

# ML4Jets 2020 @ NYU

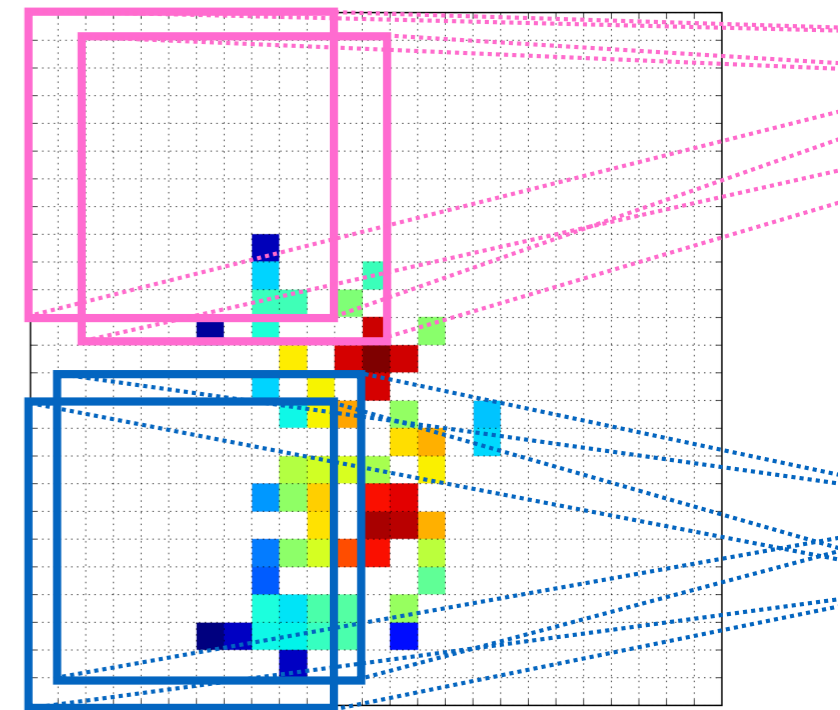
<https://indico.cern.ch/event/809820>

Benjamin Nachman

*Lawrence Berkeley National Laboratory*



**BERKELEY  
EXPERIMENTAL  
PARTICLE  
PHYSICS**



**ATLAS LBNL  
Group Meeting  
Feb. 25, 2020**

# Brief history



## Machine Learning for Jet Physics

11-13 December 2017  
Lawrence Berkeley National Laboratory  
US/Pacific timezone

## Machine Learning for Jet Physics

14-16 November 2018  
Fermilab  
America/Chicago timezone

## ML4Jets2020

15-17 January 2020  
Kimmel Center for University Life  
America/New\_York timezone

In many ways, jet physics has been leading the adaptation and development of advanced ML in HEP

This workshop series was born at LBNL in 2017



# Community challenges



One of the outcomes of the 2017 workshop was the need for a community comparison study of top tagging algorithms.

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SciPost Physics

Submission

## The Machine Learning Landscape of Top Taggers

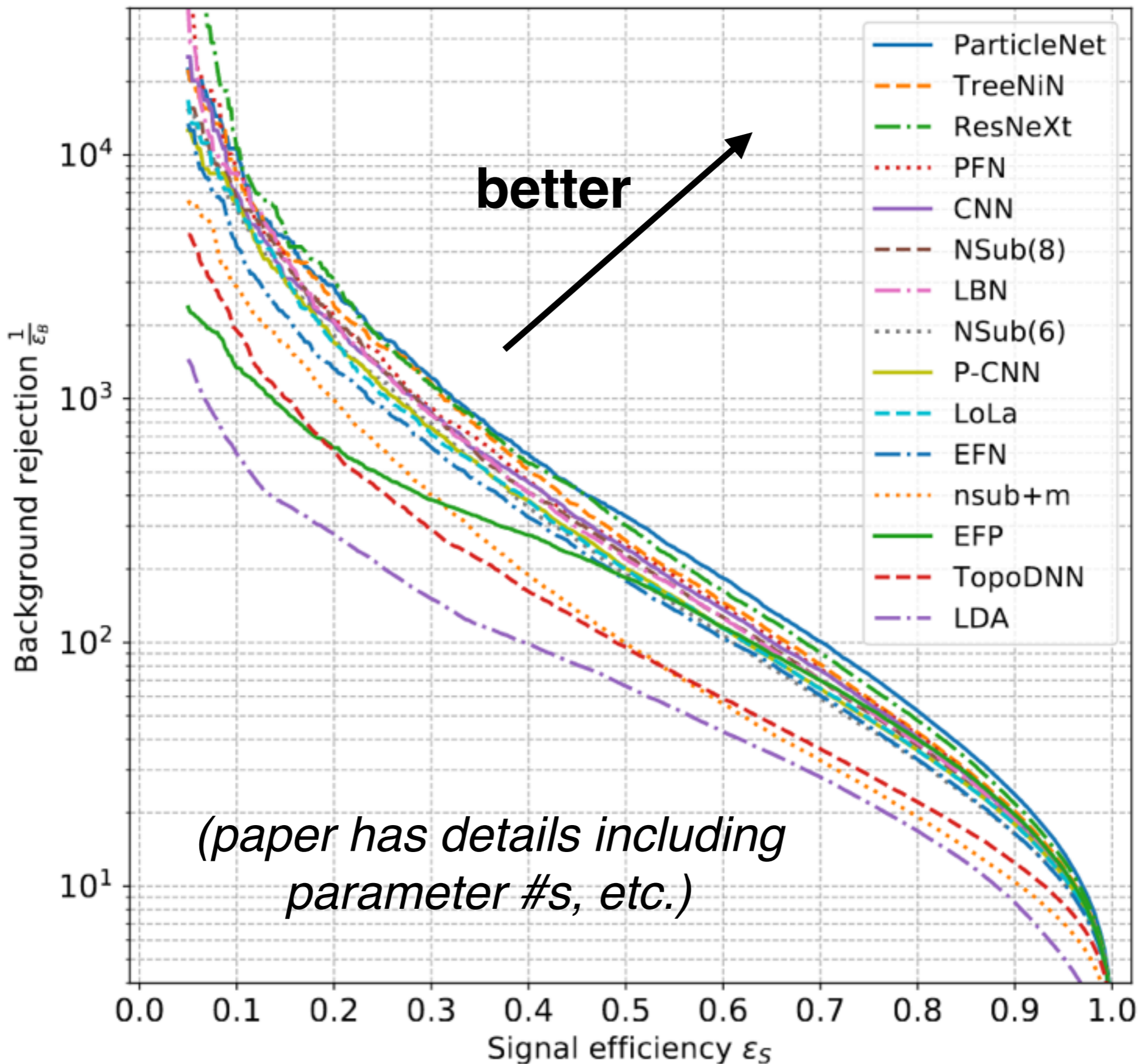
G. Kasieczka (ed)<sup>1</sup>, T. Plehn (ed)<sup>2</sup>, A. Butter<sup>2</sup>, K. Cranmer<sup>3</sup>, D. Debnath<sup>4</sup>, B. M. Dillon<sup>5</sup>, M. Fairbairn<sup>6</sup>, D. A. Faroughy<sup>5</sup>, W. Fedorko<sup>7</sup>, C. Gay<sup>7</sup>, L. Gouskos<sup>8</sup>, J. F. Kamenik<sup>5,9</sup>, P. T. Komiske<sup>10</sup>, S. Leiss<sup>1</sup>, A. Lister<sup>7</sup>, S. Macaluso<sup>3,4</sup>, E. M. Metodiev<sup>10</sup>, L. Moore<sup>11</sup>, B. Nachman,<sup>12,13</sup> K. Nordström<sup>14,15</sup>, J. Pearkes<sup>7</sup>, H. Qu<sup>8</sup>, Y. Rath<sup>16</sup>, M. Rieger<sup>16</sup>, D. Shih<sup>4</sup>, J. M. Thompson<sup>2</sup>, and S. Varma<sup>6</sup>

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re<sup>11</sup>,  
D. Shih<sup>4</sup>,

# Community challenges



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One of the outcomes of the 2018 workshop was the need for a community challenge for anomaly detection.

# Community challenges

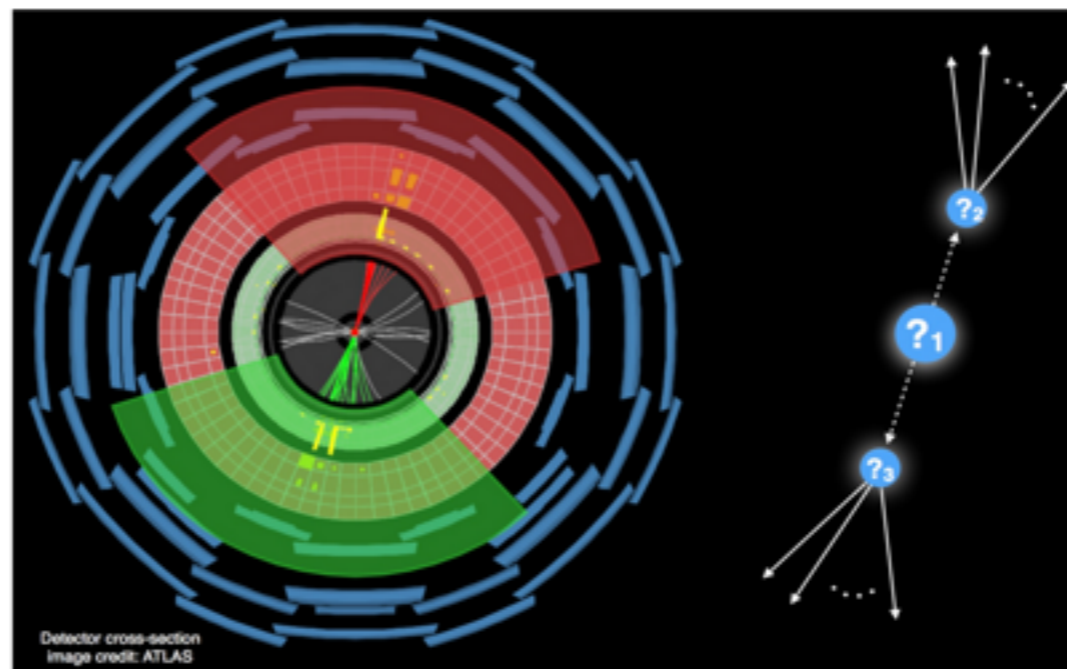


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One of the outcomes of the 2018 workshop was the need for a community challenge for anomaly detection.

More on this  
in a bit...

LHCOlympics2020



Detector cross-section  
Image credit: ATLAS

# Community challenges



One of the outcomes of the 2017 workshop was the need for a community comparison study of top tagging algorithms.

One of the outcomes of the 2018 workshop was the need for a community challenge for anomaly detection.

One of the outcomes of the 2020 workshop was the need for a community challenge for unfolding.

**Stay tuned!**

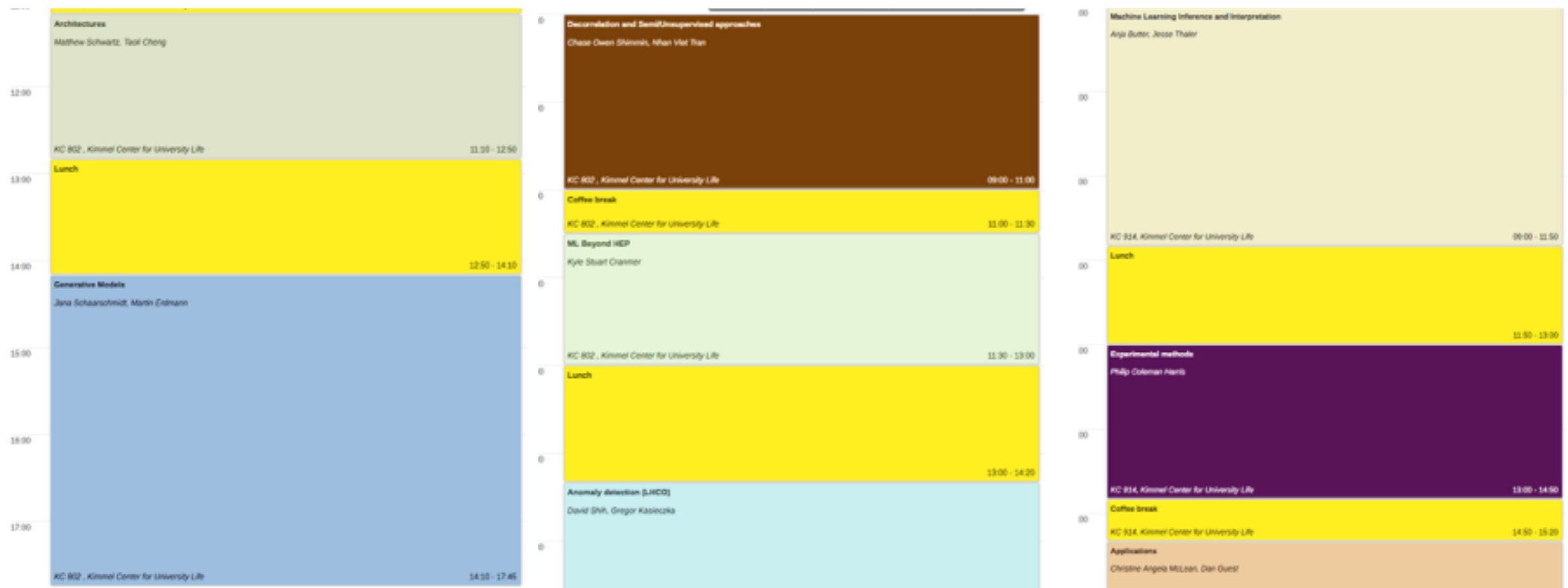


# 2020 Edition: Overview



There was a packed agenda with three very full days of interesting talks!

I won't review every talk ... please take a look at the slides for all the contributions and for details. These slides are some personal highlights.



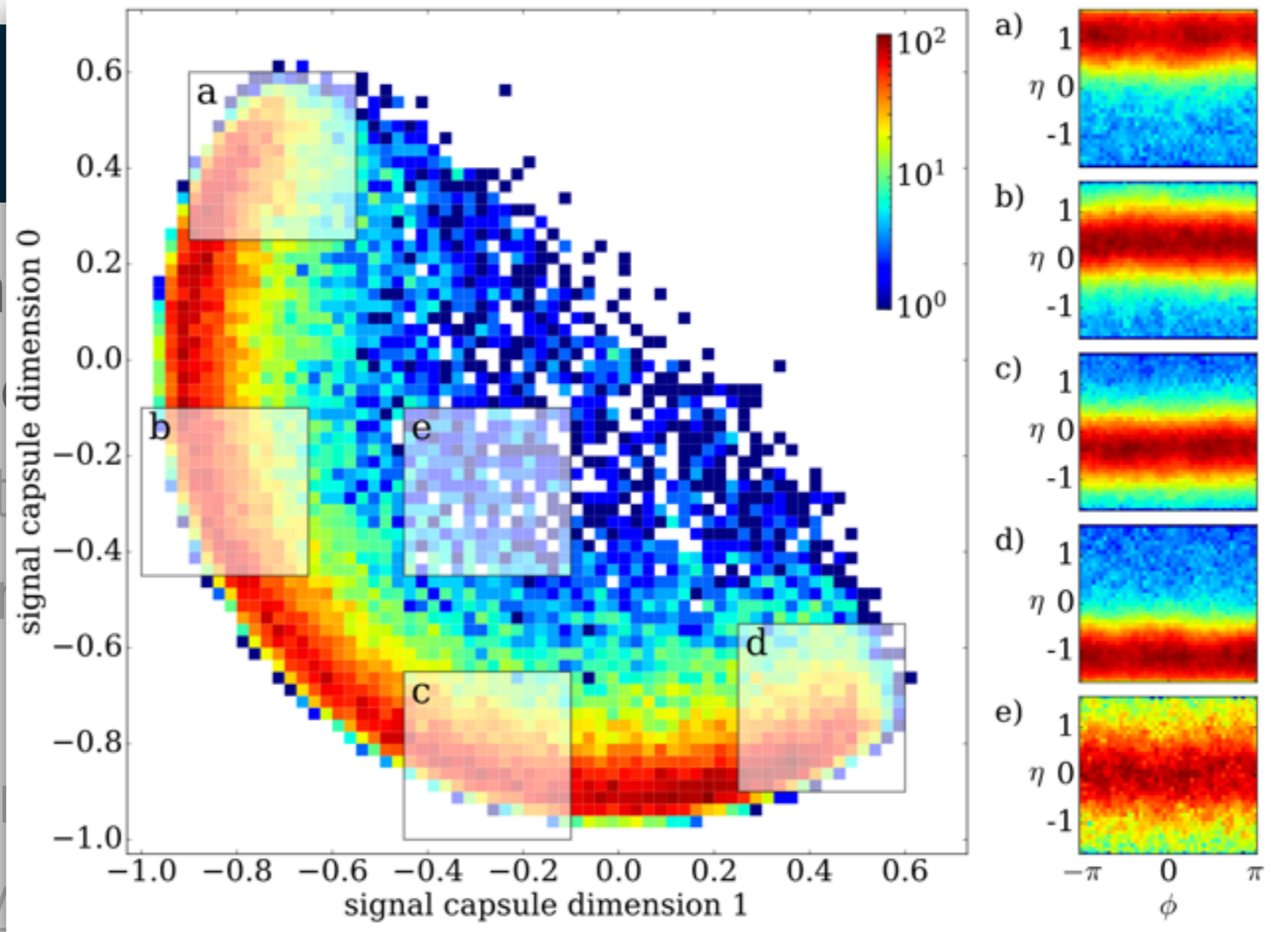
# Architectures - Highlights

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- Lorentz covariant networks (more on next slide)
- Yet another particle cloud architecture
  - Jet constituents are permutation invariant thanks to QM ... need an architecture that acts on sets. There are now a few of these based on Deep Sets (MIT group) and various graph networks (UCSB and now also University of Zurich)
- A first study of “capsule networks” in HEP. These networks try to learn directions orthogonal to classification directions in feature space. Supposed to be interpretable.

