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Searching for New Physics with Deep Autoencoders

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Based on M. Farina, YN and D. Shih, arXiv:1808.08992 [hep-ph].

Physics Opportunities and Advanced Tools, HKUST, 2019

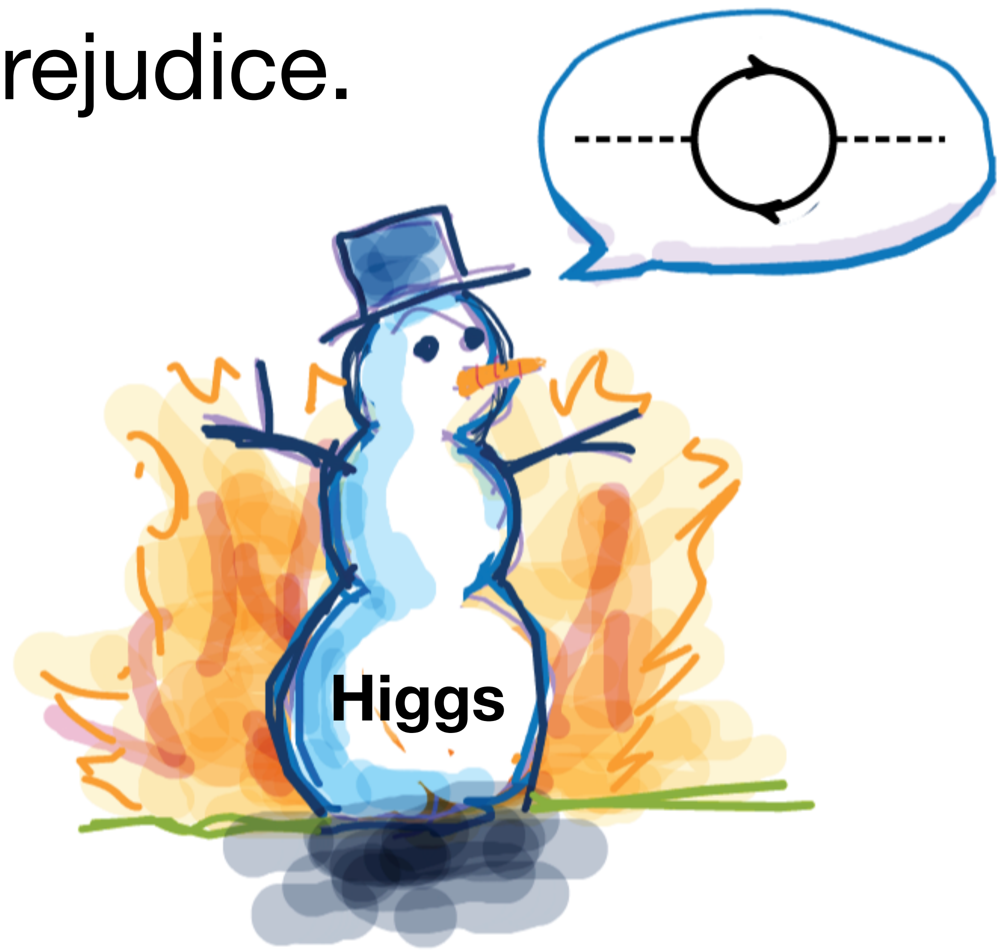
Expected Physics

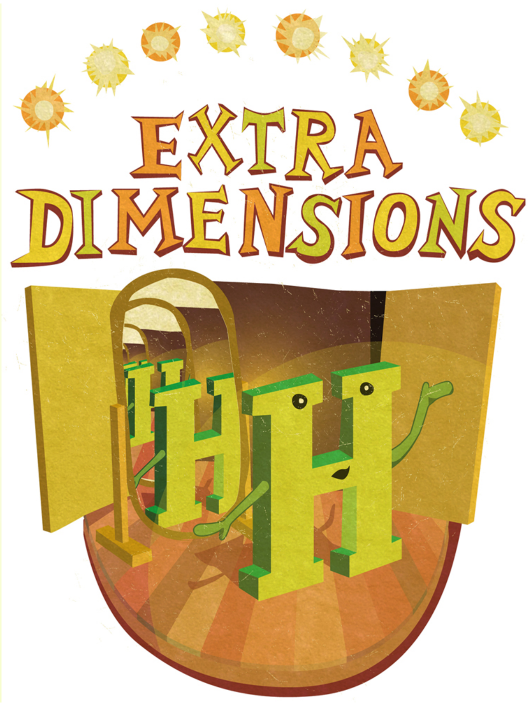
We have considered many possibilities of BSM physics with top-down theory prejudice.

In particular, many are motivated by **the naturalness problem**.

Our candidates are :

Supersymmetry, Composite Higgs, Extra dimension, …

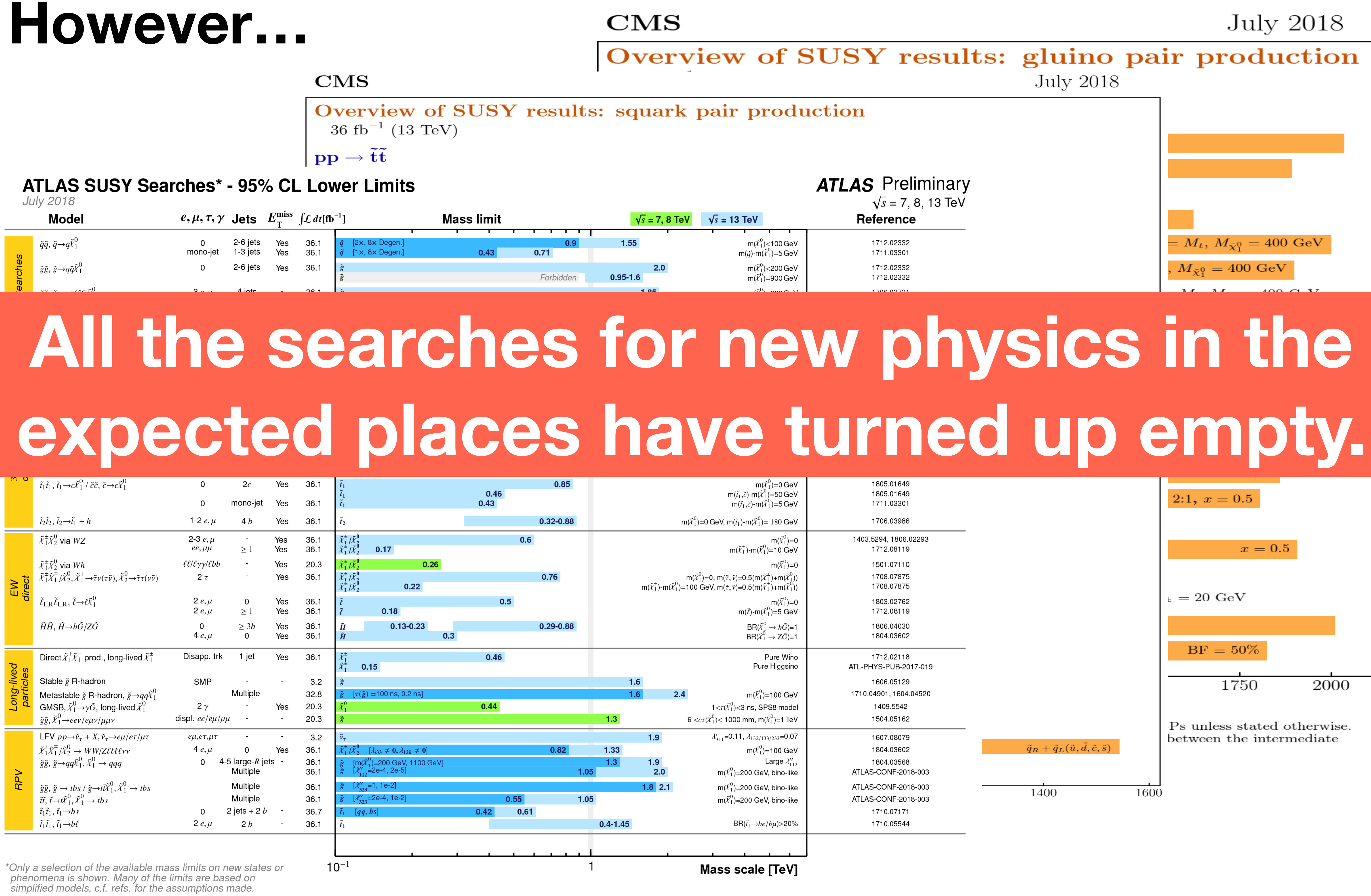




…

Status of Searches

However…



All the searches for new physics in the expected places have turned up empty.

Unexpected Physics

We may need to prepare well for unexpected physics.

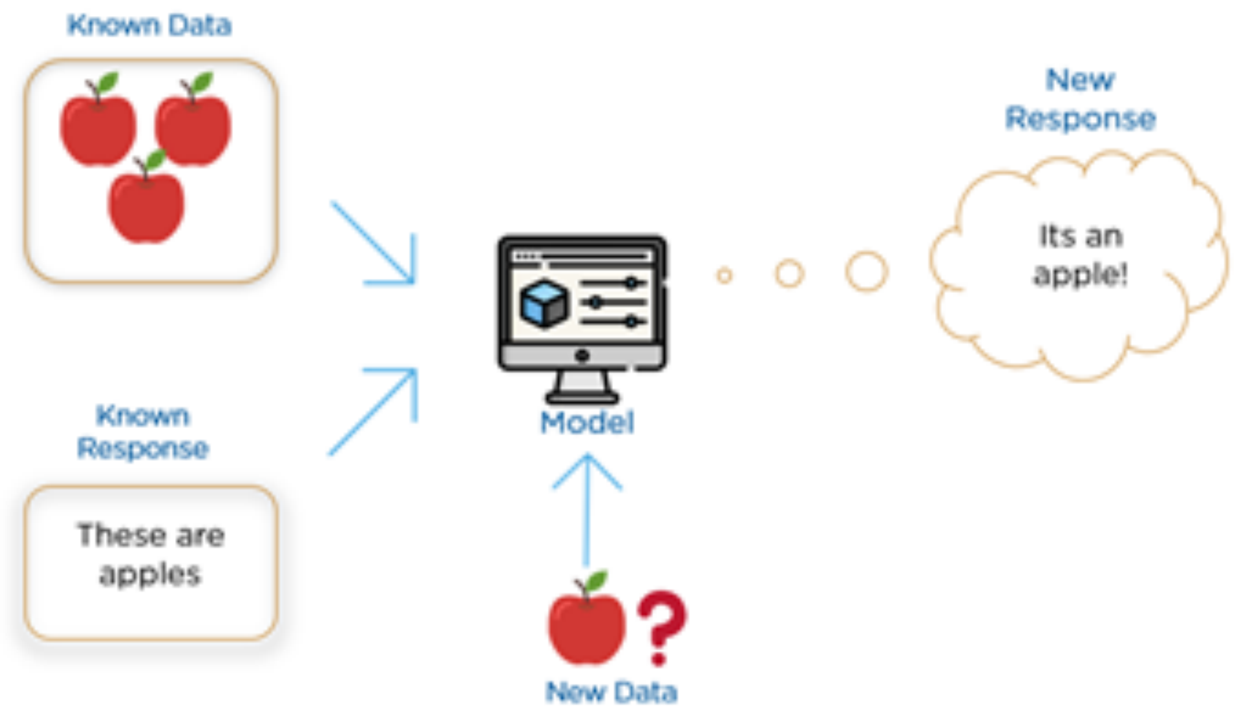
Can we find new physics without knowing what we're looking for ??

Machine Learning can help !

