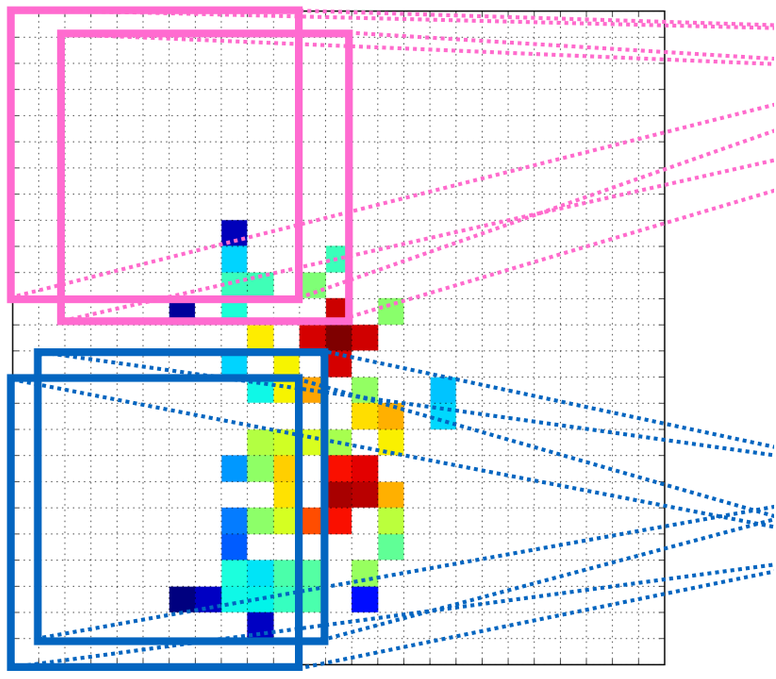
Jack Collins, Kiel Howe, **BPN**, Phys. Rev. Lett. 121, 241803 (2018)

# Weakly Supervised Learning for Classification and Anomaly Detection in High-Energy Physics


Benjamin Nachman

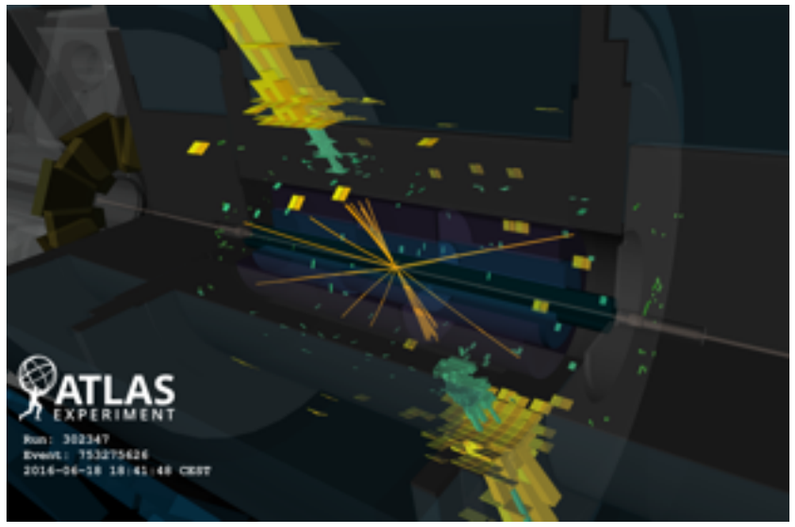
*Lawrence Berkeley National Laboratory*

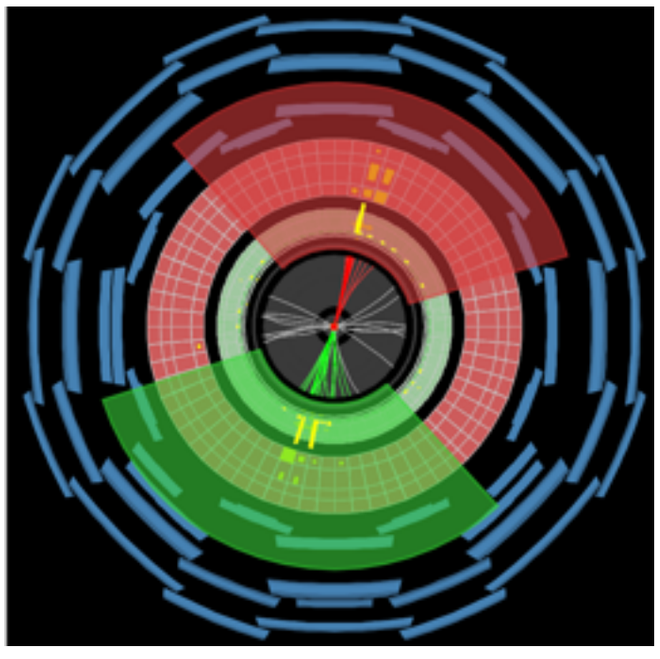
BERKELEY LAB

BERKELEY EXPERIMENTAL PARTICLE PHYSICS

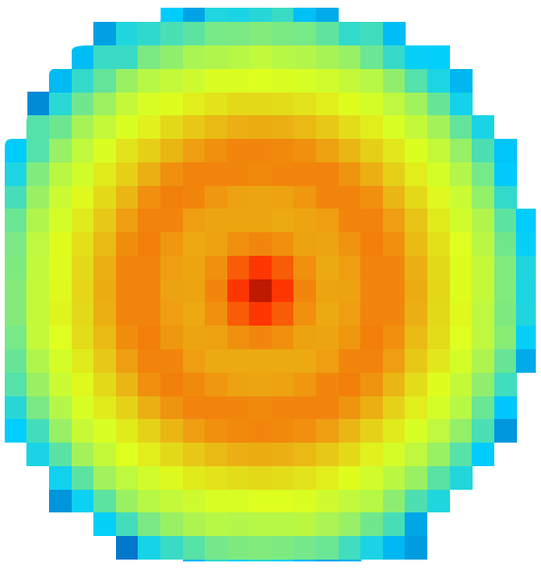
UCR Data Science Seminar
January 17, 2019




The goal of HEP is to identify the smallest length-scale structures in nature.

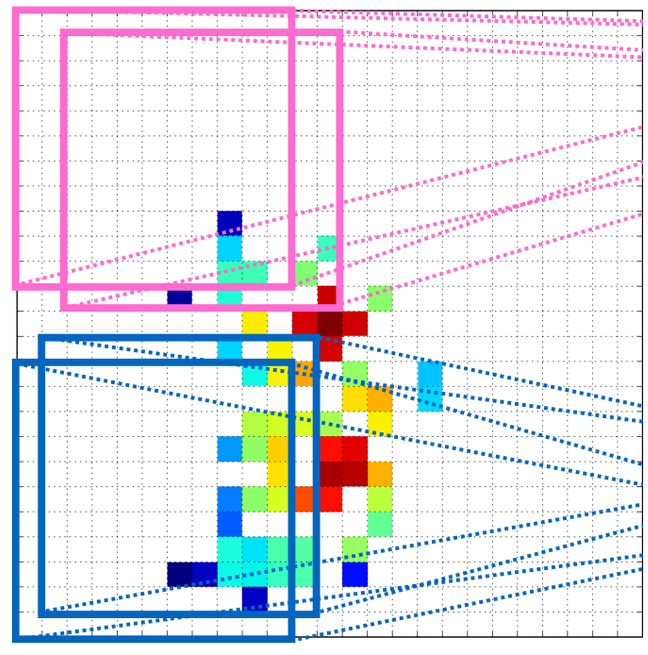


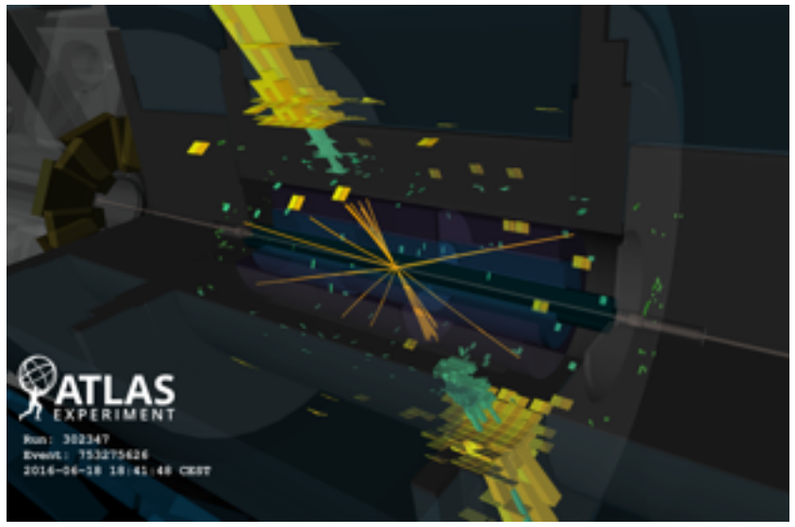
This is a complex data mining problem.
**Simulations** used extensively for analysis.



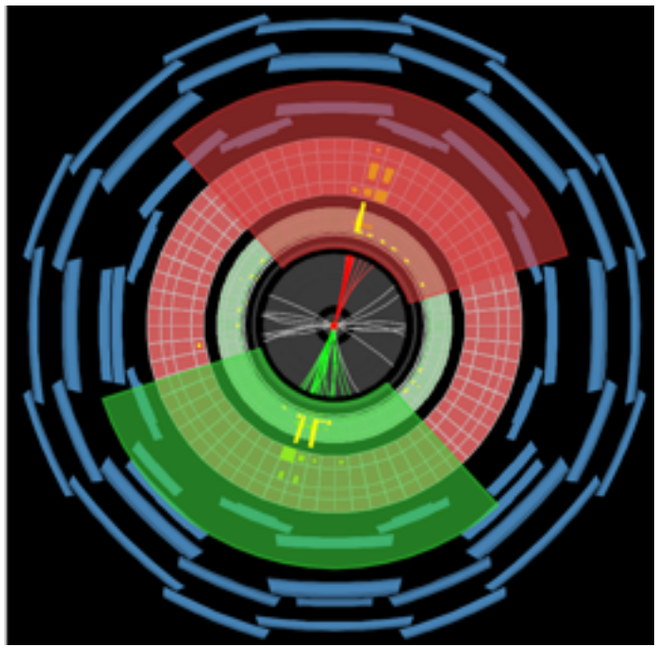
ML is used across physics. Learning from data is critical for **robustness** and **optimality**.

Despite an impressive and extensive program, we have found nothing new yet.



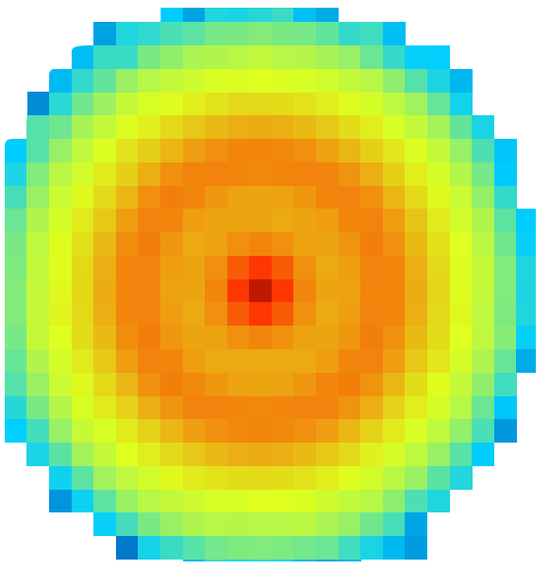



The goal of HEP is to identify the smallest length-scale structures in nature.



# High Energy Physics at the LHC

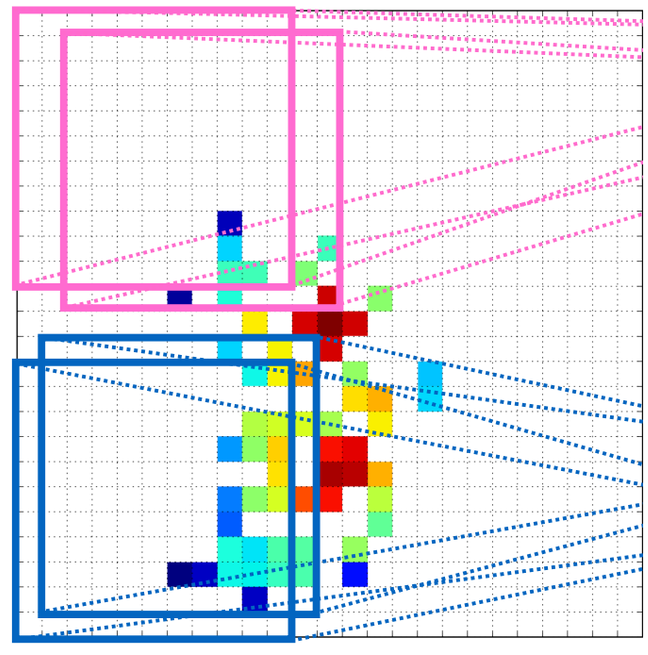
This is a complex data mining problem. Simulations used extensively for analysis.



# ML for classification

ML is used across physics. Learning from data is critical for robustness and optimality.

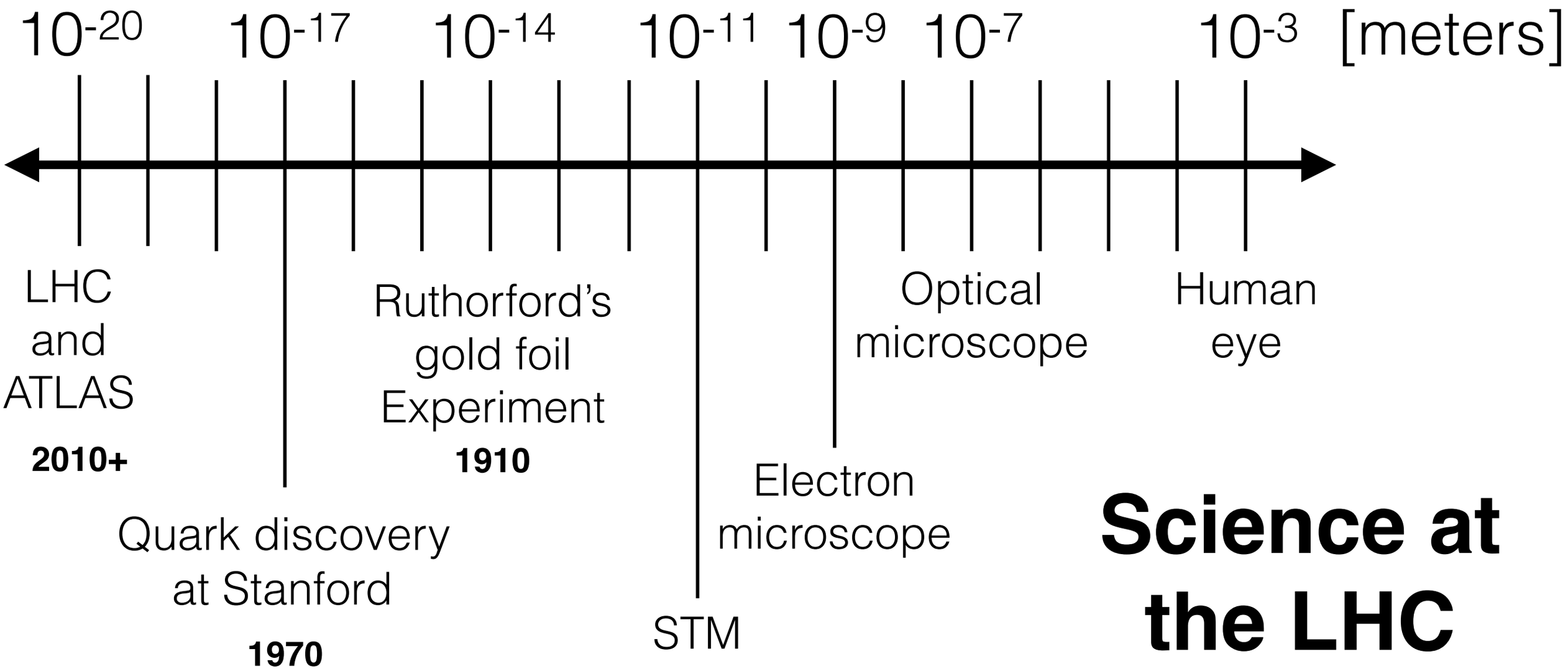
# Weak supervision to apply ML to unlabeled data



Despite an impressive and extensive program, we have found nothing new yet.

# Anomaly detection for the unknown

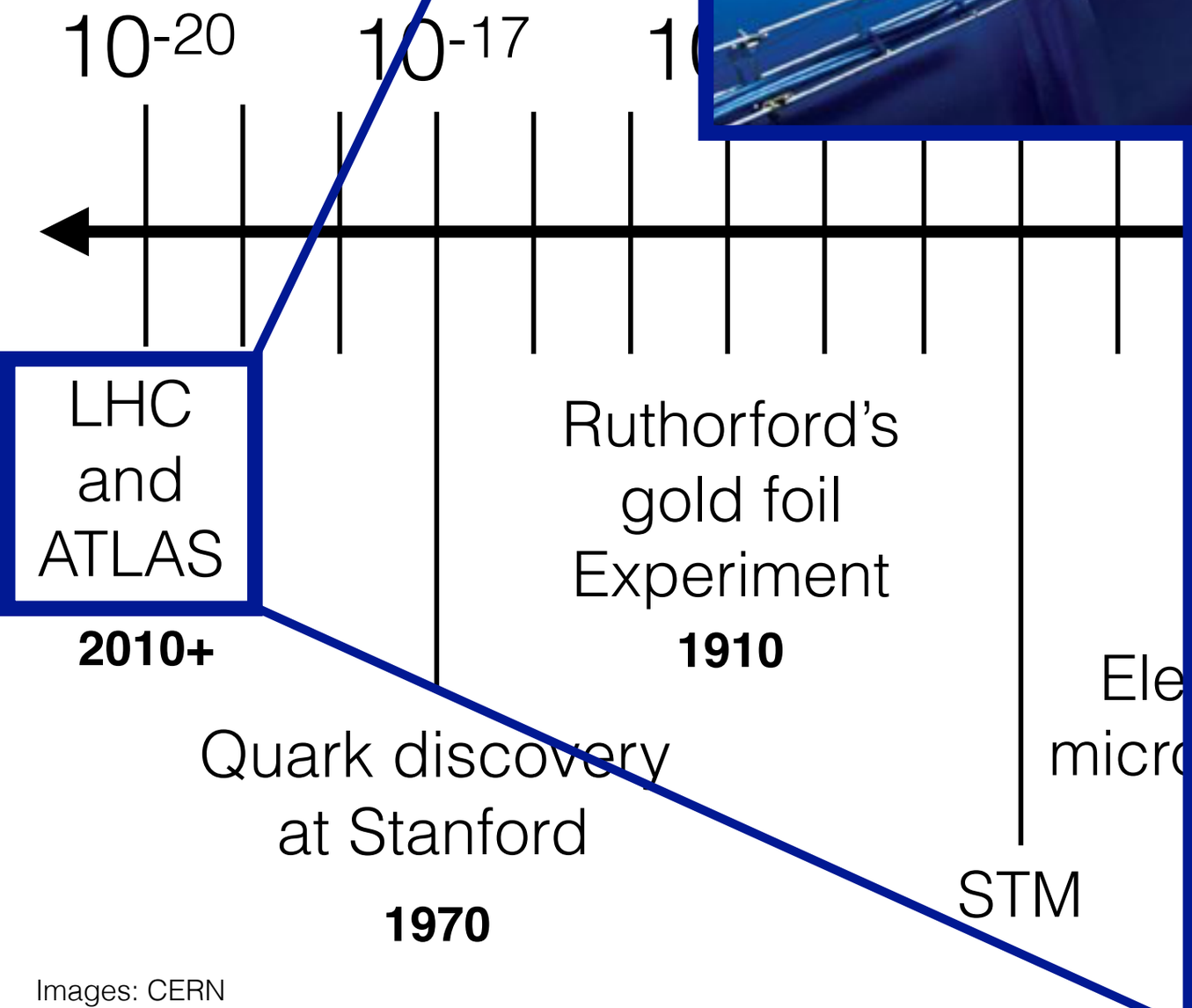
Goal: **We want to study the structure of the smallest building blocks of matter.** For this, we need the most powerful microscope ever built!




**Science at the LHC**

***20 mile beam line and a 5 story detector***

**access to a new frontier!**



Images: CERN

# High Energy Physics at the LHC

*Center-of-mass energy = 13 TeV*

Deposits in our calorimeters

99.9999997% speed of light

Reconstructed trajectories of charged particles

ATLAS EXPERIMENT

Run: 302347
Event: 753275626
2016-06-18 18:41:48 CEST

In total: 100 million readout channels !

# High Energy Physics at the LHC

One of the critical goals of the LHC is to identify new, massive particles

*p*

?

*p*

Remember $E = mc^2$:
(need lots of E to make new particles with a lot of m!)

# High Energy Physics at the LHC

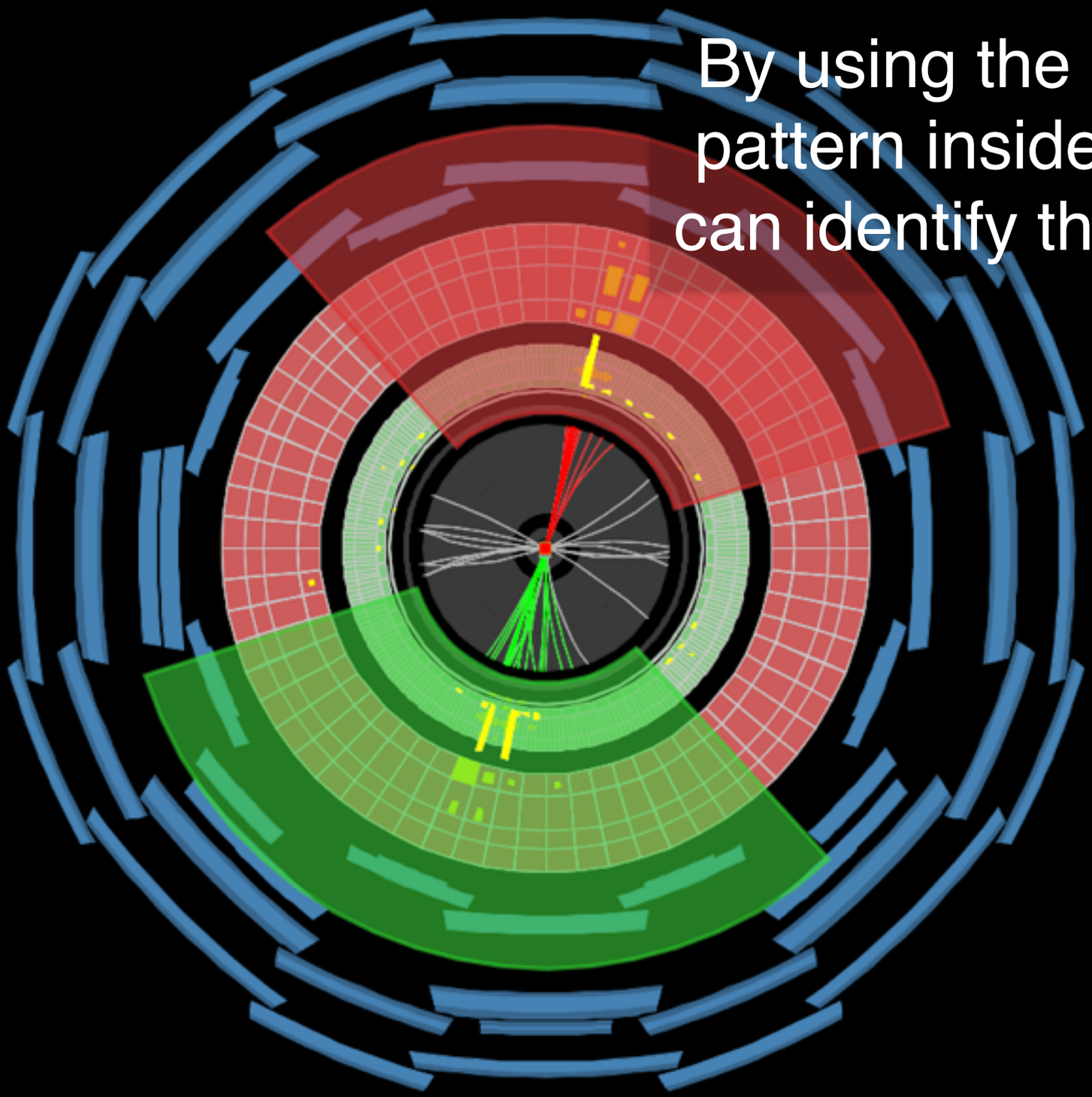
One of the critical goals of the LHC is to identify new, massive particles

The decay of the new particles often result in **jets**

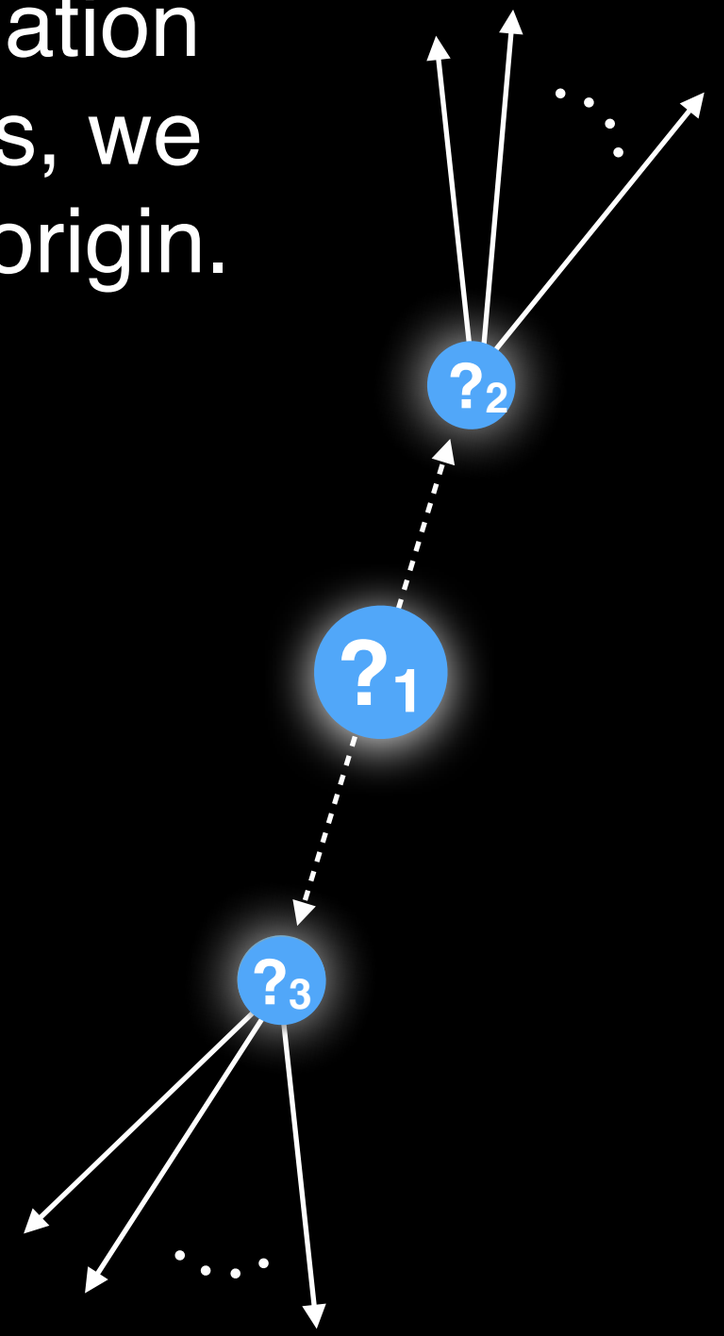
Remember $E = mc^2$:
(need lots of E to make new particles with a lot of m!)

# Jets as a tool for discovery





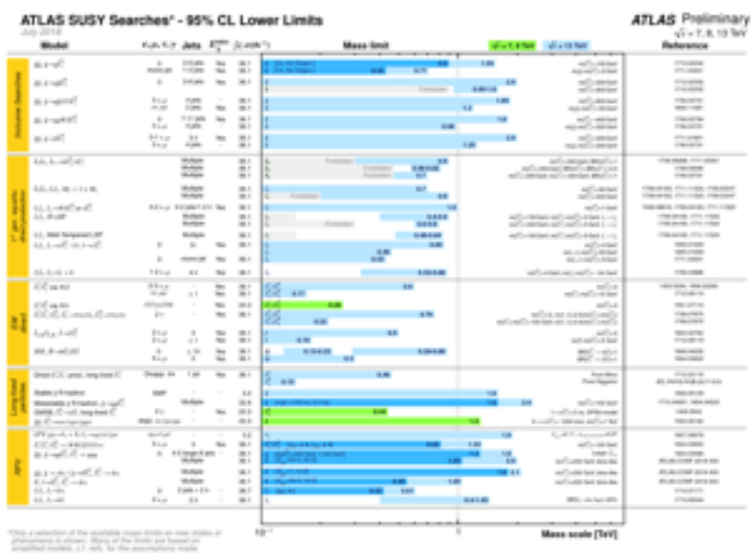
By using the radiation pattern inside jets, we can identify their origin.

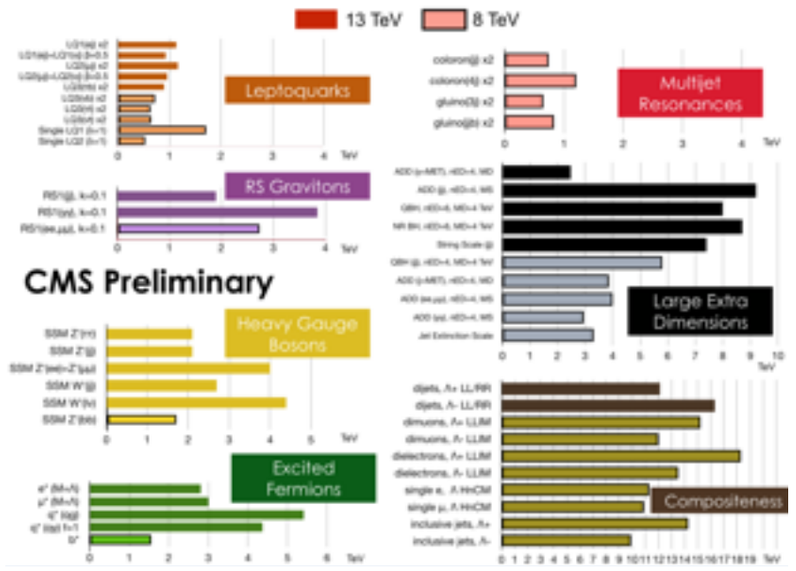


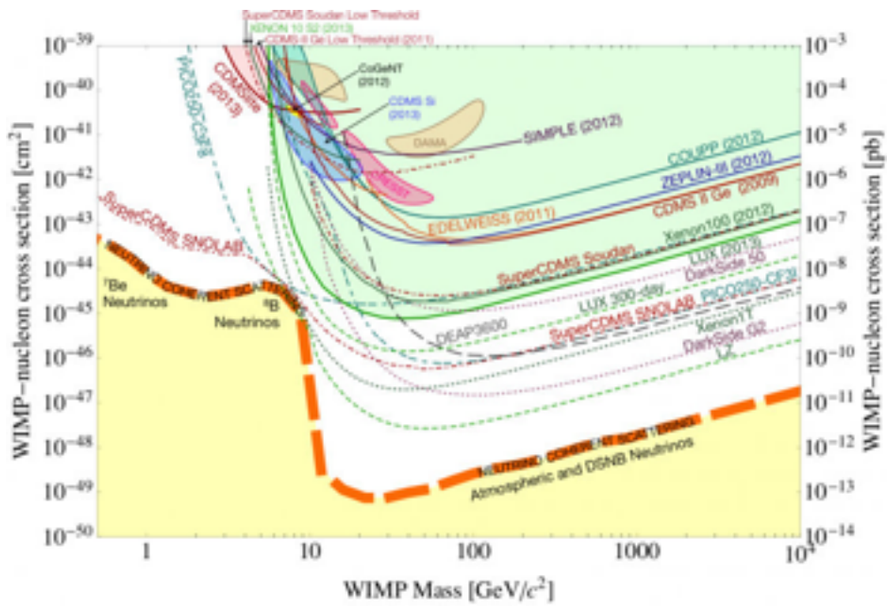
# …and what have we found? Nothing.



We have performed hundreds of hypothesis tests and have never rejected the null (the Standard Model)




**Three possibilities**

There is nothing new

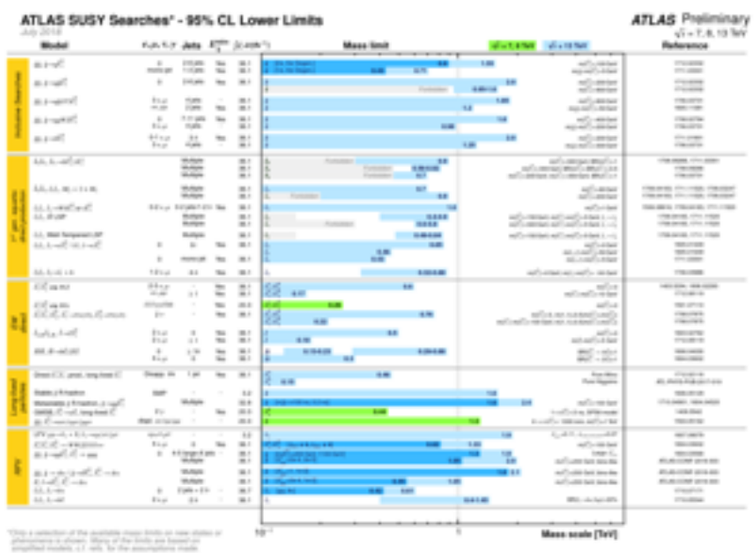
Patience! (new stuff is just rare)

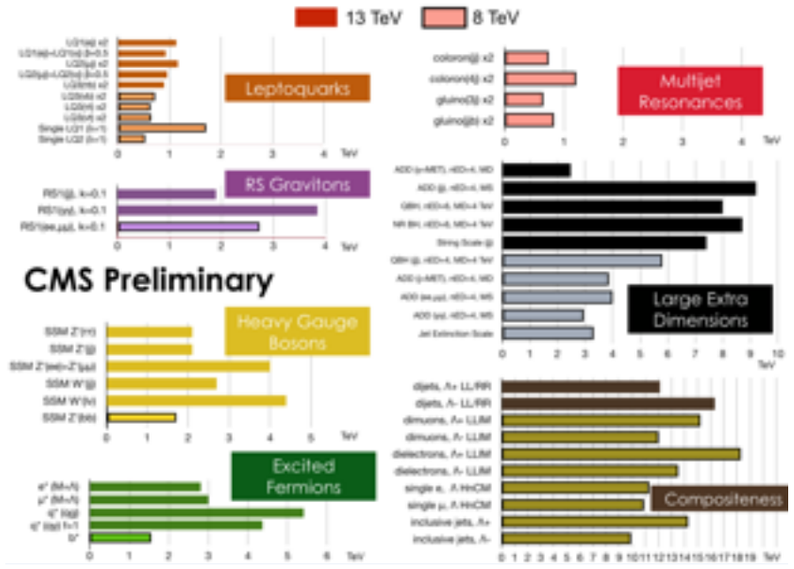
We are just not looking in the right place

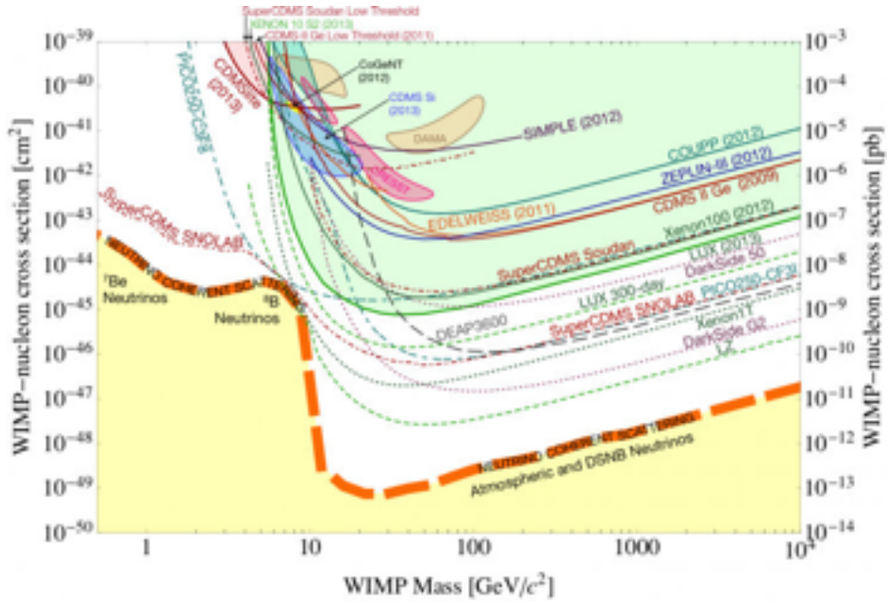
# …and what have we found? Nothing.



We have performed hundreds of hypothesis tests and have never rejected the null (the Standard Model)

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# Searching for new particles / forces



background / signal model independent

| Most searches at the LHC (with or without ML) | Data versus simulation (“general search”) |
|---|---|
| CWoLa Hunting (focus of this talk) | Autoencoders |

# Searching for new particles / forces



background / signal model independent

CWoLa
(focus of

Data versus simulation

Most searches at the LHC
(with or without ML)

*Usually, one has a model of new particle production. Run simulations with that model and of the background and compare with data. Compare data and simulation.*

# Searching for new particles / forces



background / signal model independent

Most searches at the LHC
(with or without ML)

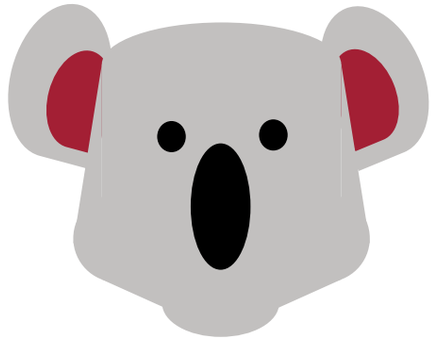
coders

## Data versus simulation
## (“general search”)

*Another approach is to remain signal model agnostic and simply compare the data with our simulation of the Standard Model.*

# Searching for new particles / forces





background / signal model independent

| Most searches at the LHC (with or without ML) | Data versus simulation (“general search”) |
|---|---|
| CWoLa Hunting (focus of this talk) | Autoencoders |

New ideas: use machine learning to find new signals.

# Training Directly on (unlabeled) Data



I hope I've convinced you that it is important to have an open mind when looking at data.

Now, let's take a step back and discuss why it is important to train on data **in general**.

*Intermezzo: Learning directly from data*

- Why it is important to learn directly from data
- How to learn without labels

# The importance of training on data



**Let's start with a small thought experiment.**

*Are these equivalent?*

(1) train in simulation & calibrate in data

(2) train in data

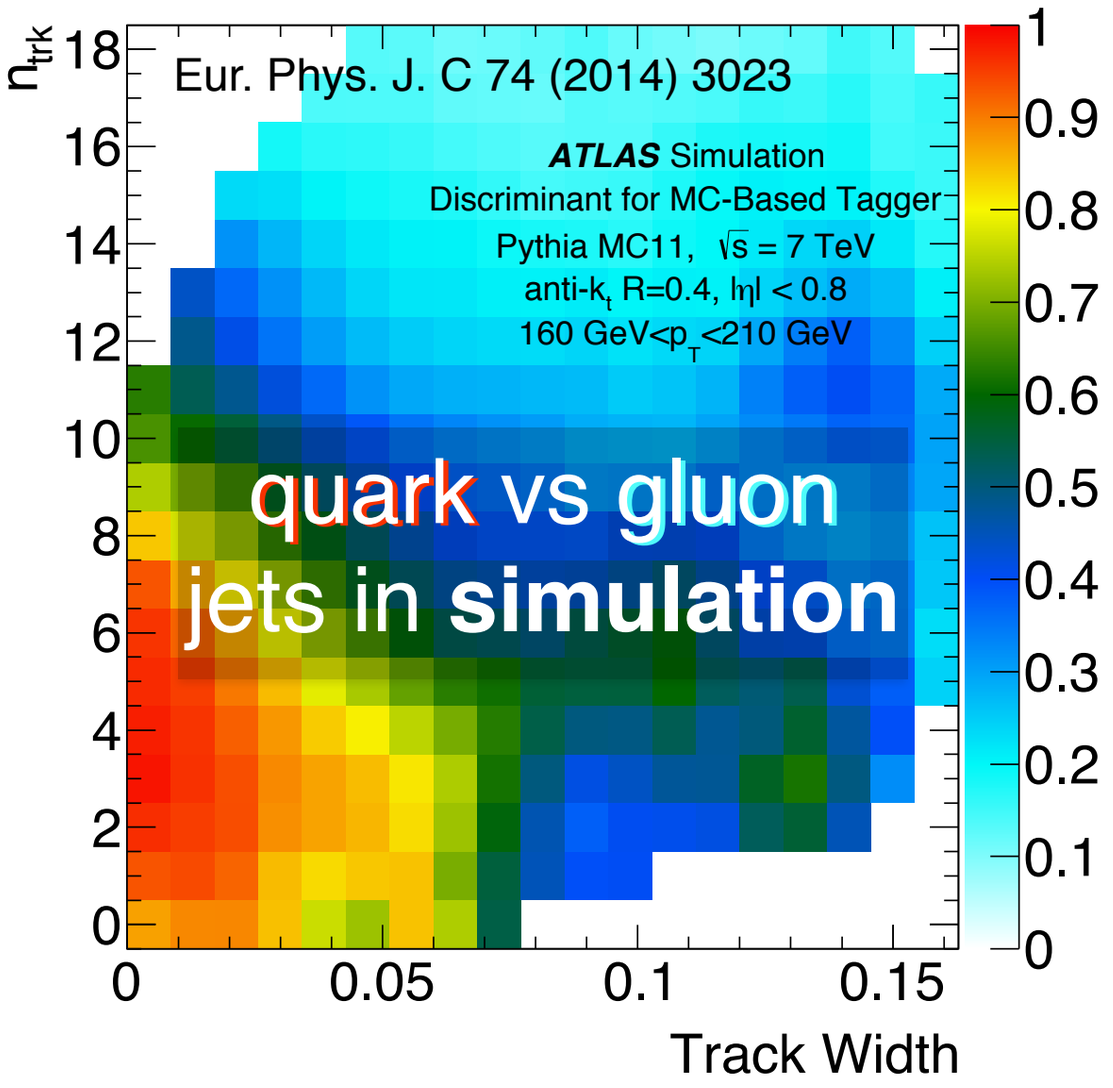
← what we mostly do right now

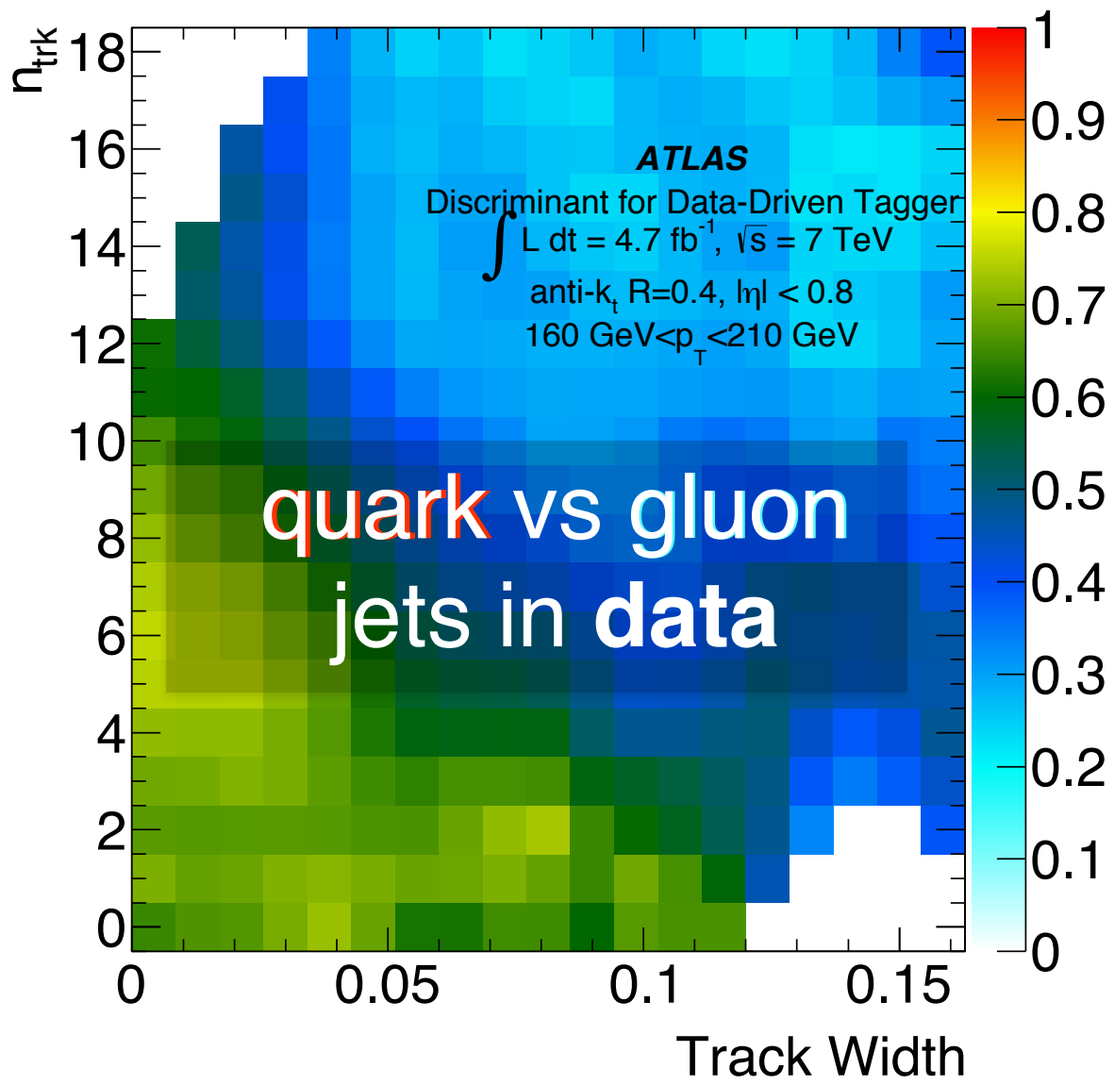
calibration = adjust TPR/FPR to match data

# Background and Motivation



Usual paradigm: train in simulation, validate on data, test on data.