# Architectures -

- Lorentz covariant
- Yet another particle
- Jet constituent
- QM ... need an
- are now a few
- group) and var
- also University



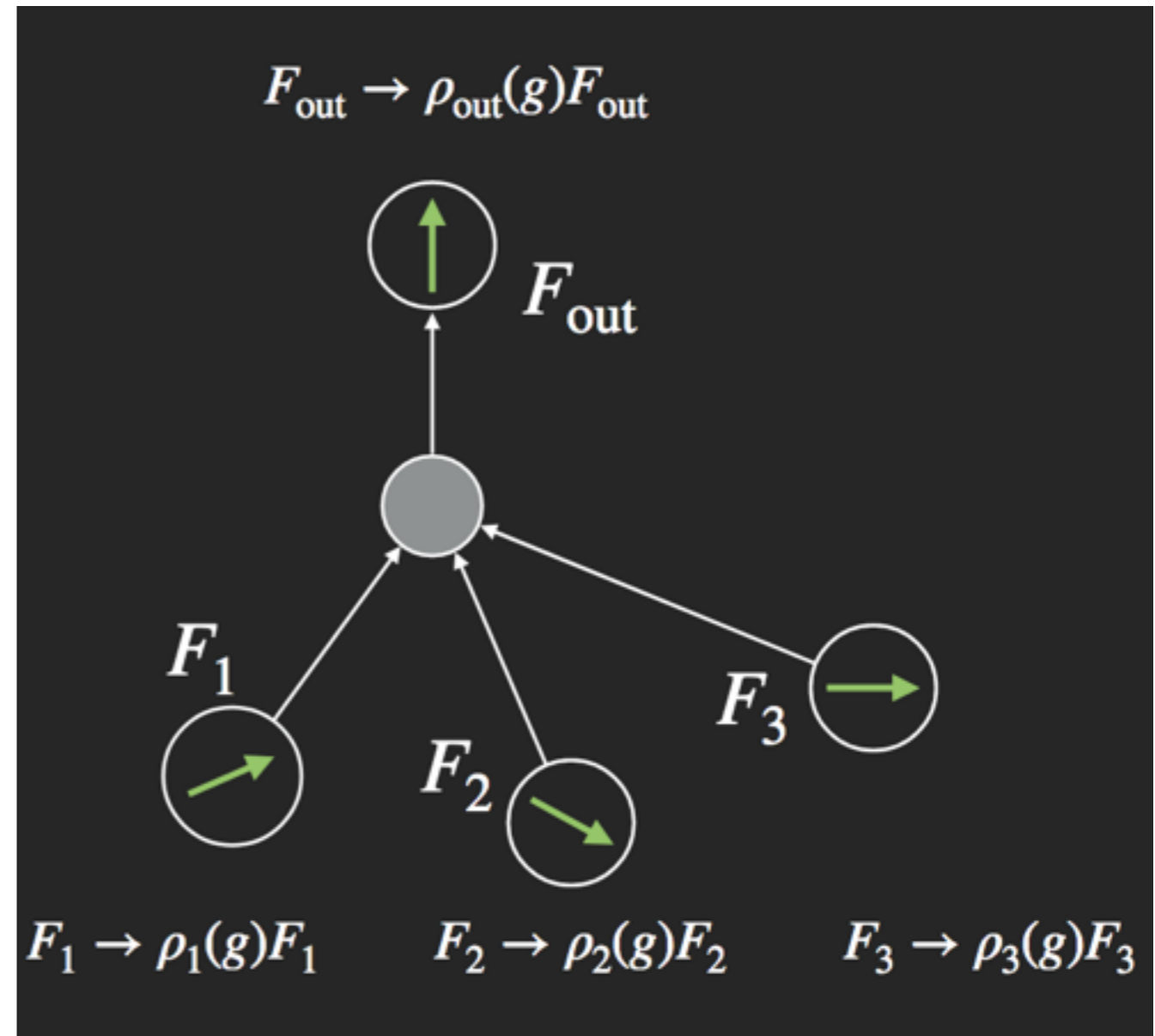
- A first study of “capsule networks” in HEP. These networks try to learn directions orthogonal to classification directions in feature space. Supposed to be interpretable.

**Classifier = length in capsule space**

New architecture that is Lorentz covariant - output is in a representation of the Lorentz group and transforms with the input

...e.g. for classification, output is a scalar (Lorentz invariant)

No need to preprocess as it is already invariant under translations along  $\eta$  (boosts in  $z$ ), etc.

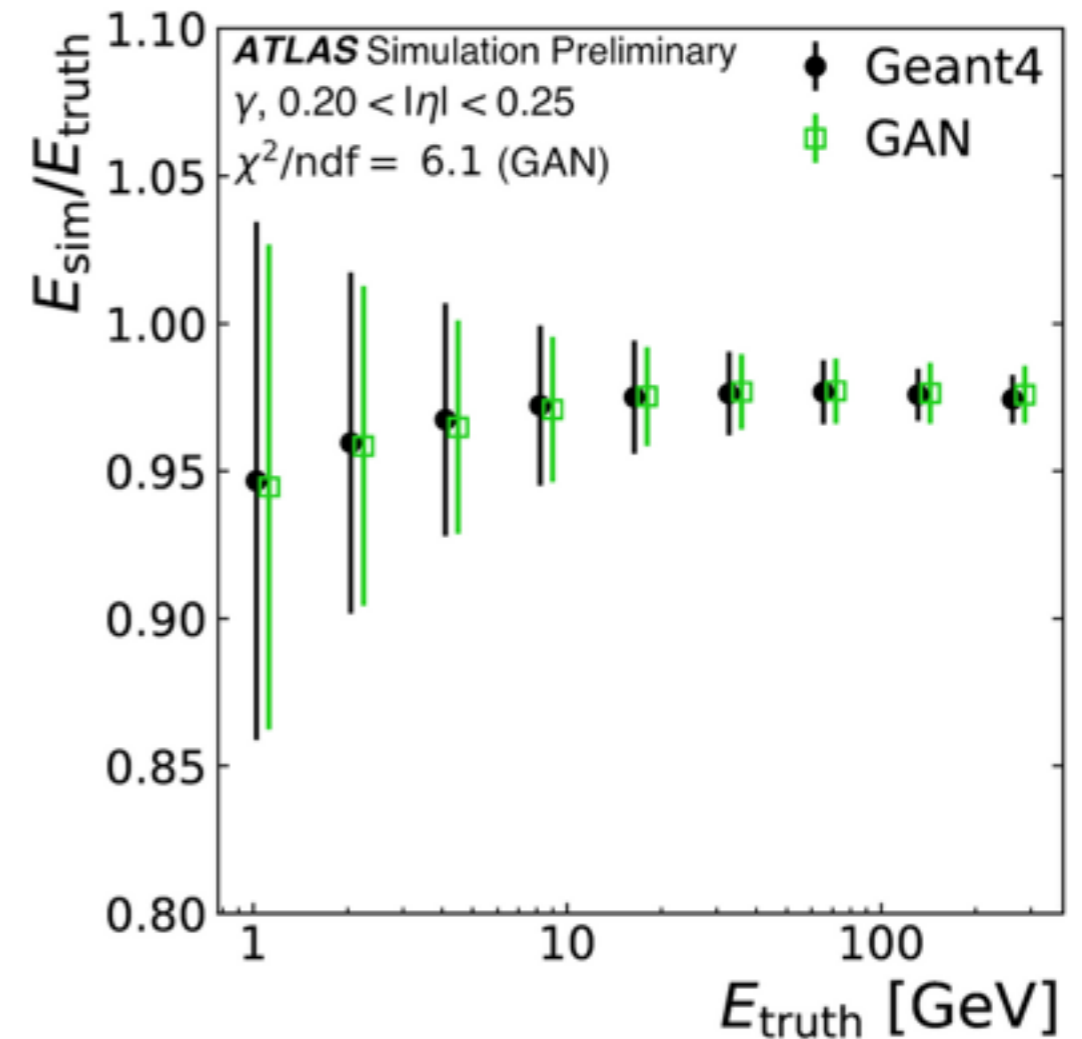
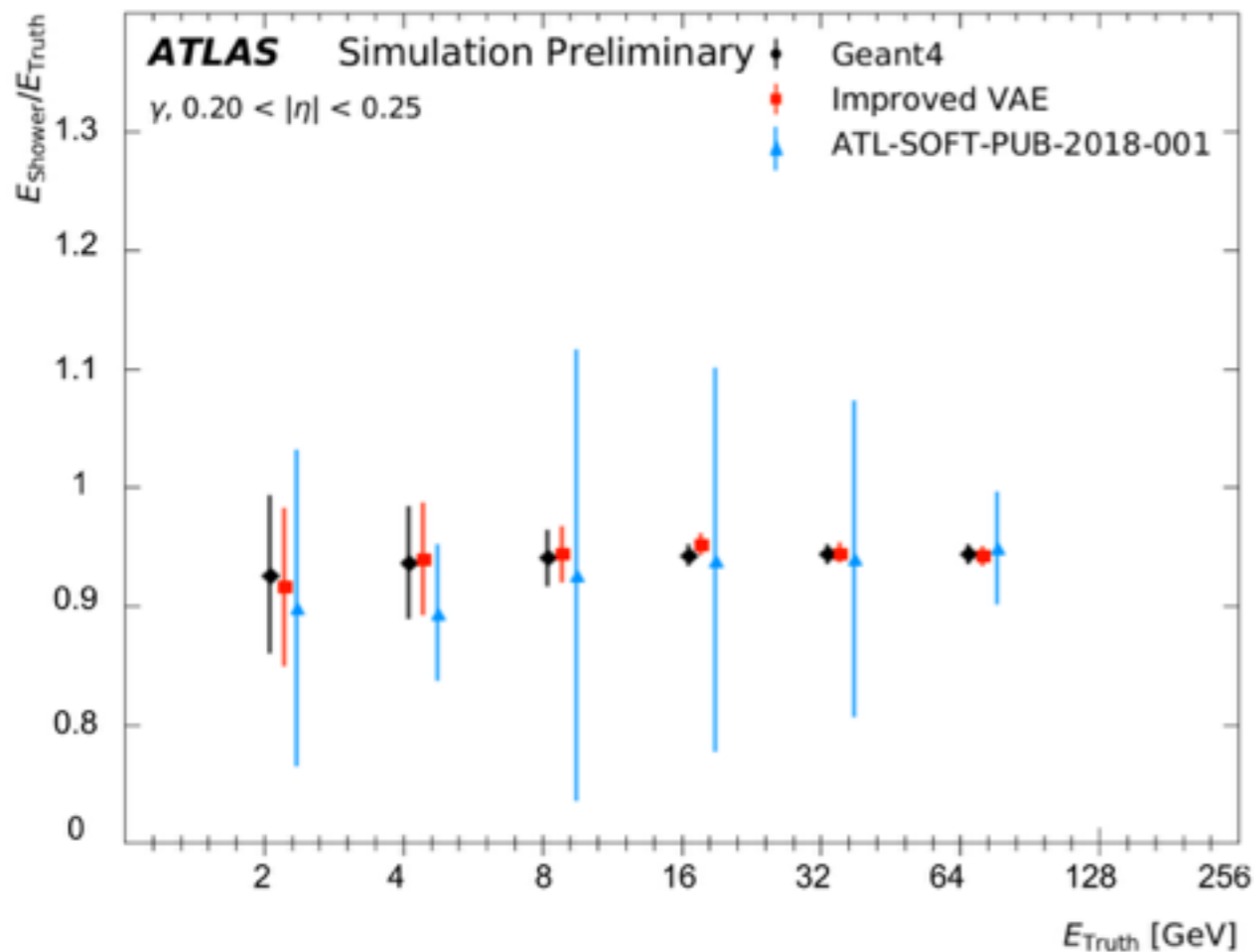


Demonstrated to be in the same ballpark as other top tagging algorithms, but with **way fewer parameters.**

# Generative models - Highlights

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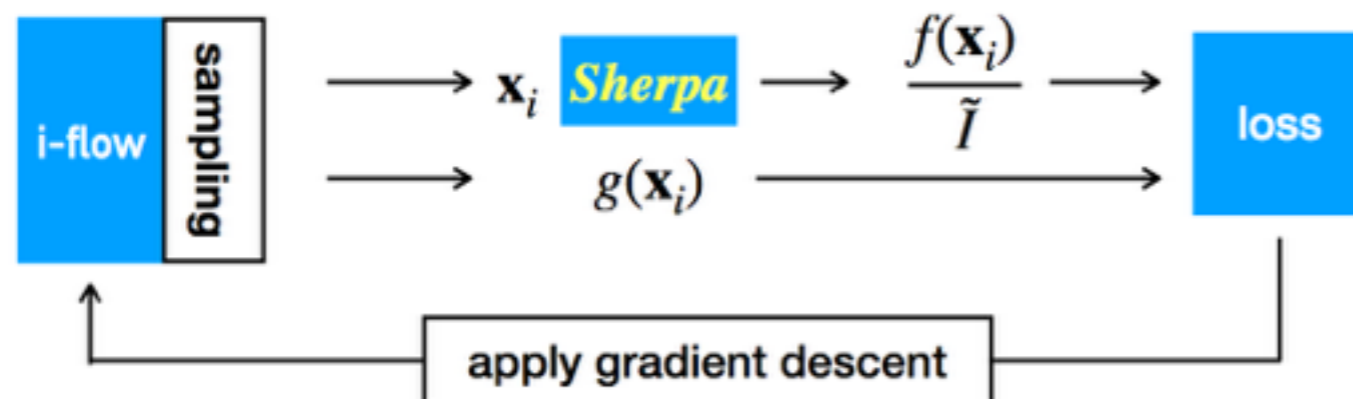
- Calorimeter simulation from ATLAS and CALICE
  - Rapid improvements in fidelity



(two different deep generative models)

- Calorimeter simulation from ATLAS and CALICE
  - Rapid improvements in fidelity
- As a “non-parameteric” fitting function (next slide)
- For unbinned event subtraction (2 slides from now)
- For phase space integration

