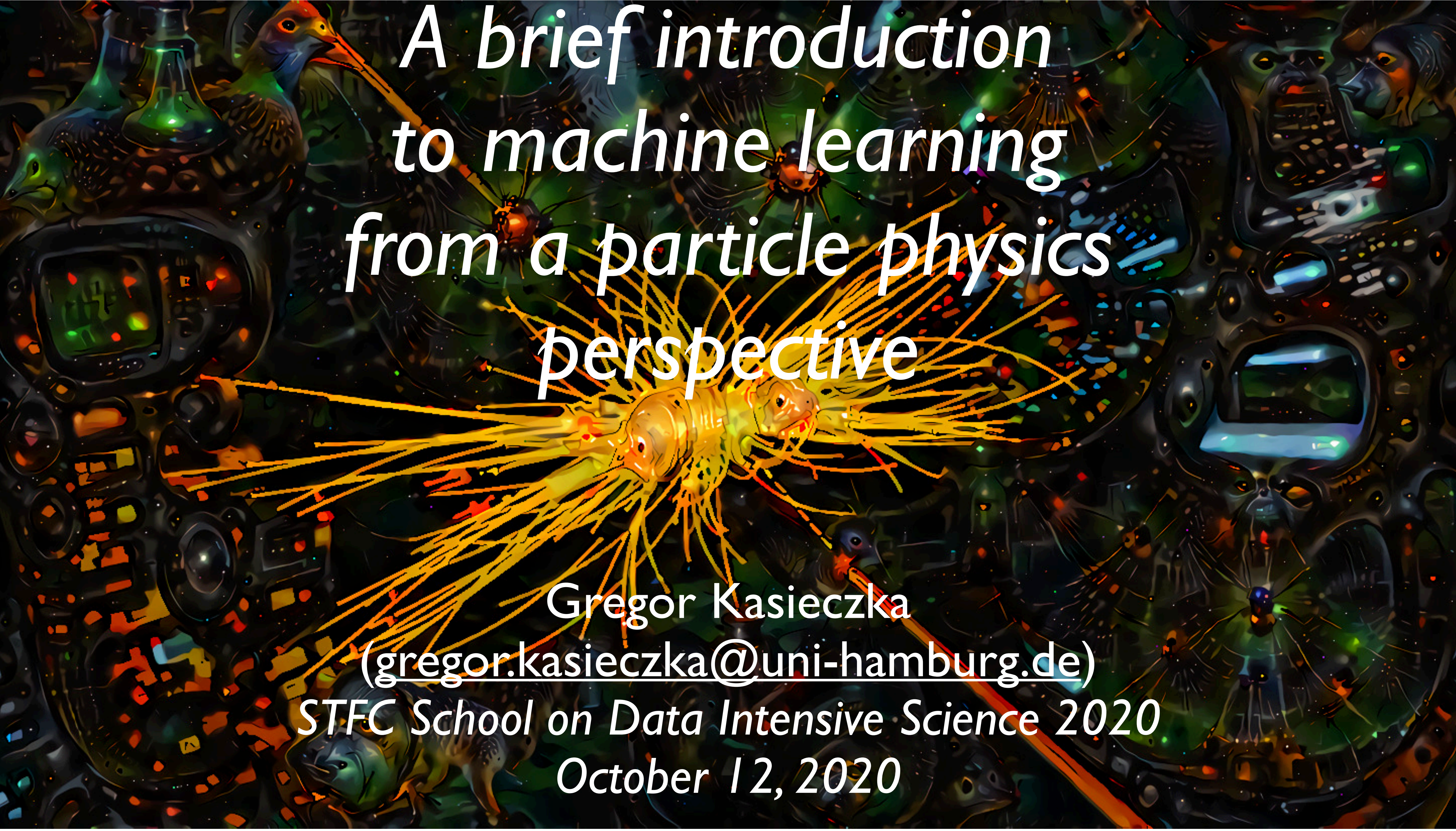

# A brief introduction to machine learning from a particle physics perspective

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*October 12, 2020*

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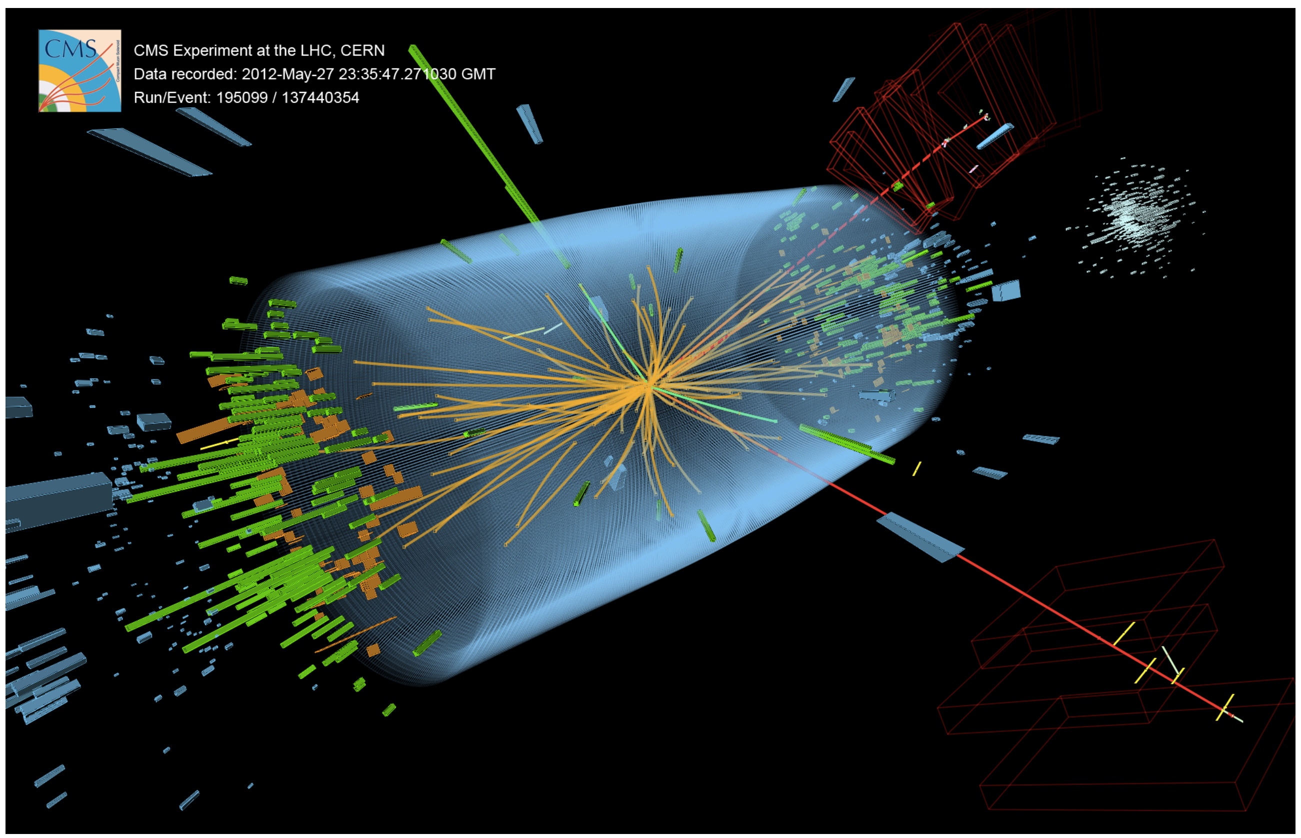
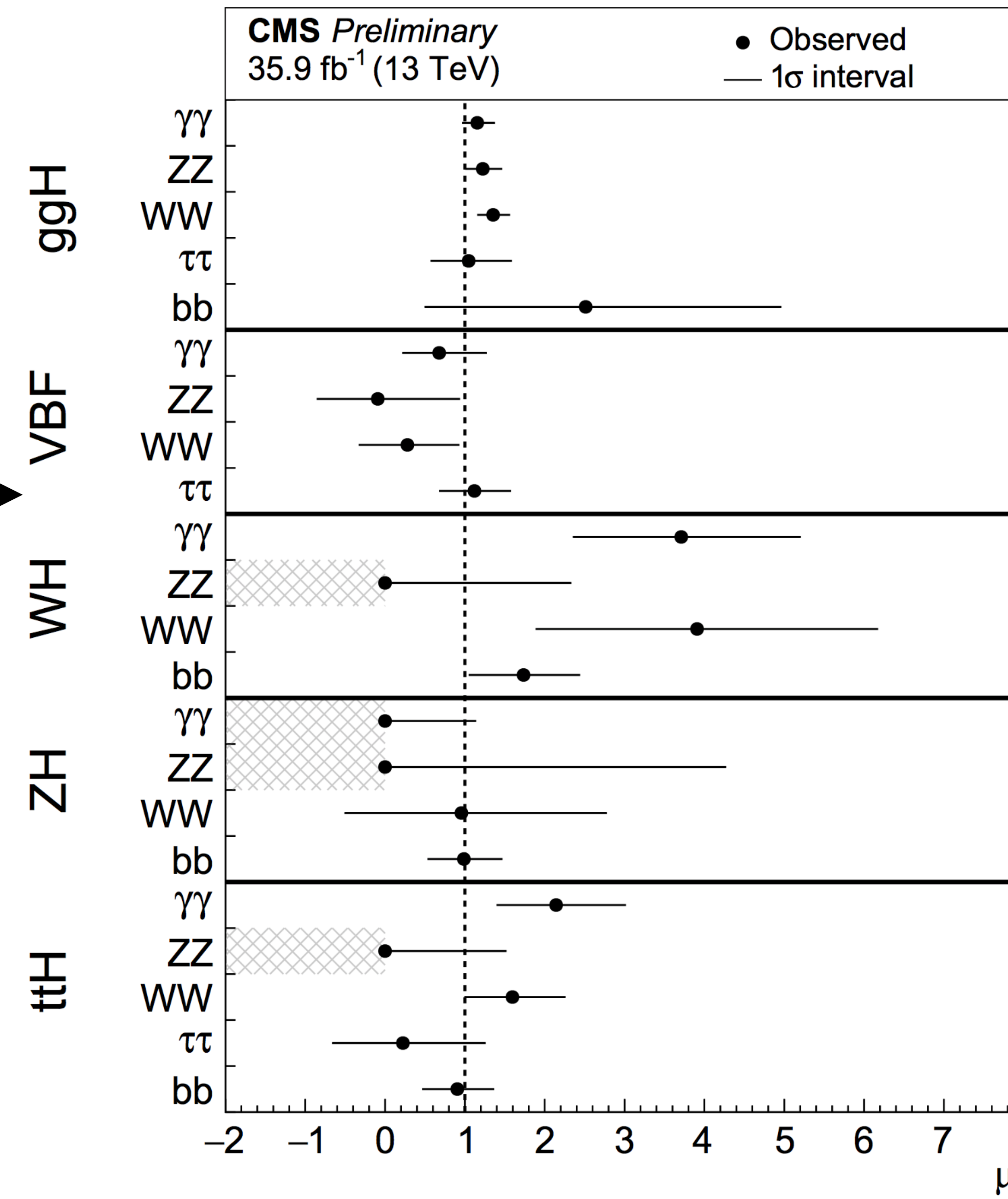
# Higgs Boson: Discovery to Precision…

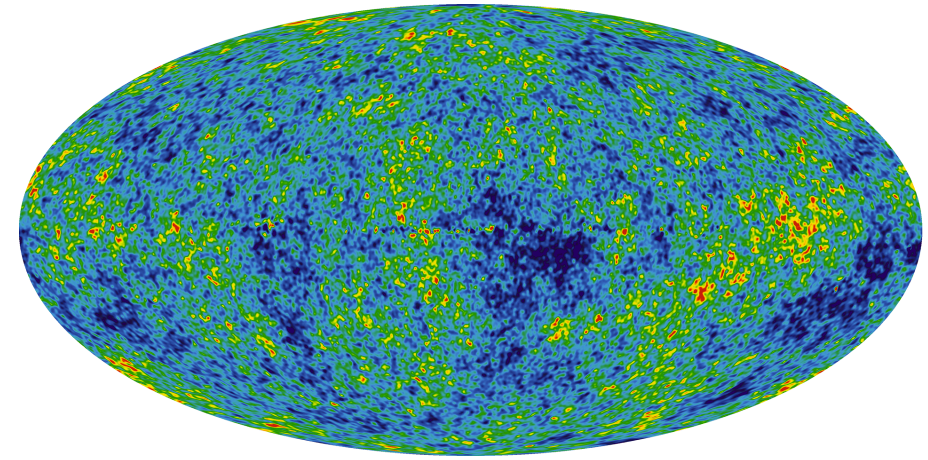



***2012: Discovery of the Higgs boson***

Now

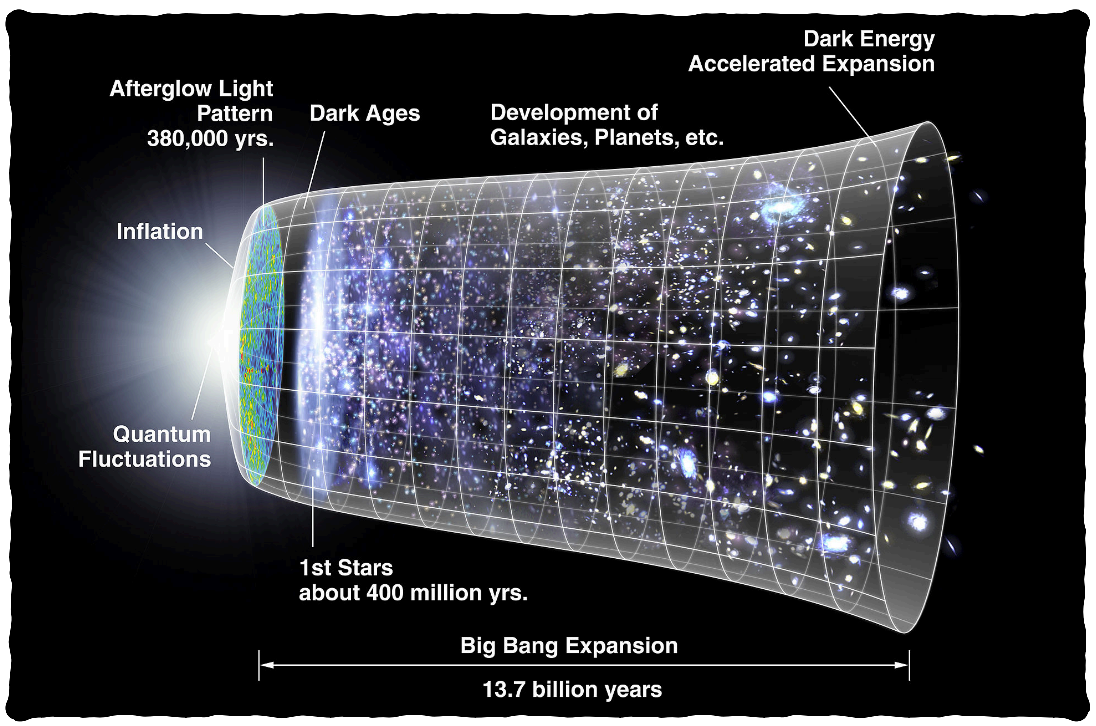


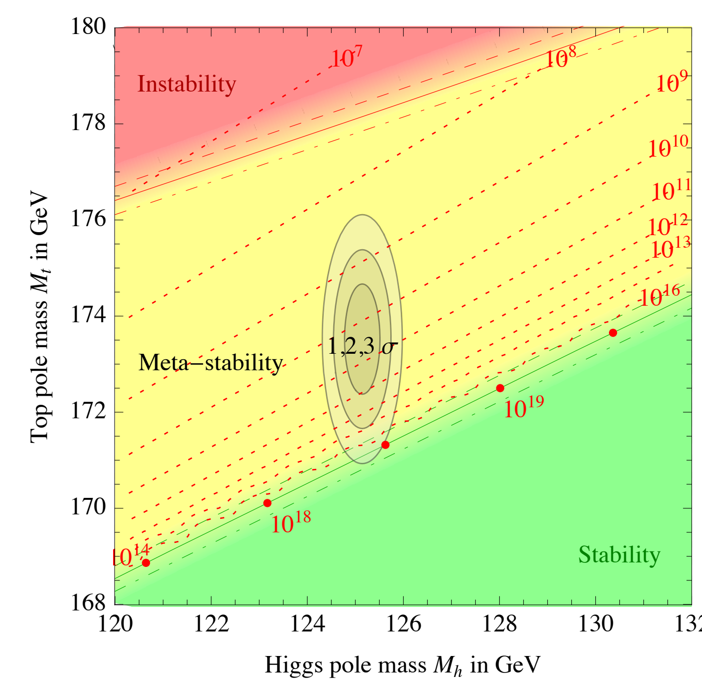
**Why are neutrinos massive?**



**What are the origins of the LHCb flavour anomaly?**

**What is the nature of dark matter & dark energy?**



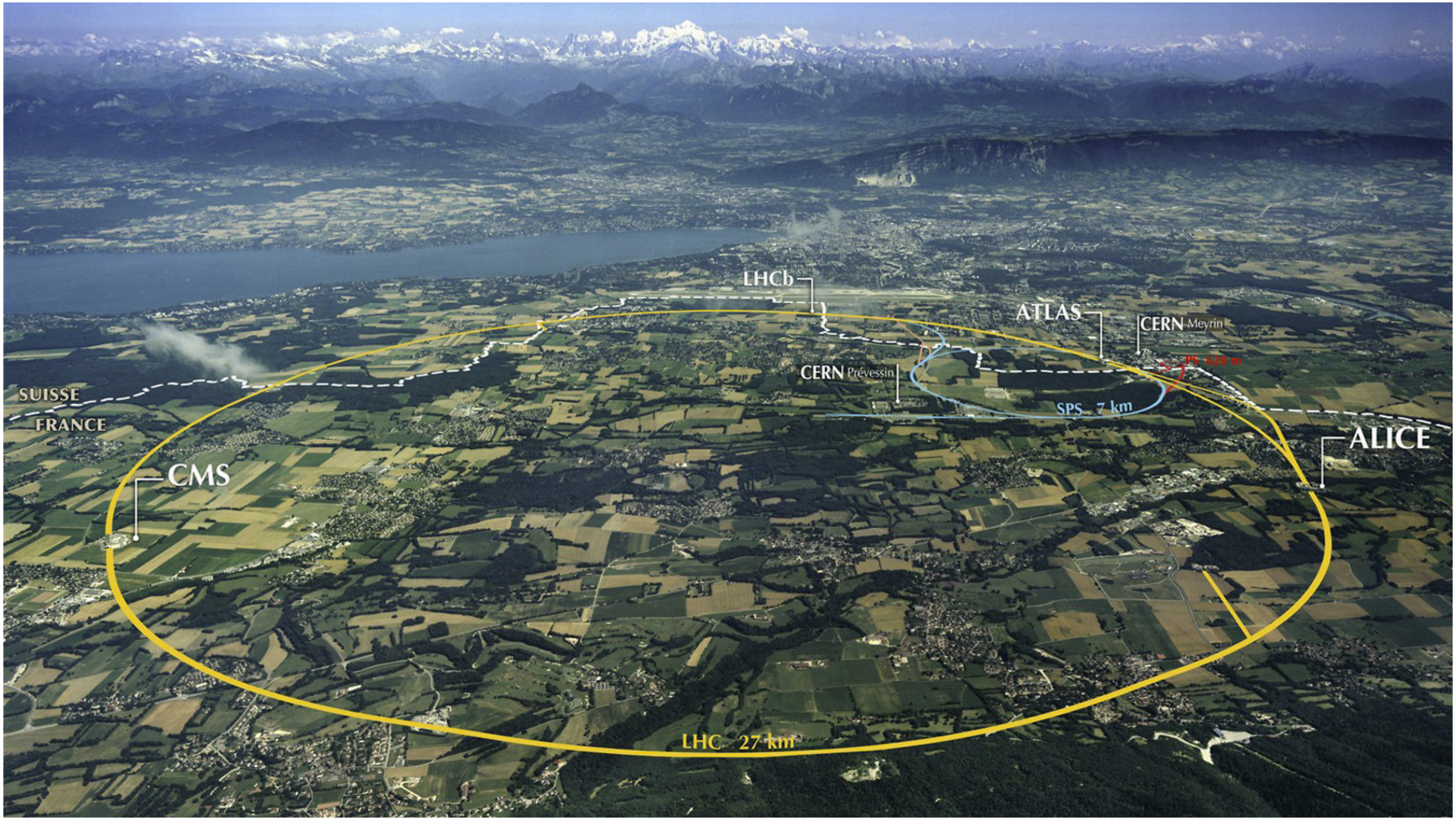




**Is the electroweak vacuum stable?**

**Why is there more matter than anti-matter?**

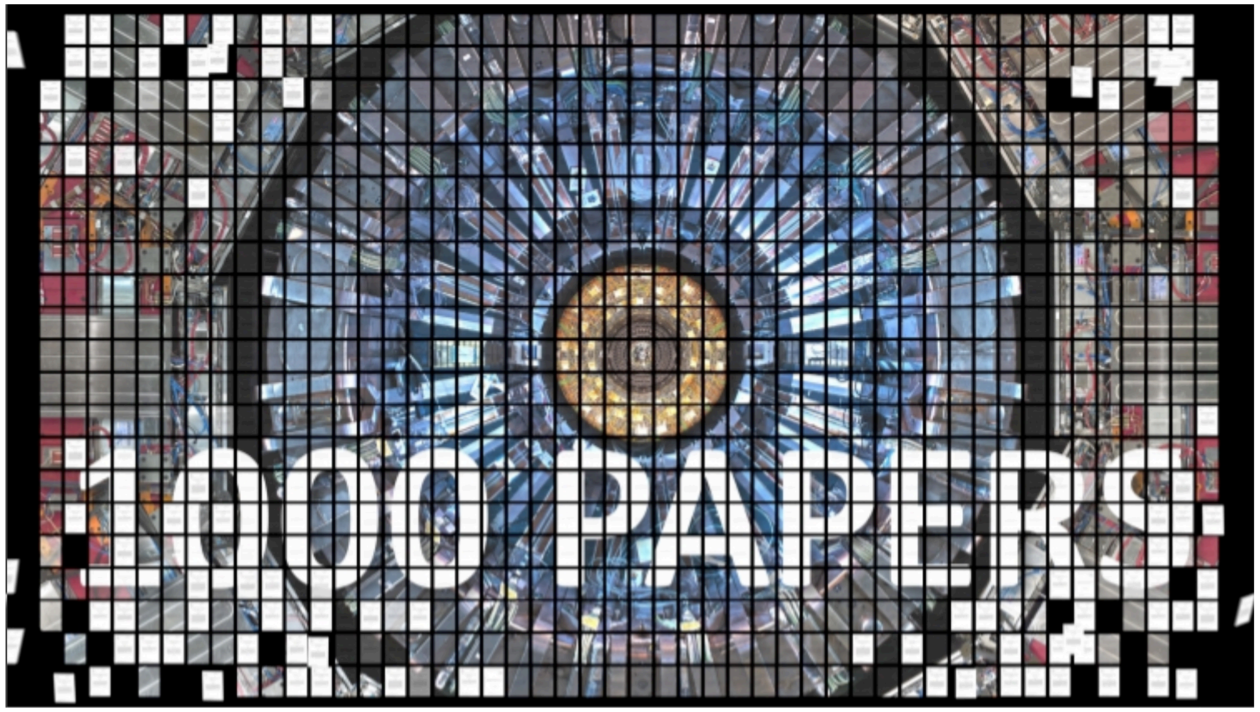
**How can the Higgs boson be light when the mass receives large quantum corrections?**

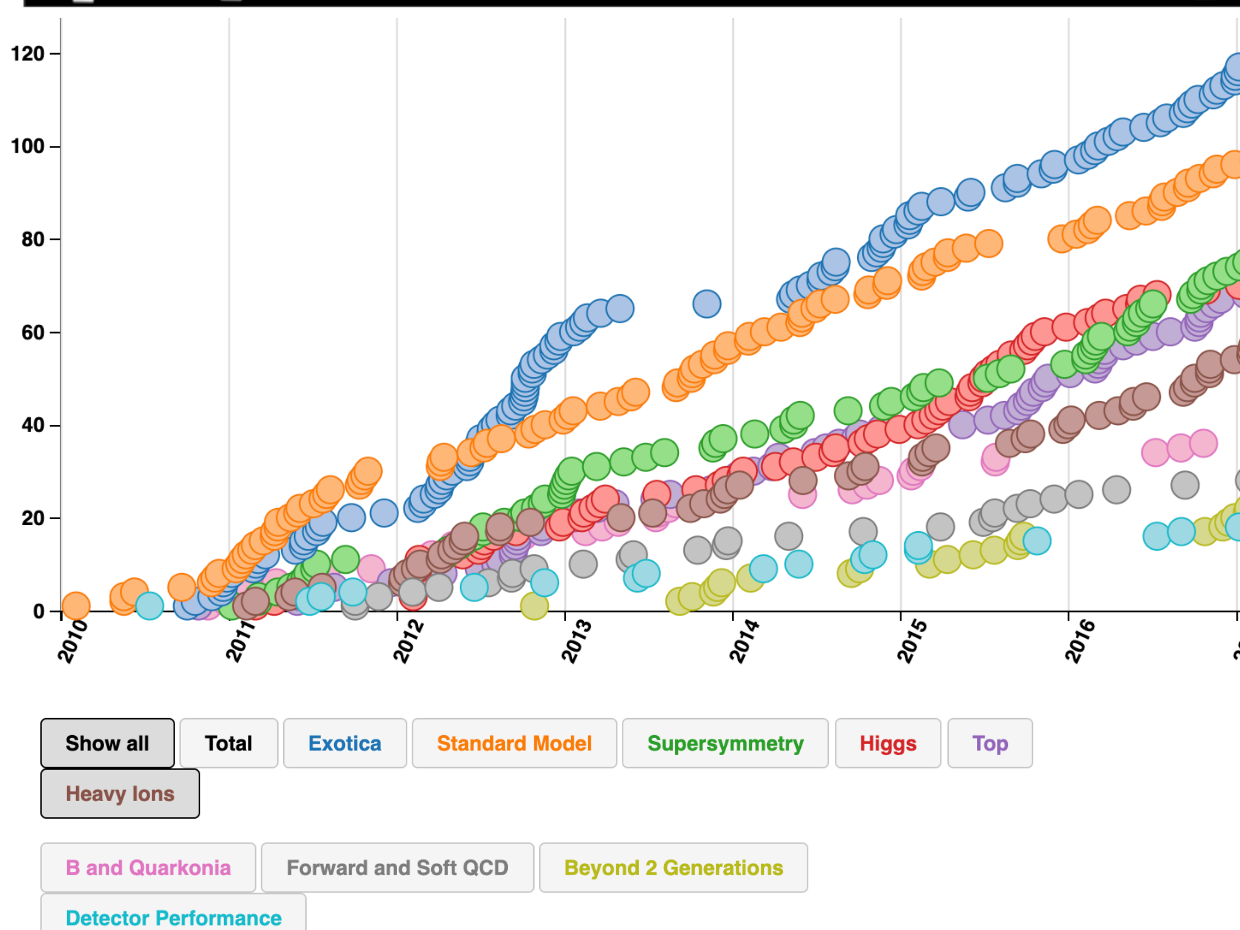
**What are the details of cosmic inflation?**



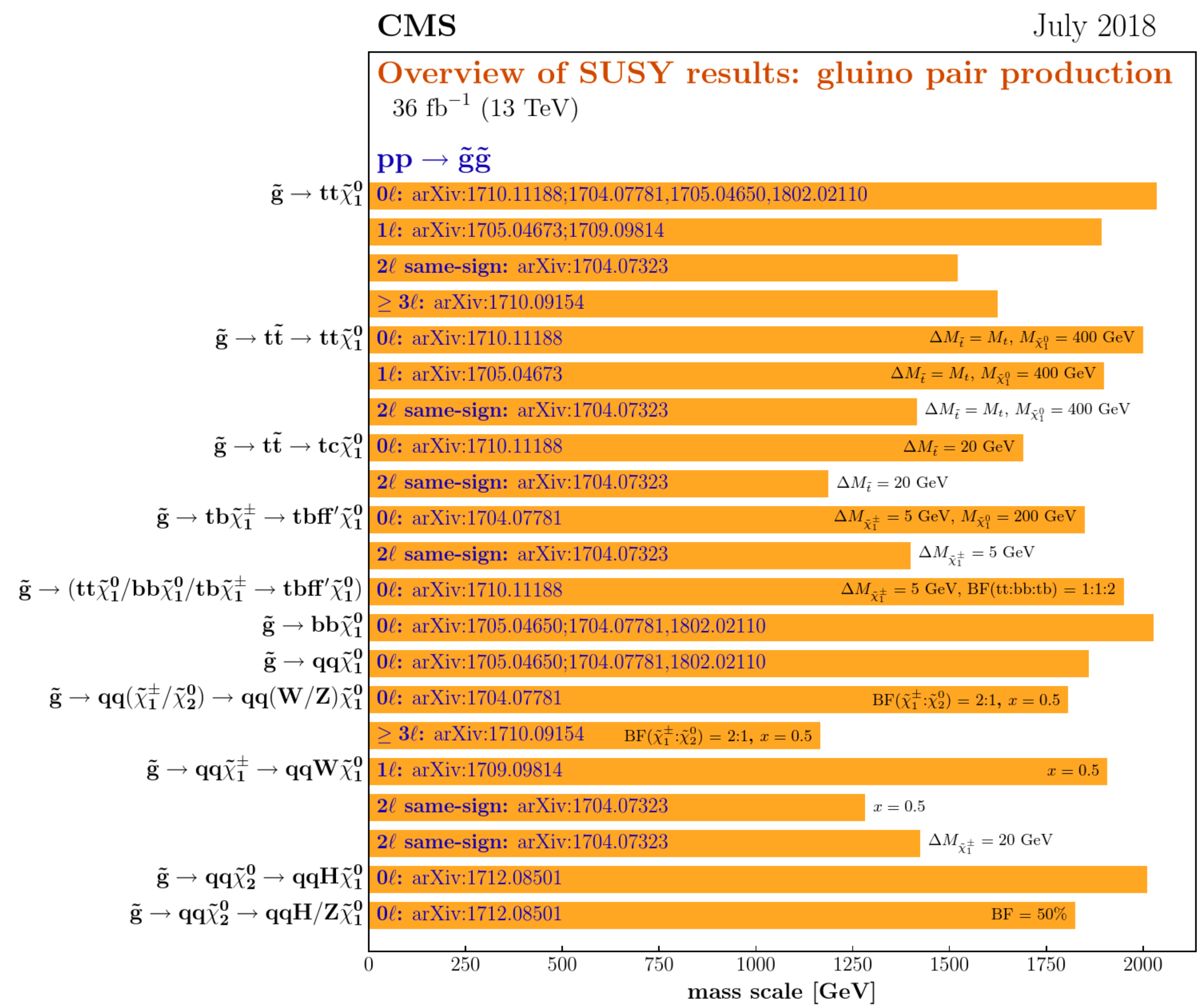

- *LHC: 27 km circumference*
- *Collide protons with a centre-of-mass energy of 13 TeV (99.999999% of speed of light)*
- *40 Million collisions/second in ATLAS/CMS*
- *~25 Petabyte collision data/year / experiment*
- *Planned High Luminosity Upgrade (HL-LHC)*
- *Higher data rate, higher pile-up*
  - *Big data challenges ahead!*
- *Begin operation O(2026)*

# Many results…




# …but no new physics so far



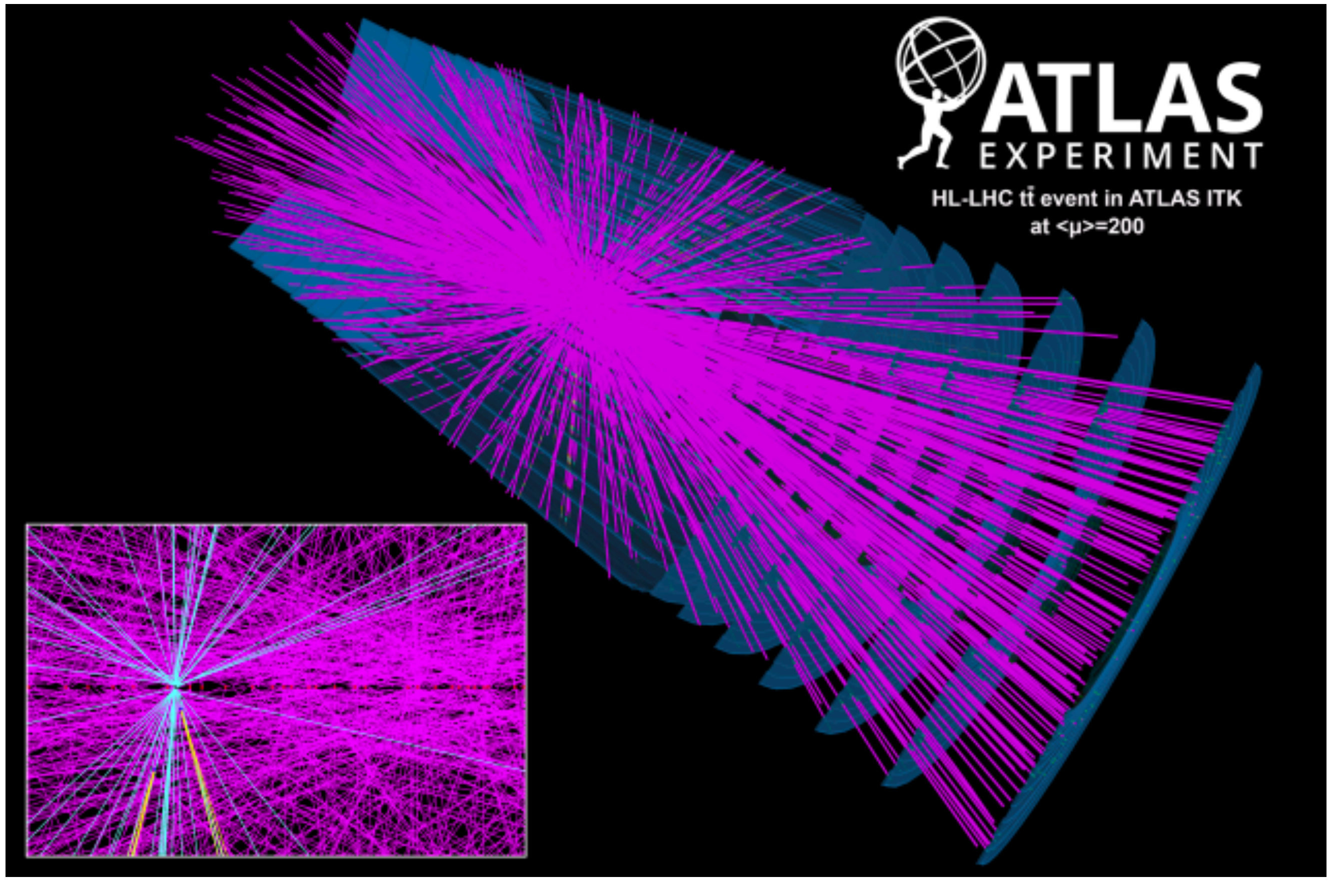

Selection of observed limits at 95% C.L. (theory uncertainties are not included). Probe **up to** the quoted mass limit for light LSPs unless stated otherwise. The quantities $\Delta M$ and $x$ represent the absolute mass difference between the primary sparticle and the LSP, and the difference between the intermediate sparticle and the LSP relative to $\Delta M$, respectively, unless indicated otherwise.

