Representation Learning of Collider Events

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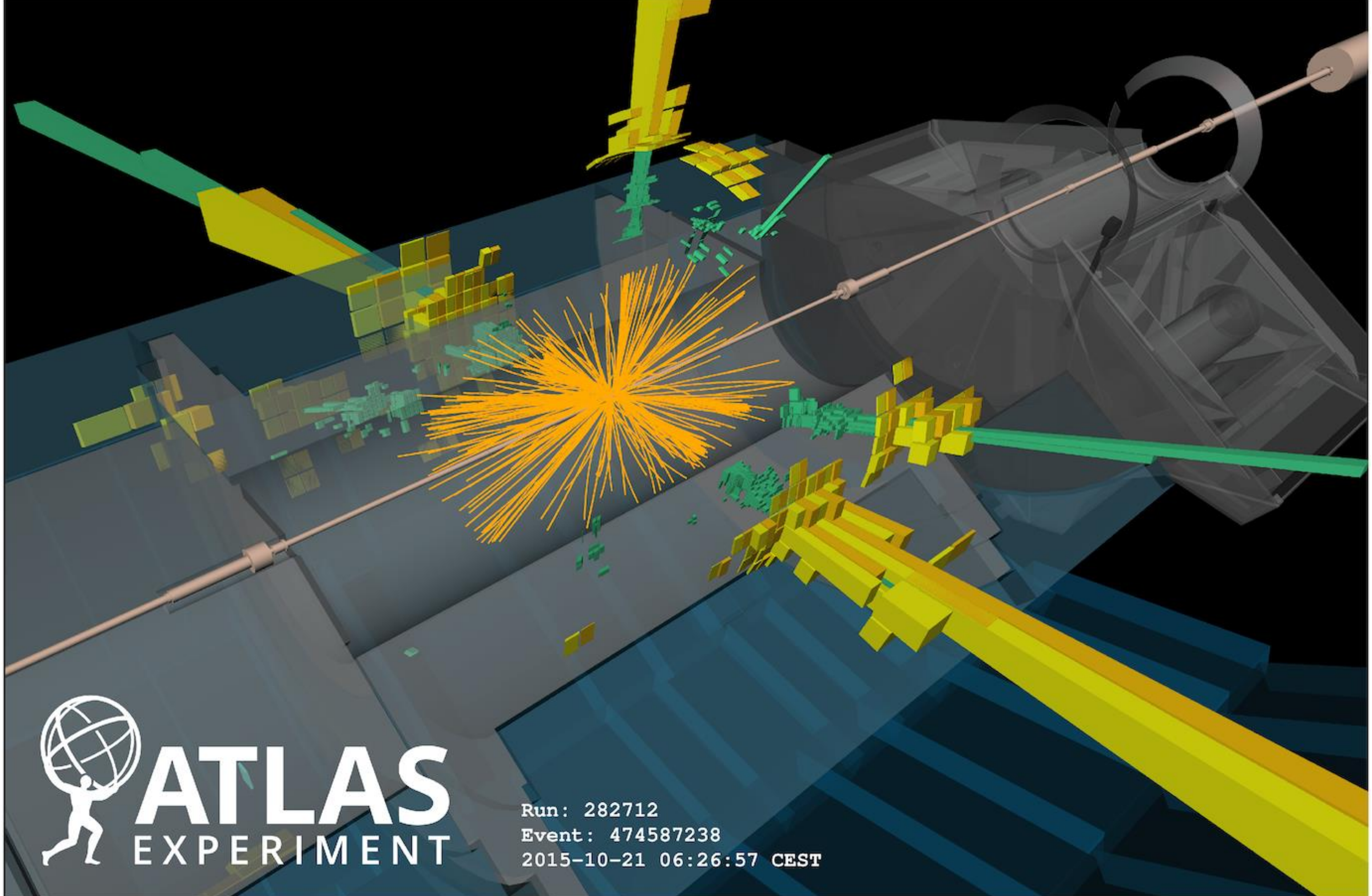
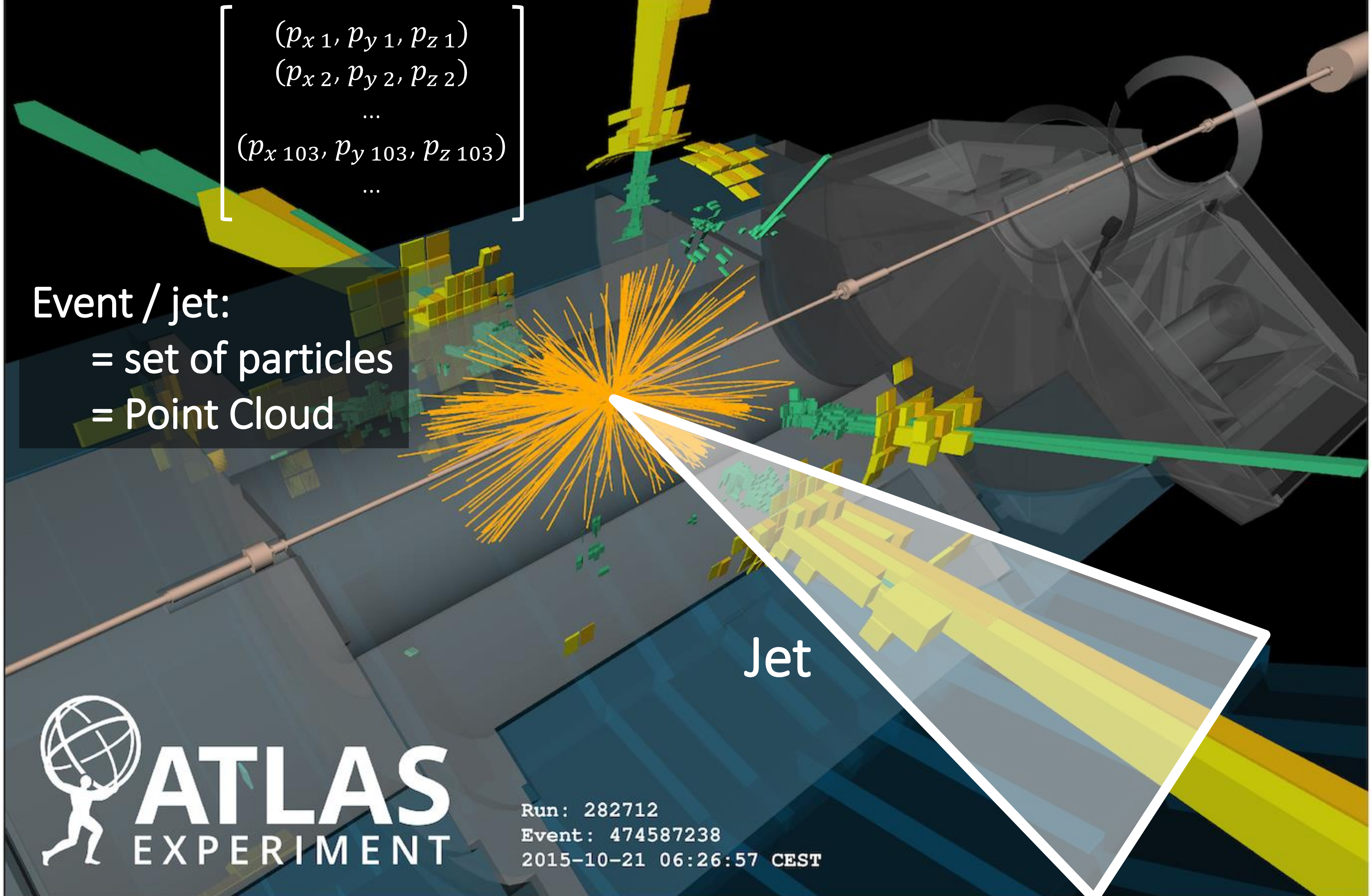

