

Deep learning for LHC classification, regression, generation, and beyond

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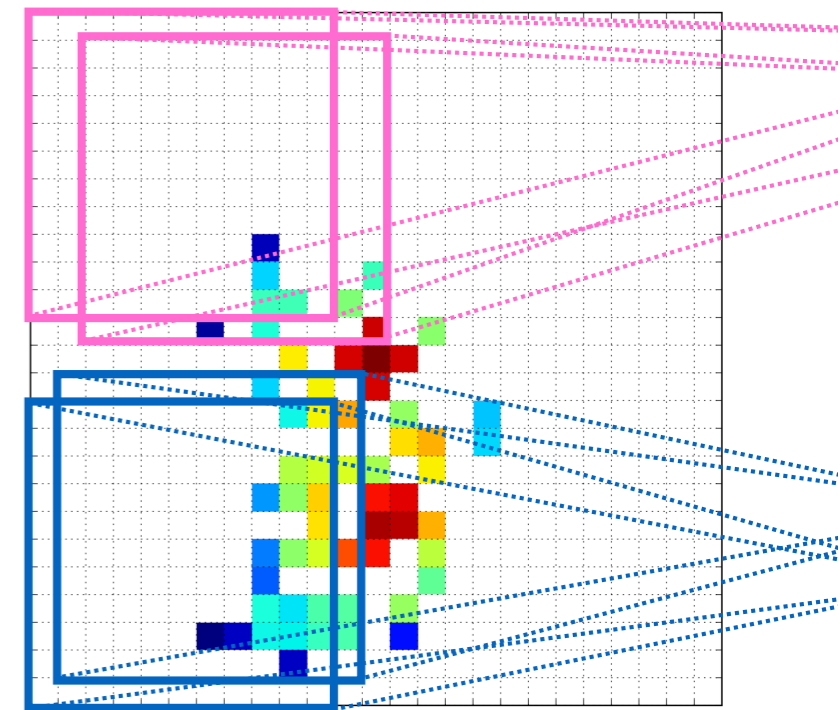
@bpnachman



bnachman



**BERKELEY
EXPERIMENTAL
PARTICLE
PHYSICS**



DANCE 2019
October 29, 2019

Deep learning for LHC classification, regression, generation, and **beyond**

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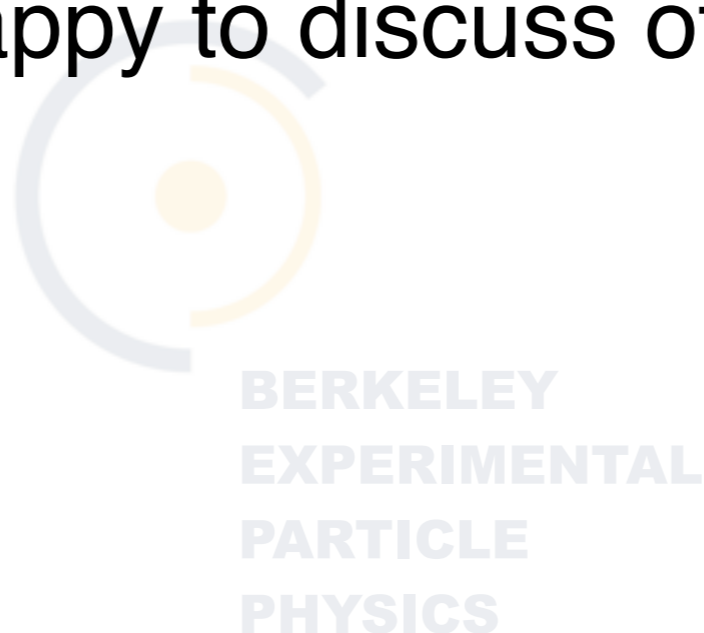
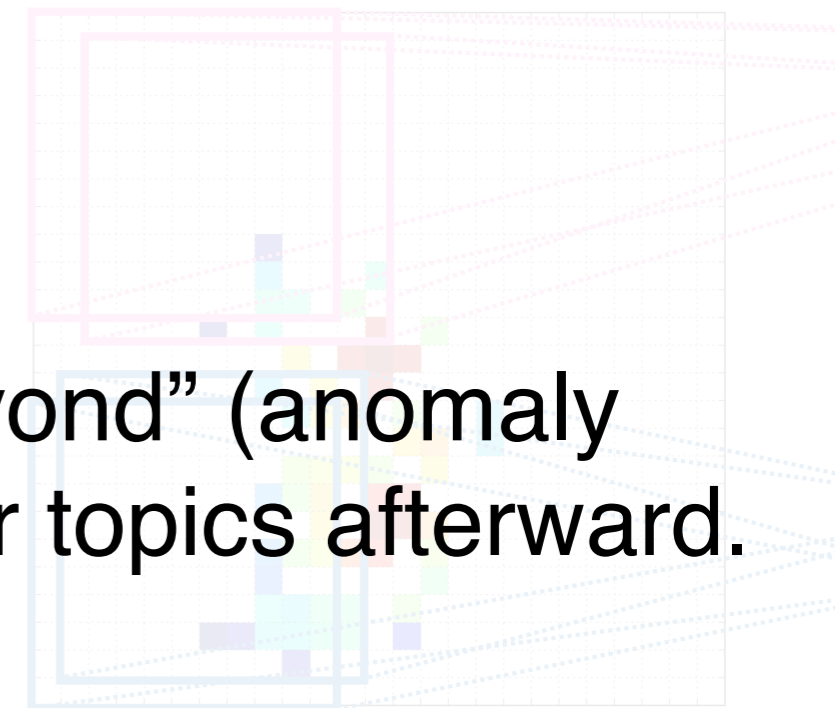
cern.ch/bnachman

[@bnachman](https://twitter.com/bnachman)

[bnachman](https://github.com/bnachman)

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...today I will mostly talk about the “beyond” (anomaly detection), but I am happy to discuss other topics afterward.



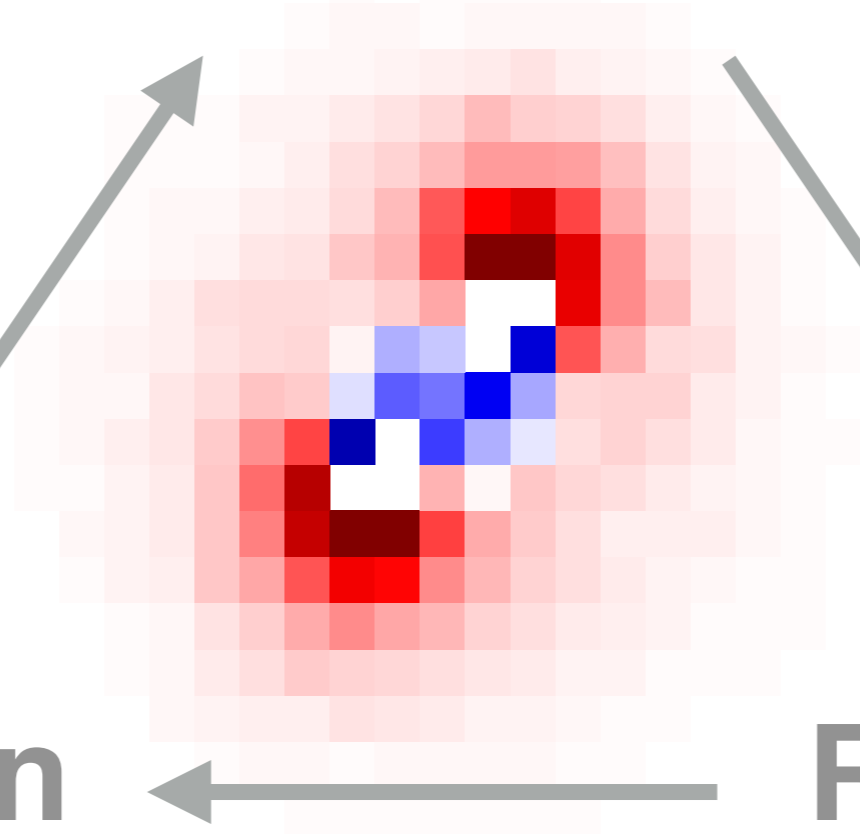
DANCE 2019
October 29, 2019

full supervision / weak supervision

Classification

provide
examples
for training

arbitrarily
many
categories

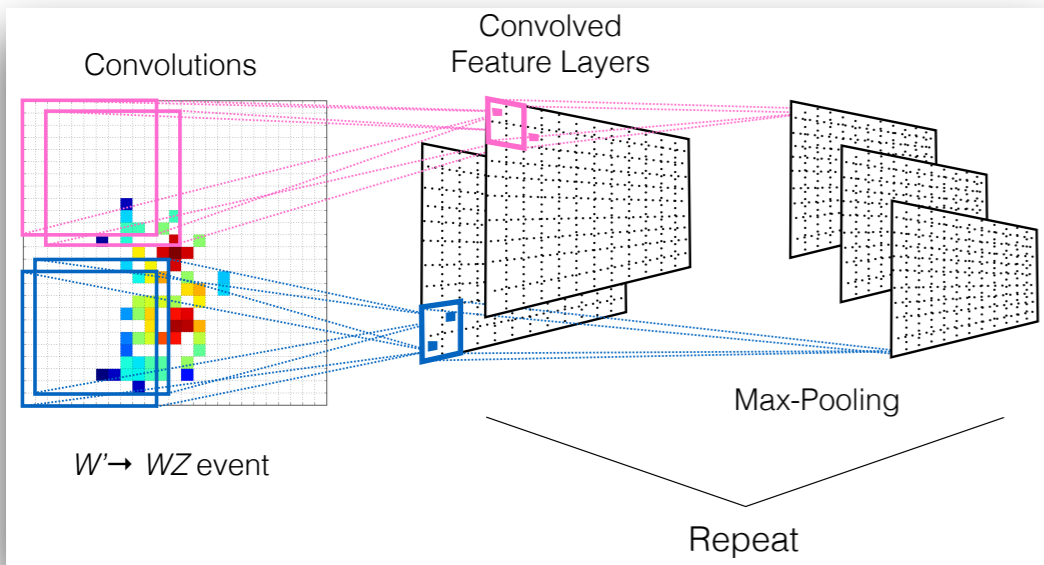


Generation

Regression

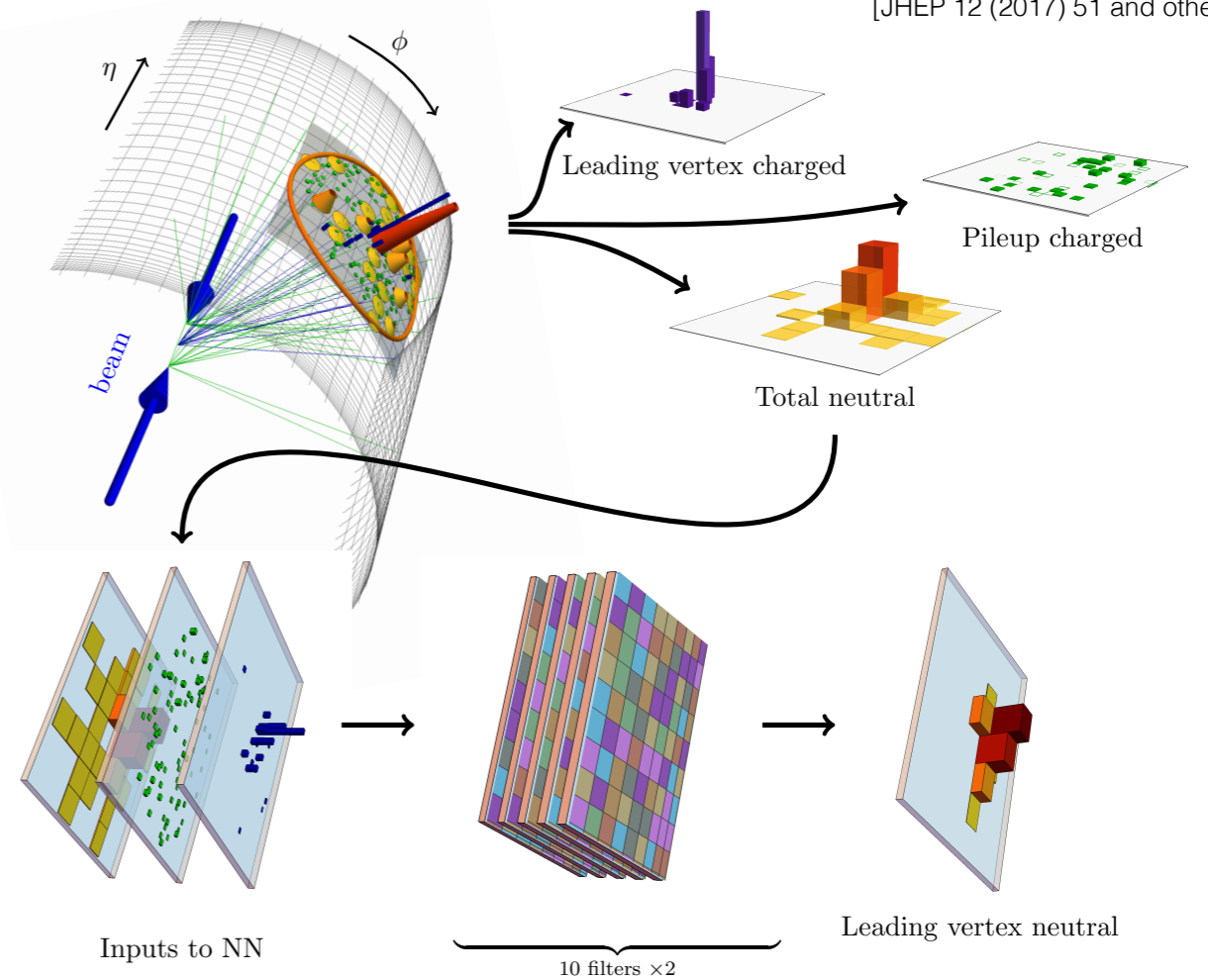
map noise
to structure

[JHEP 07 (2016) 069 and papers that cite it]



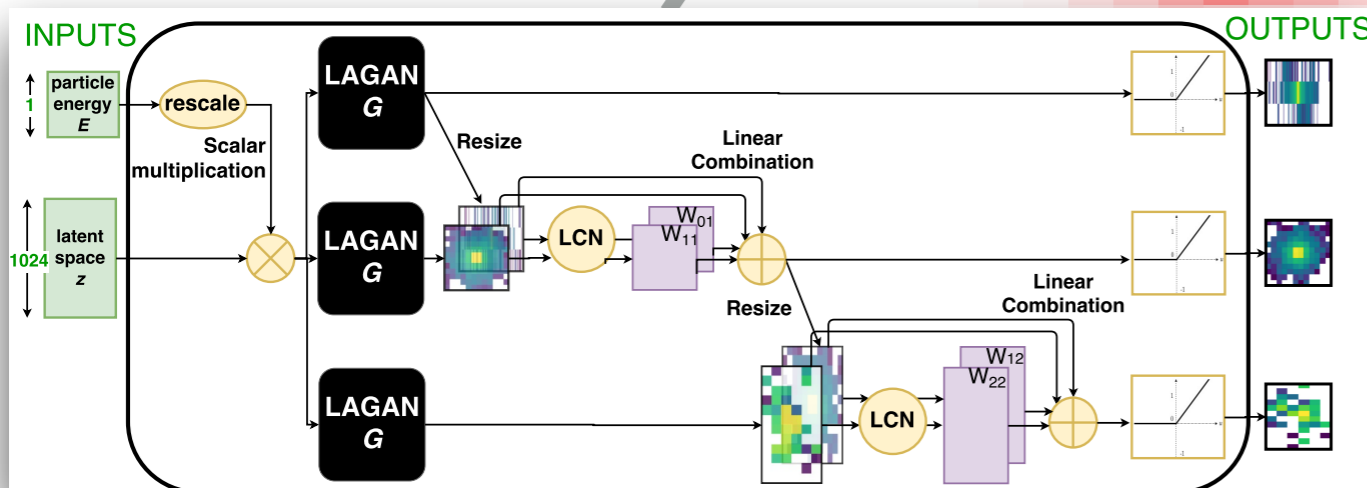
Representing detectors as images

[JHEP 12 (2017) 51 and others]



Convolutional Neural Networks for Noise Mitigation

[PRL 120 (2018) 042003 and papers that cite it]



Generative Adversarial Networks to accelerate simulation

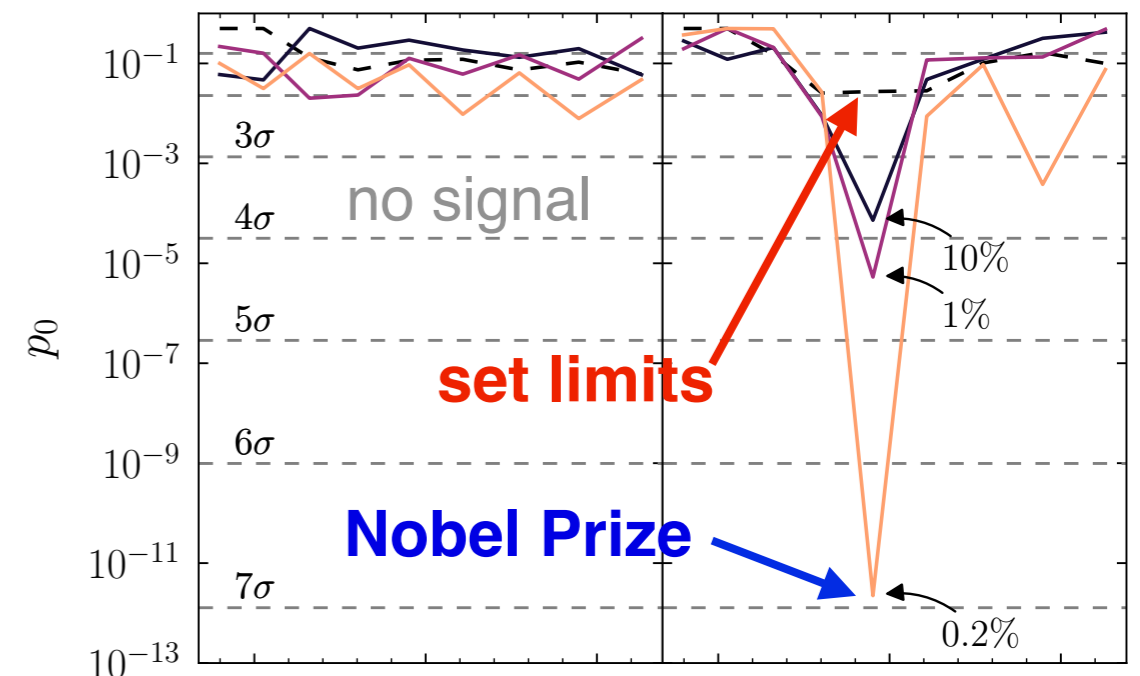
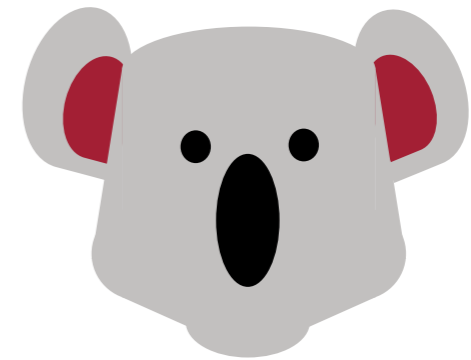
Regression

Many places where these are already part of collaboration workflows ... many other places where this is still active work!

Outline for today

5

- Uncertainties in a NN-based analysis
- Searches at the LHC
- Learning without labels
- Model agnostic searches
- The future





“But what are the uncertainties on the NN”?

- question asked by every review board

“But what are the uncertainties on the NN”?

- question asked by every review board

- Before this can happen, need to better understand statistical and systematic properties of DNN based discriminators

3. Absence of rigorous treatment of statistical/systematic errors

(snippets from yesterday's slides)

Uncertainties for a NN-based analysis



Precision / Optimality: $\text{NN}(\mathbf{x}) \neq \frac{p_{\text{true}}(\mathbf{x}|\text{S+B})}{p_{\text{true}}(\mathbf{x}|\text{B})}$

limited training statistics

$p_{\text{train}}(\mathbf{x}) \neq p_{\text{true}}(\mathbf{x})$

inaccurate training data

$\text{NN}(\mathbf{x})|_{p_{\text{true}}=p_{\text{train}}} \neq \frac{p_{\text{true}}(\mathbf{x}|\text{S+B})}{p_{\text{true}}(\mathbf{x}|\text{B})}$

model/optimization flexibility

Statistical uncertainty

Systematic uncertainty

limited prediction statistics

$p_{\text{prediction}}(\mathbf{x}) \neq p_{\text{true}}(\mathbf{x})$

inaccurate prediction data

Accuracy / Bias: $p_{\text{prediction}}(\text{NN}) \neq p_{\text{true}}(\text{NN})$

High-dimensional Uncertainty



One word of caution: current paradigm for uncertainties may be too naive for hypervariate analysis!

(truly end-to-end)

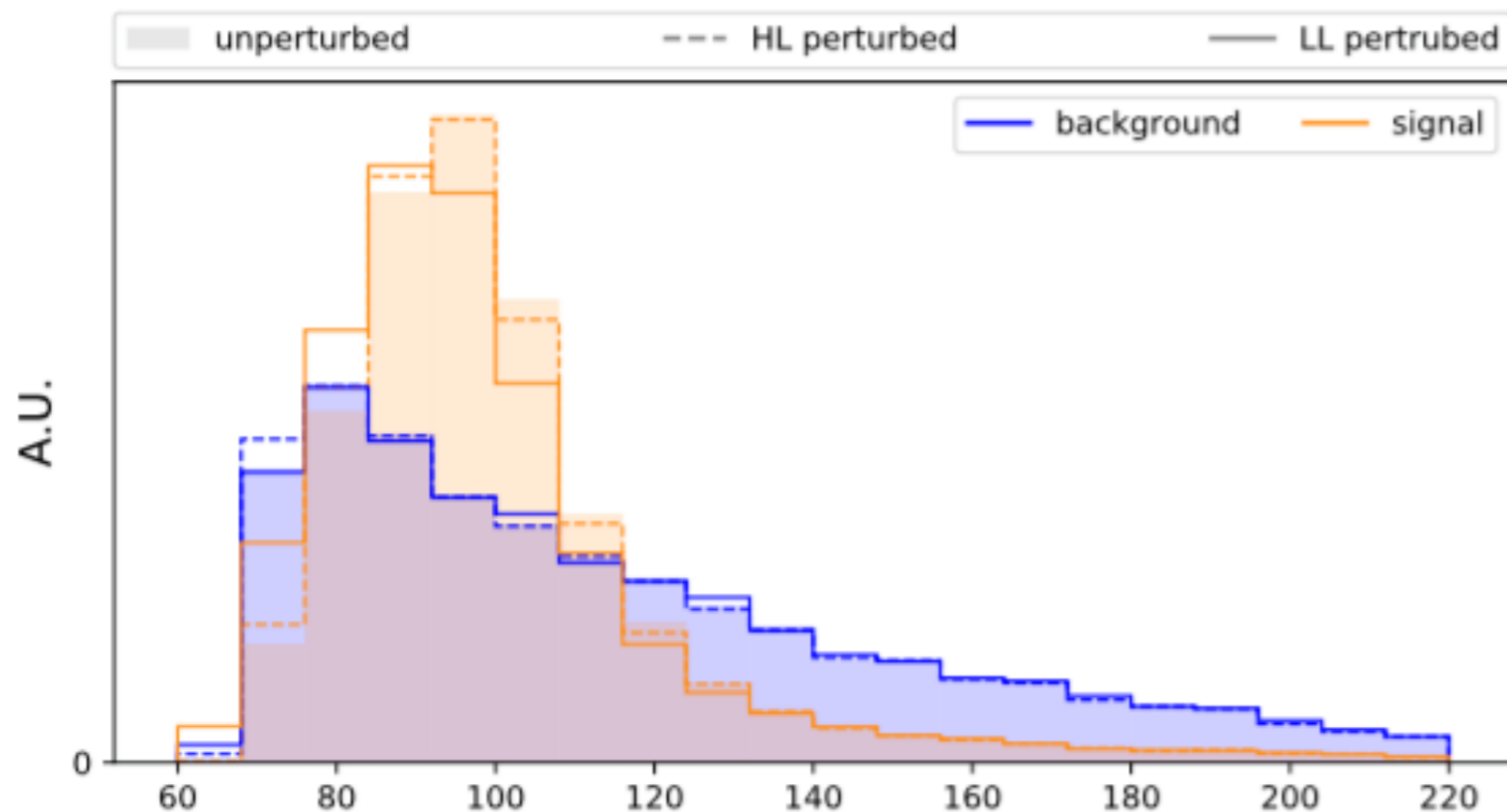
e.g. for some uncertainties, we often compare two different models - one nuisance parameter.

High-dimensional Uncertainty

10

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e.g. for some uncertainties, we often compare two different models - one nuisance parameter.



Borrowing ideas from **AI safety**, one can show that small perturbations can make big changes in NN output while preserving “control region” performance.

Some observable we want to validate

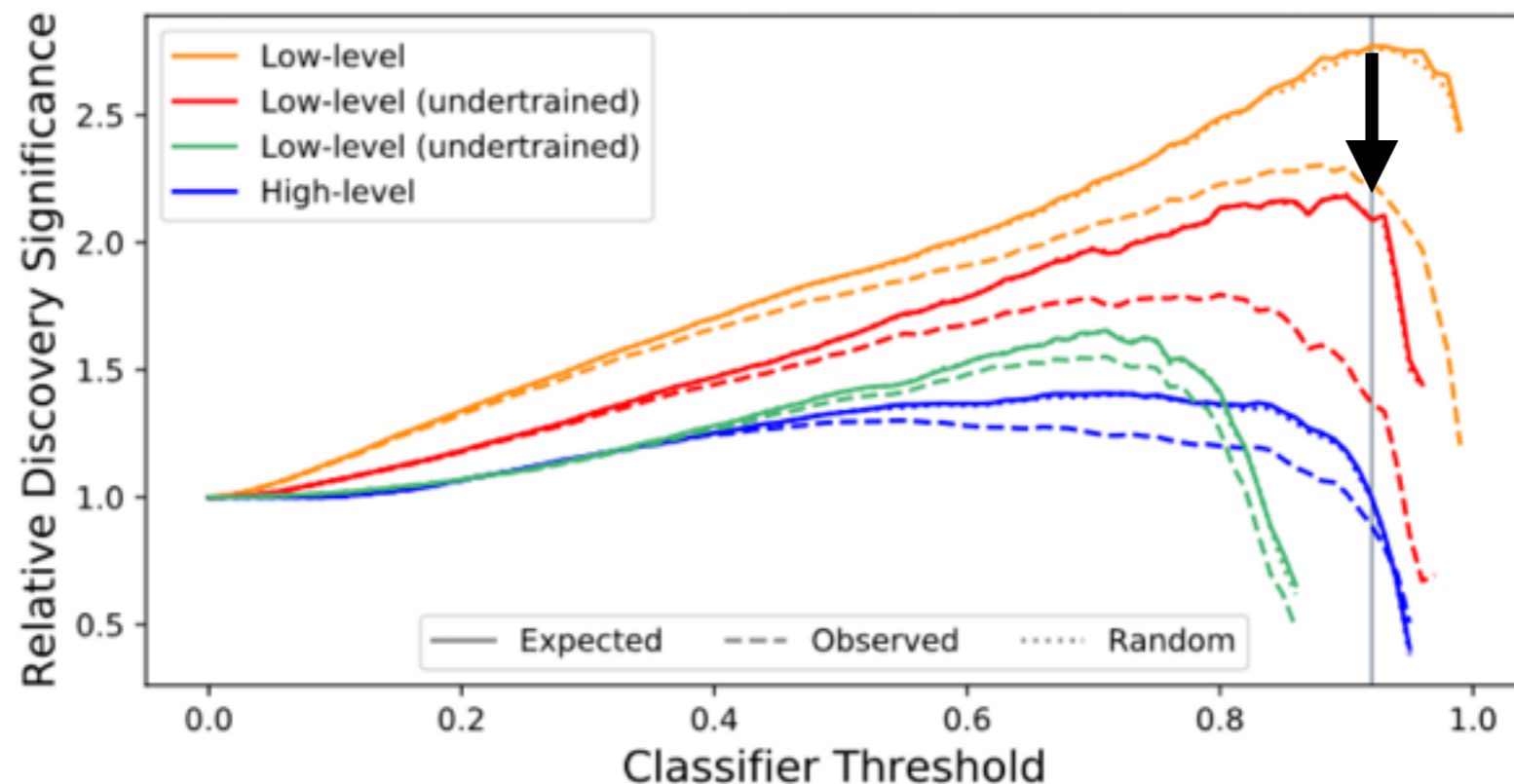
[1910.08606]

High-dimensional Uncertainty

11

One word of caution: current paradigm for uncertainties may be too naive for hypervariate analysis!

e.g. for some uncertainties, we often compare two different models - one nuisance parameter.



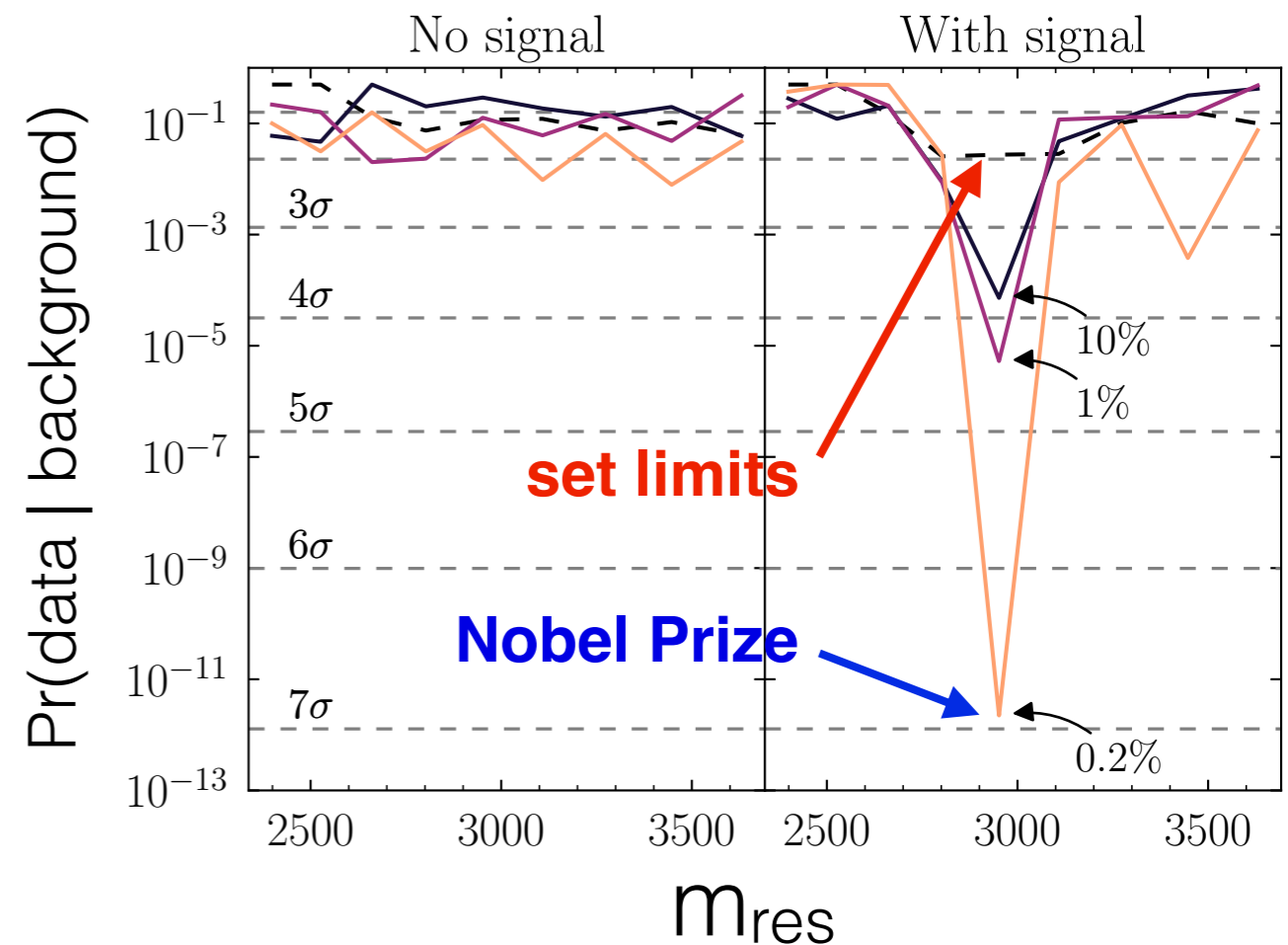
Borrowing ideas from **AI safety**, one can show that small perturbations can make big changes in NN output while preserving “control region” performance.

How to get around this?