**http://cms.web.cern.ch/org/physics-papers-timeline**

# Why?

- Precision measurements and searches for new physics need
  - better tools to identify and measure particles and processes
  - higher accuracy and speed
- Finding unknown signatures and measurements need
  - new ways of analysing data
- Future data taking with higher collision rates needs:
  - faster reconstruction and triggering
  - faster event generation and detector simulation

(a) promising answer: **Deep Learning**

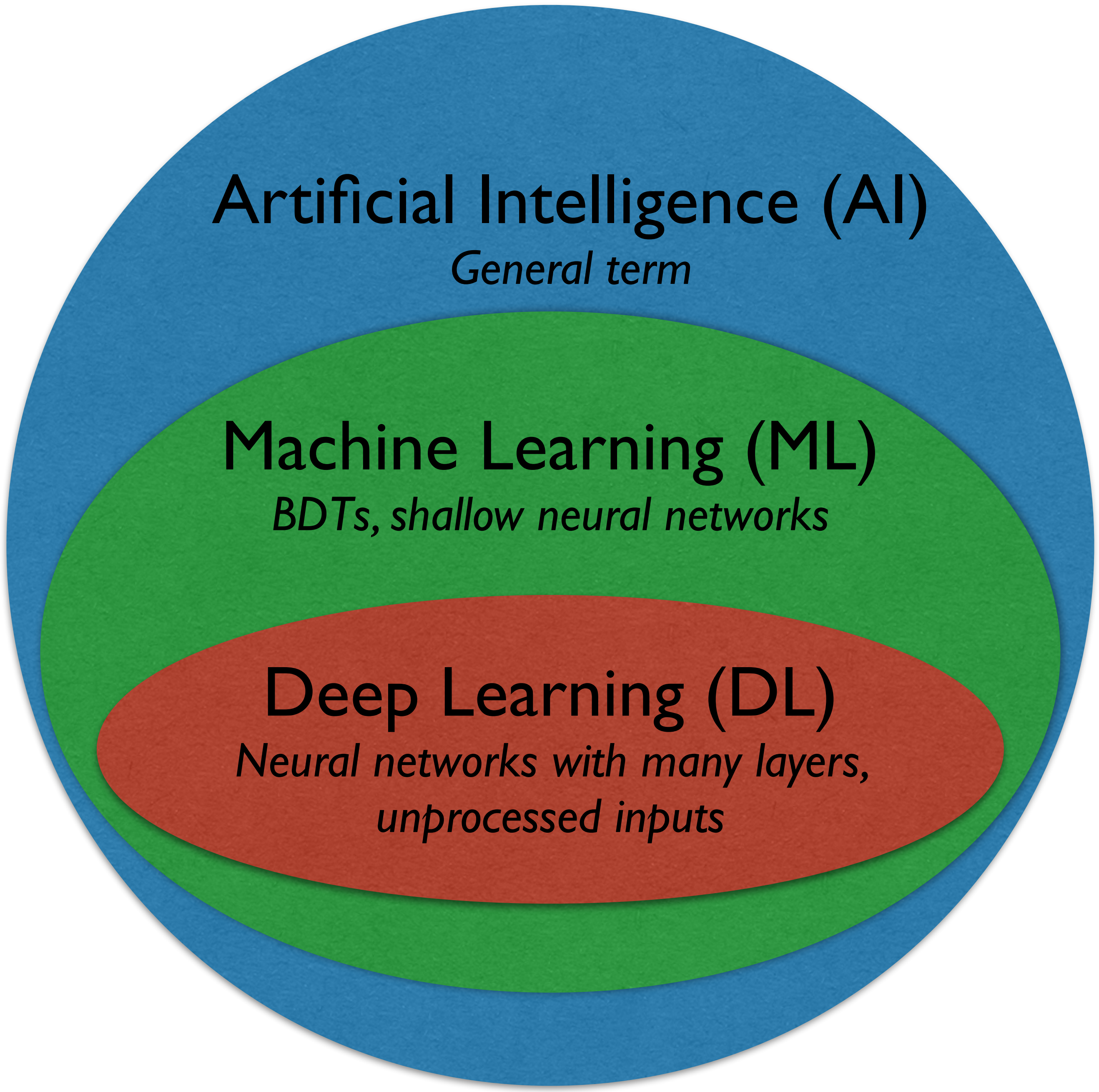


# Program

- The basics
- Supervised particle tagging & architectures
- Generative models
- Unsupervised searches
- Some final words

# The basics

# Terminology

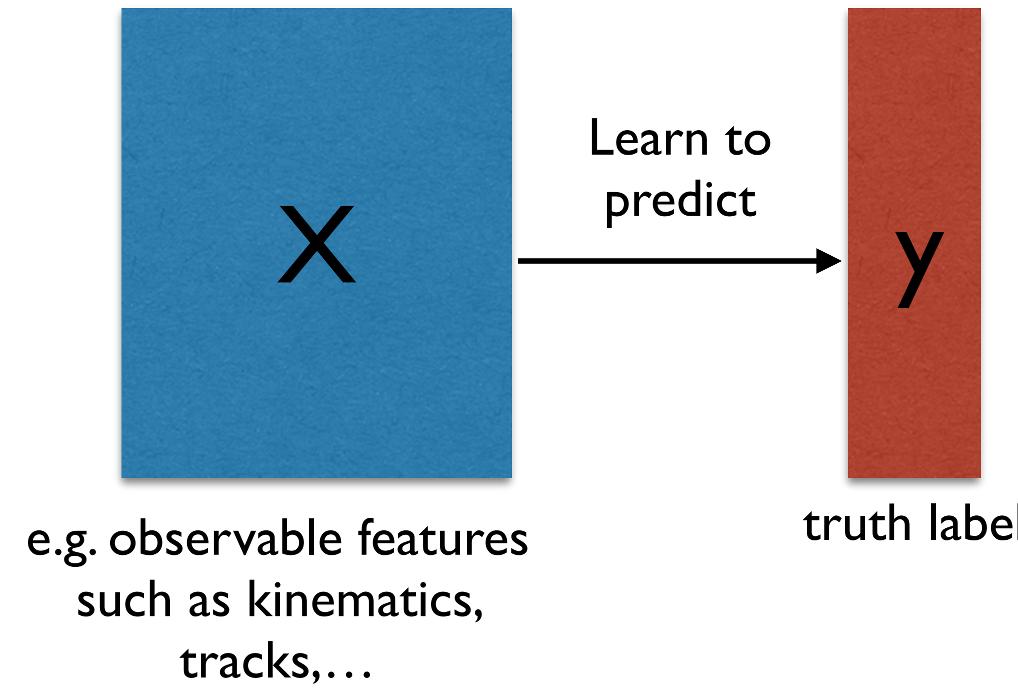


# Tasks

## Supervised Learning

**Attempt to infer some target *(truth label)*: classification (*jet flavour tagging*) or regression (*energy calibration*)**

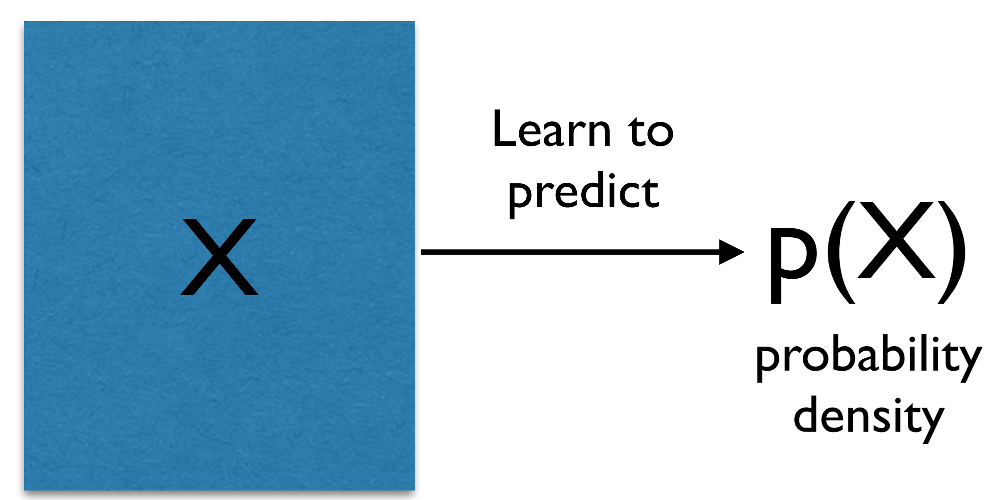
**Need training dataset with known labels (typically from MC simulation)**

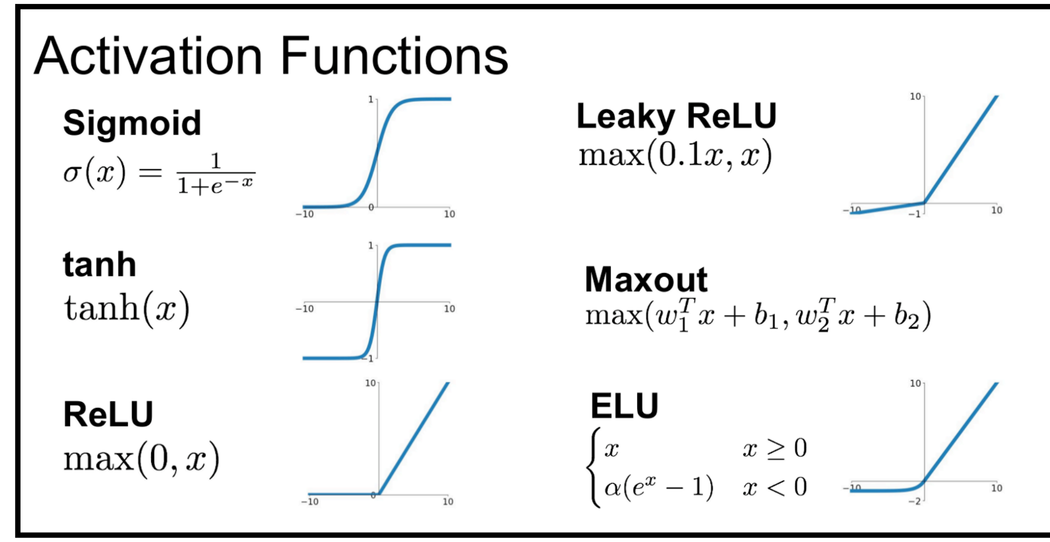


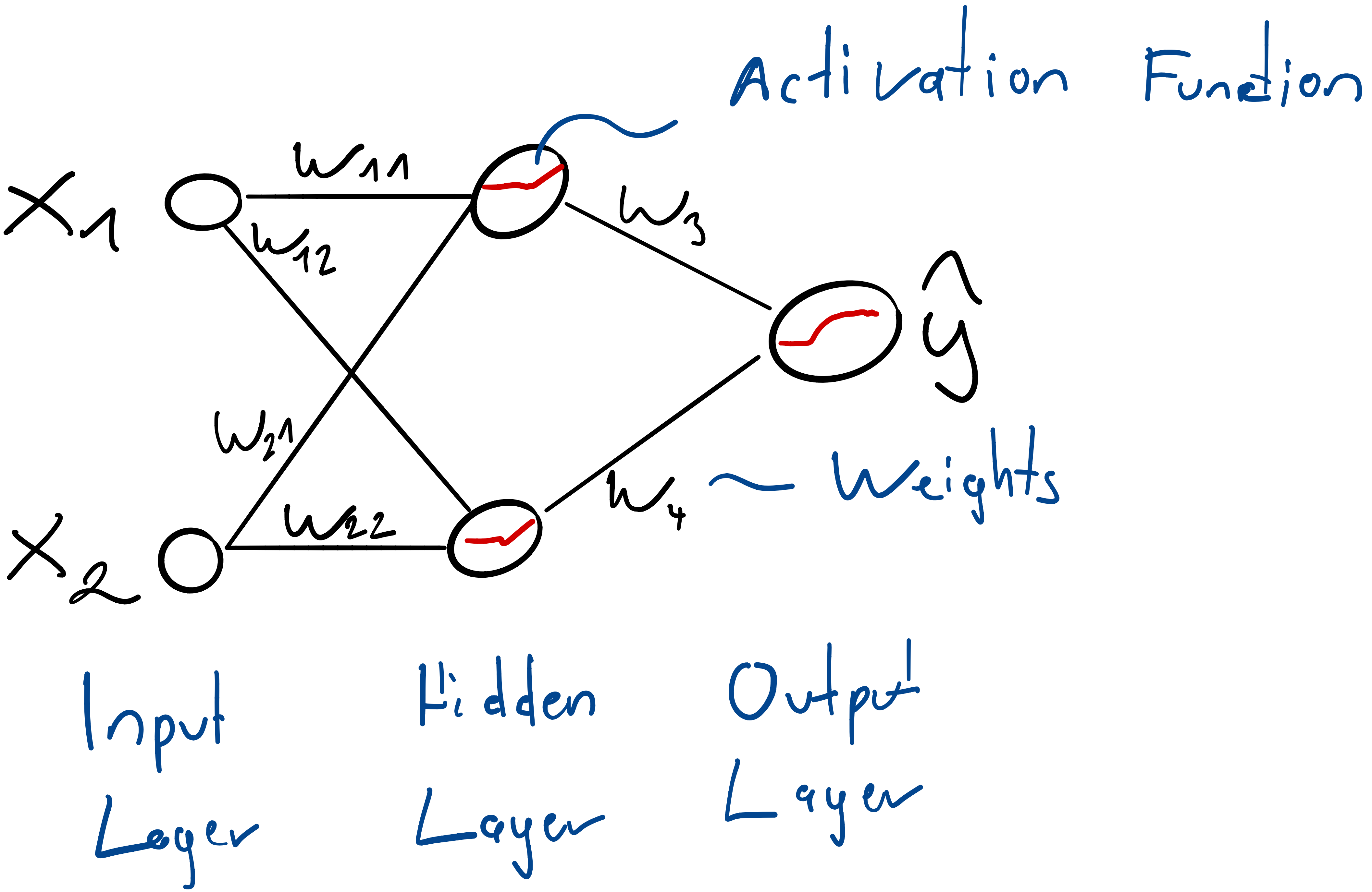

## Unsupervised

**No target, learn the probability distribution**

**Useful for generative models and anomaly detection.**




Activation Functions
Sigmoid
$\sigma(x) = \frac{1}{1+e^{-x}}$
Leaky ReLU
$\max(0.1x, x)$
tanh
$\tanh(x)$
Maxout
$\max(w_1^T x + b_1, w_2^T x + b_2)$
ReLU
$\max(0, x)$
ELU
$\begin{cases} x & x \geq 0 \\ \alpha(e^x - 1) & x < 0 \end{cases}$


Activation Function
$x_1$
$x_2$
$w_{11}$
$w_{12}$
$w_{21}$
$w_{22}$
$w_3$
$w_4$
$\hat{y}$
Weights
Input Layer
Hidden Layer
Output Layer

# How do networks learn?

- *Backpropagation + Gradient descent*
- Pass input ($x_1, x_2, \dots$) to networks
- From output ($\hat{y}$) and true value (y) calculate optimisation target (*loss function L*)
- For example: Mean Squared Error (MSE) for regression:

$$L(y, \hat{y}) = (y - \hat{y})^2$$

- Find gradient of loss function with respect to weights
- Use gradient to find new weights

$$w_{t+1} = w_t - \eta \frac{\partial L}{\partial w_t} \equiv w_t - \eta \nabla L(w_t)$$

*Learning rate*

- Practically, this is taken care of by an optimiser algorithm *(e.g. Adam as default)*

# Classification Loss

- Classification loss function: **Cross entropy** between true labels (p) and network output (q): $H(p,q) = -\sum p_i \ln q_i$

- Rewrite as: $$-\sum p_i \ln q_i = H(p) + D_{KL}(p||q)$$

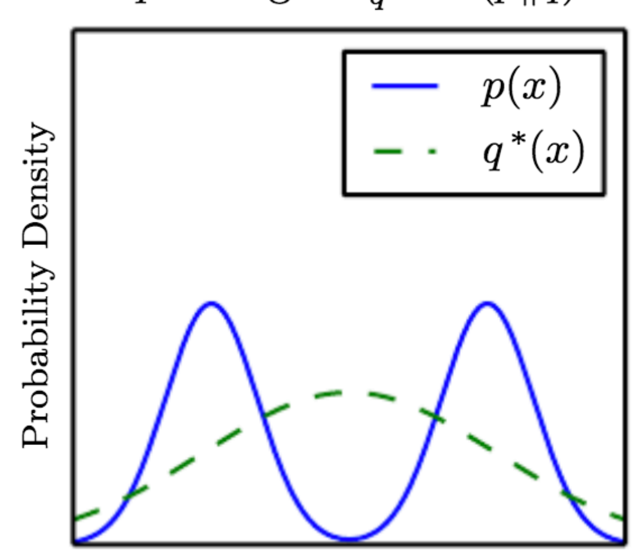
$$H(p) = -\sum p_i \ln p_i$$

- Entropy: *Average amount of information produced by measurements of random variable (Notice similarity to Gibbs entropy)*

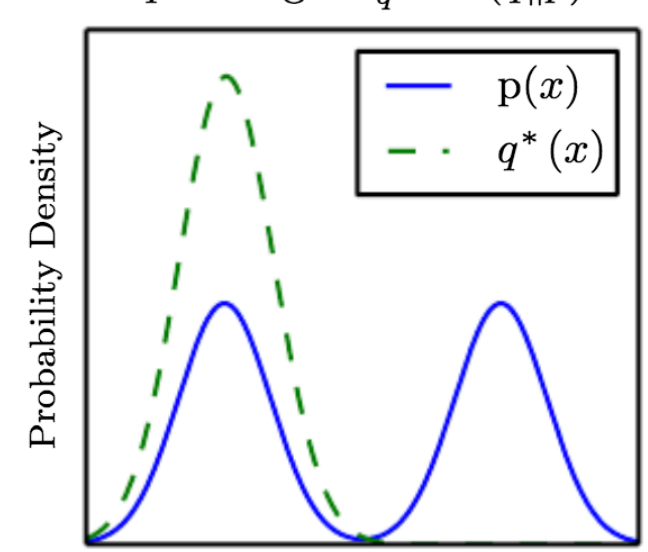
Kullback-Leibler Divergence:
(measure of difference between two distributions)

$$D_{\mathrm{KL}}(p||q) = -\sum p(i) \log \frac{q(i)}{p(i)}$$

$q^* = \mathrm{argmin}_q D_{\mathrm{KL}}(p||q)$

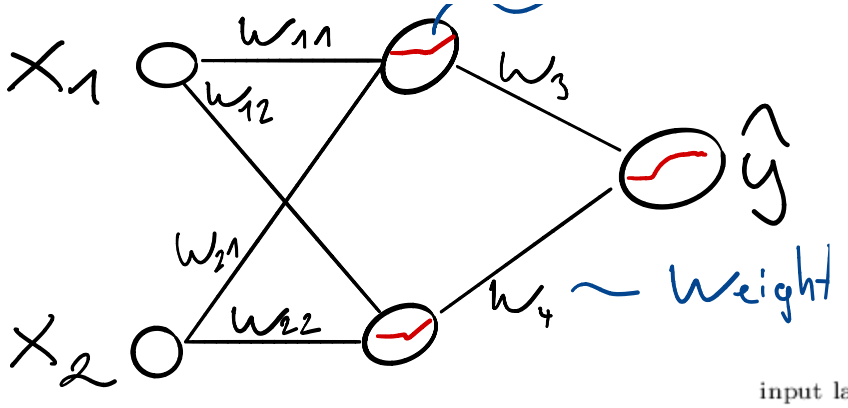



$q^* = \mathrm{argmin}_q D_{\mathrm{KL}}(q||p)$

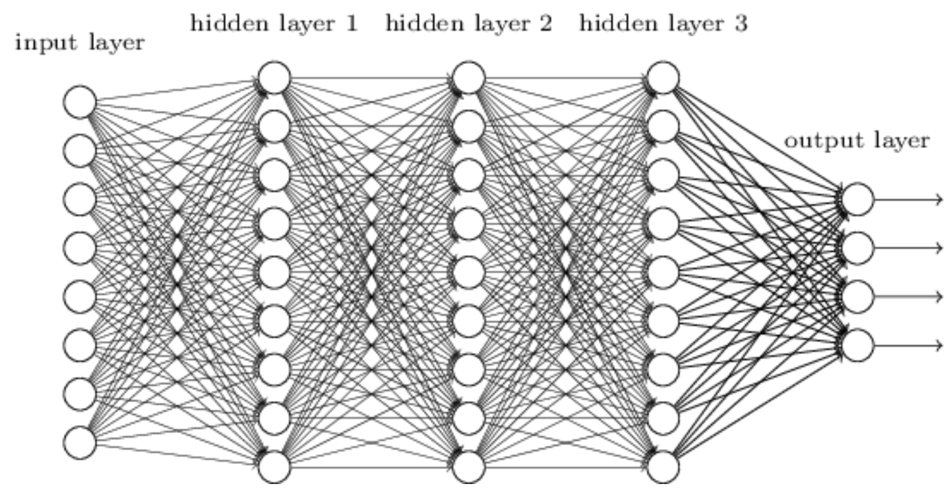



For fixed true labels, the cross entropy measures the differences bewegen truth and network prediction

# Complexity




**6 weights**

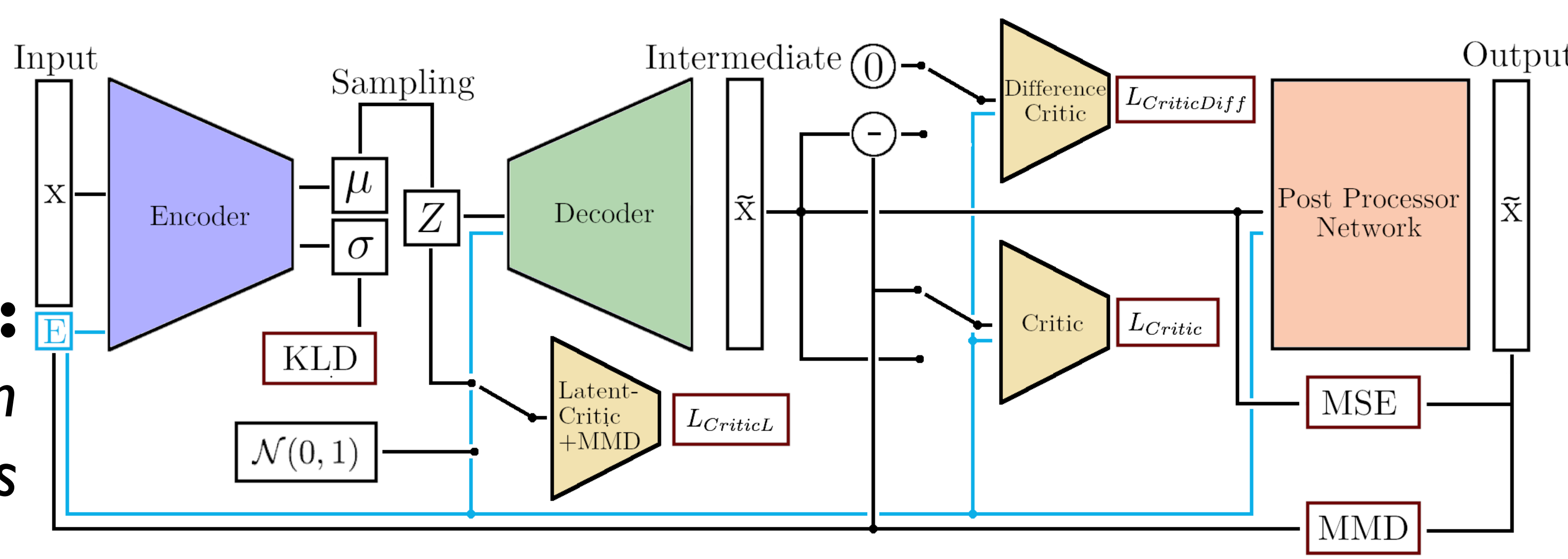



**300 weights**

| stage | output | ResNet-50 | ResNeXt-50 (32×4d) |
|---|---|---|---|
| conv1 | 112×112 | 7×7, 64, stride 2 | 7×7, 64, stride 2 |
| conv2 | 56×56 | 3×3 max pool, stride 2<br>[1×1, 64; 3×3, 64; 1×1, 256] ×3 | 3×3 max pool, stride 2<br>[1×1, 128; 3×3, 128, C=32; 1×1, 256] ×3 |
| conv3 | 28×28 | [1×1, 128; 3×3, 128; 1×1, 512] ×4 | [1×1, 256; 3×3, 256, C=32; 1×1, 512] ×4 |
| conv4 | 14×14 | [1×1, 256; 3×3, 256; 1×1, 1024] ×6 | [1×1, 512; 3×3, 512, C=32; 1×1, 1024] ×6 |
| conv5 | 7×7 | [1×1, 512; 3×3, 512; 1×1, 2048] ×3 | [1×1, 1024; 3×3, 1024, C=32; 1×1, 2048] ×3 |
| | 1×1 | global average pool<br>1000-d fc, softmax | global average pool<br>1000-d fc, softmax |
| # params. | | **25.5**×$10^6$ | **25.0**×$10^6$ |
| FLOPs | | **4.1**×$10^9$ | **4.2**×$10^9$ |

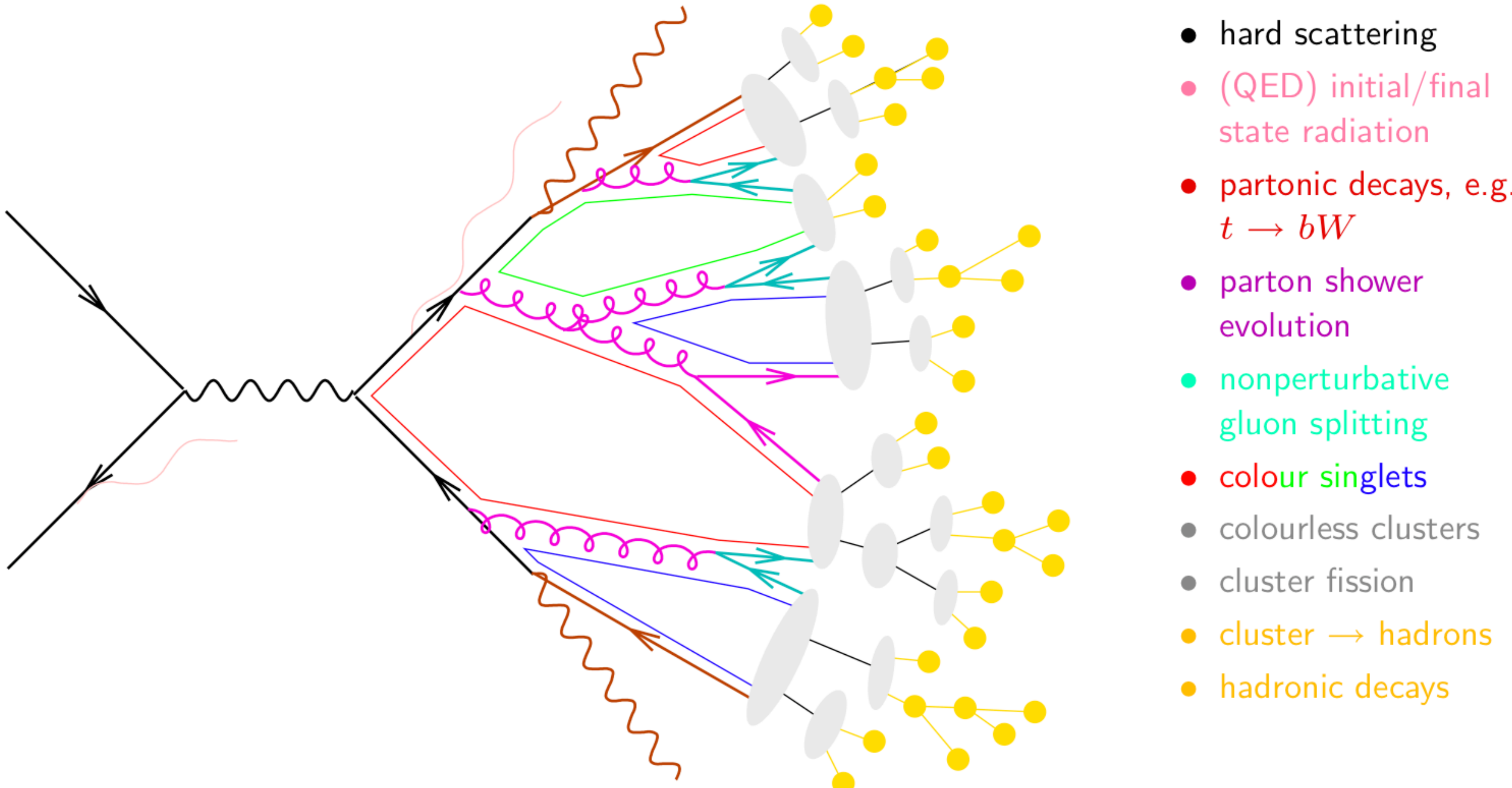
**25 million weights:**
*2016 state of the art for image classification*

Deep Learning:
Complex network + low level inputs

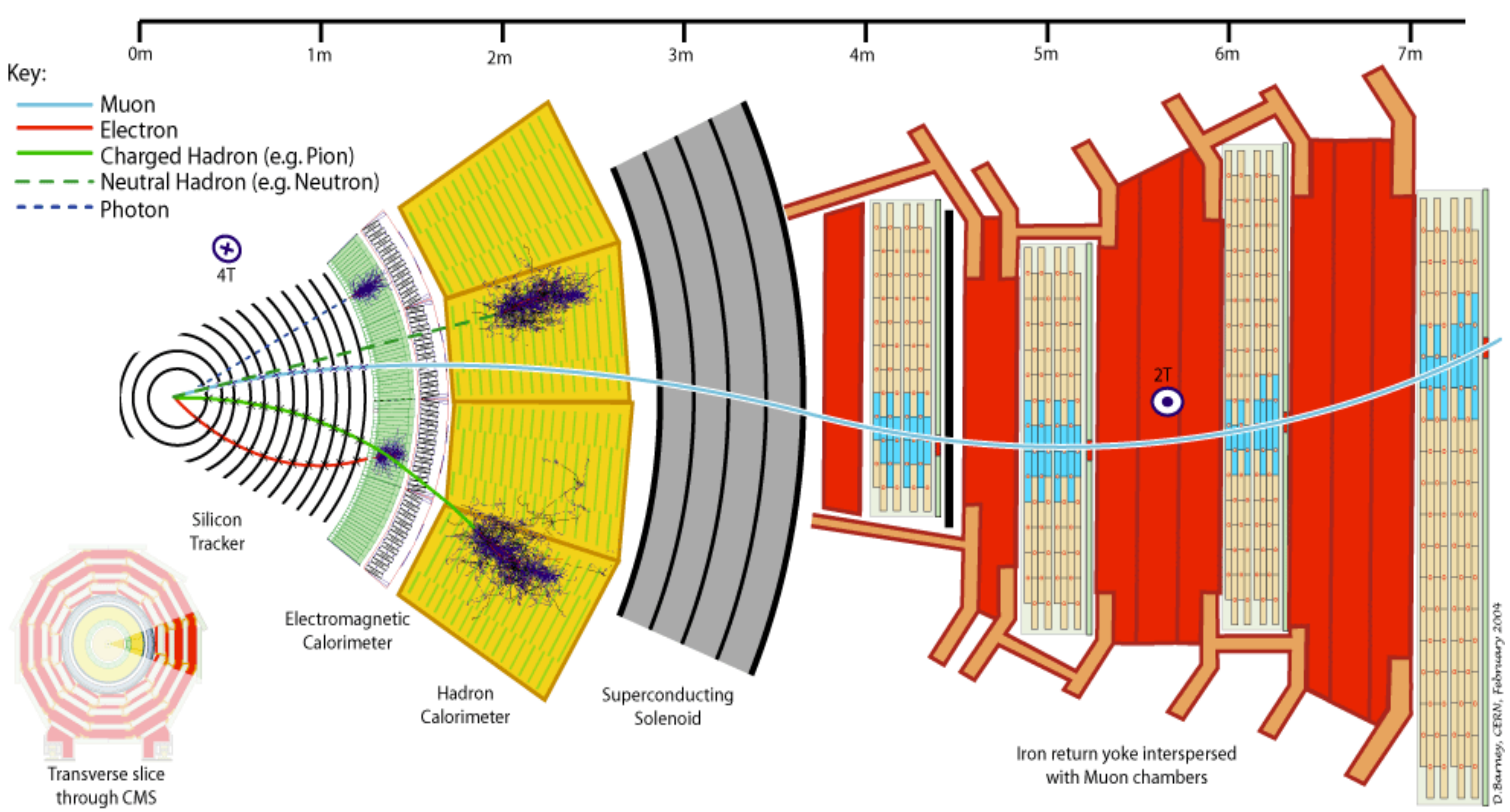



**71 million weights:**
*2020 generative network from physics*

# Supervised particle tagging & architectures



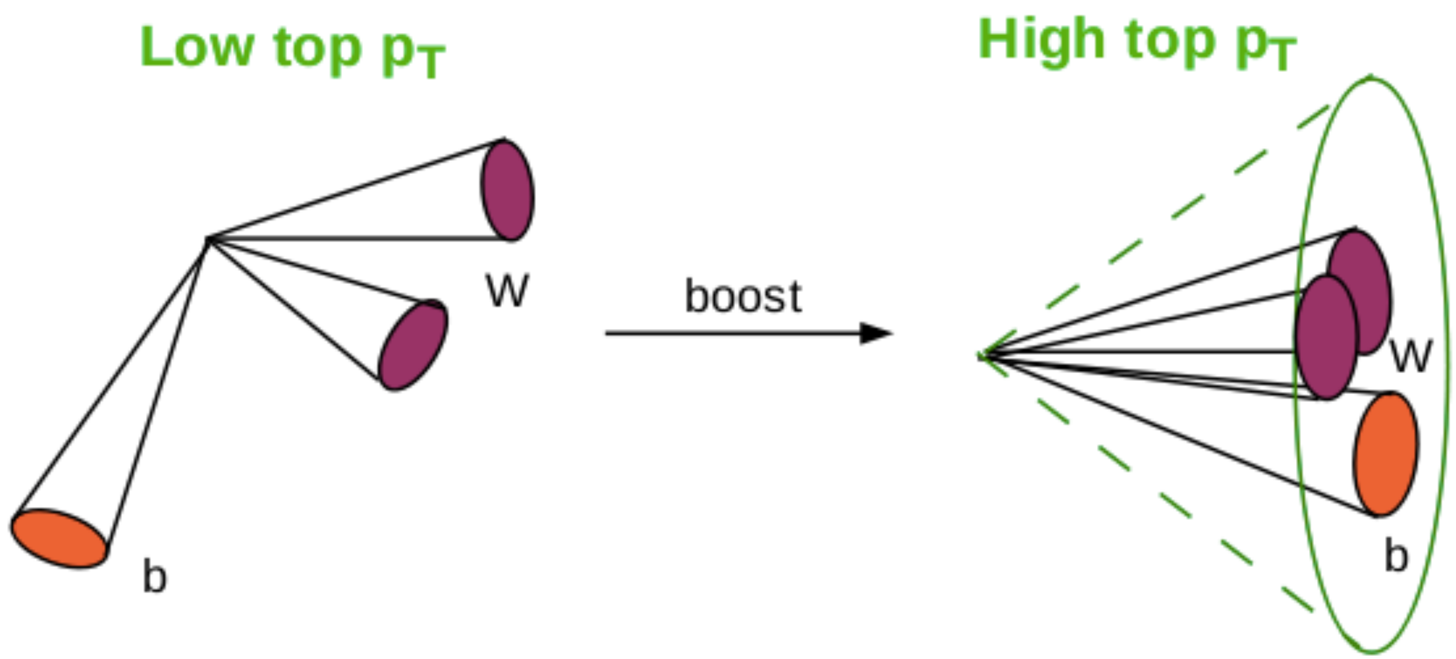

+




*We want to infer underlying physics from measurements in the detector.*

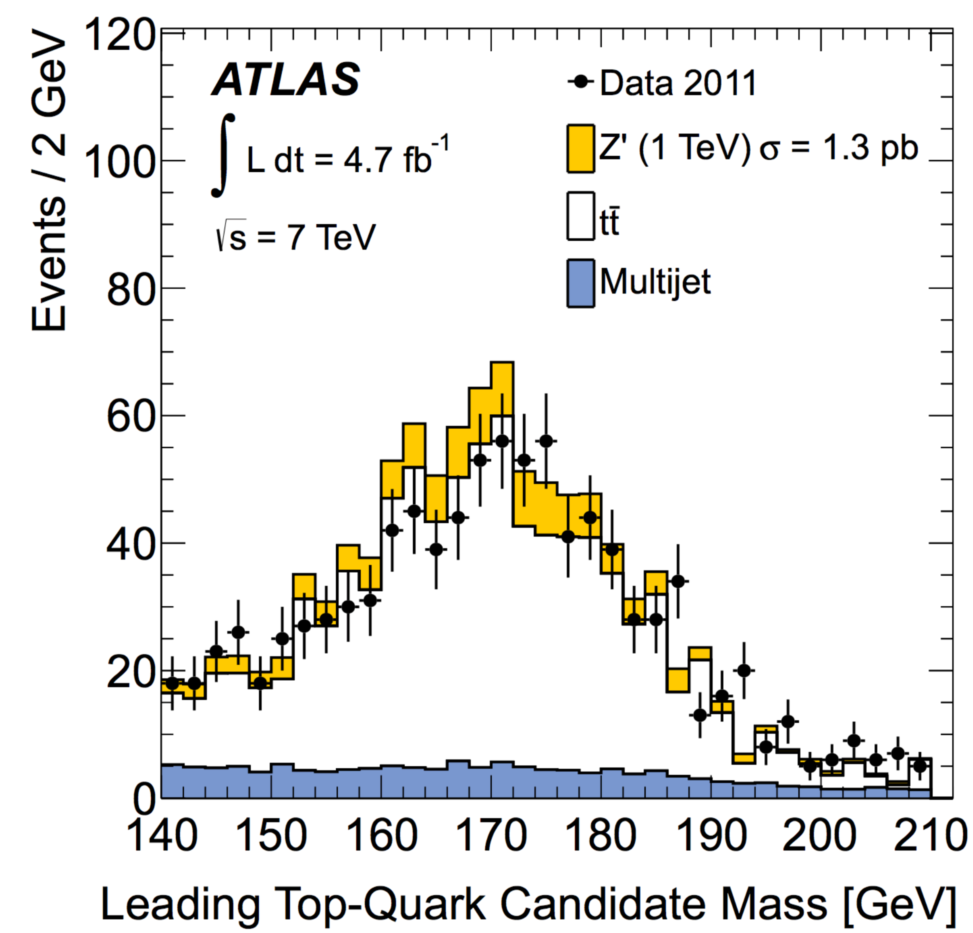
*How can deep neural networks assist us?*

# Heavy Resonance Tagging



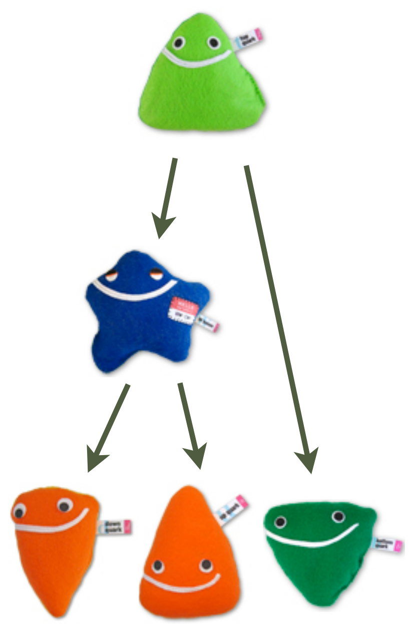

- Hadronically decaying top/Higgs/W/Z
- Contained in one (large-R) jet
- How to distinguish from light quark/gluon jets (and from each other)
- For new physics searches (and SM studies)

- Mass
  *Calculate using a grooming algorithm (eg mMDT/softdrop or pruning)*
- Centers of hard radiation
  *n-subjettiness or energy correlation functions*
- Flavour
  *b tagging of large-R jets or subjets*
- Combinations




*Towards an Understanding of the Correlations in Jet Substructure*
D Adams et al (BOOST 2013 Participants), Eur.Phys.J. C75
*Top Tagging,* T Plehn, M Spannowksy, J.Phys. G39 (2012) 083001
*Boosted Top Tagging Method Overview,* GK, Proc. Top2017

# *Top Quark*



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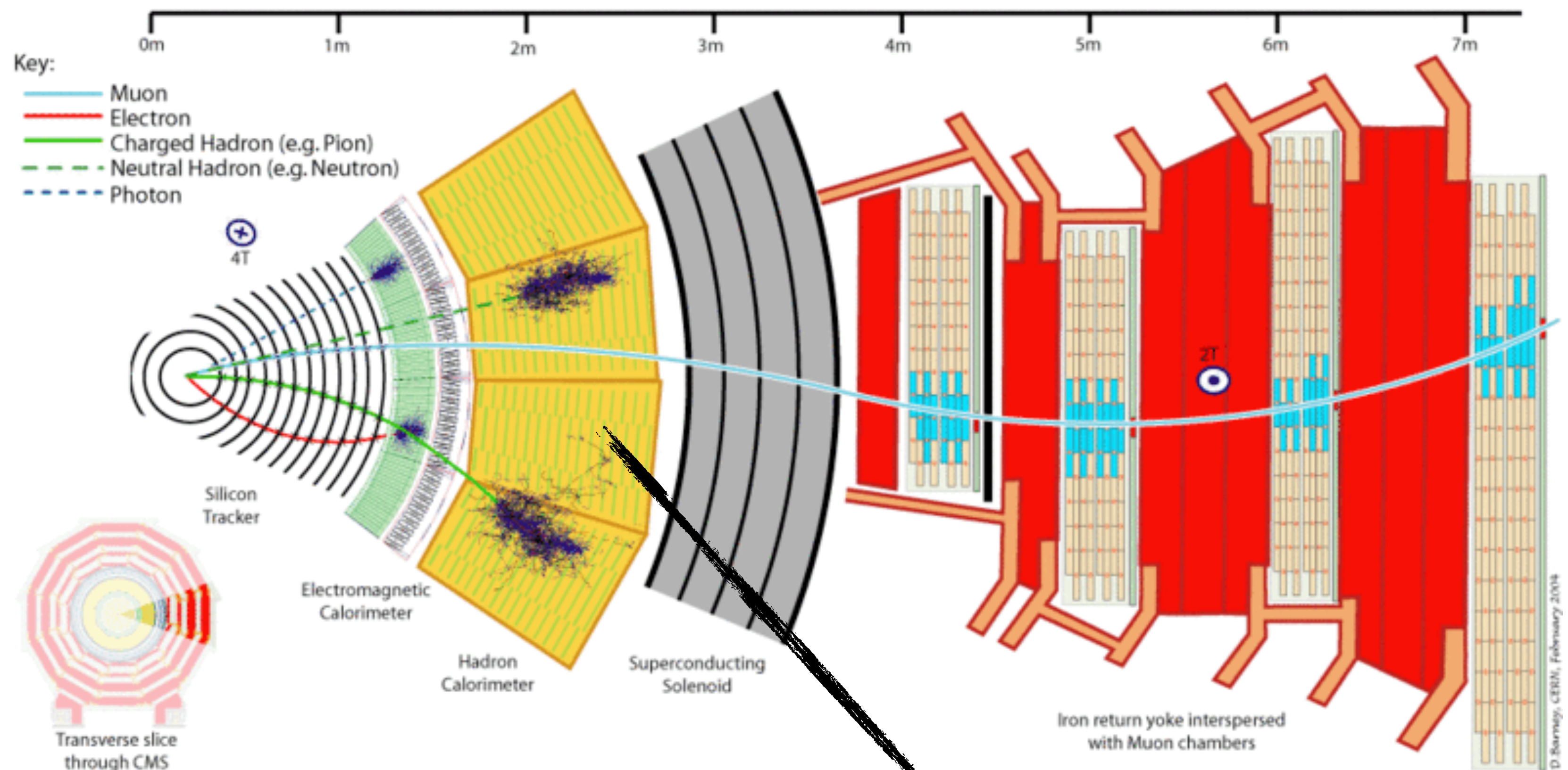
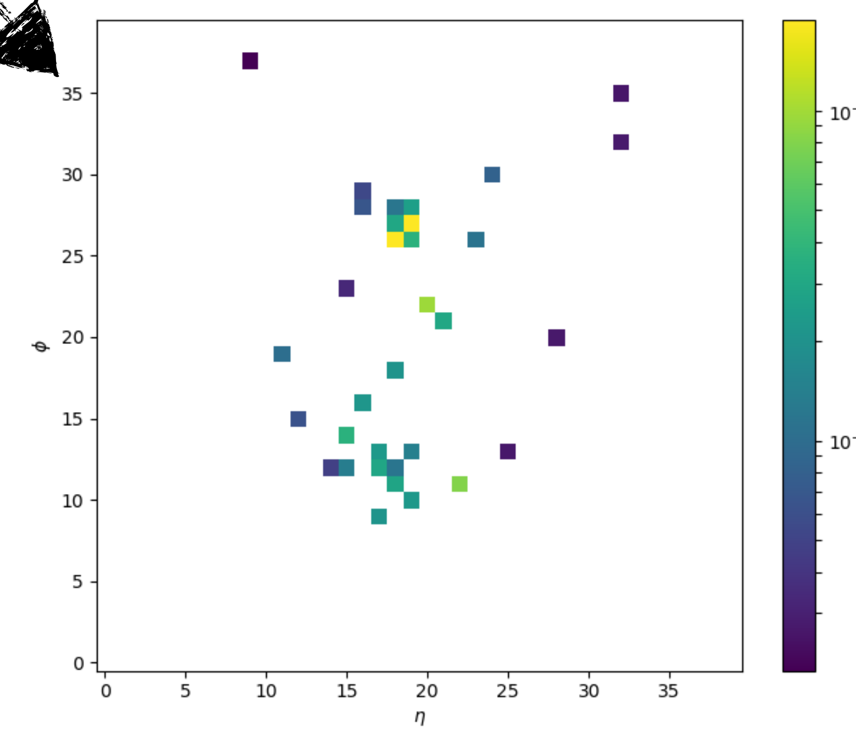