ATLAS
EXPERIMENT
Run: 282712
Event: 474587238
2015-10-21 06:26:57 CEST

$$\begin{bmatrix} (p_{x\,1}, p_{y\,1}, p_{z\,1}) \\ (p_{x\,2}, p_{y\,2}, p_{z\,2}) \\ \dots \\ (p_{x\,103}, p_{y\,103}, p_{z\,103}) \\ \dots \end{bmatrix}$$

Event / jet:

= set of particles

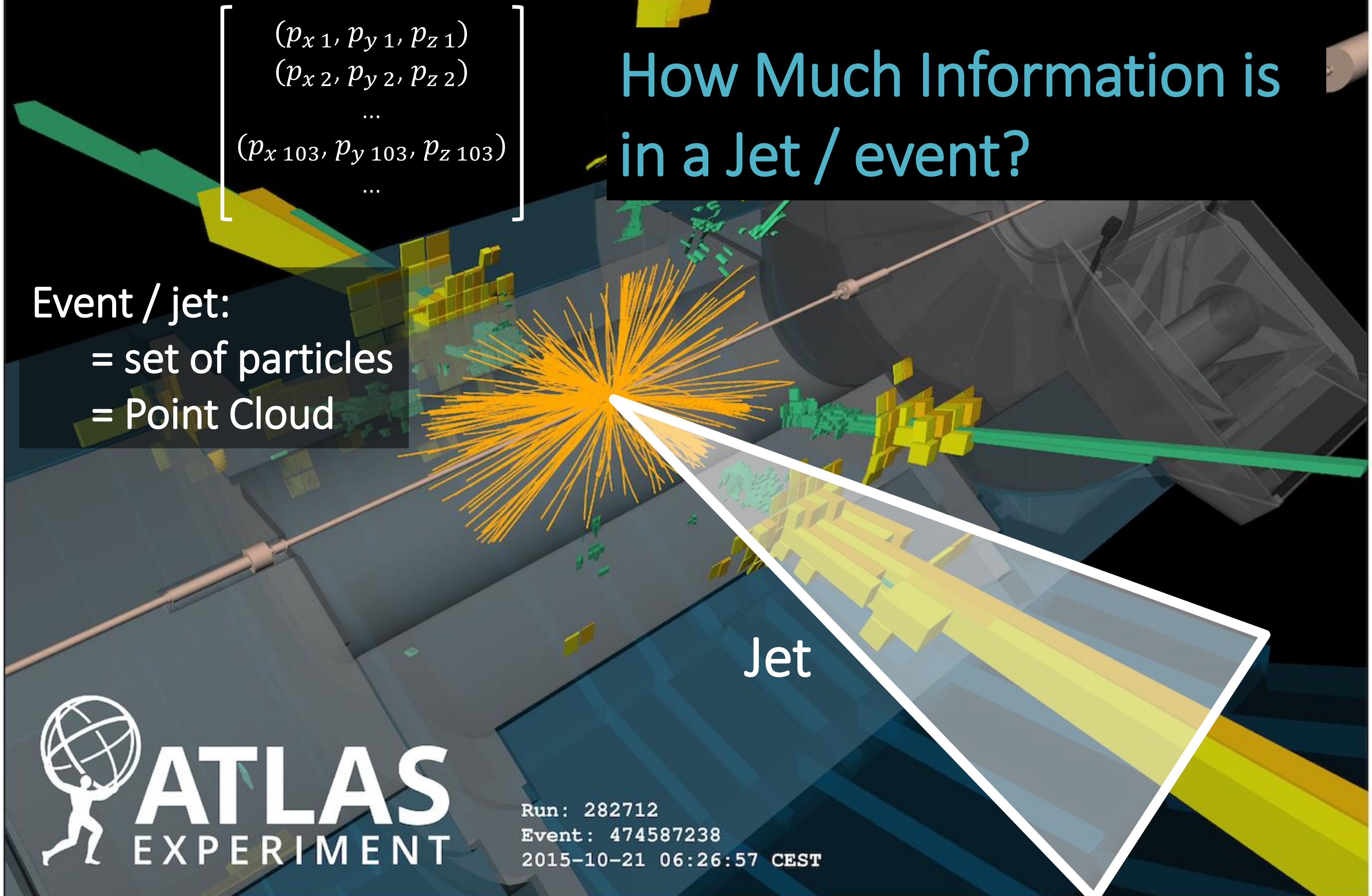
= Point Cloud



How Much Information is in a Jet / event?

$$\begin{bmatrix} (p_{x\,1}, p_{y\,1}, p_{z\,1}) \\ (p_{x\,2}, p_{y\,2}, p_{z\,2}) \\ \dots \\ (p_{x\,103}, p_{y\,103}, p_{z\,103}) \\ \dots \end{bmatrix}$$

Event / jet:
- = set of particles
- = Point Cloud



Menu

(Absolutely no substitutions)

Aperetif
How much information is in a jet?

