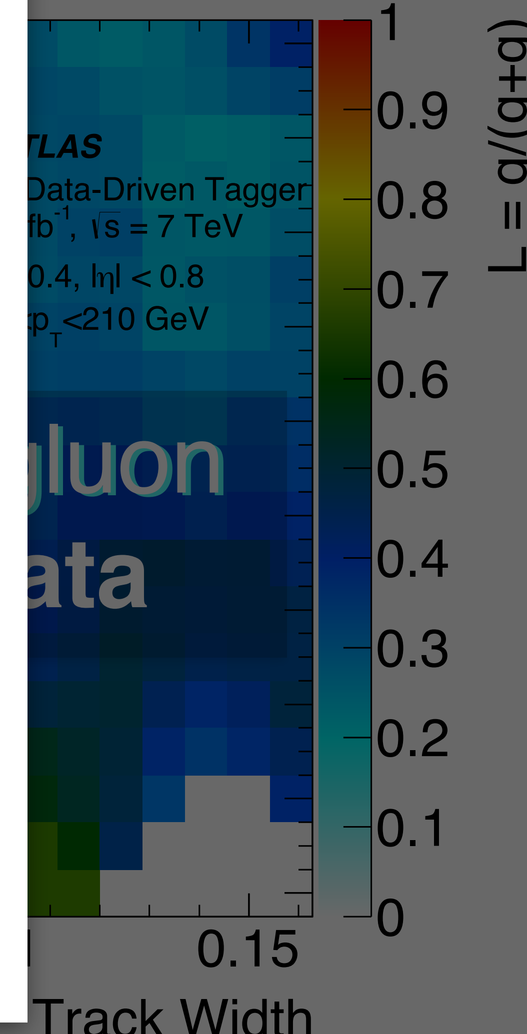
We will take about image feature vectors later today

For super n labels
label ion





Solution: Train **directly on data** using mixed samples



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…your classifier will be sub-optimal

E. Metodiev, **BPN**, J. Thaler,1708.02949
related ideas: L. Dery, **BPN**, F. Rubbo, A. Schwartzman, JHEP 05 (2017) 145

Training on data: learning when you know (basically) nothing

For supervised learning, we depend on labels

labels usually come from simulation

$$L_{M_1/M_2} = \frac{p_{M_1}}{p_{M_2}} = \frac{f_1\, p_S + (1-f_1)\, p_B}{f_2\, p_S + (1-f_2)\, p_B} = \frac{f_1\, L_{S/B} + (1-f_1)}{f_2\, L_{S/B} + (1-f_2)},$$

optimal classifier for M_1 versus M_2

optimal classifier for S versus B

What if data and simulation are very different?

