

# Boosting New Physics Searches with Deep Learning

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Accelerating the Search for Dark Matter with Machine Learning  
ICTP, Trieste

April 9, 2019

# Announcement

## SUSY2019 – SCIENTIFIC TOPICS:

- Supersymmetry: Models, Phenomenology and Experimental Results
- Unification of Forces
- Electroweak, Top and Higgs Physics
- Precision Calculations and Tools
- BSM in Flavor Physics
- Neutrino Masses: Models and Phenomenology
- Cosmology and Gravitational Waves
- Dark Matter, Astroparticle Physics
- Formal Field Theory and Strings
- Alternatives to Supersymmetry
- Machine Learning, Big Data and Quantum Information

You are invited to submit an abstract for the ML parallel session at SUSY 2019.

The deadline is TOMORROW!!



**Starts** 20 May 2019, 07:30

**Ends** 24 May 2019, 18:30

US/Central



Corpus Christi, TX, USA



[SUSY 2019](#)

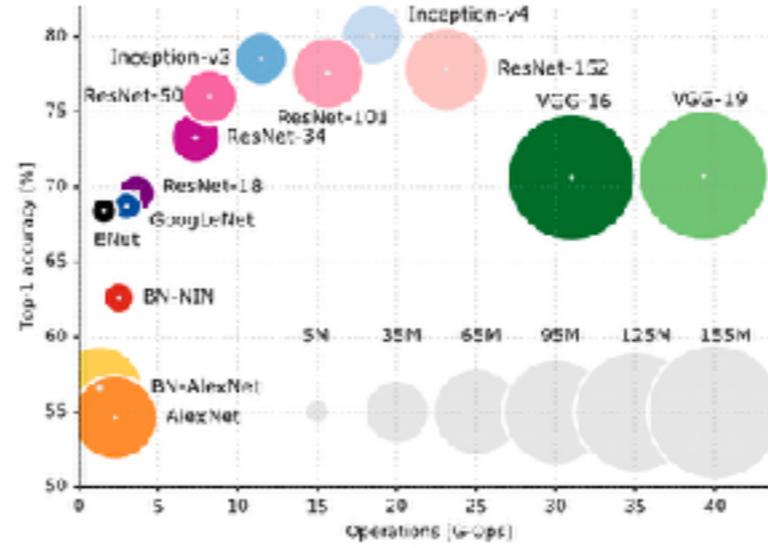
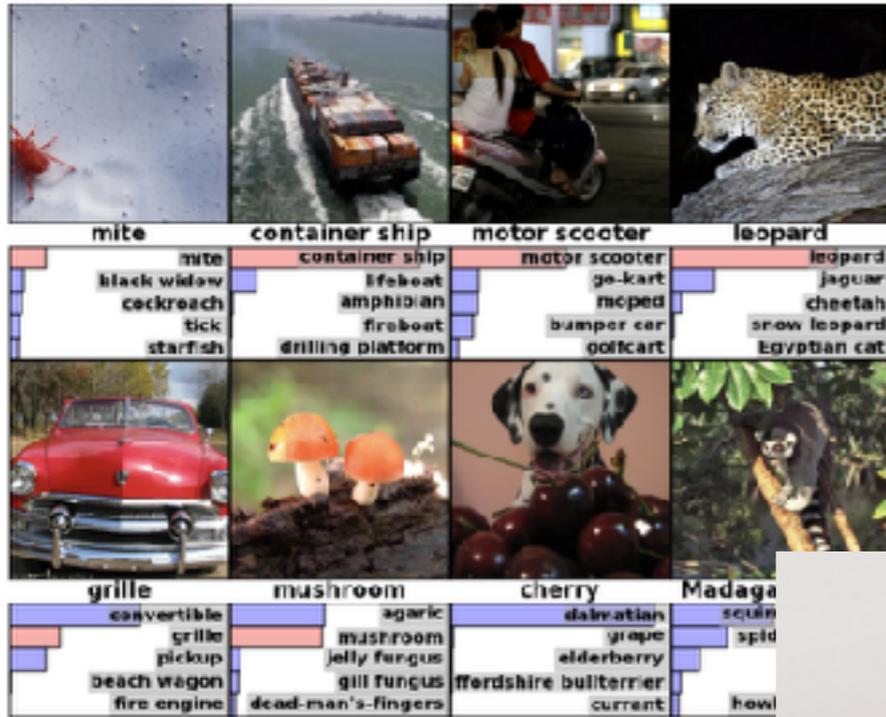


**The call for abstracts is open**

You can submit an abstract for reviewing.

[Submit new abstract](#)

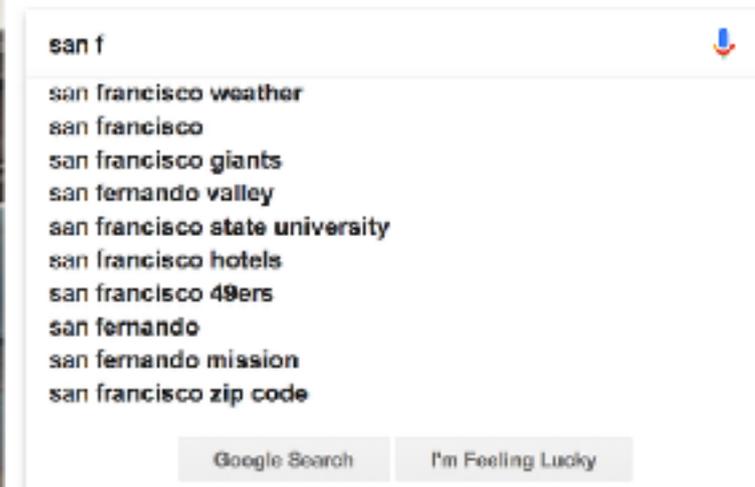
# The AI Revolution is Here



Economic growth has slowed down in recent years.

Das Wirtschaftswachstum hat sich in den letzten Jahren verlangsamt.  
Economic growth has slowed down in recent years.

La croissance économique s'est ralentie ces dernières années.



# The AI Revolution is Here

So many stunning real world successes in recent years.

Driven by:

- Growth in computational power
- Improvements in algorithms
- **Increased quantity and quality of data**

Prerequisite for deep learning: **large, complex, and well-understood datasets.**

Many real world applications are limited by  
the quality and quantity of the data.

# Big Data and Deep Learning

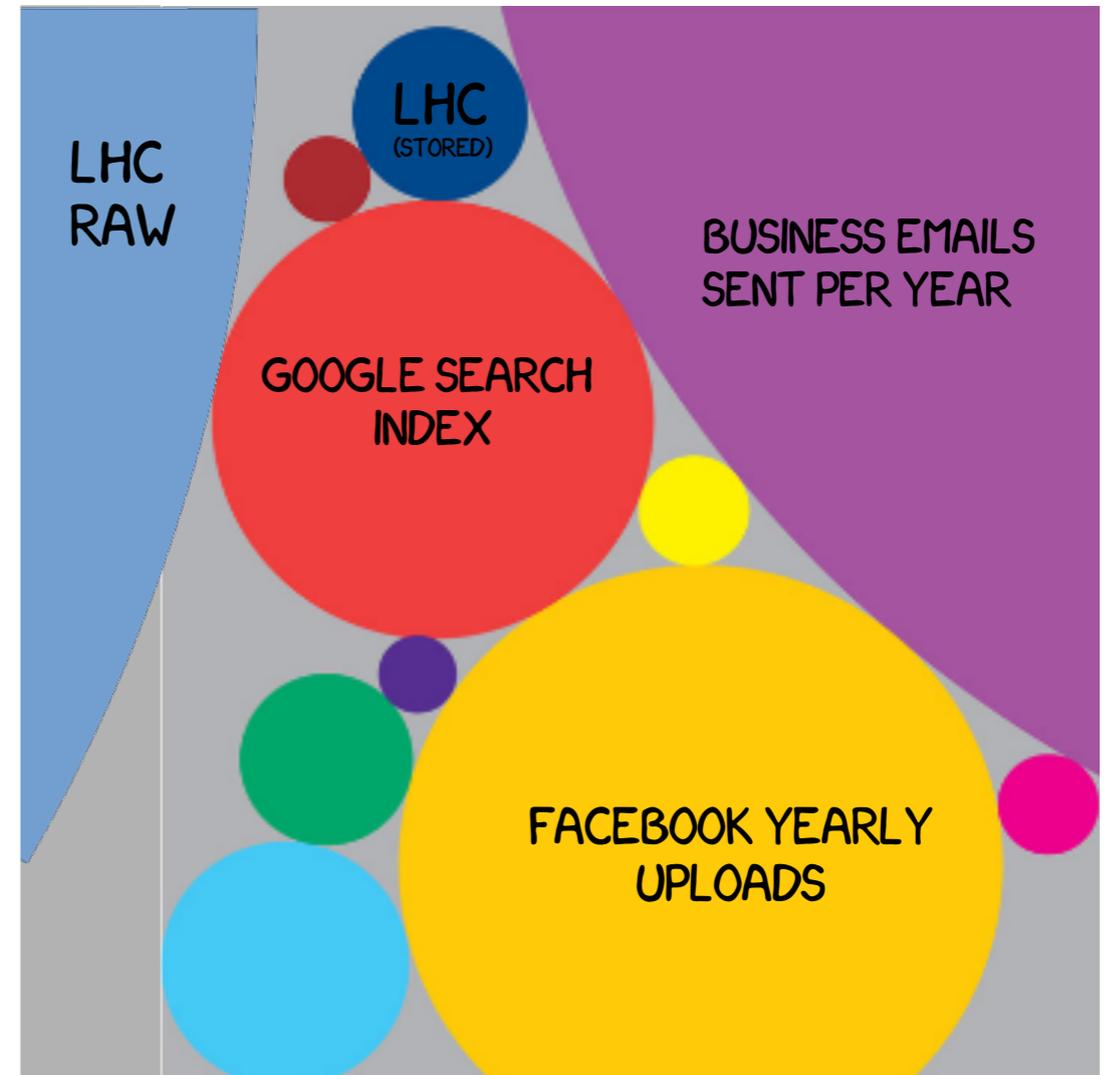
The LHC is the perfect setting for deep learning!

The data is

- large (billions of events on tape)
- complex (hundreds of particles per event)
- well-understood (Standard Model of particle physics).

Also, it is relatively easy to generate realistic simulated data.

(Madgraph, Pythia, Herwig, Delphes, GEANT,...)



<https://www.wired.com/2013/04/bigdata/>

Pasquale Musella, ETH-Zurich seminar

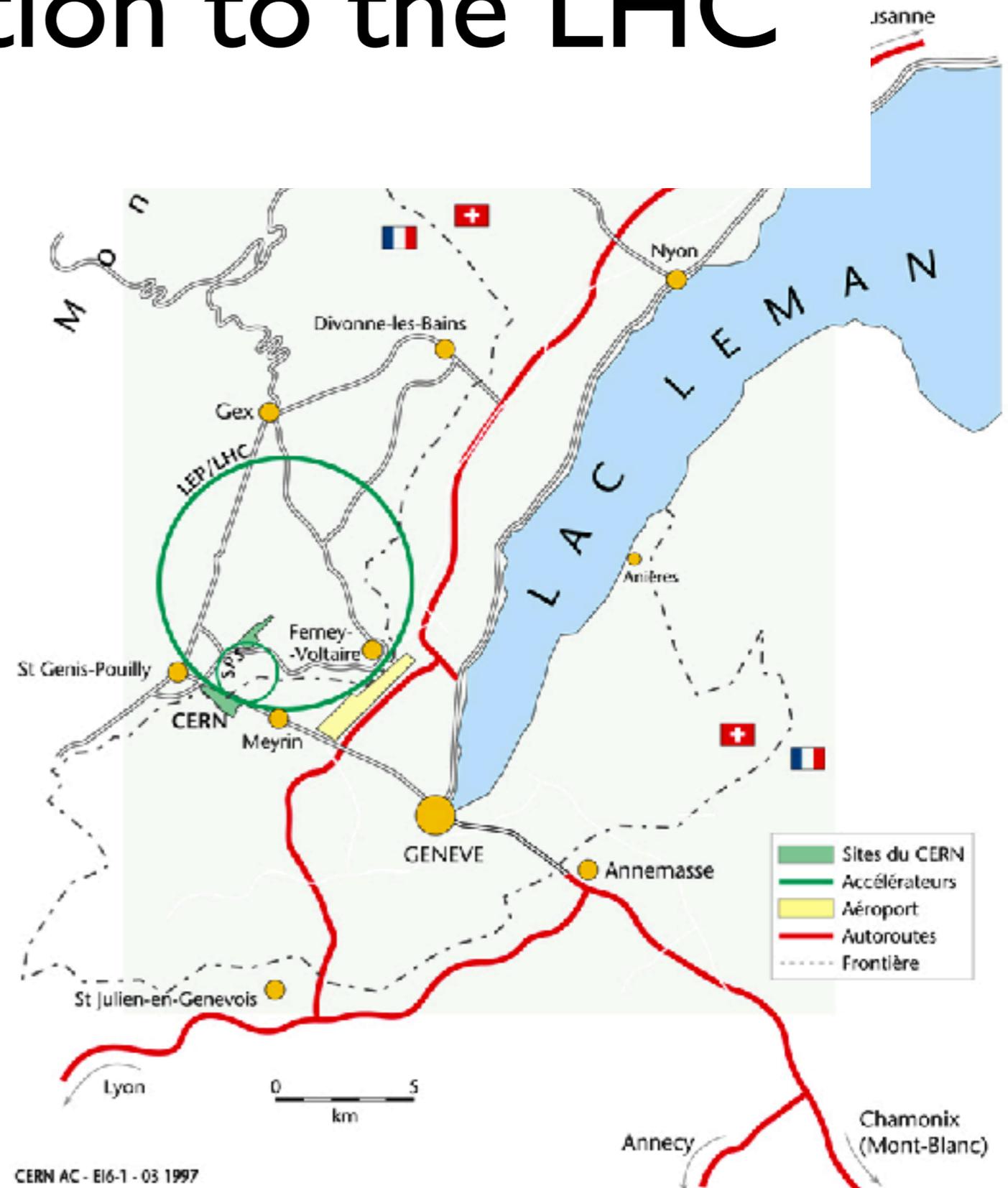
# A brief introduction to the LHC

# An introduction to the LHC

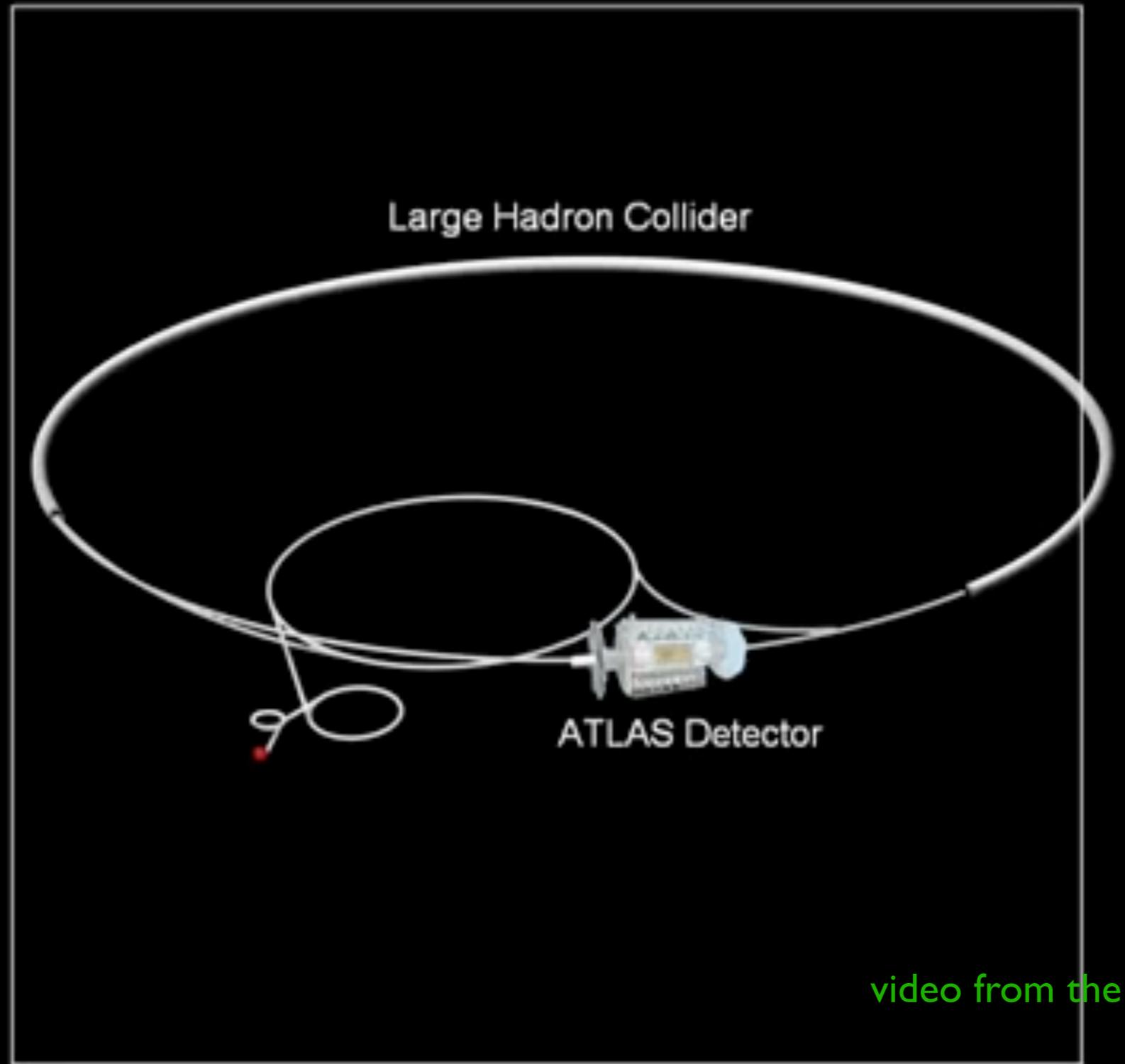
The Large Hadron Collider is the **largest** and **highest-energy** particle accelerator in the world.

It is part of CERN, located at the border of France and Switzerland, near the city of Geneva.

- 27 km long tunnel
- 100 m underground
- ~ \$10 billion
- ~5,000 scientists from ~200 countries



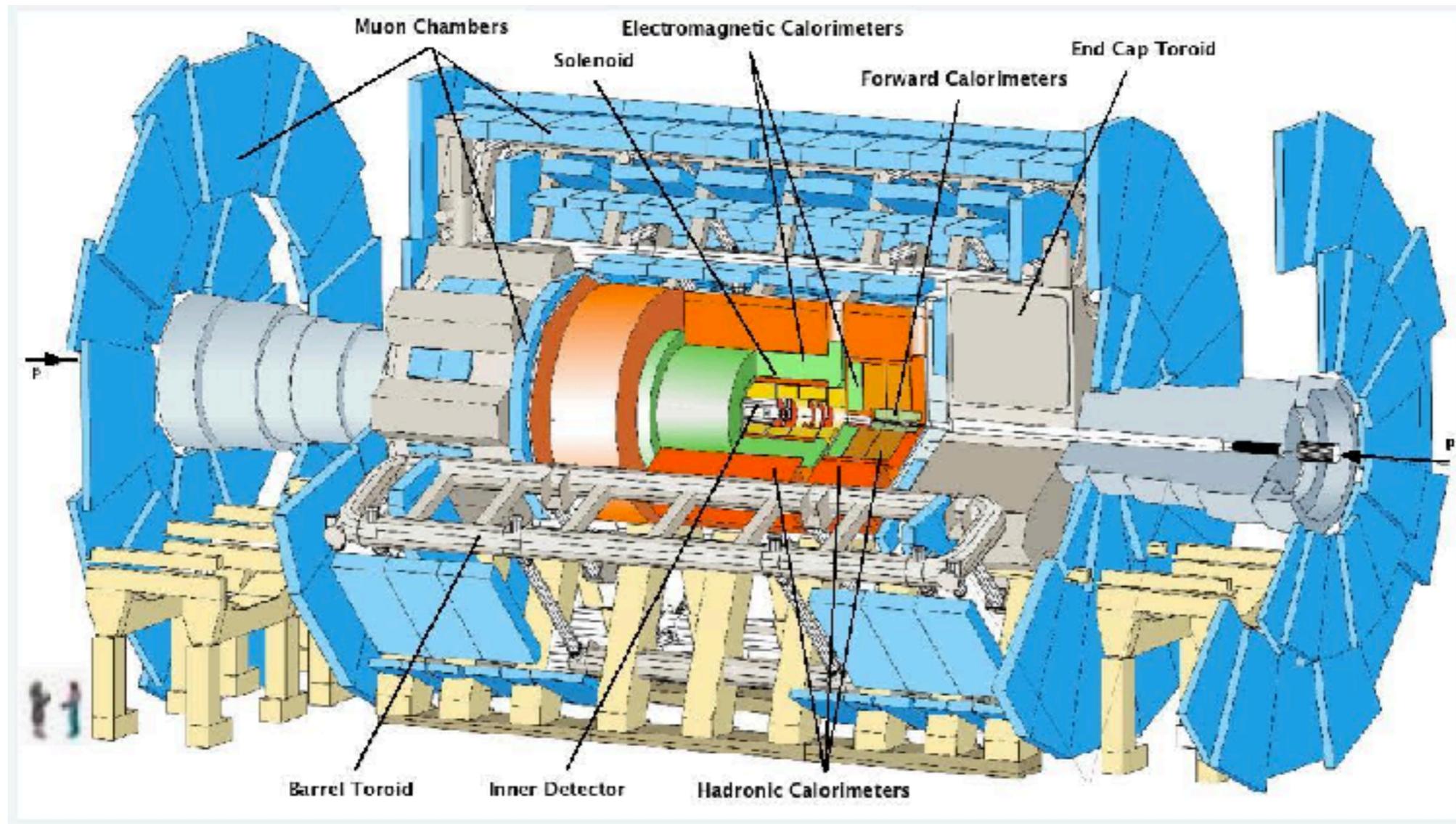
At the LHC, protons are accelerated to 99.9999991% of the speed of light, and collided together at four interaction points (ATLAS, CMS, LHCb, ALICE)