*(jet images by C Daza)*

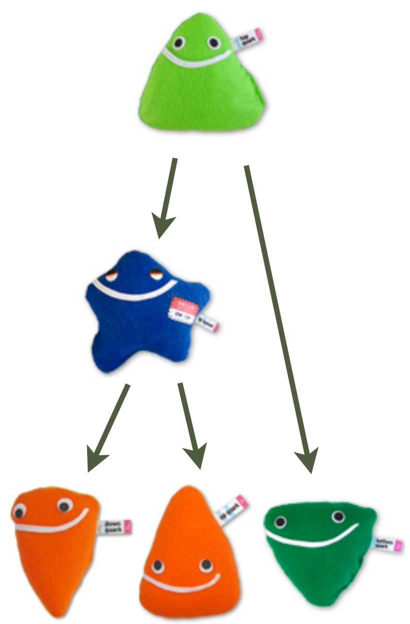
- *Measure particle energies in calorimeter*
- *Reconstruct jet from individual measurements*
- *Image preprocessing*
  - *center, rotate, mirror, pixelate, trim, normalise*

=




1 image

# Top Quark



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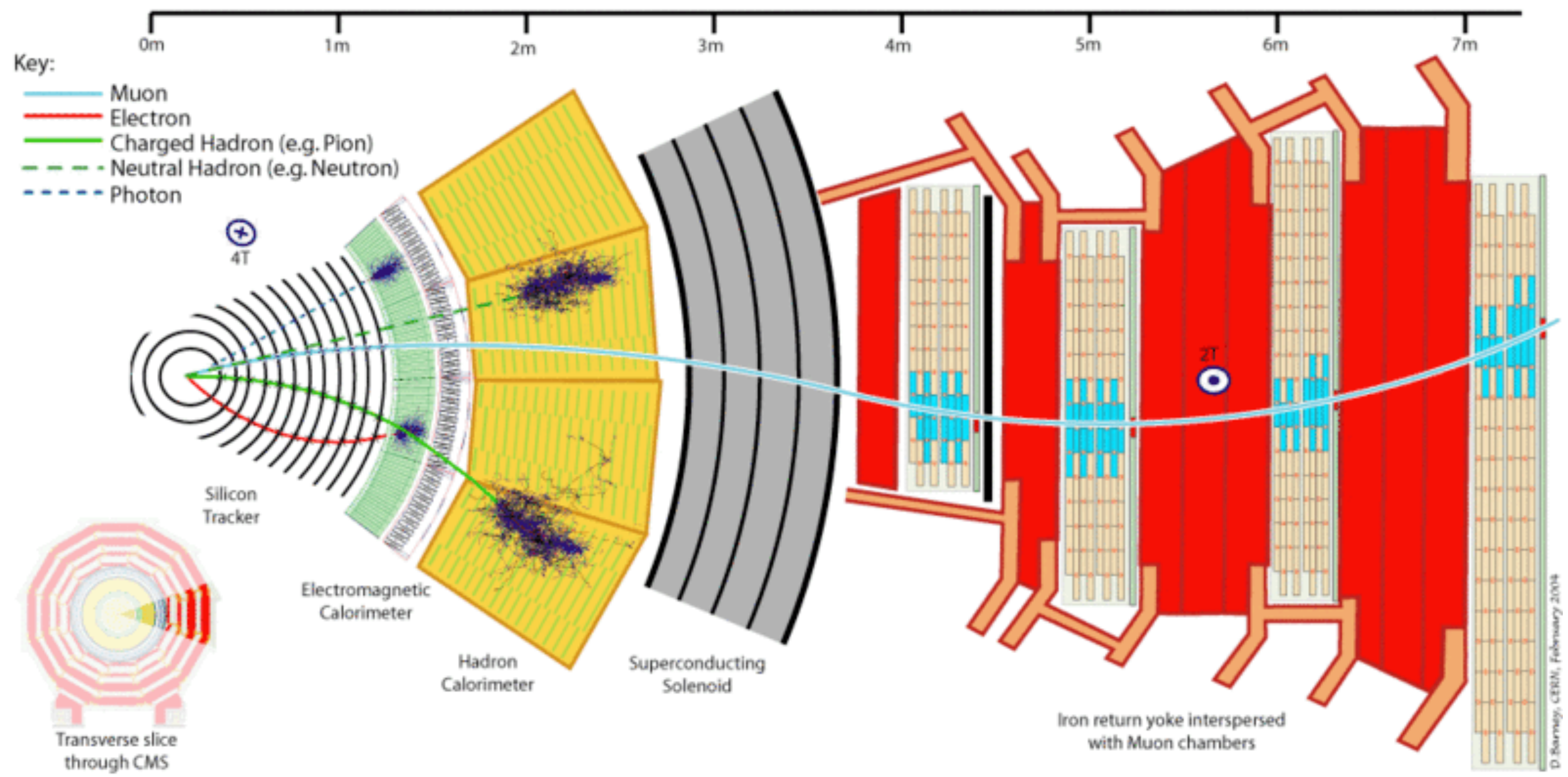


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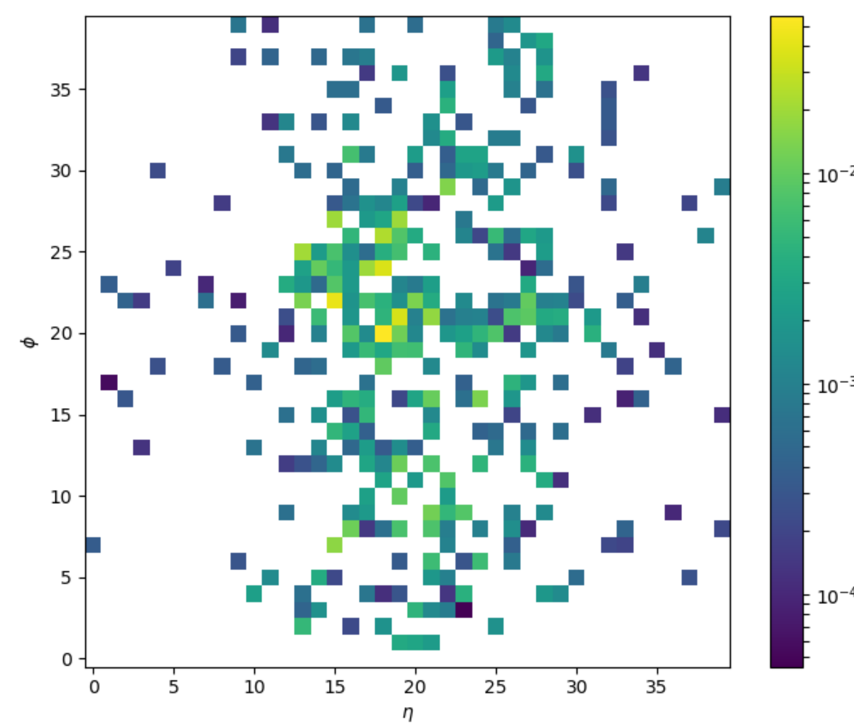
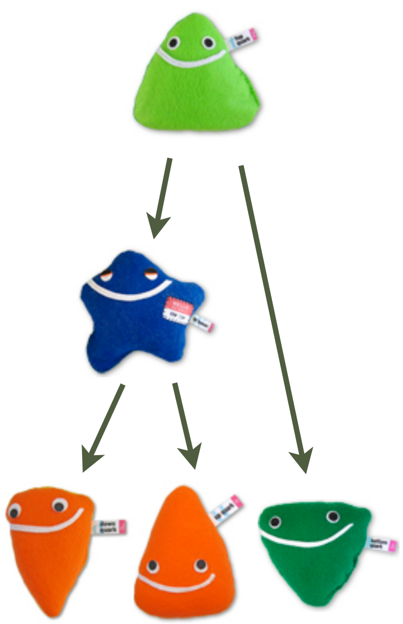



10 image average

# Top Quark



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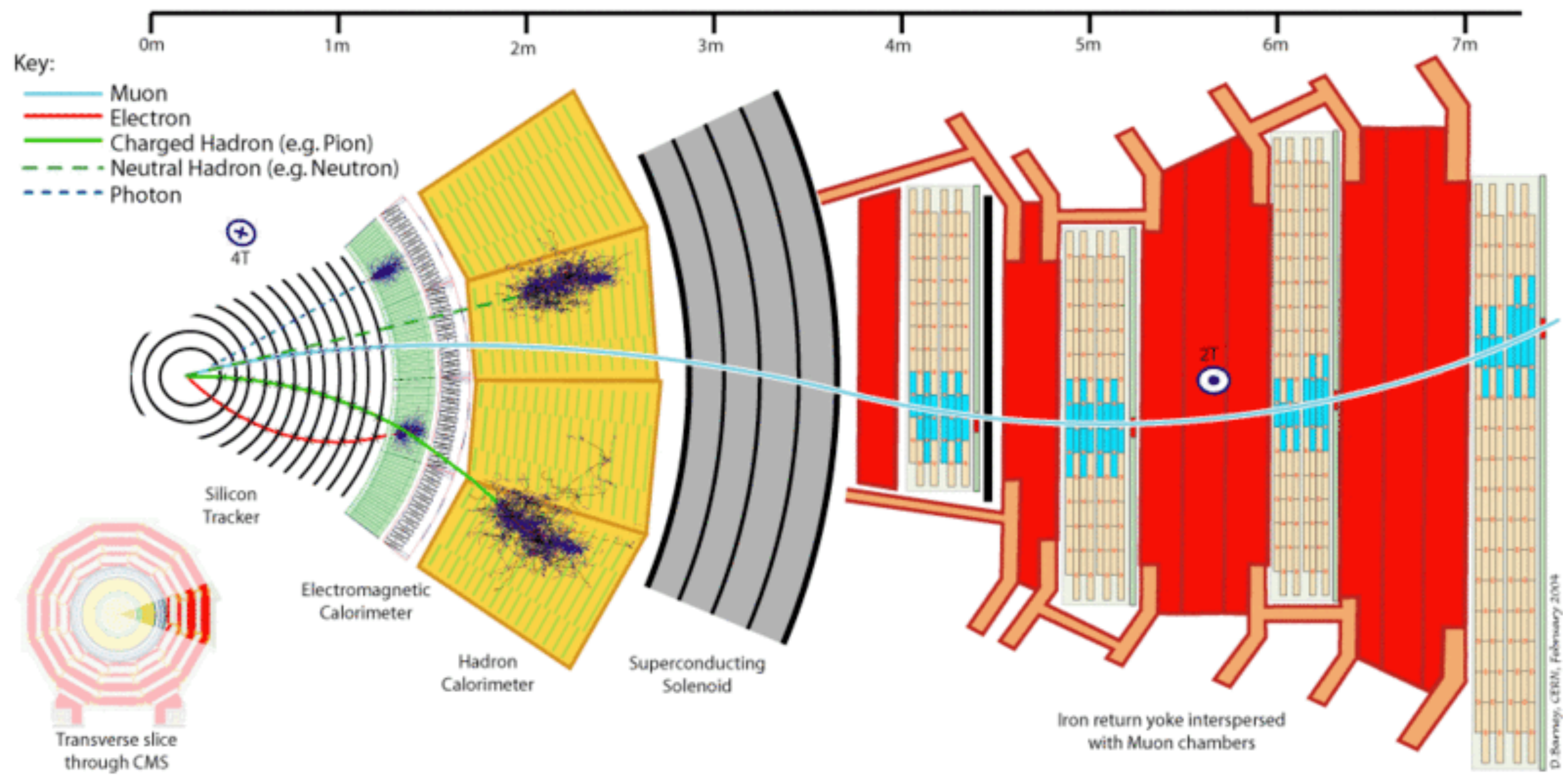


(jet images by C Daza)

- Measure particle energies in calorimeter
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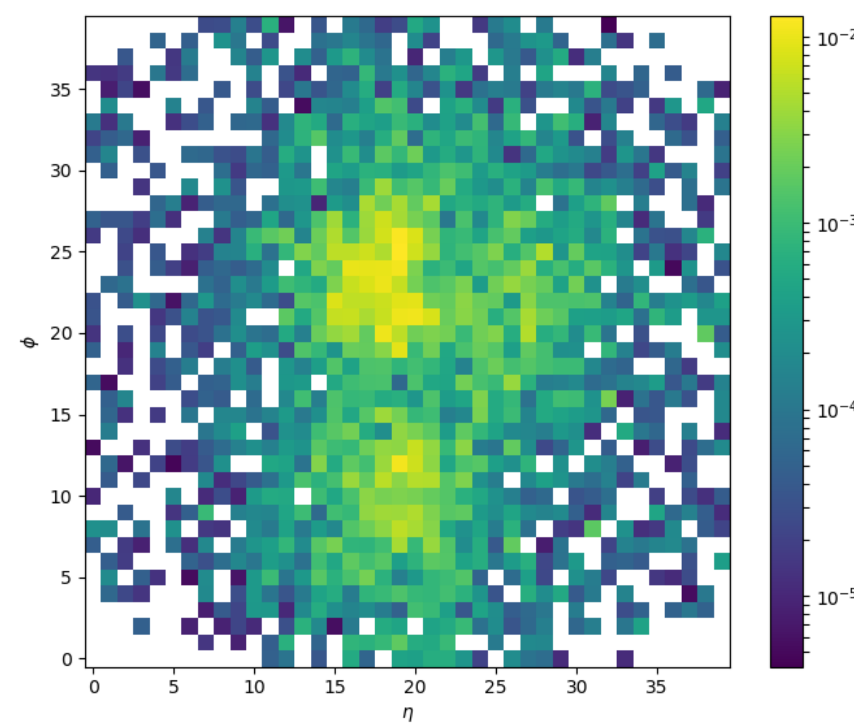
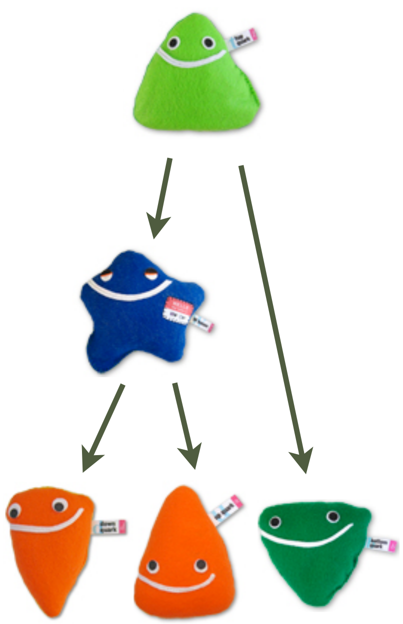
=




100 image average

# Top Quark



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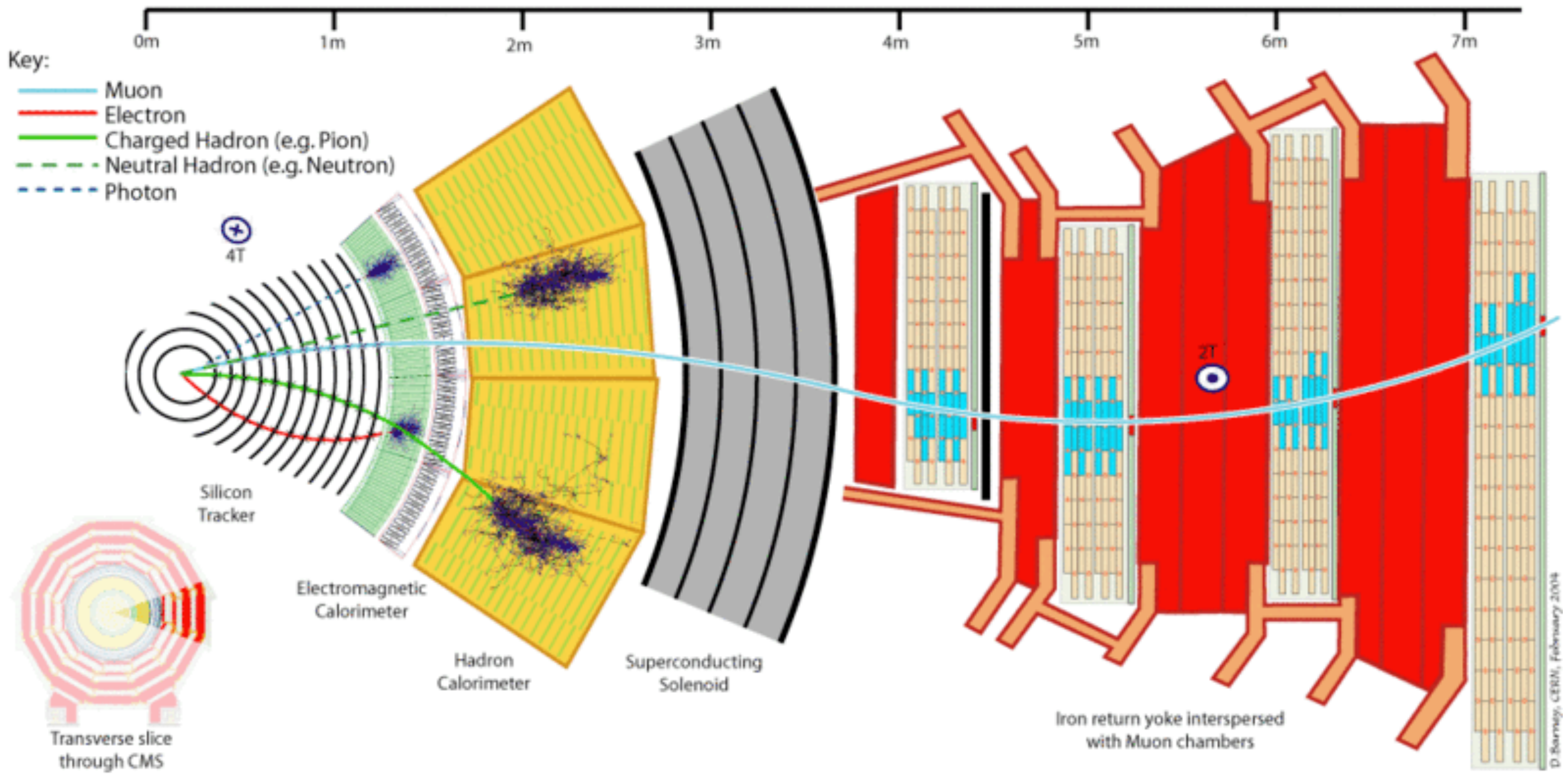
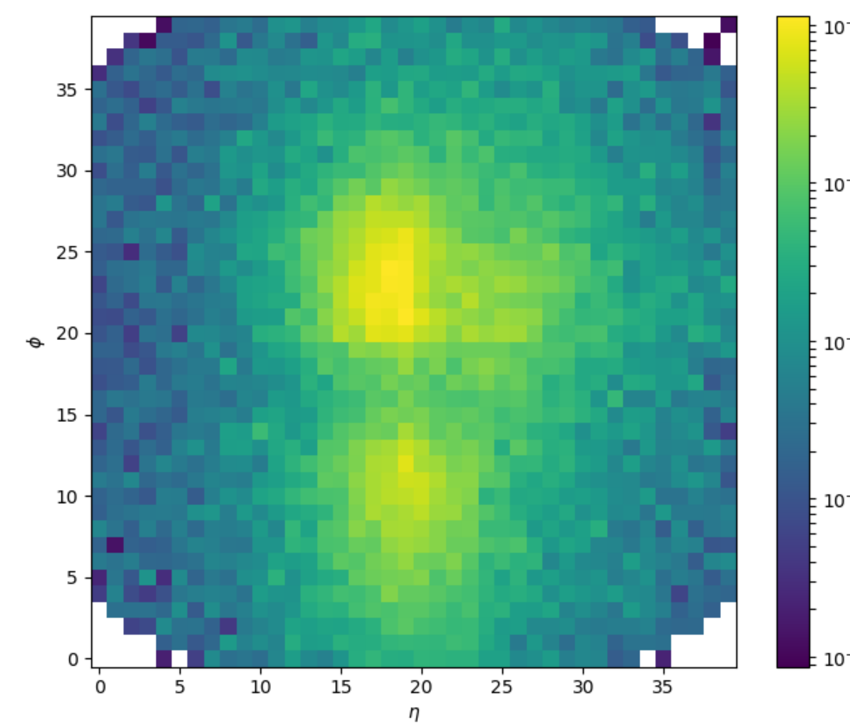



- *Measure particle energies in calorimeter*
- *Reconstruct jet from individual measurements*
- *Image preprocessing*
  - *center, rotate, mirror, pixelate, trim, normalise*

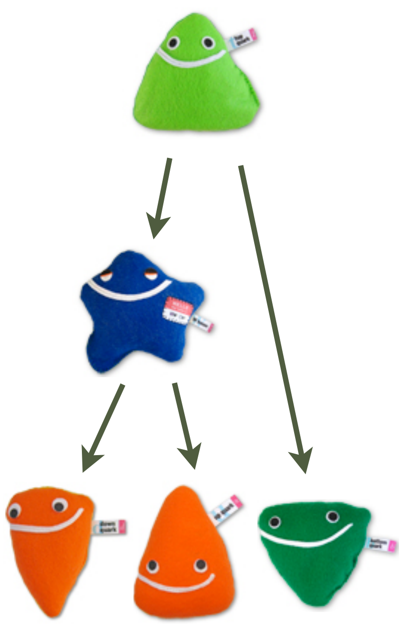
=

*(jet images by C Daza)*




1000 image average

# Top Quark



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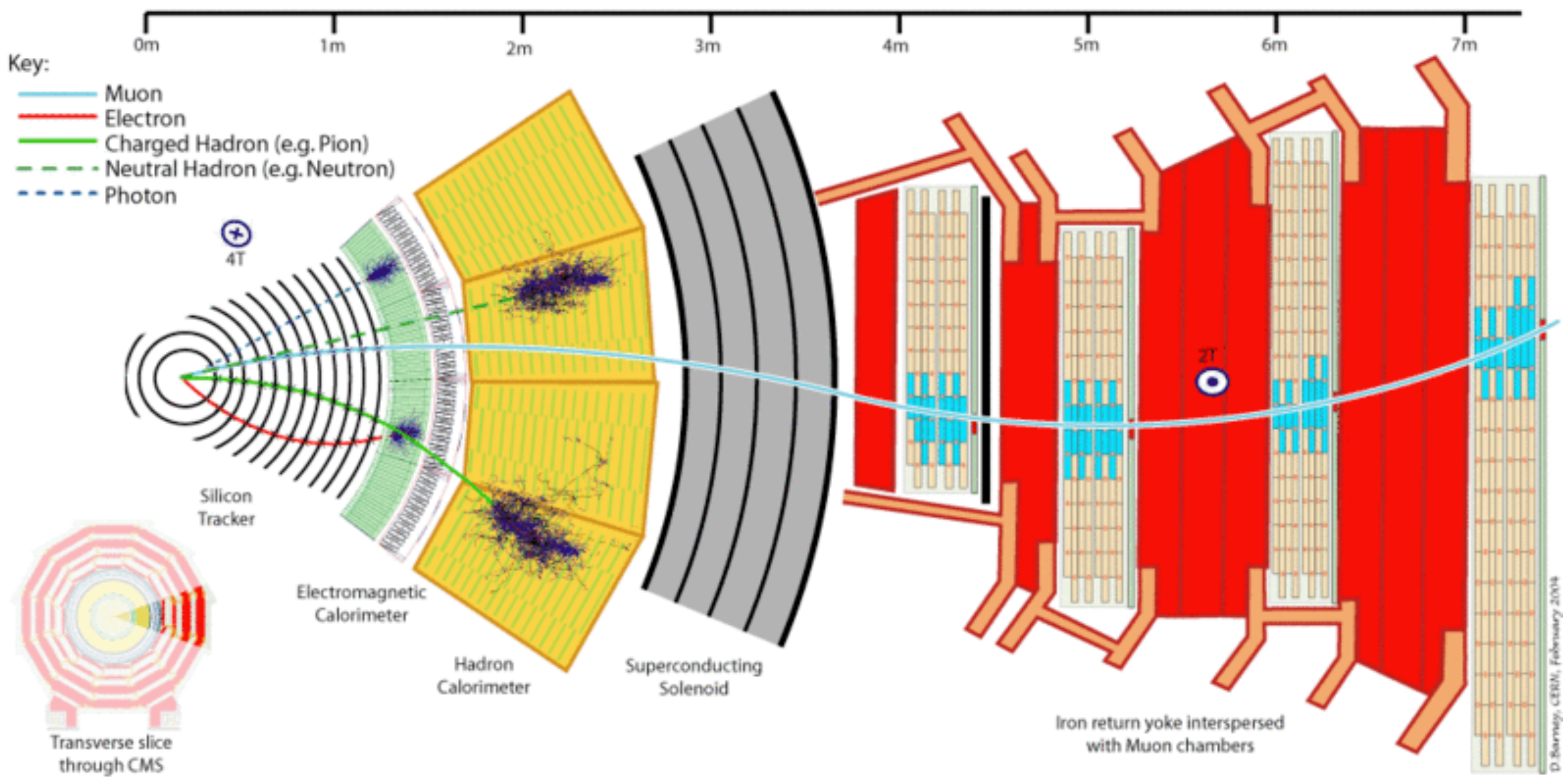


(jet images by C Daza)

- *Measure particle energies in calorimeter*
- *Reconstruct jet from individual measurements*
- *Image preprocessing*
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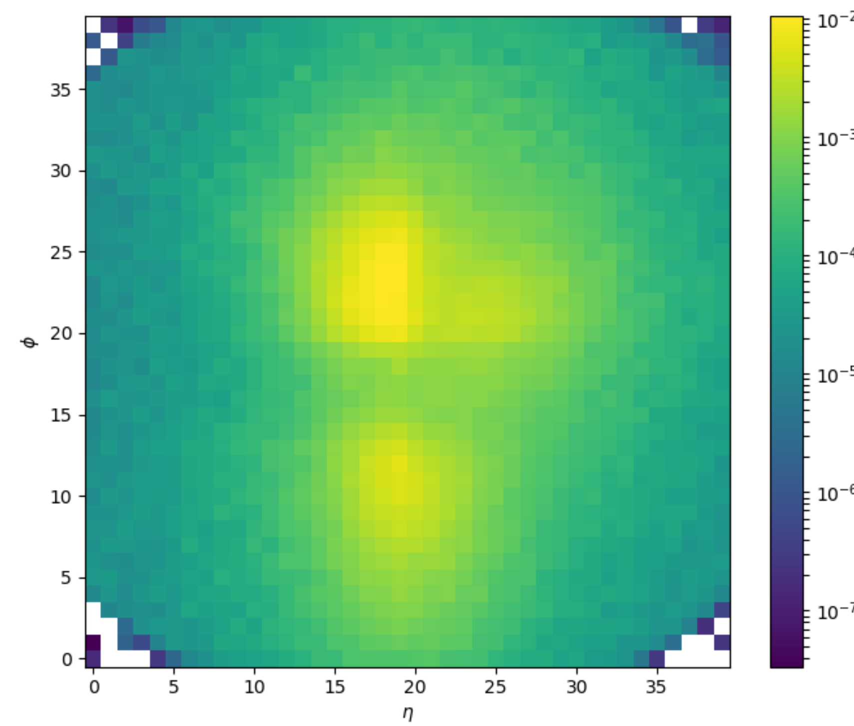
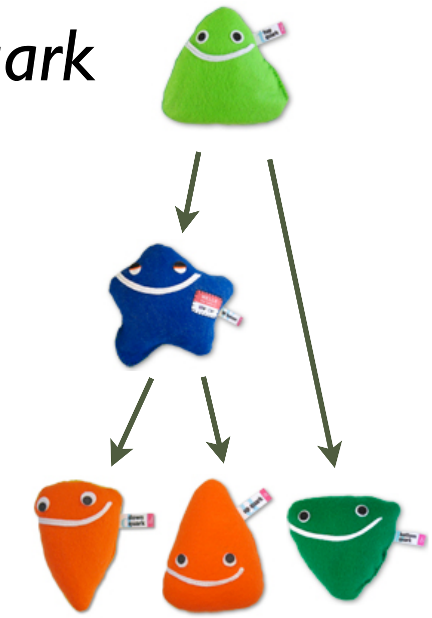
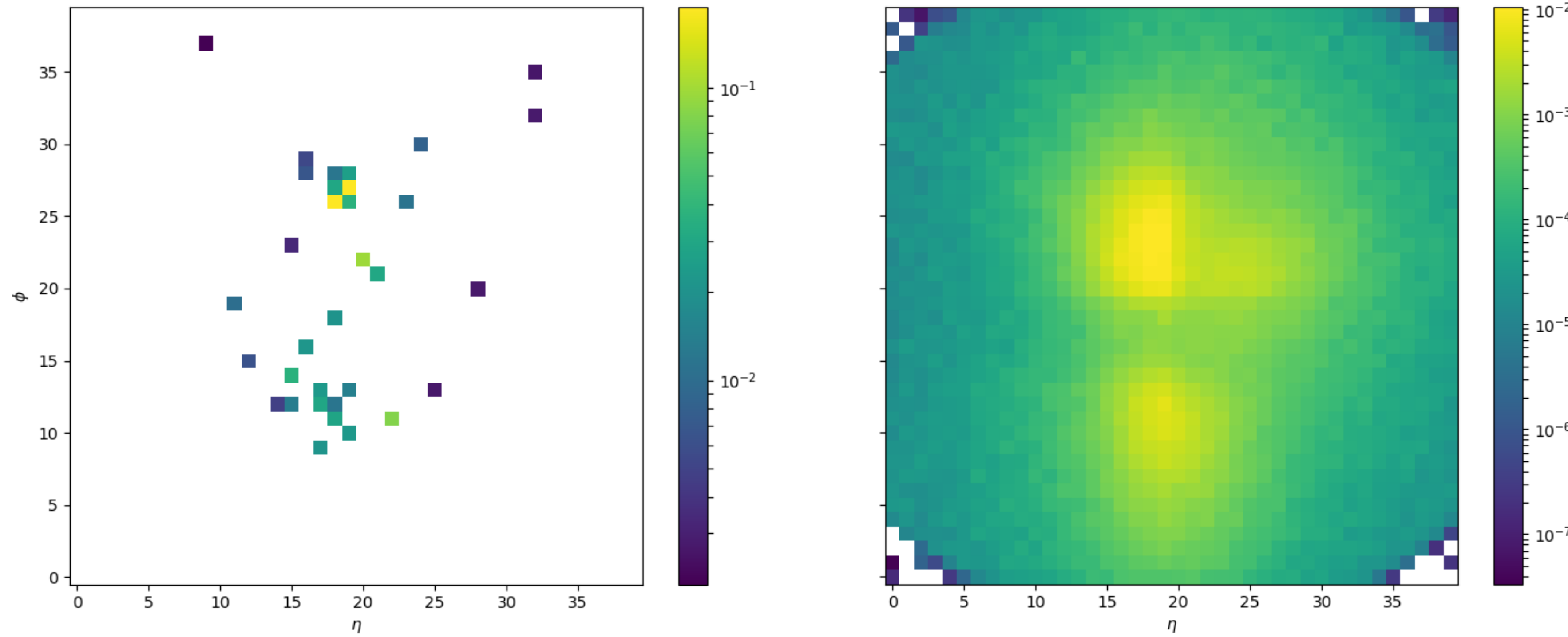



10000 image average

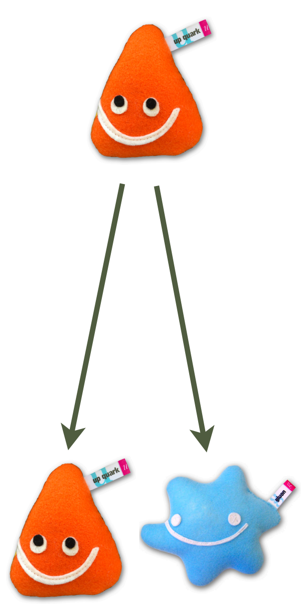
*Top Quark Jet*

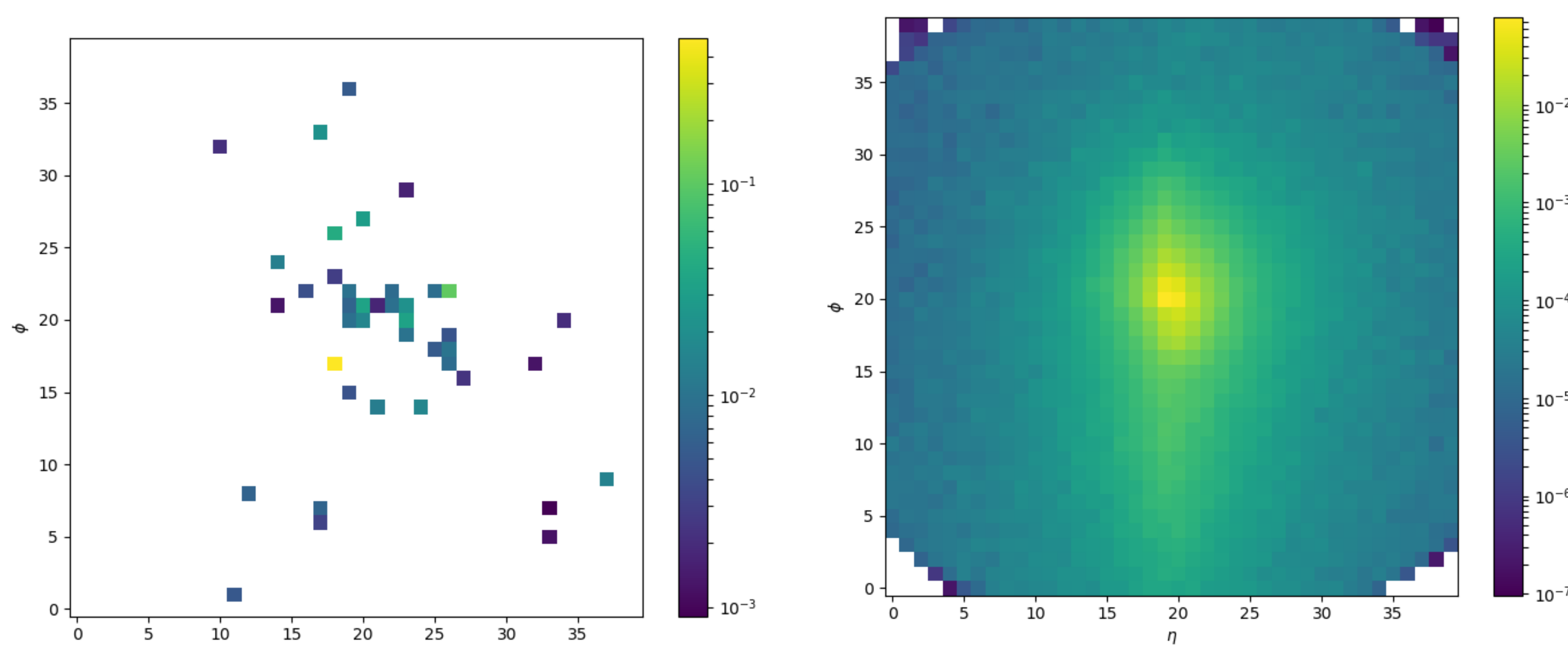




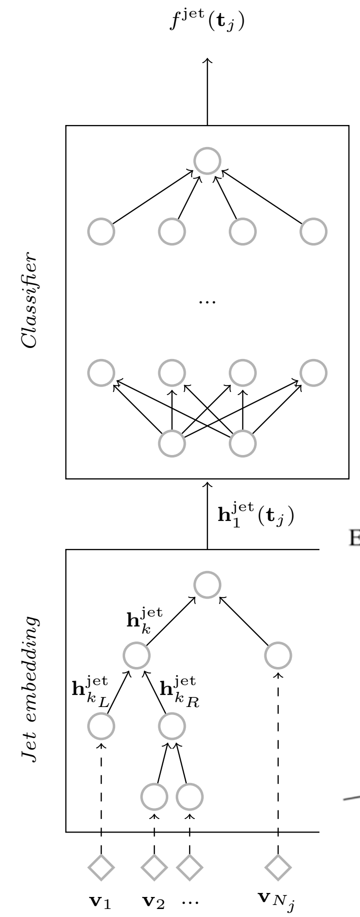
- *Binary classification task*
- *Fully supervised learning (using simulation)*
- *40x40 Pixels, $E_T$*
- *Perfectly suited for deep learning algorithms*