Appetizer
Autoencoder Introduction

Fish Course
The Metric Space of Collider Events

Cheese Selection
Application to top jets

Dessert
Mystery Special

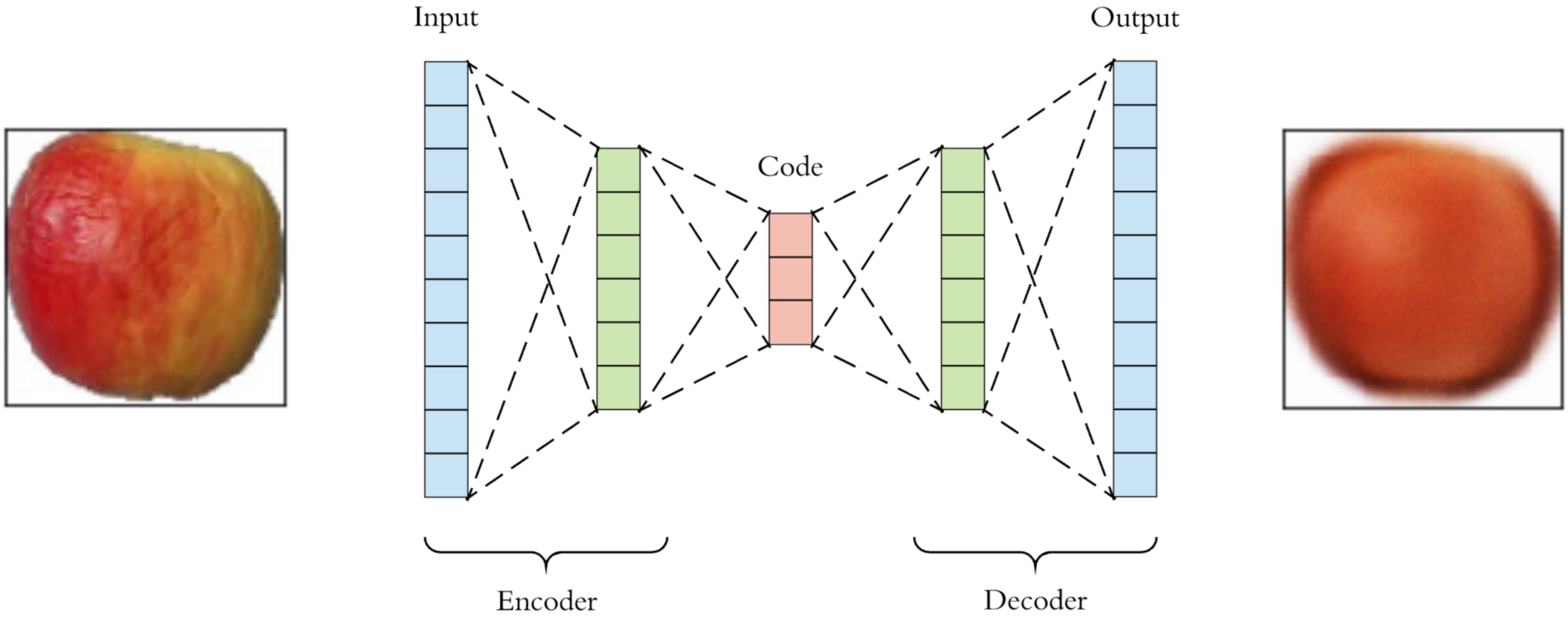
Digestif
Conclusions

Main Course
The Variational Autoencoder:
a pedagogical introduction

Appetizer

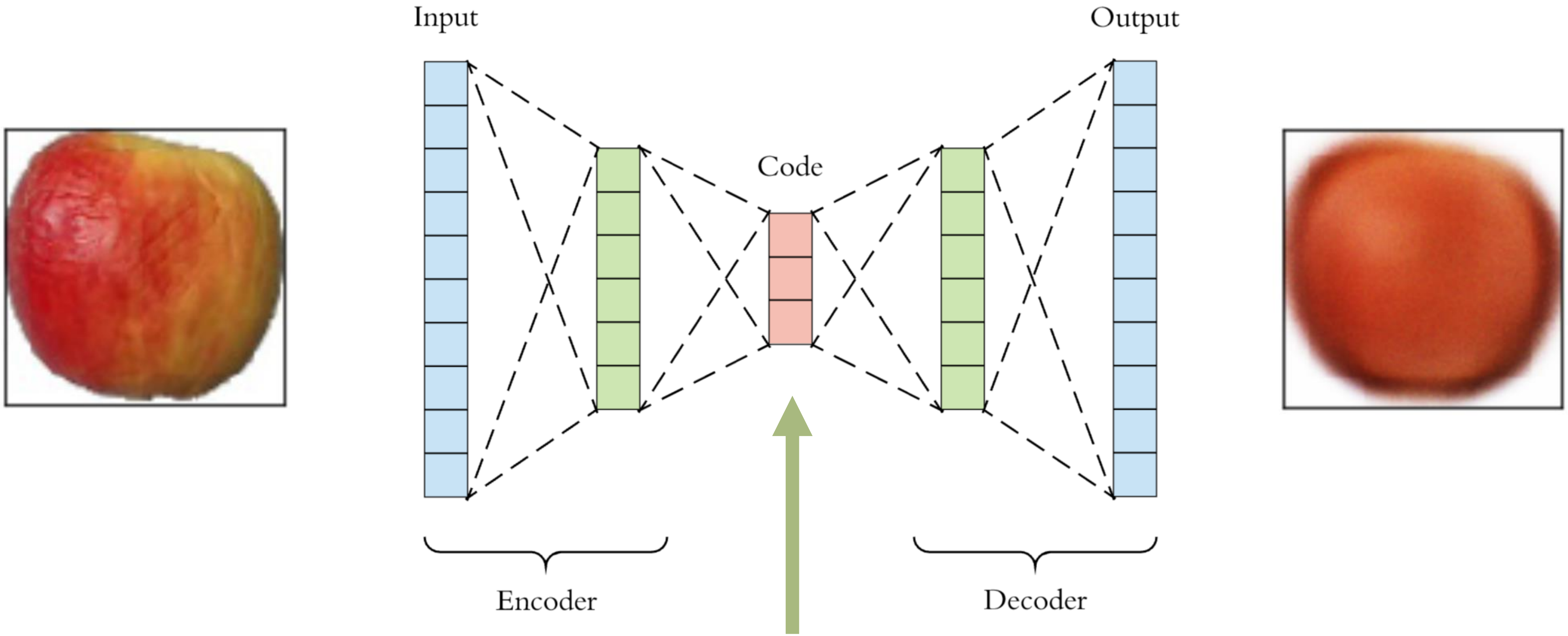
Autoencoder introduction

The Plain Autoencoder



Loss = |Output – Input| *(what is this for jets?)*

The Plain Autoencoder



Latent space =?= Learnt representation

Fish Course

The Metric Space of Collider Events

The Space of Collider Events

Jesse Thaler

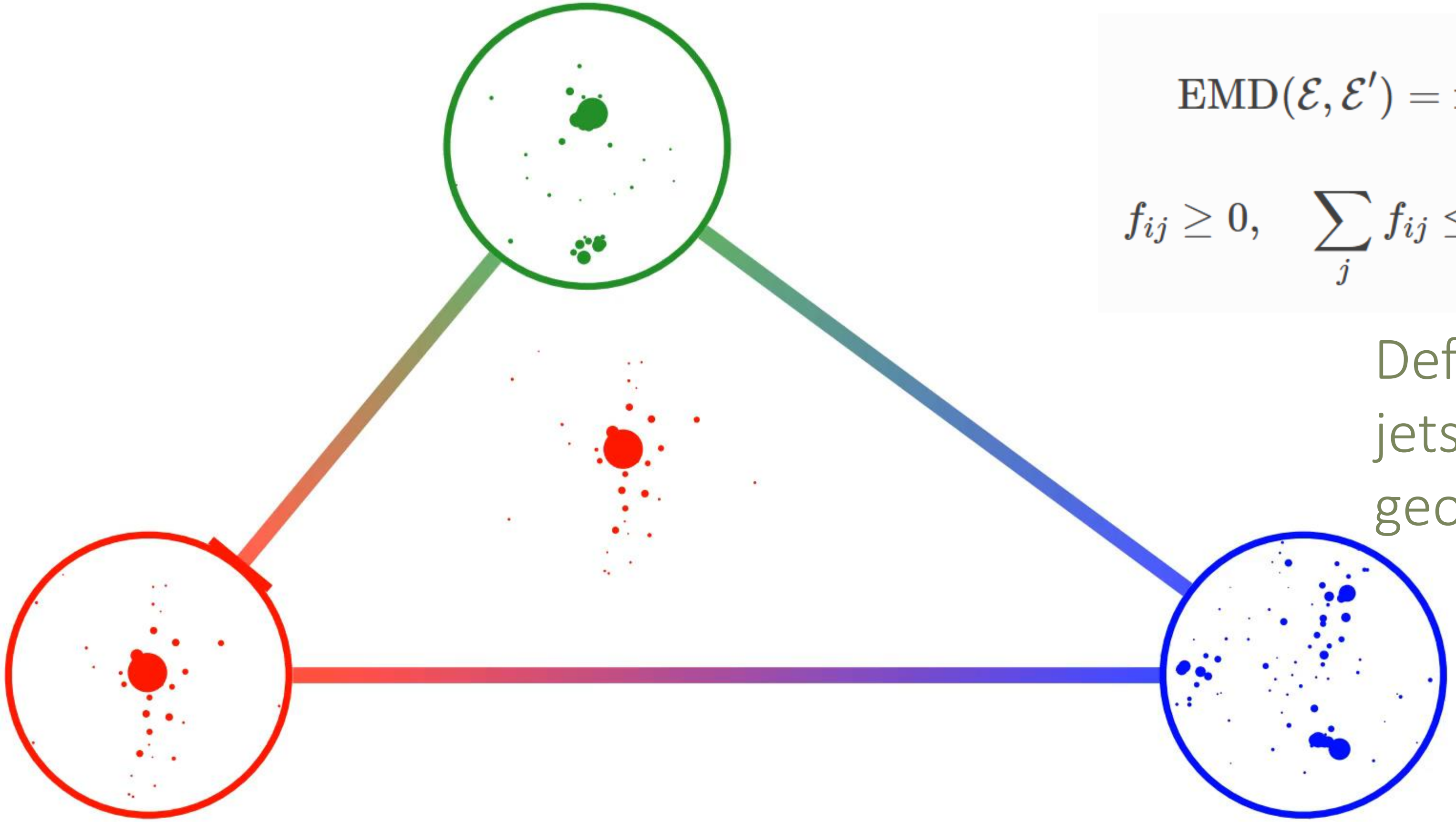
MIT

with Patrick Komiske & Eric Metodiev, 1902.02346

EPP Theory Seminar, SLAC — April 24, 2019

Earth Movers Distance

*Cost to transform one jet into another = Energy * distance*



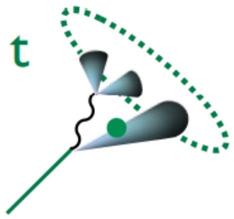
$$\mathrm{EMD}(\mathcal{E},\mathcal{E}') = \min_{\{f_{ij}\}} \sum_{ij} f_{ij}\frac{\theta_{ij}}{R} + \left|\sum_i E_i - \sum_j E'_j\right|,$$

$$f_{ij} \geq 0, \quad \sum_j f_{ij} \leq E_i, \quad \sum_i f_{ij} \leq E'_j, \quad \sum_{ij} f_{ij} = E_{\min},$$

Defines a metric space in which jets or collider events form a geometric manifold.

Taken from https://energyflow.network/docs/emd/, Eric Metediov, Patrick Komiske III, Jesse Thaler

