

Machine Learning in Particle Physics

Benjamin Nachman

Lawrence Berkeley National Laboratory

bpnachman.com

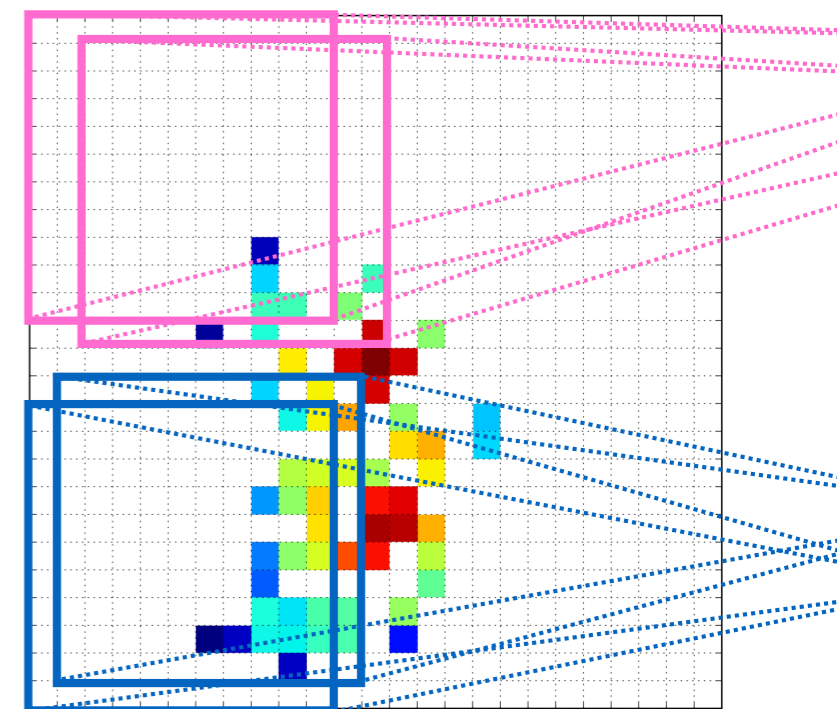


@bpnachman



bnachman

bpnachman@lbl.gov



UC Berkeley Physics
Physics 290E
February 23, 2022

Questions in fundamental physics

2

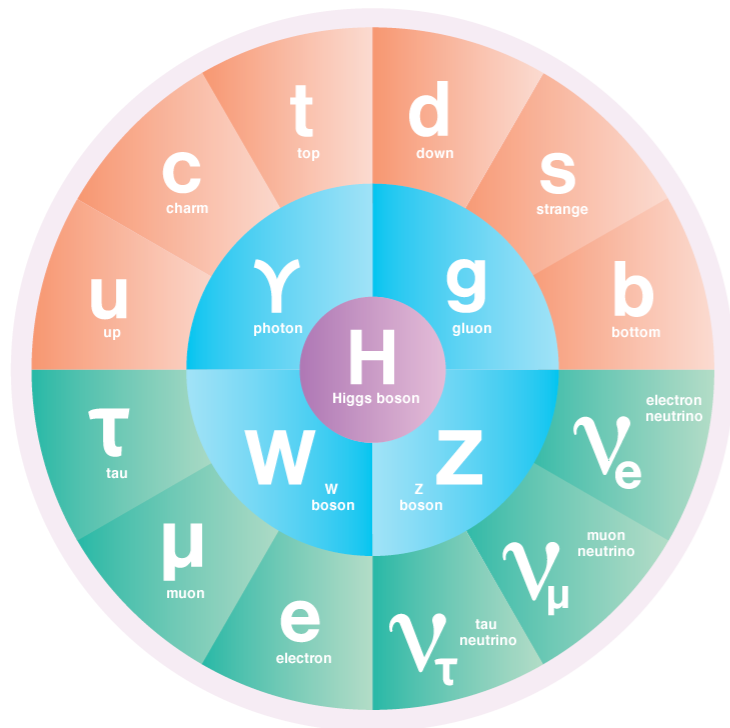
Theoretical and experimental questions motivate a deep exploration **of the fundamental structure of nature**

Why is the Higgs boson so light?

Hierarchy problem

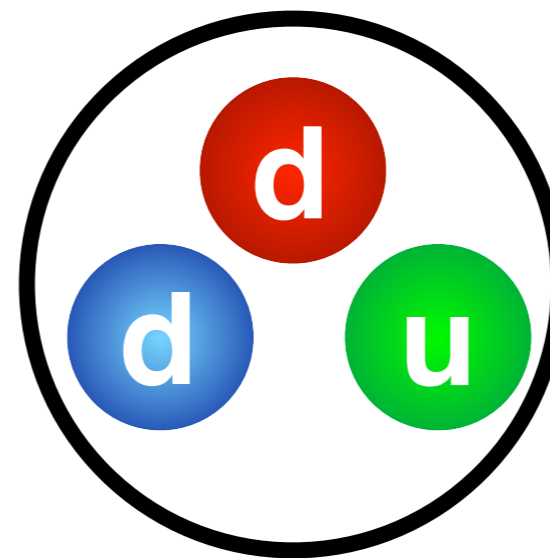
Why do neutrons have no dipole moment?

Strong CP



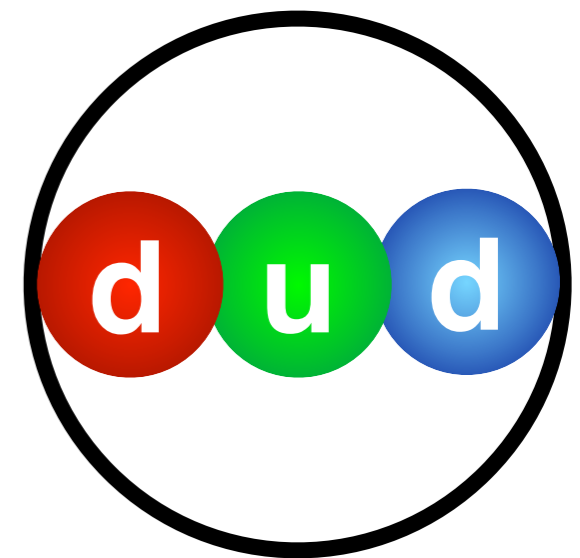
See also: quantum gravity

Neutron



>99% of pictures on the internet

Neutron



Reality

image source: symmetry magazine

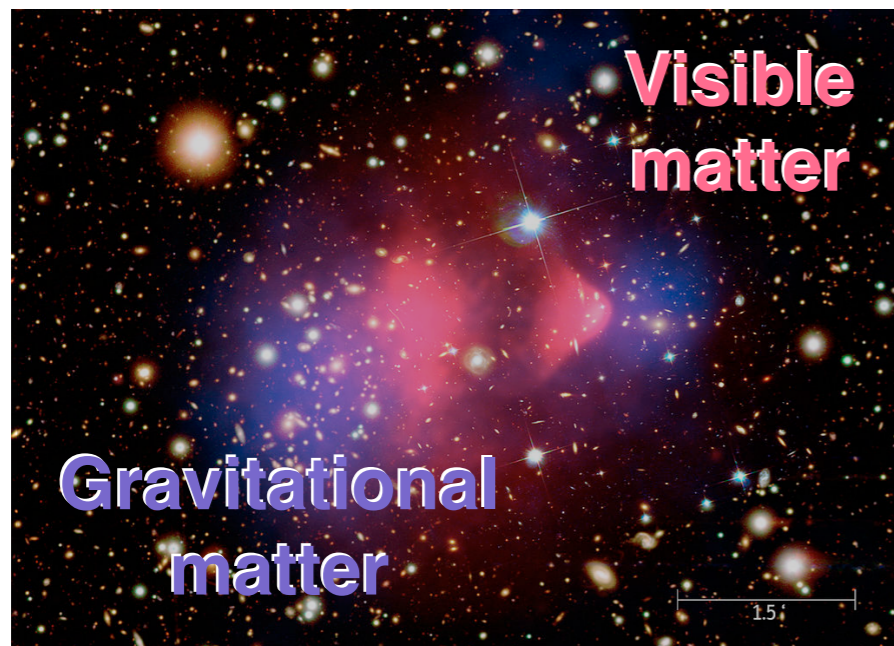
Questions in fundamental physics

3

Theoretical and **experimental** questions motivate a deep exploration **of the fundamental structure of nature**

What is the extra gravitational matter?

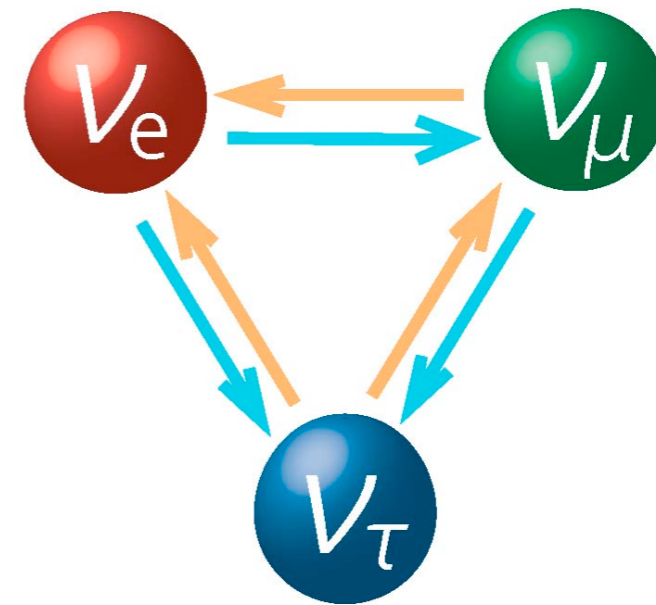
Dark Matter



See also: dark energy

Why do neutrinos have a mass?

Flavor puzzles



See also: Where did all the anti-particles go? (Baryogenesis)

Questions in fundamental physics



Theoretical and **experimental** questions motivate a deep exploration **of the fundamental structure of nature**

Dark matter

Hierarchy problem

Strong CP

Flavor puzzles

Baryogenesis

Dark energy

We have performed thousands of hypothesis tests & have **no significant evidence** for physics beyond the Standard Model

Questions in fundamental physics

5

Theoretical and **experimental** questions motivate a deep exploration **of the fundamental structure of nature**

Dark matter

Hierarchy problem

Strong CP

Flavor puzzles

Baryogenesis

Dark energy

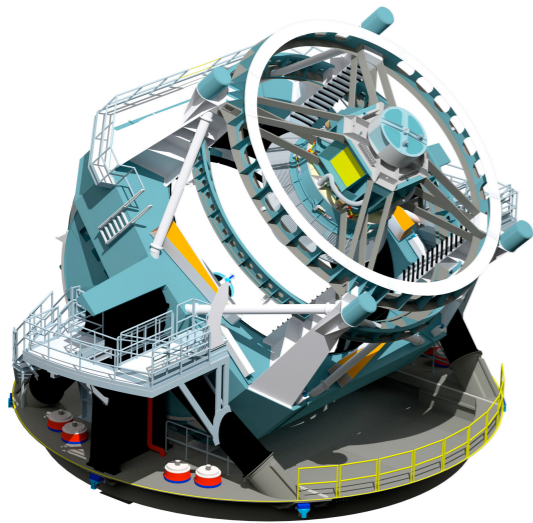
We have performed thousands of hypothesis tests & have **no significant evidence** for physics beyond the Standard Model

We will need new tools to explore our data in new ways!

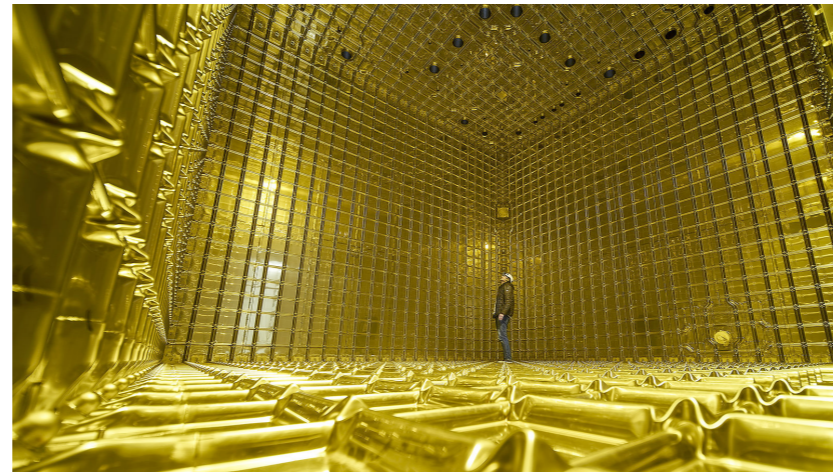
New tools: detectors



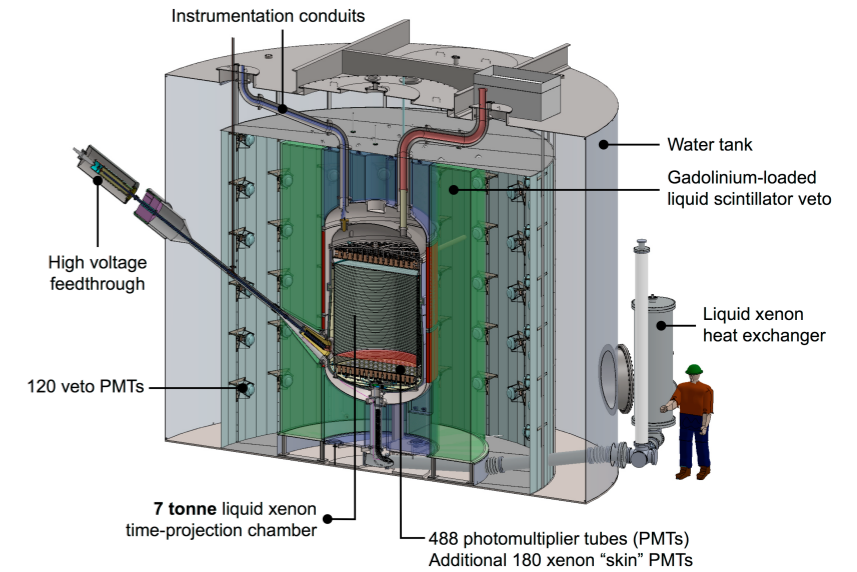
Dark matter/energy with LSST



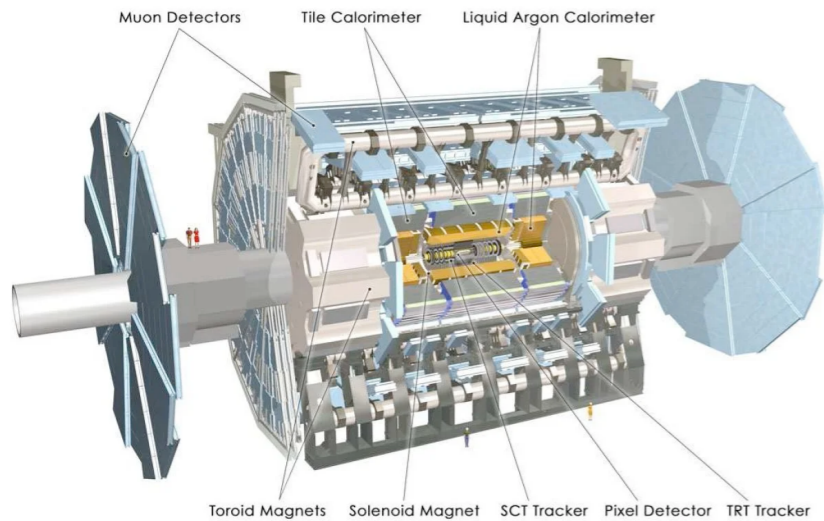
Fermilab neutrino experiments



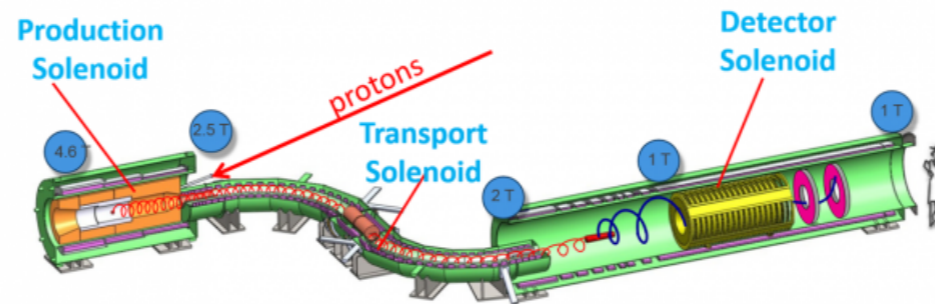
Dark Matter with LZ



Large Hadron Collider



Mu2e experiment



+ others !

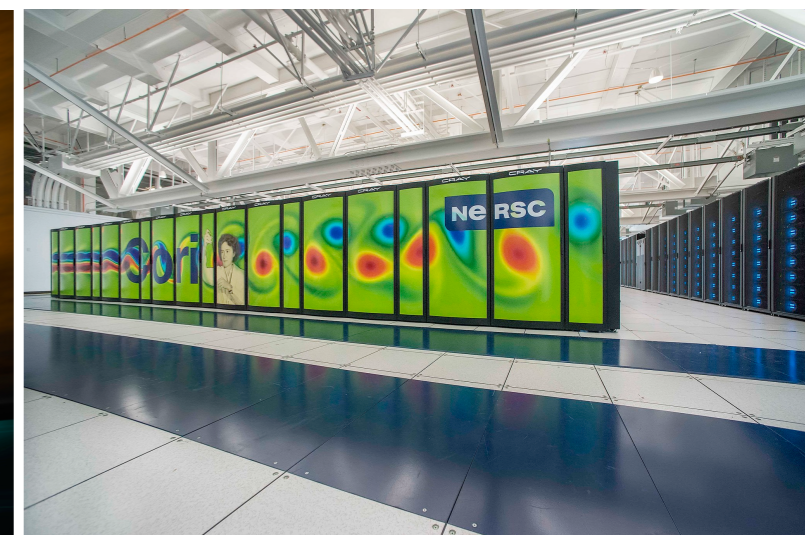
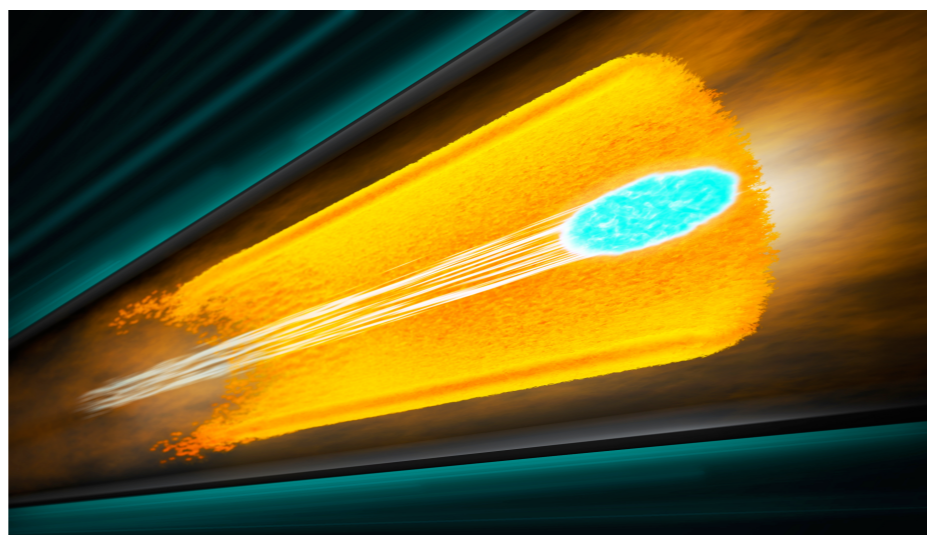
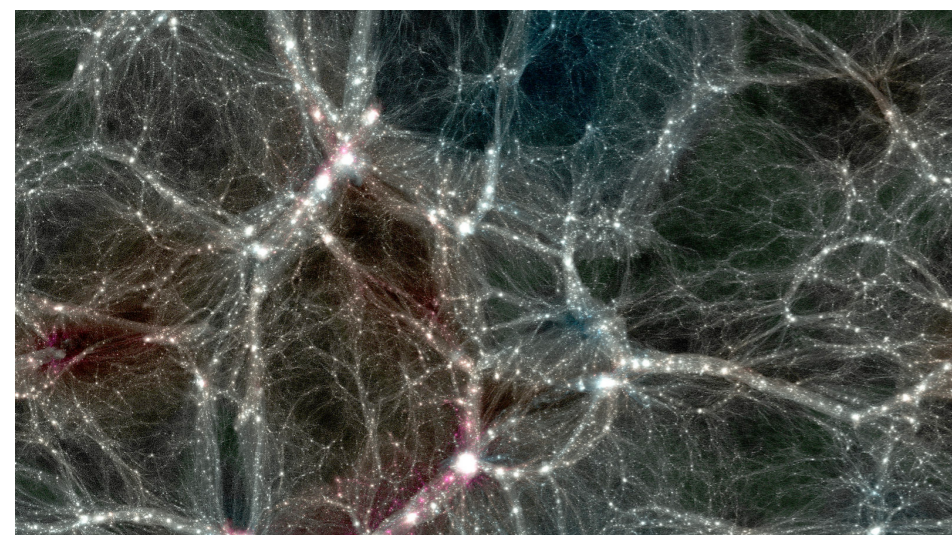
New tools: methodology



N-body simulations

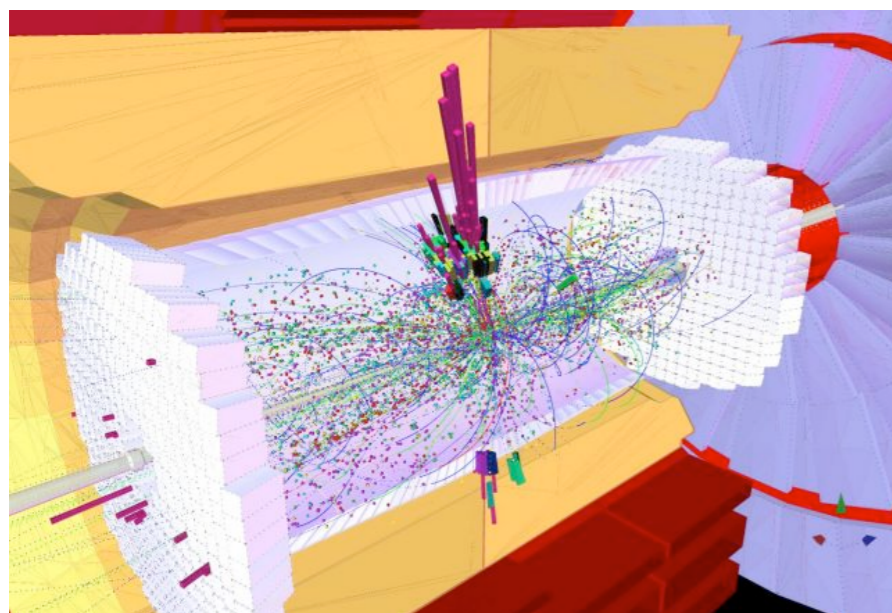
Advanced accelerators

Supercomputers



Material Simulations

Theory Calculations



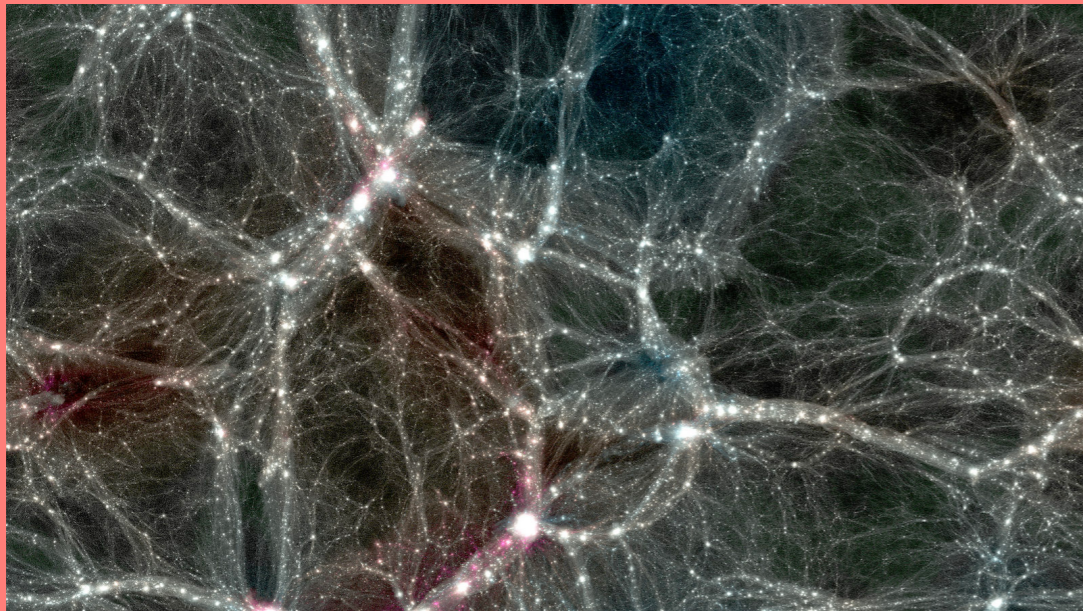
$$2\text{Im} \left(\text{Diagram with wavy lines and a dashed vertical line} \right) = \int d\Pi \left| \text{Diagram with wavy lines} \right|^2$$

+ others !

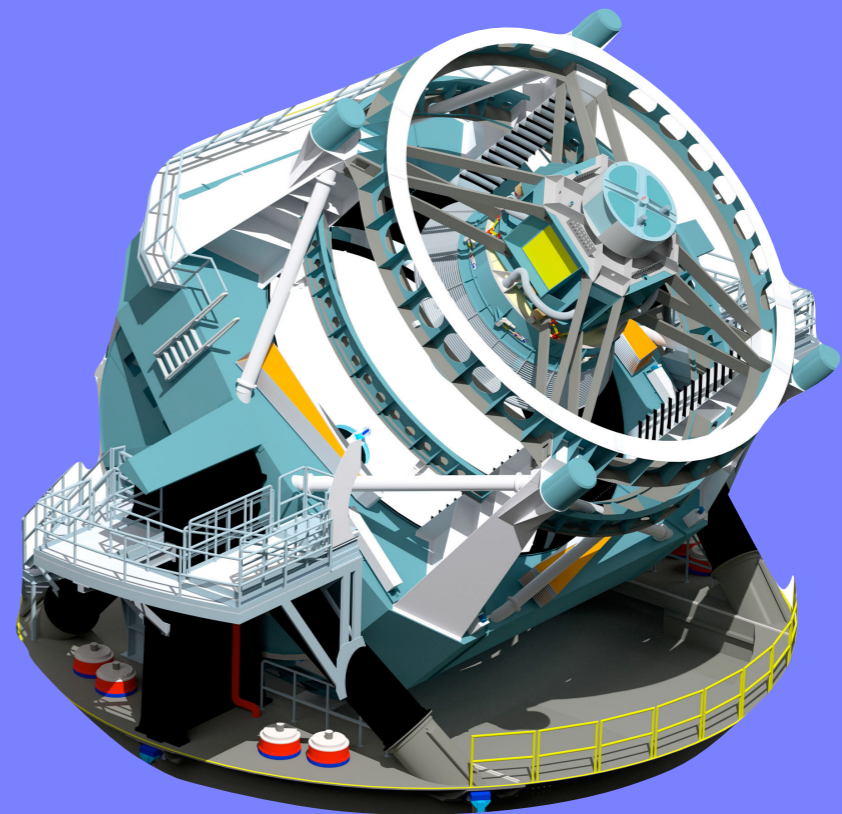
A *hyper* challenge



Key **challenge** and **opportunity**: *hypervariate phase space*
& *hyper spectral data*



Methodology



Detectors

A *hyper* challenge

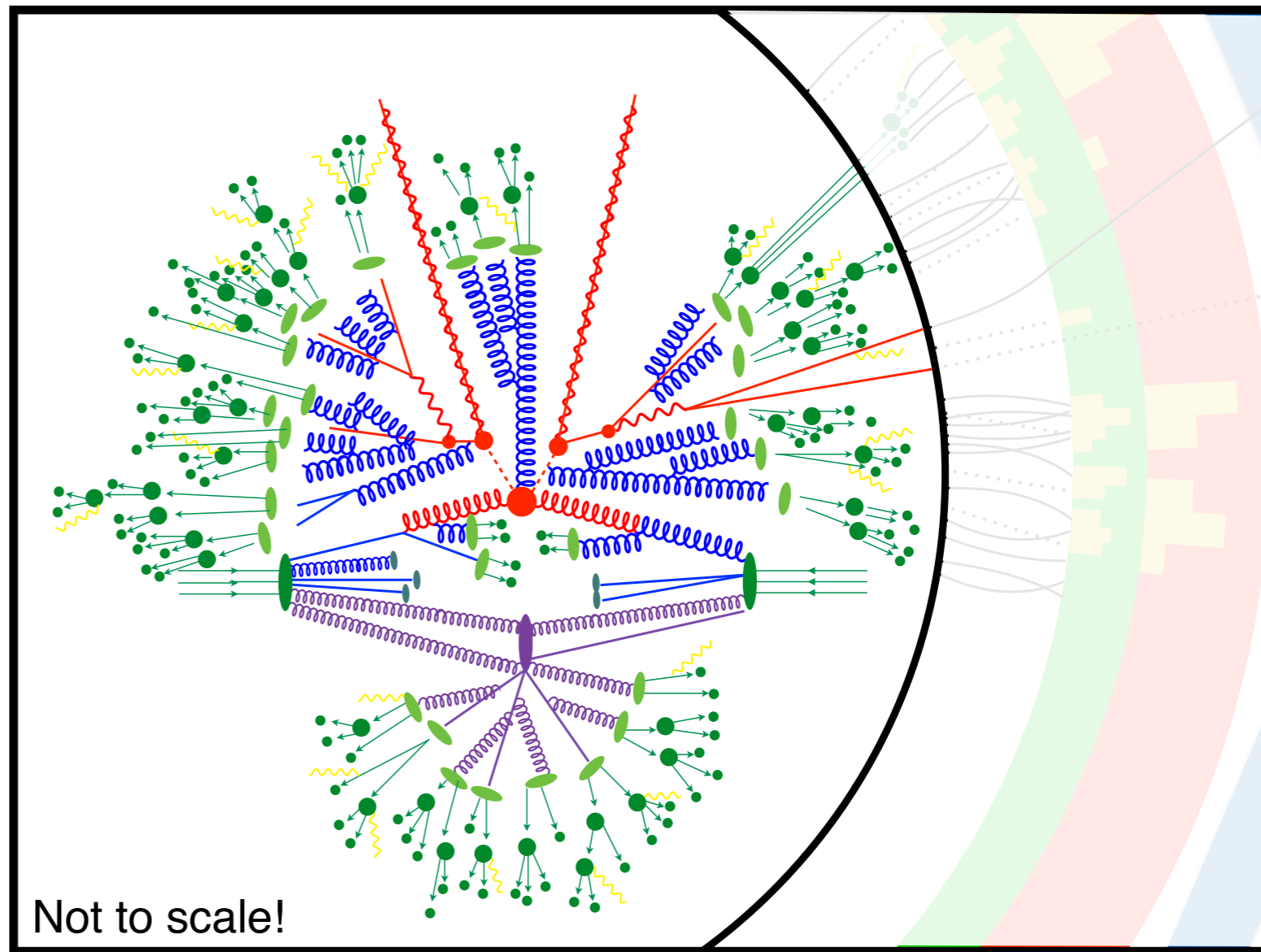


Key **challenge** and **opportunity**: *hypervariate phase space*
& *hyper spectral data*

Typical collision events
at the LHC produce
O(1000+) particles

We detect these
particles with
O(100 M)
readout channels

Image inspired by JHEP 02 (2009) 007



Not to scale!

A *hyper* challenge

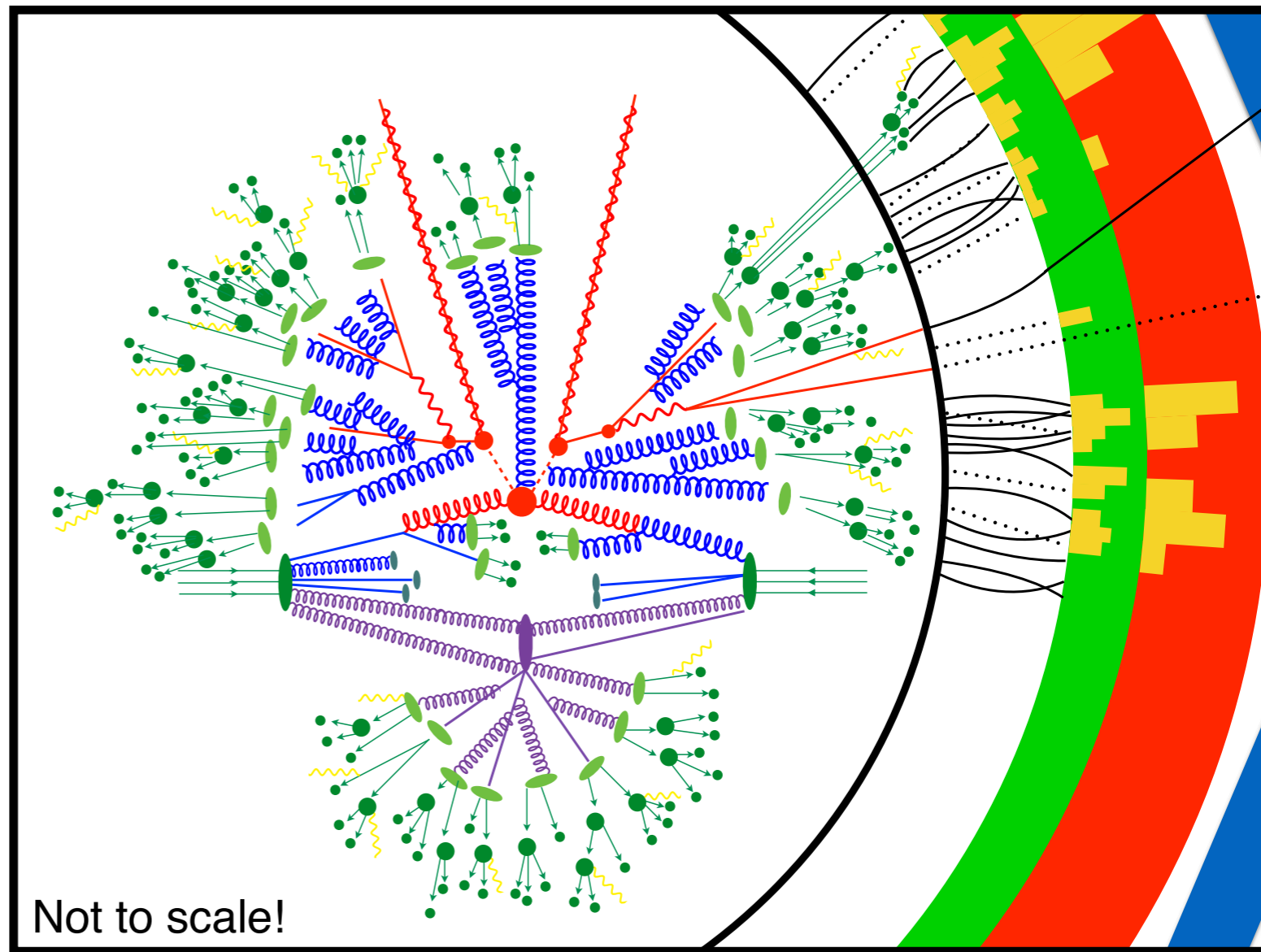
10

Key **challenge** and **opportunity**: *hypervariate phase space*
& *hyper spectral data*

Typical collision events
at the LHC produce
O(1000+) particles

We detect these
particles with
O(100 M)
readout channels

Image inspired by JHEP 02 (2009) 007



Not to scale!

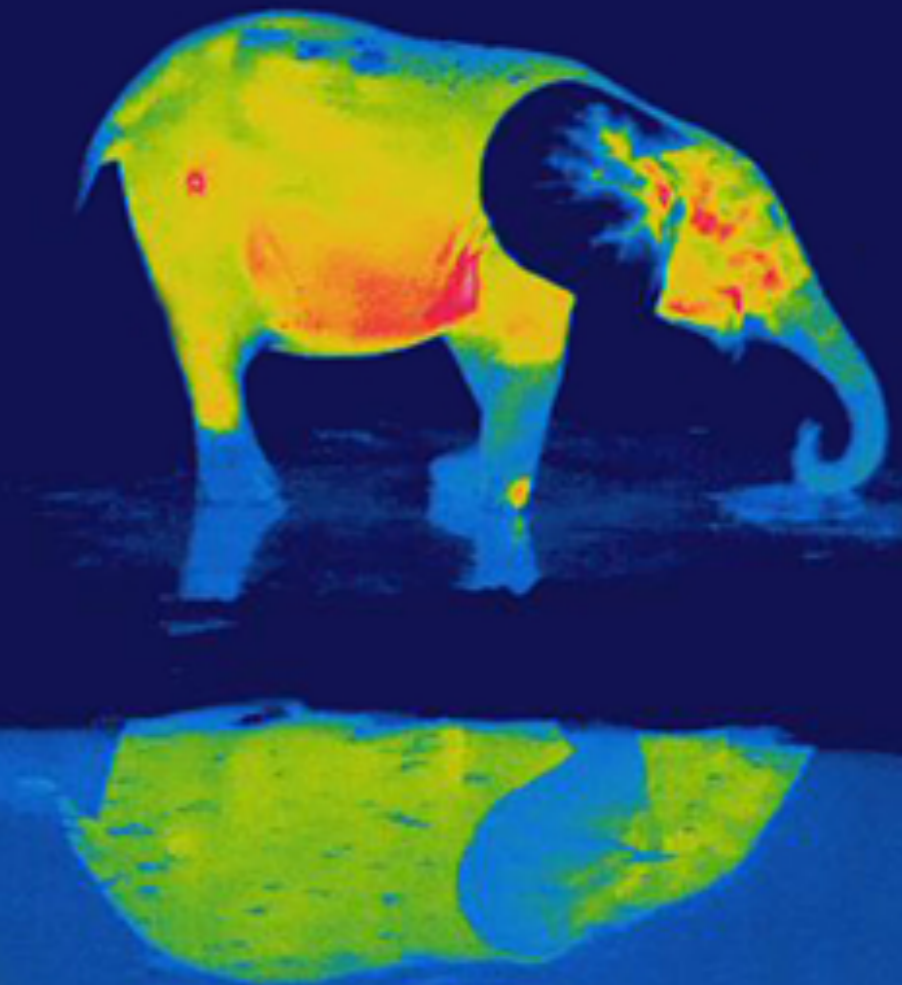
Hypervariate vision with deep learning

11

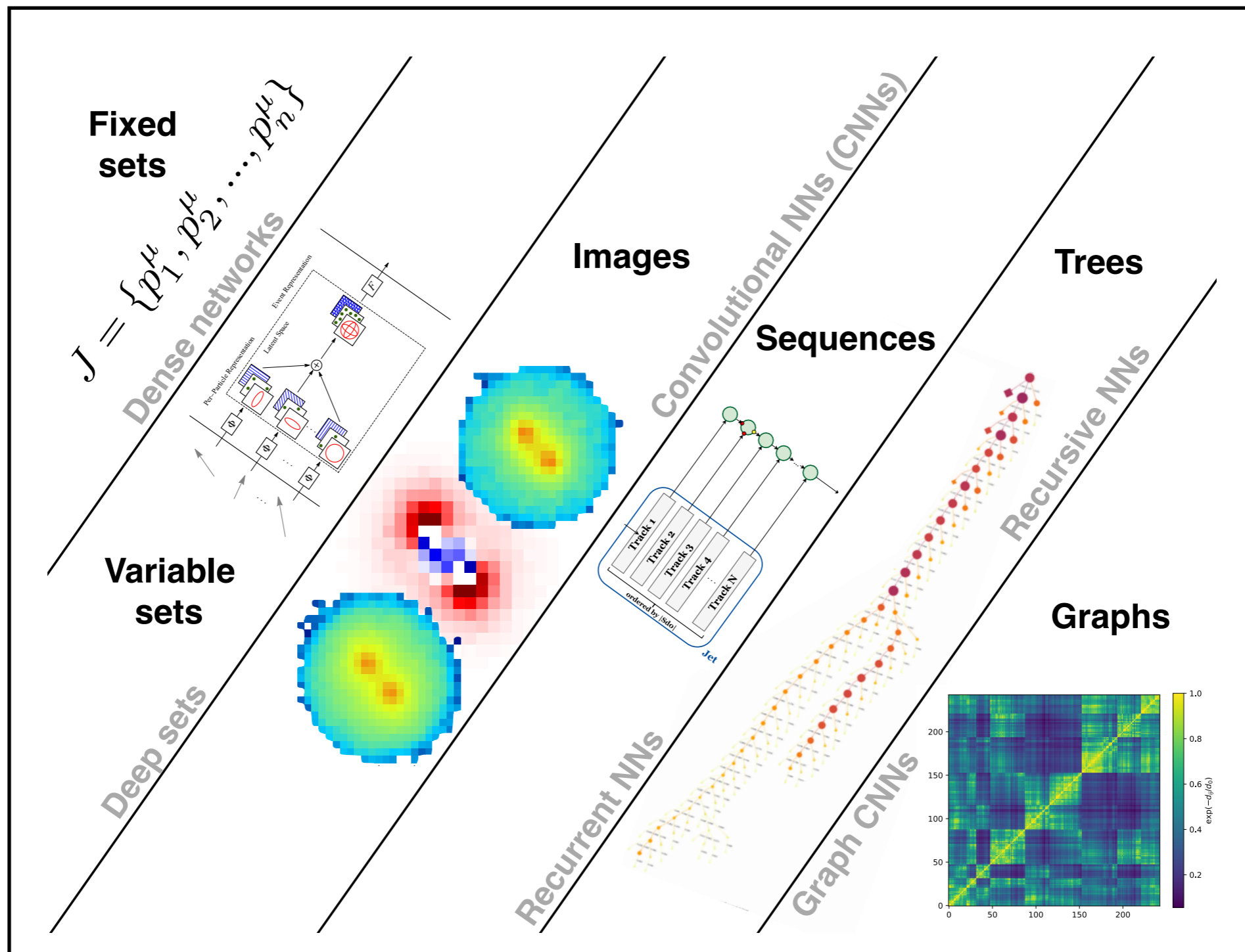
We have been conducting “multivariate” analysis of collision events for many years

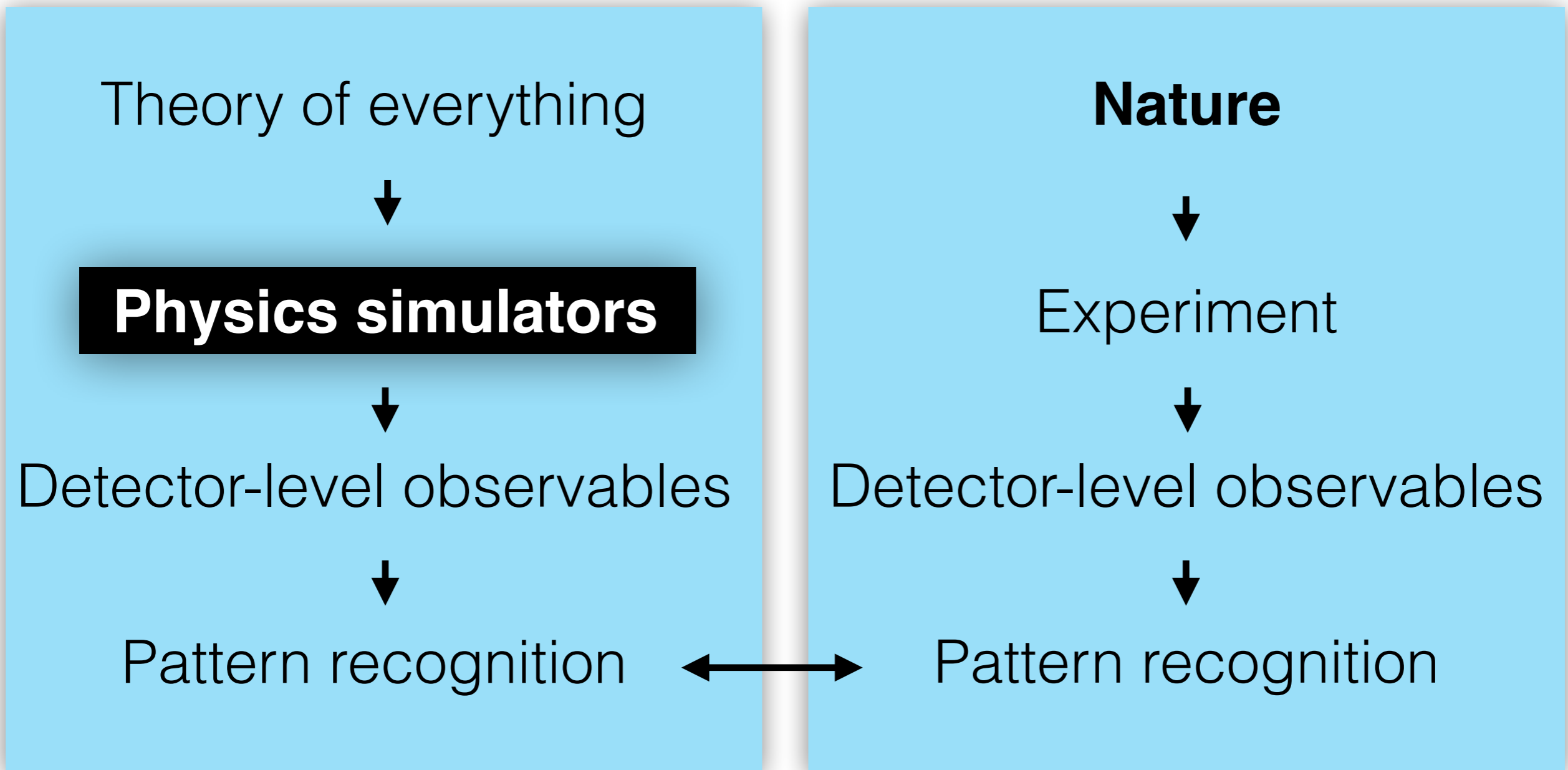
However, recent advances have opened up a **new way** of looking at our data. This **hypervariate vision** will lead to a deeper understanding of nature and perhaps surprises along the way...

Everyone is aware that there must be new physics, but maybe we need hypervariate vision to see it?

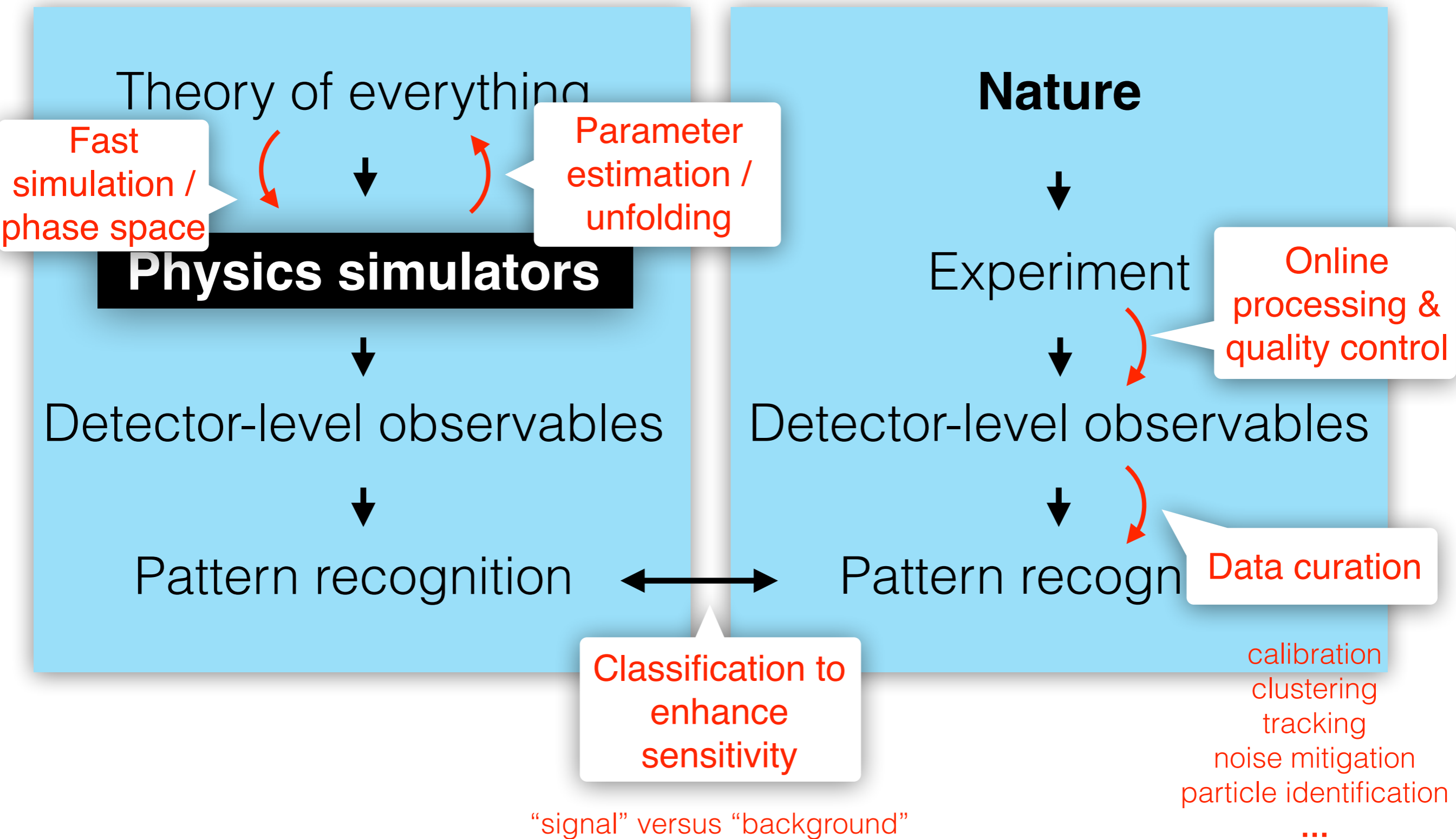


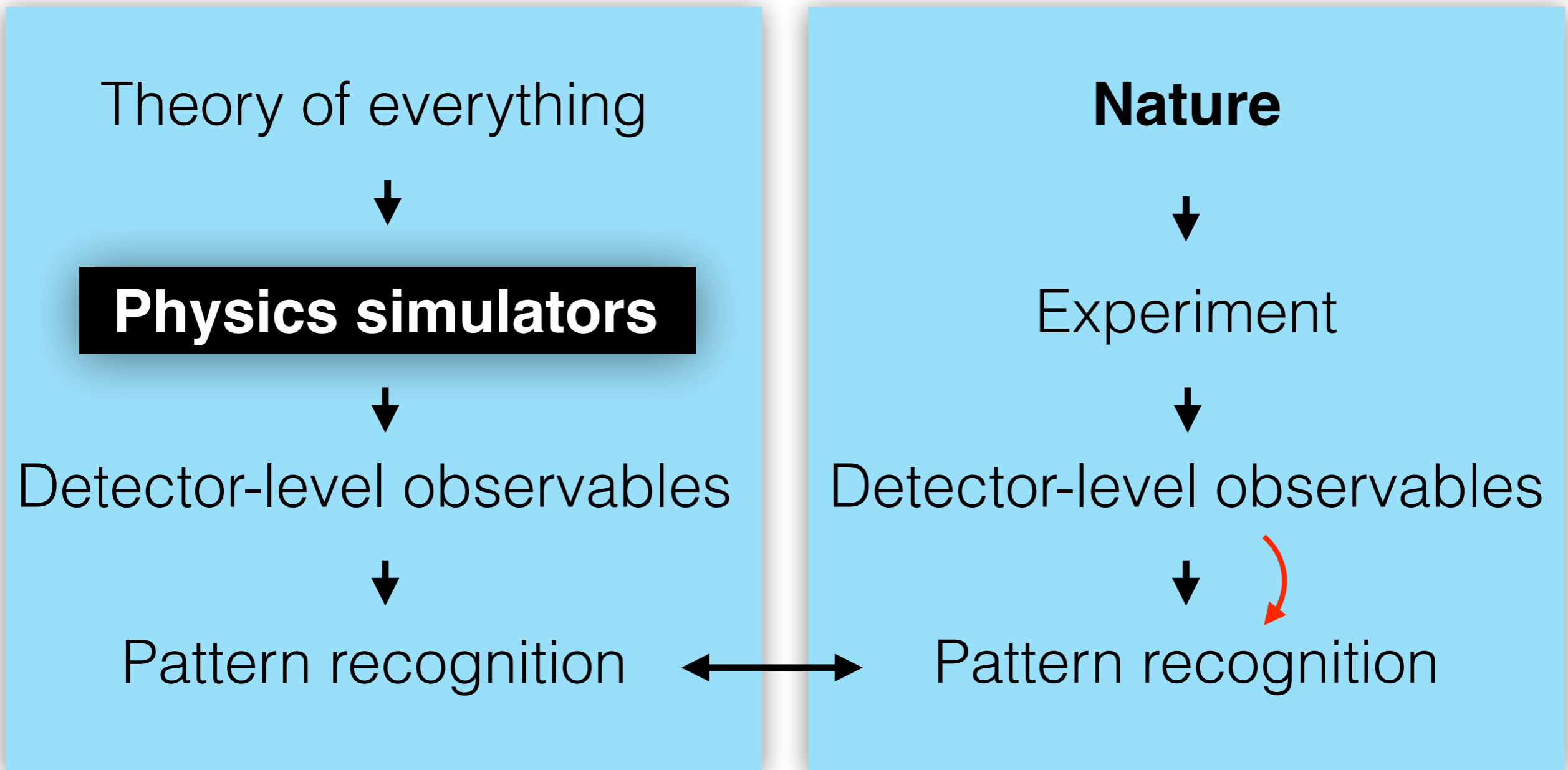
Representing our data



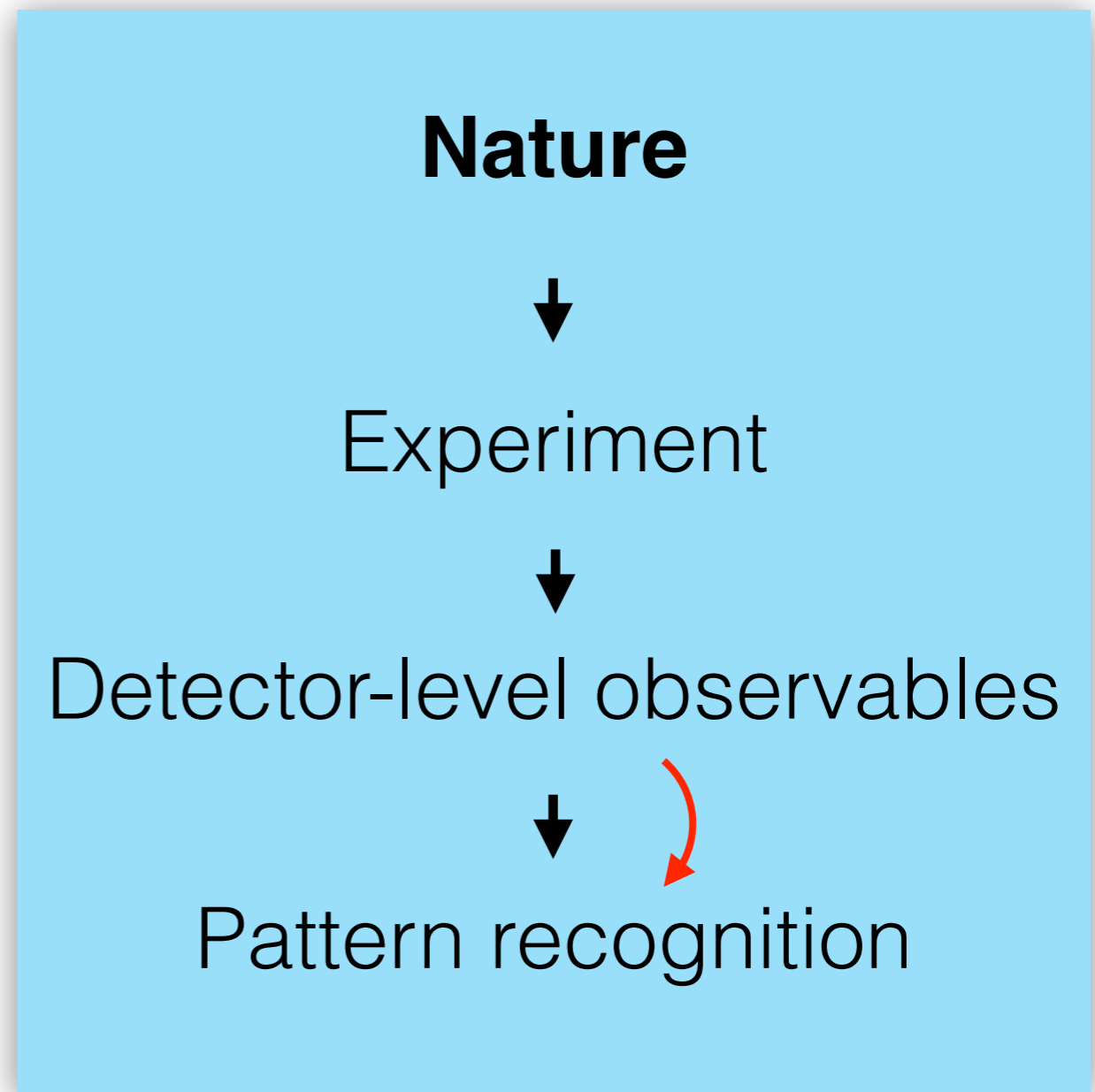
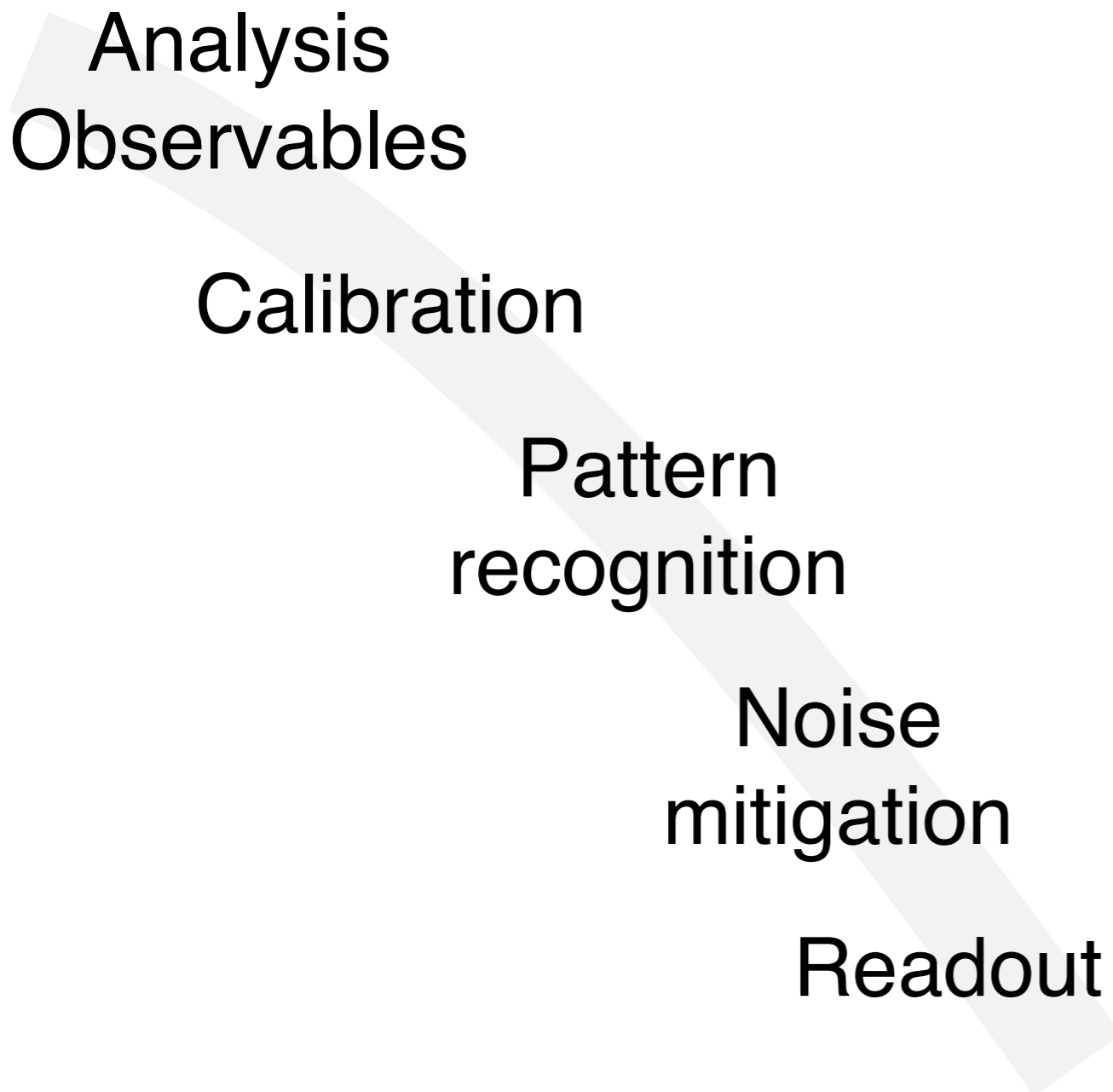