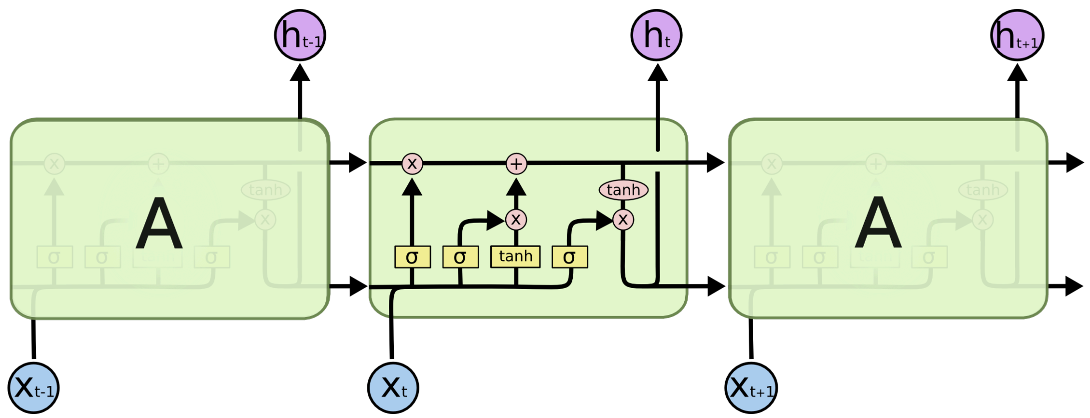
*QCD Jet*

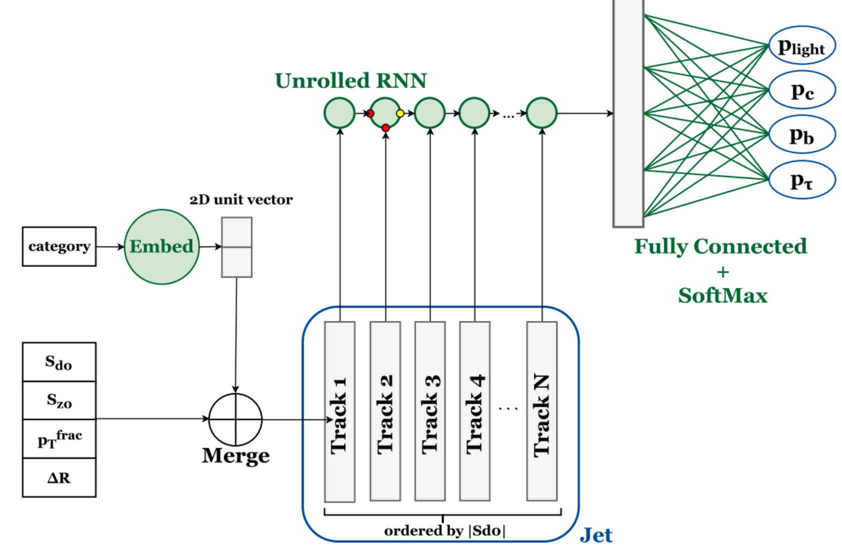


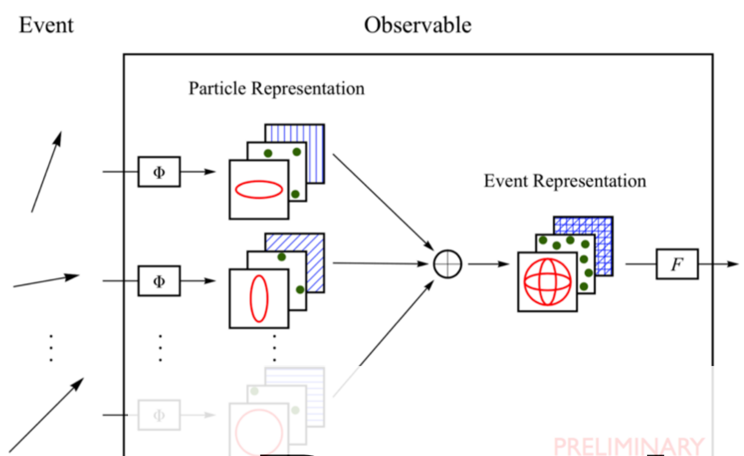


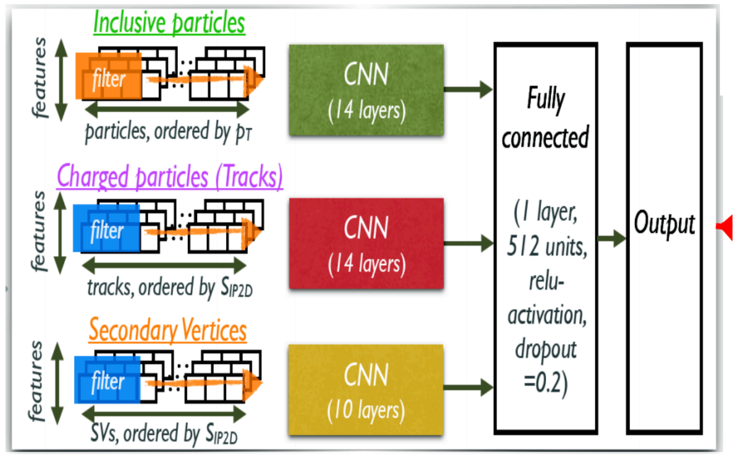
# Possible Approaches

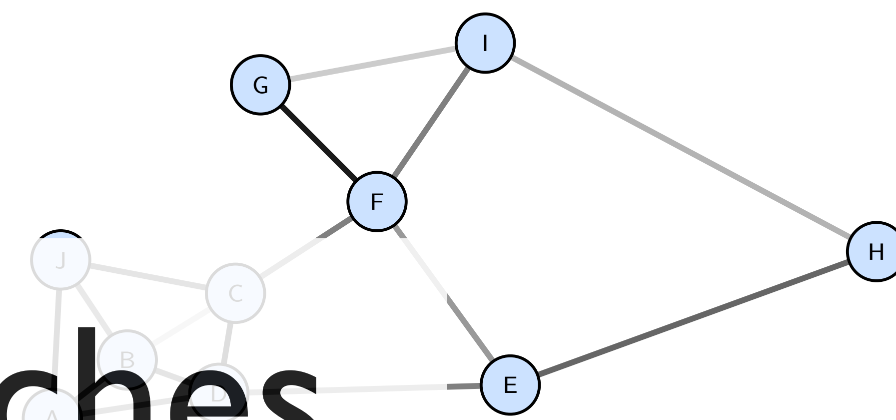


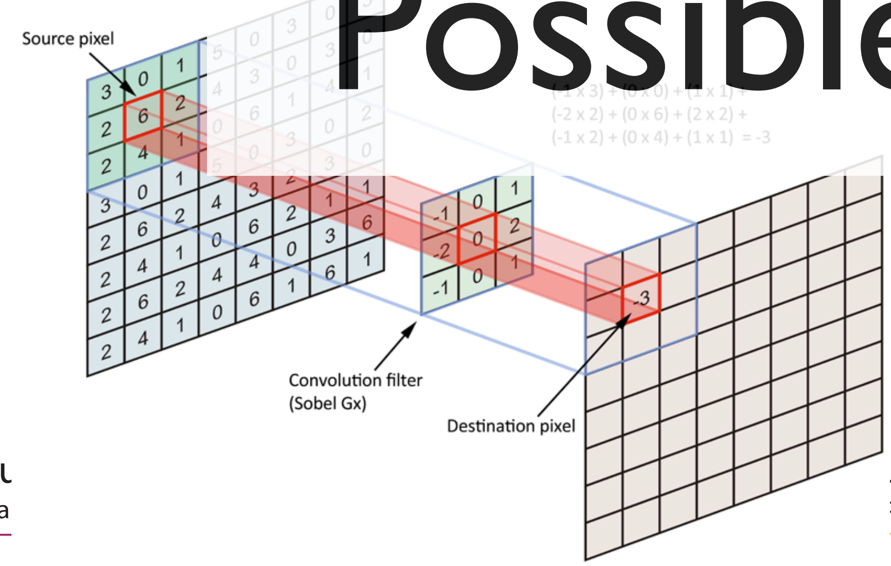



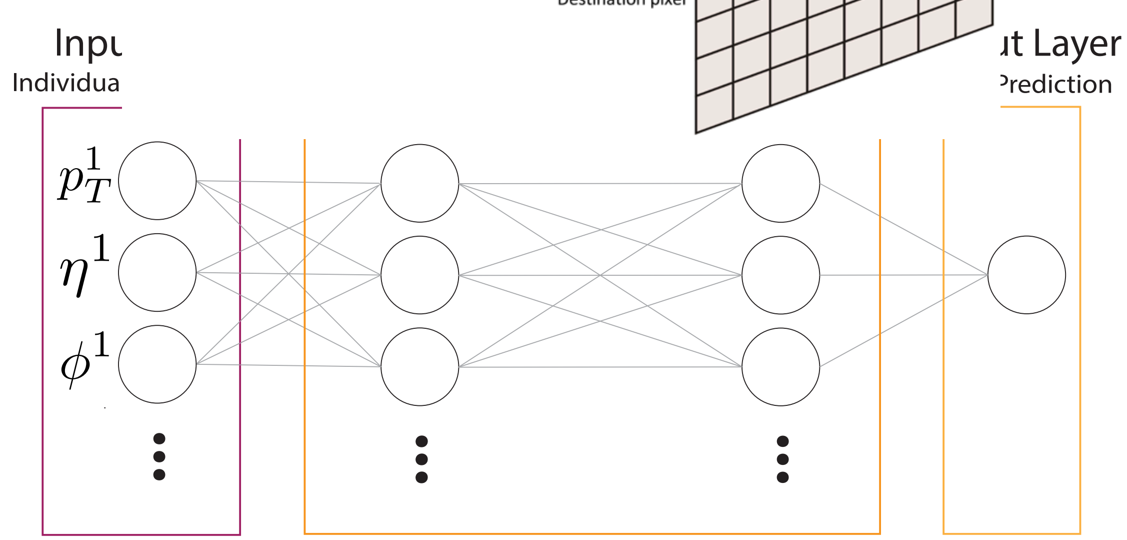



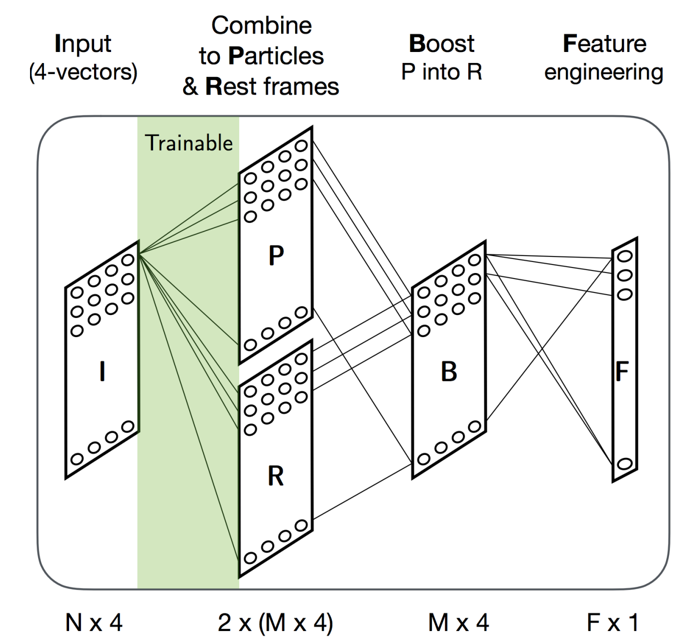

$$k_{\mu,i} = \begin{pmatrix} E_0 & E_1 & \cdots & E_N \\ p_{x,0} & p_{x,1} & \cdots & p_{x,N} \\ p_{y,0} & p_{y,1} & \cdots & p_{y,N} \\ p_{z,0} & p_{z,1} & \cdots & p_{z,N} \end{pmatrix}$$

Combination Layer (**CoLa**): create linear combinations:

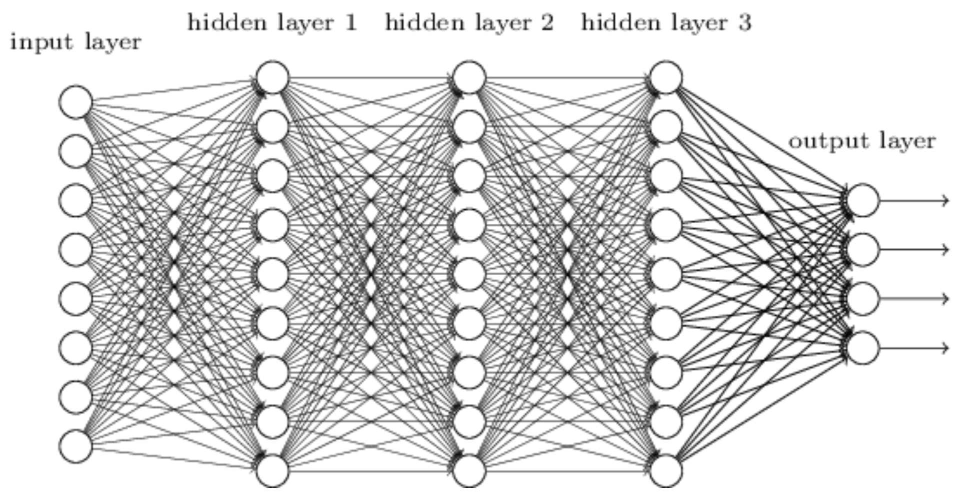
$$k_{\mu,i} \xrightarrow{\text{CoLa}} \widetilde{k}_{\mu,j} = k_{\mu,i}\, C_{ij}$$

Lorentz Layer (**LoLa**): Use resulting matrix to extract physics features.
Main assumption is the Minkowski metric

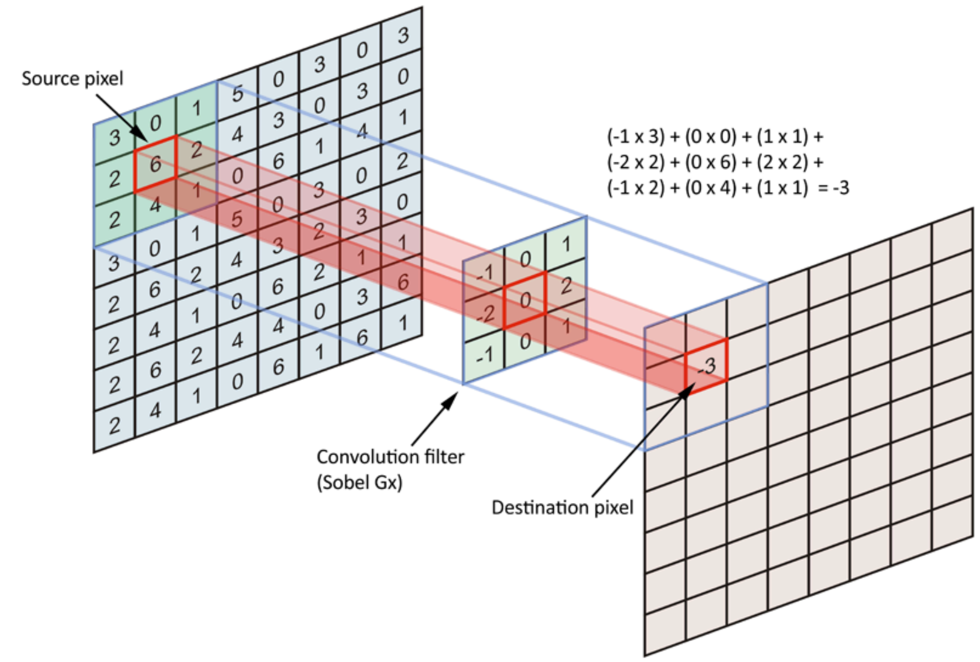
$$\widetilde{k}_{\mu,i} \rightarrow \sum_j (\widetilde{k}_i - \widetilde{k}_j)_\mu (\widetilde{k}_i - \widetilde{k}_j)_\nu \eta^{\mu\nu} B_{ij}$$



## High-level: Fully Connected

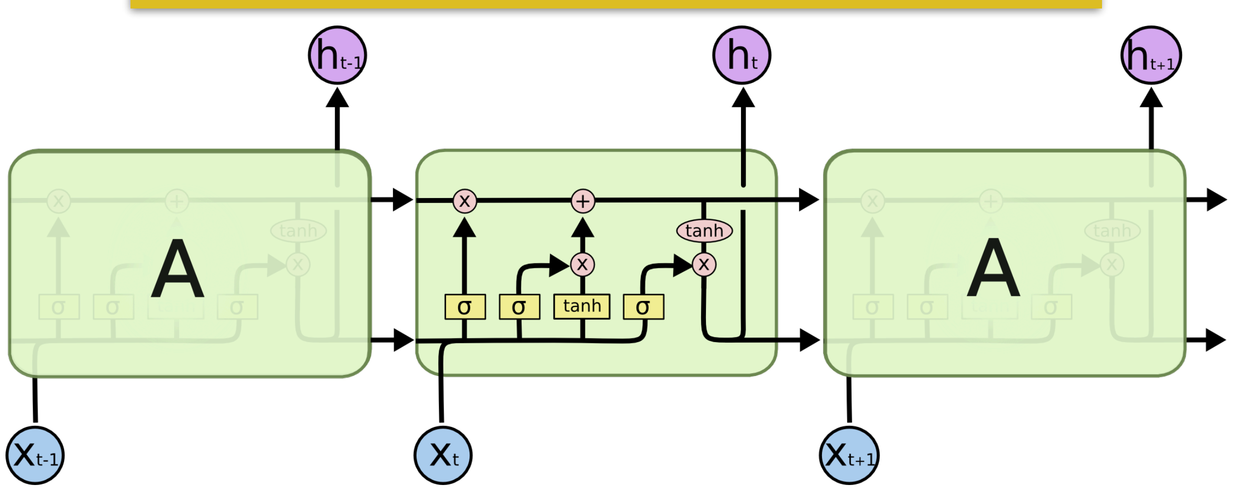



## Regular grid: Convolution

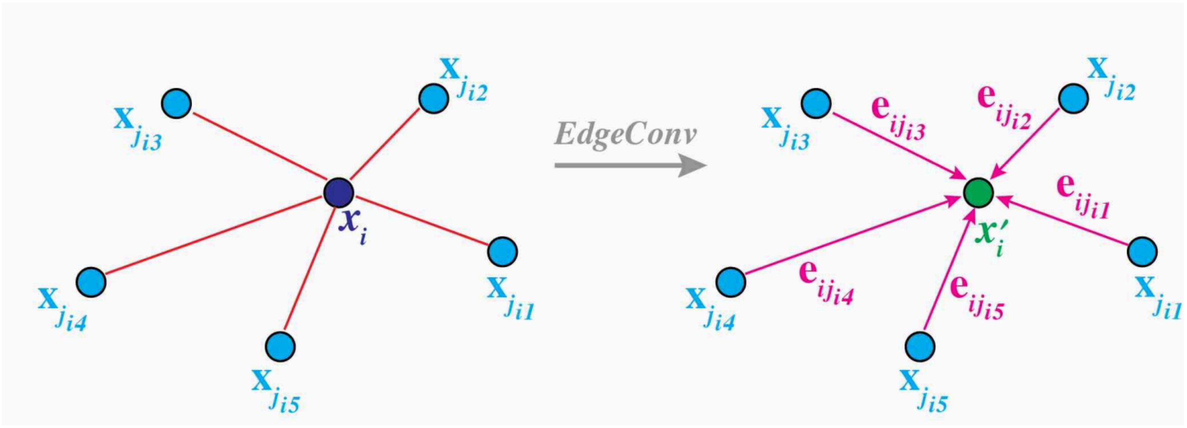



# Representation

## Time series: Recurrent

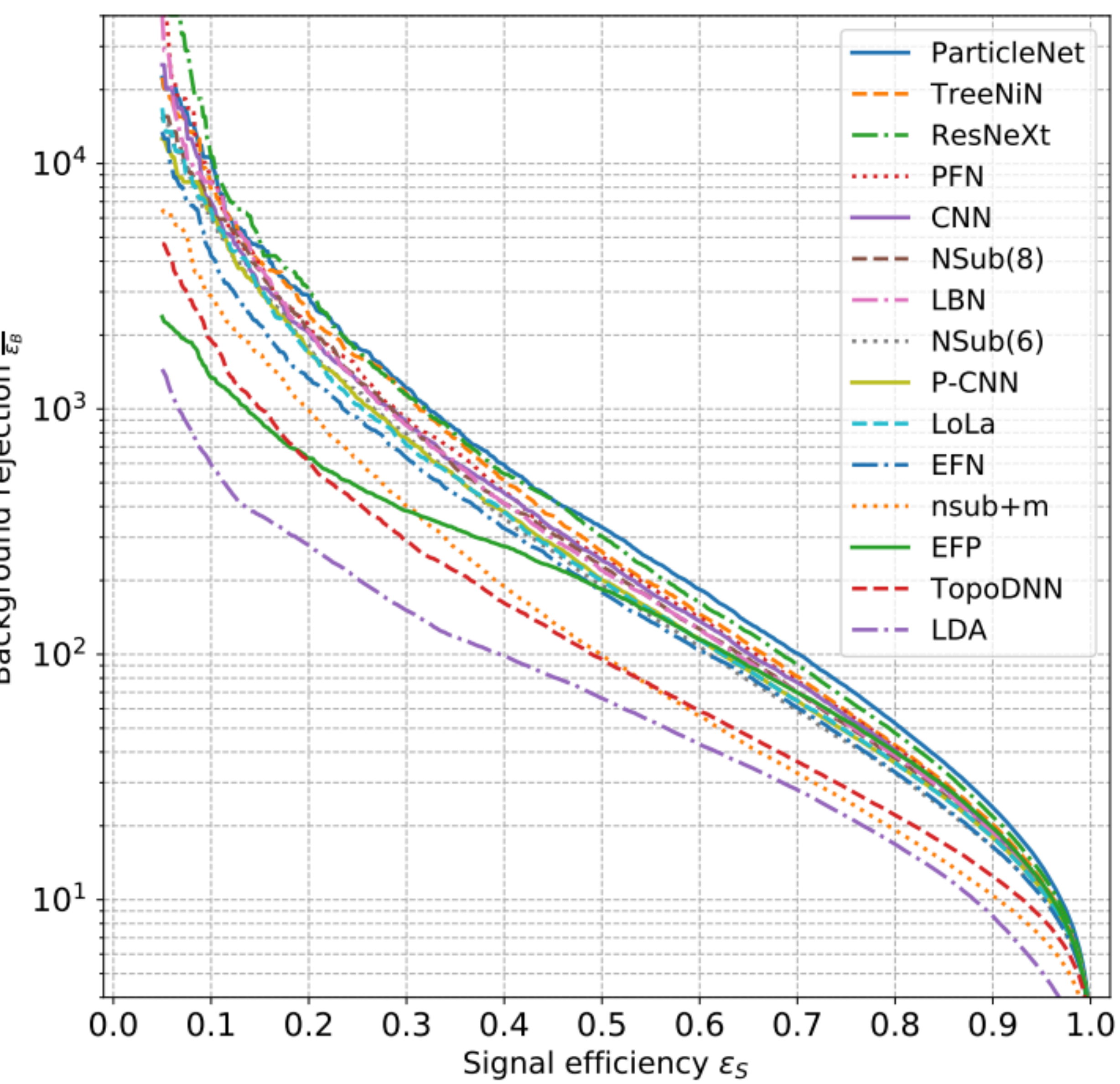



## Point cloud: Sets & Graphs



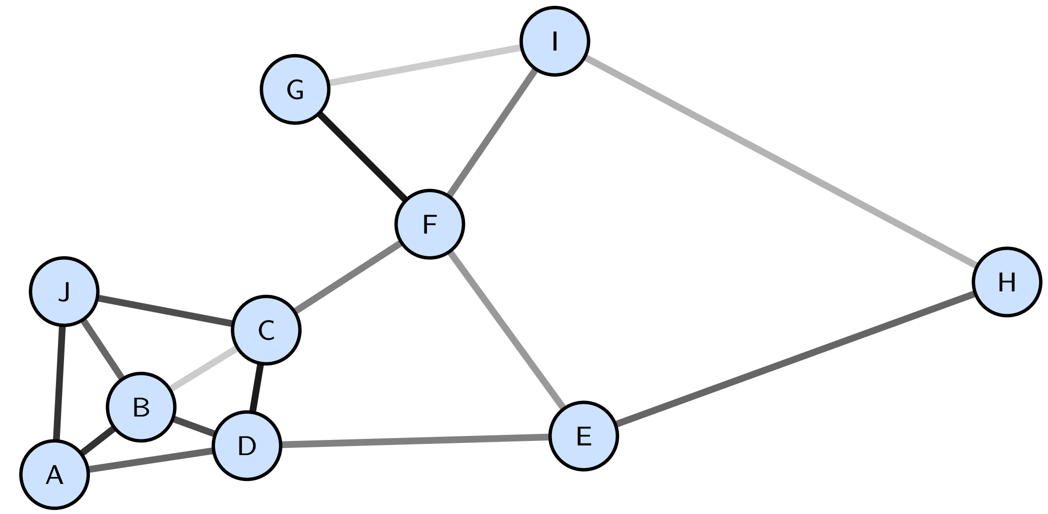
# Results

**Community performance comparison (toy dataset public): 1902.09914**

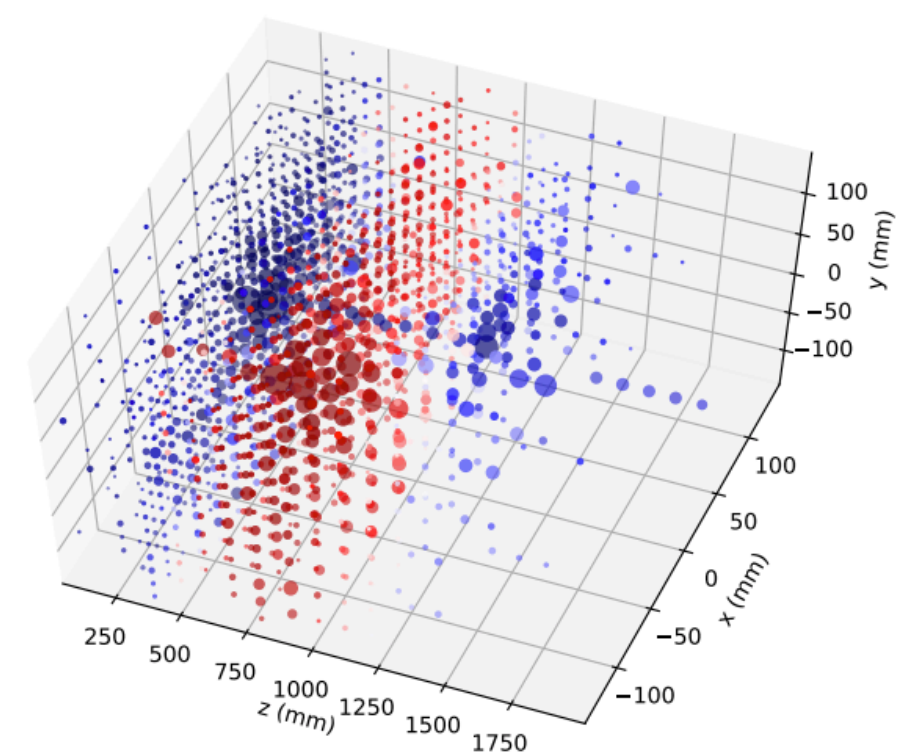


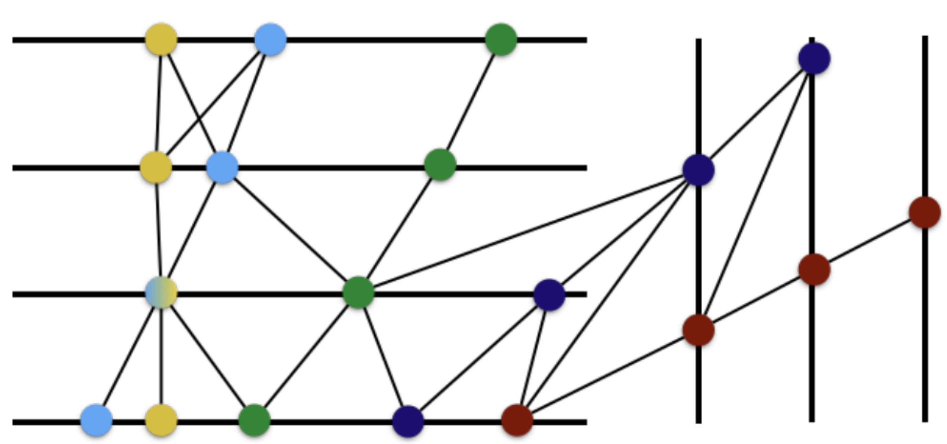

- Great test-bed to compare different data representations
    - (and, of course, useful for new physics searches, top/Higgs measurements)
- Still surprising gains in performance
    - Although it needs to be seen how well these translate to data
- (Also developments in flavour tagging, not covered here)

# ParticleNet = Graphs



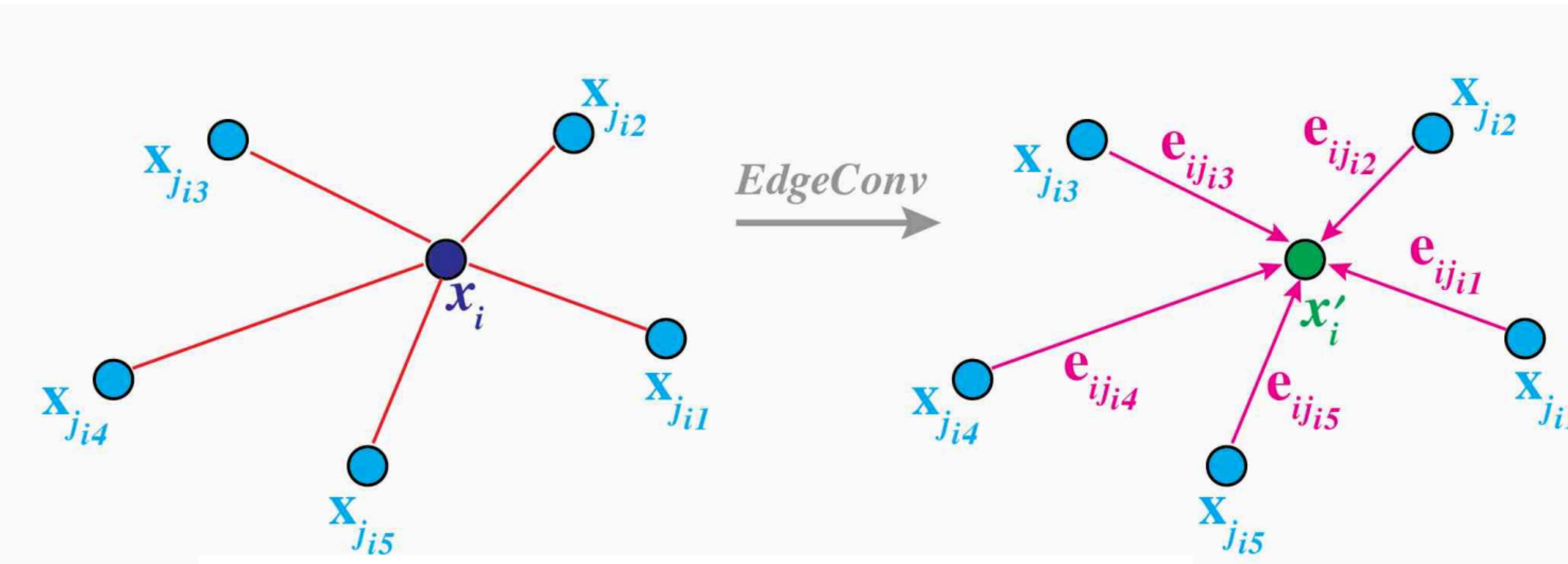

- Images are a convenient representation, but do not capture real structure of our measurements
- Alternative: Graphs
    - Vertex: Particle
    - Edge: Distance (for example geometric)
- Active development of graphs on CS side, but already HEP applications:
    - Particle Net (best performing top tagger in community s based on EdgeConv) (1902.08570)
    - Calorimeter Clustering (1902.07987)
    - Tracking (1810.06111)



1902.08570
1801.07829

# Closer look

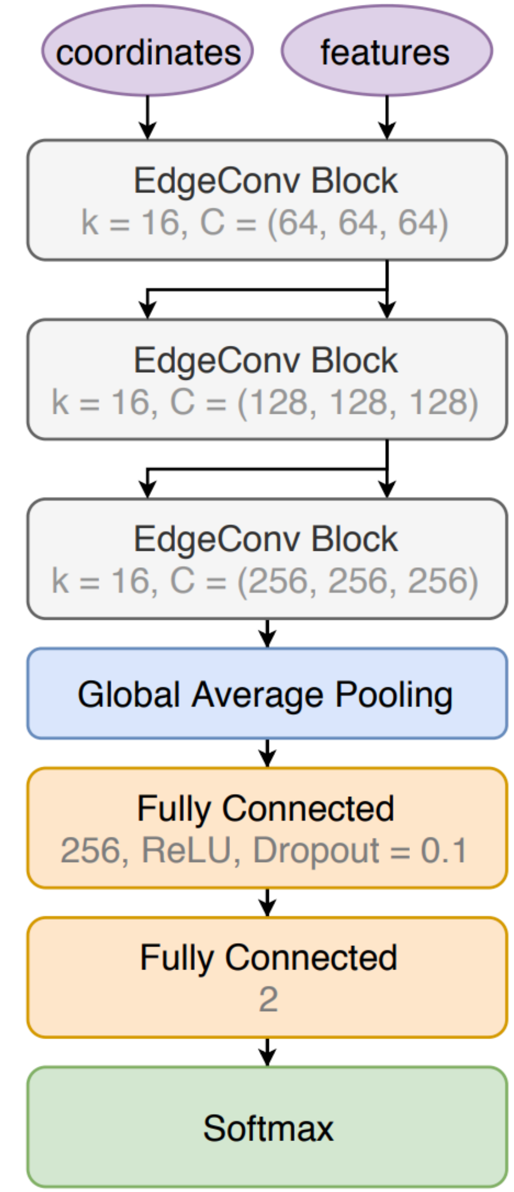


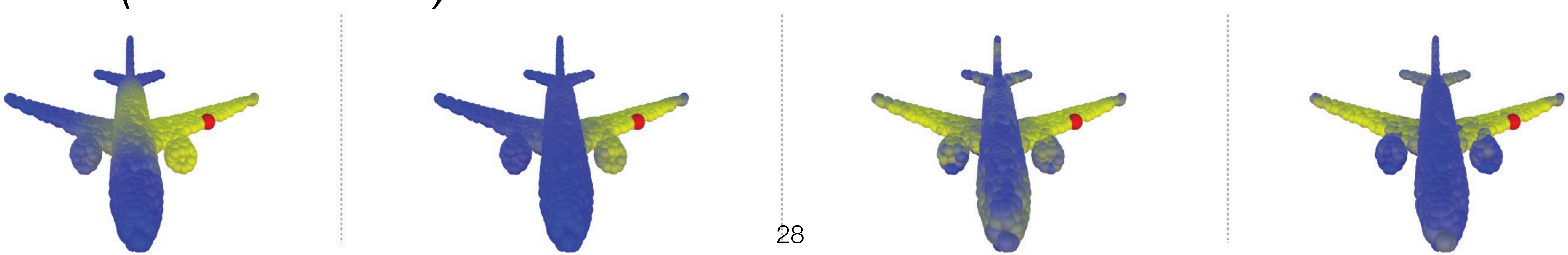

$$\boldsymbol{x}'_i = \underset{j=1}{\overset{k}{\square}} \boldsymbol{h}_{\boldsymbol{\Theta}}(\boldsymbol{x}_i, \boldsymbol{x}_{i_j})$$

*Aggregation function (sum or max)*

*Neural network*

$$\boldsymbol{h}_{\boldsymbol{\Theta}}(\boldsymbol{x}_i, \boldsymbol{x}_{i_j}) = \bar{\boldsymbol{h}}_{\boldsymbol{\Theta}}(\boldsymbol{x}_i, \boldsymbol{x}_{i_j} - \boldsymbol{x}_i)$$



# Generative models

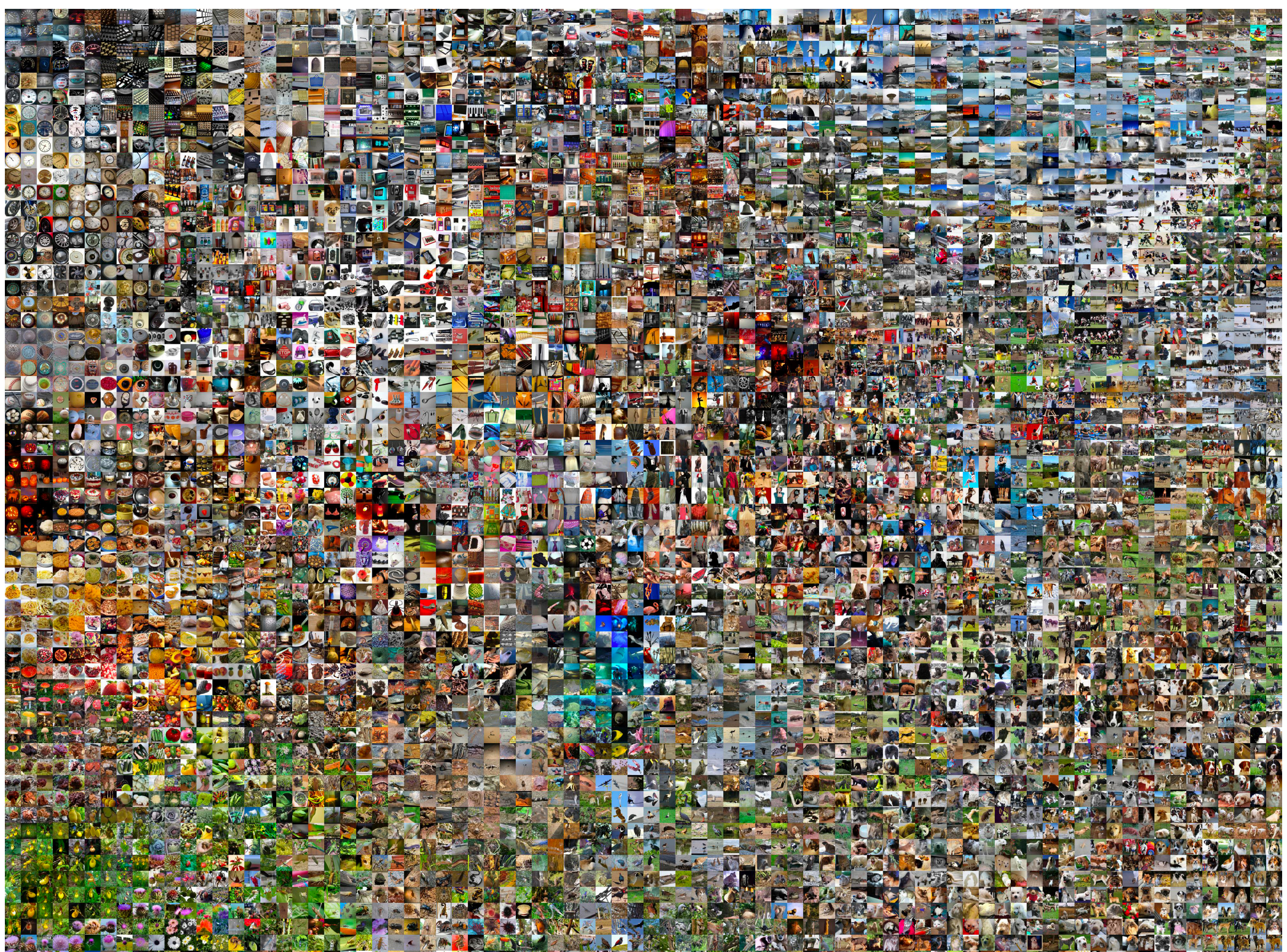
# Generative Networks

*Large Scale GAN Training for High Fidelity Natural Image Synthesis*, A Brock, J Donahue, K Simonyan, 1809.11096

https://www.thispersondoesnotexist.com/

# Generators

We **have**:
many images
(or collision events,
or detector readouts, …)



*wired.com*

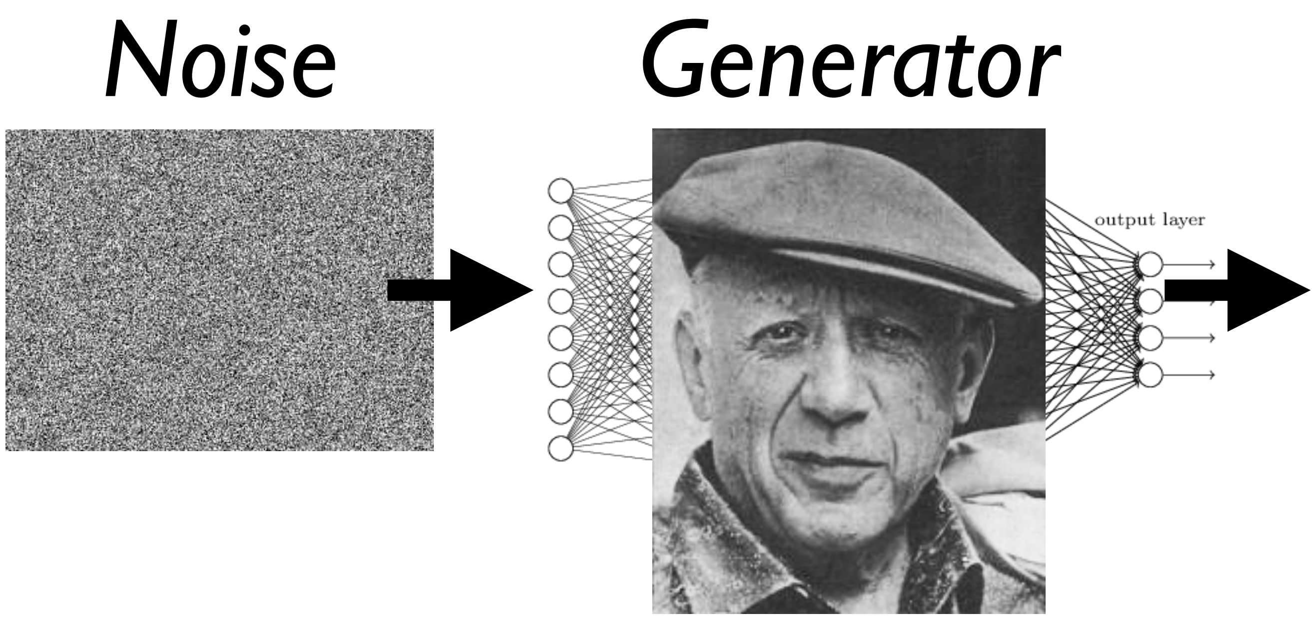
We **want**: more images.

(Specifically: New examples that are similar to the examples, but not exact copies)

How to encode in neural net?