## i-flow + Sherpa: Phase Space Integration

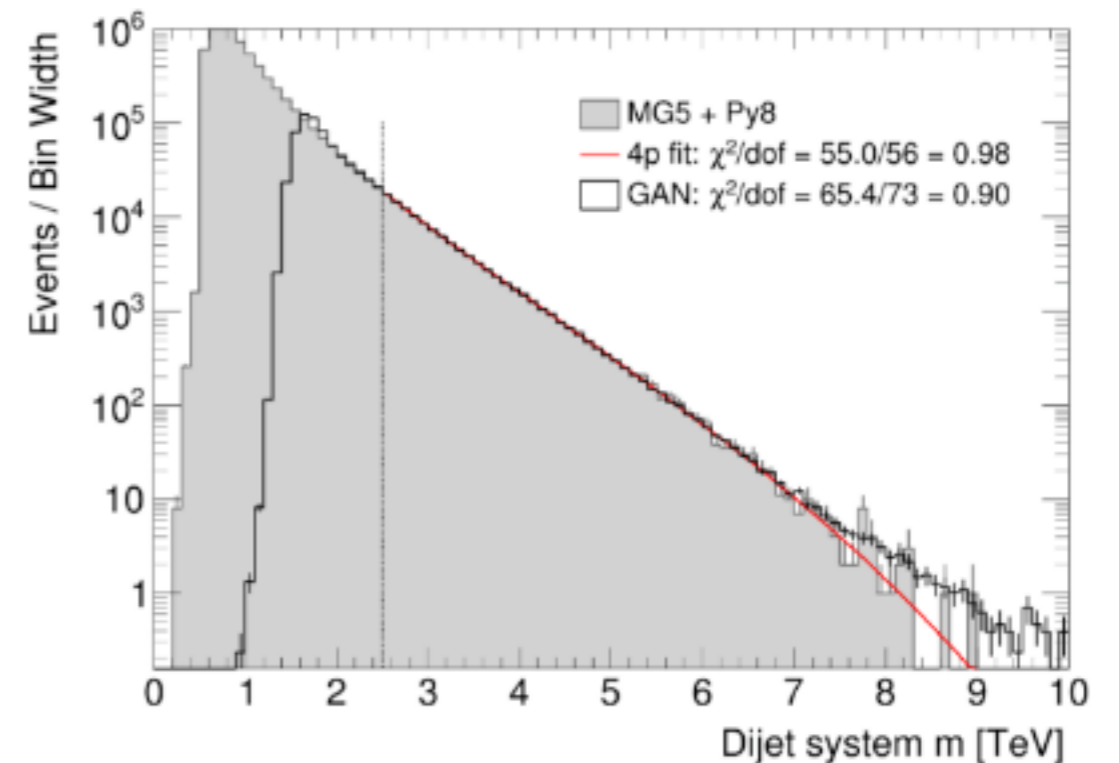
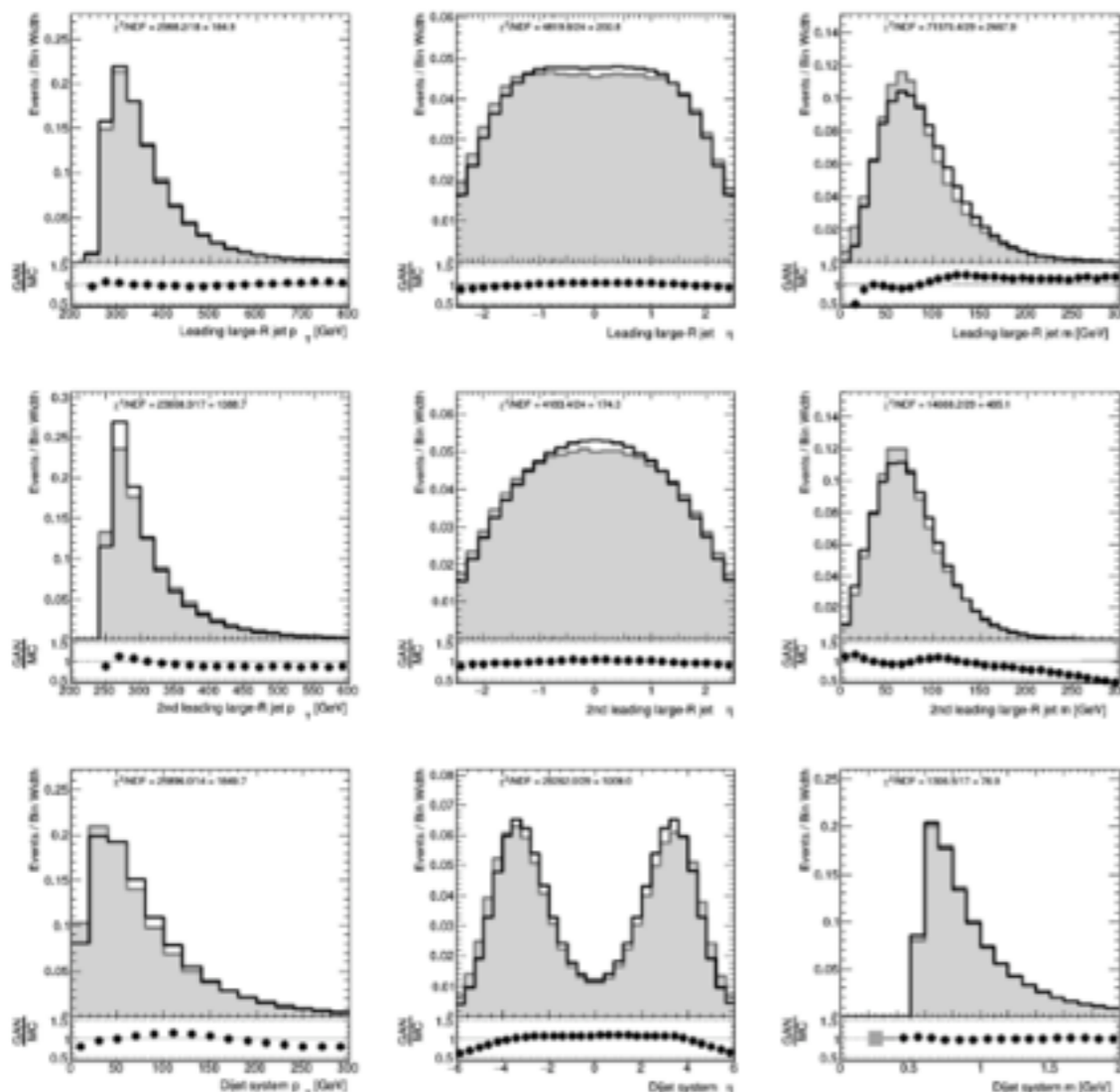


Preliminary results for unweighting efficiency are promising compared to state-of-the-art (VEGAS and FOAM)

# Generative models - Dijet GAN

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Generative NN's are good at interpolating - can they be used to learn good ~non-parameteric fitting functions?

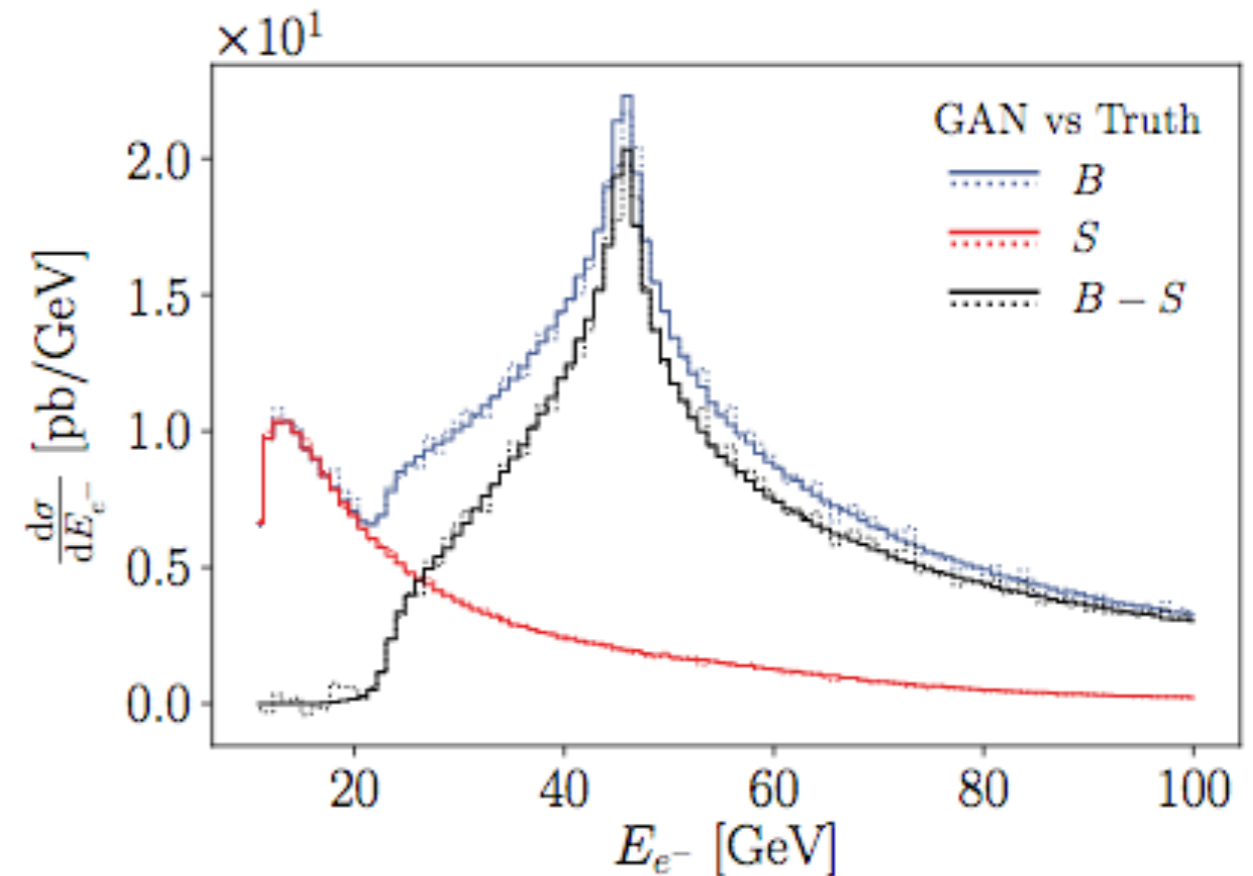


Seems to be effective at  $m_{jj}$  but not yet achieving precision in the additional jet kinematic features.

Perhaps could be useful for conditional generation as well, i.e. after making cuts.

Proposal to use GANs to do unbinned event subtraction

Idea: learn to generate  $S$  and  $X$  where  $S$  and  $X$  have to sum in distribution to  $B$ .  
This will make  $X = B - S$ .



I'm not sure what the killer application is, but it seems like a very nice idea and maybe can be used for subtracting backgrounds for scale factors, unfolding, ...



- Decorrelation
  - Why do we need to decorrelate? Might want a classifier to not sculpt bumps, so need classifier to be  $\sim$ uncorrelated with e.g.  $m_J$ .
  - Decorrelation in CMS (next slide)
  - A new decorrelation scheme (2 slides)
- Optimal transport
  - How do define how close two jets are to each other?
  - Structure discovery with autoencoders (3 slides)
  - Generalization of energy movers' distance

# Decorrelation - CMS

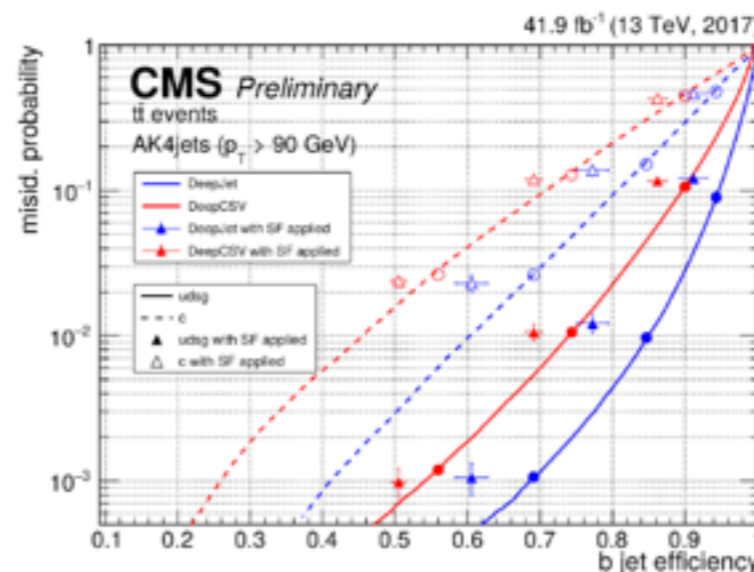
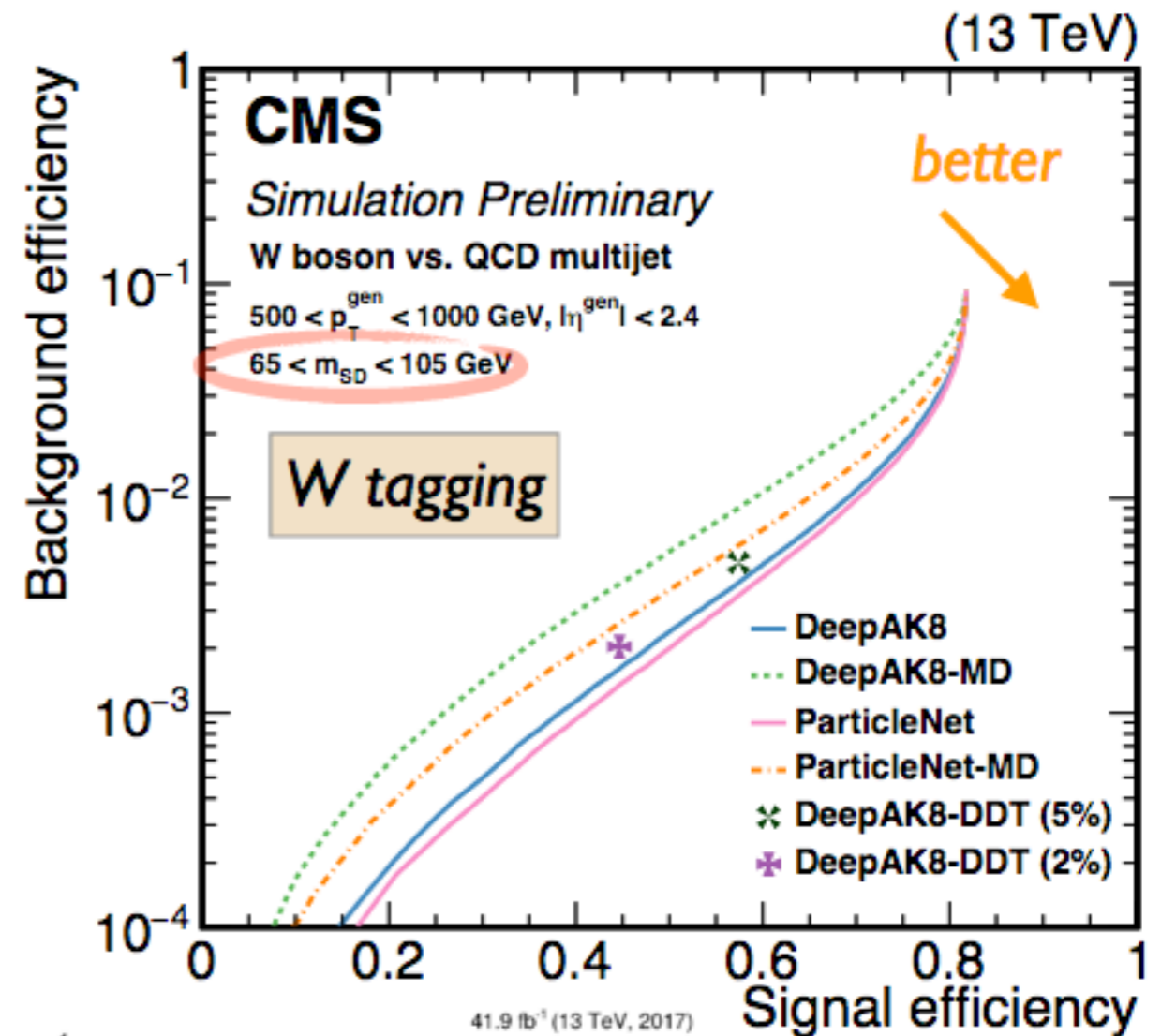
18

CMS presented many results with state-of-the-art taggers and various decorrelation schemes.

DDT + NN only works for a fixed WP  
(can always decorrelate “by hand” in one place)

They are using rather complex networks compared to what we are doing - they have more power, but do they understand their uncertainties?