Visualizing Top Quark Evolution



500 GeV

Top Quark

↓ Decay
EMD: 161.1 GeV

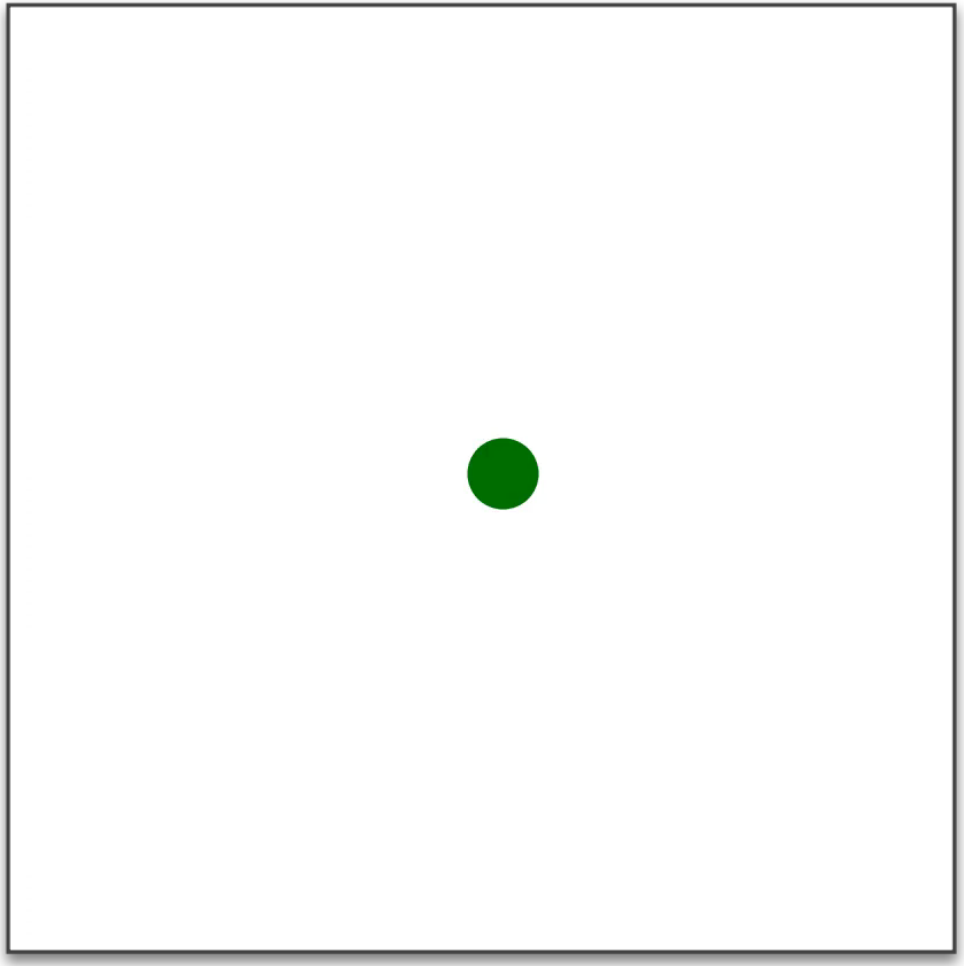
Three Quarks

↓ Showering
EMD: 47.1 GeV

Partons

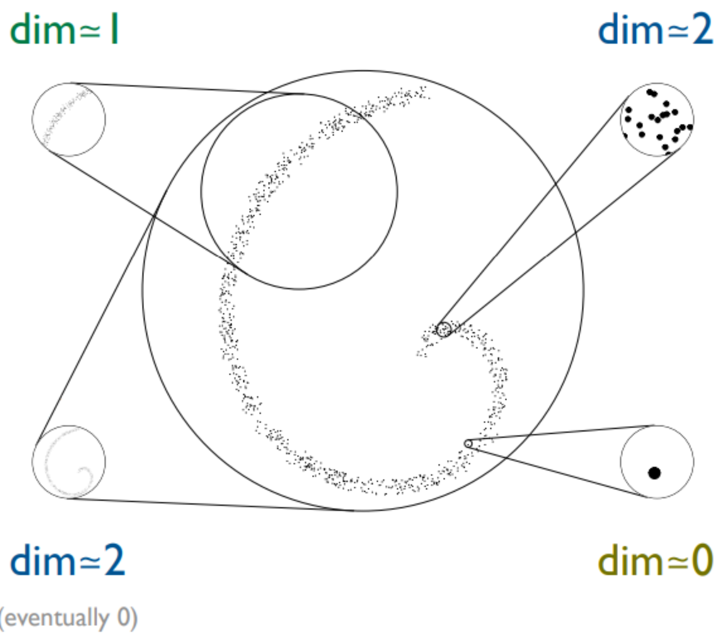
↓ Hadronization
EMD: 27.0 GeV

Hadrons



Quantifying Dimensionality

Correlation Dimension: $\dim(Q) = Q \frac{\partial}{\partial Q} \ln \sum_i \sum_j \Theta\big(\mathrm{EMD}(\mathcal{E}_i, \mathcal{E}_j) < Q\big)$



$$N_{\text{neighbors}}(r) \sim r^{\text{dim}}$$

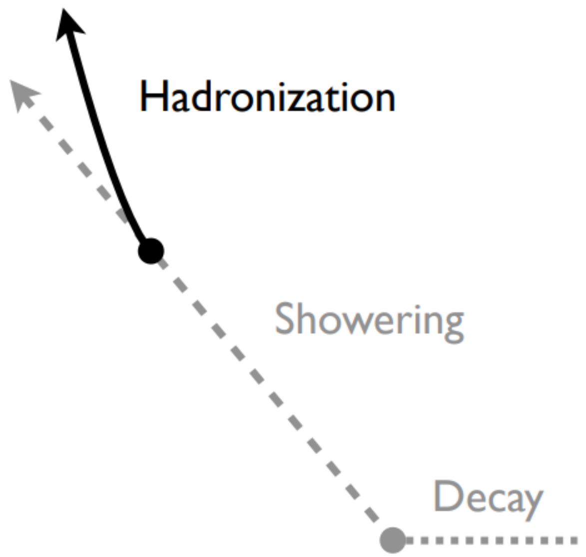
$$\Downarrow$$

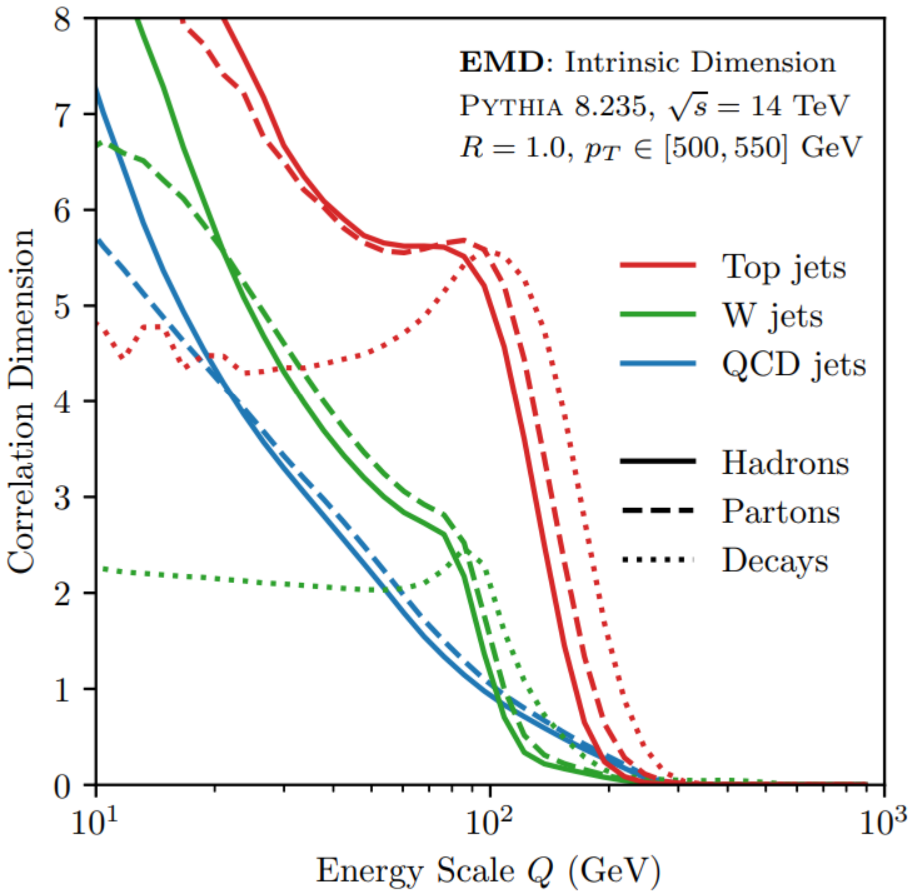
$$\dim(r) \sim r \frac{\partial}{\partial r} \ln N_{\text{neighbors}}(r)$$

[Grassberger, Procaccia, PRL 1983; Kégl, NIPS 2002]

Hadron-Level Dimension

$$\dim(Q) = Q\frac{\partial}{\partial Q}\ln\sum_i\sum_j\Theta(\text{EMD}(\mathcal{E}_i,\mathcal{E}_j) < Q)$$





Increasing complexity: multi-body phase space
perturbative emissions
non-perturbative dynamics

[Komiske, Metodiev, JDT, 1902.02346]

Preliminary Calculation

Leading Log:

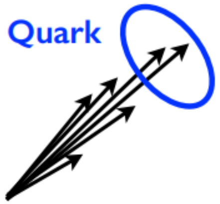
(single log, since dim has derivative)