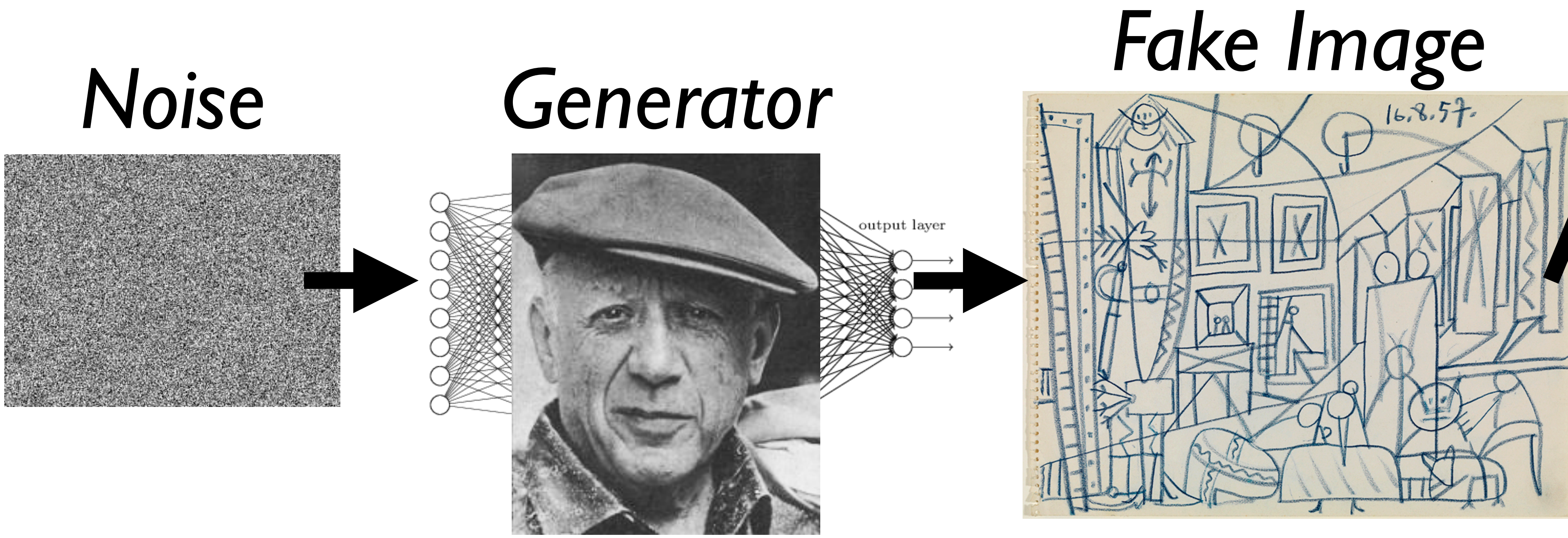
# Alternating Training

Train Generator
Freeze Discriminator
*Then*
Train Discriminator
Freeze Generator

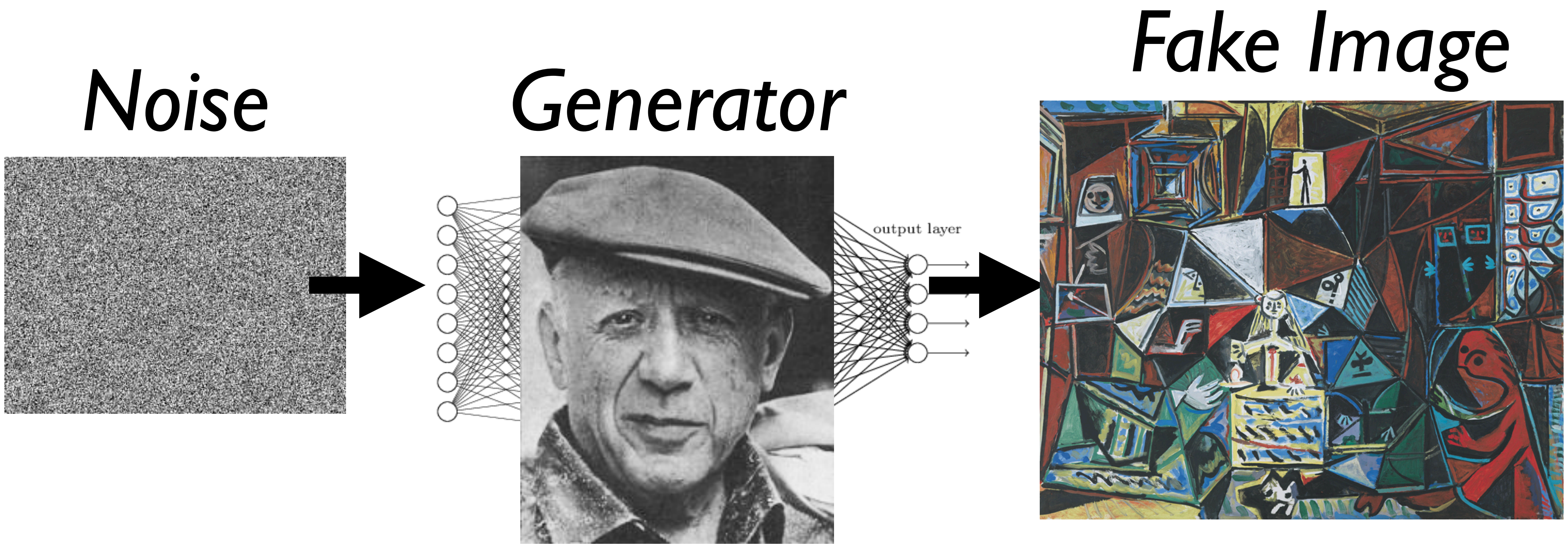
# Alternating Training

Train Generator
Freeze Discriminator
*Then*
Train Discriminator
Freeze Generator

# Alternating Training

Train Generator
Freeze Discriminator
*Then*
Train Discriminator
Freeze Generator

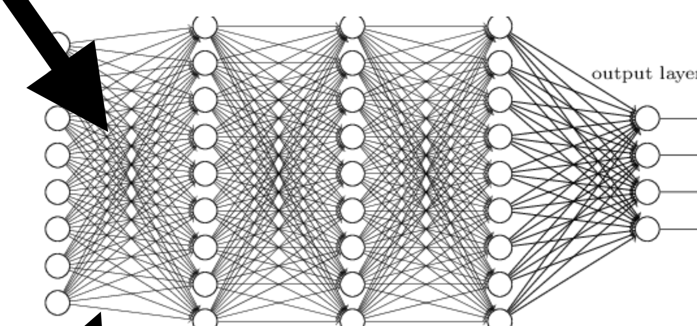



# Alternating Training

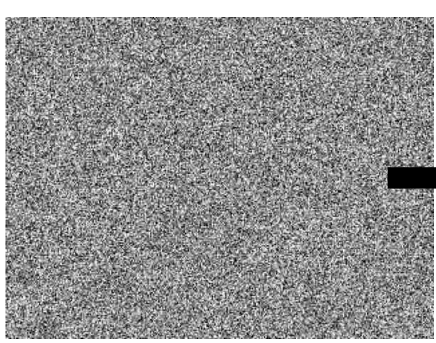
Train Generator
Freeze Discriminator
*Then*
Train Discriminator
Freeze Generator

*Real Images*

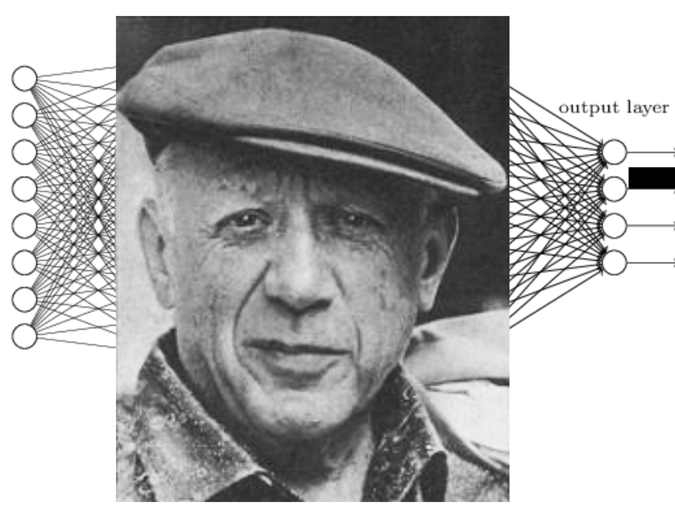
*Discriminator*




*Noise*

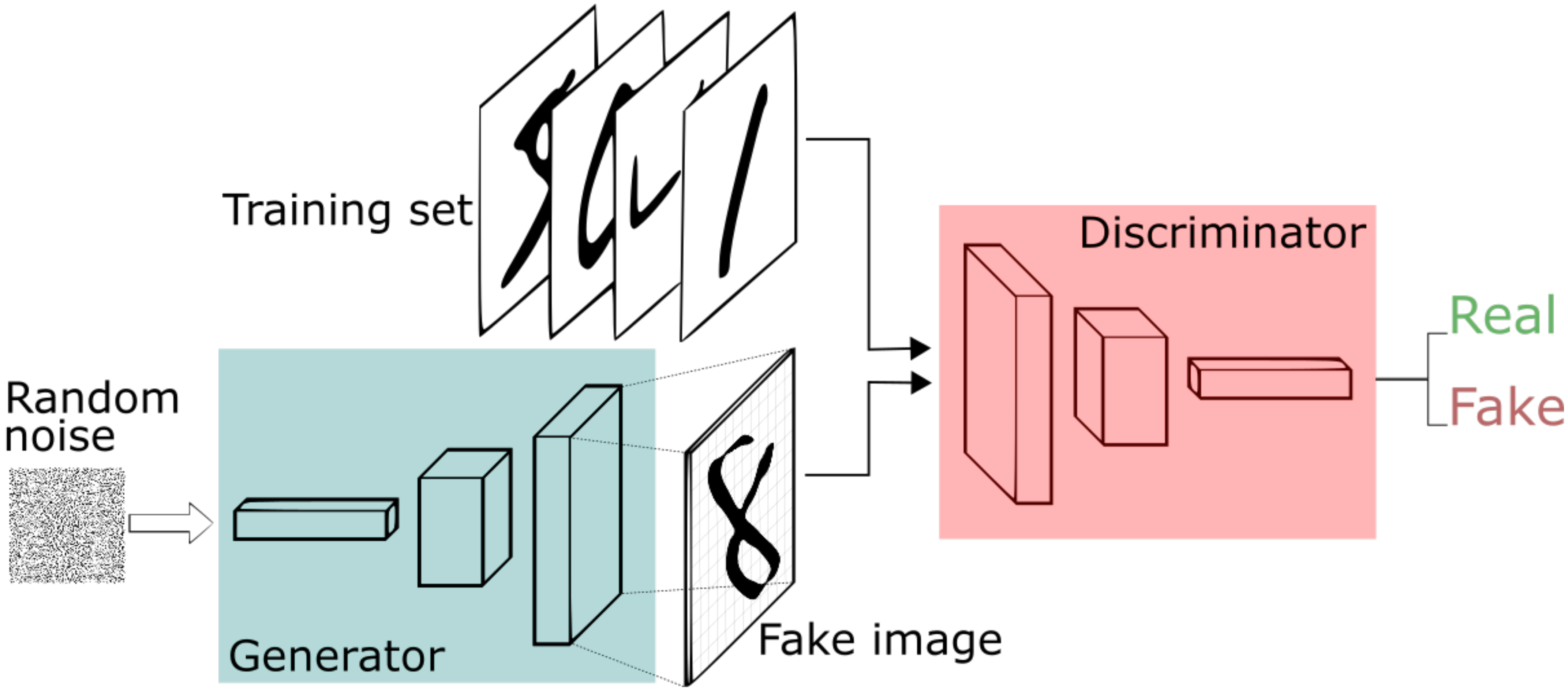


*Generator*




*Fake Image*

# Generative Adverserial




$$\min_G \max_D V(D,G) = \mathbb{E}_{\boldsymbol{x}\sim p_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z}\sim p_{\boldsymbol{z}}(\boldsymbol{z})}[\log(1 - D(G(\boldsymbol{z})))]$$

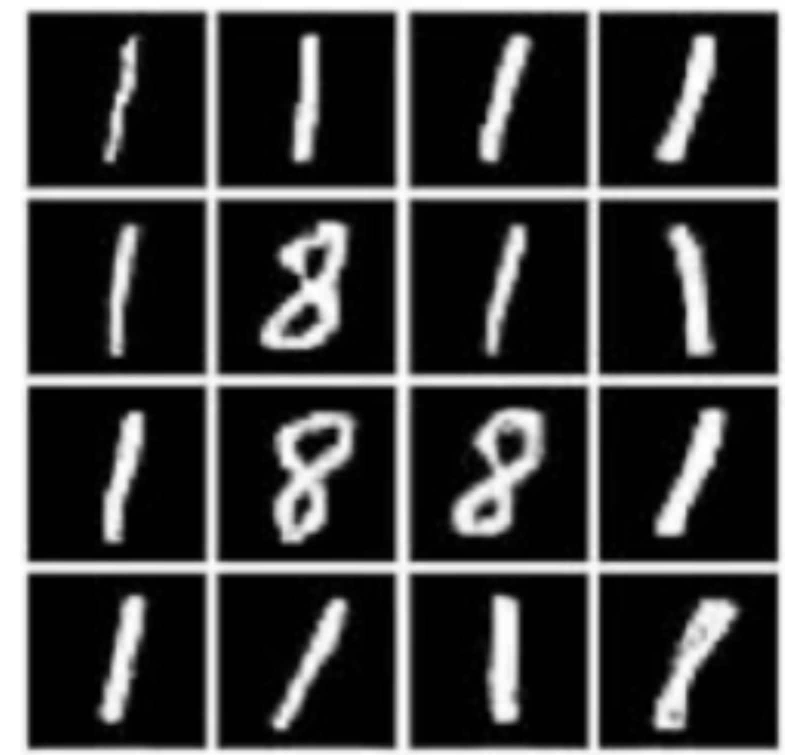
*Real Samples*

*Generated Fake Samples*

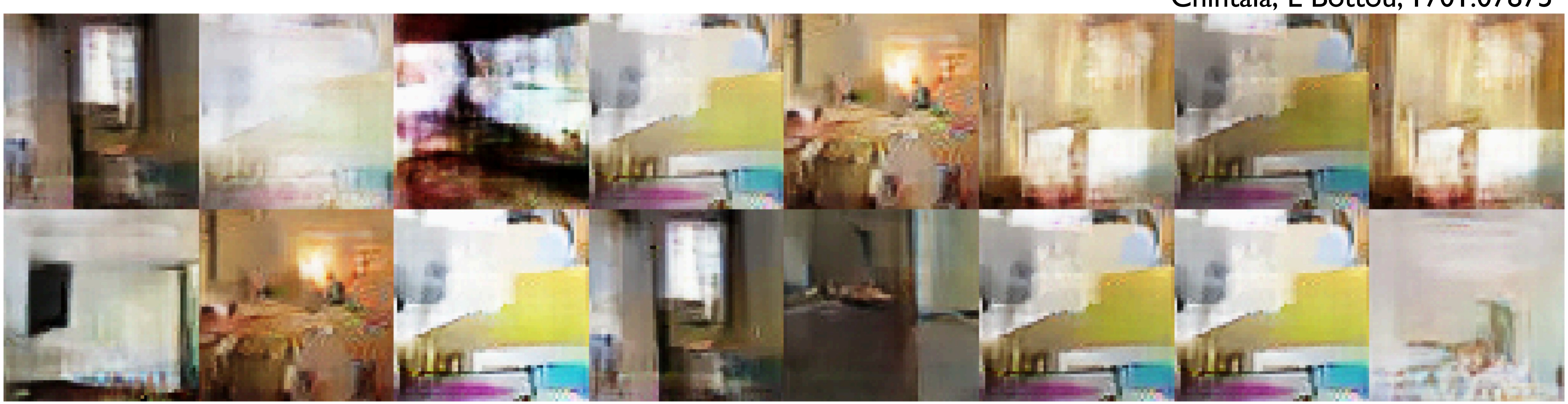
*Generative Adversarial Networks*
IJ Goodfellow et al
1406.2661

# GAN Problems

- Stability and convergence of learning
- Generator & Discriminator matching
  - Vanishing gradient
  - (use small momentum in training)
- Mode collapse
- Hard to interpret loss
  - Not correlated to image quality
- Similar to issues with adversarial training



*lilianweng*
*Wasserstein GAN,* M Arjovsky, S Chintala, L Bottou, 1701.07875

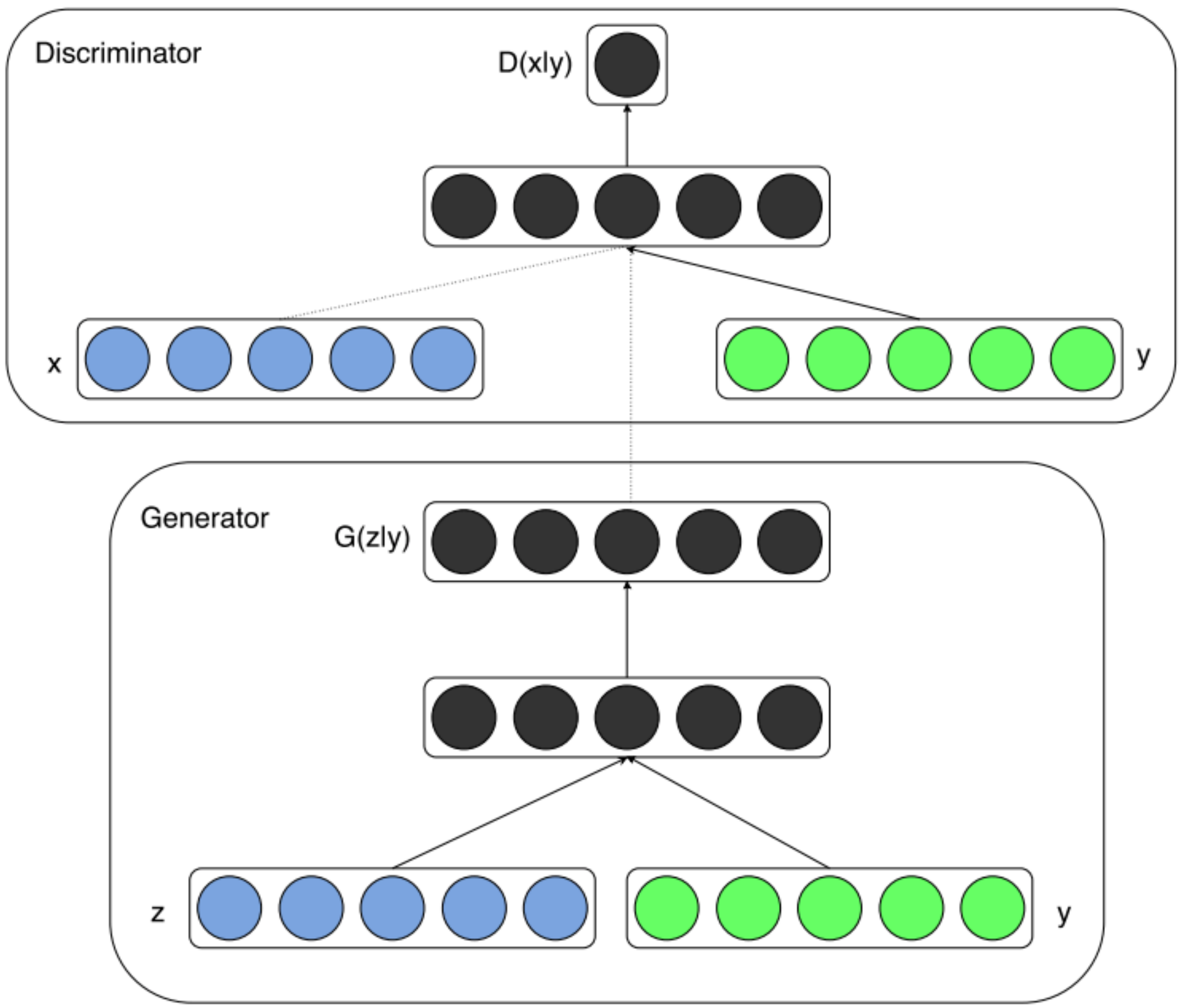


# Label Conditioning

- To improve usefulness (and training) of GANs:
  - Provide information on picture we are simulating (label y)
  - Use this information in training of generator and discriminator conditioning

$$\log D(x) + \log(1 - D(G(z)) \to \log D(x|y) + \log(1 - D(G(z|y'))$$

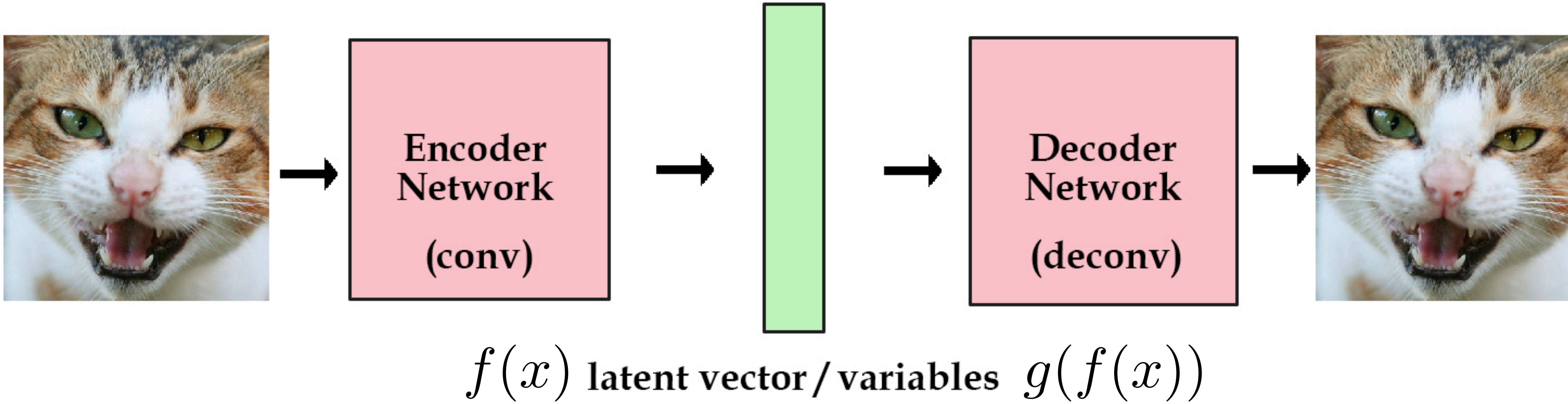
- Counteract mode collapse
- Key for physics application (labels: energy, particle type, …)




*Conditional Generative Adversarial Nets*
M Mirza, S Osindero
1411.1784

# Variational Autoencoder

# Autoencoder

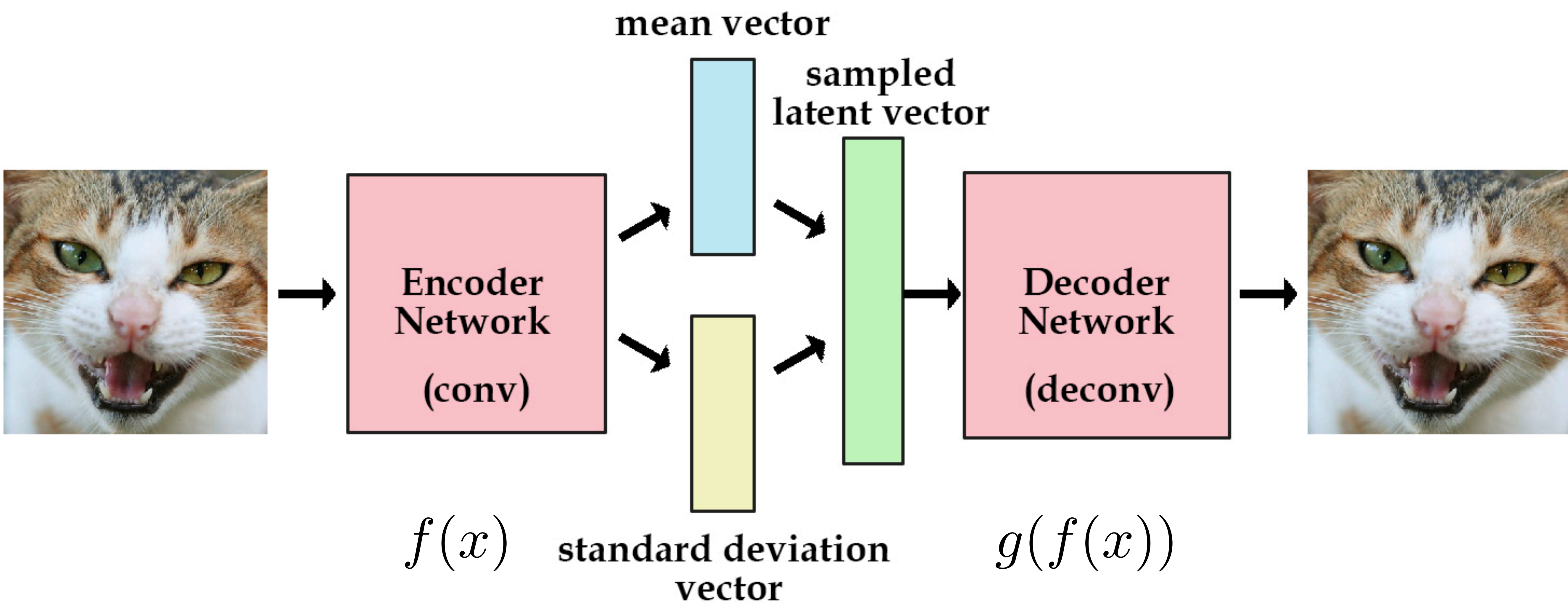



$$L = (\hat{y} - g(f(x)))^2$$

- Self-supervised learning
- *Latent space/bottleneck* with compressed representation (remember yesterday!)
- Dimension reduction
- Denoising
- Anomaly detection (later today!)

*kvfrans*
*deeplearningbook.org*

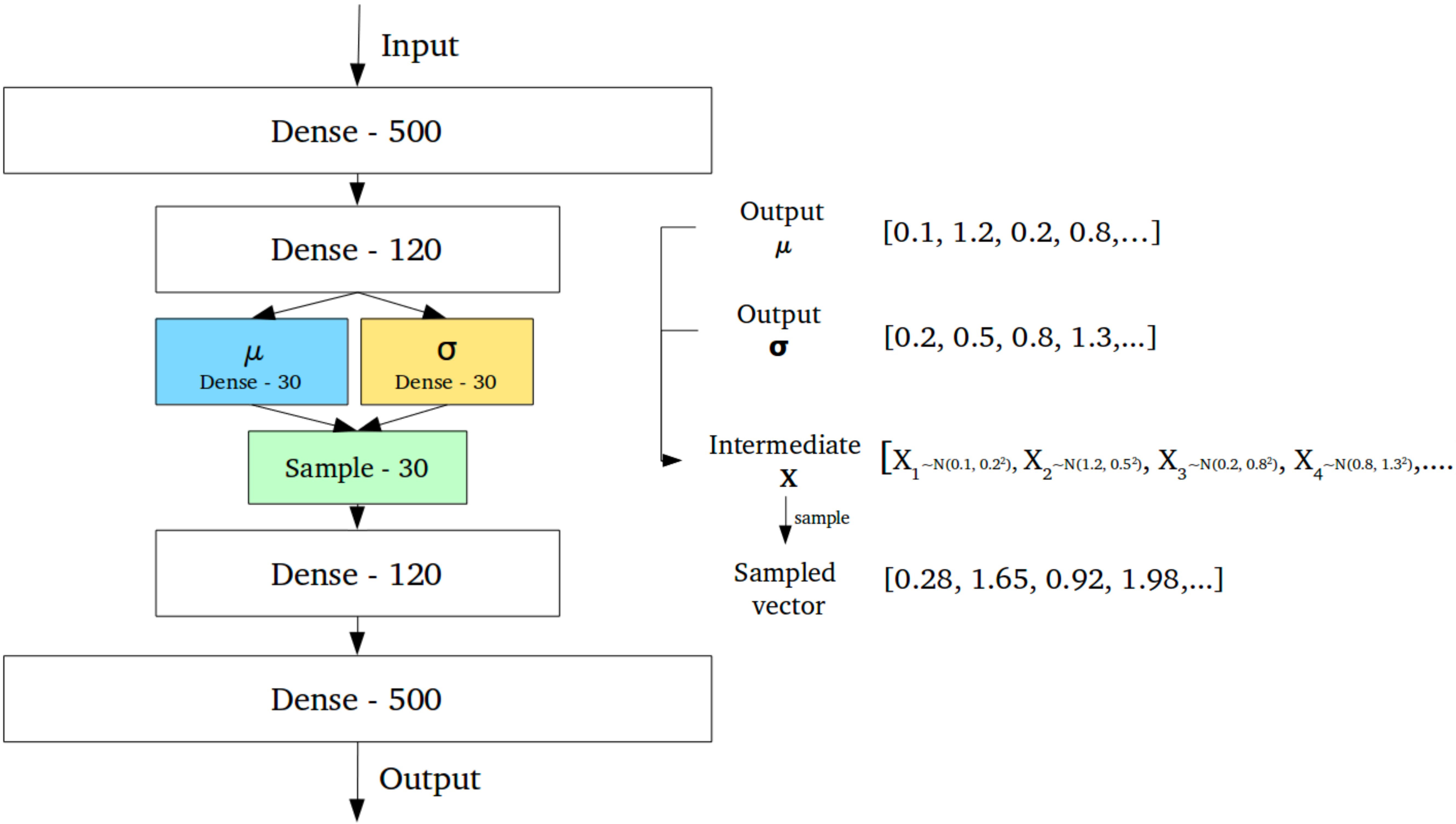
# Variational Autoencoder




- Want to sample from latent space
- Split into mean and standard deviation
- Add penalty term (Kullback-Leibler divergence)
  so mean/std are close to unit Gaussian

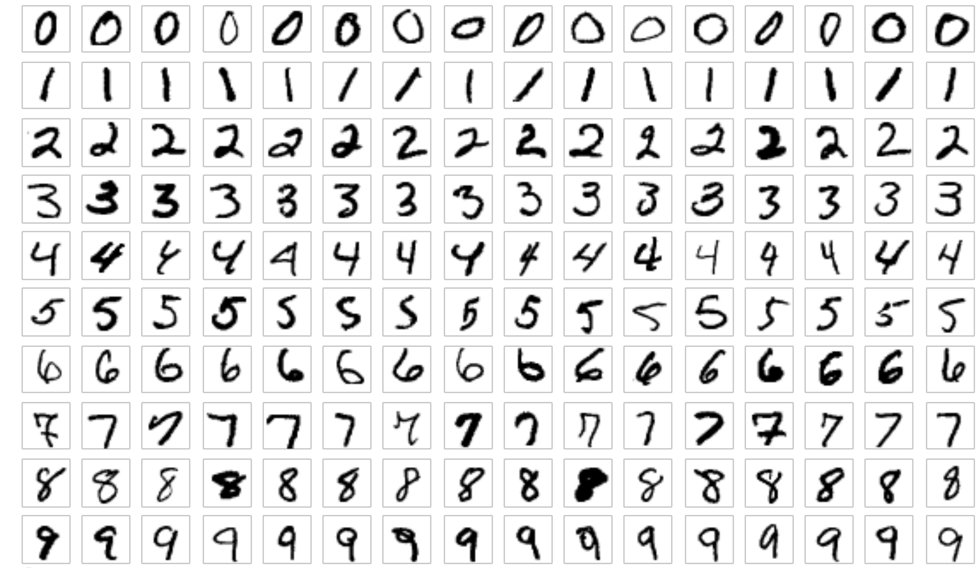
*kvfrans*
*towardsdatascience.com*

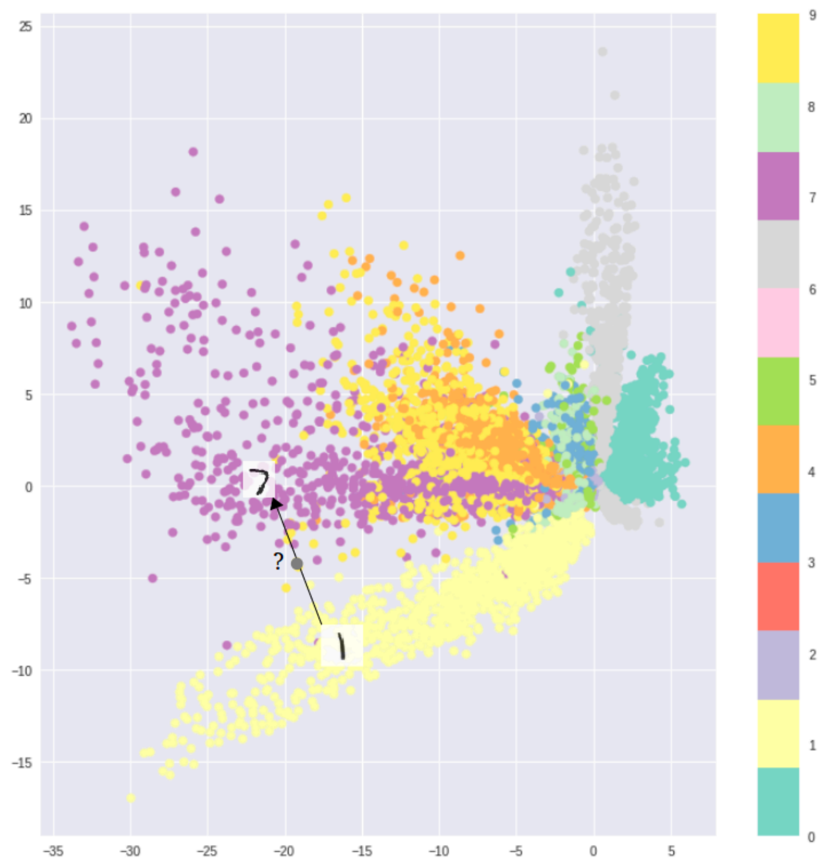
# Concrete



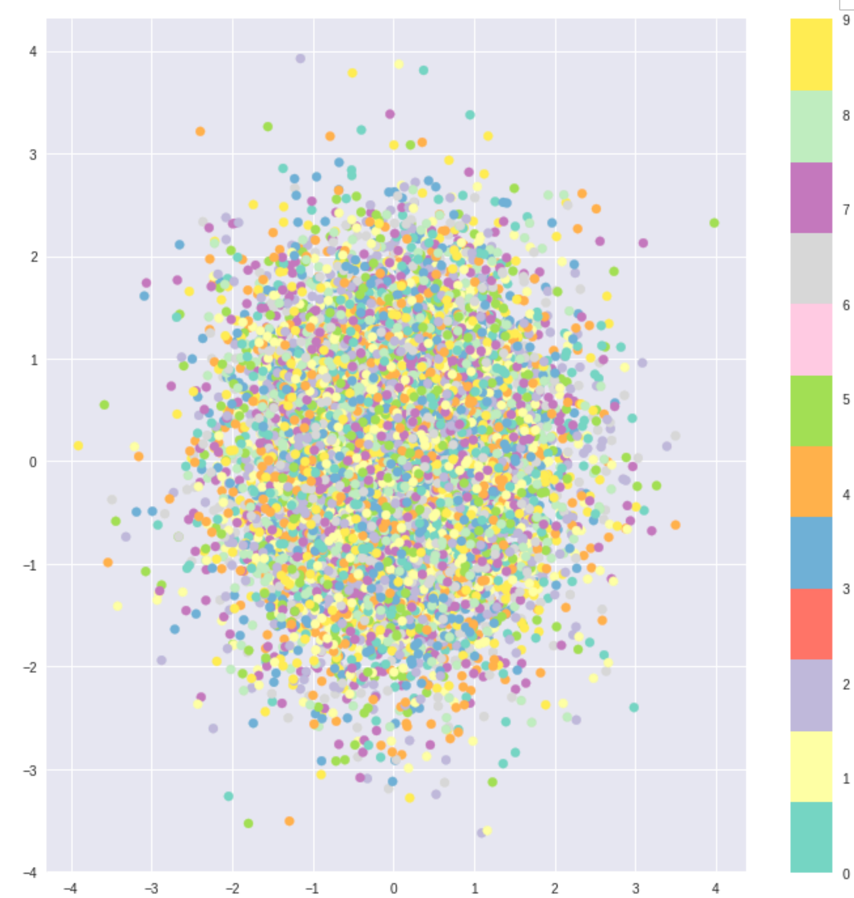

towardsdatascience.com

# Variational Autoencoder

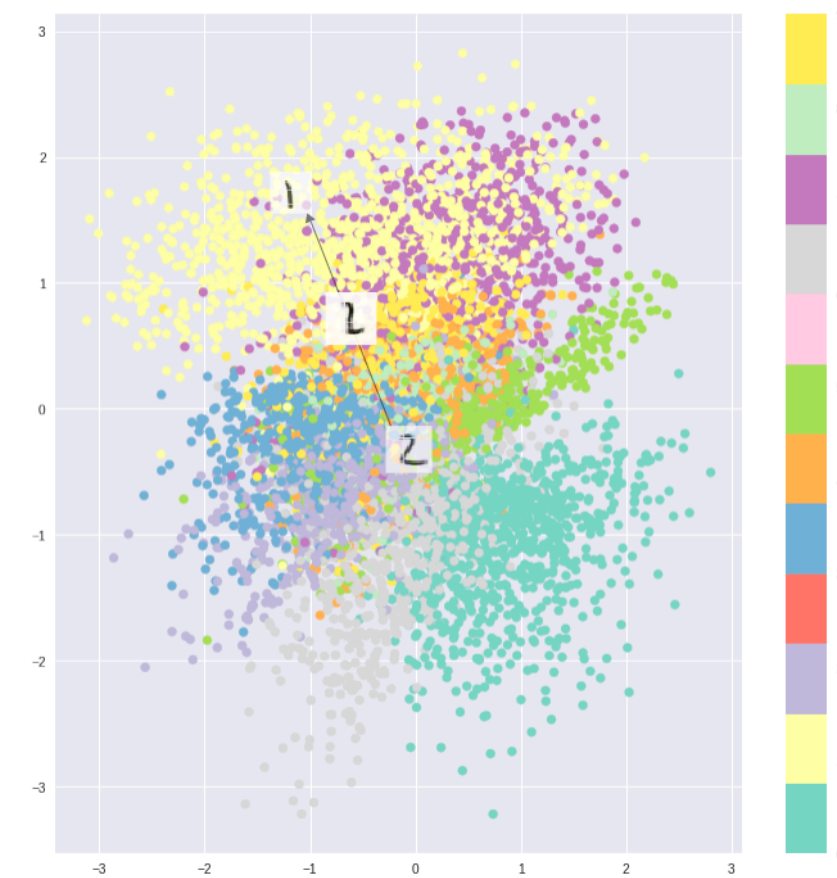




*Reconstruction Loss Only*



*KL Loss Only*



*Combined Loss*

$$L = (\hat{y} - g(f(x)))^2$$

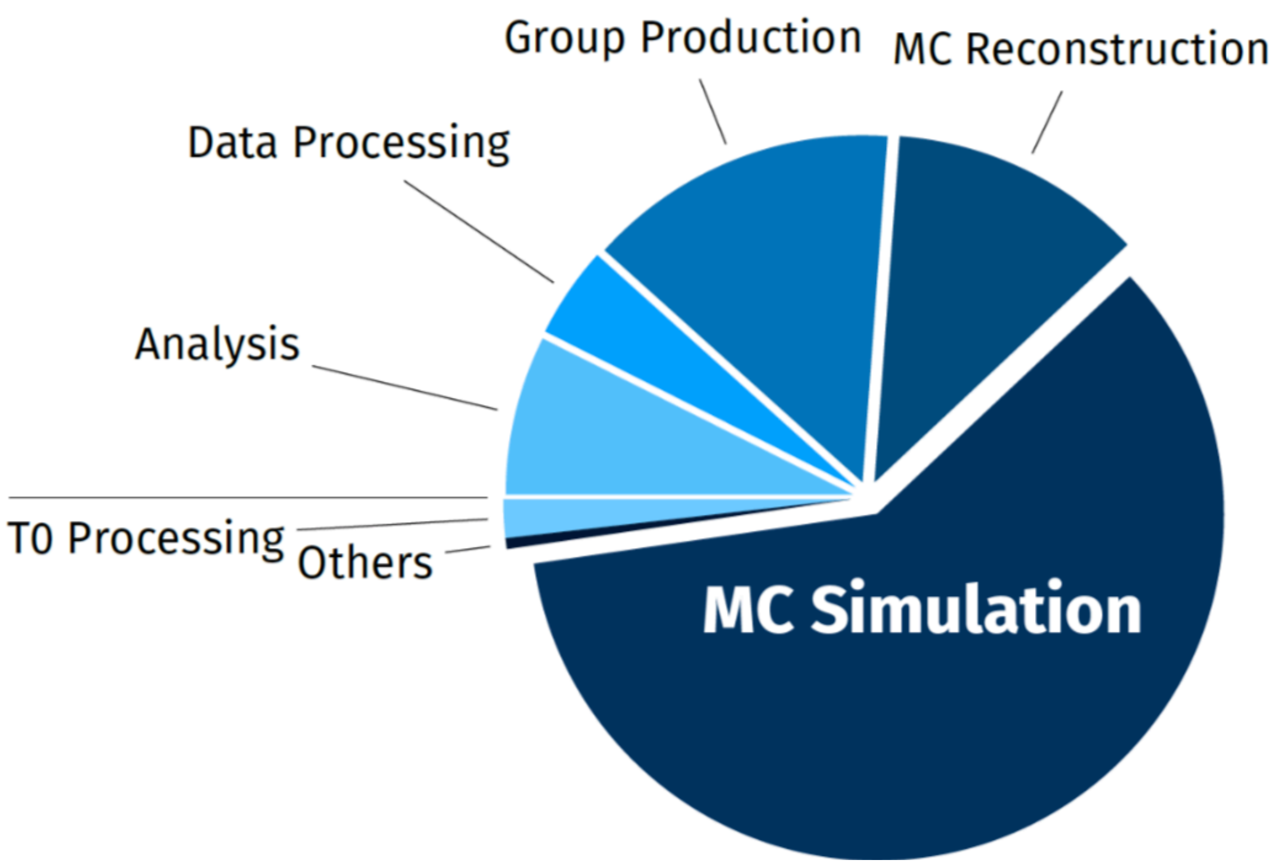
$$\frac{1}{2}\sum_{j=1}^{J}\left(1 + \log((\sigma_j)^2) - (\mu_j)^2 - (\sigma_j)^2\right)$$