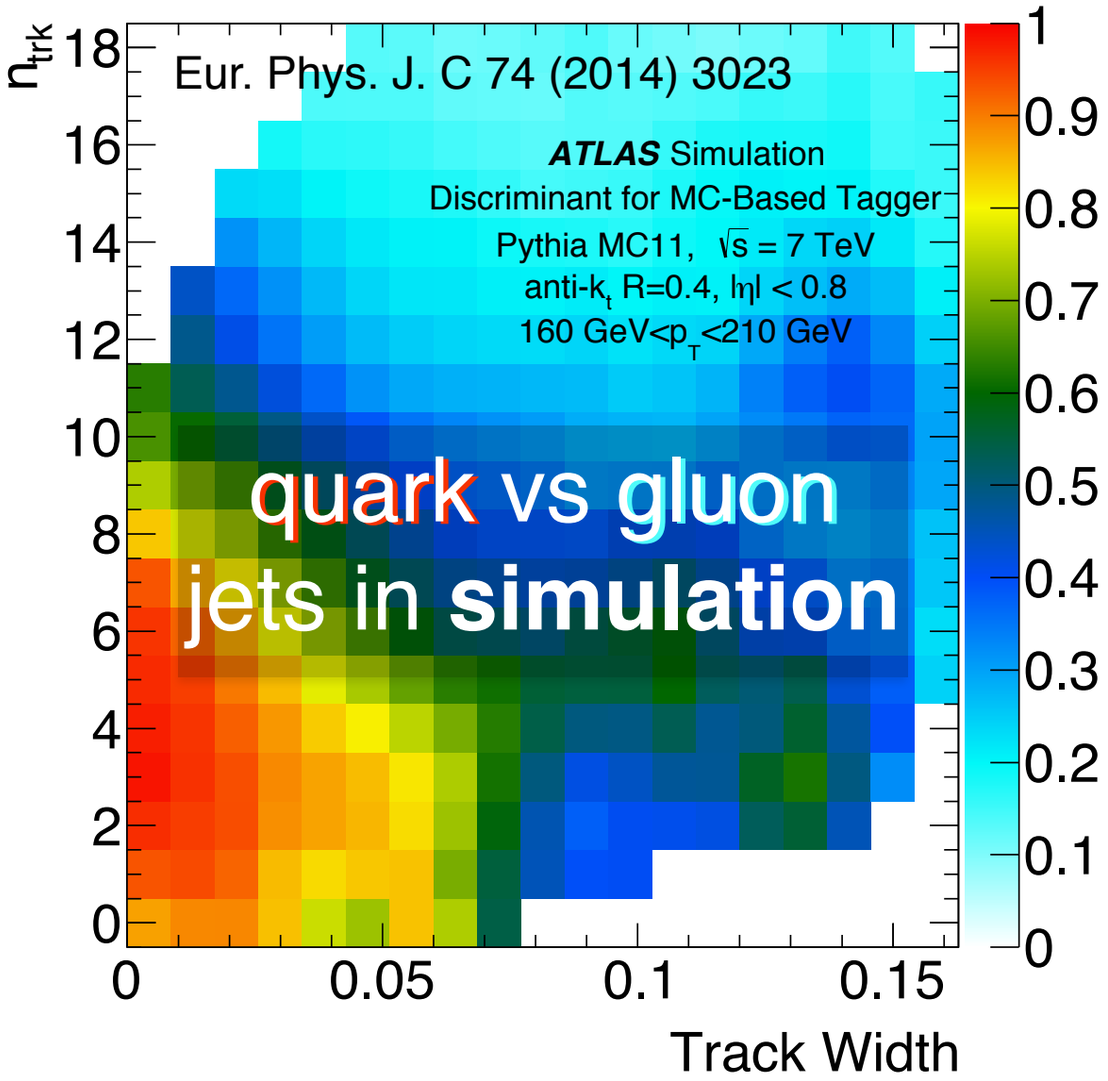

If data and simulation differ, this is sub-optimal!

**(answer from previous slide is no!)**

# Background and Motivation



Usual paradigm: **train in simulation**, validate on data, test on data.




Recall: optimal classifier (by Neyman-Pearson NP) is a threshold cut on the likelihood ratio.

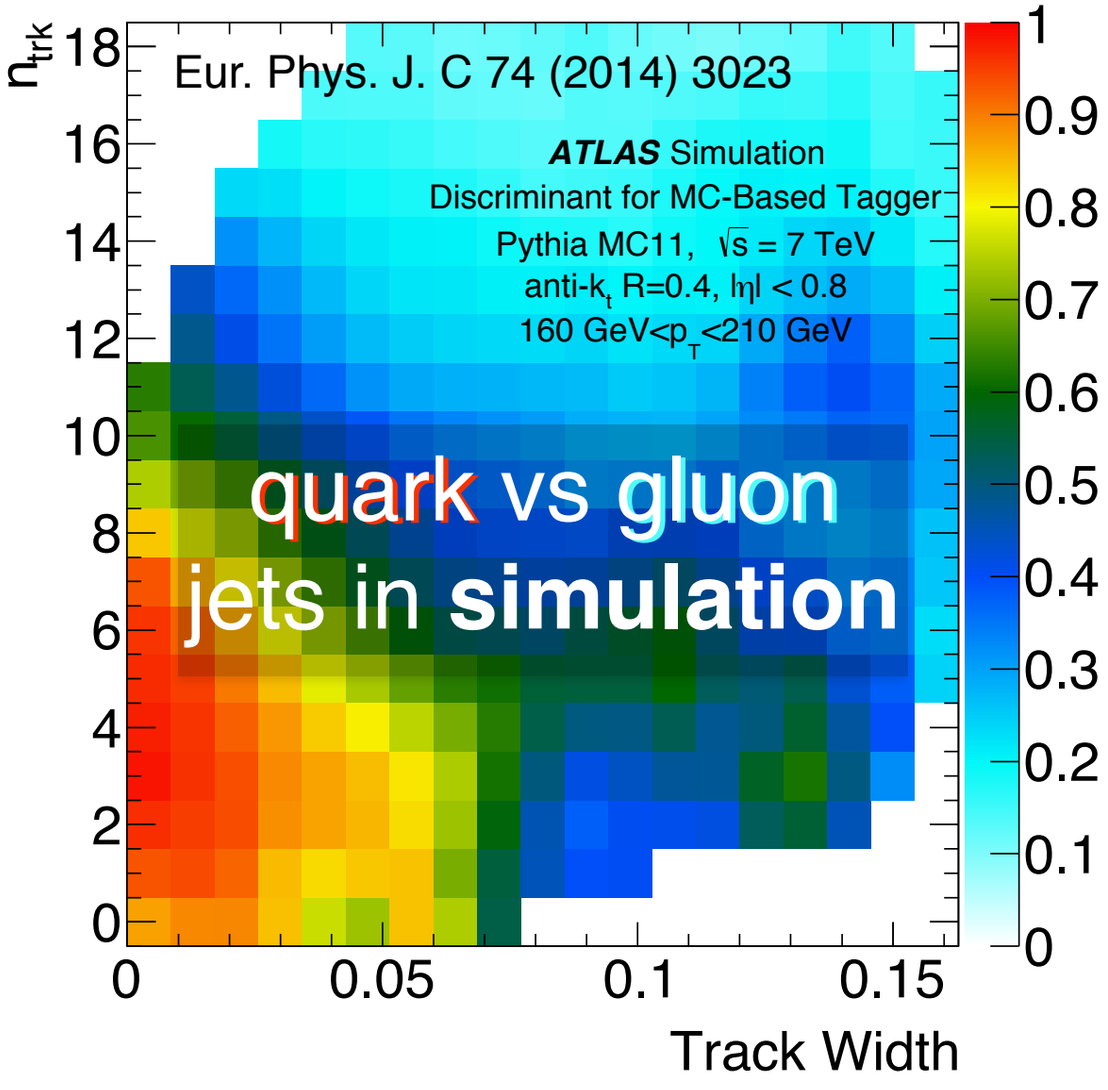
For a 2D feature space, no need for a NN or BDT - can use a histogram to “train” the classifier.

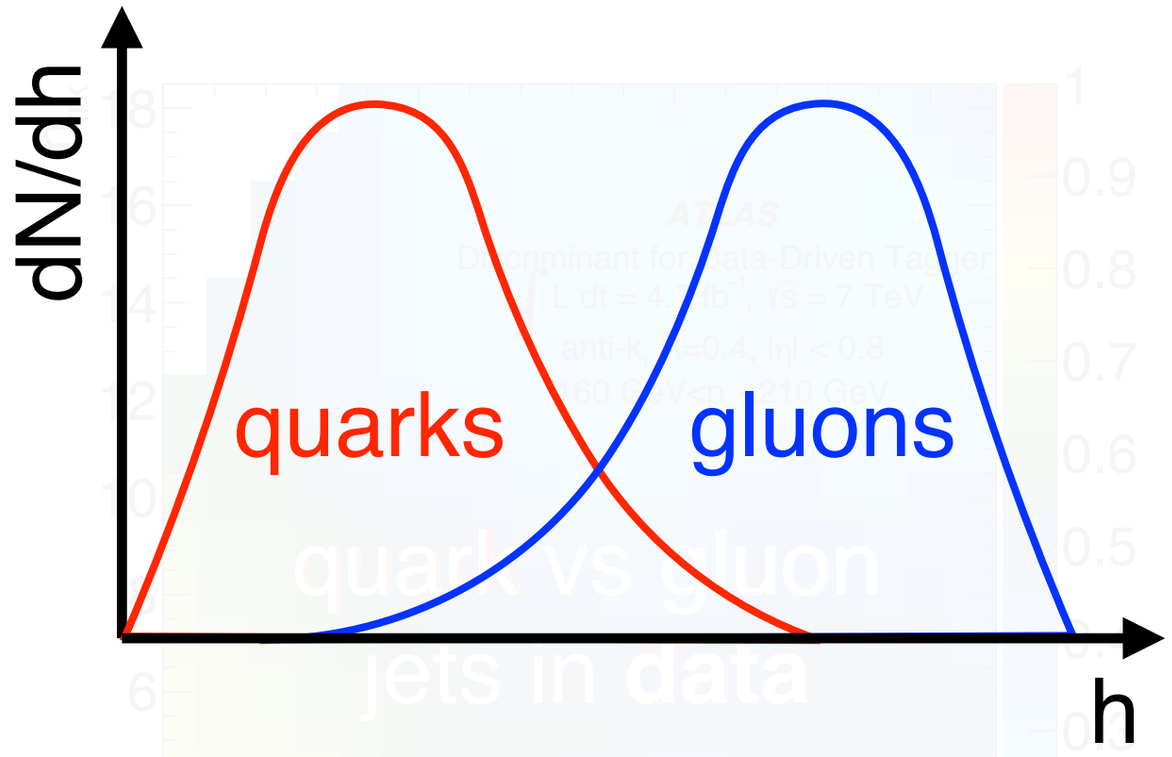
$h(n_{trk}, \text{Track Width}) \rightarrow [0,1]$

# Background and Motivation



Usual paradigm: **train in simulation**, validate on data, test on data.

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# Background and Motivation



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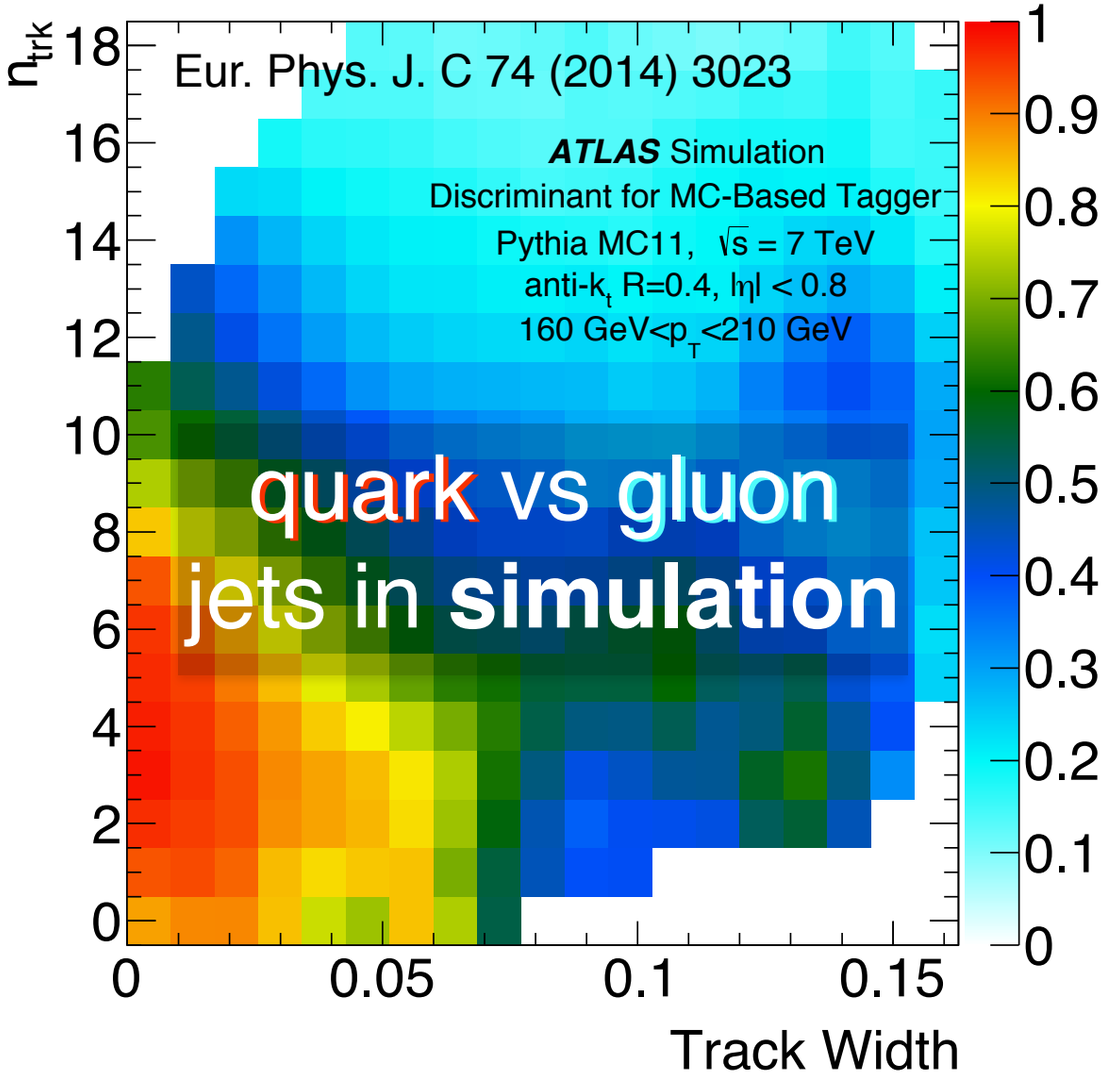
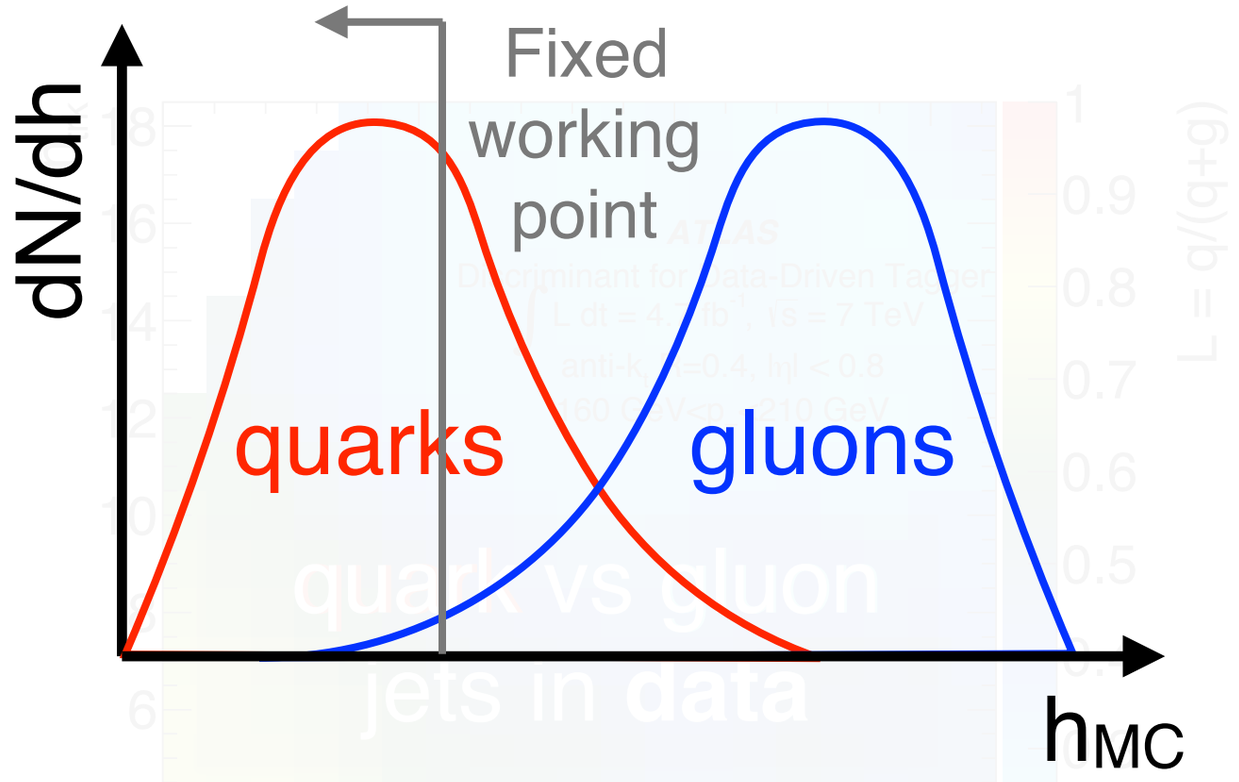


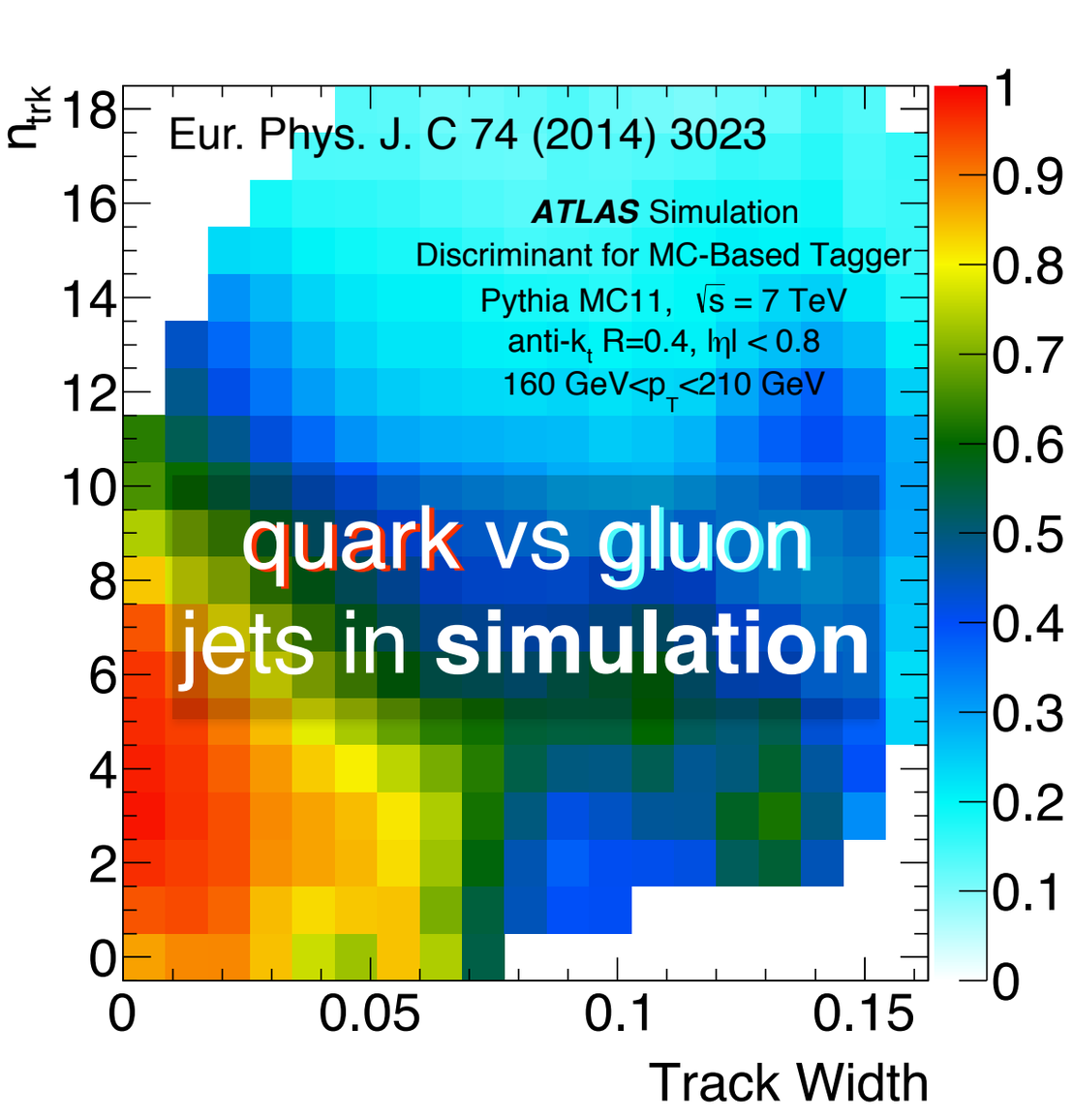

For a 2D feature space, no need for a NN or BDT - can use a histogram to “train” the classifier.

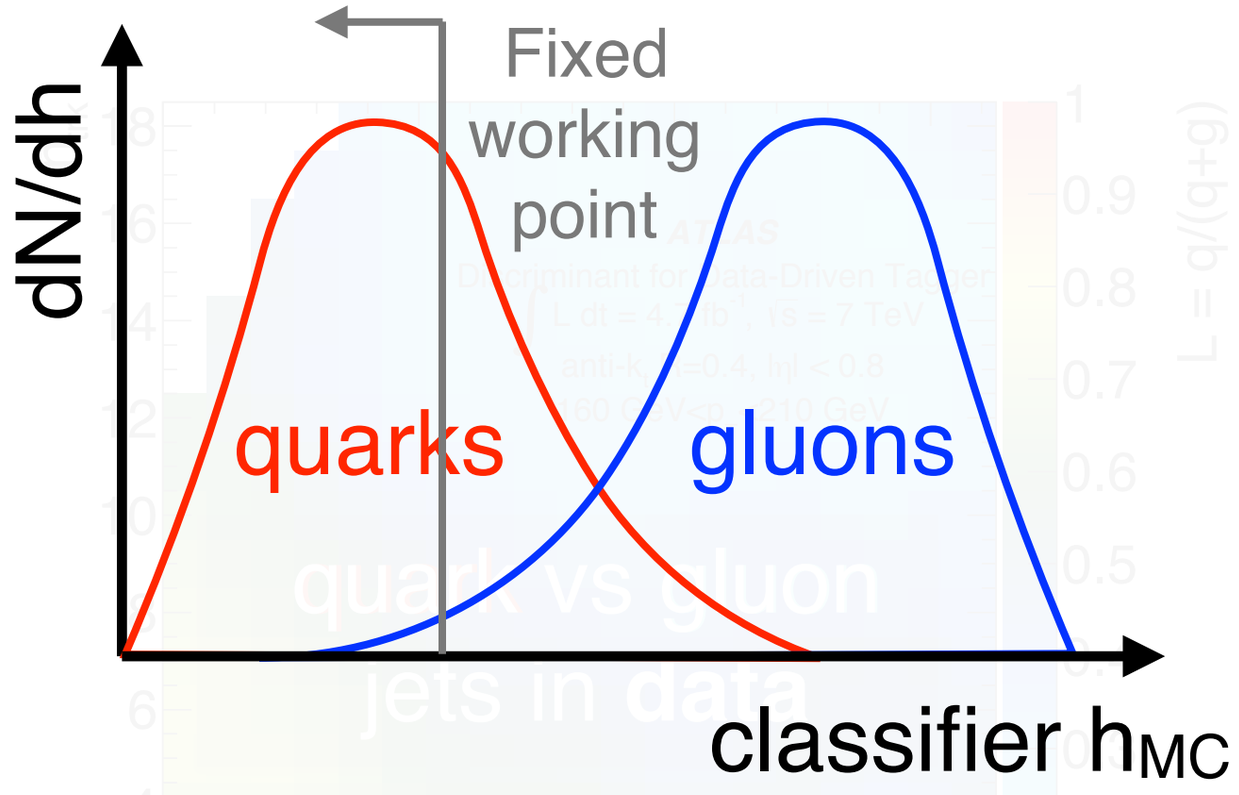
$h_{MC}(n_{trk}, \text{Track Width}) \rightarrow [0,1]$

# Background and Motivation



Usual paradigm: **train in simulation**, validate on data, test on data.




WP in simulation:

$\varepsilon_{signal,MC}$, $\varepsilon_{back,MC}$

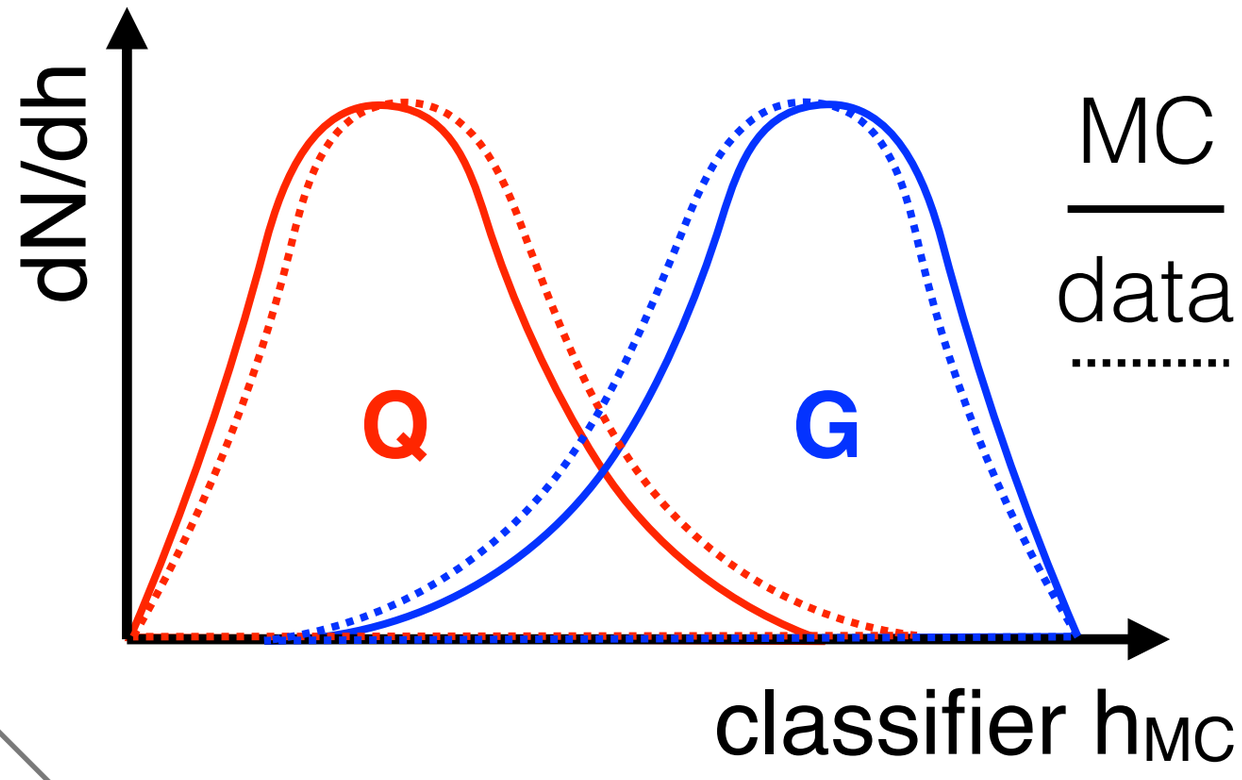
# Background and Motivation



Usual paradigm: train in simulation, **validate on data**, test on data.

Determine the performance of the WP in data.






How did we get this?

dijets = $f_q$ x **Q** + (1-$f_q$) x **G**

Z+jets = $g_q$ x **Q** + (1-$g_q$) x **G**

2 equations, 2 unknowns (**Q**, **G**)

two event samples with different q/g fractions

(N.B. f & g from simulation and selection can't bias Q and G)

# Background and Motivation



Usual paradigm: train in simulation, **validate on data**, test on data.

Determine the performance of the WP in data.

How did we get this?

dijets = $f_q$ x **Q** + (1-$f_q$) x **G**

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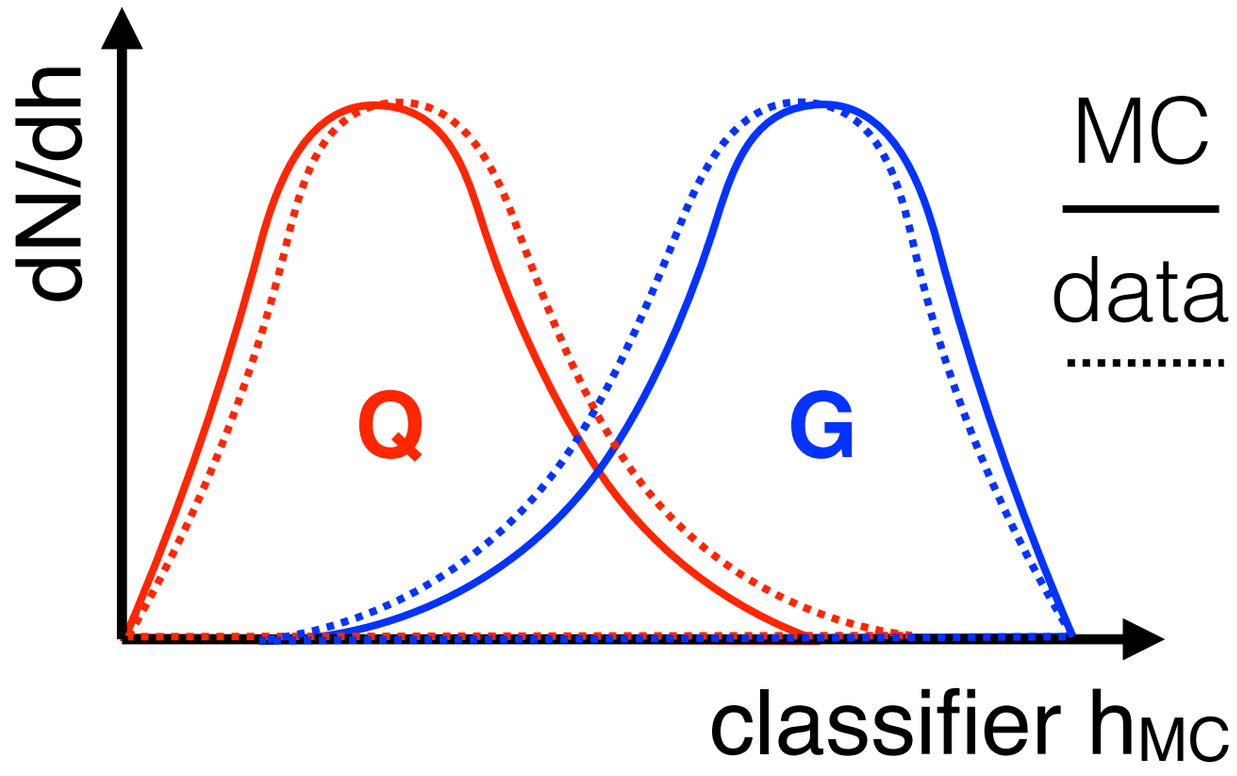
2 equations, 2 unknowns (**Q**, **G**)




WP in data:

$\varepsilon_{signal,data}$, $\varepsilon_{back,data}$

Can correct the MC to have the same performance as data.

# Background and Motivation



Usual paradigm: train in simulation, validate on data, **test on data**.

Once we have scale factors (& their uncertainty), we can ensure that our analysis will be **accurate**.

…so what is the problem?

*remember my claim from earlier:*

If data and simulation differ, this is sub-optimal!

This is an **accuracy** versus **precision** problem. It is "easy" to achieve accuracy through calibration, but the results may not be the best one possible.

# Background and Motivation



In this 2D feature space, we can actually derive $h_{data}$.

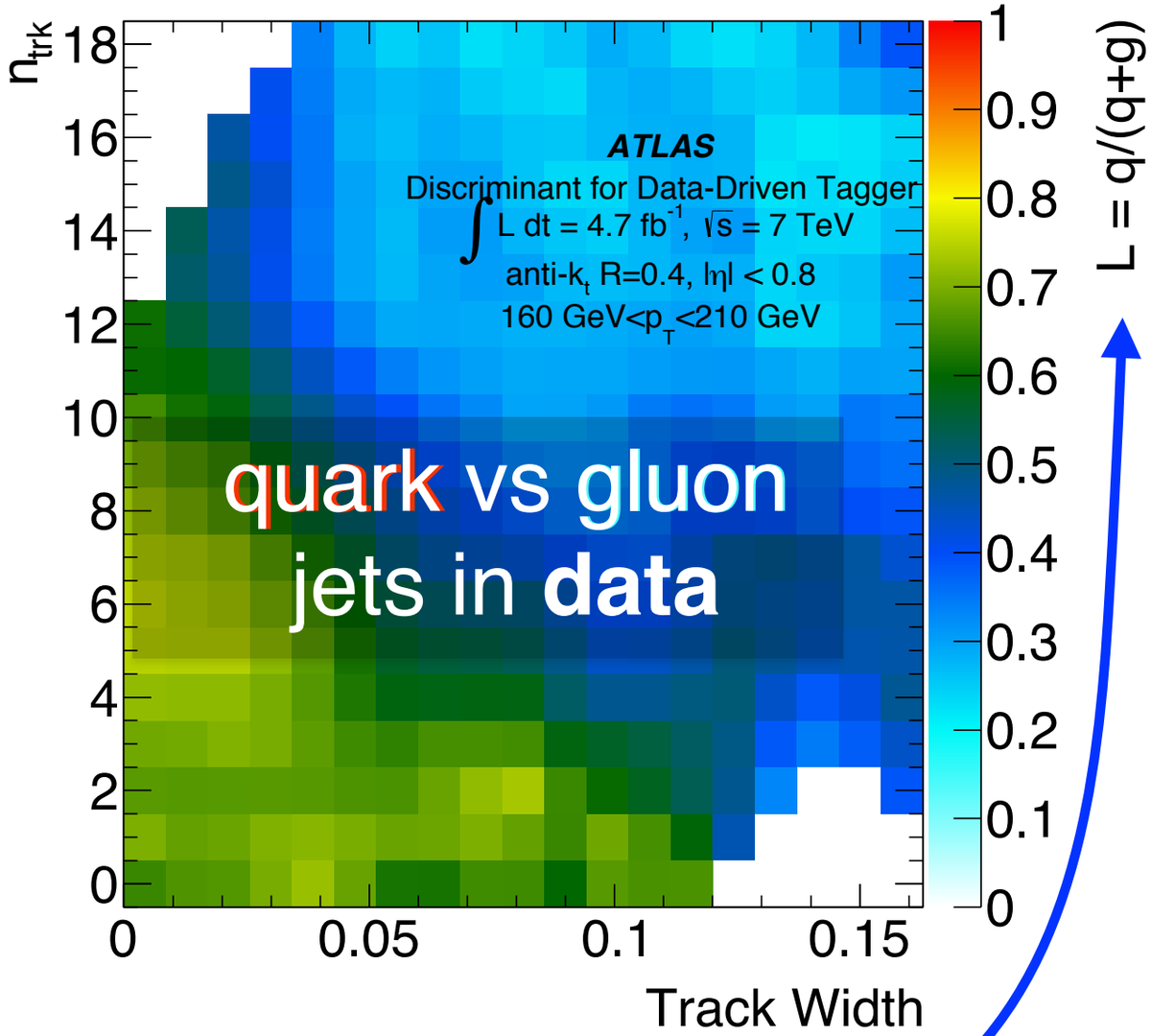
Using the same trick as earlier:

dijets = $f_q$ x Q + (1-$f_q$) x G

Z+jets = $g_q$ x Q + (1-$g_q$) x G

2 equations, 2 unknowns (Q, G)

(now Q and G are 2D histograms)




*in general:*

$h_{MC}(n_{trk}, \text{Track Width}) \neq h_{data}(n_{trk}, \text{Track Width})$

# Take it to the extreme

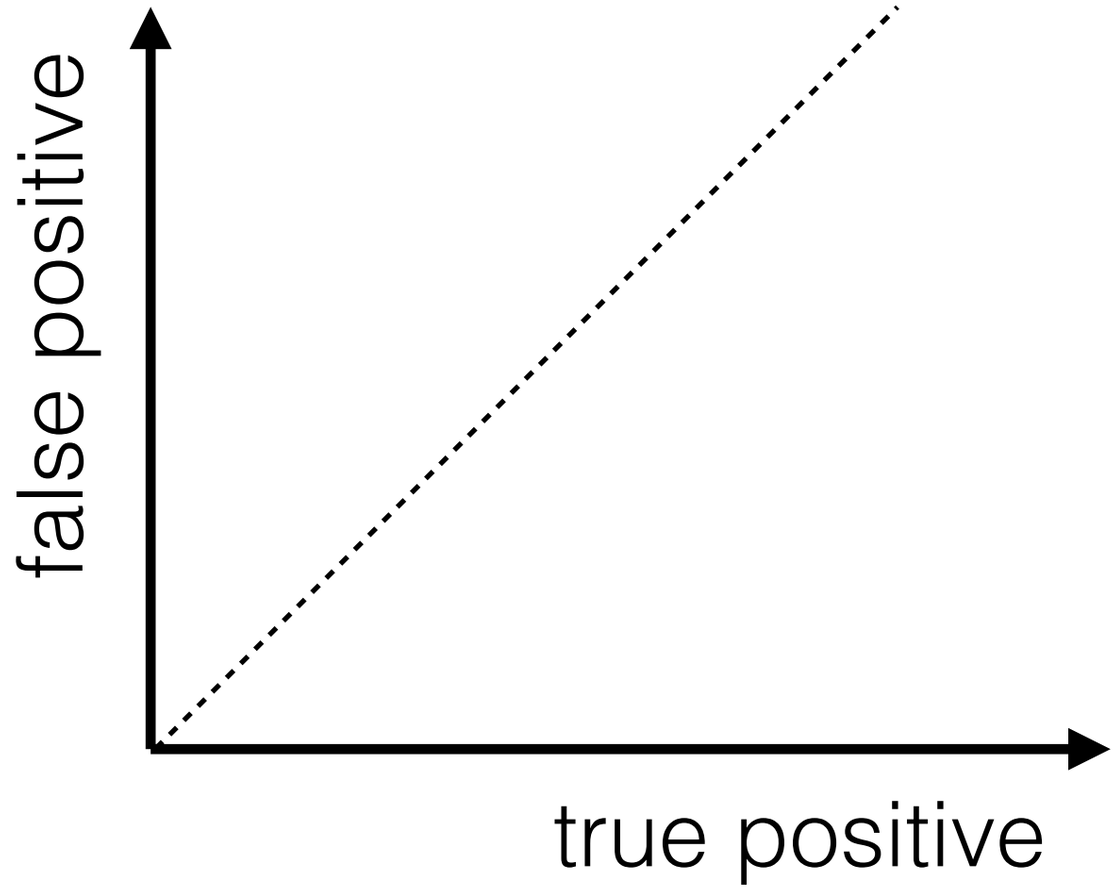


To stress this point, suppose that $h_{MC}$ is the random classifier:

$h_{MC}$ = 0 if you pick a random number x in [0,1] and $x < \varepsilon$

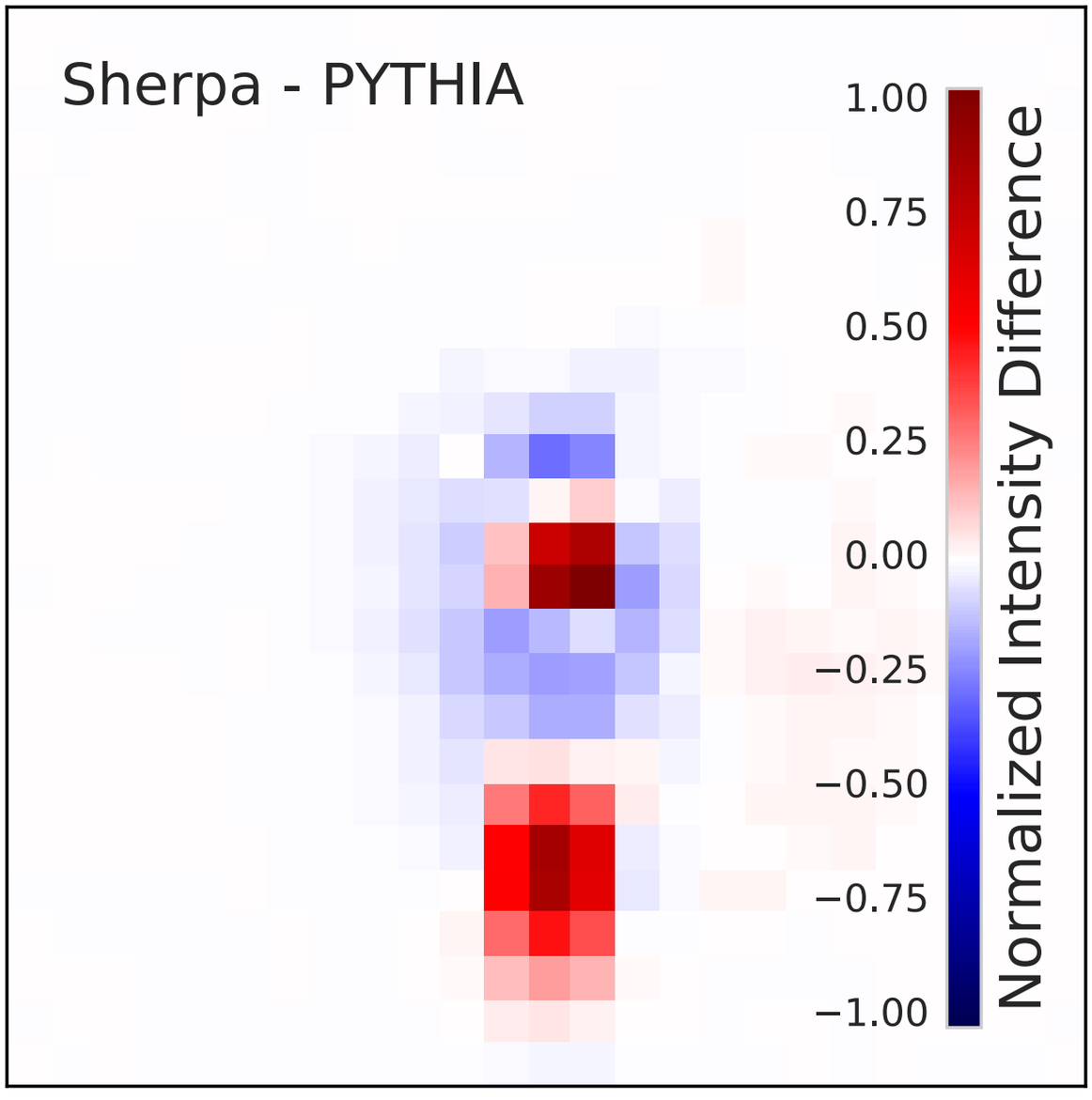
1 otherwise

We can calibrate this classifier in data, but clearly, it is sub-optimal !!