12

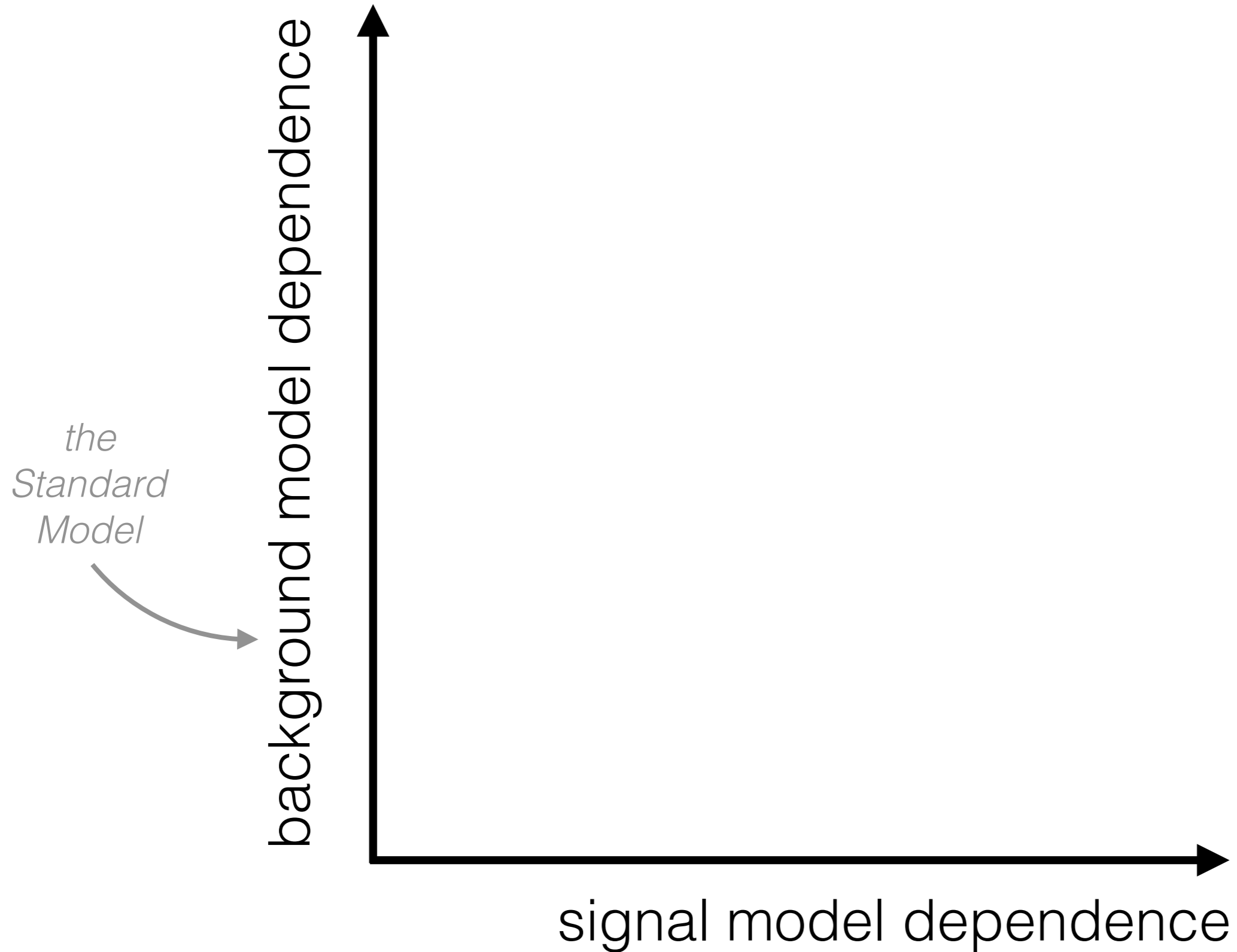
Work hard to understand the true nuisance parameters in the hypervariate parameter space.

Don't use simulation!
(focus for the rest of the talk
though not always possible!)



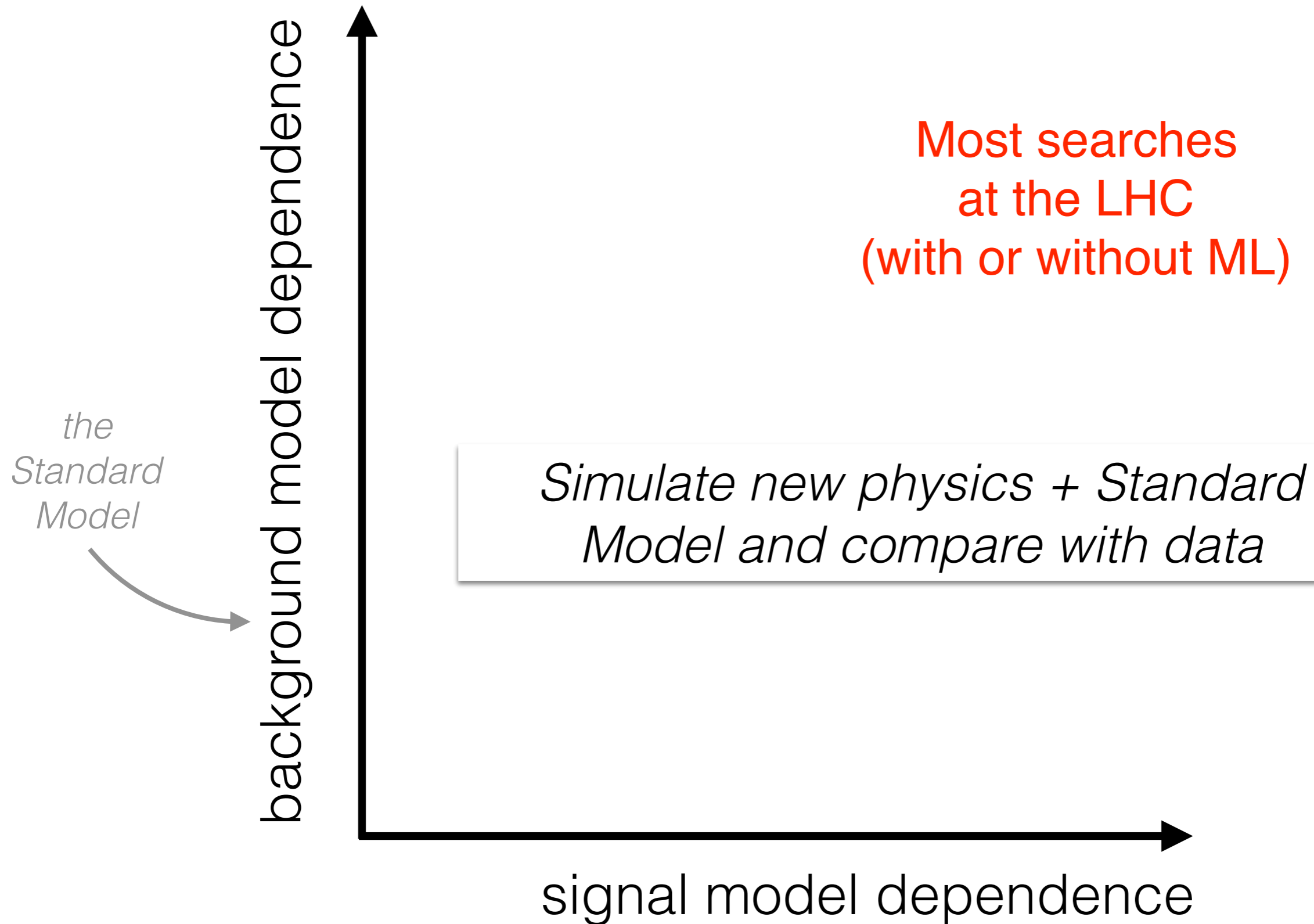
Searching for new particles / forces

13



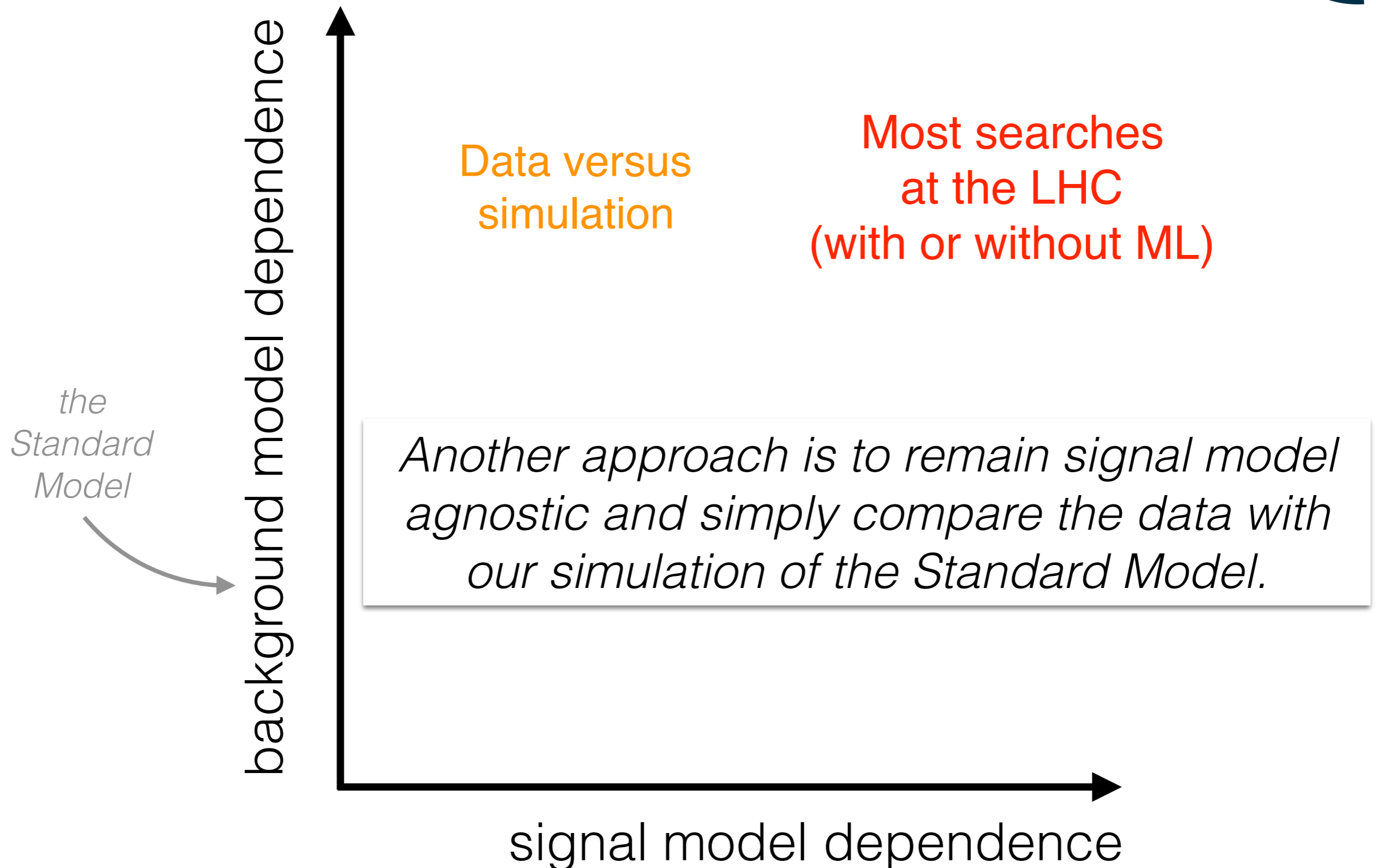
Searching for new particles / forces

14



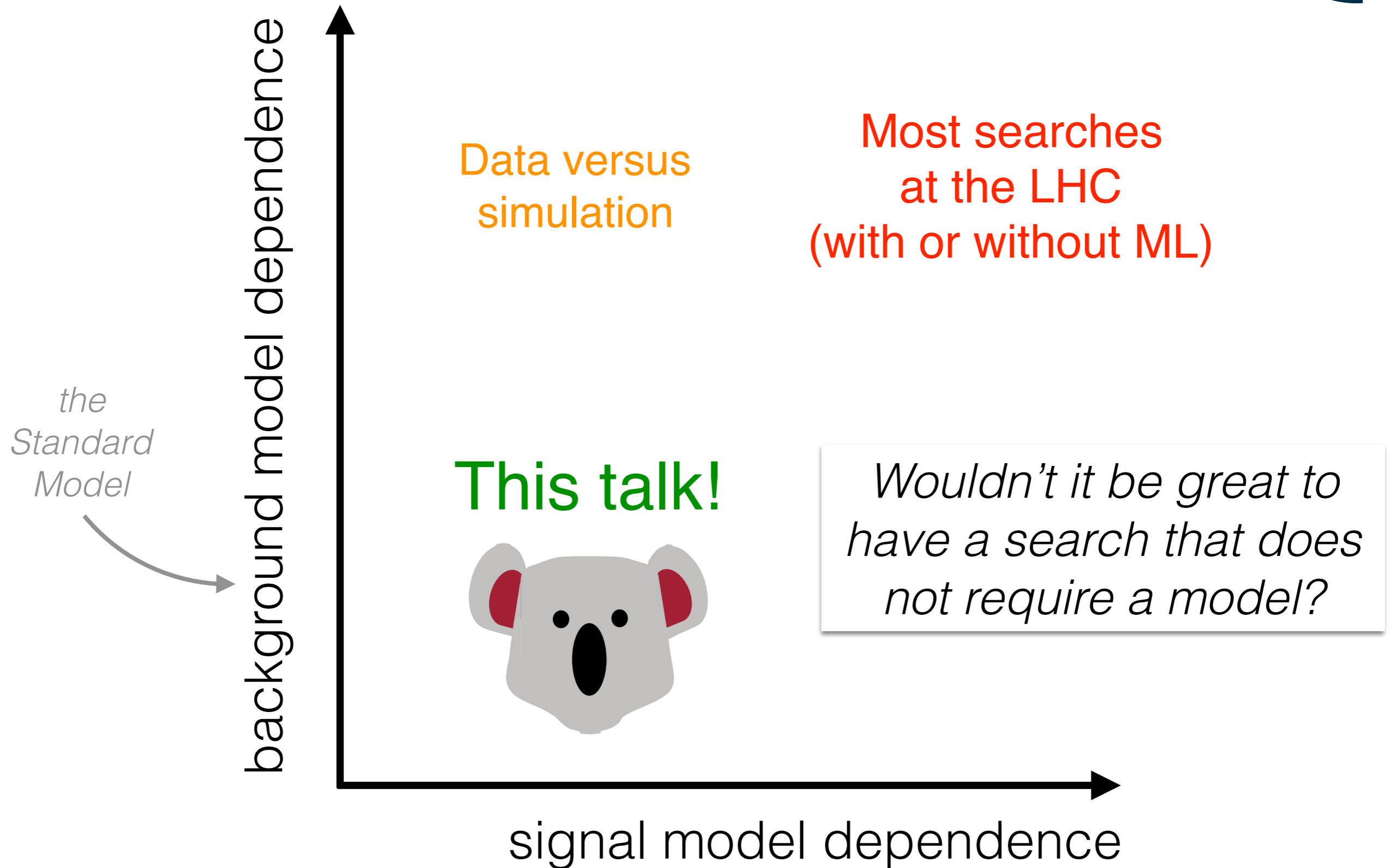
Searching for new particles / forces

15



Searching for new particles / forces

16



Searching for new particles / forces

17

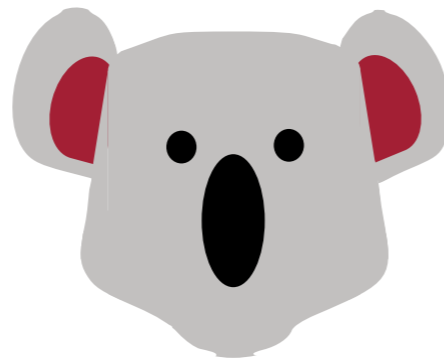
background model dependence

The question then becomes:

**how to train a classifier directly on data,
without a particular signal model in mind?**

*the
Standard
Model*

This talk!



*Wouldn't it be great to
have a search that does
not require a model?*

signal model dependence

What is the problem?

18

Why can't I just pay some physicists to label events and then train a neural network using those labels?



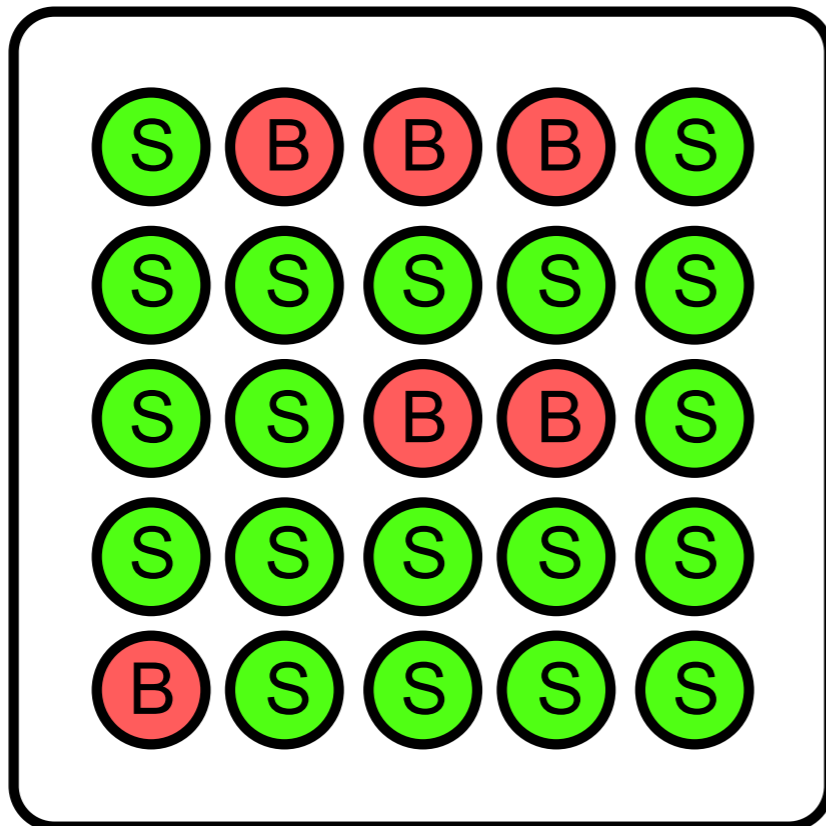
Image credit: pixabay.com

Answer: this is not cats-versus-dogs ... thanks to quantum mechanics it is **not possible to know** what happened.

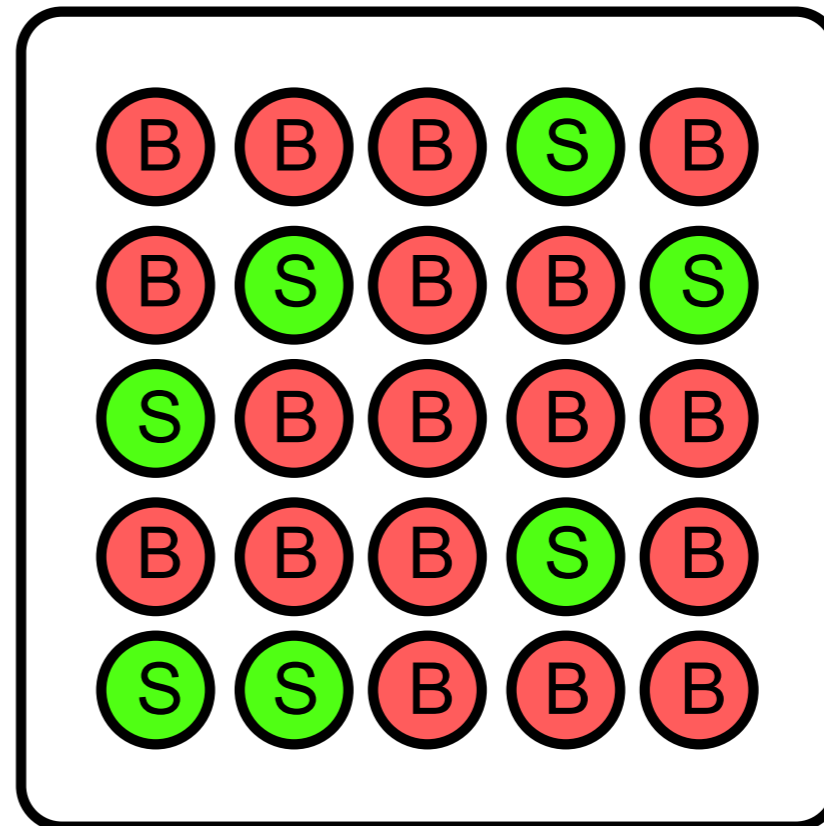
What is the problem?

The data are unlabeled and in the best case, come to us as mixtures of two classes (“signal” and “background”).

Mixed Sample 1



Mixed Sample 2



(we don't get to observe the color of the circles)

What is the problem?

20

The data are unlabeled and in the best case, come to us as mixtures of two classes (“signal” and “background”).

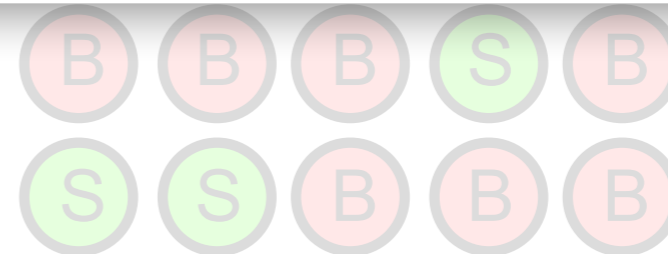
Mixed Sample 1



Mixed Sample 2

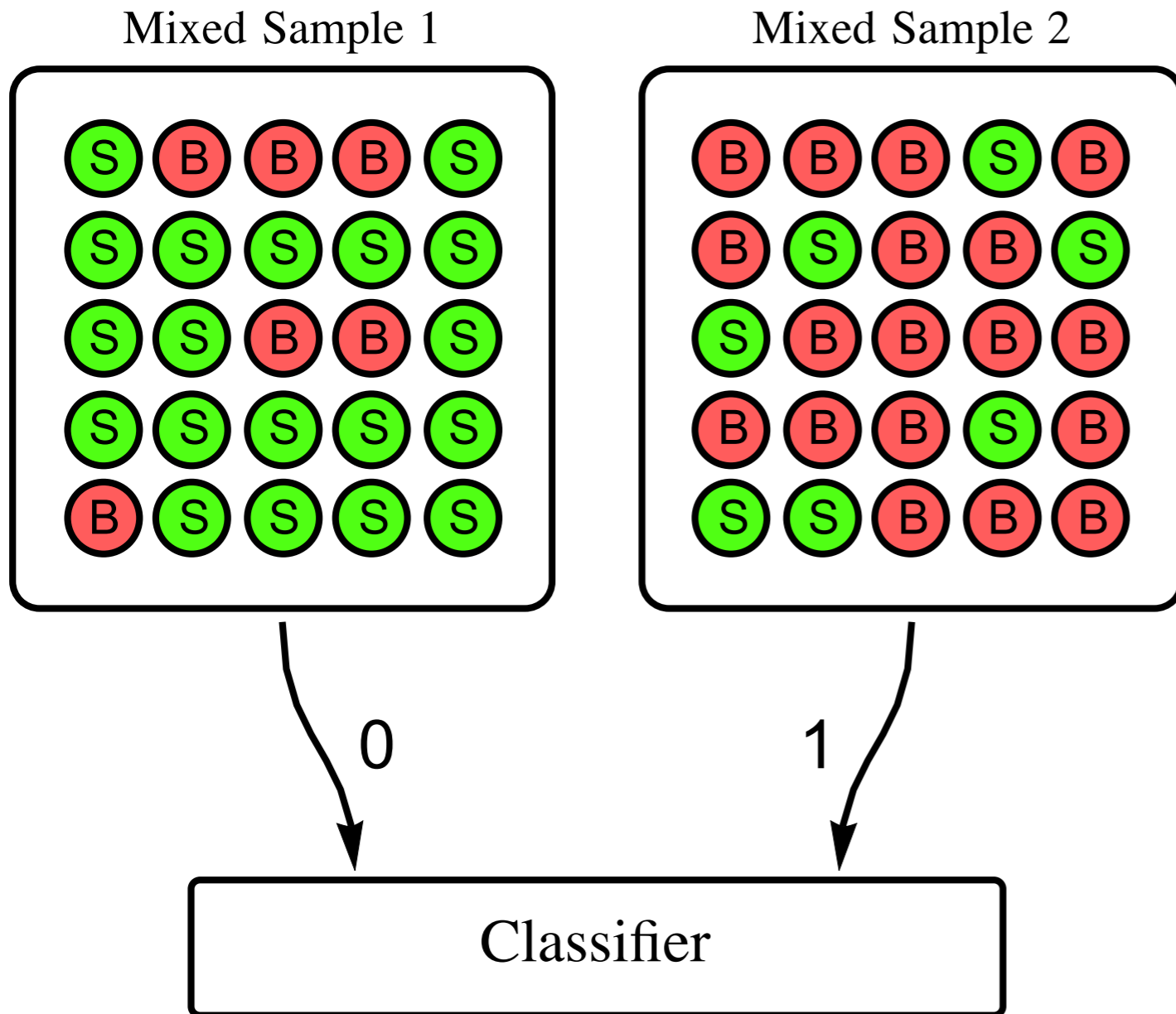


Can we do without any label info?



(we don't get to observe the color of the circles)

Classification Without Labels



Yes !

[Komiske, Metodiev, **BPN**, Schwartz, PRD 98 (2018) 011502]

[Cohen, Freytsis, Ostdiek, JHEP 02 (2018) 034]

[Metodiev, **BPN**, Thaler, JHEP 10 (2017) 51]

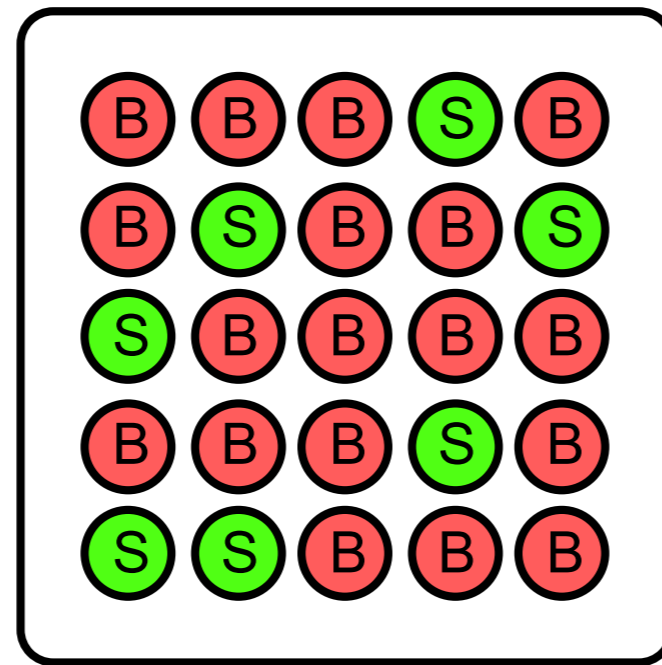
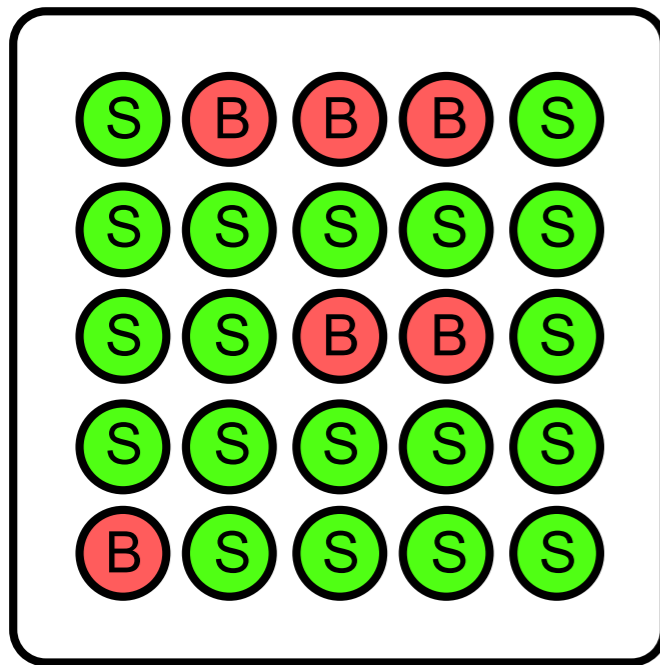
[Dery, **BPN**, Rubbo, Schwartzman, JHEP 05 (2017) 145]

Classification Without Labels

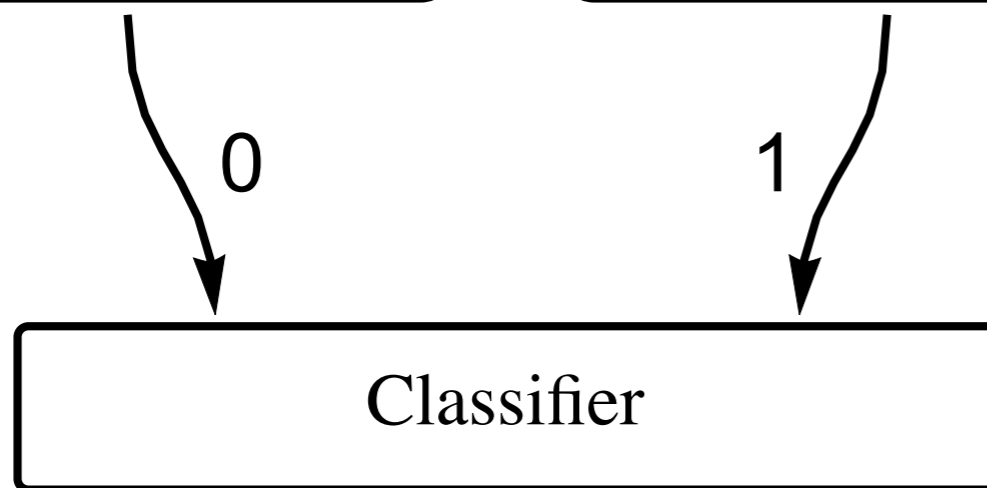


Mixed Sample 1

Mixed Sample 2



Yes !



[Komiske, Metodiev, **BPN**, Schwartz, PRD 98 (2018) 011502]

[Cohen, Freytsis, Ostdiek, JHEP 02 (2018) 034]

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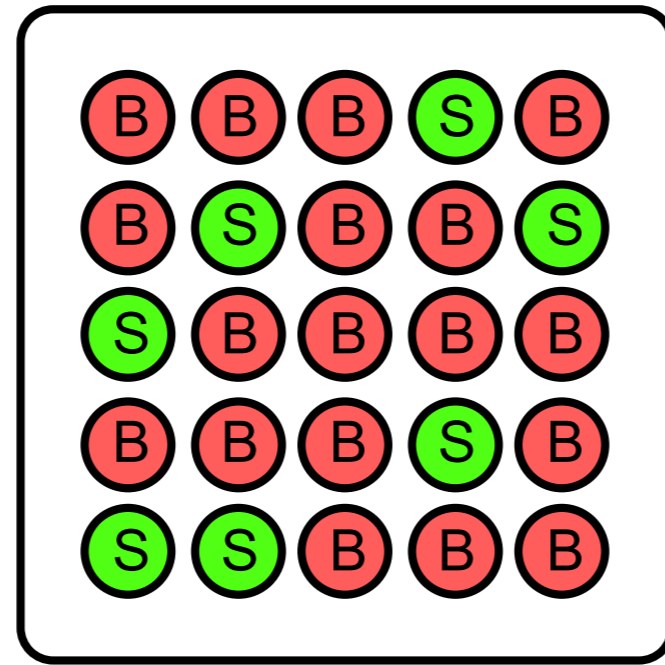
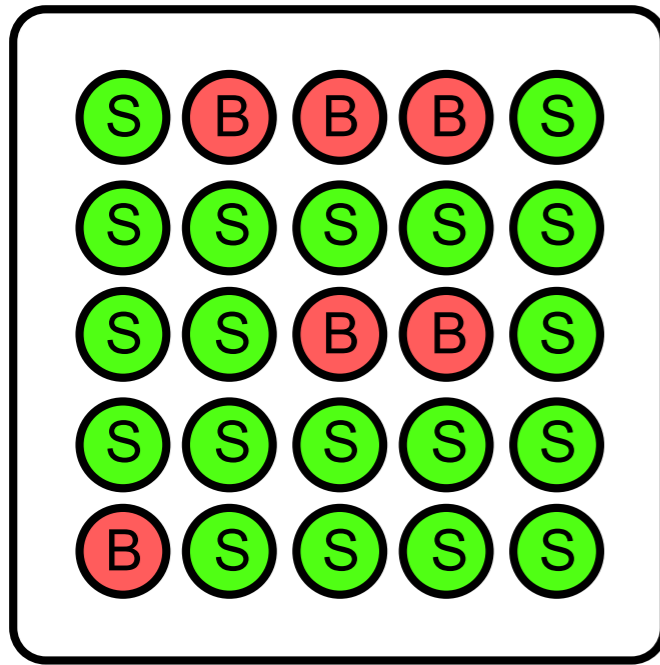
Classification Without Labels



23

Mixed Sample 1

Mixed Sample 2



0

1

Classifier

Yes !

One can show that this procedure asymptotically converges to the optimal classifier (with labels).