kvfrans

*1312.6114*

*towardsdatascience.com*

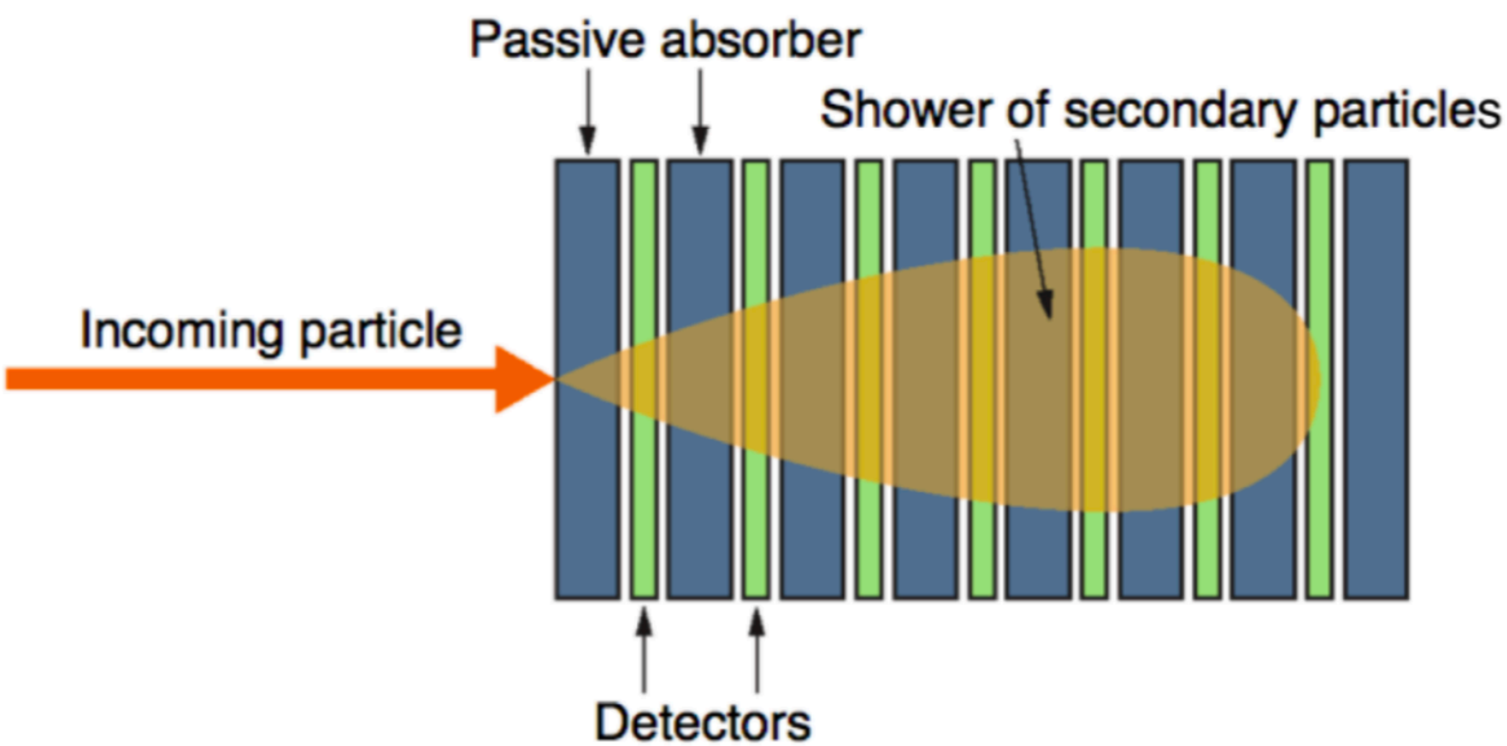
# Physics Uses

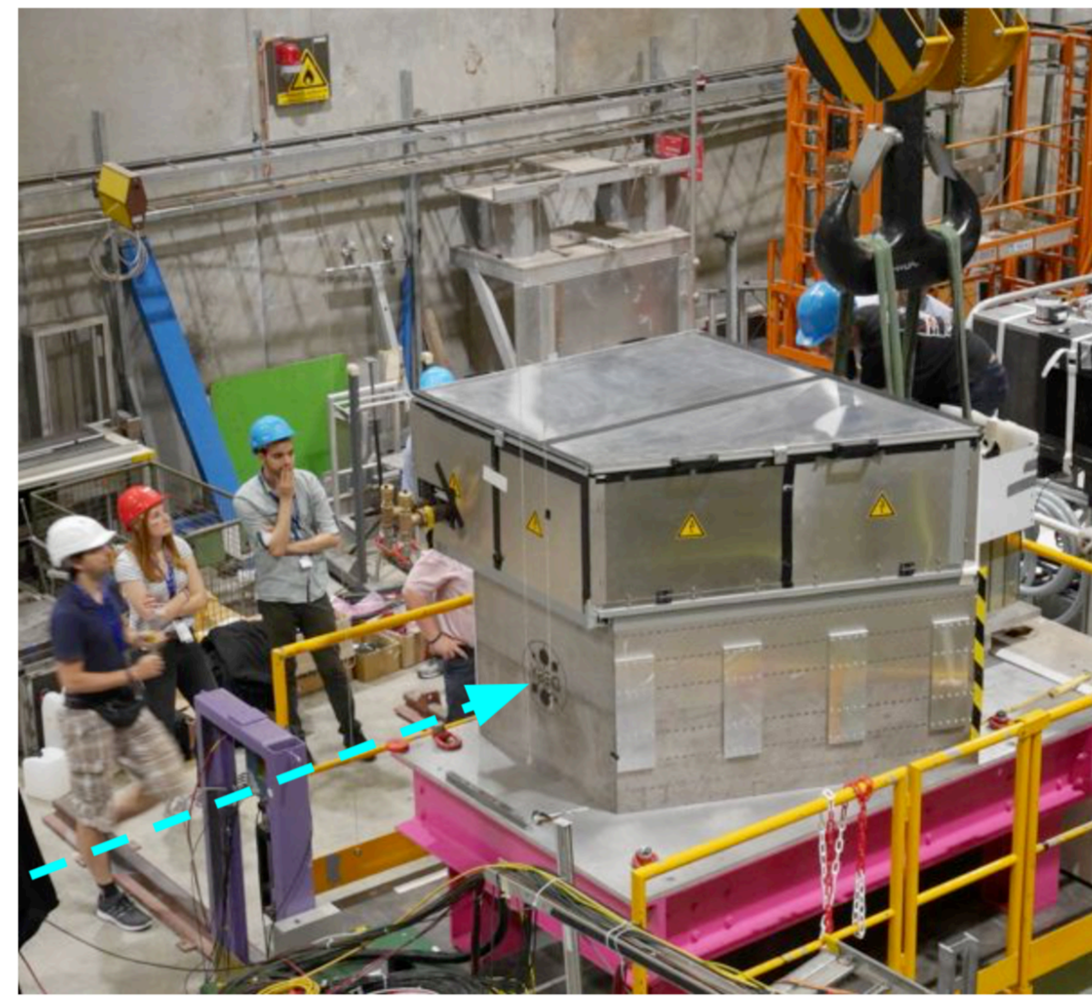



*Tobias Golling, Hammer&Nails 19*

# Particle Showers

Main motivation:
*Fast simulation of interaction between particles and detector material*
Started by CaloGAN (1705.02355)

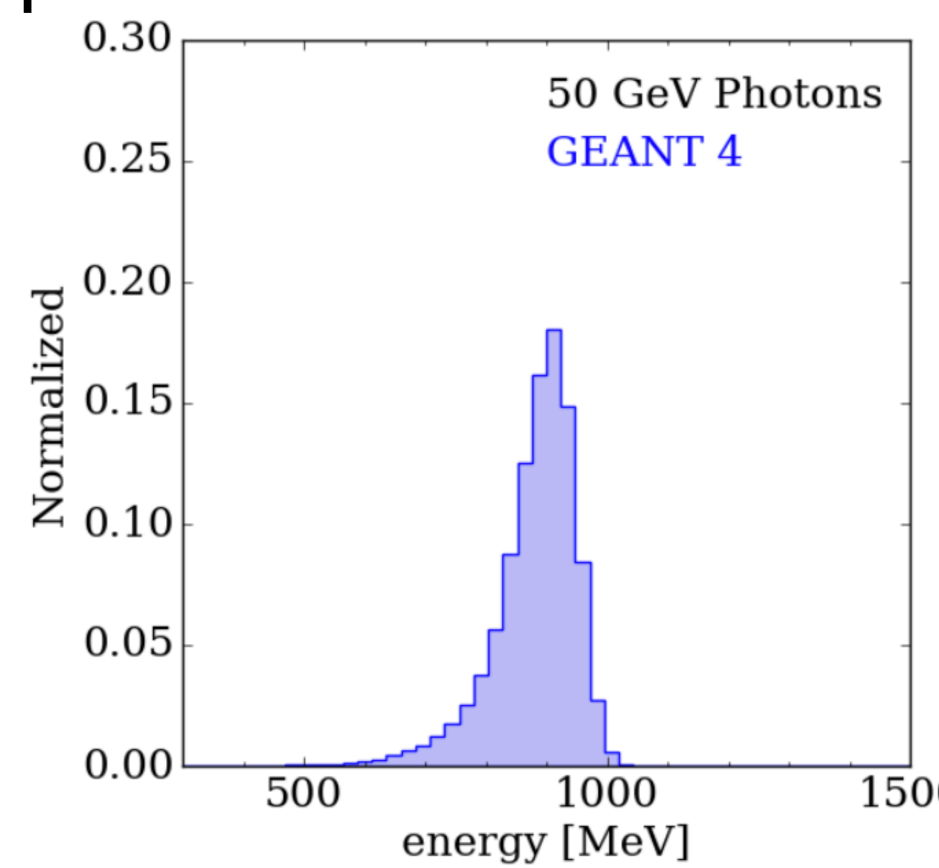


Generative models are also applied to:
*phase space integration and sampling, event generation, ….*

# Additional Challenges

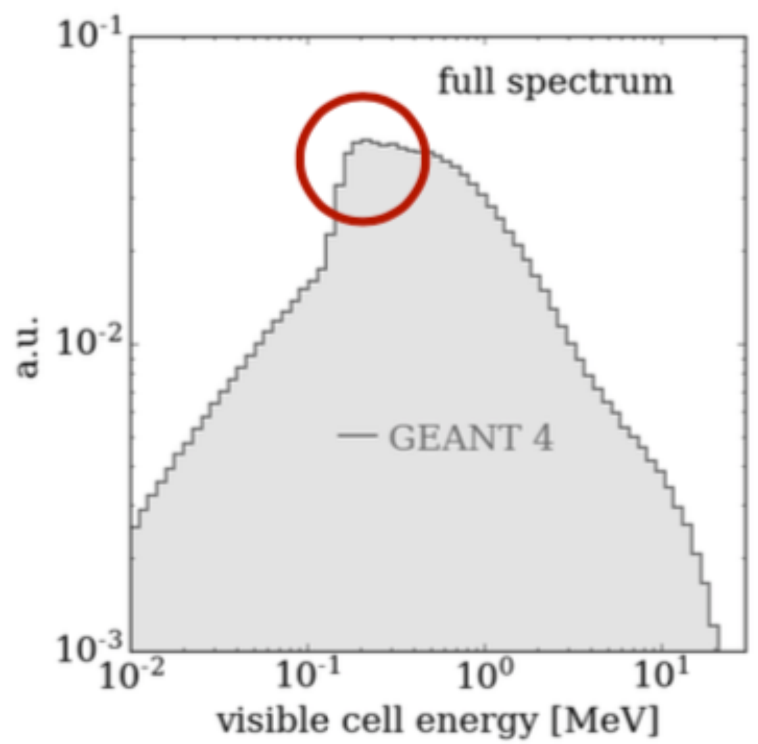
- How to evaluate convergence of models?
- Correctly model differential distributions
- Condition on a large number of quantities (energy, particle type, impact position, angle, …)
- Other considerations:
  Coverage (do I produce example for all phase space?)
  Saliency (is this a good example of the desired type of event)
  Mode collapse
  Overfitting

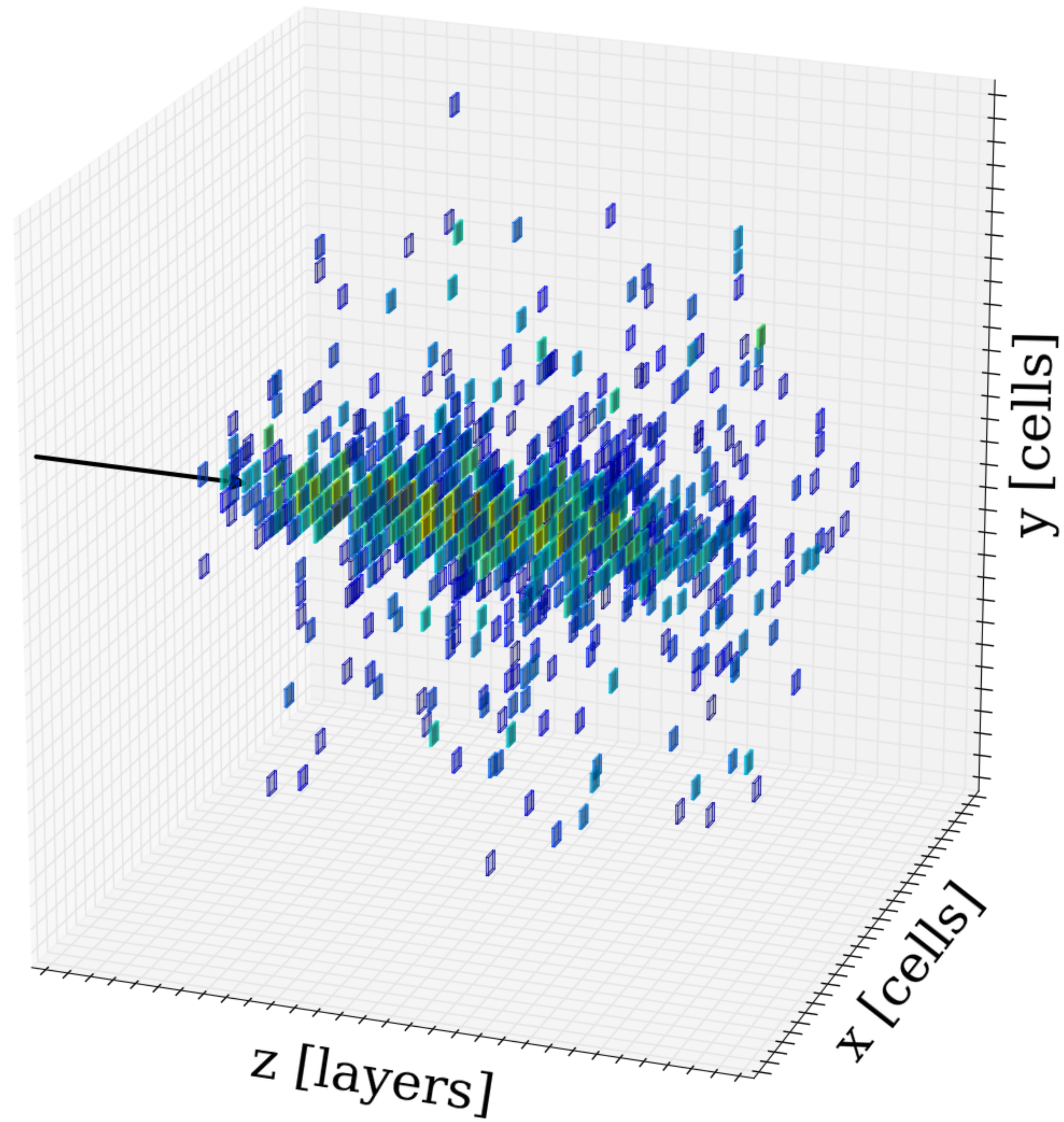


# Concrete Problem

**Describe photon showers in high granularity calorimeter prototype**

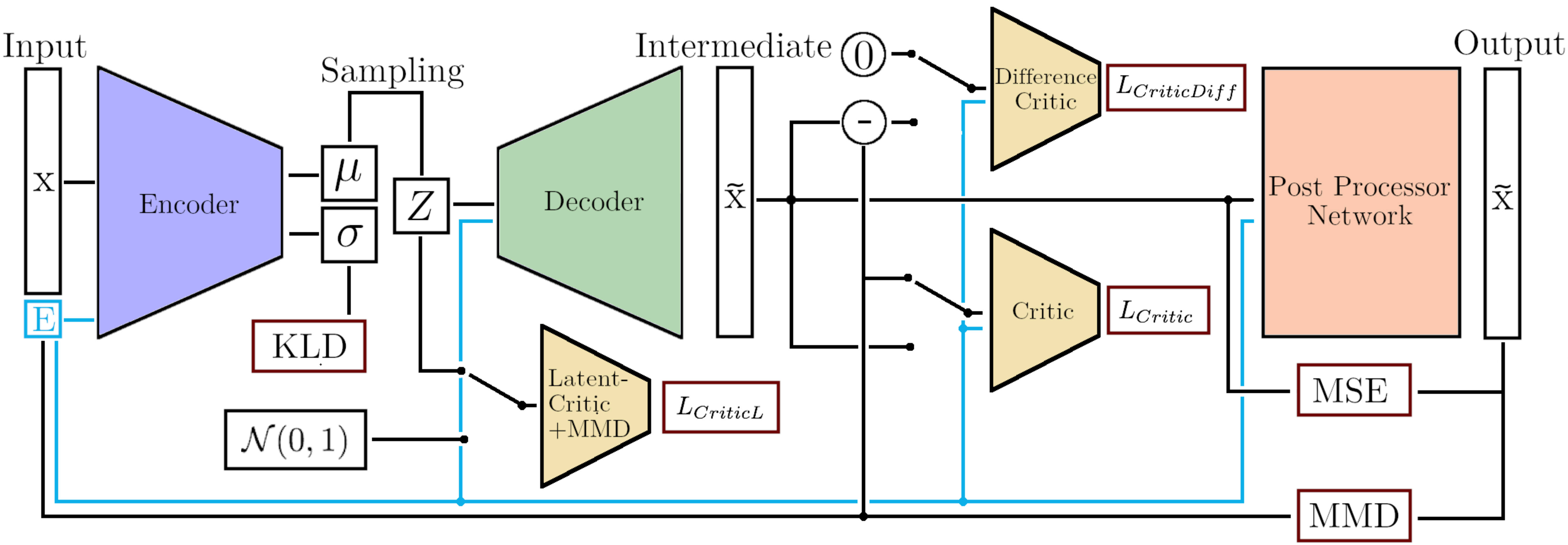
- 30x30x30 cells (Si-W)
- Photon energies from 10 to 100 GeV
- Use 950k examples (uniform in energy) created with GEANT4 to train



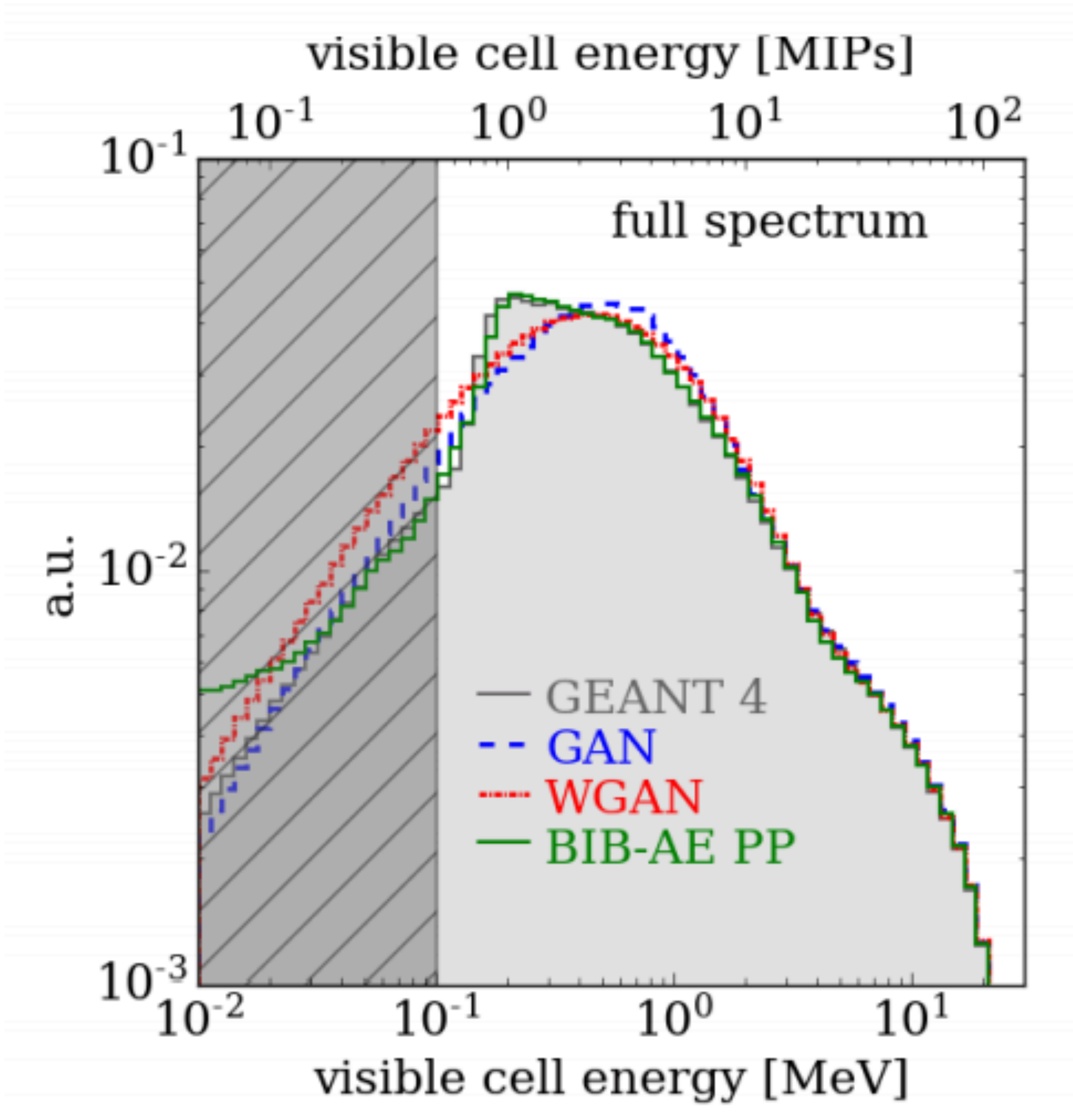

- Not only model individual images but also **differential distributions**

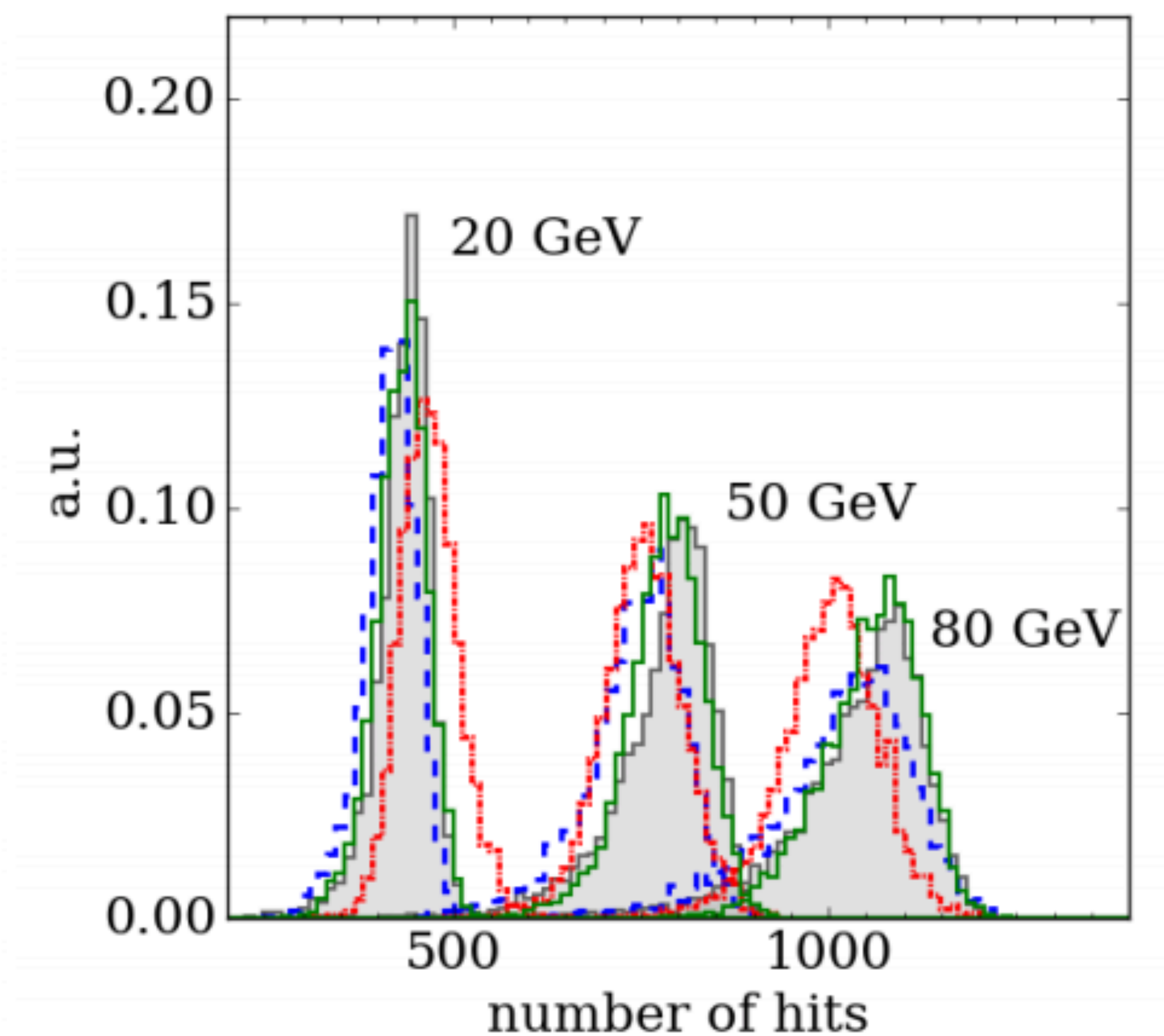
# Architecture




- BIB-AE (based on 1912.00830) with added post-processing
- Unifies features of GAN and VAE
- 71M trainable parameters

# Result



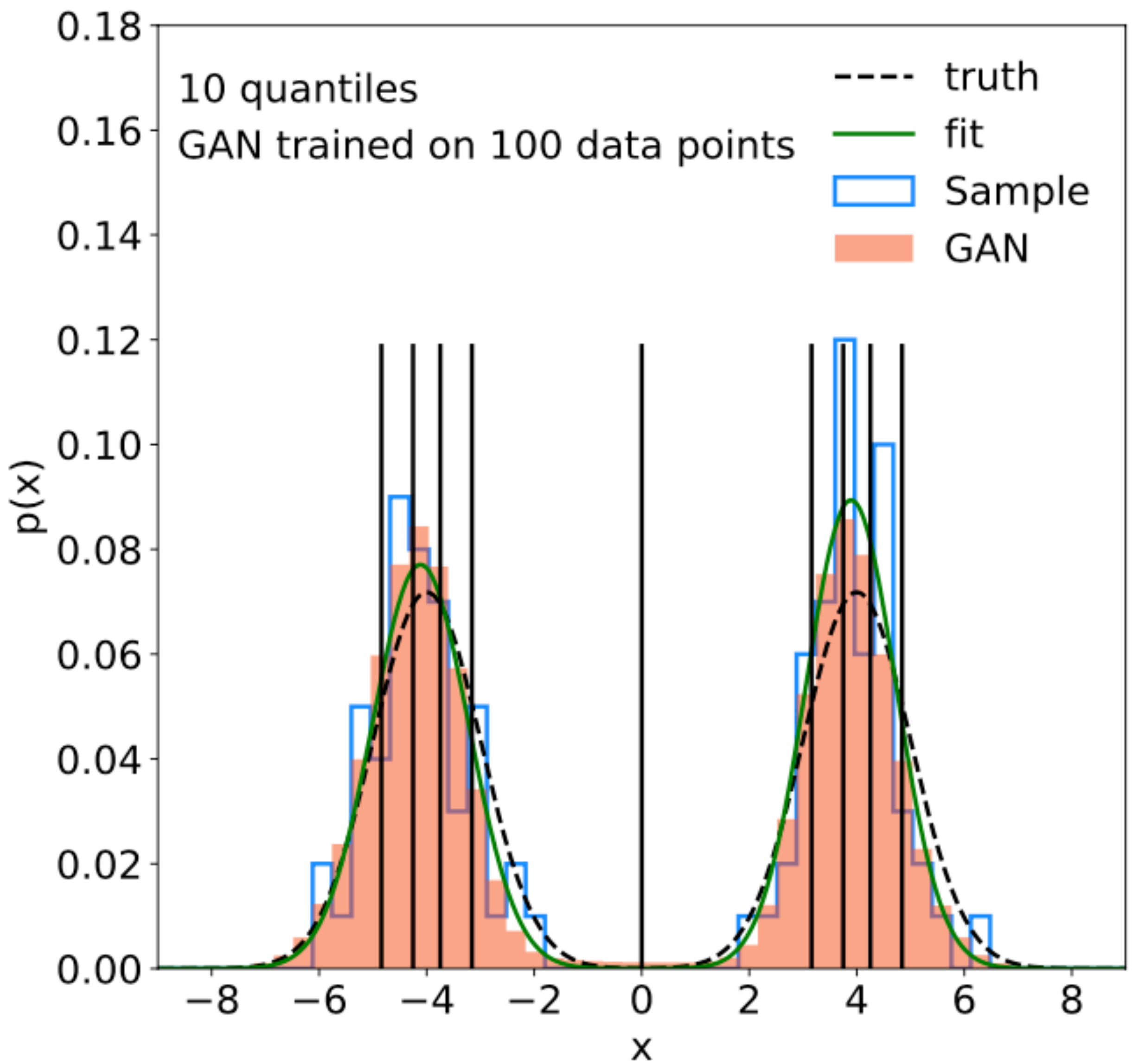



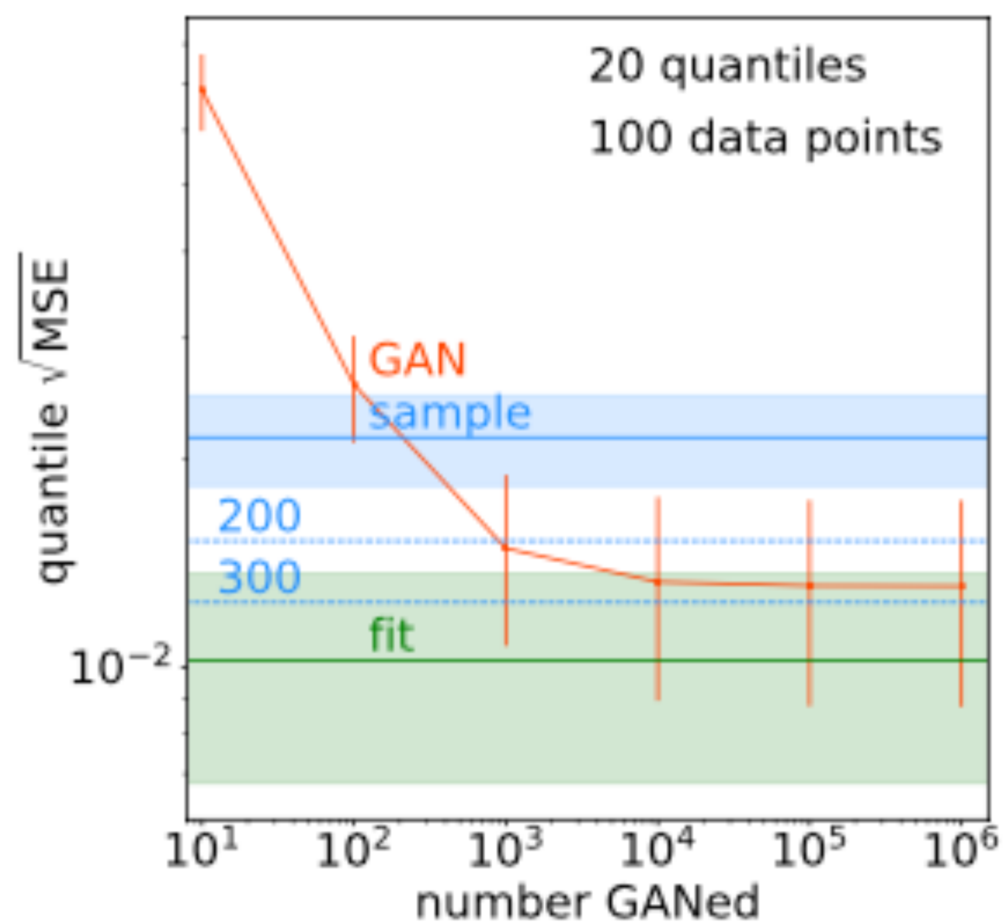

*Can now learn differential distributions*
*Still room to improve*

# Limitations of Generative Models

- Generative models are powerful in quickly producing more examples, still need training examples
- Machine learning is great at interpolation, but it cannot do magic
- Expect to simulate typical examples, do not trust the tails of distributions without verification
- Can networks **amplify?**