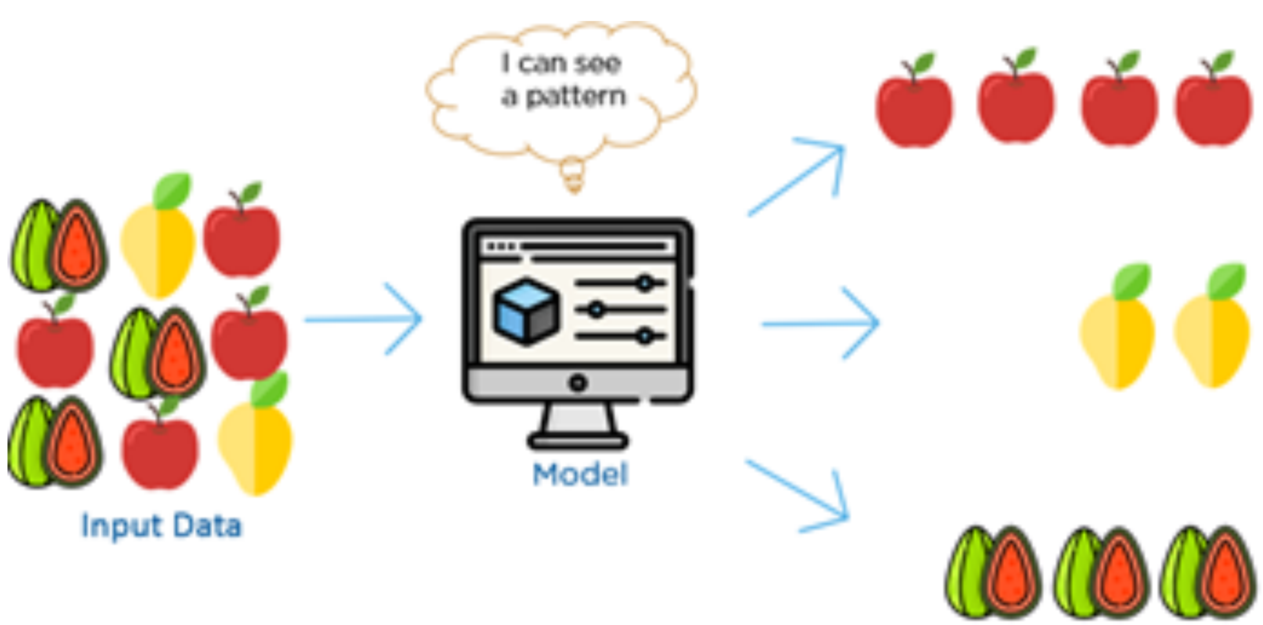
ML Algorithms

Machine learning algorithms can be classified into :

- **Supervised learning**
  - ✓ Learn from labeled data.
  - ✓ Machine can answer if new data is an apple or not.

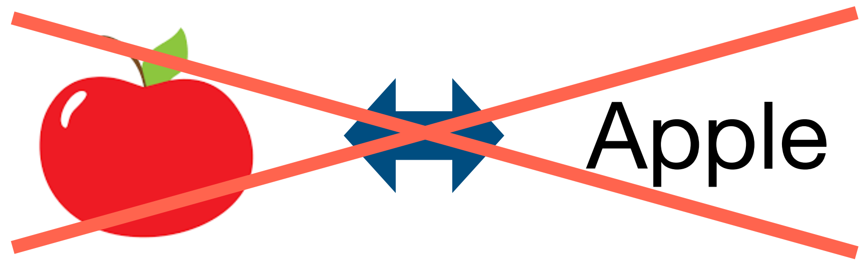


- **Unsupervised learning**
  - ✓ Learn from unlabeled data.
  - ✓ Machine looks for patterns and extracts features in data.



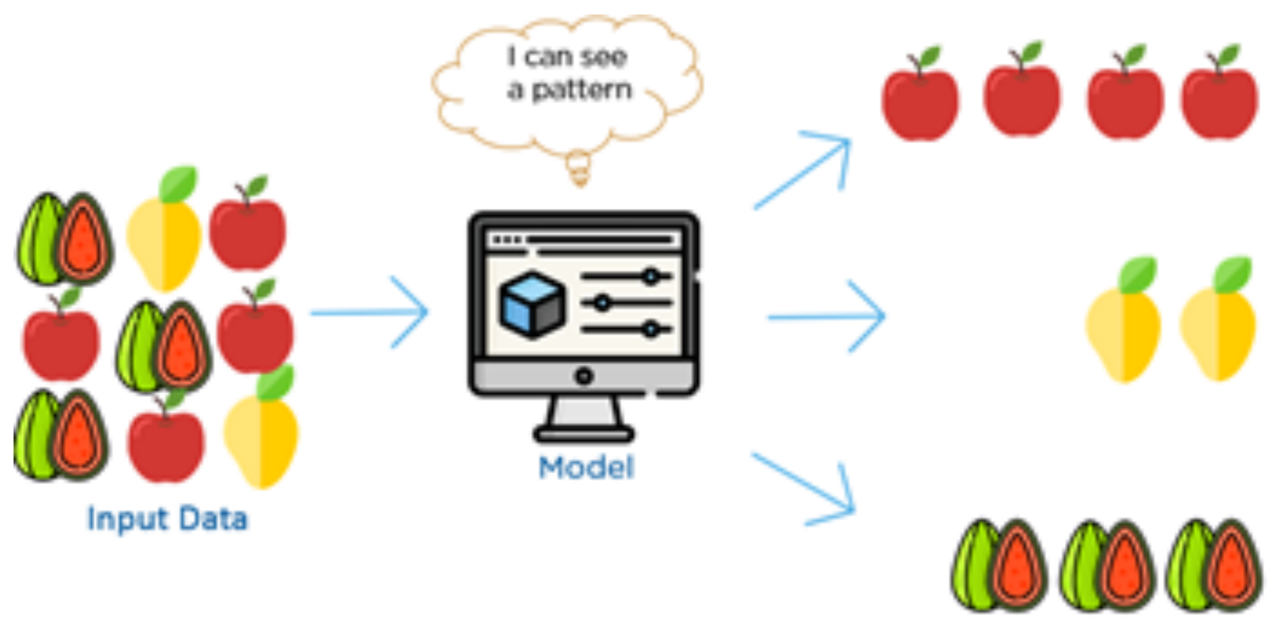
Search for Unexpected

We don't know what we're looking for and cannot attach a label to new physics.



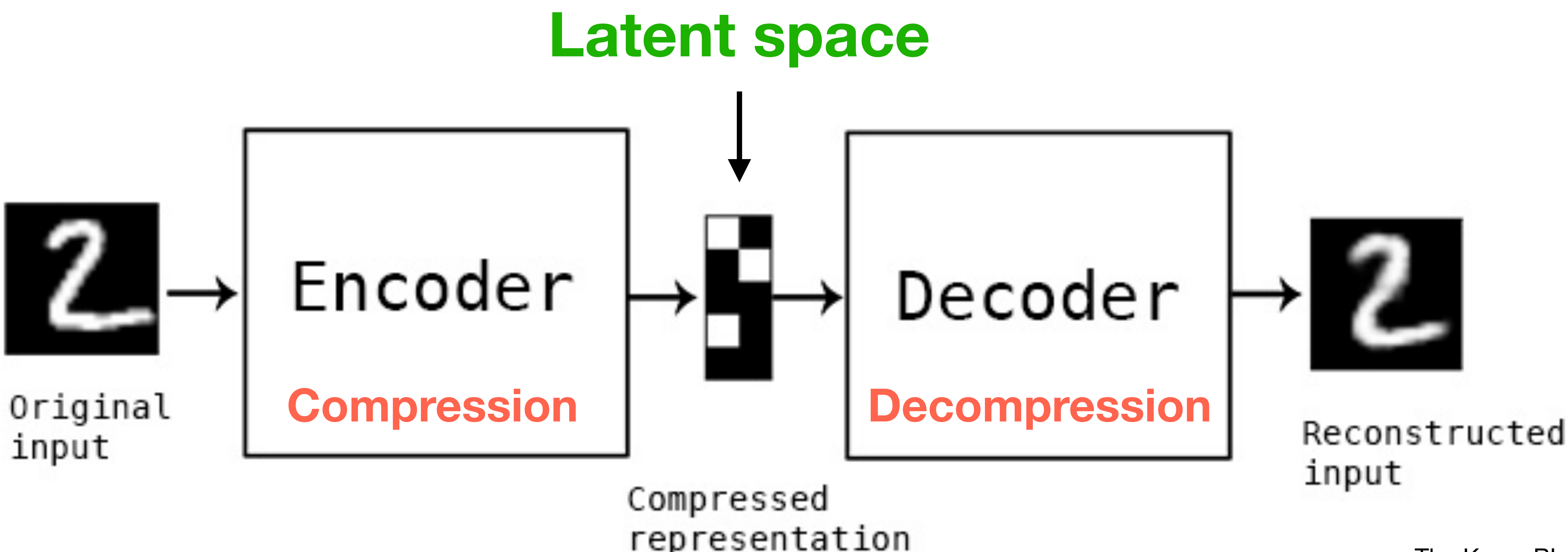
Unsupervised learning comes into play !

- **Unsupervised learning**
  - ✓ Learn from unlabeled data.
  - ✓ Machine looks for patterns and extracts features in data.



Autoencoder

Autoencoder is an unsupervised learning algorithm that maps an input to a latent compressed representation and then back to itself.

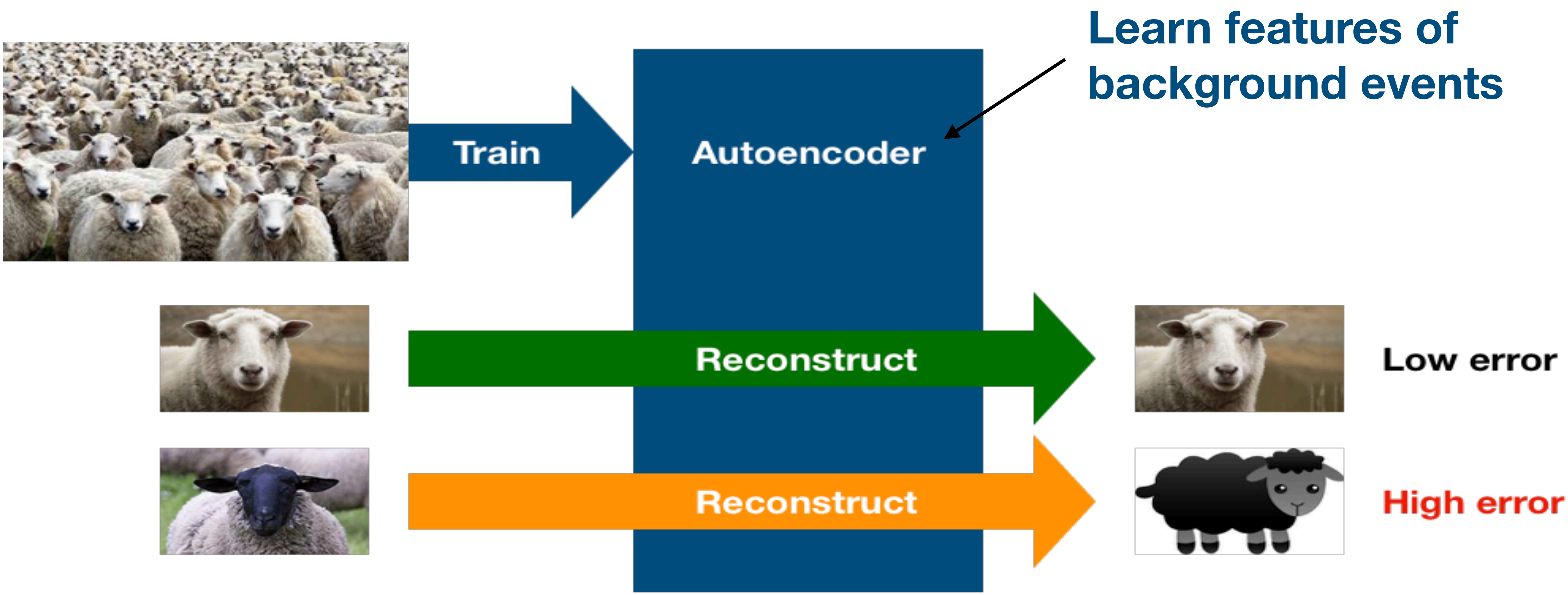


The Keras Blog

By learning how to reproduce original input, autoencoder extracts features of input data.

Anomaly Detection

Autoencoder learns to map background events back to themselves.