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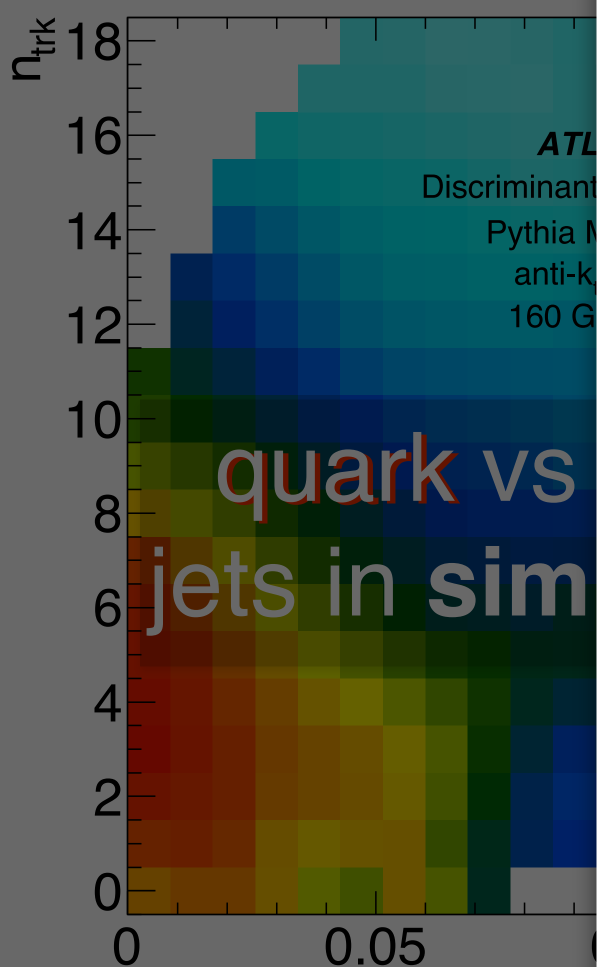
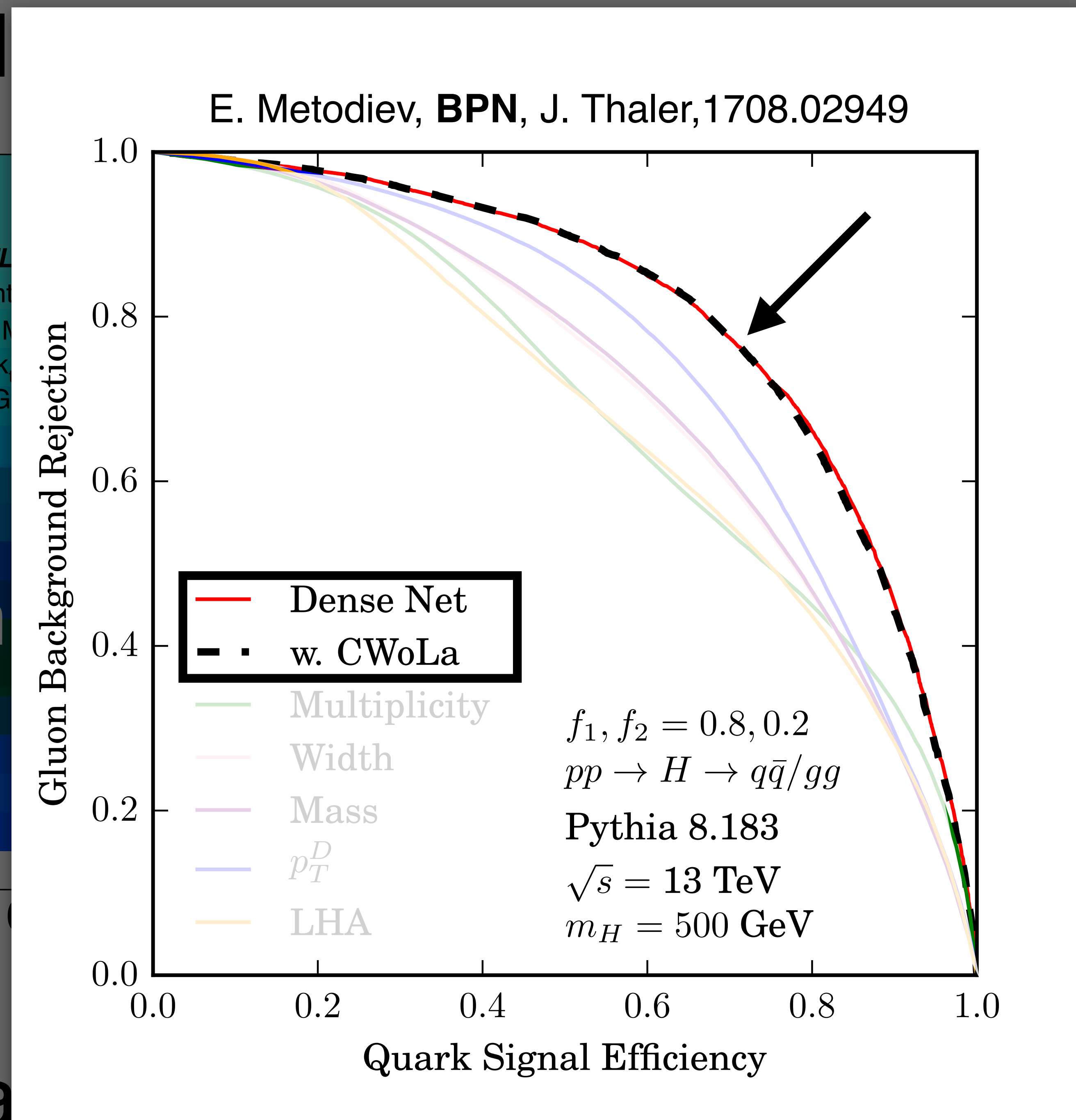
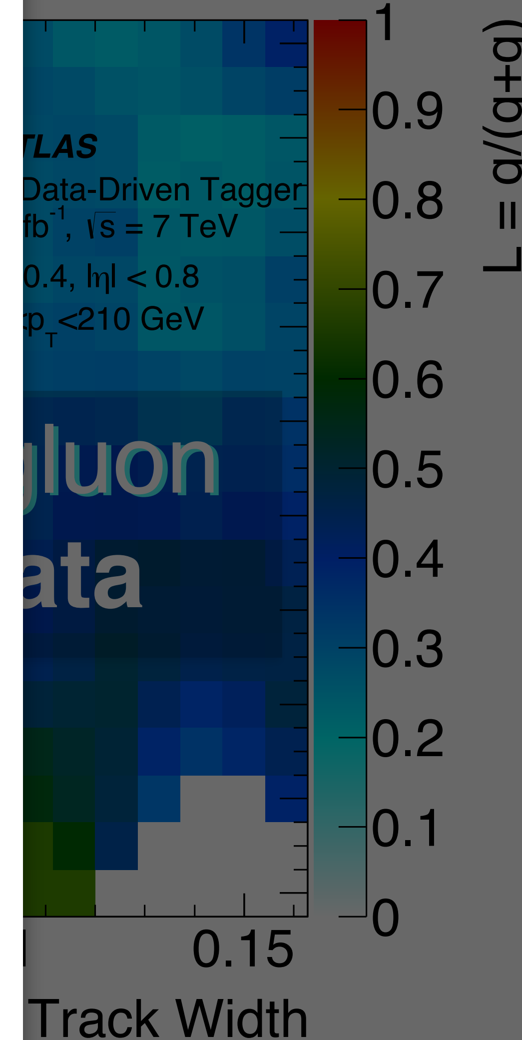
label   ion