video from the ATLAS experiment

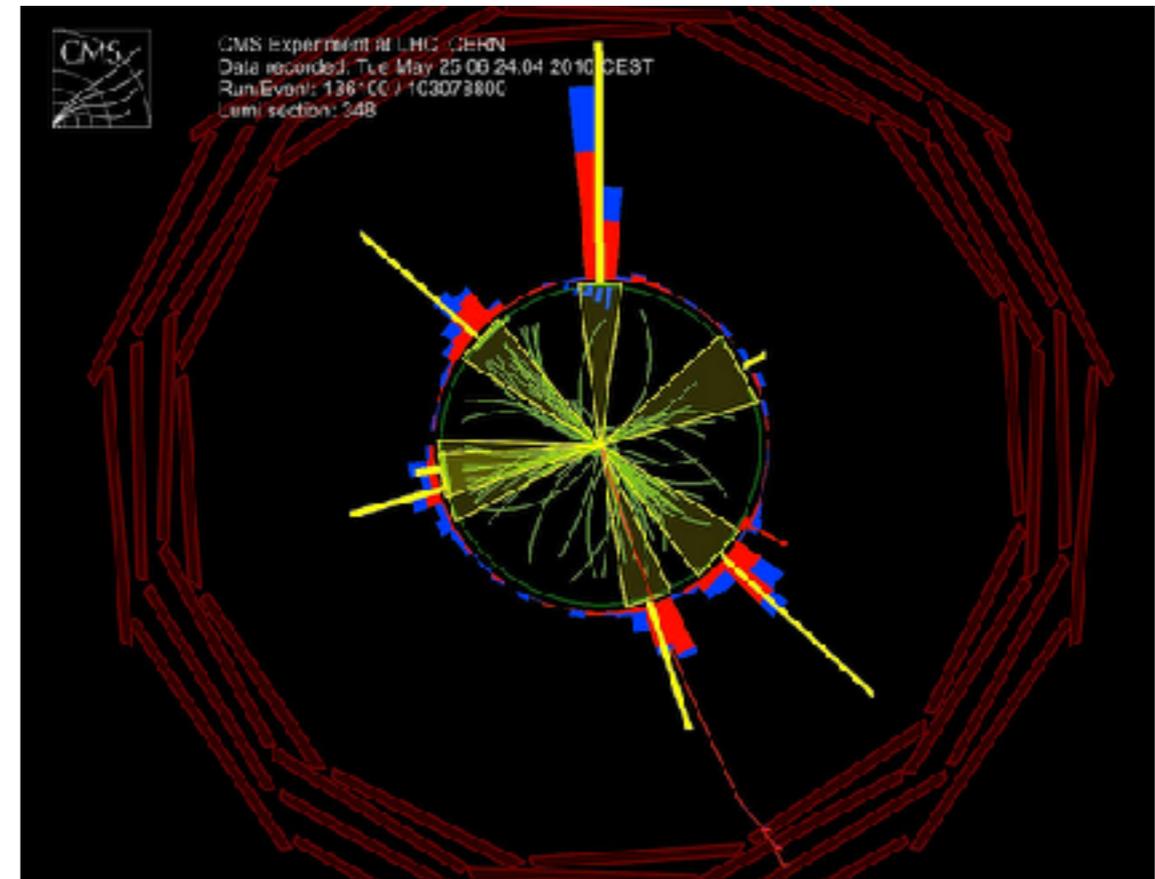
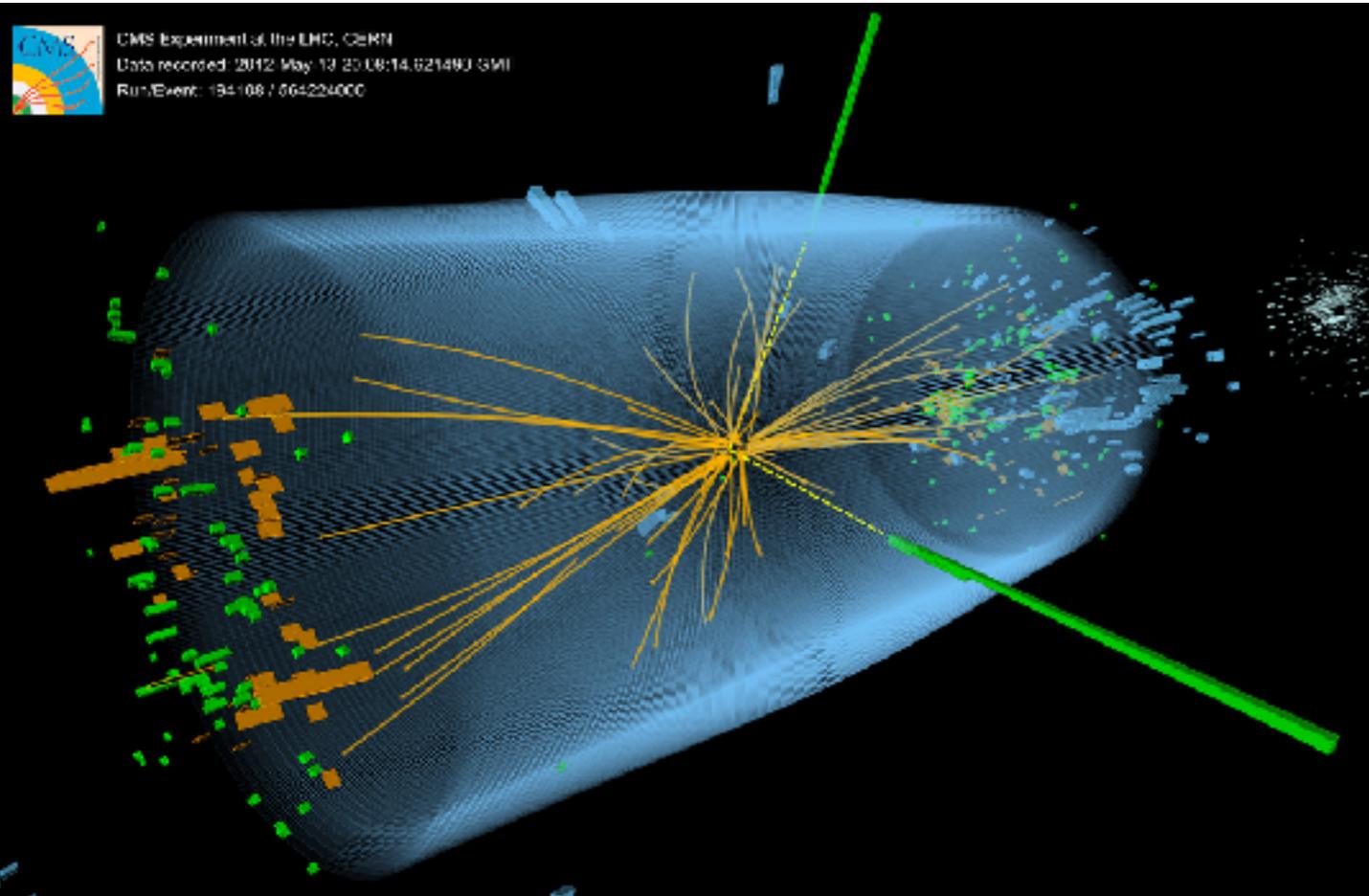
Beam energy: 6.5 TeV / proton  
~ 300 trillion protons (in ~3000 bunches) in each beam  
25 ns bunch spacing

# An LHC Detector



Detector is cylindrical (symmetric around beam axis)

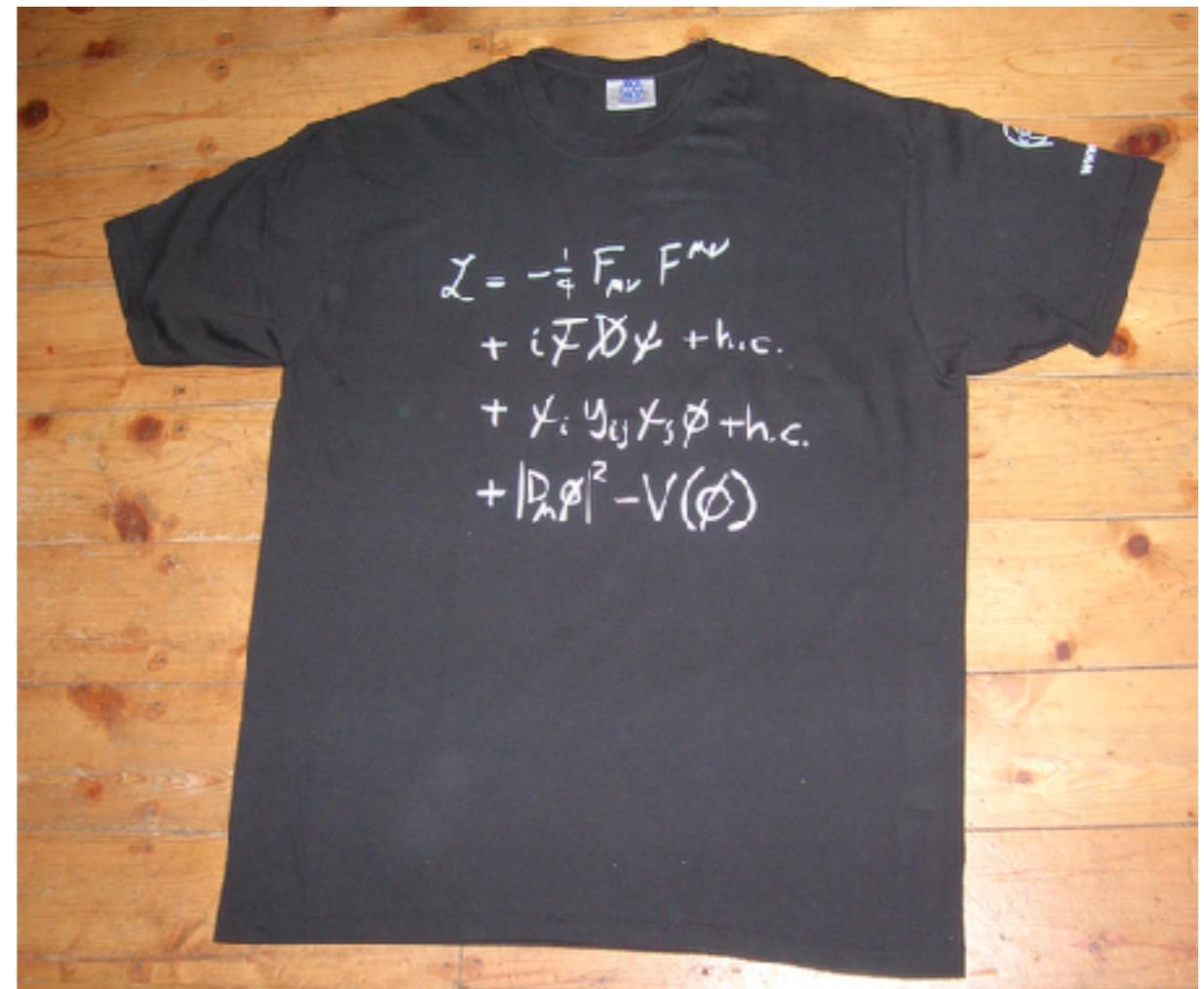
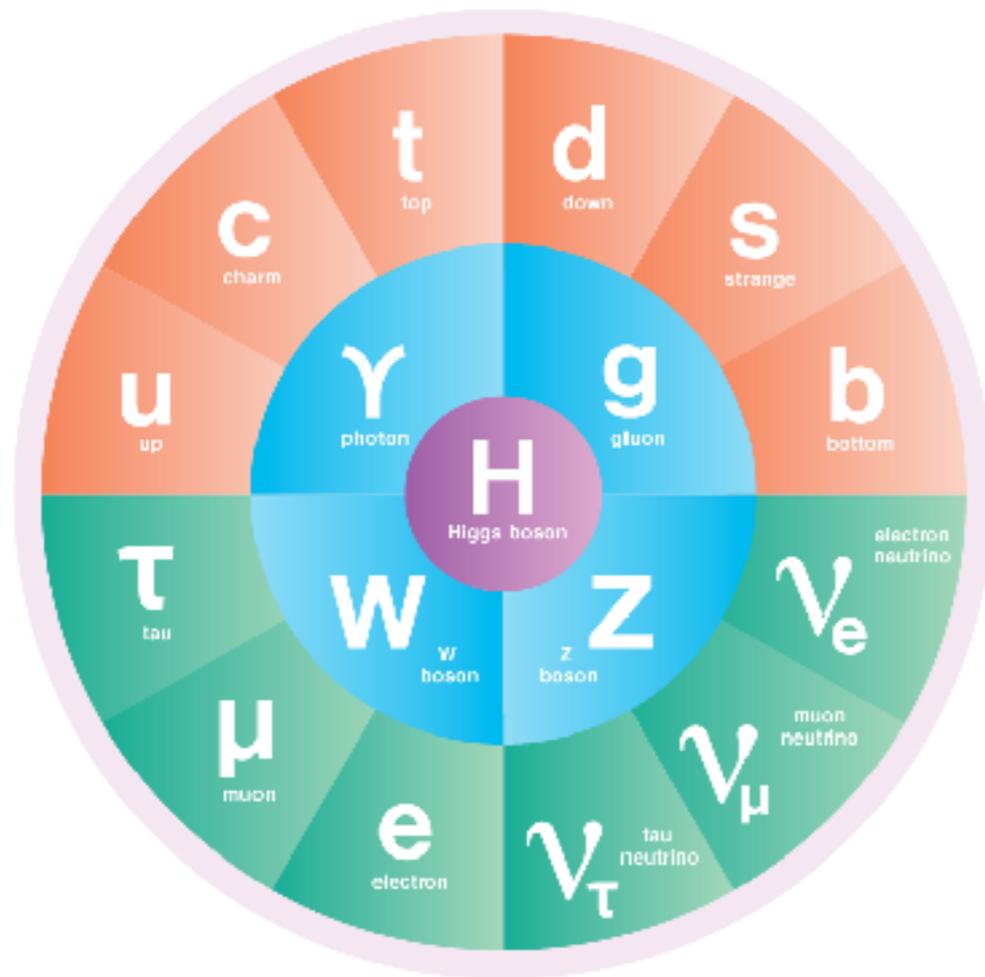
# Collision events at the LHC

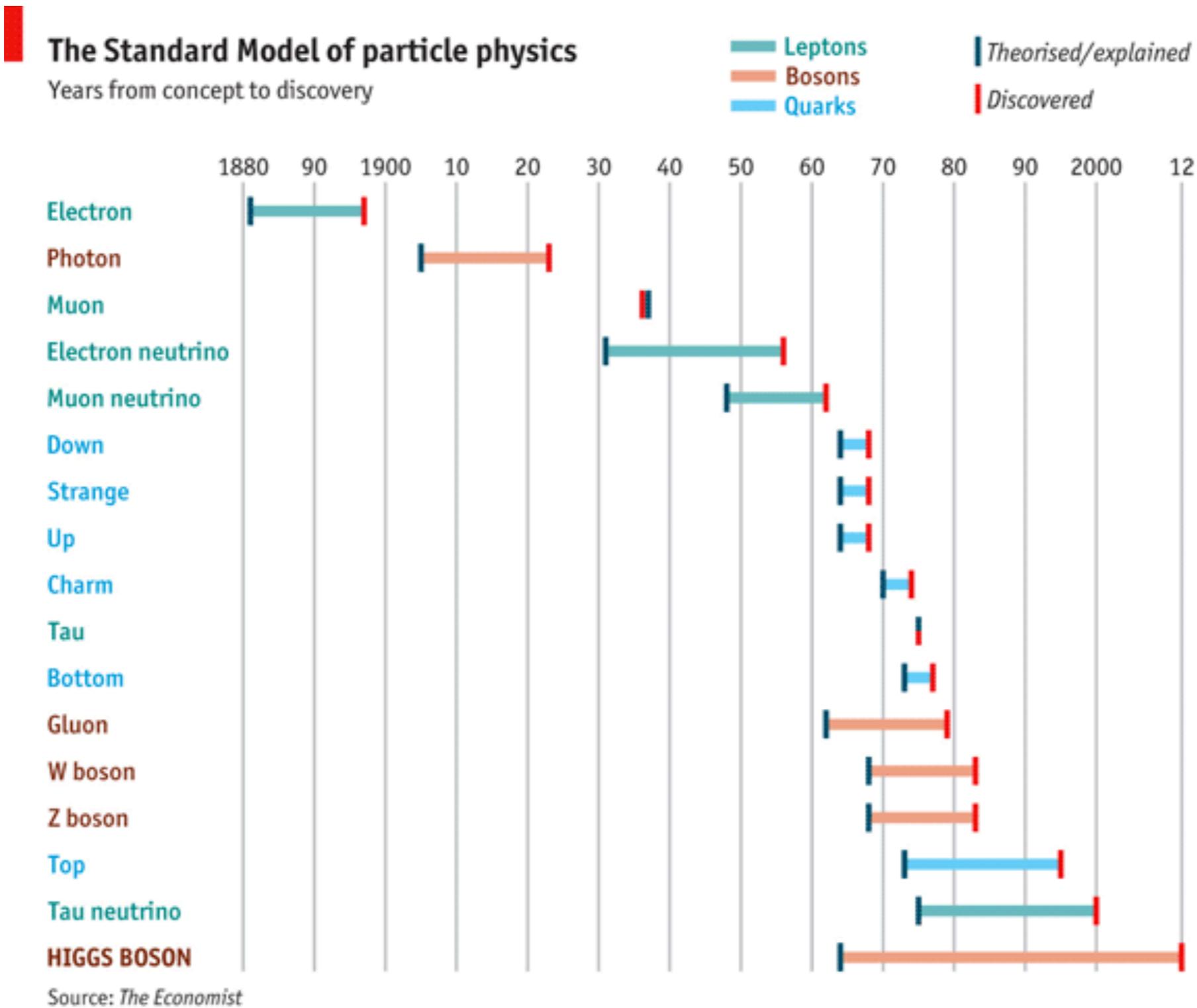


raw event rate  $\sim$  GHz  $\Rightarrow$   $\sim$  100 Hz after “triggering”  
data rate:  $\sim$  1 GB/s  $\sim$  several PB/year

**What is all this for?**

# The Standard Model of Particle Physics



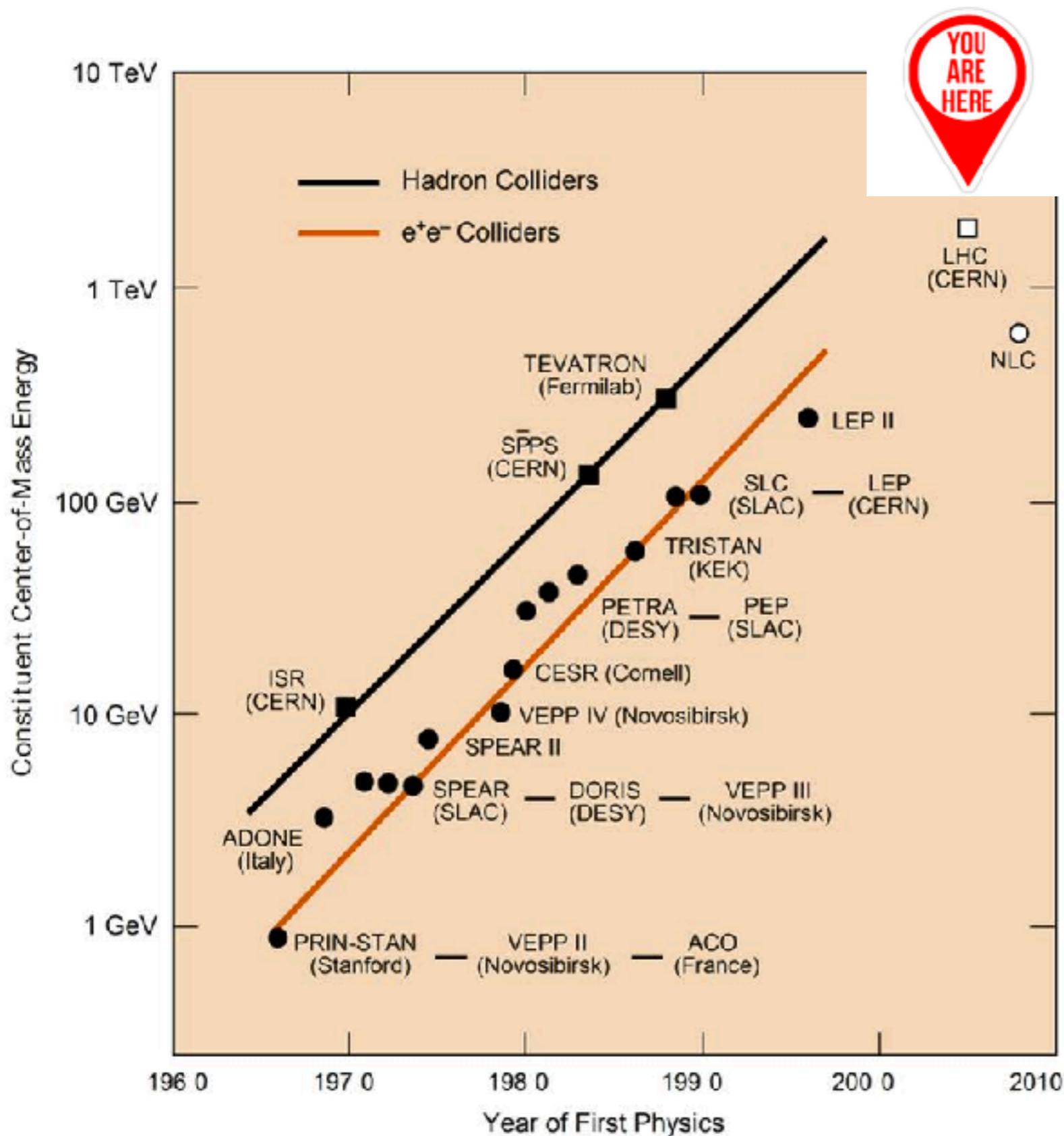


Was established in the 1970s...

... and people have been trying (and failing) to break it ever since.

**What else is there beyond the  
Standard Model?**

**What is the next layer of fundamental  
matter and interactions?**



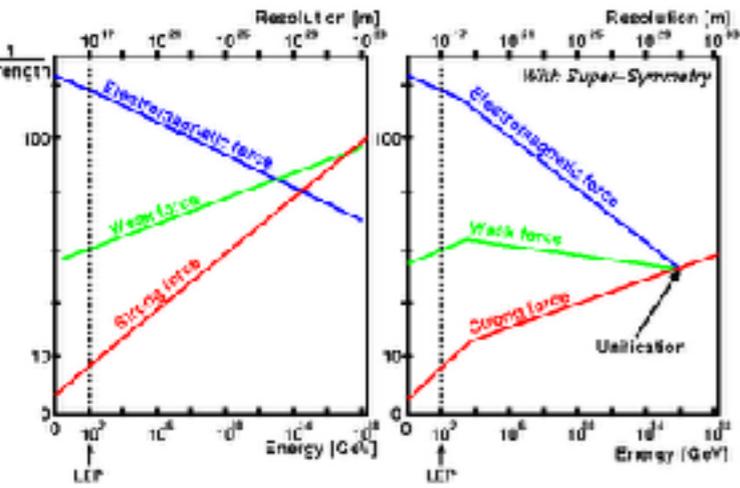
The main tool in the search for new physics beyond the SM is the **particle collider**.