# One more slide about why it matters






J. Barnard, E. Dawe, M. Dolan, N. Rajcic,
Phys. Rev. D 95 (2017) 014018

Especially important for **deep learning** using subtle features → hard to model!

*radiation pattern inside a particular type of jet - same physics, different simulators!*

# Achieving the Optimal Classifier



Two ways around the problems mentioned earlier:

(1) Derive the classifier in MC, but don't let it use information that is not present in data.

"Learning to pivot"

*G. Louppe, M. Kagan, K. Cranmer, 1611.01046*

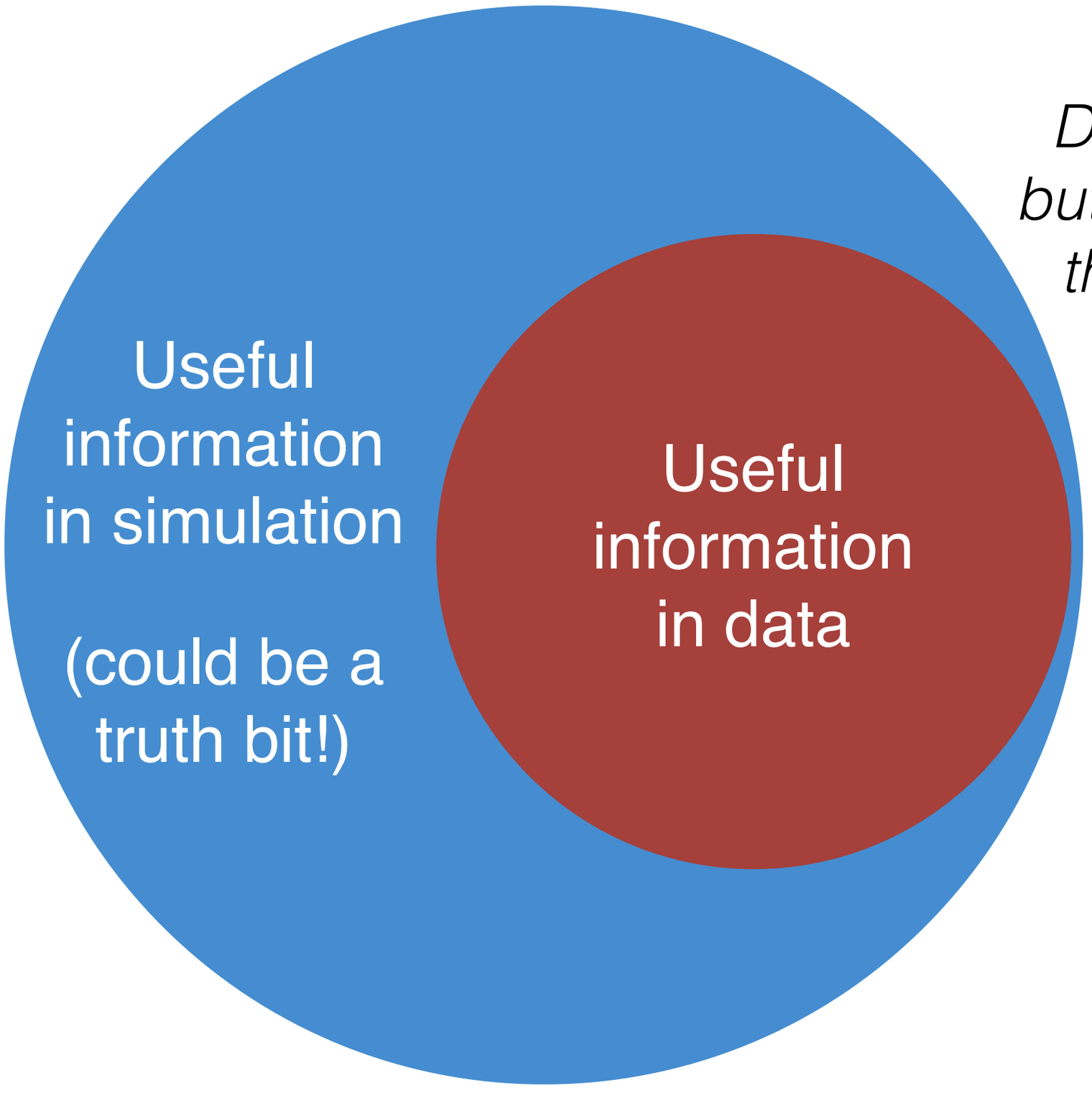
(2) Train on unlabeled data.

"Weak supervision"

*L. Dery, **BPN**, F. Rubbo, A. Schwartzman, JHEP 05 (2017) 145*
*E. Metodiev, **BPN**, J. Thaler, JHEP 10 (2017) 174*

# When option 1 works






Option 1:

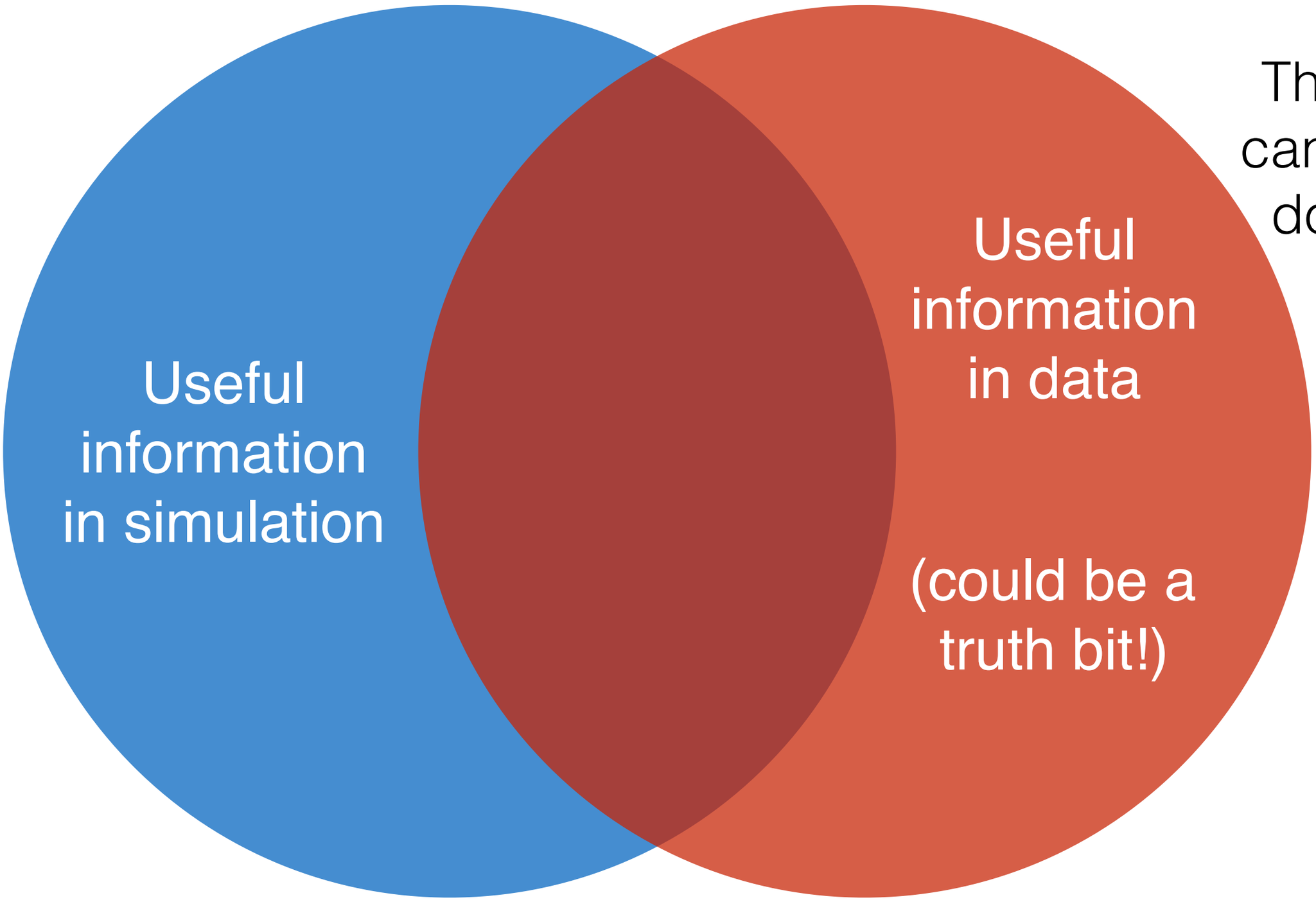
*Derive the classifier in MC, but don't let it use information that is not present in data.*

Classifier can't use information from simulation that is not useful in data and can learn the (data) optimal classifier.

# When option 1 is sub-optimal



The simulation can't use what it doesn't know.



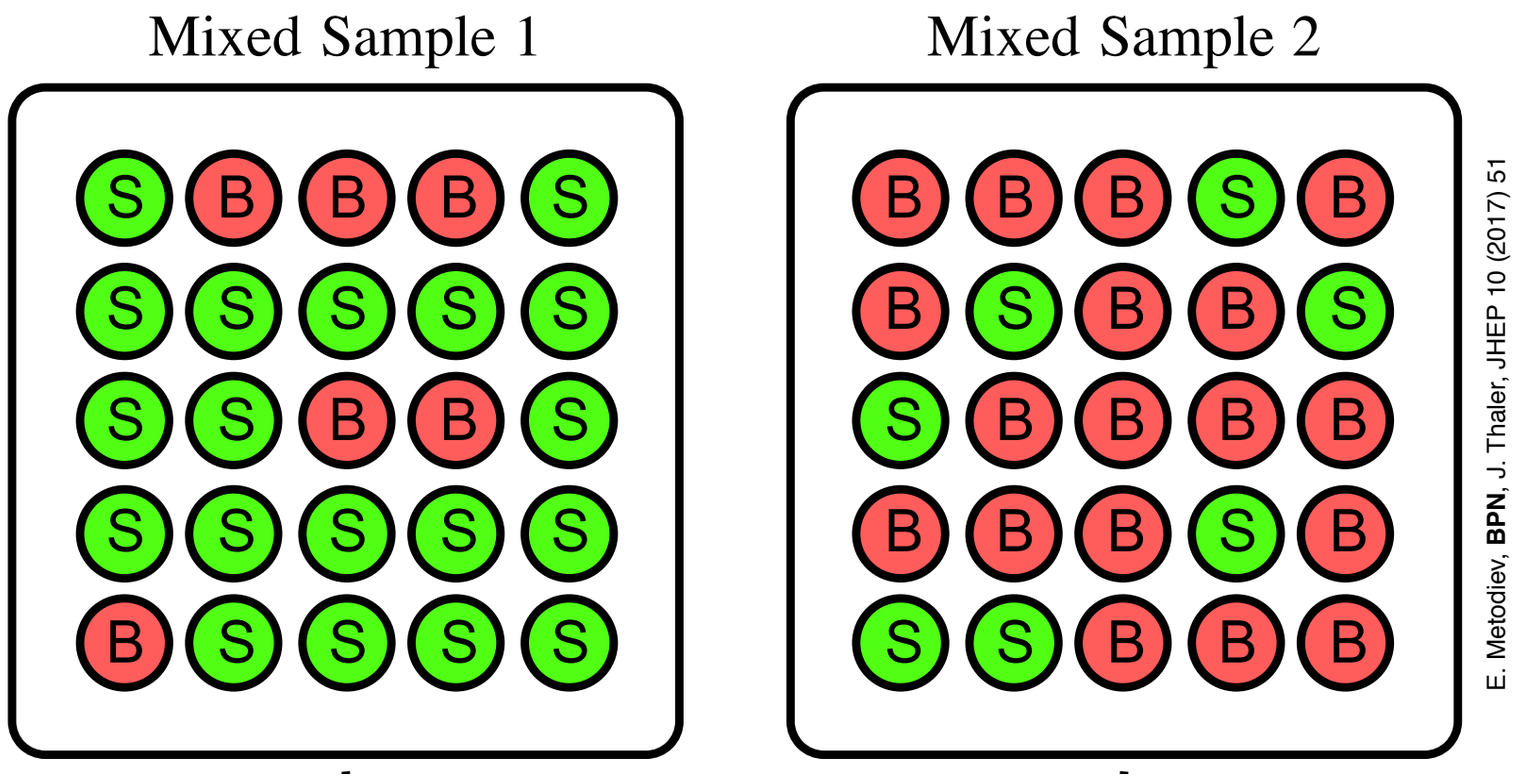

…many other applications of this approach, such as reducing sensitivity to systematic uncertainties, unwanted correlations between features, etc.

# Option 2: Learn from data!



Challenge is that data are **unlabeled**.

**The setup**: suppose you have (at least) two mixed samples, each composed of two classes (say **q** and **g**).




**Assumption**: The two classes are well-defined i.e. **q** in sample 1 is statistically identical to **q** in sample 2.

There is an interesting connection between what I'm calling "weak supervision" and the topic of "label noise".

# Weak sup. option 1: Use class proportions



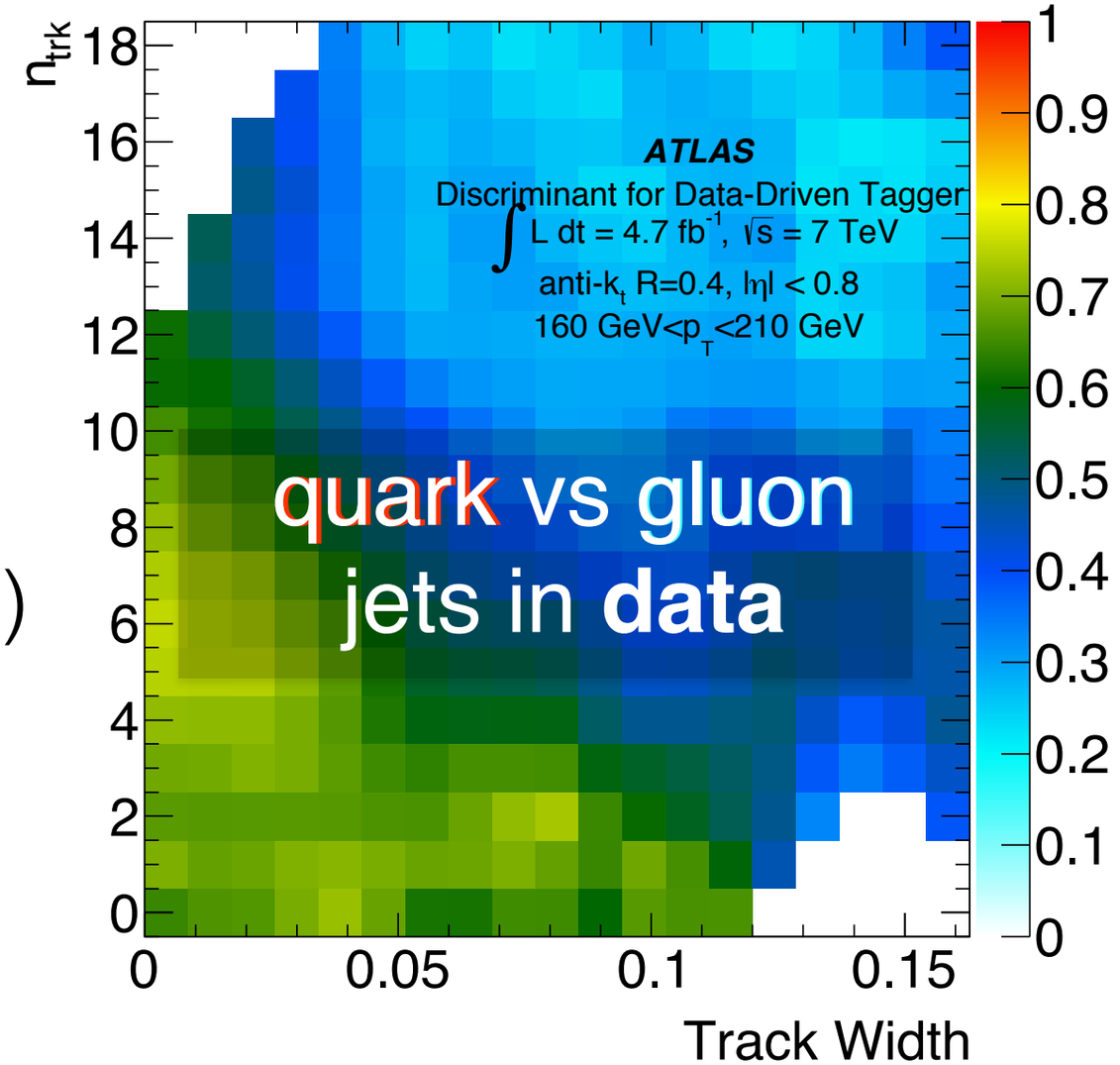
Remember this plot?

$$\text{dijets} = f_q \times Q + (1-f_q) \times G$$

$$\text{Z+jets} = g_q \times Q + (1-g_q) \times G$$

two equations, two unknowns (Q, G)

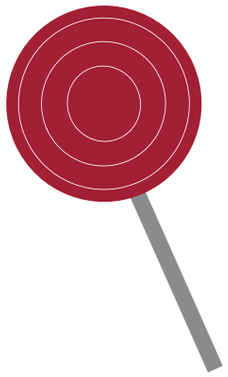
We often know f, g
(from ME + PDF) much better than
full radiation pattern inside jets.




This doesn’t work well when you have more than 2 observables because the templates become sparse.

# Method 1: Learn from Proportions





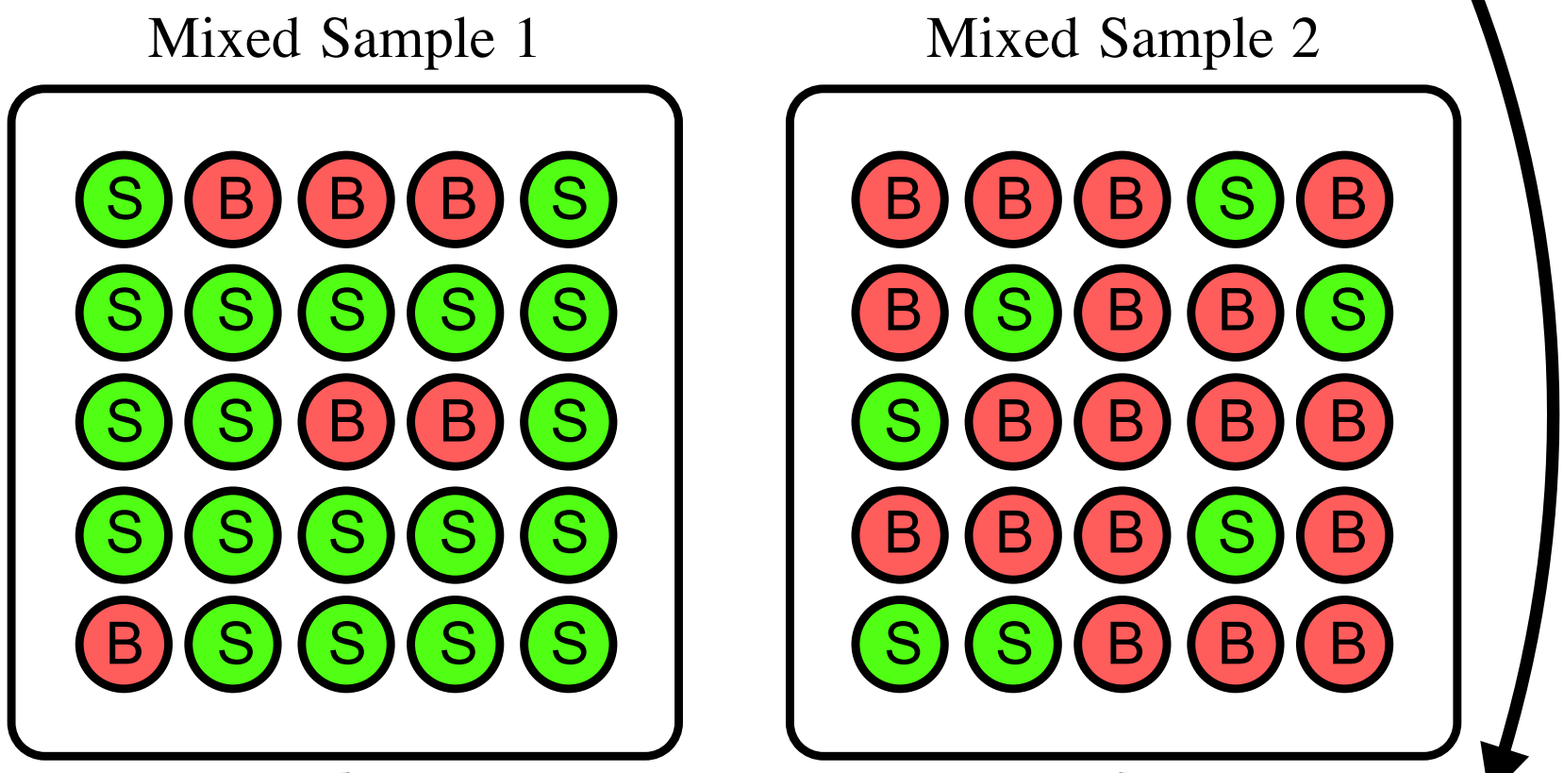
$$f_{\text{full}} = \text{argmin}_{f':\mathbb{R}^n \to \{0,1\}} \sum_{i=1}^{N} \ell\left(f'(x_i) - t_i\right)$$

loss fcn. labels

**LoLiProp**

*Learning from Label Proportions*

Solution: Train using class proportions. Work "on average"



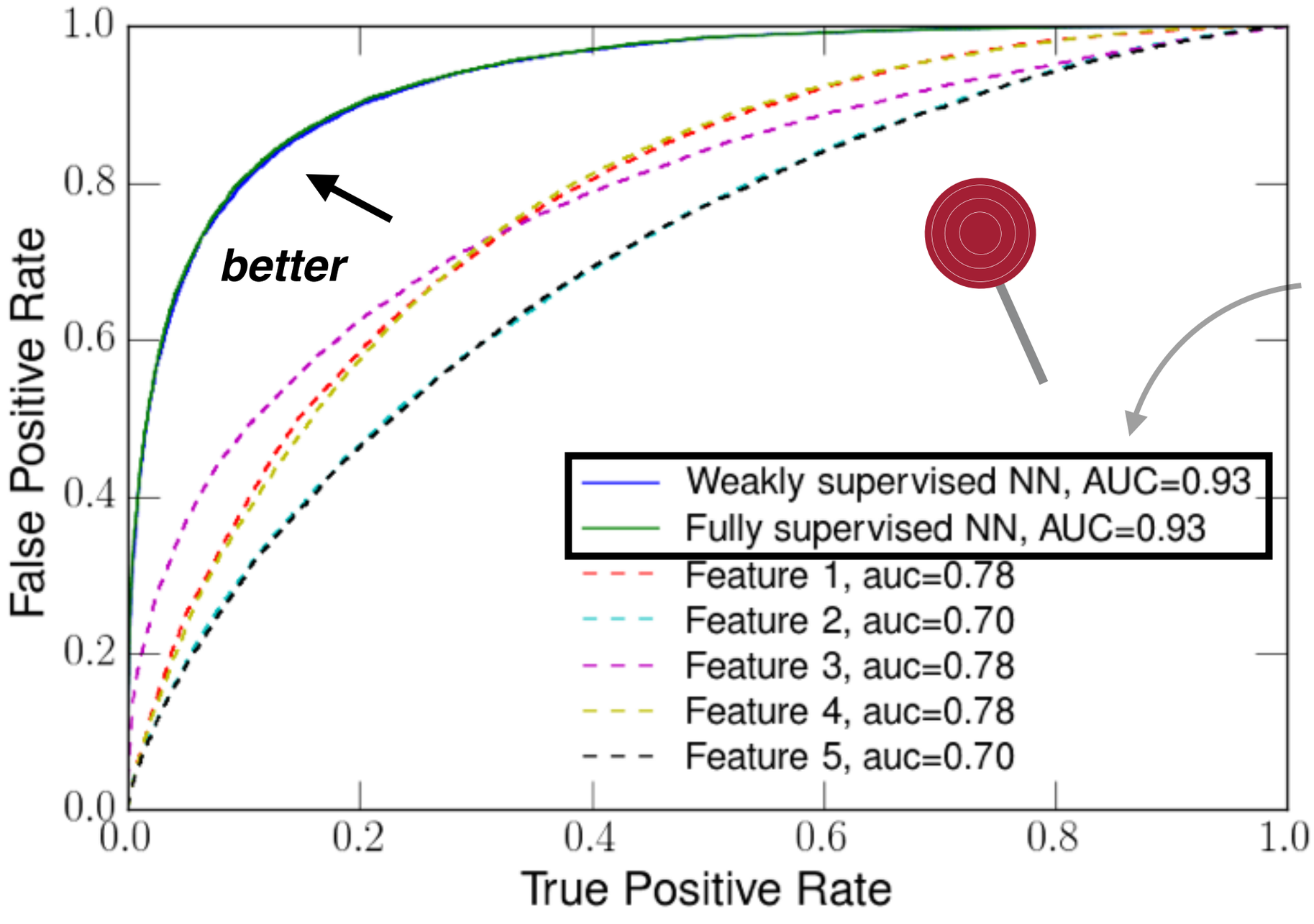

$$f_{\text{weak}} = \text{argmin}_{f':\mathbb{R}^n \to [0,1]} \ell\left(\sum_{i=1}^{N} \frac{f'(x_i)}{N} - y\right)$$

proportions

L. Dery, **BPN**, F. Rubbo, A. Schwartzman, JHEP 05 (2017) 145

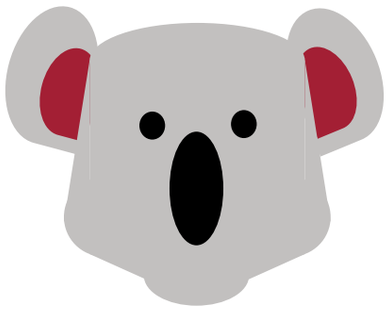
# Works!




1.0
0.8
0.6
0.4
0.2
0.0
False Positive Rate
0.0
0.2
0.4
0.6
0.8
1.0
True Positive Rate
better
area under
the curve
Weakly supervised NN, AUC=0.93
Fully supervised NN, AUC=0.93
Feature 1, auc=0.78
Feature 2, auc=0.70
Feature 3, auc=0.78
Feature 4, auc=0.78
Feature 5, auc=0.70

# Method 2: Learning without Proportions

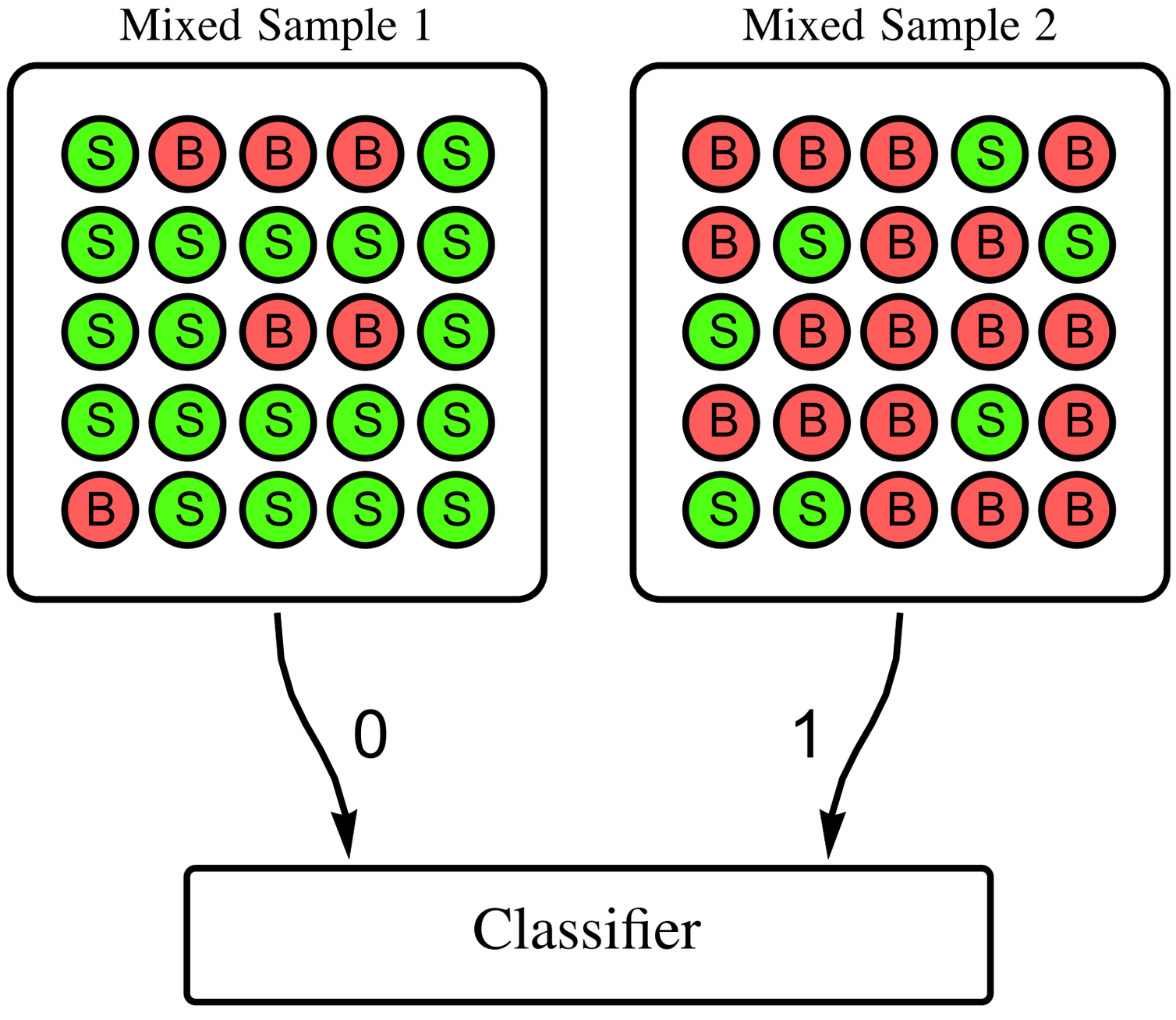




**CWoLa**

*Classification Without Labels*

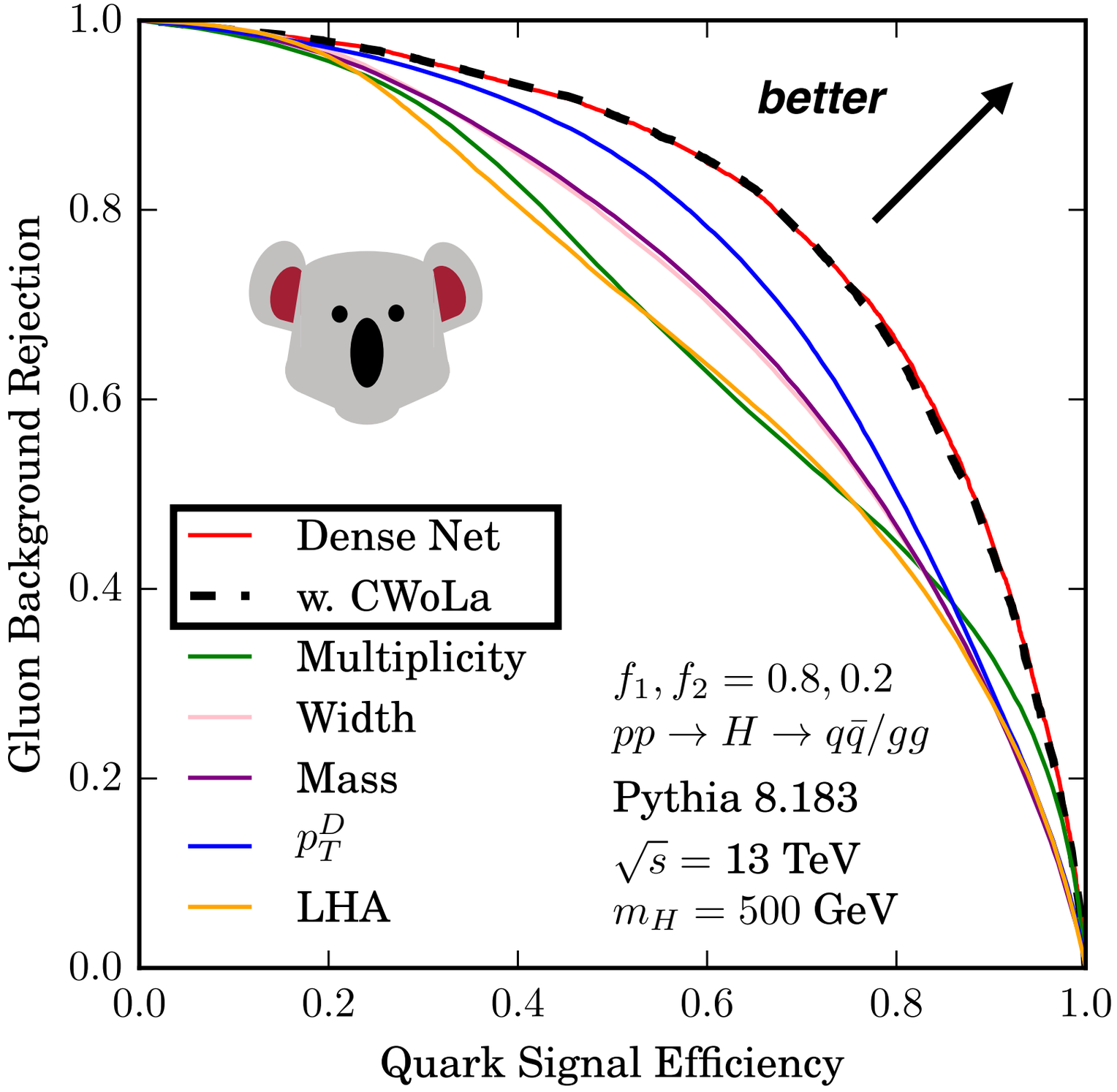
Solution: Train **directly on data** using mixed samples




E. Metodiev, **BPN**, J. Thaler, JHEP 10 (2017) 51

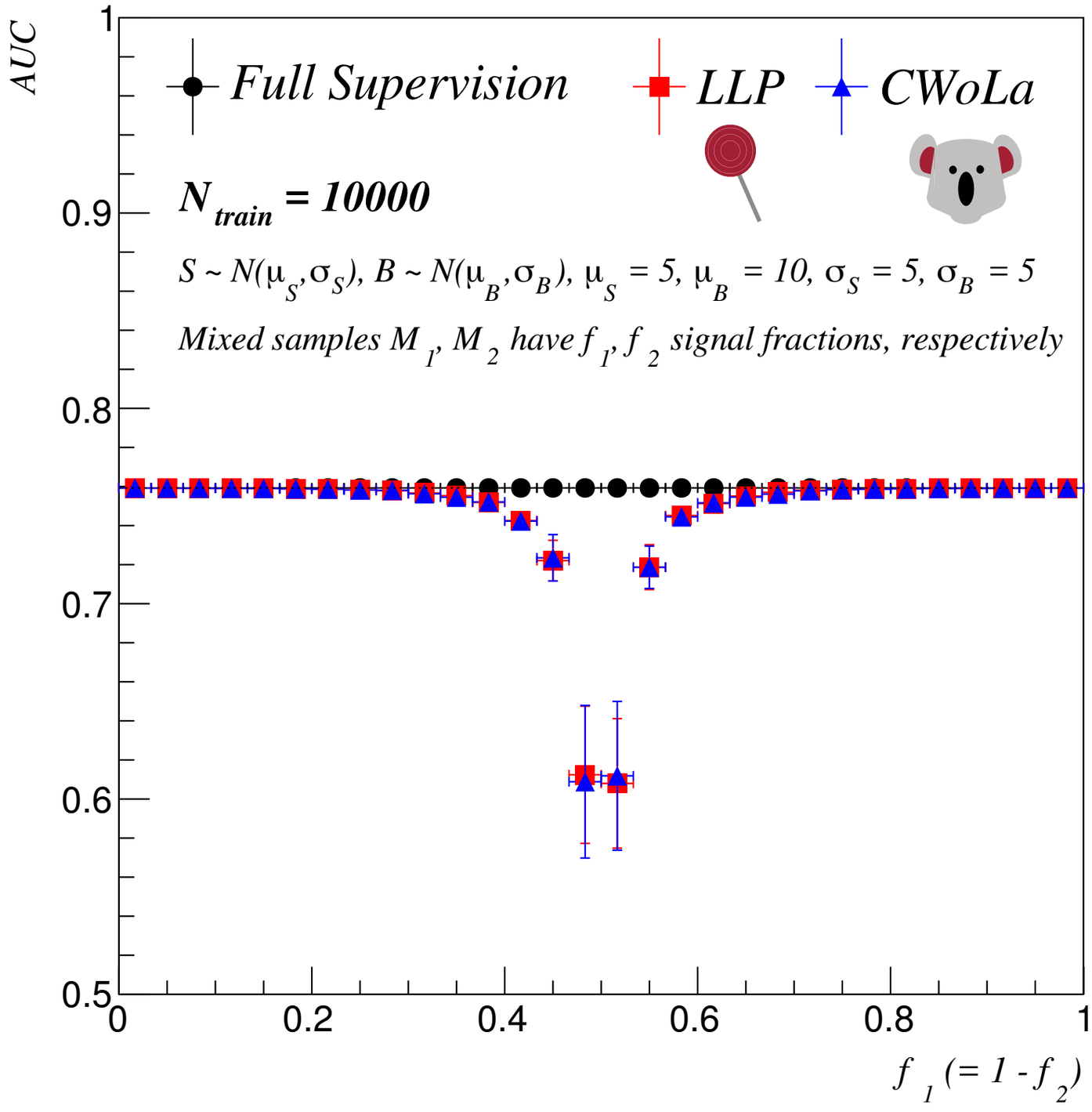
# Works!