(large scale factors →)



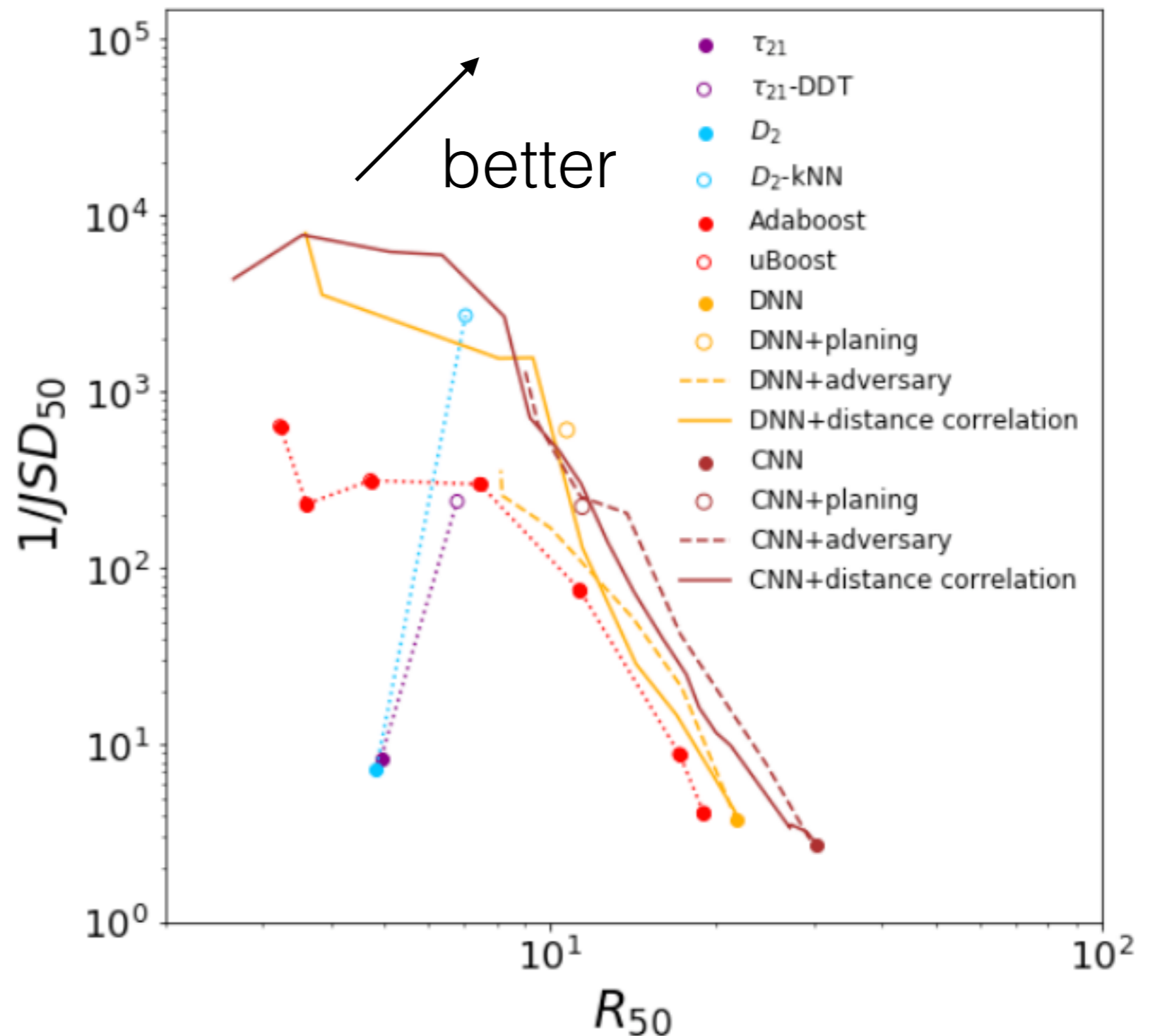
# Decorrelation - DisCo

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New alternative to adversarial decorrelation using “Distance Correlation”

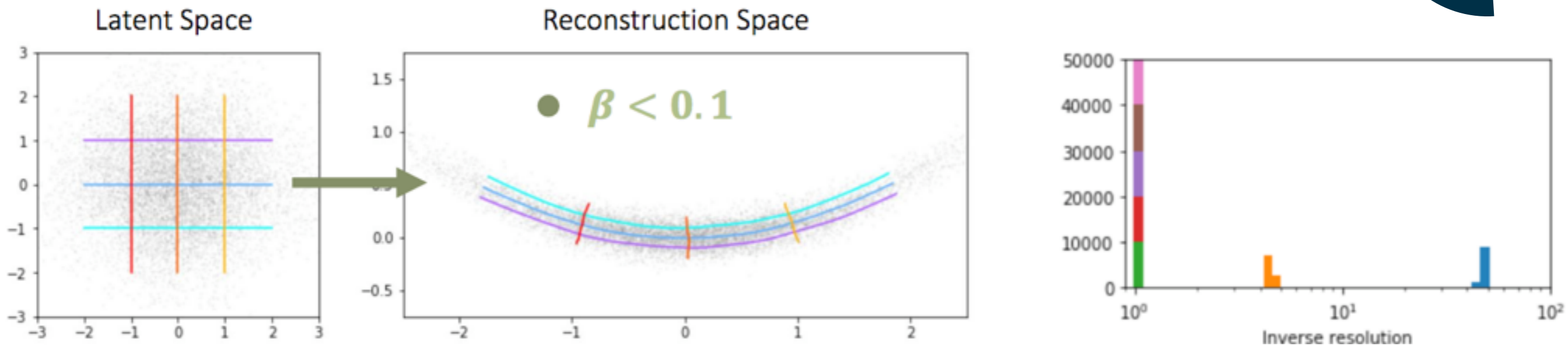
Much easier to train because not minimax ... also has only one additional parameter (not a whole NN’s worth)

They did a nice recast of the ATLAS result as their benchmark!



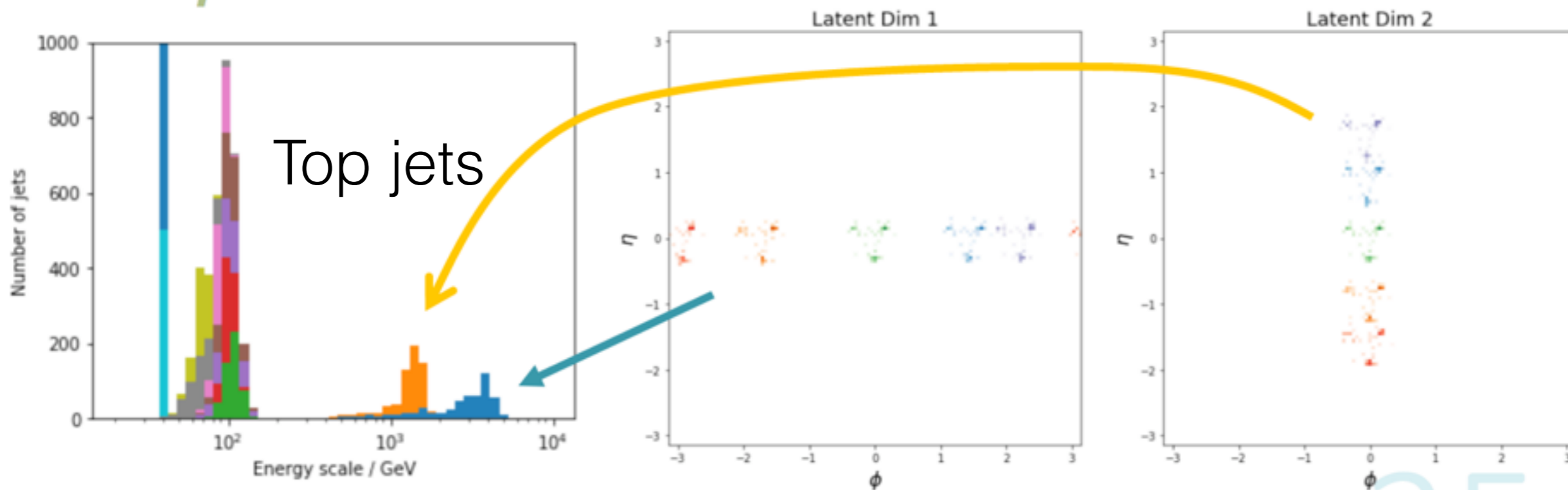
# Semi-supervised - VAEs to find structure

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$\beta = 40 \text{ GeV}$

$\beta$  is the cost for encoding information



Physical scales in a problem can be automatically discovered

# Anomaly detection - Highlights



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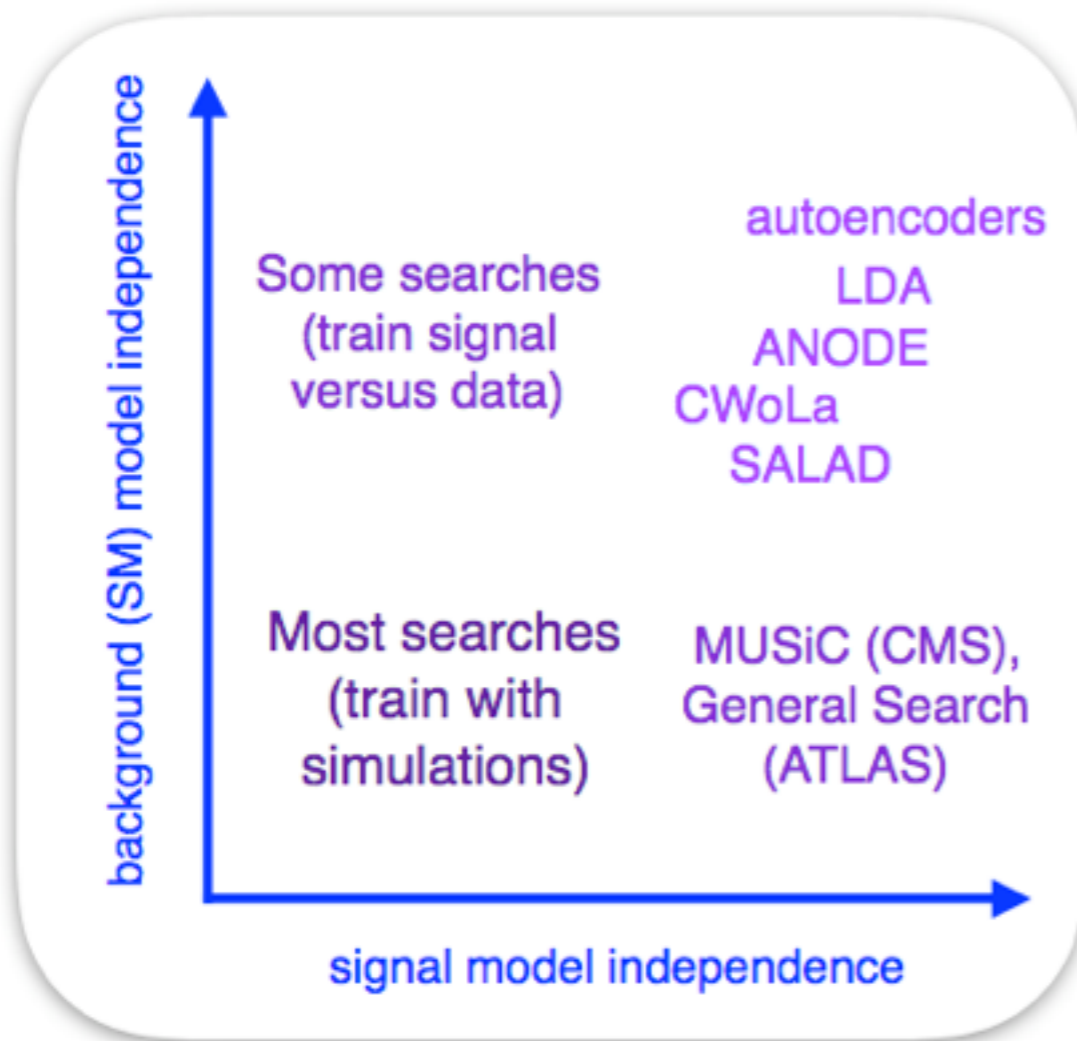
- This session was special - we still had talks of new ideas, but additionally heard LHC Olympics solutions
- At the end of the session, we unveiled the first of three “black boxes” with simulations that may or may not have had added signal.
- We heard very positive feedback especially from ATLAS/ CMS experimentalists who told us that this was a great exercise for them to prepare for data analyses

# Anomaly detection - New methods

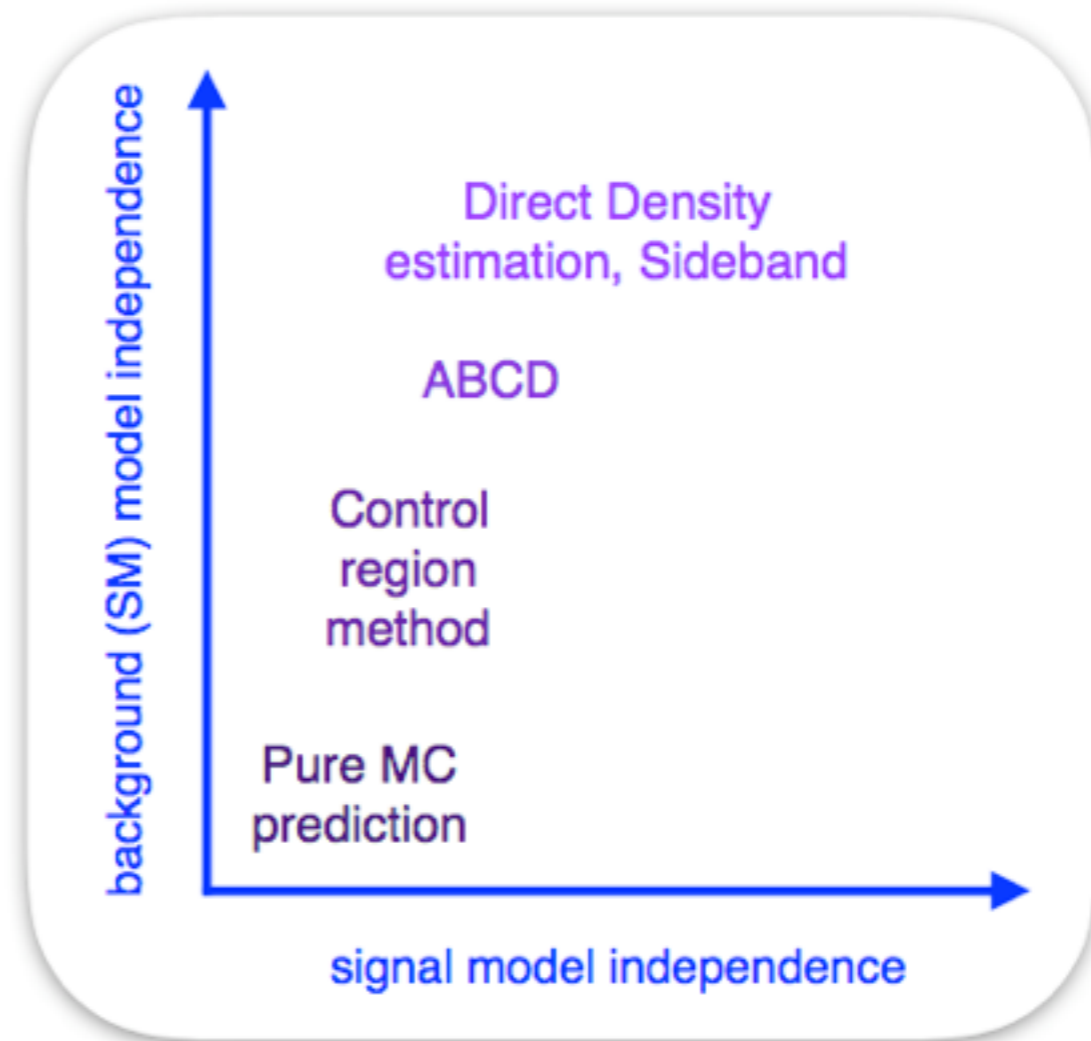
22

Many new methods were presented in the anomaly detection session!