[Komiske, Metodiev, **BPN**, Schwartz, PRD 98 (2018) 011502]

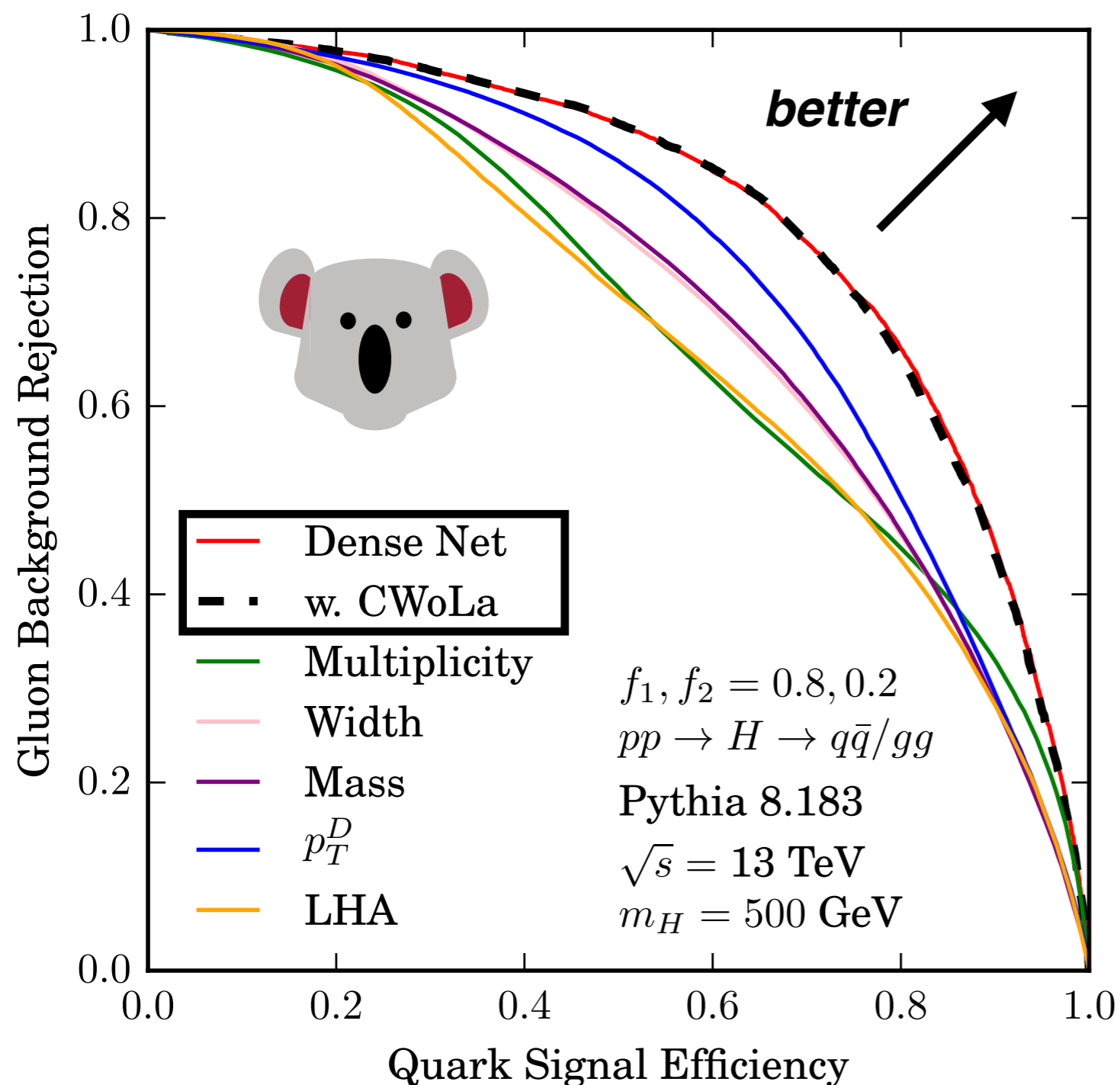
[Cohen, Freytsis, Ostdiek, JHEP 02 (2018) 034]

[Metodiev, **BPN**, Thaler, JHEP 10 (2017) 51]

[Dery, **BPN**, Rubbo, Schwartzman, JHEP 05 (2017) 145]

Classification Without Labels

24



In practice, it also seems to work well, often approaching the case with 100% label information (fully supervised)

What if we know even less?



25

There are many uses for CWoLa when you know the two classes. What if you don't - can we use CWoLa to **hunt for new** particles without a signal model in mind?

What if we know even less?

26

There are many uses for CWoLa when you know the two classes. What if you don't - can we use CWoLa to **hunt for new** particles without a signal model in mind?

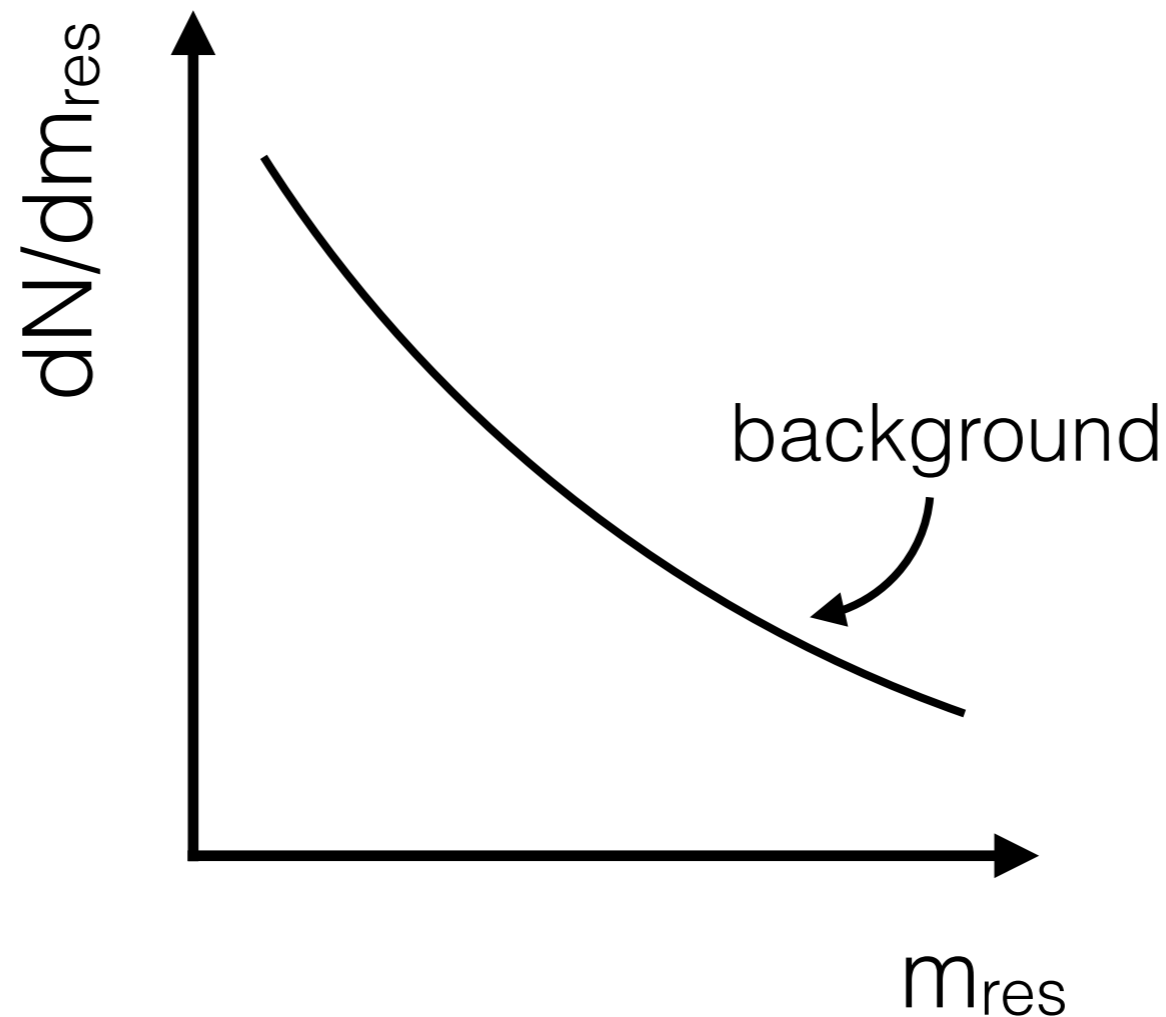


Yes!
...CWoLa hunting

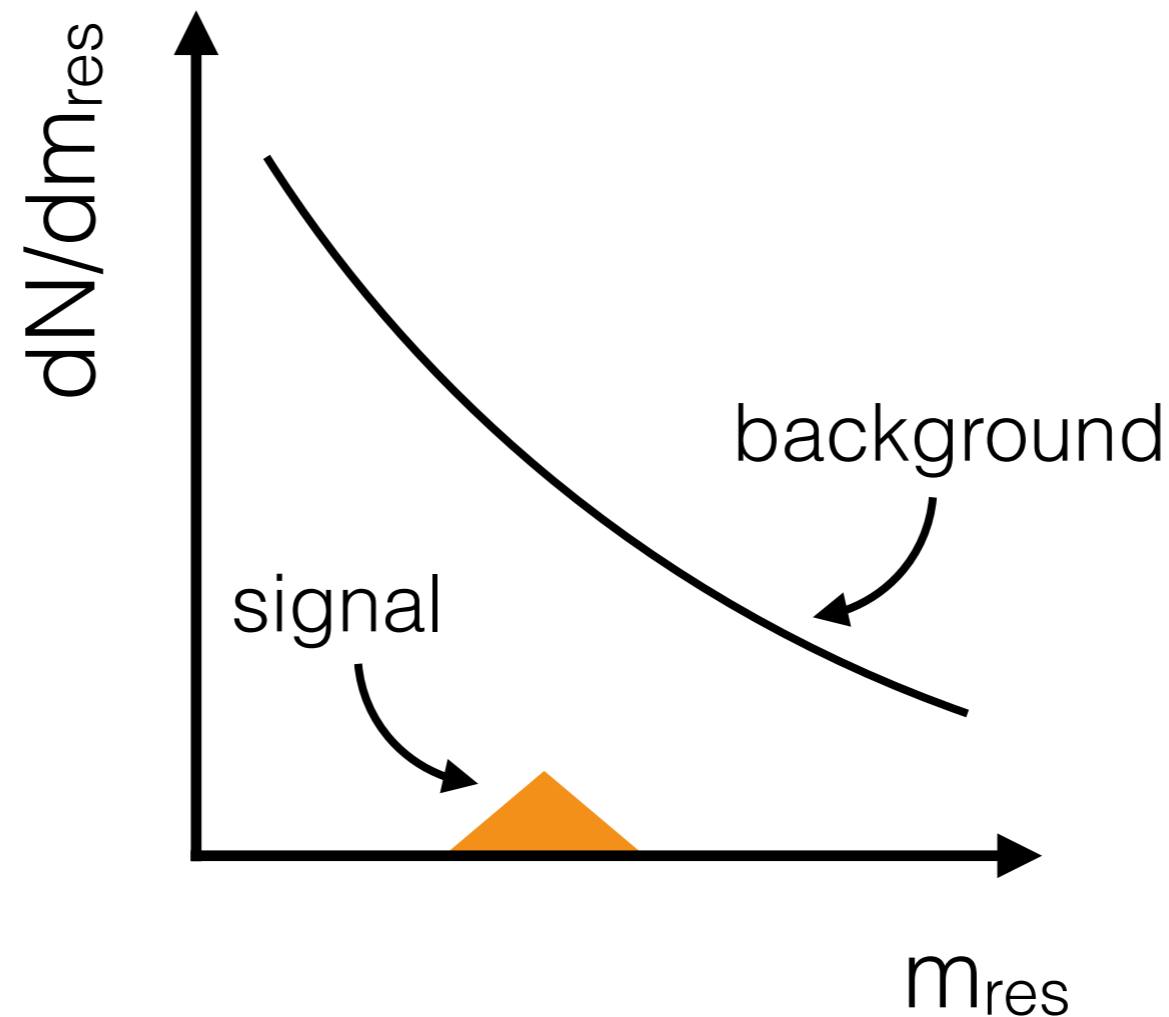
[J. Collins, K. Howe, **BPN**
PRL 121 (2018) 241803]

[J. Collins, K. Howe, **BPN**
PRD 99 (2019) 014038]

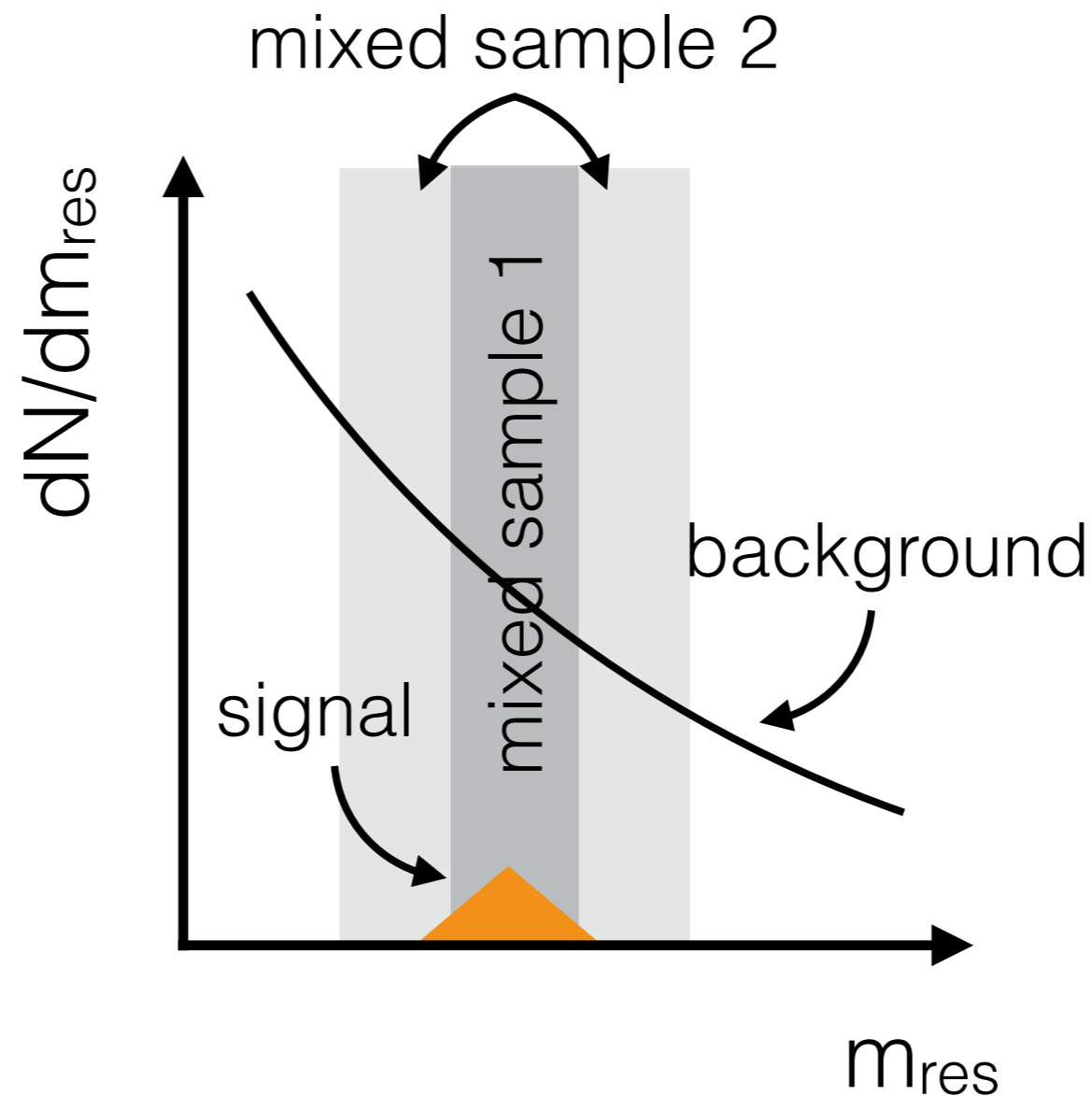
*Image from *The Courier Mail*. Koala is actually being freed - I do not condone violence against these animals!



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



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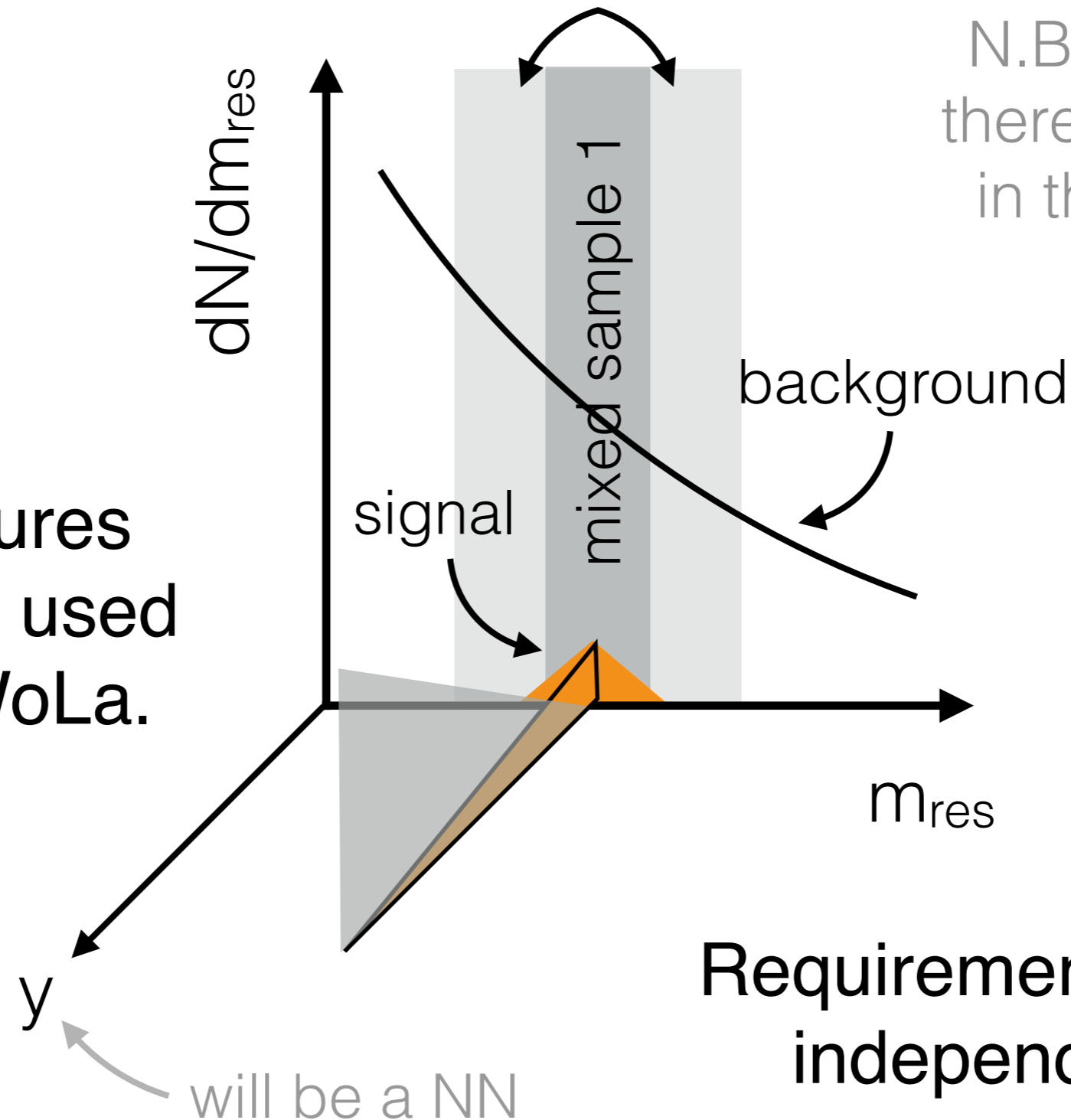


We don't know where the signal is, but for a given hypothesis, we can make signal windows and sidebands.

CWoLa Hunting for new particles

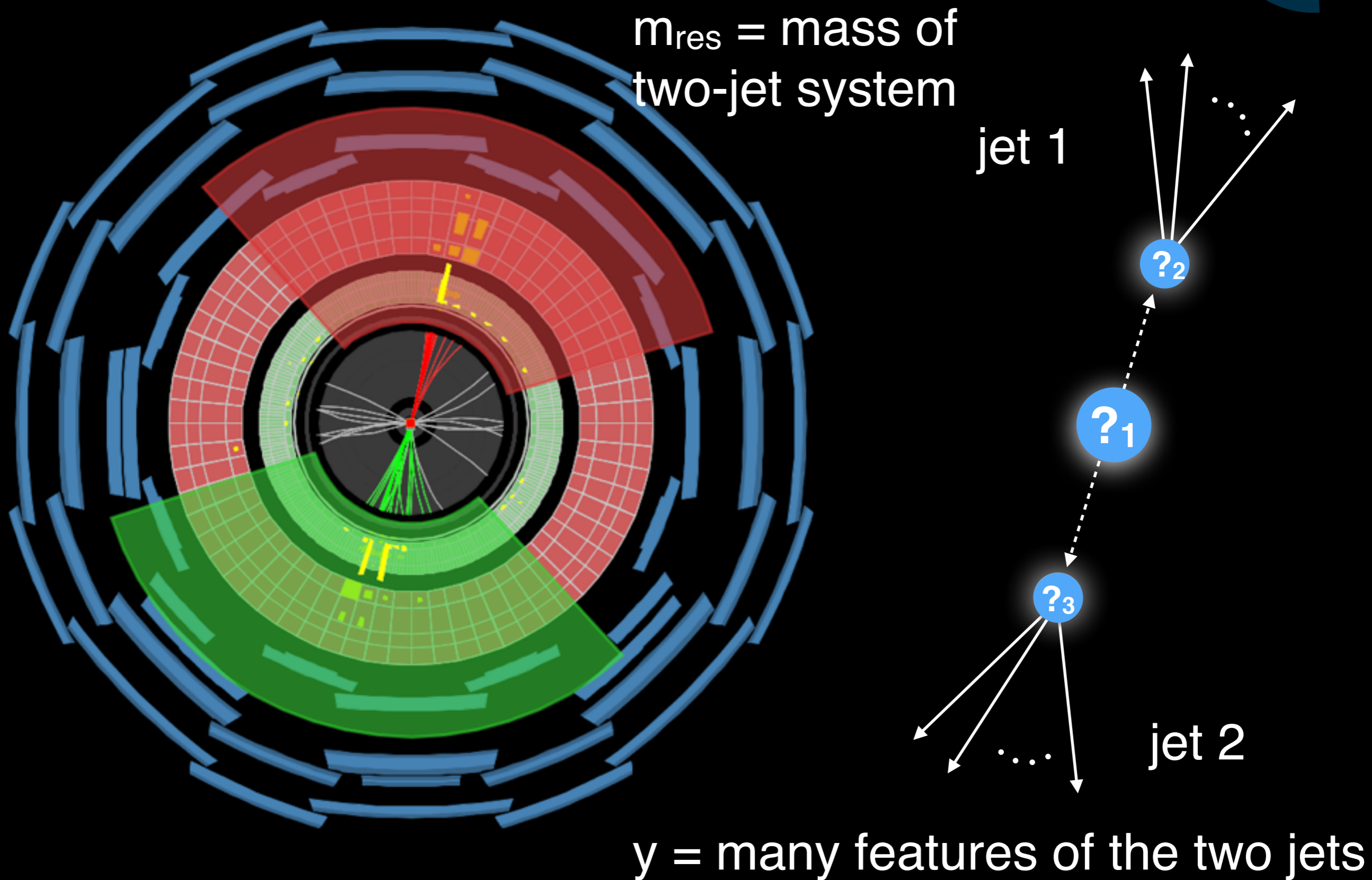
30

mixed sample 2



Example: two-jet search

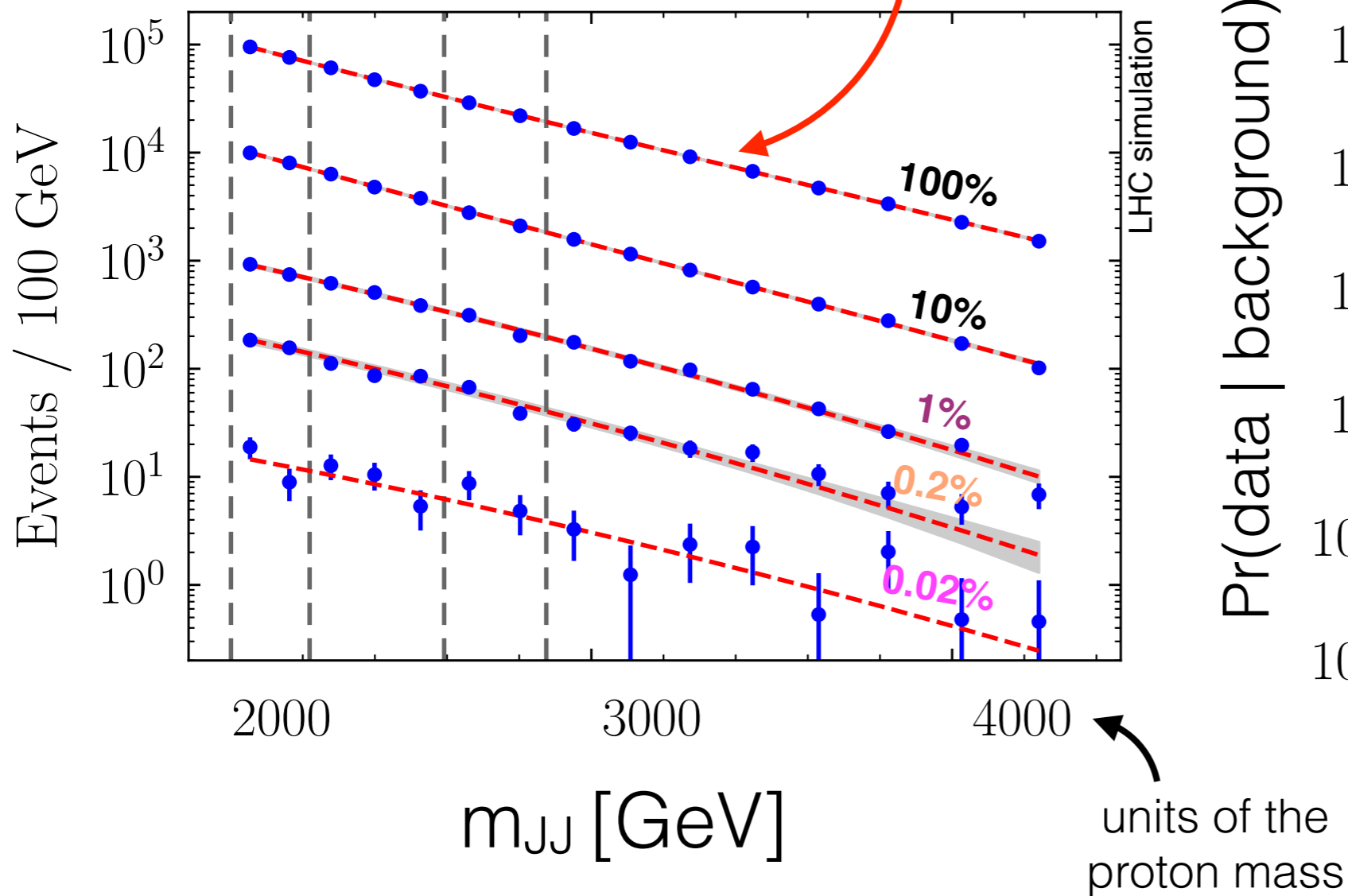
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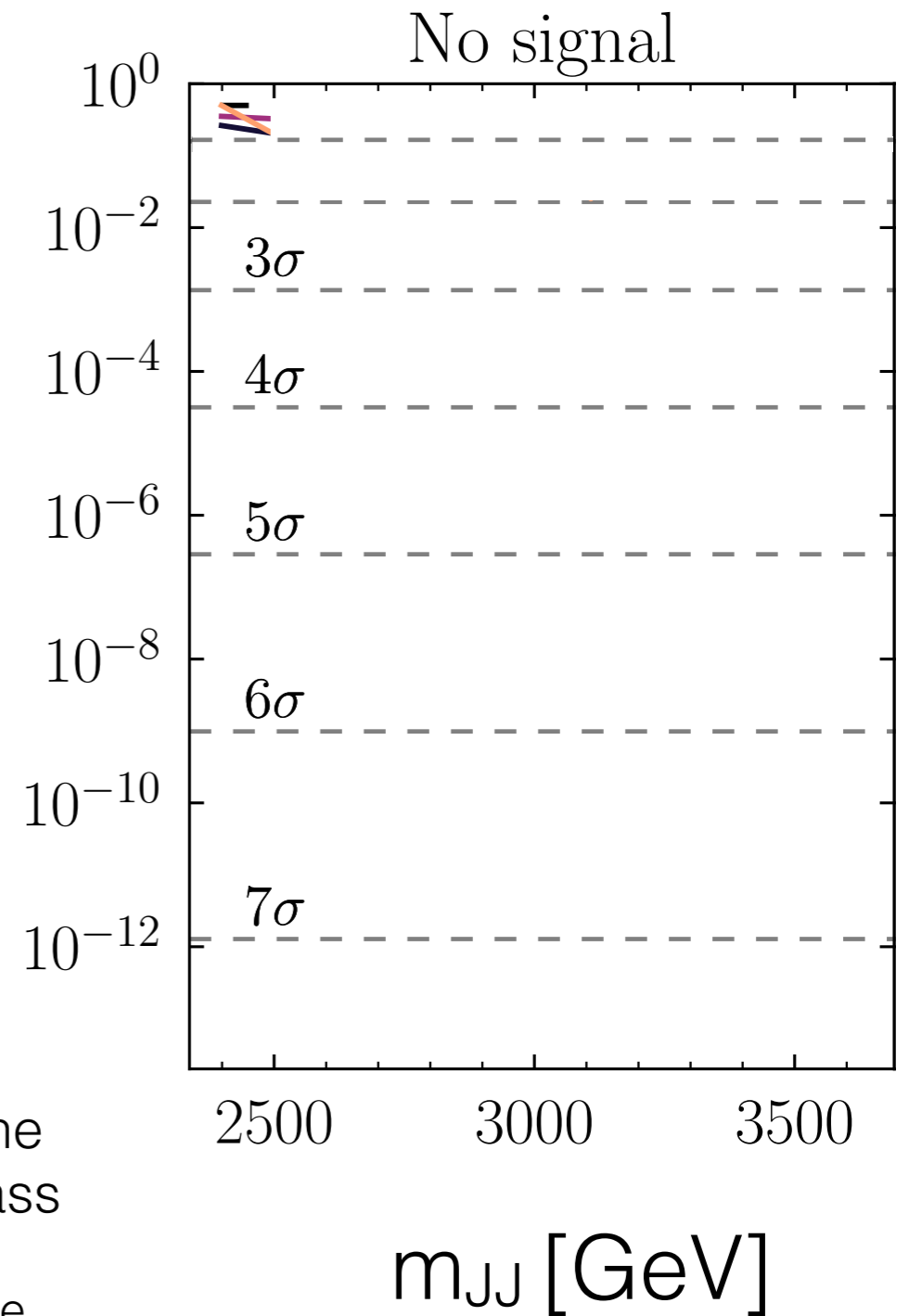
Example: two-jet search

sidebands

standard parametric fit to background.