1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
Gluon Background Rejection
Quark Signal Efficiency
better
Dense Net
w. CWoLa
Multiplicity
Width
Mass
$p_T^D$
LHA
$f_1, f_2 = 0.8, 0.2$
$pp \to H \to q\bar{q}/gg$
Pythia 8.183
$\sqrt{s} = 13$ TeV
$m_H = 500$ GeV

# A note about training statistics






signal fraction of mixed sample 1

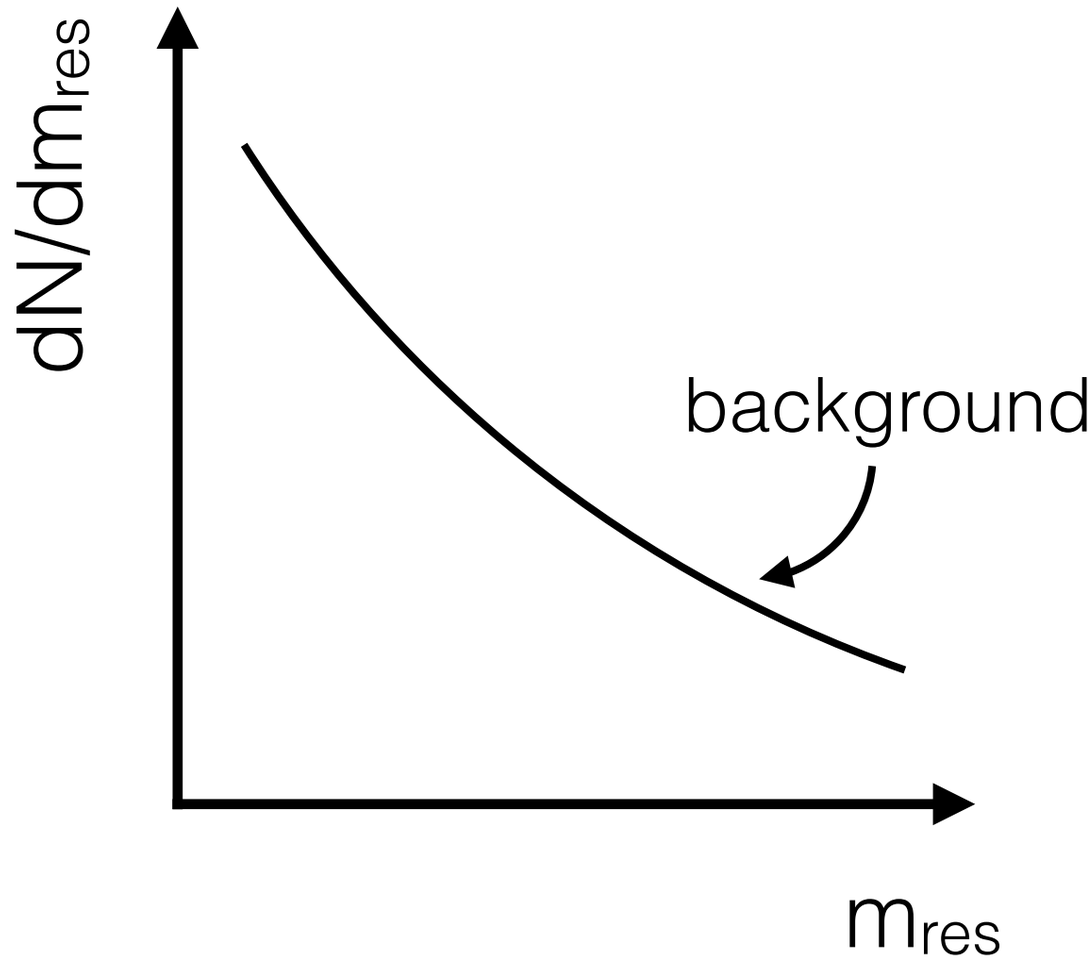
Can't learn when the two proportions are the same.

The more similar they are, the worse the performance.

(lower effective statistics)

# CWoLa Hunting for new particles

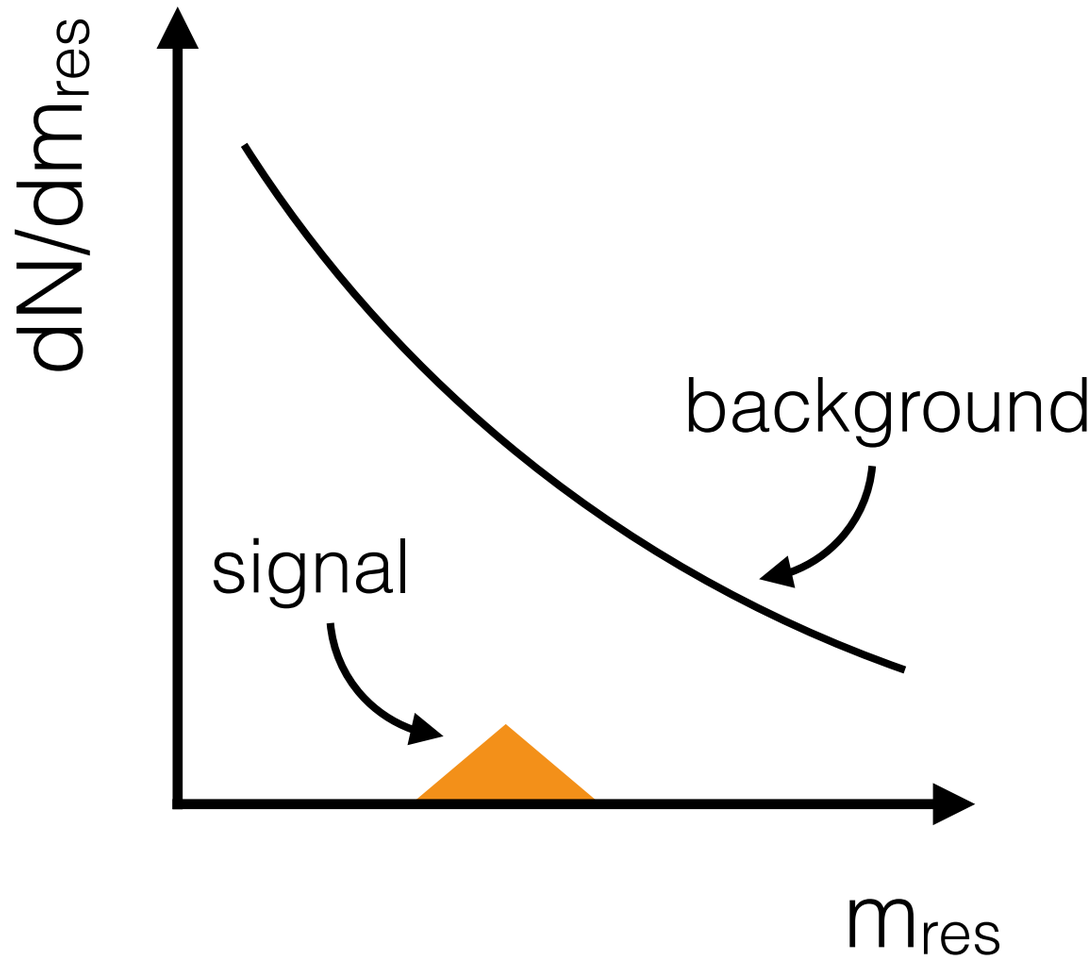





Assumption: there is a feature that we know about where the background is smooth and the signal (if it exists) is localized.

# CWoLa Hunting for new particles

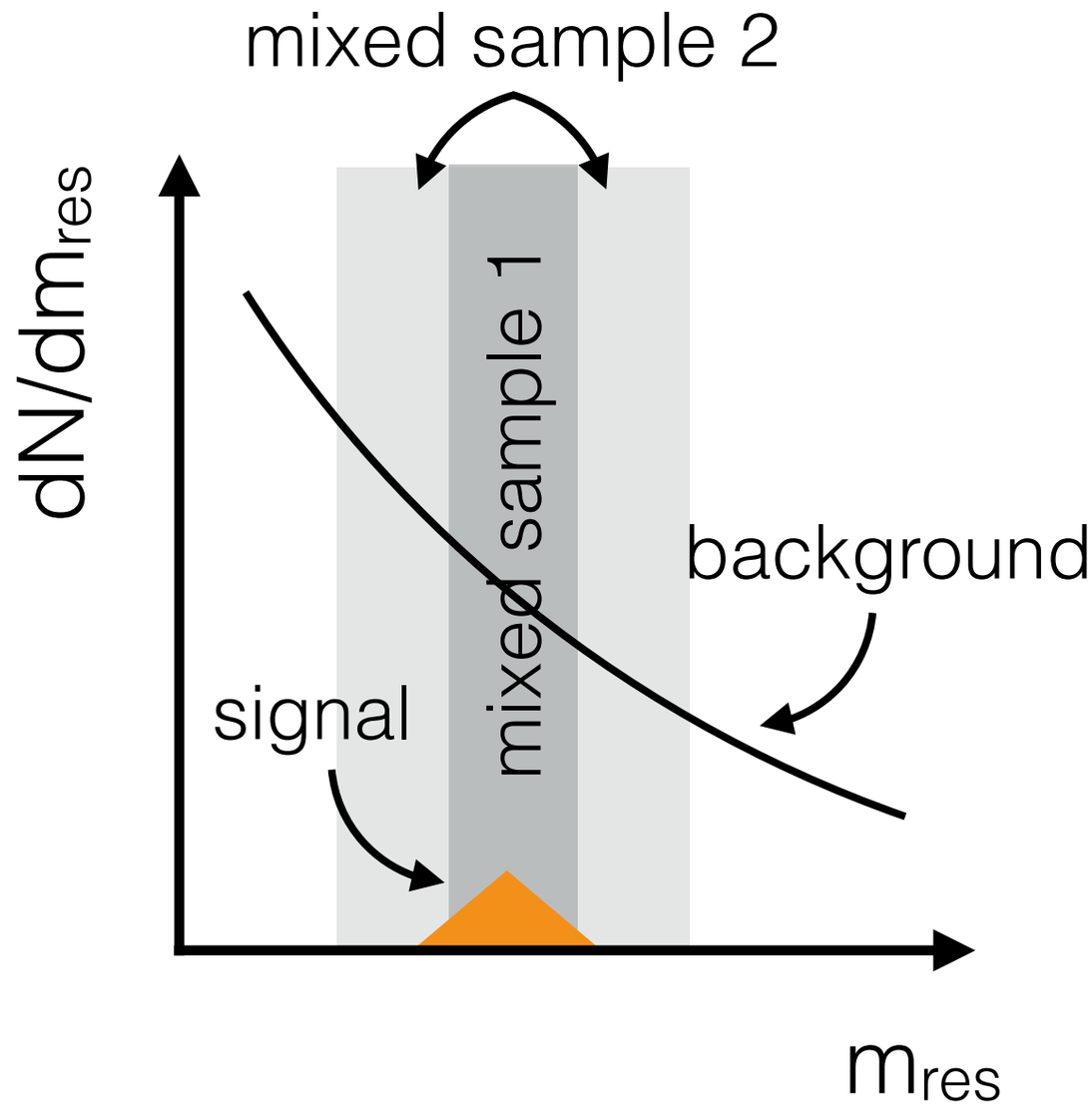





Assumption: there is a feature that we know about where the background is smooth and the signal (if it exists) is localized.

# CWoLa Hunting for new particles

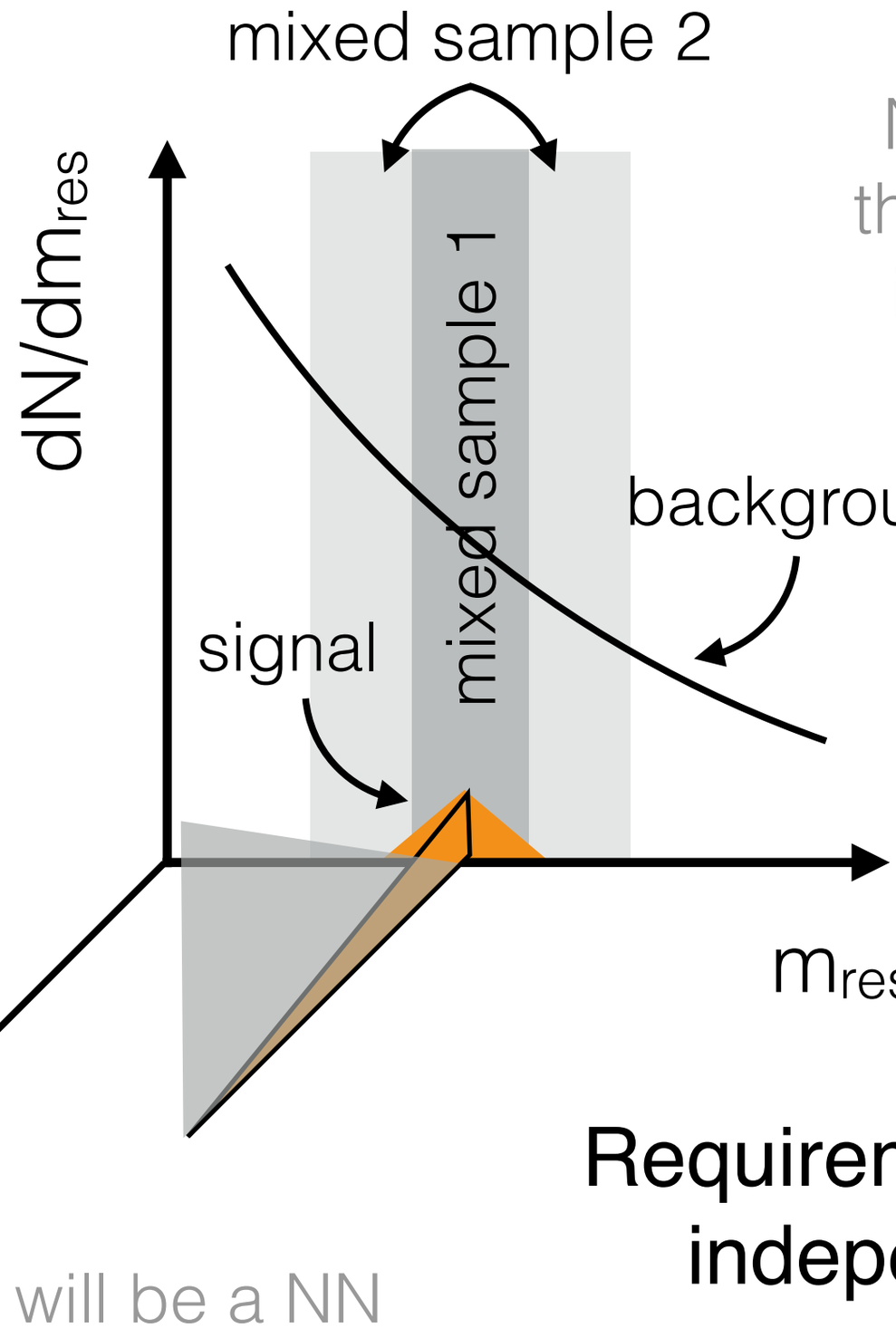





We don’t know where the signal is, but for a given hypothesis, we can make signal windows and sidebands.

# CWoLa Hunting for new particles






N.B. it is okay that there is some signal in the sidebands!

Other features can then be used to train CWoLa.

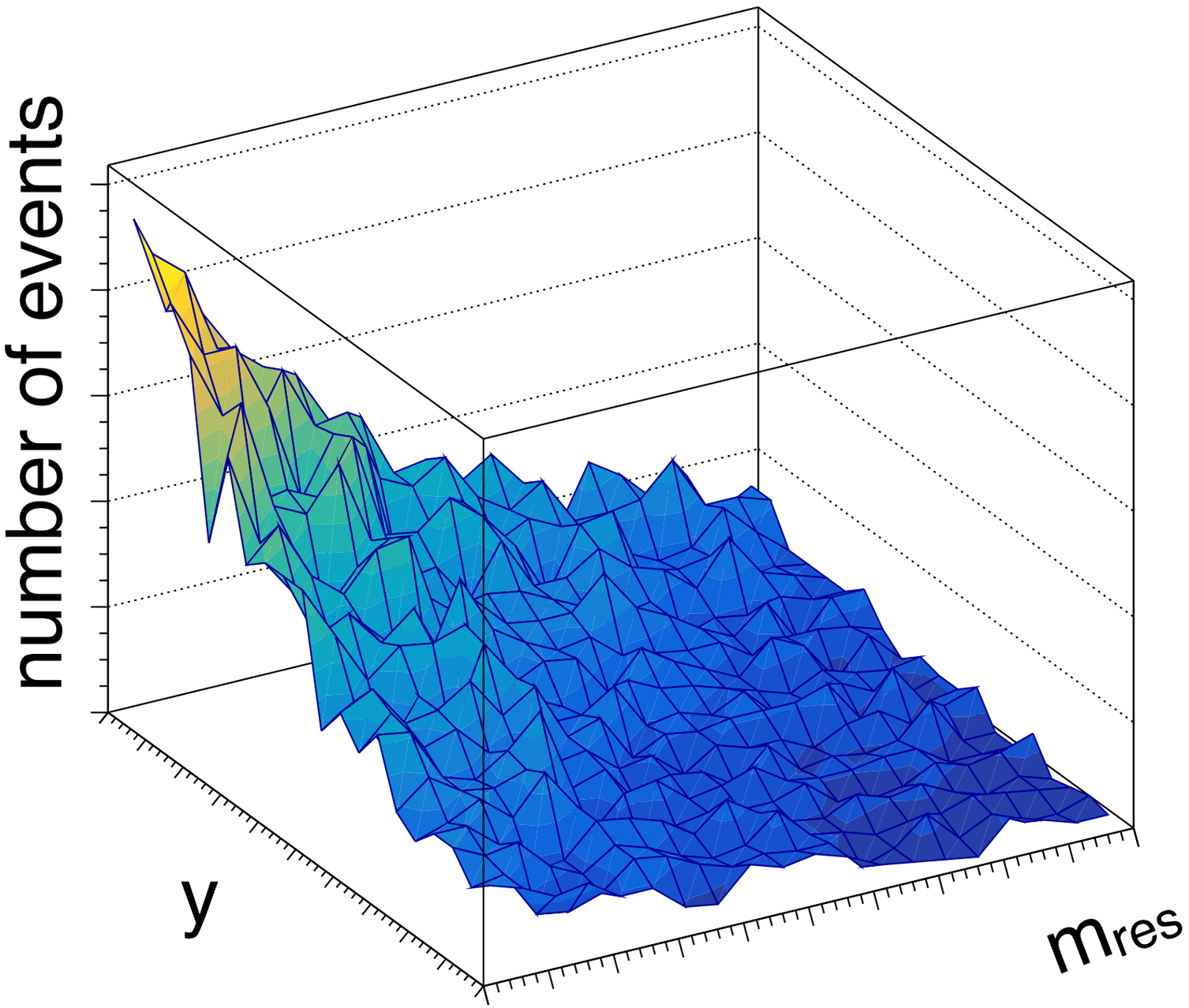
Requirement: y is (nearly) independent of $m_{res}$.

# Overtraining & Look Elsewhere Effect*



Naively, pay a huge LEE penalty because y can be high-dimensional.

*i.e. you will sculpt lots of bumps!*



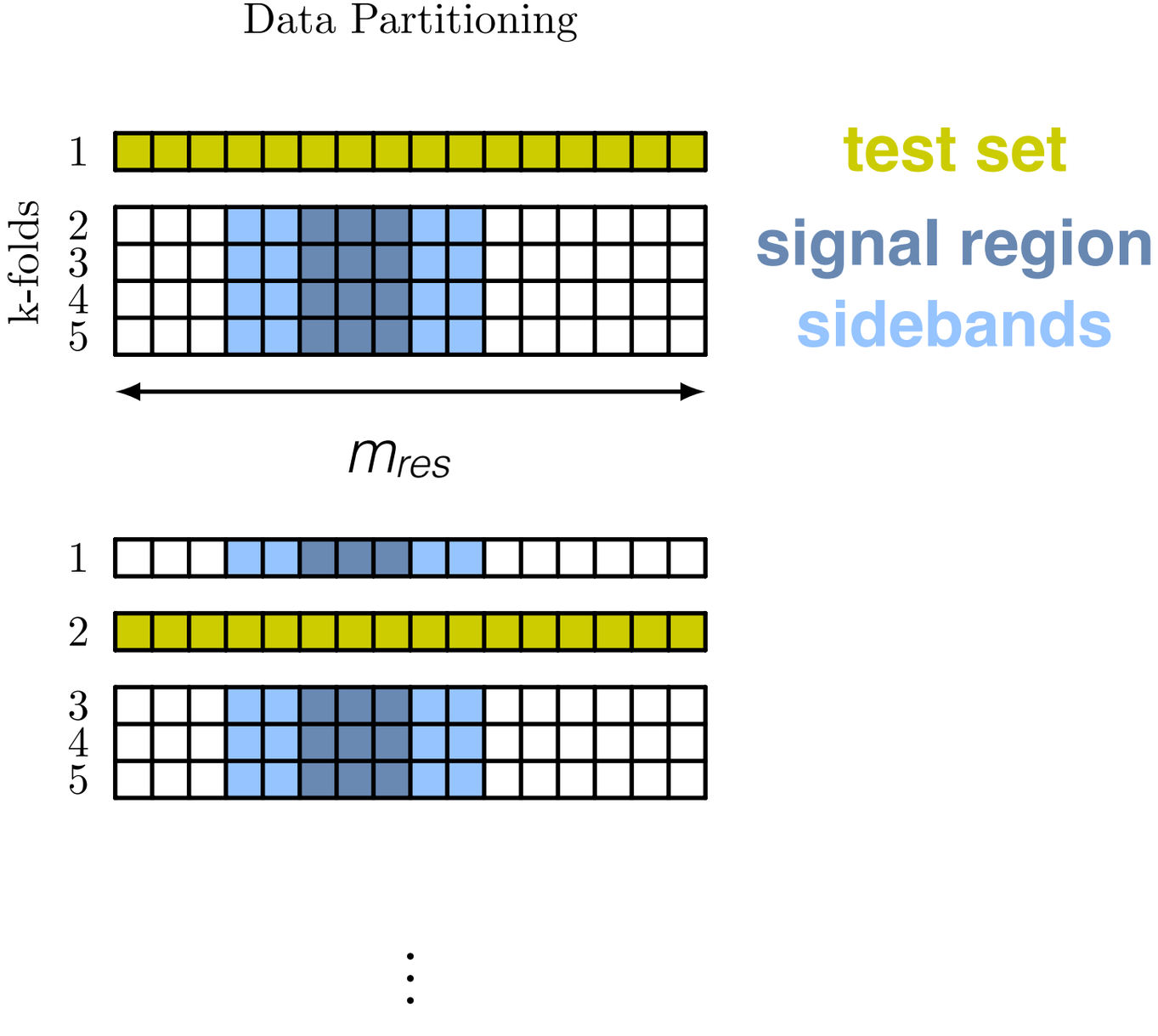

Solution: **(nested) cross-training**

*you may know this as the multiple comparisons problem

# Nested cross-training

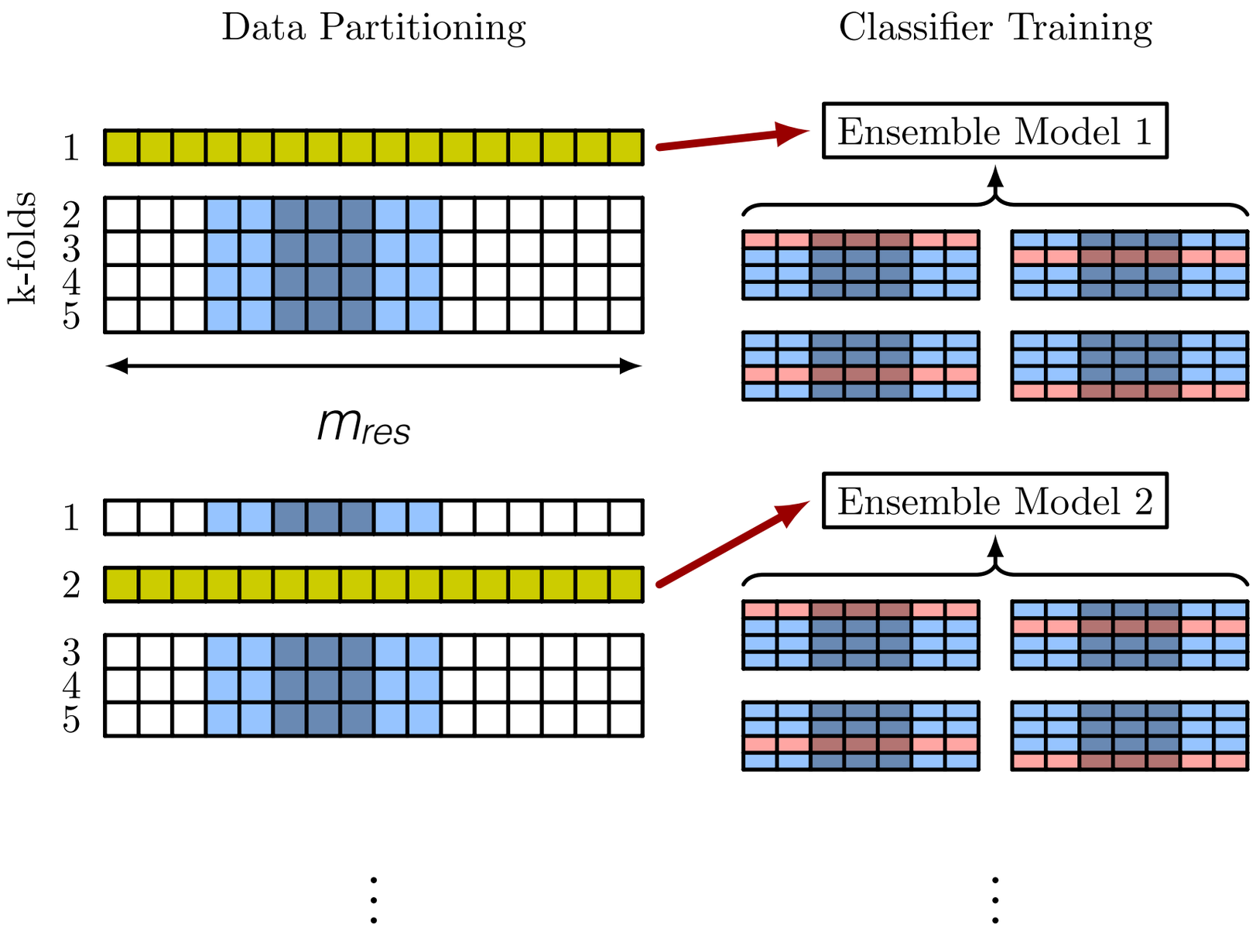


(1) Divide the entire dataset into k-folds.



# Nested cross-training

## (2) Train CWoLa classifiers.



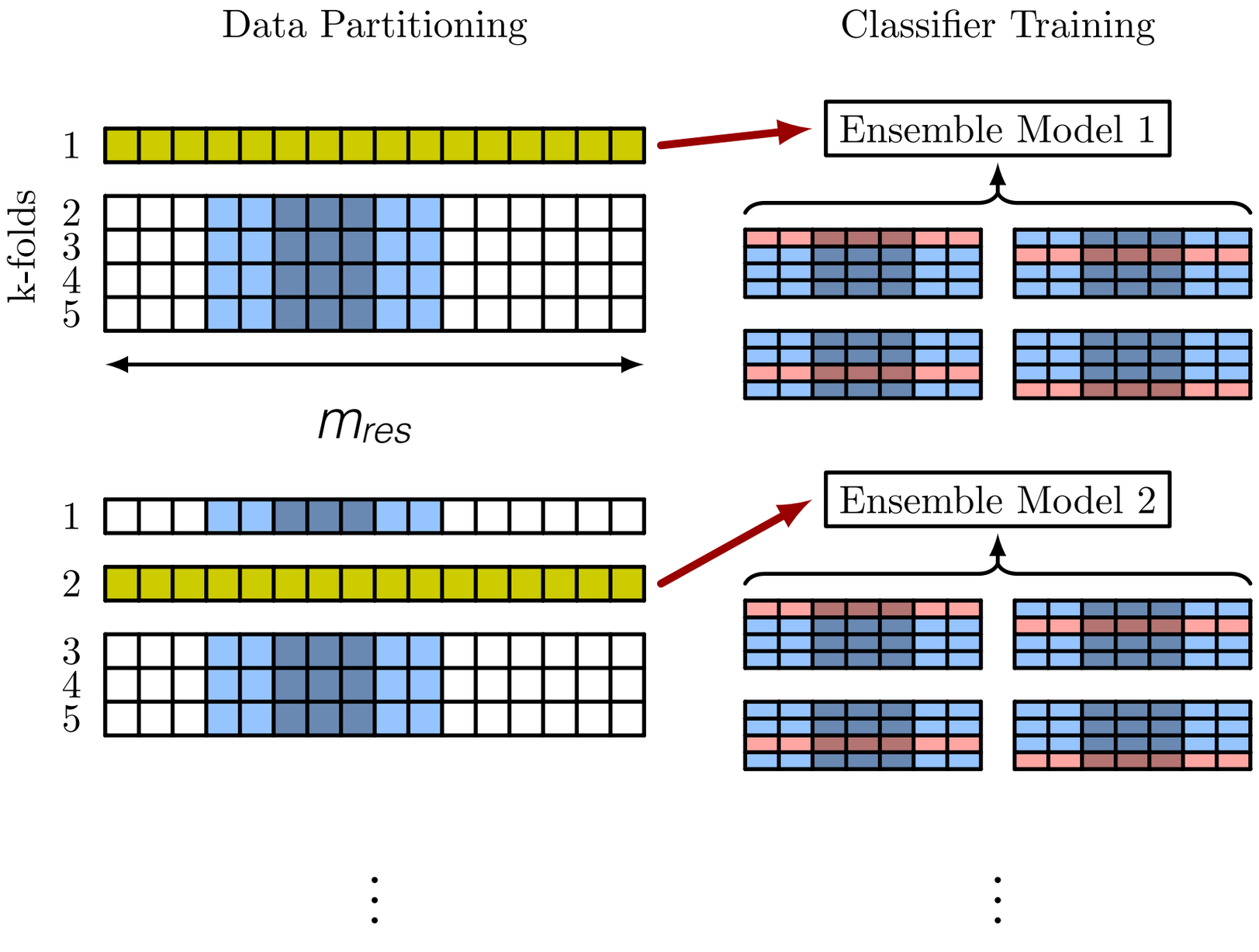

Train signal versus sideband k-1 times

rotating the validation set

*In practice, also train many networks with a different initialization and take the best one per k-1 rotation.*

# Nested cross-training

## (2) Train CWoLa classifiers.

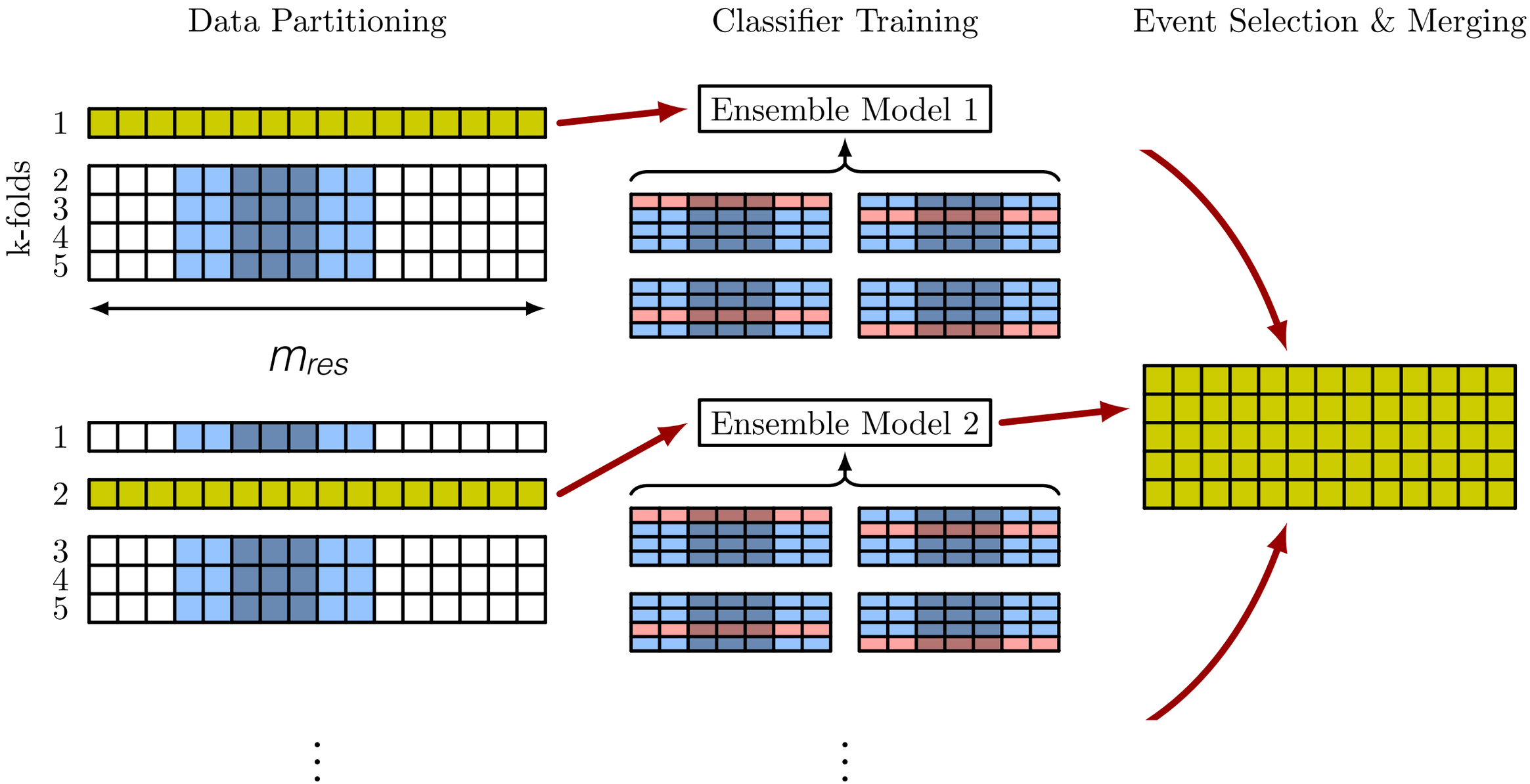



The Ensemble Model is just the average of the four networks.

*Data fluctuations will cancel destructively while signal interferes constructively.*

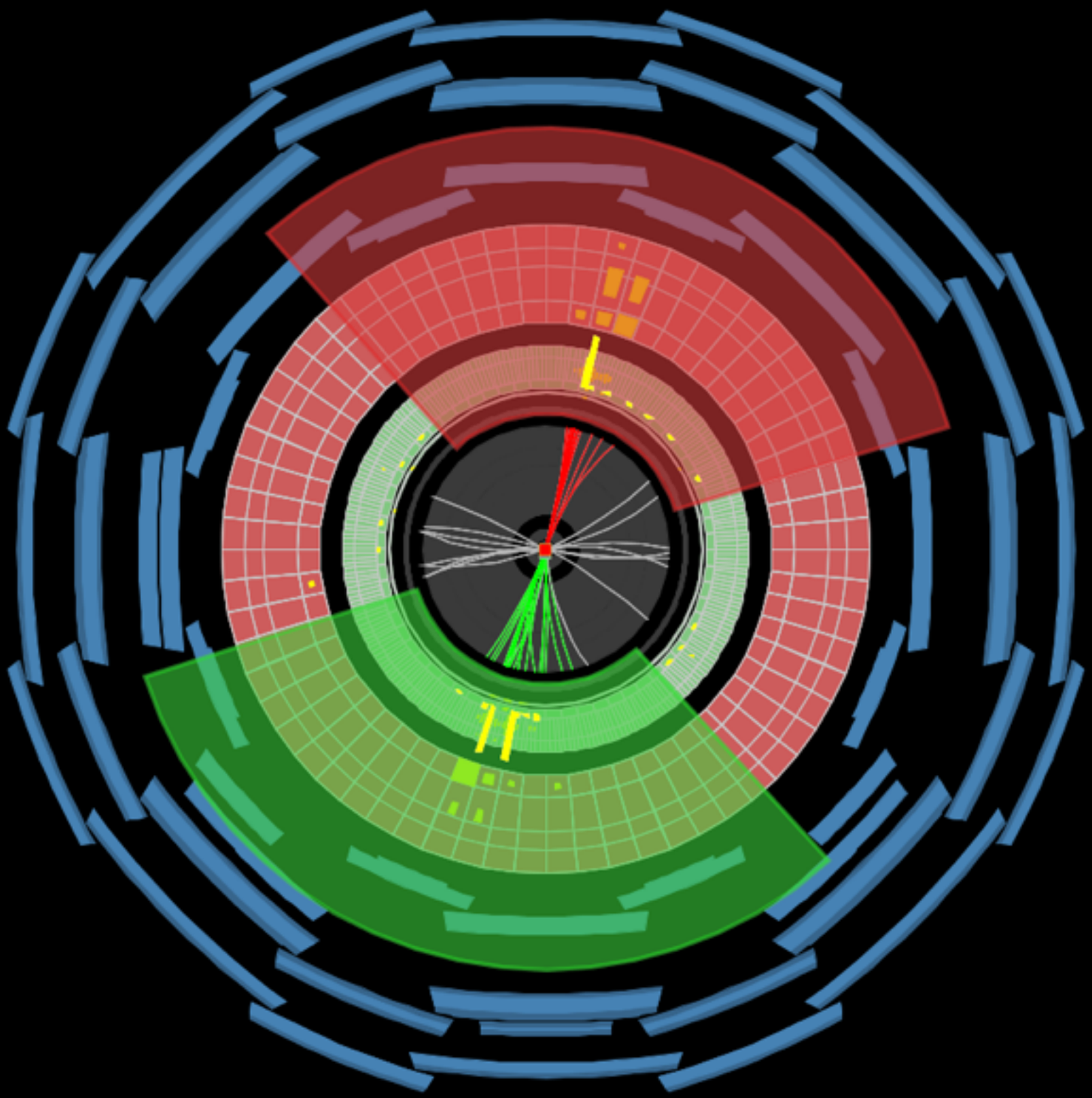
# Nested cross-training

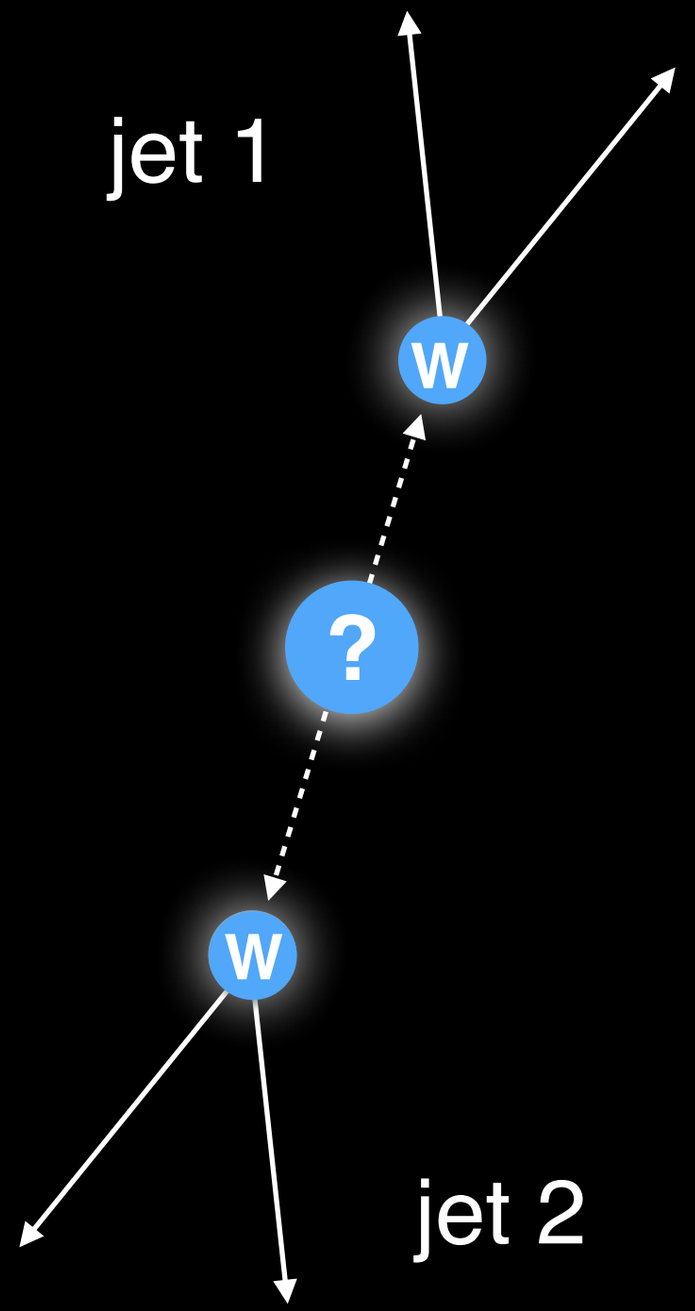
(3) Apply classifiers to holdout test sets and sum.