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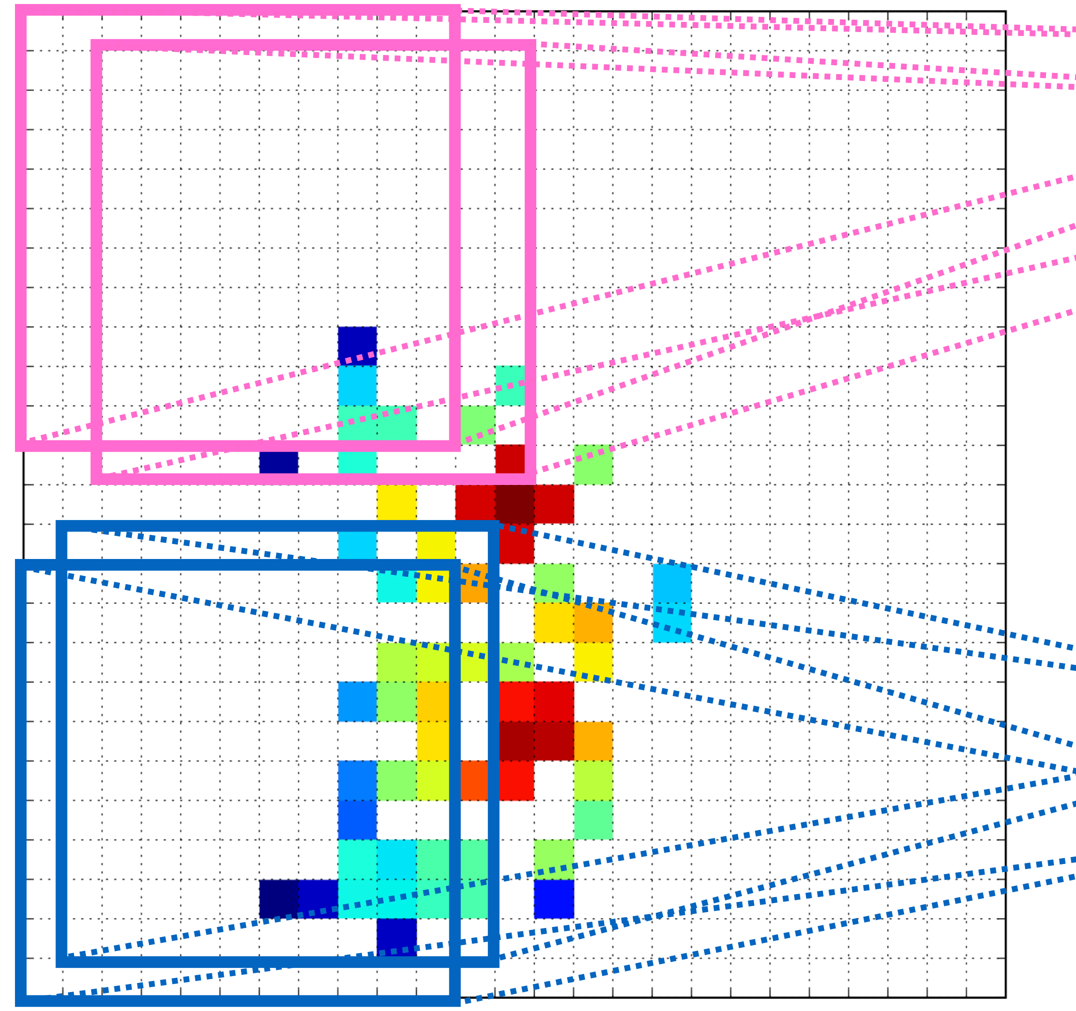
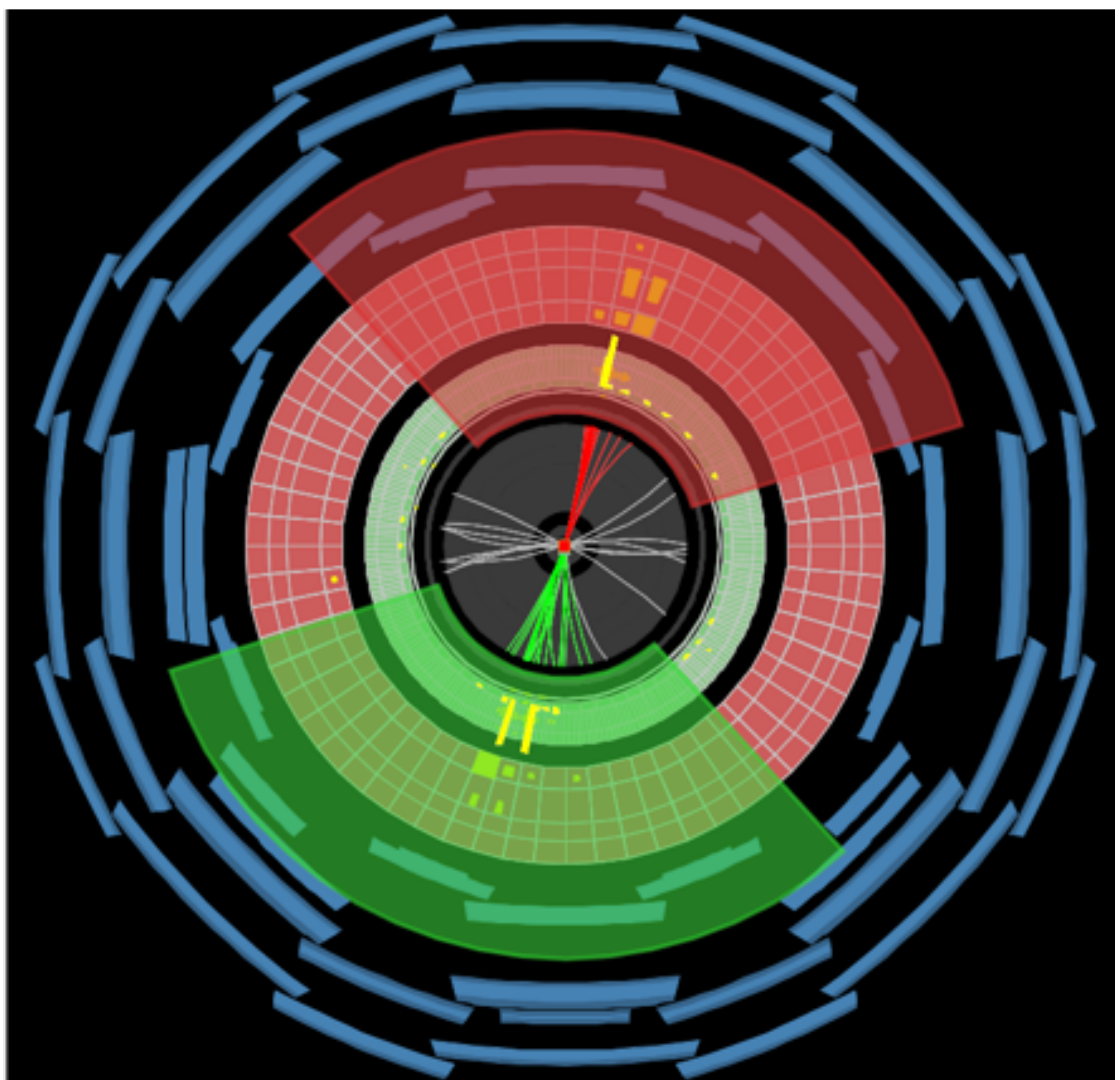
The future

(D)NN's are powerful tools that will help us fully exploit the physics potential of our experiments.





We must be cautious to apply the right tool for the right job.

The more you know, the less black the boxes will be…