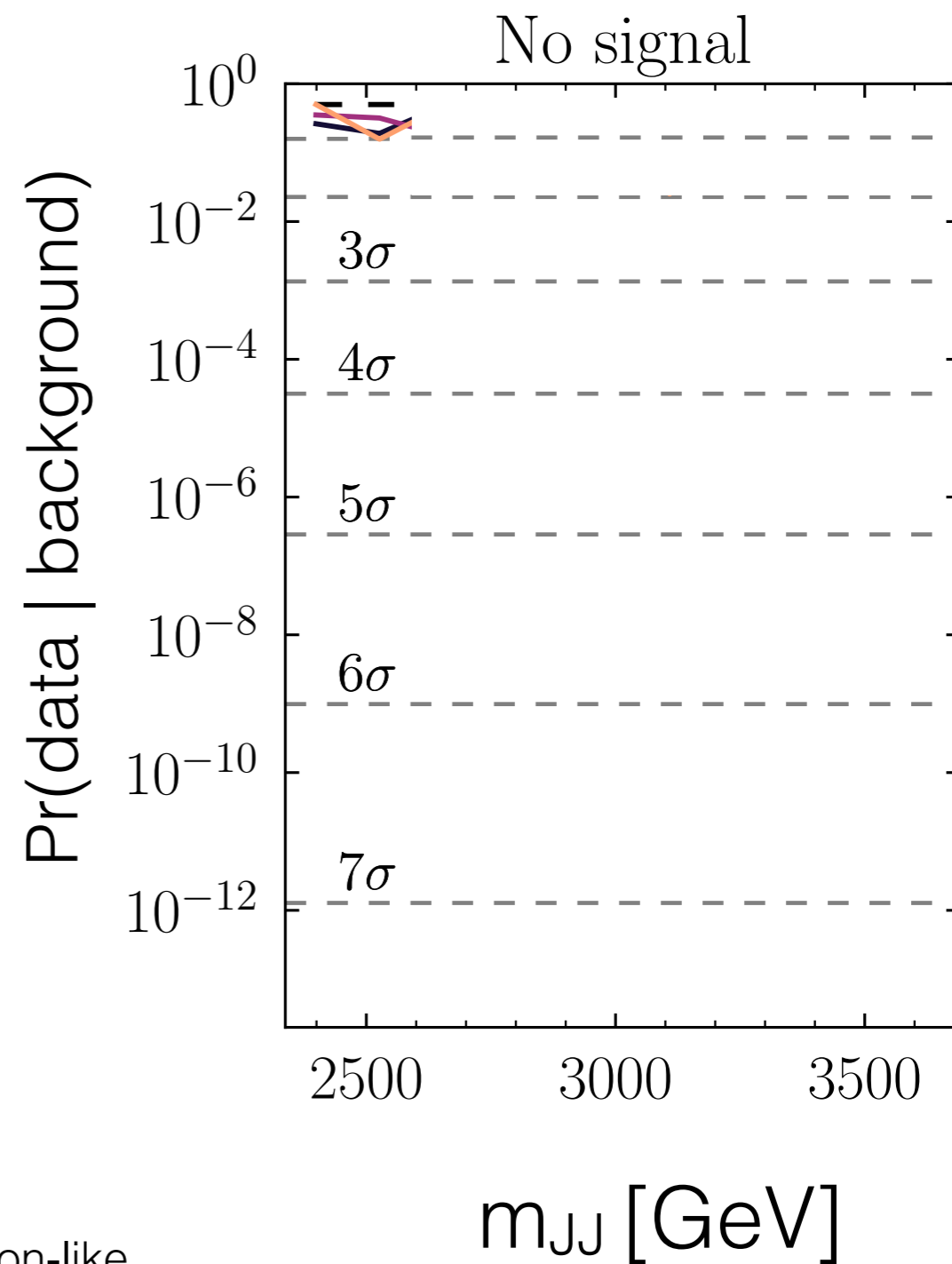
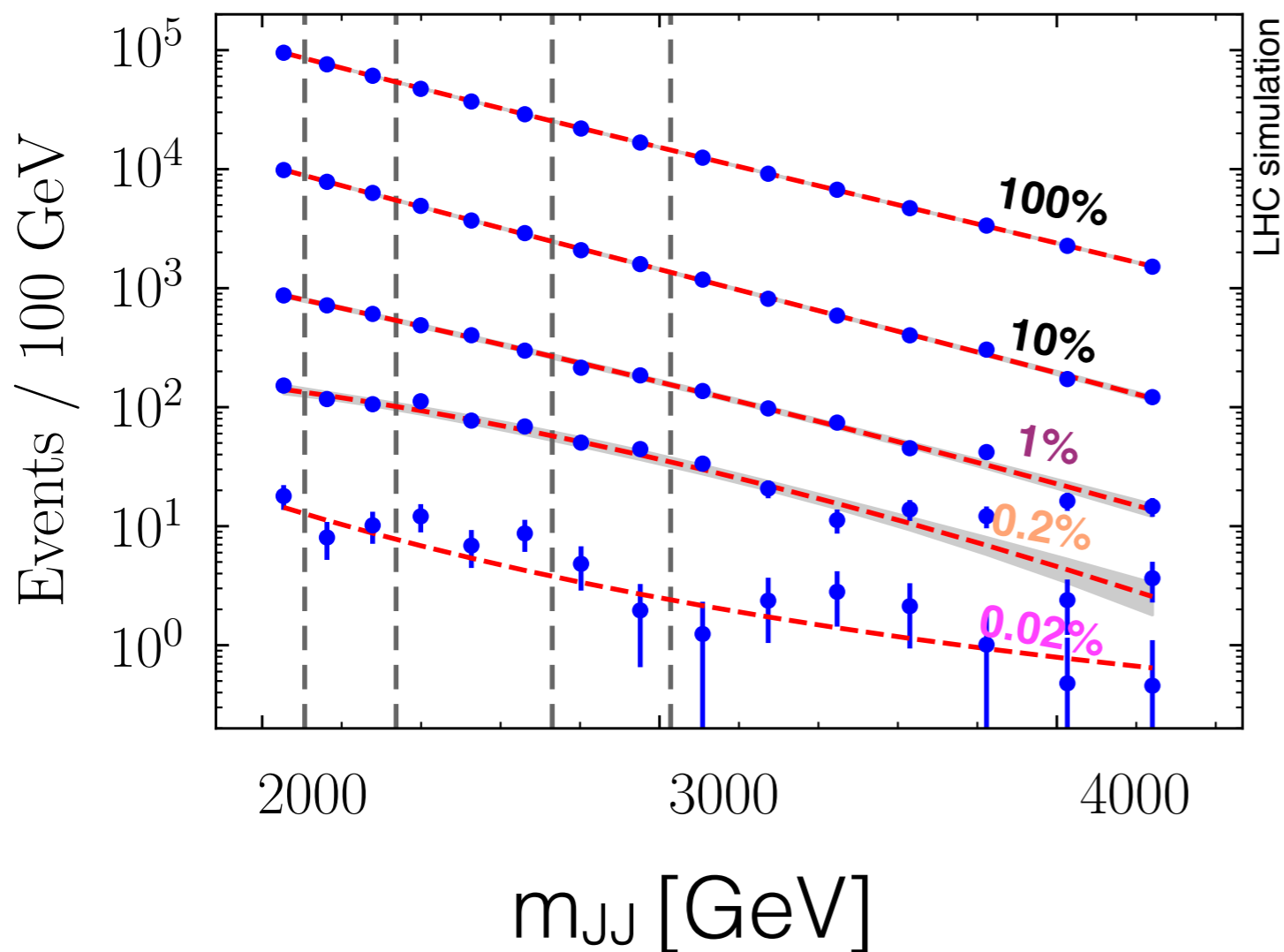
Pr(data | background)



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

Example: two-jet search

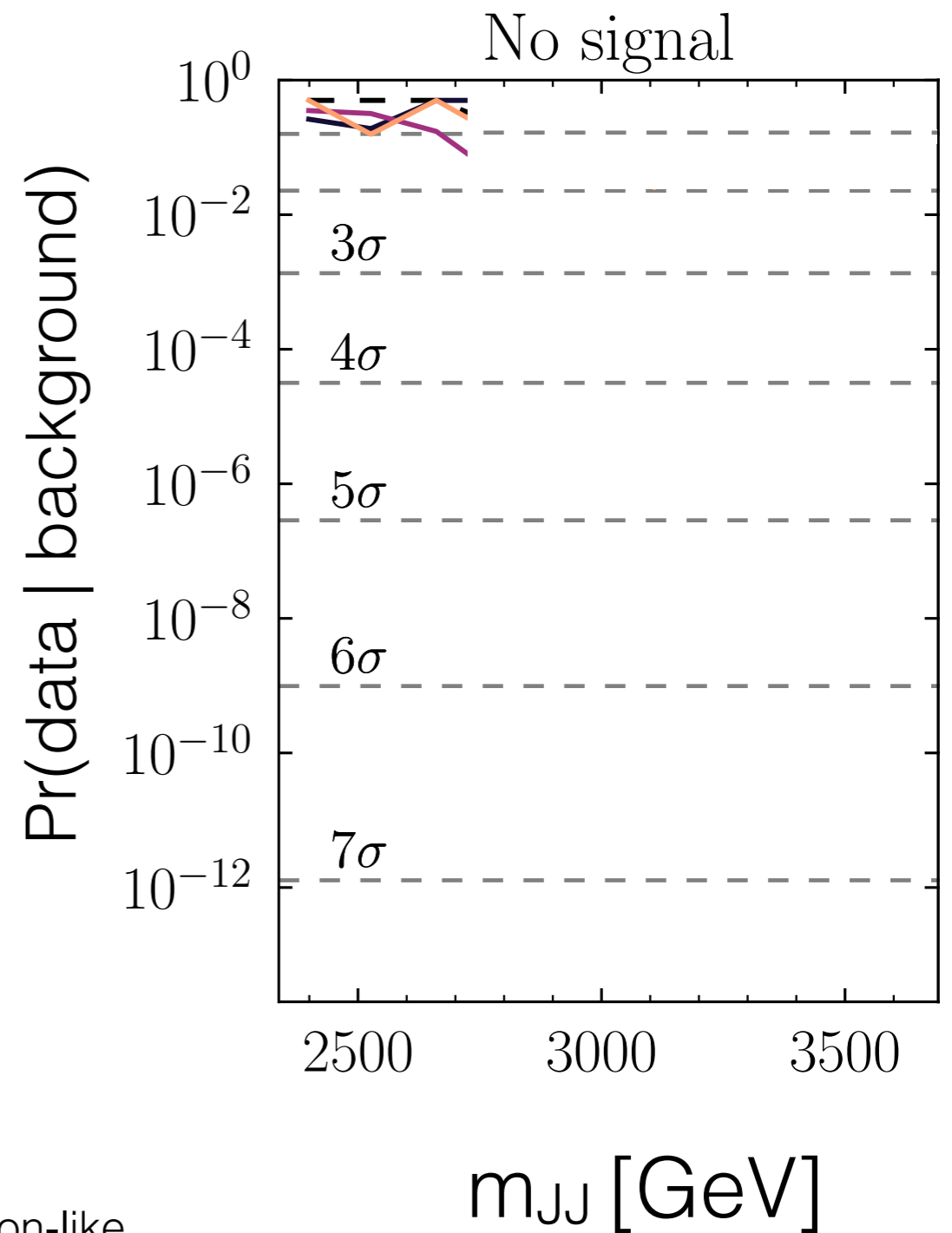
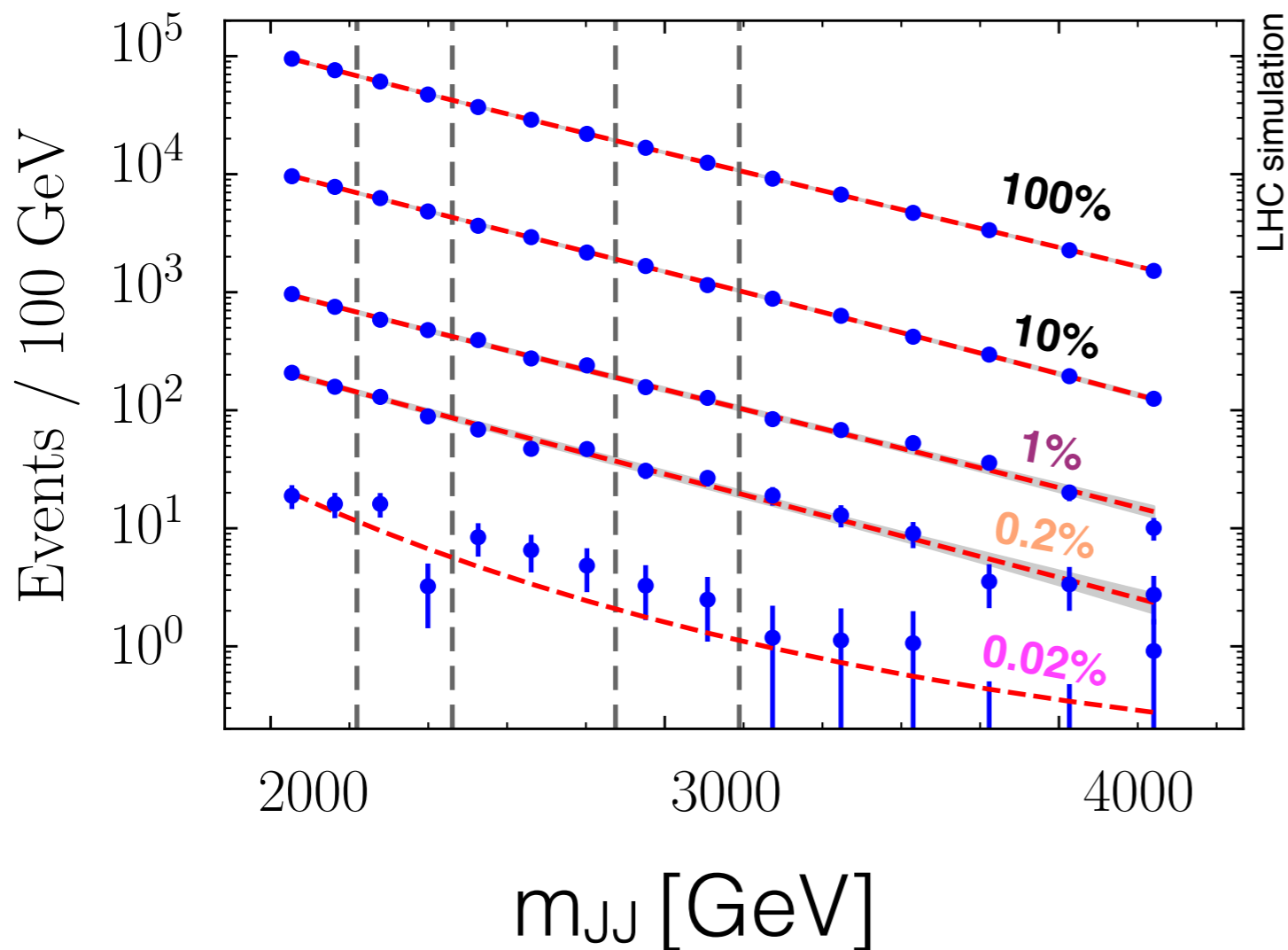
33



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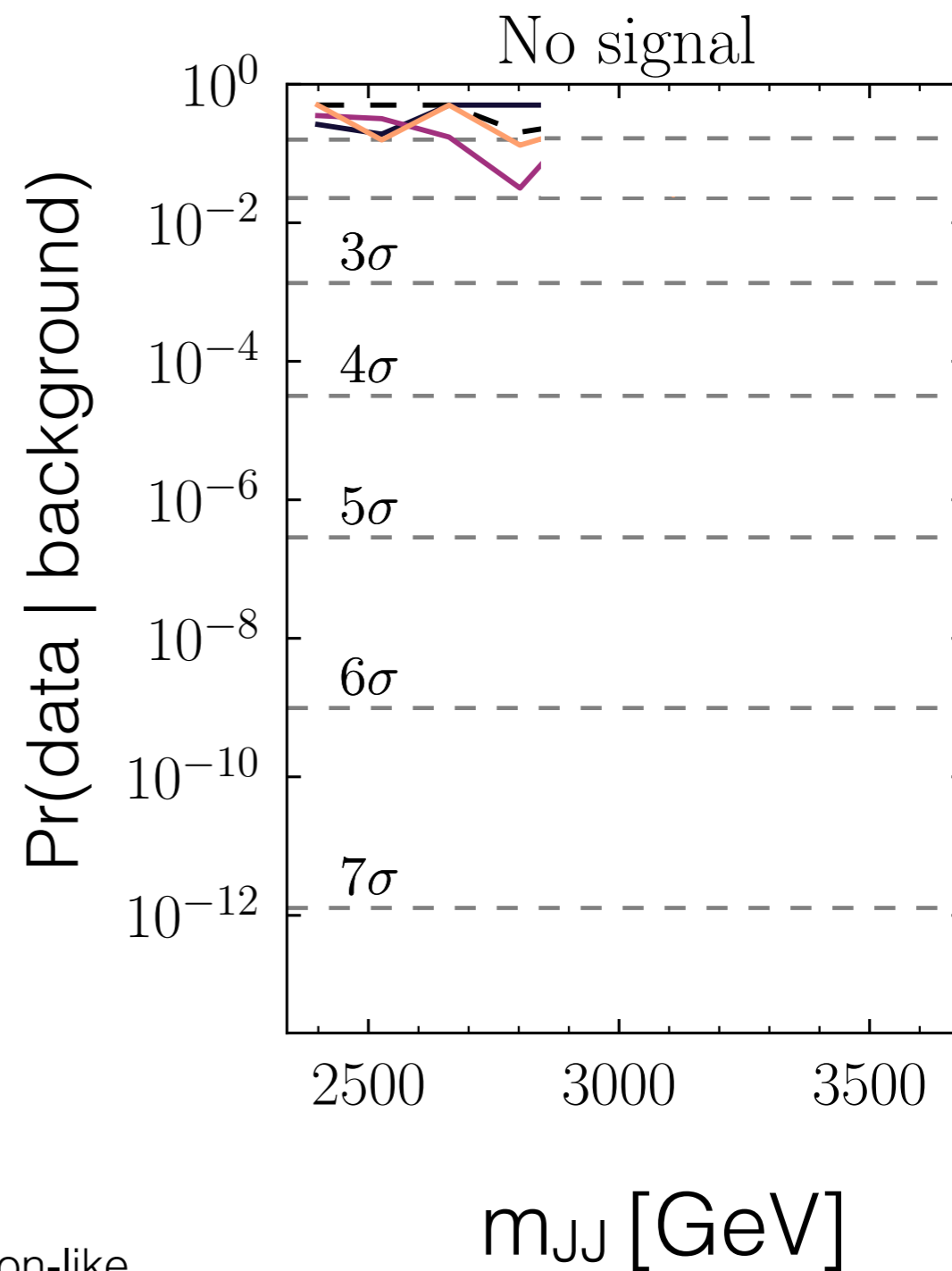
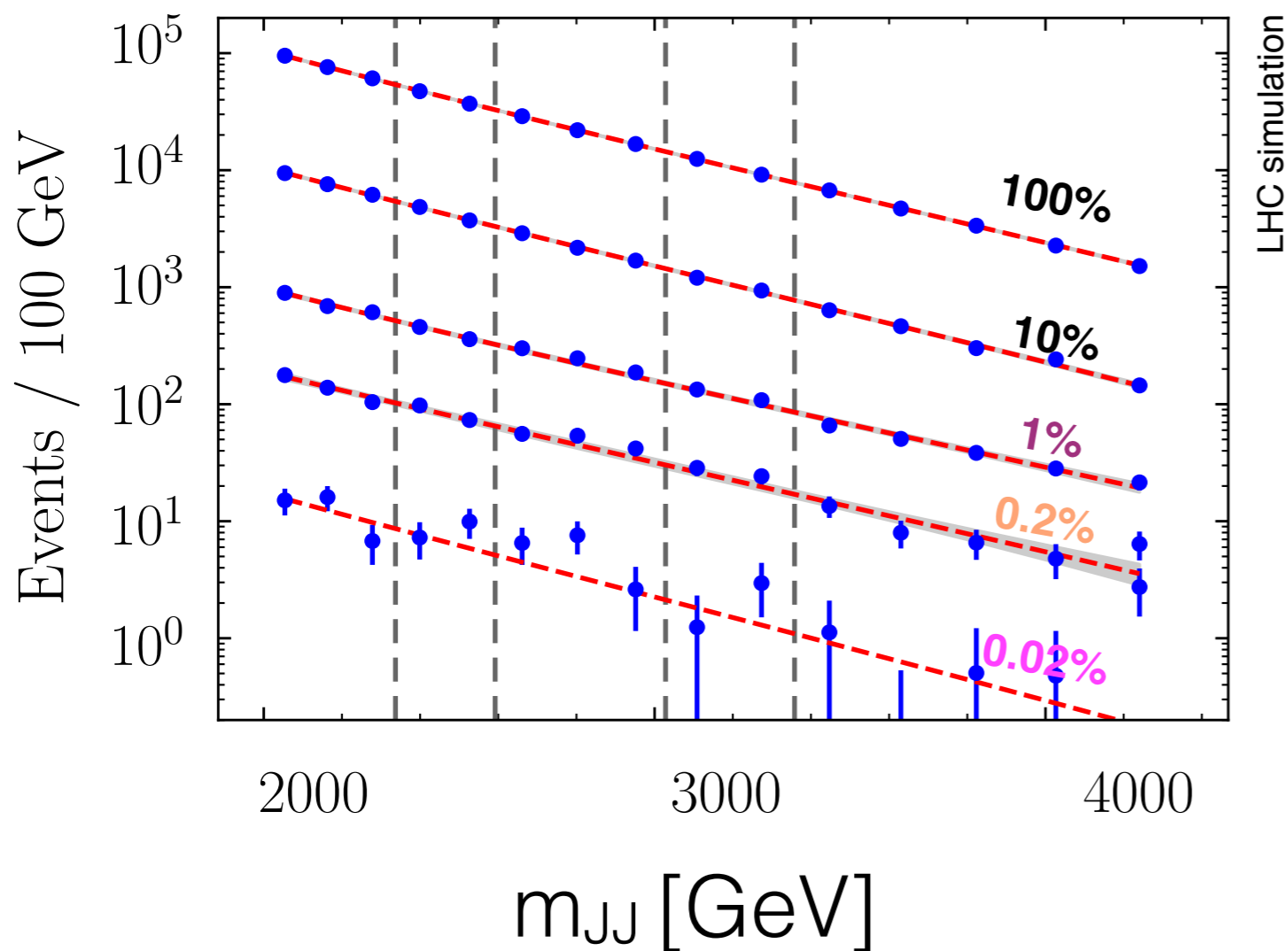
34



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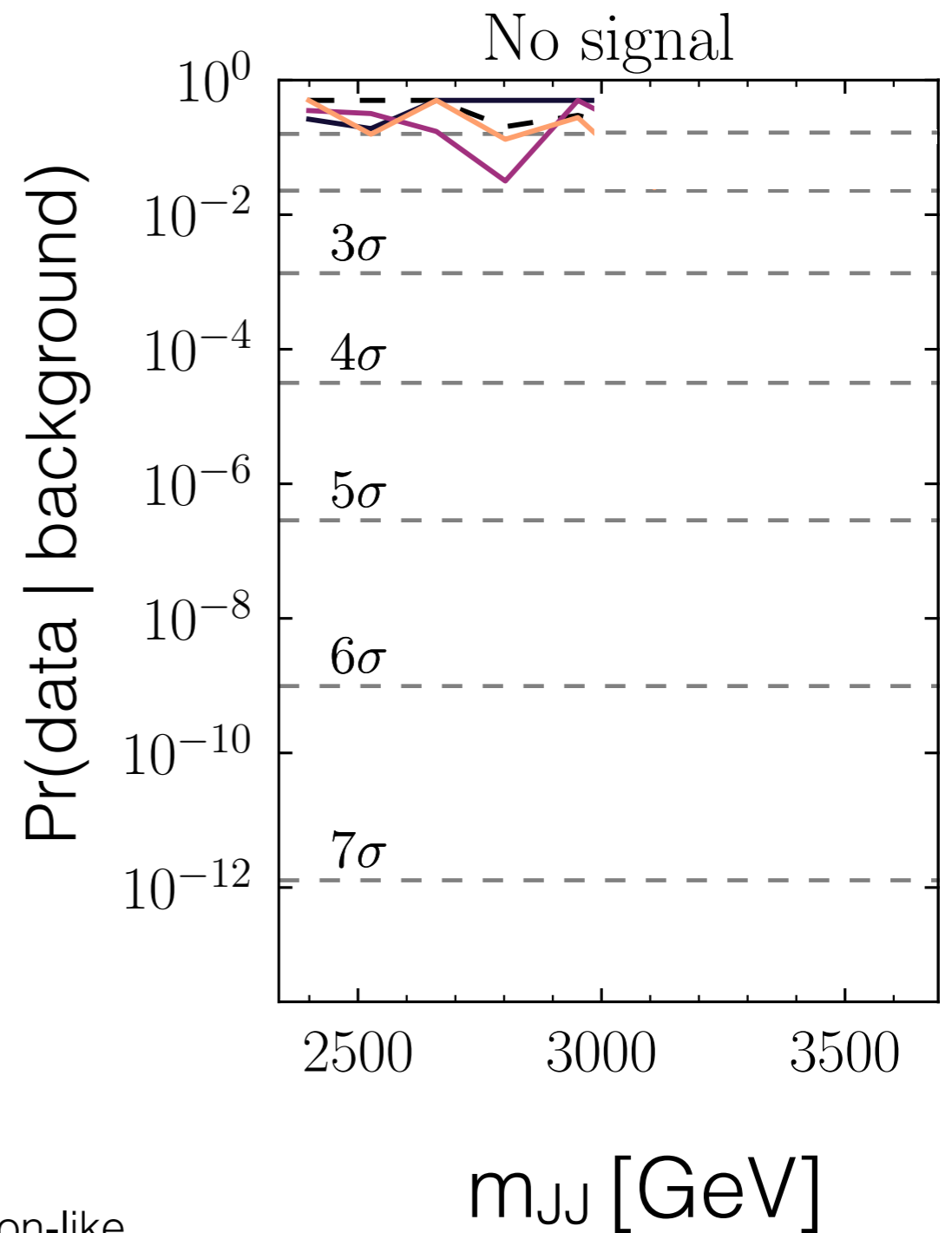
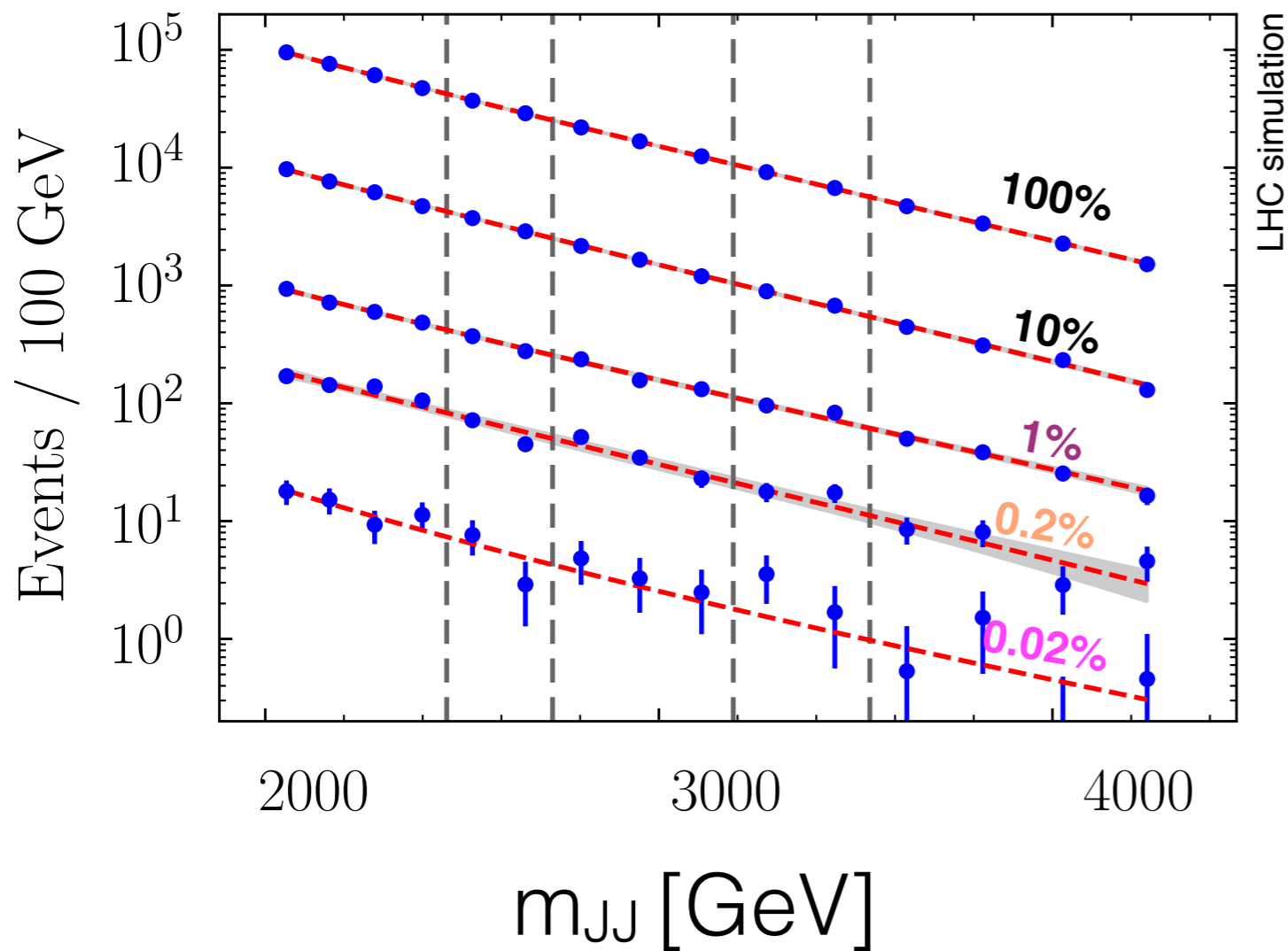
35



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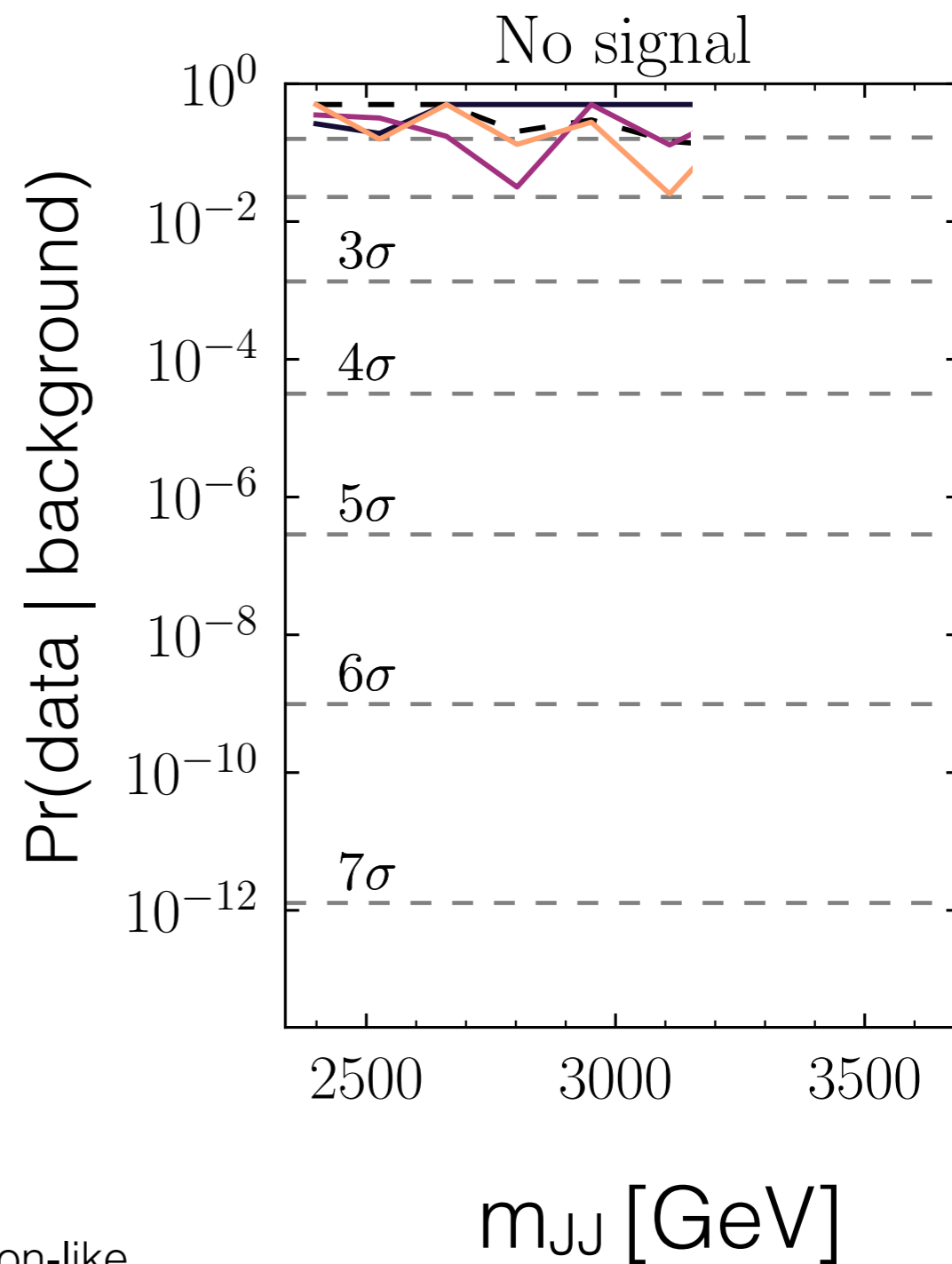
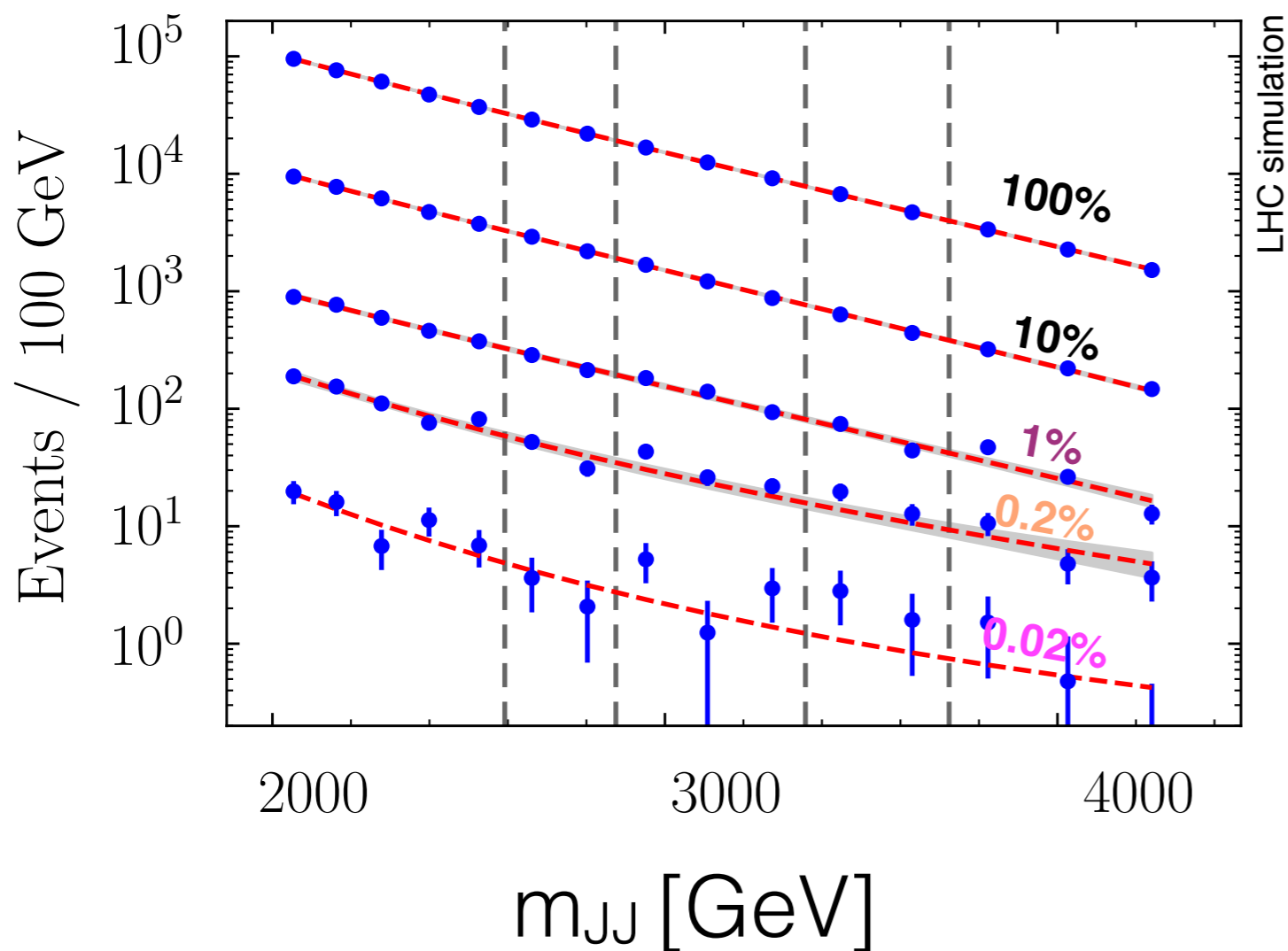
36