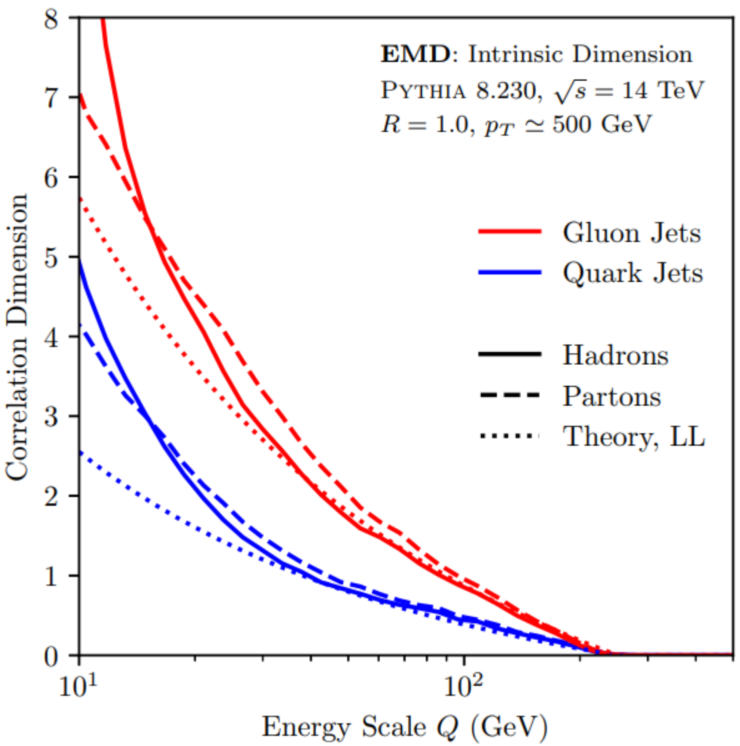
$$\mathrm{dim}_i(Q) \simeq -\frac{8\alpha_s}{\pi} C_i \ln\frac{Q}{p_T}$$