# Amplification 1D

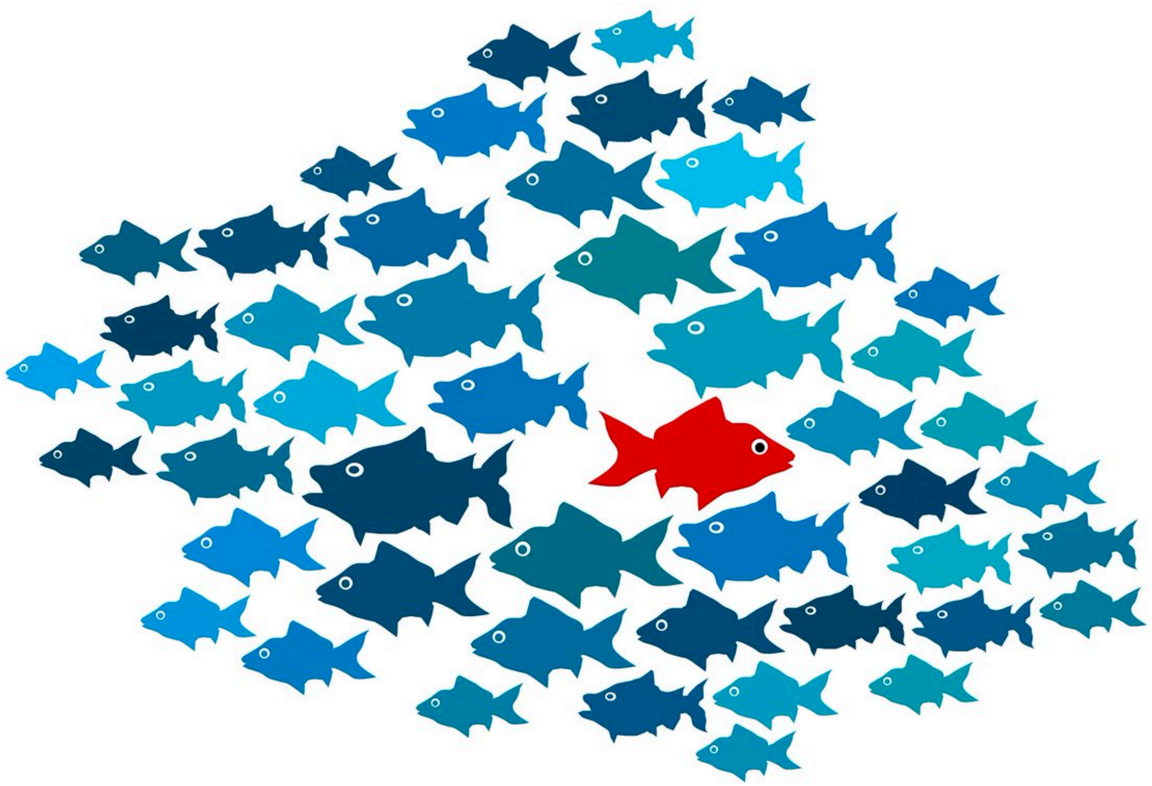


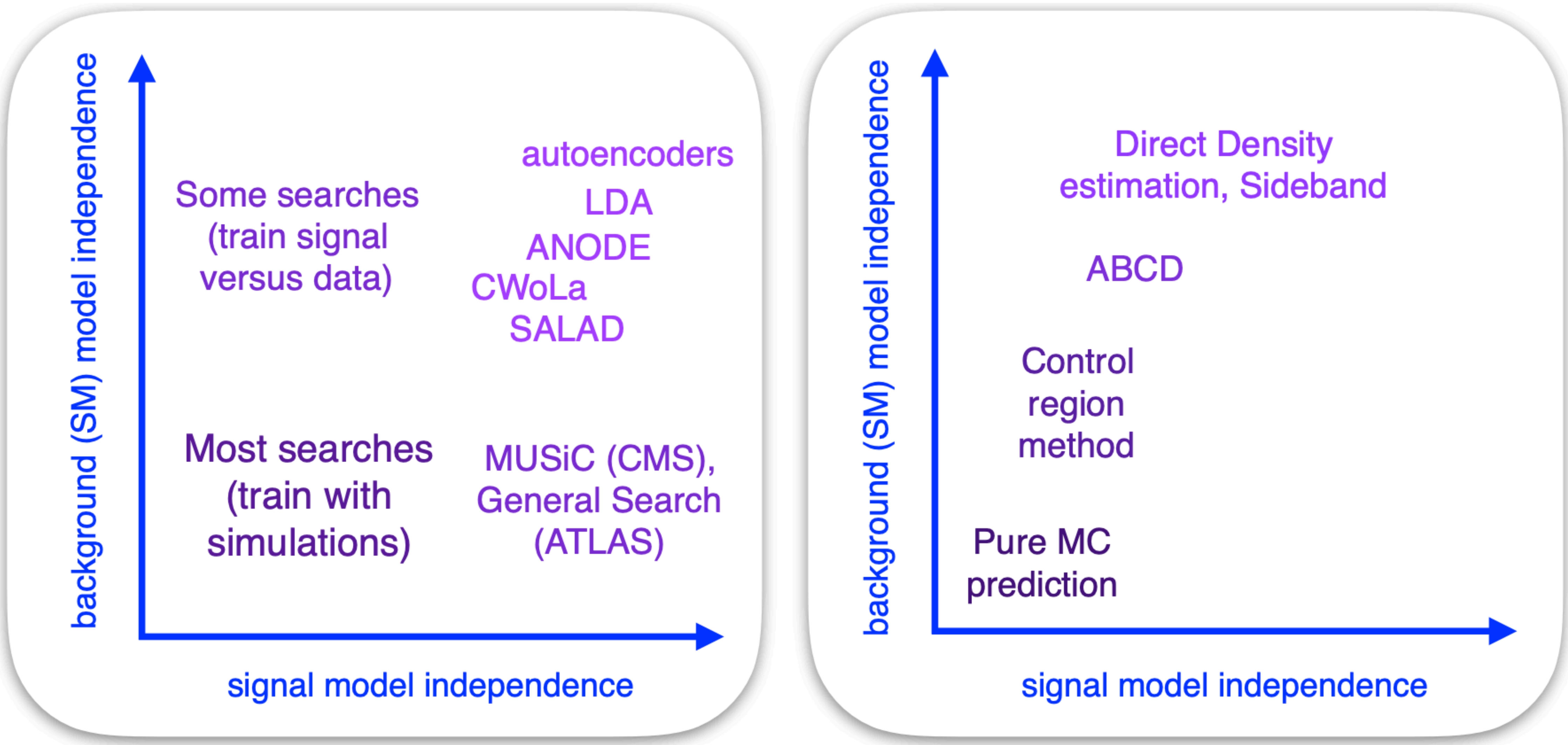

*Improve statistics of training sample by interpolation*

# Unsupervised Searches

# Can we look for new physics, without knowing what to look for?



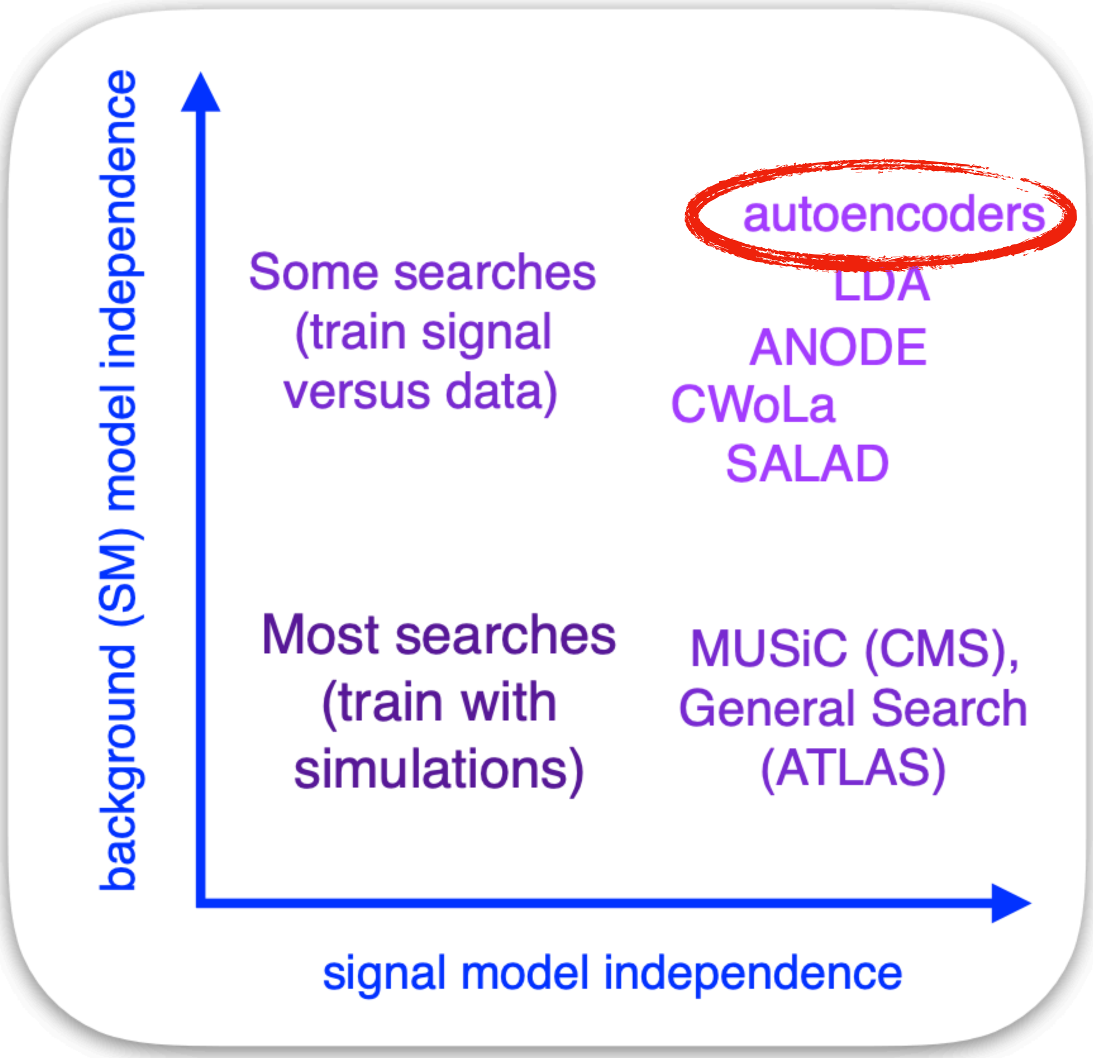
# Approaches



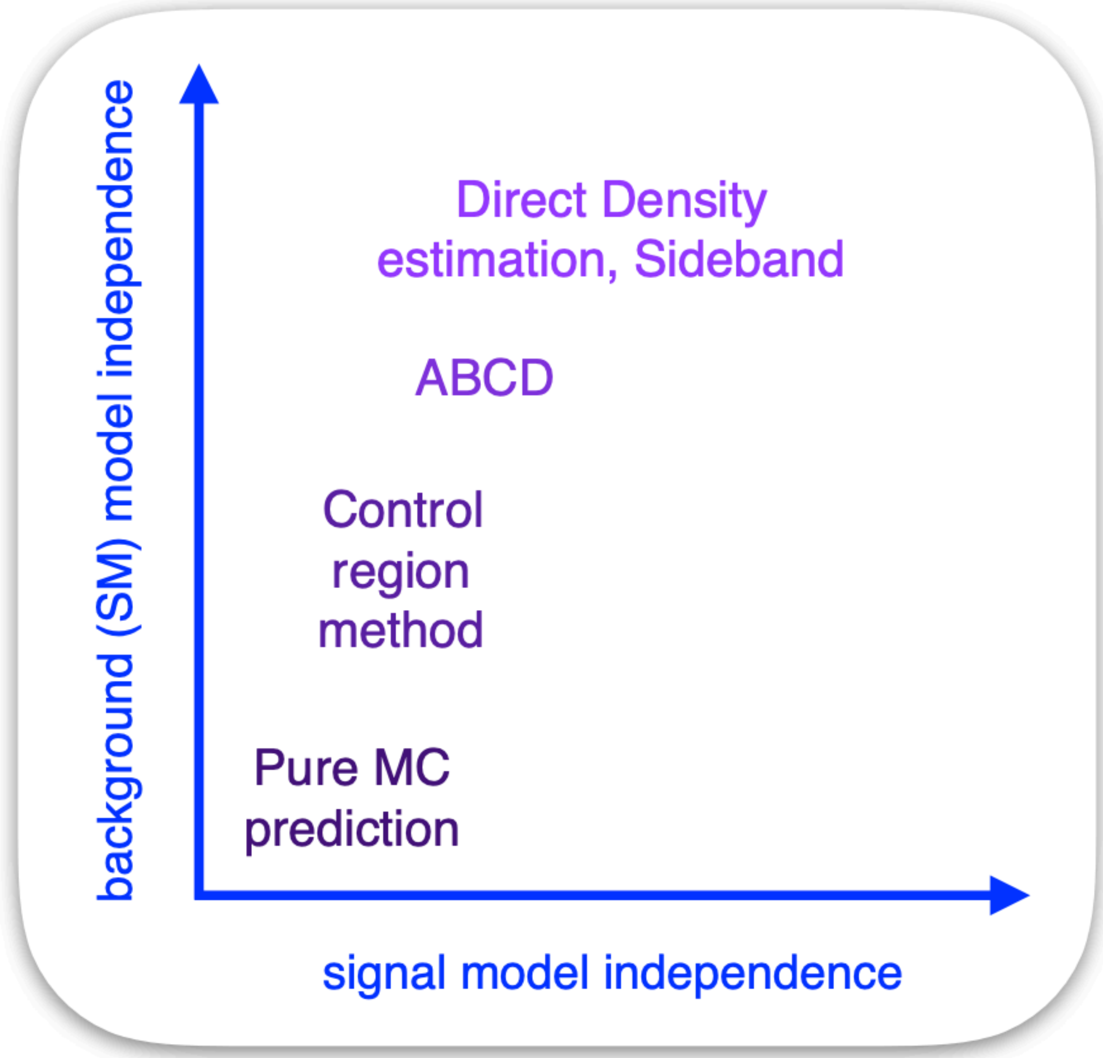

(a) Signal sensitivity (b) Background specificity

***From Ben Nachman, David Shih, 2001.04990***

# Approaches



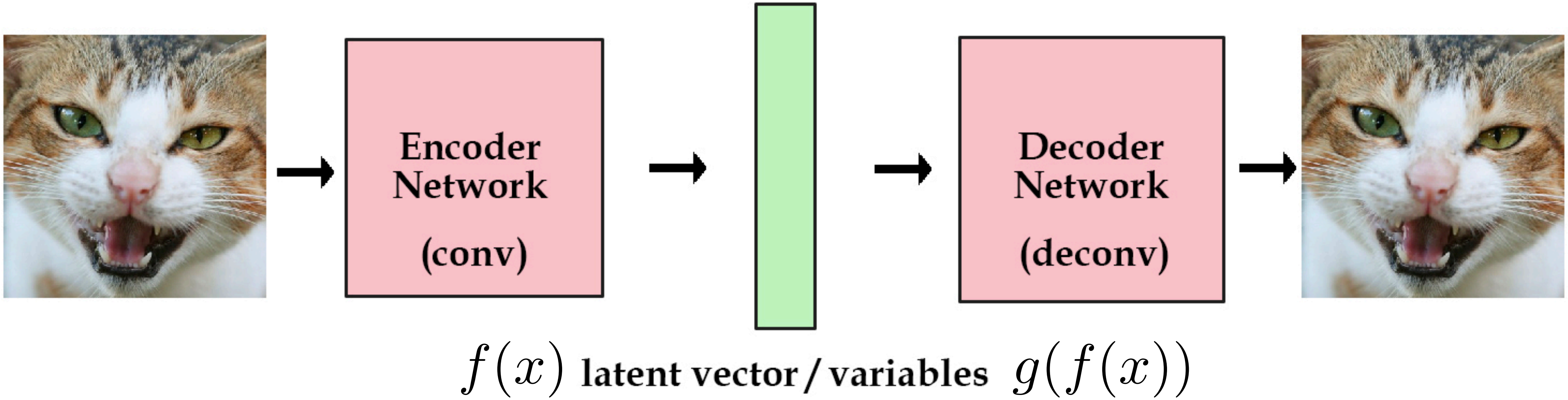

(a) Signal sensitivity




(b) Background specificity

***From Ben Nachman, David Shih, 2001.04990***

# Autoencoder

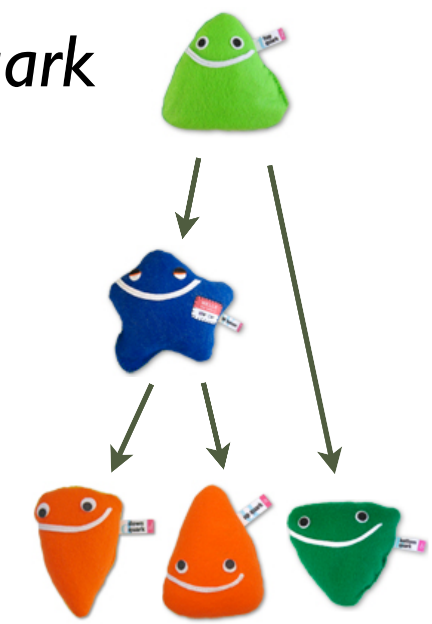



$$L = (\hat{y} - g(f(x)))^2$$

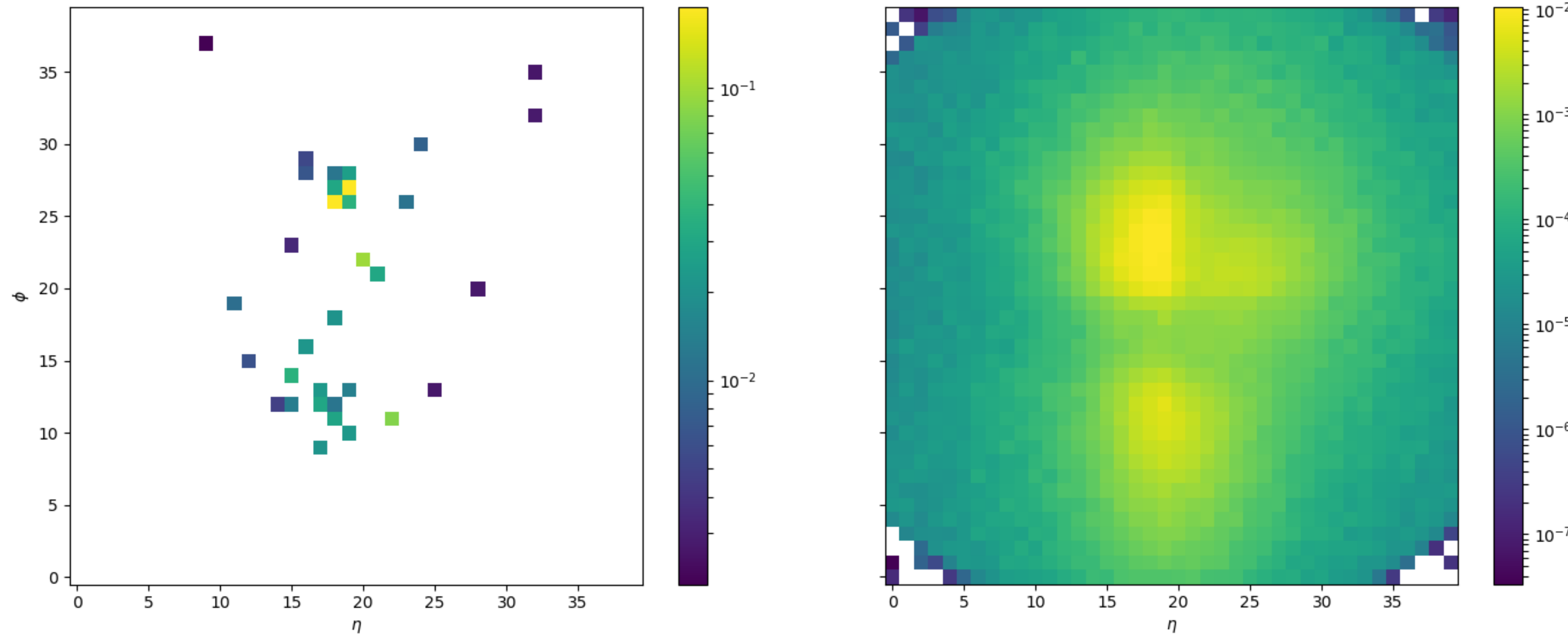
- Weakly supervised learning
- *Latent space/bottleneck* with compressed representation
- Dimension reduction
- Denoising

*kvfrans*
*deeplearningbook.org*

*Top Quark Jet*

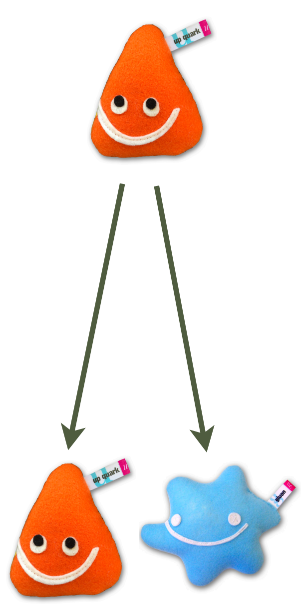


=

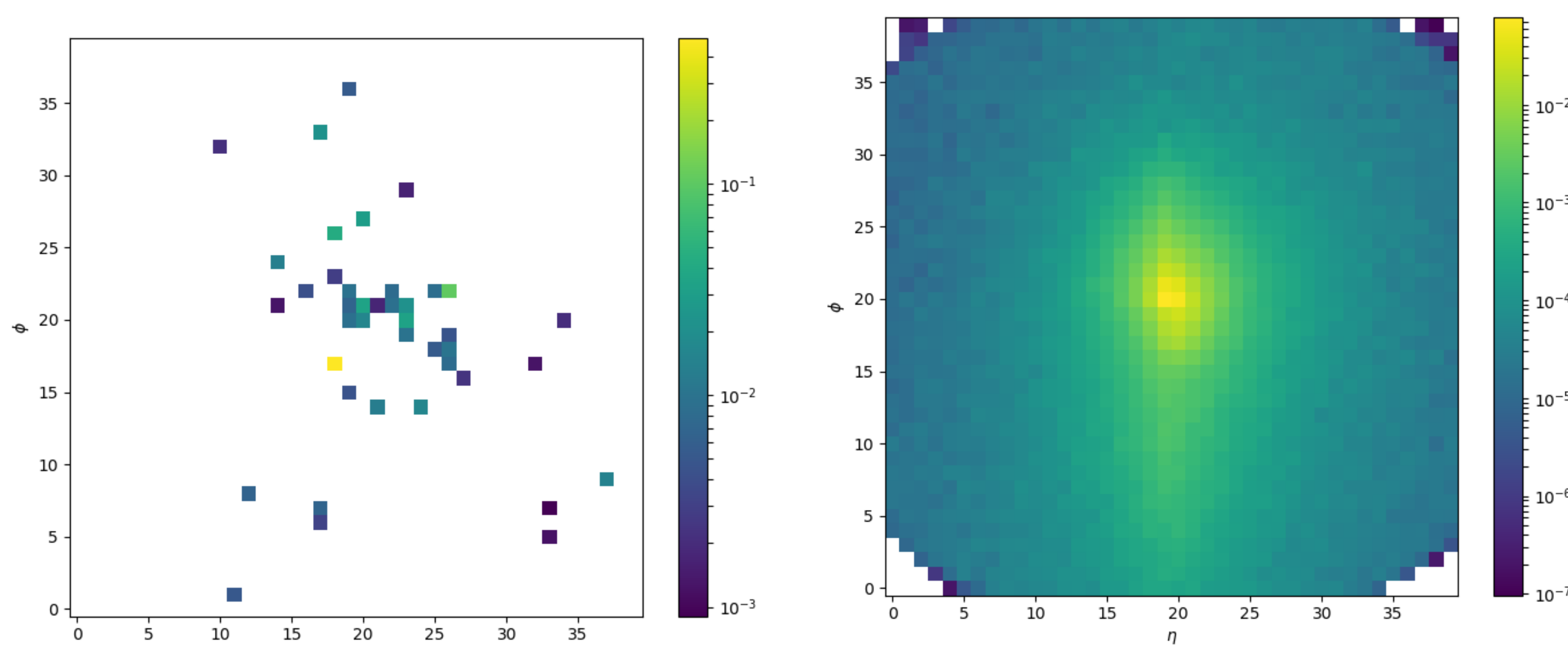



# Remember Jet Images

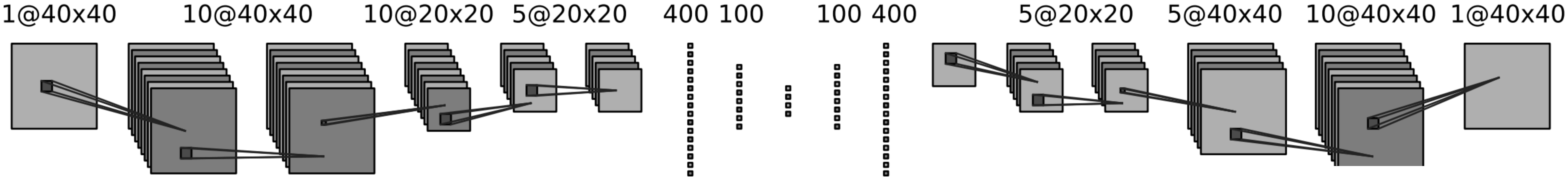
*QCD Jet*

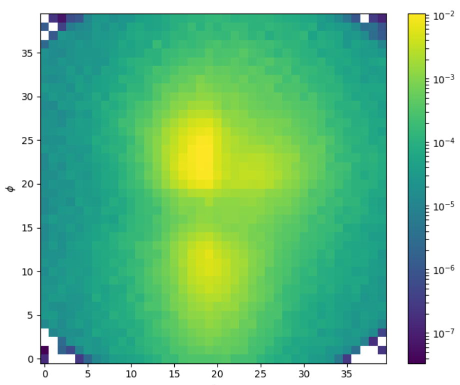


=

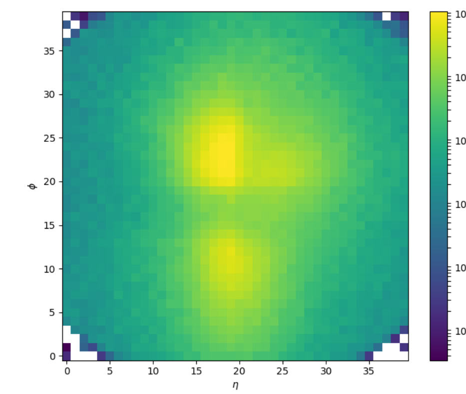


# Autoencoder

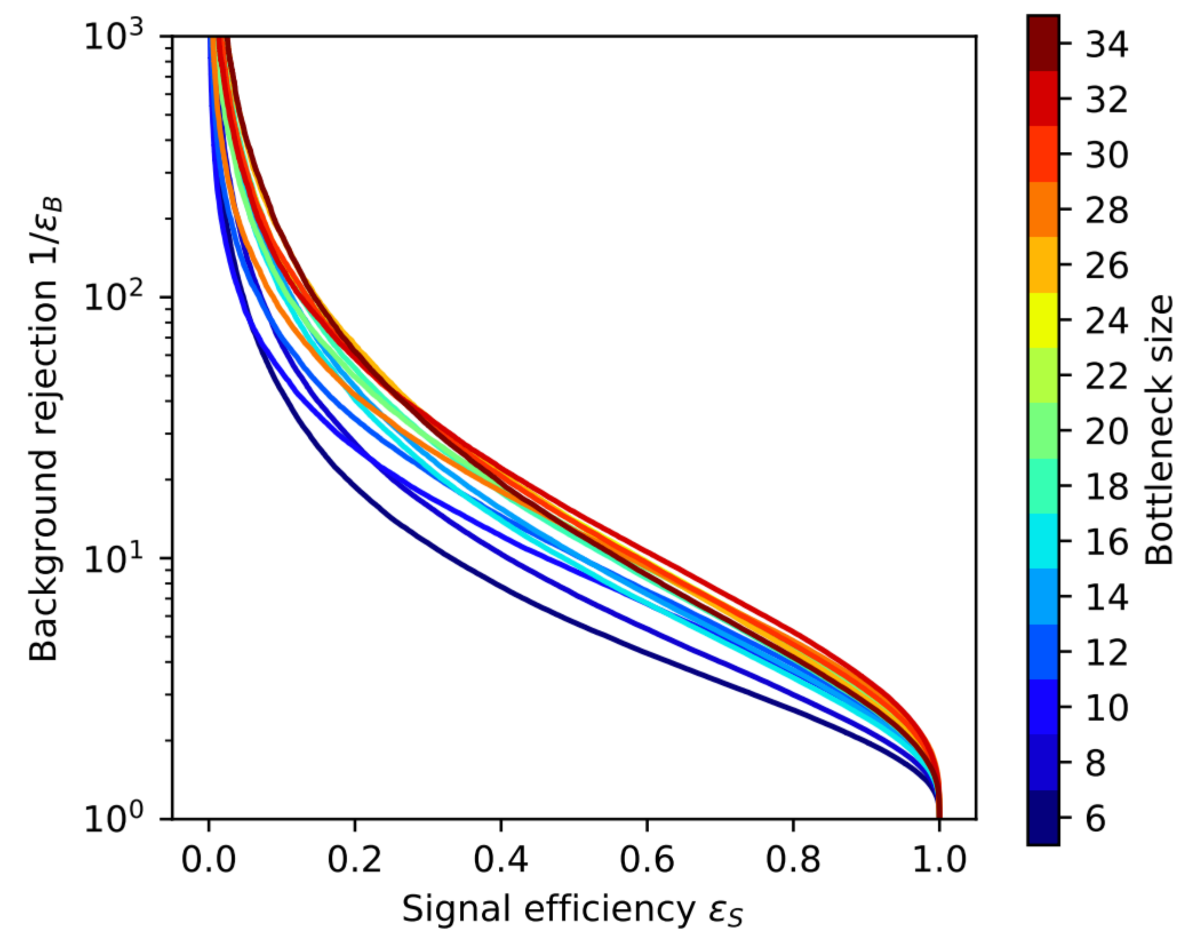


$$L_{\text{auto}} = \sum_{1600\ \text{pixels}} \left( k_T^{\text{norm,in}} - k_T^{\text{auto}} \right)^2$$



- Train on pure QCD light quark/ gluon jets and apply to top tagging
- Top quarks/ new physics identified as anomaly




*QCD or What?*
T Heimel, GK, T Plehn, JM Thompson, 1808.08979
*Searching for New Physics with Deep Autoencoders*
M Farina, Y Nakai, D Shih, 1808.08992

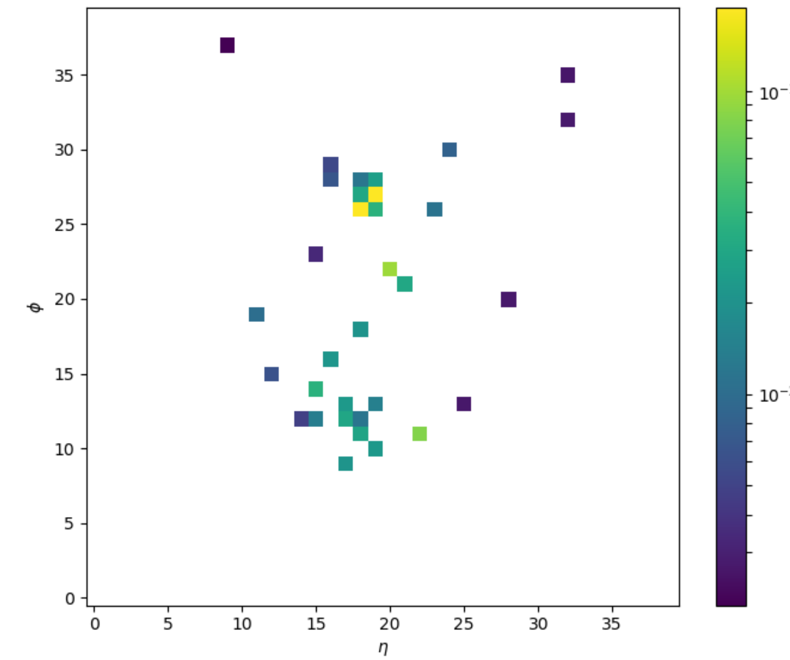
# Caveats

- Anomaly score for a given signature depends on complexity of signal/background in addition to training data

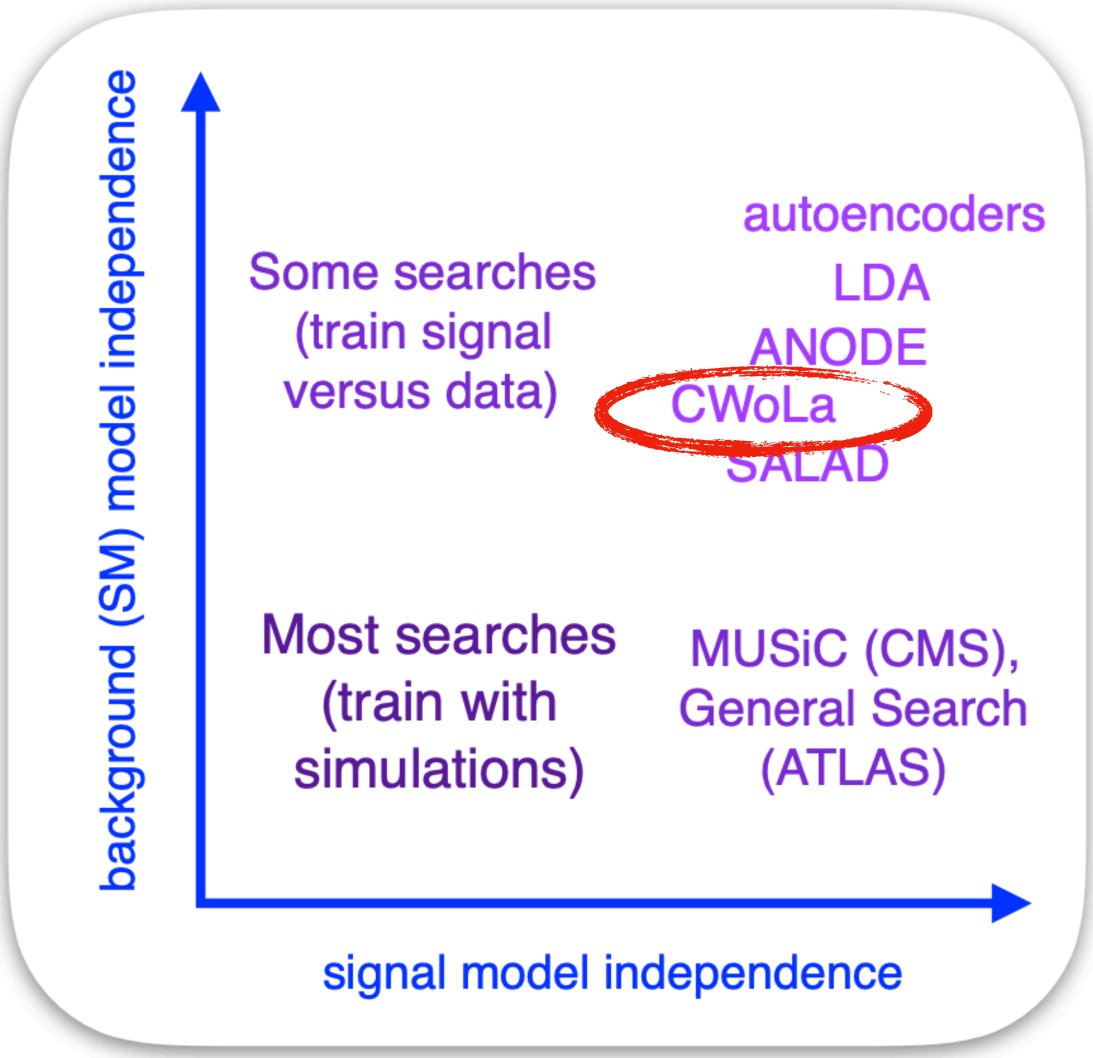
- We are not looking for individual anomalous events but anomalous regions of phase space

- Usual L2 difference not optimal as loss:

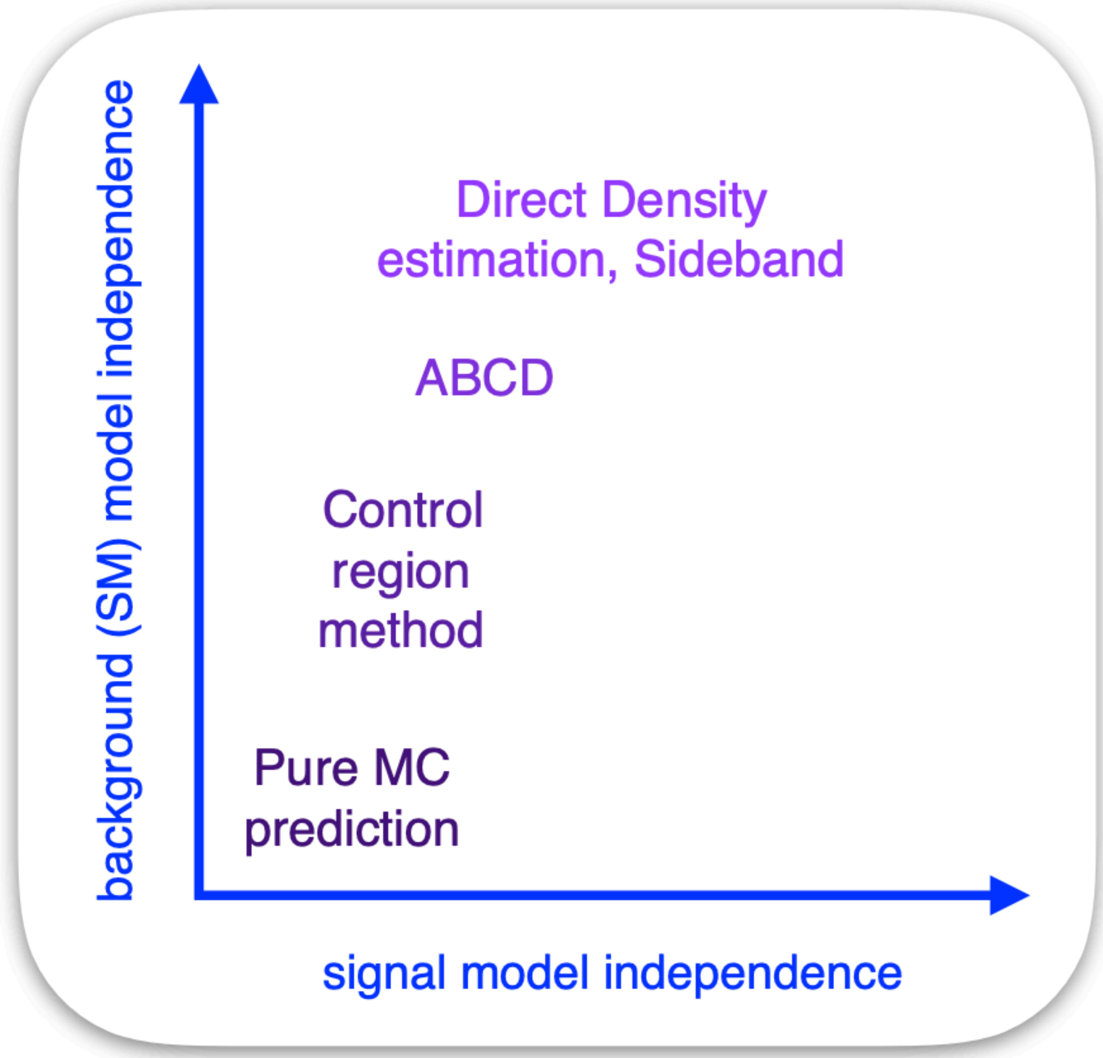
  - Different distributions of pixels compatible with same physics



# Approaches



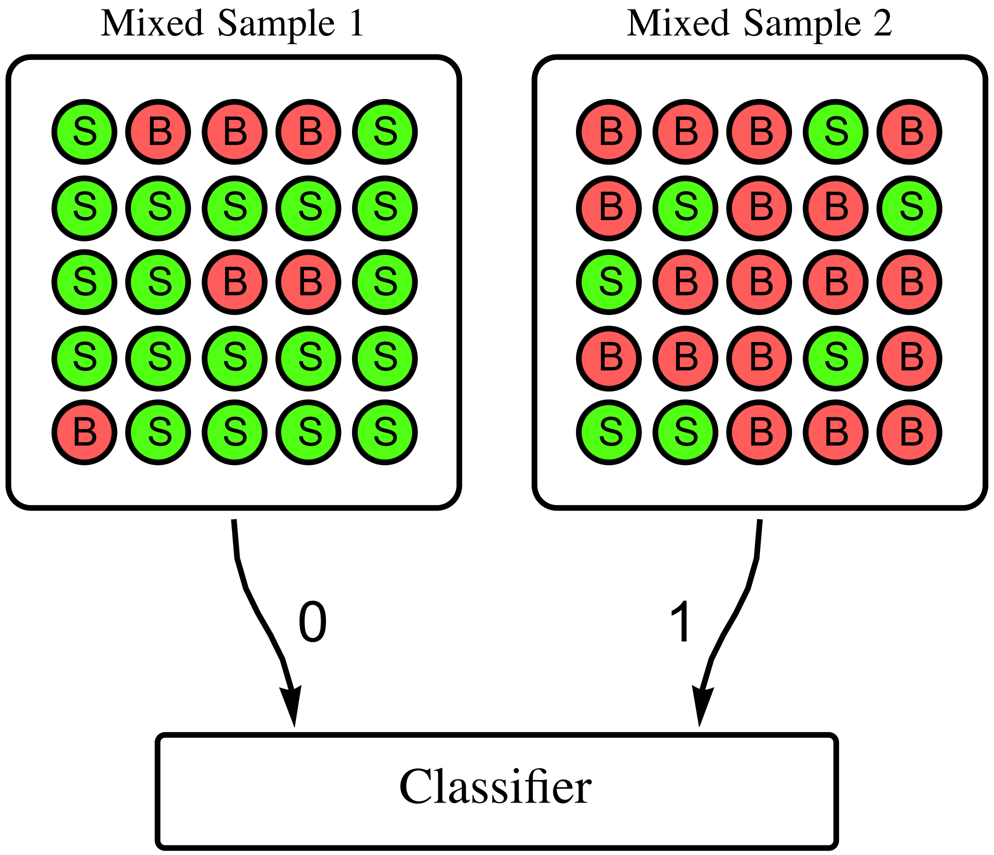

(a) Signal sensitivity




(b) Background specificity

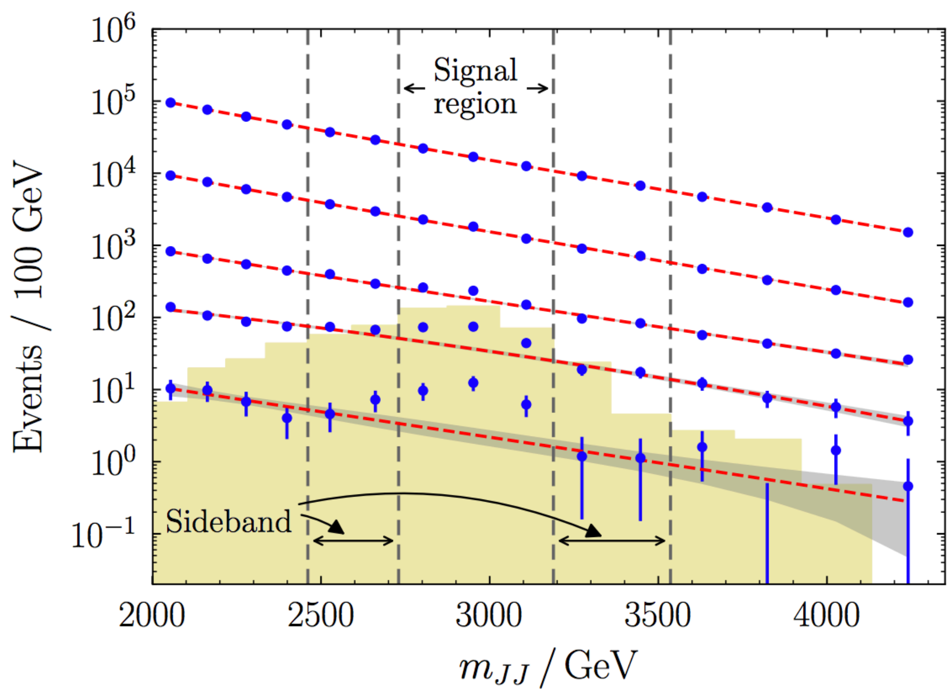
***From Ben Nachman, David Shih, 2001.04990***

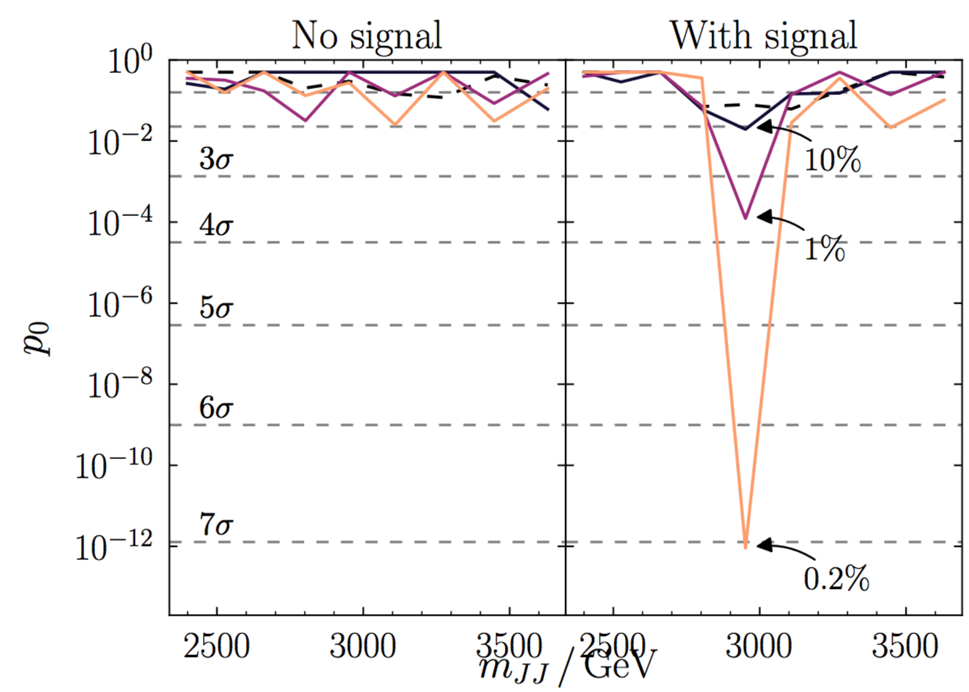
# CWola Hunting




$$L_{M_1/M_2} = \frac{p_{M_1}}{p_{M_2}} = \frac{f_1\, p_S + (1-f_1)\, p_B}{f_2\, p_S + (1-f_2)\, p_B} = \frac{f_1\, L_{S/B} + (1-f_1)}{f_2\, L_{S/B} + (1-f_2)}$$