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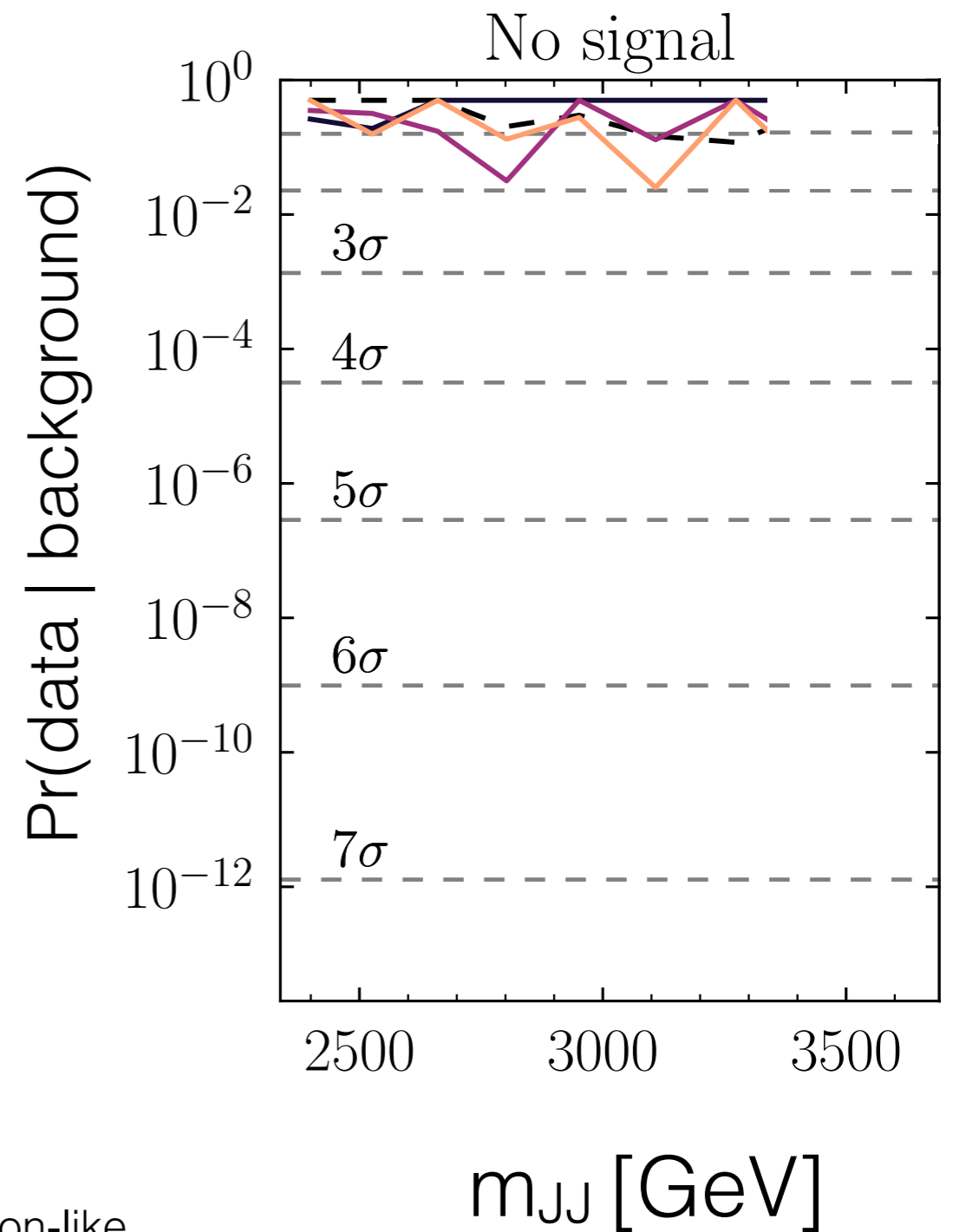
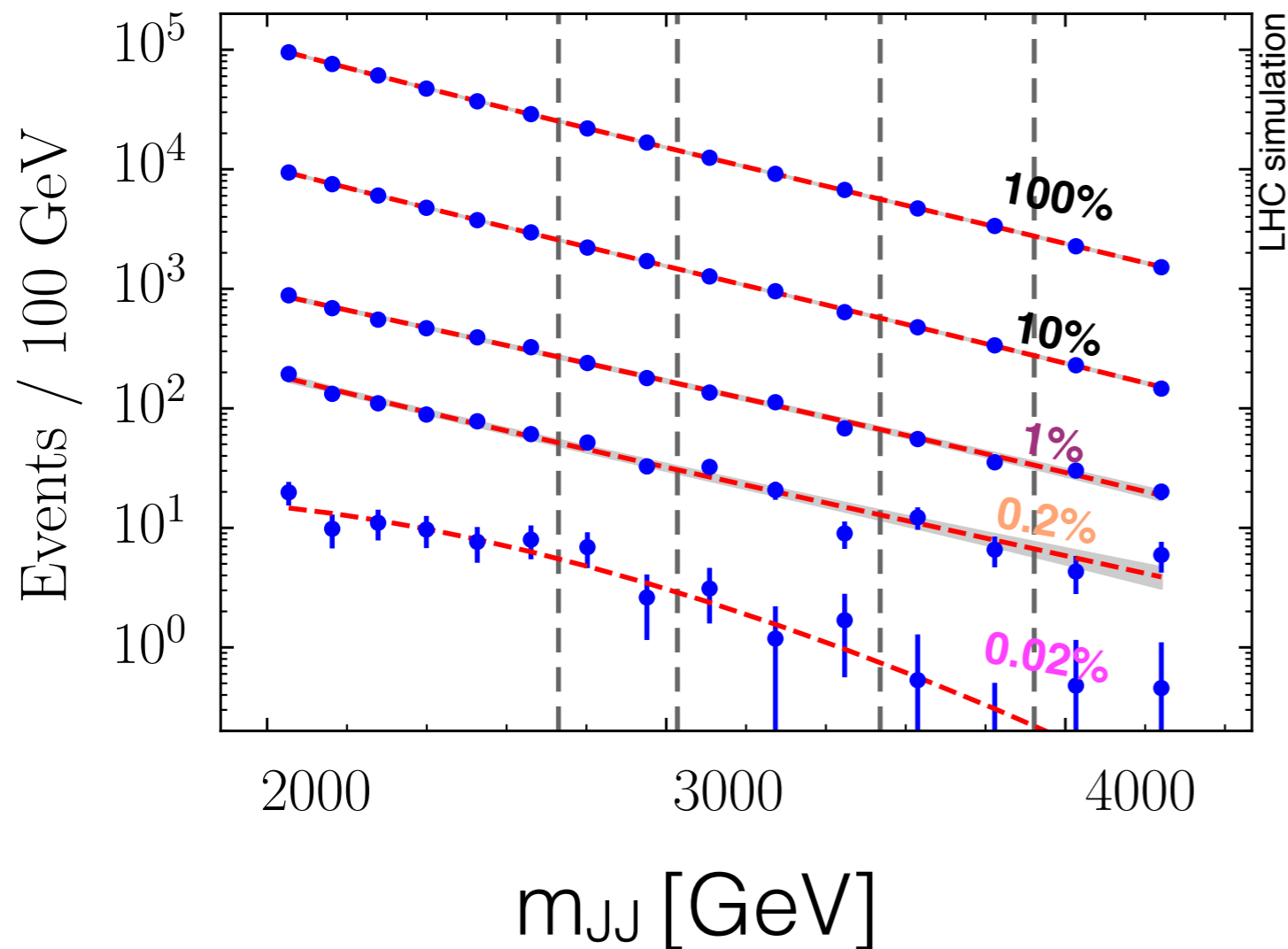
37



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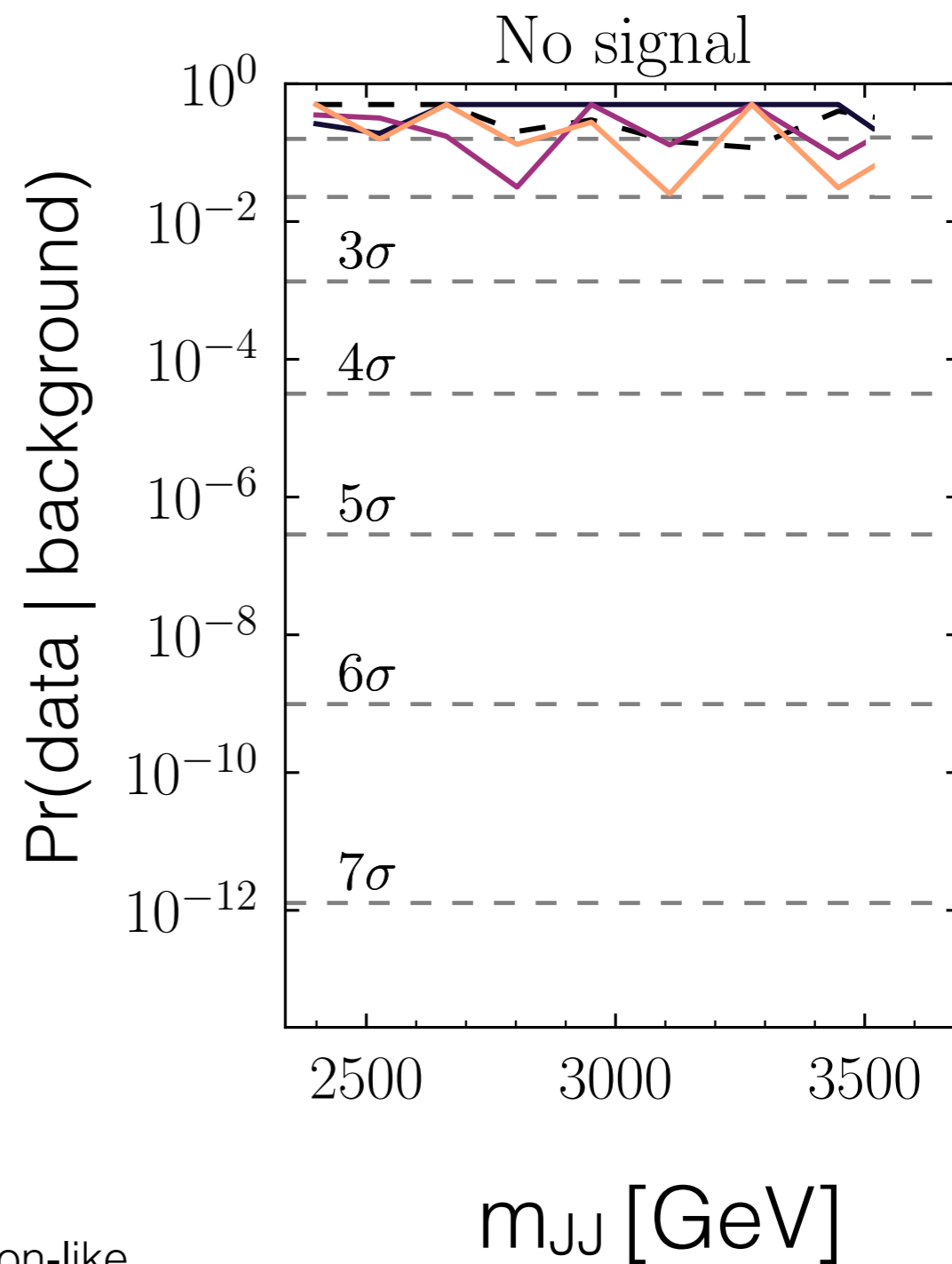
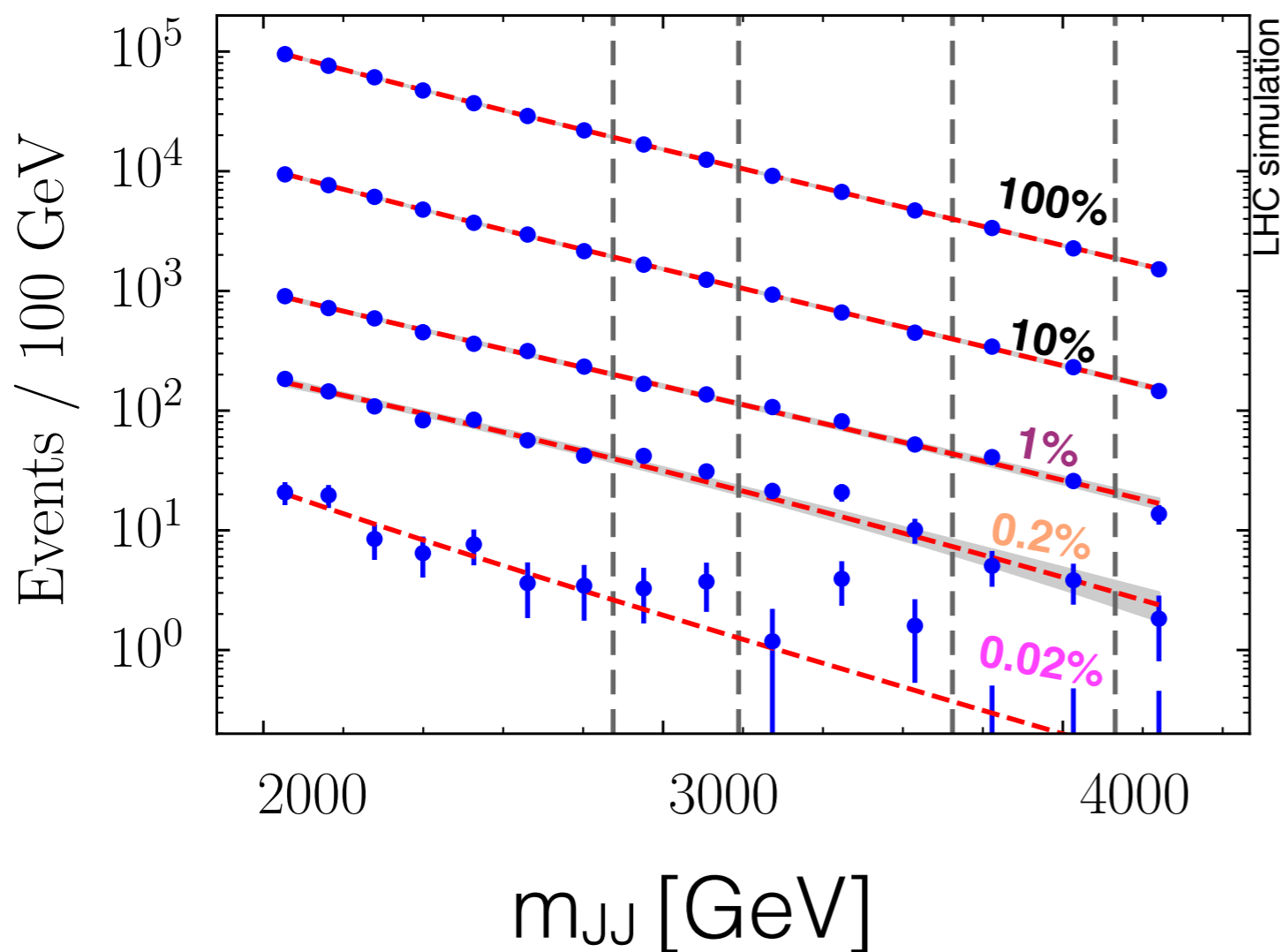
38



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Example: two-jet search

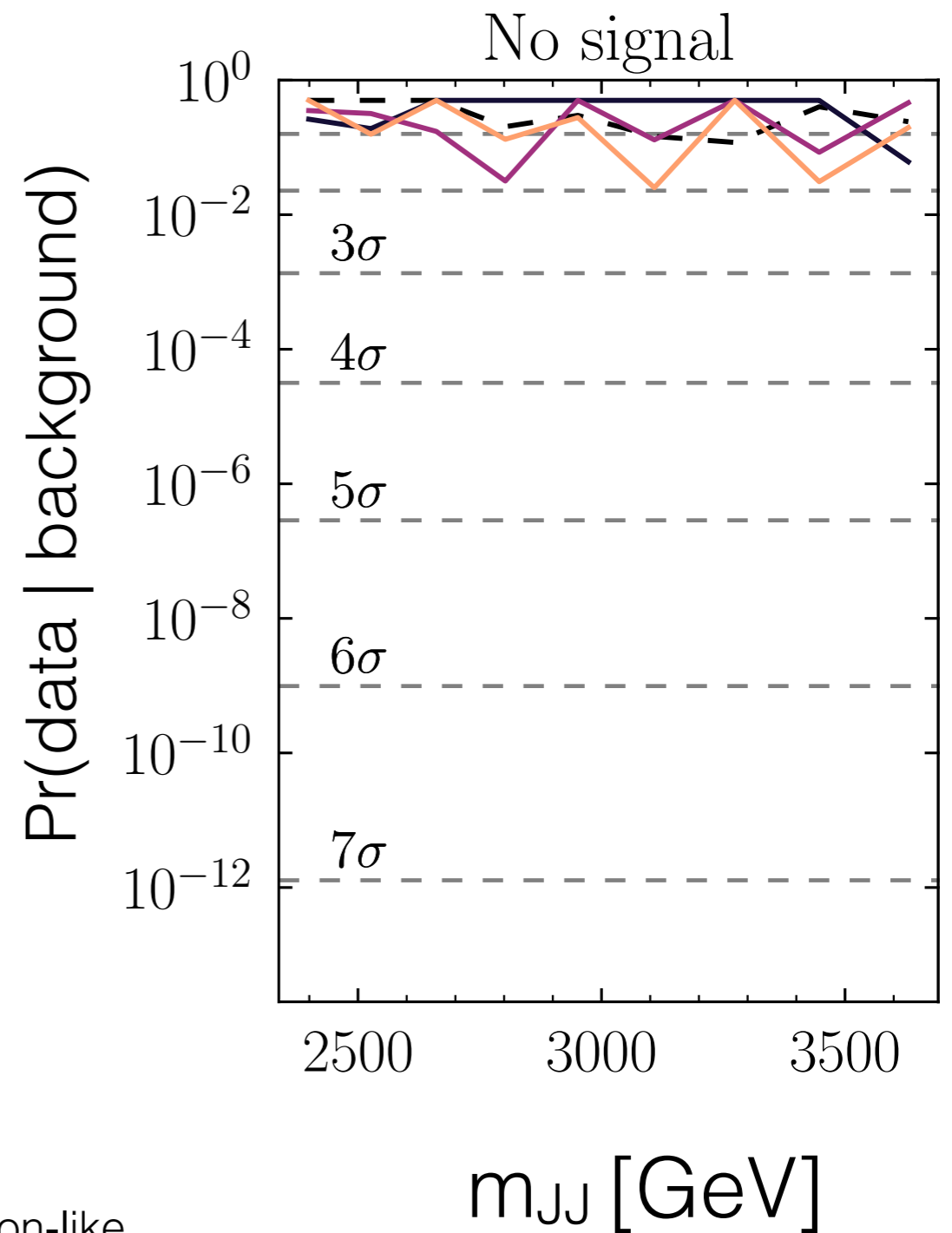
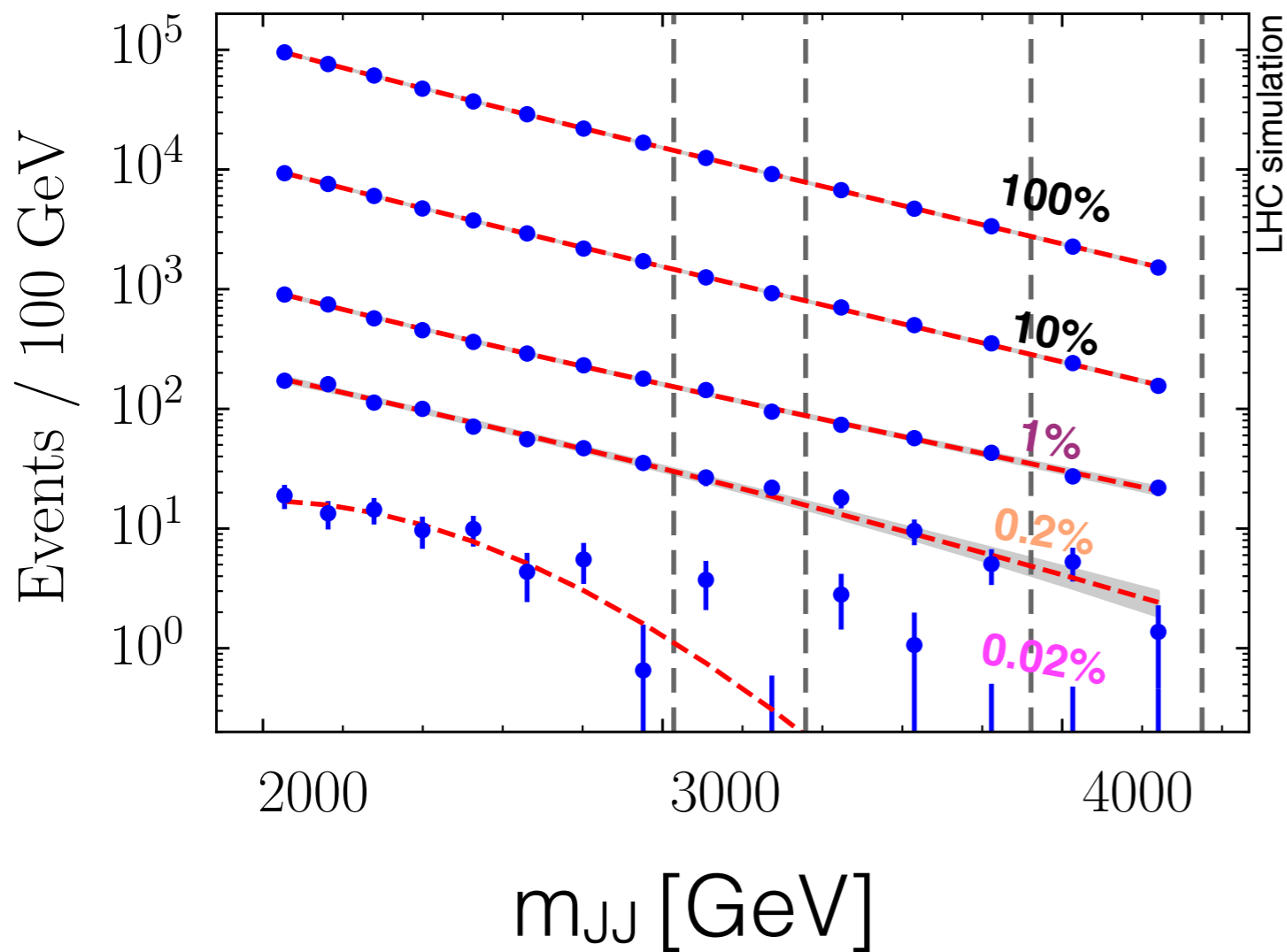
39



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Example: two-jet search

40

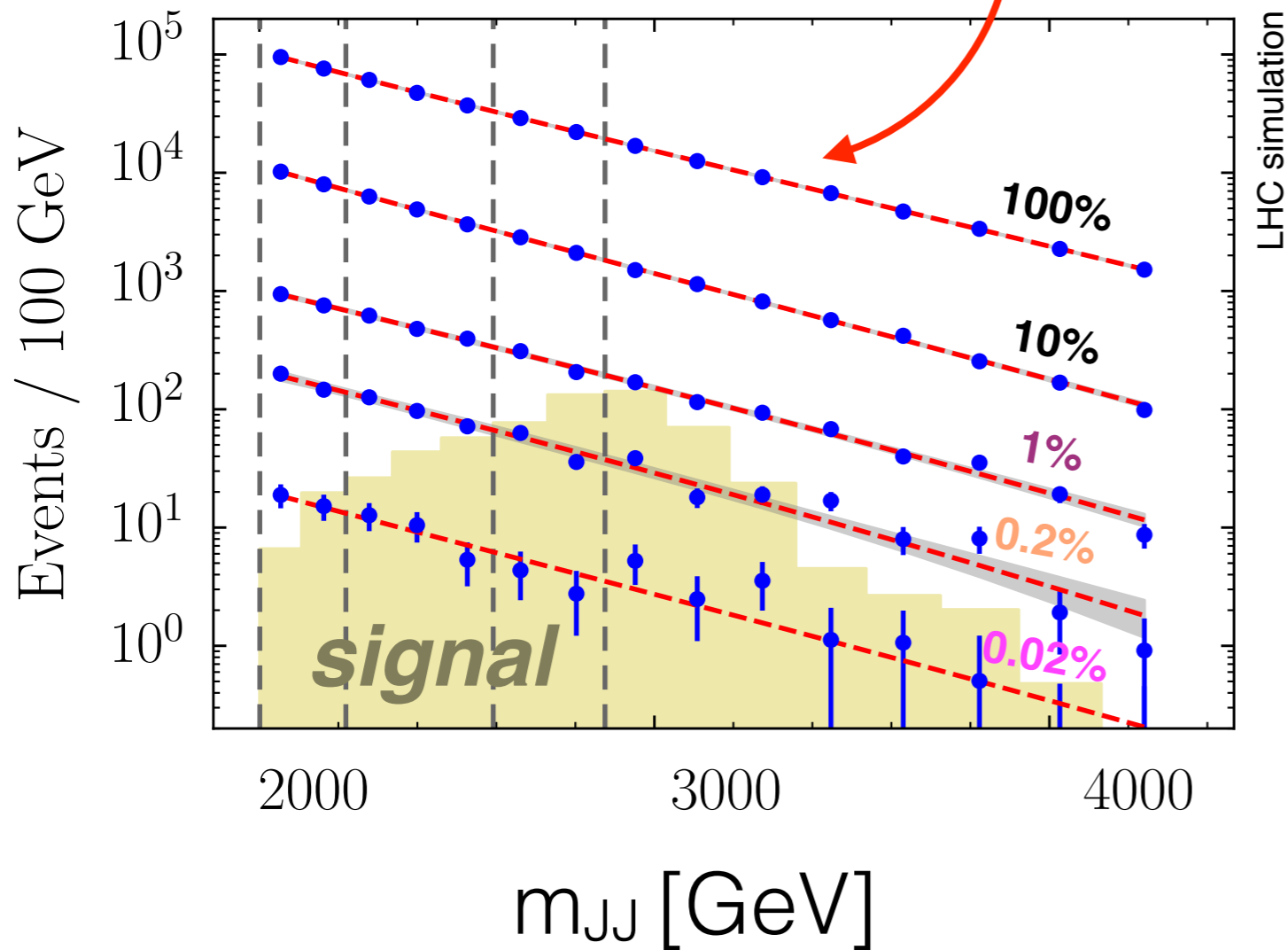


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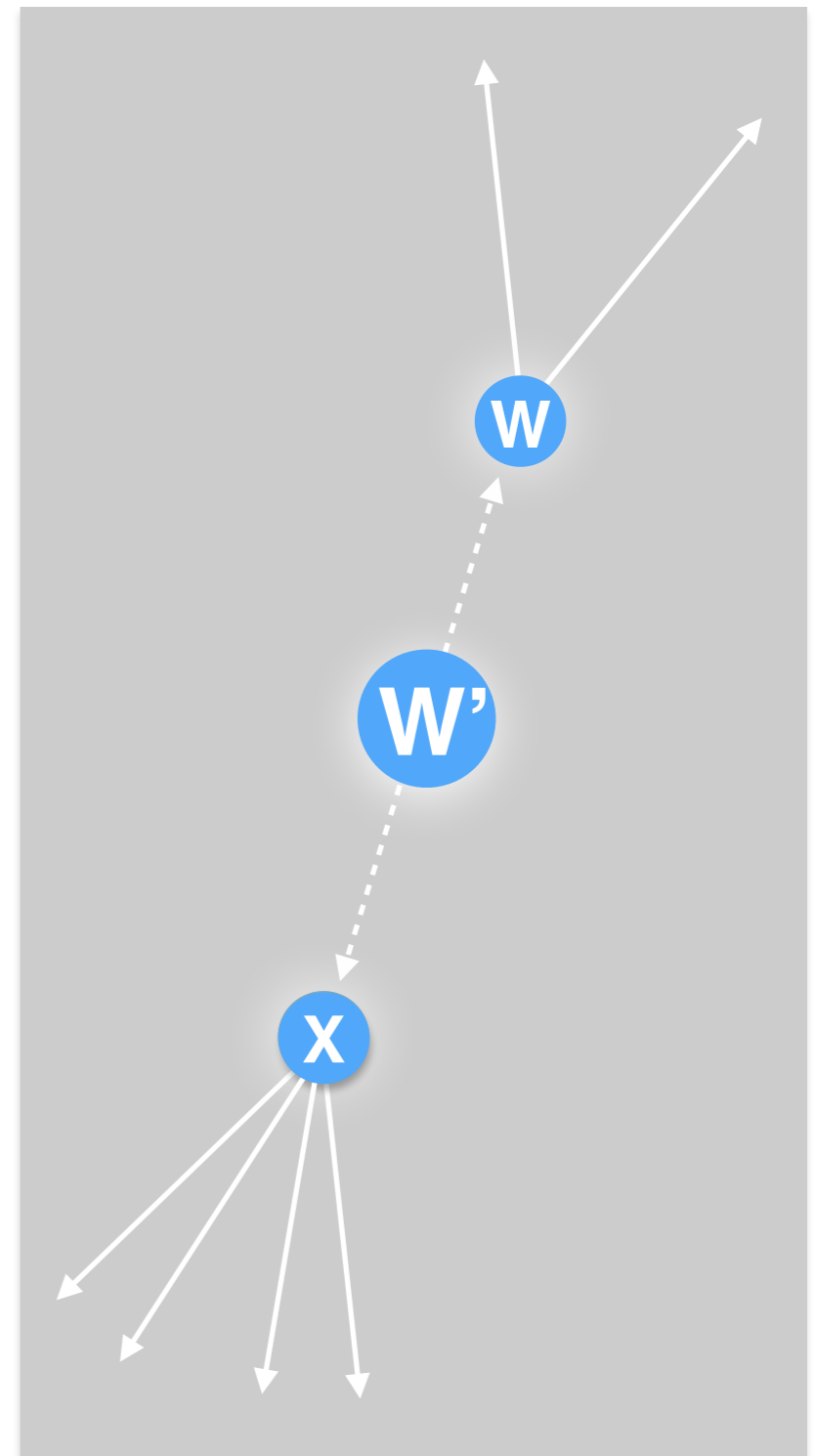
...and when there is a signal?

sidebands

standard parametric
fit to background.