Data analysis in particle physics + ML

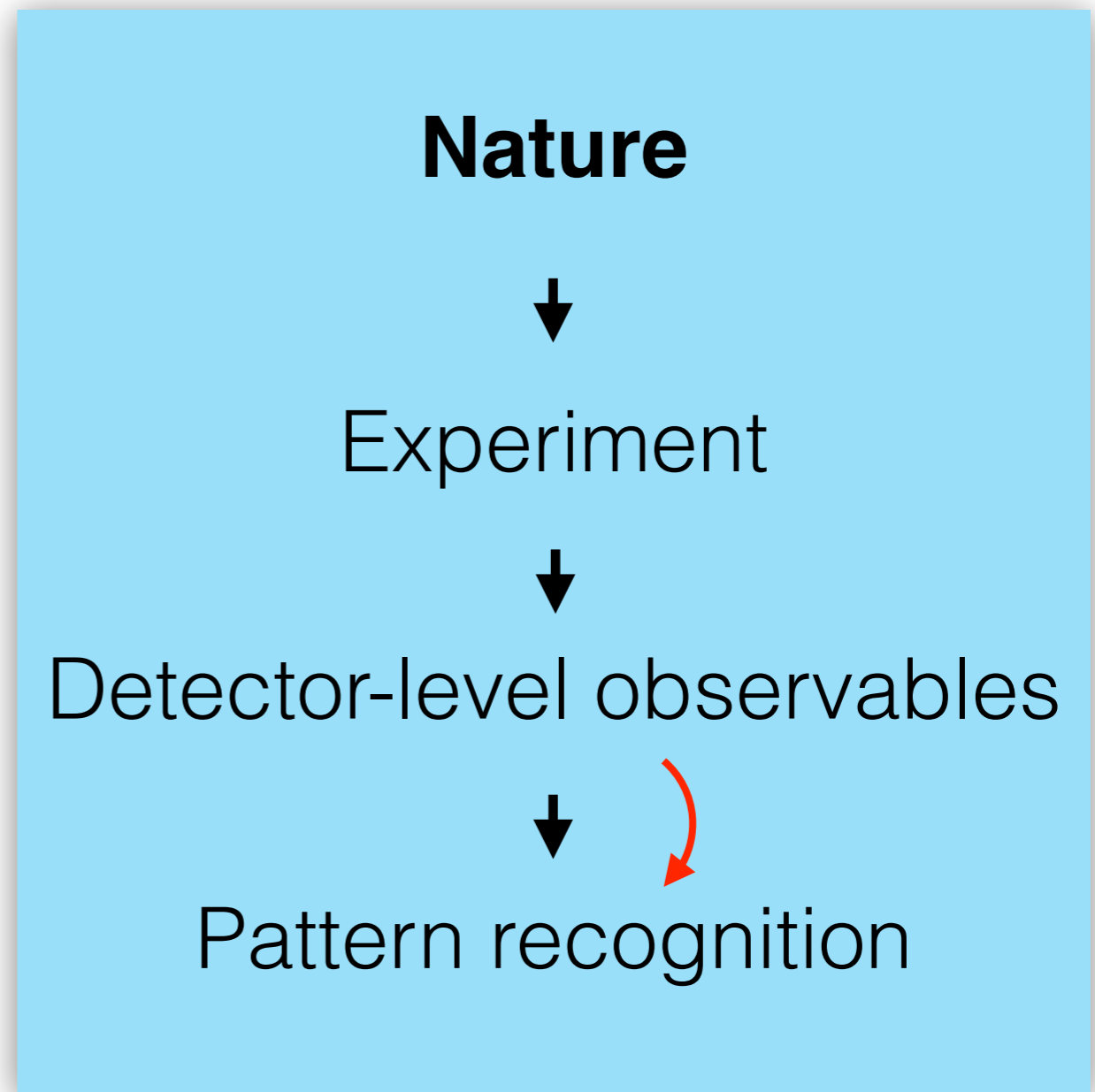
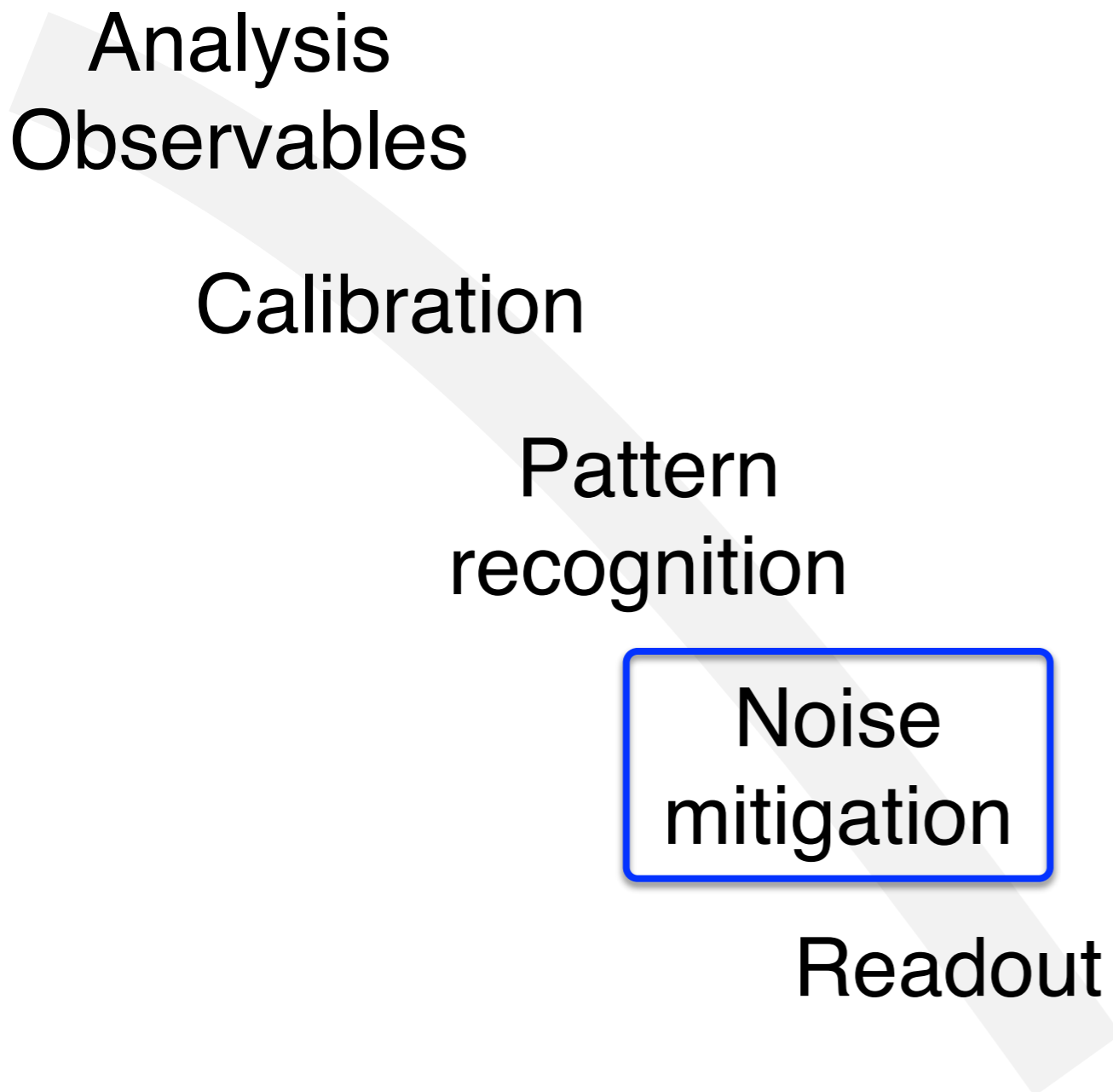




This is where most machine learning is being applied.



This is where most machine learning is being applied.

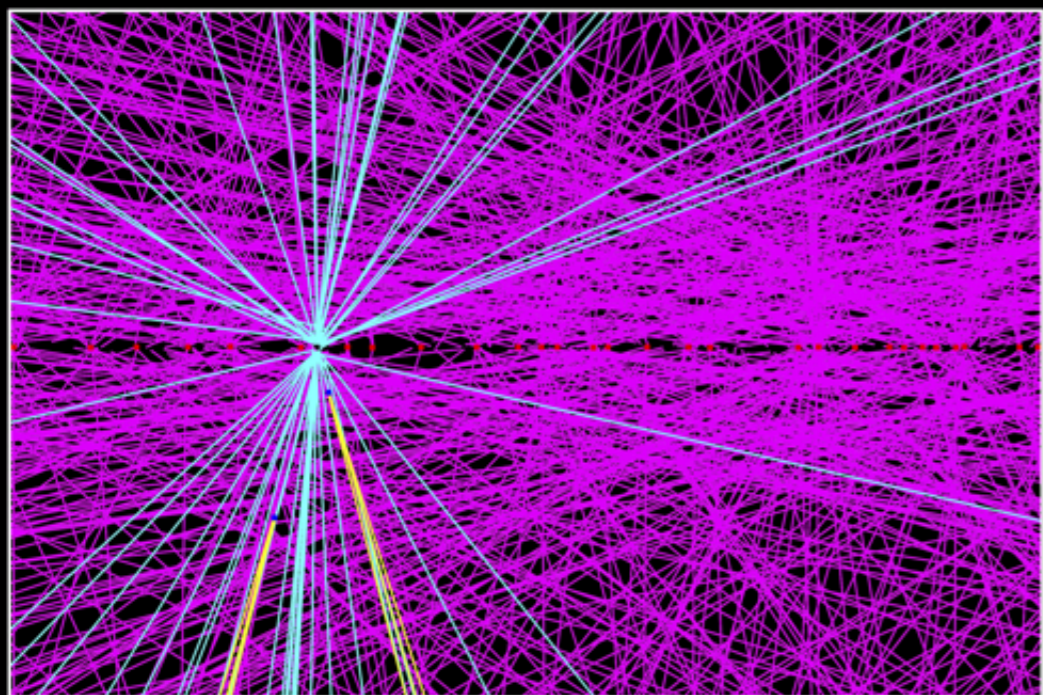
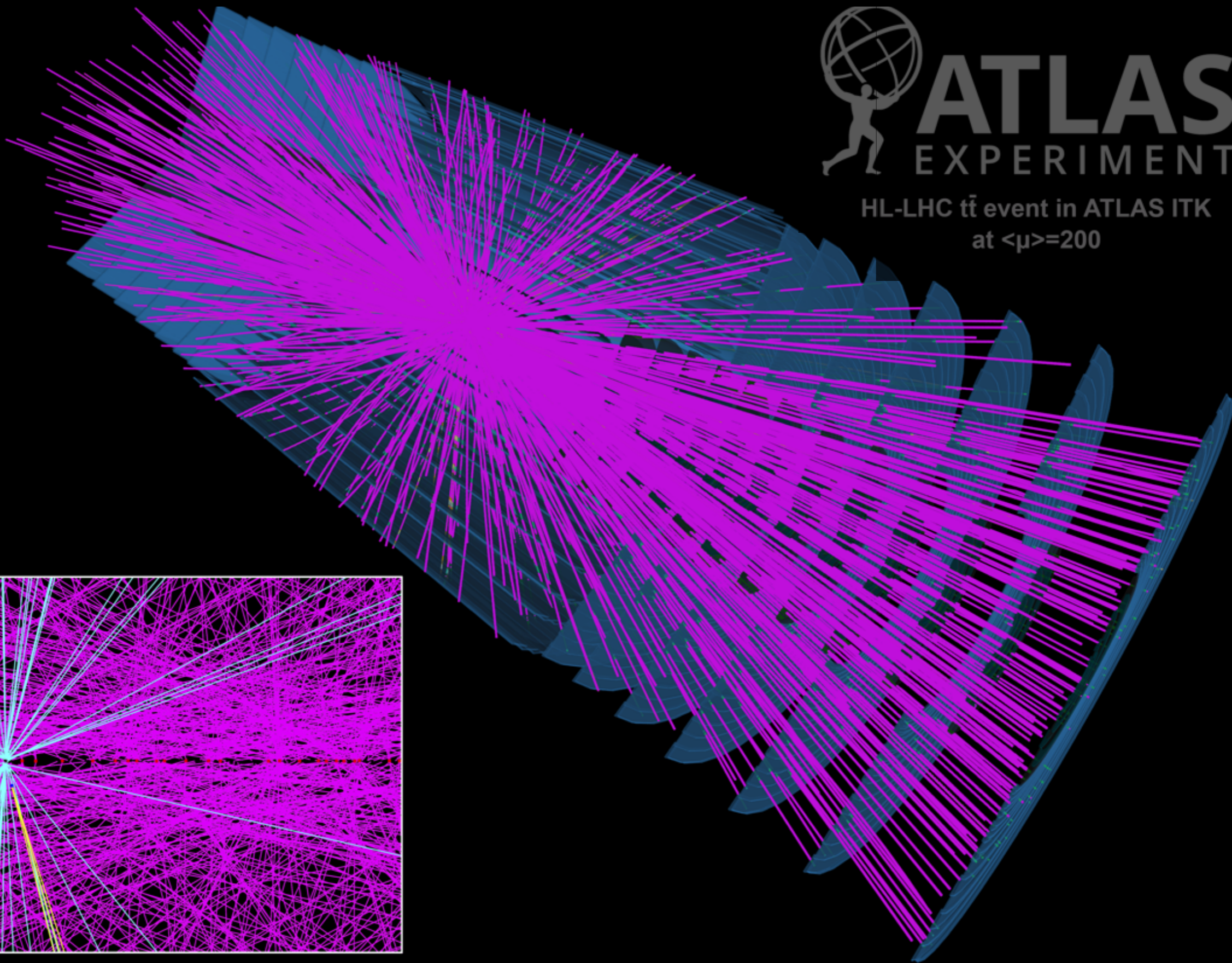


This is where most machine learning is being applied.

Example: Removing Noise

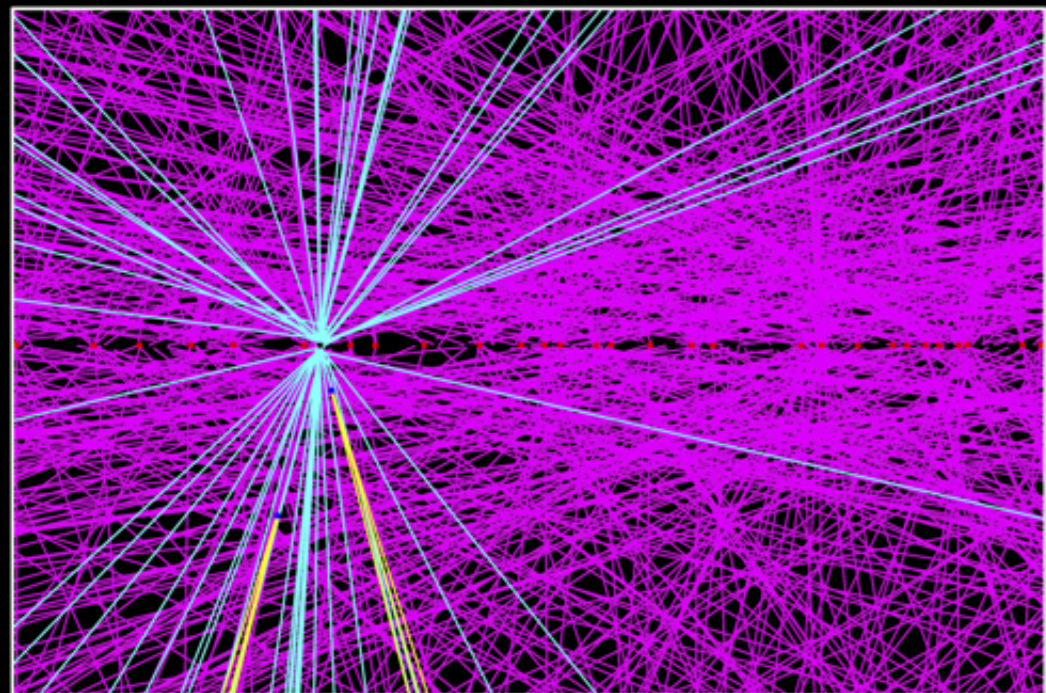


HL-LHC $t\bar{t}$ event in ATLAS ITK
at $\langle\mu\rangle=200$



Example: Removing Noise

pp collisions at the LHC
don't happen one at a time!

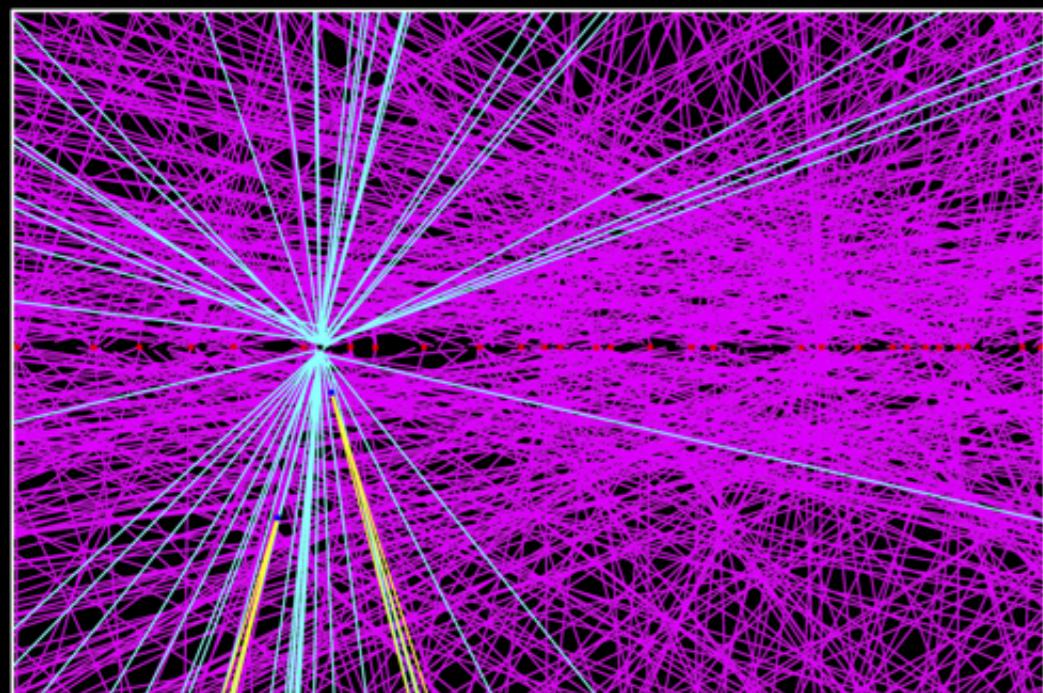


Example: Removing Noise

pp collisions at the LHC
don't happen one at a time!



the extra collisions are called **pileup** and
add soft radiation on top of our events

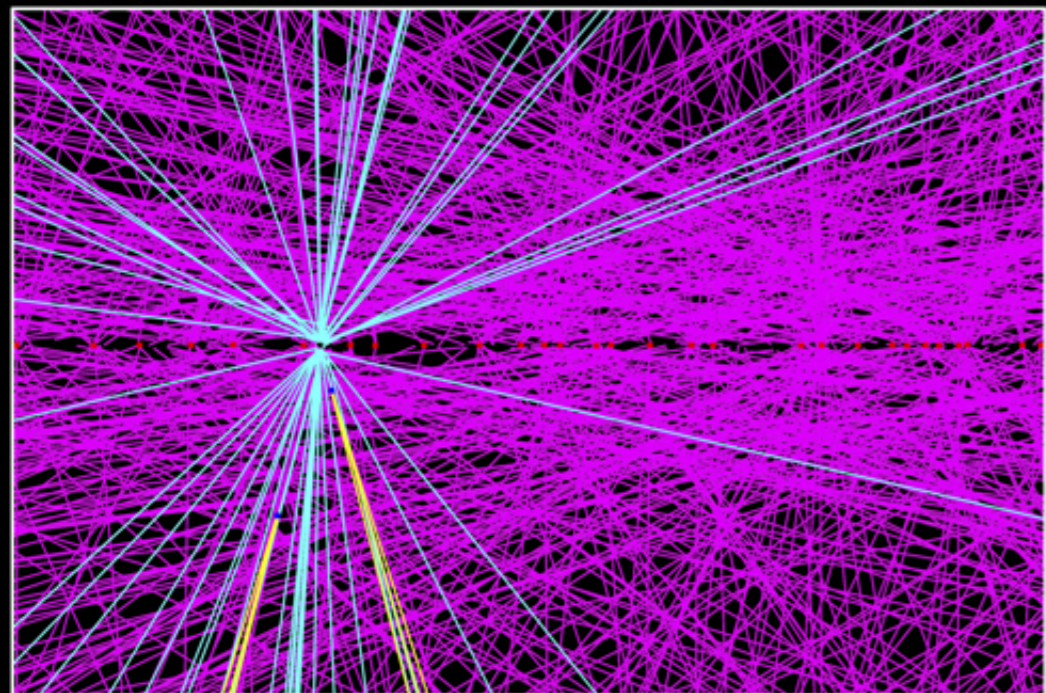


Example: Removing Noise

pp collisions at the LHC
don't happen one at a time!



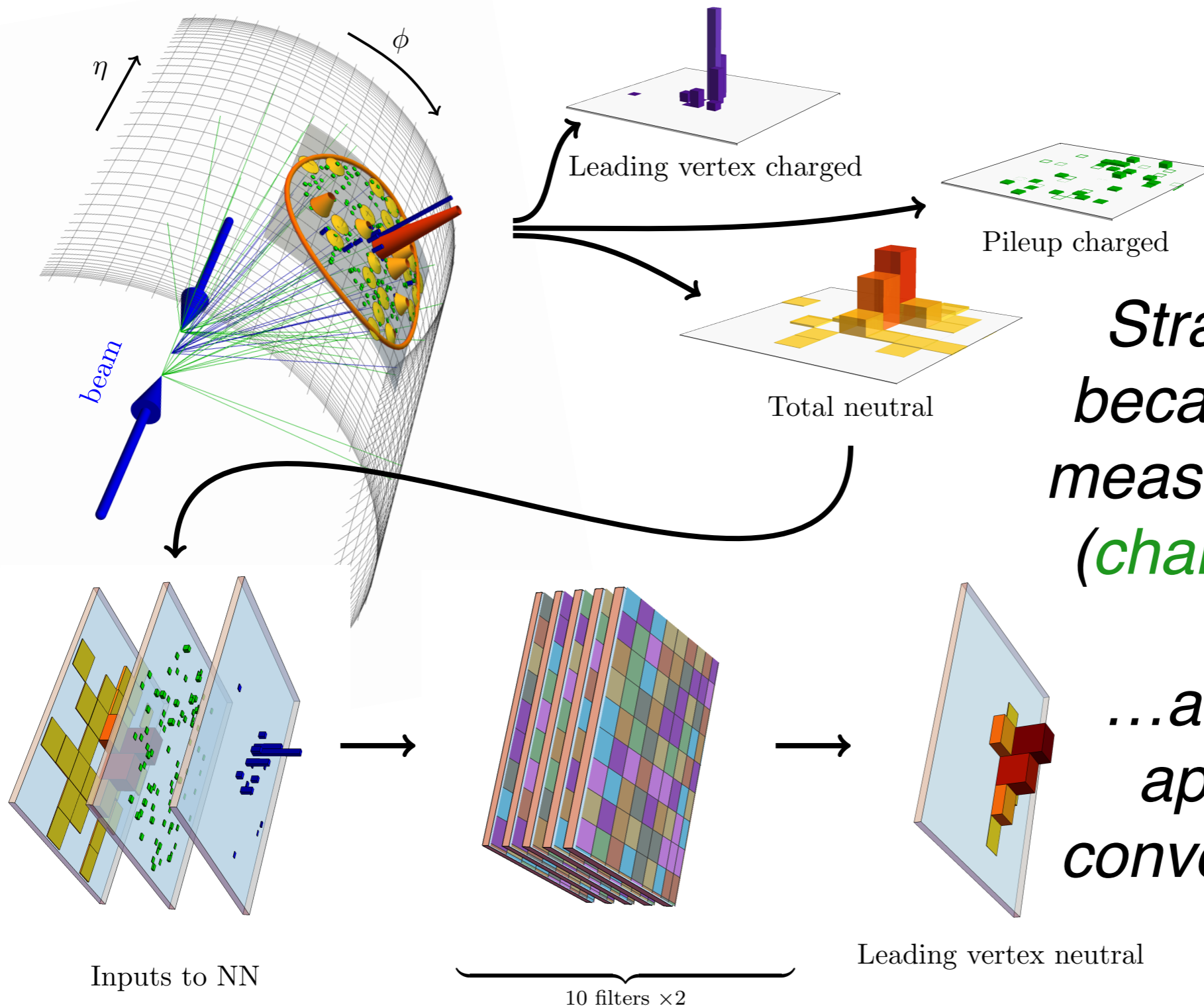
the extra collisions are called **pileup** and
add soft radiation on top of our events



this is akin to image
de-noising - we can
use ML for that!

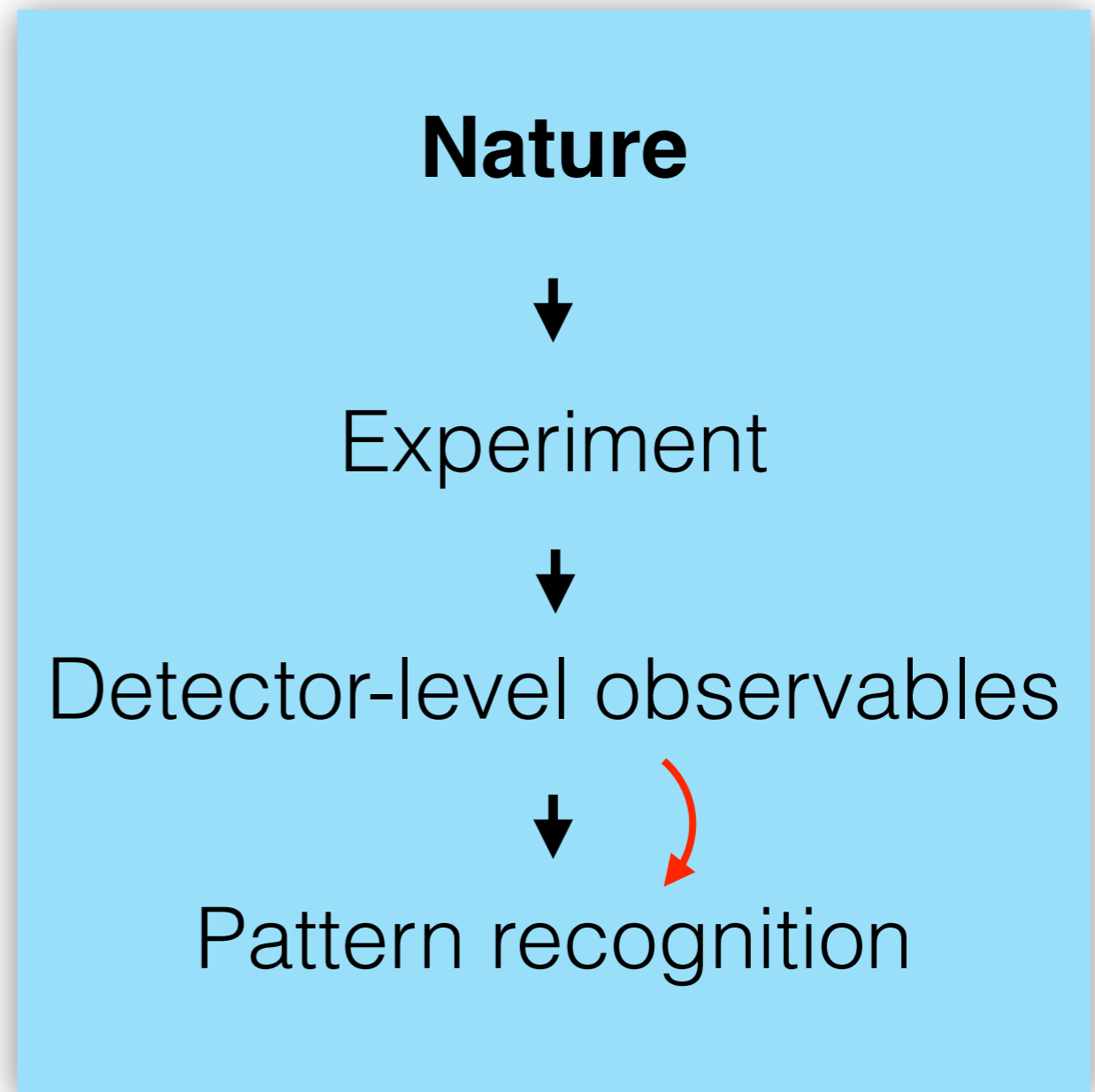
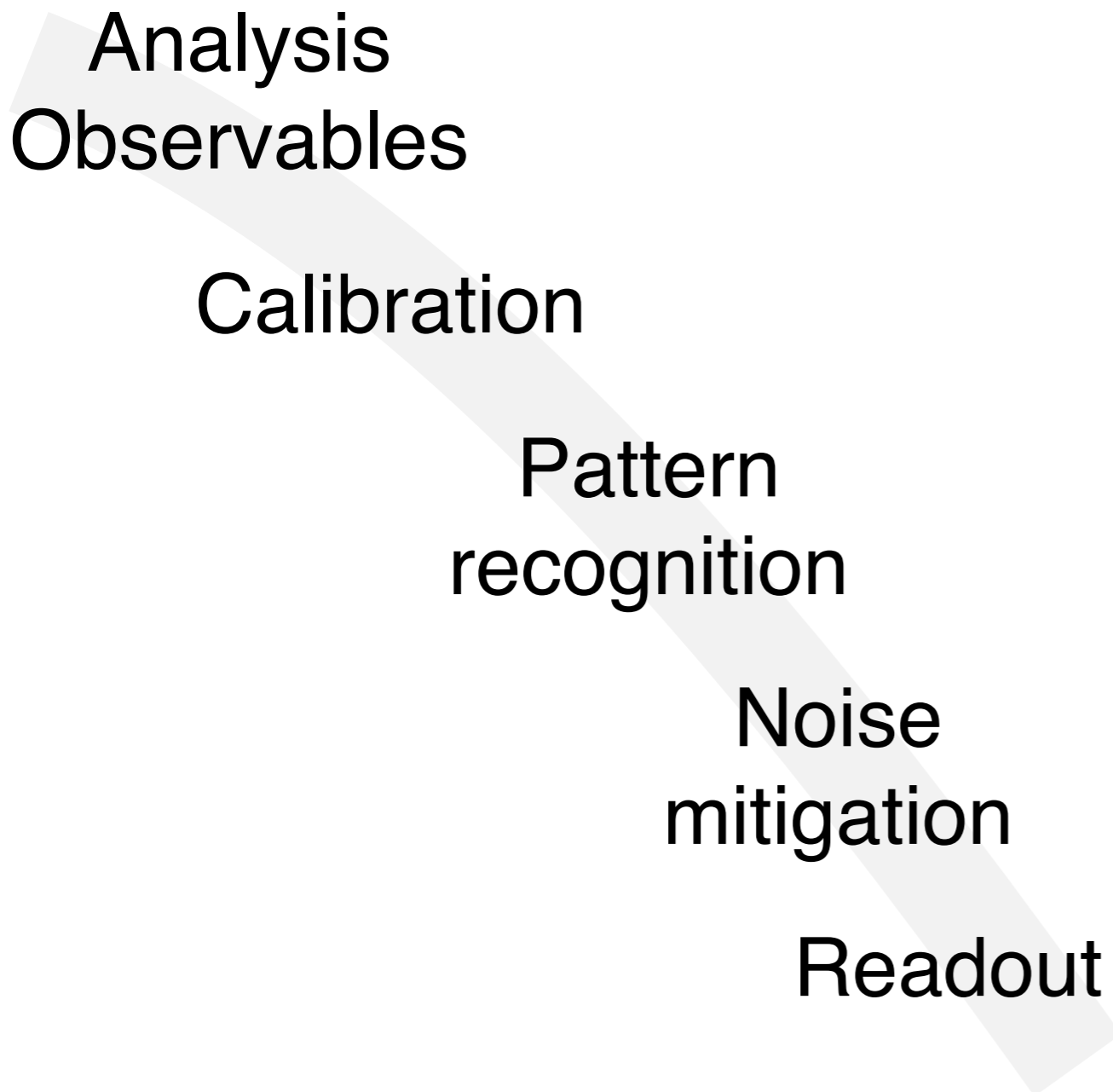
Example: Removing Noise

Image: Journal of High Energy Physics 12 (2017) 51



*Strange noise
because we can
measure $\sim 2/3$ of it
(charged pileup)*

*...also a natural
application of
convolutional NNs!*



This is where most machine learning is being applied.

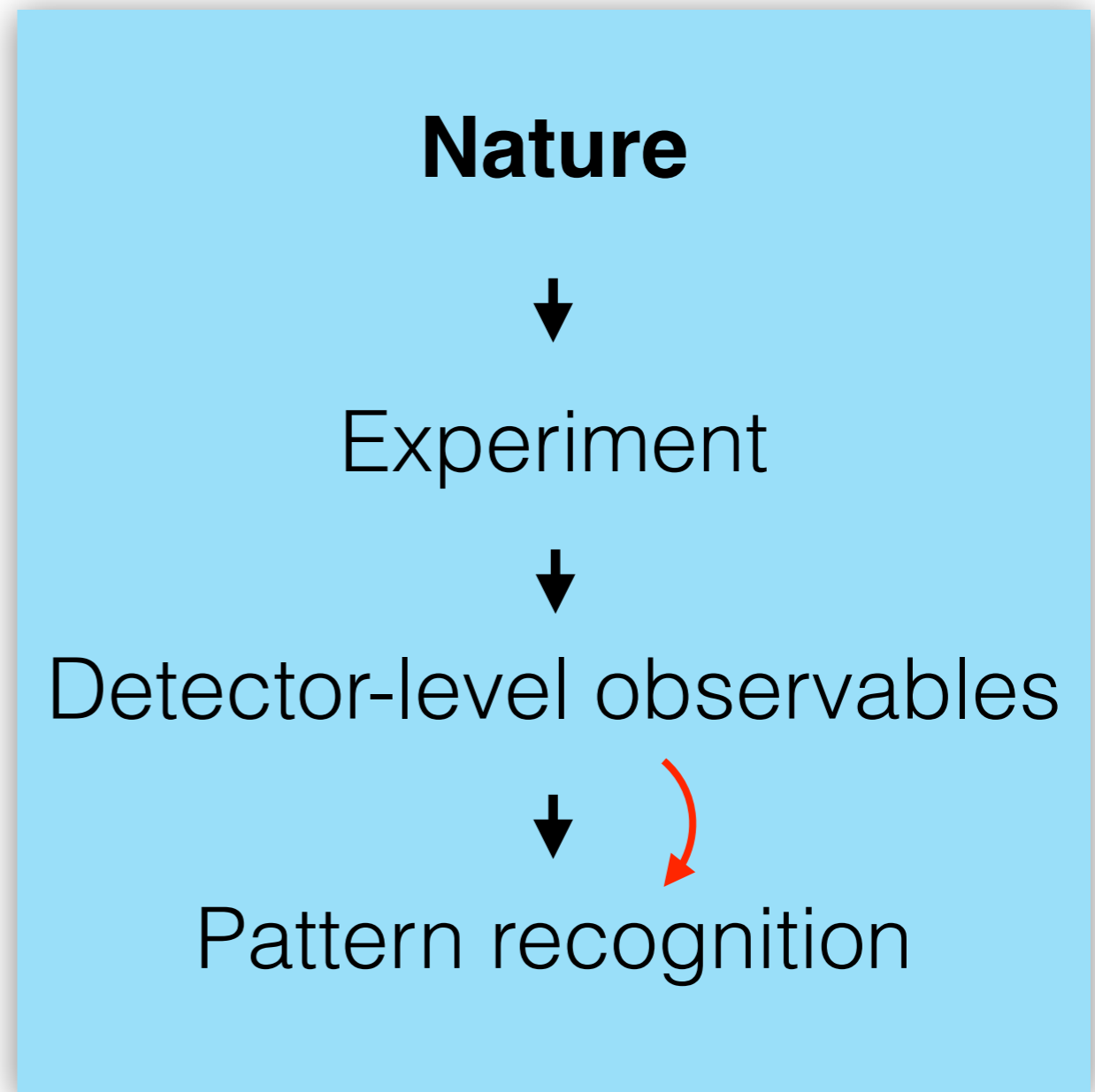
Analysis
Observables

Calibration

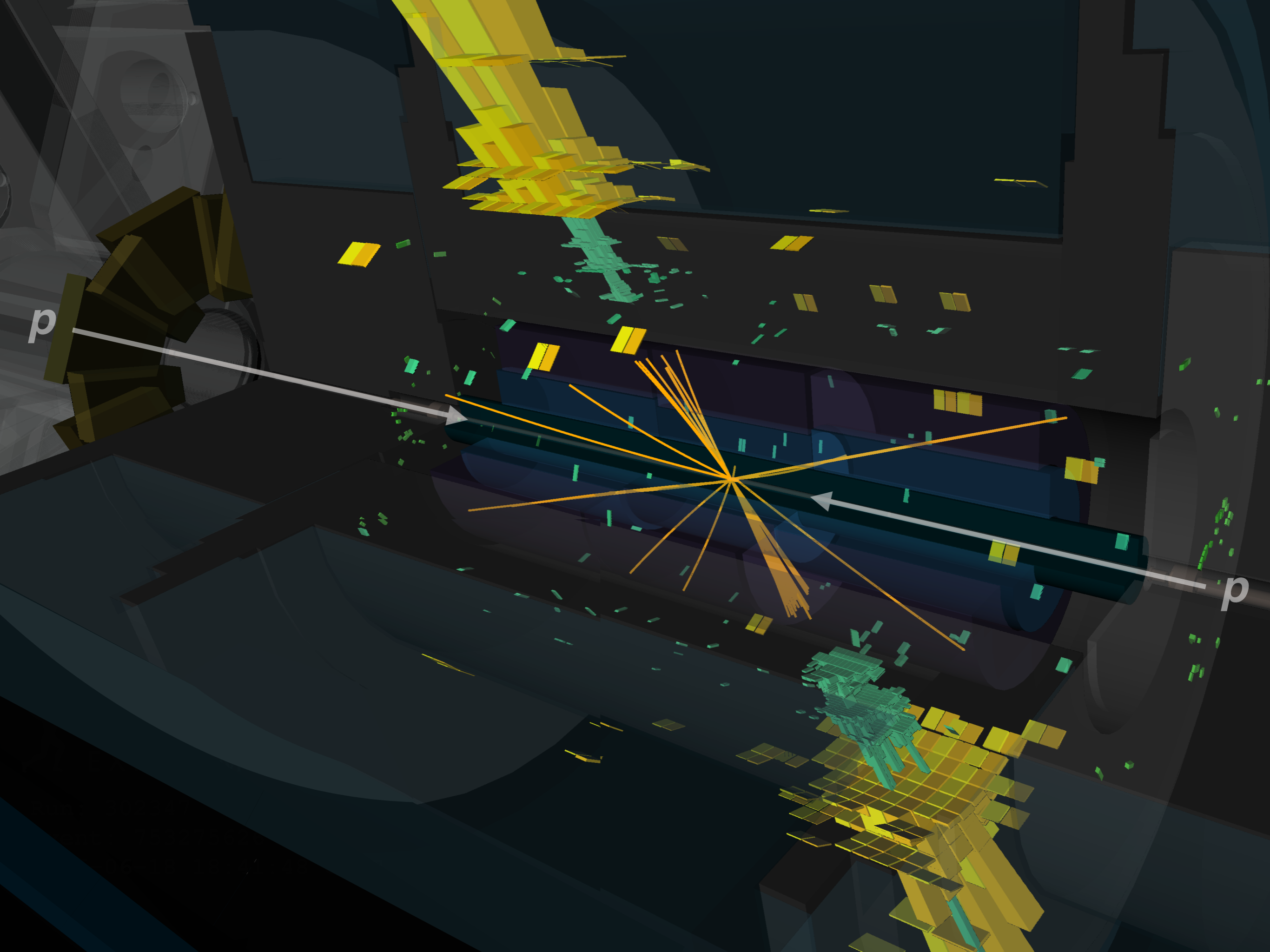
Pattern
recognition

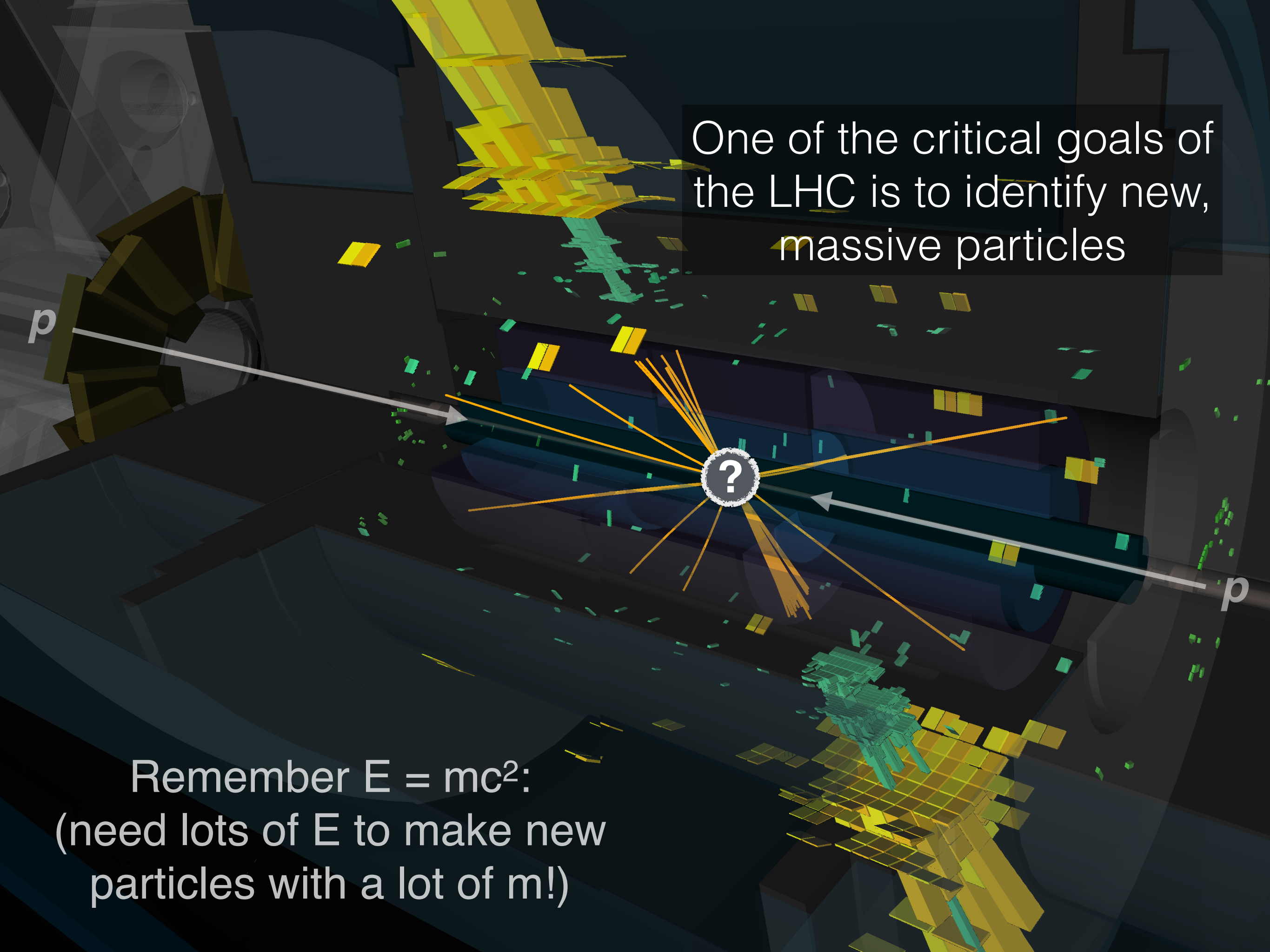
Noise
mitigation

Readout



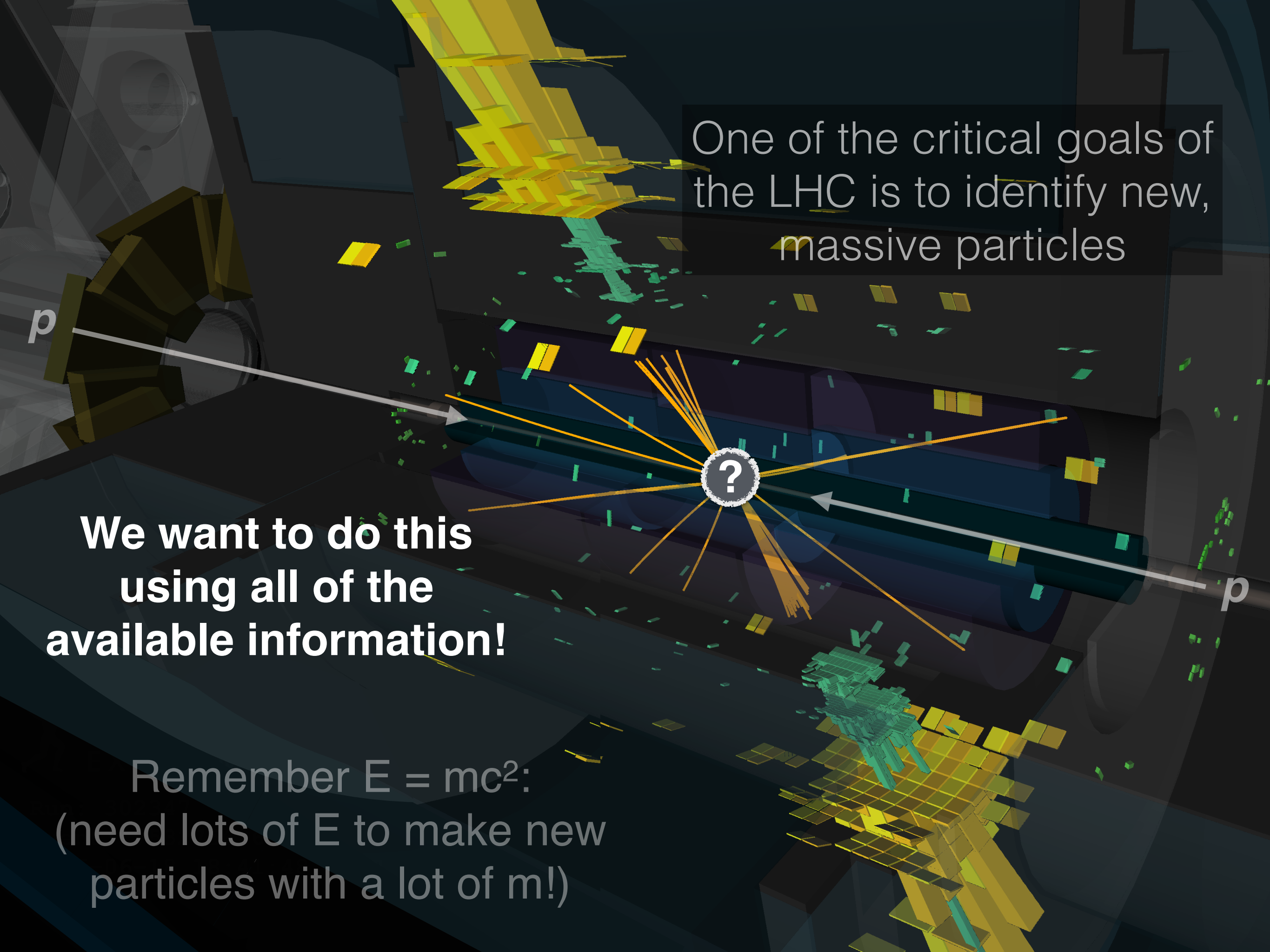
This is where most machine learning is being applied.