By smashing together elementary particles at higher and higher energies, we hope to create new particles.

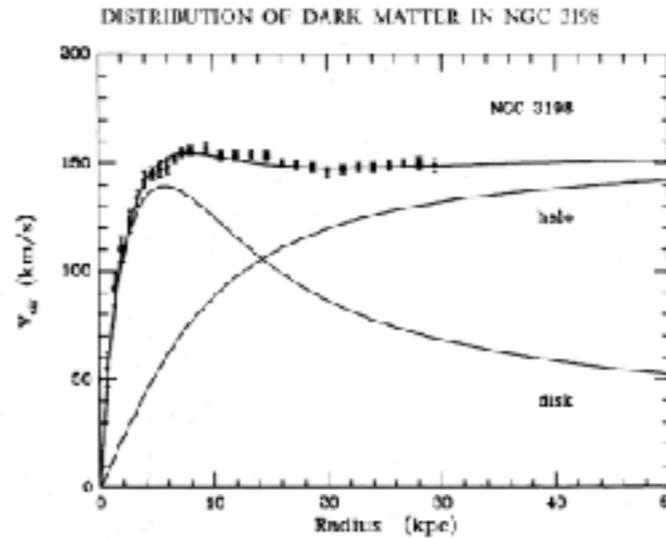
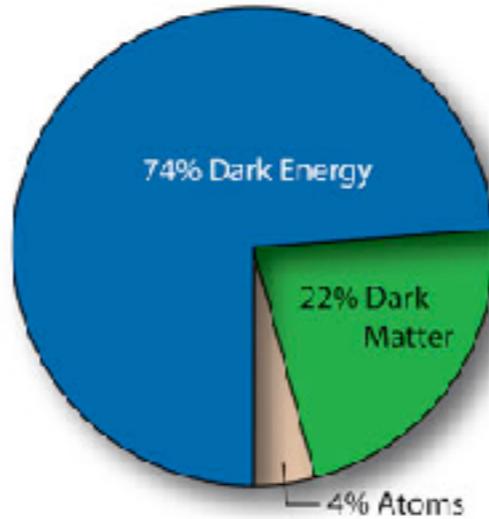
We attempt to “see” these new particles by studying the collision debris with very powerful detectors.

# We know there's new physics out there...

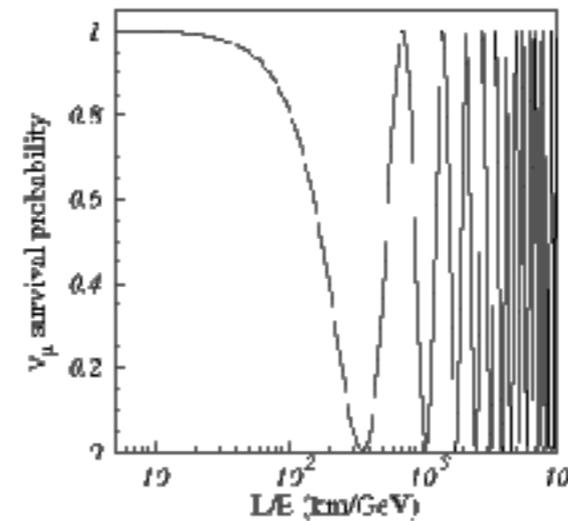
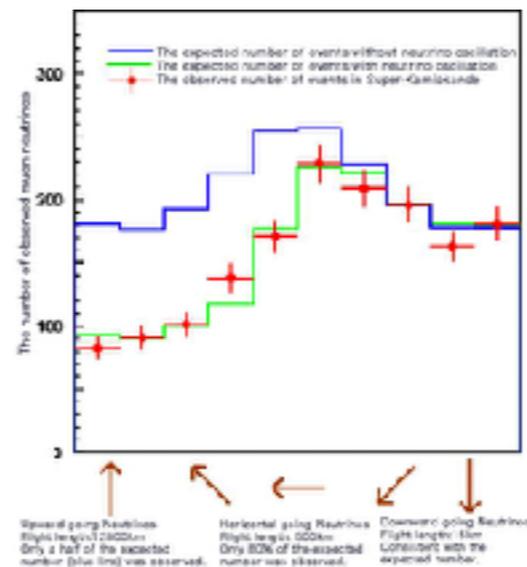
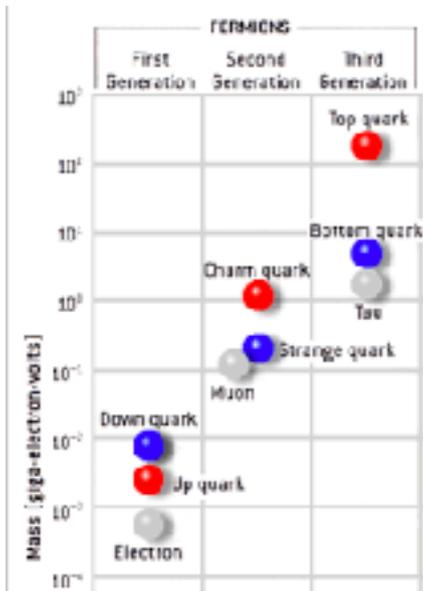
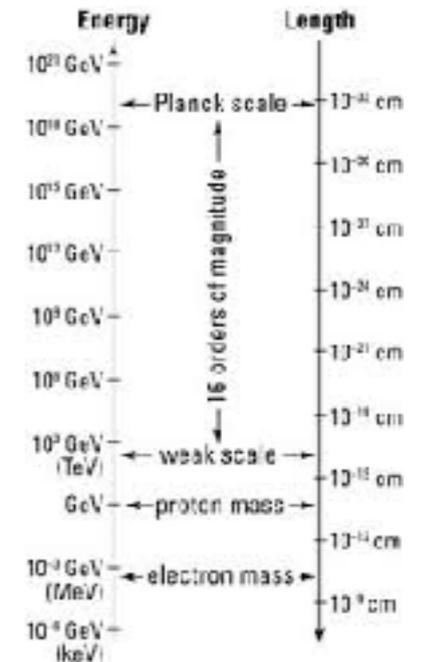
grand unification



dark matter



hierarchy problem



flavor puzzle

neutrino masses

strong CP problem

$$\mathcal{L} \supset \theta \frac{\alpha_s}{8\pi} G_{\mu\nu} \tilde{G}^{\mu\nu}$$

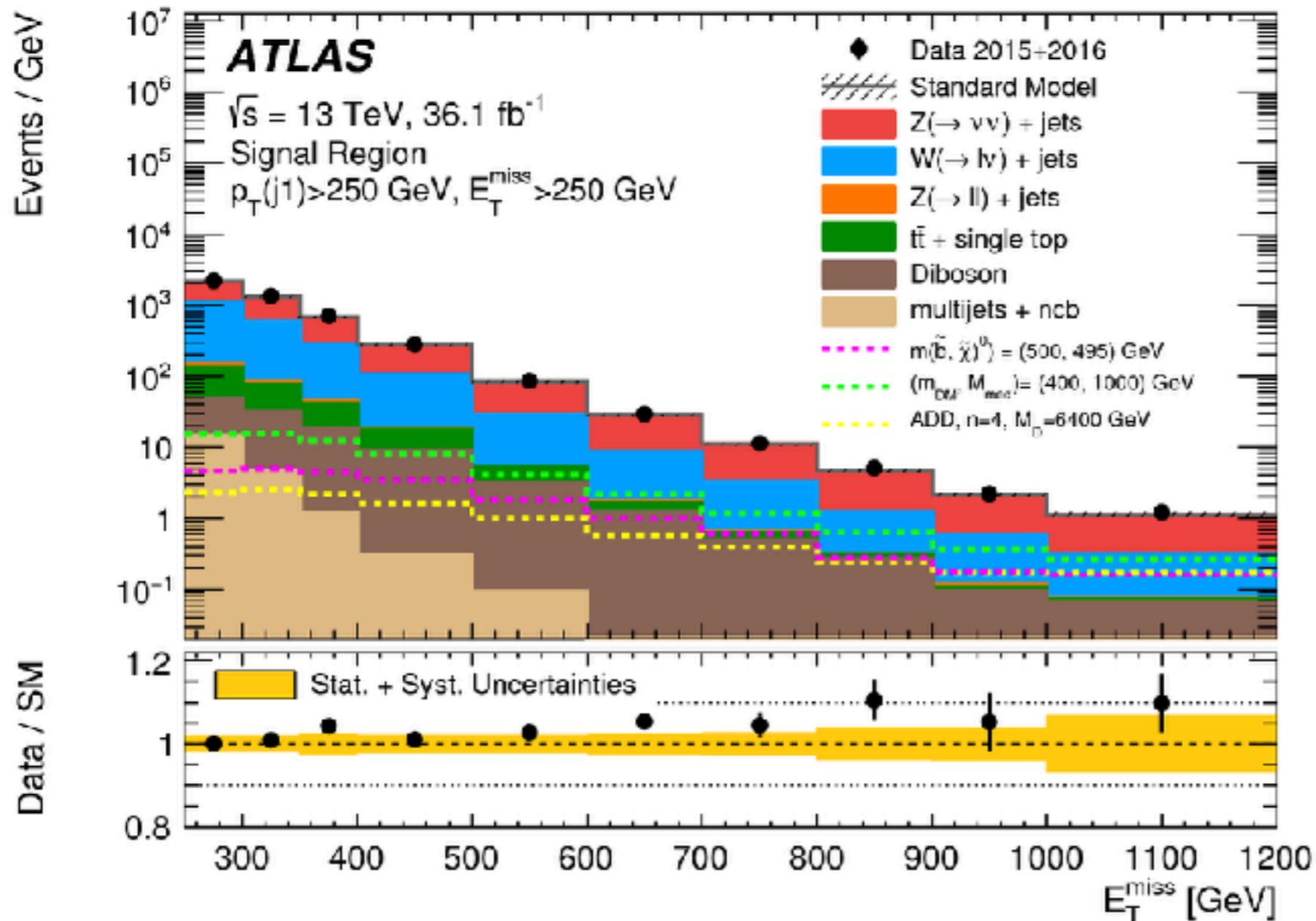
$$\theta \lesssim 10^{-10}$$







# What does a typical search for new physics look like at the LHC?



- Identify a “signal region” in the phase space, **motivated by some model**, where one expects S/N to be greatly enhanced.
- Estimate SM background using combination of simulations and data-driven methods (control regions)
- Compare data to SM prediction: announce discovery significance or set a limit on the model

This generally assumes we know what we're looking for.

- ➔ ML can still help in this case, by improving S/N — supervised learning, classification, regression

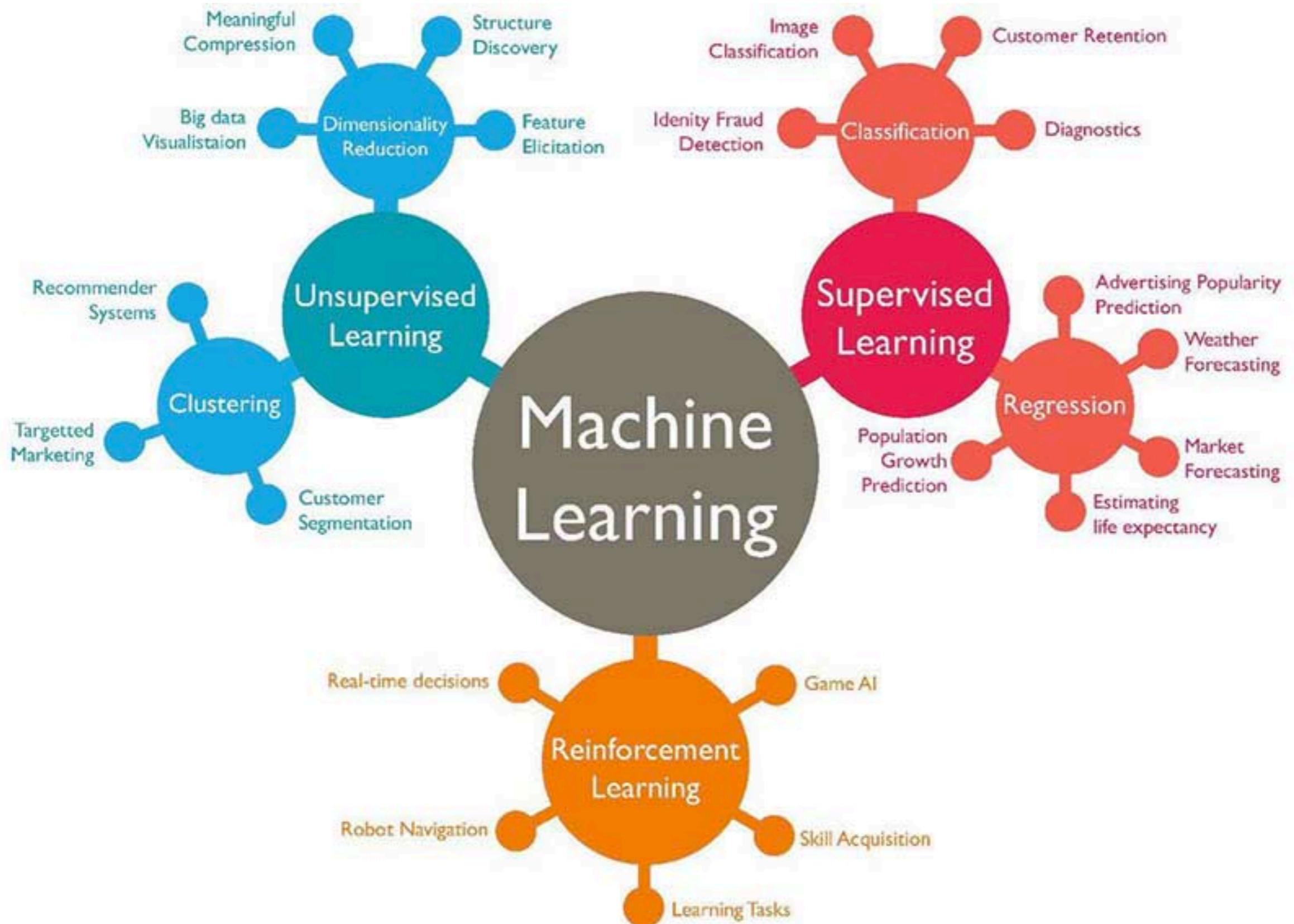
What if we don't know what we're looking for? Can we find the unexpected signal buried underneath all this raw data?

- ➔ ML can help in this case — unsupervised learning, clustering, anomaly detection

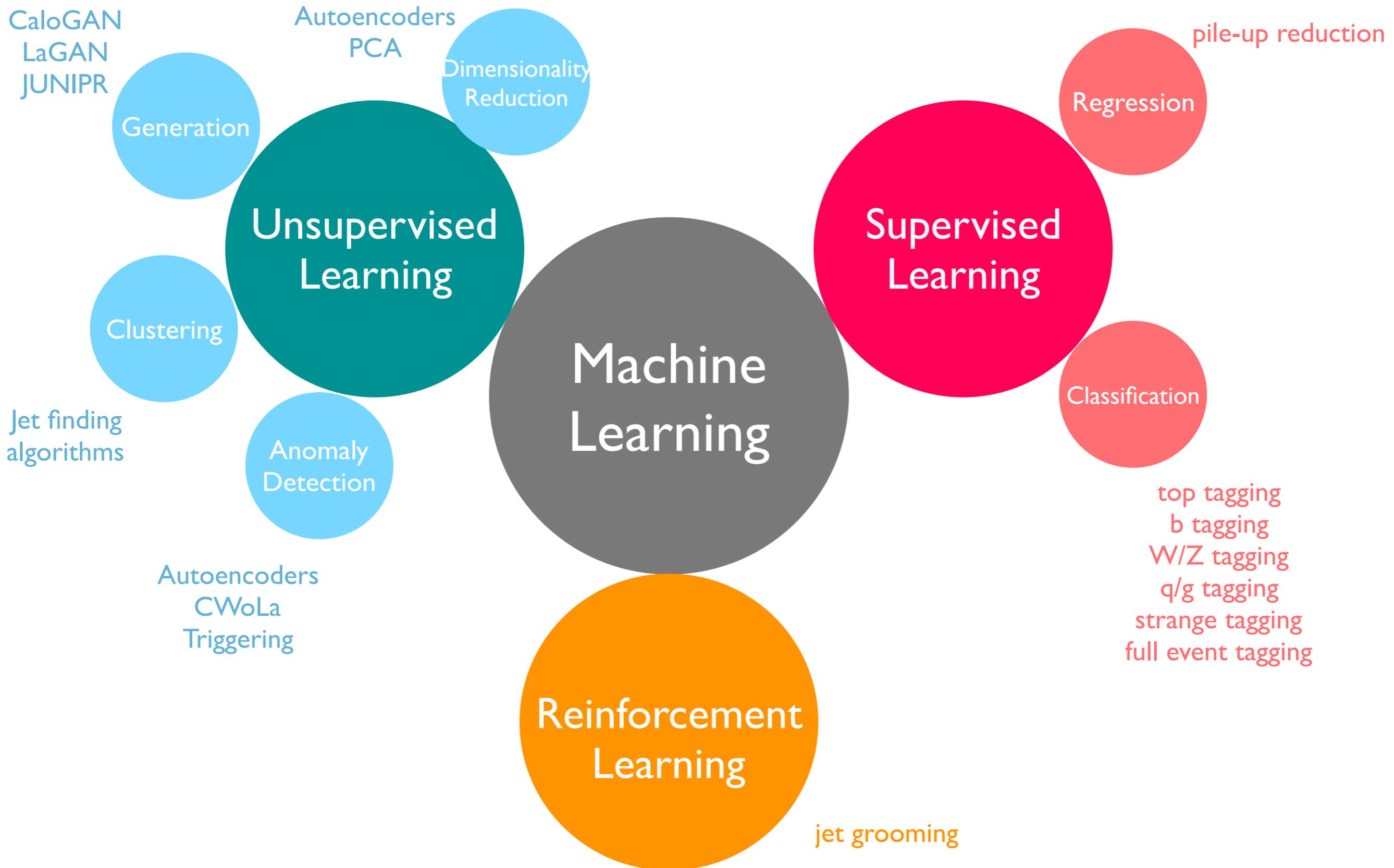
A promising path forward:

Adapt sophisticated ML tools developed for real-world applications in order to improve data analysis at the LHC

# The Landscape of ML



# The Landscape of ML @ LHC

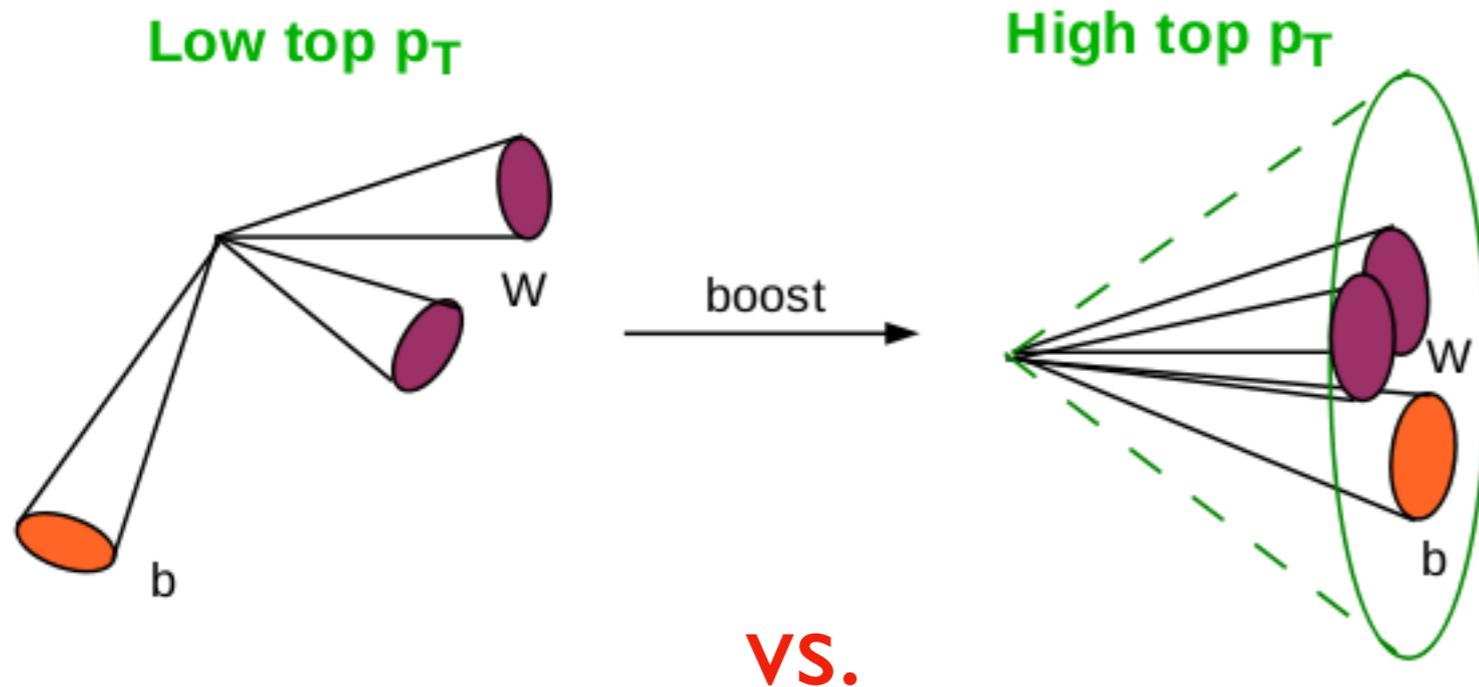


# Recent progress in ML @ LHC

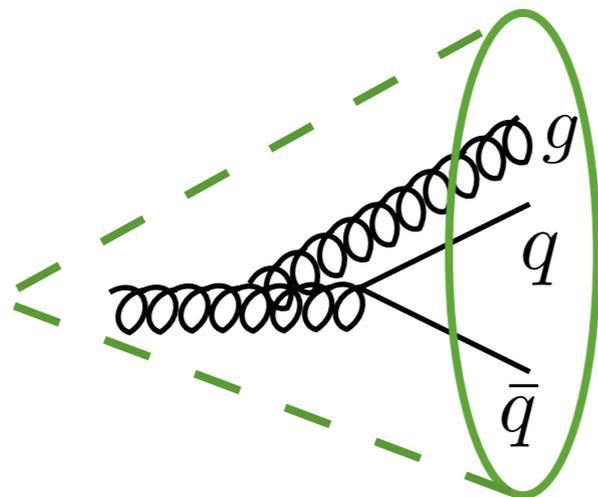
- Huge performance gains, especially for object classification
- Exploring the possibilities of learning physics directly from the data
- Developing new and unconventional ways of searching for new physics

In the rest of this talk, I will focus on some recent works that touch upon these points.