*from Nachman & DS 2001.04990*



(a) Signal sensitivity

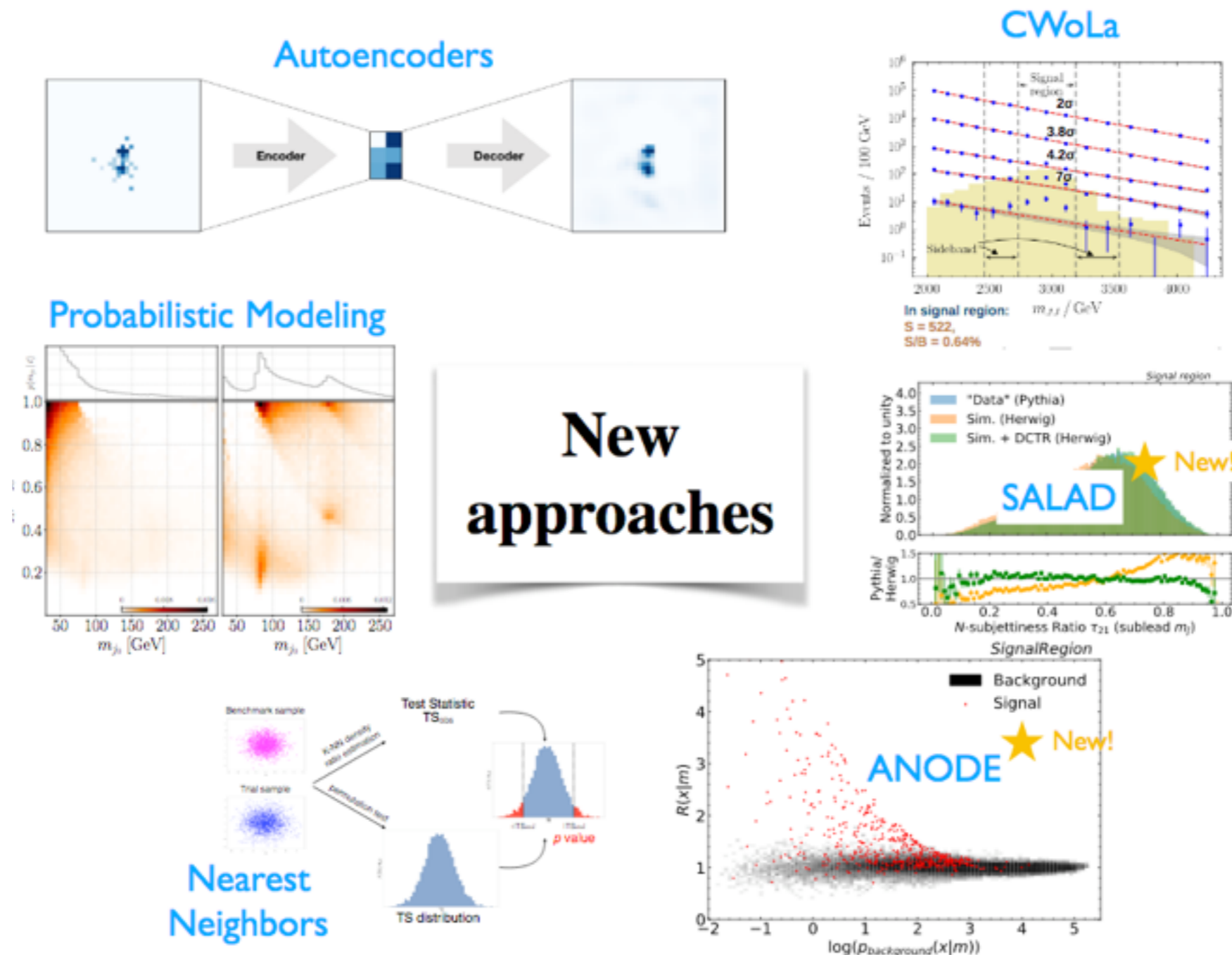


(b) Background specificity

# Anomaly detection - New methods

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Many new methods were presented in the anomaly detection session!



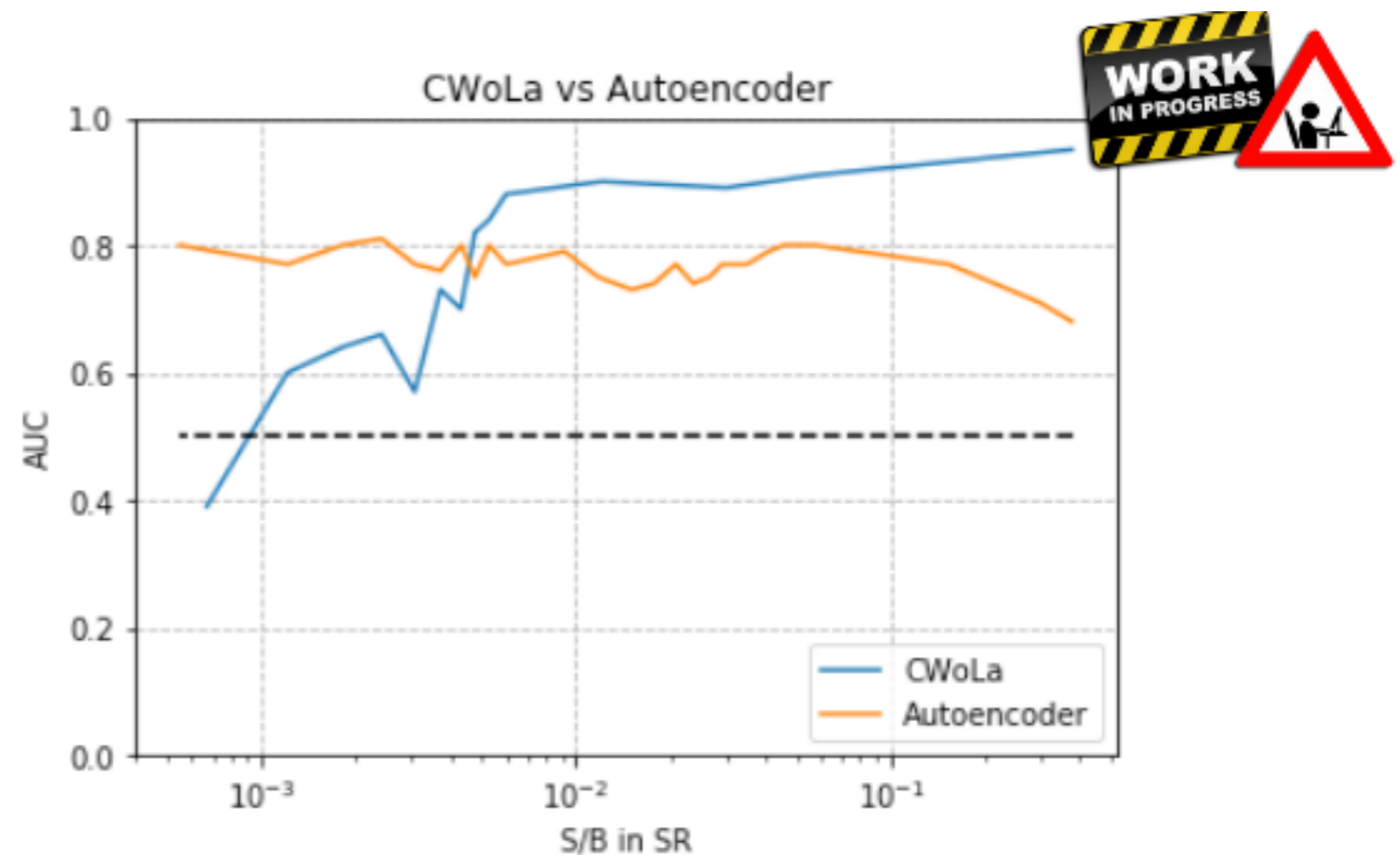
# Anomaly detection - Tradeoffs

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No algorithm will work best everywhere!

It is likely that we will need multiple approaches

This is just one plot that shows the complimentary between a semi-supervised approach and an unsupervised approach



The semi-supervised approach does better when there is enough signal while the unsupervised one doesn't use signal at all so is independent of S/B.



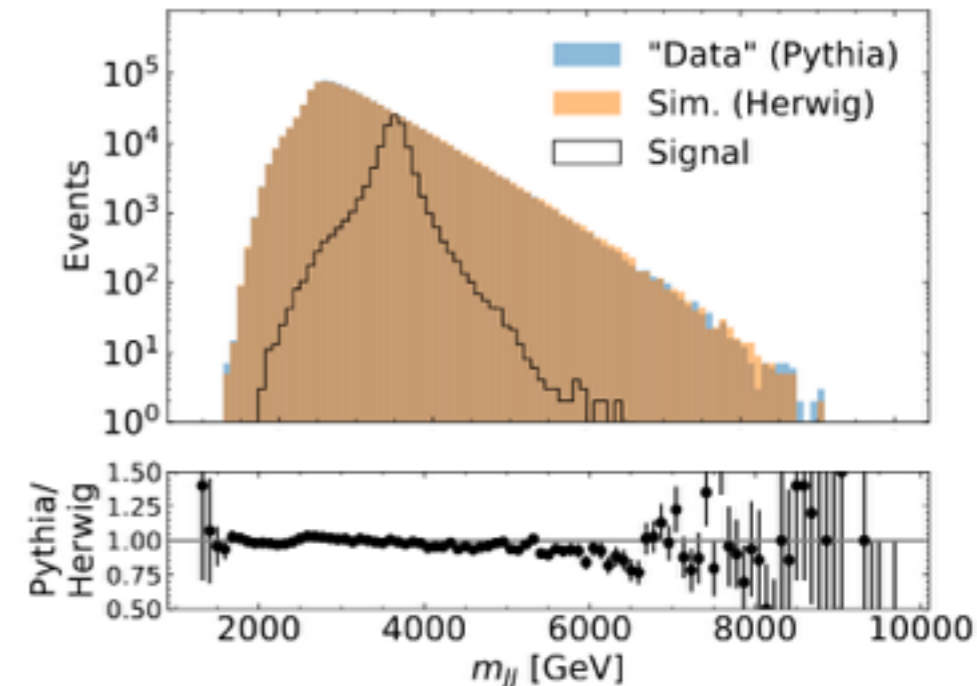
## LHC Olympics 2020: Black Boxes

Organizers: Gregor Kasieczka, Ben Nachman & David Shih

Three black boxes of simulated data were prepared:

- 1 million events each
- 4-vectors of every reconstructed particle (hadron) in the event
- Particle ID, charge, etc not included
- Single R=1 jet trigger  $p_T > 1.2$  TeV
- Black boxes are meant to be representative of actual data, meaning they are mostly background and may contain signals of new physics

In addition, a sample of 1M QCD dijet events (produced with Pythia8 and Delphes3.4.1) was provided as a background sample.



<https://doi.org/10.5281/zenodo.3547721>

# Anomaly detection - LHC Olympics

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## Box 1

Signal: 834 events

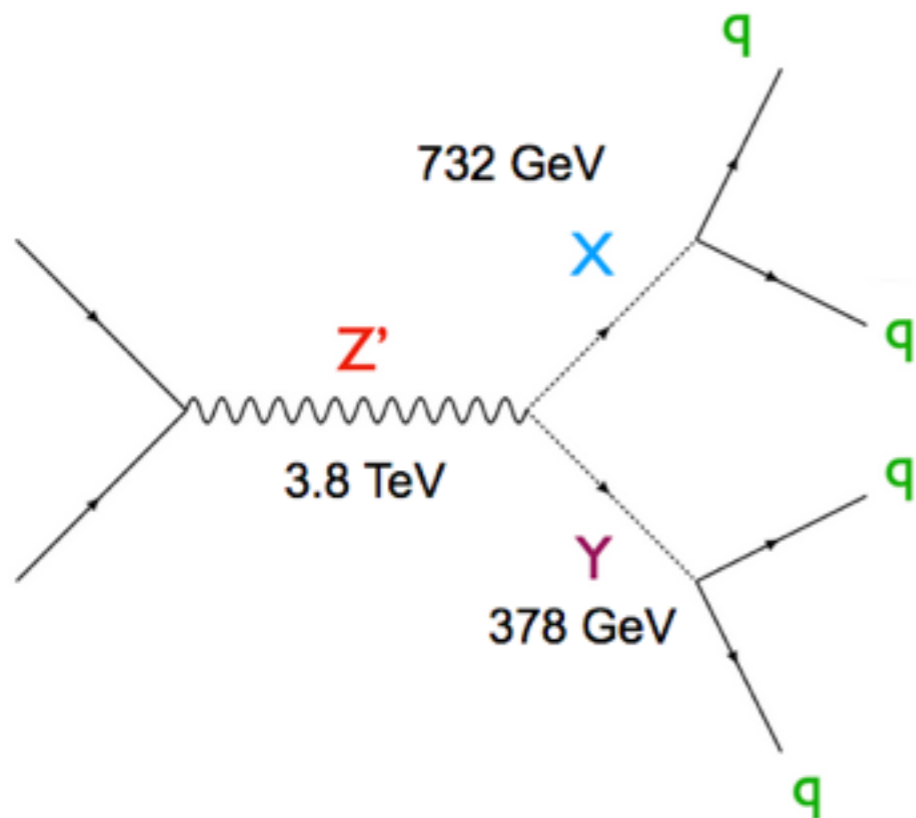
$Z' \rightarrow XY$ ;  $X, Y \rightarrow qq$

(same topology as R&D dataset)

$m_{Z'} = 3823 \text{ GeV}$

$m_X = 732 \text{ GeV}$

$m_Y = 378 \text{ GeV}$



# Anomaly detection - LHC Olympics

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## Box 1

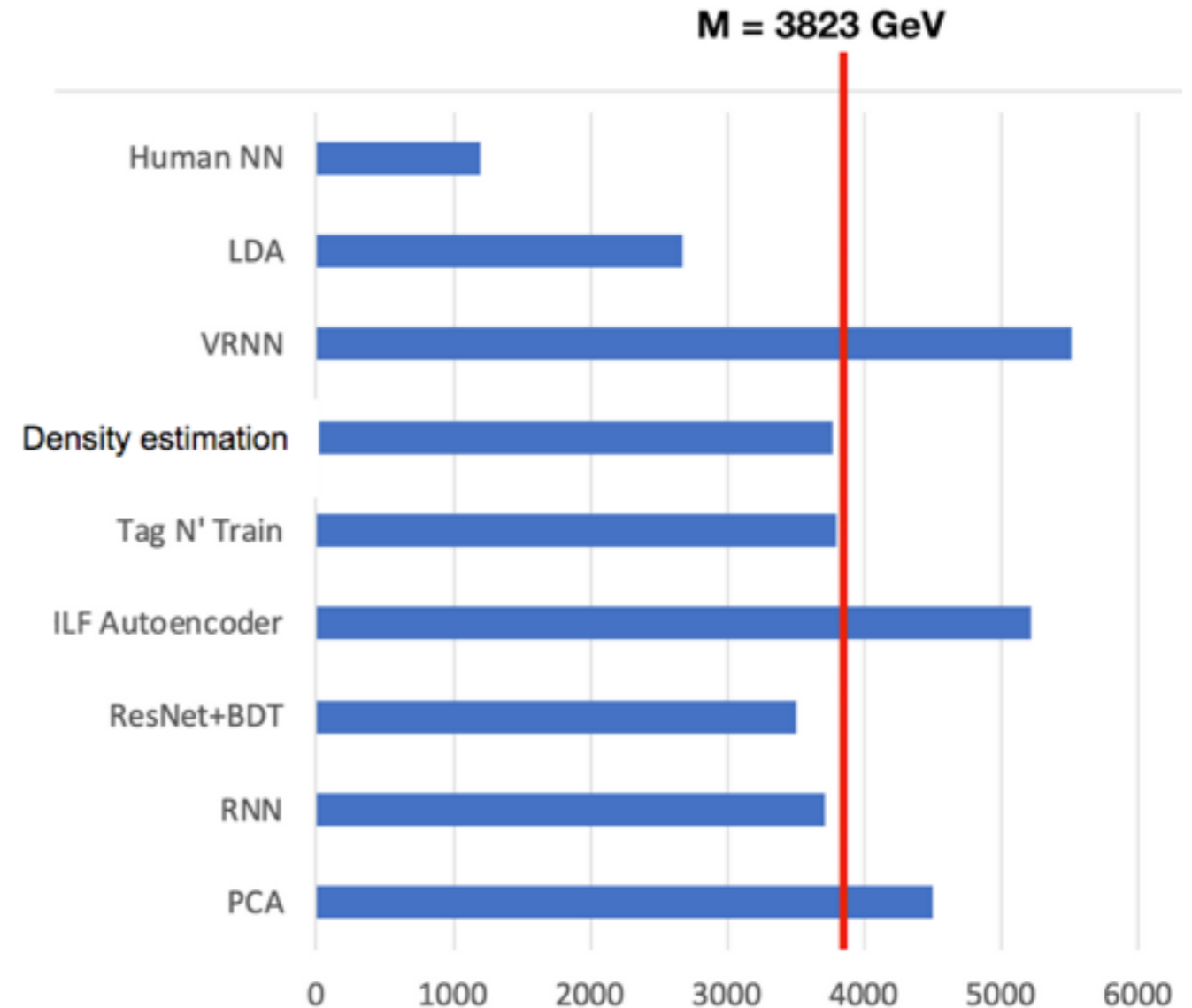
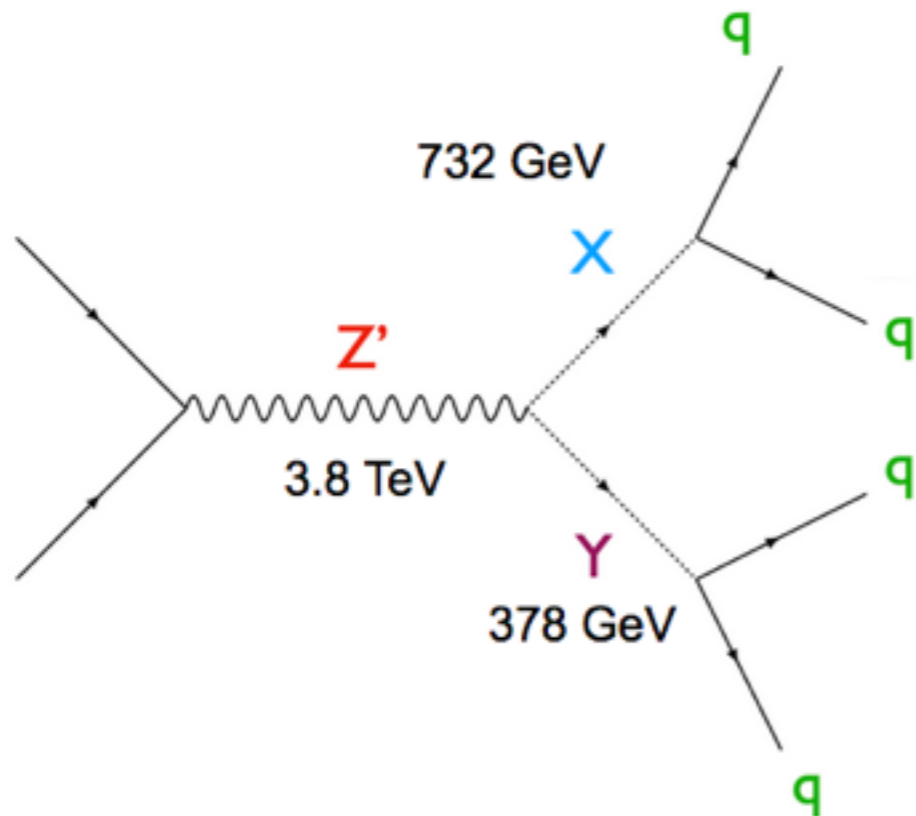
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# Anomaly detection - LHC Olympics