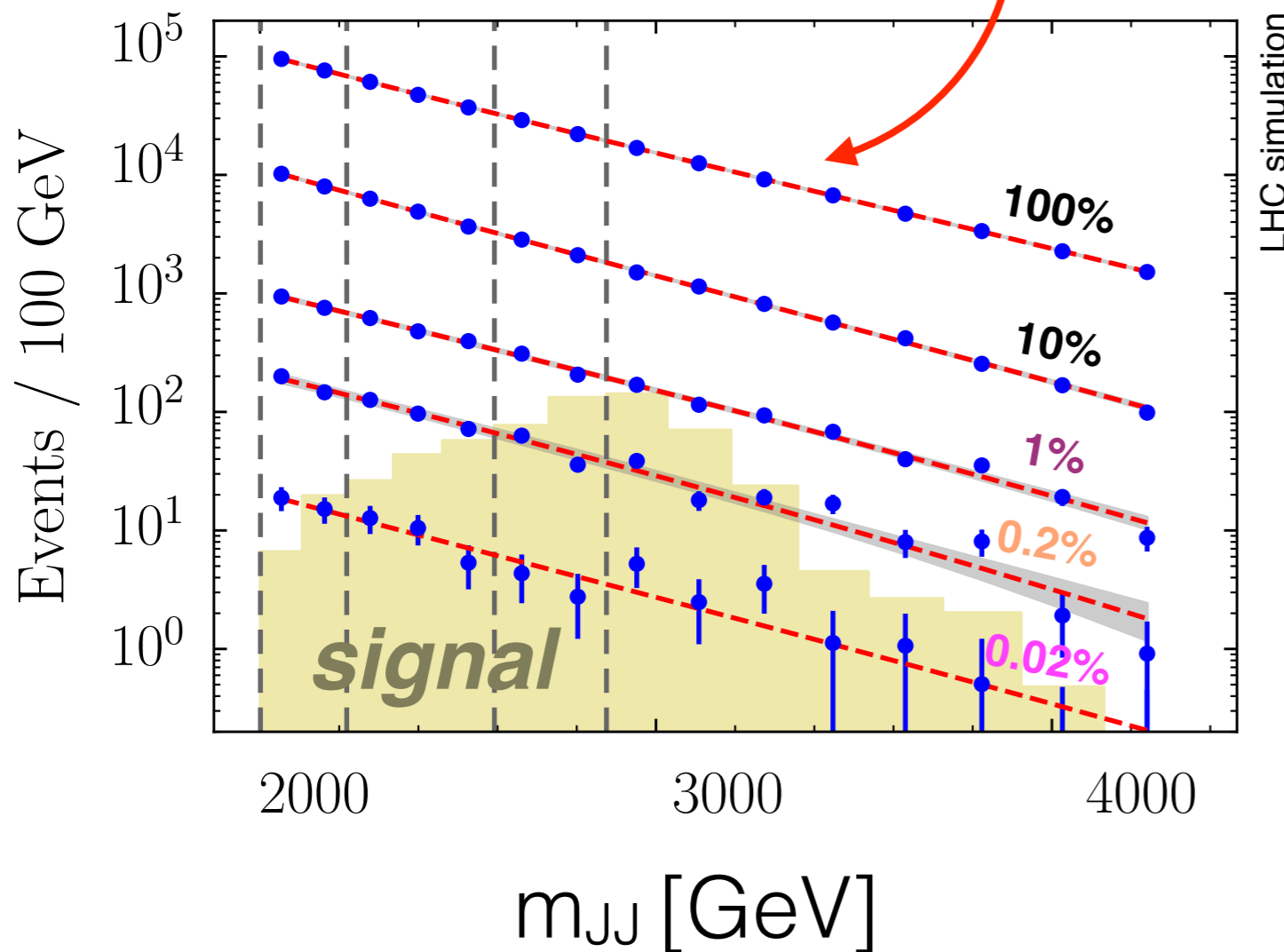
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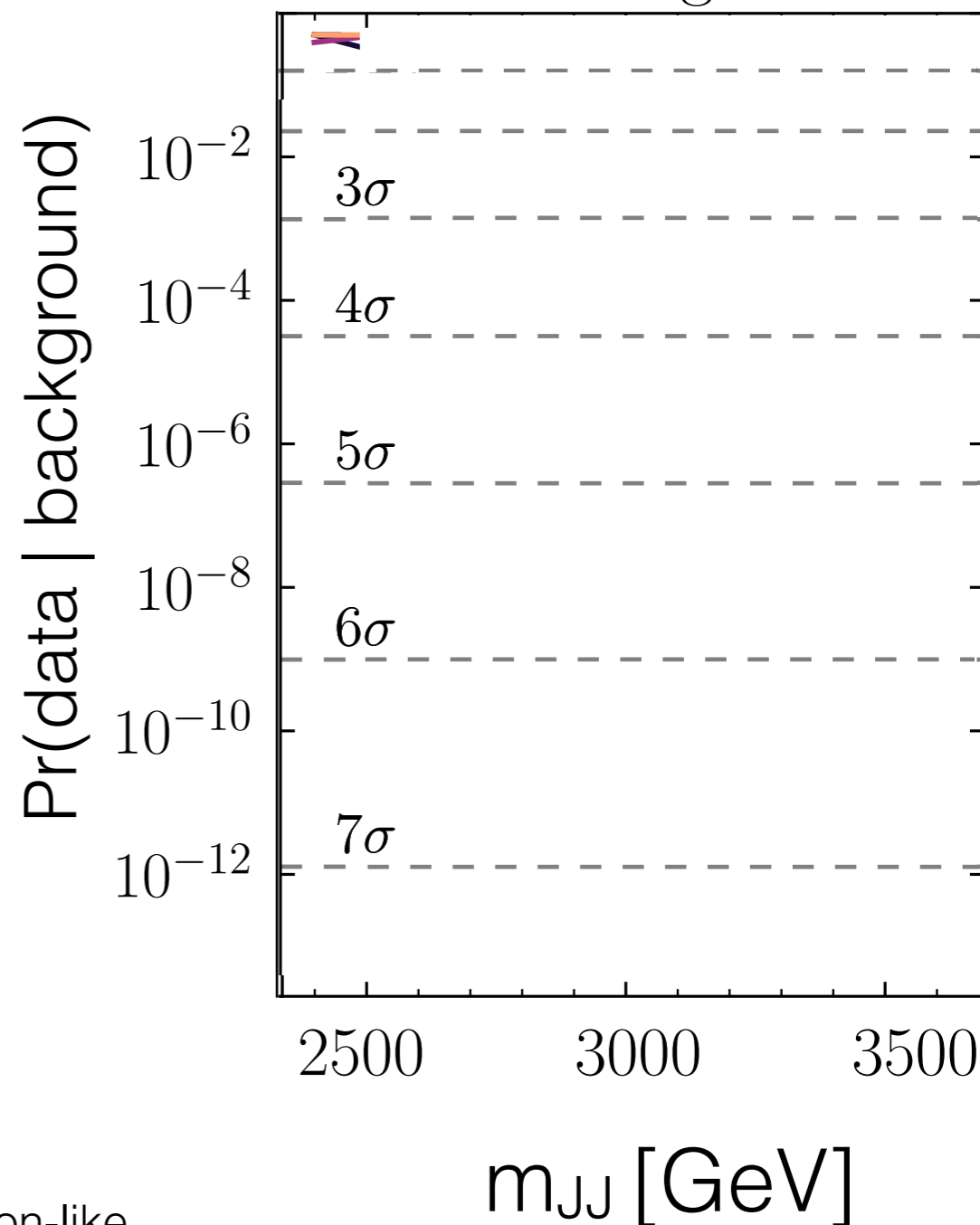
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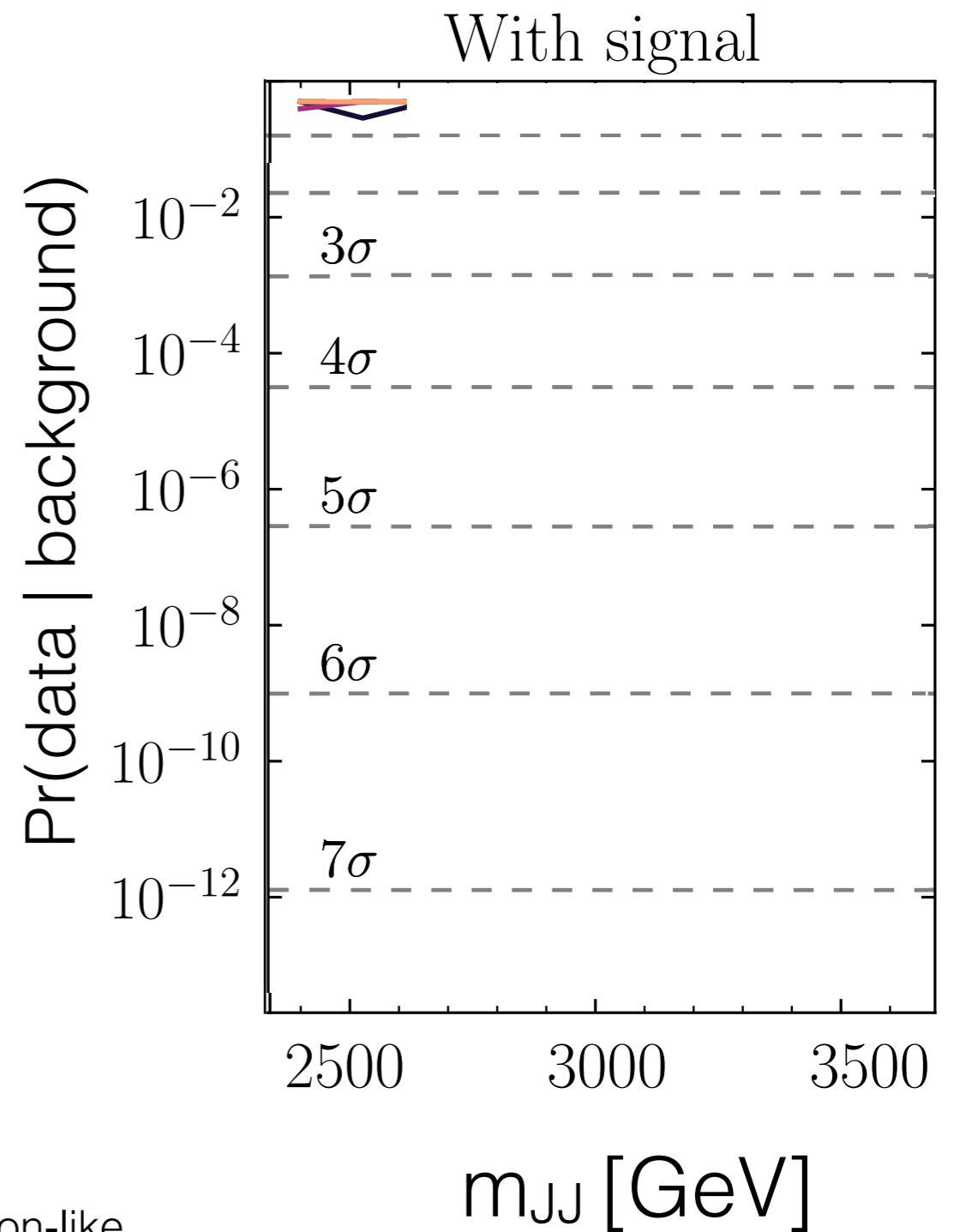
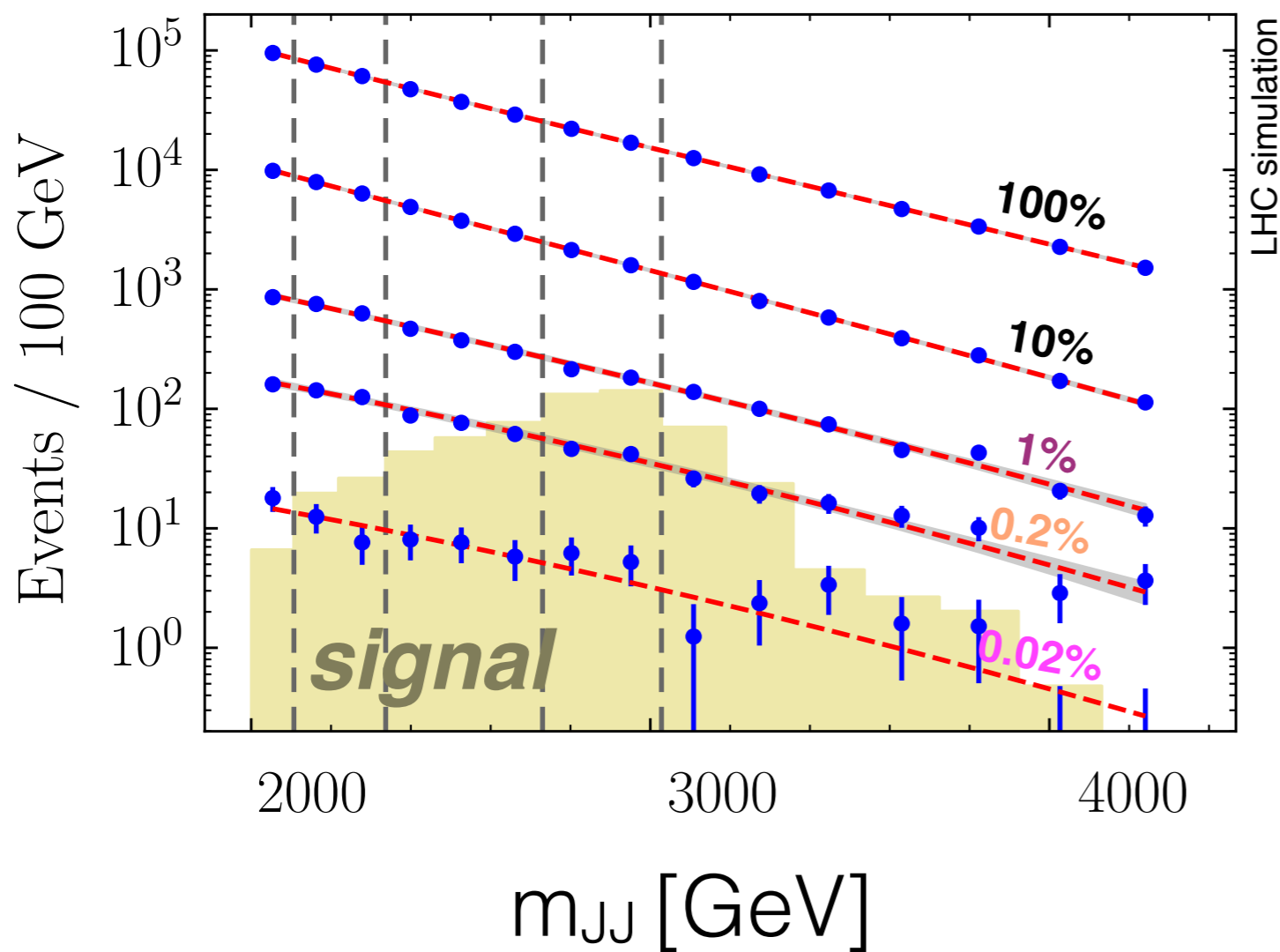


With signal



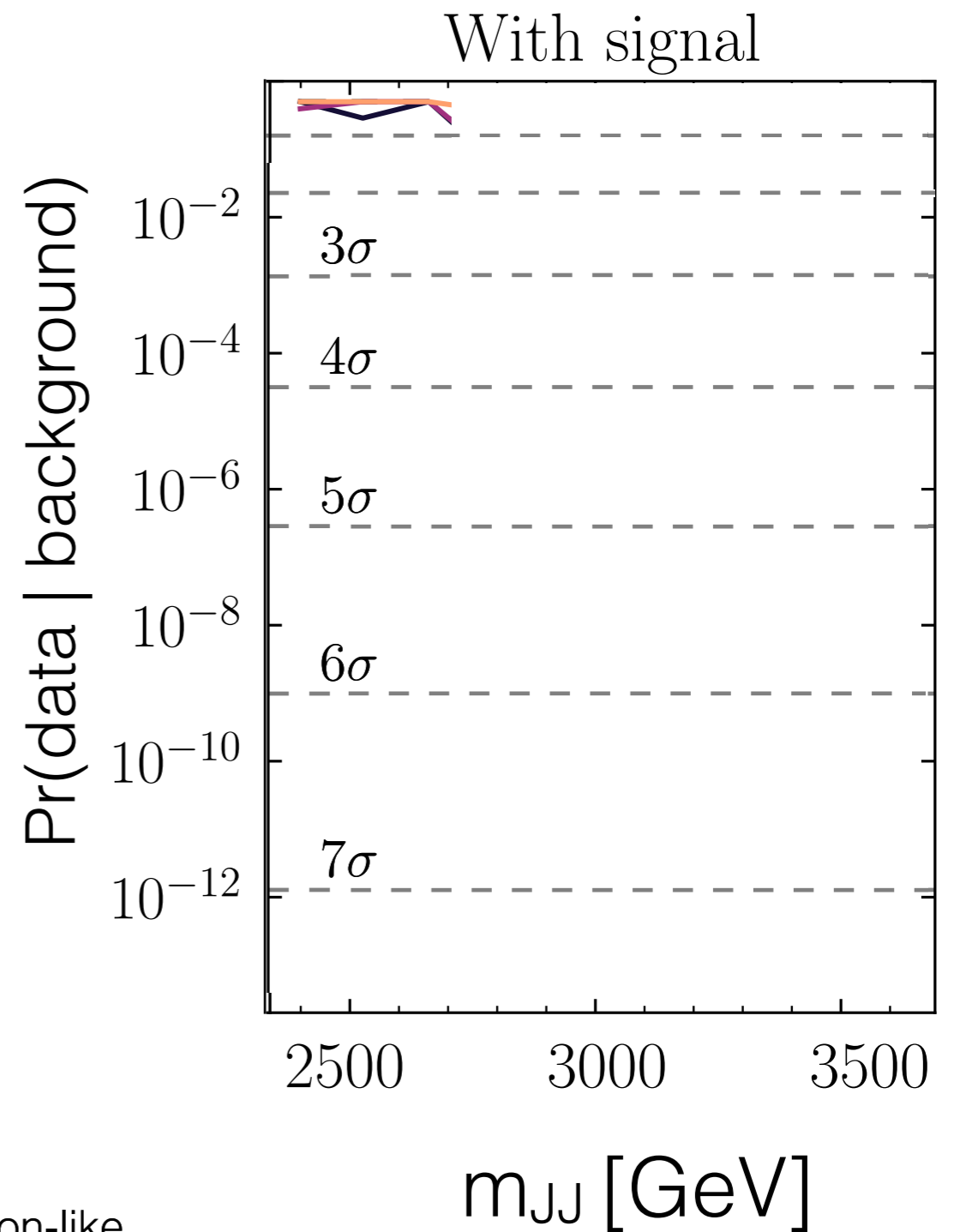
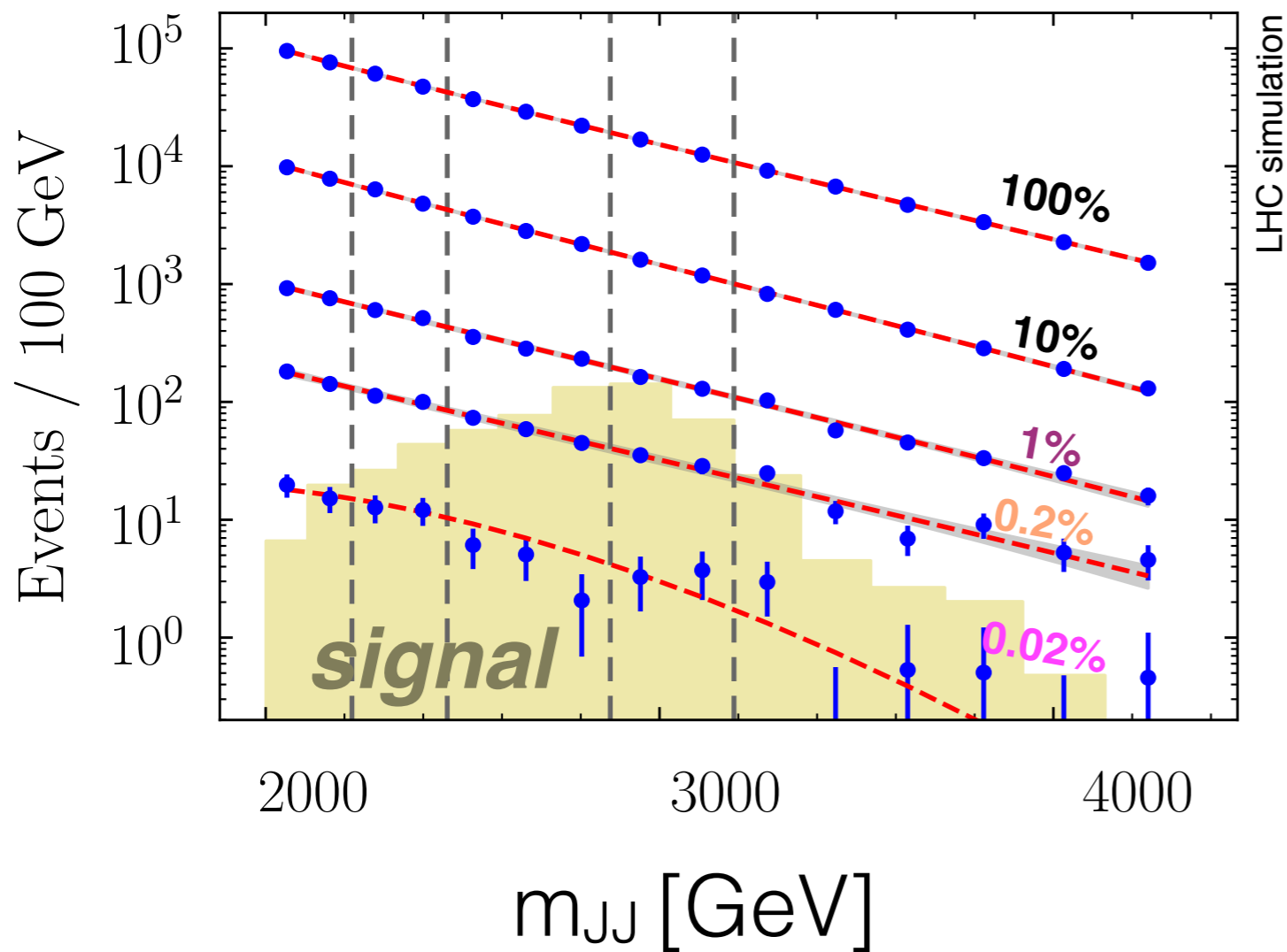
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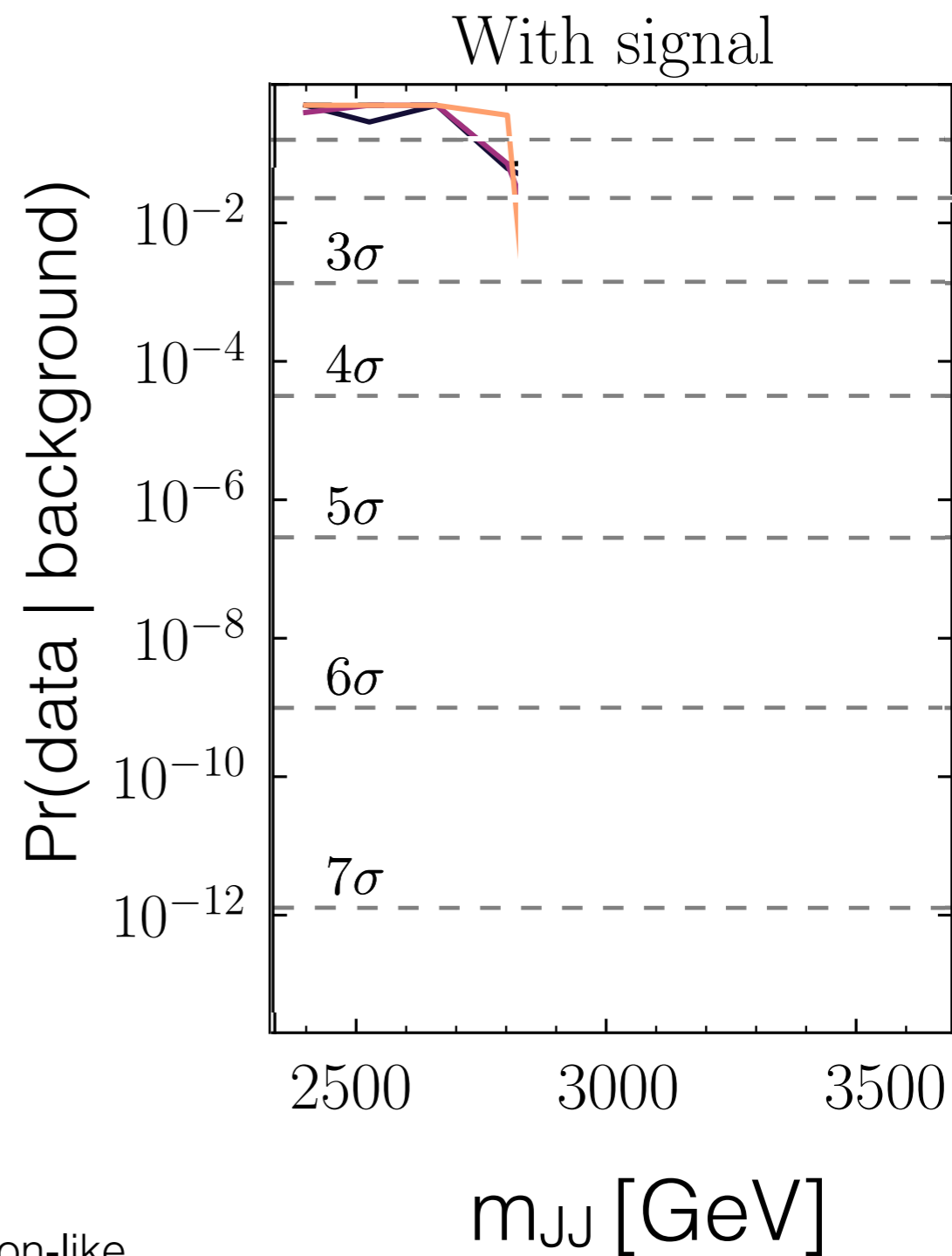
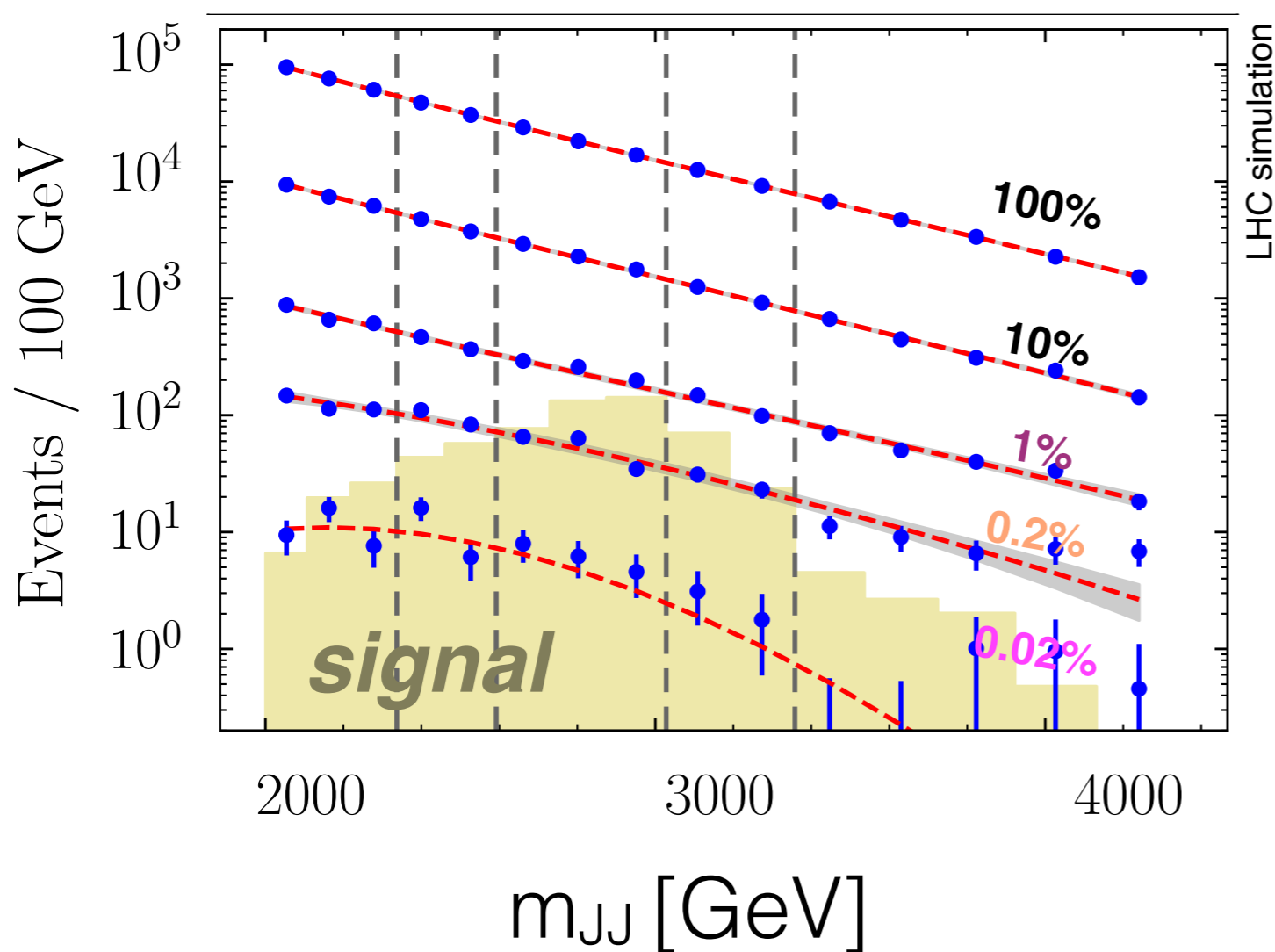
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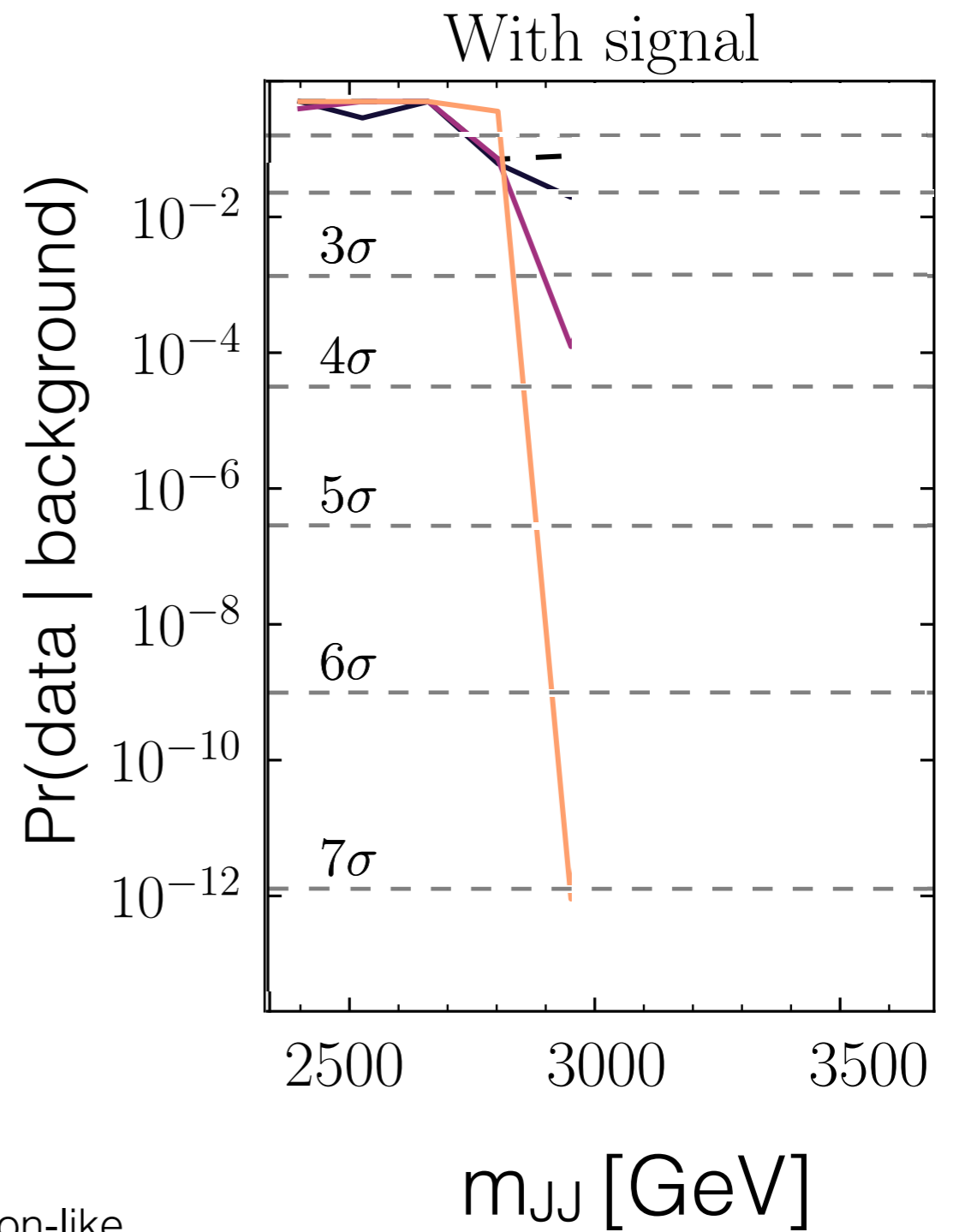
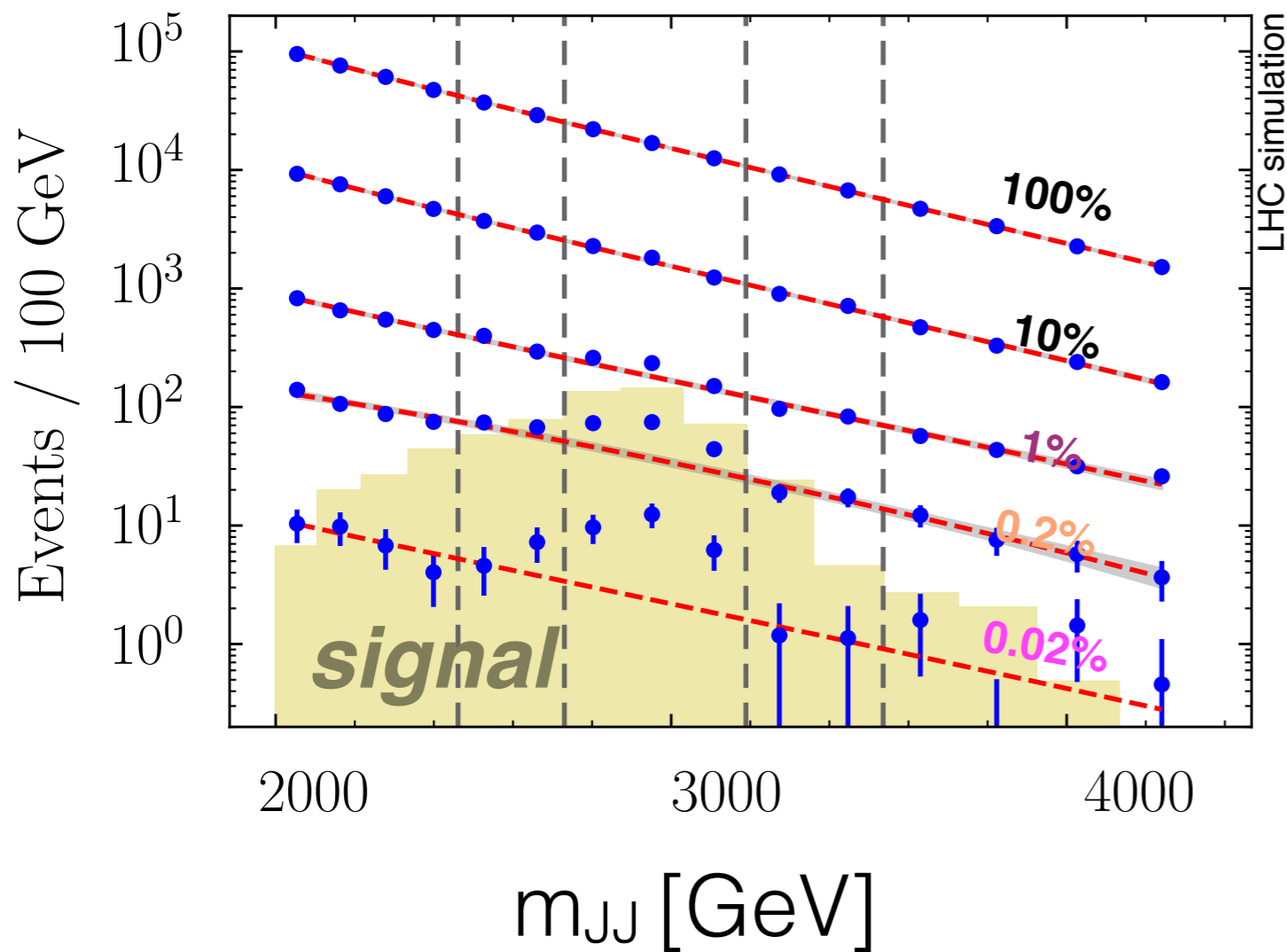
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- most 0.2% signal-region-like

...and when there is a signal?