# A benchmark problem: boosted top tagging

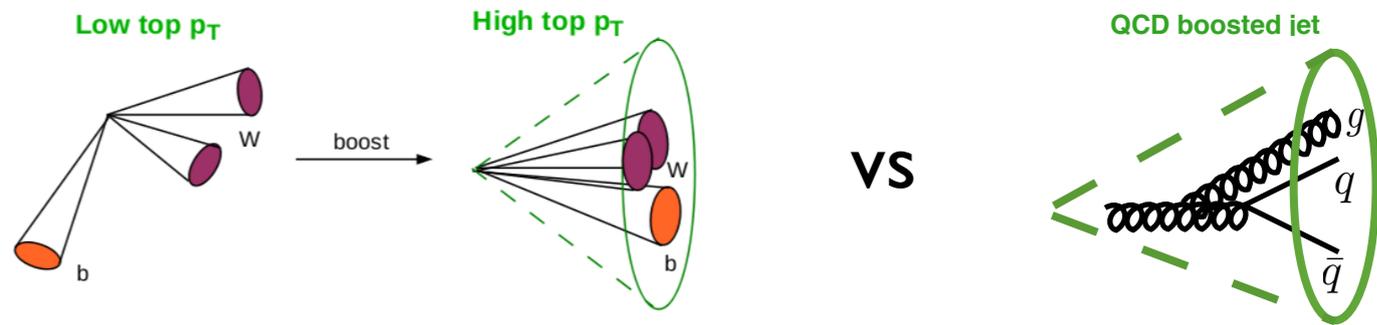


QCD boosted jet

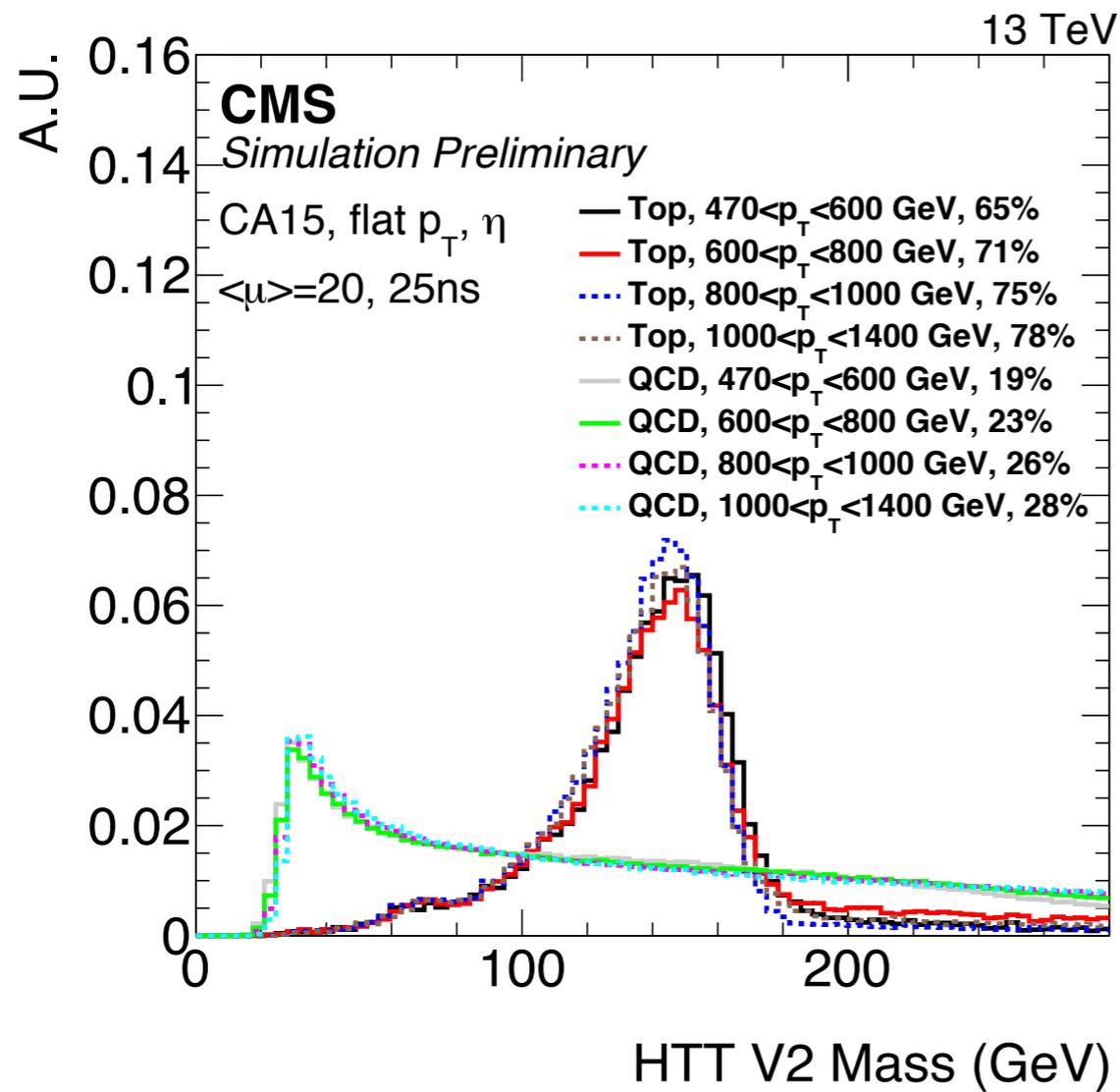


How to differentiate between these two types of jets?

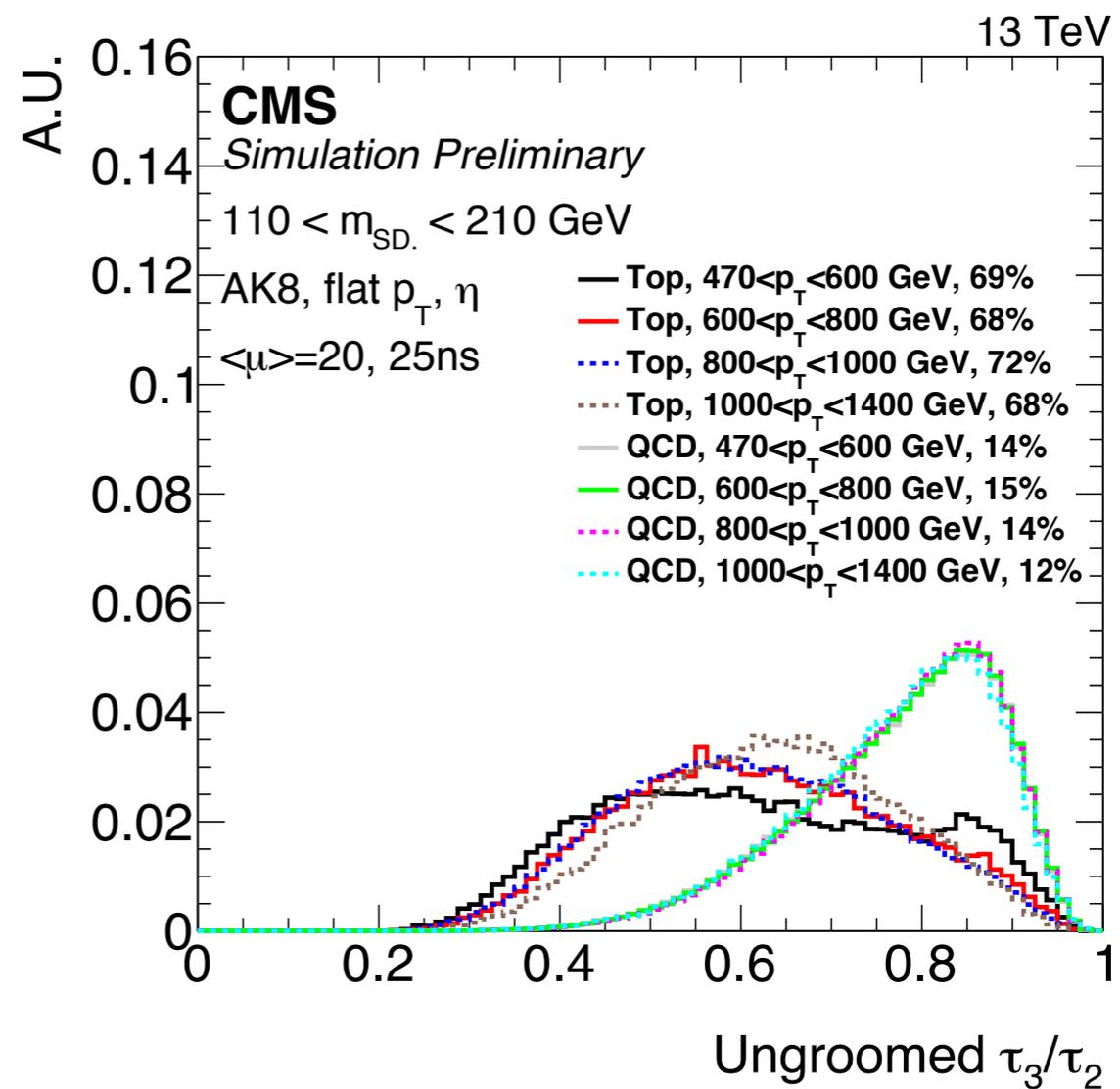
This is a straightforward supervised classification problem in ML.



Some obvious ideas:



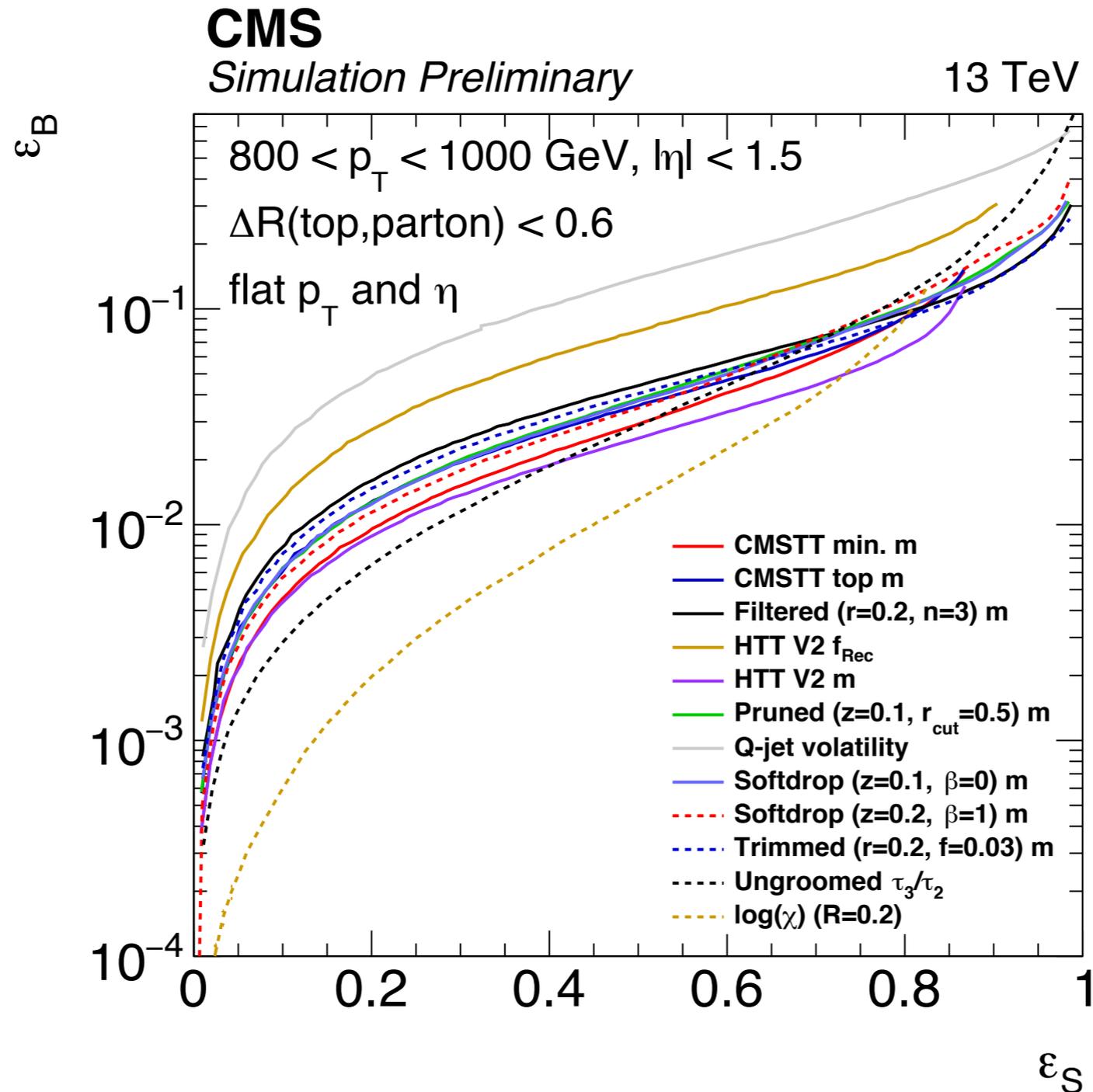
jet mass ( $m_{\text{top}}$  vs 0)



jet substructure (3 vs 1)

# State of the art with cuts on kinematic quantities:

QCD jet  
mistag rate



“ROC curve”

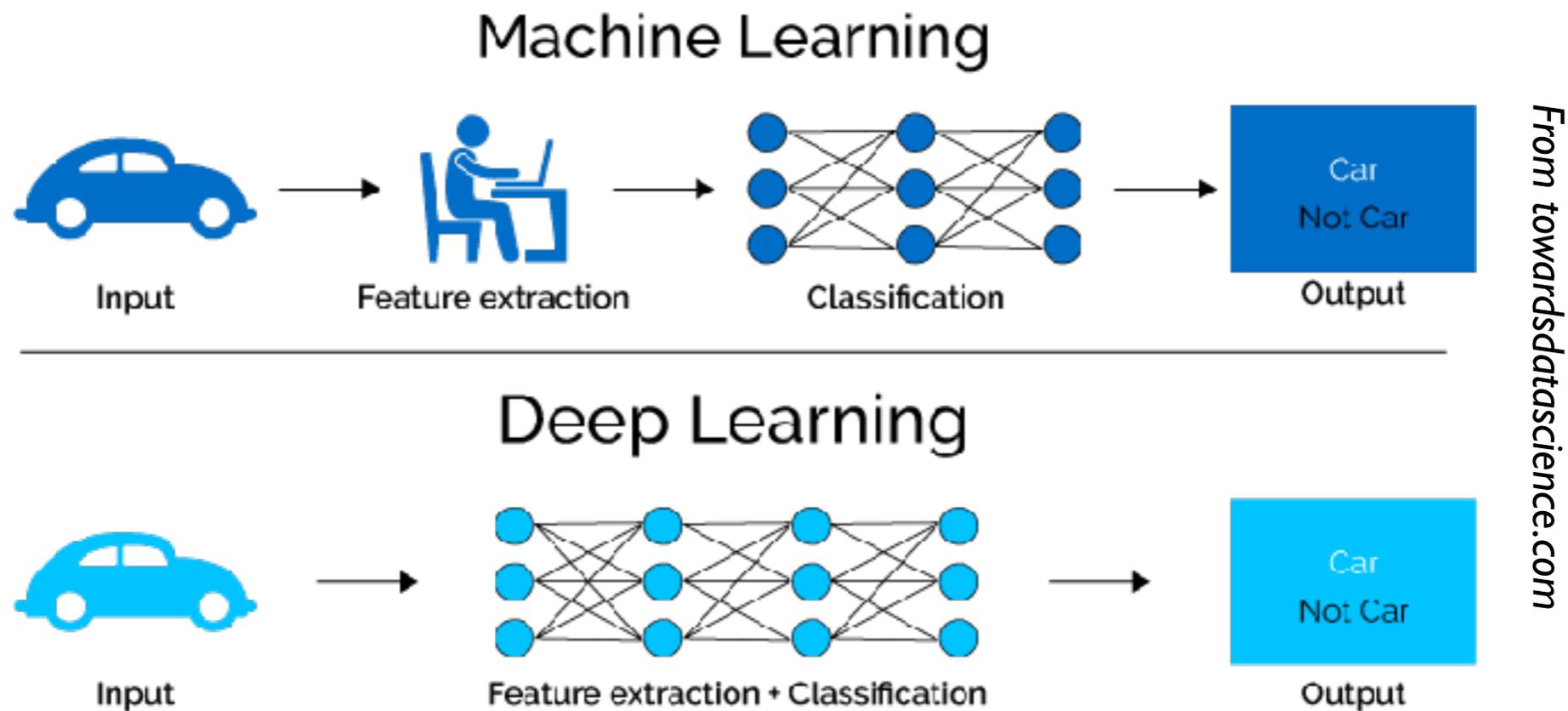
top tagging efficiency

Can deep learning do better??

# Automated Feature Engineering

By training on raw, low-level inputs, deep learning can achieve much better performance.

Deep neural networks automate and optimize the process of “feature engineering”.



Jet constituents



Deep learning algorithm



Top or QCD

# Data Representations

Although deep learning capable of building features from raw data, how we represent the data can still matter a lot.

In the case of jets, some popular options are

- Four vectors (DNNs)
- Sequences (RNNs, LSTMs)
- Binary trees (RecNNs)
- Graphs (point clouds)
- Images (CNNs)

# Jet Images

Can think of a jet as an **image in eta and phi**, with

- Pixelation provided by calorimeter towers
- Pixel intensity =  $p_T$  recorded by each tower

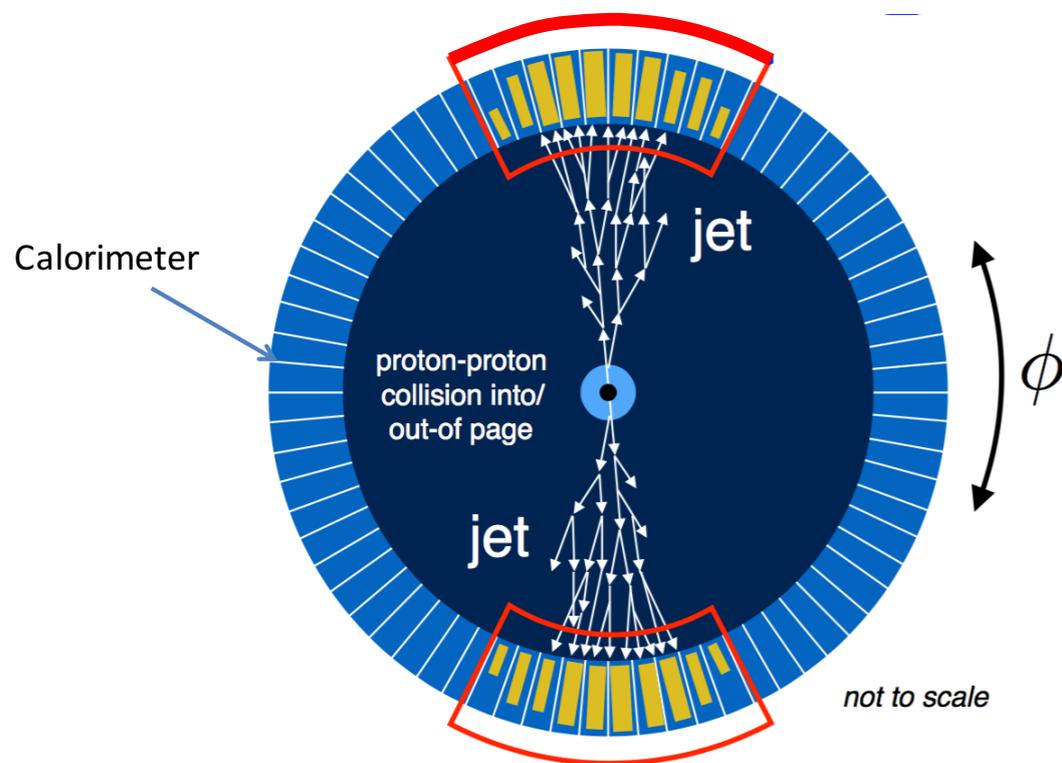
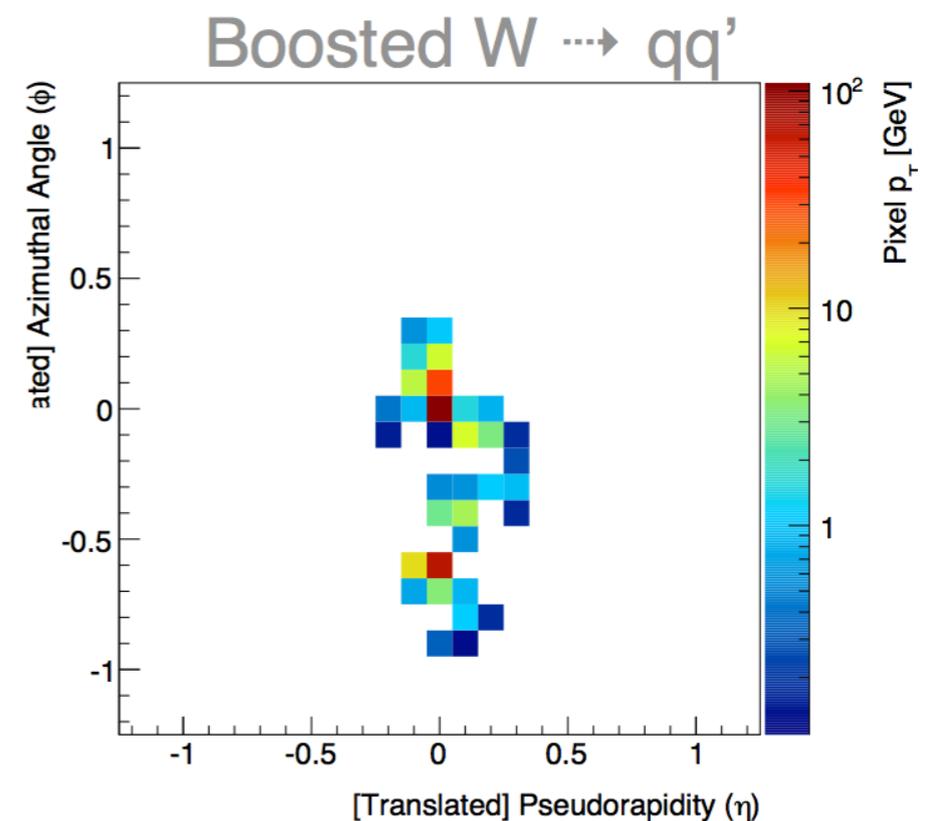