*Distinguishing mixed samples is equivalent to signal/background classification!*



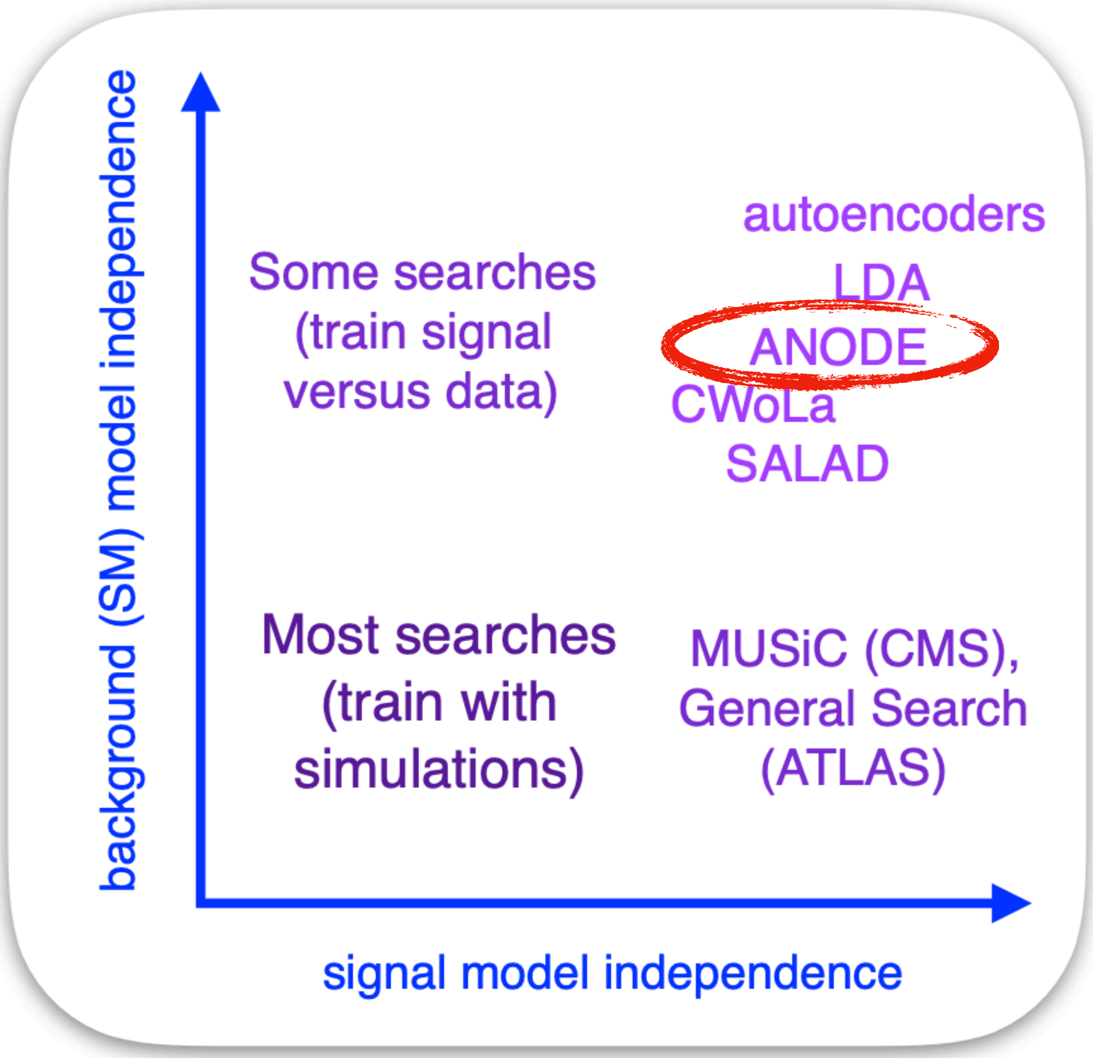




- Assume signal is resonant in one variable
- Define signal region and sidebands
- Train classifier and look for excess

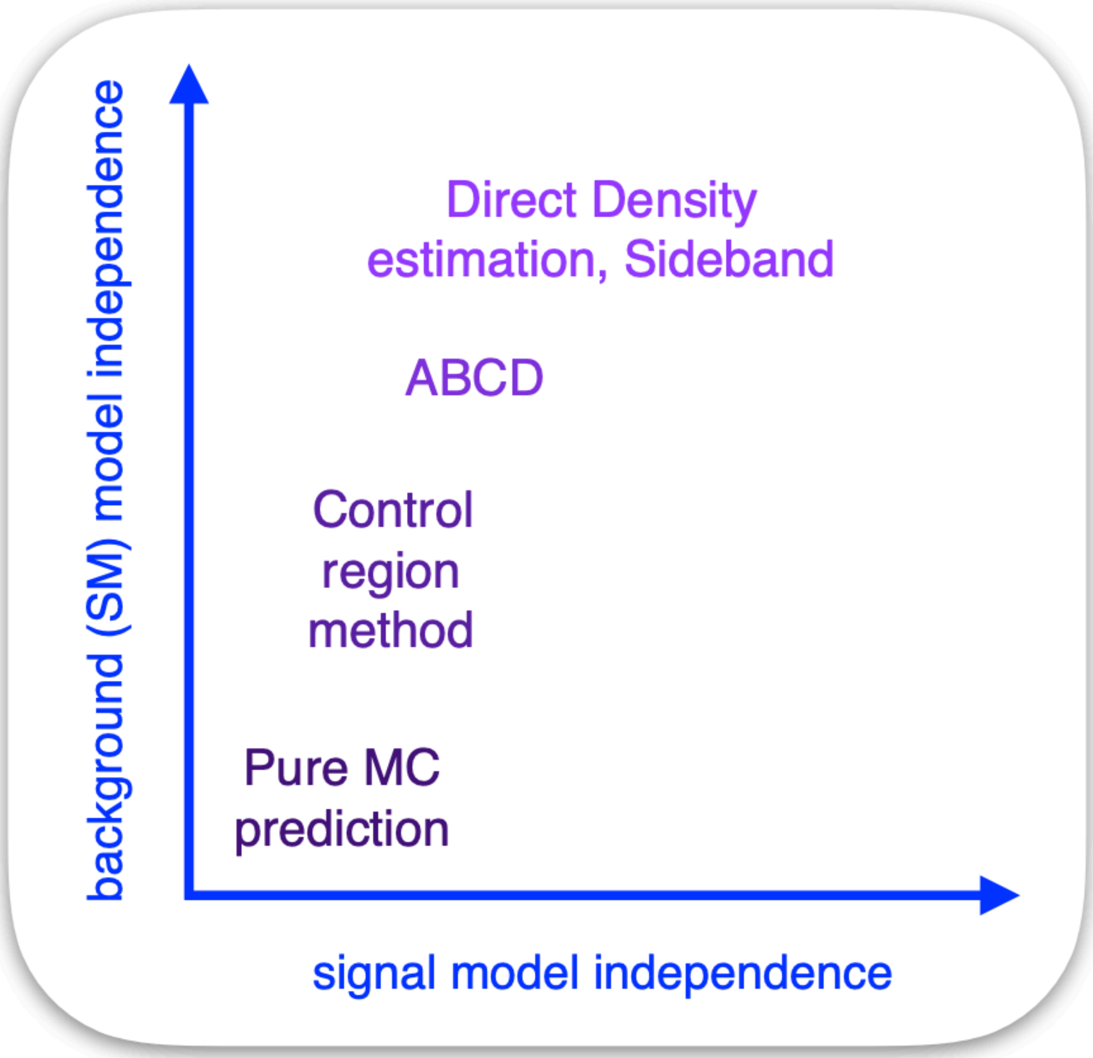


*Classification without labels: Learning from mixed samples in high energy physics*, EM Metodiev, B Nachman, J Thaler, 1708.02949
*Anomaly Detection for Resonant New Physics with Machine Learning*
JH Collins, K Howe, B Nachman
1805.02664

# Approaches




(a) Signal sensitivity



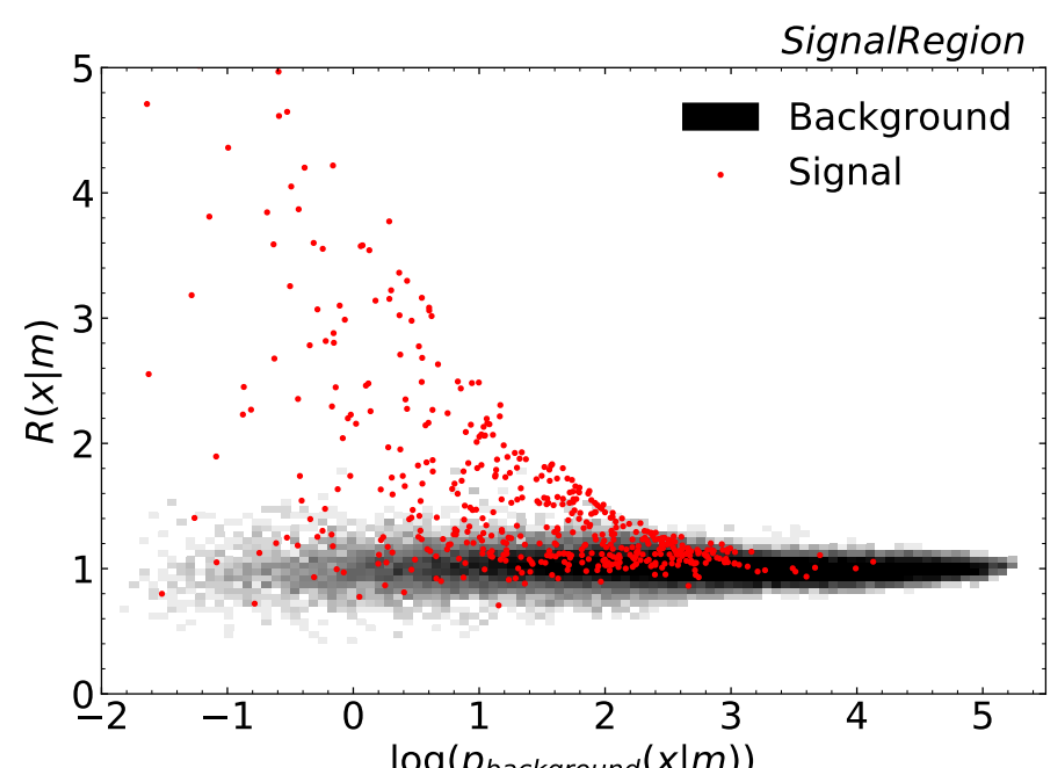

(b) Background specificity

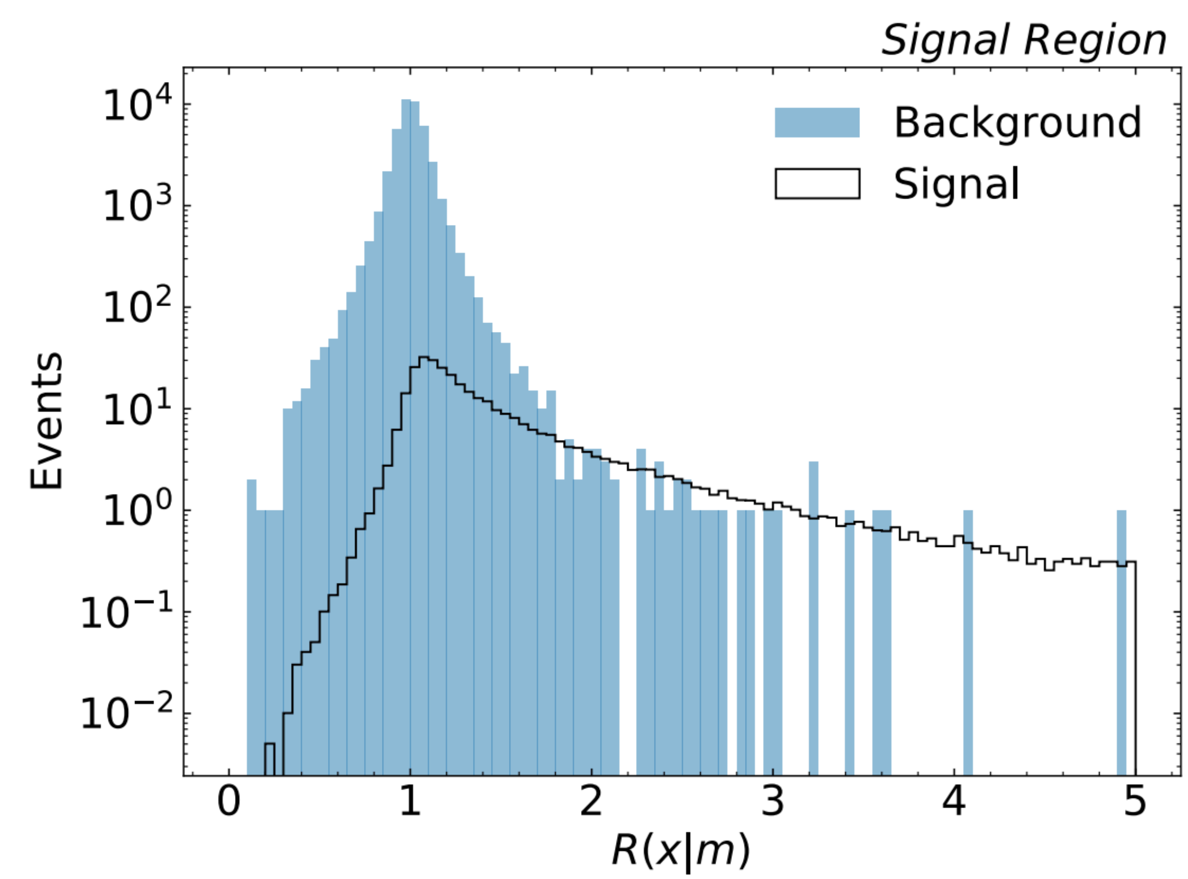
***From Ben Nachman, David Shih, 2001.04990***

# ANODE: ANOmaly detection with Density Estimation

*An anomaly is a local over density of events*

- Build density estimator in sideband region $P_{SB}$
- Extrapolation to signal region gives background estimate $P_{SB}$ -> $P_{BG}$
- Build density estimator in signal region $P_{SR}$
- Likelihood ratio $R=P_{SR}/P_{BG}$
- *Density estimation via MAF (1705.07057) (Masked Autoregressive Flow)*




*Anomaly Detection with Density Estimation*, B Nachman, D Shhih 2001.04990

# Other Ideas

- Naively Autoencoder more sensitive to outliers (out-of-data examples), density estimation more sensitive to anomalies in distributions
- One could also look for density anomalies in the latent space of autoencoders
- Also very interesting for non-HEP applications:
  - Data quality monitoring
  - Predictive maintenance
  - Credit card fraud
  - …..
- Exciting topic to start now!

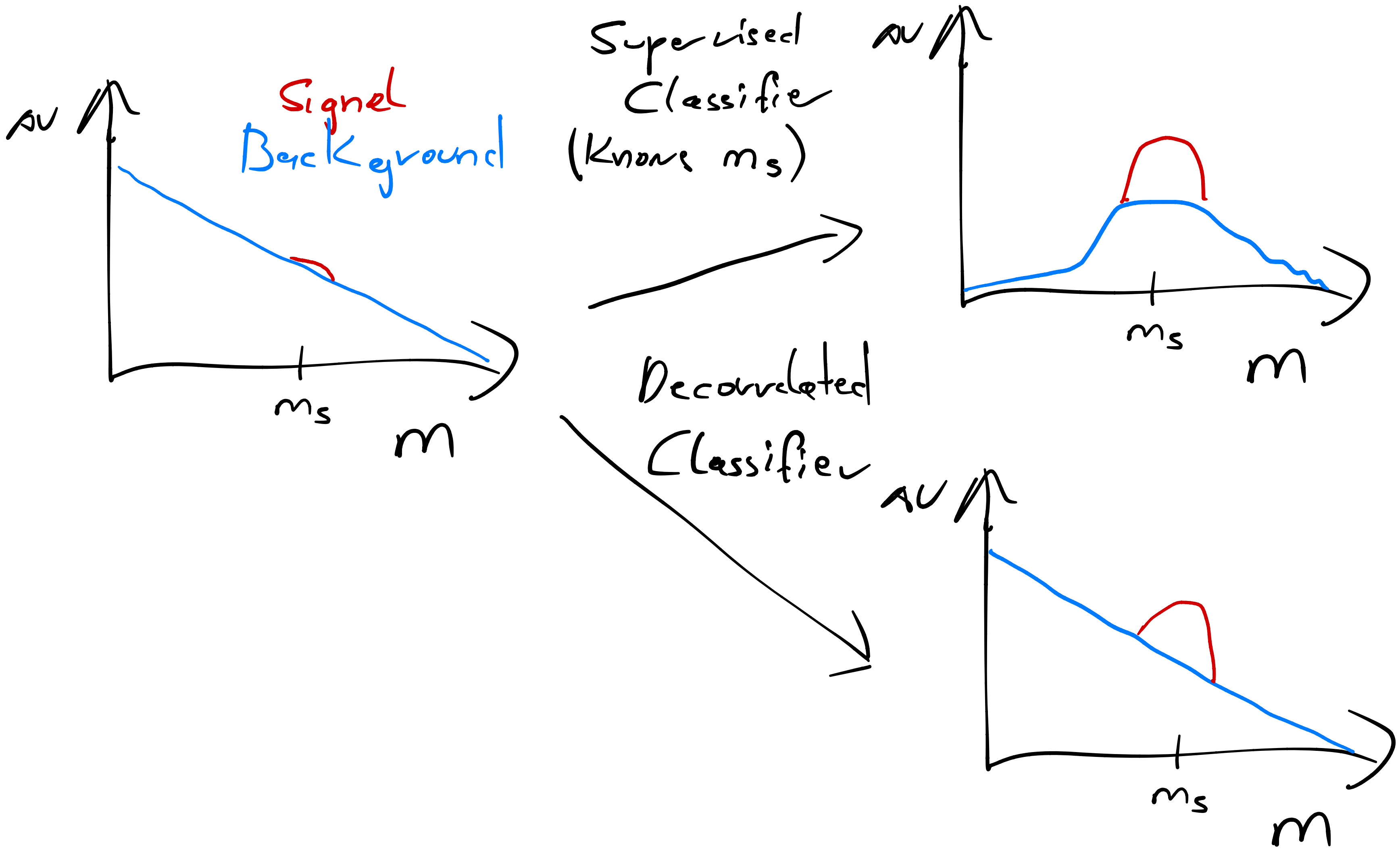
# LHC Olympics 2020

- For more on anomaly detection see material at the recent workshop: https://indico.desy.de/e/anomaly2020

# Some final words

# Correlation

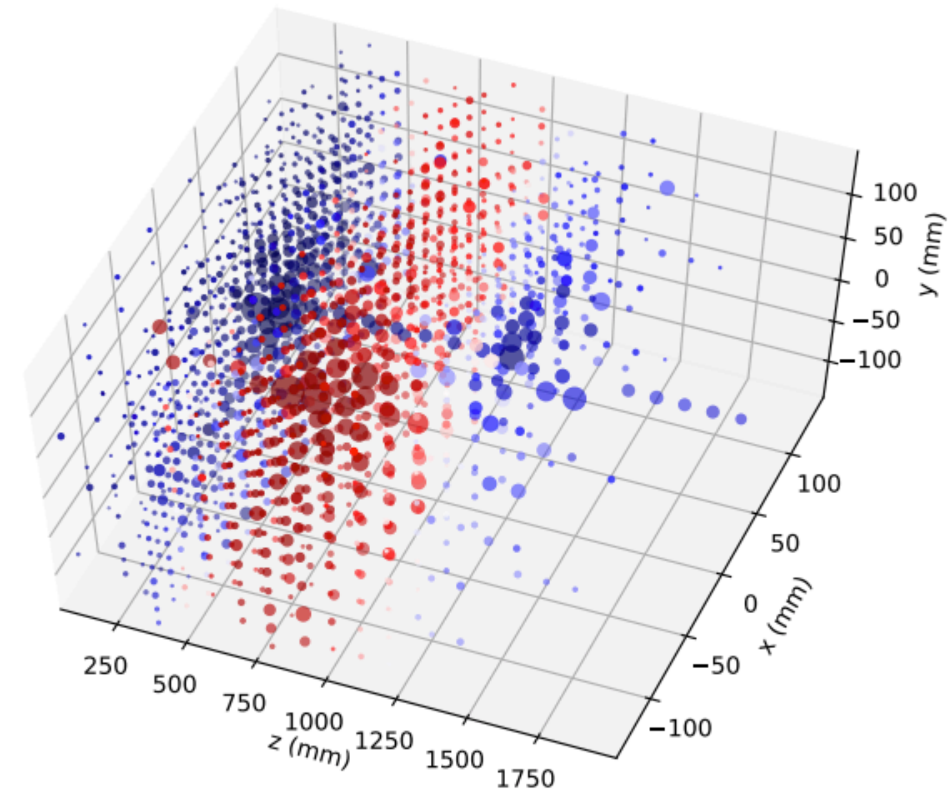
*Against a variable or data vs simulation*



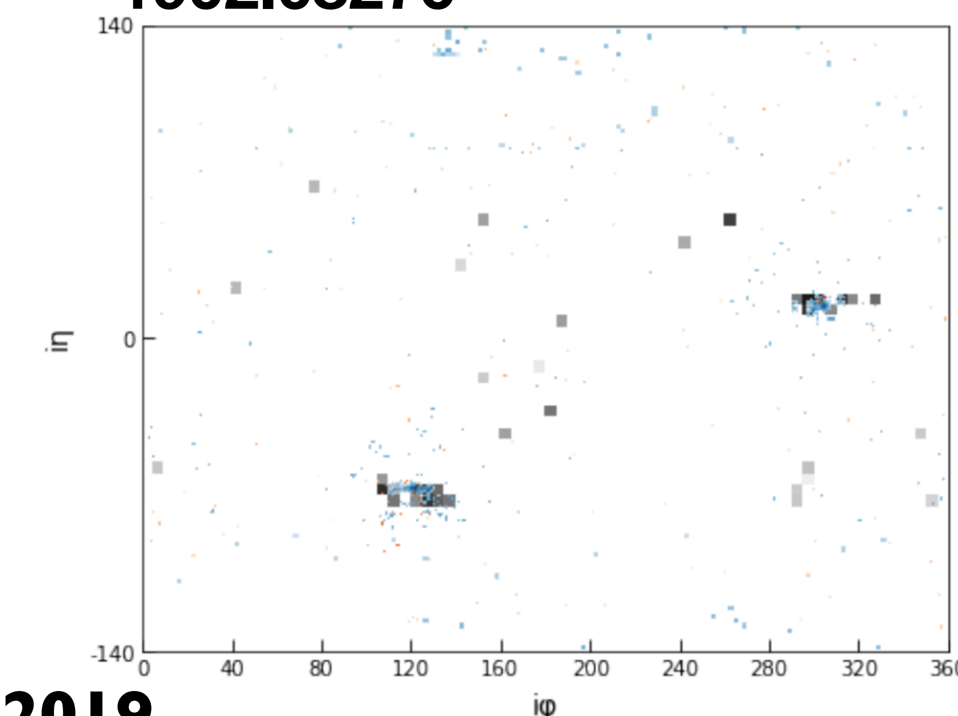

- Large number of ideas including planing (1908.08959), adversarial training (1611.01046,1703.03507), DisCo (2001.05310),…

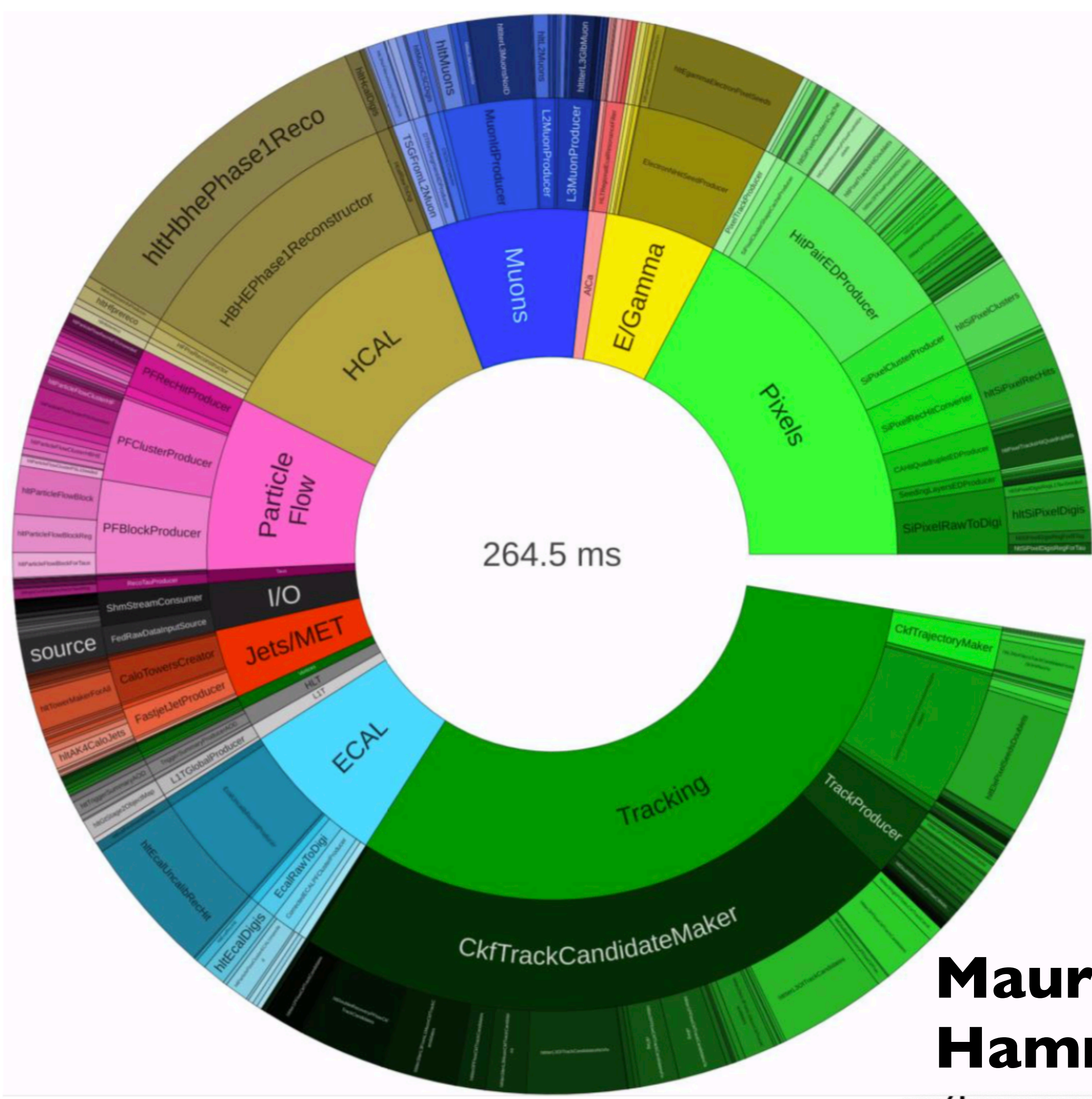
# Low Level Reconstruction

- Replace traditional algorithms for reconstruction, object ID and calibration with deep learning
- Increase physics performance and/or resource usage
- Superficially less attractive, potentially much more useful
- End-to-end learning?




1902.08276

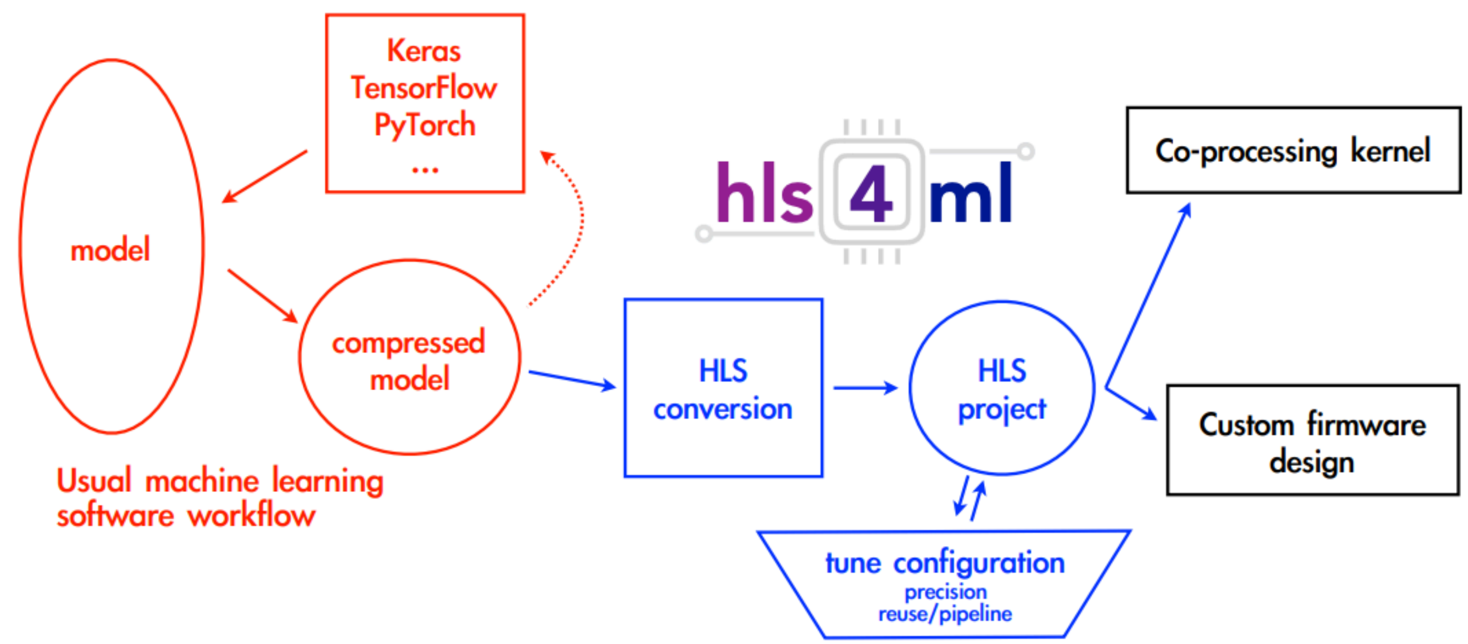


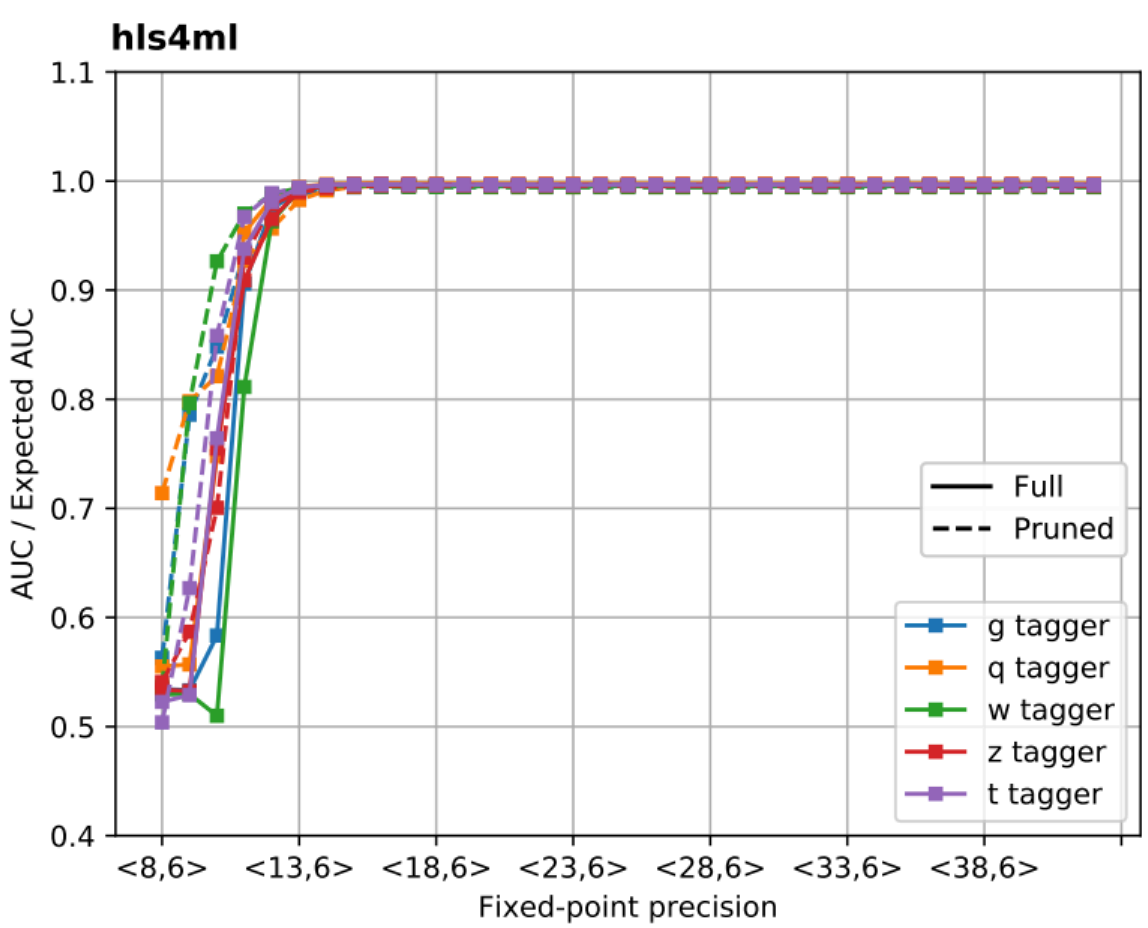



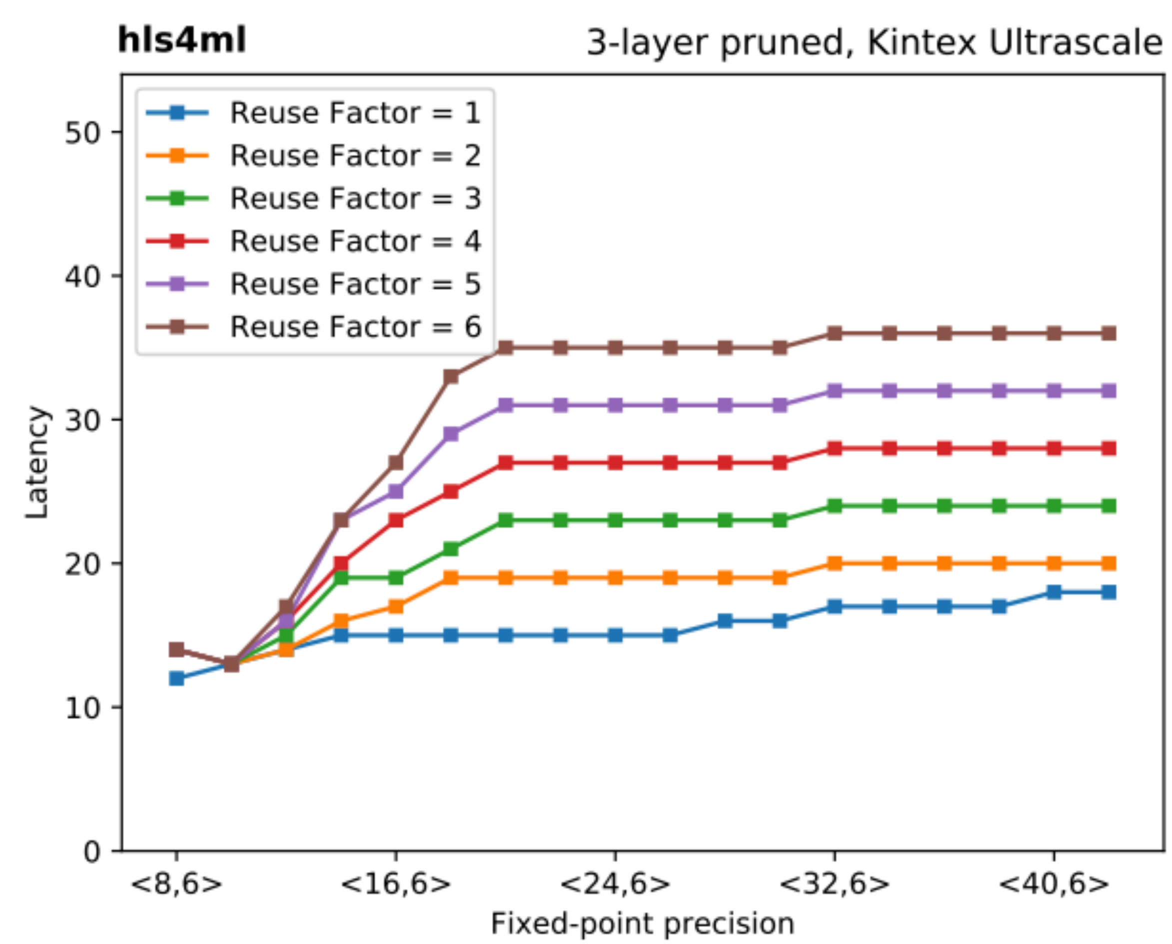

**Maurizio Pierini**
**Hammers&Nails 2019**

# Fast Decisions

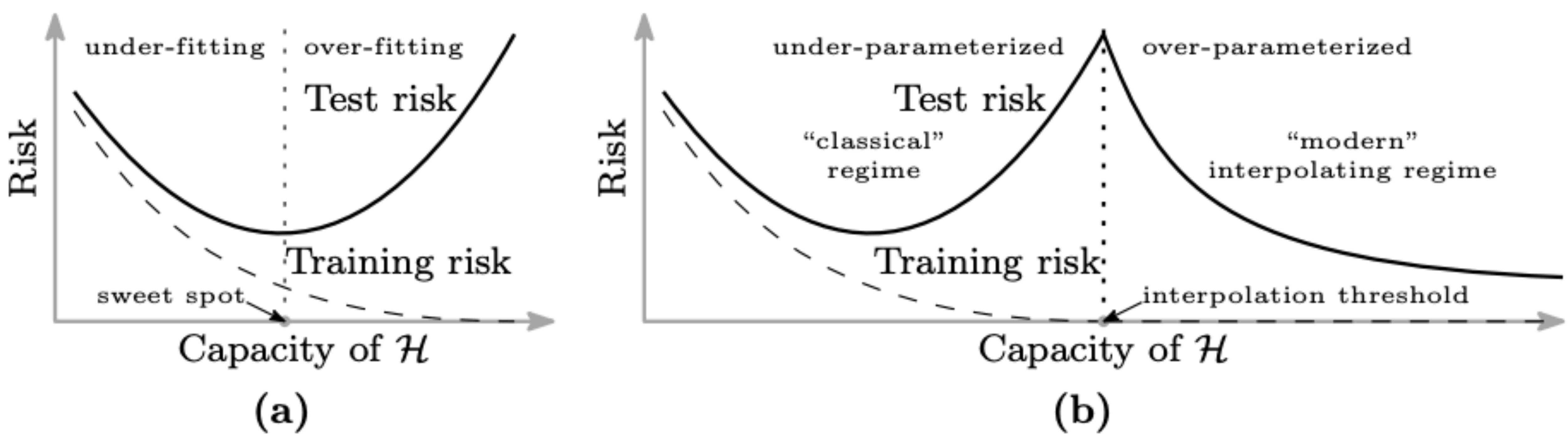
- Use neural networks in L1 Trigger
- Trained offline using normal tools, then translated and optimised for running on FPGAs



# Overtraining




**1812.11118**

# Conclusions

- Deep Learning for particle physics is rapidly developing solutions to a wide range of problems
  - Object and Event classification
  - Anomaly detection
  - Robustness and uncertainties
  - Fast reconstruction and simulation
- Further reading
  - Basic concepts: http://www.deeplearningbook.org/
  - Overview of ML in HEP papers: https://iml-wg.github.io/HEPML-LivingReview/

*Thank you!*