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

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



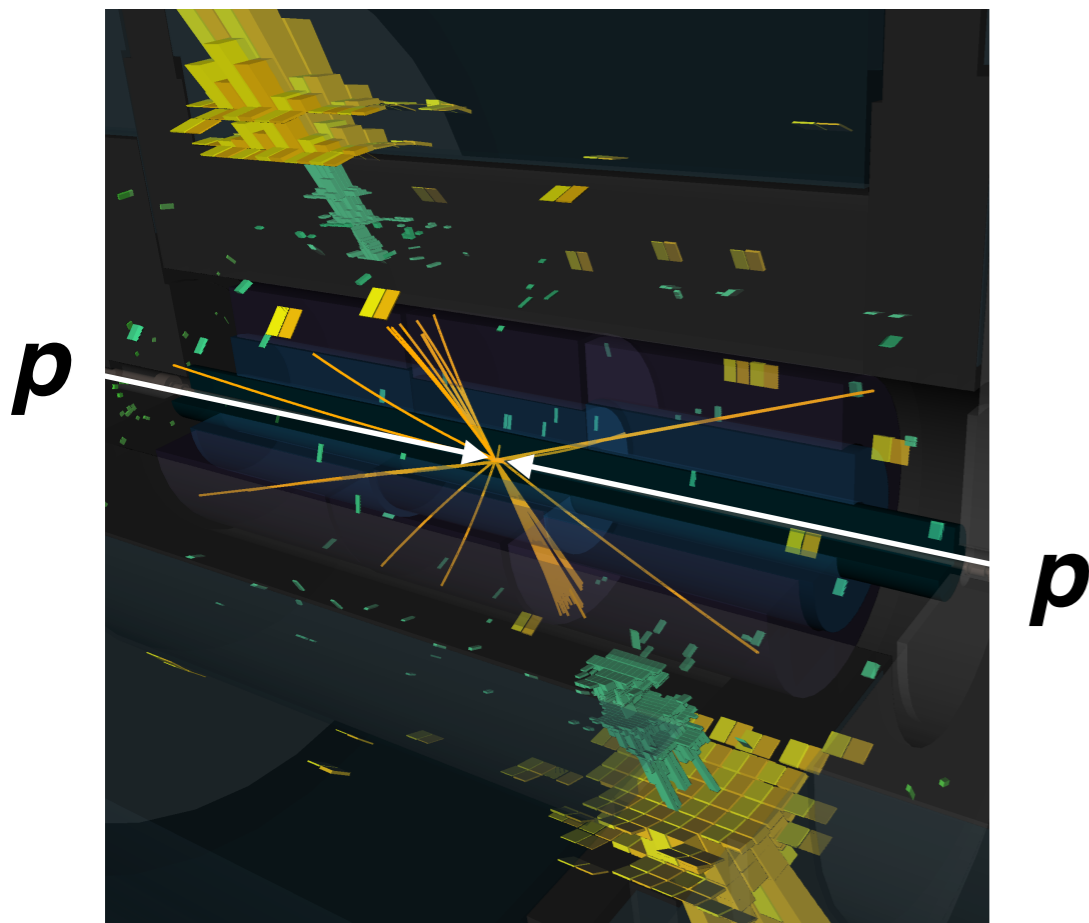
One of the critical goals of the LHC is to identify new, massive particles

We want to do this using all of the available information!

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

Analyzing collider events with ML

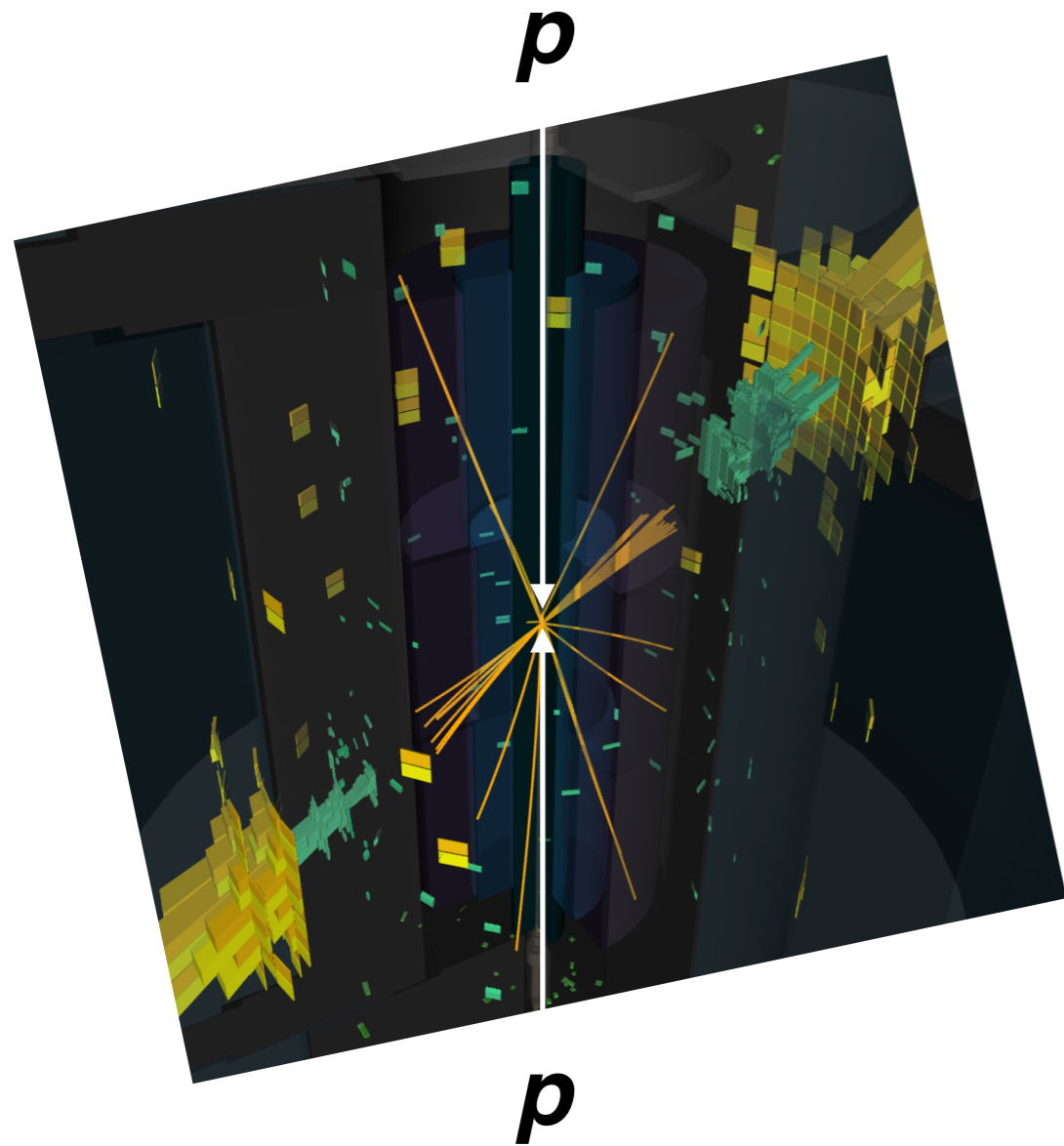
28



Think of an event as an image + convolution neural network
 $O(100) \times O(100)$ pixels = $O(10^4)$ dimensions! (state-of-the-art image processing tool)

Analyzing collider events with ML

29

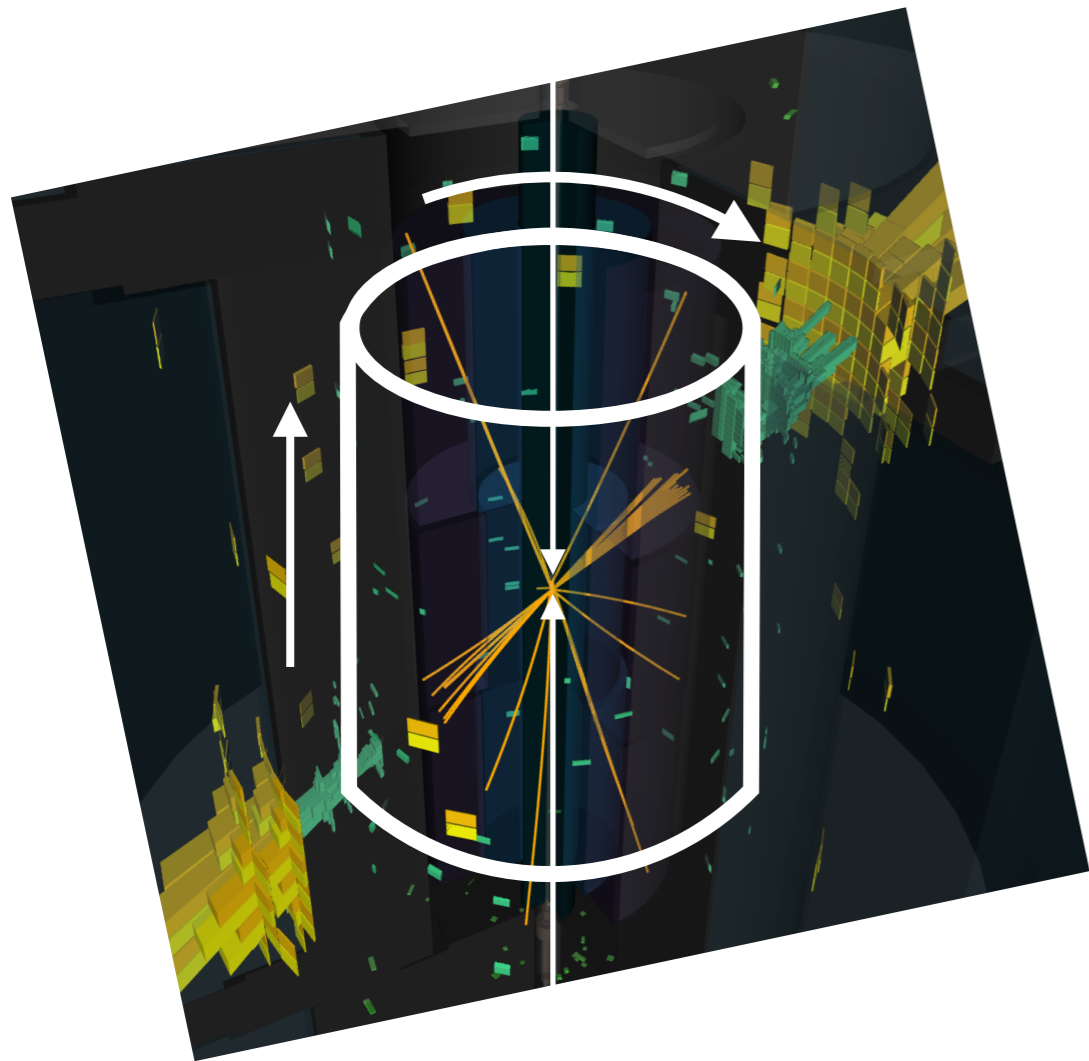


Think of an event as an image + convolution neural network

$O(100) \times O(100)$ pixels = $O(10^4)$ dimensions! (state-of-the-art image processing tool)

Analyzing collider events with ML

30

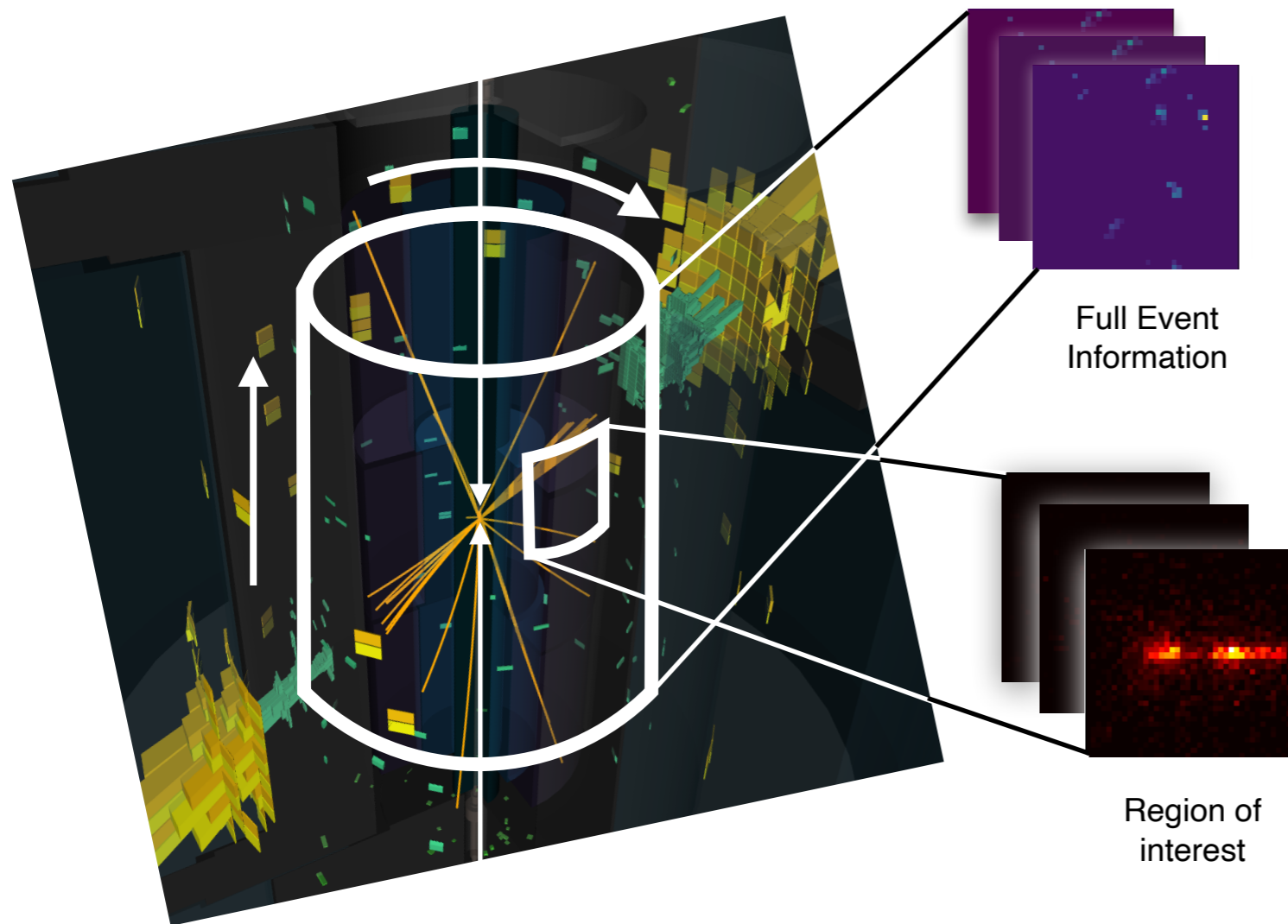


Think of an event as an image + convolution neural network

$O(100) \times O(100)$ pixels = $O(10^4)$ dimensions! (state-of-the-art image processing tool)

Analyzing collider events with ML

31

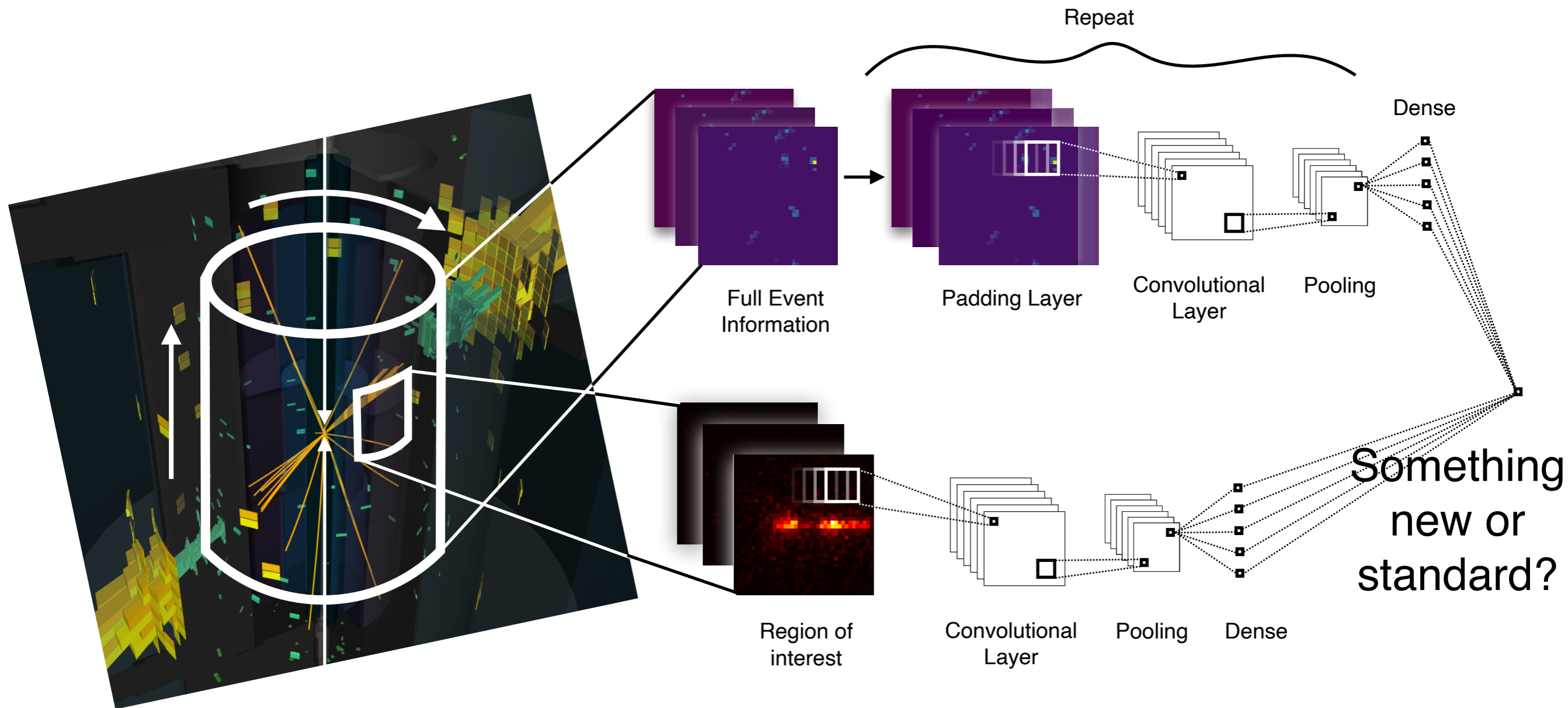


Think of an event as an image + convolution neural network

$O(100) \times O(100)$ pixels = $O(10^4)$ dimensions! (state-of-the-art image processing tool)

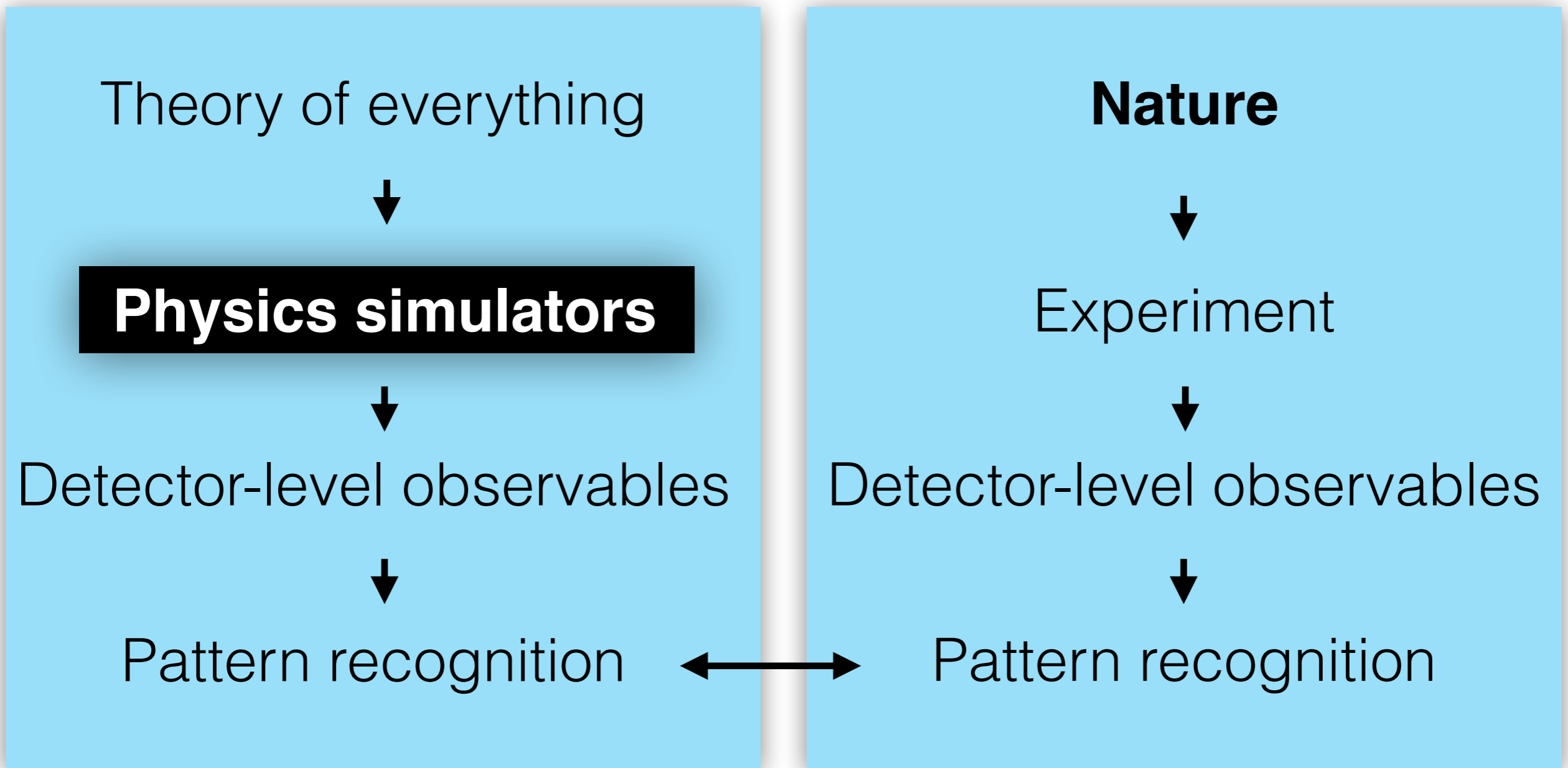
Analyzing collider events with ML

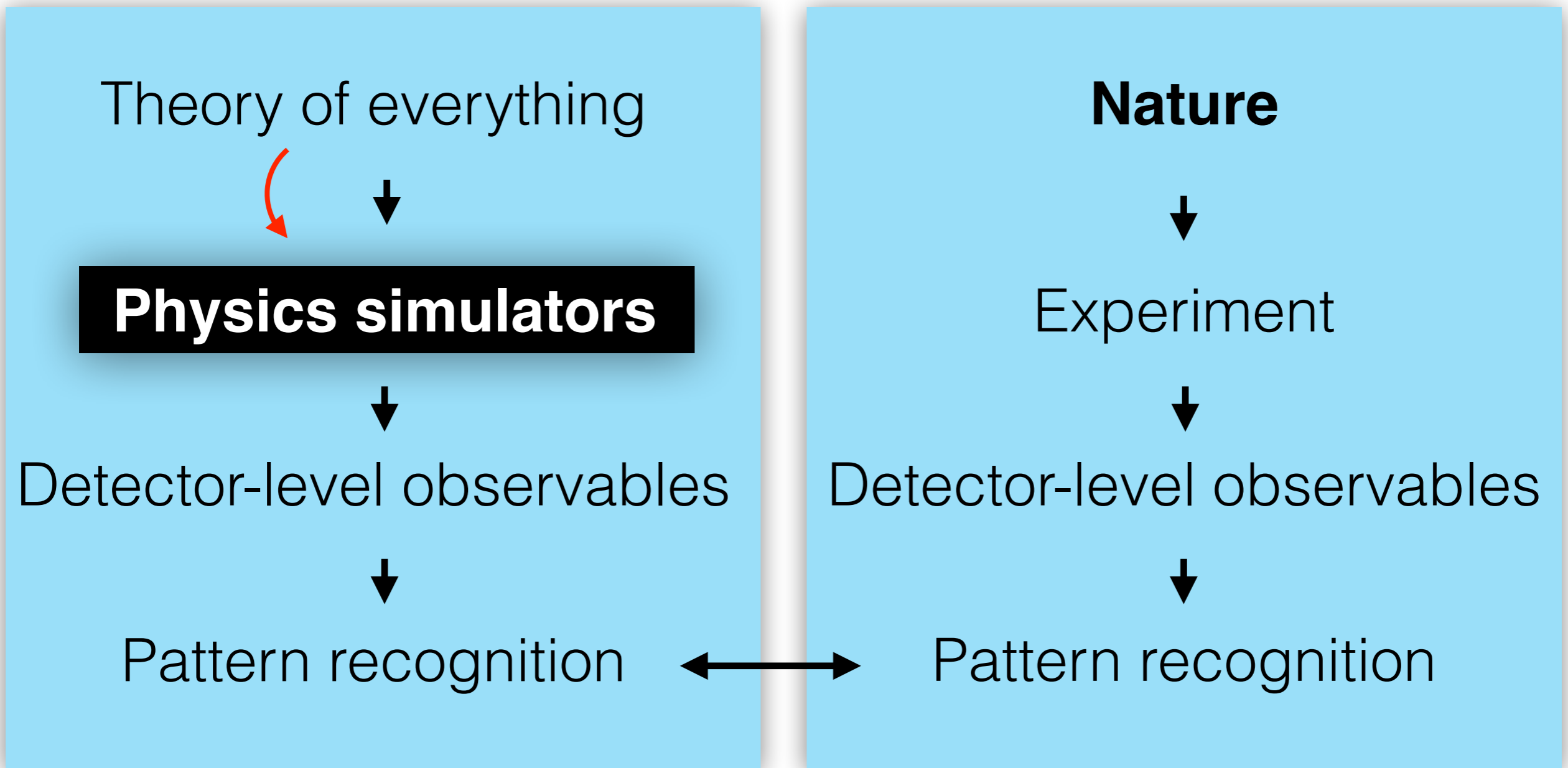
Image: Journal of High Energy Physics 10 (2018) 101



Think of an event as an image + convolution neural network

$O(100) \times O(100)$ pixels = $O(10^4)$ dimensions! (state-of-the-art image processing tool)

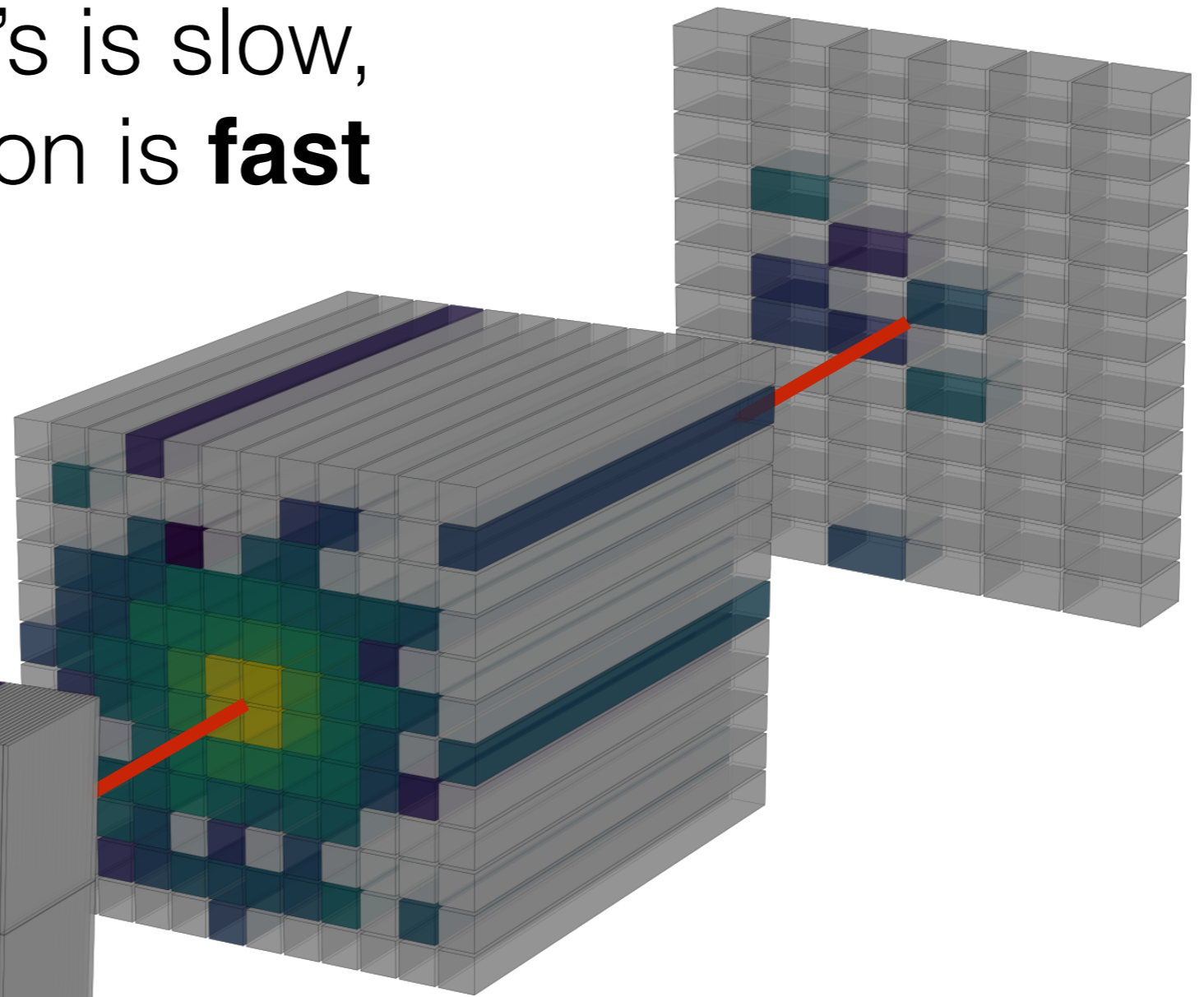
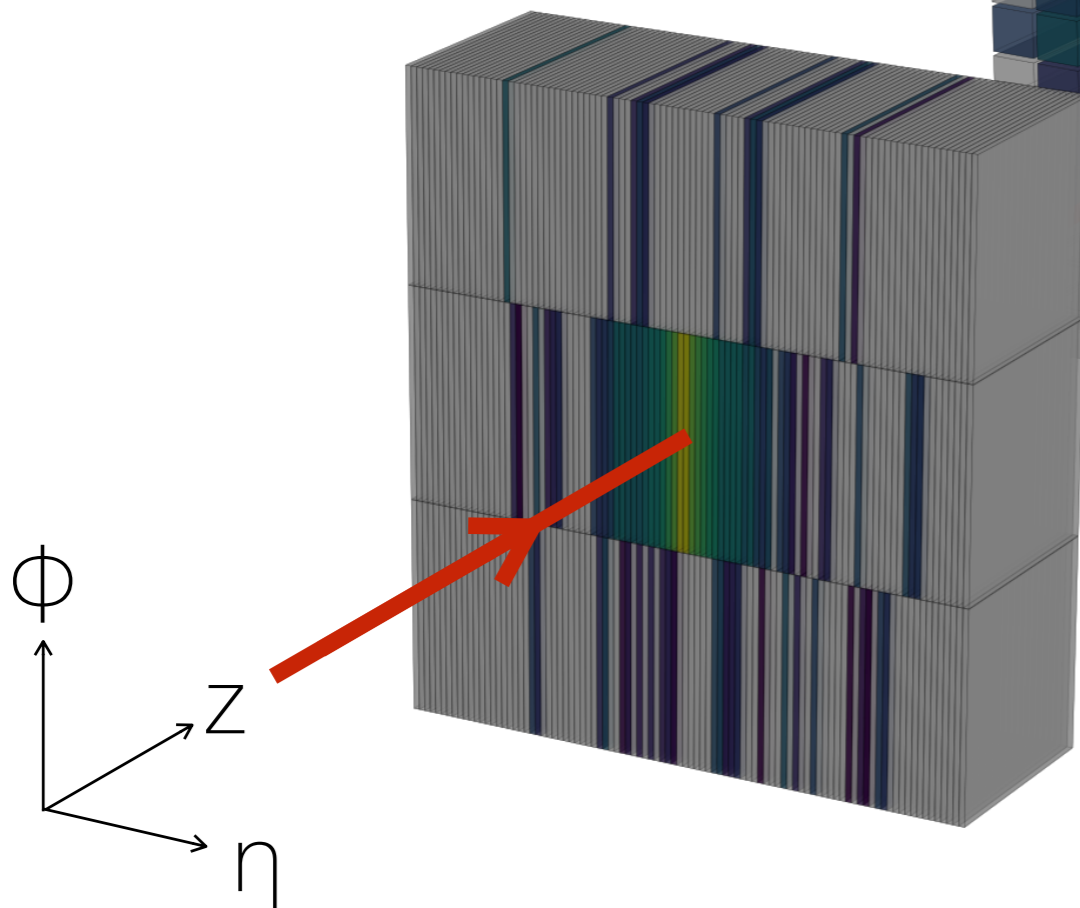




A growing toolkit called “generative models” are being developed to accelerate or augment simulations.

Training NN's is slow,
but evaluation is **fast**

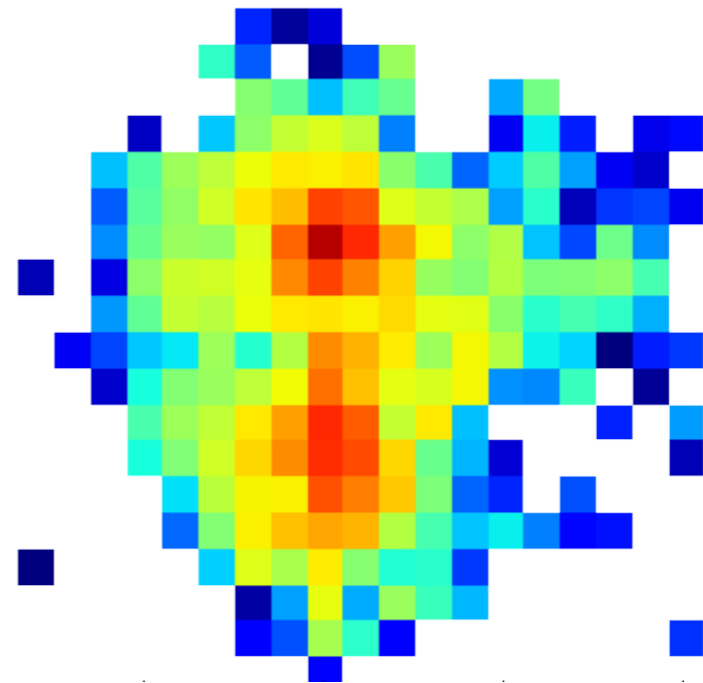
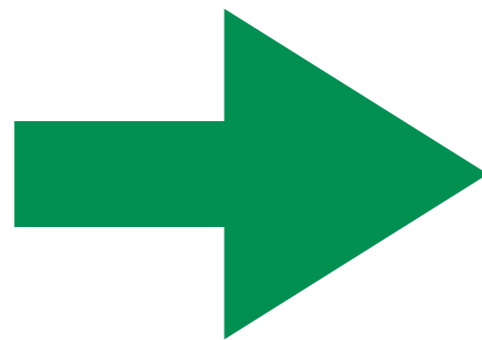
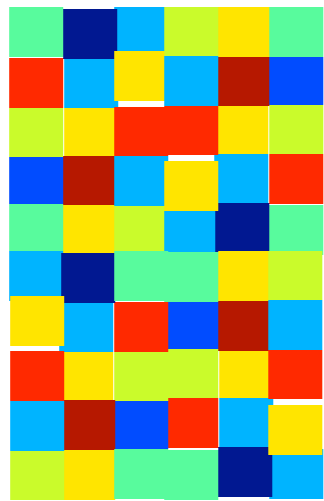
Physics-based
simulations are
often **slow**



What if we can learn to
simulate with a NN?

Can we combine our physics-simulator with deep learning?

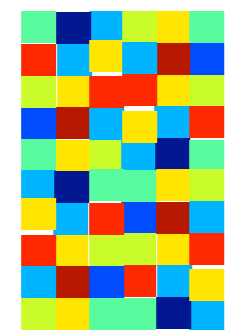
A **generator** is nothing other than a function that maps random numbers to structure.



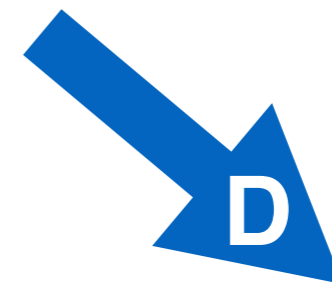
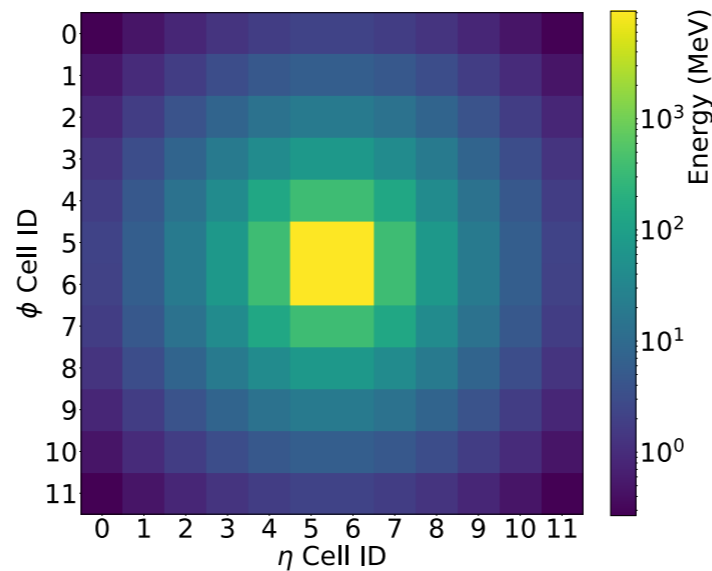
A deep learning solution: GANs

37

Generative Adversarial Networks (GAN):
*A two-network game where one **maps noise to images** and one **classifies images as fake or real**.*

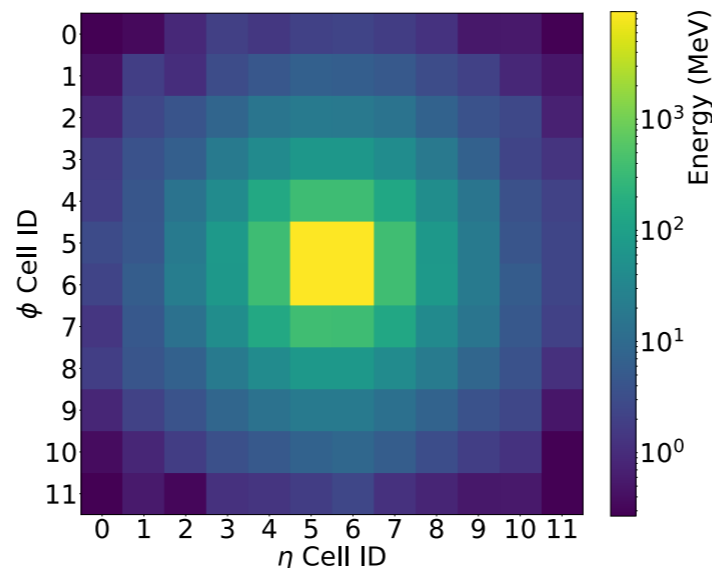


noise

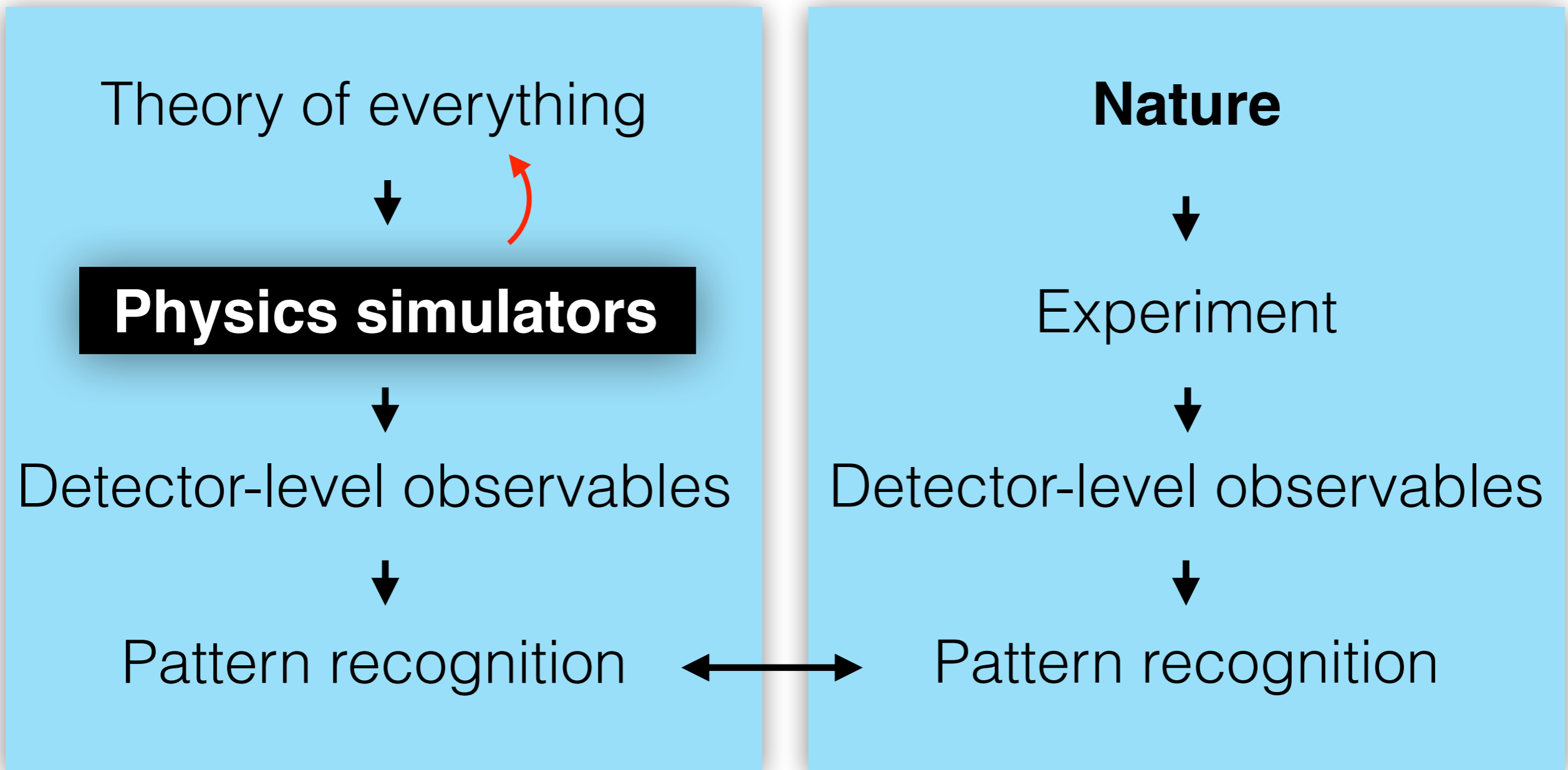


{real, fake}

When **D** is maximally confused, **G** will be a good generator



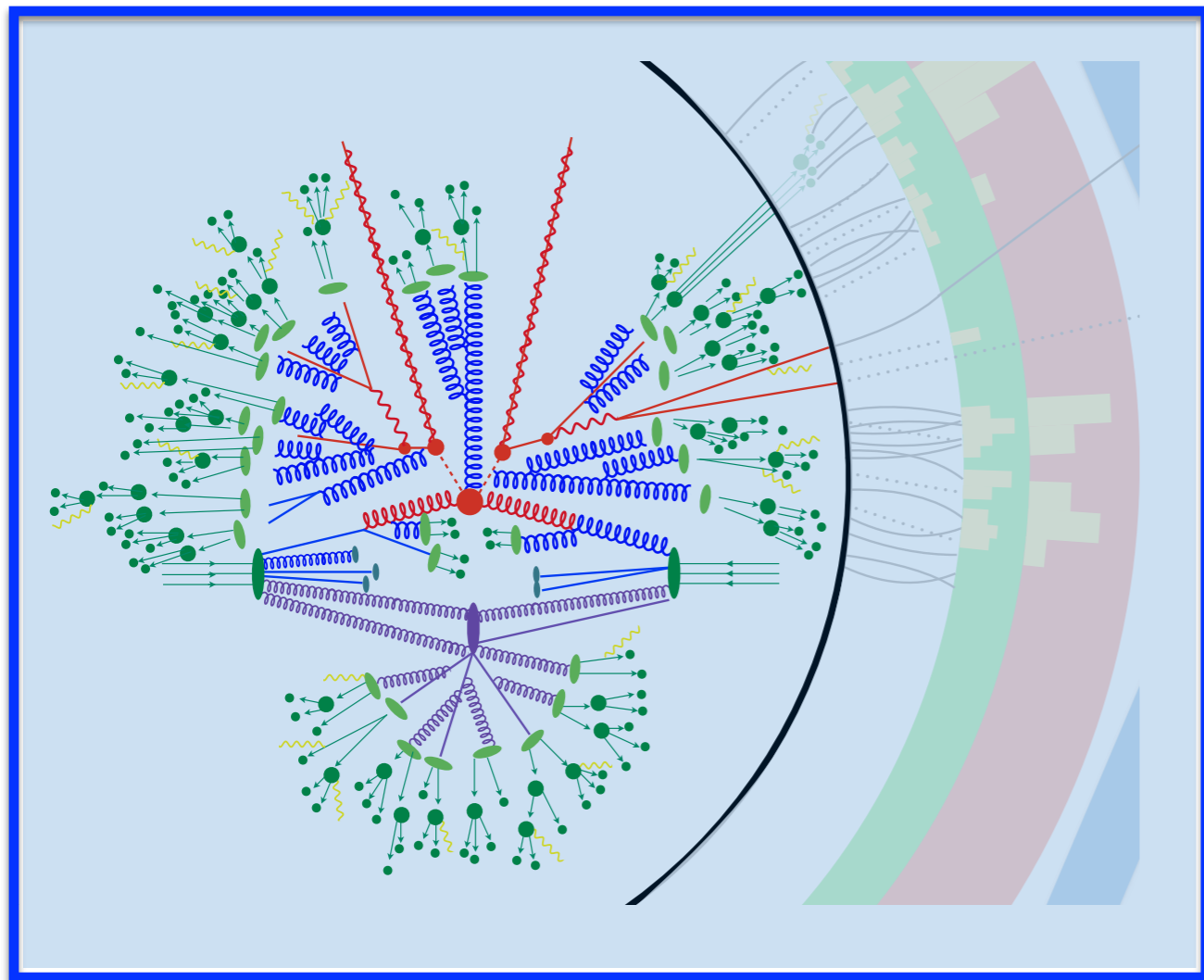
Physics-based simulator



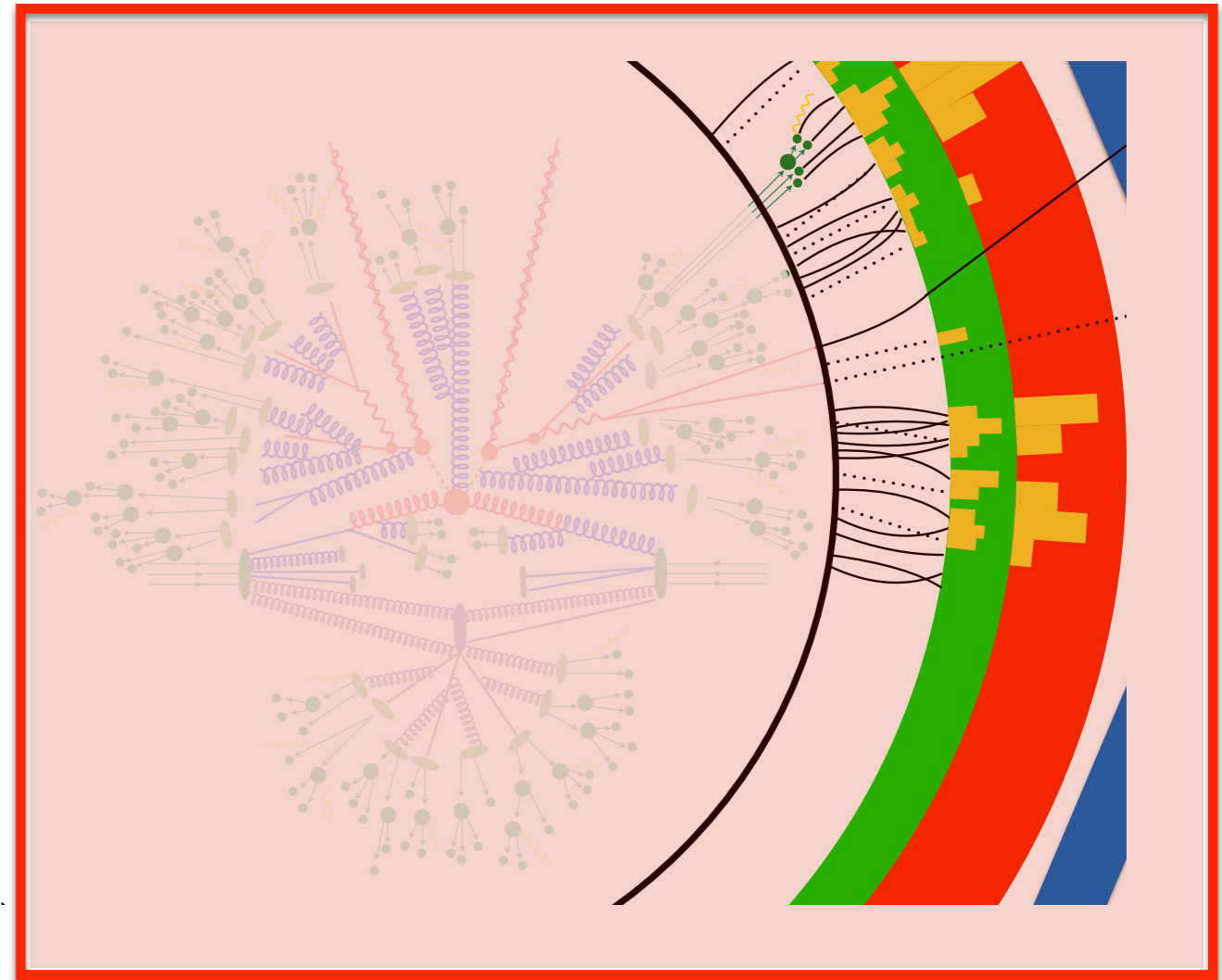
Simulators are a unique and powerful aspect of particle physics, but, they do not allow us to go “backwards” !!

The Inference Challenge

Want this



Measure this

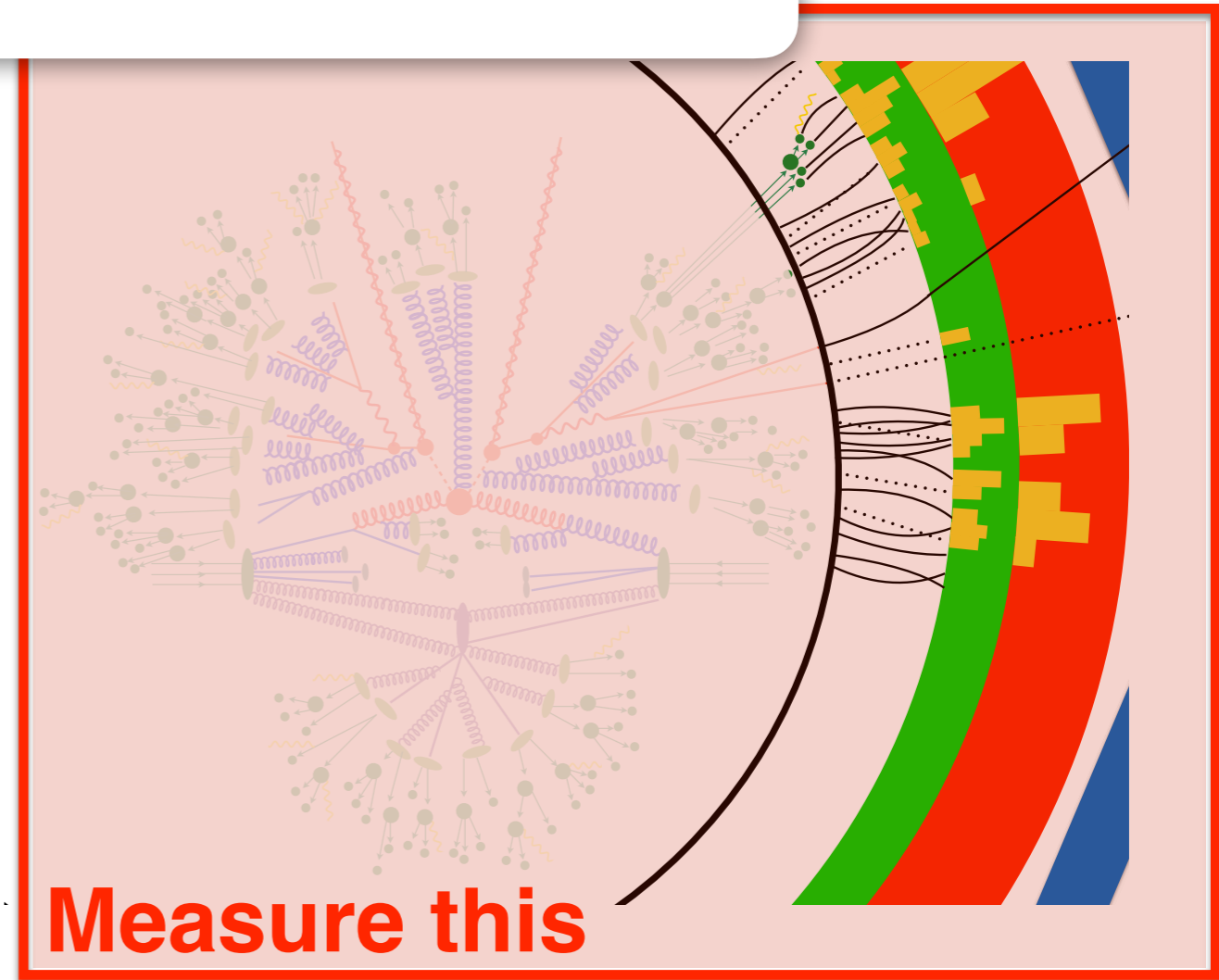
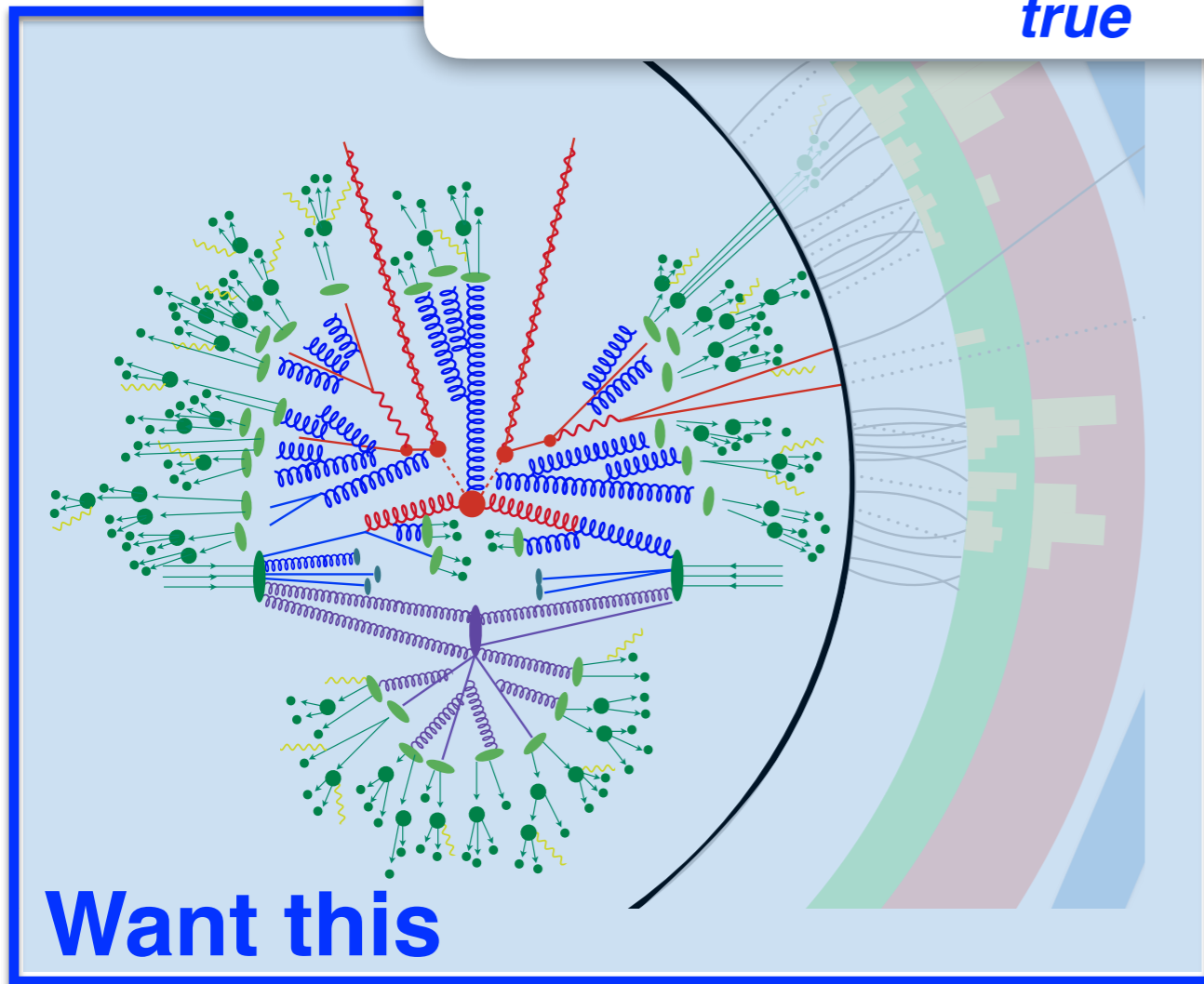


The Inference Challenge

40

If you know $p(\textit{meas.} / \textit{true})$, could do maximum likelihood, i.e.

$$\textit{unfolded} = \underset{\textit{true}}{\operatorname{argmax}} p(\textit{measured} / \textit{true})$$



The Inference Challenge

41

If you know $p(\mathit{meas.} \mid \mathit{true})$, could do maximum likelihood, i.e.

$$\mathit{unfolded} = \underset{\mathit{true}}{\operatorname{argmax}} p(\mathit{measured} \mid \mathit{true})$$



Challenge: **measured** is hyperspectral and **true** is hypervariate ... $p(\mathit{meas.} \mid \mathit{true})$ is **intractable** !