Figure credit:  
B. Nachman



Should be able to apply “off-the-shelf” NNs developed for image recognition to classify jets at the LHC! [de Oliveira et al 1511.05190](#)

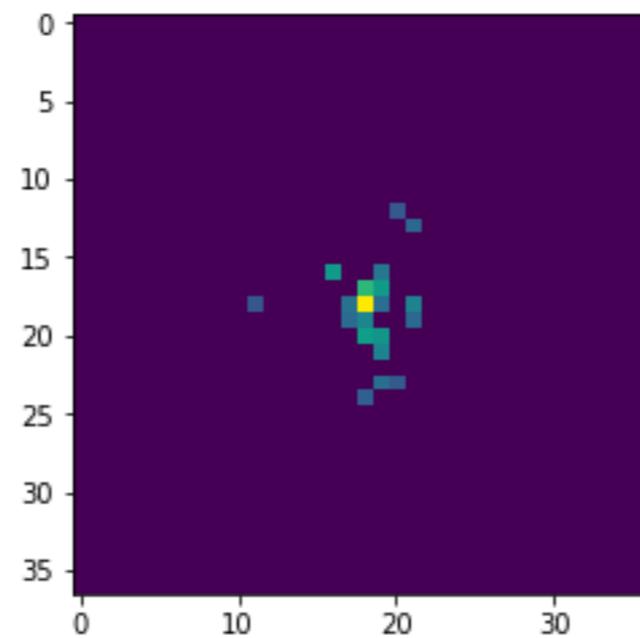
# Top Tagging with CNNs

Macaluso & DS 1803.00107

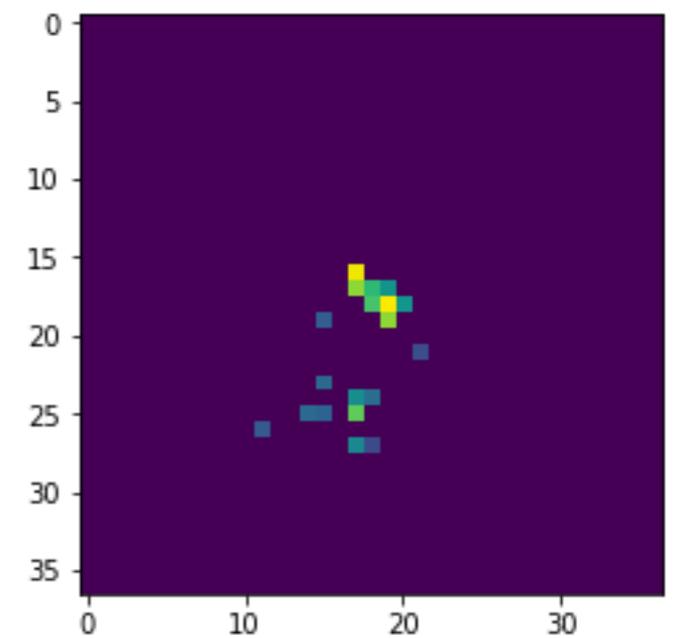
Individual images very sparse

	CMS
Jet sample	13 TeV $p_T \in (800, 900)$ GeV, $ \eta  < 1$ PYTHIA 8 and DELPHES particle-flow match: $\Delta R(t, j) < 0.6$ merge: $\Delta R(t, q) < 0.6$ 1.2M + 1.2M
Image	$37 \times 37$ $\Delta\eta = \Delta\phi = 3.2$
Colors	$(p_T^{neutral}, p_T^{track}, N_{track}, N_{muon})$

QCD



Tops



Building on previous “DeepTop” tagger of [Kasieczka et al 1701.08784](#)

Other approaches also promising (DNNs, RecNNs, RNNs, LSTMs, GNNs, ...)

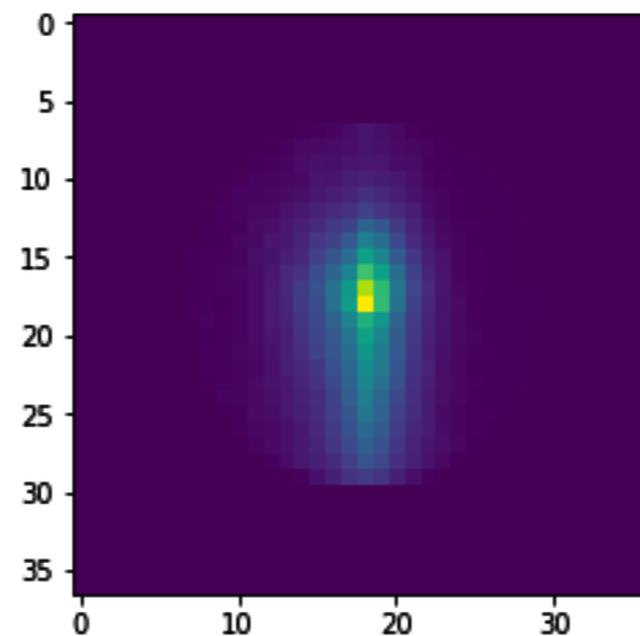
# Top Tagging with CNNs

Macaluso & DS 1803.00107

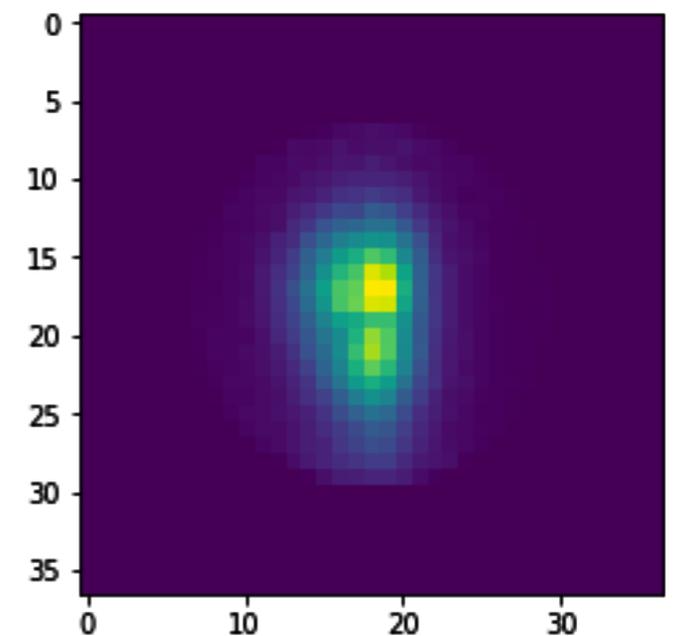
Average images clearly different

	CMS
Jet sample	13 TeV $p_T \in (800, 900)$ GeV, $ \eta  < 1$ PYTHIA 8 and DELPHES particle-flow match: $\Delta R(t, j) < 0.6$ merge: $\Delta R(t, q) < 0.6$ 1.2M + 1.2M
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QCD



Tops

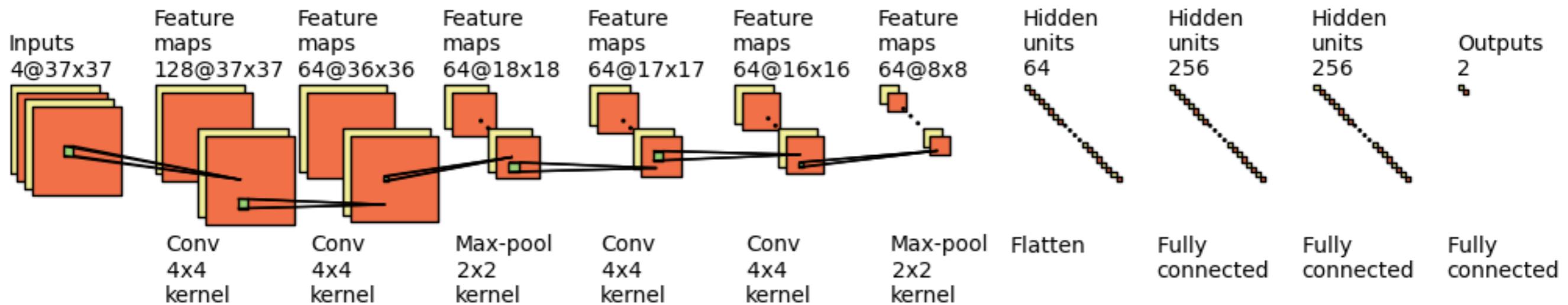


Building on previous “DeepTop” tagger of [Kasieczka et al 1701.08784](#)

Other approaches also promising (DNNs, RecNNs, RNNs, LSTMs, GNNs, ...)

# Top Tagging with CNNs

Macaluso & DS 1803.00107



AdaDelta

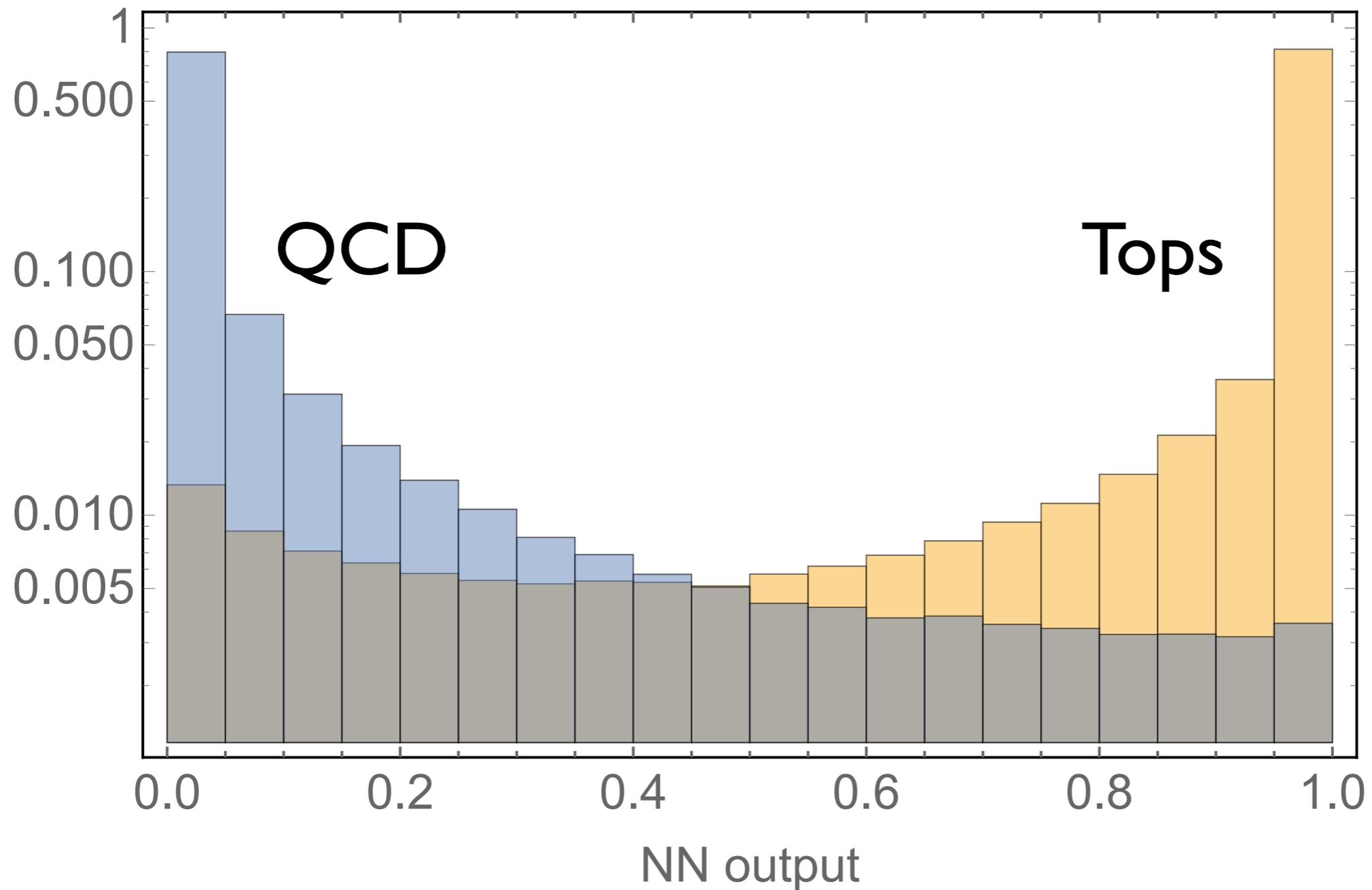
$\eta = 0.3$  with annealing schedule

minibatch size=128

cross entropy loss

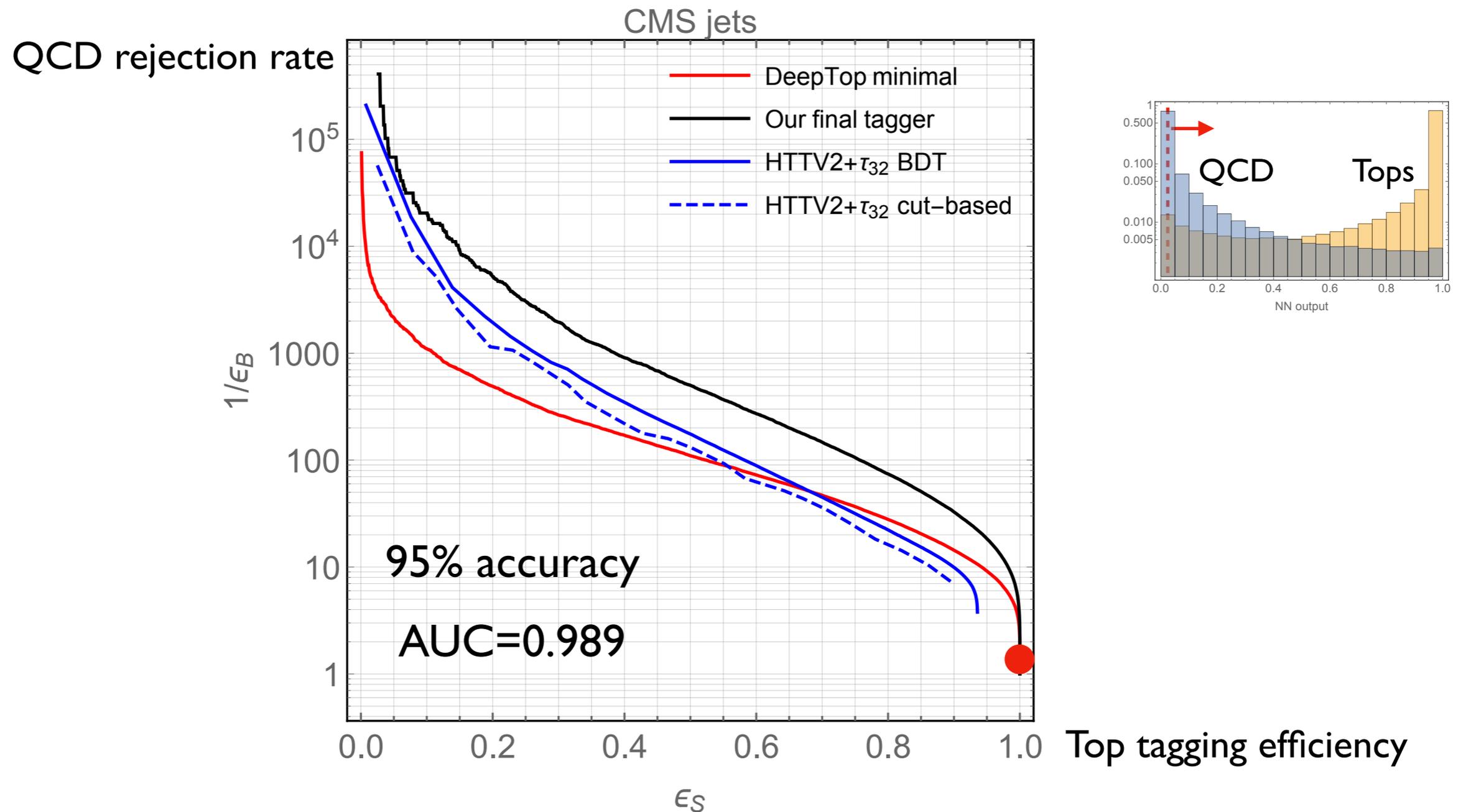
# Top Tagging with CNNs

Macaluso & DS 1803.00107



# Top Tagging with CNNs

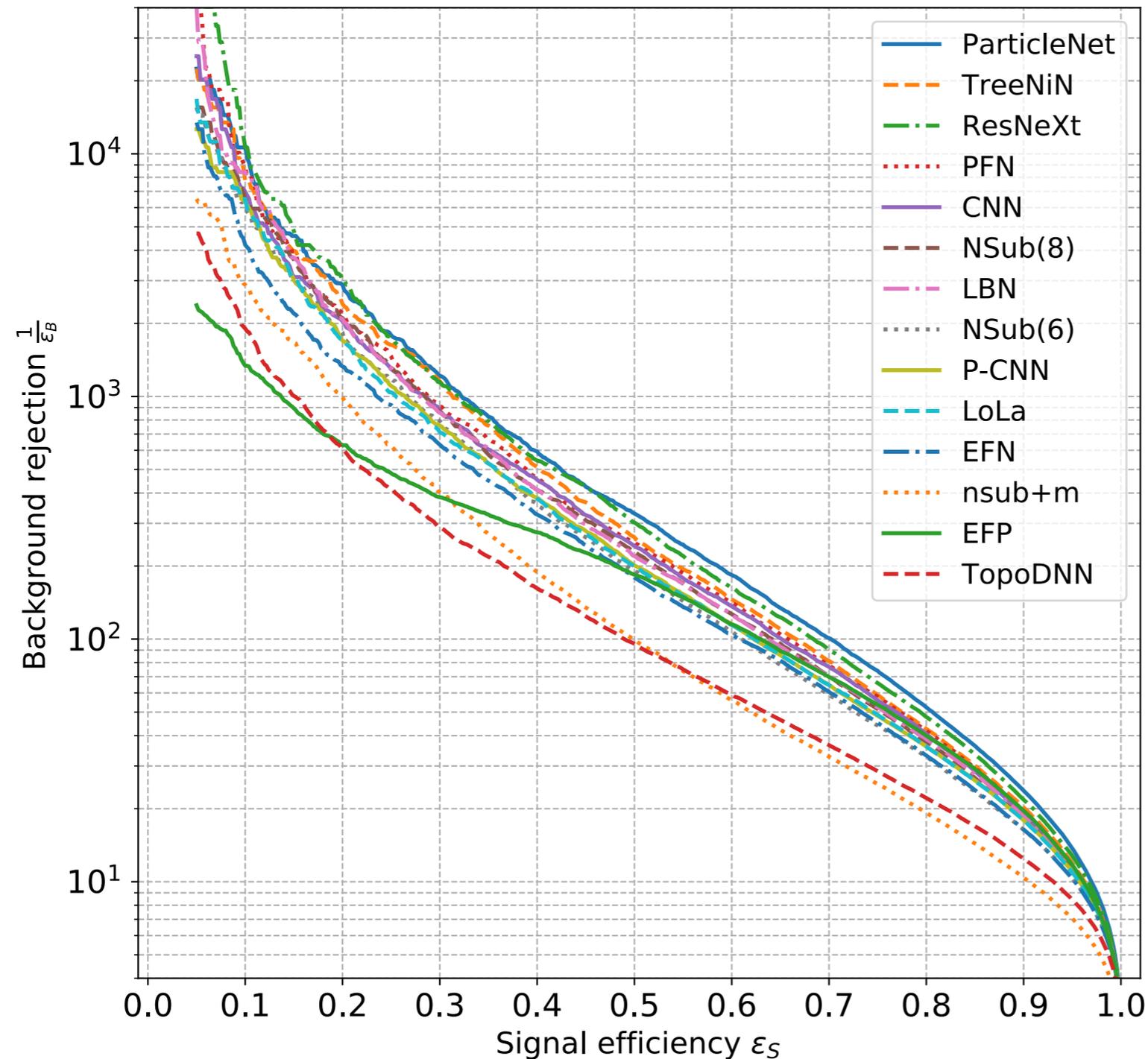
Macaluso & DS 1803.00107



Can achieve factor of  $\sim 3$  improvement over cut-based approaches and BDTs!

# Community top tagging comparison

Kasieczka, Plehn et al [1902.09914](#)



Apples-to-apples  
comparison of various  
deep learning top taggers  
on a common dataset.

# Community top tagging comparison

Kasieczka, Plehn et al 1902.09914

	AUC	Accuracy	$1/\epsilon_B$ ( $\epsilon_S = 0.3$ )	#Parameters
CNN [16]	0.981	0.930	780	610k
ResNeXt [32]	0.984	0.936	1140	1.46M
TopoDNN [18]	0.972	0.916	290	59k
Multi-body $N$ -subjettiness 6 [24]	0.979	0.922	856	57k
Multi-body $N$ -subjettiness 8 [24]	0.981	0.929	860	58k
RecNN	0.981	0.929	810	13k
P-CNN	0.980	0.930	760	348k
ParticleNet [45]	0.985	0.938	1280	498k
LBN [19]	0.981	0.931	860	705k
LoLa [22]	0.980	0.929	730	127k
Energy Flow Polynomials [21]	0.980	0.932	380	1k
Energy Flow Network [23]	0.979	0.927	600	82k
Particle Flow Network [23]	0.982	0.932	880	82k
GoaT (see text)	0.985	0.939	1440	25k



Further improvements to our CNN are possible.  
Have we found the optimal tagger??

# Supervised vs Unsupervised ML

Top tagging is a prime example of supervised machine learning.

It is a straightforward classification task with fully-labeled (QCD or top) datasets.

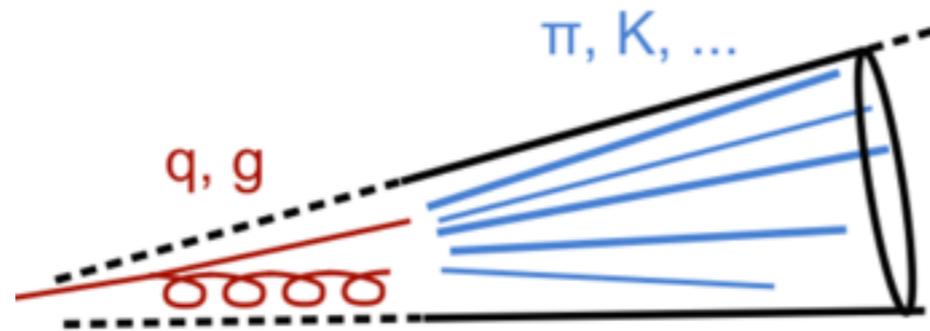
What if the data is not labeled — e.g. it is the actual LHC data and not simulation?