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## Box 1

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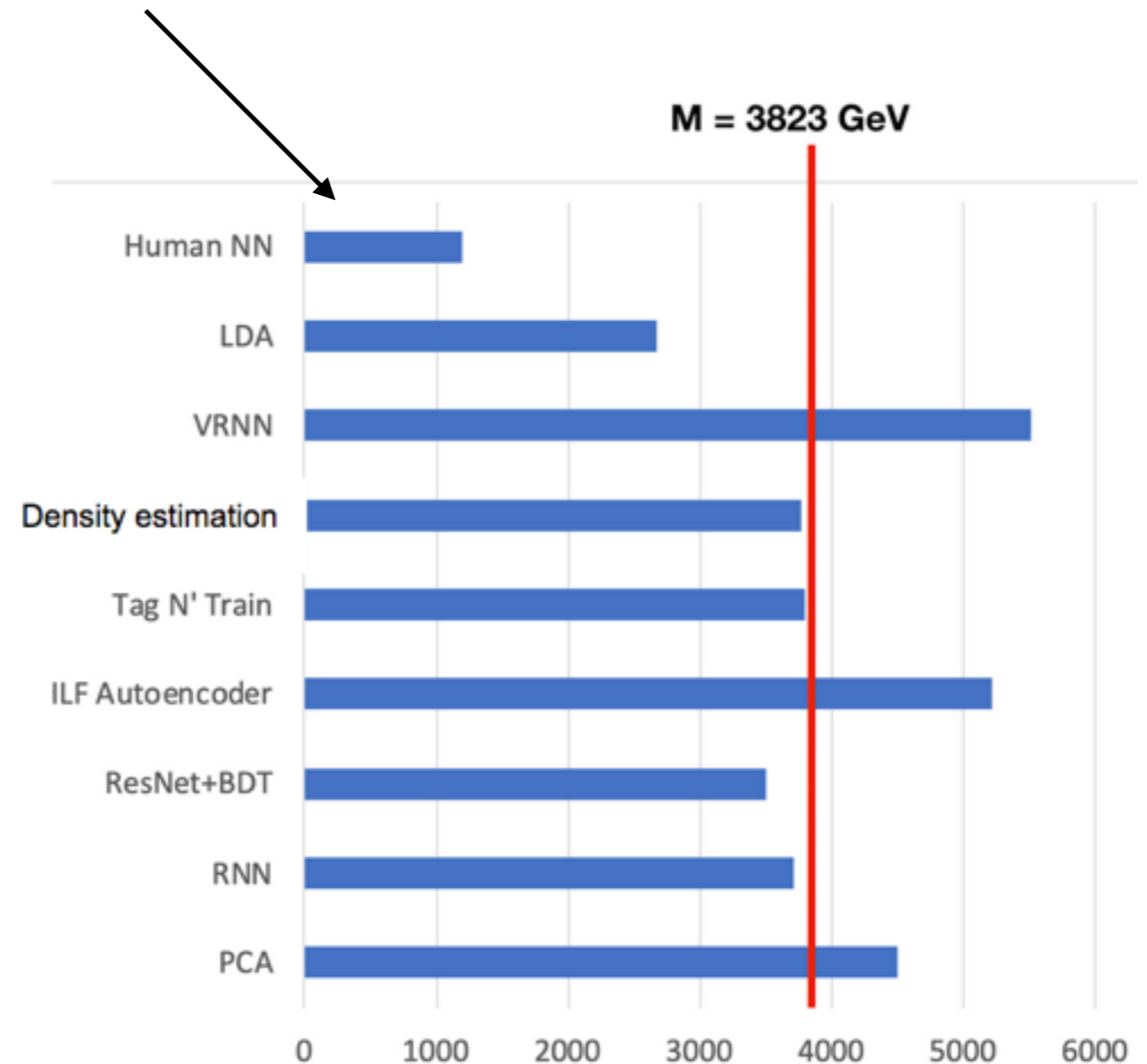
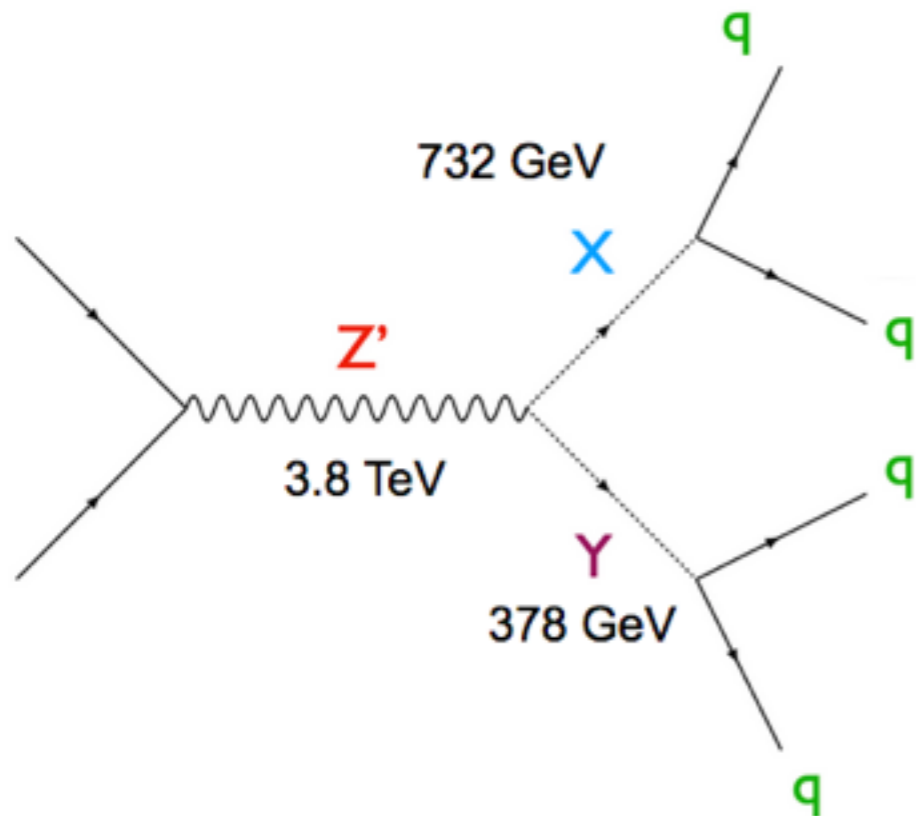
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Look at 1000 histograms



# Anomaly detection - LHC Olympics

## Box 1

Signal: 834 events

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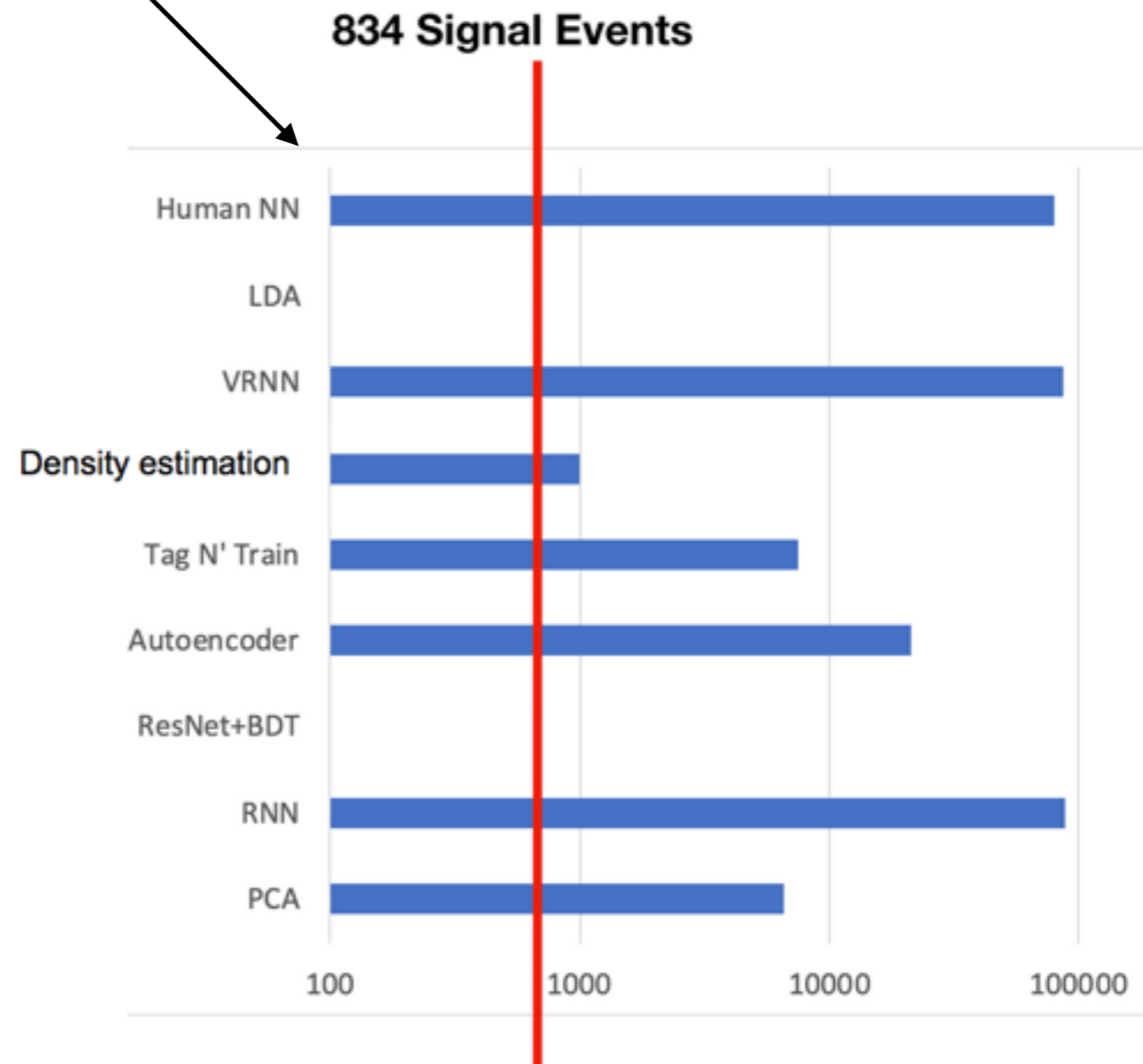
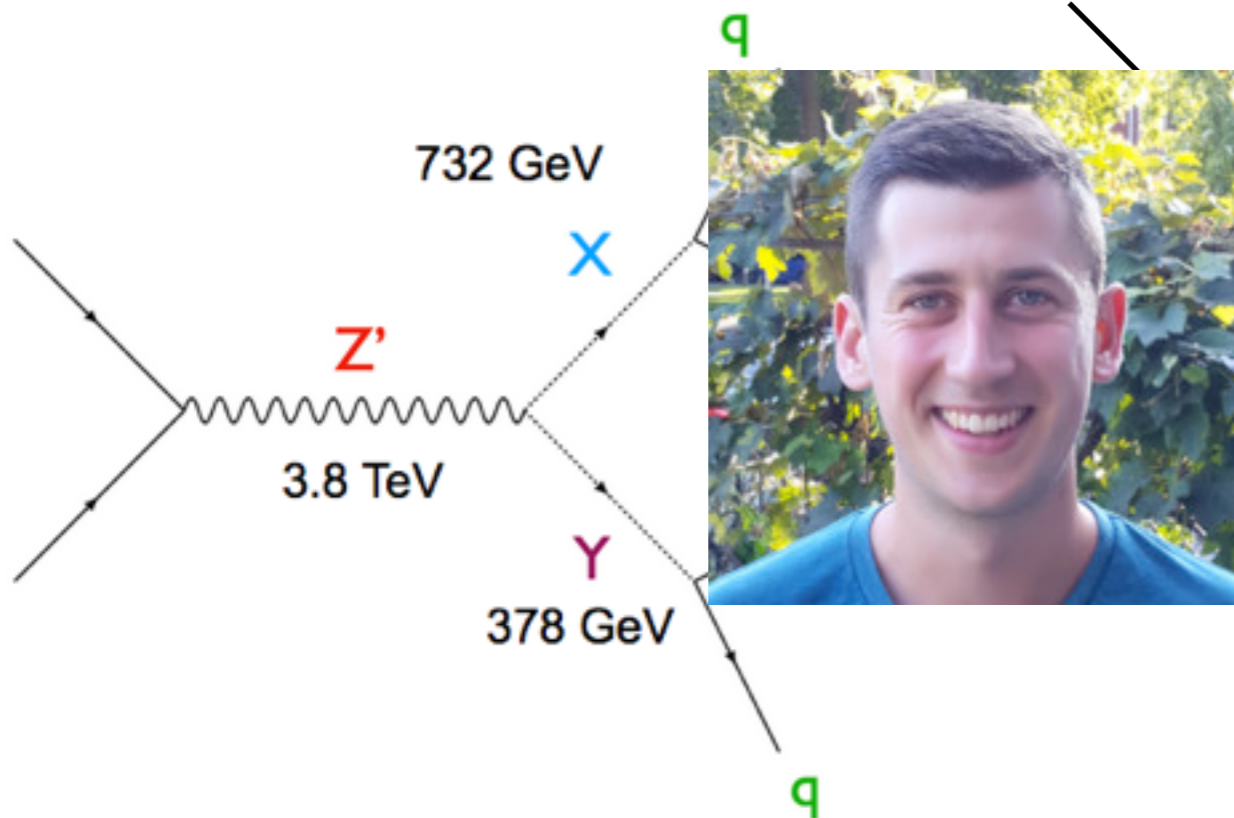
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Look at 1000 histograms

UCB  
Cosmology  
team



# LHC Olympics: next steps



- There will be another mini workshop just before BOOST where boxes 2 and 3 will be unveiled.