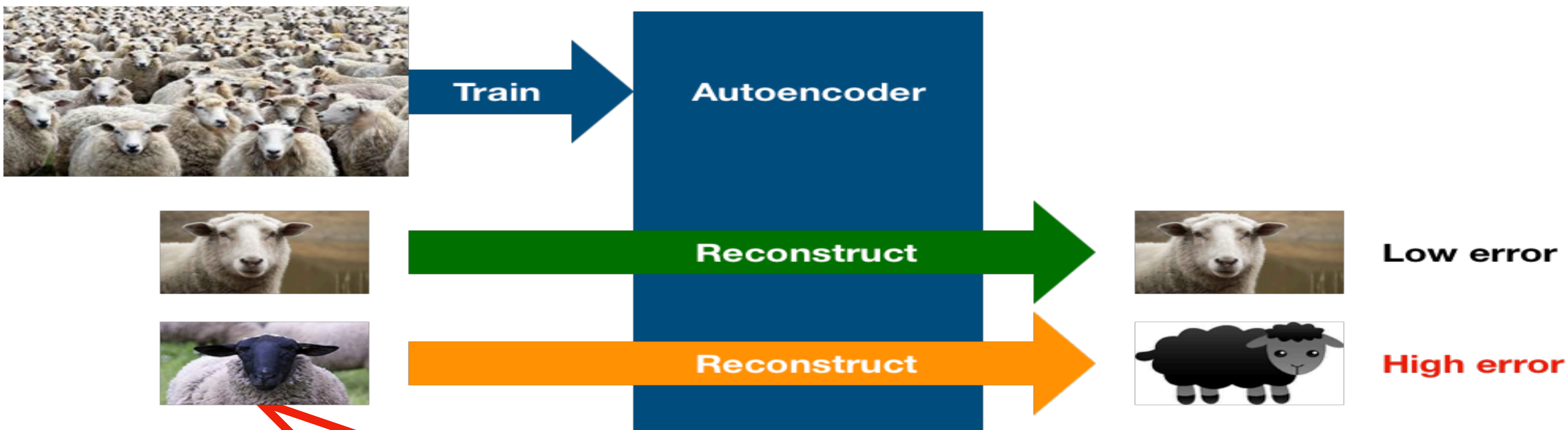


Autoencoder <u>fails to</u> reconstruct anomalous events that it has never encountered.

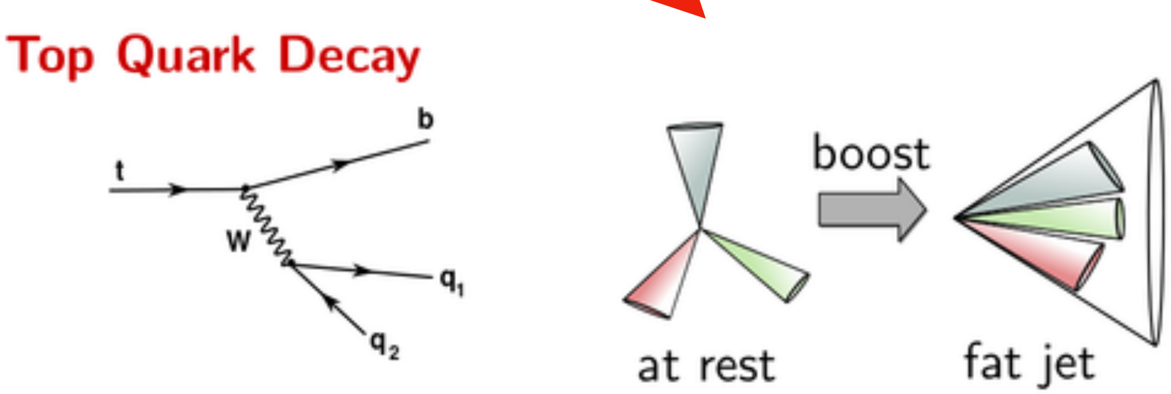
Signal the existence of anomaly !

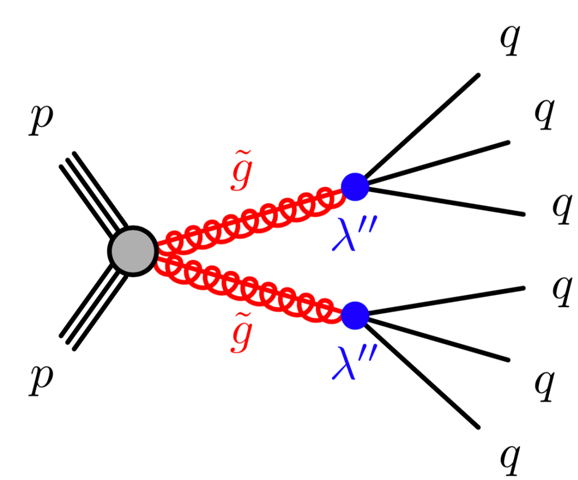
Anomalous Jet Detection

The idea is general, but concentrate on detection of anomalous jets as the first baby step.



Our examples of anomalies :





Top jets

Gluino jets

Sample Generation

Generate jet samples by using PYTHIA for hadronization and Delphes for detector simulation.

Background : QCD jets $p_T \in [800,\ 900]$ GeV $|\eta| < 1$

Signal jets: top jets, RPV gluino jets $m_{\tilde{g}} = 400$ GeV
(decay to 3 light quark jets)

Match requirement : heavy resonance is within the fat jet, $\Delta R < 0.6$

Merge requirement : the partonic daughters of heavy resonance is within the fat jet, $\Delta R < 0.6$

We use sample sizes of 100k events for training and testing.
(The performance seems to saturate.)

Jet Images

Focus on jet images (2D of eta and phi) as inputs to autoencoder.

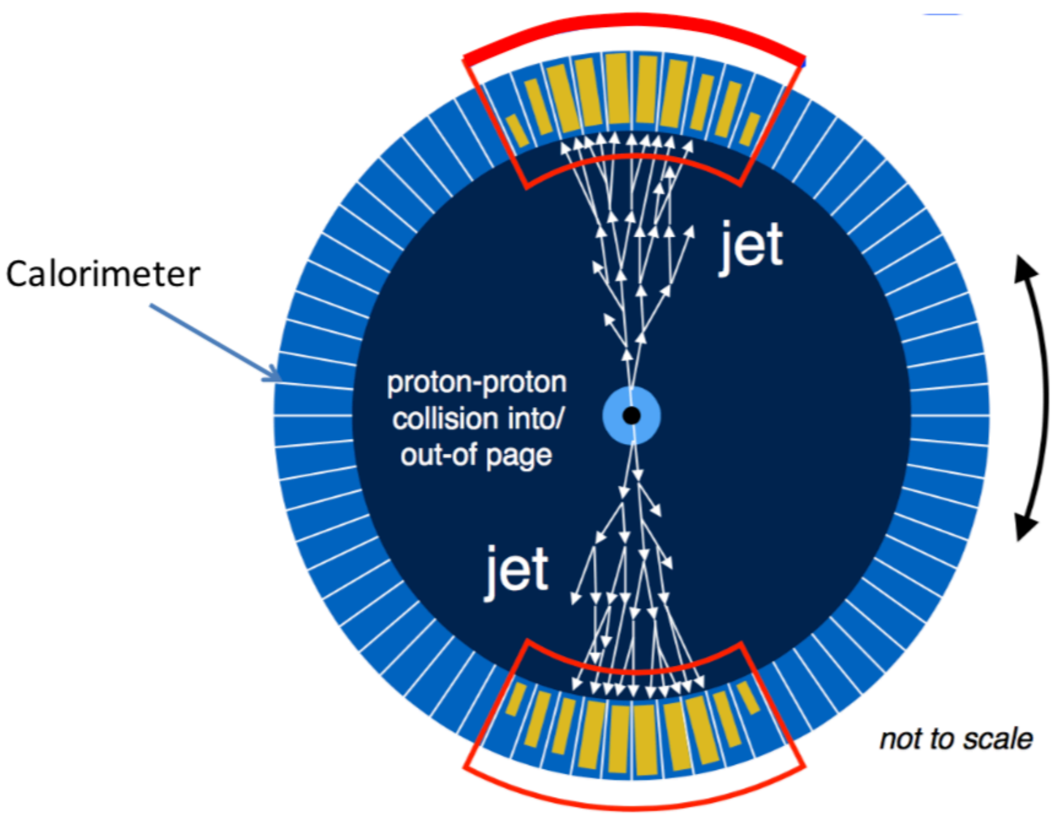
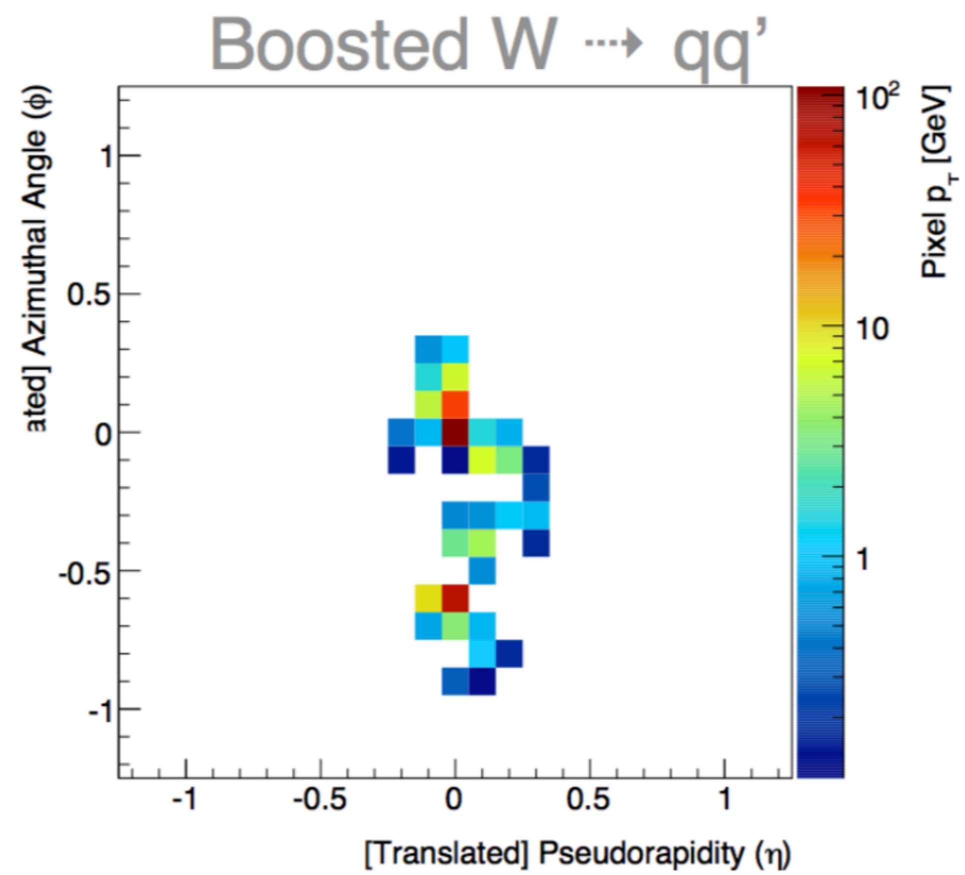


Figure credit:
B. Nachman



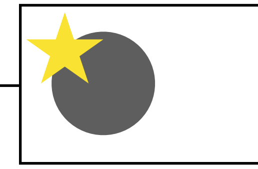
✓ Pixelation is provided by calorimeter towers.

✓ Pixel intensity is pT recorded by each tower.

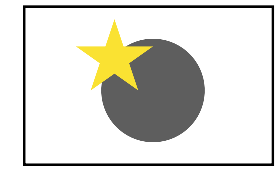
Jet Images

To improve performance…

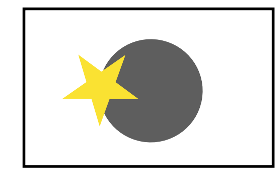
Image pre-processing



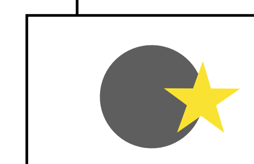
1. Shift an image so that the centroid is at the origin



2. Rotate the image so that the major principal axis is vertical



3. Flip the image so that the maximum intensity is in the upper right region



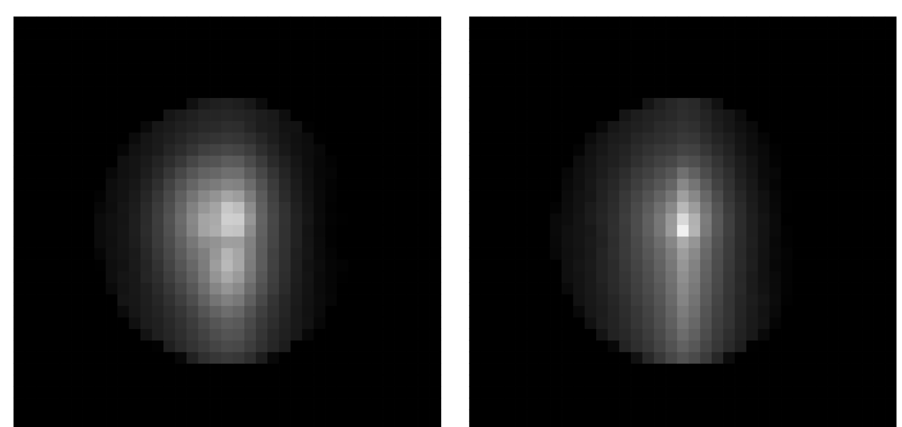
4. Normalize the image to unit total intensity