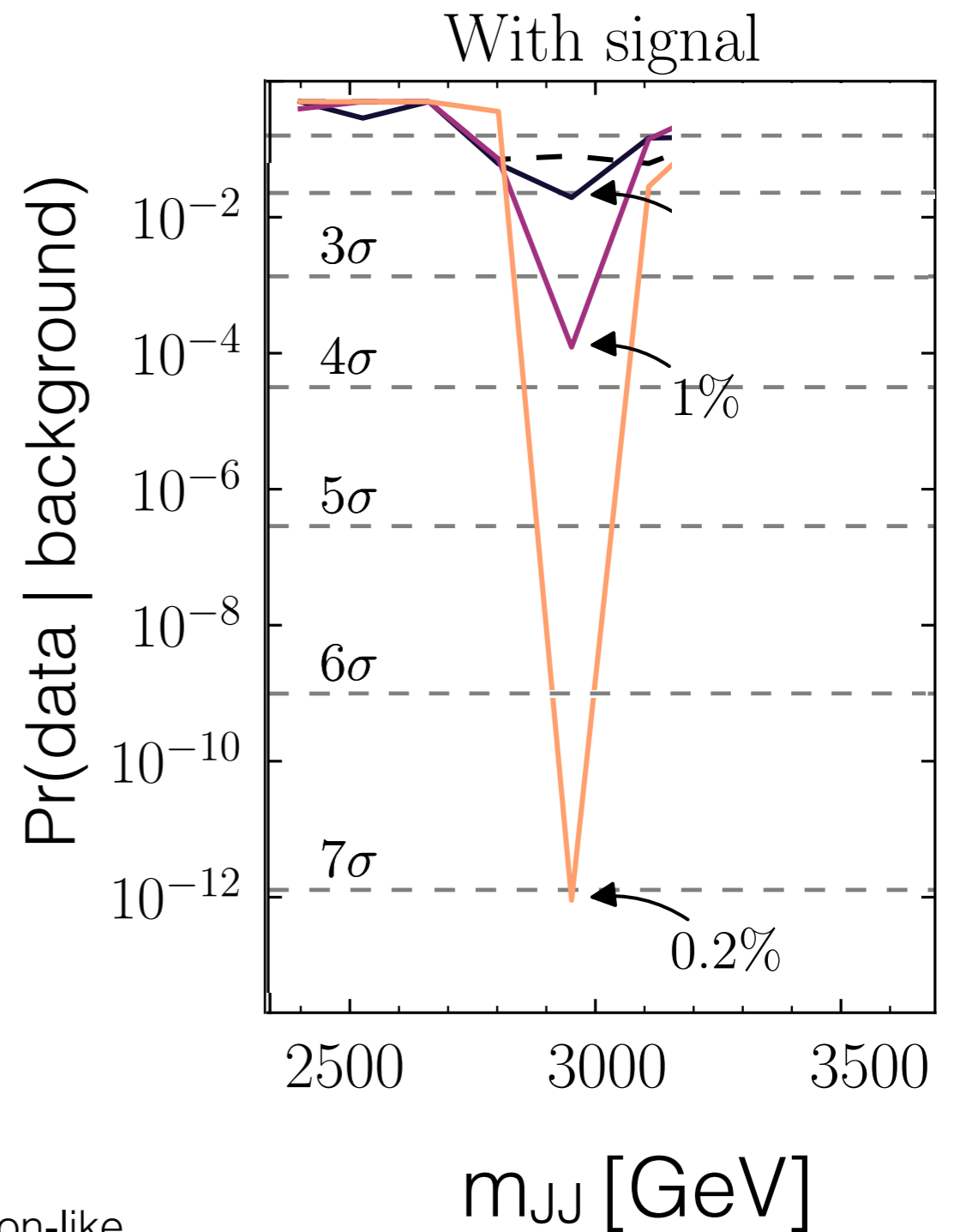
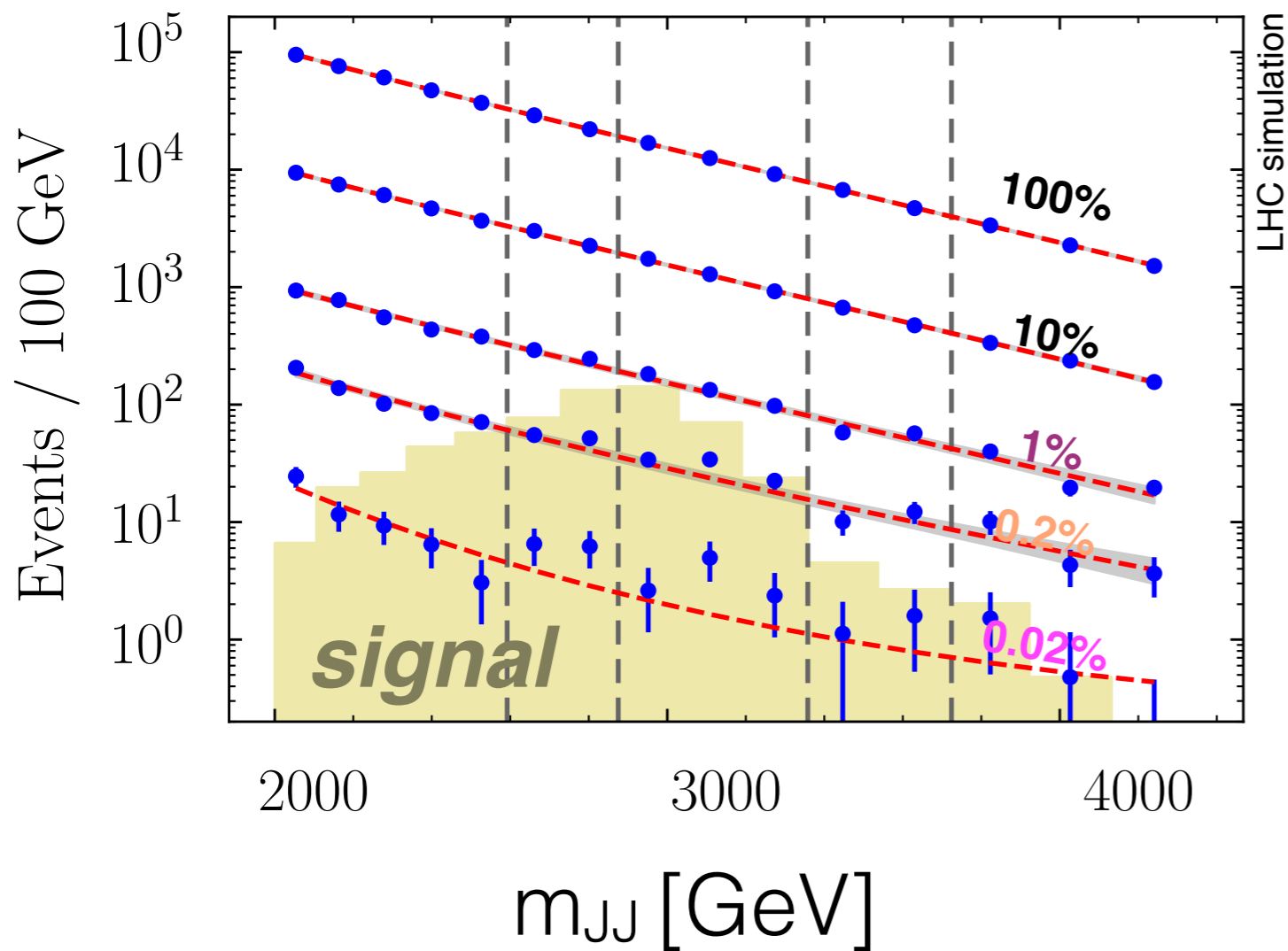
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

...and when there is a signal?



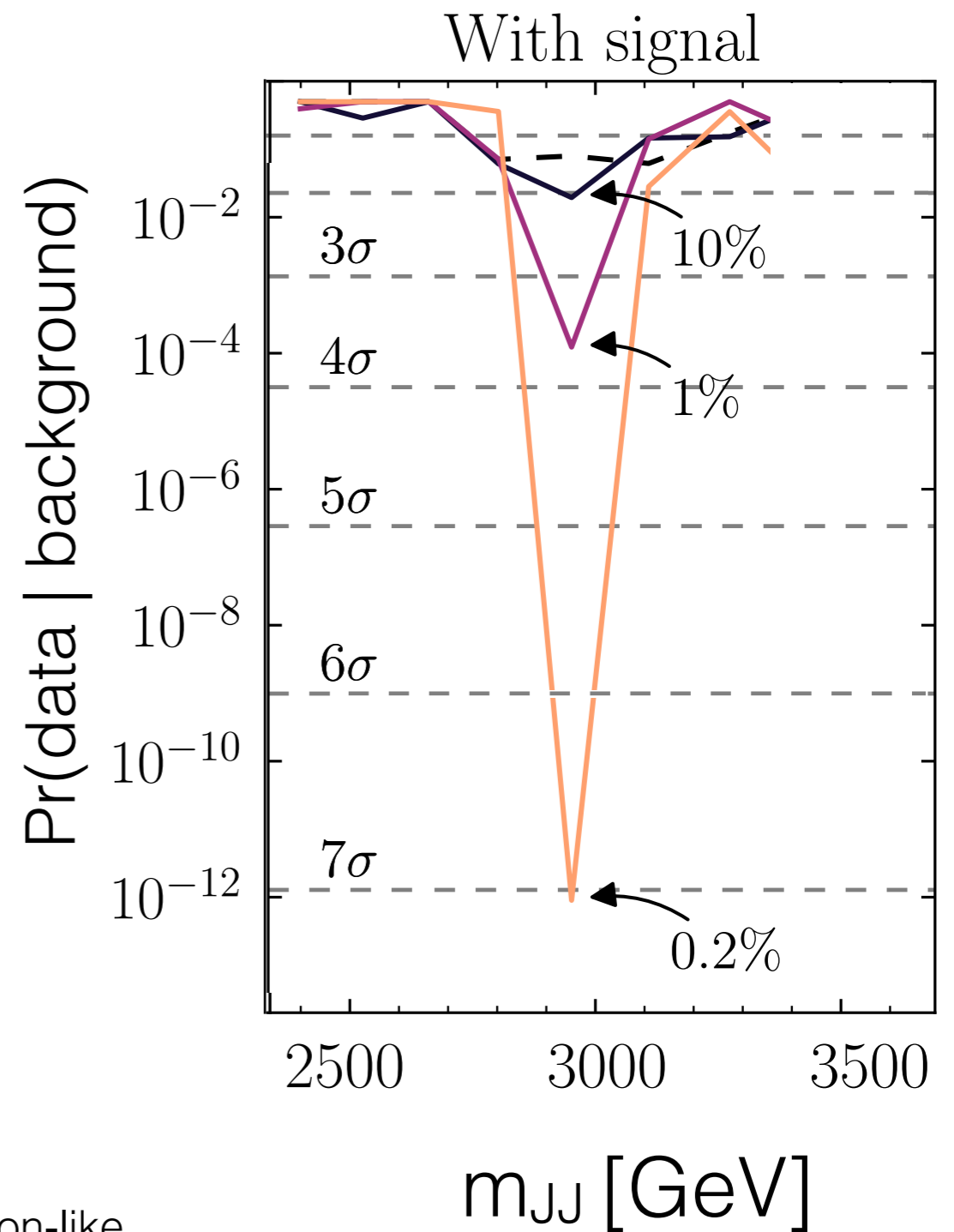
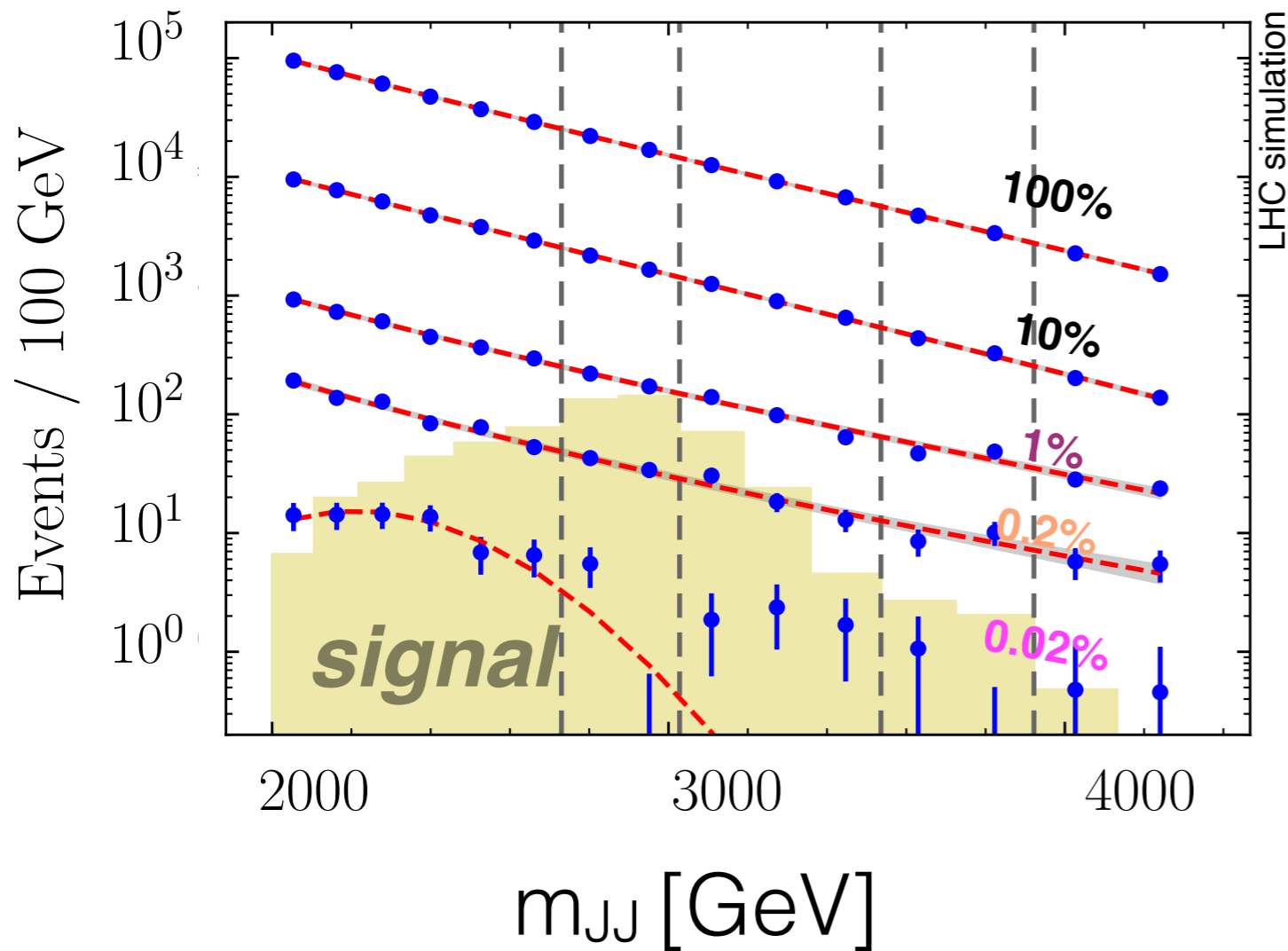
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

...and when there is a signal?



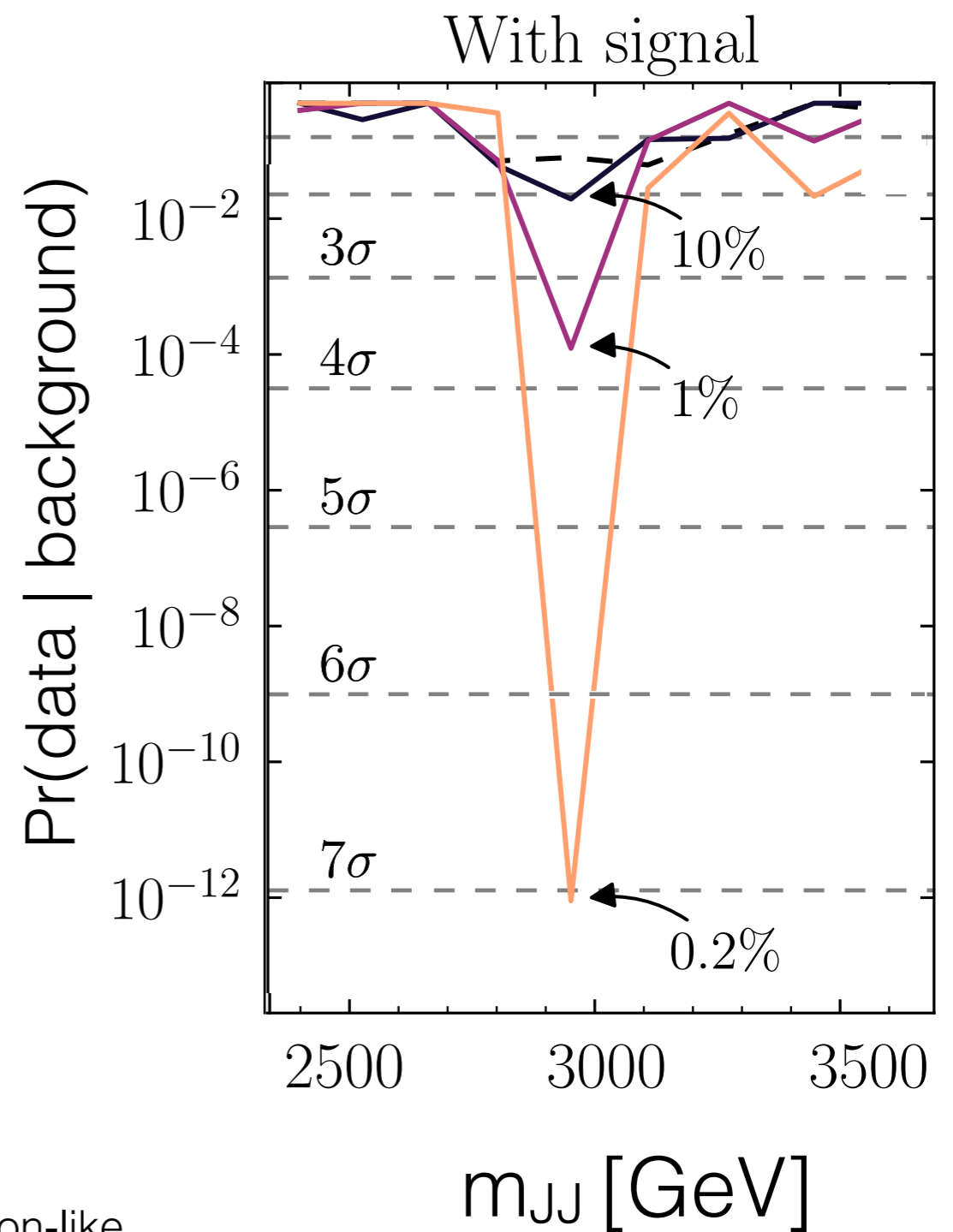
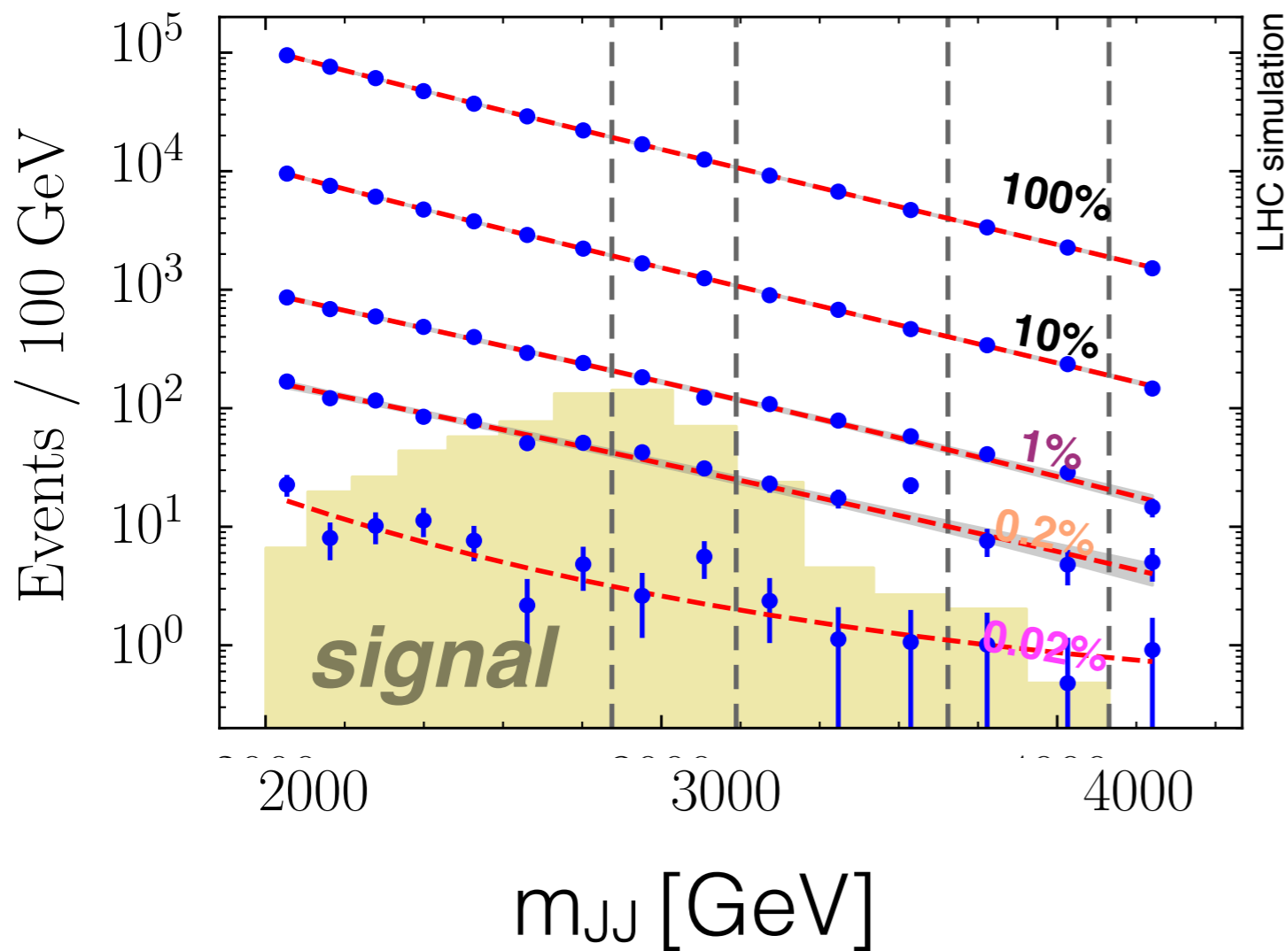
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

...and when there is a signal?



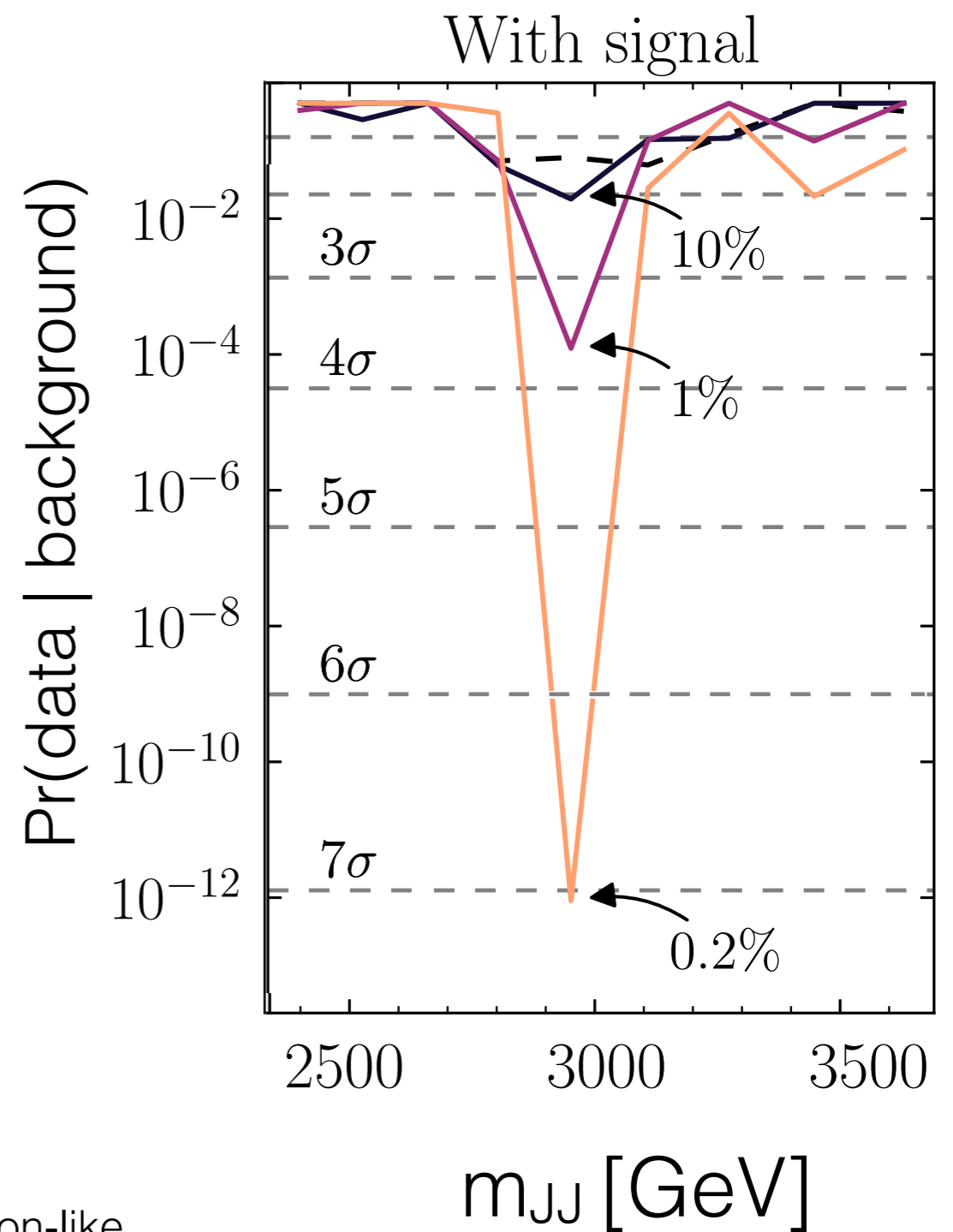
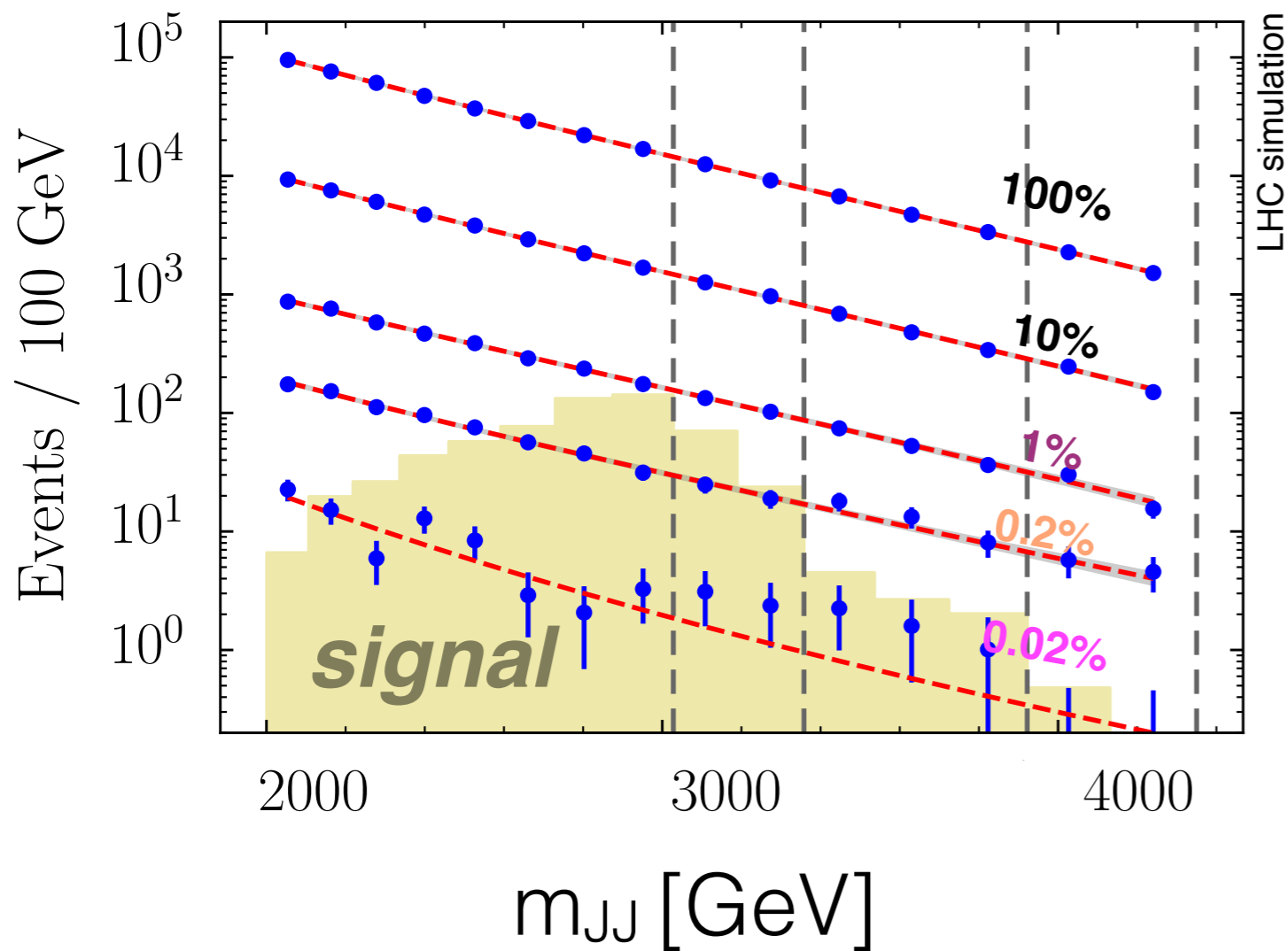
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

...and when there is a signal?



- 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?



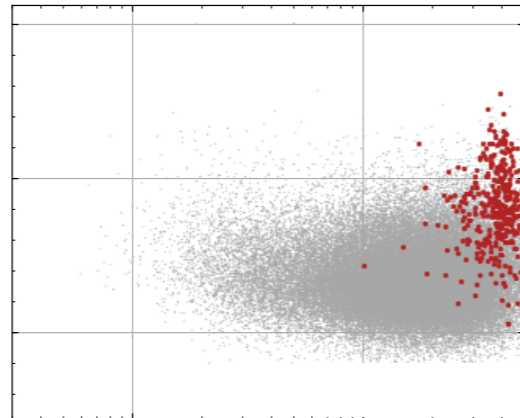
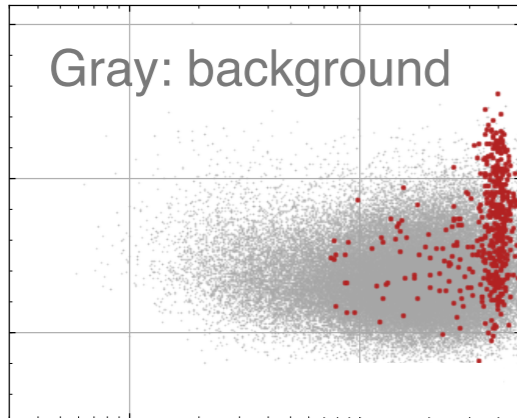
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

What is the network learning?