# Example: two-jet search

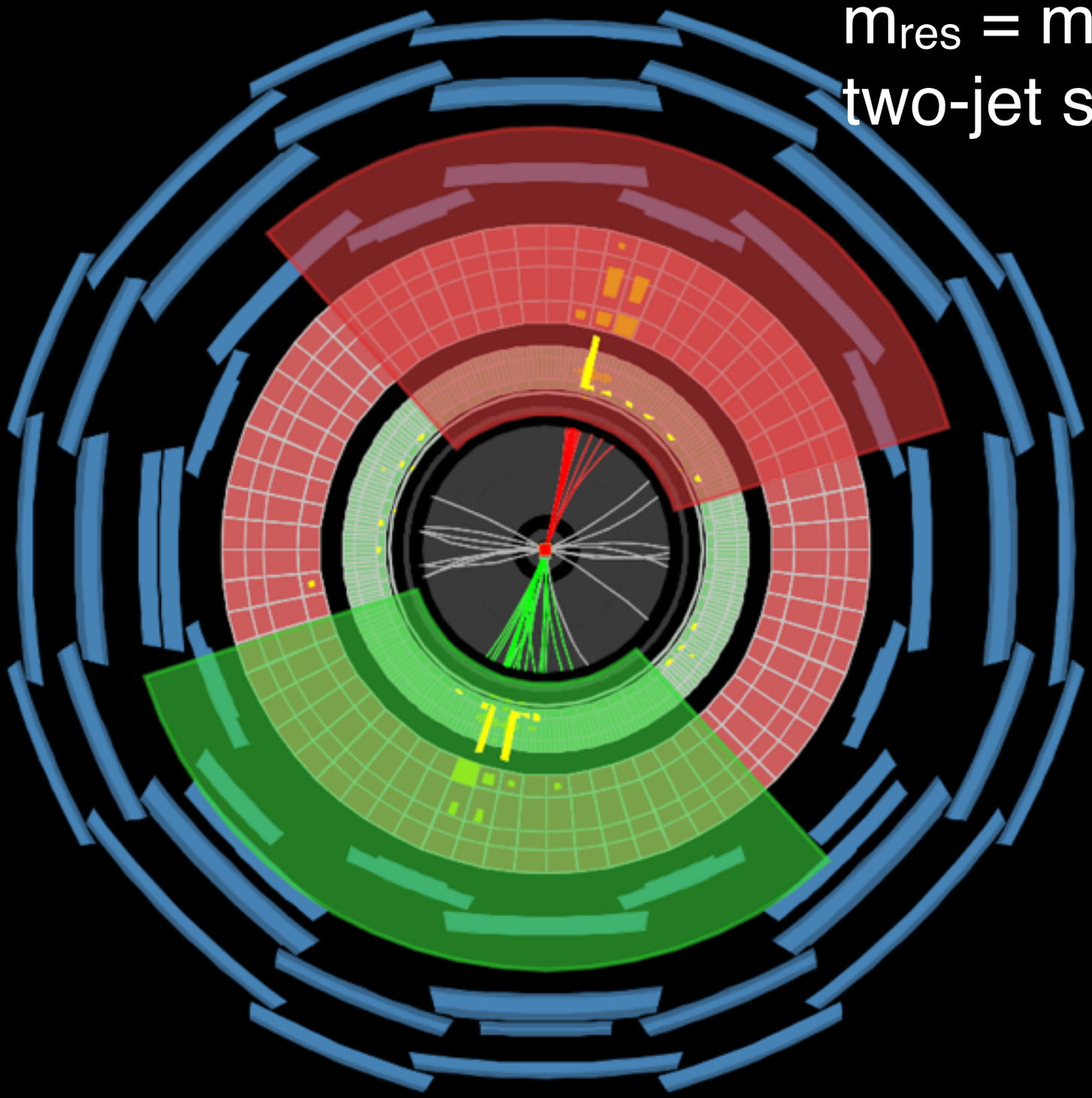


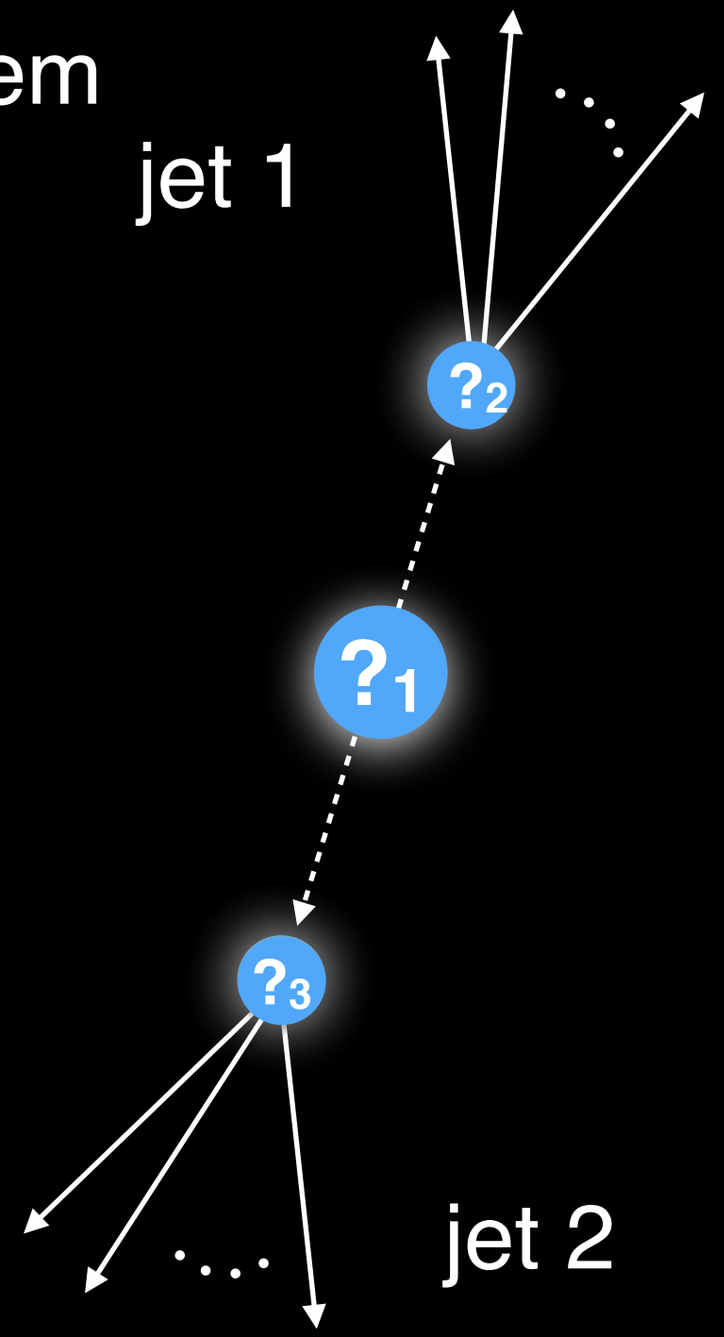




# Example: two-jet search

$m_{res}$ = mass of two-jet system

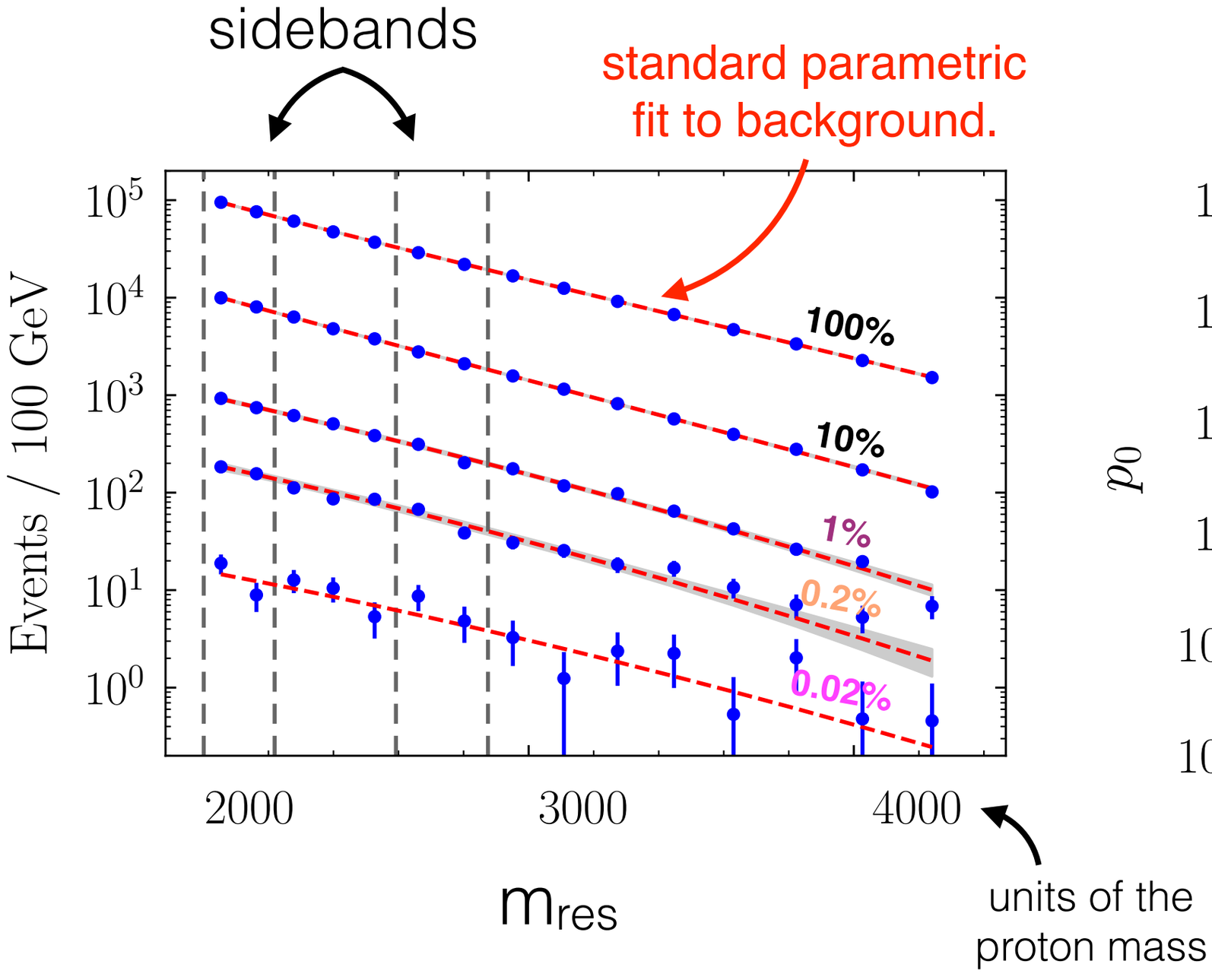


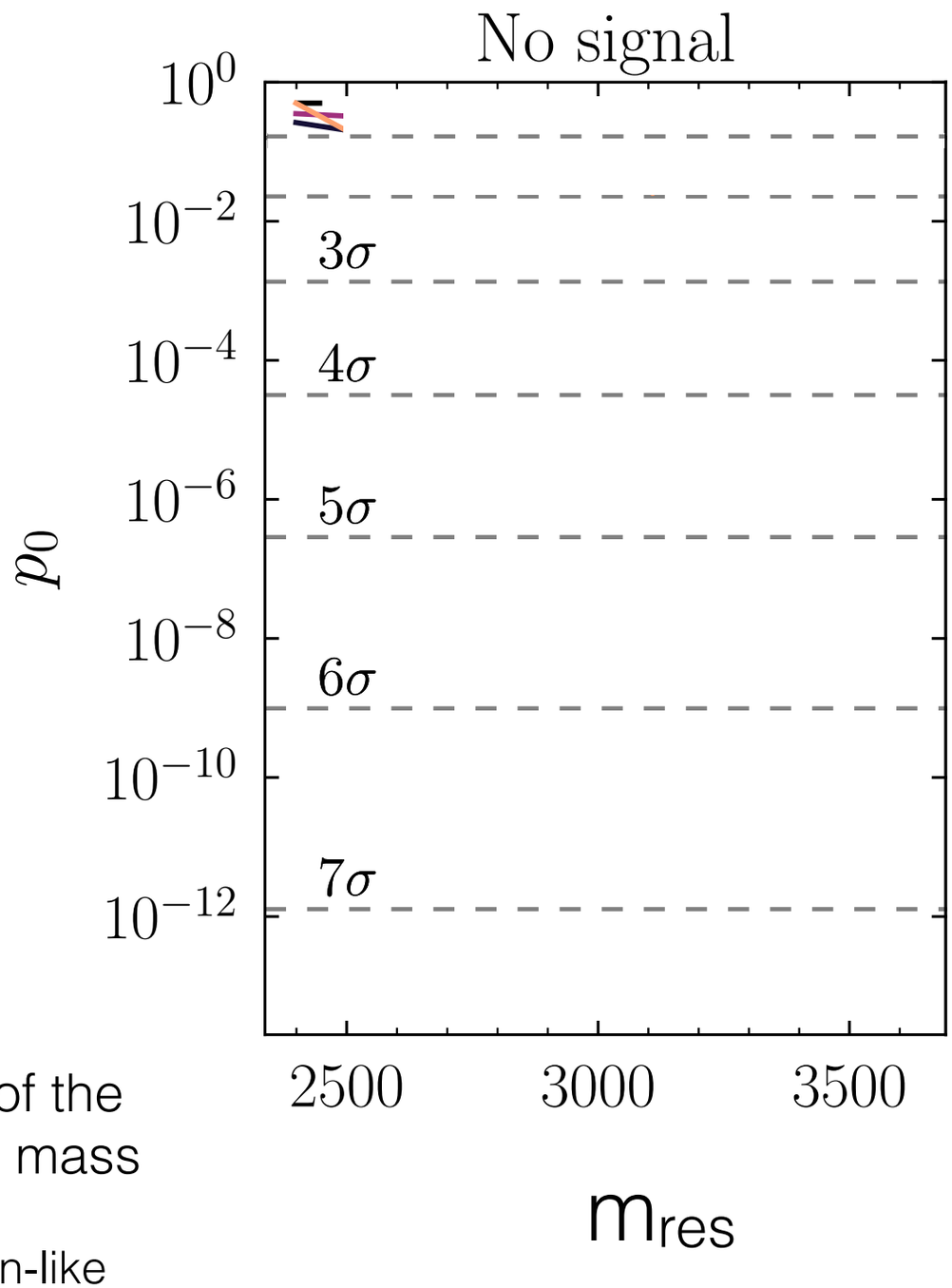



y = many features of the two jets

# Example: two-jet search






no cut on NN

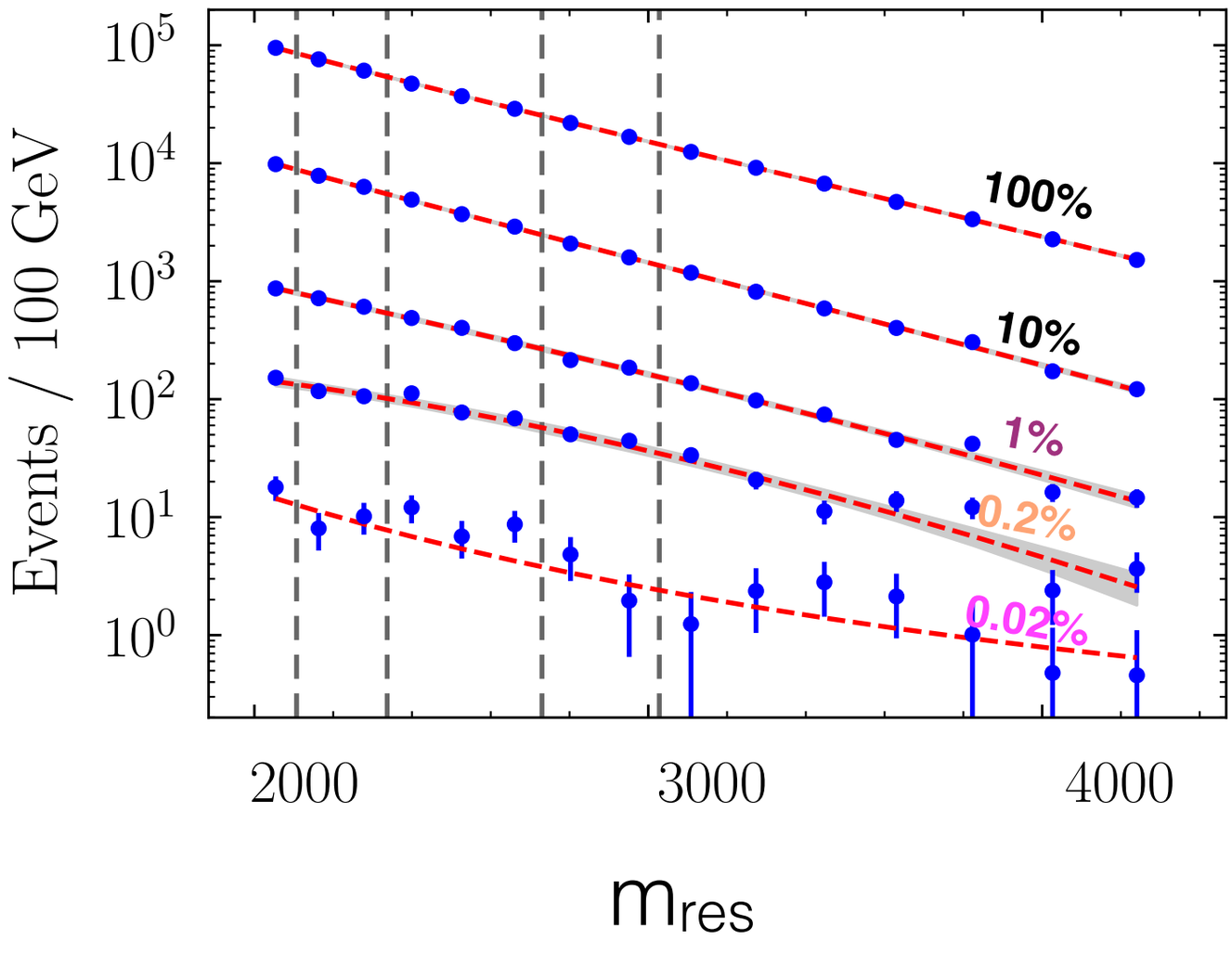
most 10% signal-region-like

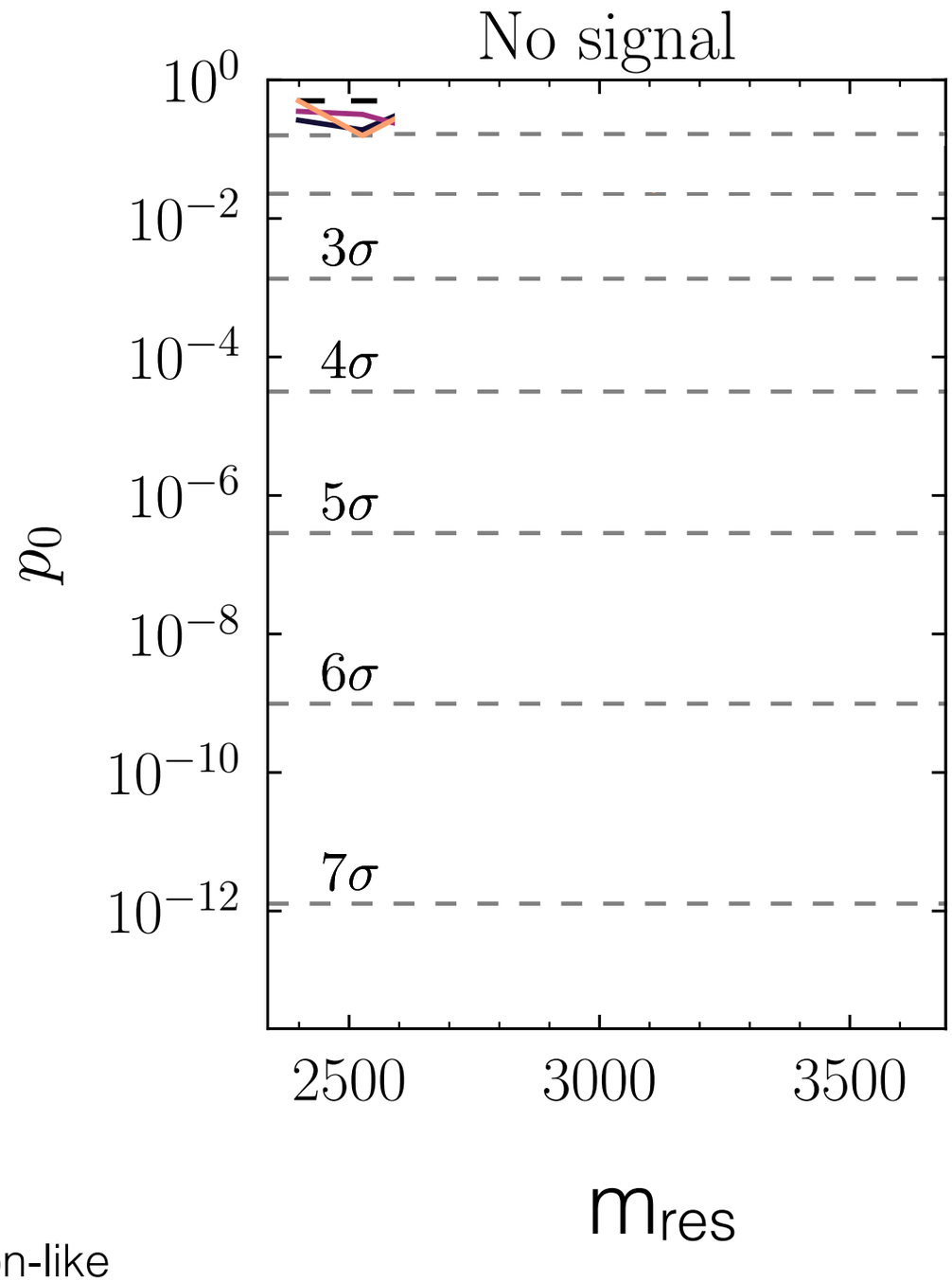
most 1% signal-region-like

most 0.2% signal-region-like

# Example: two-jet search



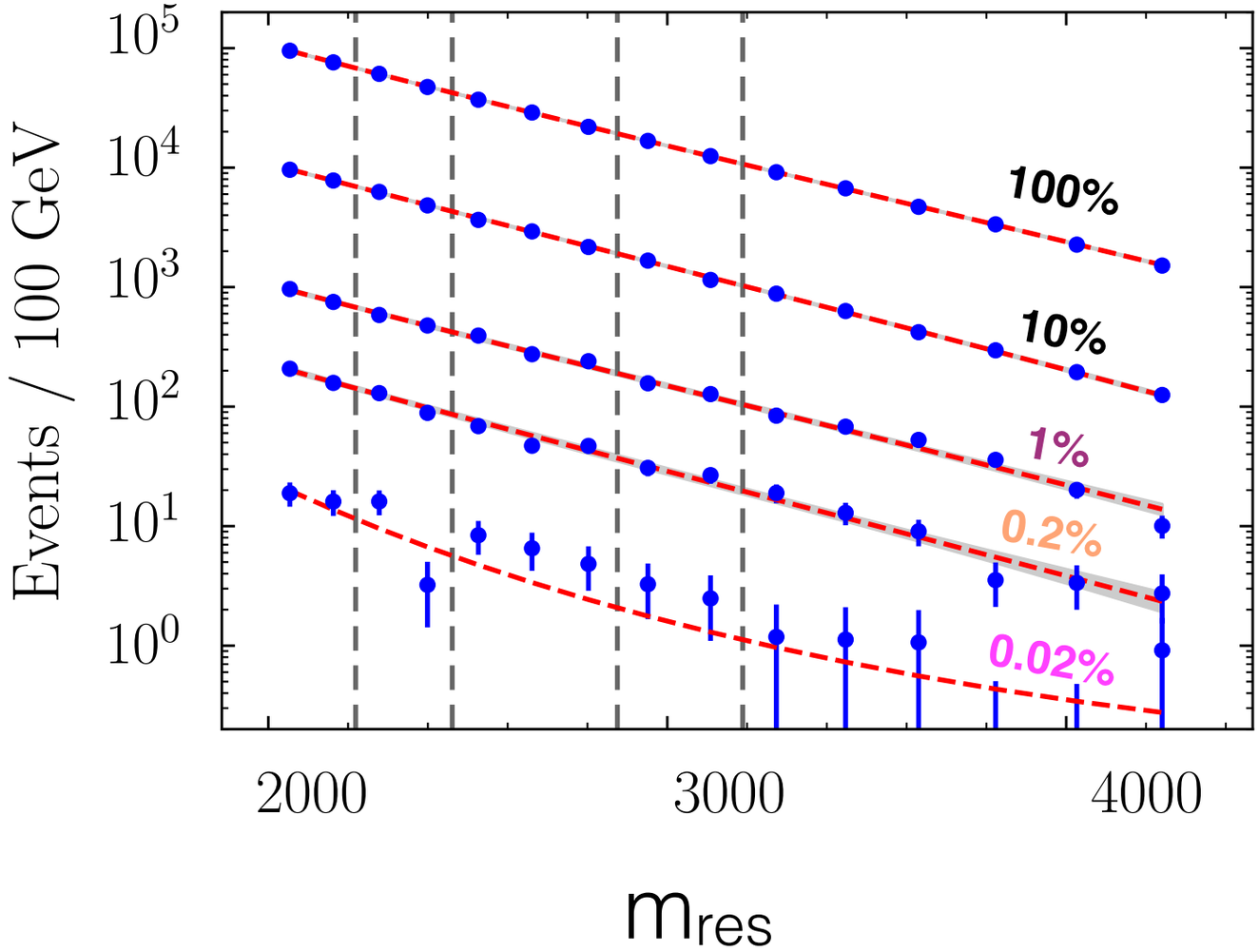


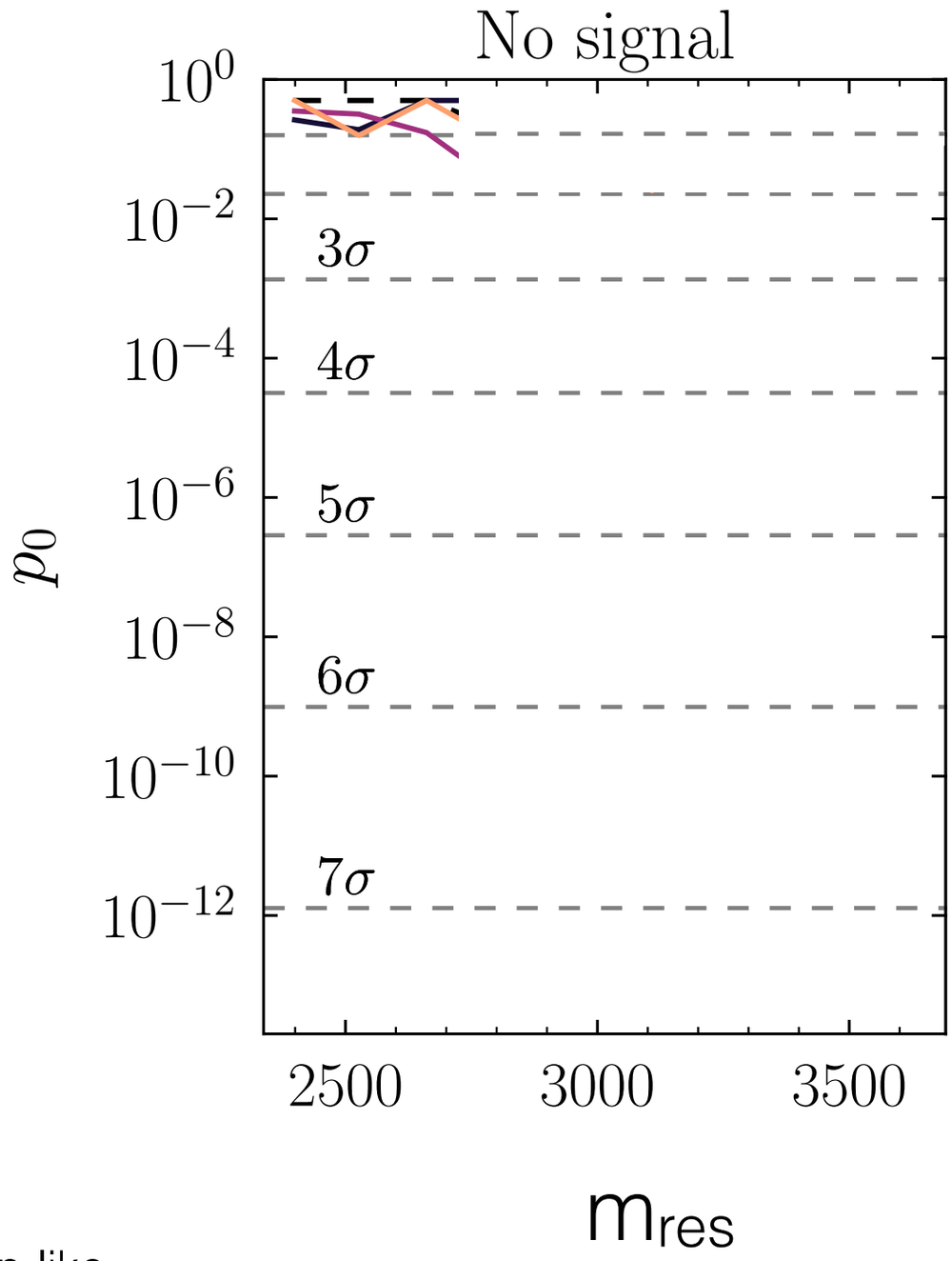




- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

# Example: two-jet search

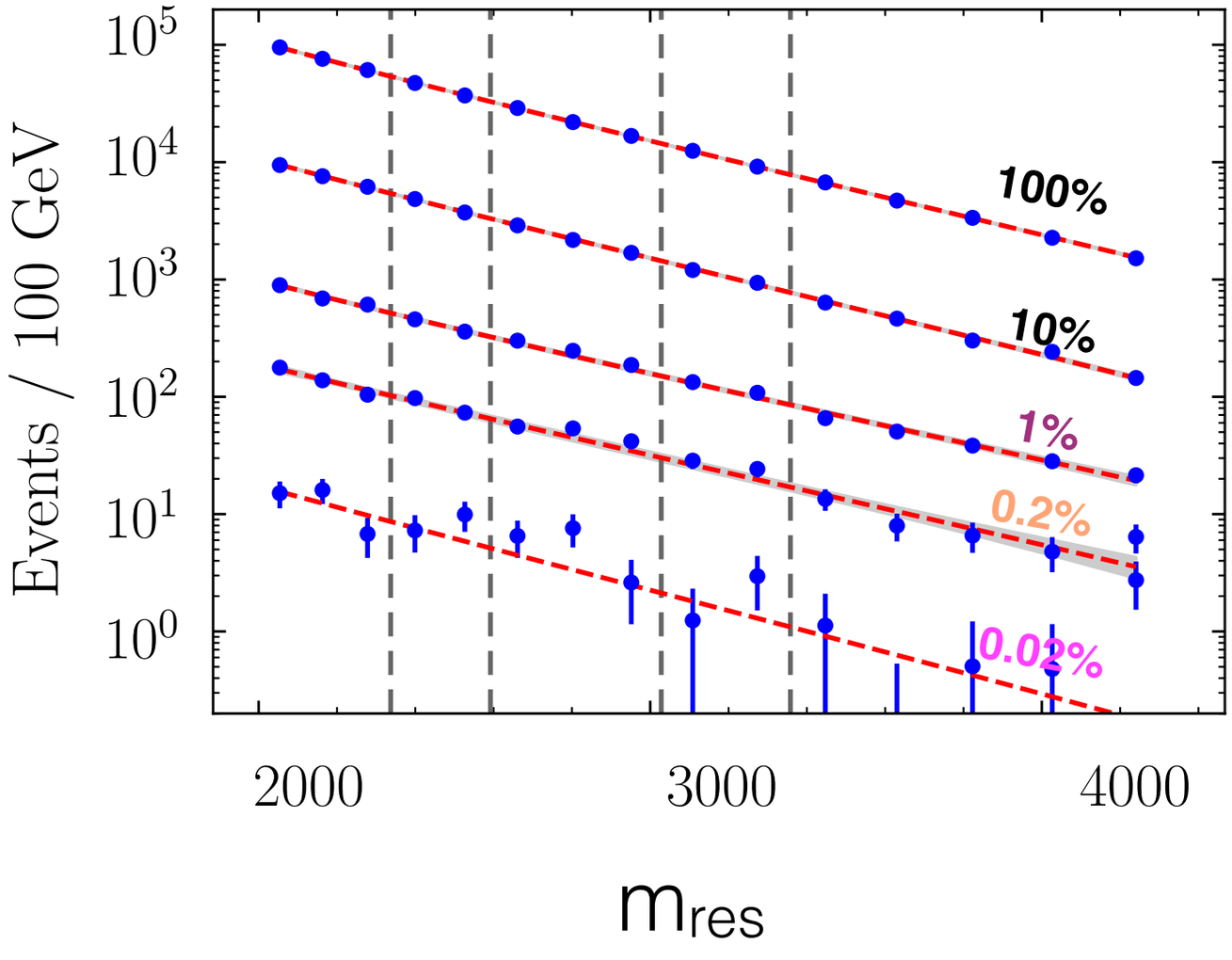


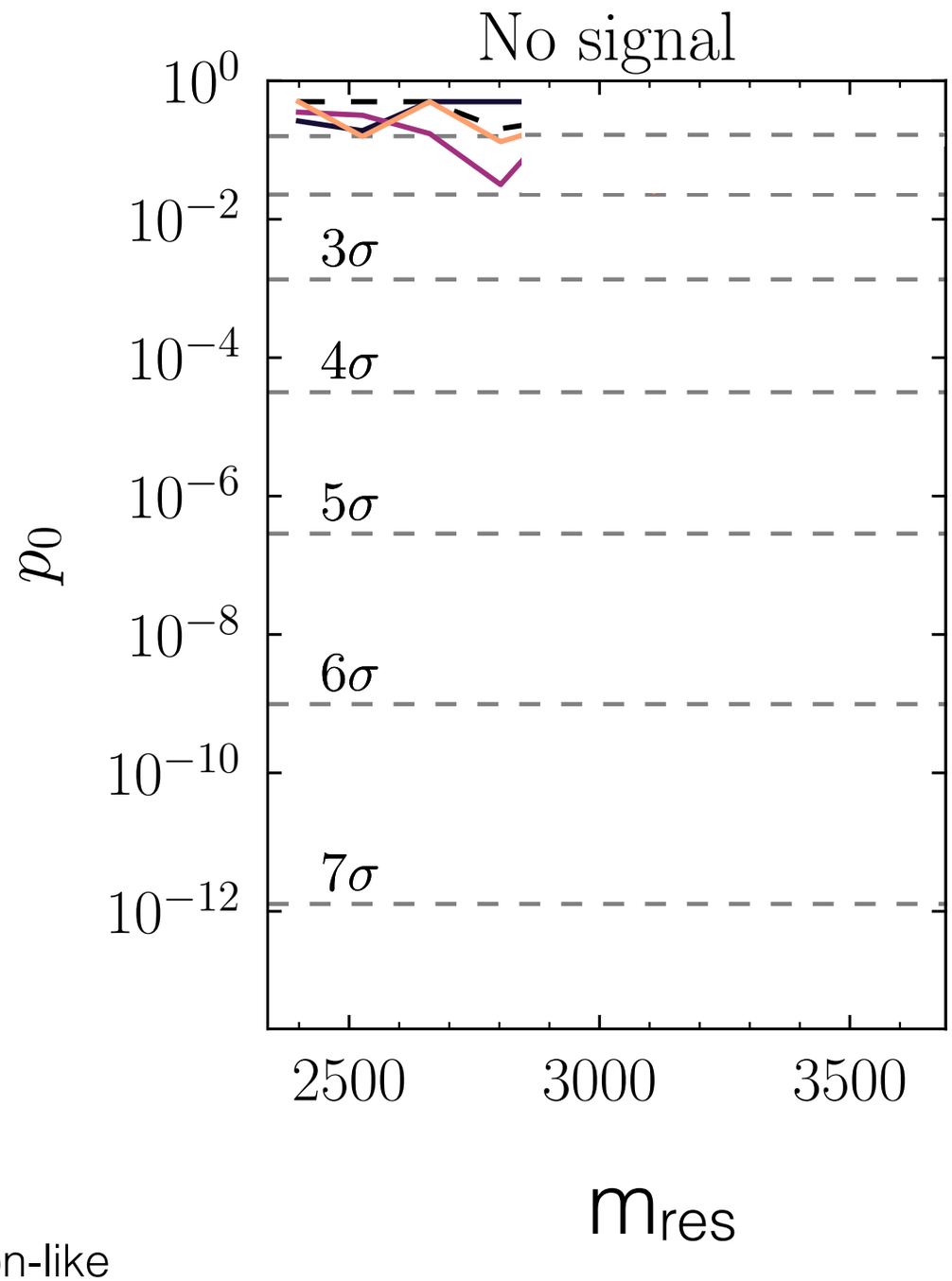



# Example: two-jet search






no cut on NN

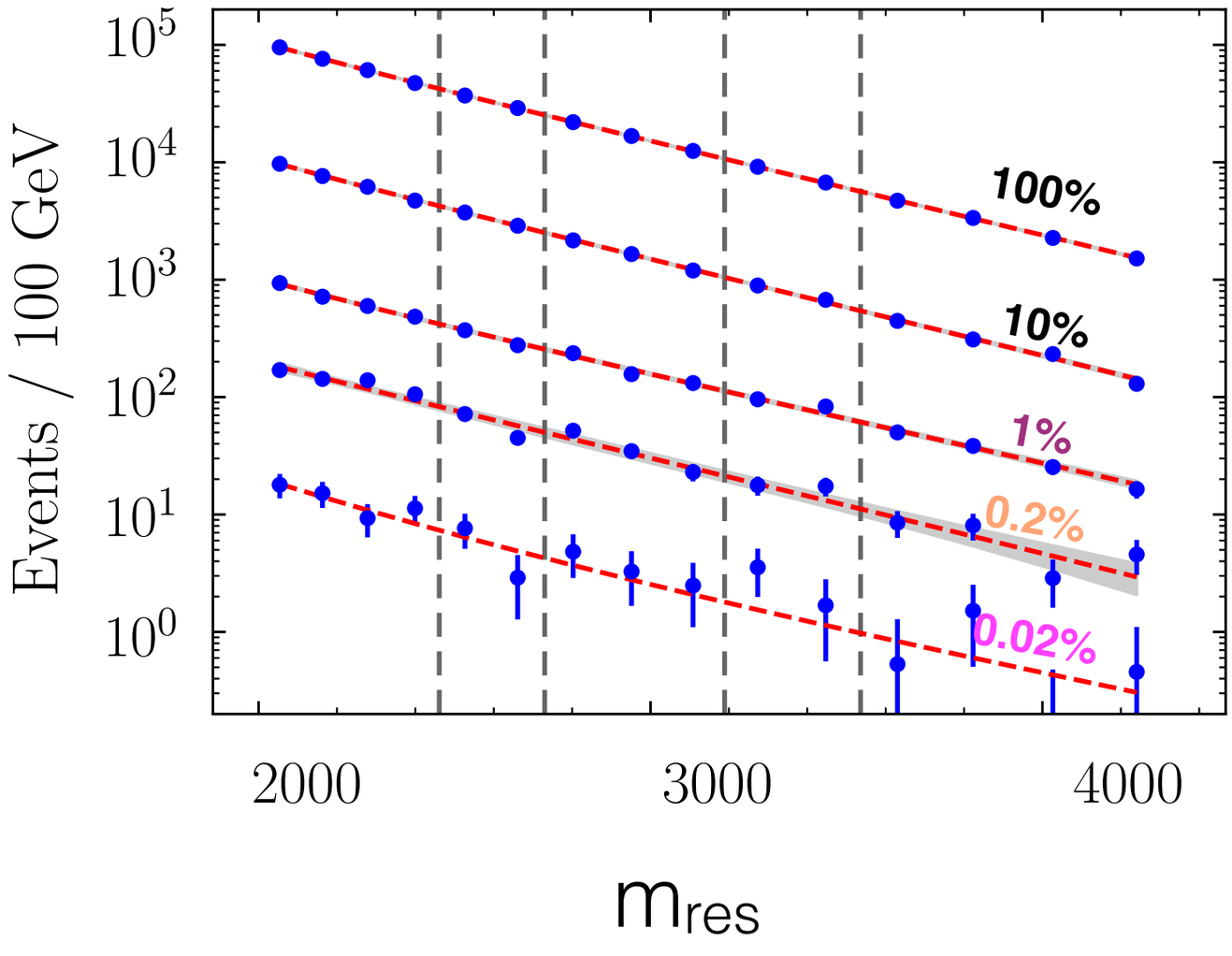
most 10% signal-region-like

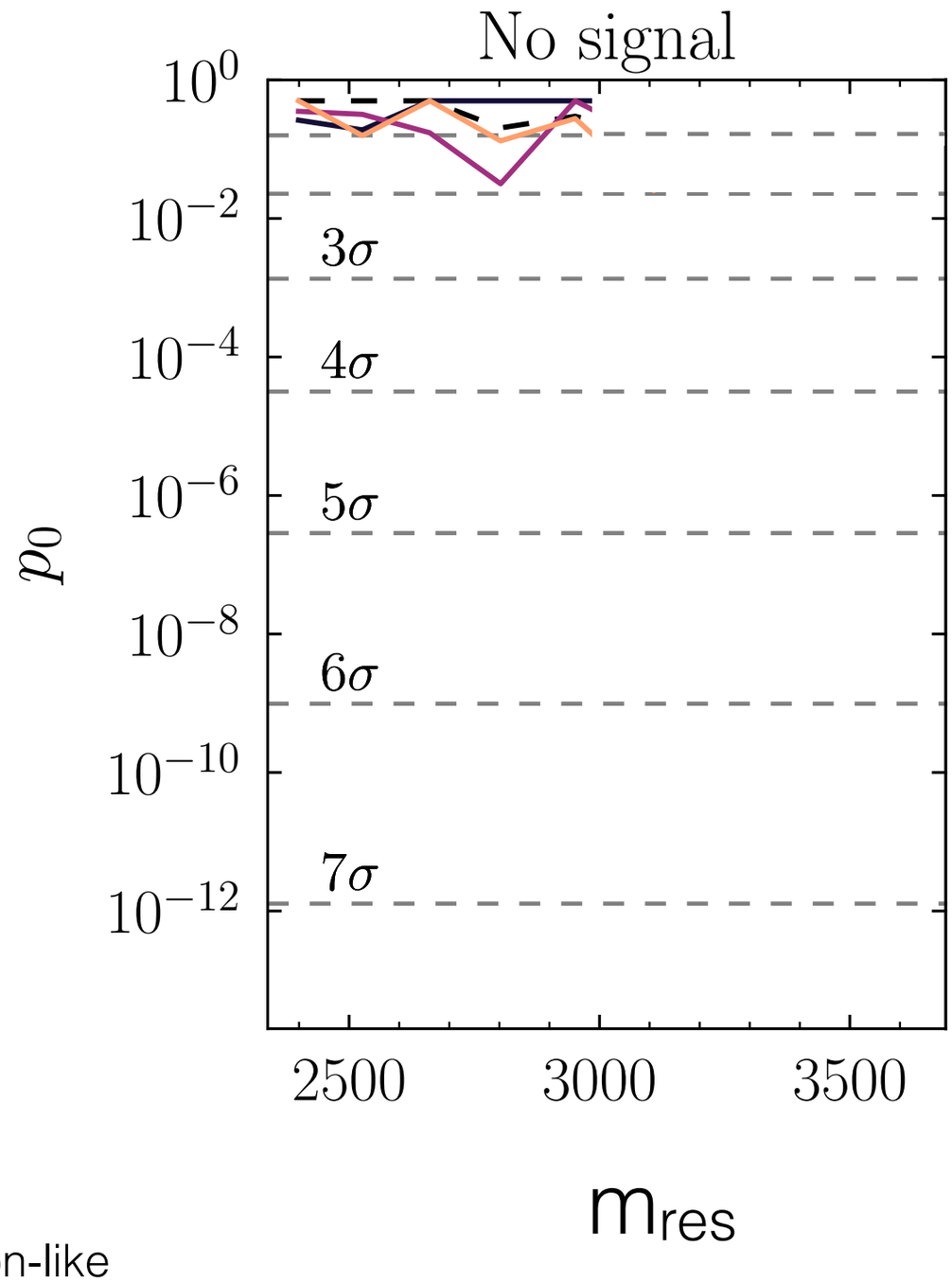
most 1% signal-region-like

most 0.2% signal-region-like