Can we apply ideas from unsupervised ML to discover patterns and features in the data?

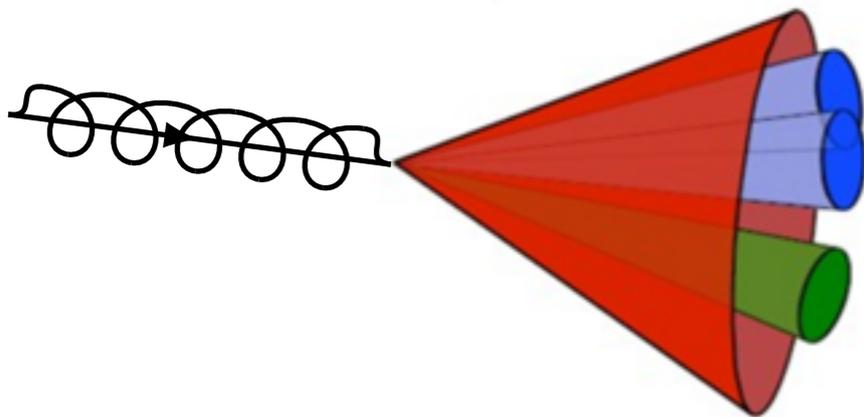
Can we discover unexpected new physics this way?

# Statement of the problem

Consider a collection of jets at the LHC. [See Jesse and Anders talks for more on jets.]



Most will be from SM processes (quark/gluon showering and hadronization).



But a small fraction could be from an unknown (heavier) new physics particle with exotic properties.

How can we use ML algorithms to discover the exotic new particle without knowing what it looks like?

# Statement of the problem

This is a standard **anomaly detection problem** in data science!

Train directly on the data



unsupervised anomaly detection (clustering)

Train on background-only (would probably need simulations for this)

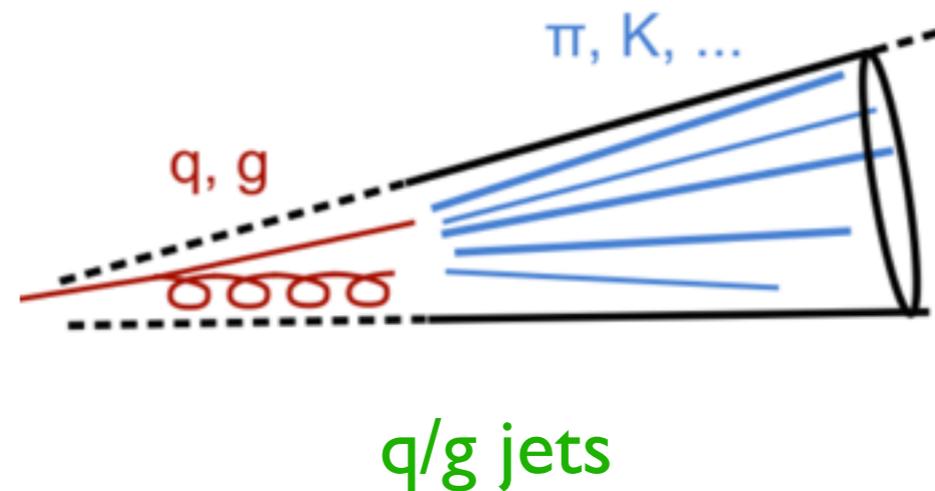


weakly-supervised anomaly detection (“one-class classification”)

# Sample definitions

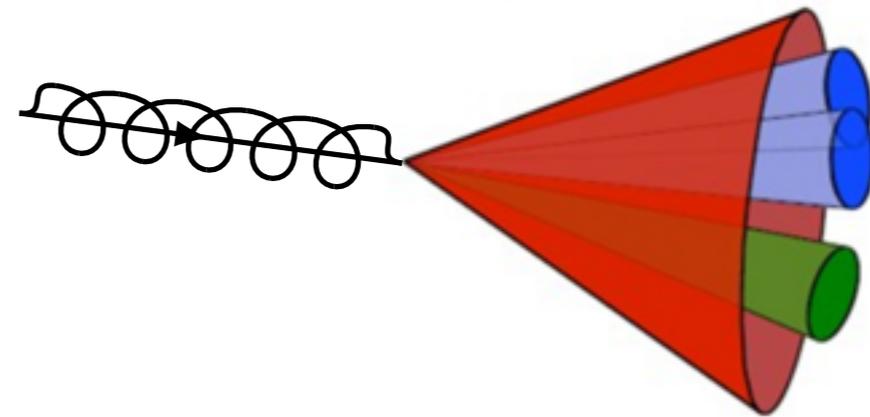
Same jet specifications as for top tagging study. We used:

- q/g jets as background, and
- boosted tops and 400 GeV gluinos (decaying via RPV) as signal



We simulated

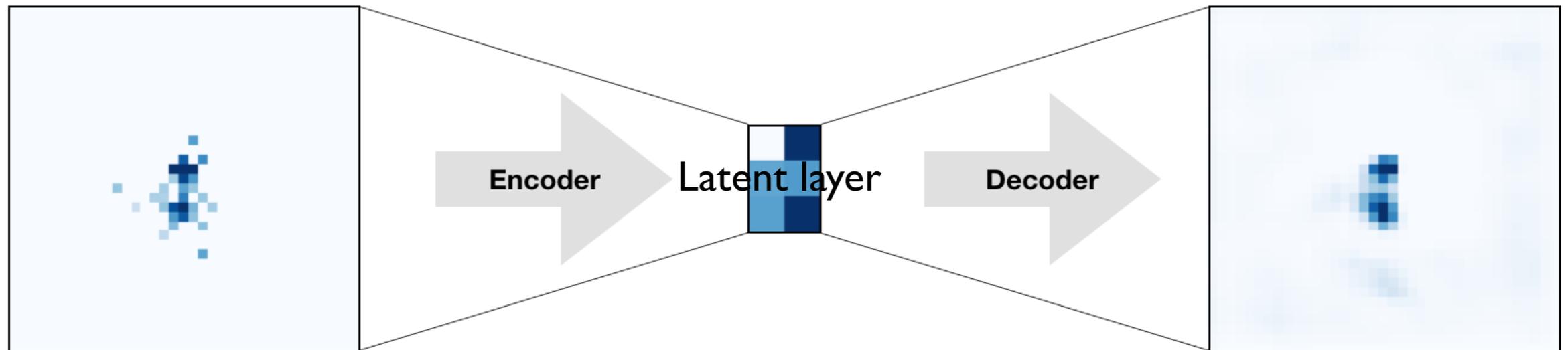
- 1.2M jets of each type
- using standard, open-source particle physics tools [Pythia8 and Delphes]
- and turned them into 37x37 grayscale images.



boosted tops and RPV gluinos

# A promising idea: deep autoencoders

Heimel et al I808.08979; Farina, Nakai & DS I808.08992



An autoencoder maps an input into a “latent representation” and then attempts to reconstruct the original input from it.

The encoding is lossy, so the decoding cannot be perfect.

Some previous approaches:

Aguilar-Saavedra et al, "A generic anti-QCD jet tagger" I709.01087

Collins et al, "CWoLa Hunting" I805.02664

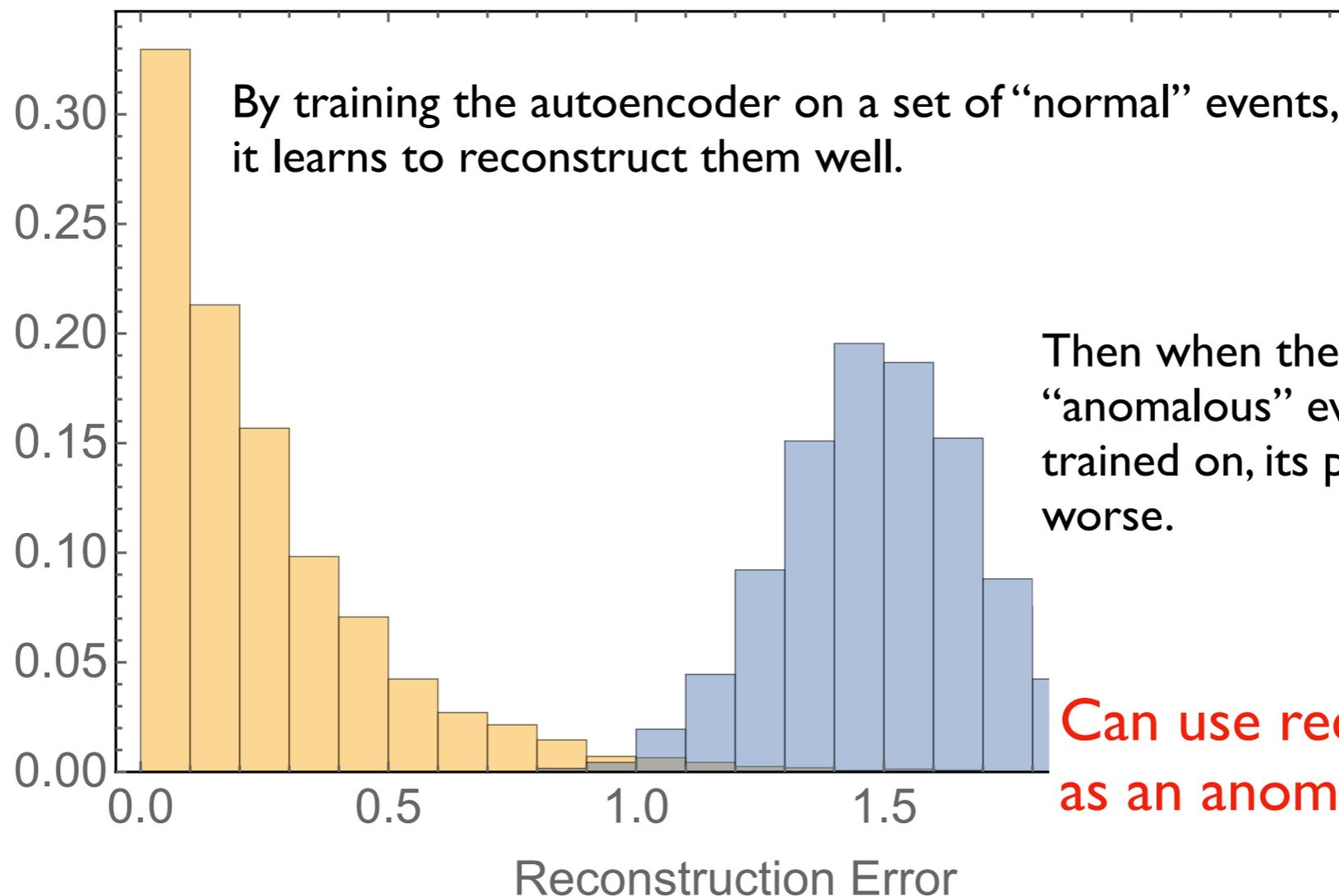
Hajer et al "Novelty Detection Meets Collider Physics" I807.10261

# Deep autoencoders for anomaly detection

Heimel et al I808.08979; Farina, Nakai & DS I808.08992

Quantify AE performance using reconstruction error:

$$L = \frac{1}{N} \sum_{i=1}^N (x_i^{in} - x_i^{out})^2$$

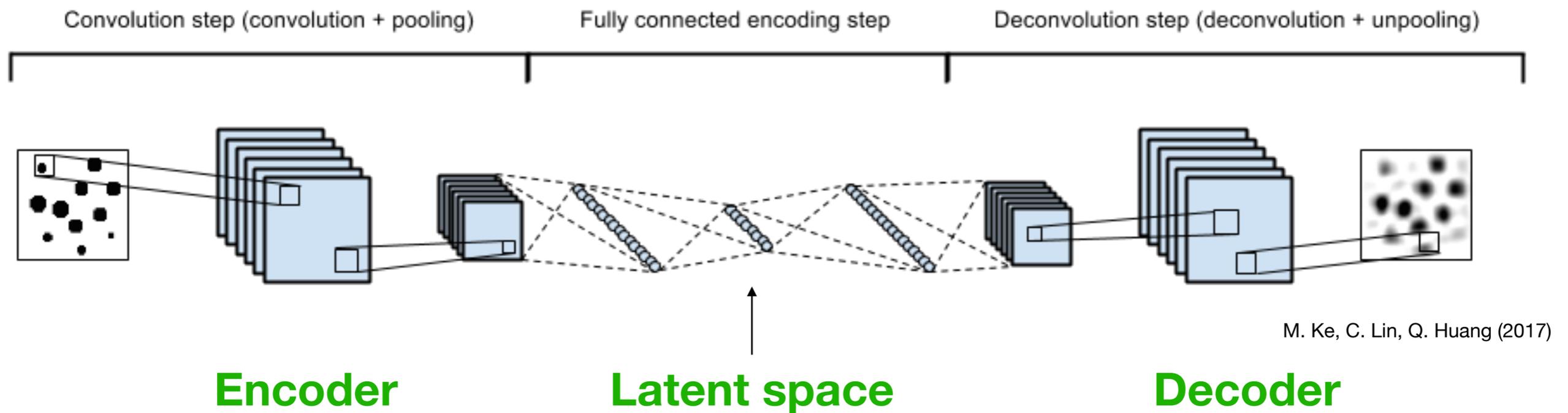


By training the autoencoder on a set of “normal” events, it learns to reconstruct them well.

Then when the autoencoder encounters “anomalous” events that it was not trained on, its performance should be worse.

Can use reconstruction error as an anomaly threshold!

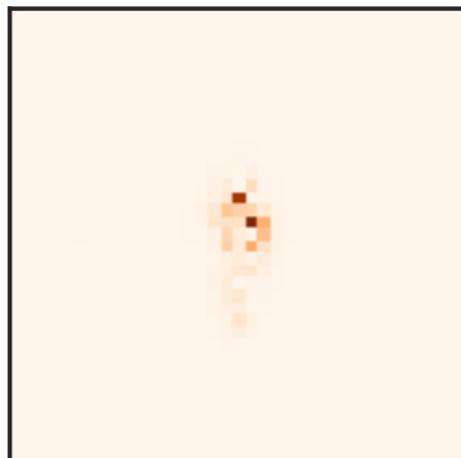
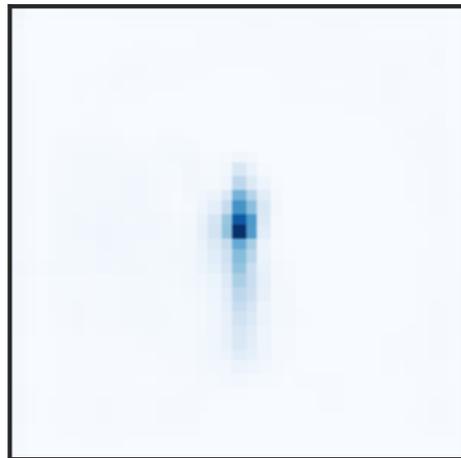
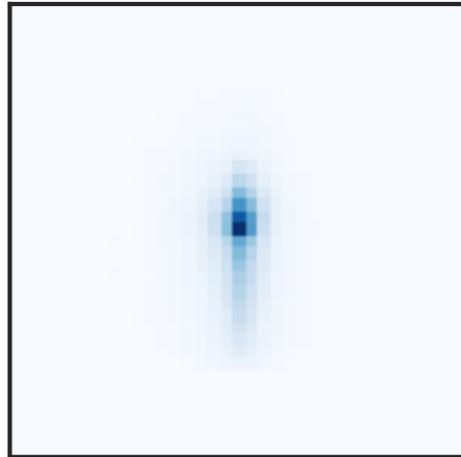
# Autoencoder architecture



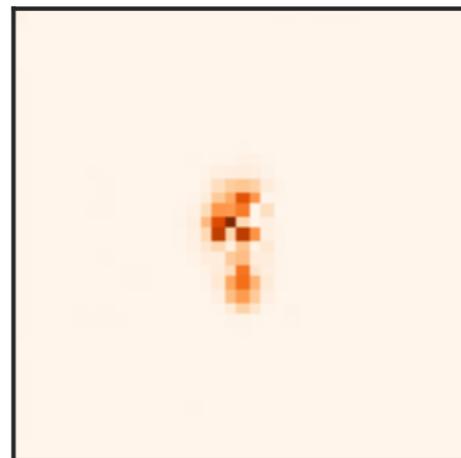
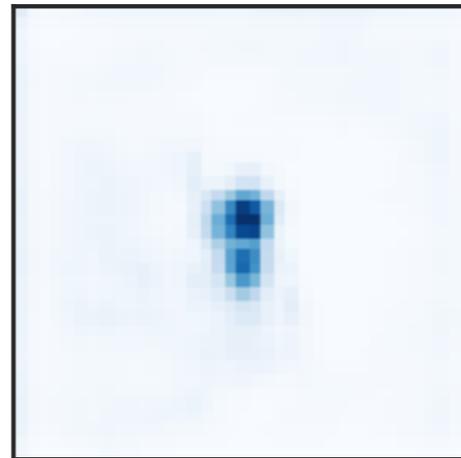
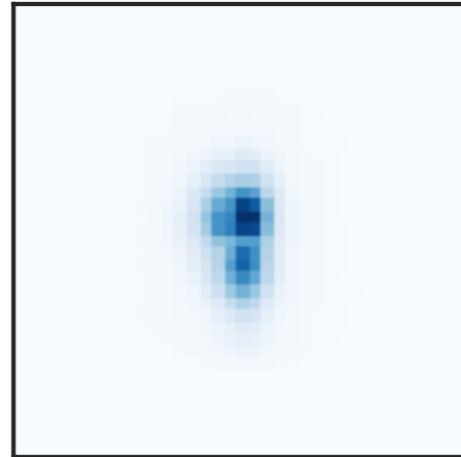
128C3-MP2-128C3-MP2-128C3-32N-6N-32N-12800N-128C3-US2-128C3-US2-1C3

Performance should be worse on “anomalous” events that autoencoder was not trained on.

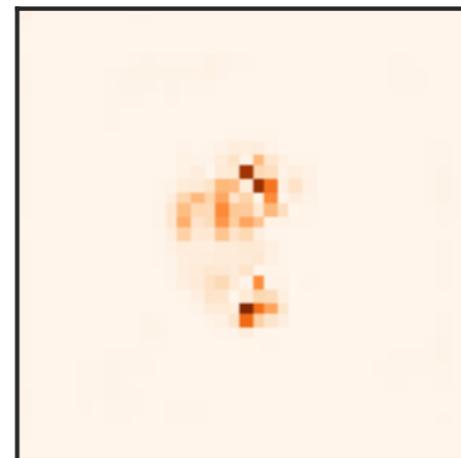
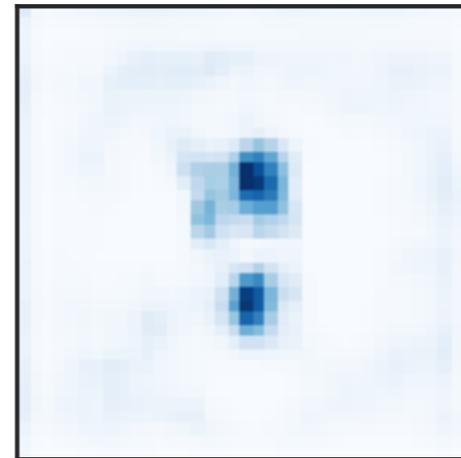
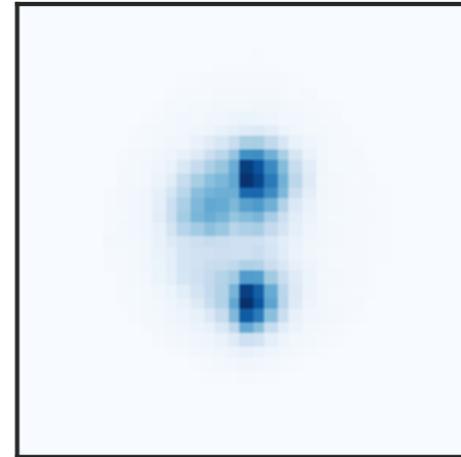
QCD



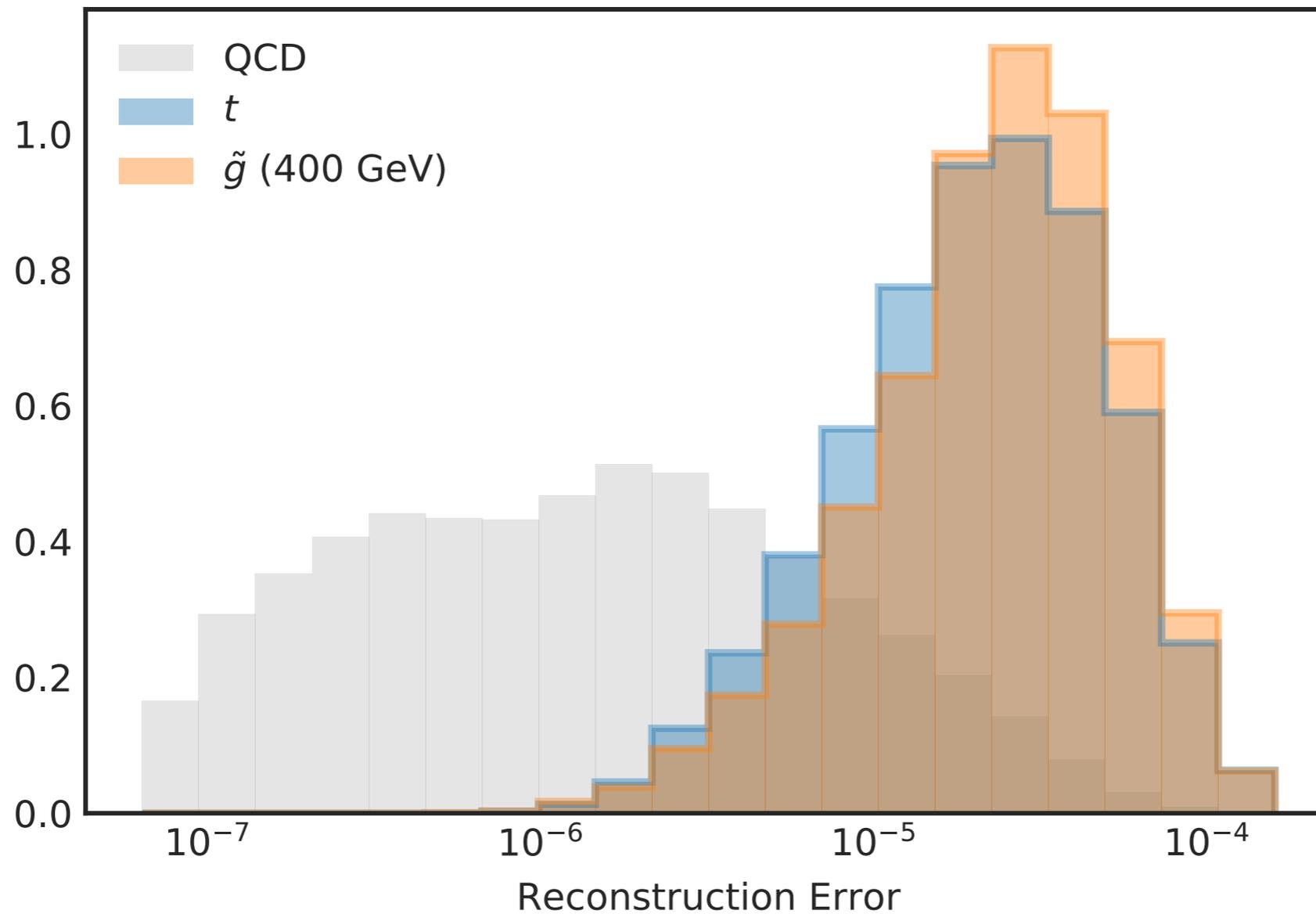
tops



gluinos



Can use reconstruction error as an anomaly threshold.