Truth signal

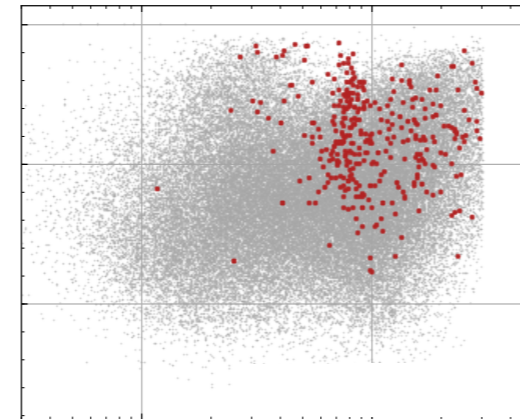
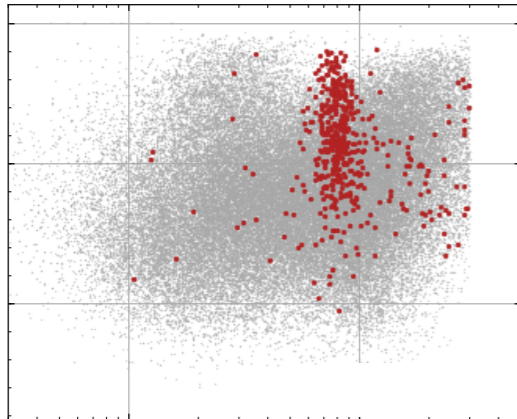
classifier
cut at 0.2%

Pr(4 prongs)



Heavier
Jet

Pr(2 prongs)

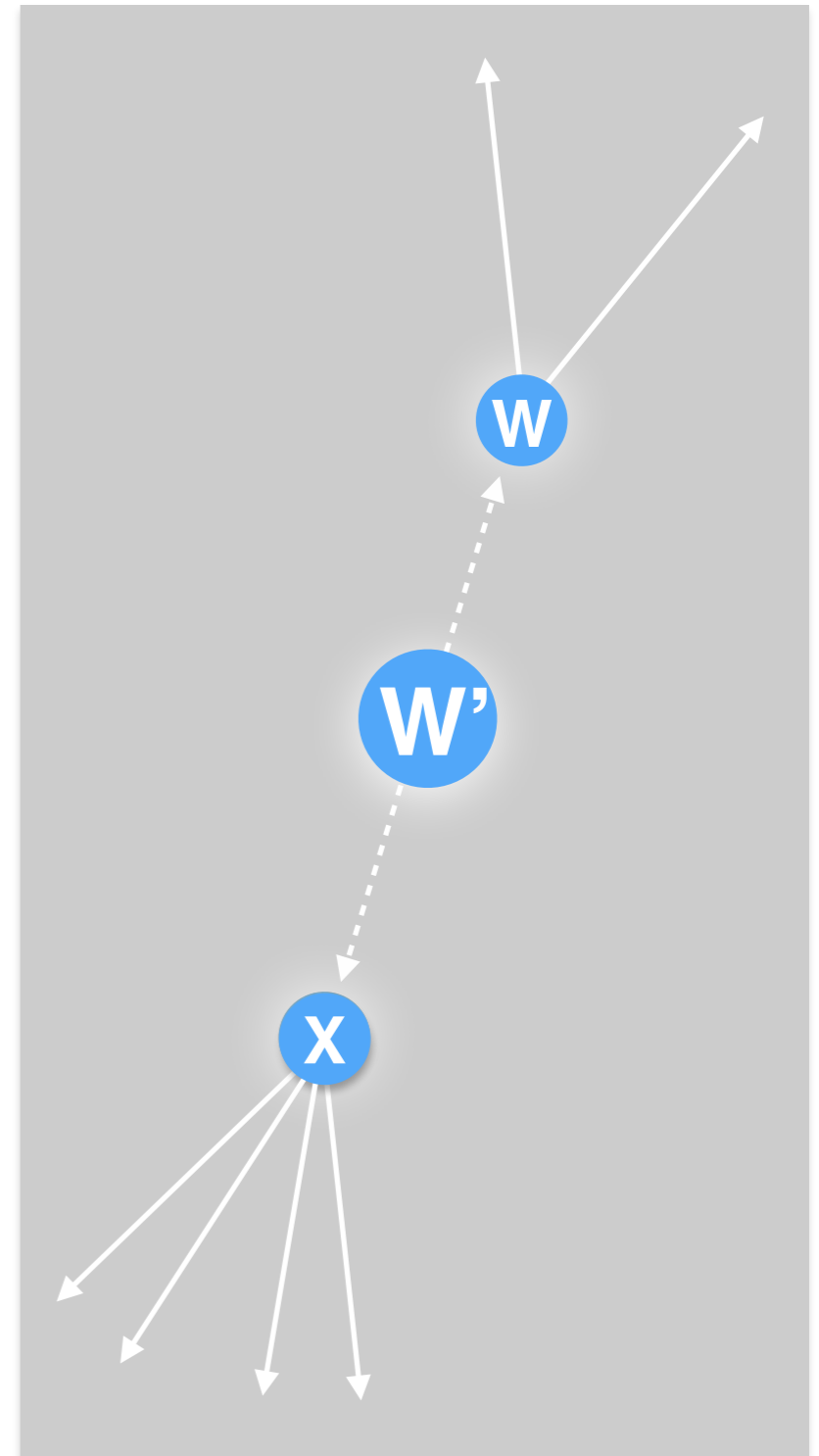


Lighter
Jet

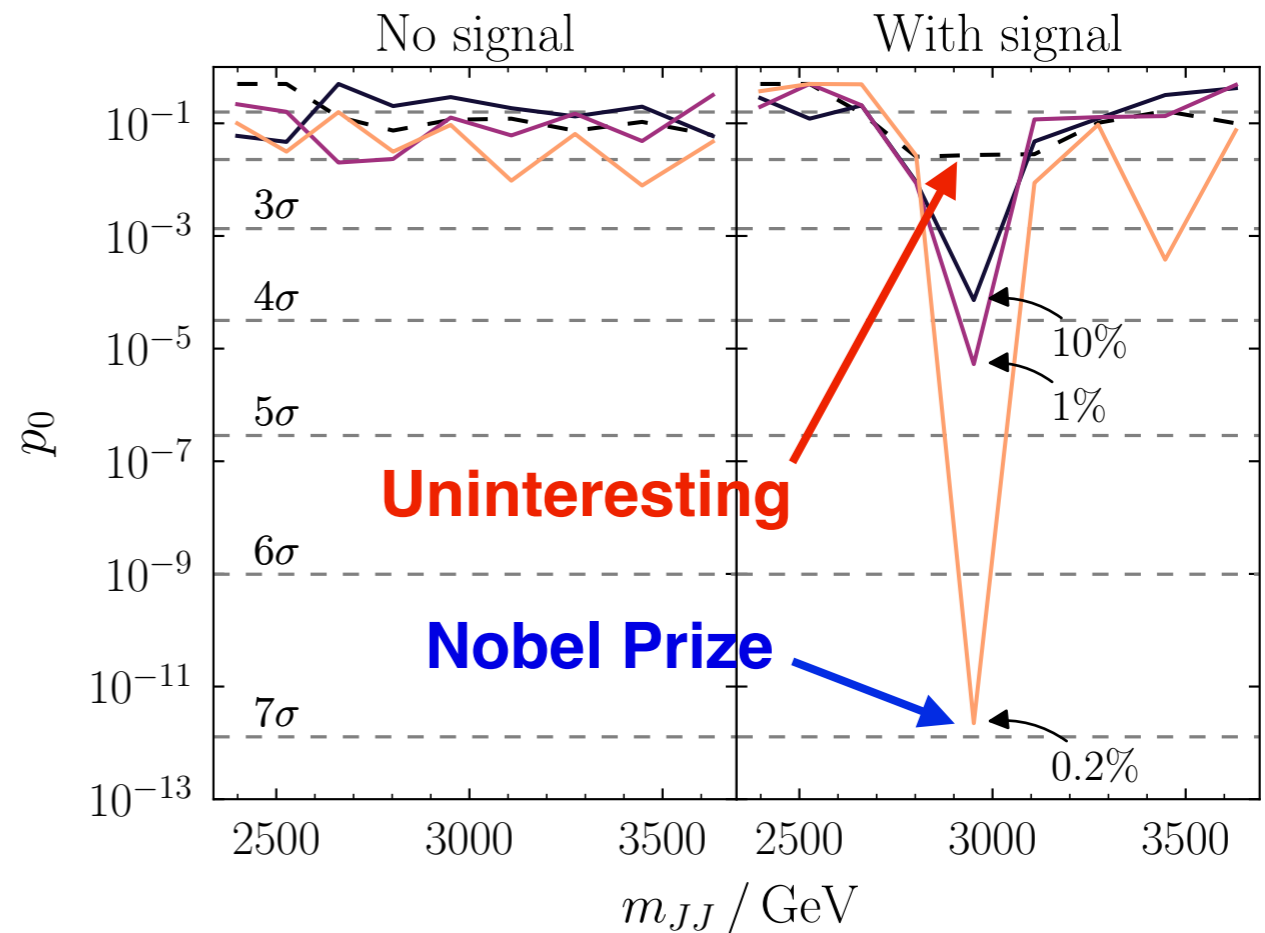
Mass

Mass

Learns to find the signal !



Deep learning has a great potential to **enhance**, **accelerate**, and **empower** HEP analyses.



Today, I have told you about an application for anomaly detection at the LHC. I would love to hear your thoughts on the applicability to DM/Neutrinos!!

Backup

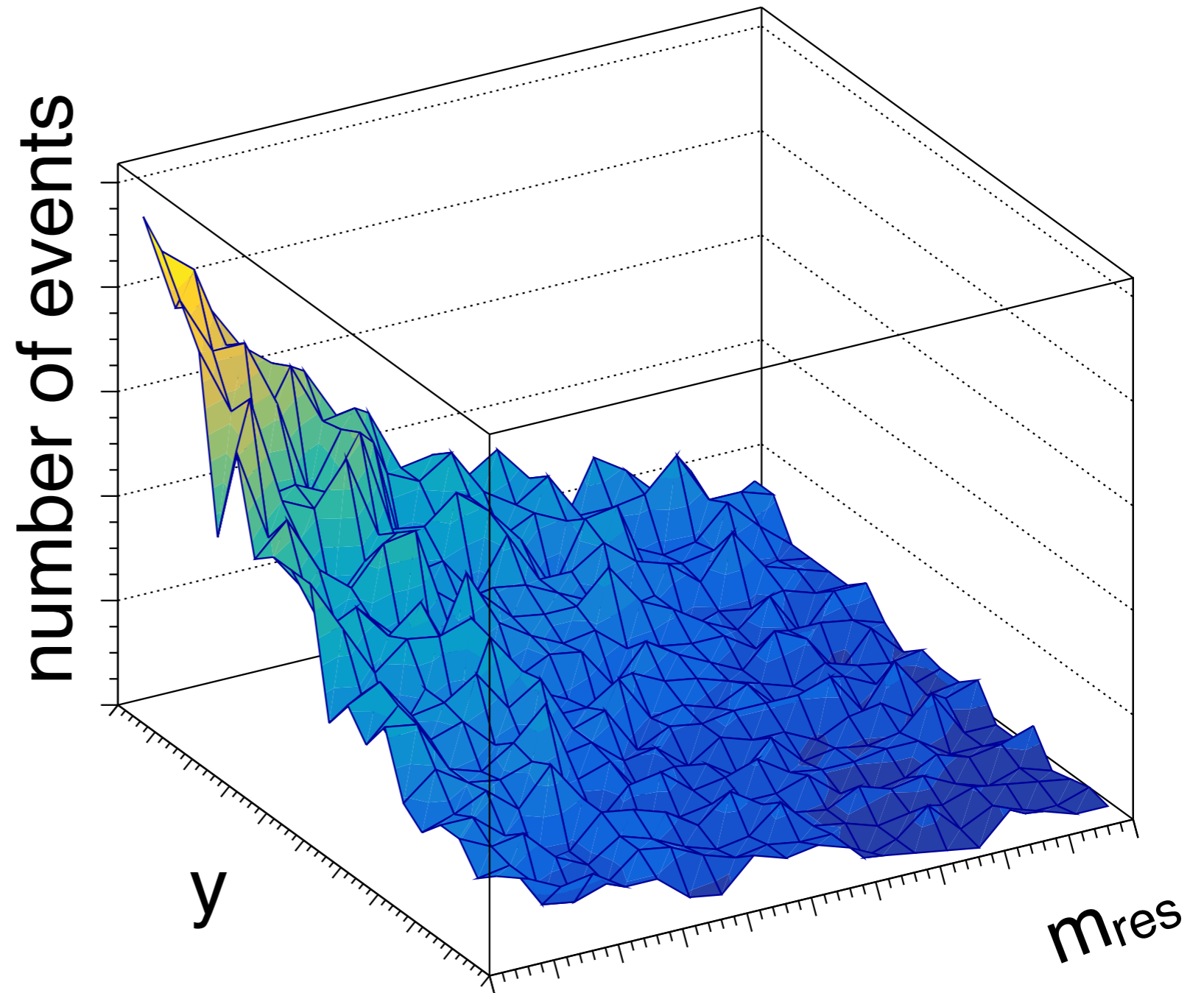


Overtraining & Look Elsewhere Effect*

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

i.e. you will sculpt lots of bumps!



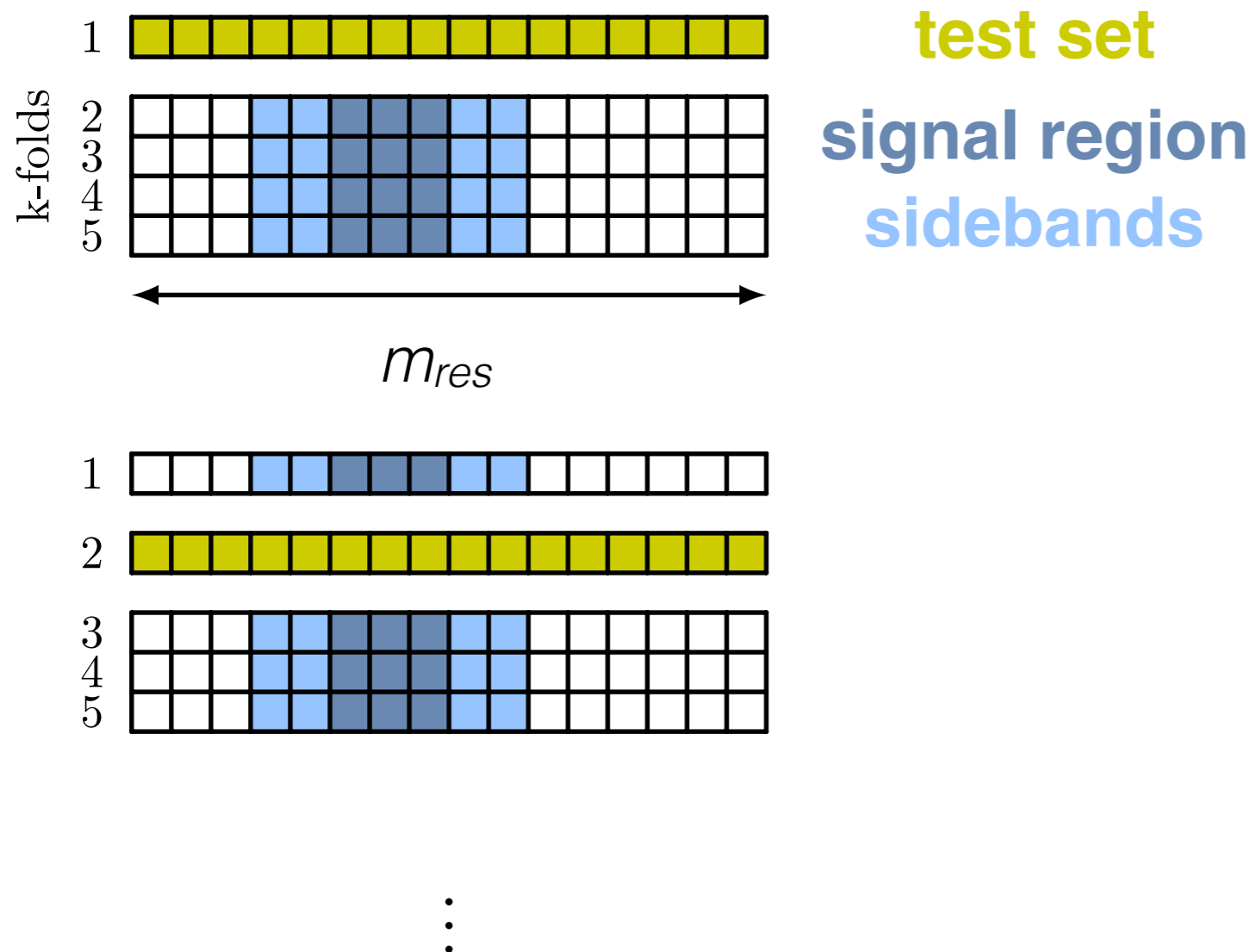
*you may know this as the multiple comparisons problem

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

Nested cross-training

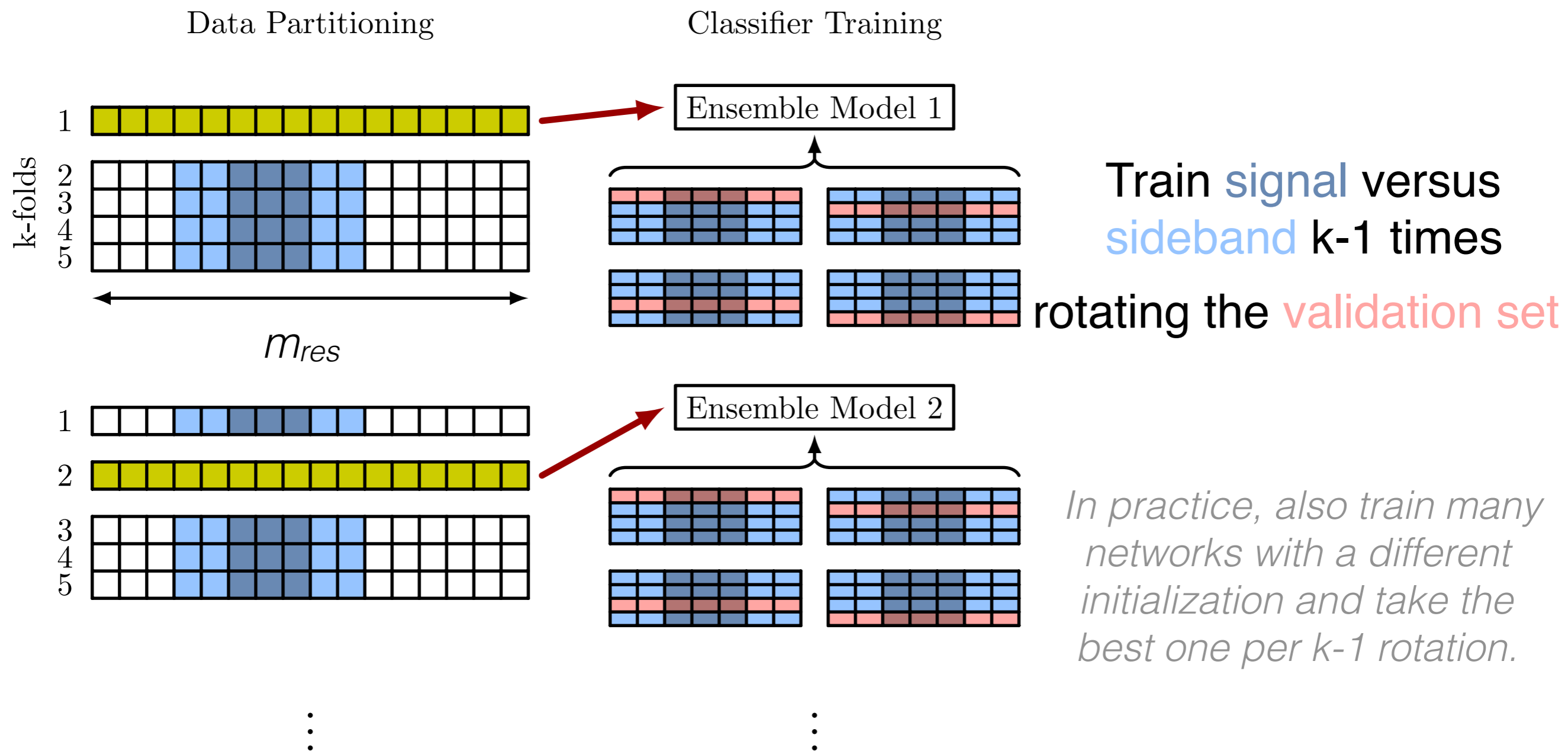
(1) Divide the entire dataset into k-folds.

Data Partitioning



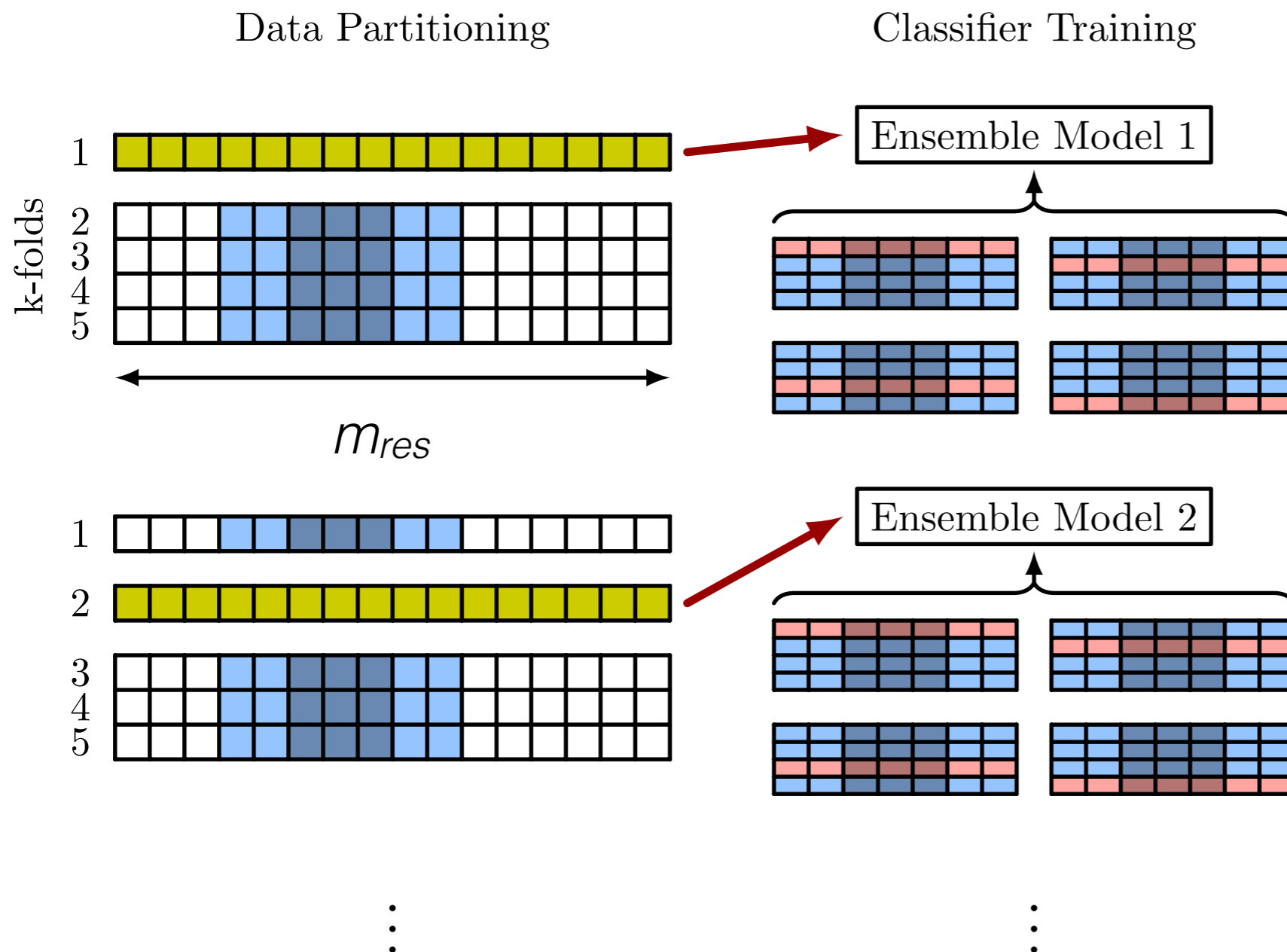
Nested cross-training

(2) Train CWoLa classifiers.



Nested cross-training

(2) Train CWoLa classifiers.

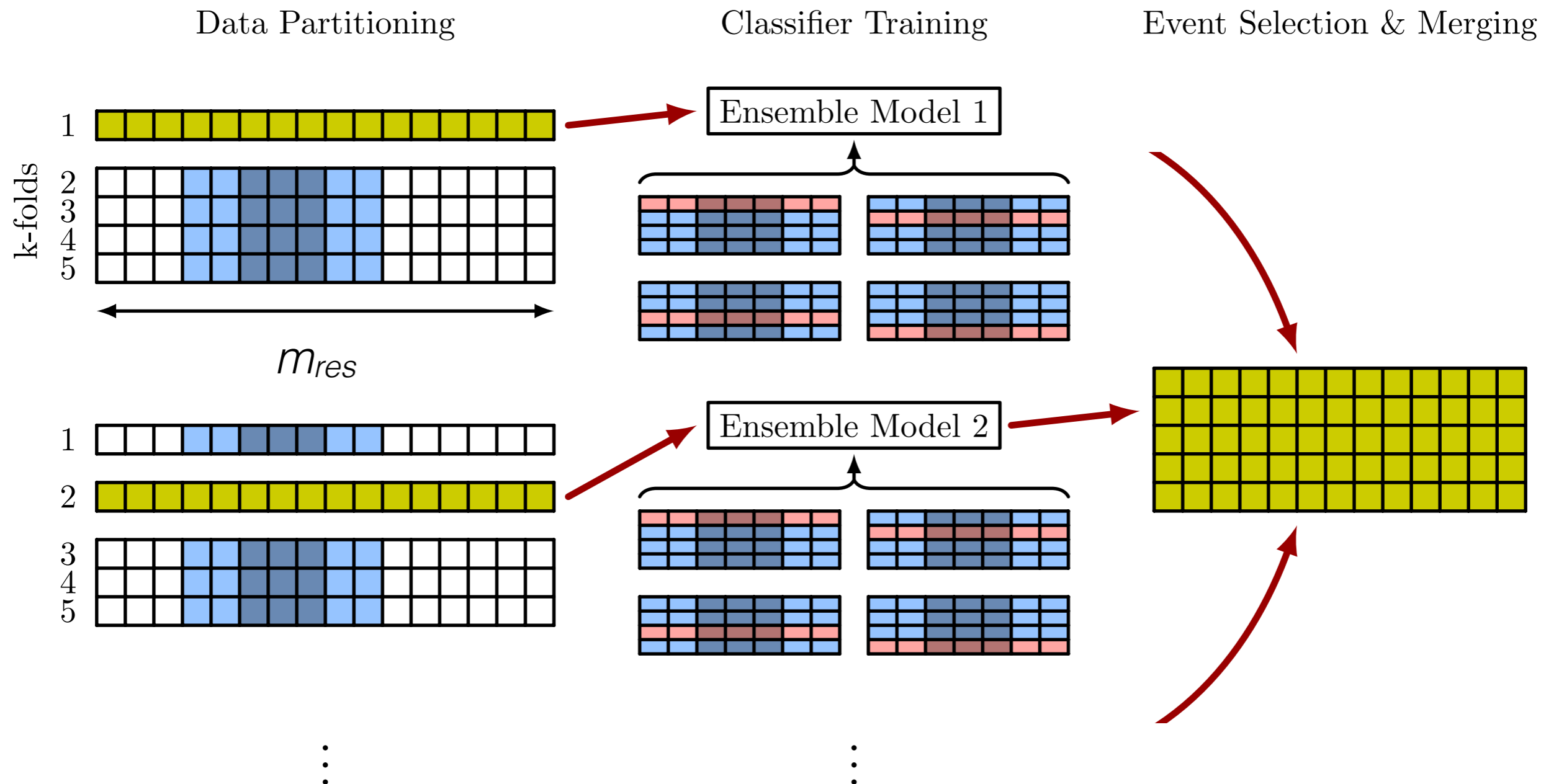


The **Ensemble Model** is just the average of the four networks.

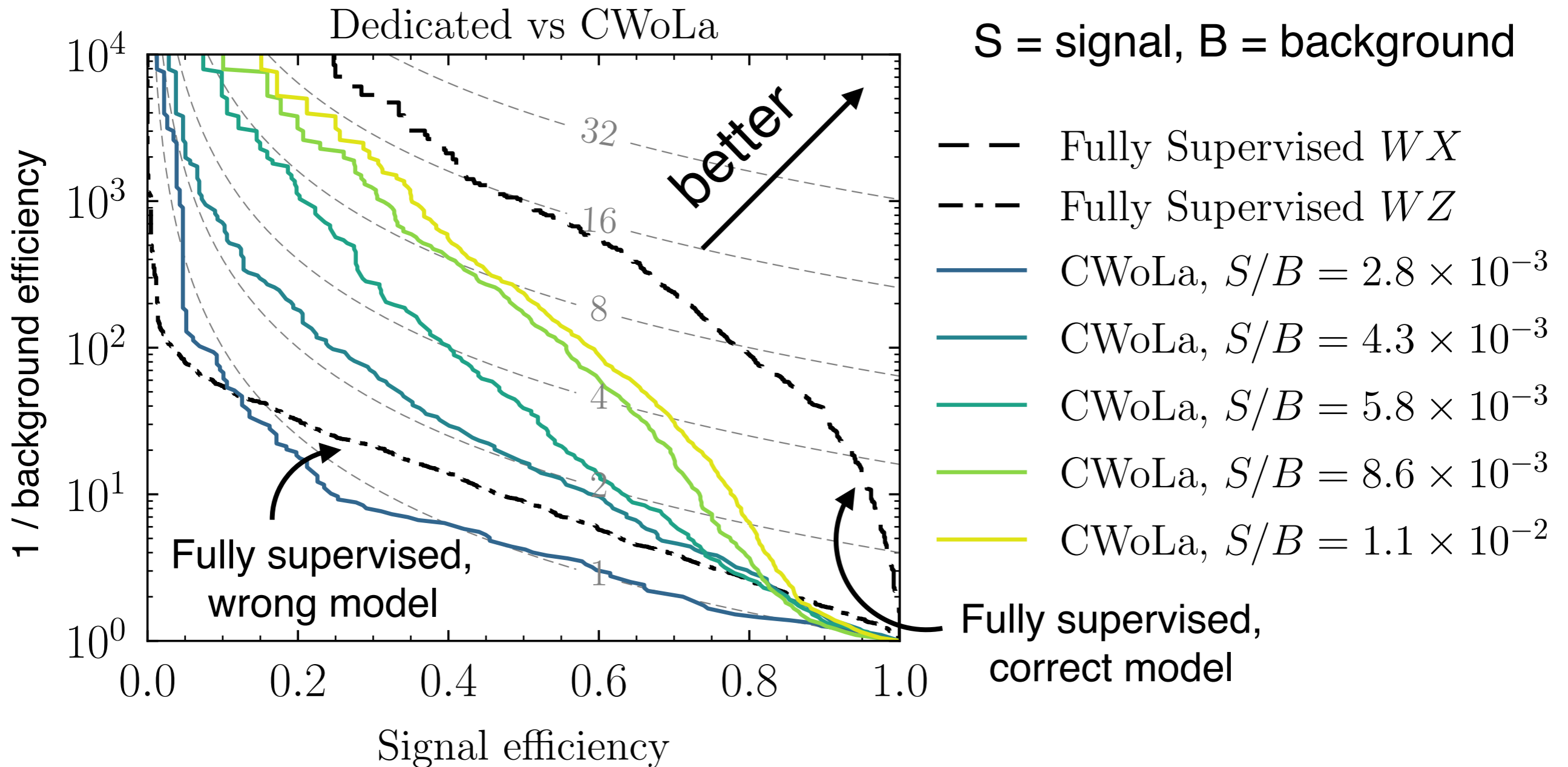
Data fluctuations will cancel destructively while signal interferes constructively.

Nested cross-training

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



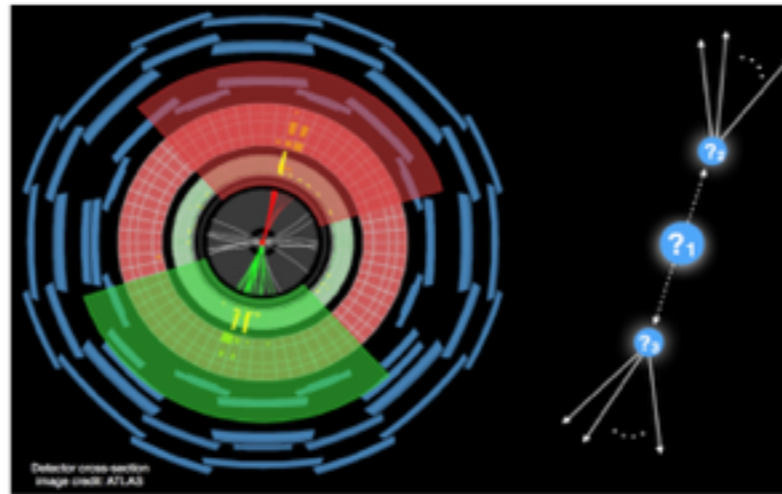
CWoLa hunting vs. Full Supervision



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!

- Overview
- Timetable
- Participant List
- LHC Olympics 2020
- Slack channel

LHC Olympics 2020



Despite an impressive and extensive effort by the LHC collaborations, there is currently no convincing evidence for new particles produced in high-energy collisions. At the same time, there has been a growing interest in machine learning techniques to enhance potential signals using all of the available information.

In the spirit of the first LHC Olympics (circa 2005-2006) [1st, 2nd, 3rd, 4th], we are organizing the 2020 LHC Olympics. Our goal is to ensure that the LHC search program is sufficiently well-rounded to capture "all" rare and complex signals. The final state for this olympics will be focused (generic dijet events) but the observable phase space and potential BSM parameter space(s) are large: all hadrons in the event can be used for learning (be it "cuts", supervised machine learning, or unsupervised machine learning).

For setting up, developing, and validating your methods, we provide background events and a few benchmark signal models. You can download these from [ZENODO LINK]. To help get you started, we have also prepared [simple python scripts](#) to read in the data and do some basic processing.

The final test will happen 2 weeks before the ML4Jets2020 workshop. We will release new datasets where the "background" will be similar to but not identical to the one in the development set (as is true in real data!). Each of these datasets will have signal injected somewhere and it is up to you to see if you can find (a) find a signal (b) what is the mass, and (c) what is the cross section. To keep the scope limited, all signals will be of the form $X \rightarrow$ hadrons, where X is a new massive particle with an $O(\text{TeV})$ mass. The events require at least one $R = 1.0$ jet with $p_T > 1 \text{ TeV}$. For each event, we provide a list of all hadrons (p_T , eta, phi, p_T , eta, phi, ...) zero-padded up to 600 hadrons.

We strongly encourage you to publish your original research methods using these datasets (before or after) the unveiling of the results. Anyone who participates will be part of a summary paper to be prepared following the workshop.

Please do not hesitate to ask questions: we will use the [ML4Jets slack channel](#) to discuss technical questions related to this challenge.

Good luck!

Gregor Kasieczka, Ben Nachman, and David Shih