5. Pixelate the image : $\Delta\eta = \Delta\phi = 3.2$ (37 x 37 pixels)

Average images

Left : top jets

Right : QCD jets



Macaluso, Shih (2018)

Reconstruction Error

Reconstruction error : a measure for how well autoencoder reproduce the original input.

$$L(\boldsymbol{x}, \hat{\boldsymbol{x}}) = \sum_{\mathbf{37 \times 37\, pixels}} |\boldsymbol{x} - \hat{\boldsymbol{x}}|^{\mathbf{2}}$$

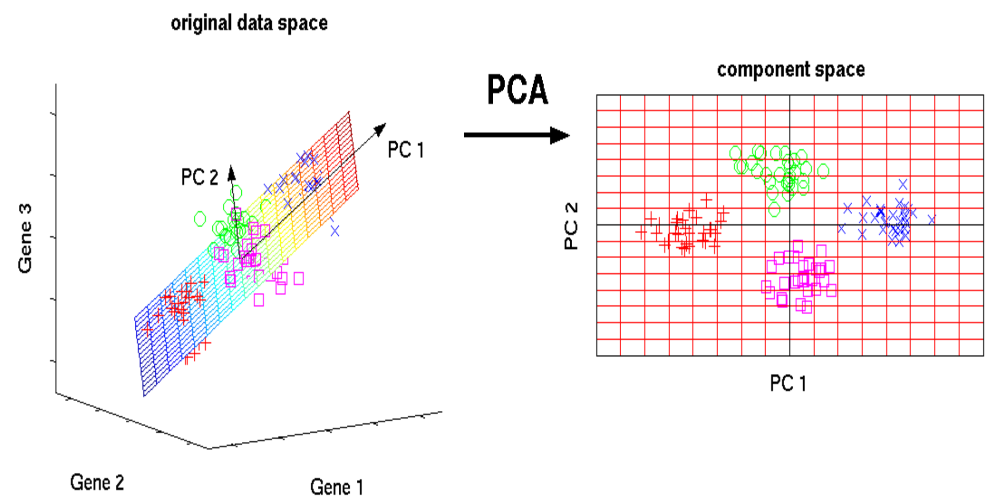
x : inputs

$\hat{x}$: outputs

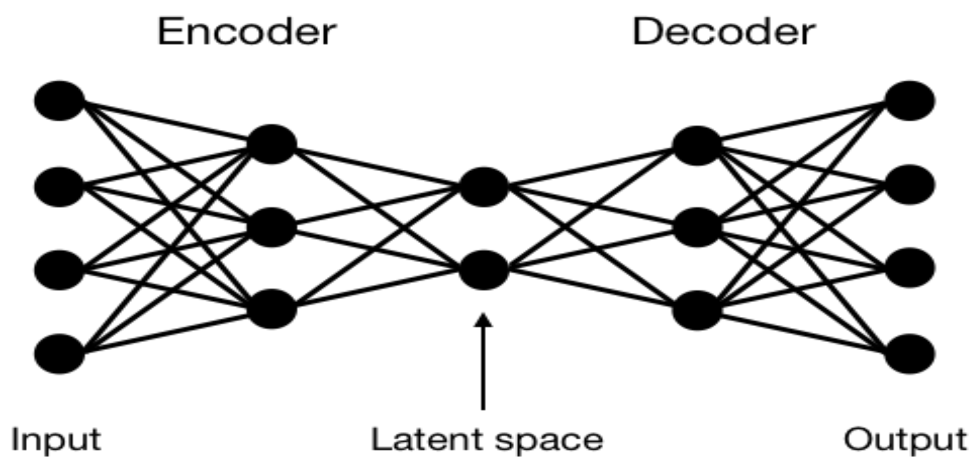
Train autoencoder to minimize reconstruction error on background events.

Our Autoencoders

We consider the following architectures :

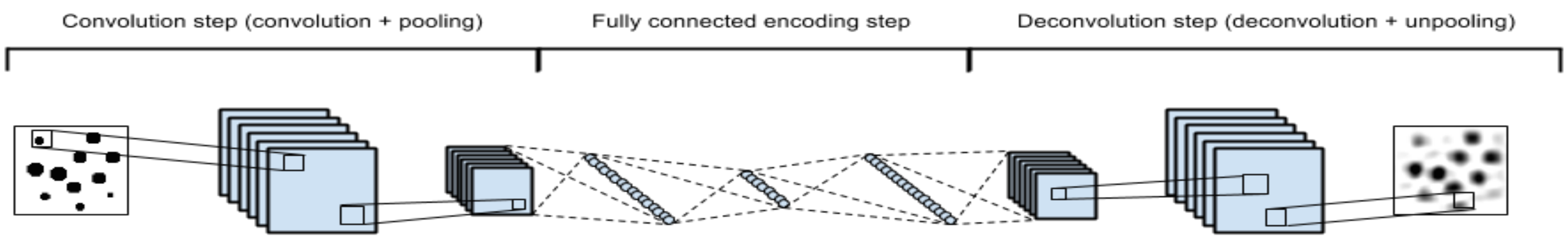


✓ **Principal Component Analysis (PCA)**



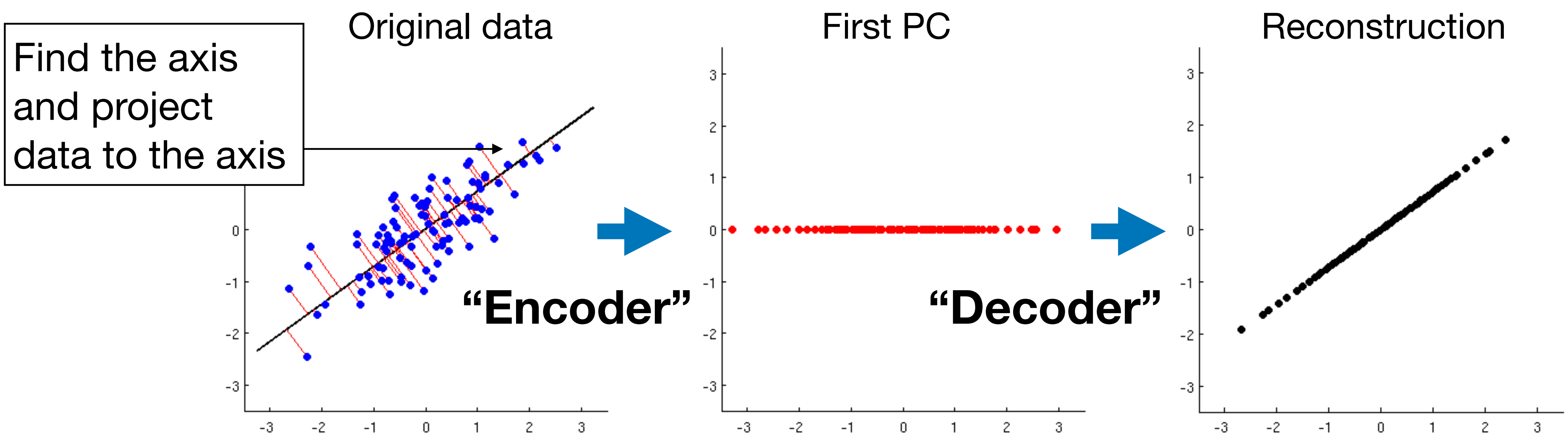
✓ **Simple (dense) autoencoder**

✓ **Convolutional autoencoder**



Principal Component Analysis

PCA is a technique to drop the least important variables by focusing on variance of data.



Eigenvectors of covariance matrix of $\boldsymbol{x}_n - \boldsymbol{c}_0 \quad (\boldsymbol{c}_0 = \sum_n \boldsymbol{x}_n / N)$ give desired axes.

$\Gamma = (\boldsymbol{e}_1 \ \boldsymbol{e}_2 \ \ldots \ \boldsymbol{e}_d)$ d : the number of principal components ($d < D$)

“PCA autoencoder”

“Encoder” : $\tilde{\boldsymbol{x}}_n = (\boldsymbol{x}_n - \boldsymbol{c}_0)\Gamma$ “Decoder” : $\boldsymbol{x}'_n = \tilde{\boldsymbol{x}}_n \Gamma^T + \boldsymbol{c}_0$

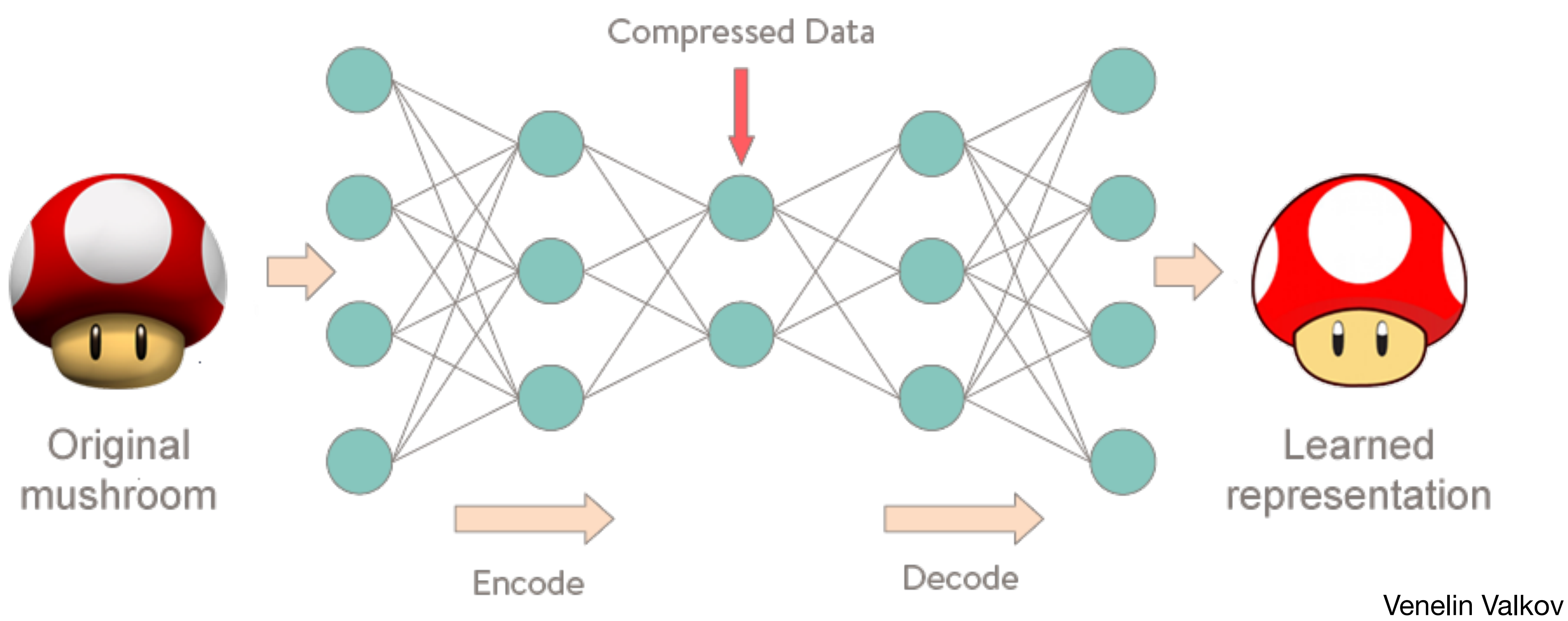
Simple Autoencoder

Autoencoder with a single dense (fully-connected) layer as encoder and as decoder.

✓ Encoder and decoder are symmetric (weights are not the same).

✓ The number of neurons in a hidden layer = 32.

✓ Flatten a jet image into a single column vector for input.