The Inference Challenge

42

If you know $p(\textit{meas.} \mid \textit{true})$, could do maximum likelihood, i.e.

$$\textit{unfolded} = \underset{\textit{true}}{\operatorname{argmax}} p(\textit{measured} \mid \textit{true})$$



Challenge: **measured** is hyperspectral and **true** is hypervariate ... $p(\textit{meas.} \mid \textit{true})$ is **intractable** !

However: we have **simulators** that we can use to sample from $p(\textit{meas.} \mid \textit{true})$

→ **Simulation-based (likelihood-free) inference** !

...an area of machine learning where particle physics is making a key contribution!

I'll briefly show you one solution to give you a sense of the power of likelihood-free inference.

I'll briefly show you one solution to give you a sense of the power of likelihood-free inference.

The solution will be built on ***reweighting***

dataset 1: sampled from $p(x)$

dataset 2: sampled from $q(x)$

Create weights $w(x) = q(x)/p(x)$ so that when dataset 1 is weighted by w , it is statistically identical to dataset 2.

I'll briefly show you one solution to give you a sense of the power of likelihood-free inference.

The solution will be built on ***reweighting***

dataset 1: sampled from $p(x)$

dataset 2: sampled from $q(x)$

Create weights $w(x) = q(x)/p(x)$ so that when dataset 1 is weighted by w , it is statistically identical to dataset 2.

What if we don't (and can't easily) know q and p ?

Fact: Neural networks learn to approximate the likelihood ratio = $q(x)/p(x)$

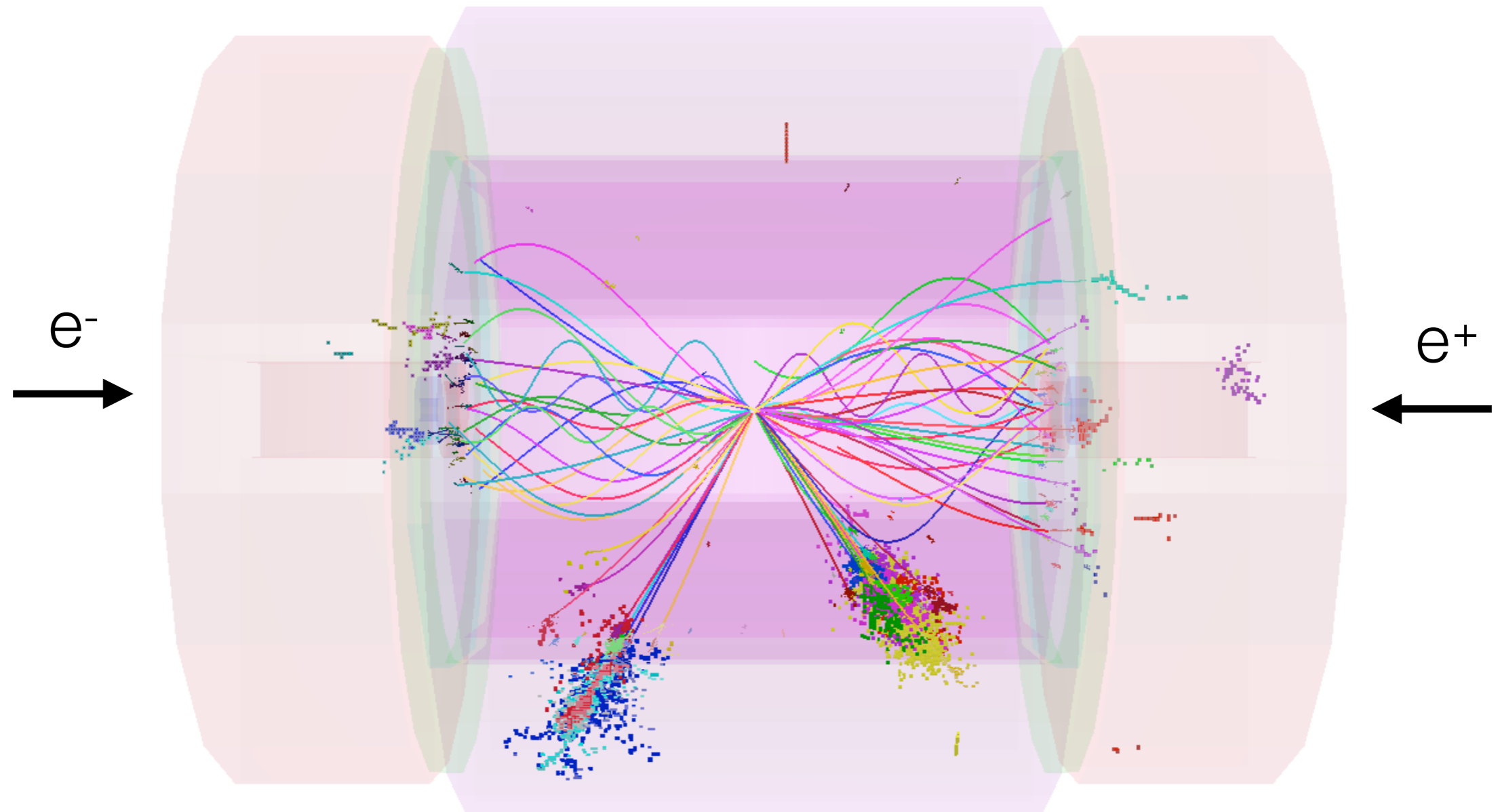
Solution: train a neural network to distinguish the two datasets!

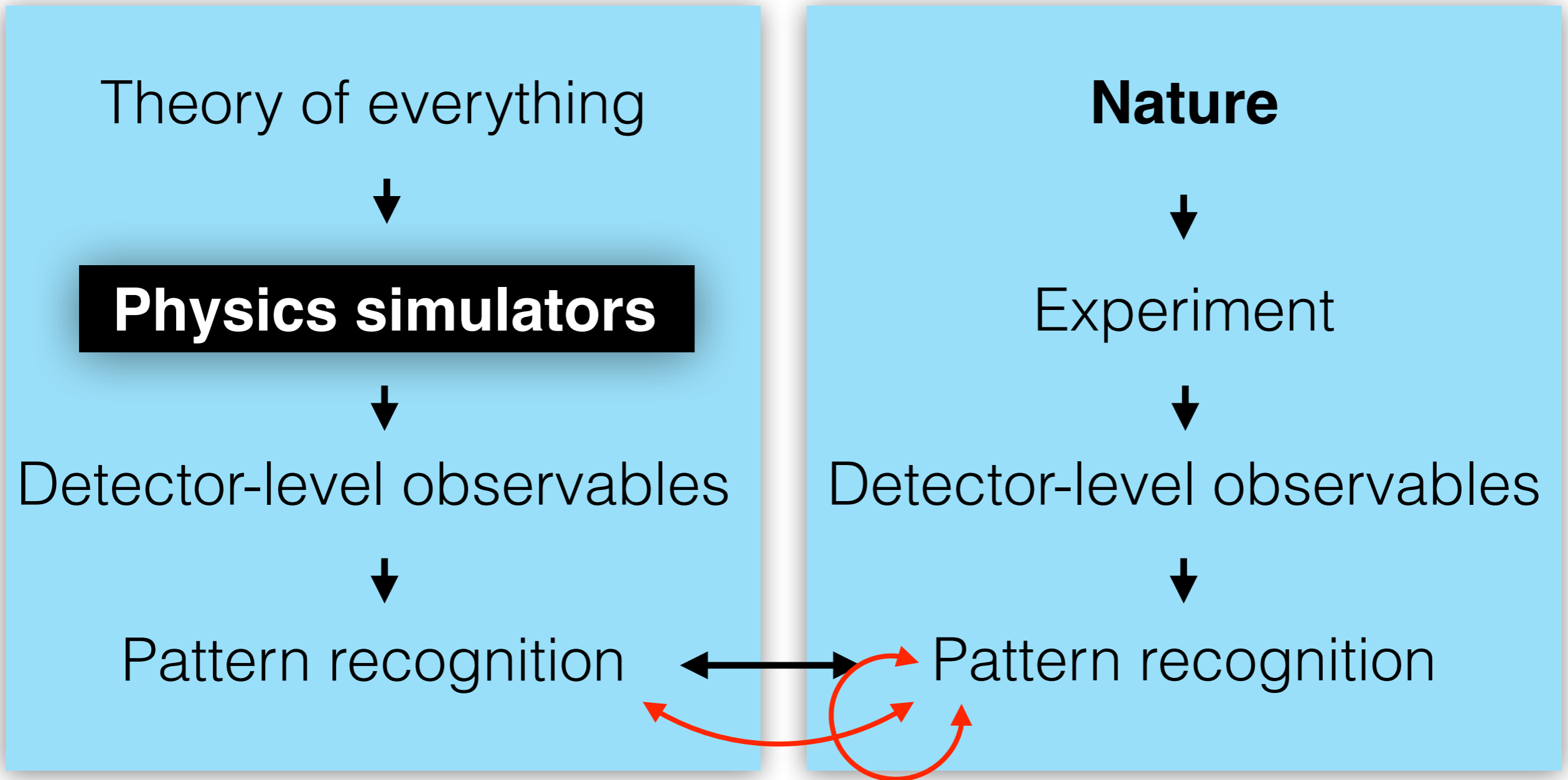
This turns the problem of **density estimation** (**hard**) into a problem of **classification** (**easy**)

Classification for reweighting

47

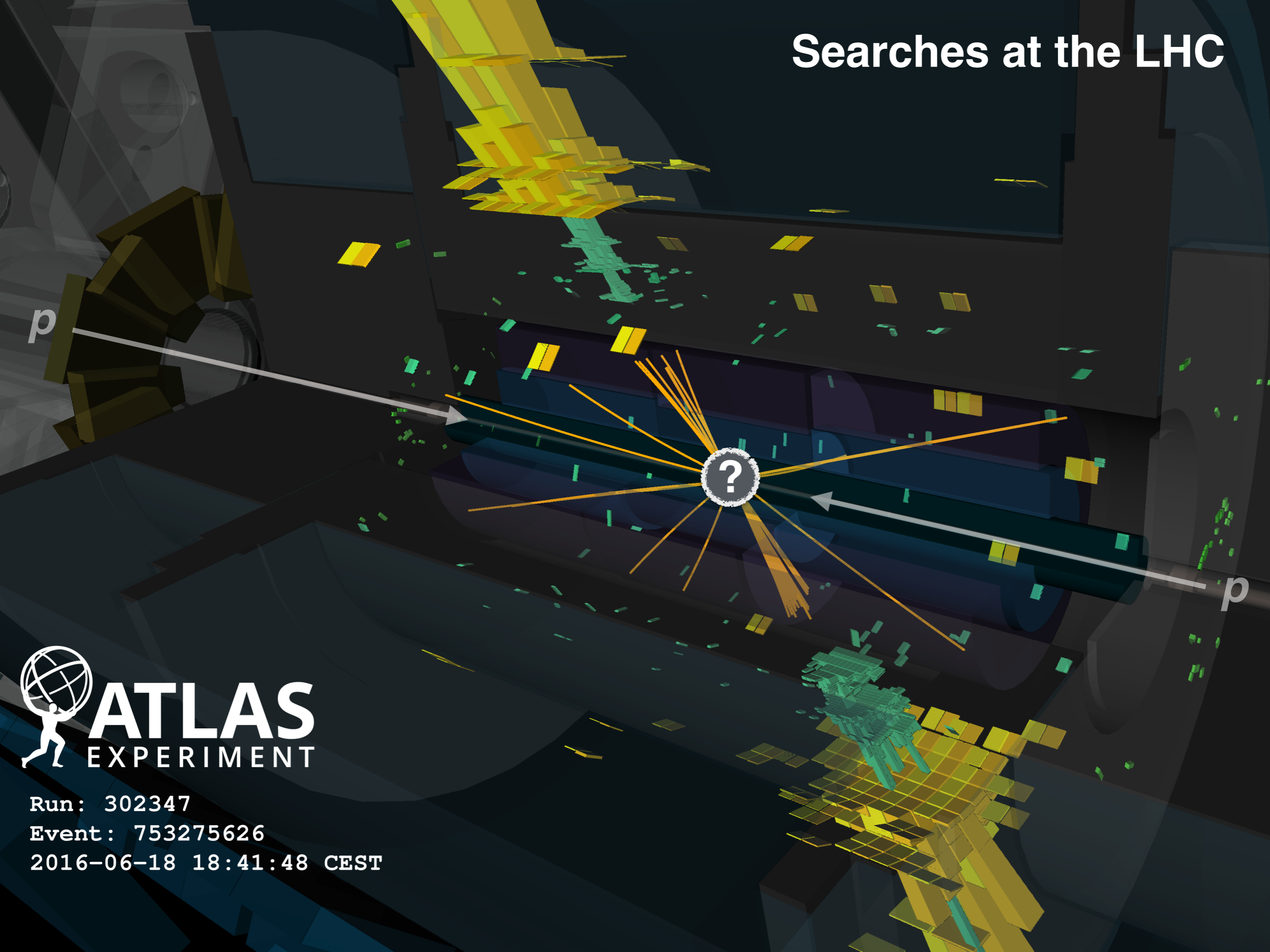
Particularly useful for particle physics, where collisions may produce a variable # of particles which are interchangeable





Anomaly detection

Searches at the LHC



 **ATLAS**
EXPERIMENT

Run: 302347

Event: 753275626

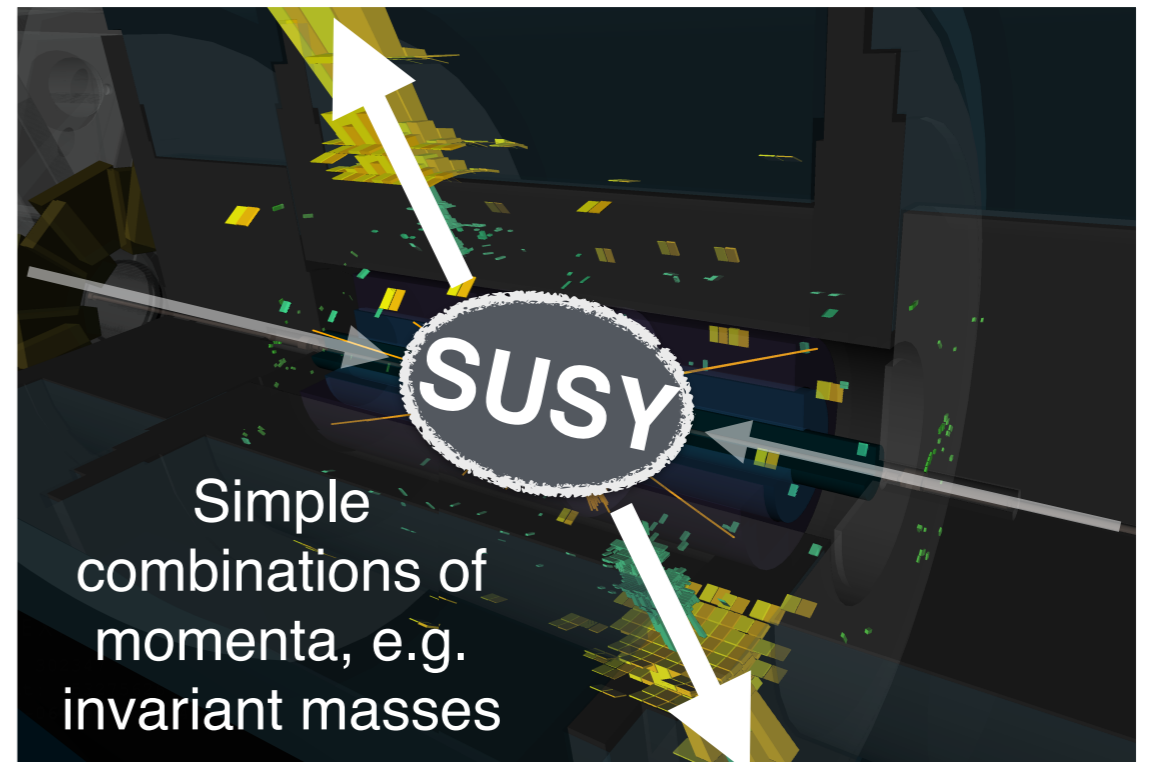
2016-06-18 18:41:48 CEST

Current Search Paradigm

50



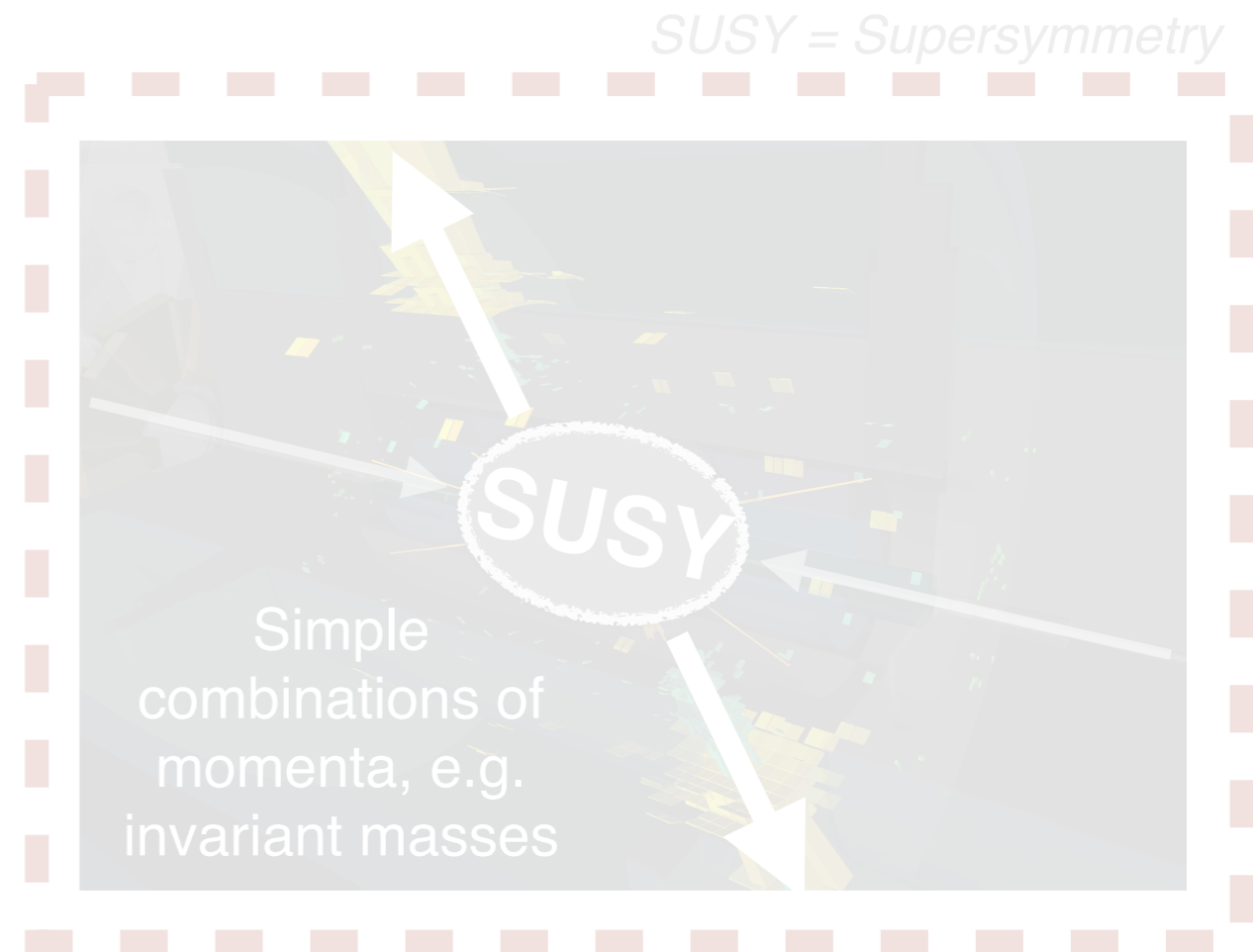
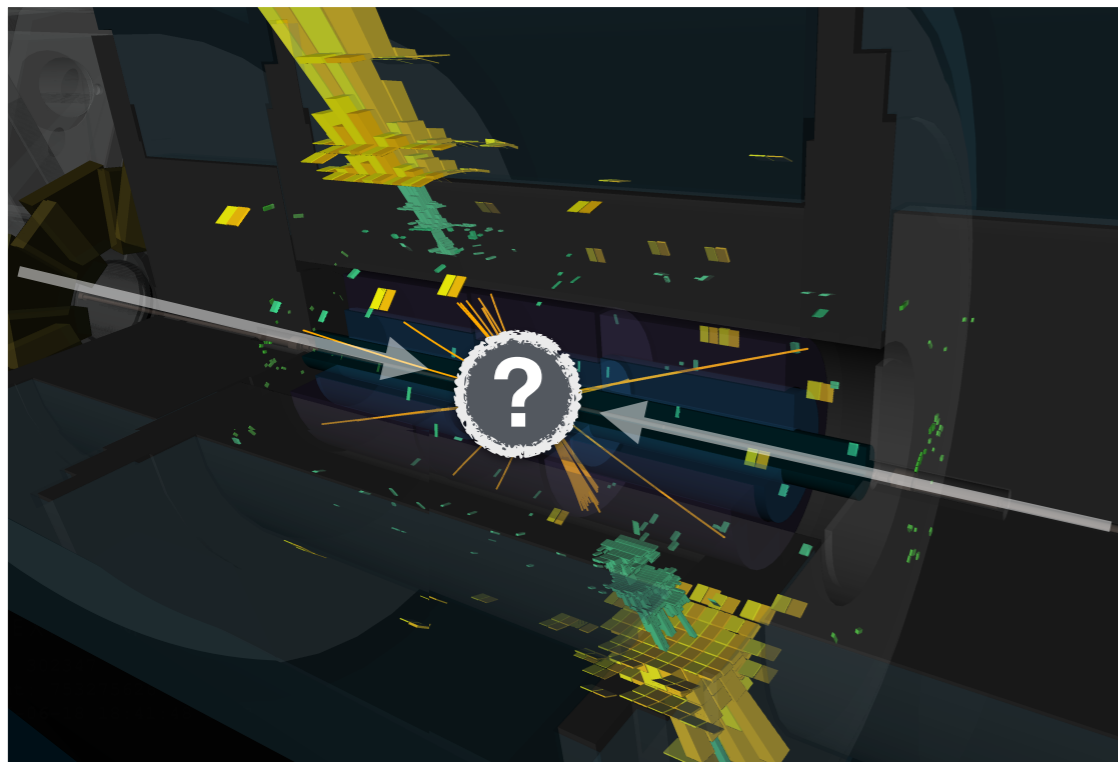
SUSY = Supersymmetry



(well-motivated) theory-biased
& low-dimensional observables

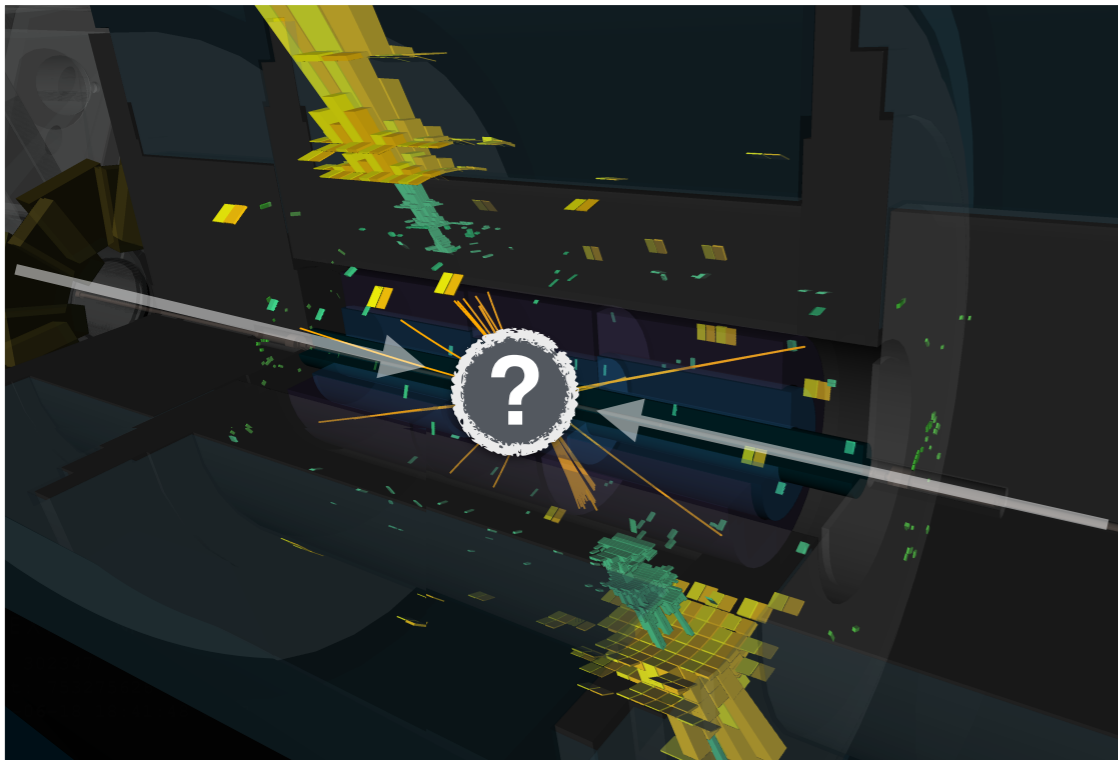
Current Search Paradigm

51



Can we relax model assumptions and explore high-dimensional feature spaces?

(well-motivated) theory-biased & low-dimensional observables



What if we are not looking in the right place for the new phenomena?!

Can we relax model assumptions and explore high-dimensional feature spaces?

What is the problem?

53

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

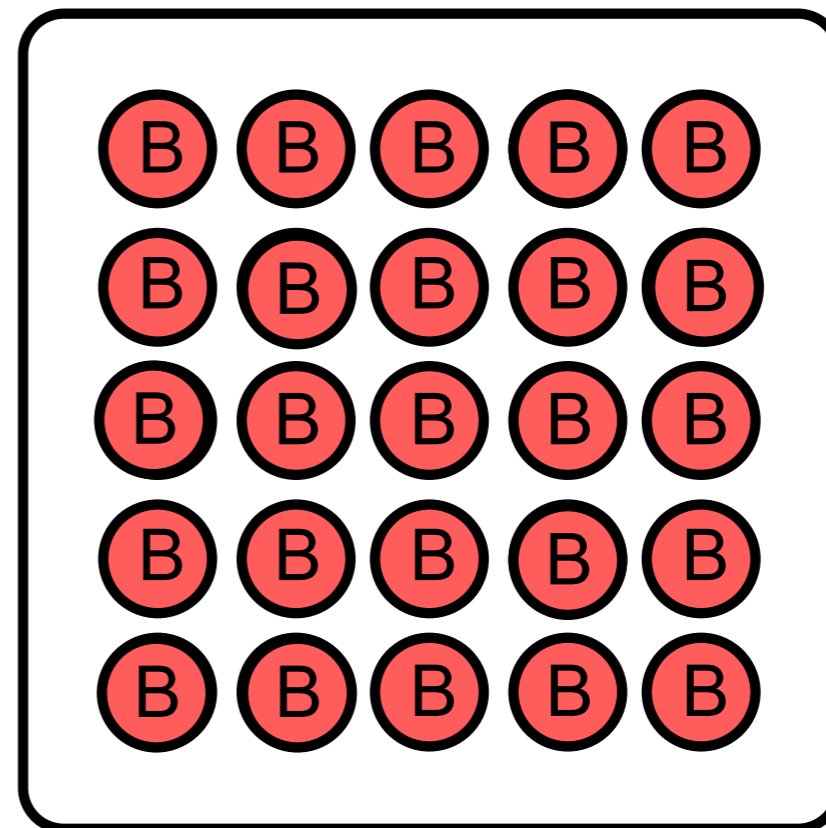
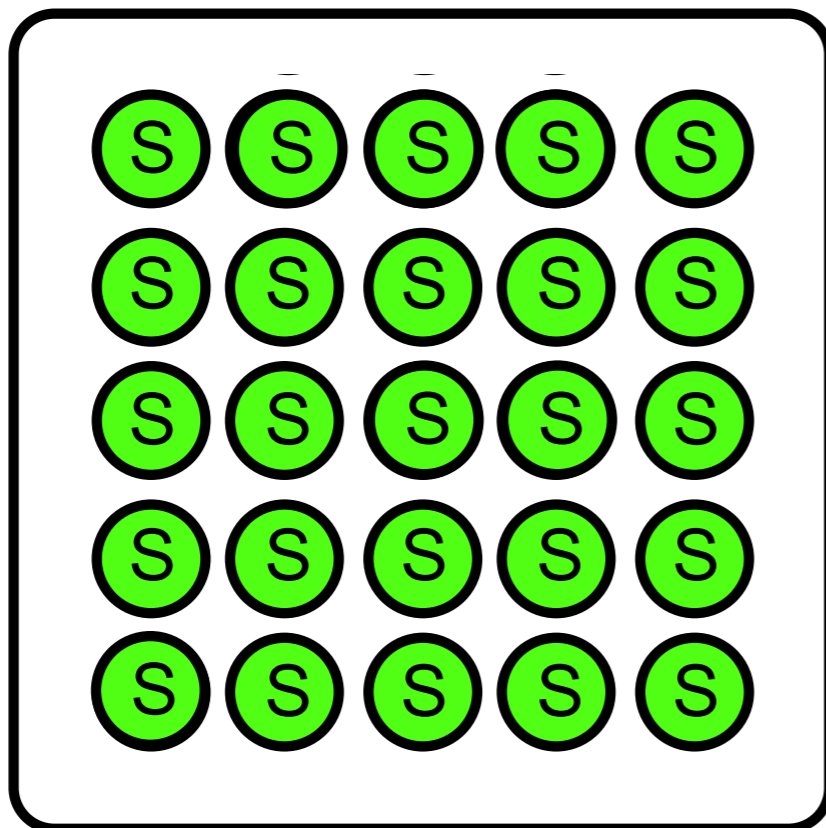


Image credit: pixabay.com

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

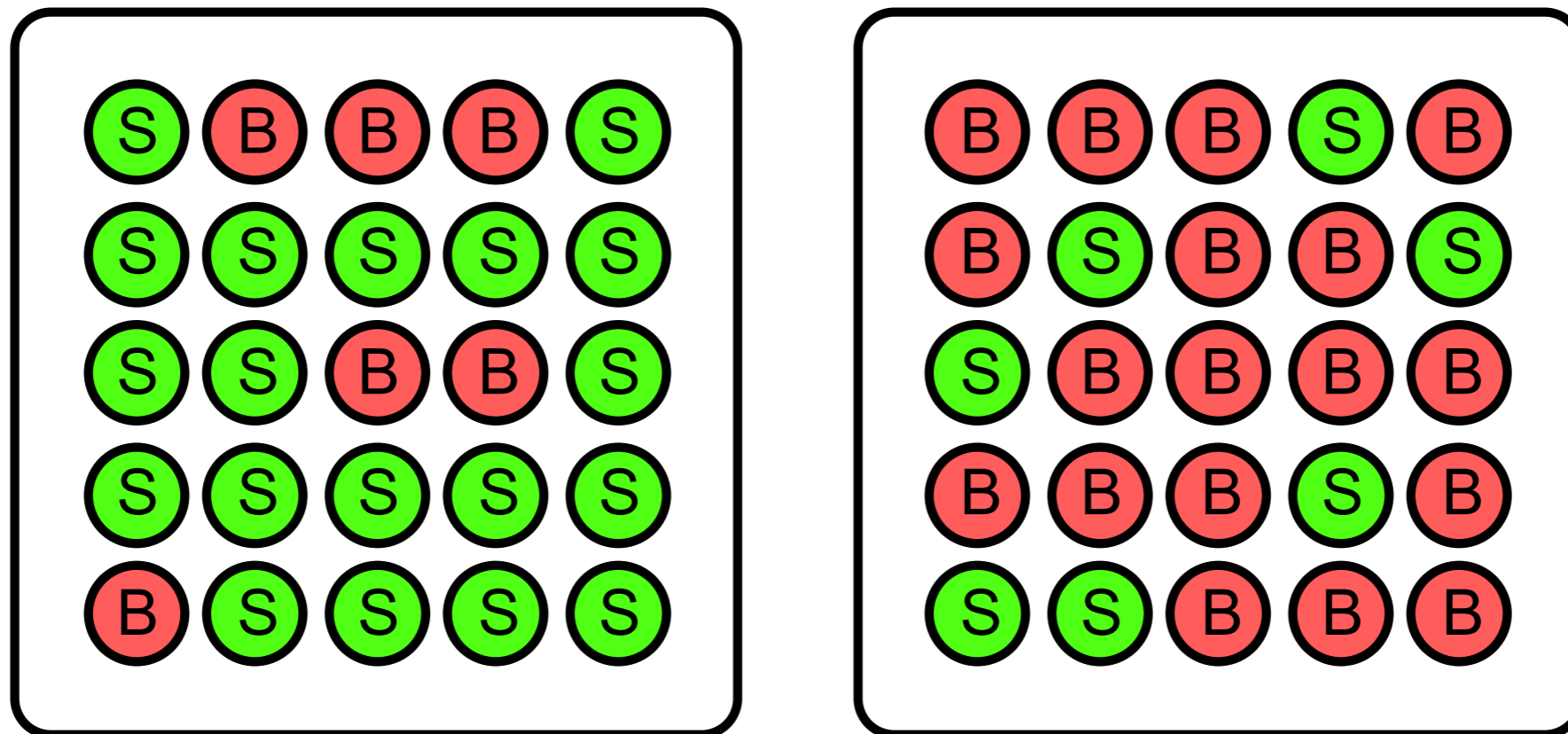
Usual case: train with labels

Usually, we train using simulations where we know which events are “**signal**” and which are “**background**”.



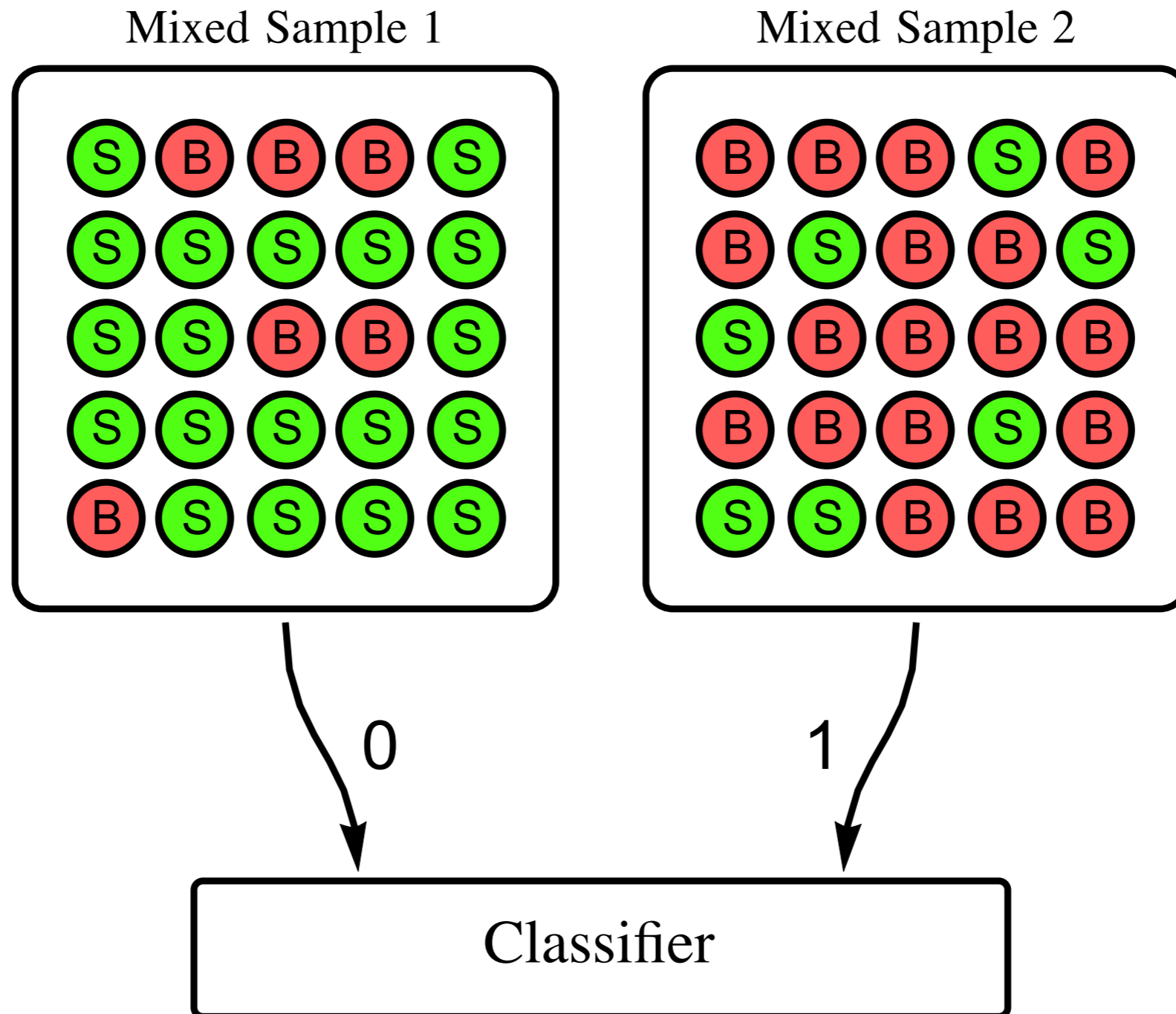
No labels, no problem!

Can we still do machine learning when reality is like this?



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

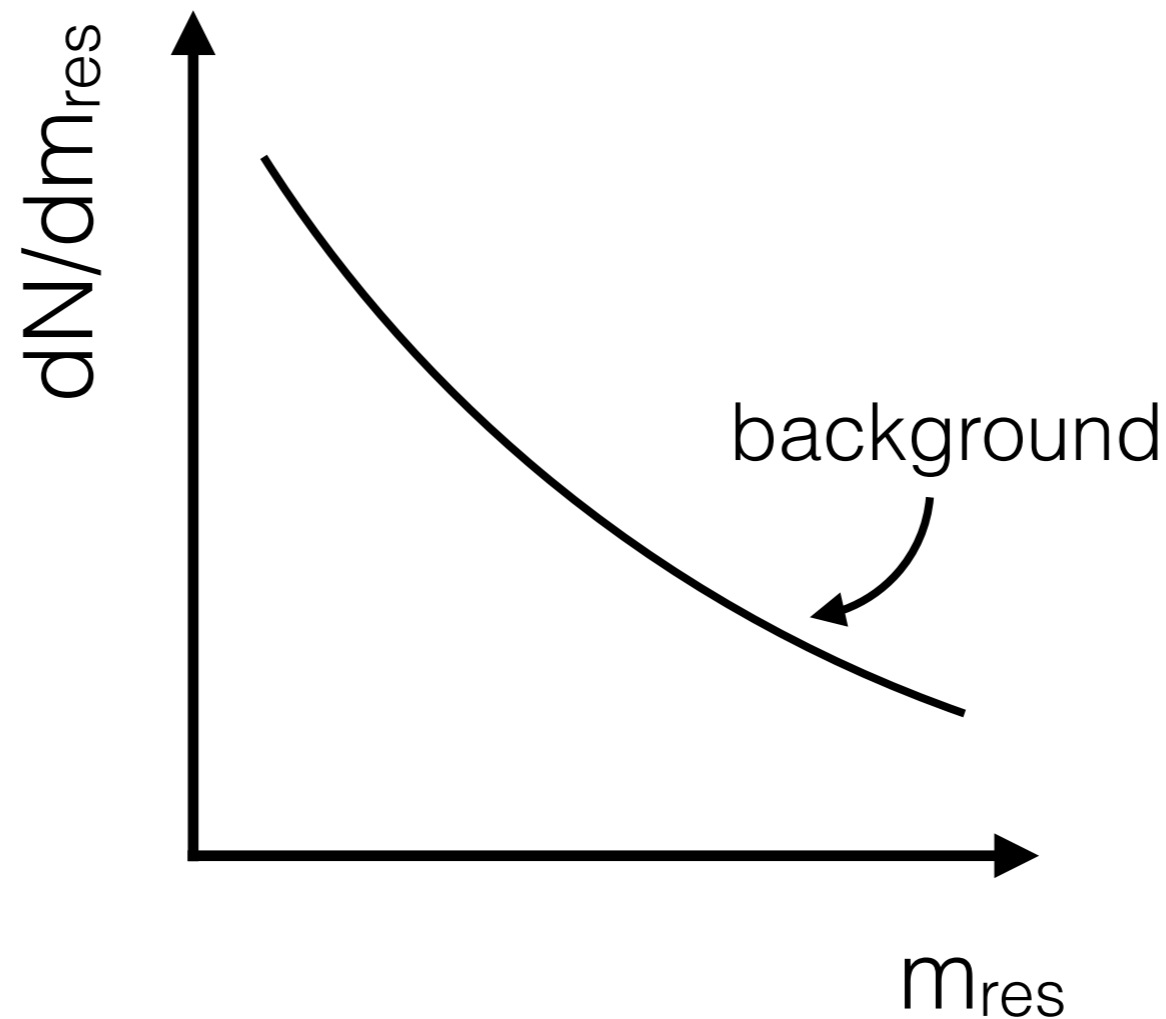
No labels, no problem!



One simple, but powerful idea: “weak supervision”

No labels, no problem!

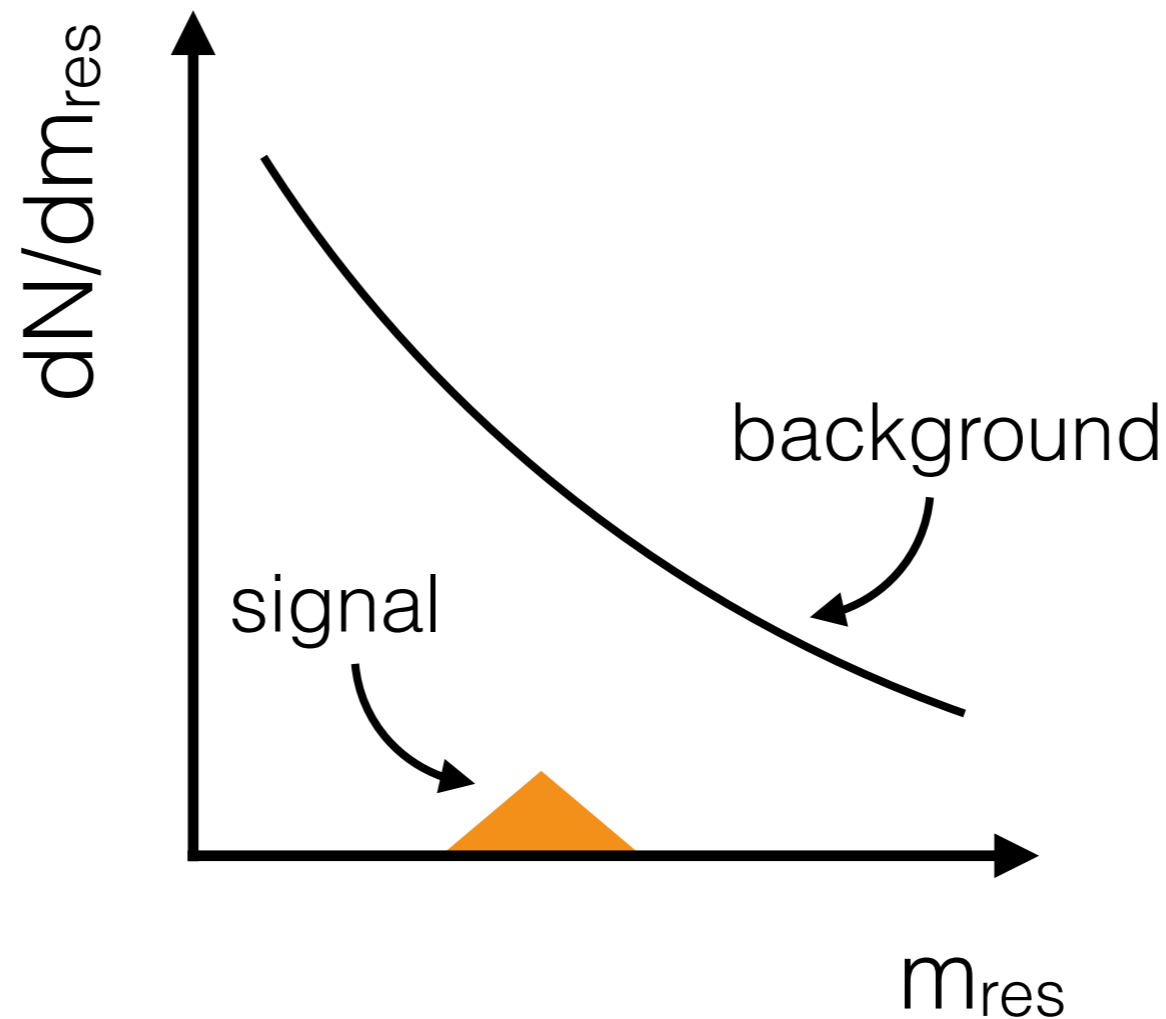
57



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

No labels, no problem!

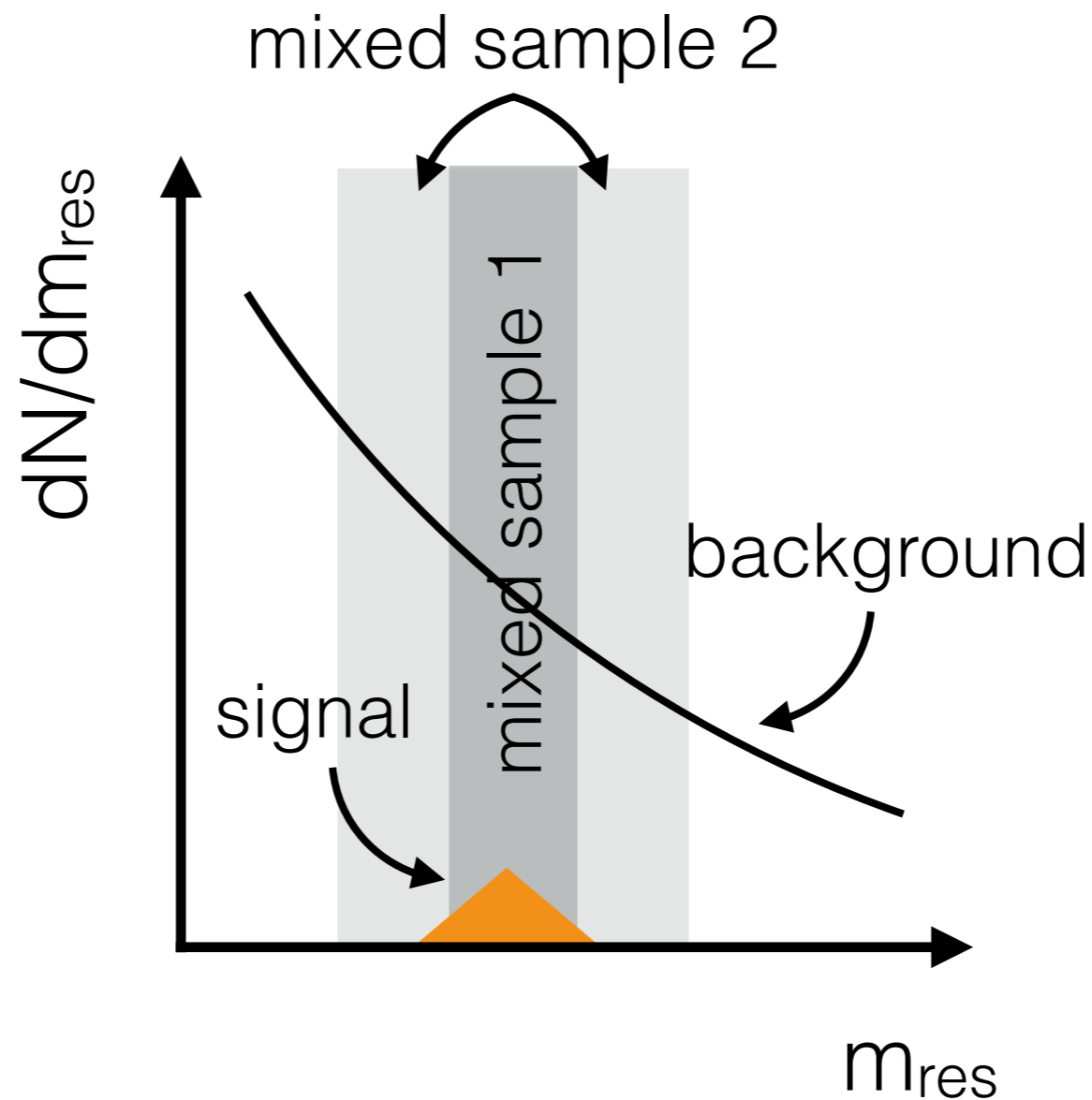
58



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

No labels, no problem!