Color Factor

$C_A = 3$

$C_F = 4/3$



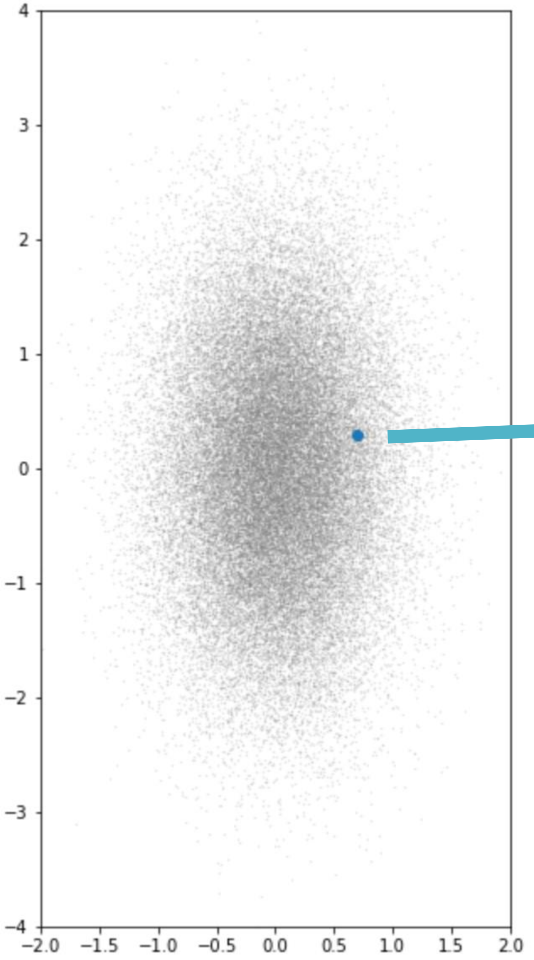


Main Course

The Variational Autoencoder

The Plain Autoencoder

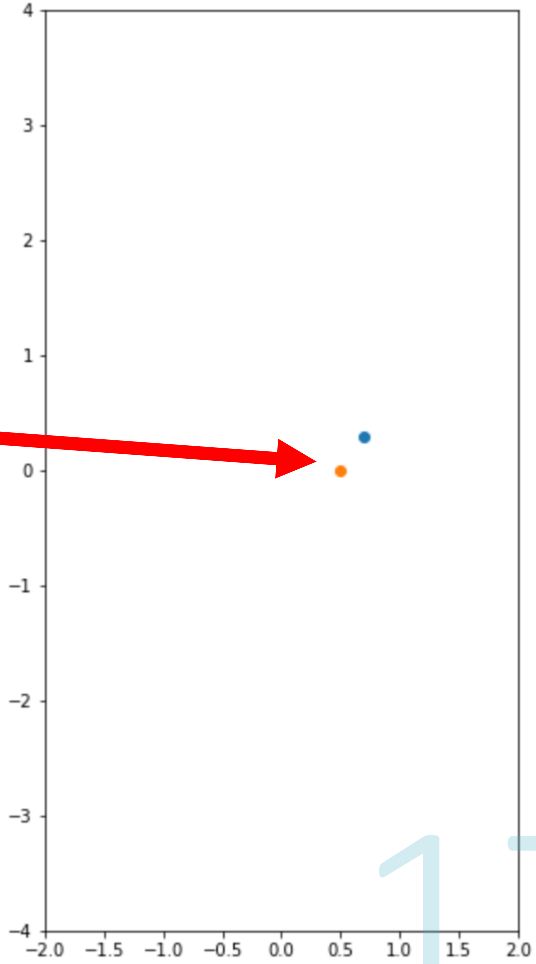
Garbage



AE

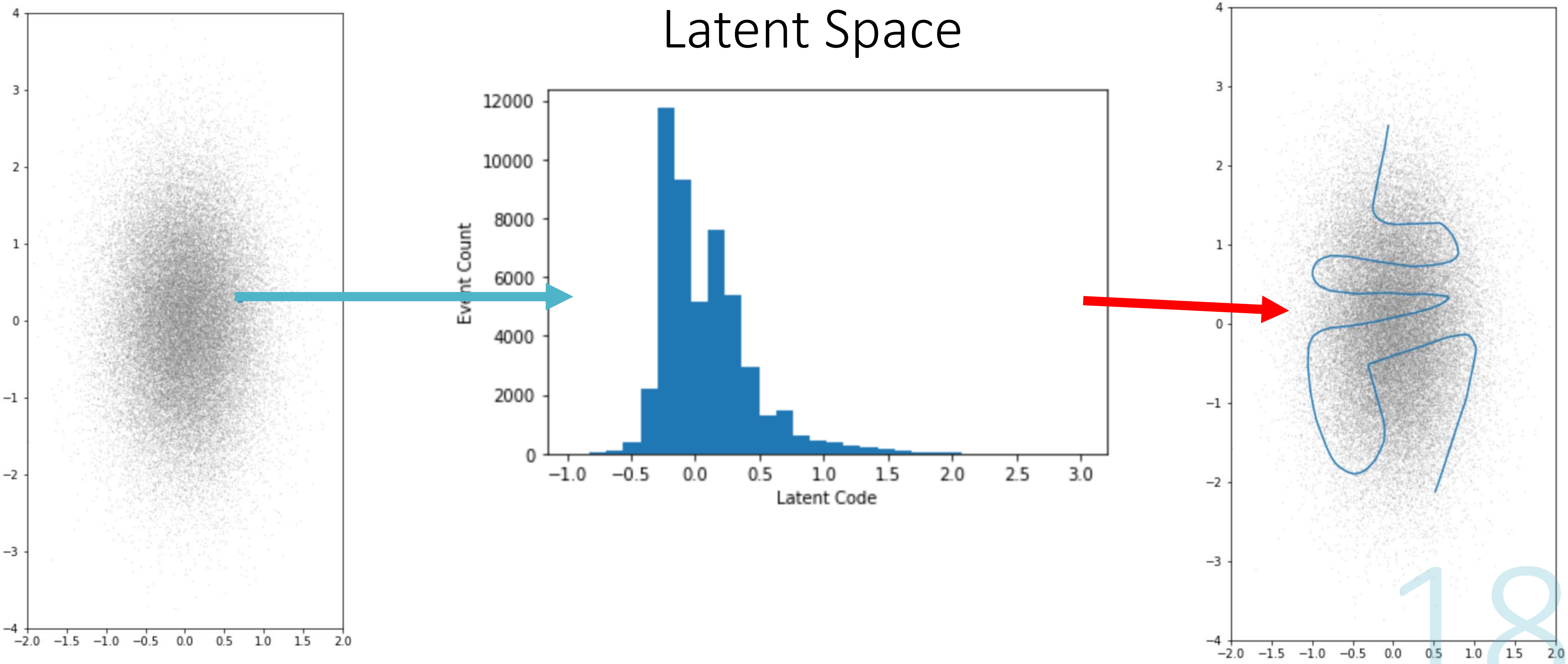
(1D latent space)

Rec. Loss = $|\boldsymbol{x}_{out} - \boldsymbol{x}_{in}|^2$



The Plain Autoencoder

Garbage

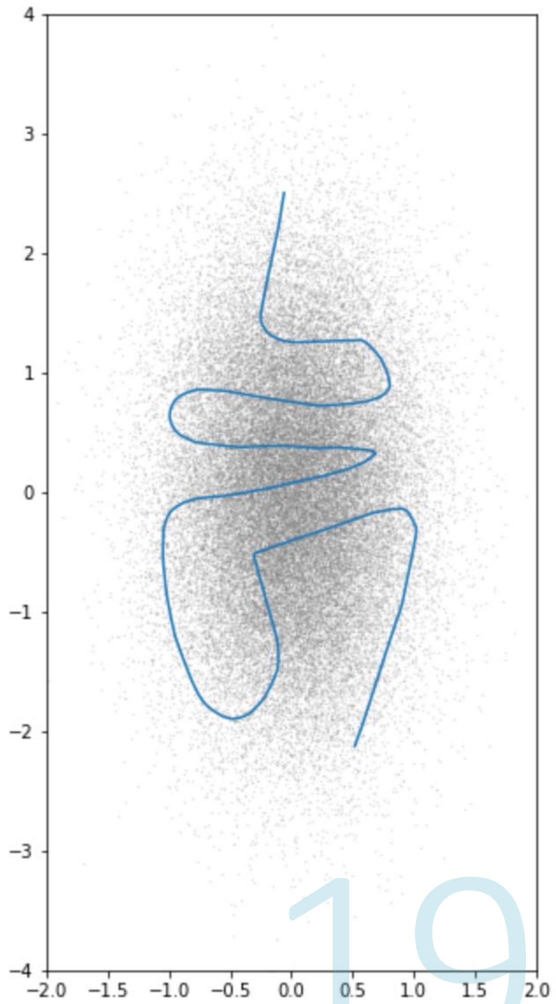


The Plain Autoencoder

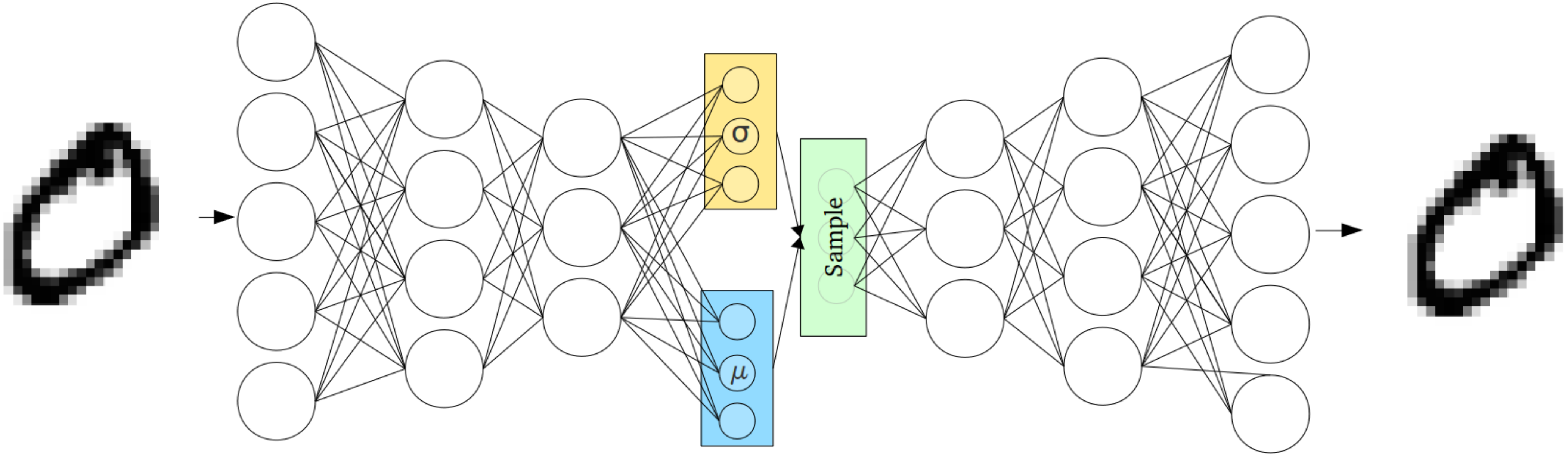
Garbage

1. The AE learns some dense packing of the data space

2. The latent representation is highly coupled with the expressiveness of the network architecture of the encoder and decoder



The Variational Autoencoder



$$\text{Loss} = \underbrace{|\boldsymbol{x}_{out} - \boldsymbol{x}_{in}|^2/\beta^2}_{\textit{Reconstruction error}} - \underbrace{\textstyle\sum_i \frac{1}{2}\left(1 + \log \sigma_i^2 - \mu_i^2 - \sigma_i^2\right)}_{KL(q(z|x)||p(z)) \sim \text{“Information cost”}}$$

The Variational Autoencoder:

Information and the loss function

$$\text{Loss} = |\boldsymbol{x}_{out} - \boldsymbol{x}_{in}|^2/\beta^2 - \sum_i \frac{1}{2}\left(1 + \log\sigma_i^2 - \mu_i^2 - \sigma_i^2\right)$$

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The Variational Autoencoder:

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1) $\boldsymbol{\beta}$ is dimensionful!