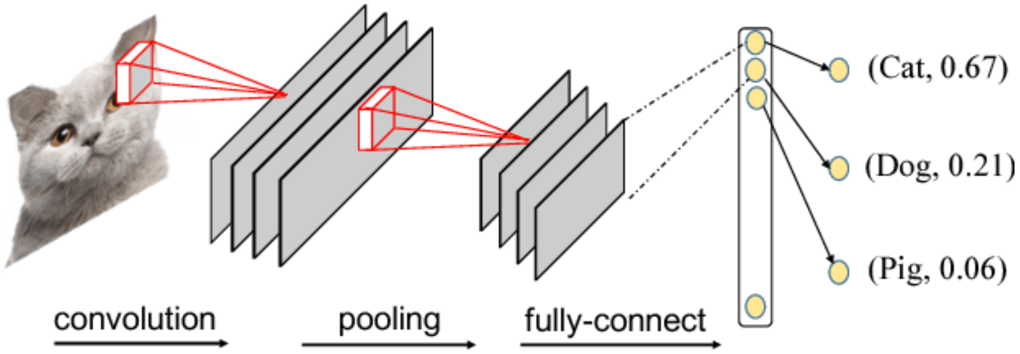


Convolutional Autoencoder

Convolutional Neural Network (CNN)

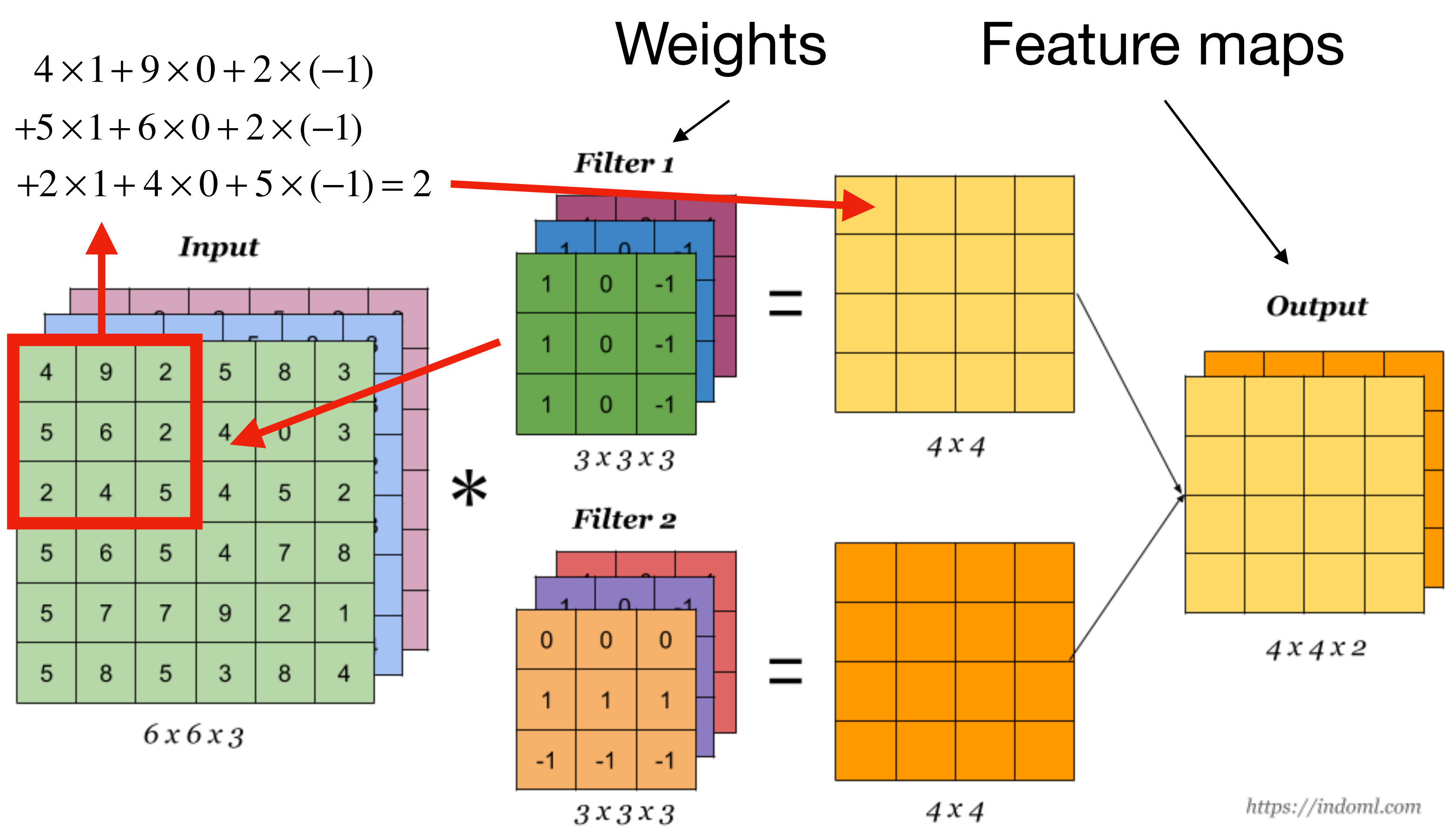
✓ Show high performance for <u>image recognitions</u>

✓ Maintain the <u>spacial information</u> of images



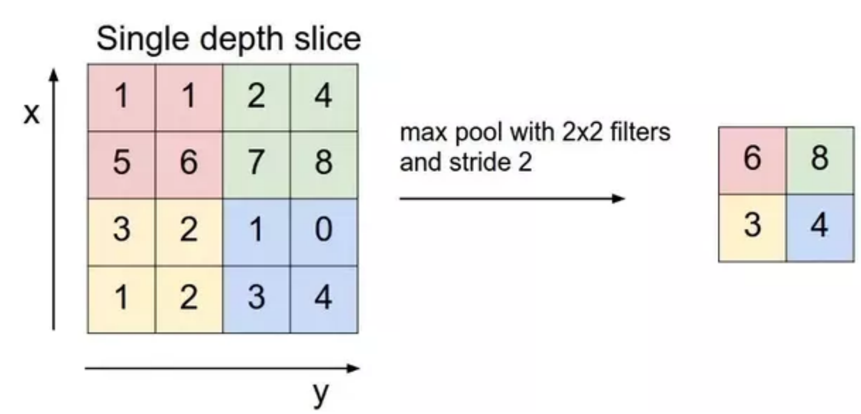
arXiv:1712.01670

Convolutional layer



Max pooling

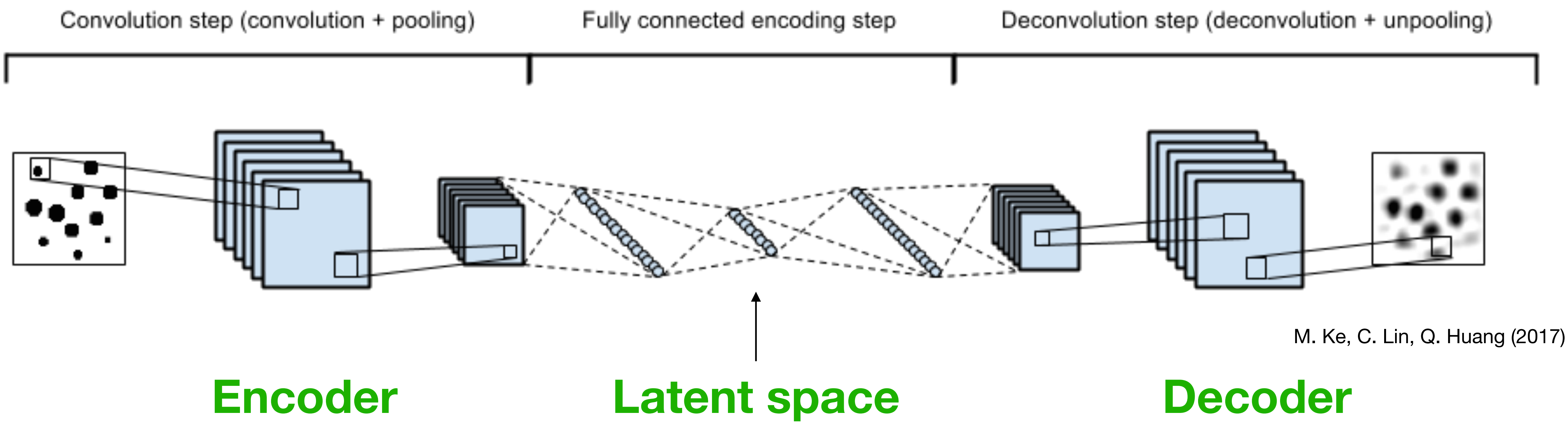
Reduce the image size



Up sampling (pooling)
also exists in autoencoder.

Convolutional Autoencoder

Autoencoder architecture :



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

128C3 : 128 filters with a 3x3 kernel

32N : a fully-connected layer with 32 neurons

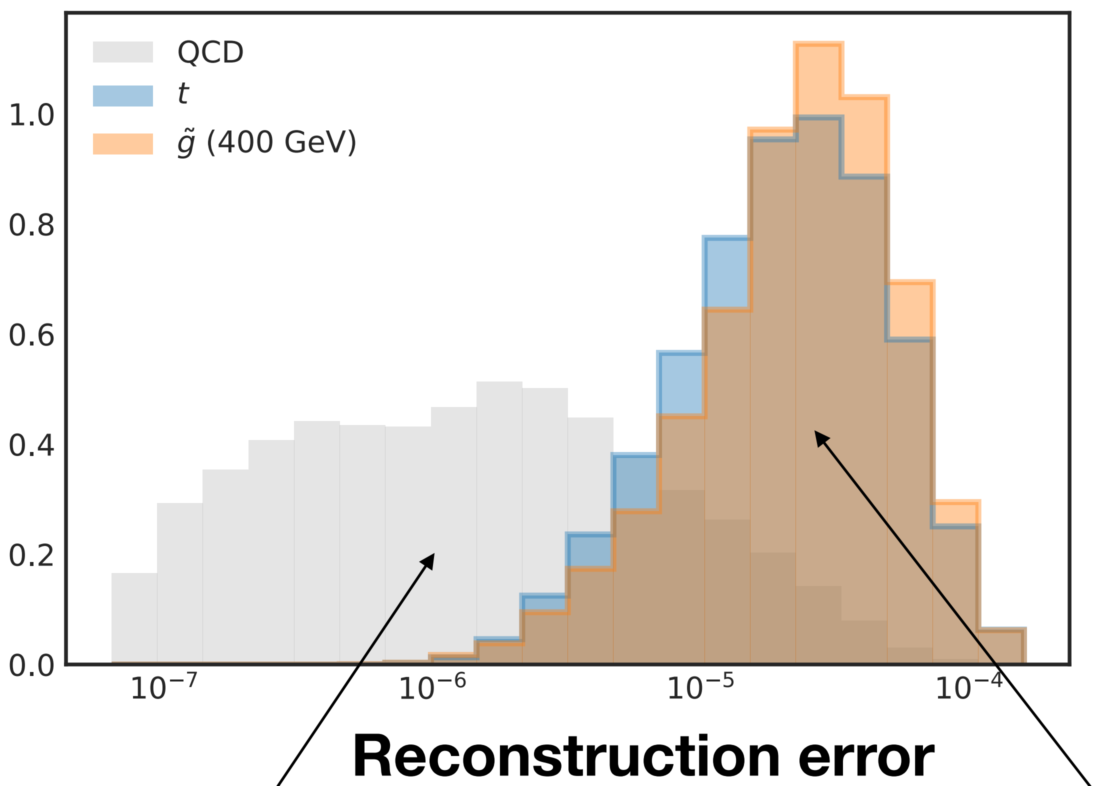
MP2 : max pooling with a 2x2 reduction factor

US2 : up sampling with a 2x2 expansion factor

Weakly-supervised mode

Weakly-supervised case with <u>pure</u> background events for training.

Convolutional autoencoder

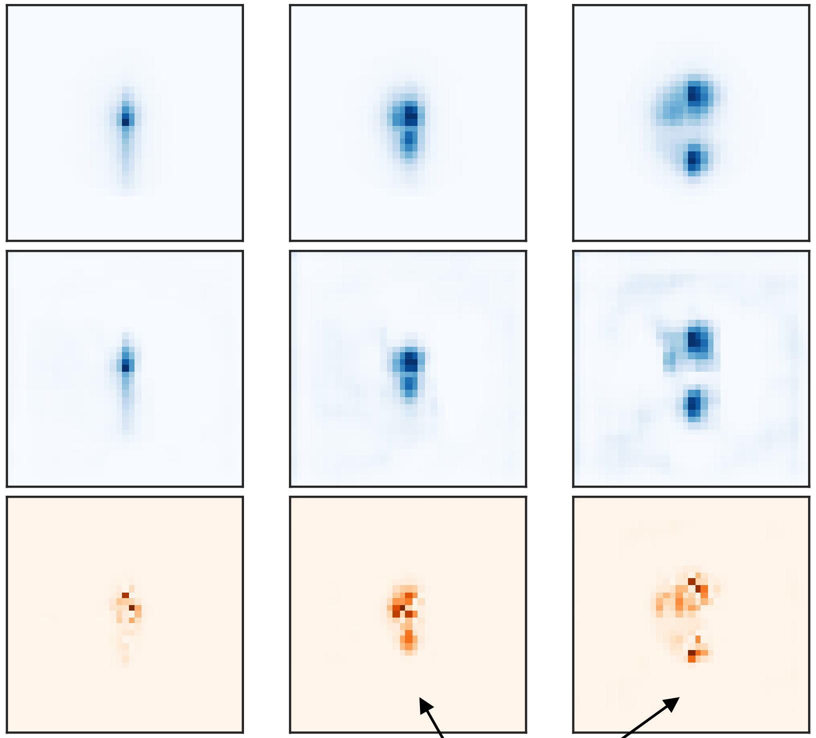


Average images QCD Top Gluino

Inputs

Outputs

Pixel-wise squared error



Autoencoder learns to reconstruct the QCD backgrounds.