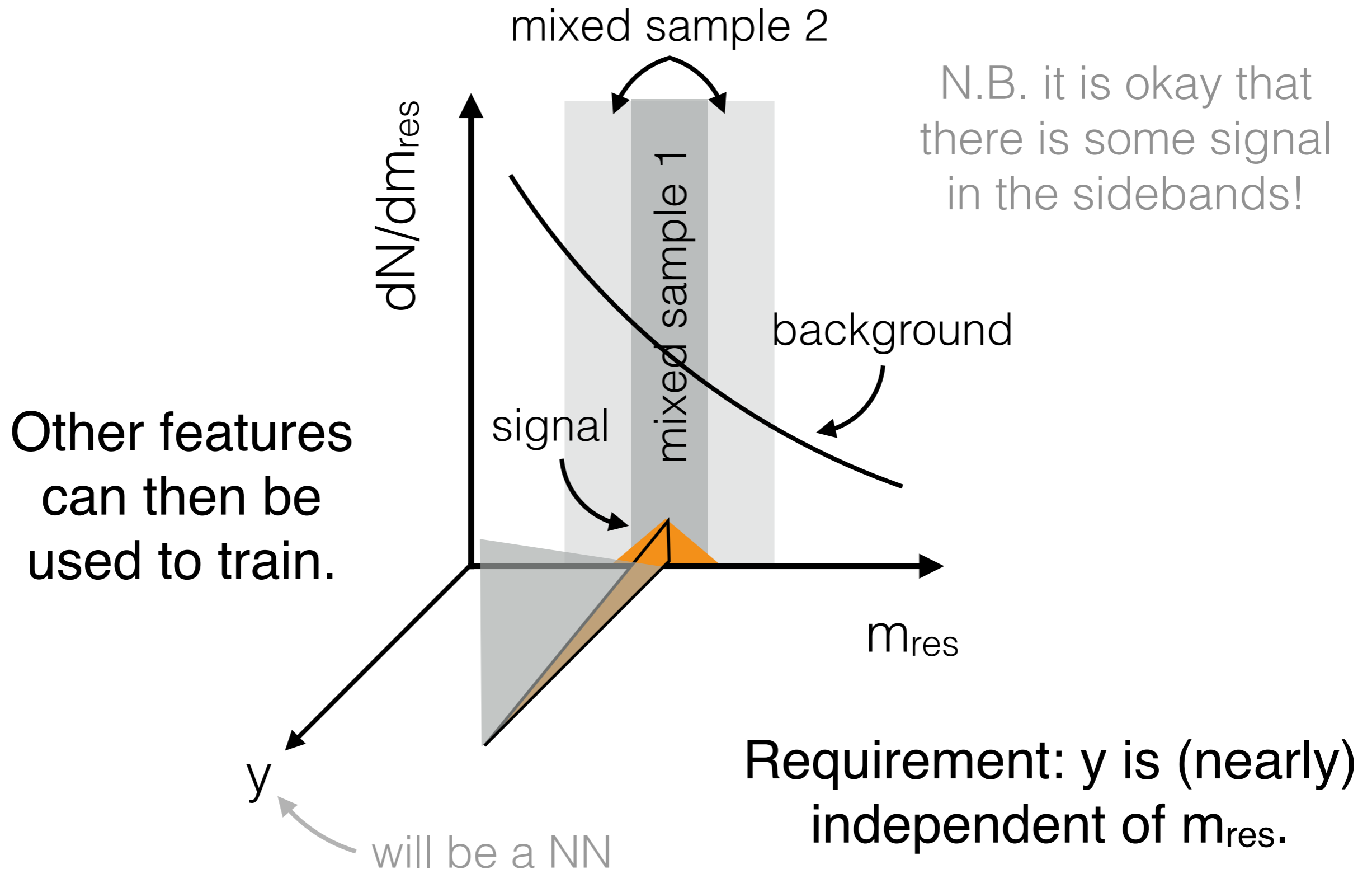
59



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

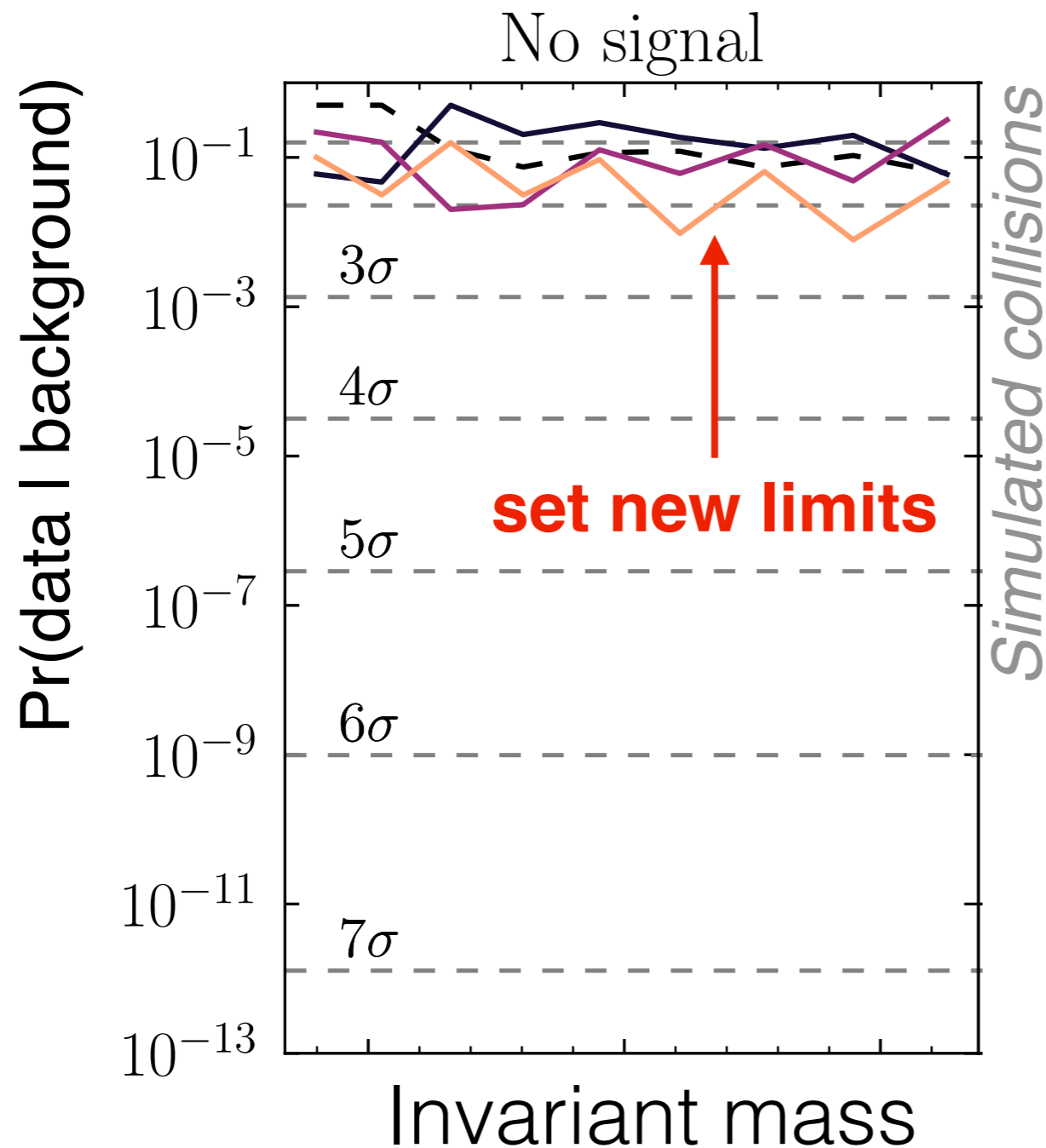
No labels, no problem!

60



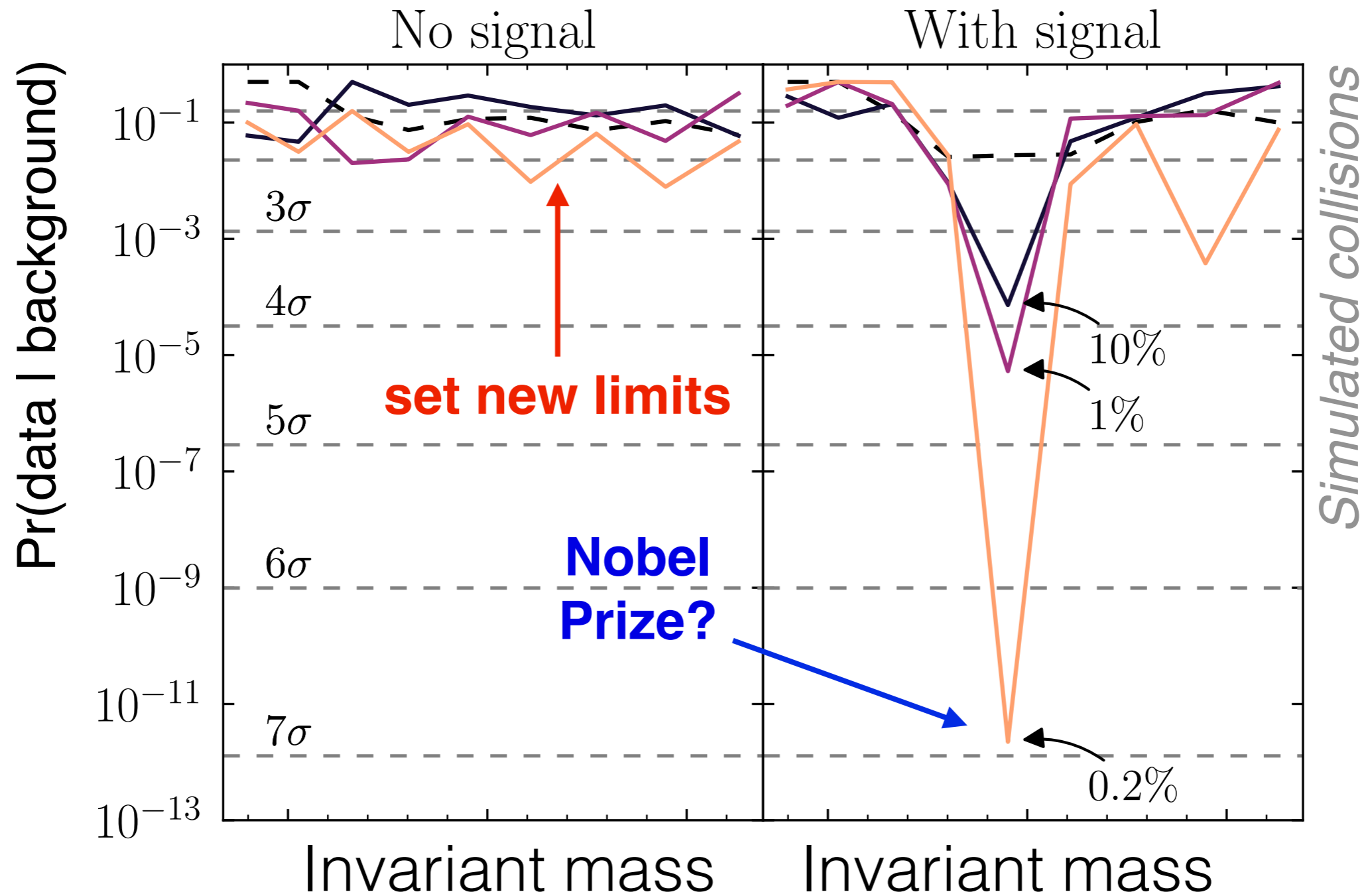
Potential of weak supervision

61

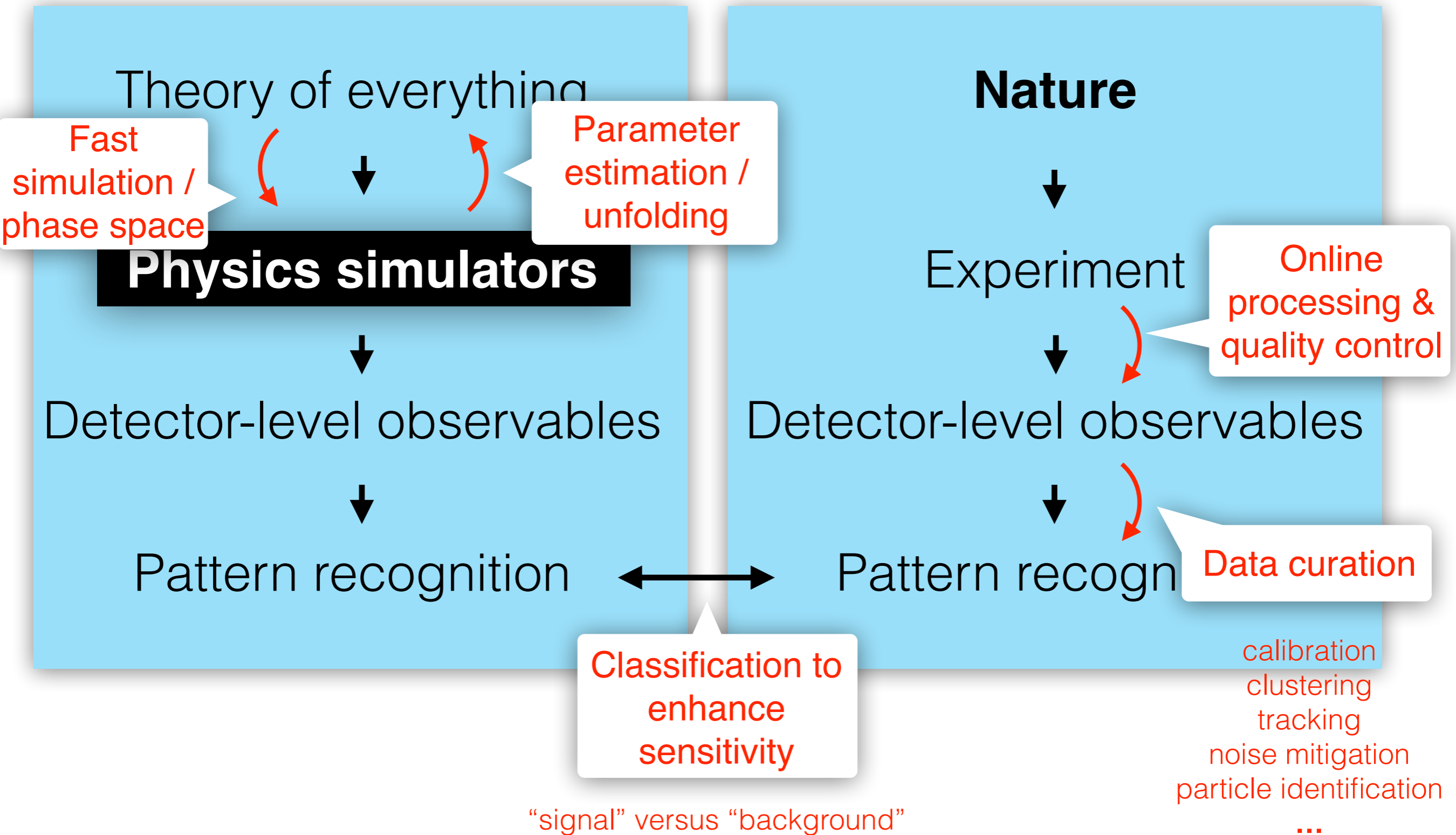


Necessary: when there is no anomaly, the procedure does not find an anomaly.

Potential of weak supervision



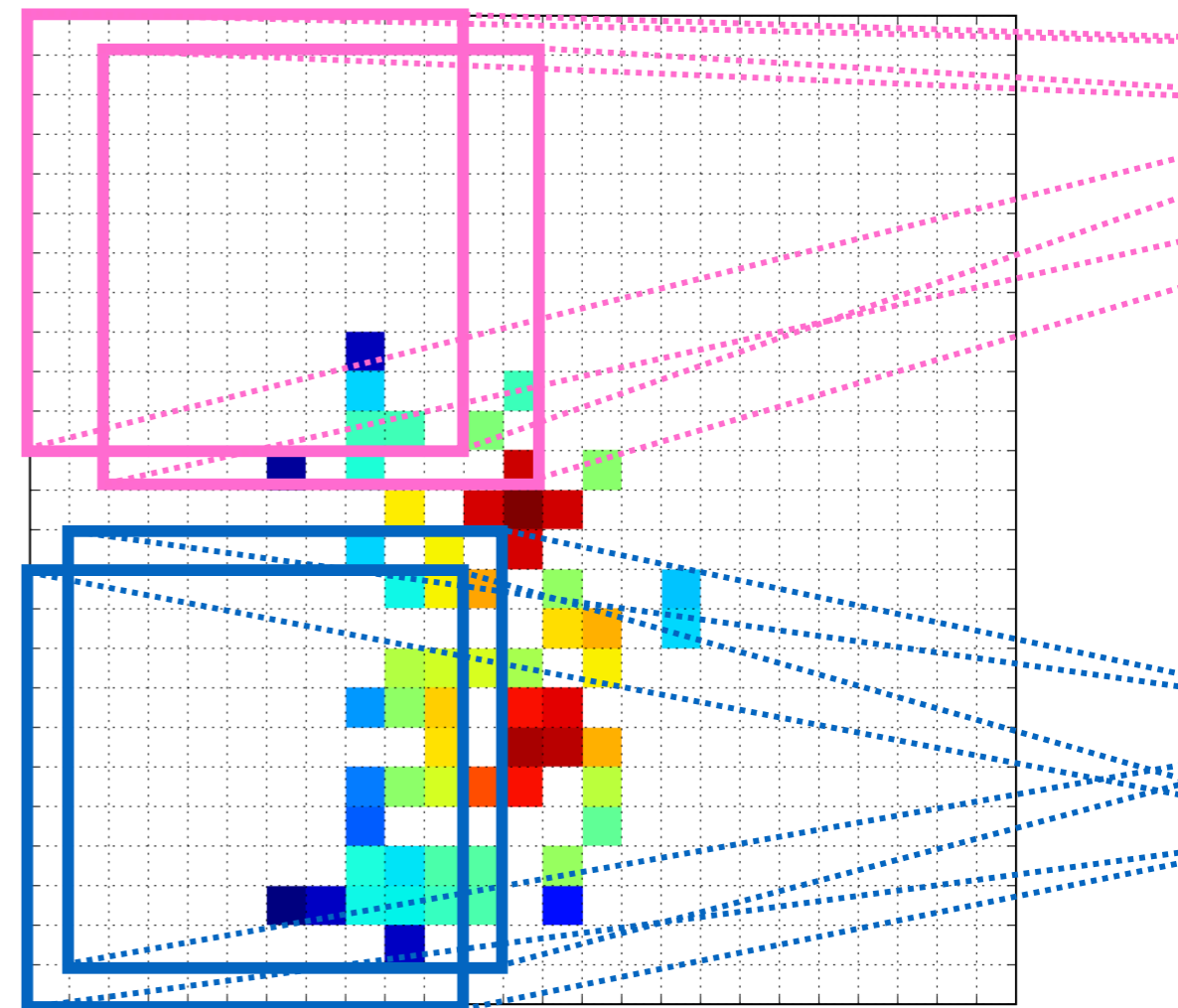
Overview: Particle physics and ML



Deep learning has a great potential to **enhance**, **accelerate**, and **empower** discoveries in particle physics.

This set of tools is growing in importance and no matter what you do, they will help you do it better.

Consider taking a statistics / statistical learning / machine learning / applied statistics course(s)!

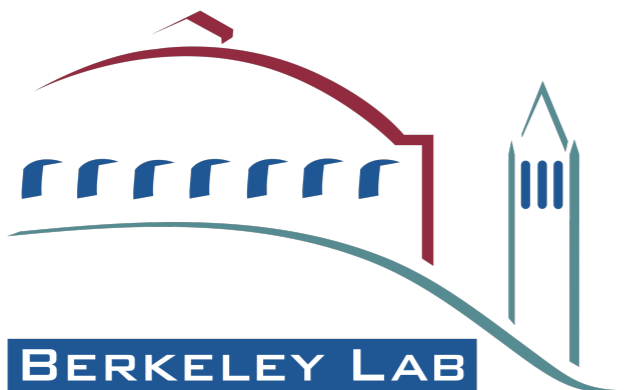


How else to get involved?

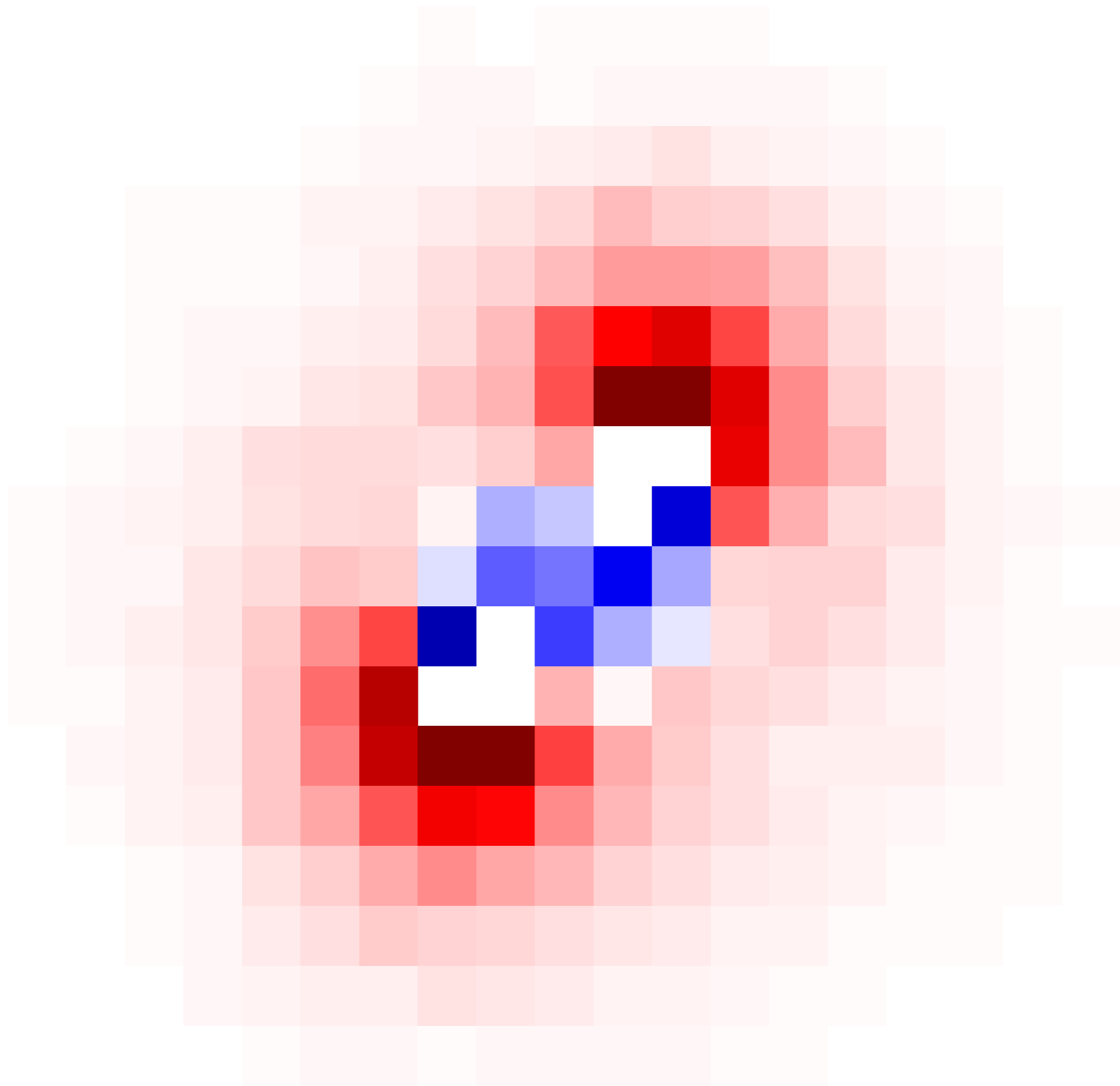
65



ML and Science Forum,
biweekly on Mondays at 11 AM

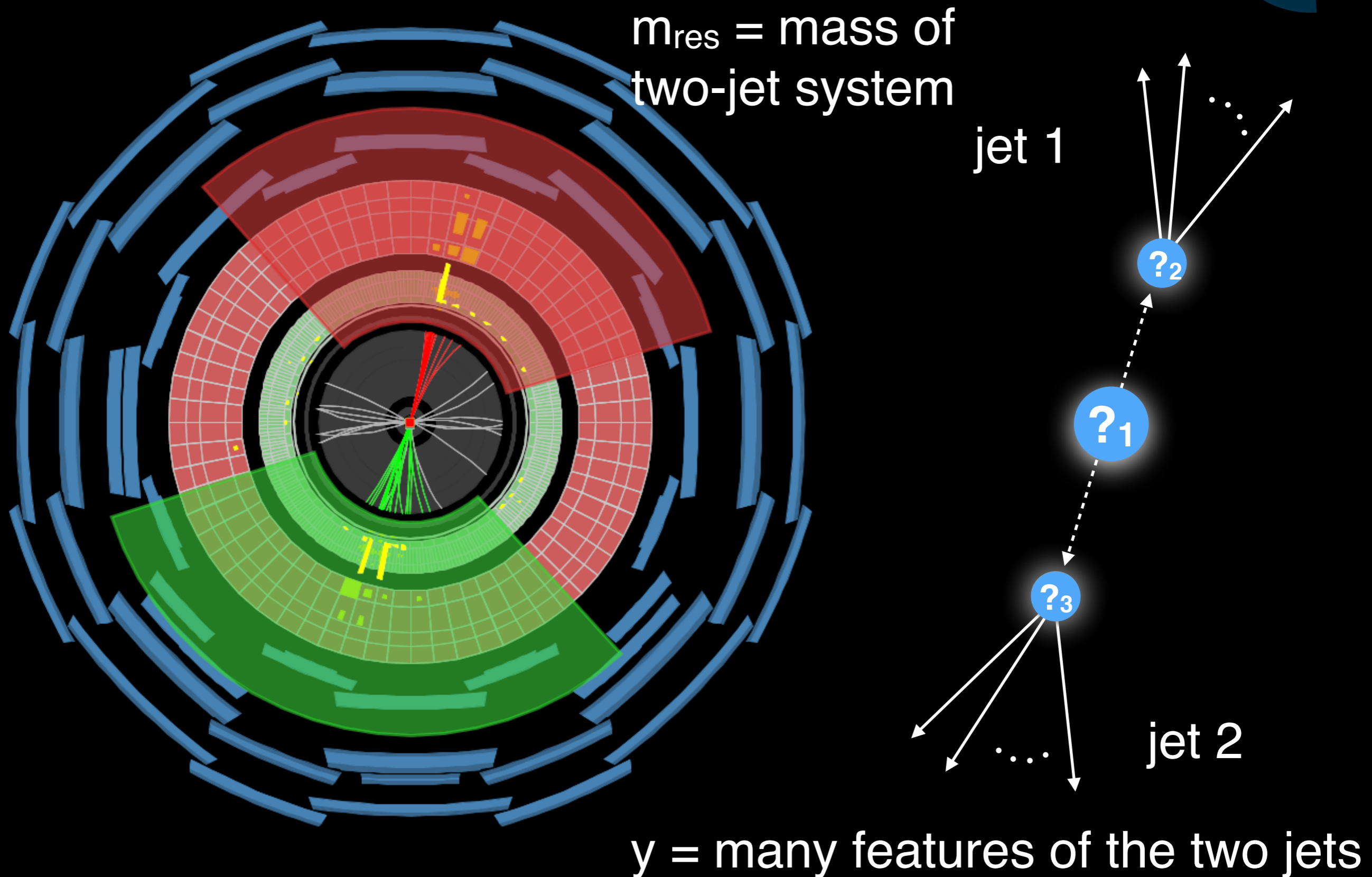


Physics Division ML meetings,
weekly on Thursdays at 1 PM
(open to all)



Fin.

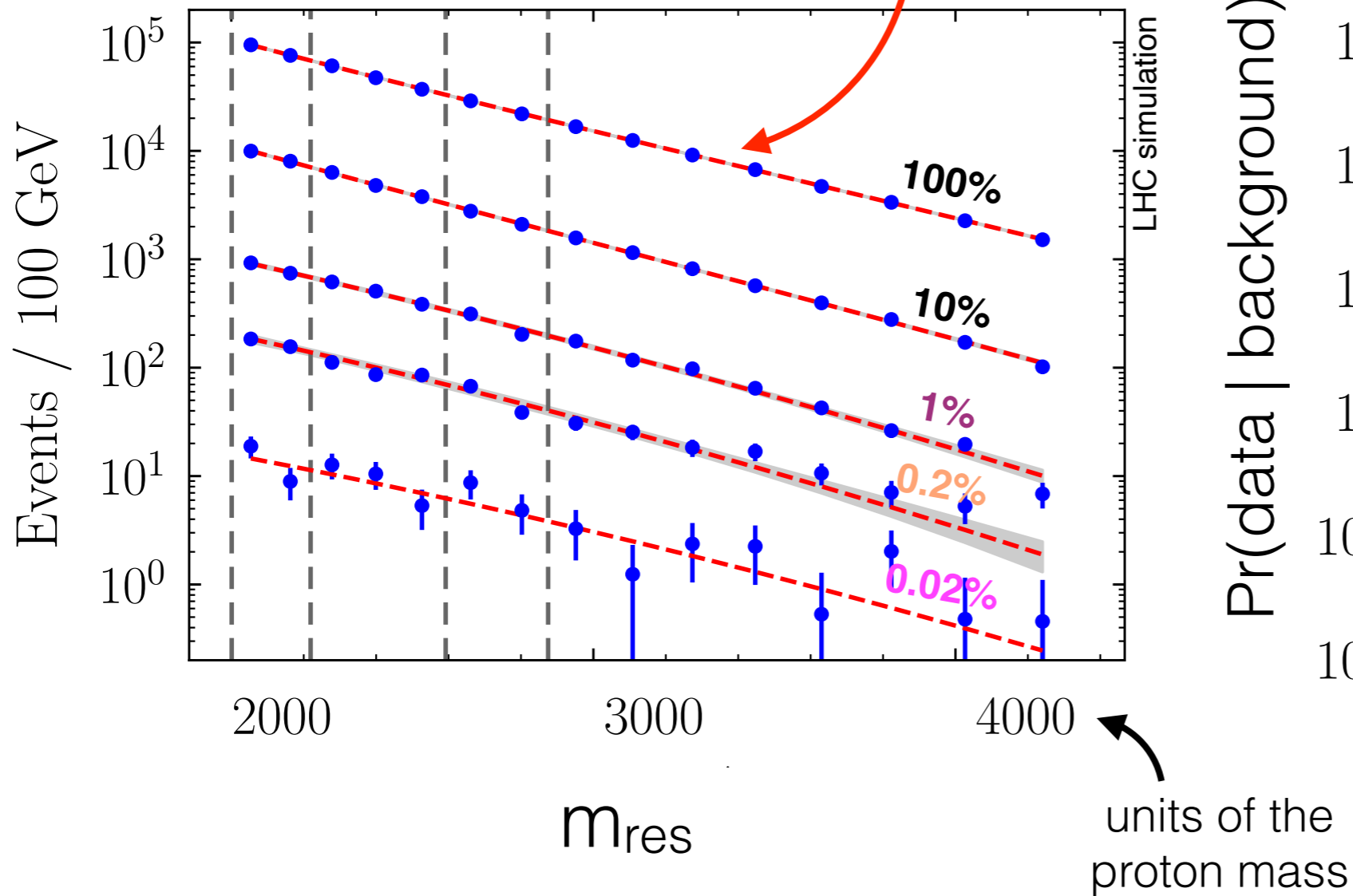
Example: two-jet search



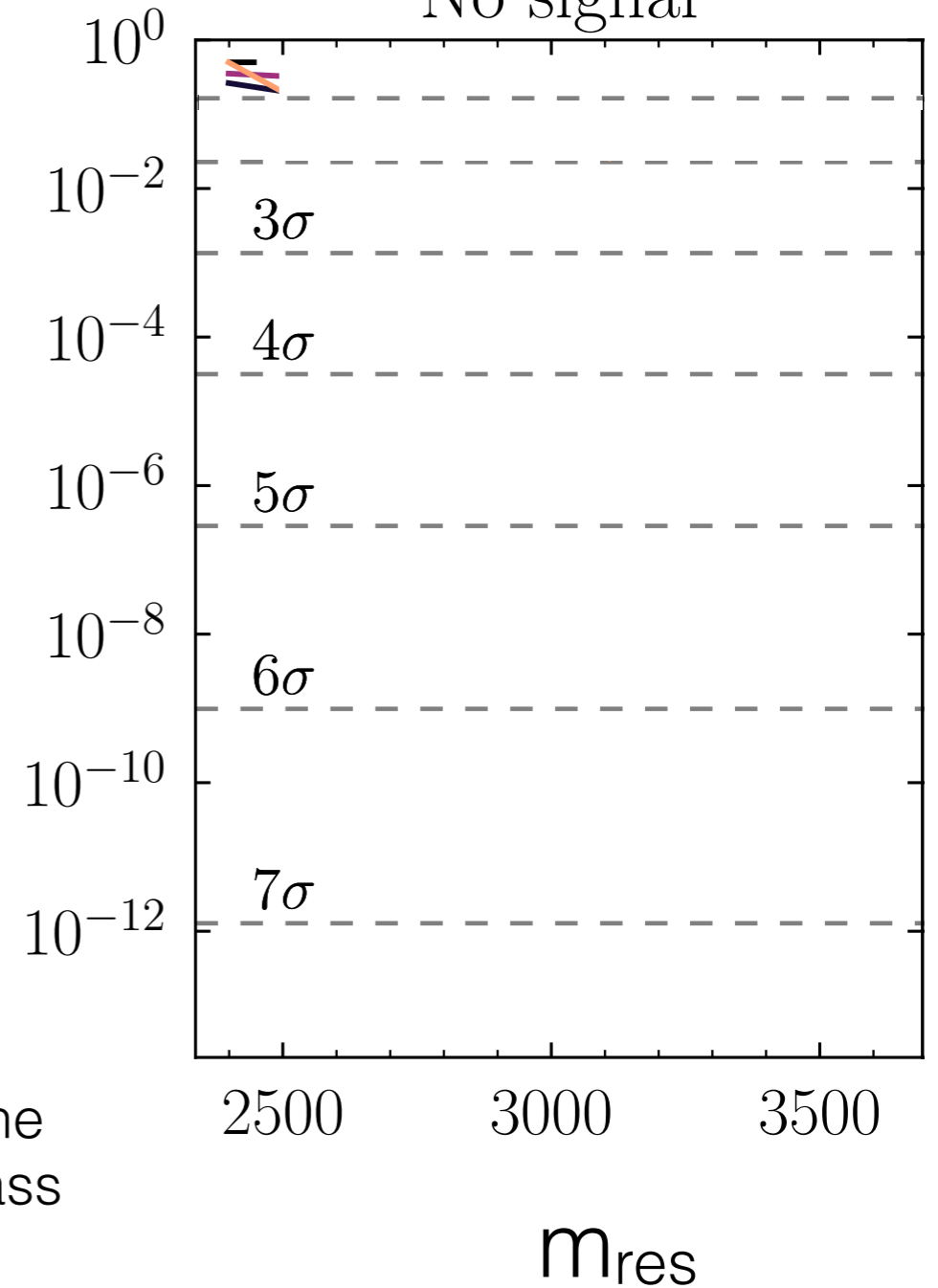
Example: two-jet search

sidebands

standard parametric fit to background.

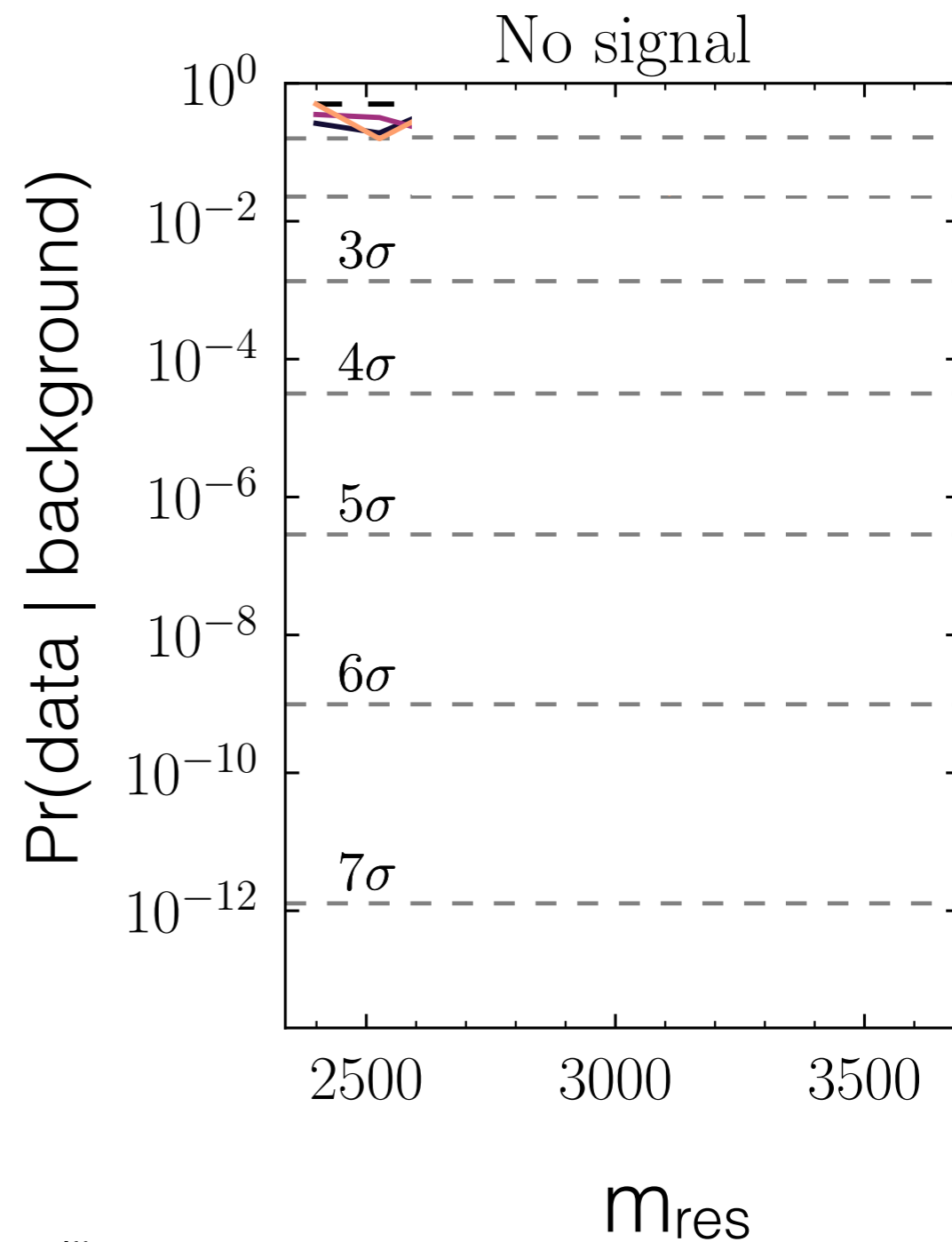
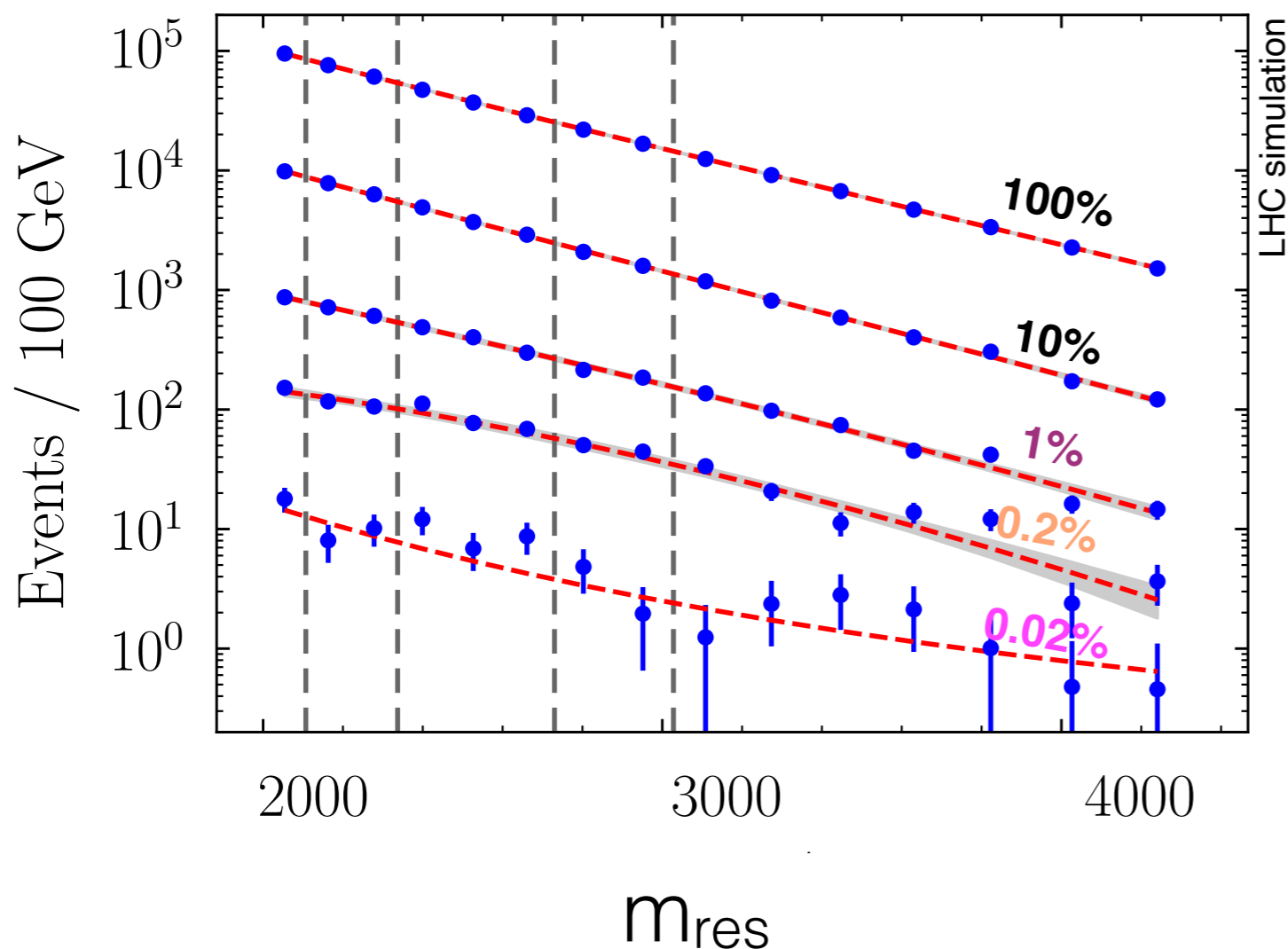


No signal



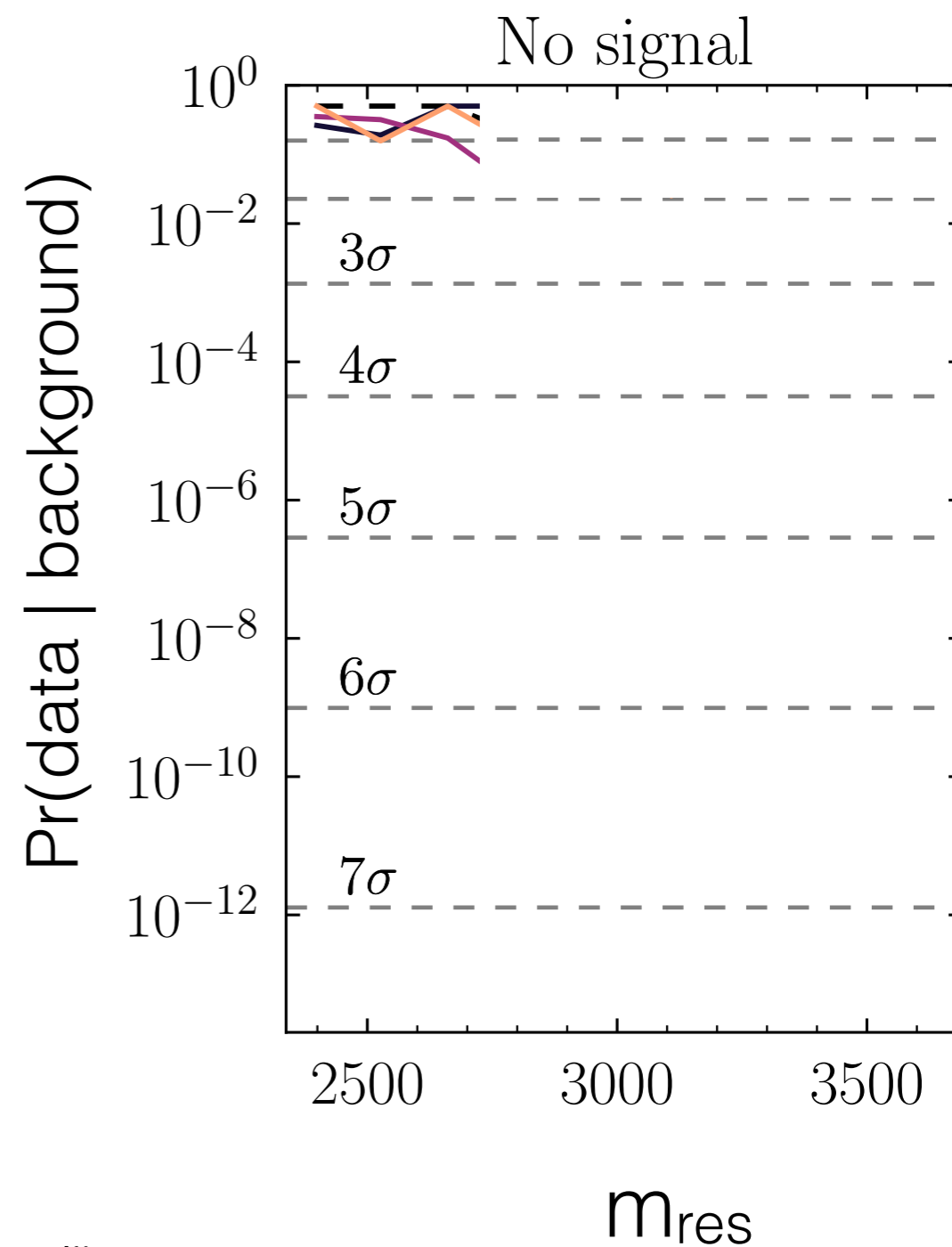
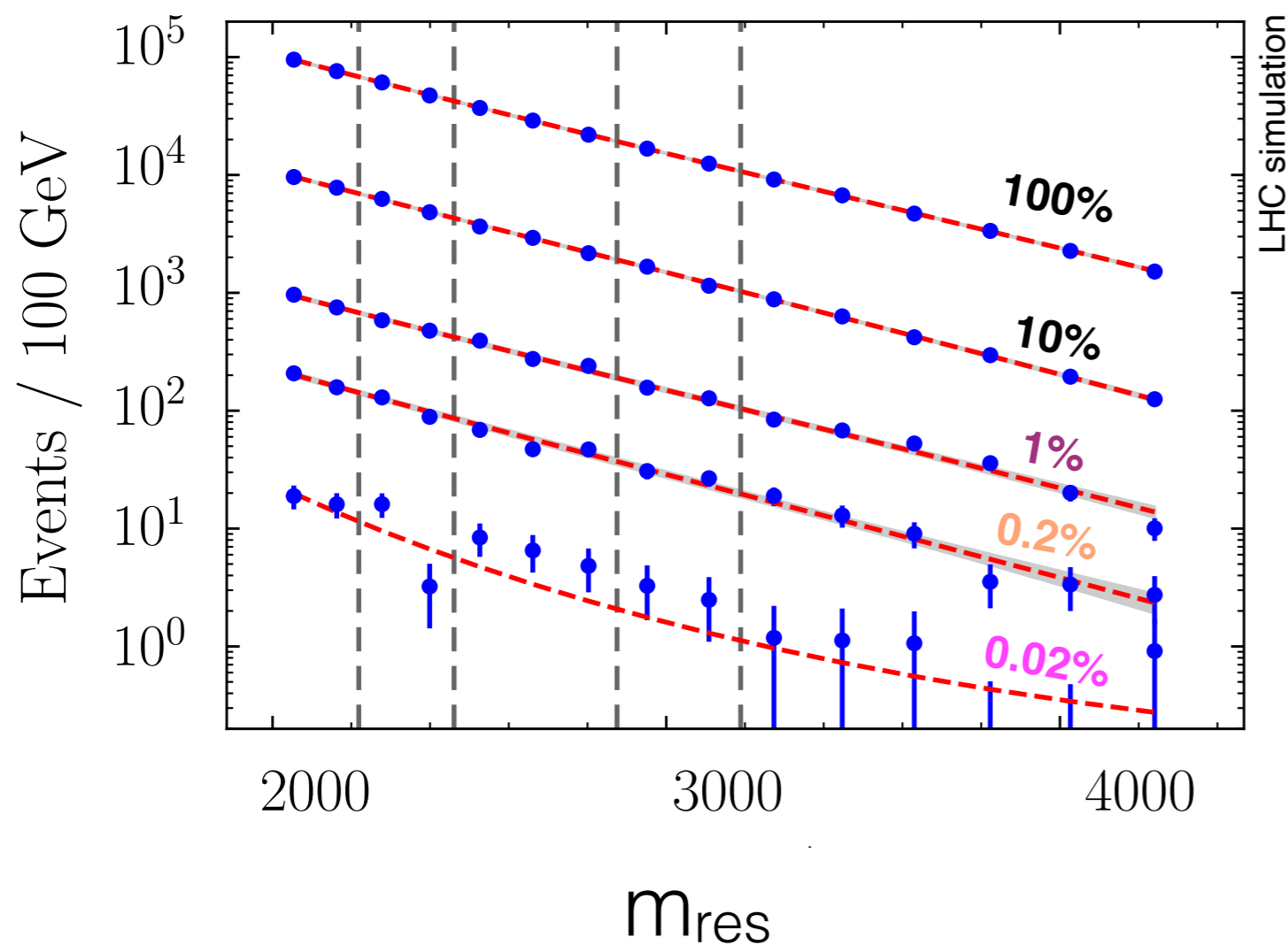
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

Example: two-jet search



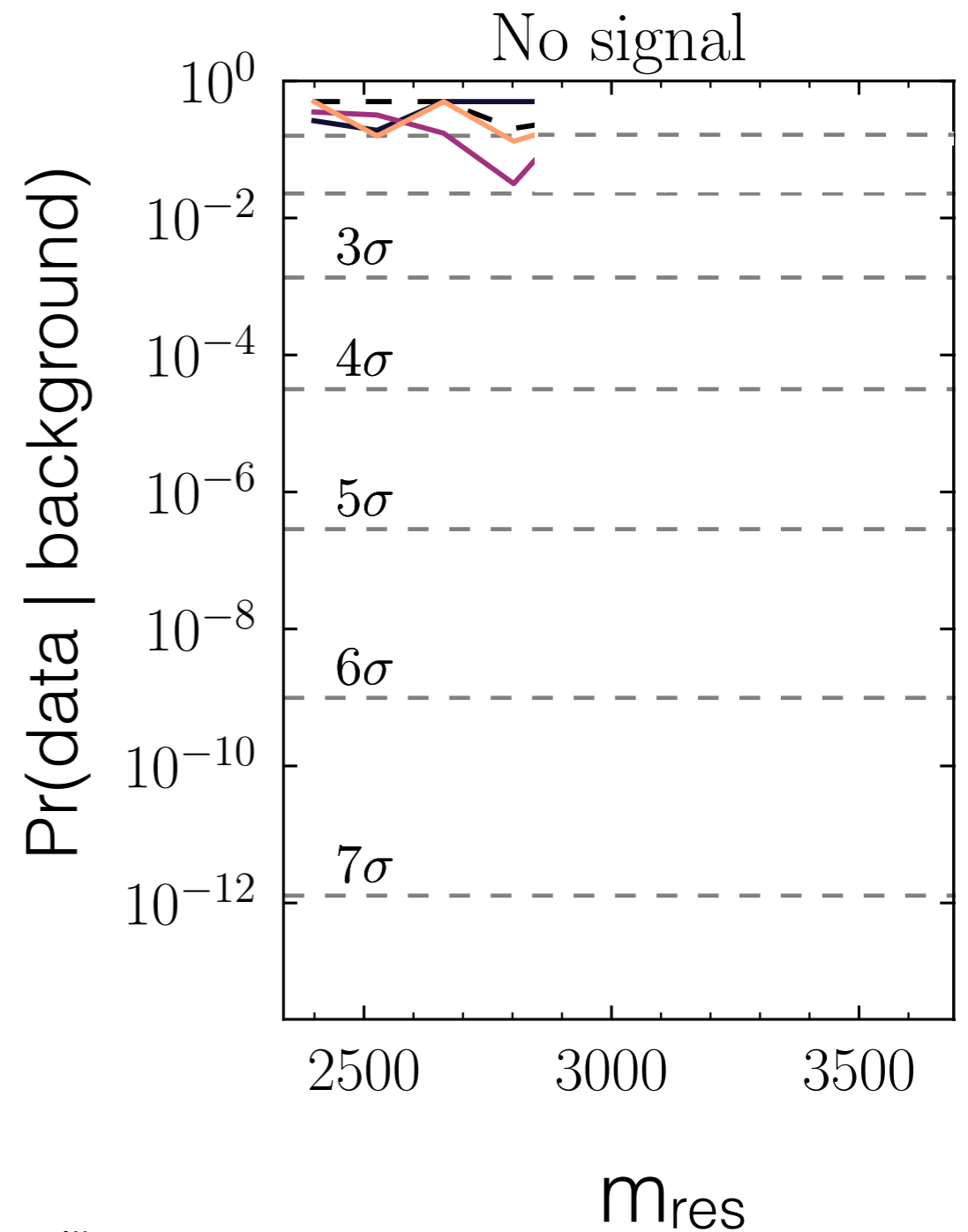
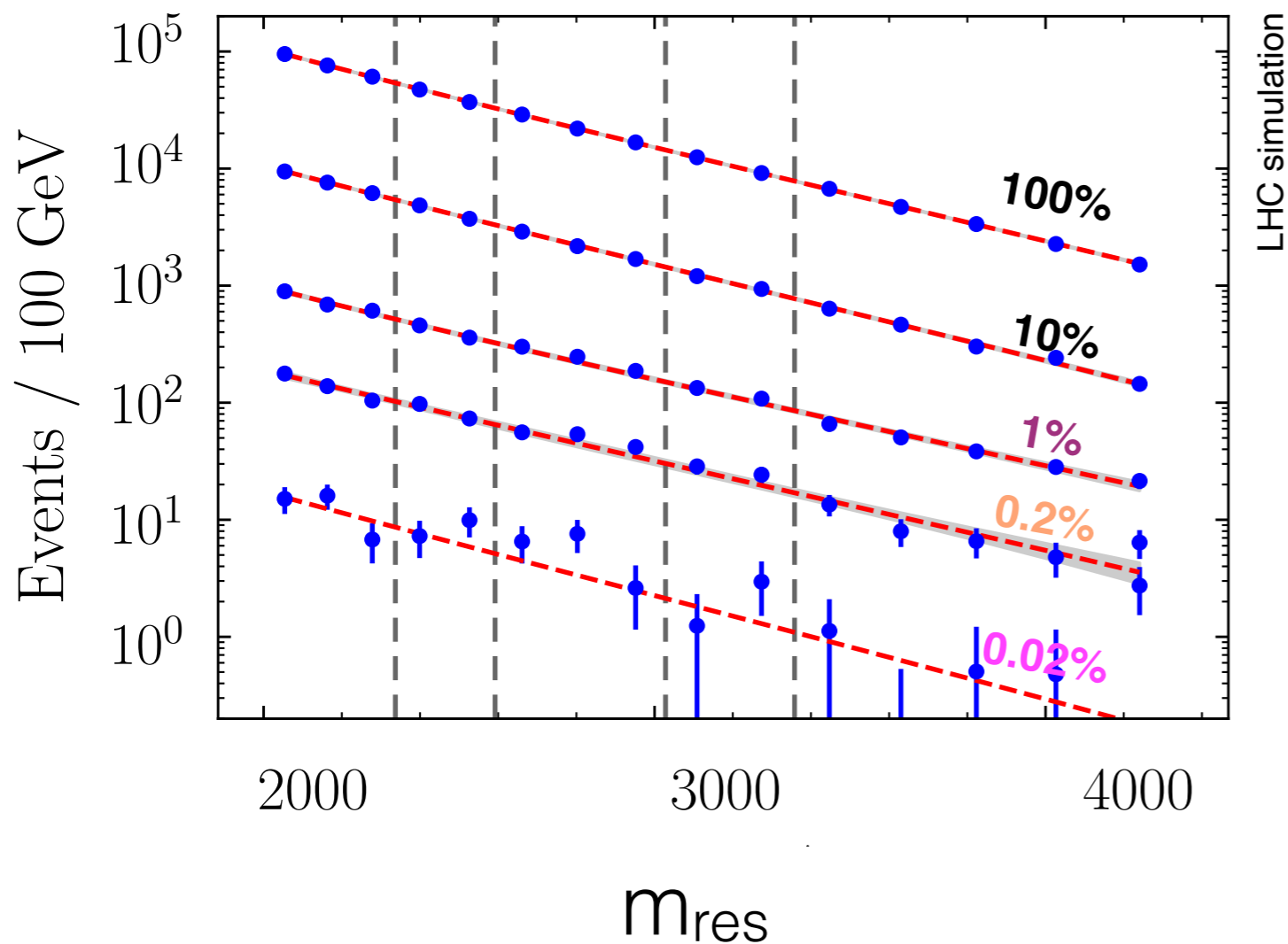
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