# Example: two-jet search

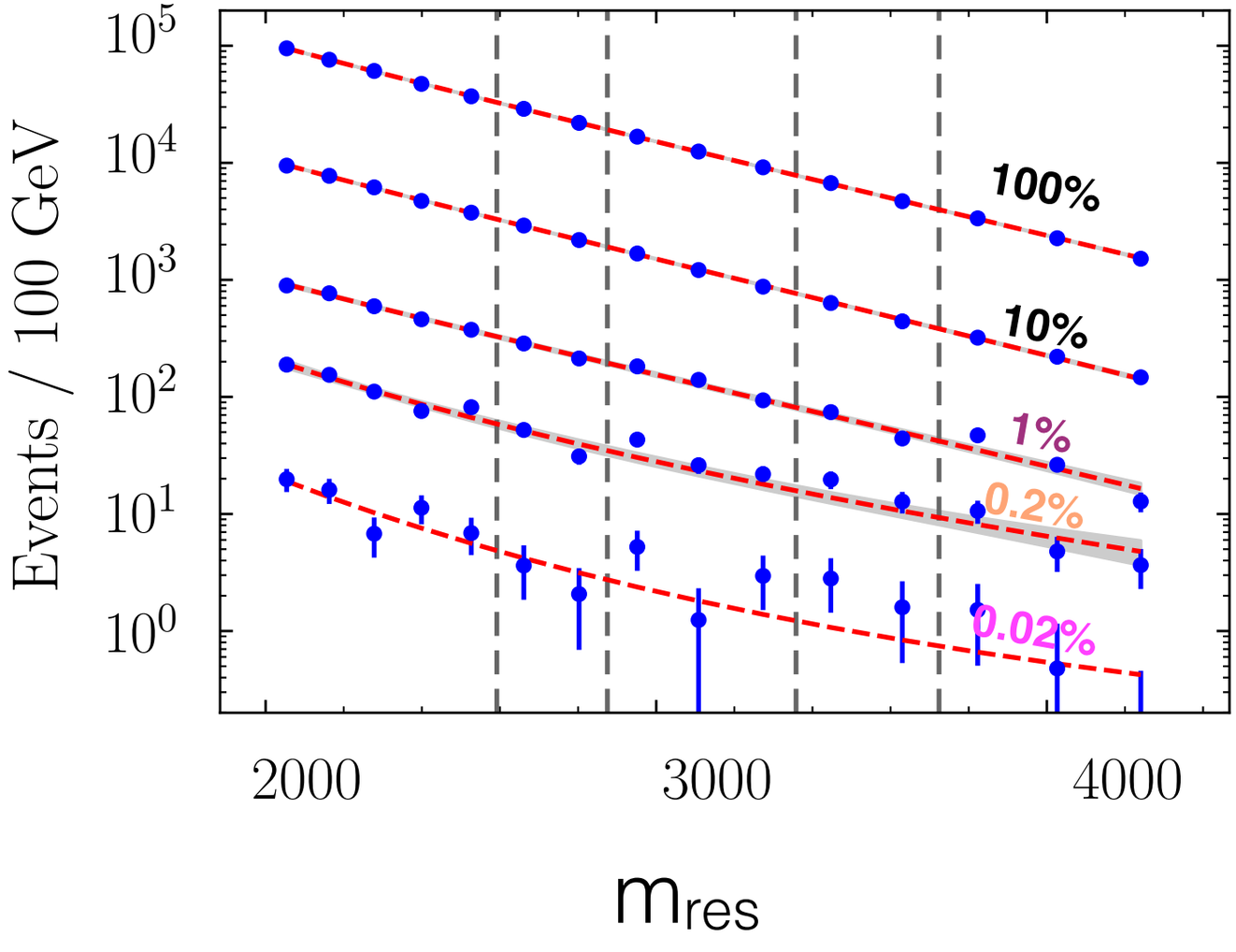


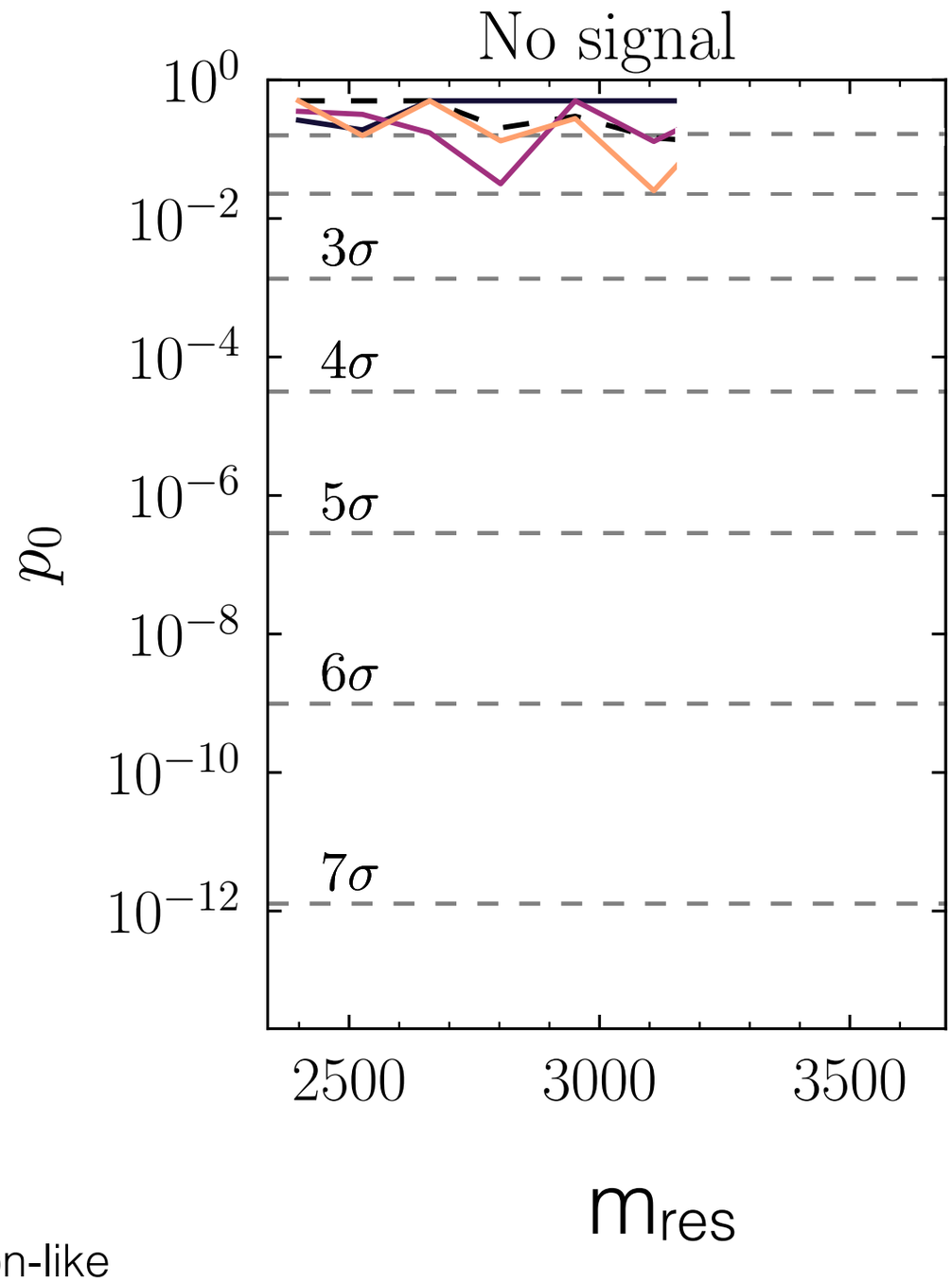



# Example: two-jet search






no cut on NN

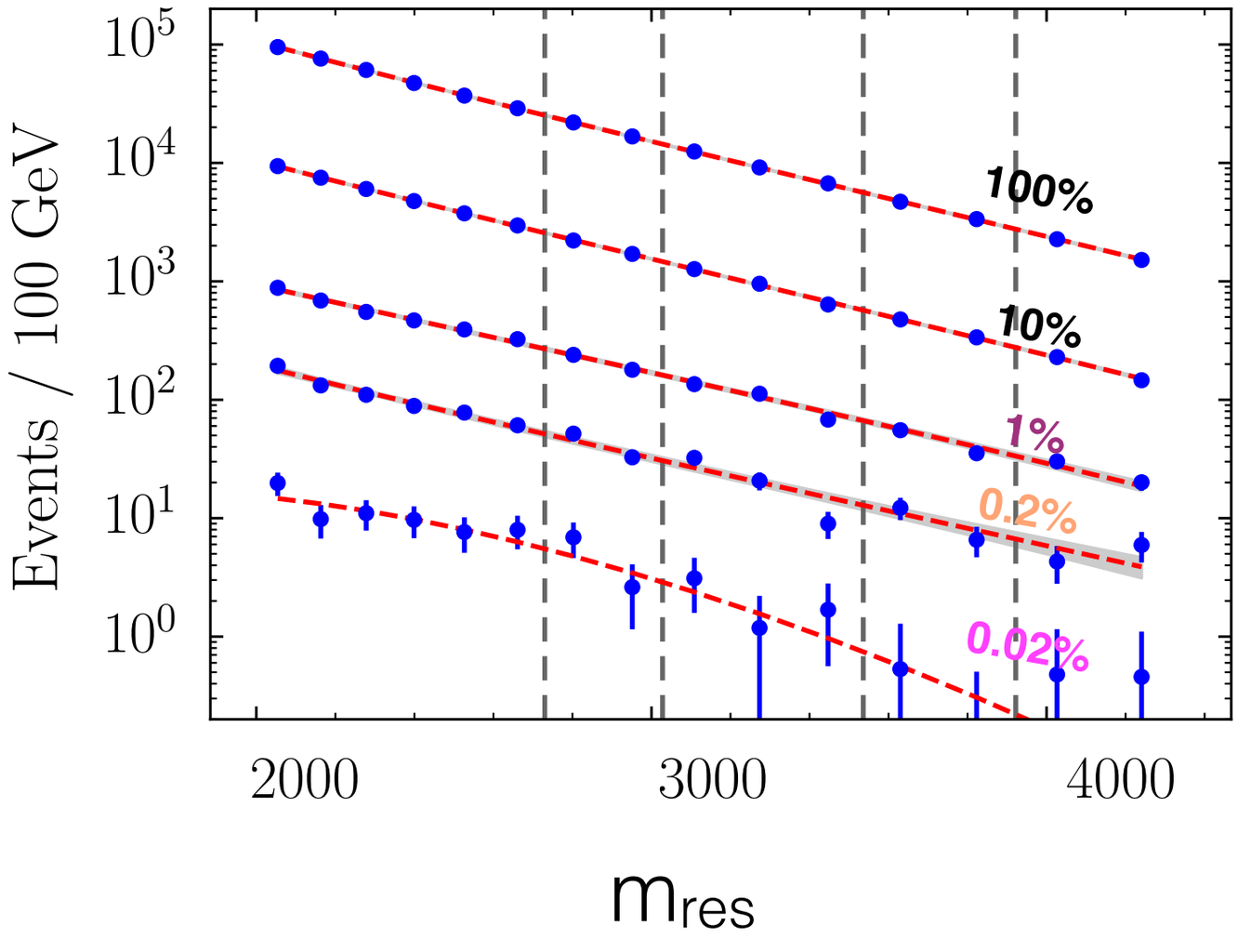
most 10% signal-region-like

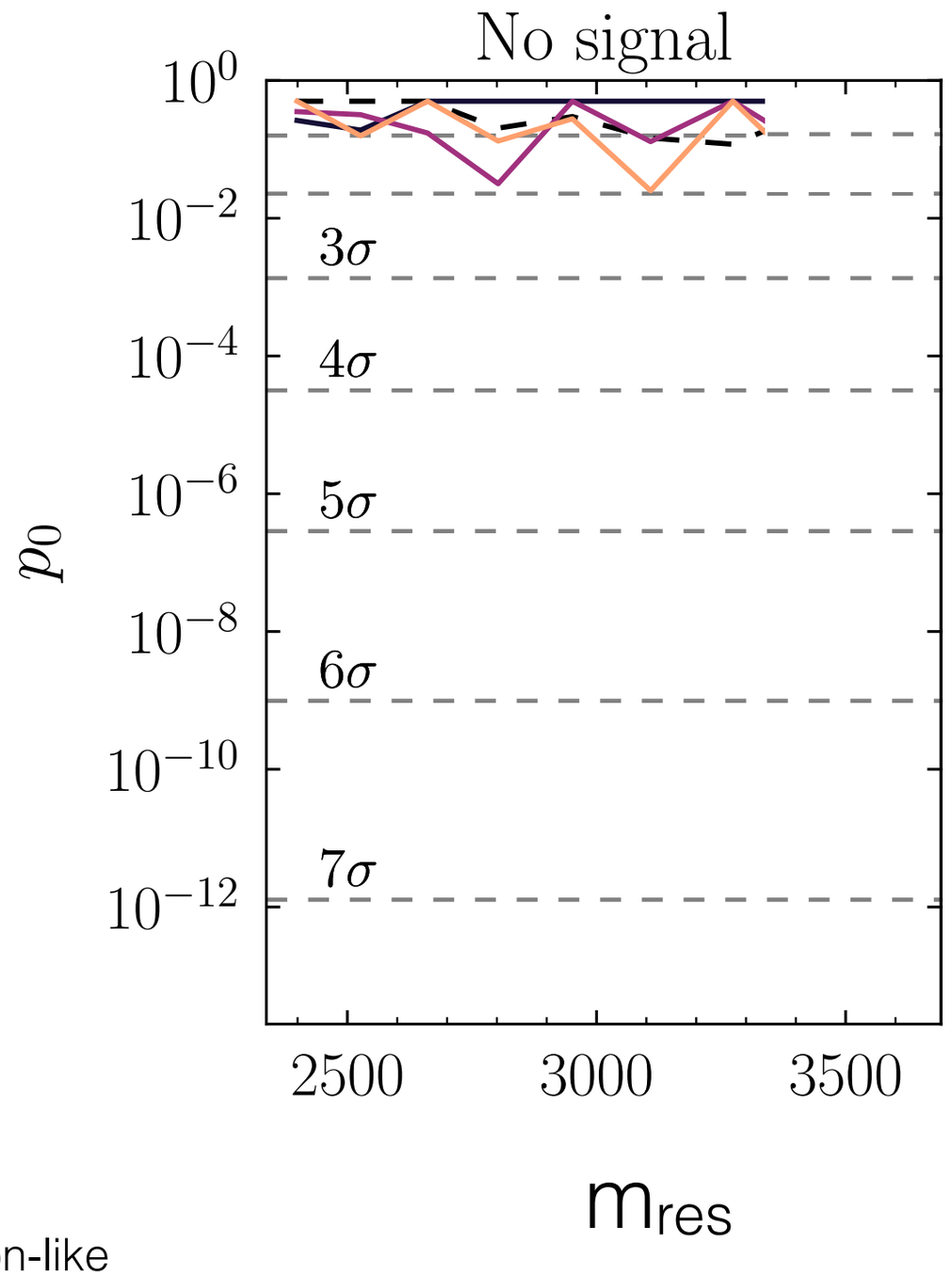
most 1% signal-region-like

most 0.2% signal-region-like

# Example: two-jet search






no cut on NN

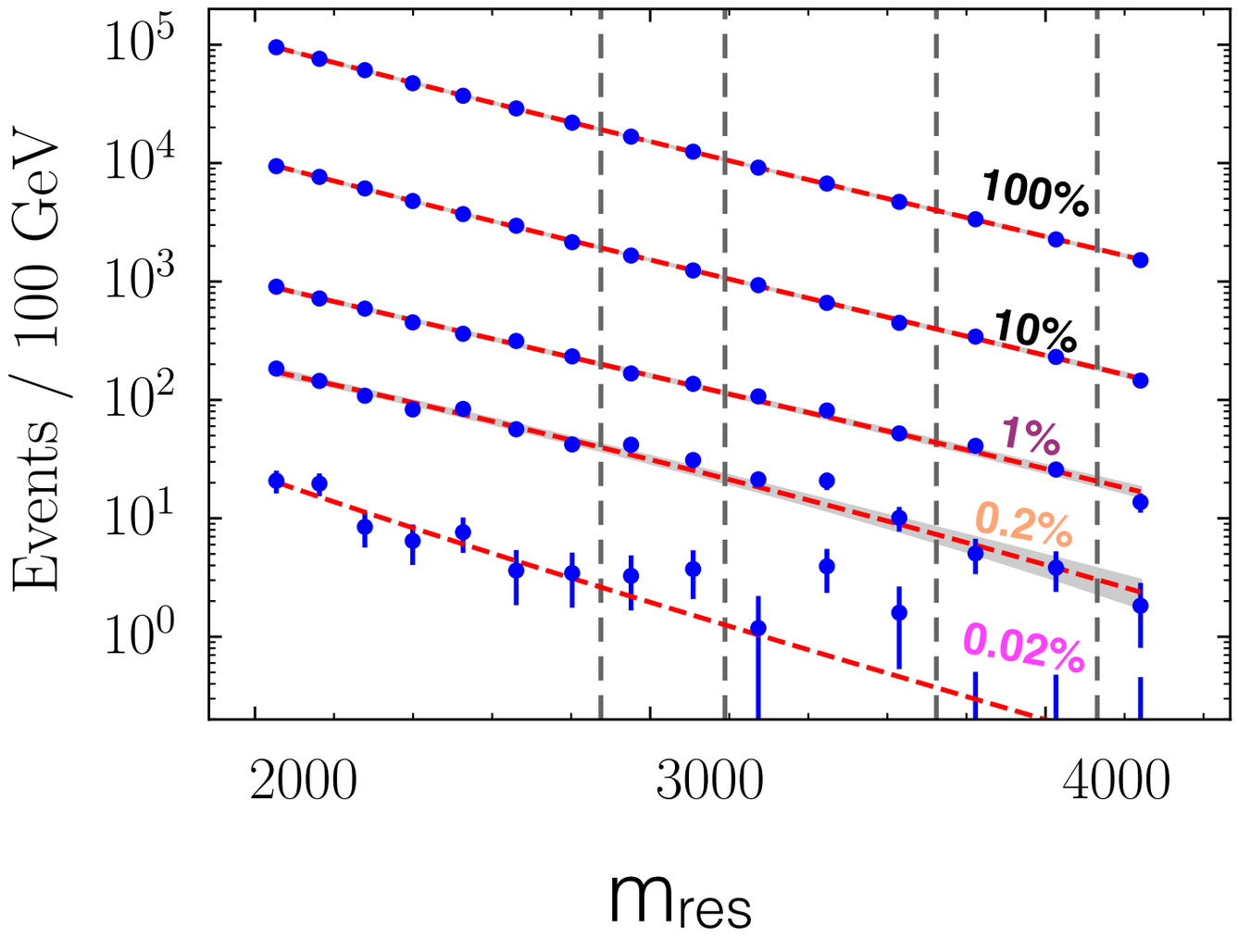
most 10% signal-region-like

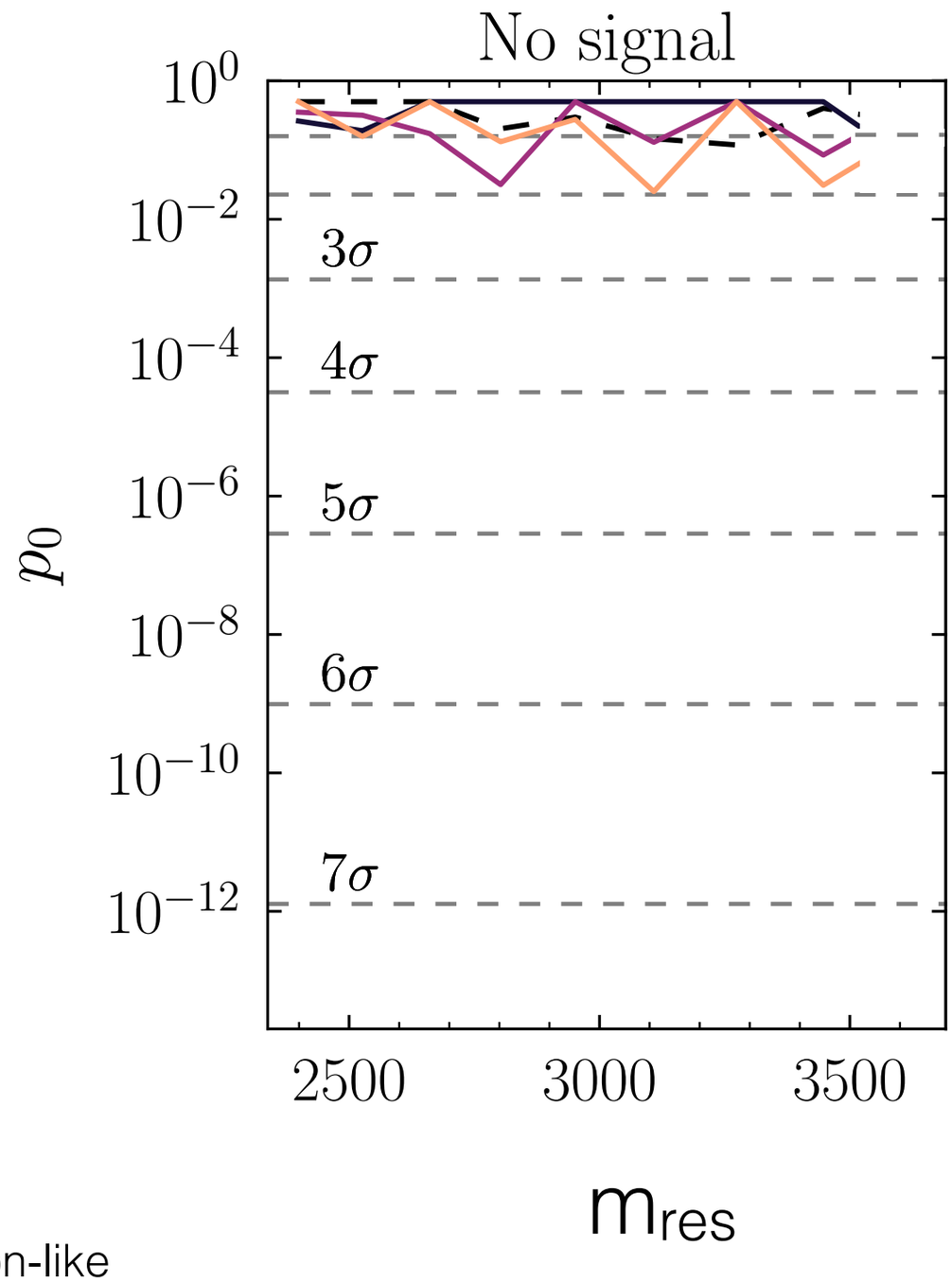
most 1% signal-region-like

most 0.2% signal-region-like

# Example: two-jet search






no cut on NN

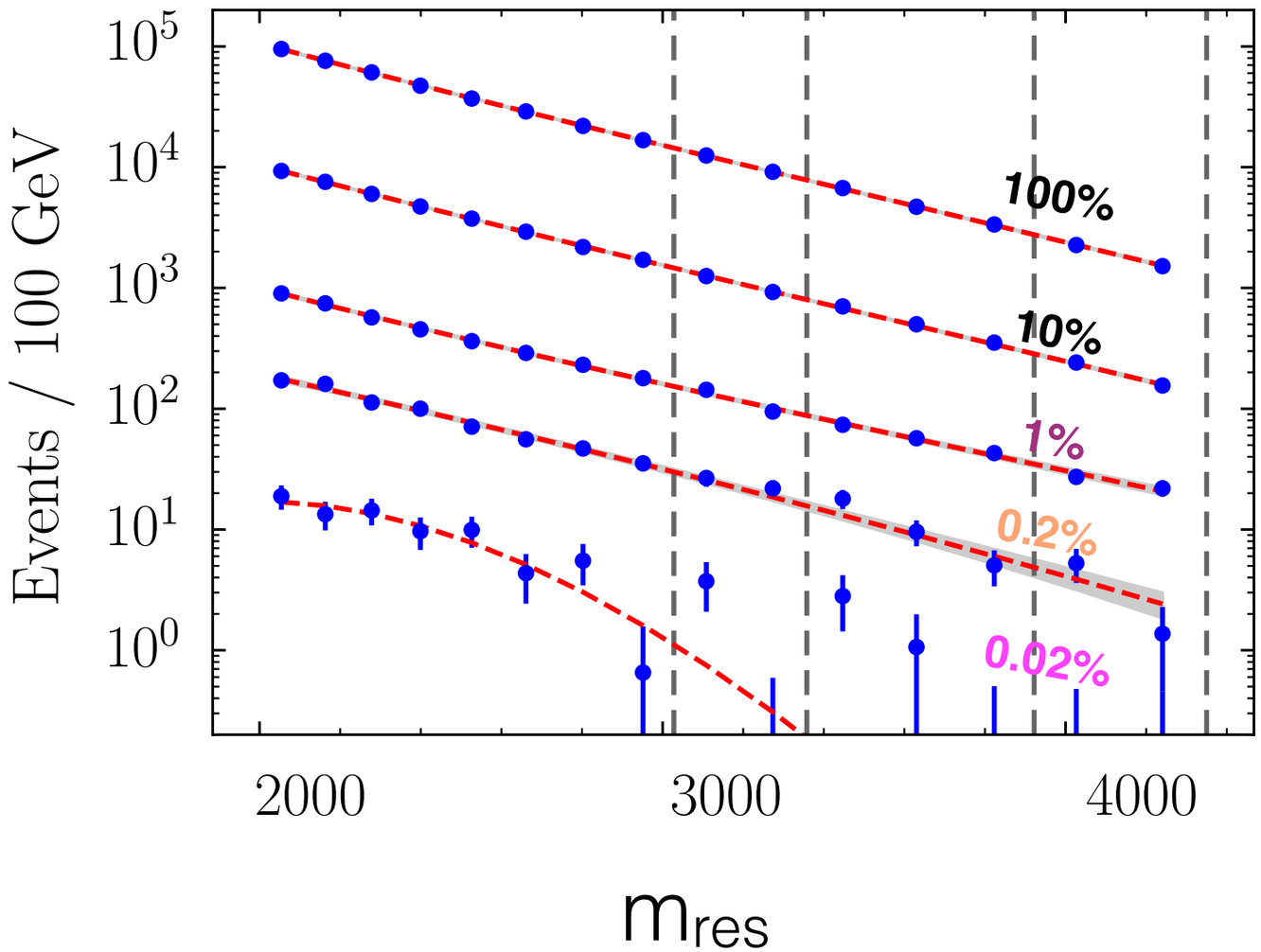
most 10% signal-region-like

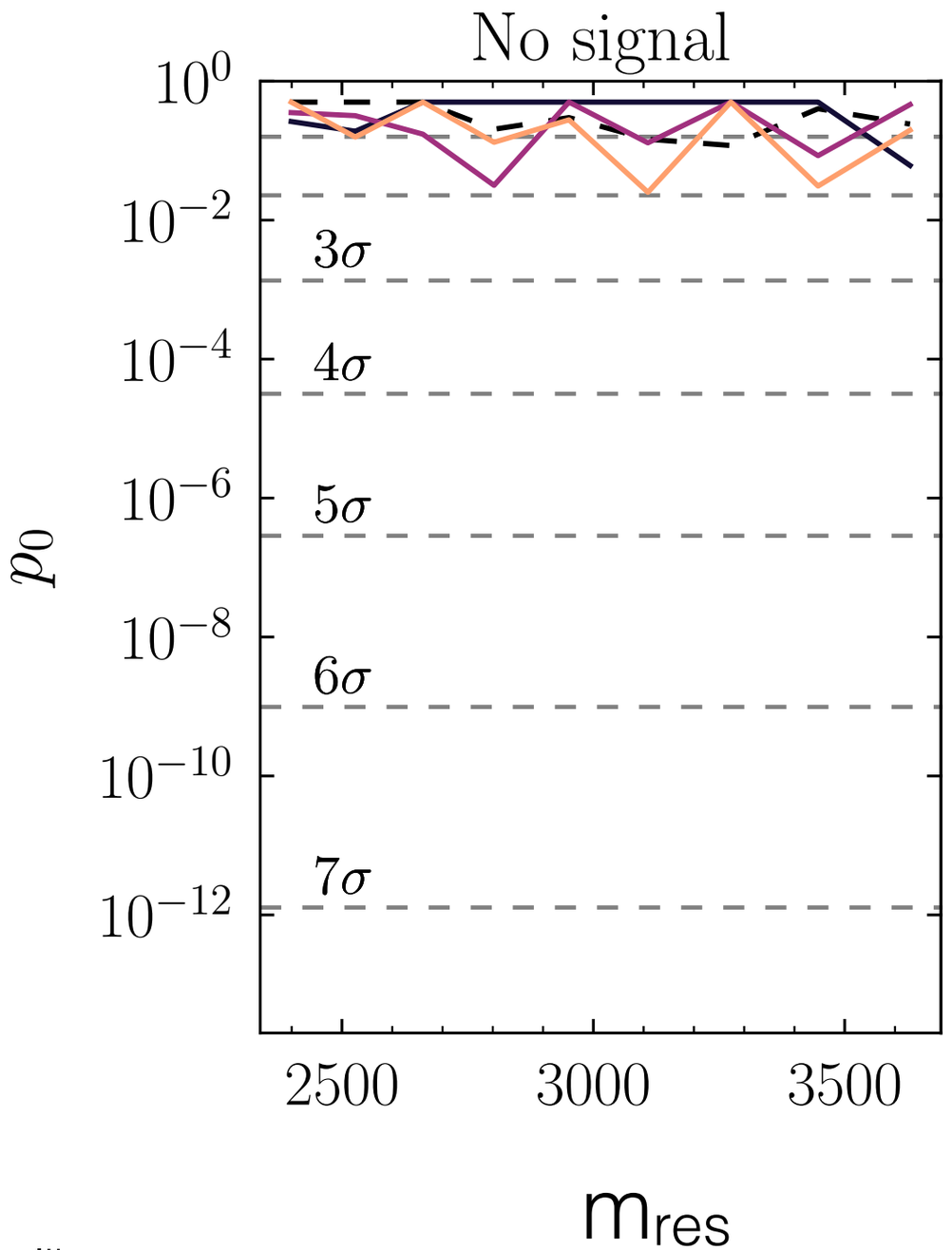
most 1% signal-region-like

most 0.2% signal-region-like

# Example: two-jet search






no cut on NN

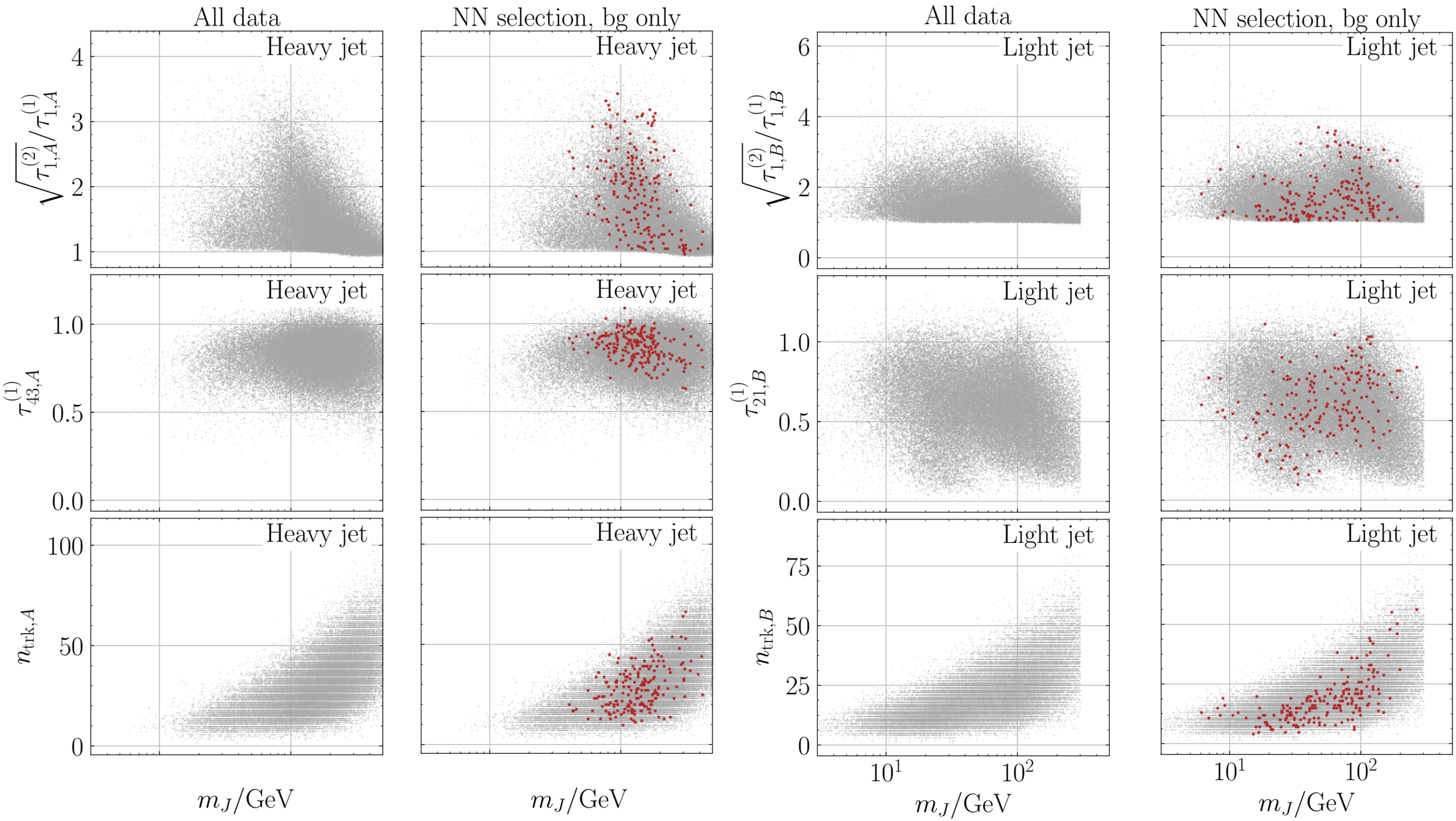
most 10% signal-region-like

most 1% signal-region-like

most 0.2% signal-region-like

# What is the network learning?

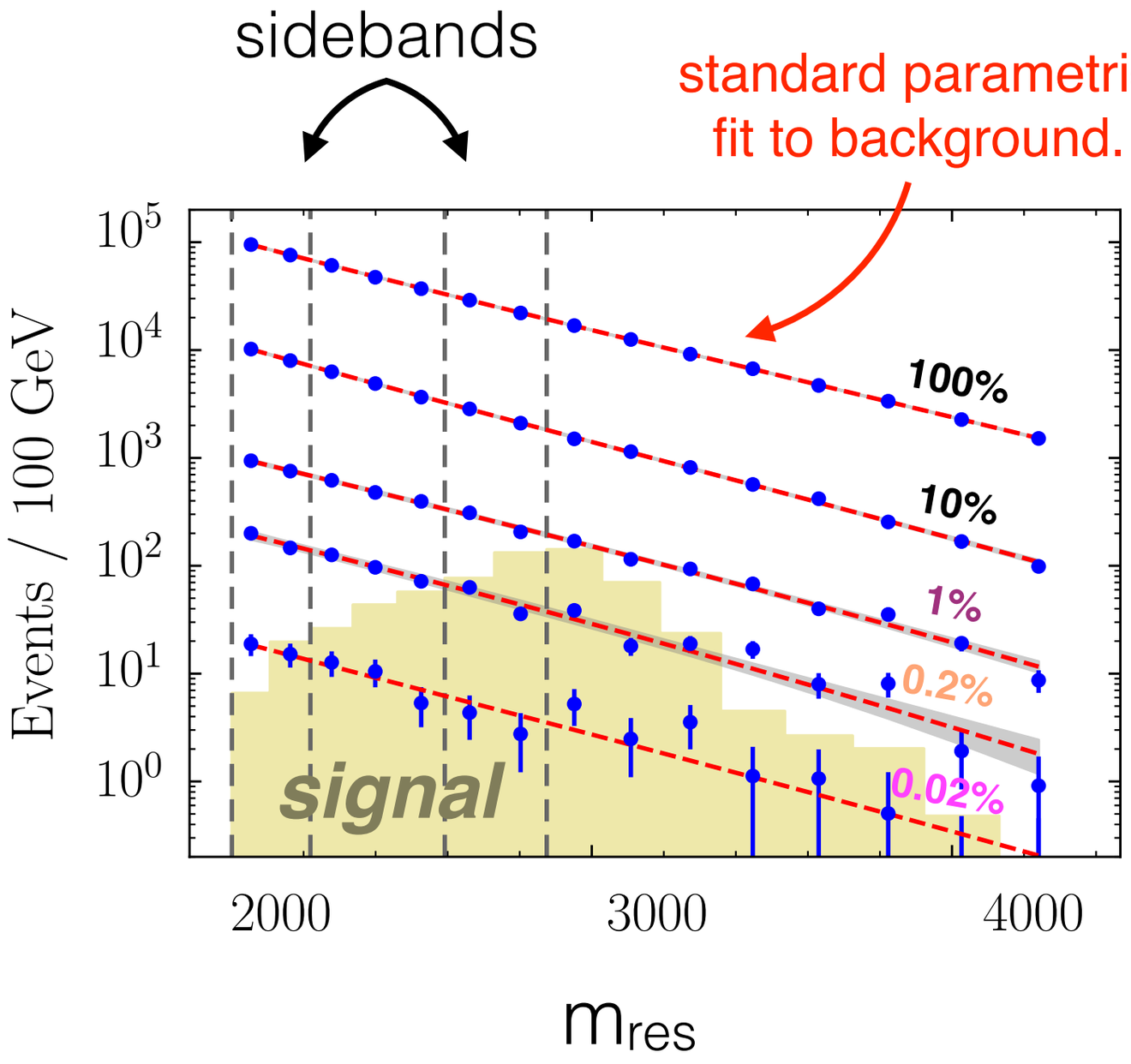