More error

Autoencoder fails to reconstruct the signals.

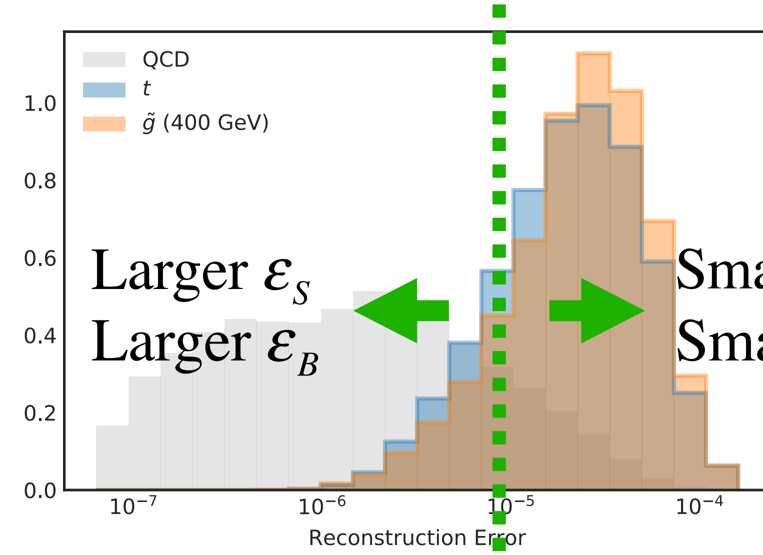
Reconstruction error is used as an anomaly threshold.

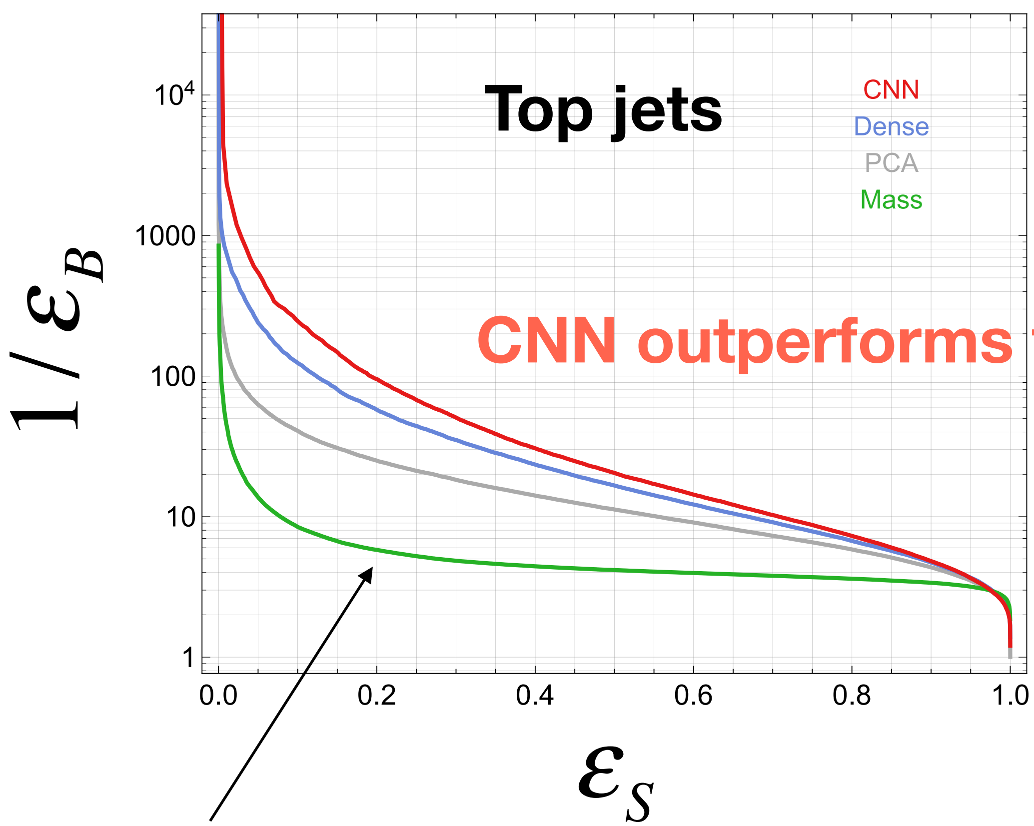
Autoencoder Performance

Performance measure :

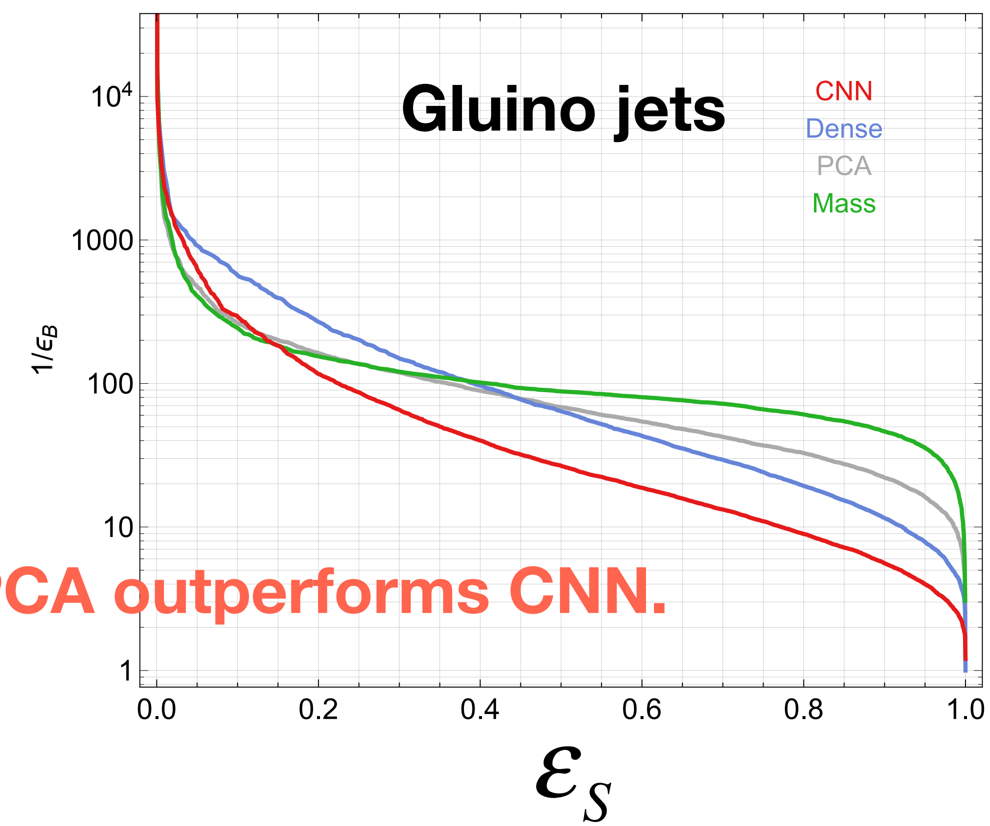
$$\varepsilon_S = \frac{\text{(Correctly classified into signals)}}{\text{(Total number of signal jets)}}$$

$$\varepsilon_B = \frac{\text{(Misclassified into signals)}}{\text{(Total number of backgrounds)}}$$





CNN outperforms the others.



PCA outperforms CNN.

Jet mass as anomaly threshold

PCA and Dense curves approach jet mass curve, suggesting <u>their reconstruction errors are highly correlated with jet mass</u>.

Choosing Latent Dimension k

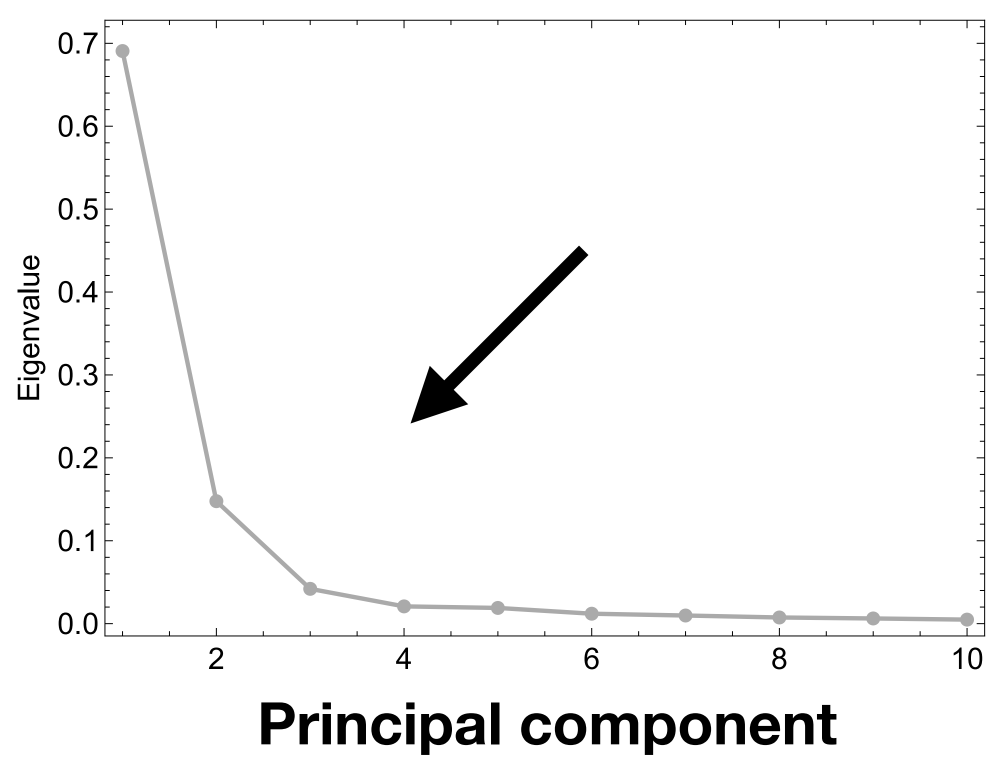
Too small k ➡ Autoencoder cannot capture all the features.

Too large k ➡ Autoencoder approaches trivial representation.

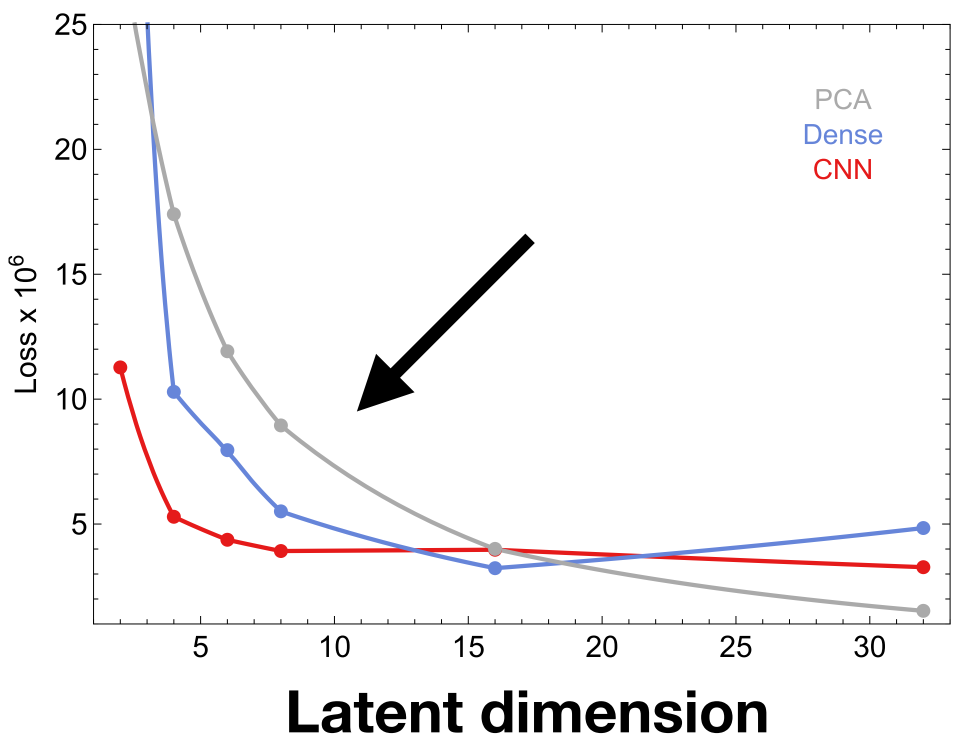
Optimizing latent dimension using a specific signal is **NOT** a good idea.