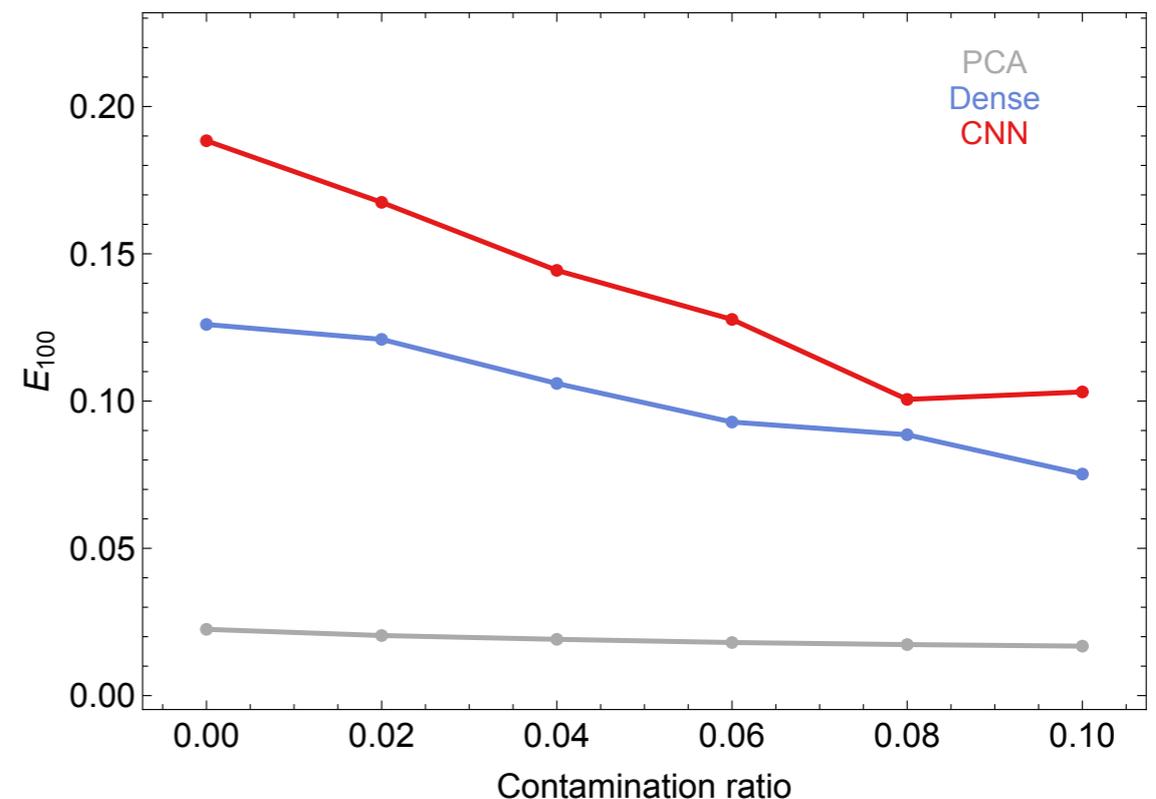
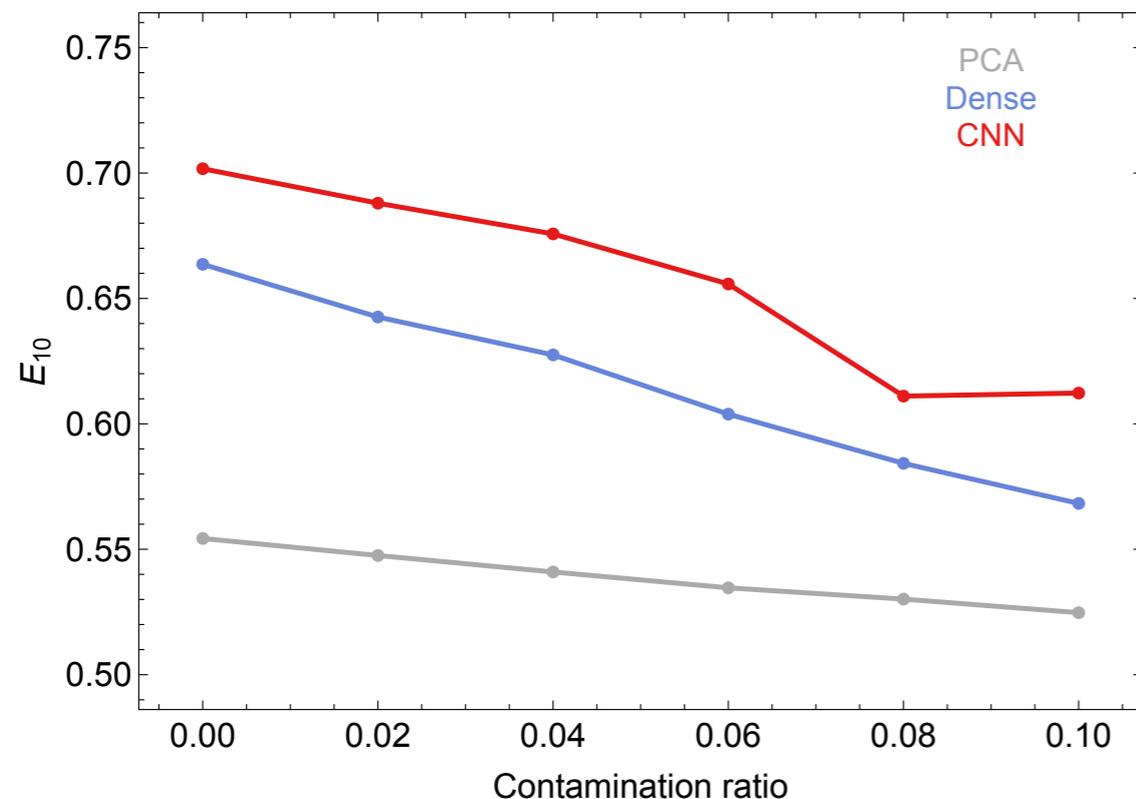


The algorithm works when trained on QCD backgrounds!

# Fully unsupervised learning

Train on sample of QCD background “contaminated” with a small fraction of signal.

Representative of actual data.

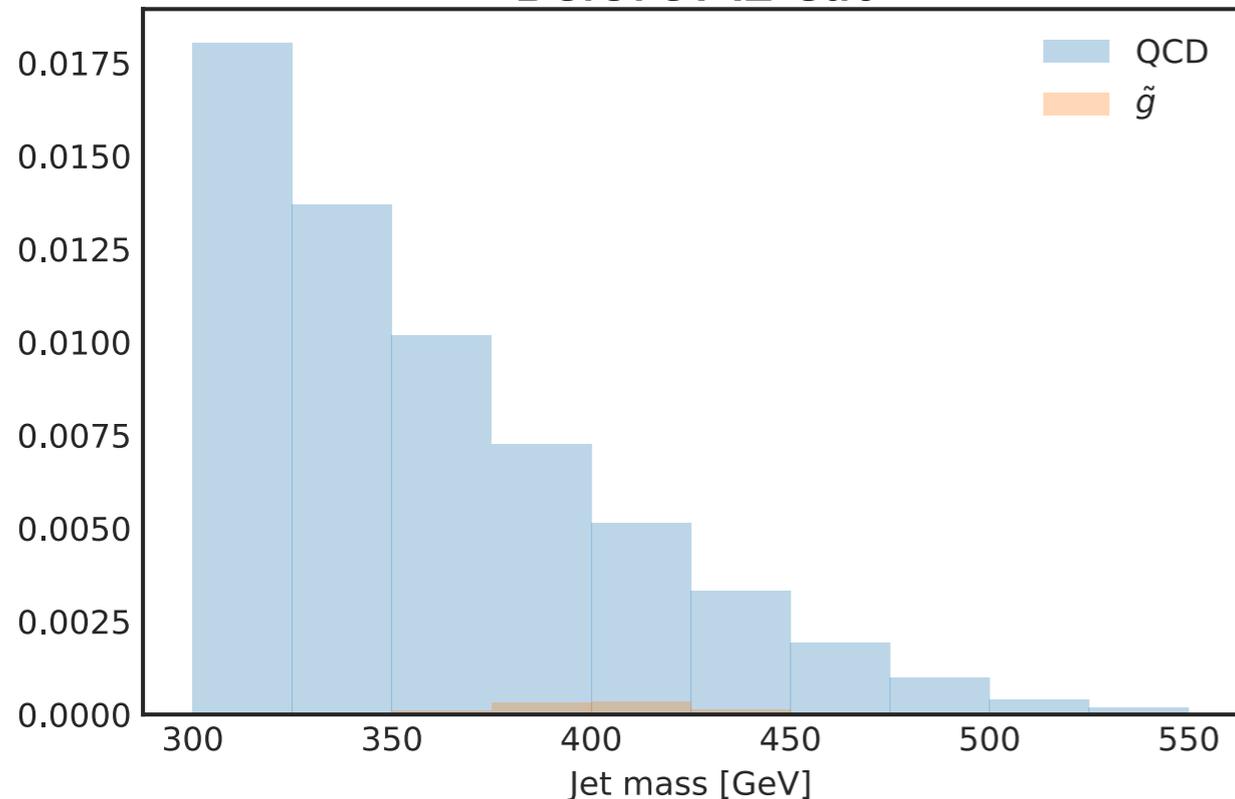


( $E_x$  = signal efficiency at bg rejection = x)

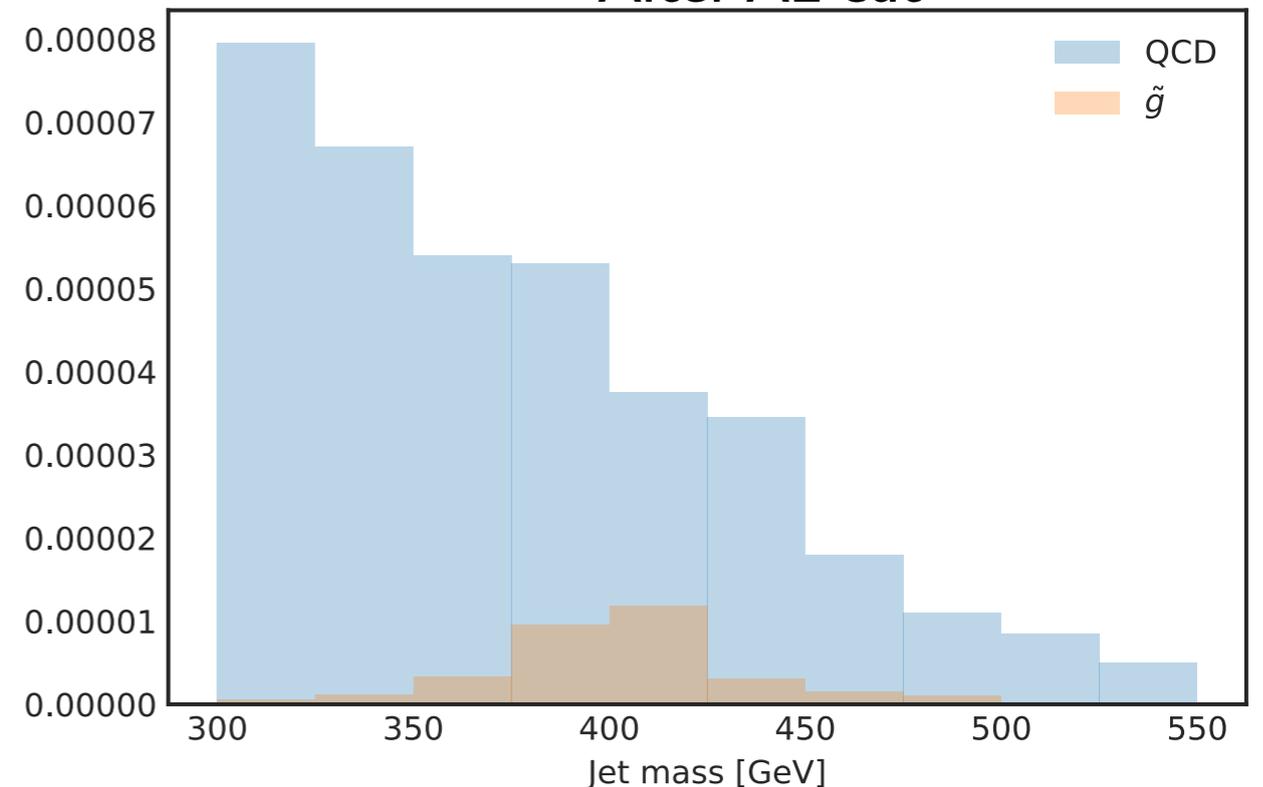
Performance of AE surprisingly robust even up to 10% contamination!

# Bump hunt with deep autoencoder

Before AE cut



After AE cut



Can train directly on data that contains 400 GeV gluinos,  
use the AE to clean away “boring” SM events,  
and improve S/N by a lot

Could really discover new physics this way!

# Summary

Deep learning has revolutionized the field of artificial intelligence and has given birth to a number of stunning real-world applications.

The revolution is coming to high-energy physics!

In this talk, we gave an overview of deep learning applications to the LHC.

Then we focused on two promising applications:

- Top tagging with jet images and CNNs (supervised learning)
  - ➡ Enormous gains in performance over cut-based and shallow ML methods.
- Deep autoencoders for open-ended anomaly detection (unsupervised learning)
  - ➡ Novel proposal for searching for new physics in the data without prejudice.

# Summary

The Standard Model has withstood the test of time for over 40 years.

Despite knowing that new physics beyond the SM is out there, we have yet to see any evidence for it at the LHC.

We need more ideas for how to search for the unexpected at the LHC.

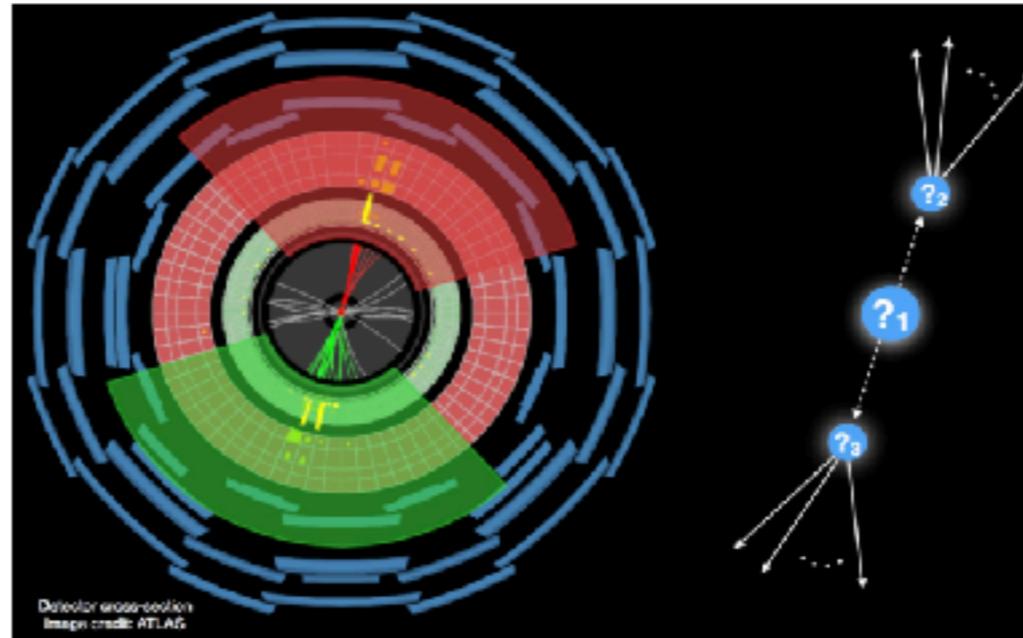
- Autoencoders for anomaly detection are a promising direction but there are surely many more!

**Input from the ML experts in the audience  
would be most appreciated!**

15-17 January 2020  
Europe/Zurich timezone

[Overview](#)[Timetable](#)[Participant List](#)[LHCOlympics2020](#)[Slack channel](#)

## LHCOlympics2020



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) [1<sup>st</sup>, 2<sup>nd</sup>, 3<sup>rd</sup>, 4<sup>th</sup>], 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 benchmark signal model. You can download these from [this page](#). 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 a new dataset where the "background" will be similar to but not identical to the one in the development set (as is true in real data!). The goal of the challenge is to see who can "best" identify BSM (yes/no, what mass, what cross-section) in the dataset. There are many ways to quantify "best" and we will use all of the submissions to explore the pros/cons of the various approaches.



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April 4, 2019

Dataset Open Access

# R&D Dataset for LHC Olympics 2020 Anomaly Detection Challenge

Gregor Kasieczka; Ben Nachman; David Shih

This is the first R&D dataset for the LHC Olympics 2020 Anomaly Detection Challenge. It consists of 1M QCD dijet events and 100k  $W \rightarrow XY$  events, with  $X \rightarrow jj$  and  $Y \rightarrow jj$ . The  $W$ ,  $X$ , and  $Y$  masses are 3.5 TeV, 500 GeV and 100 GeV respectively. The events are produced using Pythia8 and Delphes 3.4.1, with no pileup or MPI included. They are selected using a single fat-jet ( $R=1$ ) trigger with  $p_T$  threshold of 1.3 TeV.

The events are randomly shuffled together, but for the purposes of testing and development, we provide the user with a signal/background truth bit for each event. Obviously, the truth bit will not be included in the actual challenge.

These events are stored as pandas dataframes saved to compressed h5 format. For each event, all Delphes reconstructed particles in the event are assumed to be massless and are recorded in detector coordinates ( $p_T$ , eta, phi). More detailed information such as particle charge is not included. Events are zero padded to constant size arrays of 700 particles, with the truth bit appended at the end. The array format is therefore (Nevents=1.1M, 2101).

For more information, including an example Jupyter notebook illustrating how to read and process the events, see the official LHC Olympics 2020 webpage.

<https://indico.cern.ch/event/809820/page/16782-lhcolympics2020>

Files (2.8 GB) <span style="float:right">v</span>		
Name	Size	
events_anomalydetection.h5	2.8 GB	<a href="#">Download</a>

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**Publication date:**  
April 4, 2019

**DOI:**  
[DOI 10.5281/zenodo.2629073](https://doi.org/10.5281/zenodo.2629073)

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Versions

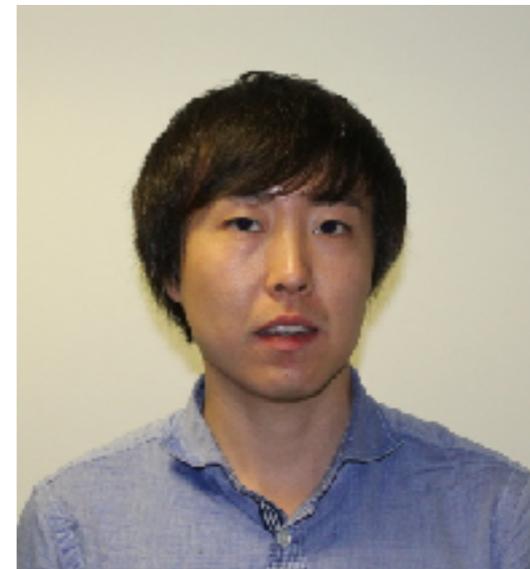
# Thanks for your attention!