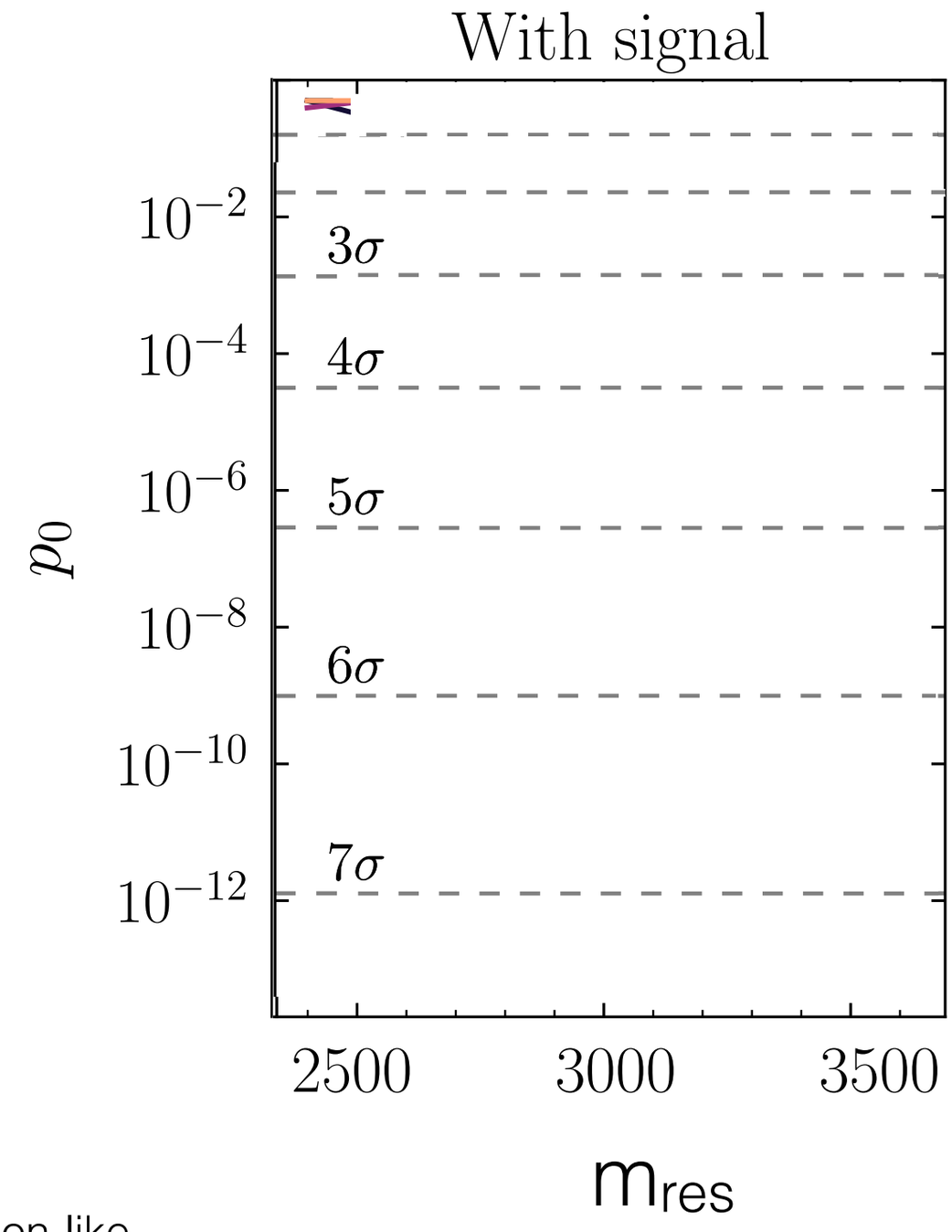



**Learns nothing … as desired !**

# …and when there is a signal?






no cut on NN

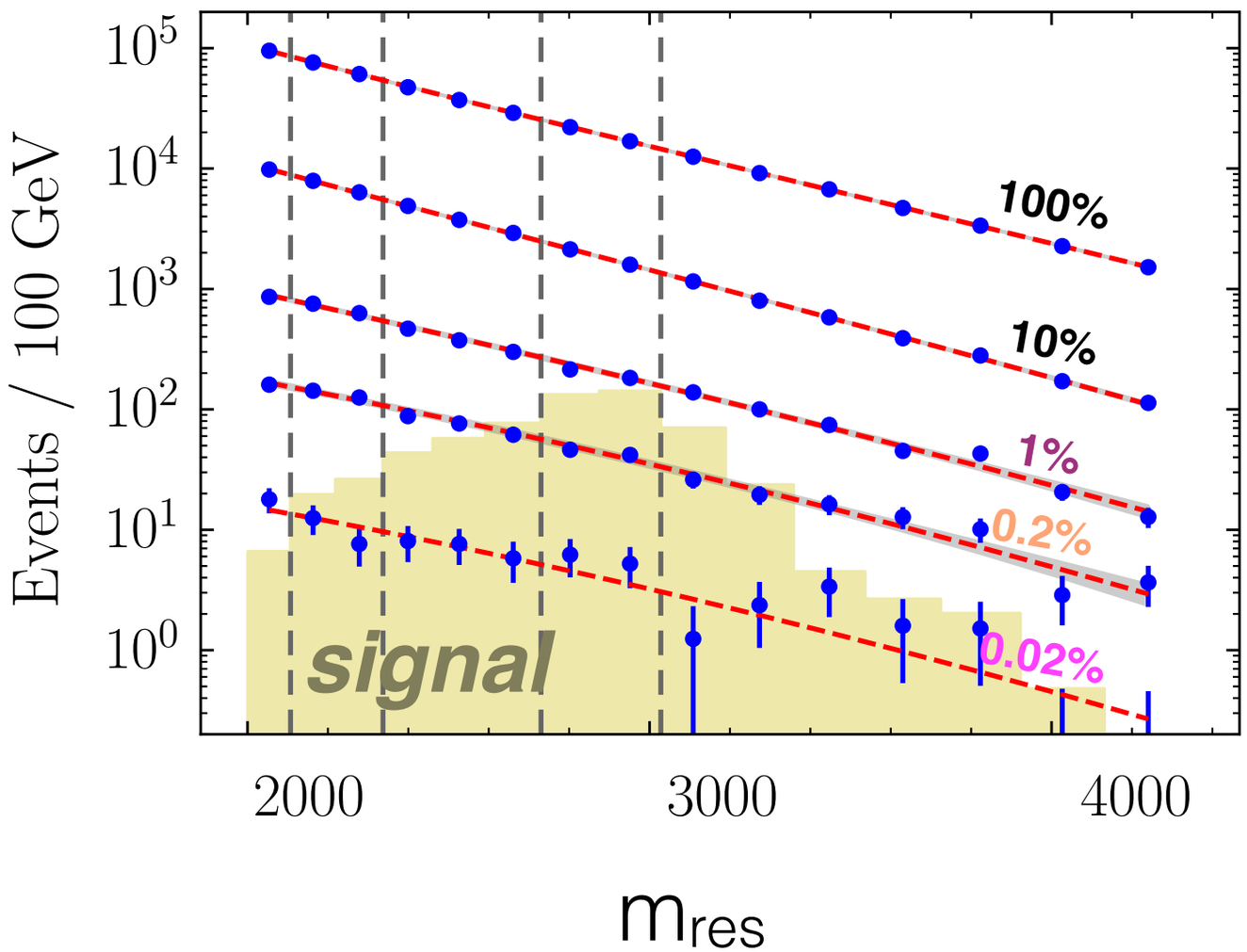
most 10% signal-region-like

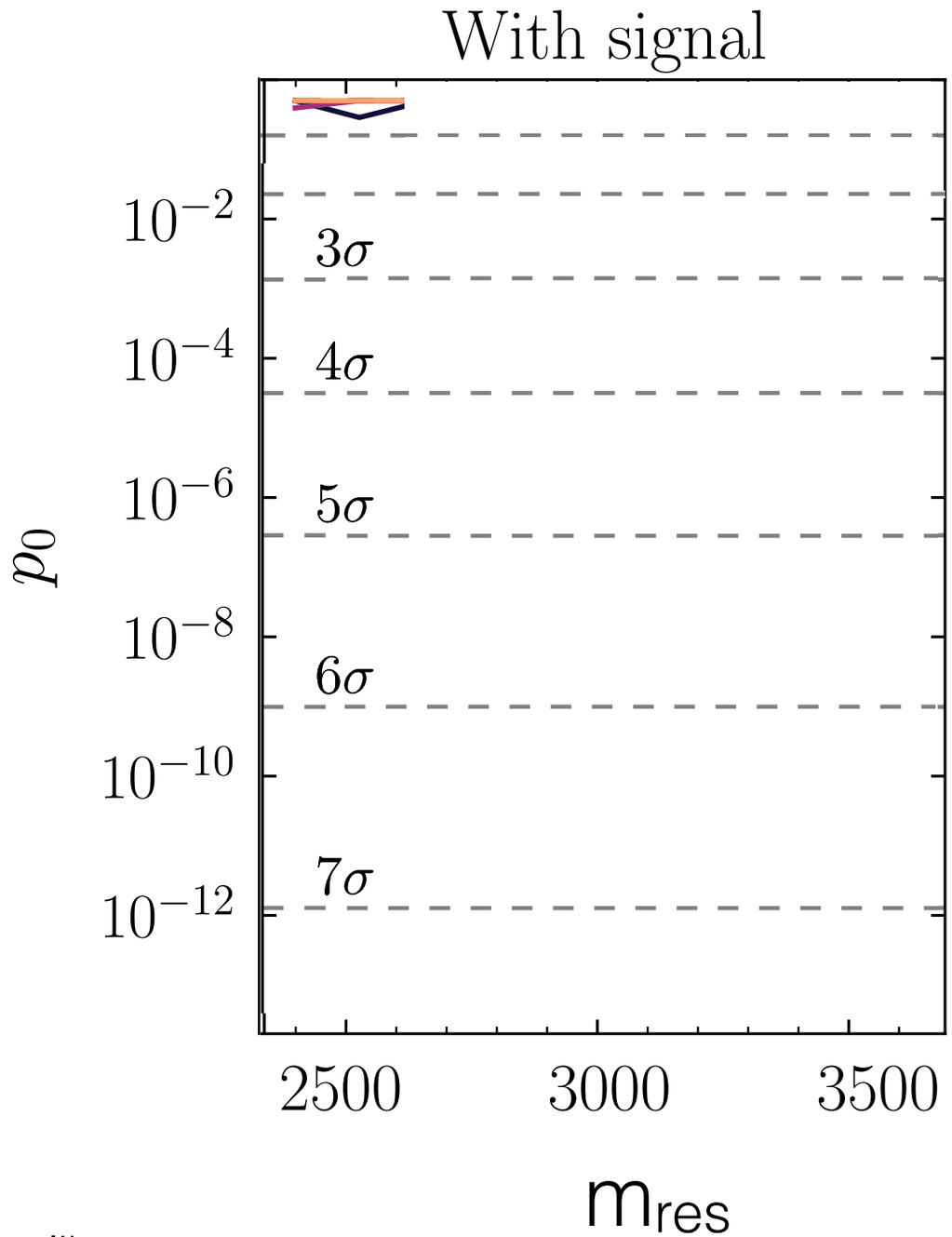
most 1% signal-region-like

most 0.2% signal-region-like

# …and when there is a signal?



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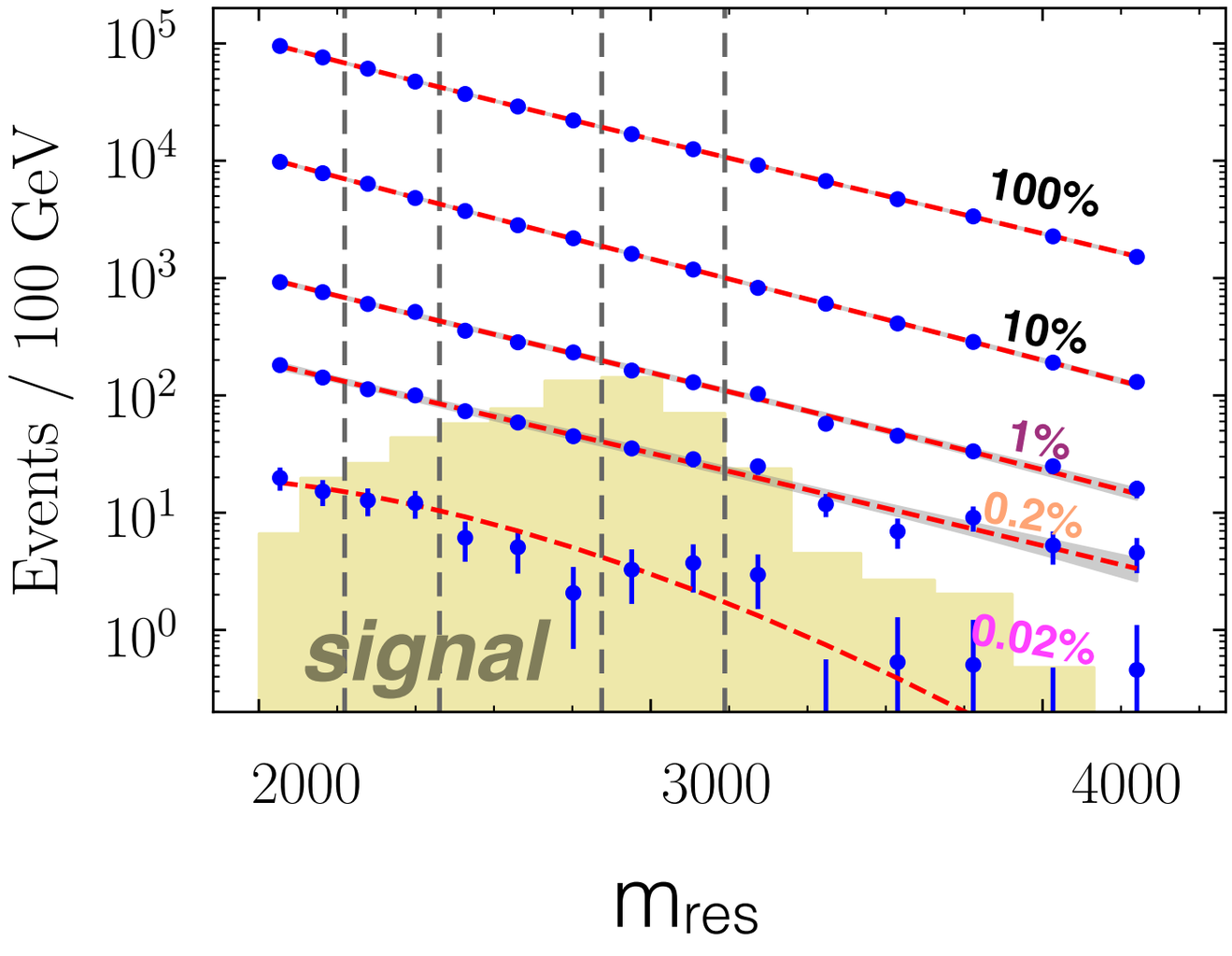


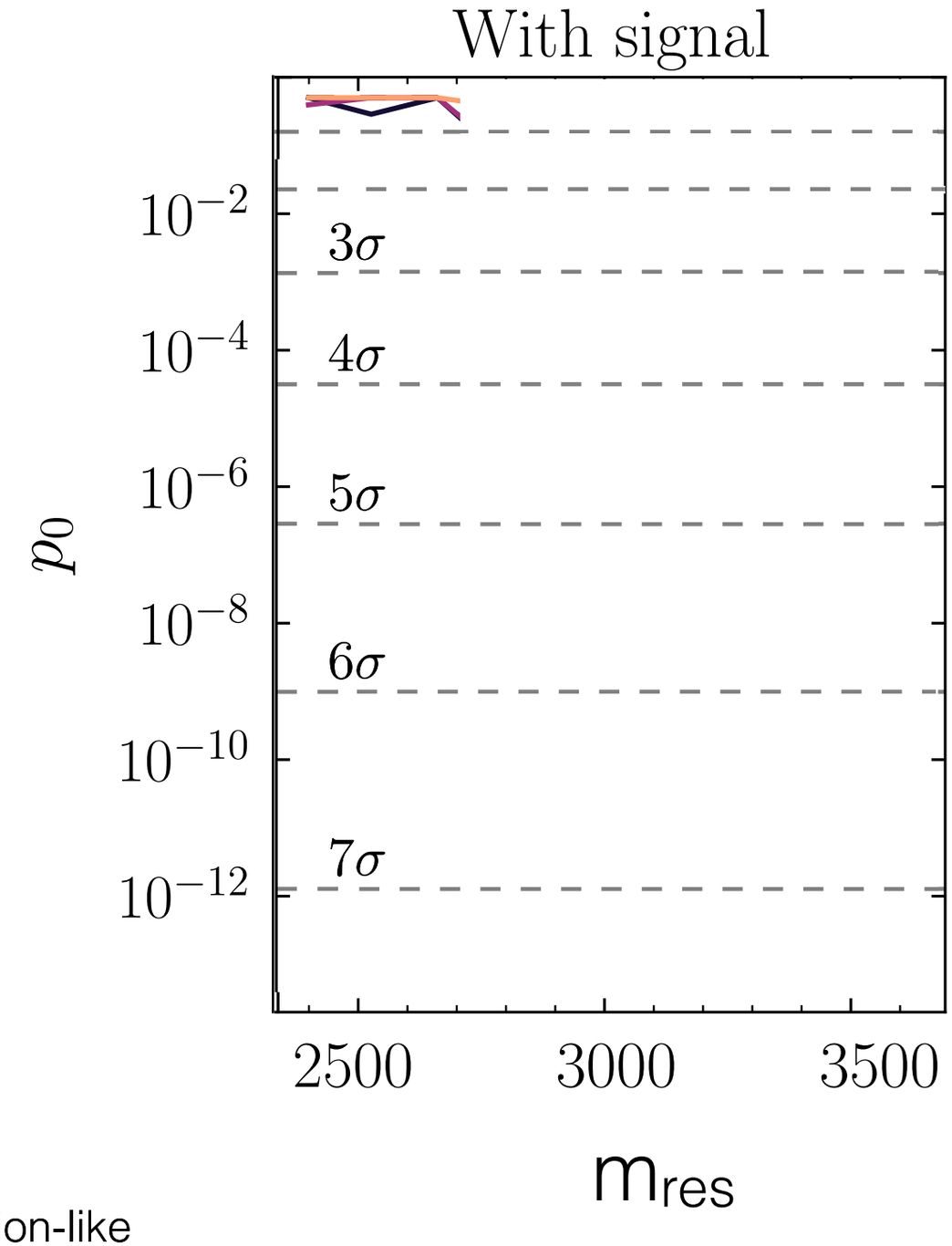


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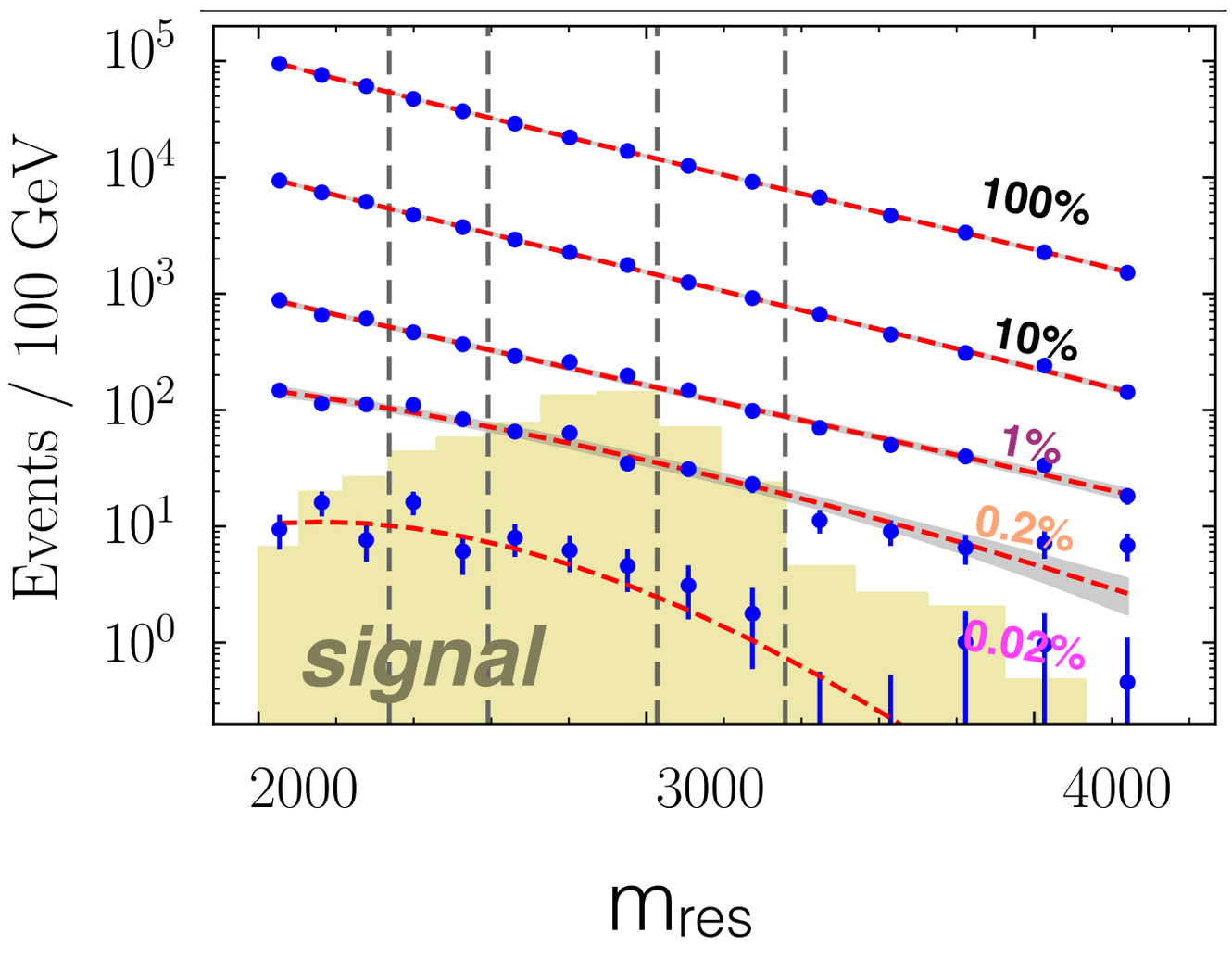


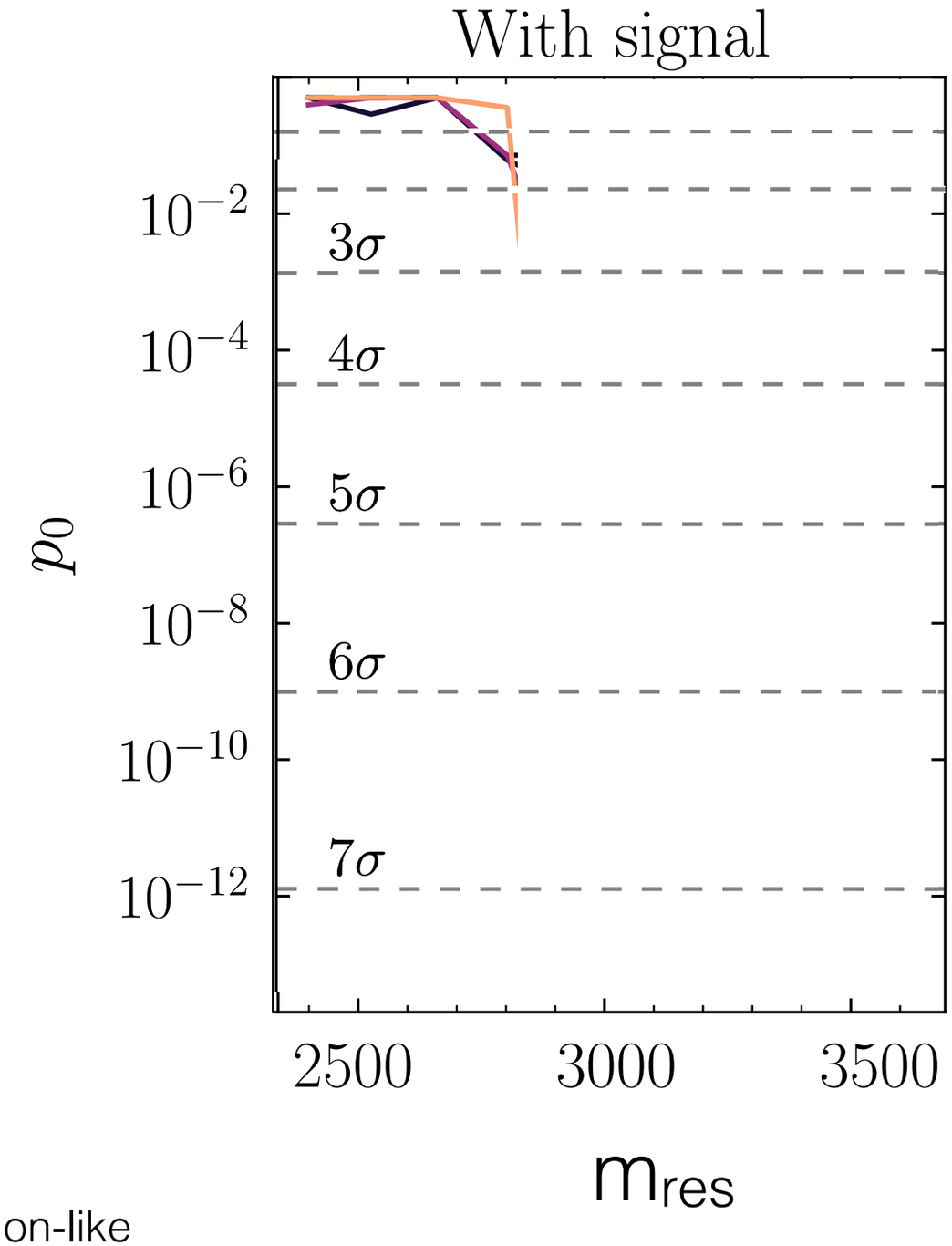


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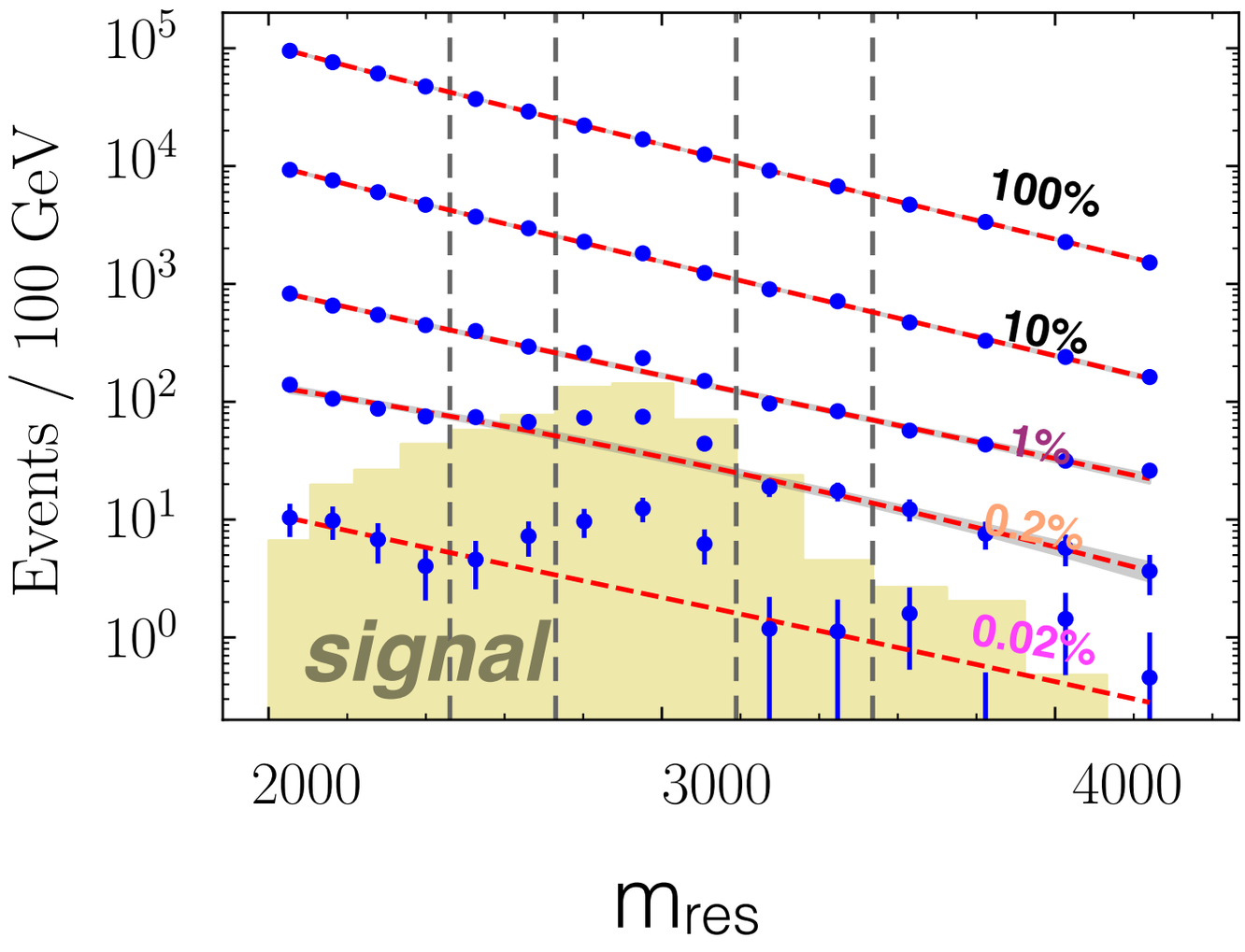


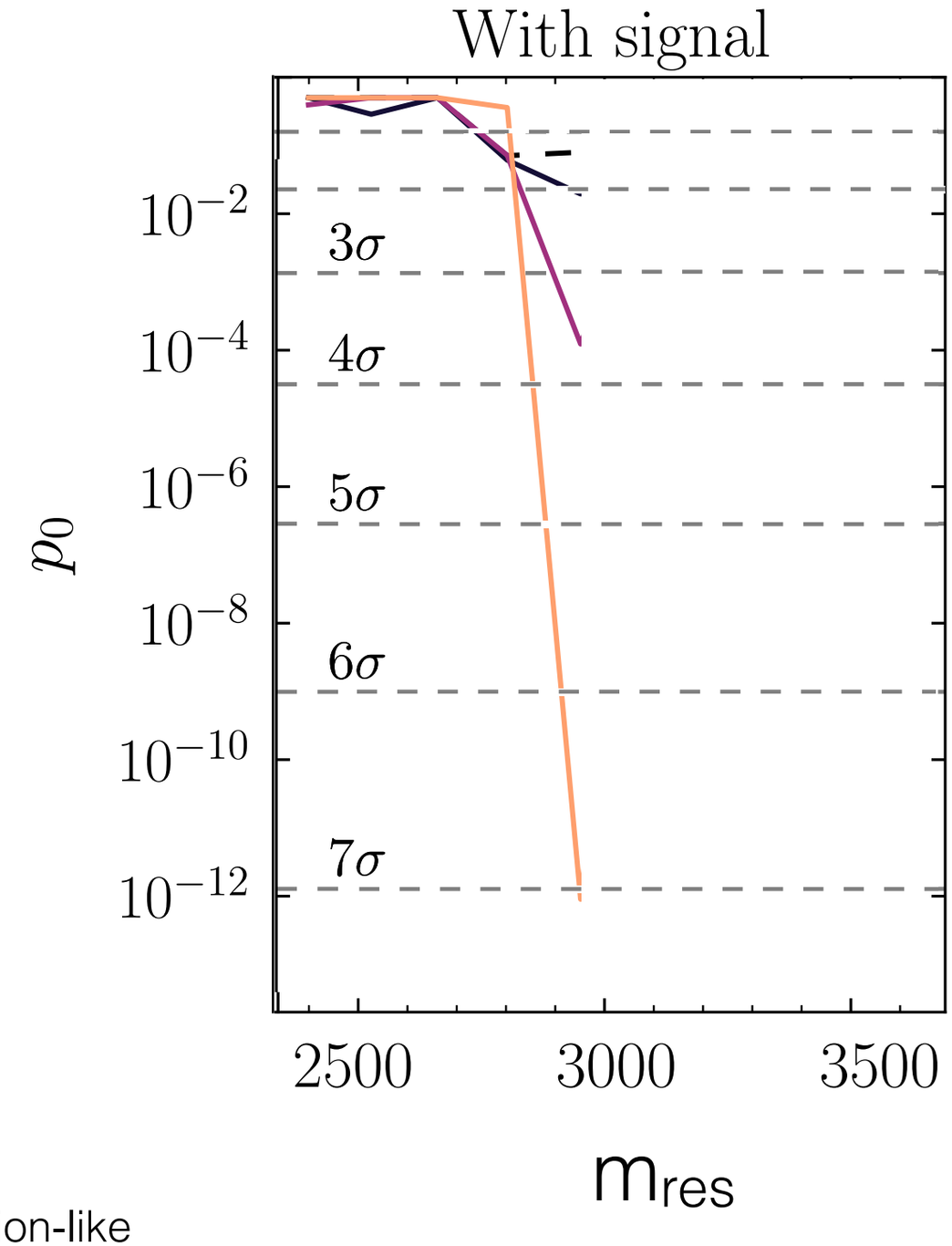


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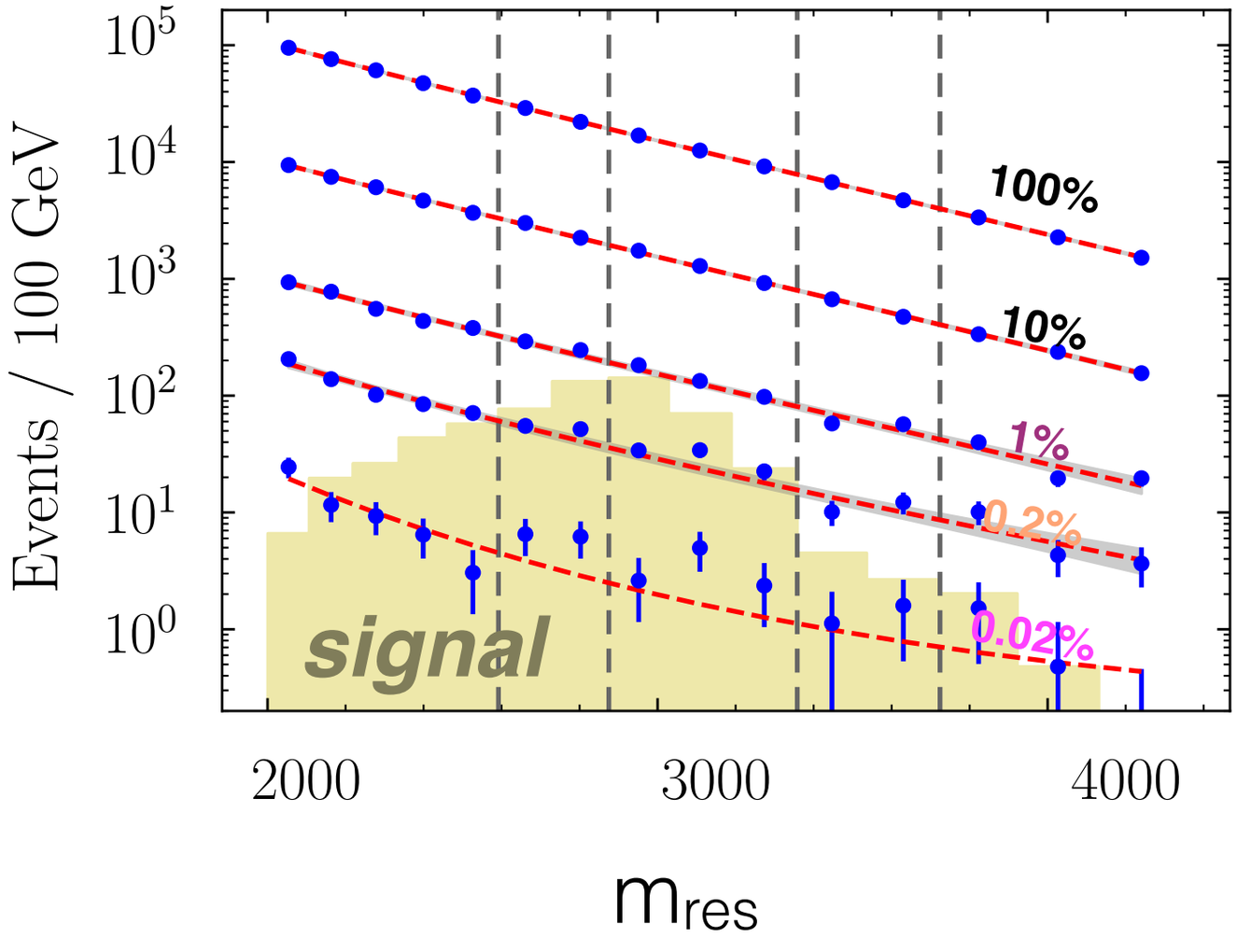


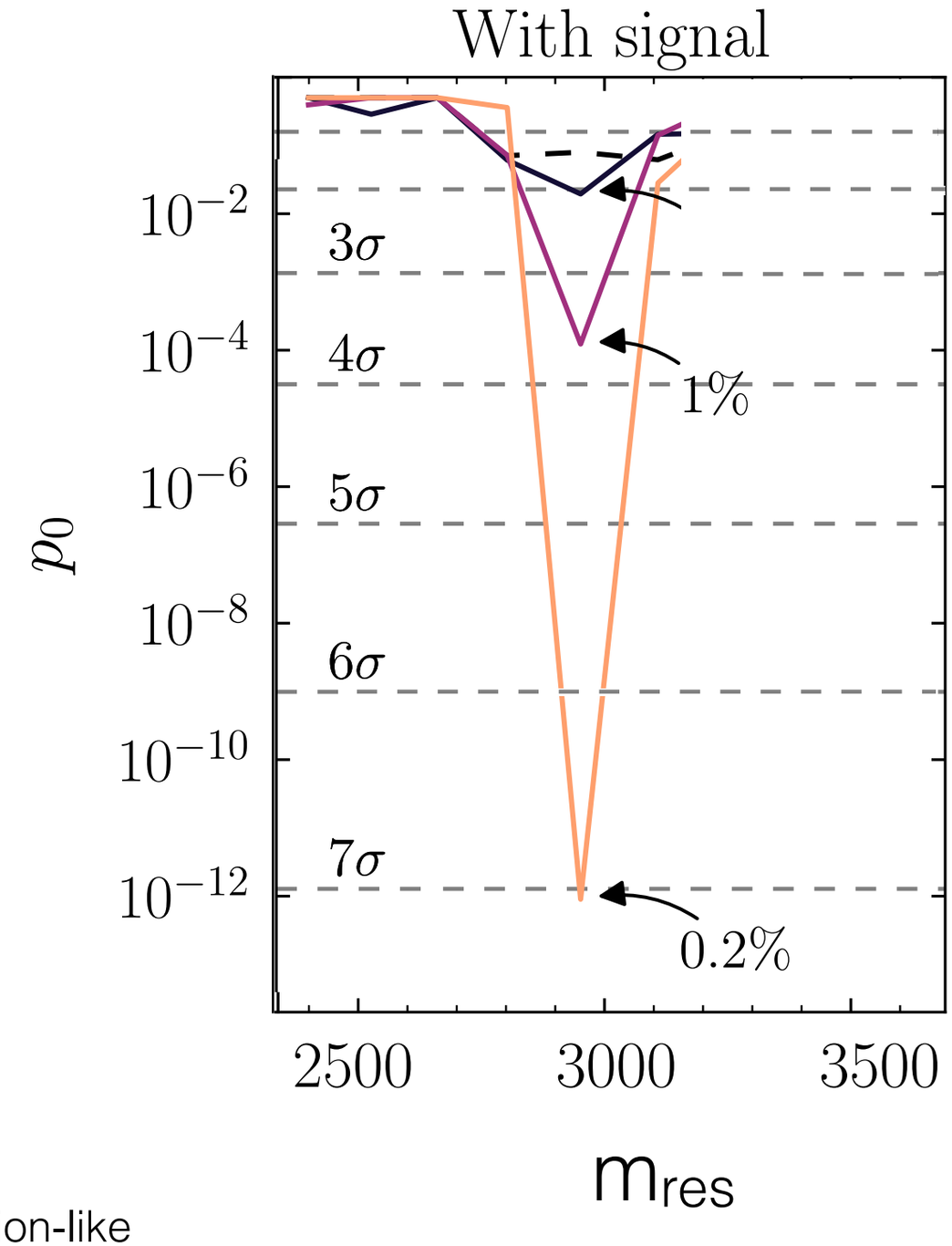


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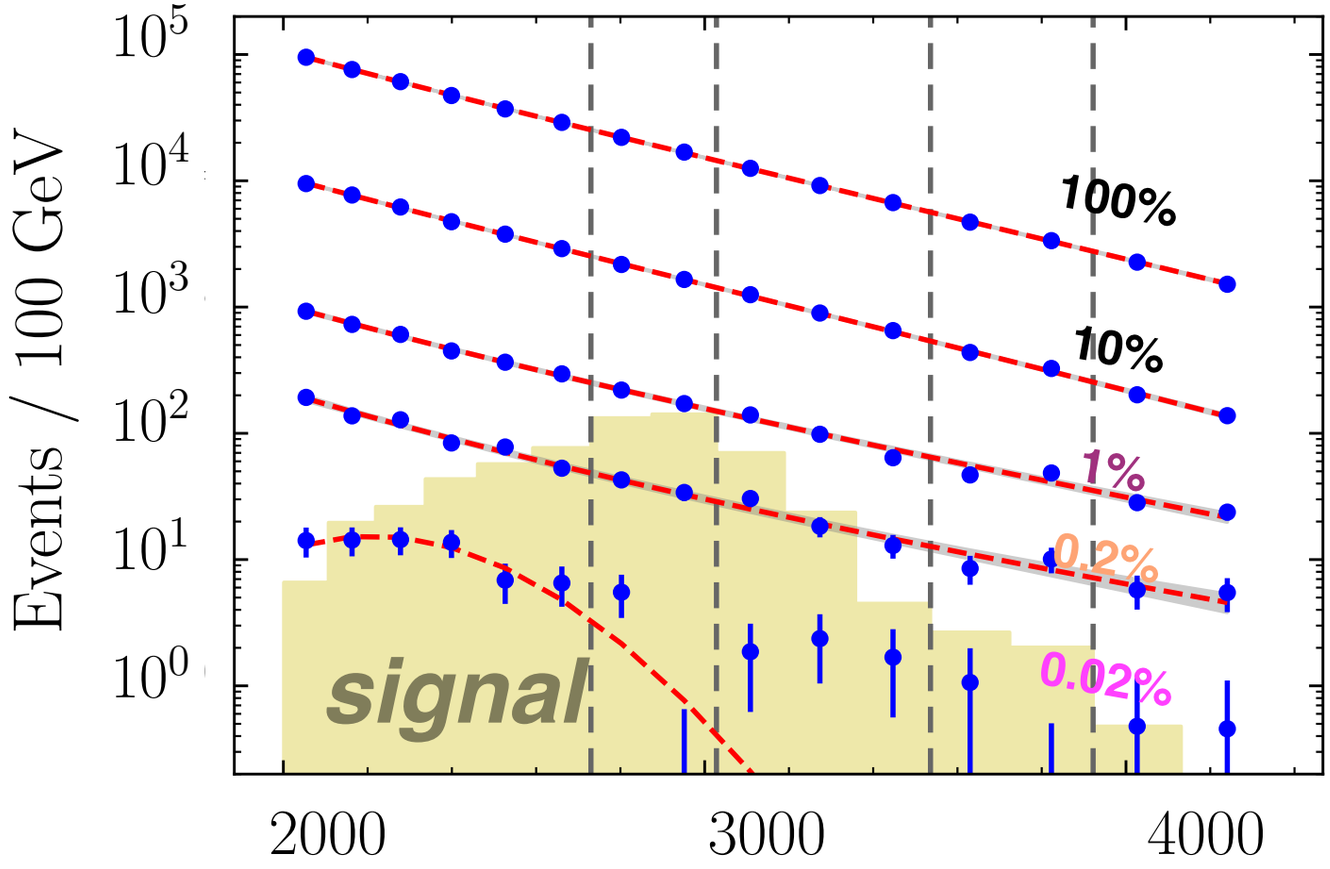