Instead, we examine PCA eigenvalues or reconstruction error vs latent dimension and look at where they are saturated.

Amount of variance ("scree plot") :



Reconstruction error :



We choose k = 6.

Robustness with Other Monte Carlo

Autoencoder really does not learn artifacts special to a Monte Carlo?

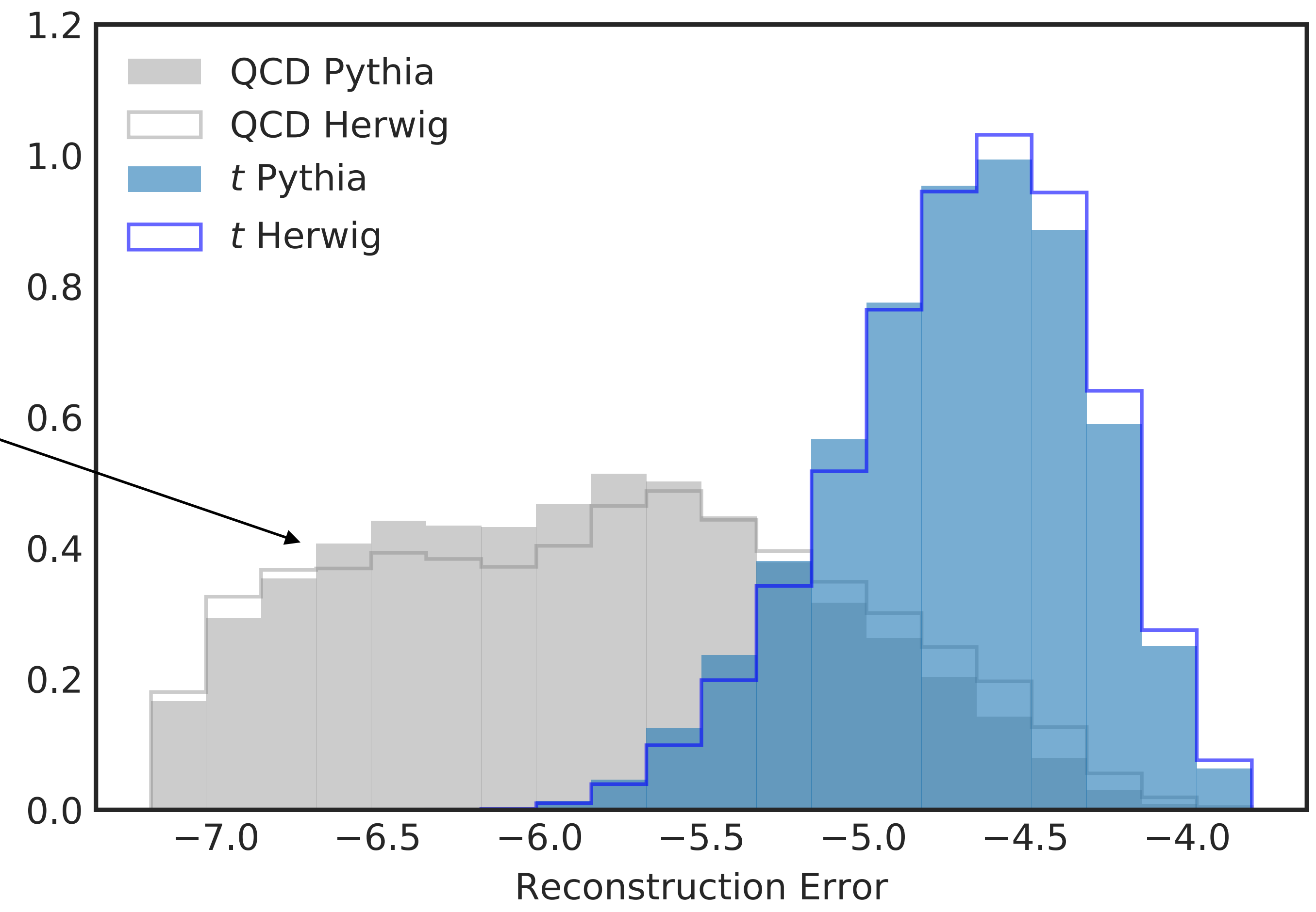
One possible check :

Evaluate autoencoder (trained on PYTHIA samples) on jet samples produced with HERWIG.

Comparison of reconstruction error (top jets, CNN)

The differences are small.

Separation between background and anomaly is preserved.



Autoencoder probably learns fundamental jet features.

Unsupervised Mode

A much more exciting possibility is…

Train autoencoder on actual data !

Actual data may contain some amount of signals.

Unsupervised Mode

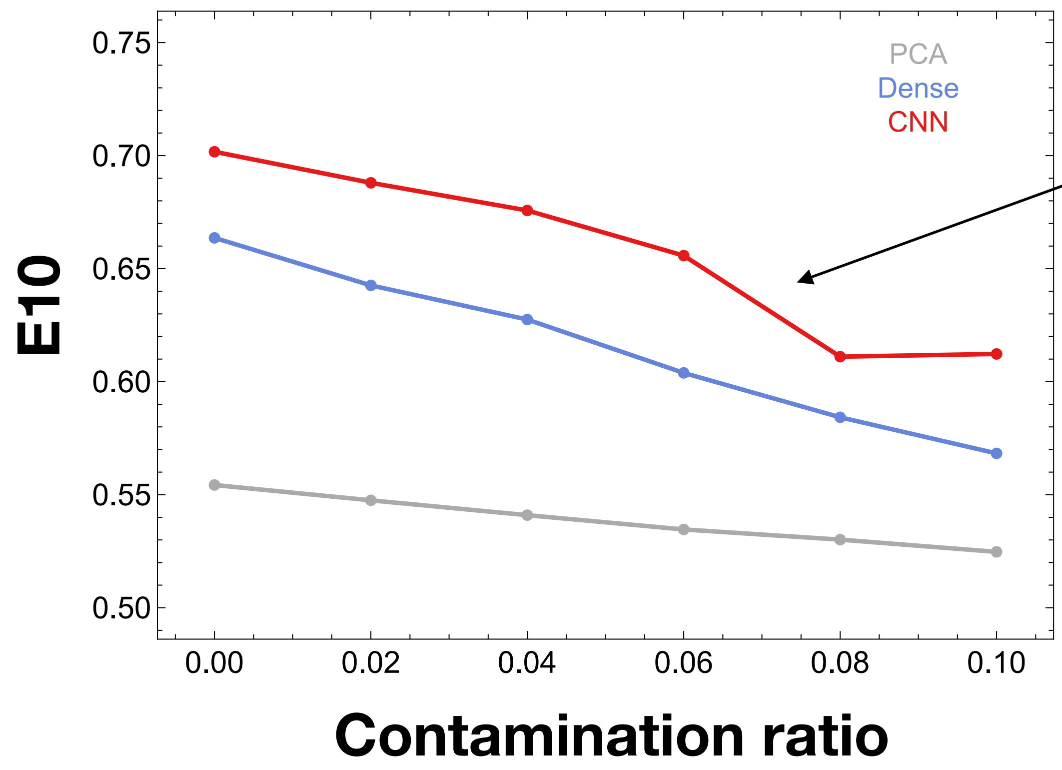
Train autoencoder on a sample of backgrounds <u>contaminated by a small fraction of signal events</u>.

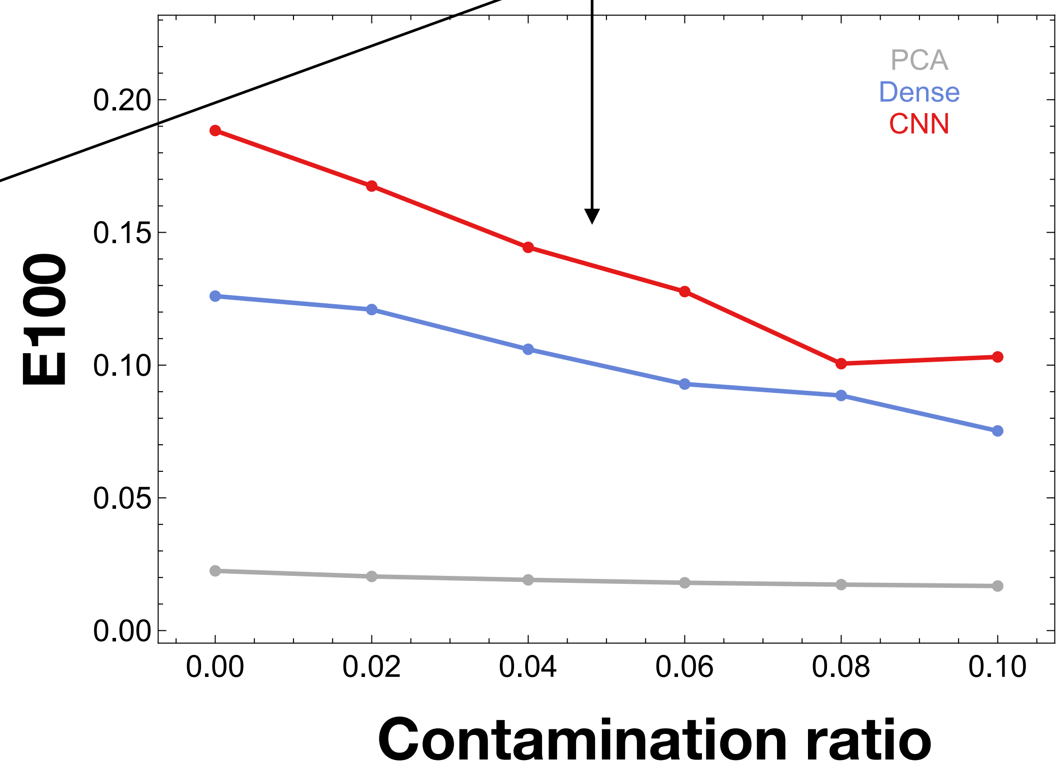
Autoencoder performance is remarkably stable against signal contamination.

$E_{10,\,100}$: the signal efficiency at 90% and 99% background rejection

Top jets for anomalous events

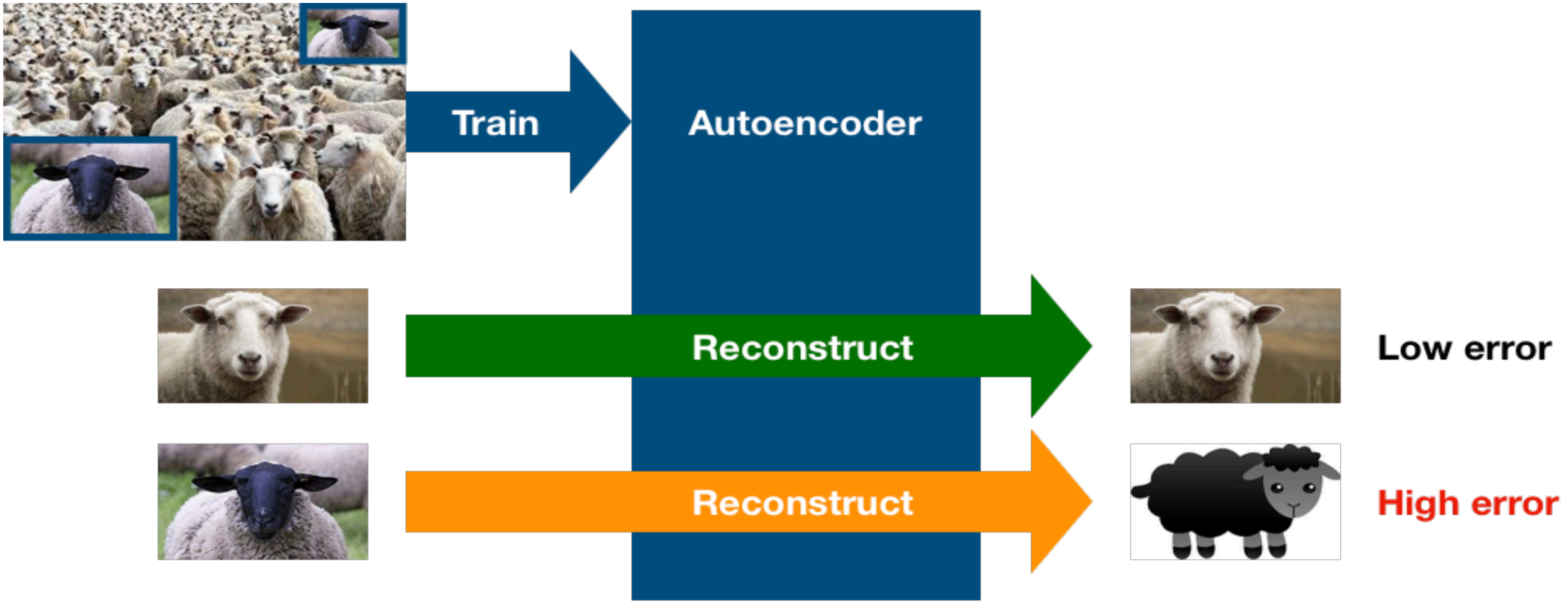
Reduction is not dramatic !