Example: two-jet search



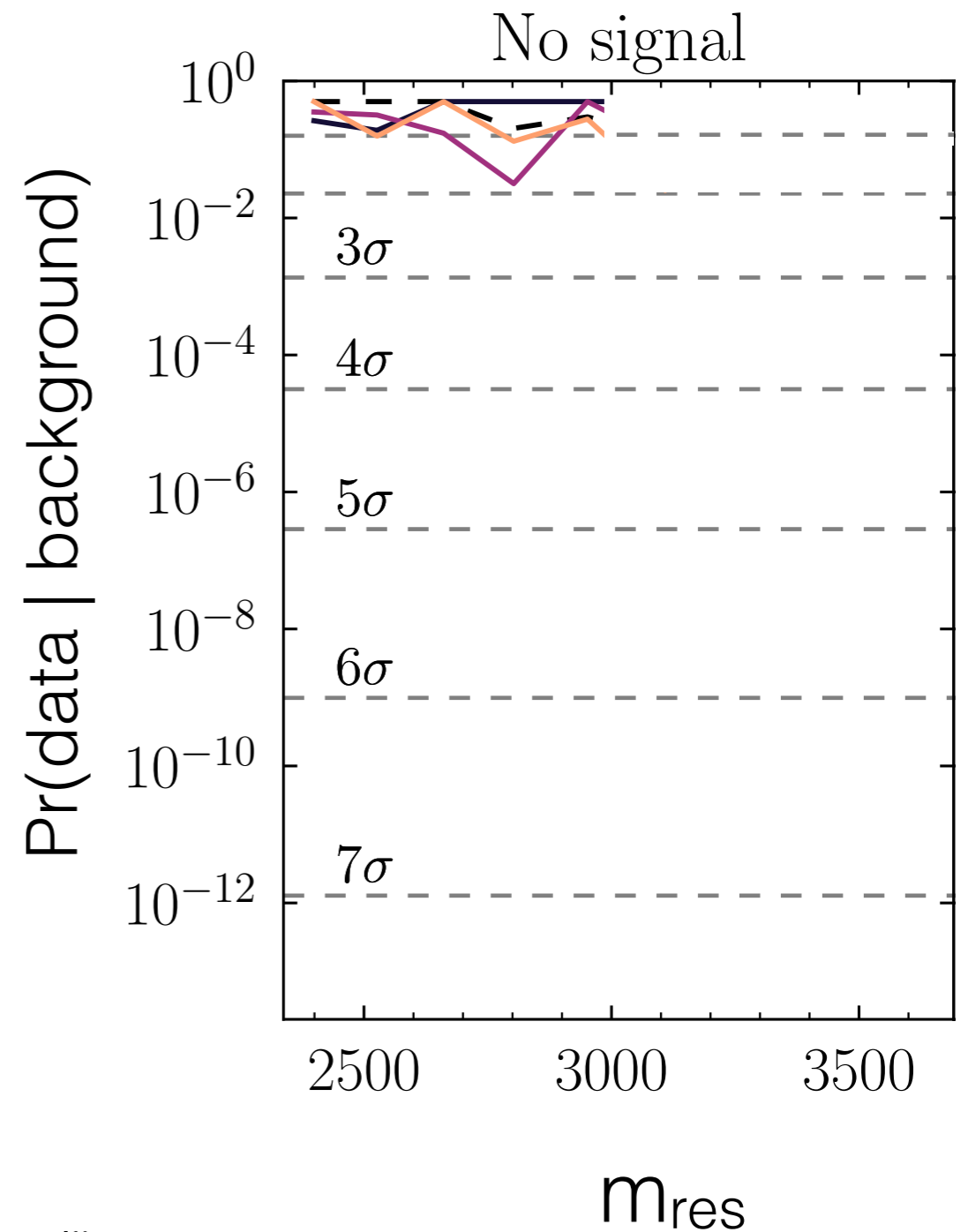
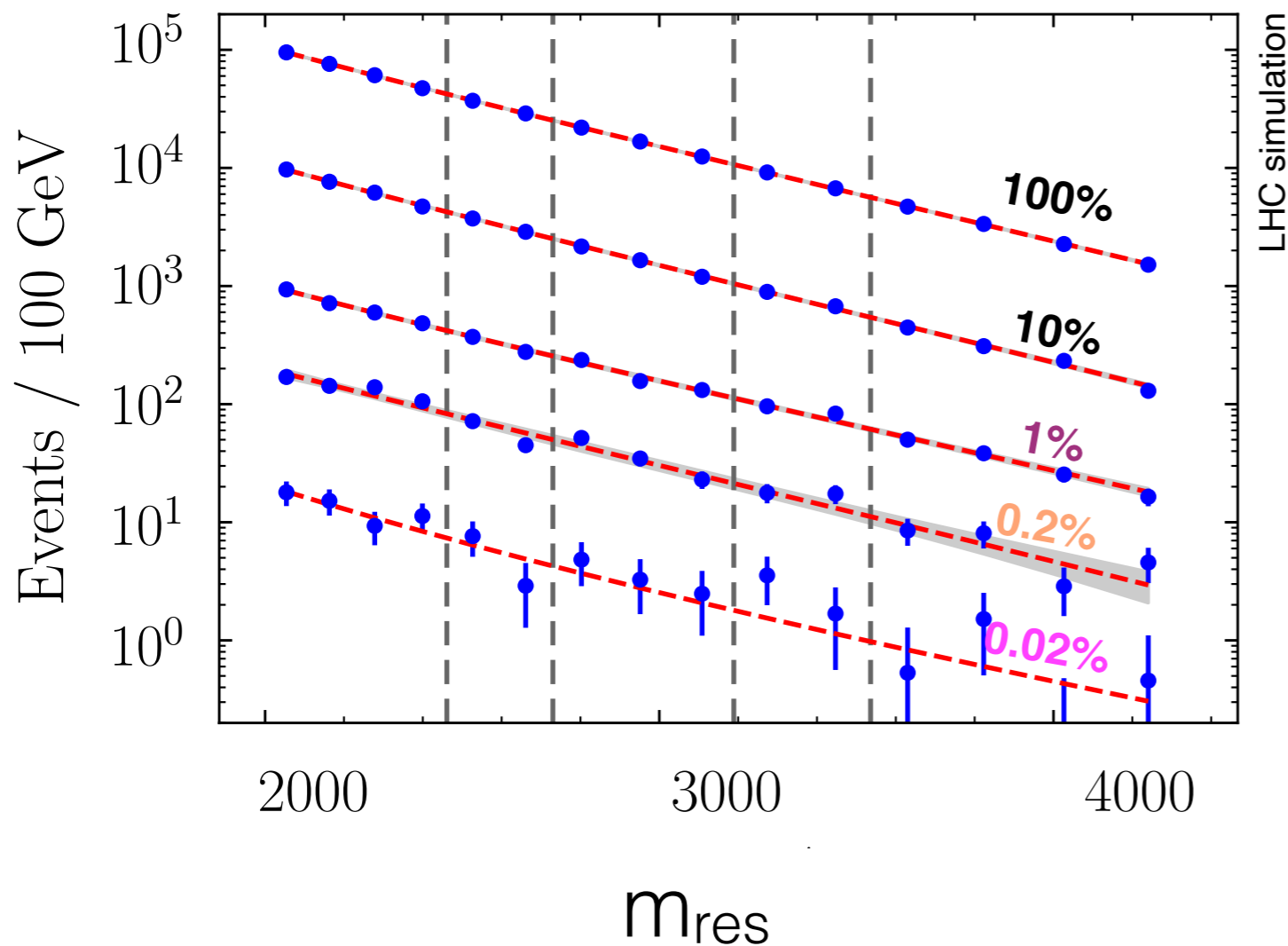
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

Example: two-jet search



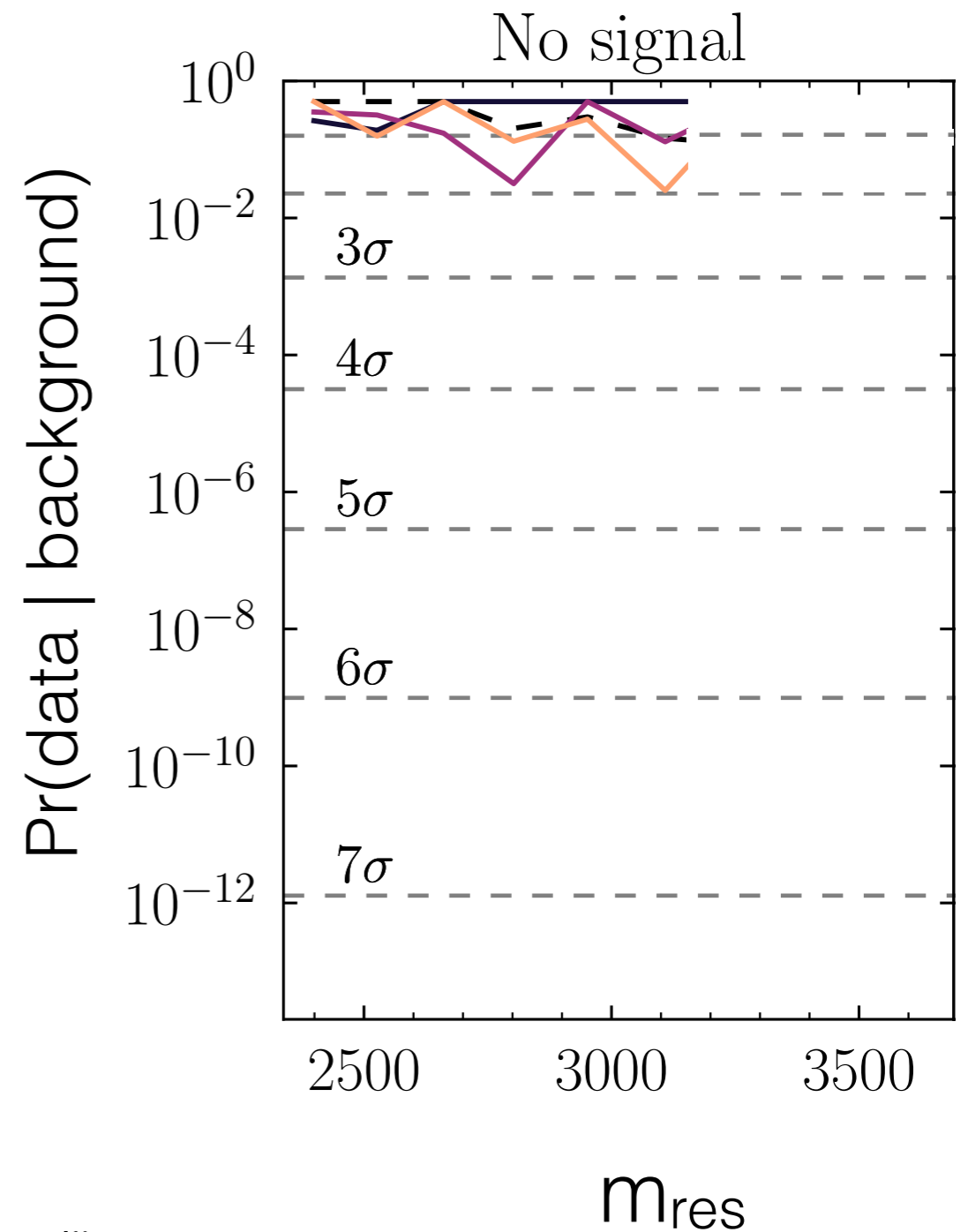
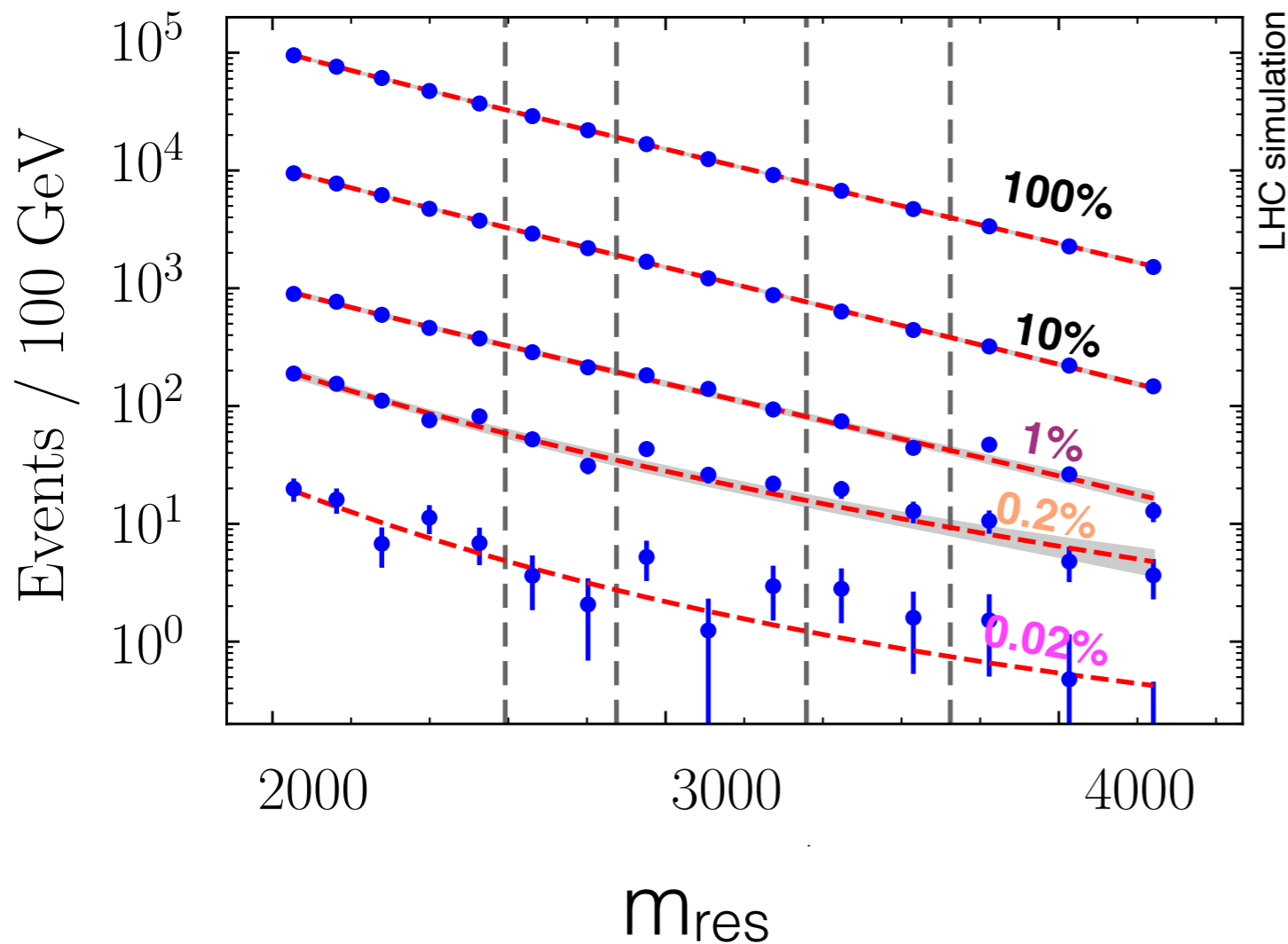
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

Example: two-jet search



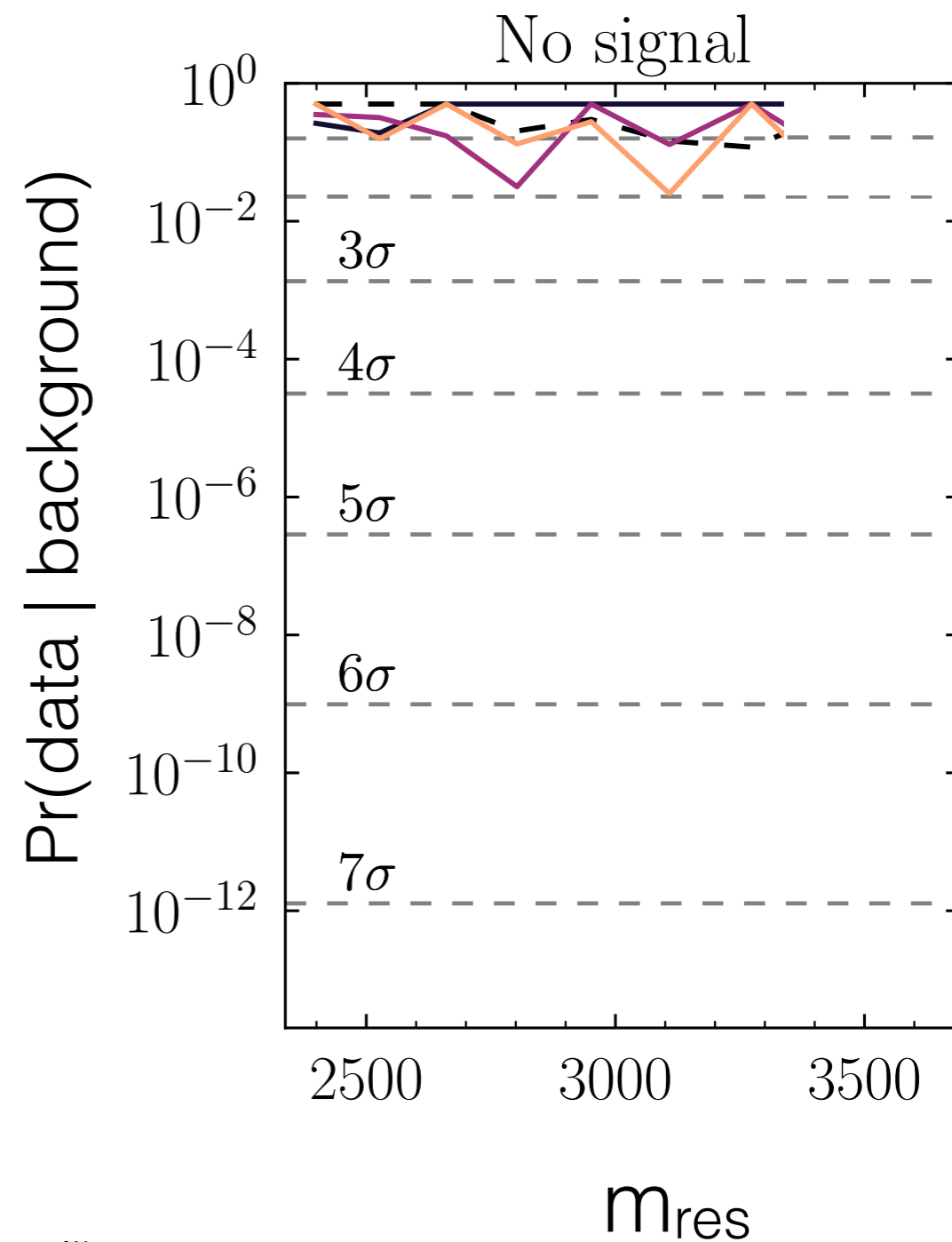
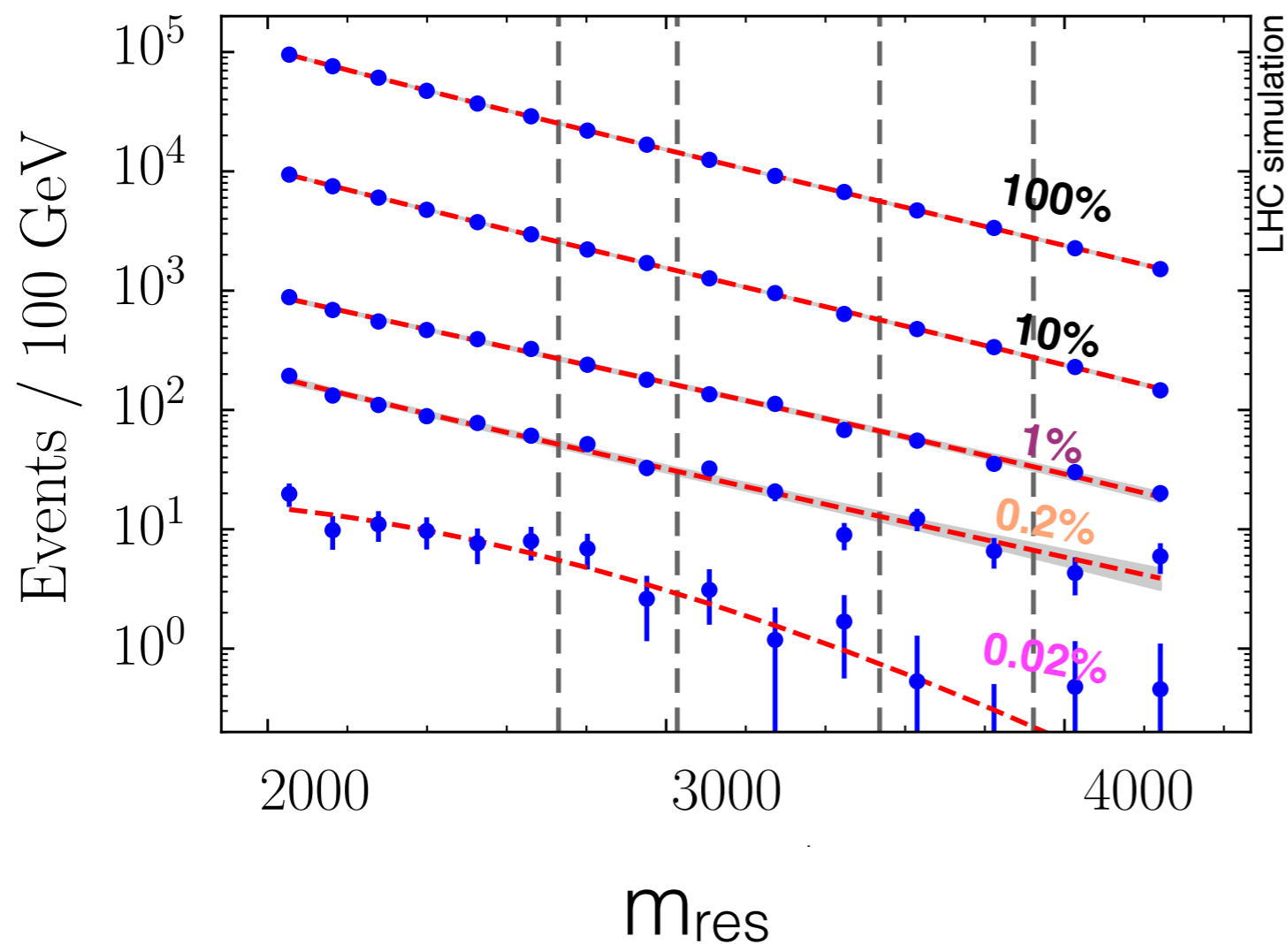
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

Example: two-jet search



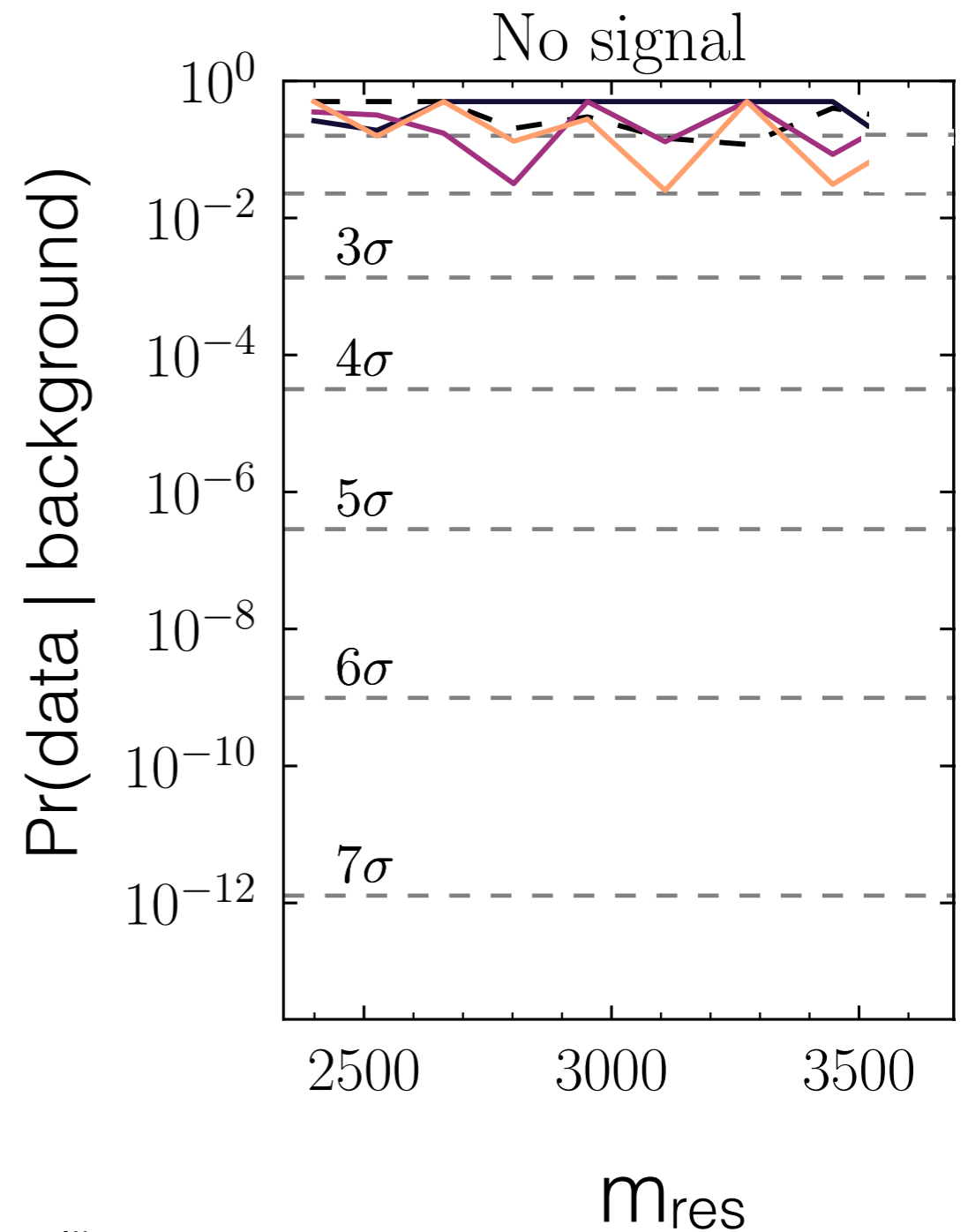
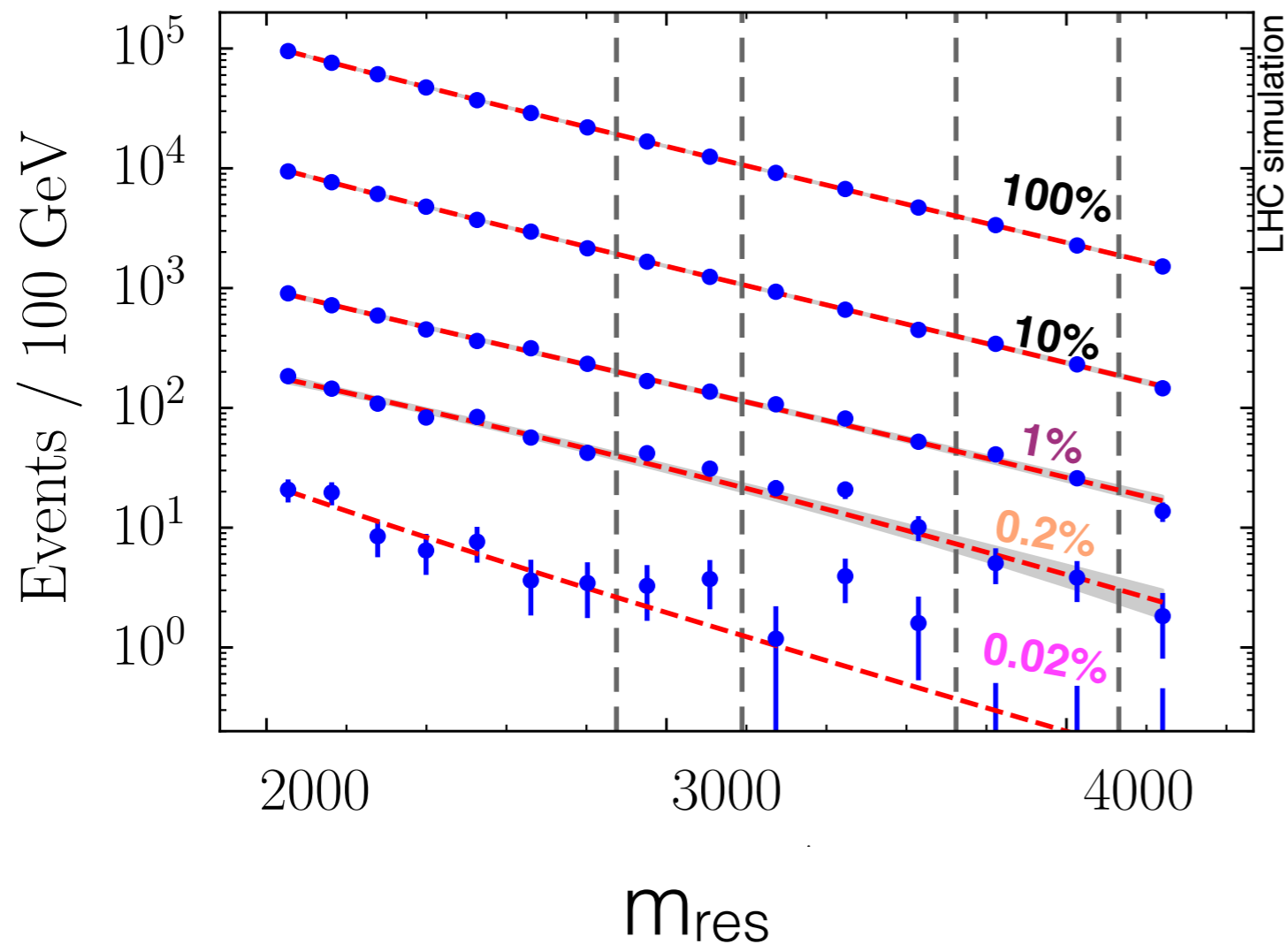
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

Example: two-jet search



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

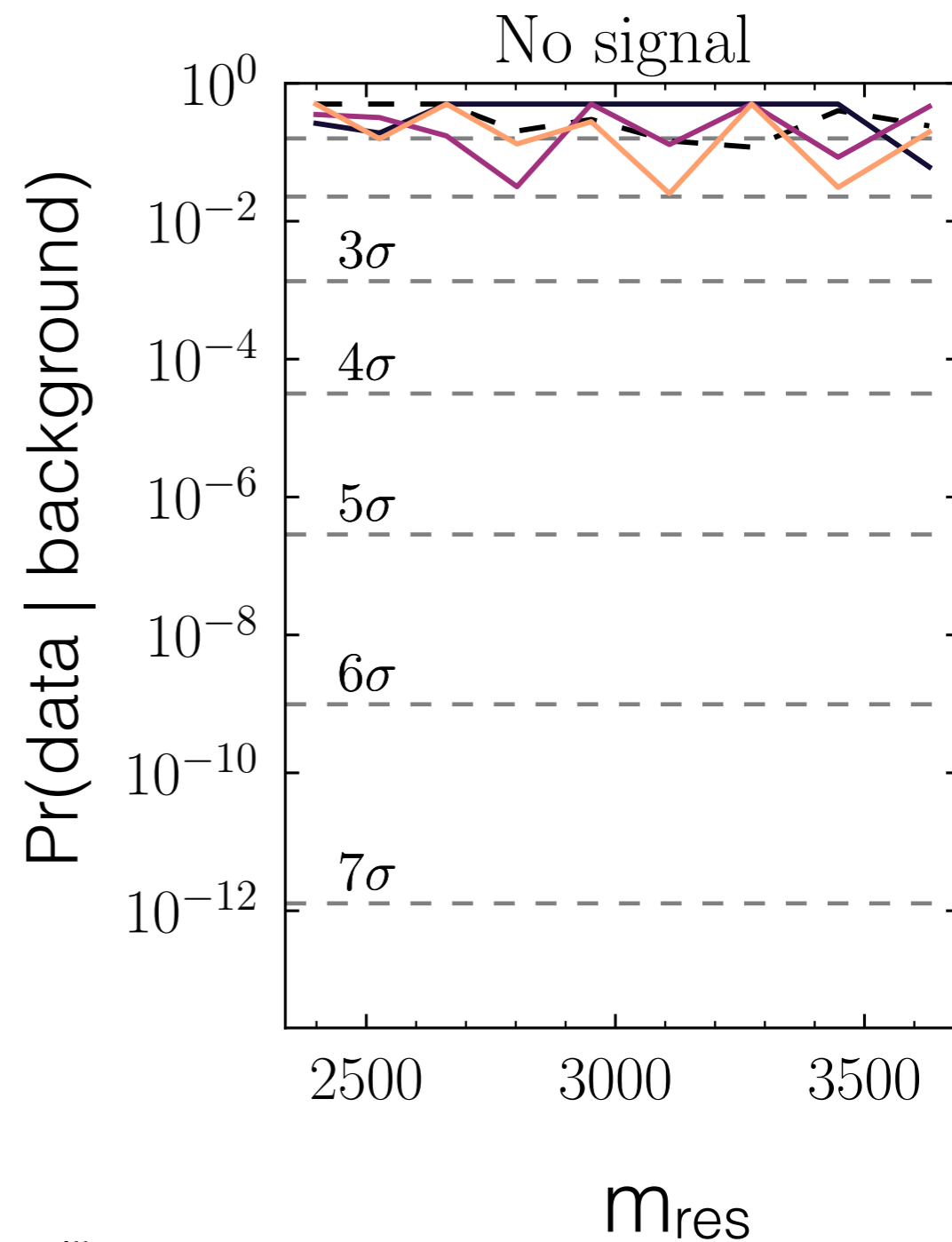
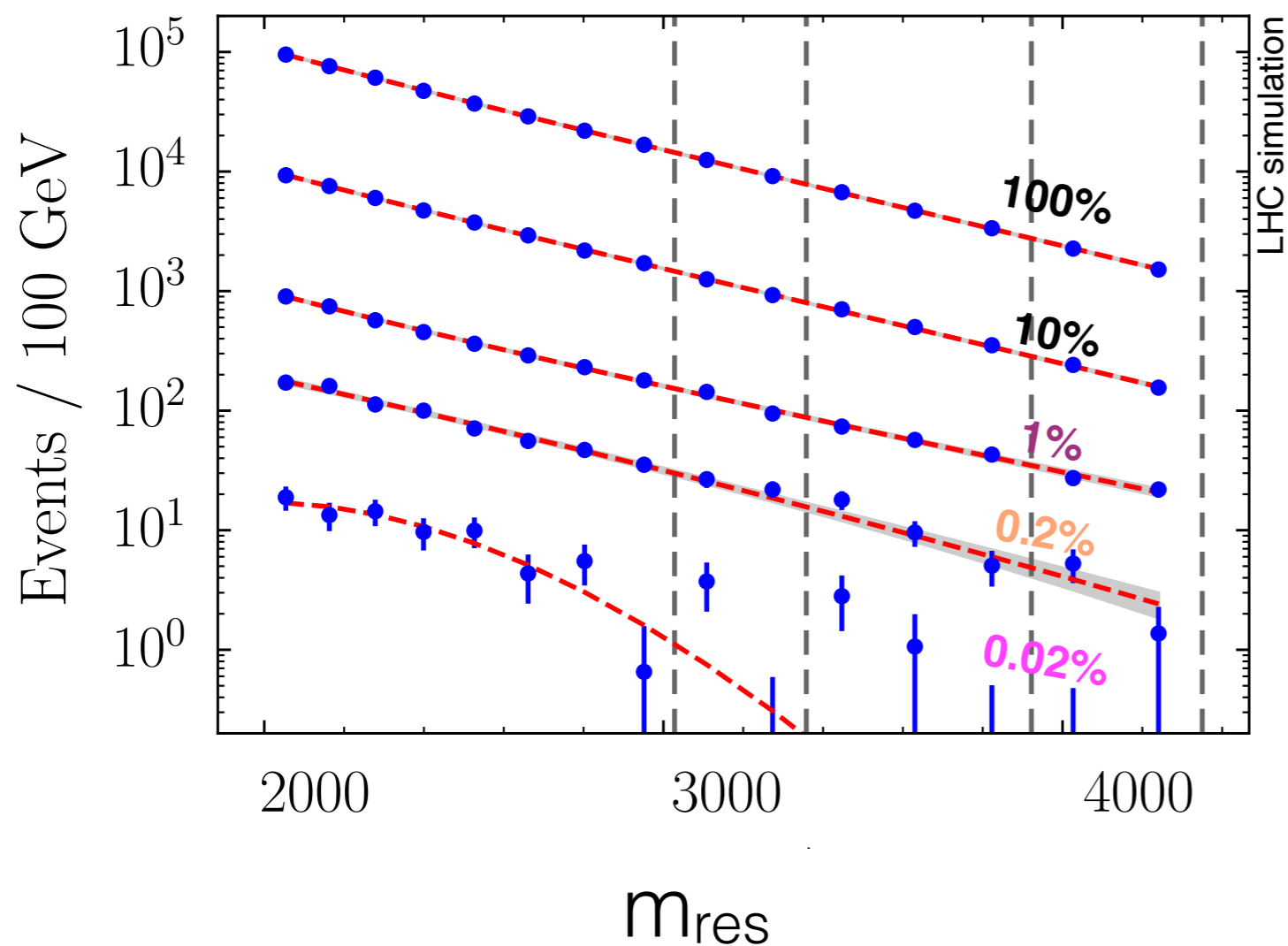
Example: two-jet search



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

Example: two-jet search

76

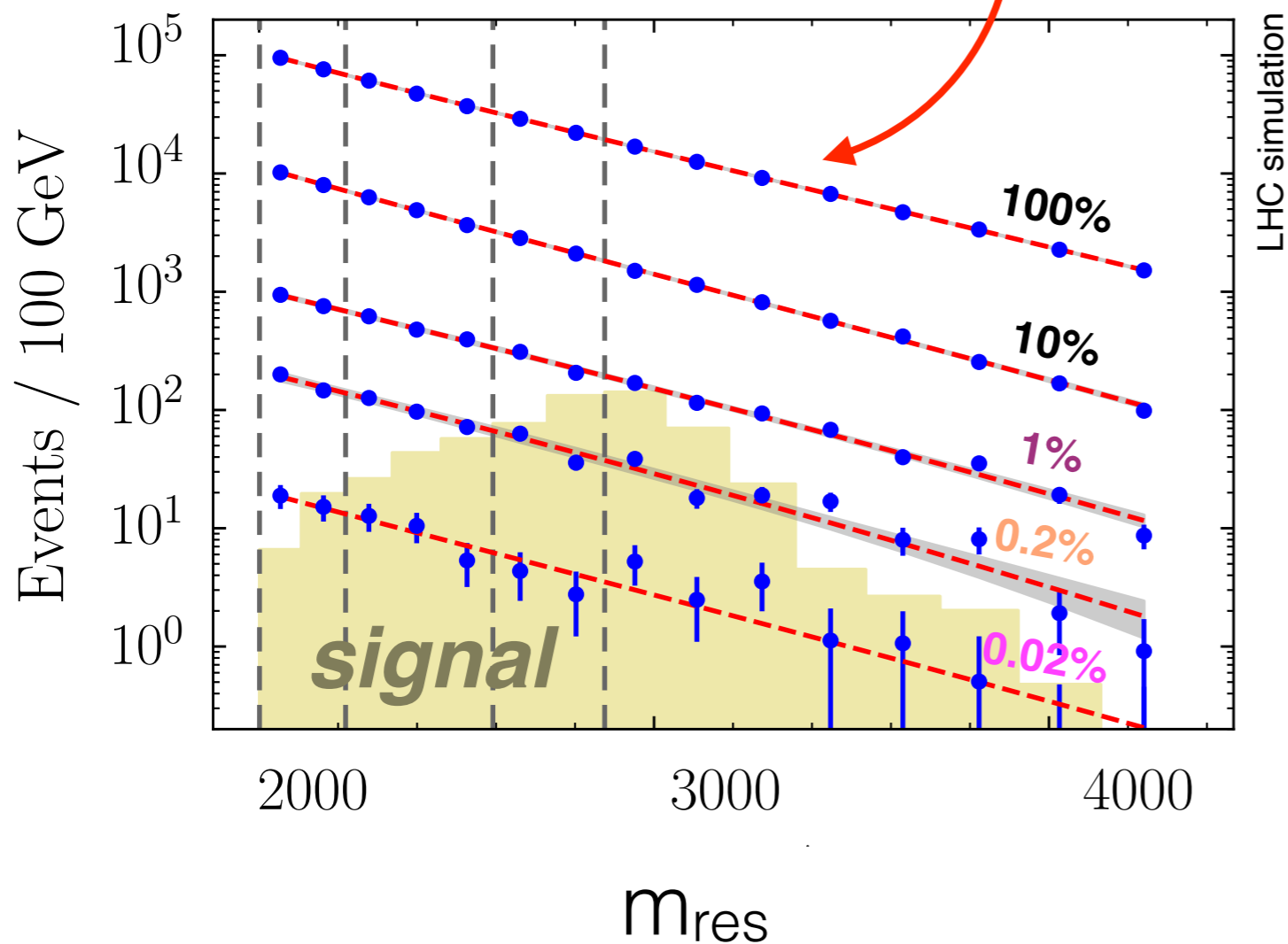


- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

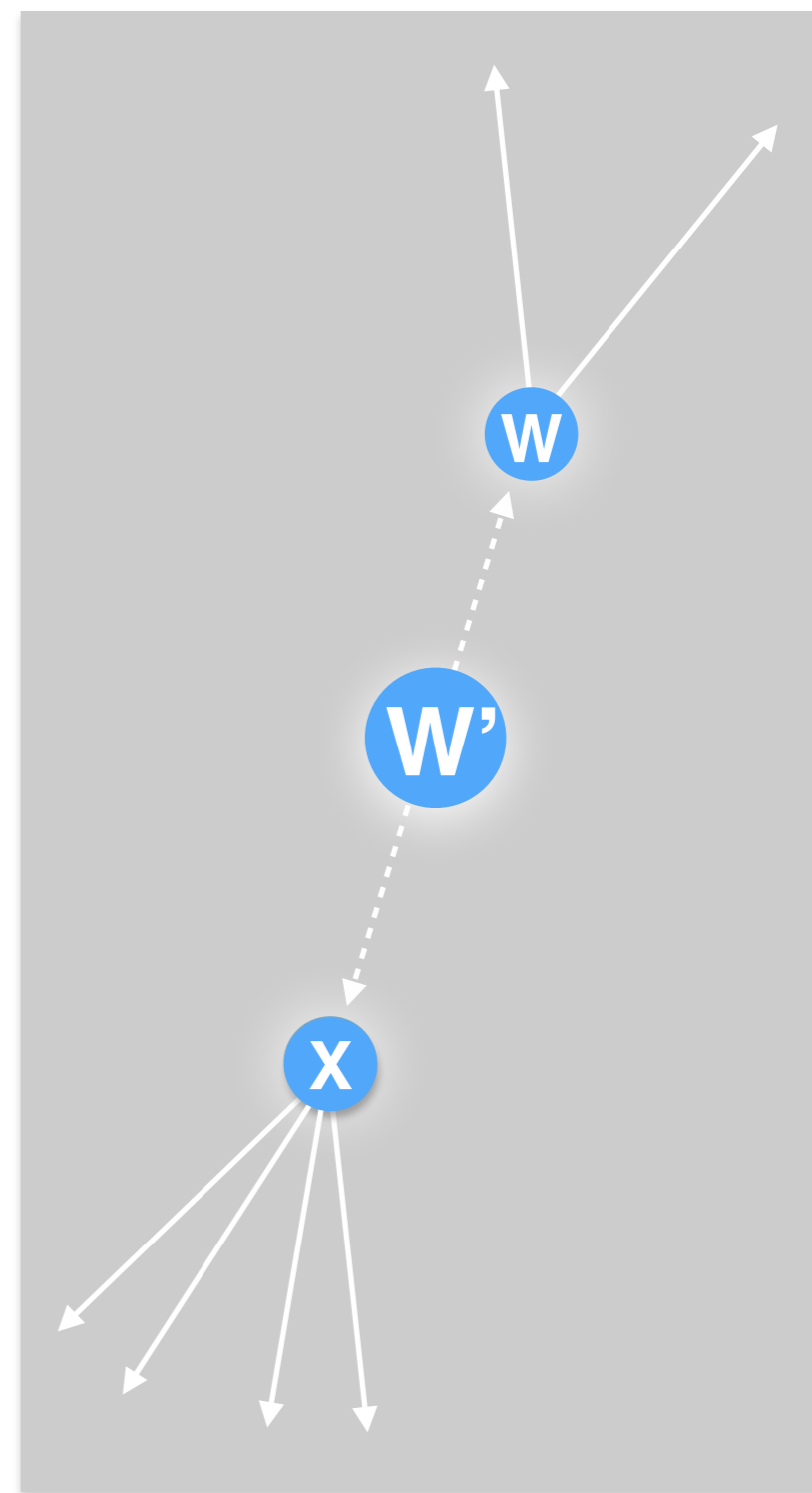
...and when there is a signal?

sidebands

standard parametric
fit to background.



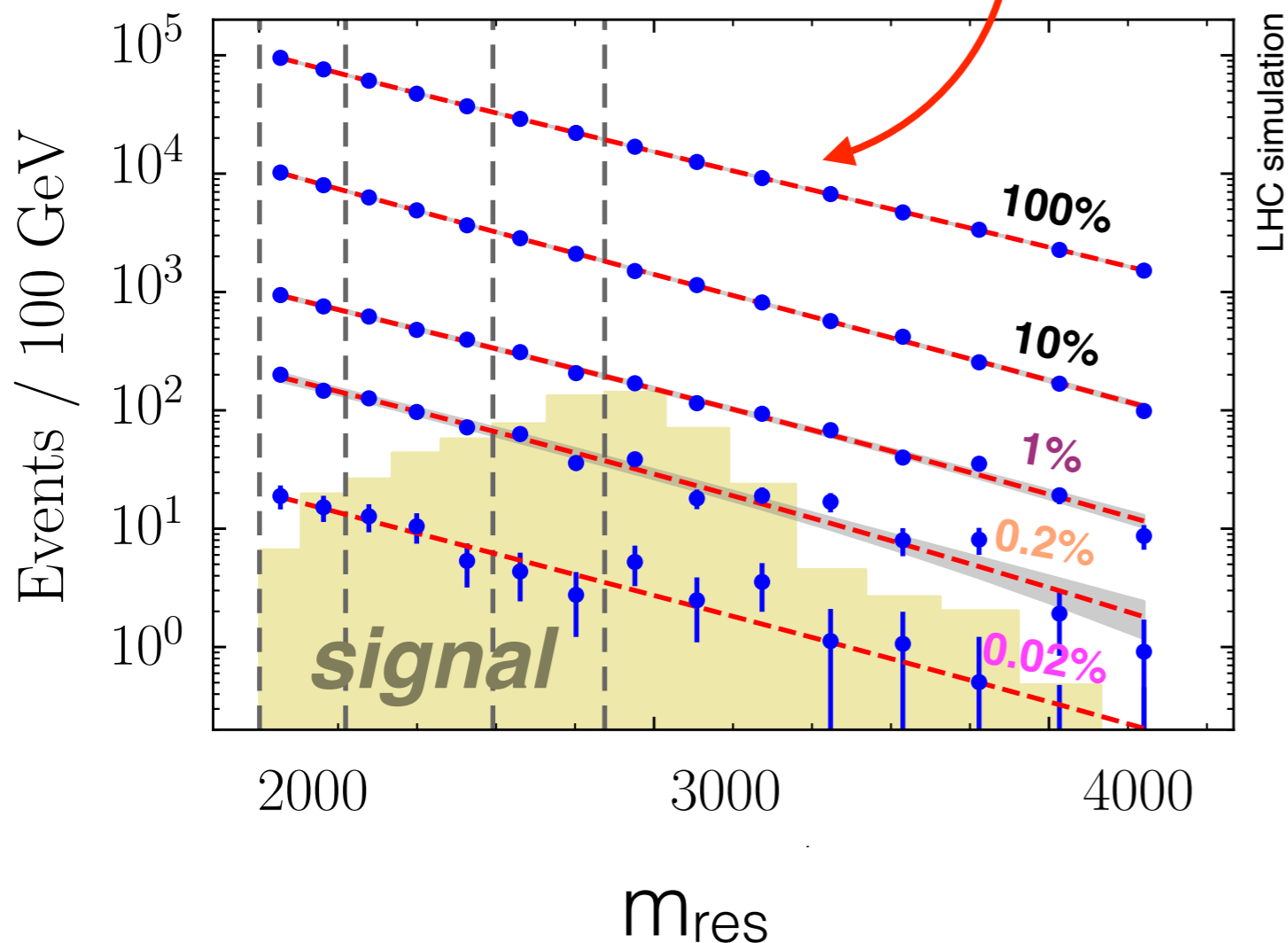
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like



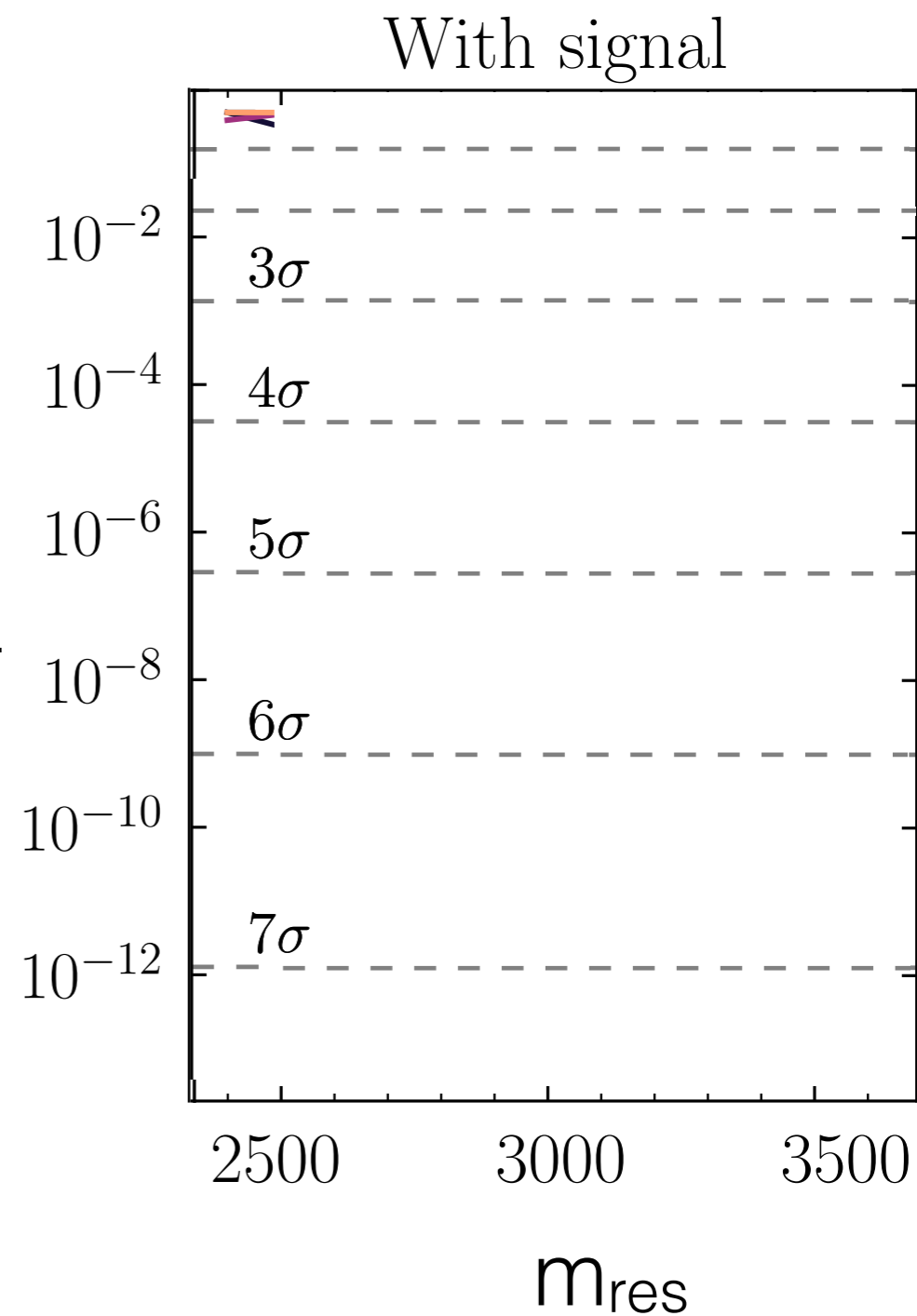
...and when there is a signal?

sidebands

standard parametric fit to background.