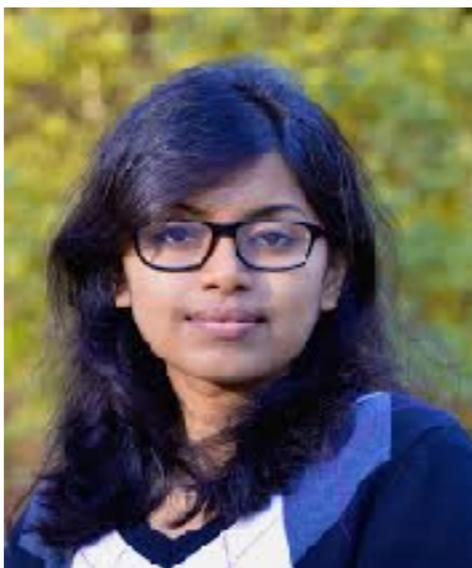
Sebastian Macaluso



Marco Farina



Yuichiro Nakai



Dipsikha Debnath



Matt Buckley



Scott Thomas

**Backup material**

# Autoencoder architectures

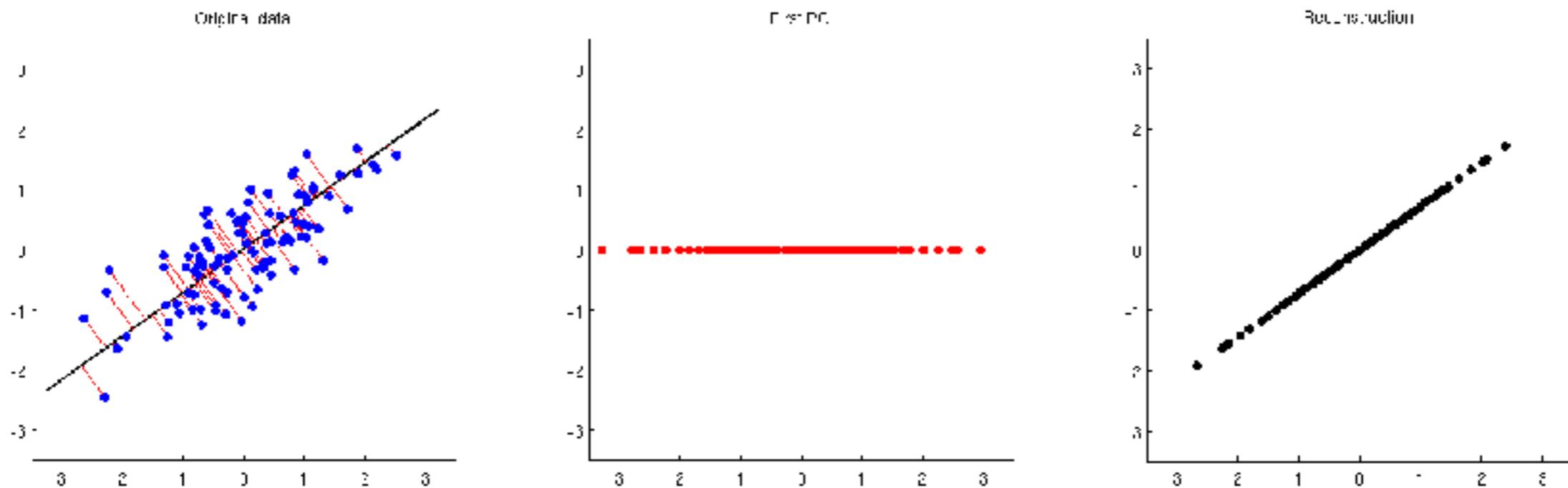
We considered three autoencoder architectures (many more are possible):

- Principal Component Analysis (PCA)
- Dense NN
- Convolutional NN

# Autoencoder architectures

We considered three autoencoder architectures (many more are possible):

- Principal Component Analysis (PCA)



Project onto the first  $d$  PCA eigenvectors

$$z = \mathcal{P}_d x_{in}$$

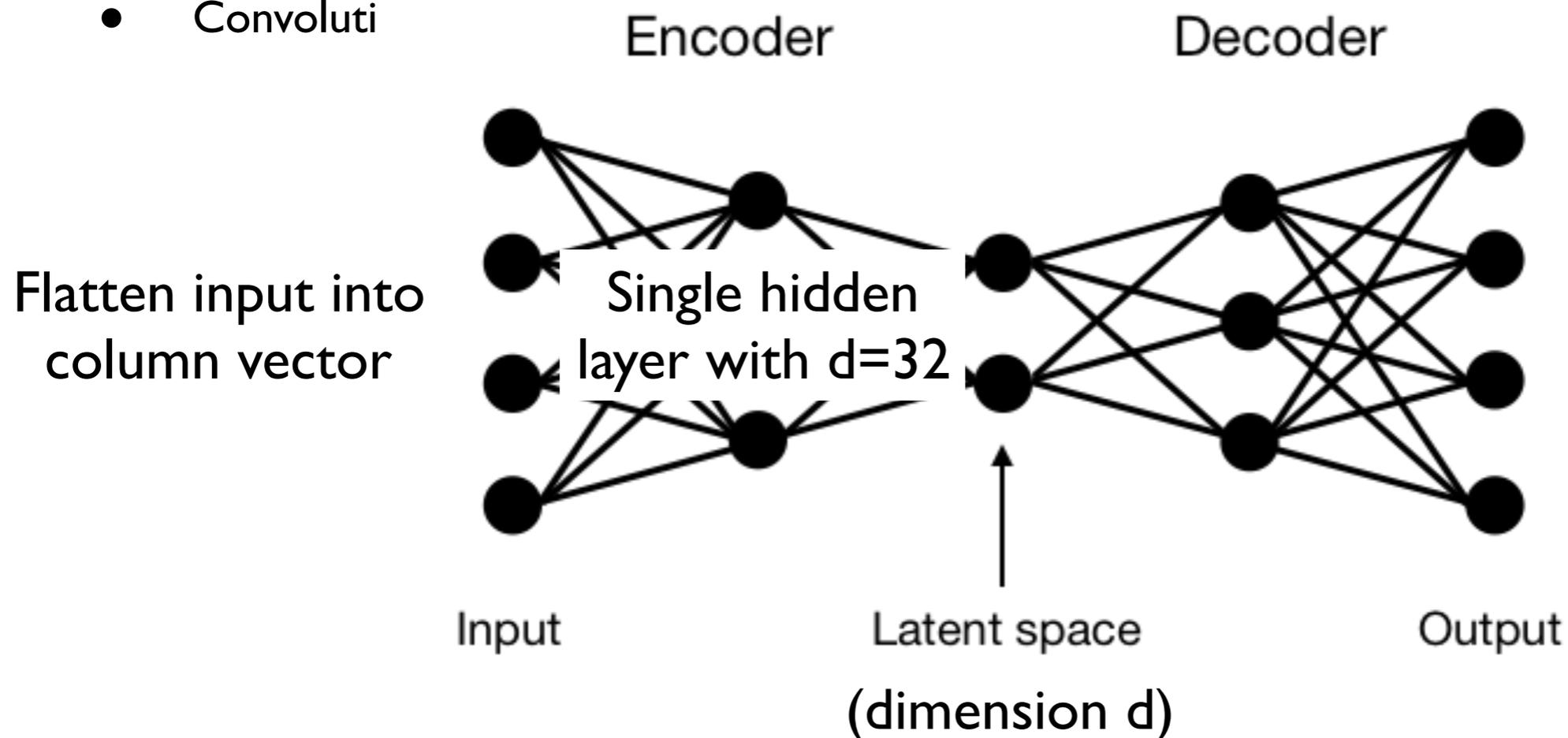
Inverse transform to reconstruct original input

$$x_{out} = \mathcal{P}_d^T z = \mathcal{P}_d^T \mathcal{P}_d x_{in}$$

# Autoencoder architectures

We considered three autoencoder architectures (many more are possible):

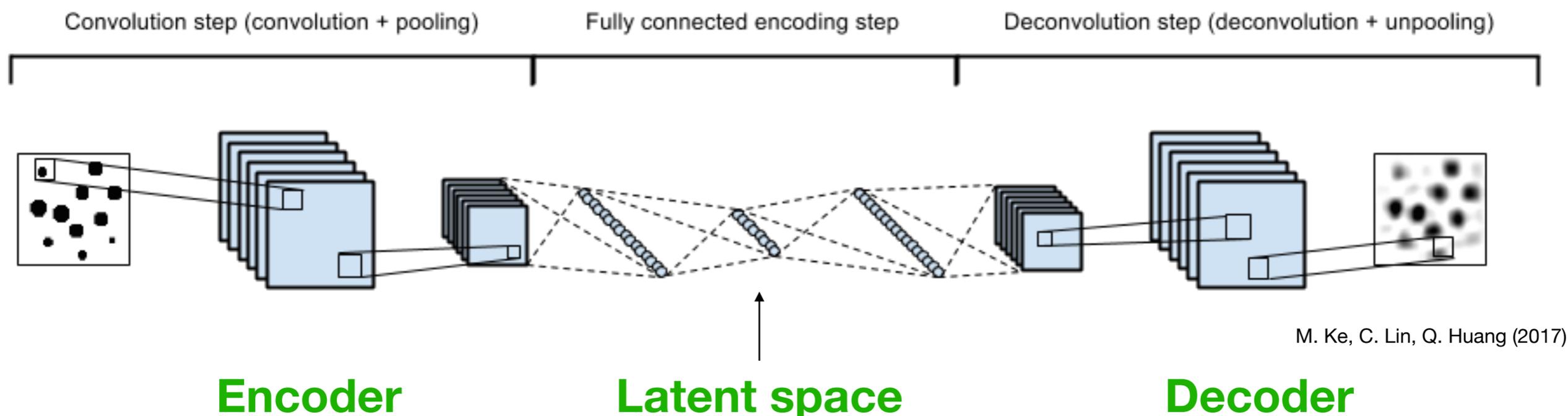
- Principal Component Analysis (PCA)
- Dense NN
- Convoluti



# Autoencoder architectures

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- Convolutional NN

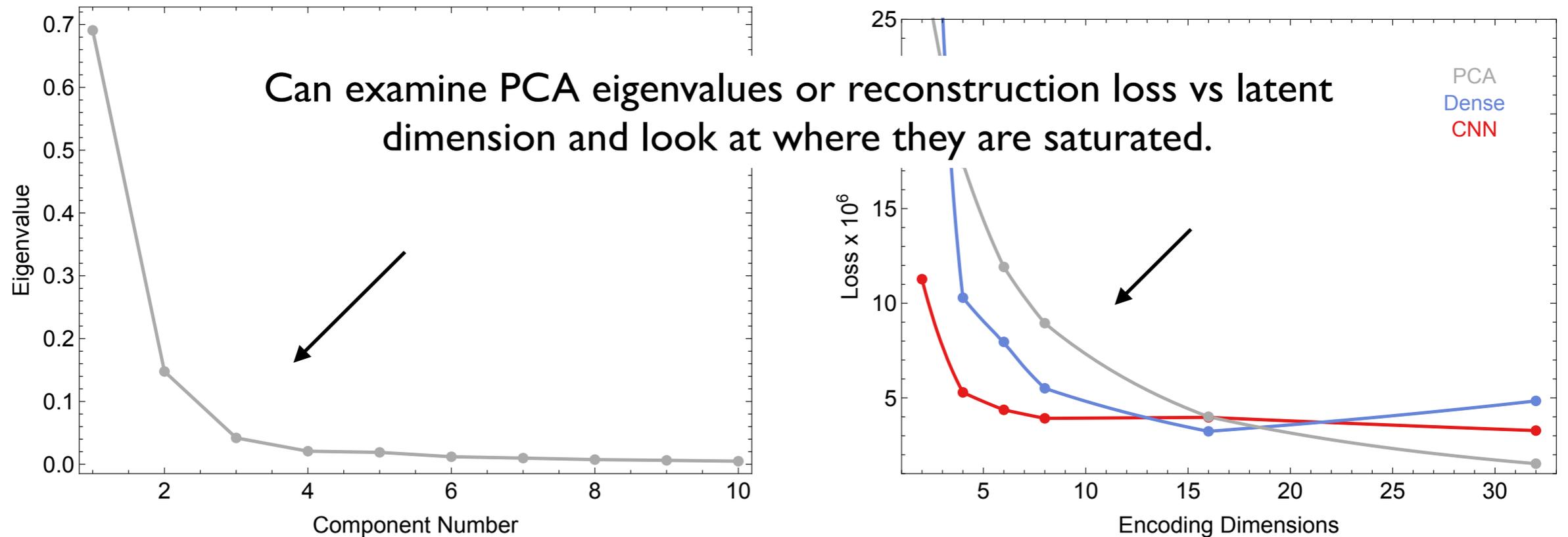


I28C3-MP2-I28C3-MP2-I28C3-32N-6N-32N-I2800N-I28C3-US2-I28C3-US2-I C3

# Choosing the latent dimension

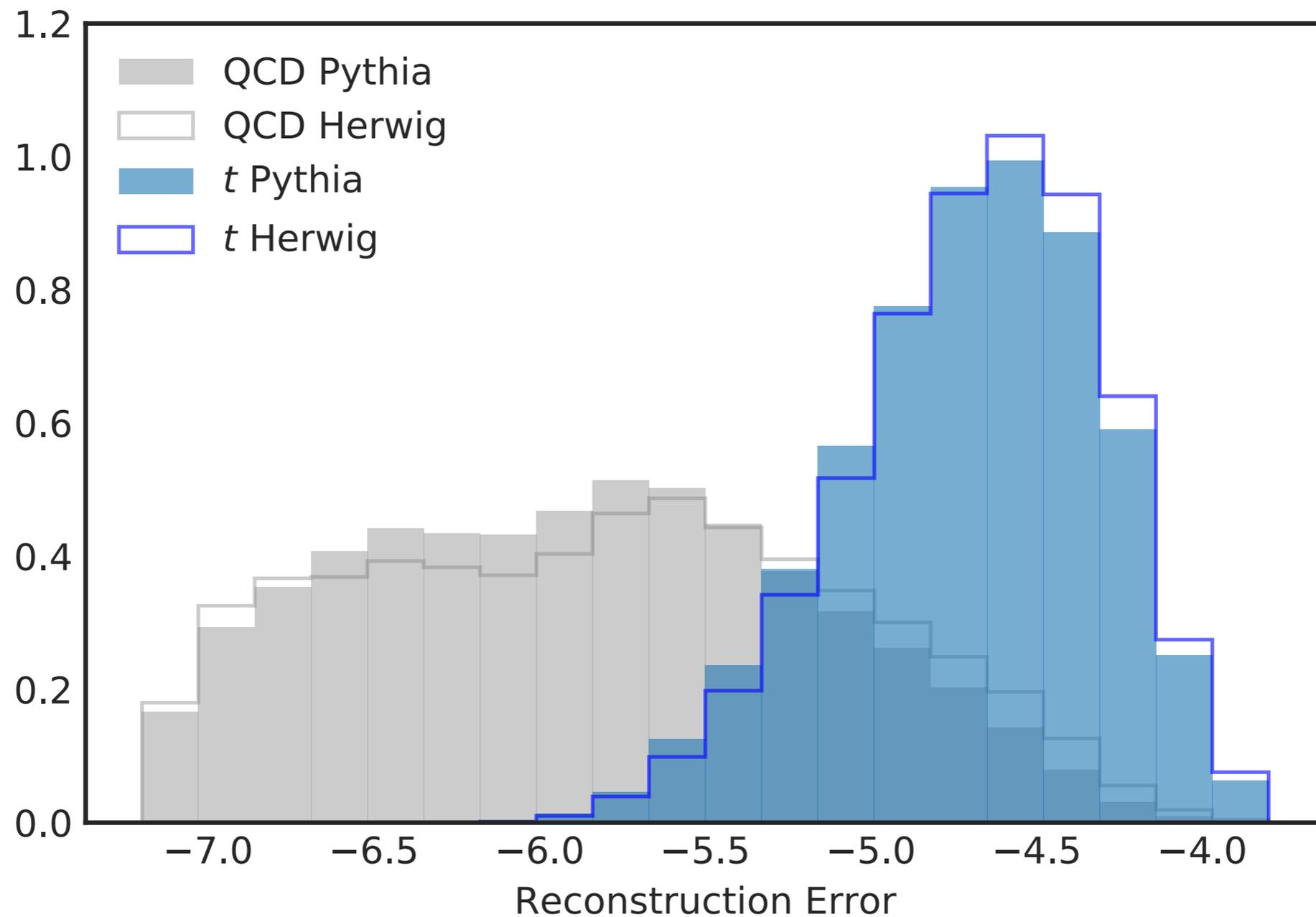
$d$  too large  $\rightarrow$  autoencoder becomes identity transform  
 $d$  too small  $\rightarrow$  autoencoder cannot learn all the features

Should choose the latent dimension in an unsupervised manner  
(ie without optimizing on a specific signal)

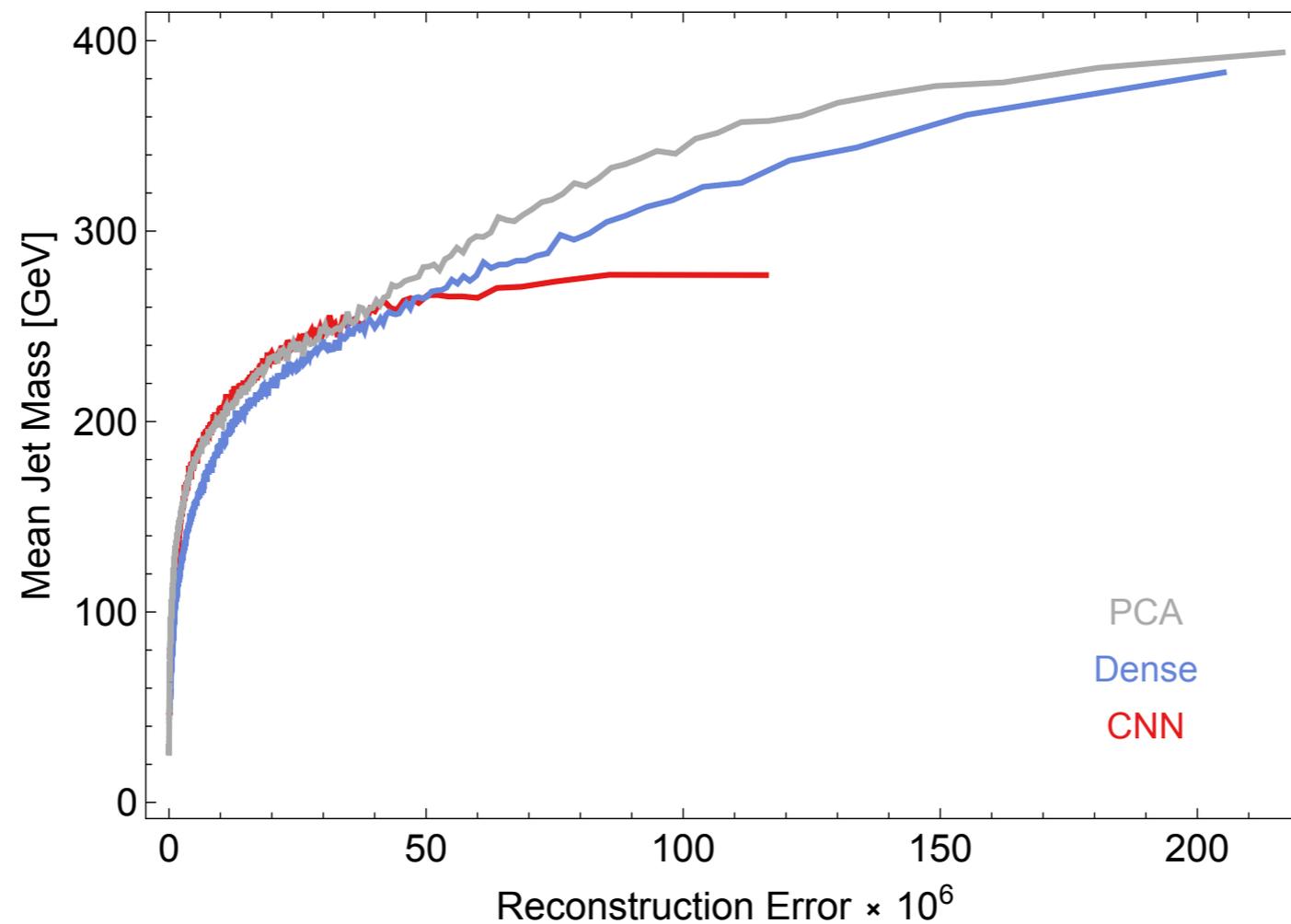


We chose  $d=6$

# Robustness with other Monte Carlo



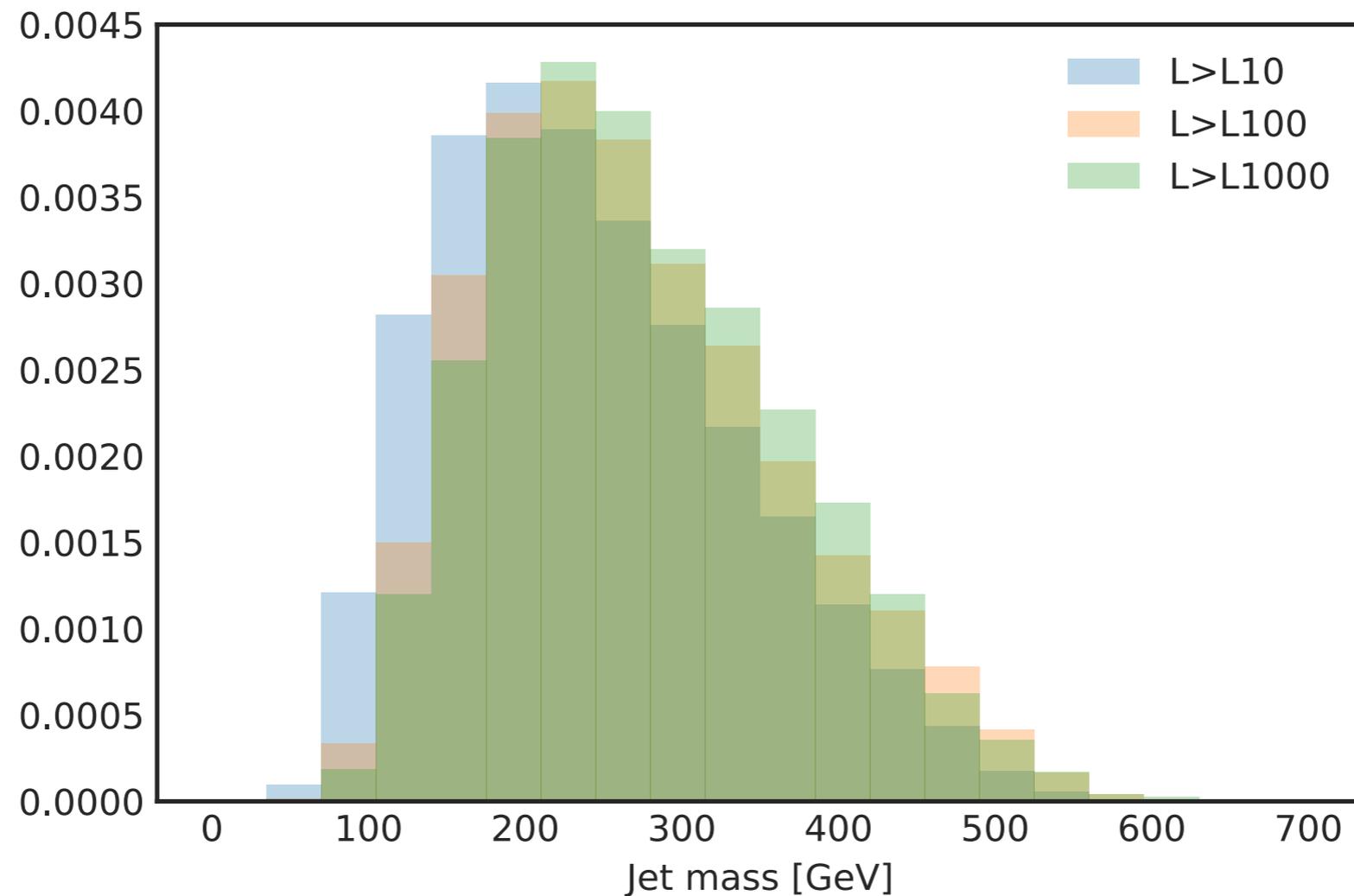
# Correlation with jet mass



Indeed, this is confirmed by looking at mean jet mass in bins of reconstruction error for the QCD background.

CNN is no longer correlated with jet mass for  $m \gtrsim 250$  GeV

# Correlation with jet mass



The QCD jet mass distribution is stable against harder cuts on the reconstruction error, for the CNN autoencoder.