Unsupervised Mode

Autoencoder learns to preferentially reconstruct backgrounds and still poorly reconstructs signals.



Autoencoder could be trained directly on data and then could potentially discover anomalies in backgrounds.

Correlation with Jet Mass

In actual new physics searches, we look for subtle signals…

It's more powerful to combine autoencoder with another variable such as <u>jet mass</u>.

Cut hard on reconstruction error to clean out the QCD background and look for a bump in jet mass distribution.

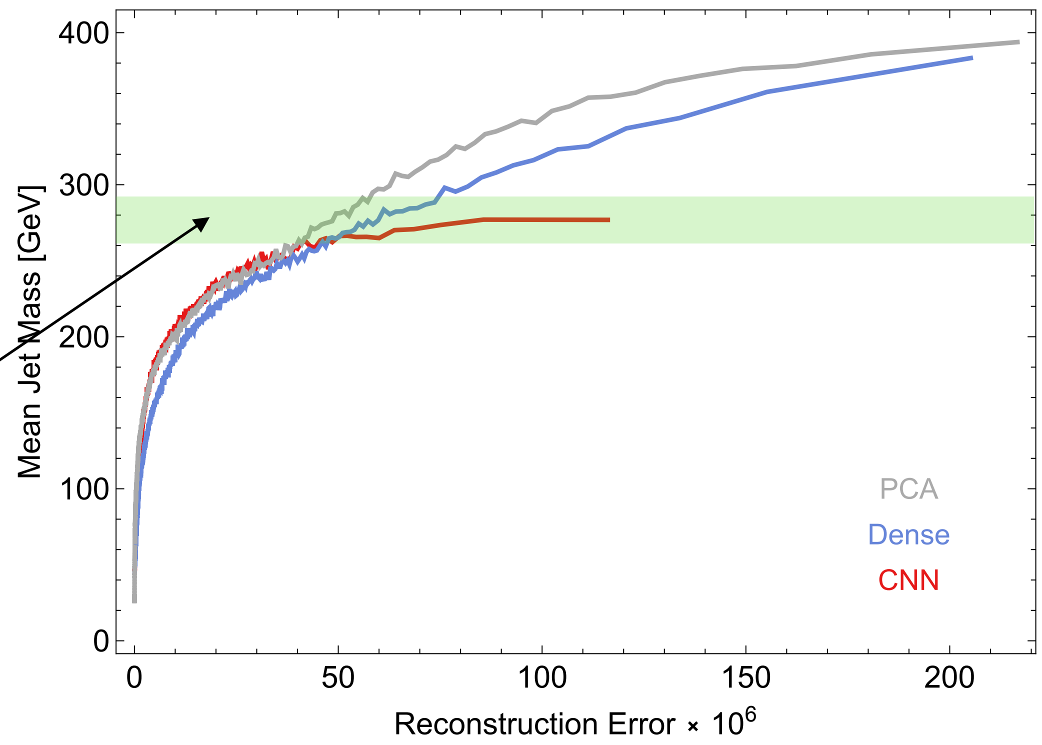
Reconstruction error should not be correlated with jet mass.

Correlation with Jet Mass

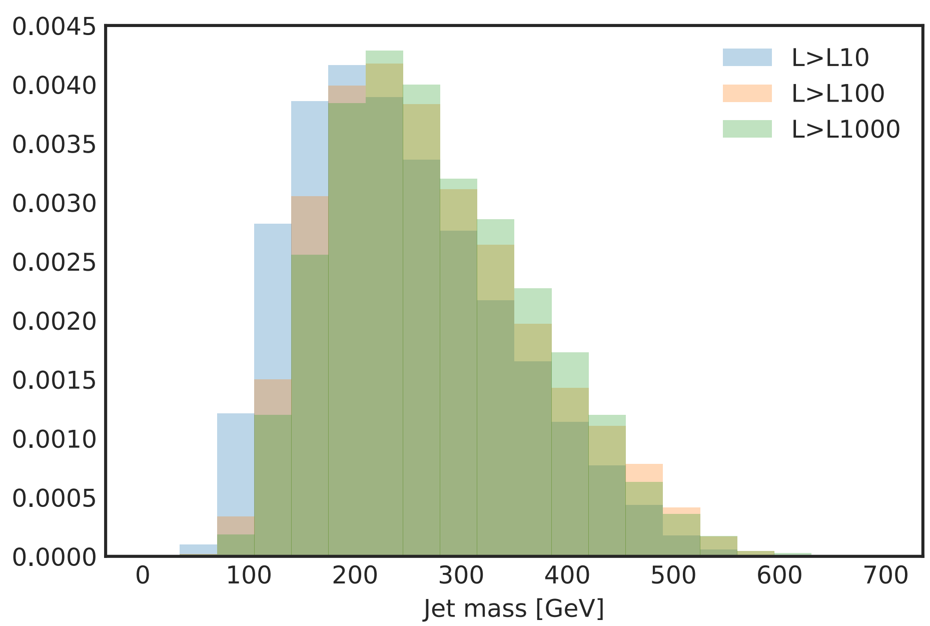
- **Mean jet mass in bins of reco error for the QCD background**

✓ For PCA and dense, reco error is correlated with jet mass.

✓ Jet mass distribution is stable against cutting on CNN loss.



- **Jet mass distributions after cuts on CNN loss**



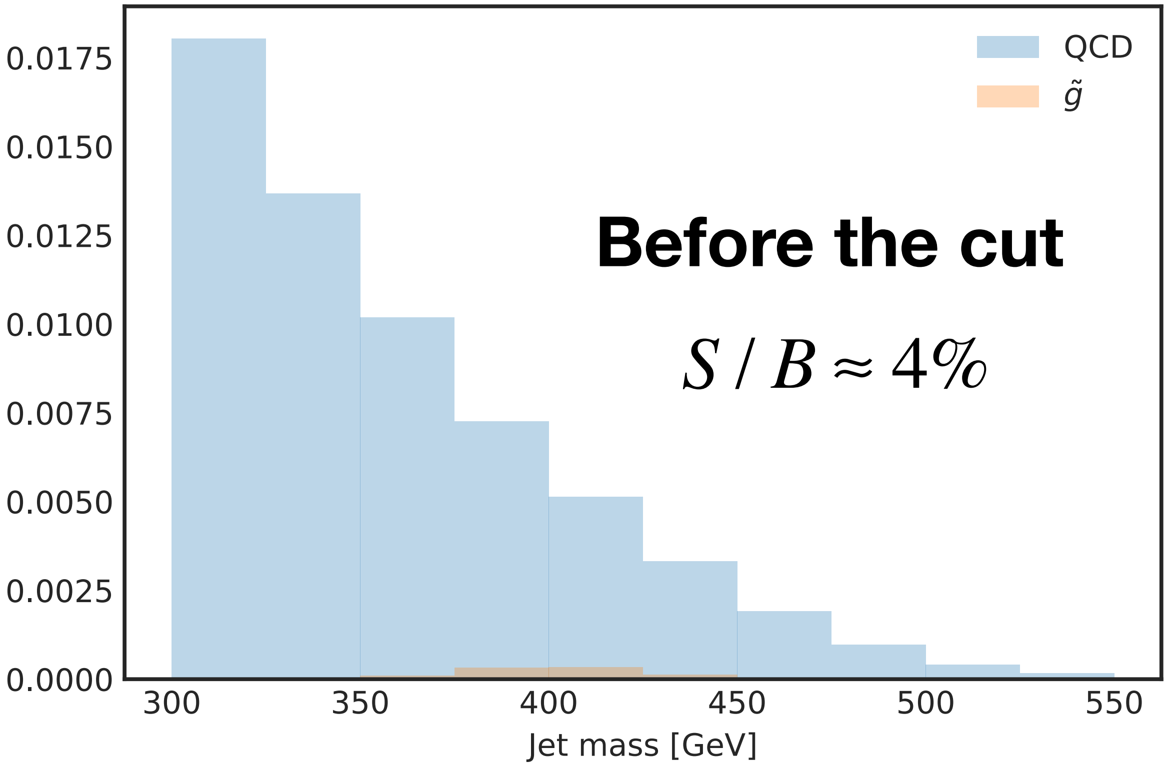
Reduce the QCD background by a factor of 10, 100 and 1000.

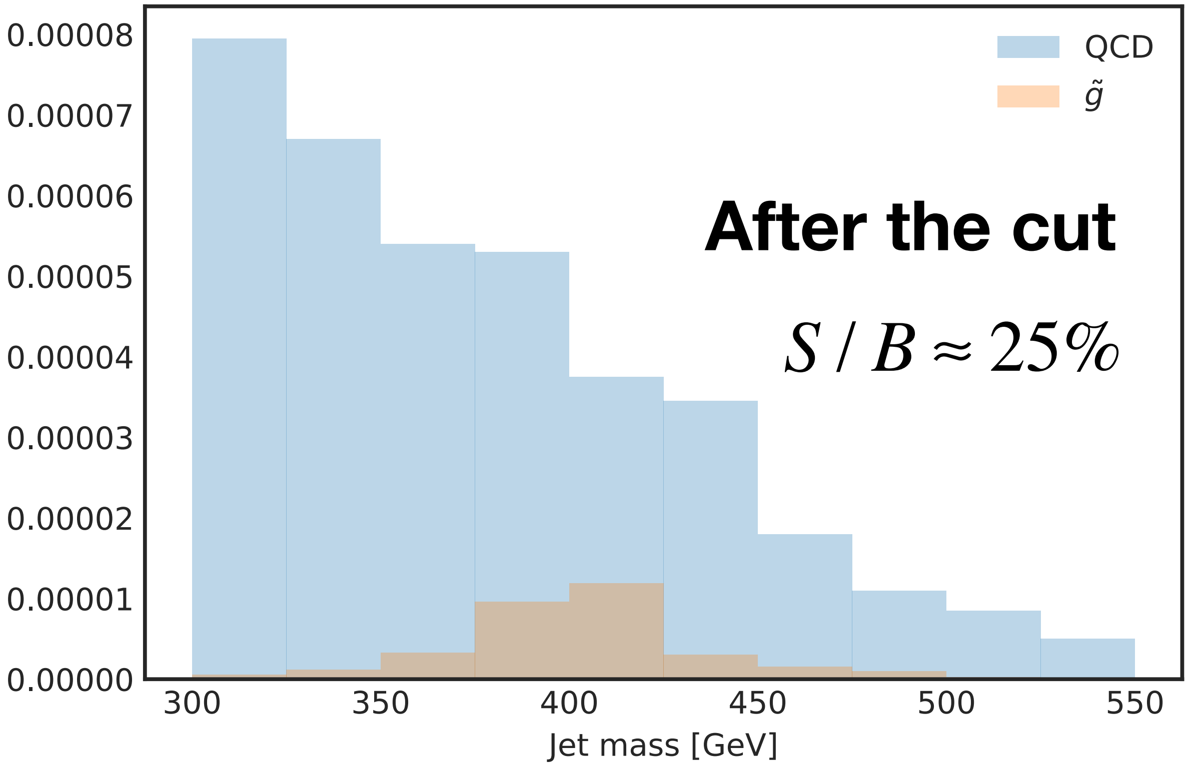
Convolutional autoencoder is useful for a bump hunt in jet mass above 300 GeV.

Bump Hunt

Thresholding on reconstruction error gives a significant improvement of S/B.

Jet mass histograms
(normalized to LO gluino and QCD cross sections)





One could plausibly discover new physics this way !

Summary

- ✓ Autoencoder learns to map background events back to themselves but fails to reconstruct signals that it has never encountered before.
- ✓ Reconstruction error is used as an anomaly threshold.
- ✓ Autoencoder performance is stable against signal contamination which enables us to train autoencoder on actual data.
- ✓ Jet mass distribution is stable against cutting on CNN loss and convolutional autoencoder is useful for a bump hunt in jet mass.
- ✓ Thresholding on reco error gives a significant improvement of S/B.

Thank you.