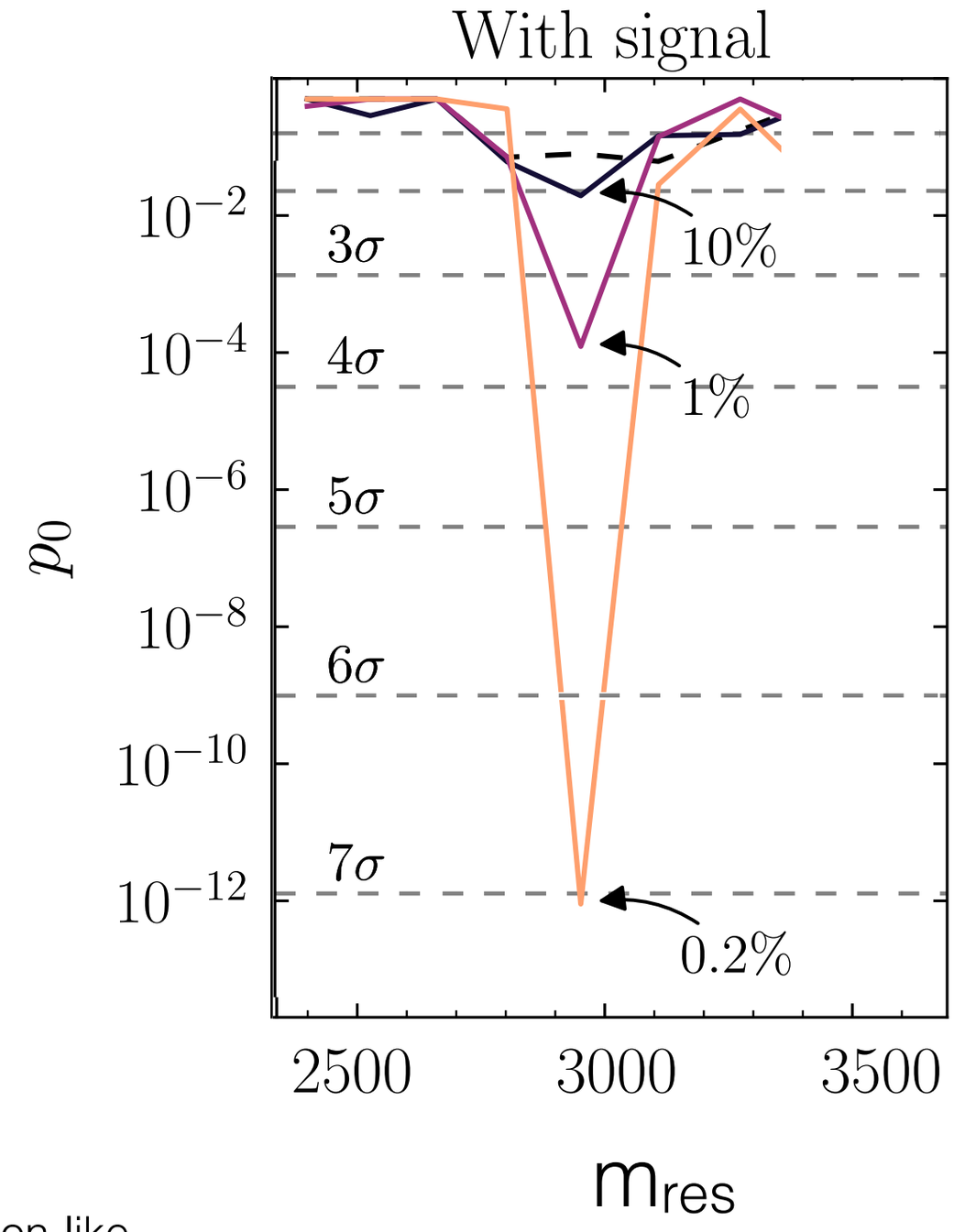


no cut on NN

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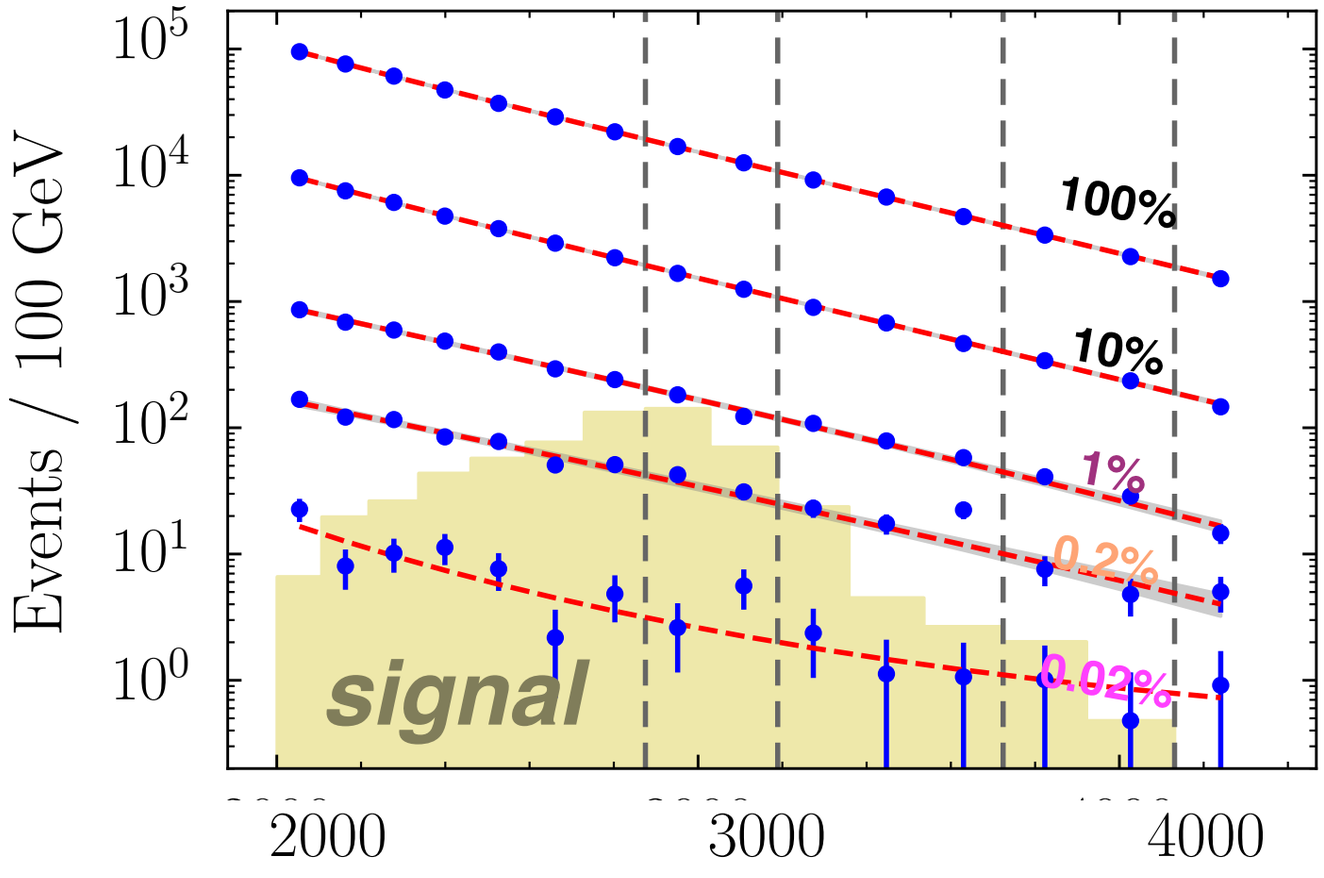


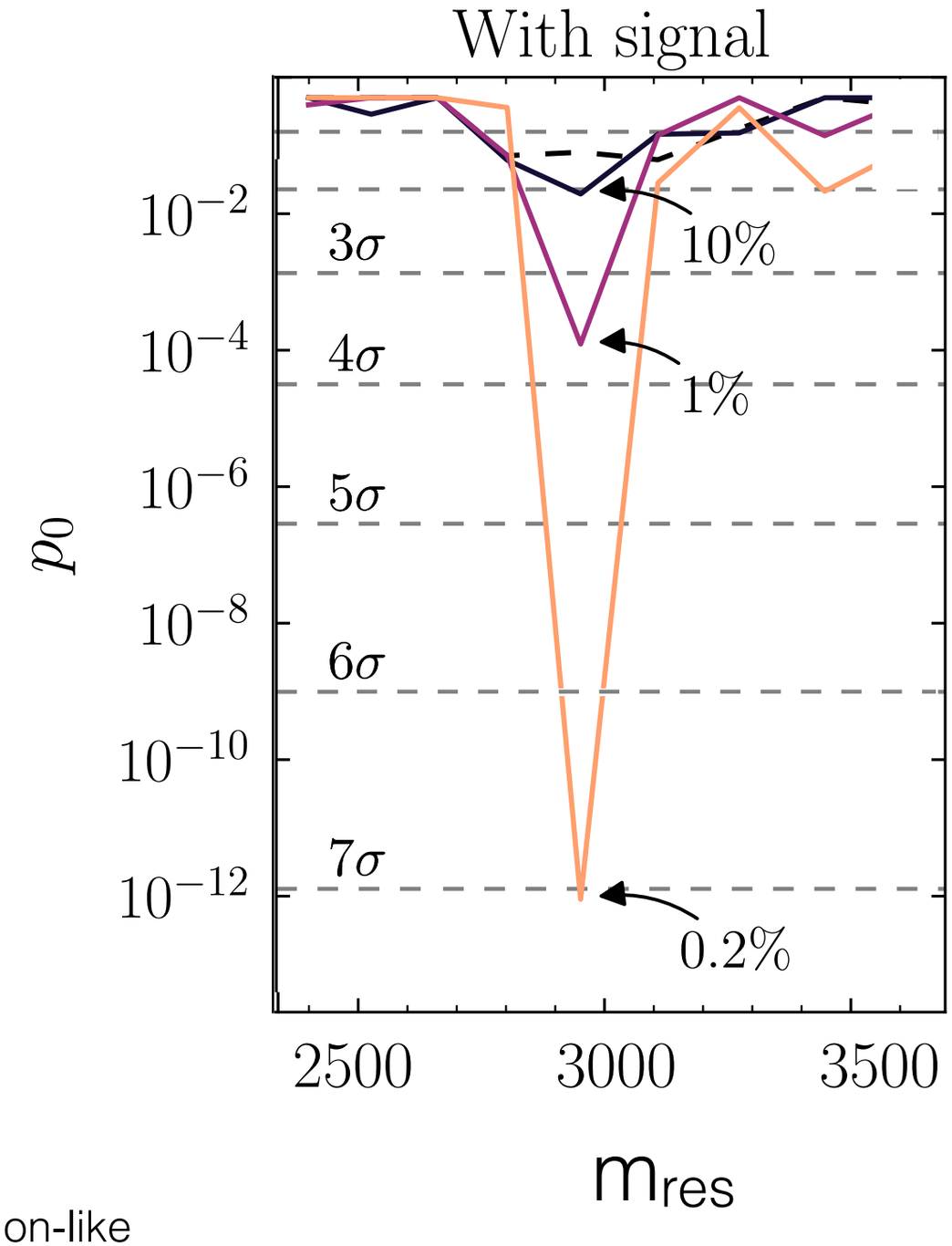


no cut on NN

most 10% signal-region-like

most 1% signal-region-like

most 0.2% signal-region-like

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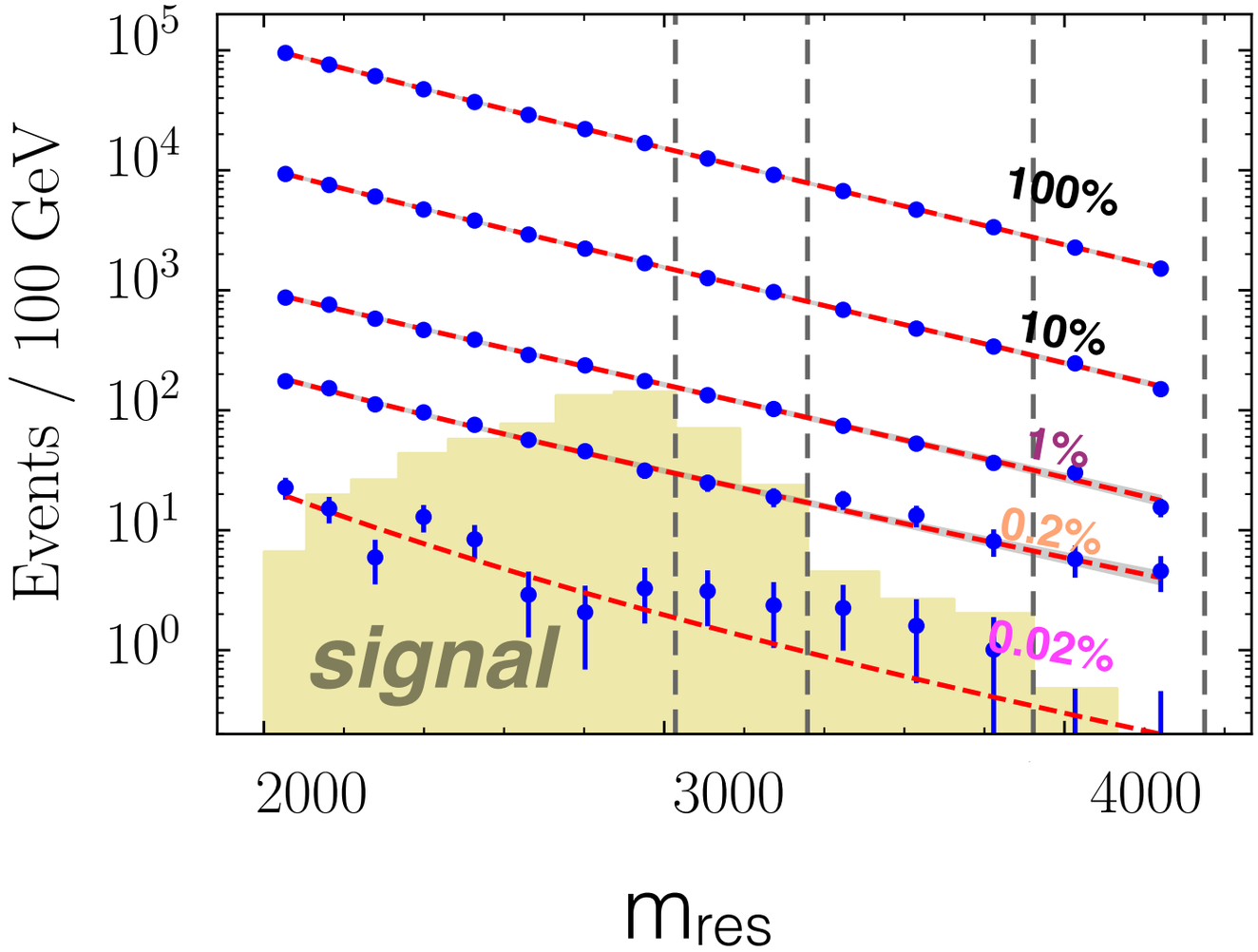
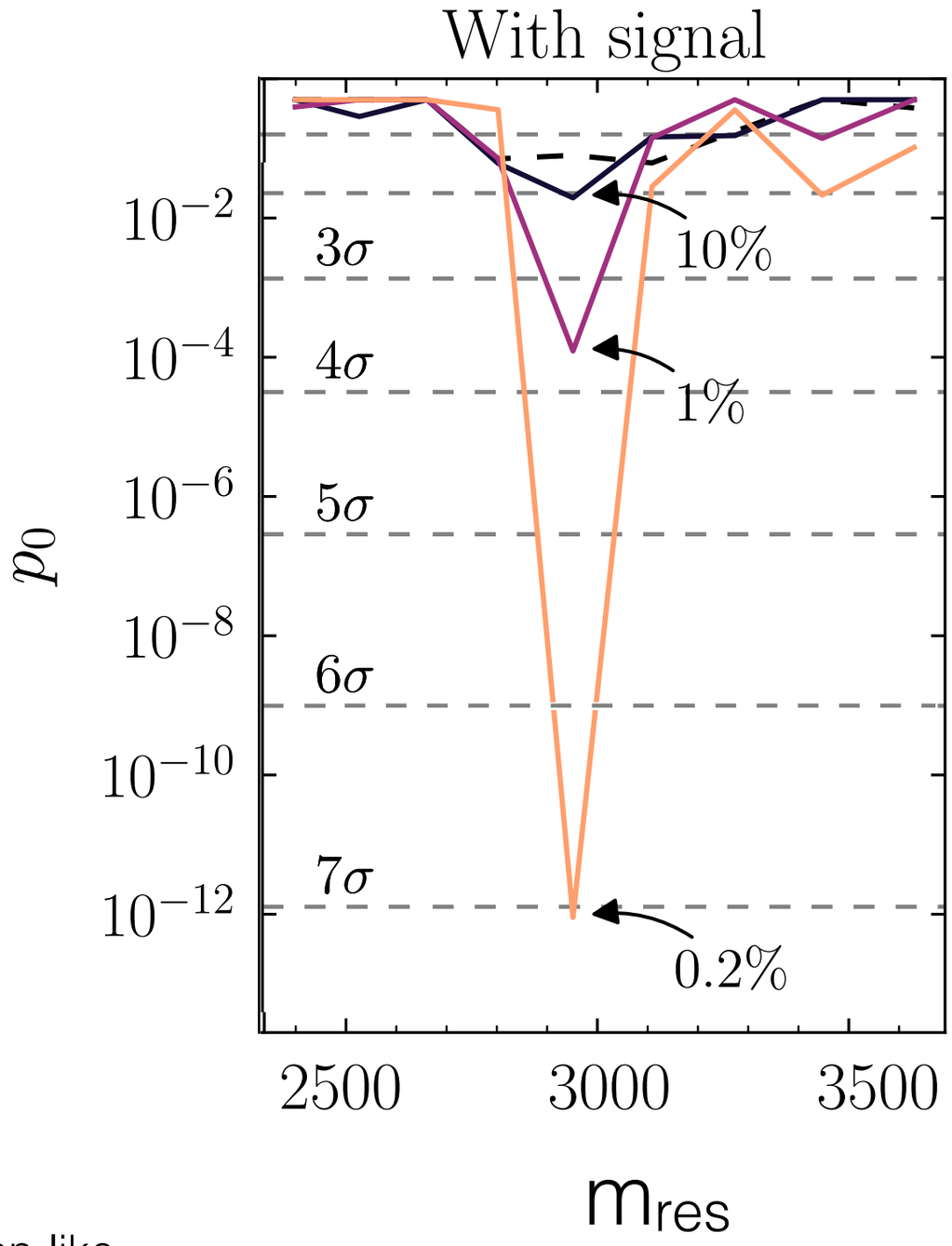



no cut on NN

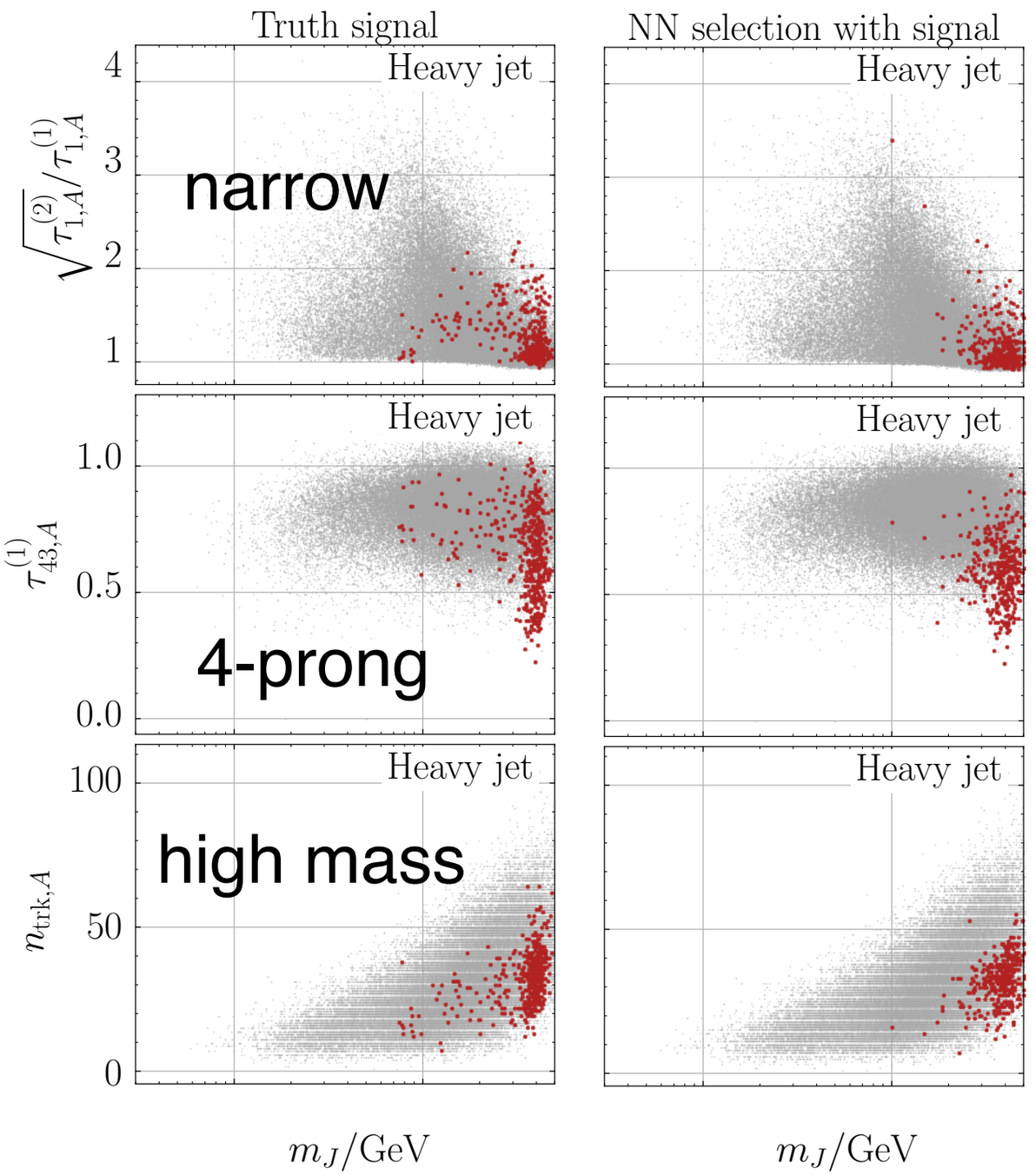
most 10% signal-region-like

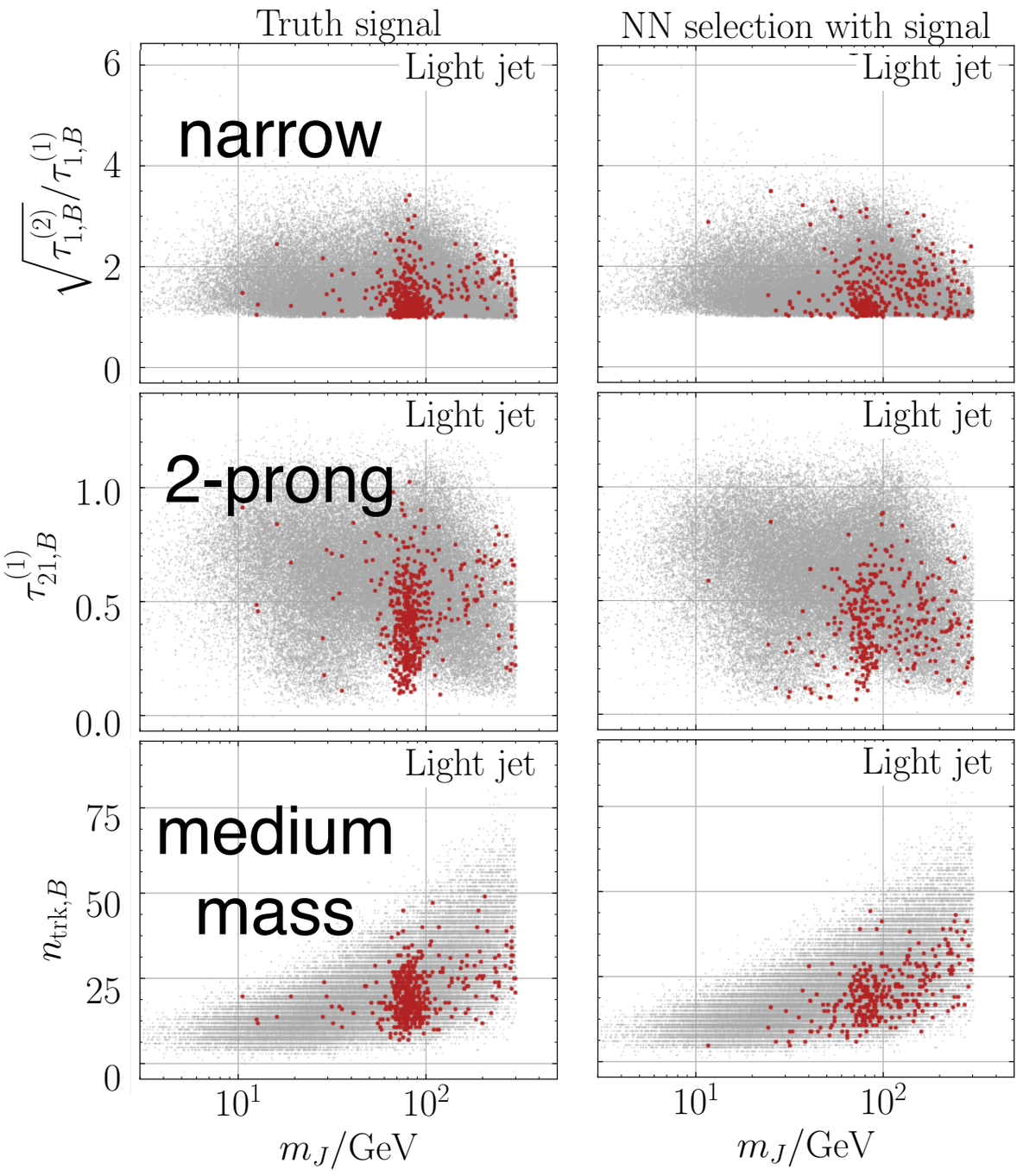
most 1% signal-region-like

most 0.2% signal-region-like

# What is the network learning?

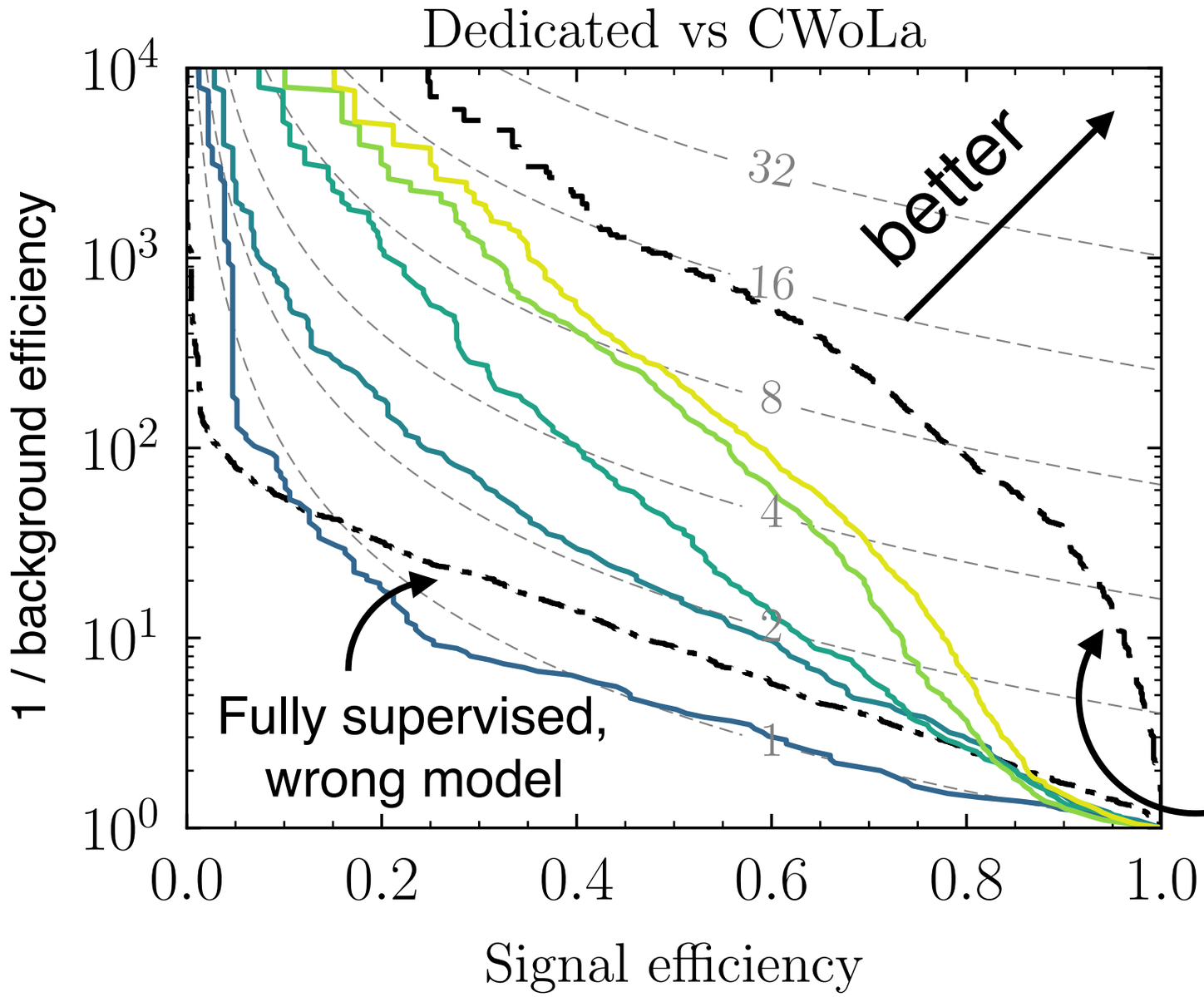





**Learns to find the signal !** **X → A(→qq) + B(→qqqq)**

# CWoLa hunting vs. Full Supervision




S = signal, B = background

- Fully Supervised $WX$
- Fully Supervised $WZ$
- CWoLa, $S/B = 2.8 \times 10^{-3}$
- CWoLa, $S/B = 4.3 \times 10^{-3}$
- CWoLa, $S/B = 5.8 \times 10^{-3}$
- CWoLa, $S/B = 8.6 \times 10^{-3}$
- CWoLa, $S/B = 1.1 \times 10^{-2}$

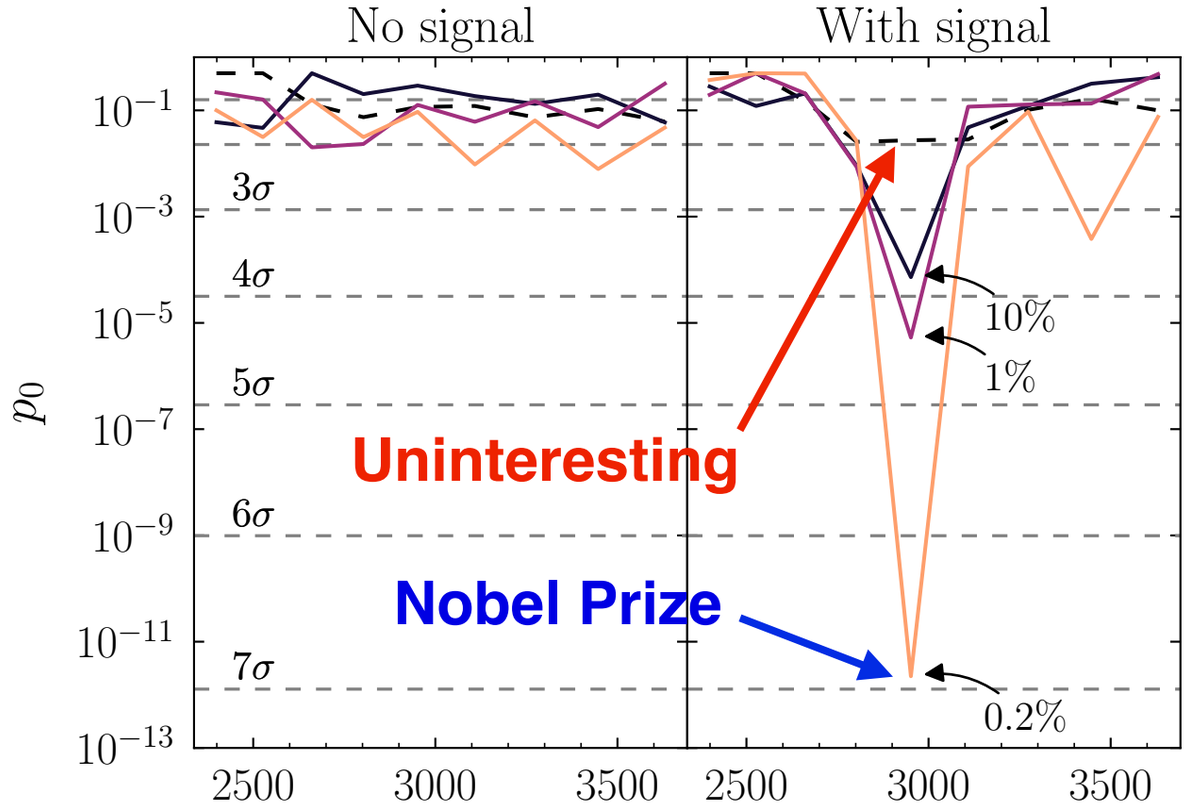
If you know what you are looking for, you should look for it. If you don't know, then CWoLa hunting may be able to catch it!

# Outlook* I

Jack Collins, Kiel Howe, **BPN**, PRL 121, 241803 (2018)



If we continue to find nothing (and even if we find something!), it is important to broaden our scope.




There may be new particles hiding, but we need **hyper-variate vision** to find it … ML can help us learn something **fundamental about nature** !

*Image from this article. This Koala is actually being freed - I do not condone violence against these animals!

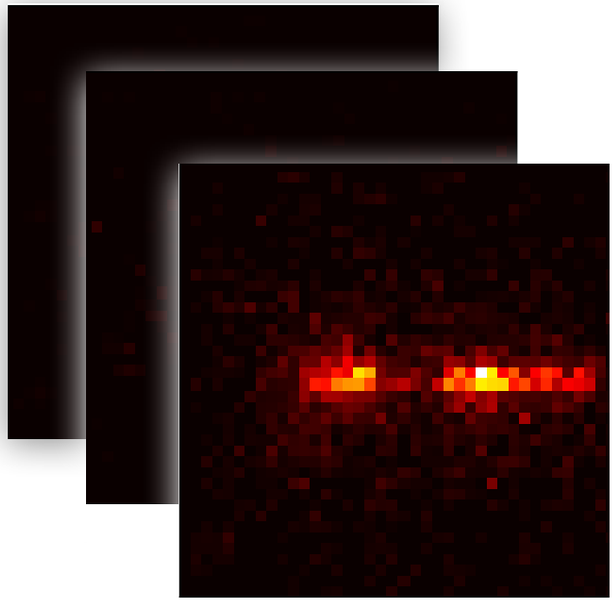
# Outlook II



*Today I've given you an example of anomaly detection with weak supervision*

*… HEP is also pushing innovative methods on many ML fronts …*

*this is just a taste of an expanding field!*



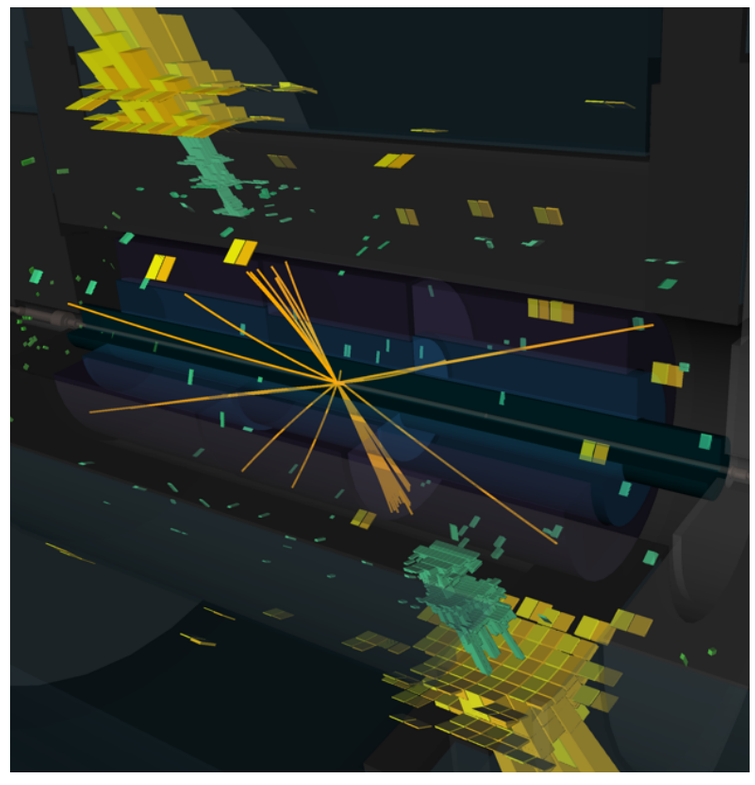
**Classification**

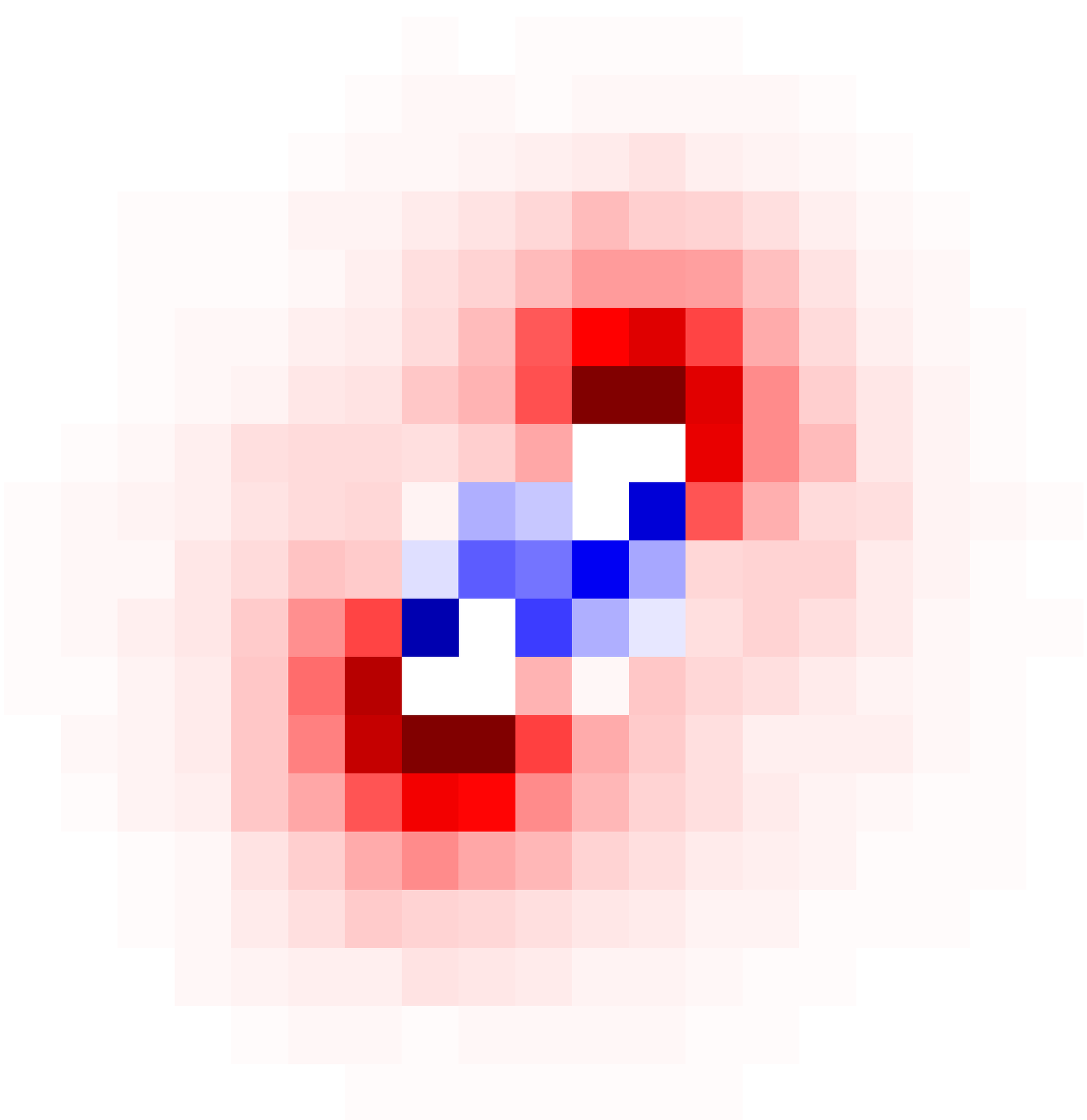
provide examples for training

arbitrarily many categories

**Generation** ← **Regression**

map noise to structure





Fin.

# Autoencoders



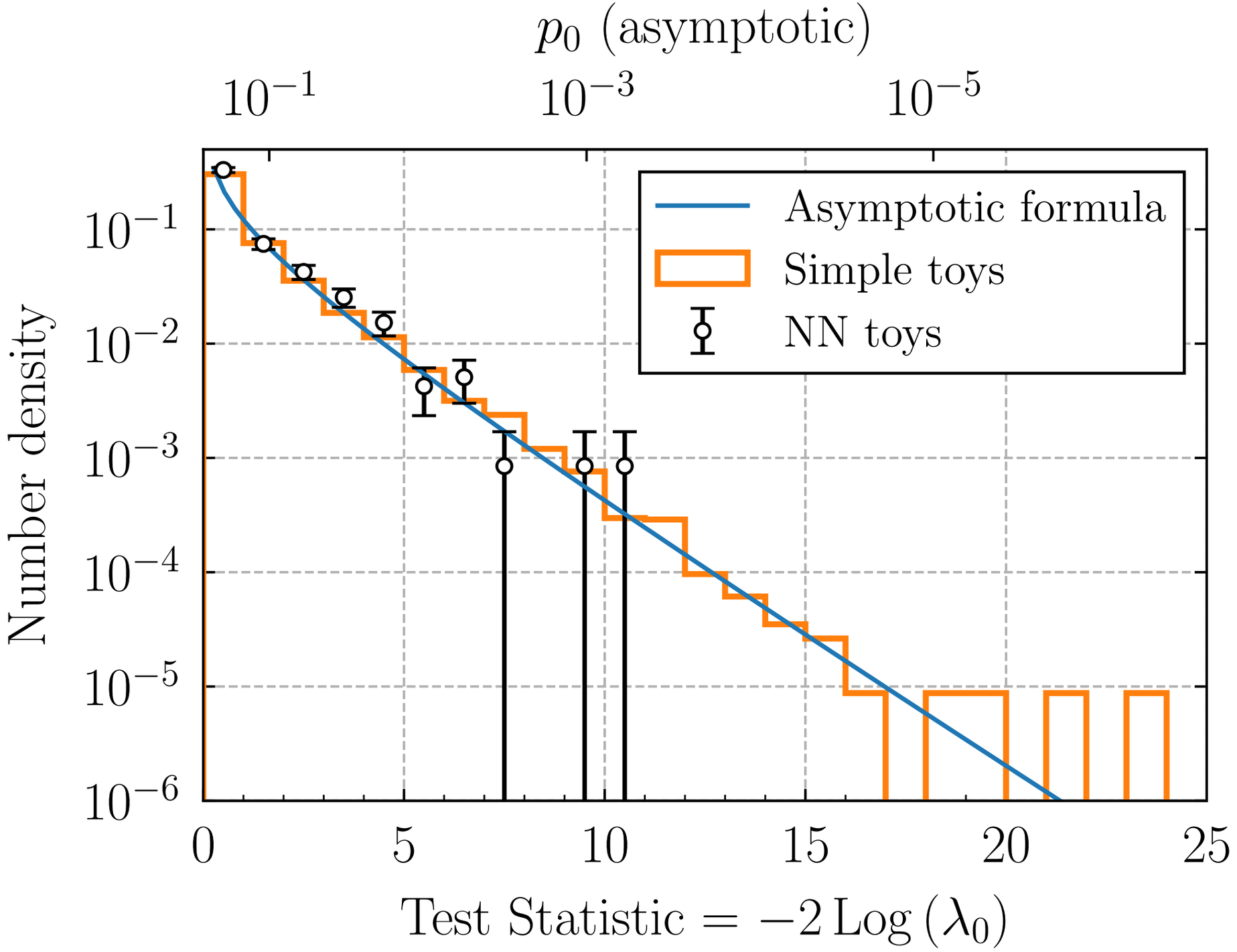
Marco Farina, Yuichiro Nakai, David Shih,
https://arxiv.org/abs/1808.08992

Theo Heimel, Gregor Kasieczka, Tilman Plehn,
Jennifer M Thompson, https://arxiv.org/abs/1808.08979

Olmo Cerri, Thong Q. Nguyen, Maurizio Pierini, Maria Spiropulu,
Jean-Roch Vlimant, https://arxiv.org/abs/1811.10276

# Statistics




$p_0$ (asymptotic)
$10^{-1}$
$10^{-3}$
$10^{-5}$
Asymptotic formula
Simple toys
NN toys
Number density
$10^{-1}$
$10^{-2}$
$10^{-3}$
$10^{-4}$
$10^{-5}$
$10^{-6}$
0
5
10
15
20
25
Test Statistic $= -2\,\mathrm{Log}\,(\lambda_0)$