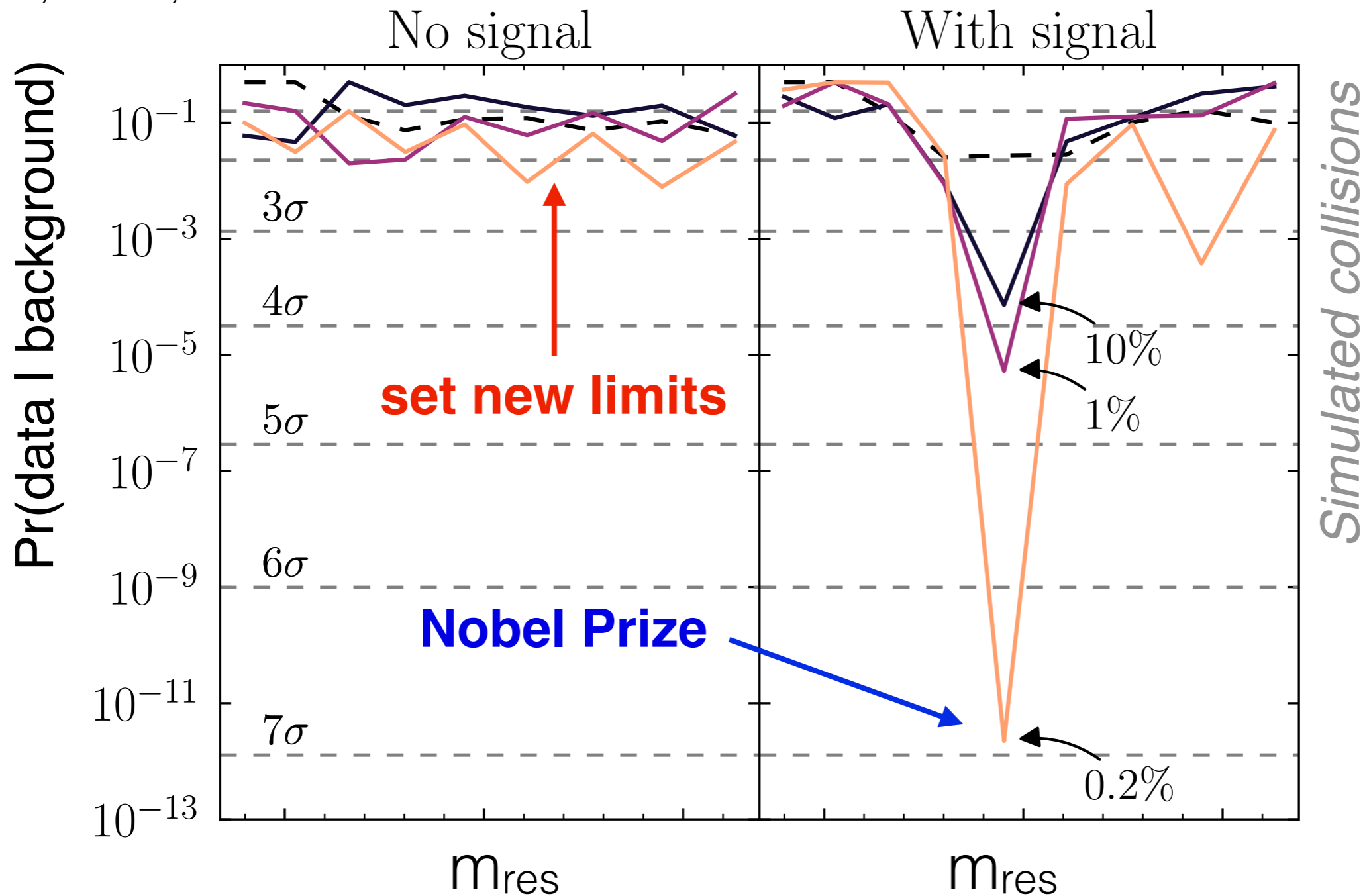
Anomaly Detection Mini-Workshop -- LHC Summer Olympics 2020

July 18, 2020  
INF/AP Lecture Hall  
Europe/Berlin timezone

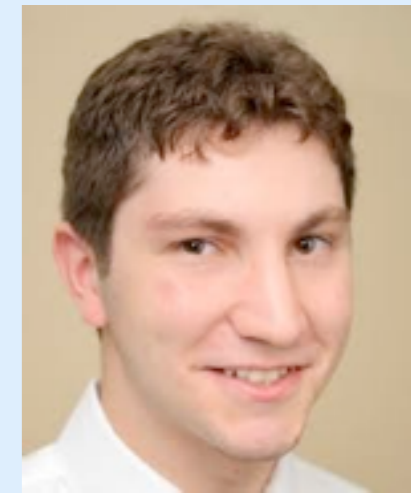
# Anomaly detection - Bonus!

[Phys. Rev. Lett. 121 \(2018\) 241803](#)

J. Collins, K. Howe, BPN



Aviv Cukierman



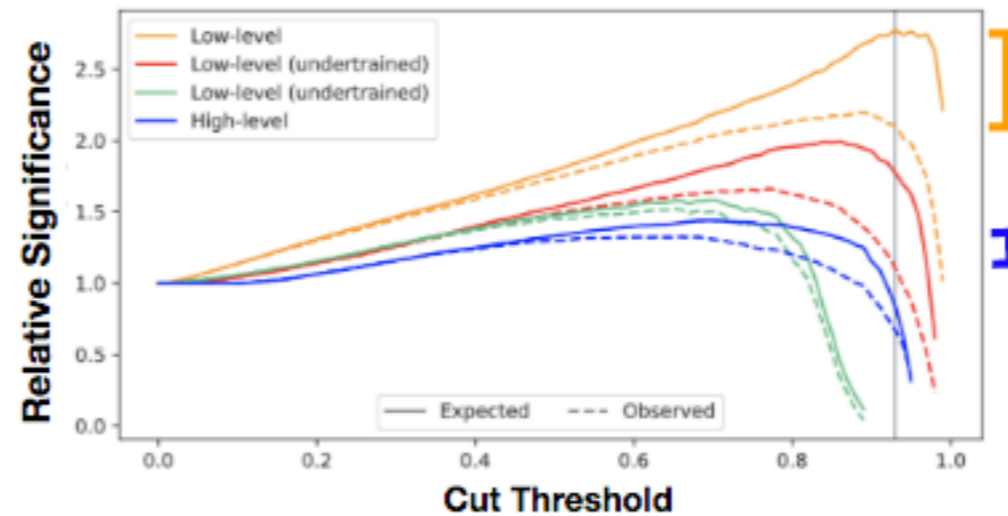
*Our first data result from **ATLAS** will come out this spring!*

- Bayesian neural networks
  - Can encode some forms of uncertainty
- High-dimensional uncertainties with AI Safety (next slide)
- Unfolding
  - A generalization of iterative Bayesian unfolding (2 slides)
  - Conditional generative model (basically learn true given reco)
- Benchmarking (3 slides)



We show that it is possible to find systematic mismodellings  $g(J) \mapsto J'$ , that confuse NN classifiers

- These effects are subtle, **remaining undetected** in control/validation regions
- Susceptibility is **reduced**, but not entirely, when using **fewer and higher-level inputs**



## What is AI Safety?

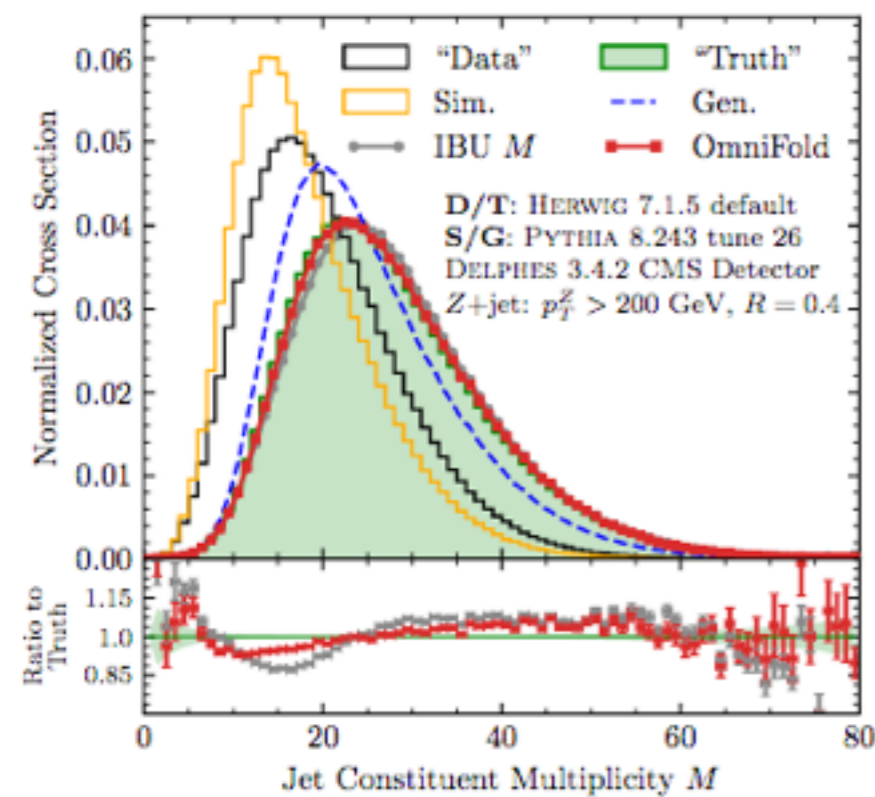
High-dimensional uncertainties are a real challenge for deploying deep networks on low-level features!



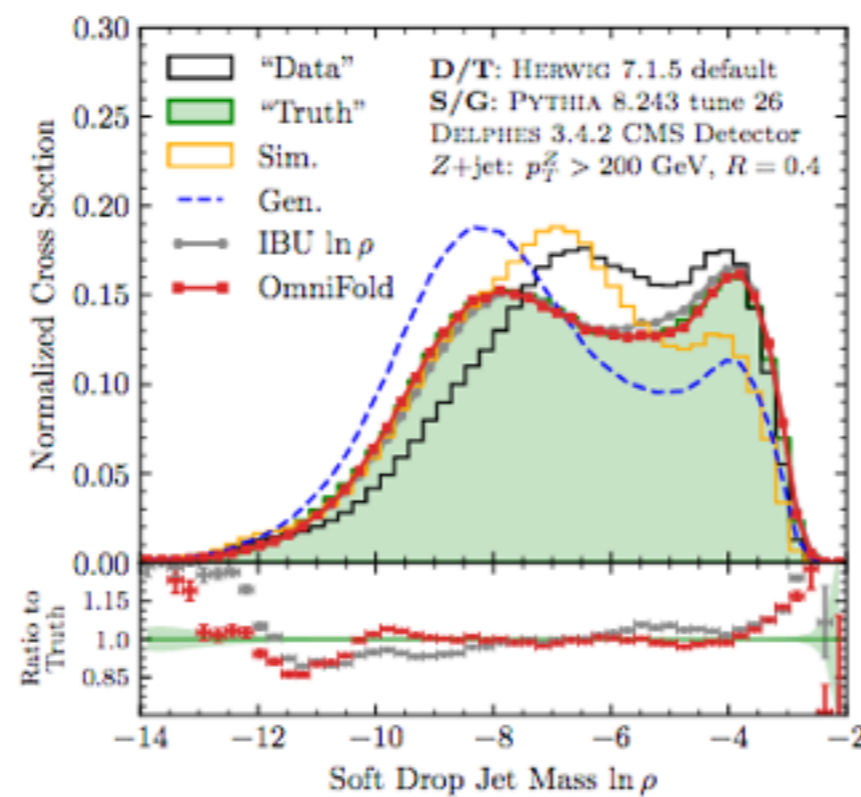
It is now possible to unfold the “full phase space” i.e. all of the 4-vectors and particle types in a single event !!

## Single **OmniFold** instantiation vs. individual applications of IBU

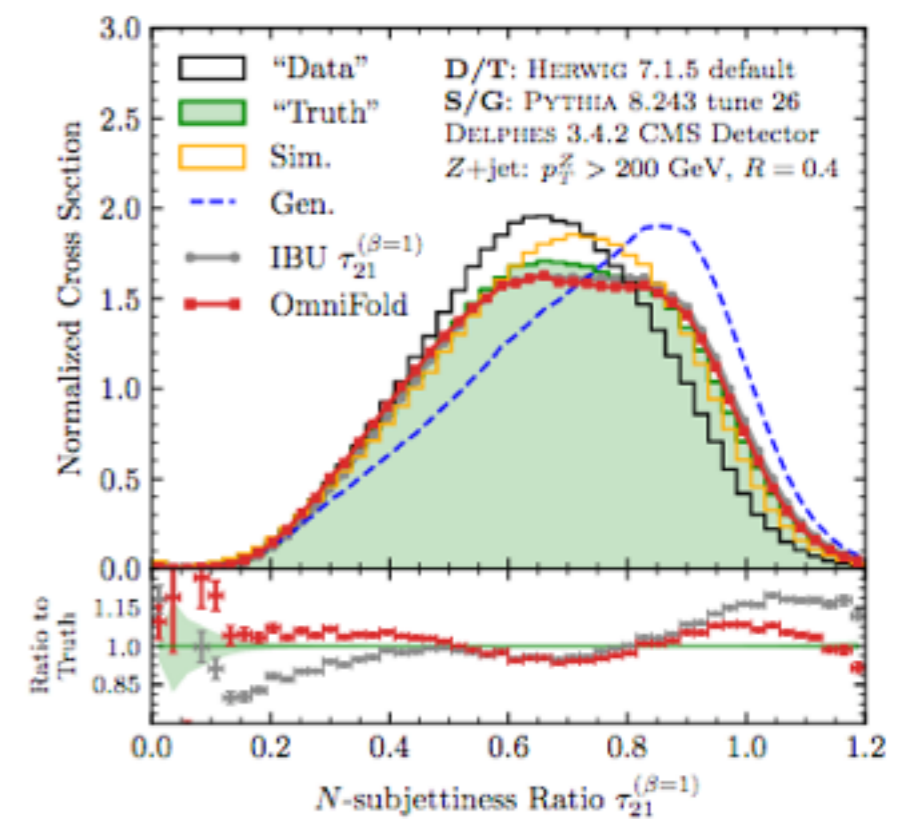
(IBU = iterative Bayesian unfolding, standard in ATLAS)



IRC unsafe



IRC safe



Sudakov safe

# Benchmarking

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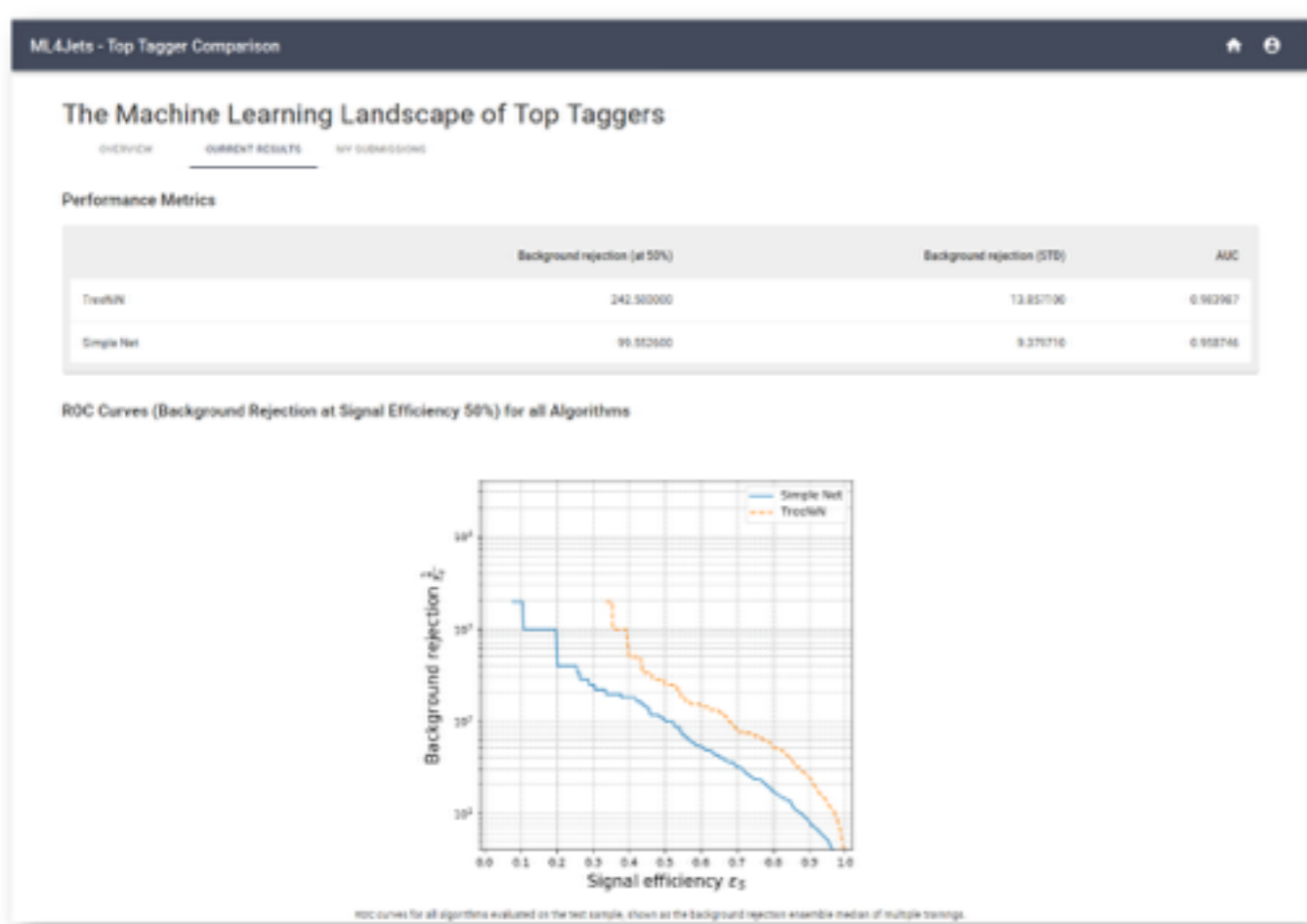
Included a live demo! Could be used for future challenges as well as for analysis in the collaboration - can we update all results at once if e.g. b-tagging is improved?