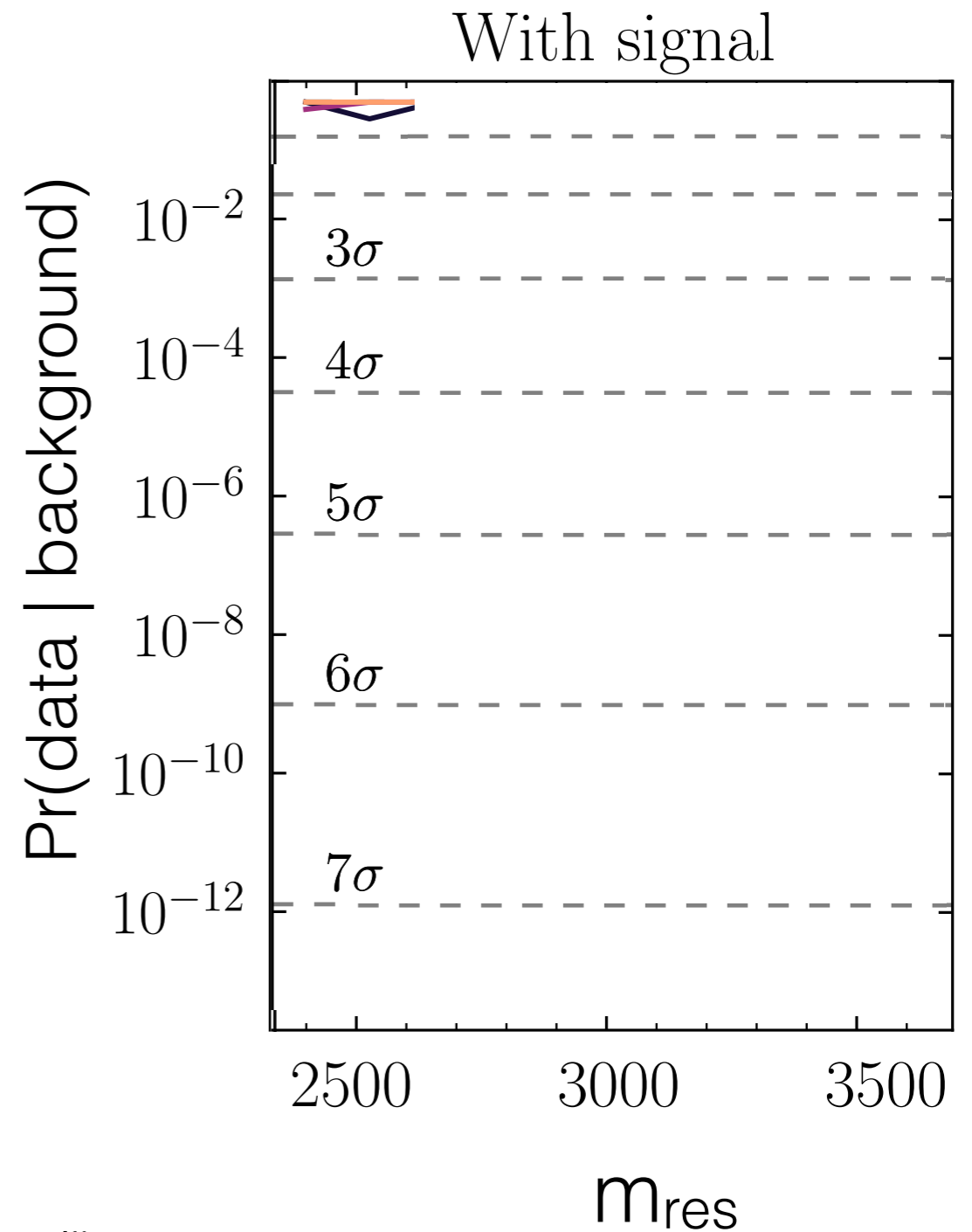
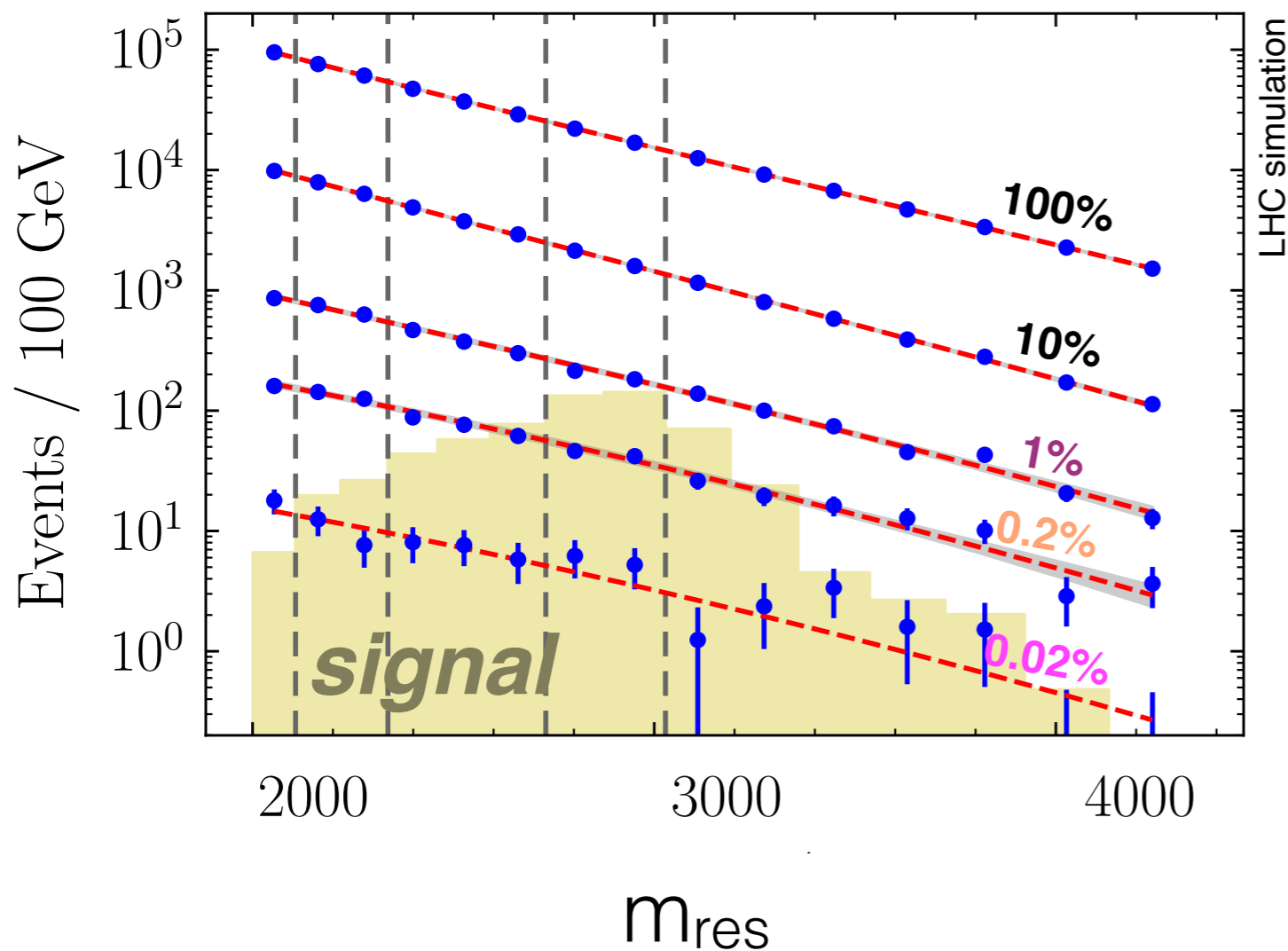


Pr(data | background)



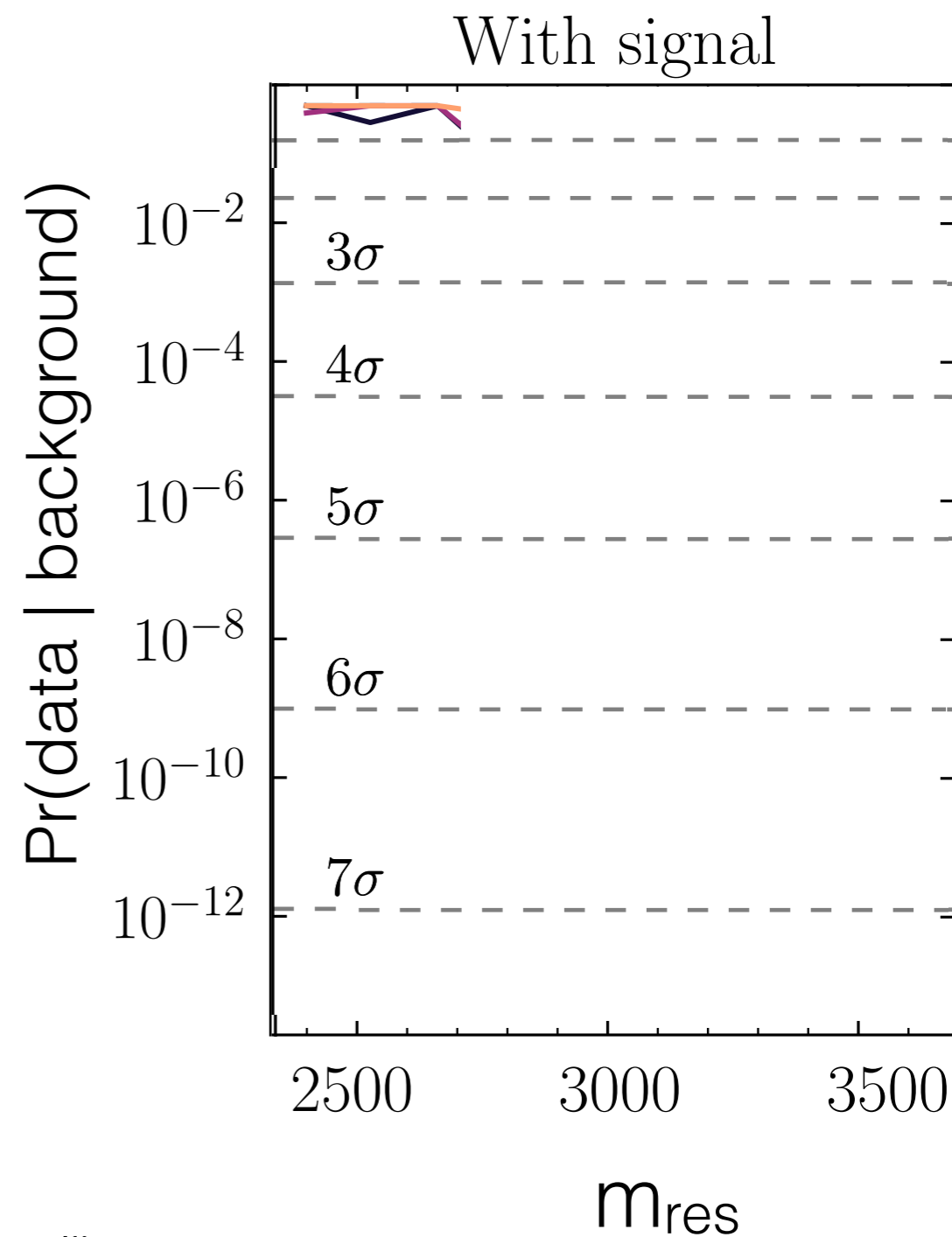
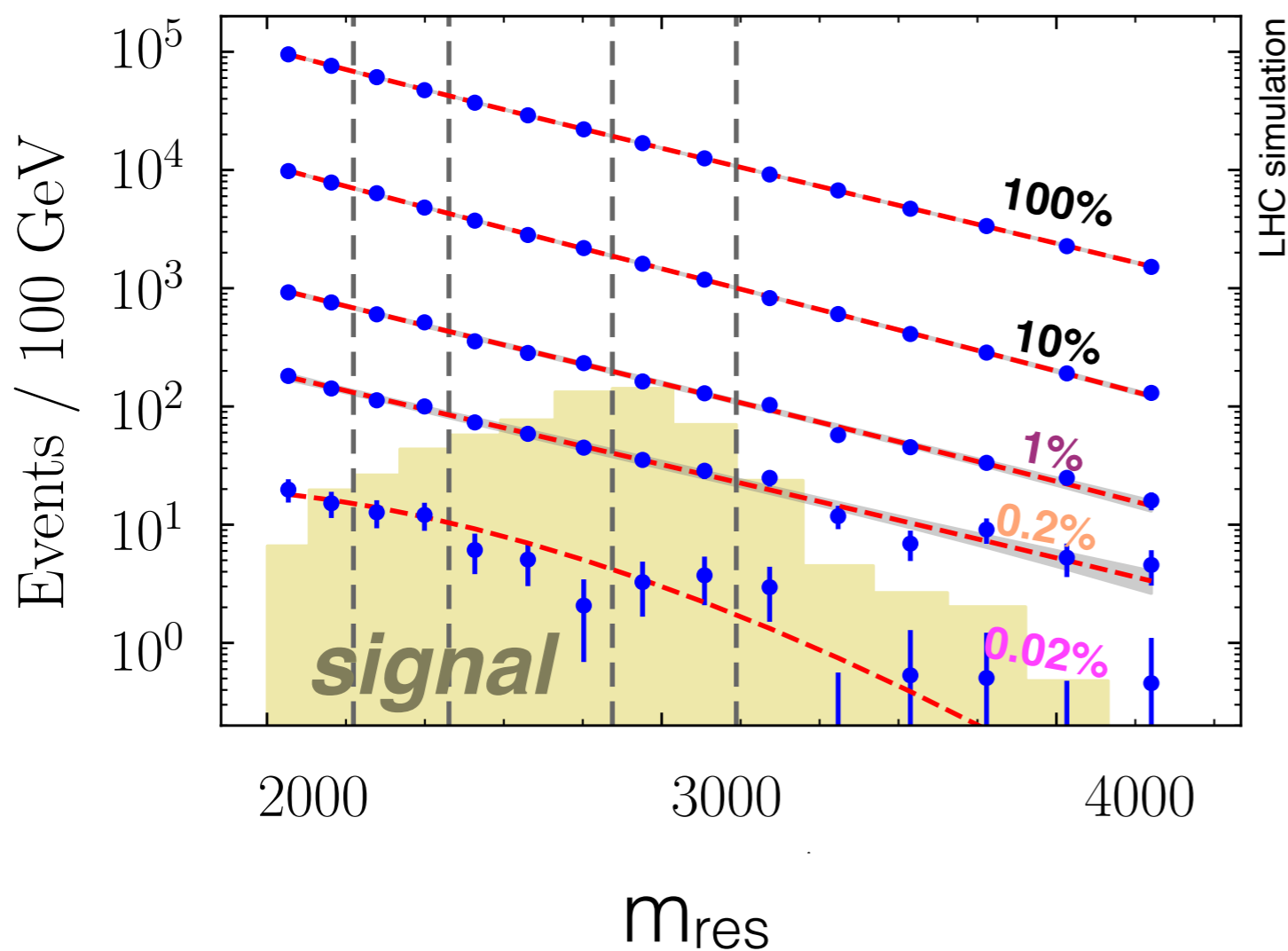
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

...and when there is a signal?



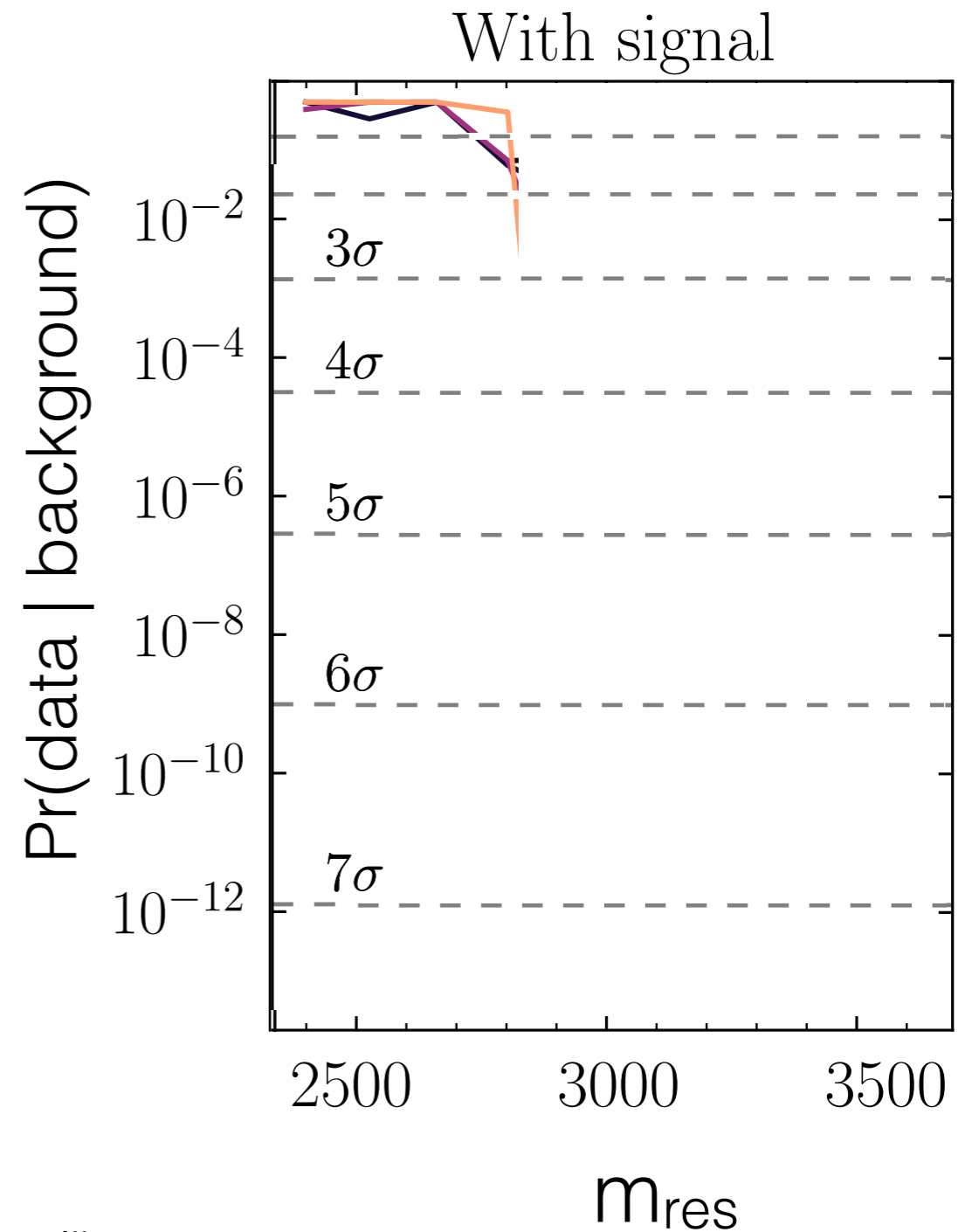
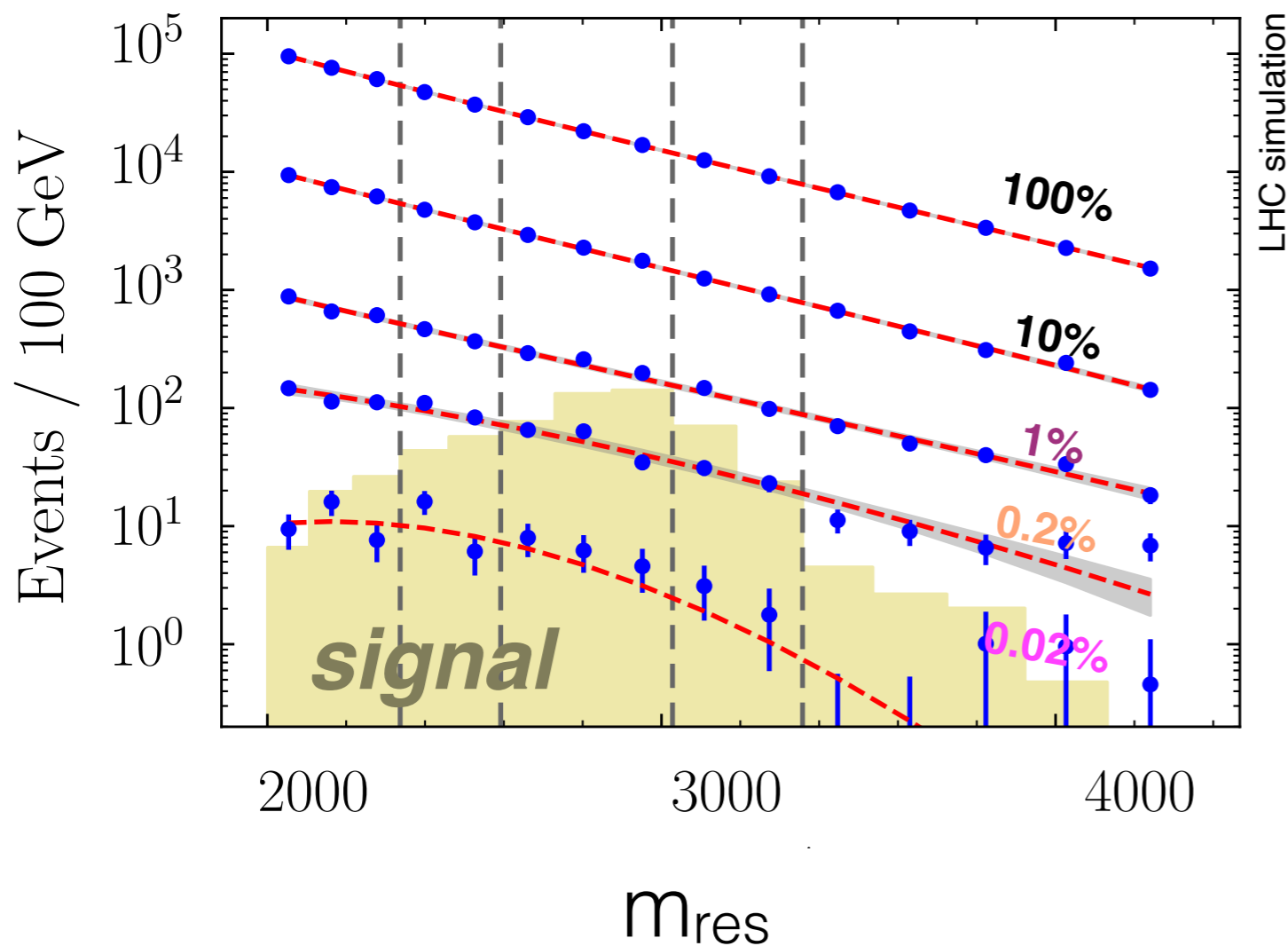
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

...and when there is a signal?



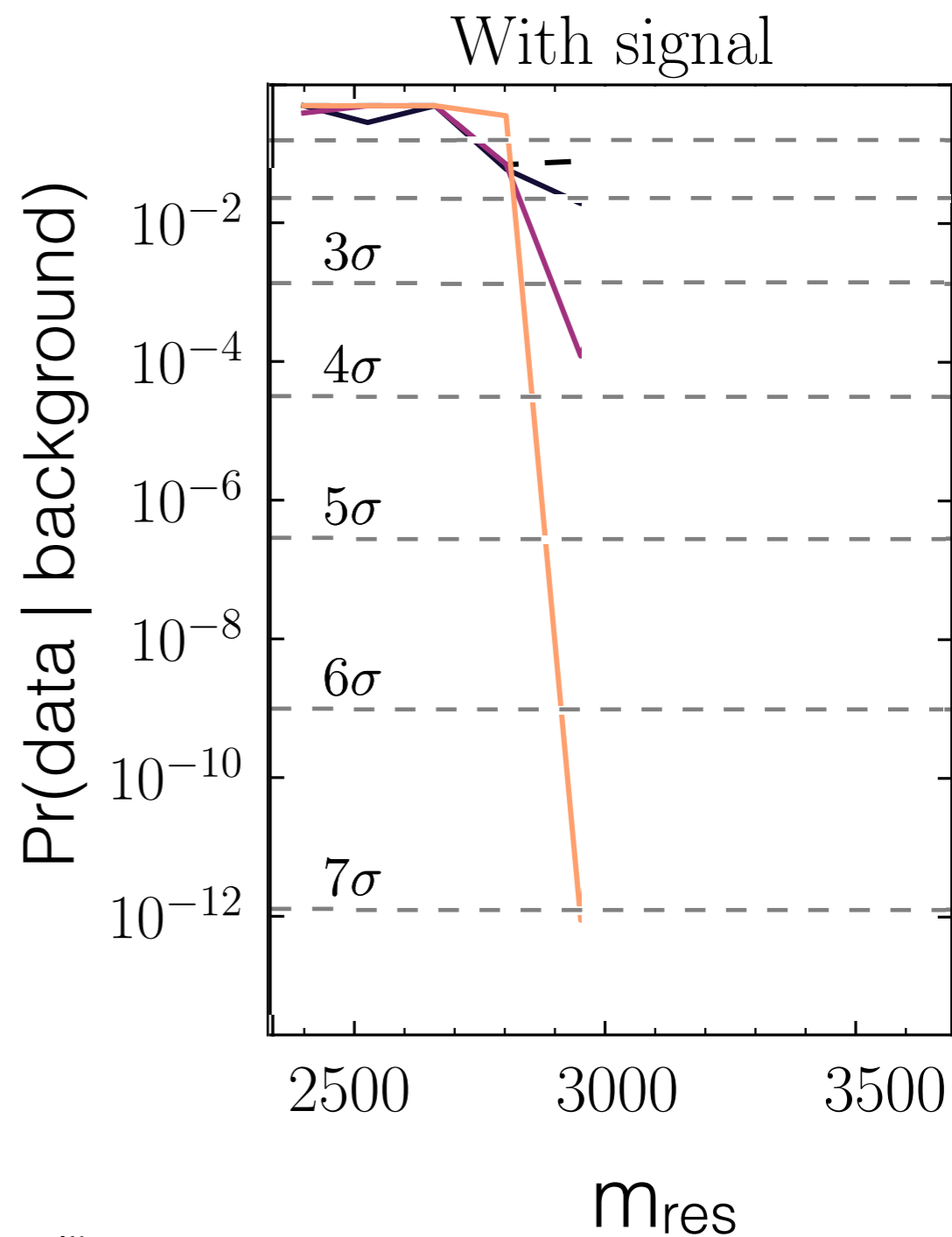
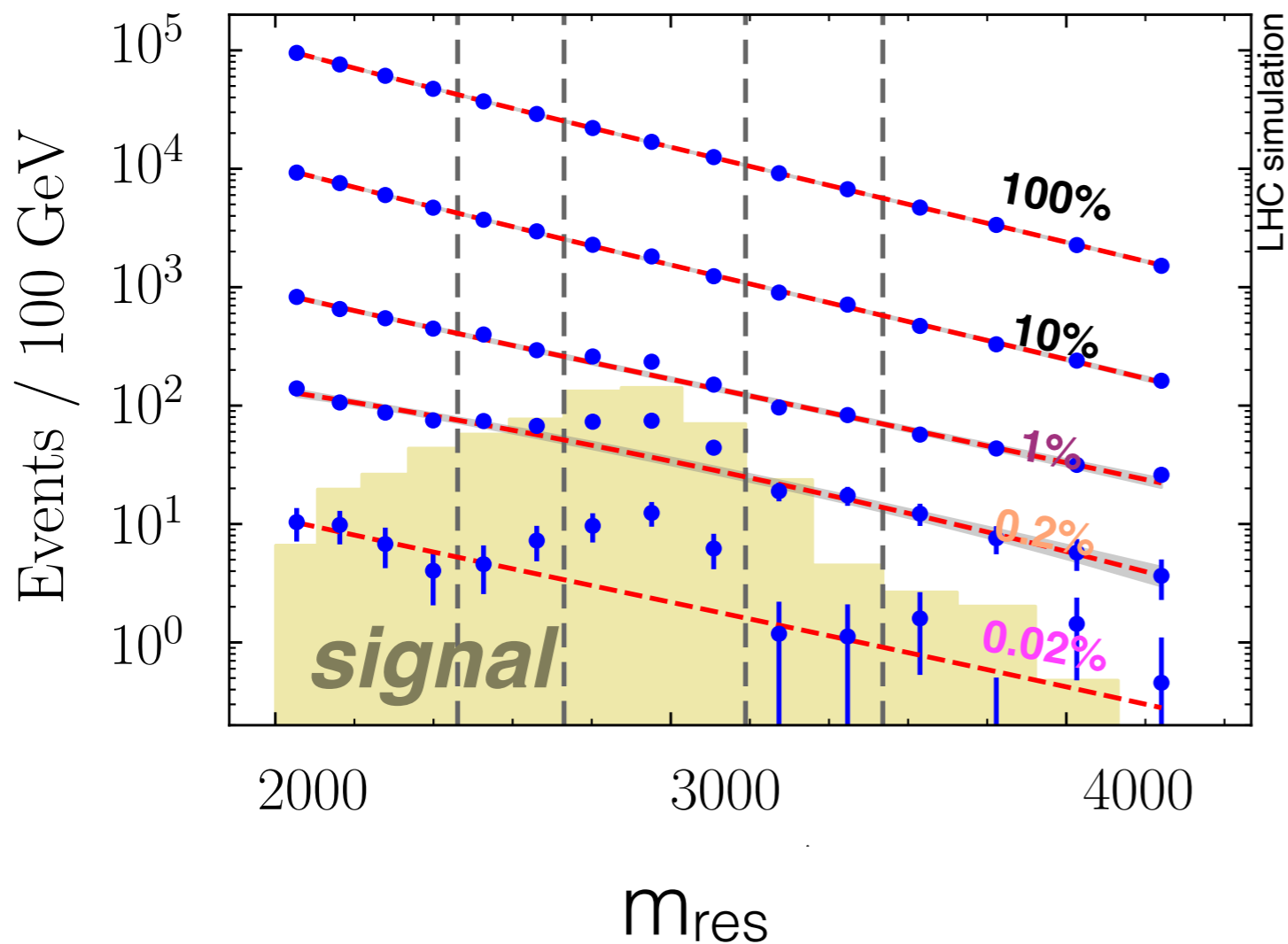
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

...and when there is a signal?



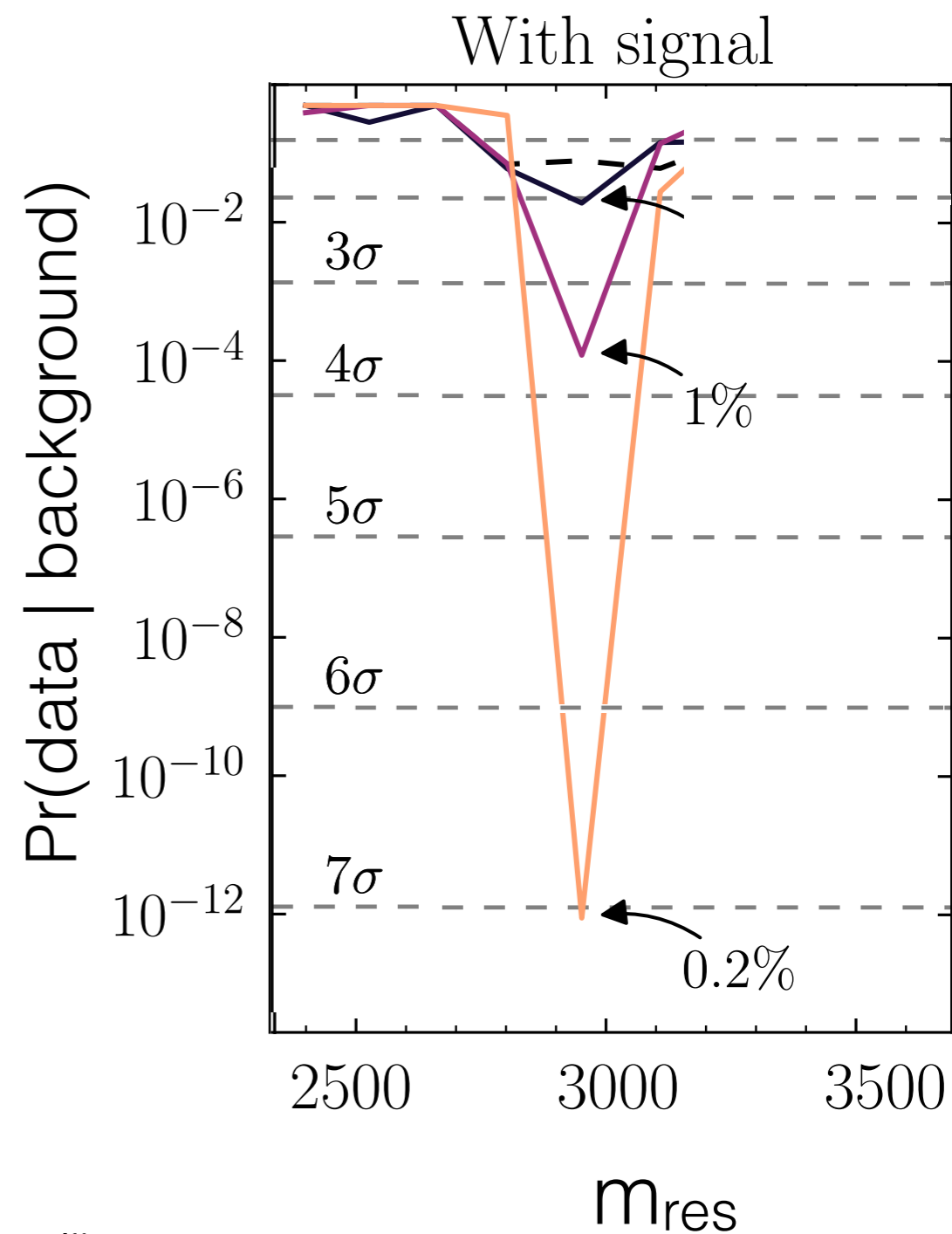
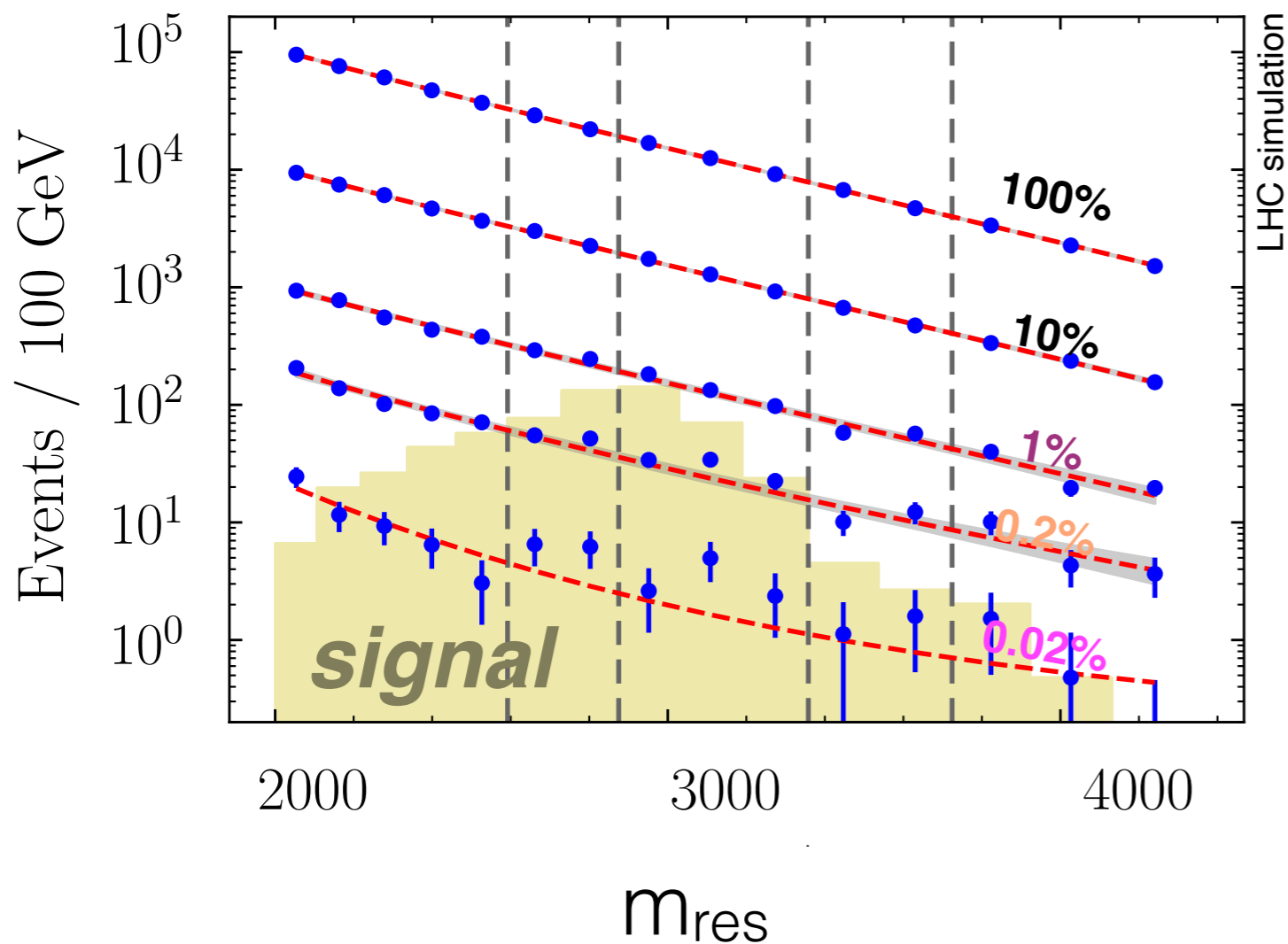
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

...and when there is a signal?



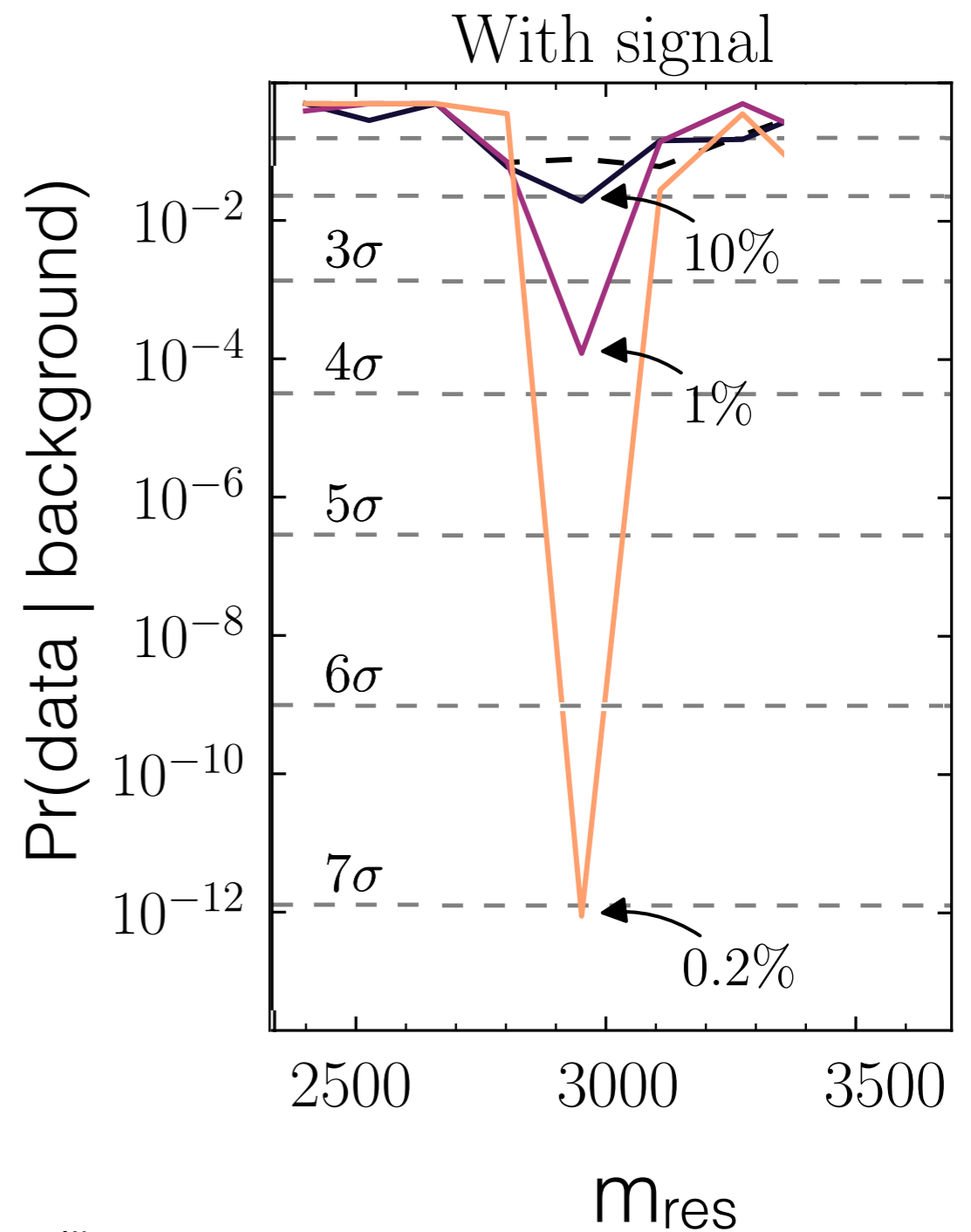
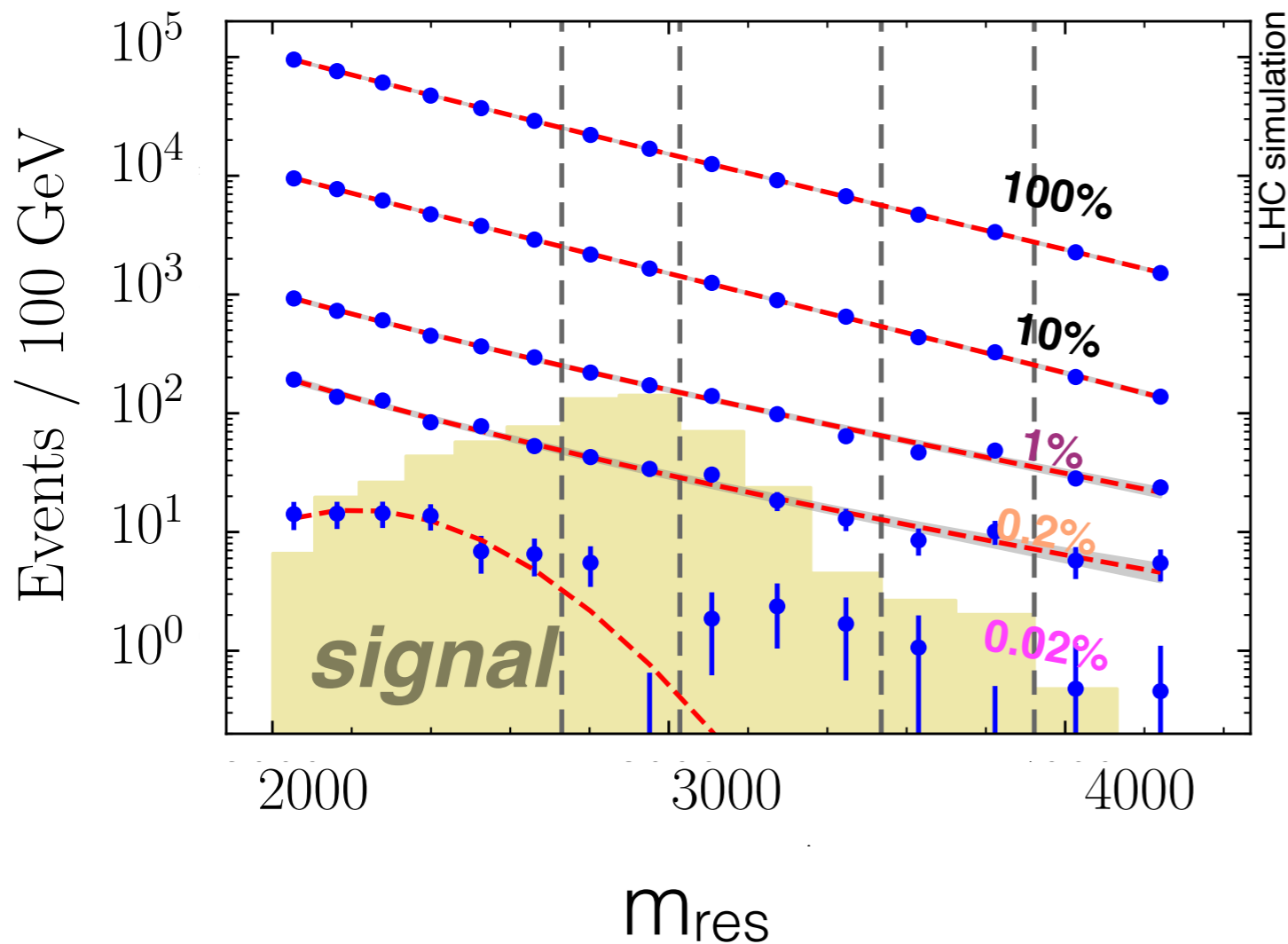
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

...and when there is a signal?



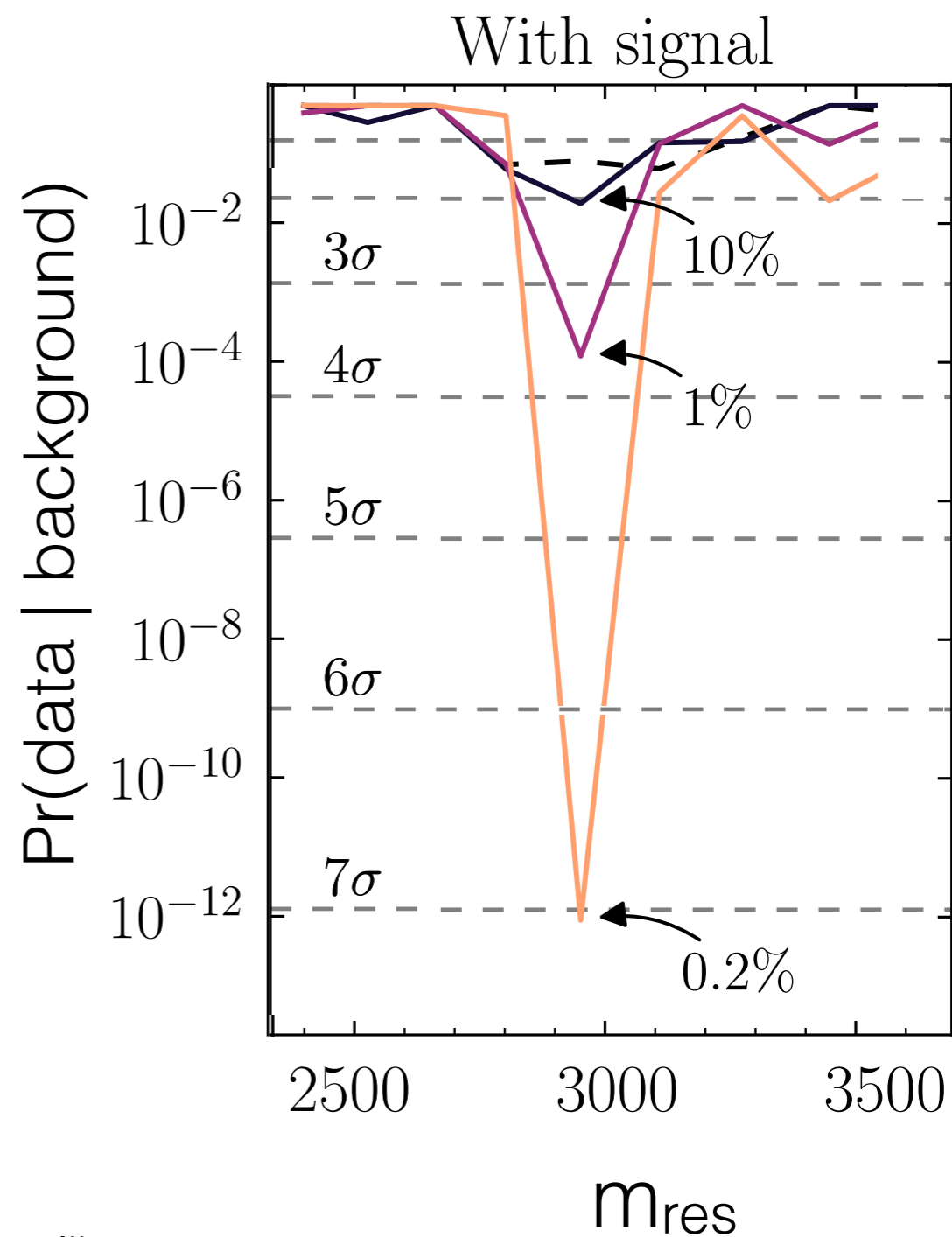
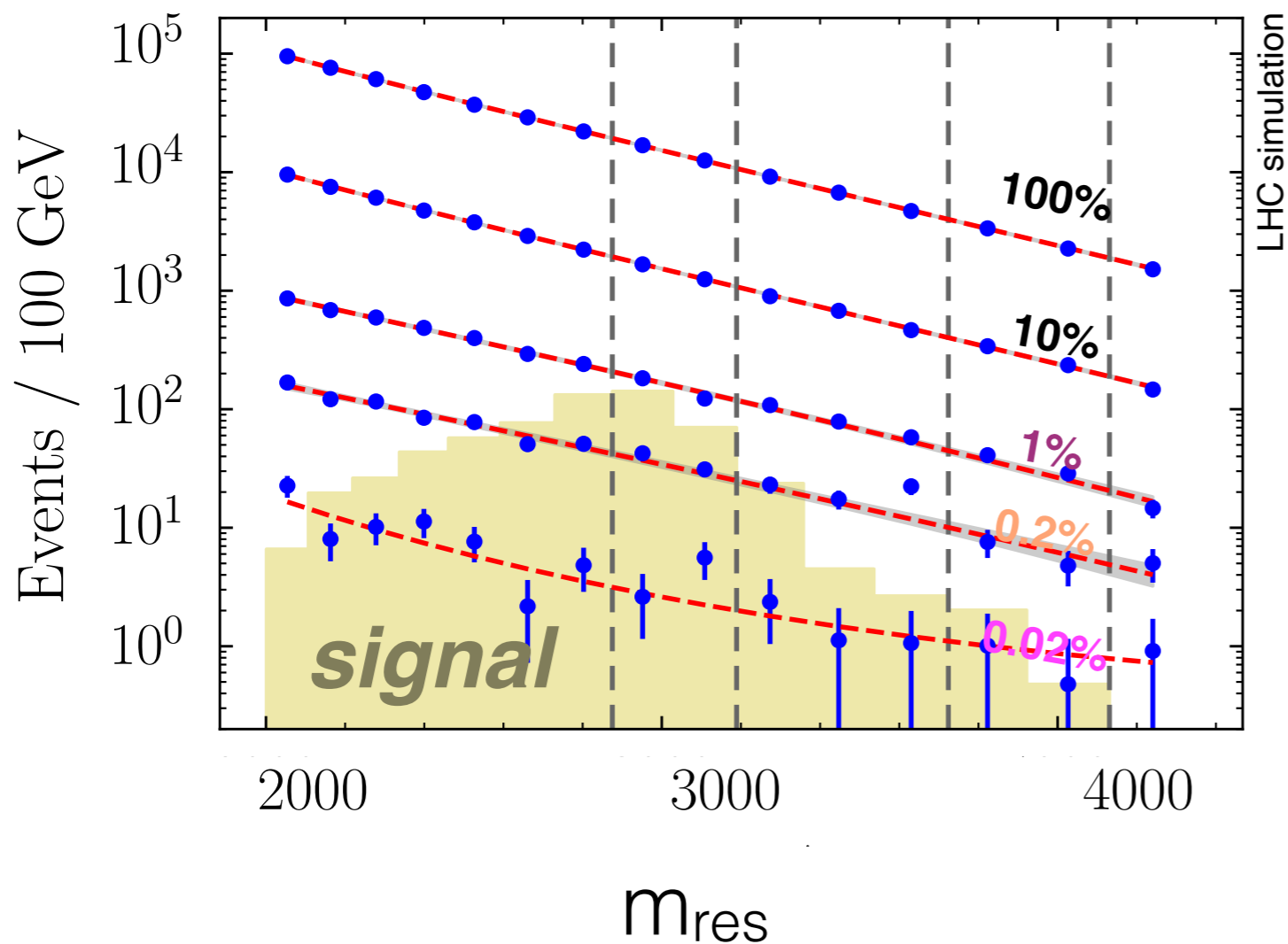
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

...and when there is a signal?