## Reproducible Open Benchmarks for Data Analysis Platform

Kyle Cranmer, Irina Espejo,  
**Sebastian Macaluso, Heiko Mueller**  
*New York University*

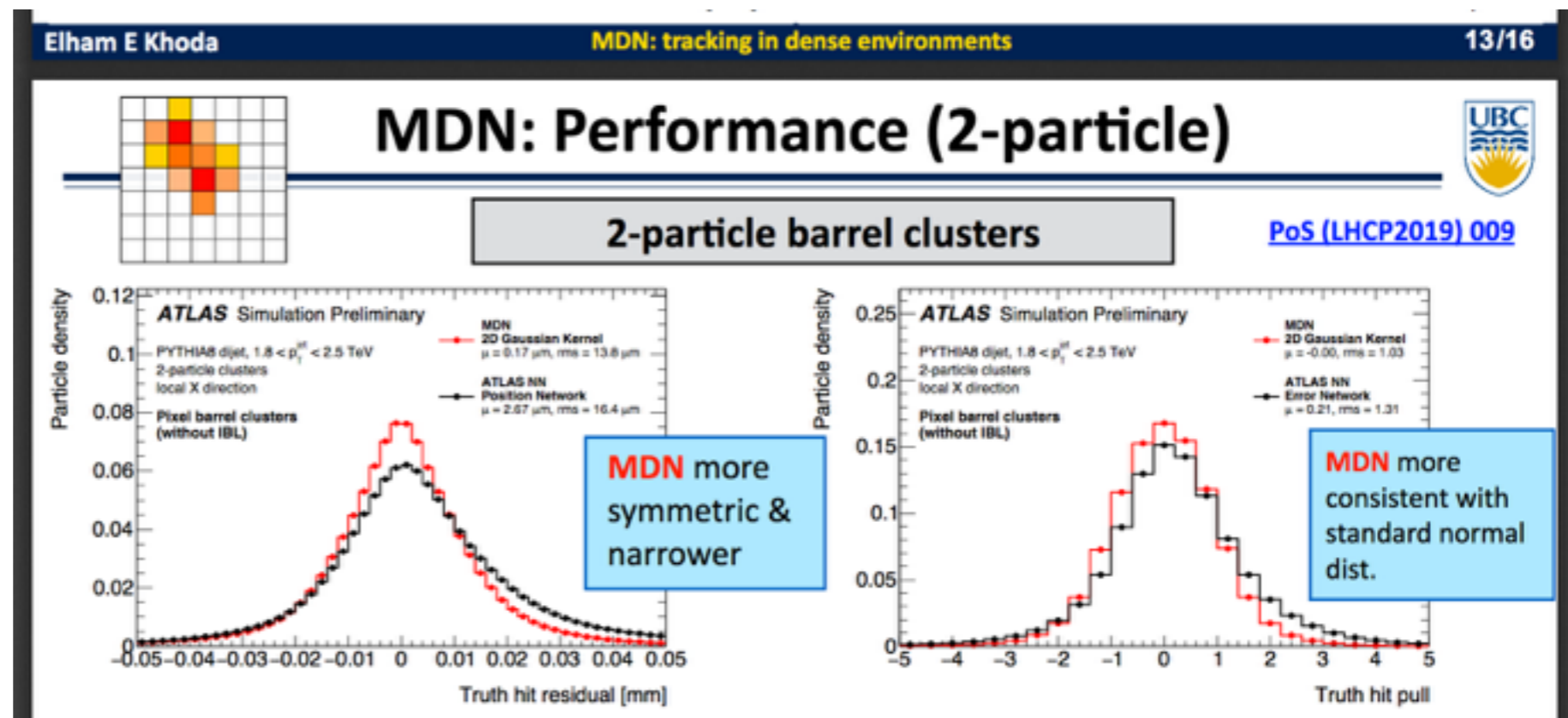
Shih-Chieh Hsu, Aaron Maritz,  
Ajay Rawat, Cha Suaysom  
*University of Washington*

(click this to see the slides)



- Vertexing with graph networks
  - Set to graph networks
- Mixture density networks for pixel clusters in dense environments

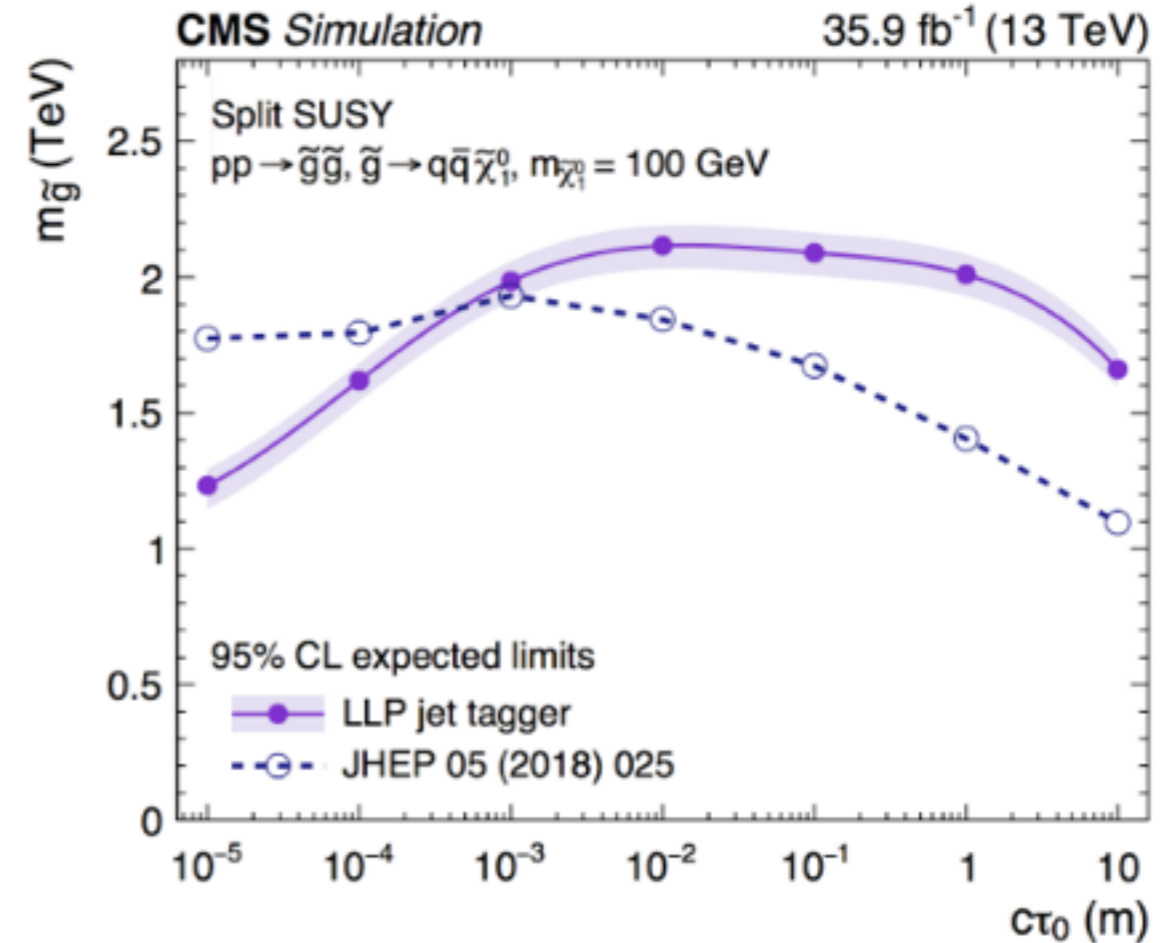
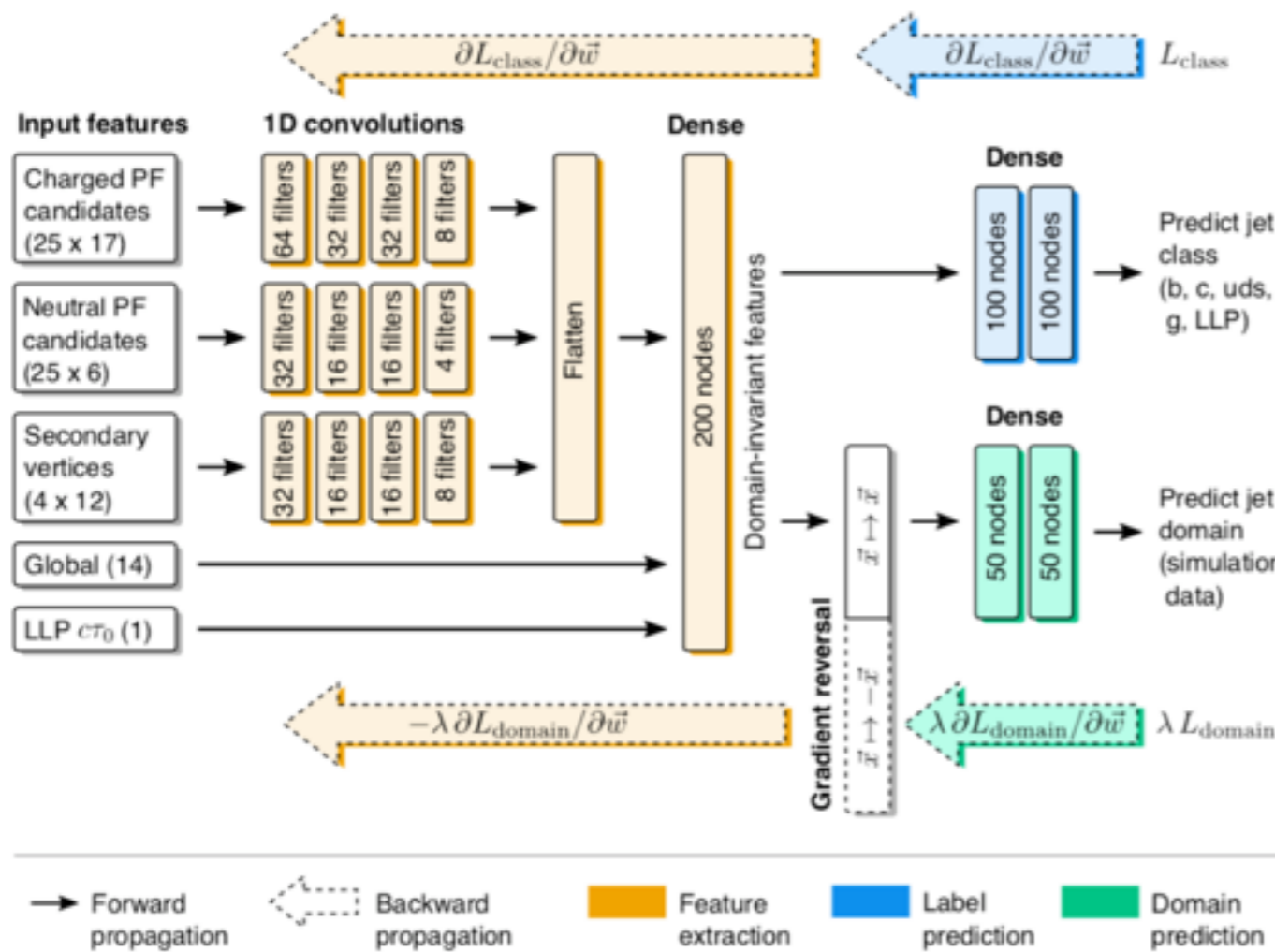
(Gaussian mixture model where mixture coefficients are NNs)



- Displaced jet tagging (next slide)

# Applications and experimental methods

Displaced jet tagging in CMS - very sophisticated!  
*high dimensional + decorelation*



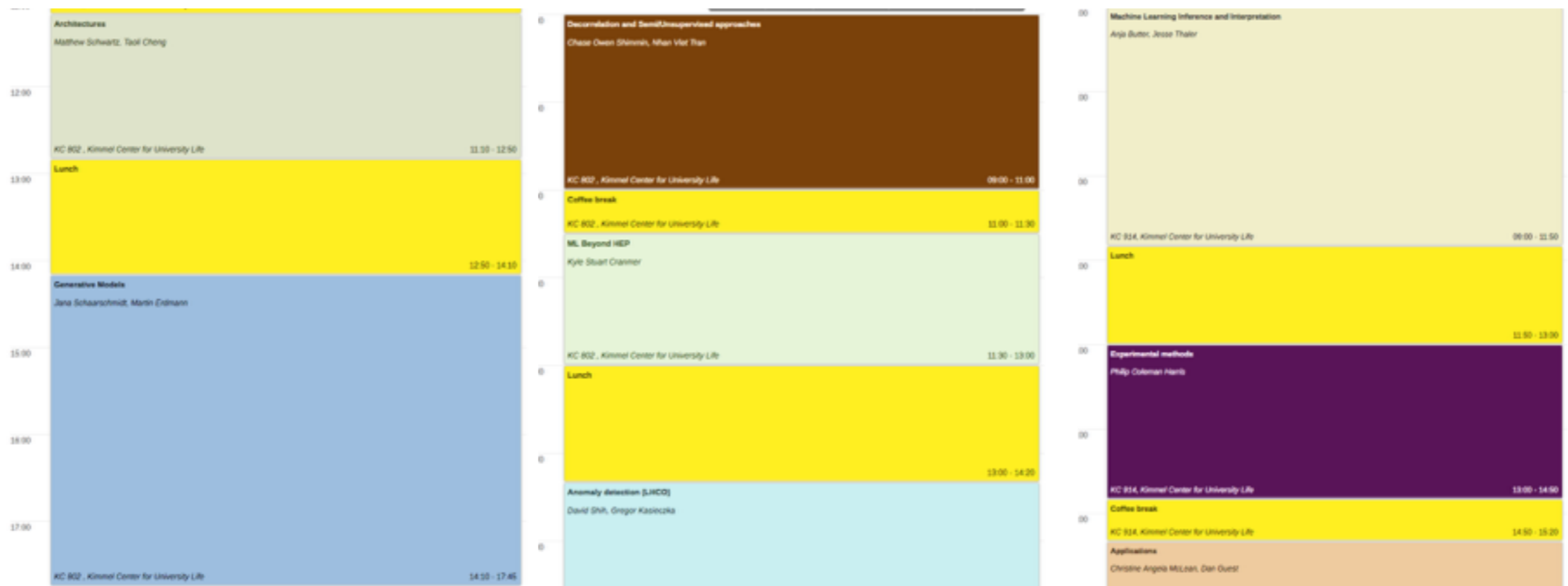
*no idea how to do signal uncertainties  
 ... and they don't either*

# Summary

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There was a packed agenda with three very full days of interesting talks!

I won't review every talk ... please take a look at the slides for all the contributions and for details. These slides are some personal highlights.



ML4Jets 20/21



Philosophenweg Heidelberg, week of Dec 14, 2020

Questions?