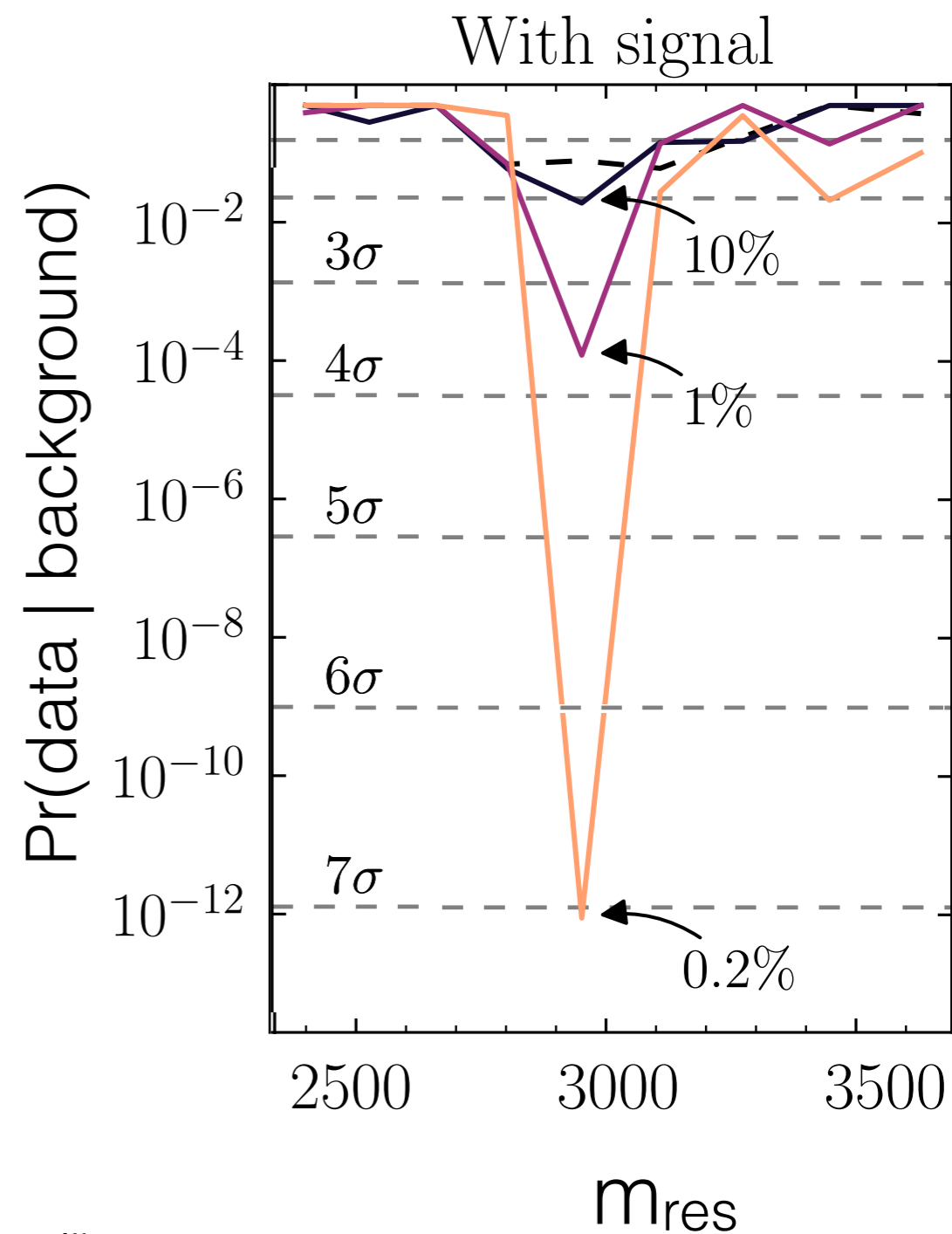
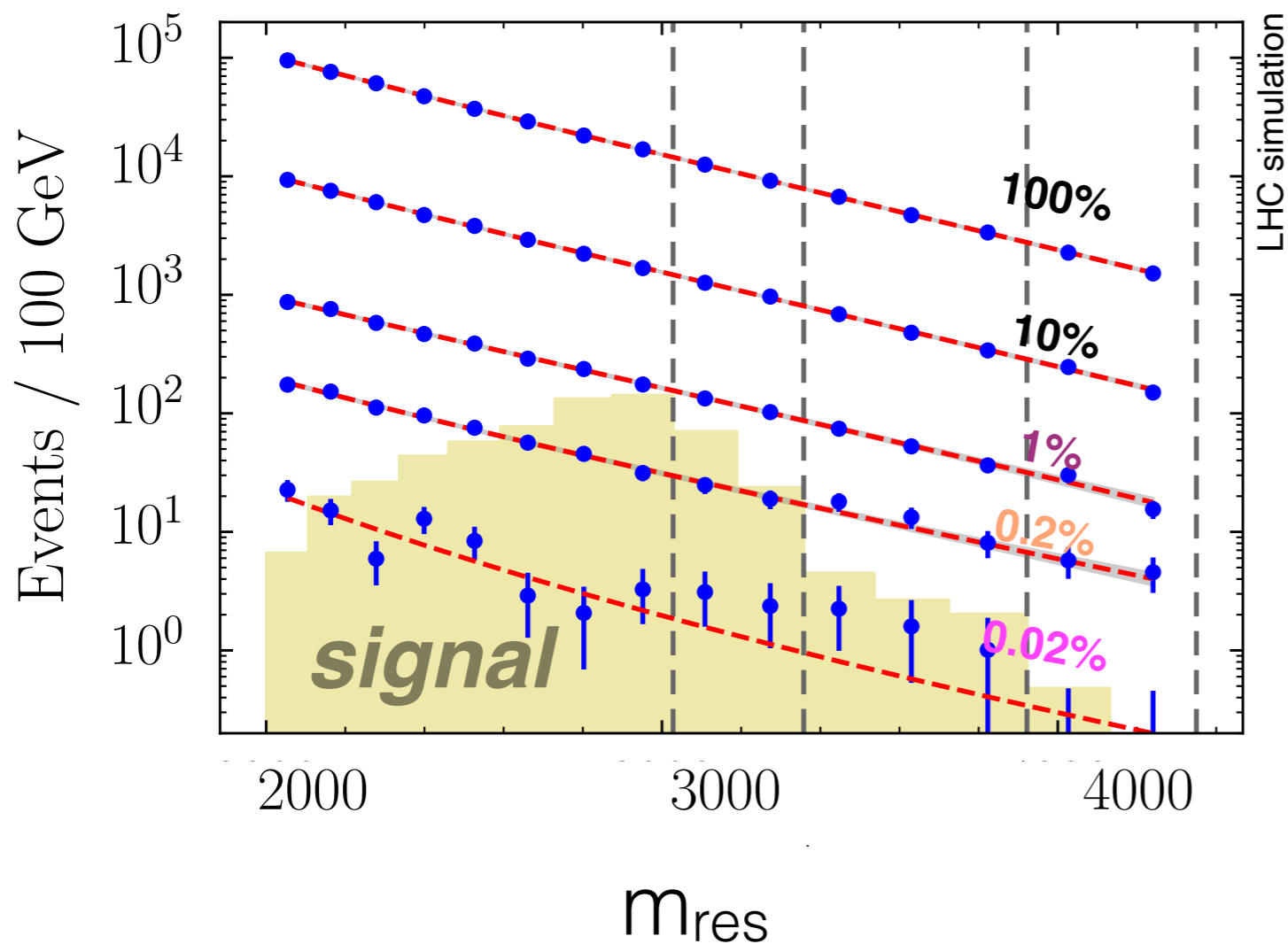
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

...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?



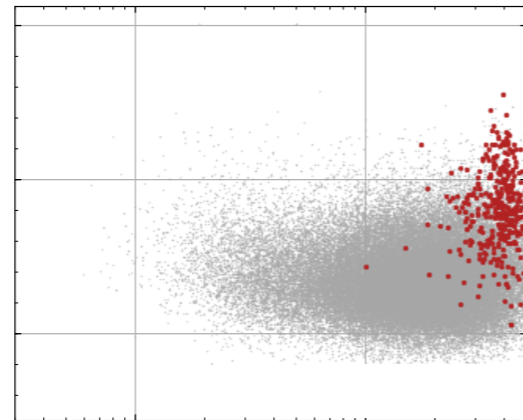
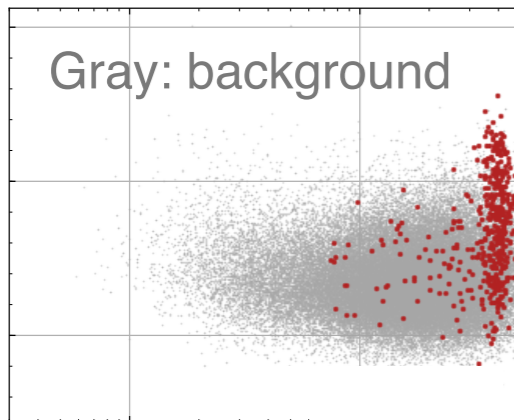
- no cut on NN
- most 10% signal-region-like
- most 1% signal-region-like
- most 0.2% signal-region-like

What is the network learning?

Truth signal

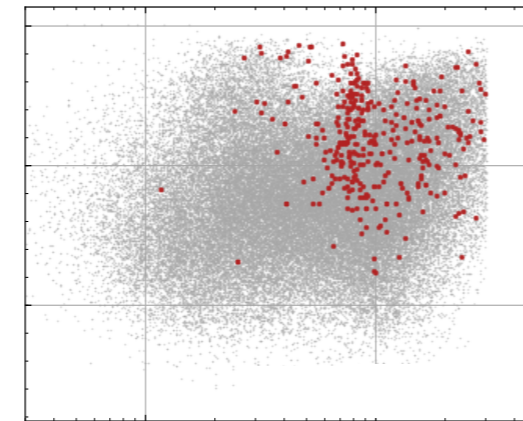
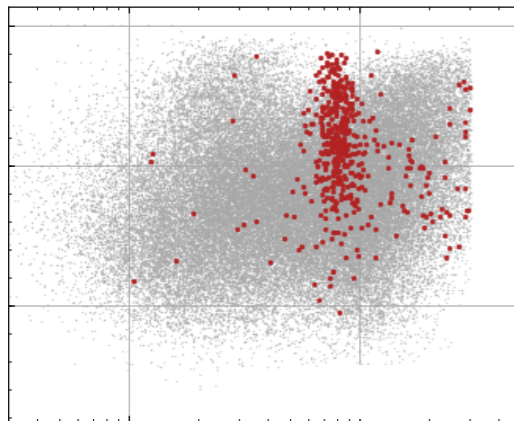
NN cut at 0.2%

Pr(4 prongs)



Heavier
Jet

Pr(2 prongs)

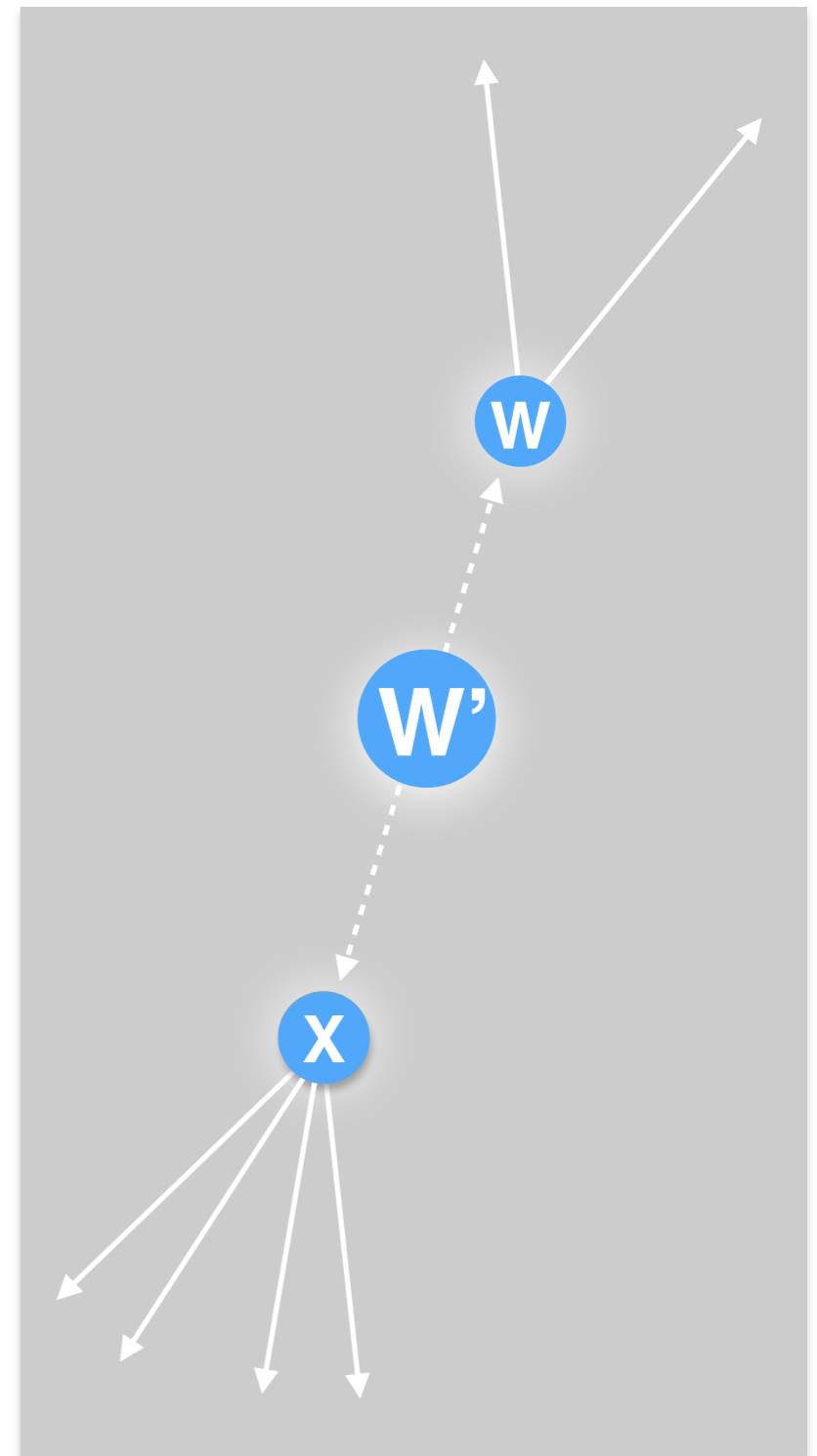


Lighter
Jet

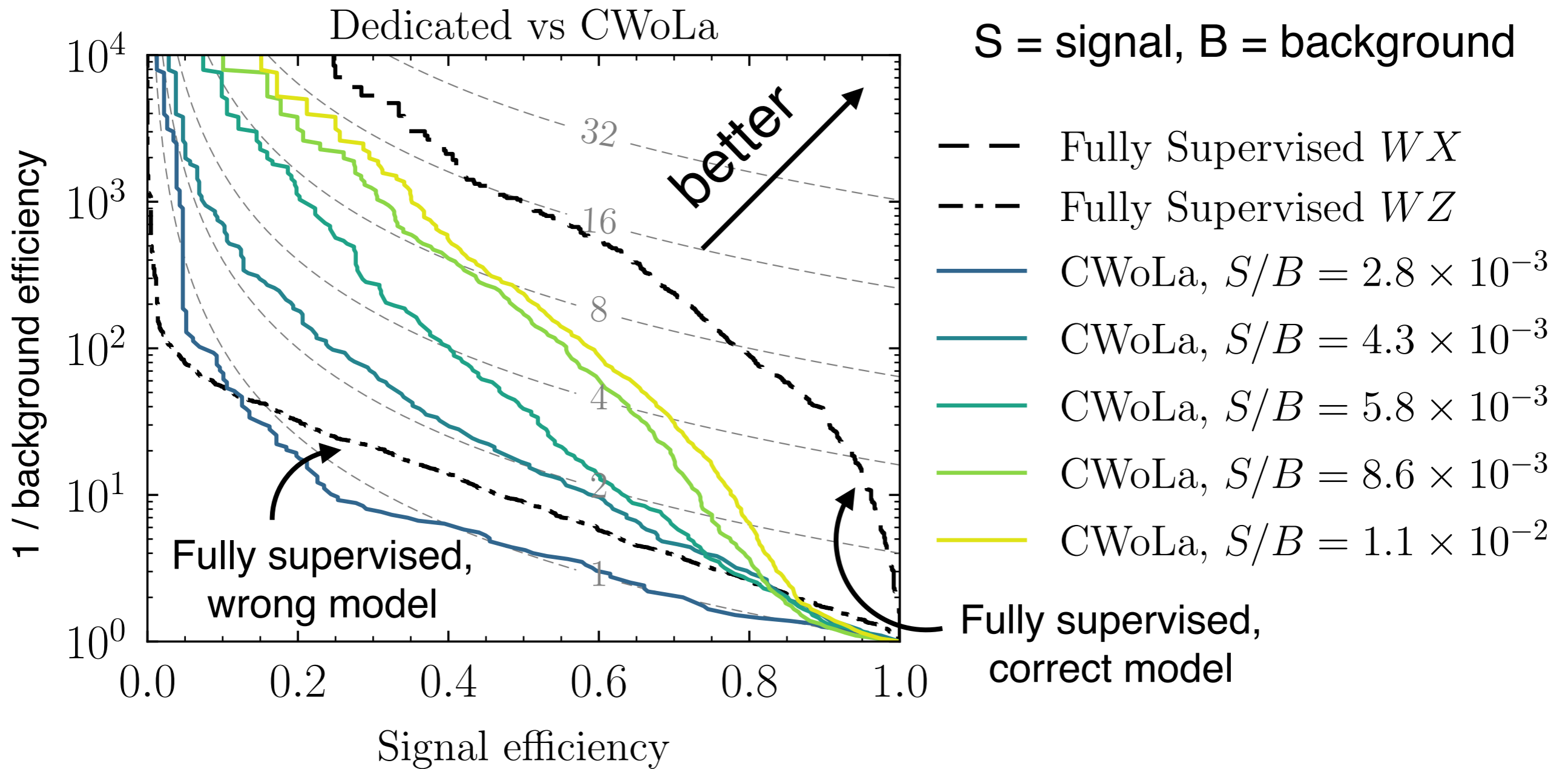
Mass

Mass

Learns to find the signal !



CWoLa hunting vs. Full Supervision

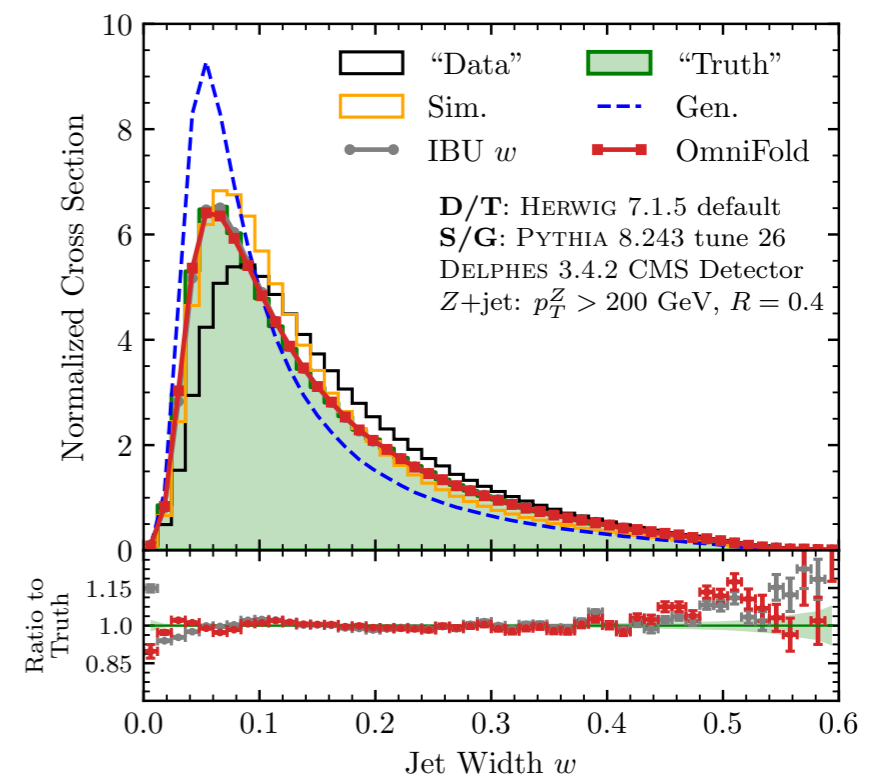
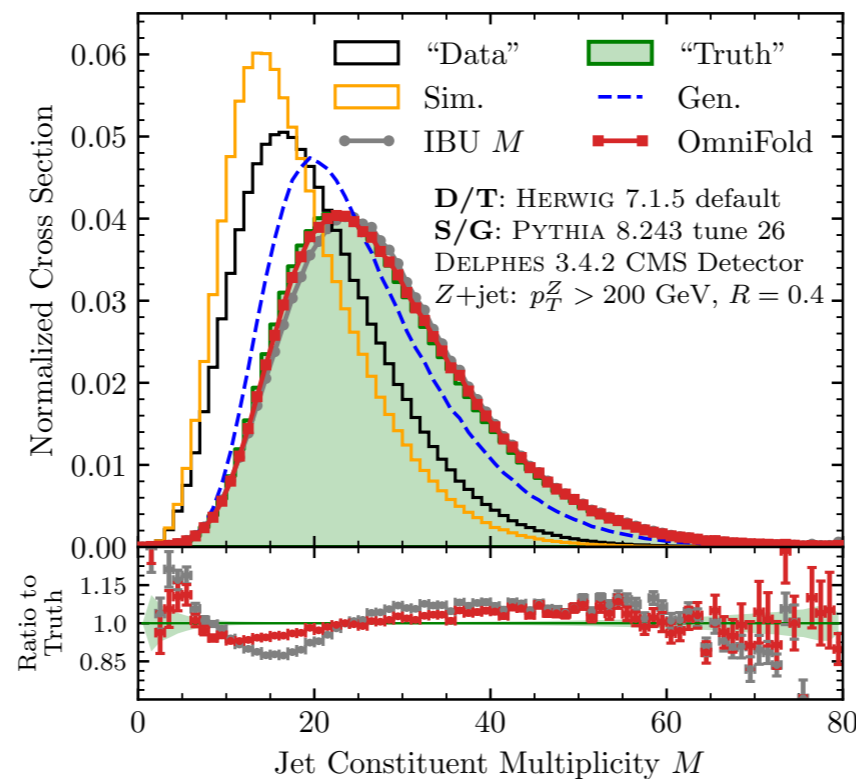
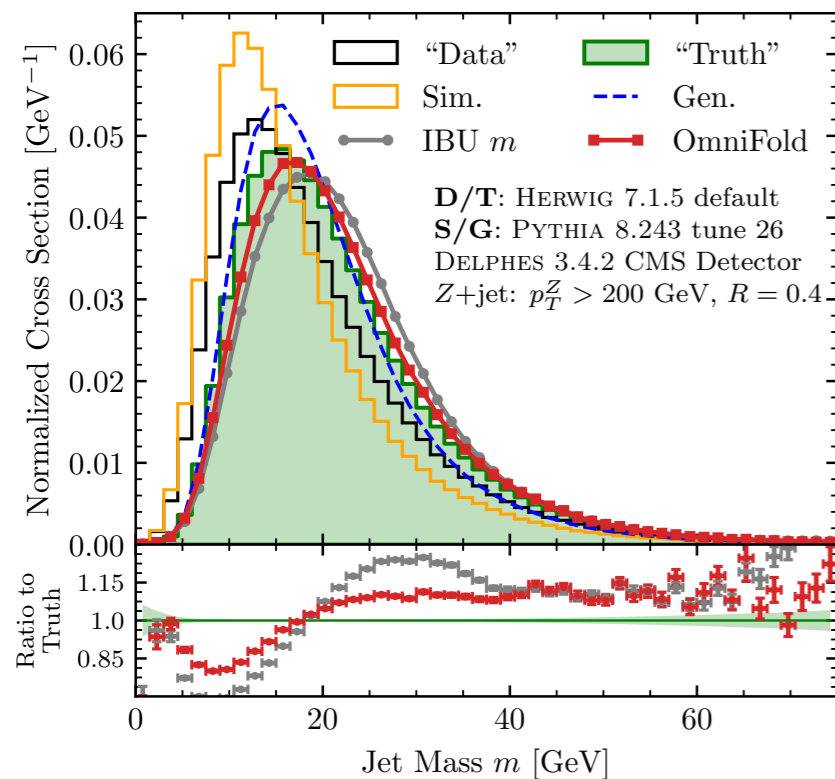


If you know what you are looking for, you should look for it. If you don't know, then CWoLa hunting may be able to catch it!

Example: Unfolding

*What if we could unfold all particles simultaneously?
We could then compute observables (and their bins)
AFTER doing the measurement (!)*

*...stick around for the second part of this
session for more discussions on this point*



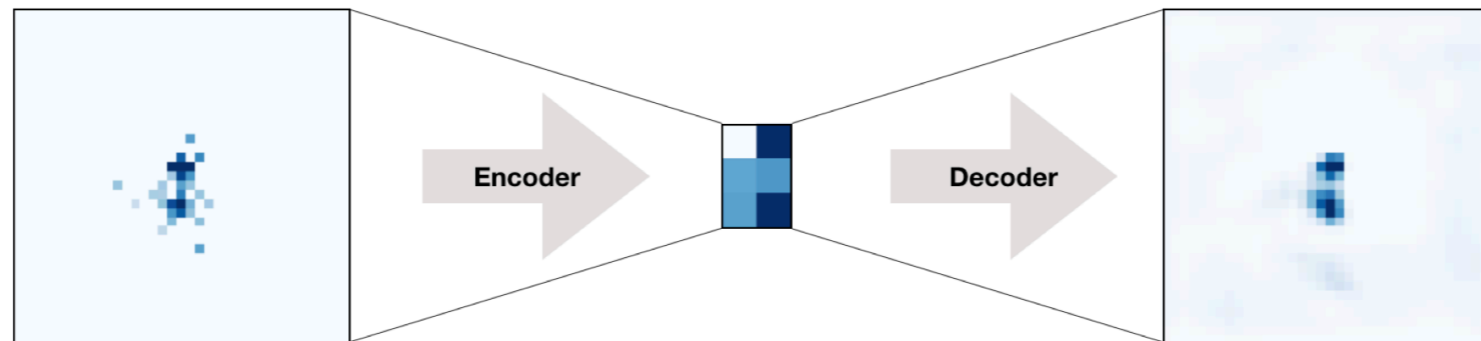
Supervision refers to the type of label information provided to the ML during training.

Unsupervised = no labels
Weakly-supervised = noisy labels
Semi-supervised = partial labels
Supervised = full label information

These categories are not exact
and the boundaries are not rigid!

Unsupervised = no labels

Typically, the goal of these methods is to look for events with low $p(\text{background})$



One strategy (autoencoders) is to try to compress events and then uncompress them. When $x = \text{uncompress}(\text{compress}(x))$, then x probably has low $p(x)$.

Weakly-supervised = noisy labels

Typically, the goal of these methods is to look for events with high $p(\textit{possibly signal-enriched})/p(\textit{possibly signal-depleted})$

e.g. Classification Without Labels (CWoLa), events in a signal region are labeled “signal” and events in a sideband are labeled “background”. These labels are “noisy” but a classifier trained with them can detect the presence of a signal.

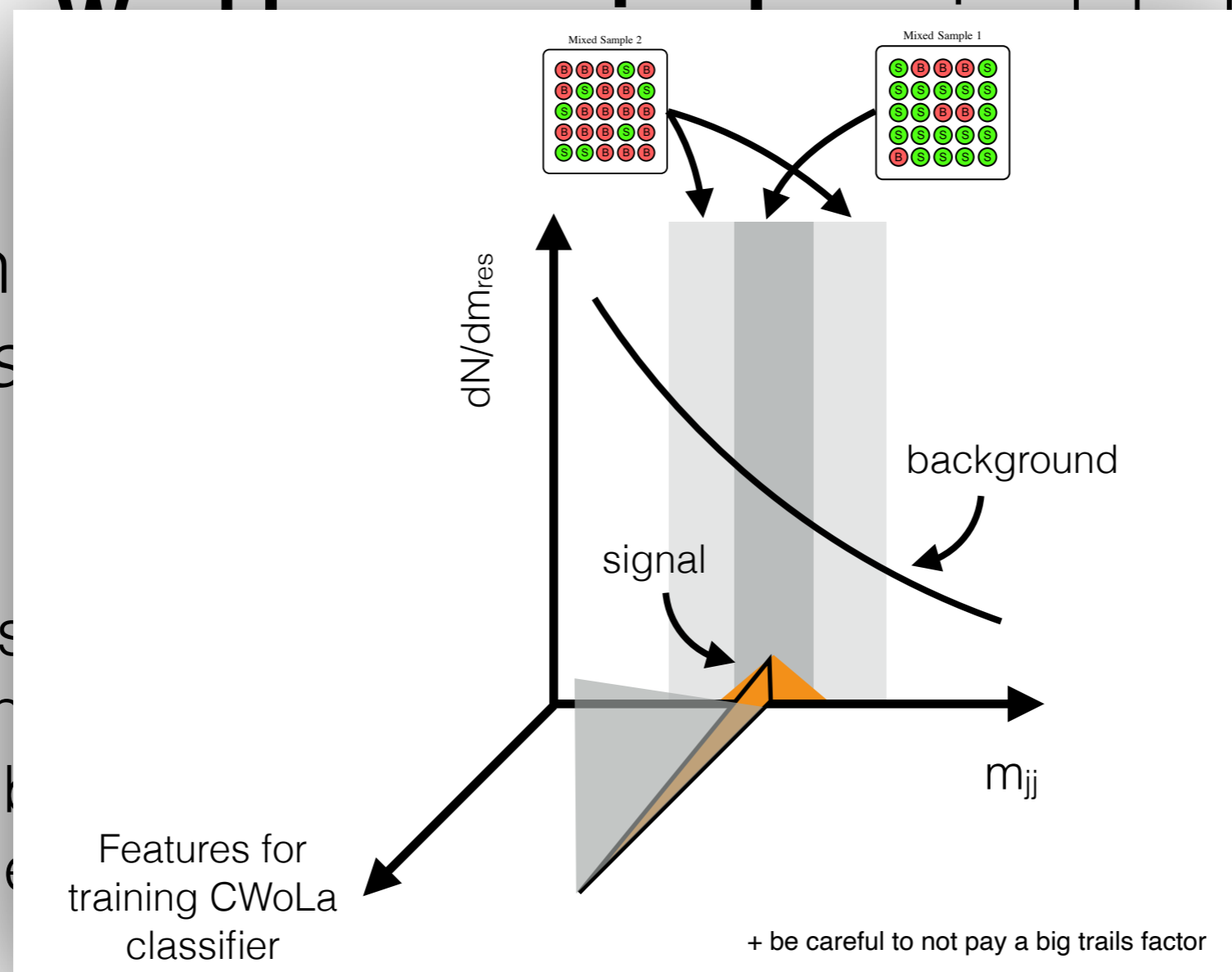
Solutions: Weakly-supervised

Typically, the
high $p(\text{poss})$

or events with
signal-depleted)

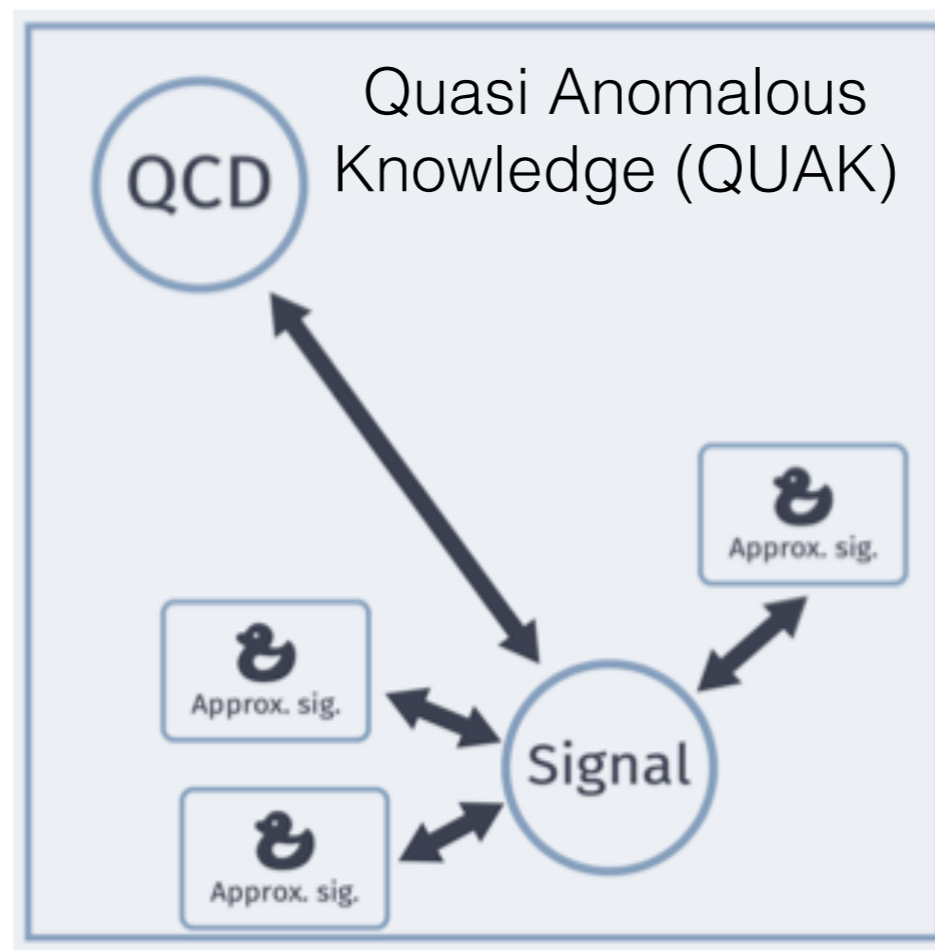
e.g. Clas
region
labeled “
traine

in a signal
band are
a classifier
signal.

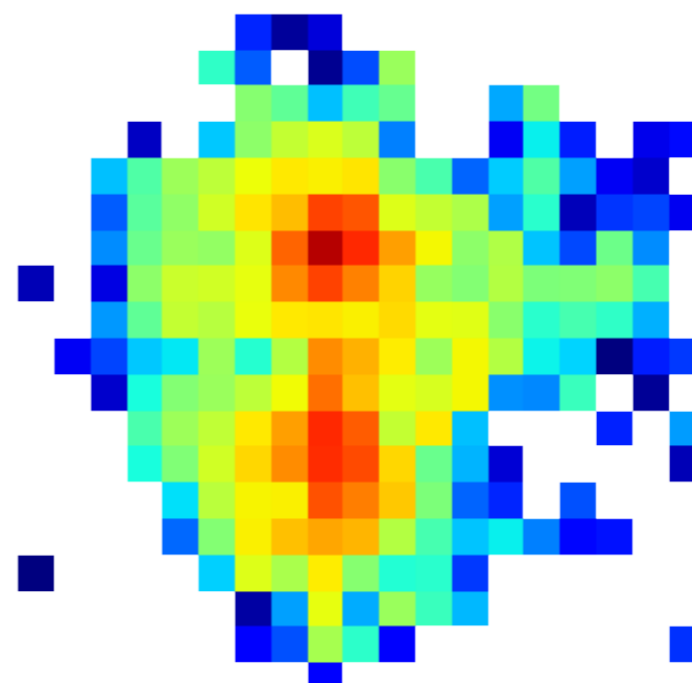
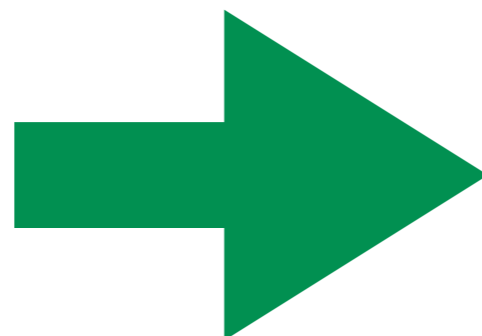
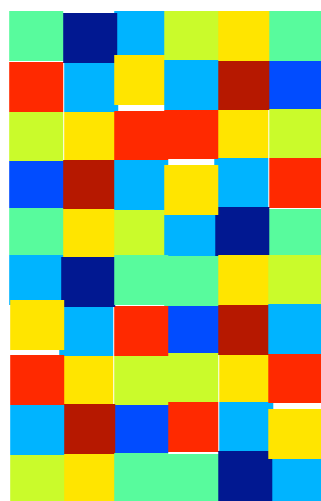


Semi-supervised = partial labels

Typically, these methods use some signal simulations to build signal sensitivity



A **generator** is nothing other than a function that maps random numbers to structure.



Deep Generative Models in HEP

96

Speeding up
slow simulation

Generating
Phase space

Estimating SM
backgrounds

Measurements
and Inference

BSM searches

N.B. being comprehensive with citations would fill up the slide - please see my link to the Living Review at the end for a comprehensive list

Deep Generative Models in HEP

97

Speeding up
slow simulation

Generating
Phase space

Estimating SM
backgrounds

Measurements
and Inference

BSM searches

N.B. being comprehensive with citations would fill up the slide - please see my link to the Living Review at the end for a comprehensive list

N.B. being comprehensive with citations would fill up the slide - please see my link to the Living Review at the end for a comprehensive list

Deep Generative Models in HEP

98

Speeding up
slow simulation

Generating
Phase space

Estimating SM
backgrounds

Measurements
and Inference

BSM searches

N.B. being comprehensive with citations would fill up the slide - please see my link to the Living Review at the end for a comprehensive list

Deep Generative Models in HEP



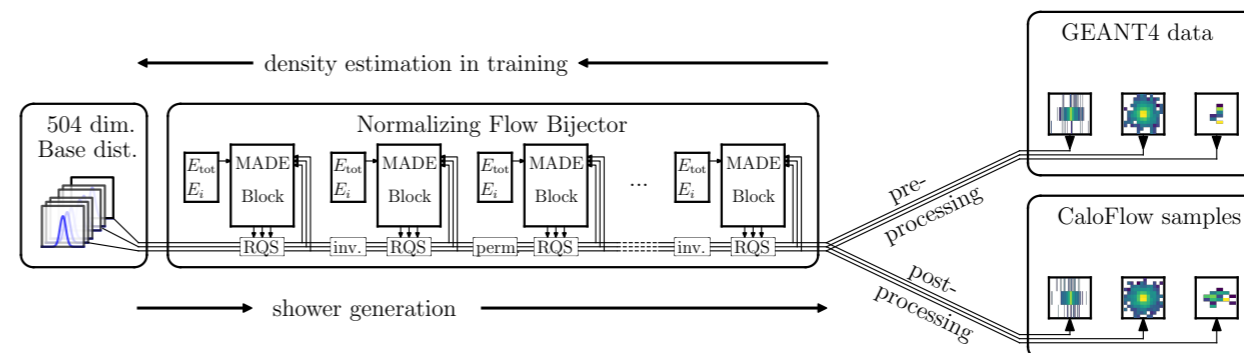
Speeding up
slow simulation

Generating
Phase space

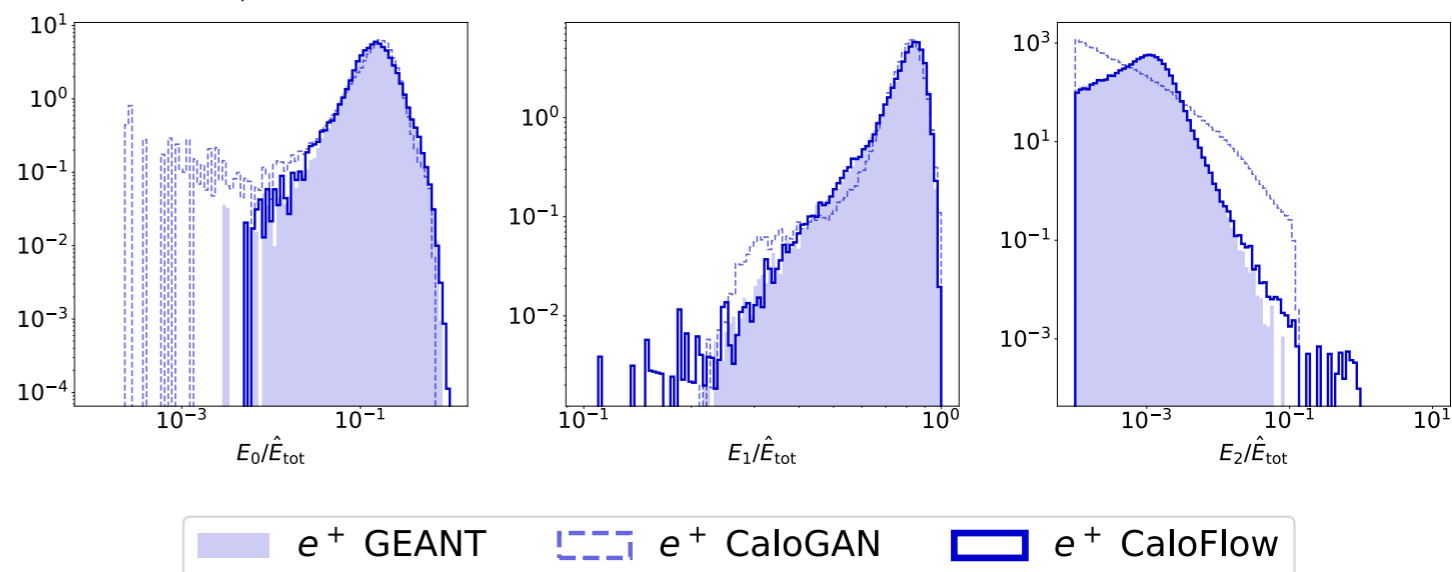
Estimating SM
backgrounds

Measurements
and Inference

BSM searches



GAN, Flow are NNs



CaloFlow: Krause and Shih, 2106.05285

CaloGAN: Paganini, Oliveira, Nachman, 1705.02355

not quite a fair comparison, but the state-of-the-art accuracy is highly non-trivial and very impressive!

N.B. being comprehensive with citations would fill up the slide - please see my link to the Living Review at the end for a comprehensive list

Deep Generative Models in HEP



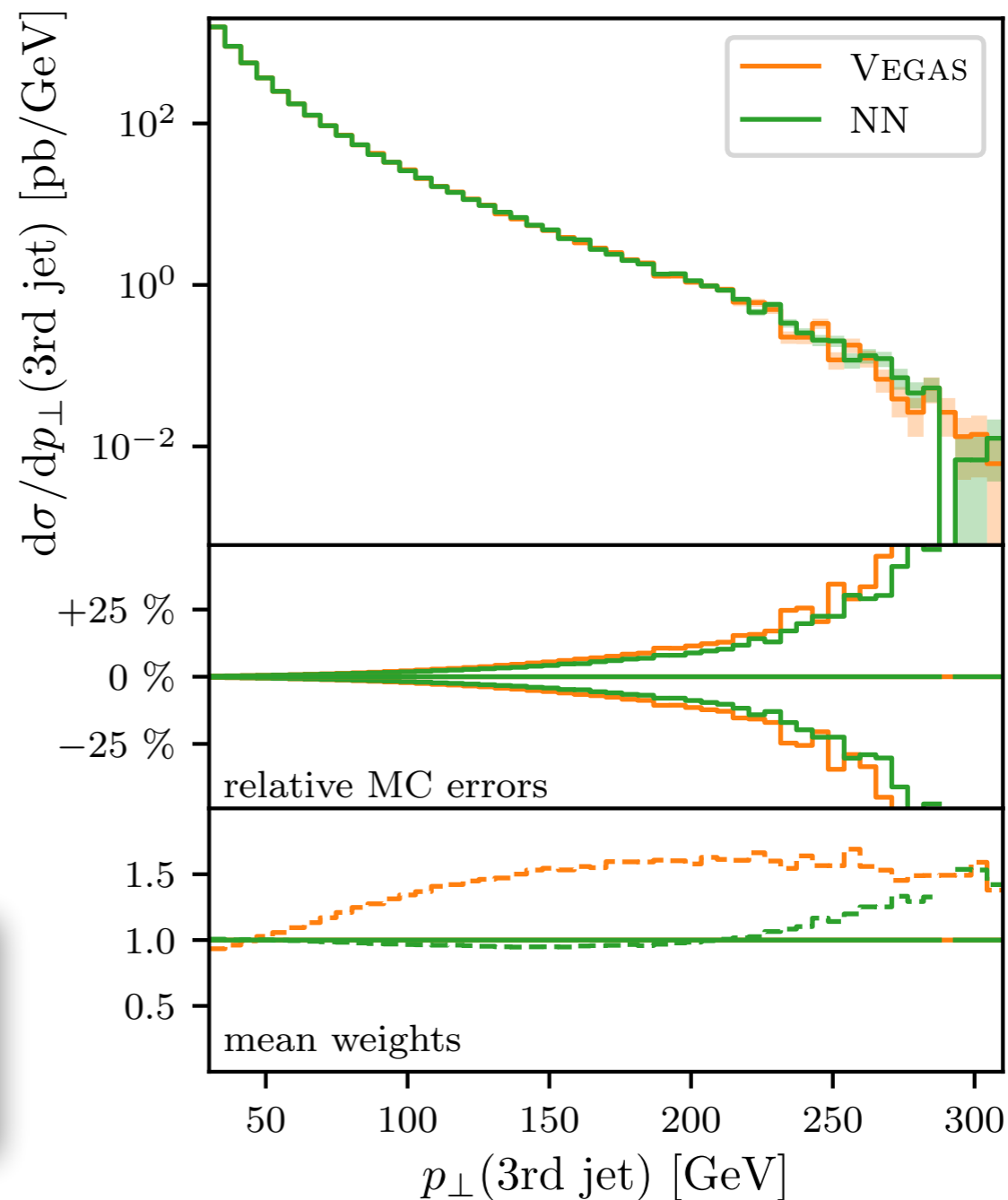
Speeding up
slow simulation

Generating
Phase space

Estimating SM
backgrounds

Measurements
and Inference

BSM searches



Bothmann et al., 2001.05478

N.B. being comprehensive with citations would fill up the slide - please see my link to the Living Review at the end for a comprehensive list

Deep Generative Models in HEP



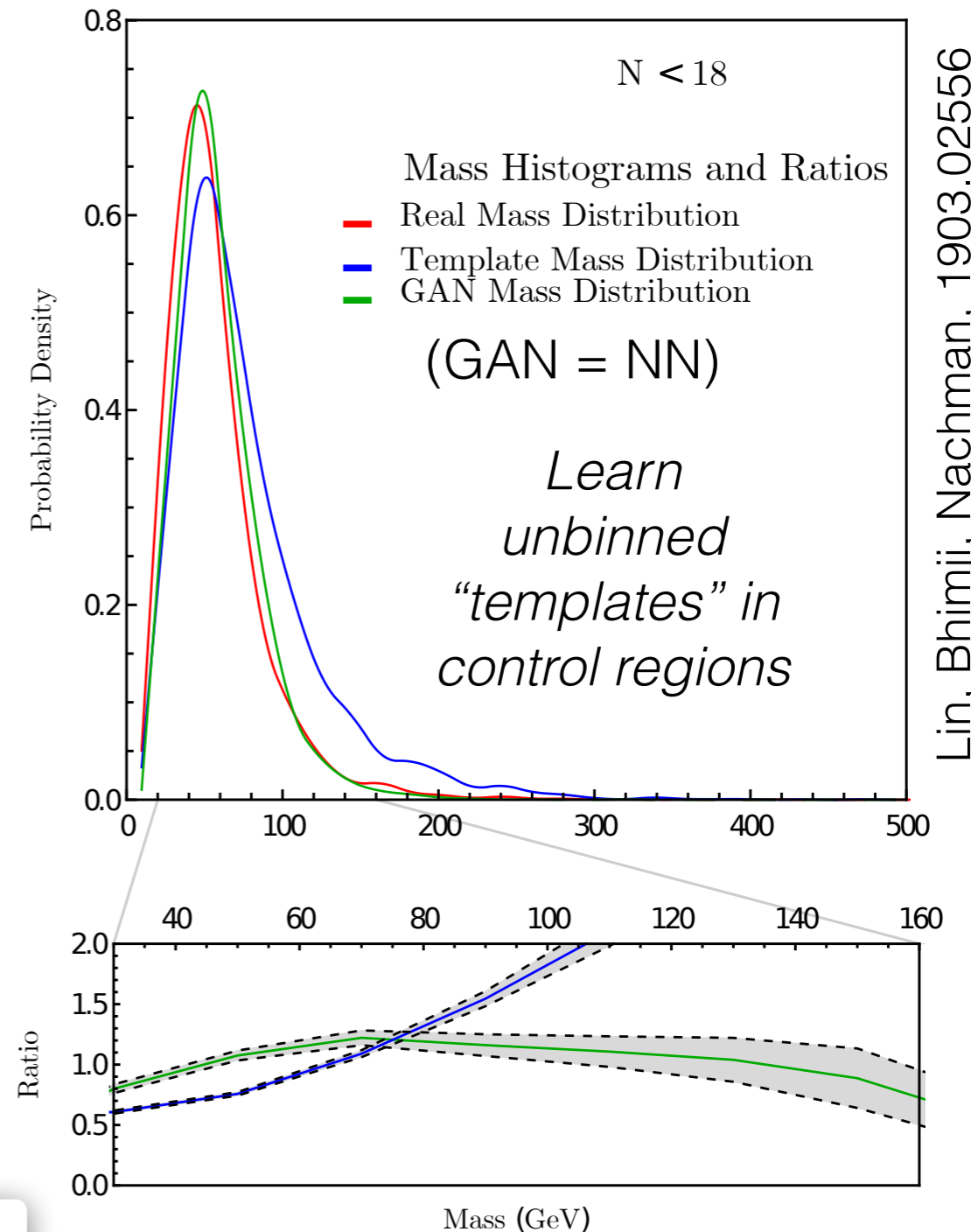
Speeding up
slow simulation

Generating
Phase space

Estimating SM
backgrounds

Measurements
and Inference

BSM searches



Lin, Bhimji, Nachman, 1903.02556

N.B. being comprehensive with citations would fill up the slide - please see my link to the Living Review at the end for a comprehensive list

Deep Generative Models in HEP

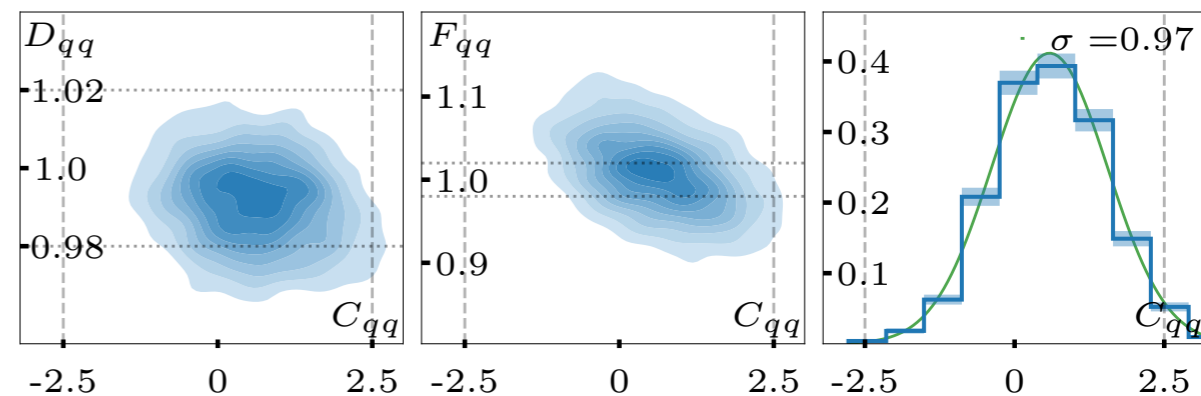
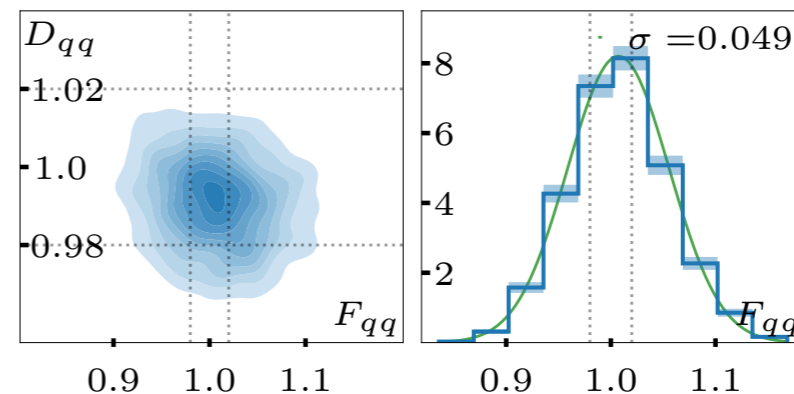
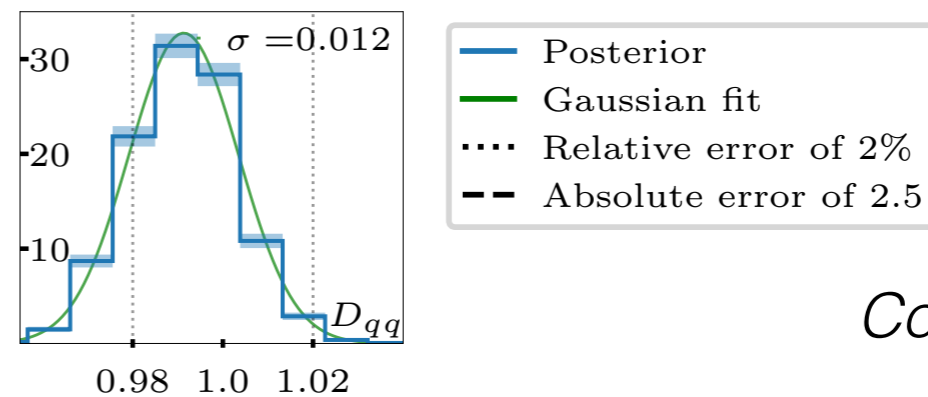
Speeding up slow simulation

Generating Phase space

Estimating SM backgrounds

Measurements and Inference

BSM searches



Coefficients of splitting functions with invertible NNs

Bieringer et al., 2012.09873

N.B. being comprehensive with citations would fill up the slide - please see my link to the Living Review at the end for a comprehensive list

Deep Generative Models in HEP

Speeding up
slow simulation

Generating
Phase space

Estimating SM
backgrounds

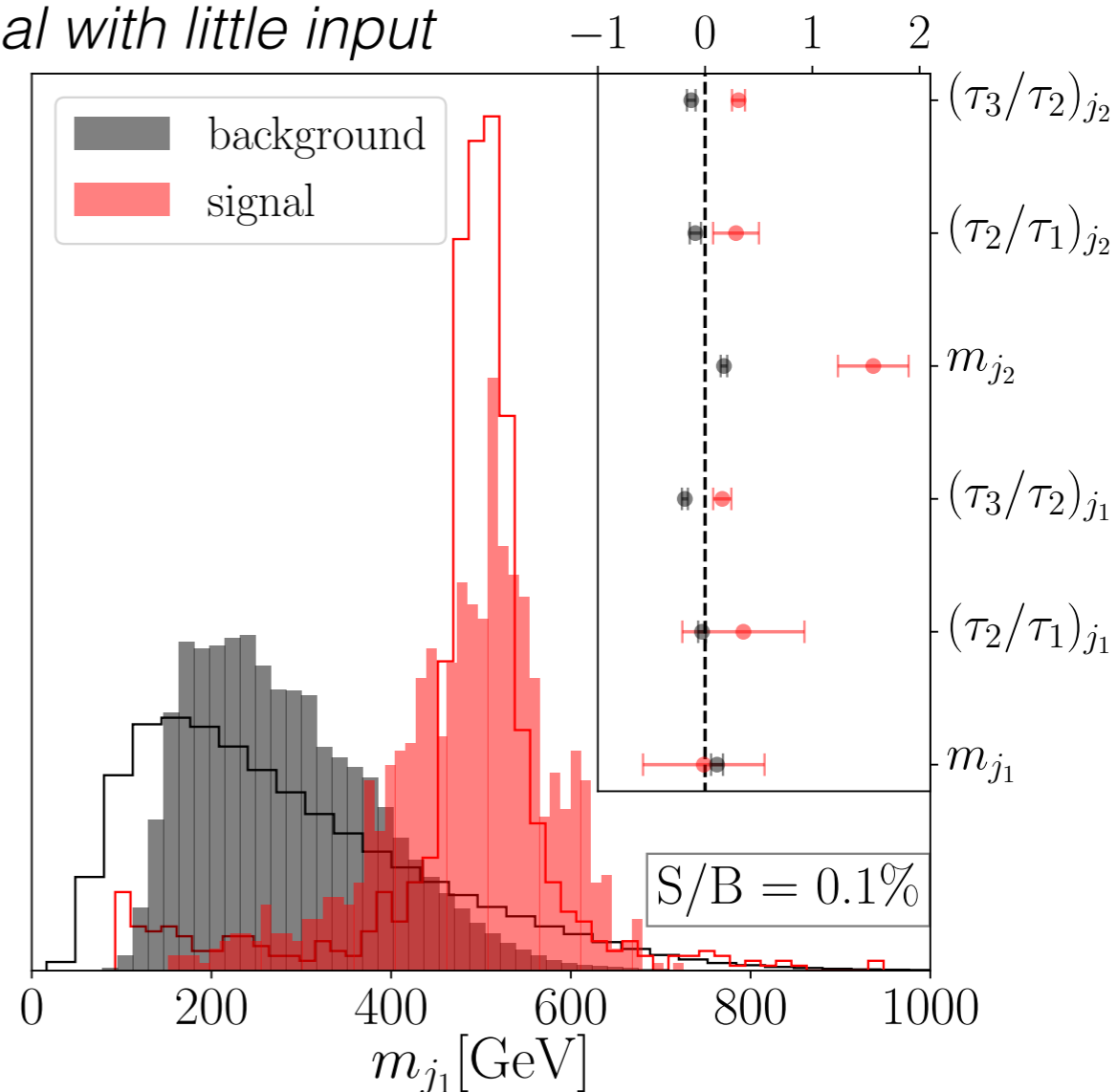
Measurements
and Inference



See also the LHC
Olympics 2020

BSM searches

*Extract features of
signal with little input*



Bortolato et al., 2103.06595

N.B. being comprehensive with citations would fill up the slide - please see my link to the Living Review at the end for a comprehensive list