The same dimension as the distance metric,
e.g. GeV.

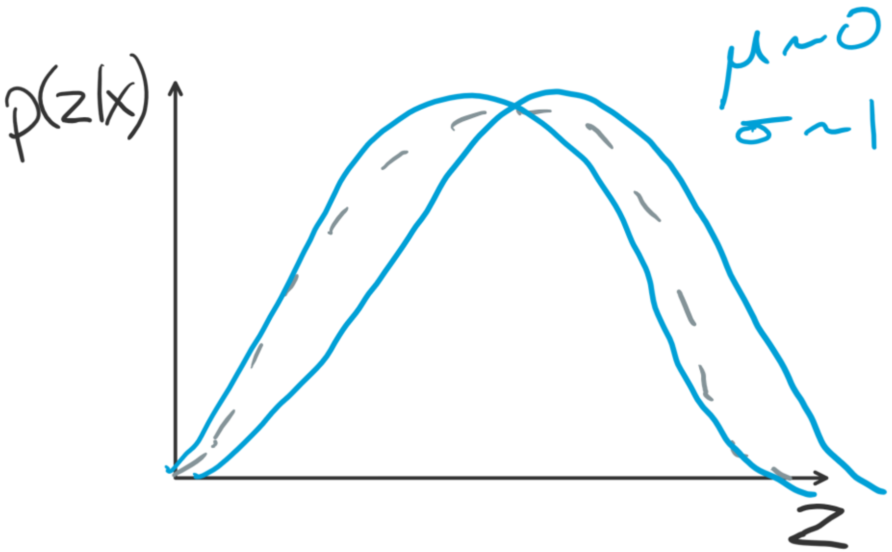
$$\text{Loss} = |\boldsymbol{x}_{out} - \boldsymbol{x}_{in}|^2 - \beta^2 \sum_i \frac{1}{2}\left(1 + \log\sigma_i^2 - \mu_i^2 - \sigma_i^2\right)$$

The Variational Autoencoder:

Information and the loss function

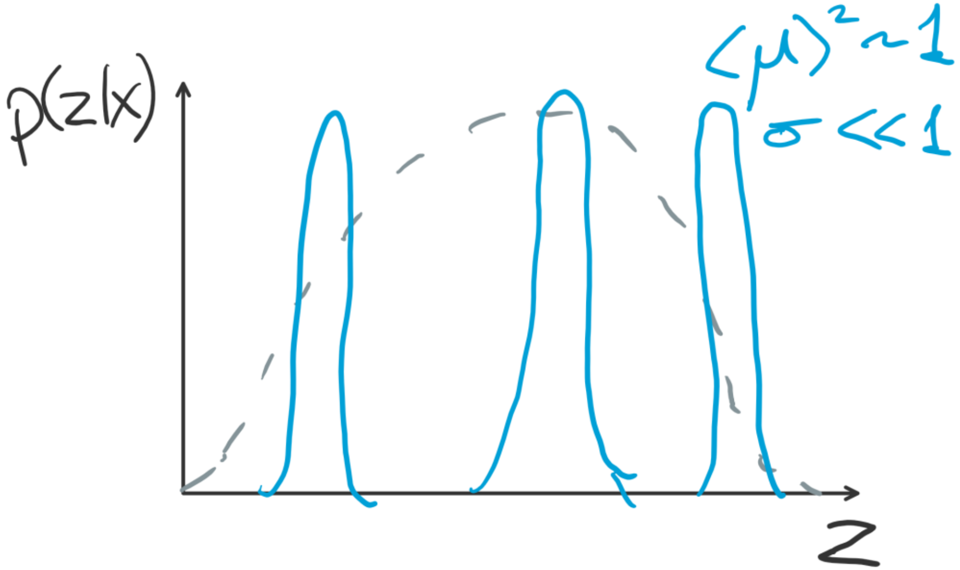
$\boldsymbol{\beta} \rightarrow \infty$

No info encoded in latent space



$\boldsymbol{\beta} \ll$ *Lengthscale*

Info encoded in latent space



$$\text{Loss} = |\boldsymbol{x}_{out} - \boldsymbol{x}_{in}|^2 - \beta^2 \sum_i \frac{1}{2}\left(1 + \log\sigma_i^2 - \mu_i^2 - \sigma_i^2\right)$$

The Variational Autoencoder:

Information and the loss function

$\boldsymbol{\beta} \rightarrow \infty$

No info encoded in latent space

$\boldsymbol{\beta} \ll$ ***Lengthscale***

Info encoded in latent space

2) $\boldsymbol{\beta}$ is the cost for encoding information

The encoder will only encode information about the input to the extent that its usefulness for reconstruction is sufficient to justify the cost.

$$\text{Loss} = |\boldsymbol{x}_{out} - \boldsymbol{x}_{in}|^2 - \beta^2 \sum_i \frac{1}{2}\left(1 + \log\sigma_i^2 - \mu_i^2 - \sigma_i^2\right)$$

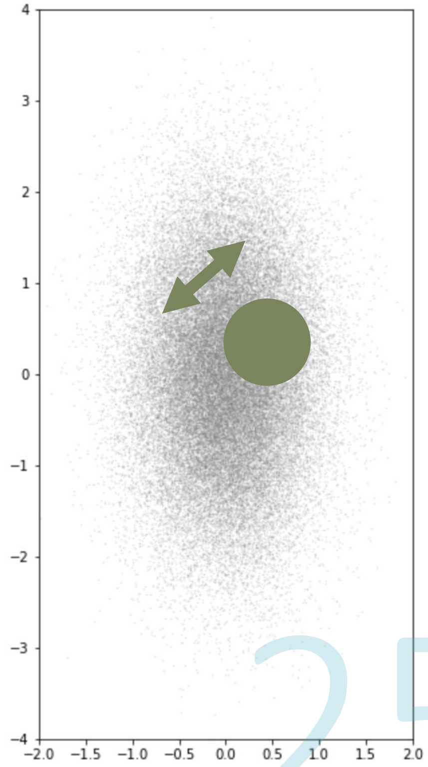
The Variational Autoencoder:

Information and the loss function

$$\text{Loss} = |\boldsymbol{x}_{out} - \boldsymbol{x}_{in}|^2/\beta^2 - \sum_i \frac{1}{2}\left(1 + \log\sigma_i^2 - \mu_i^2 - \sigma_i^2\right)$$

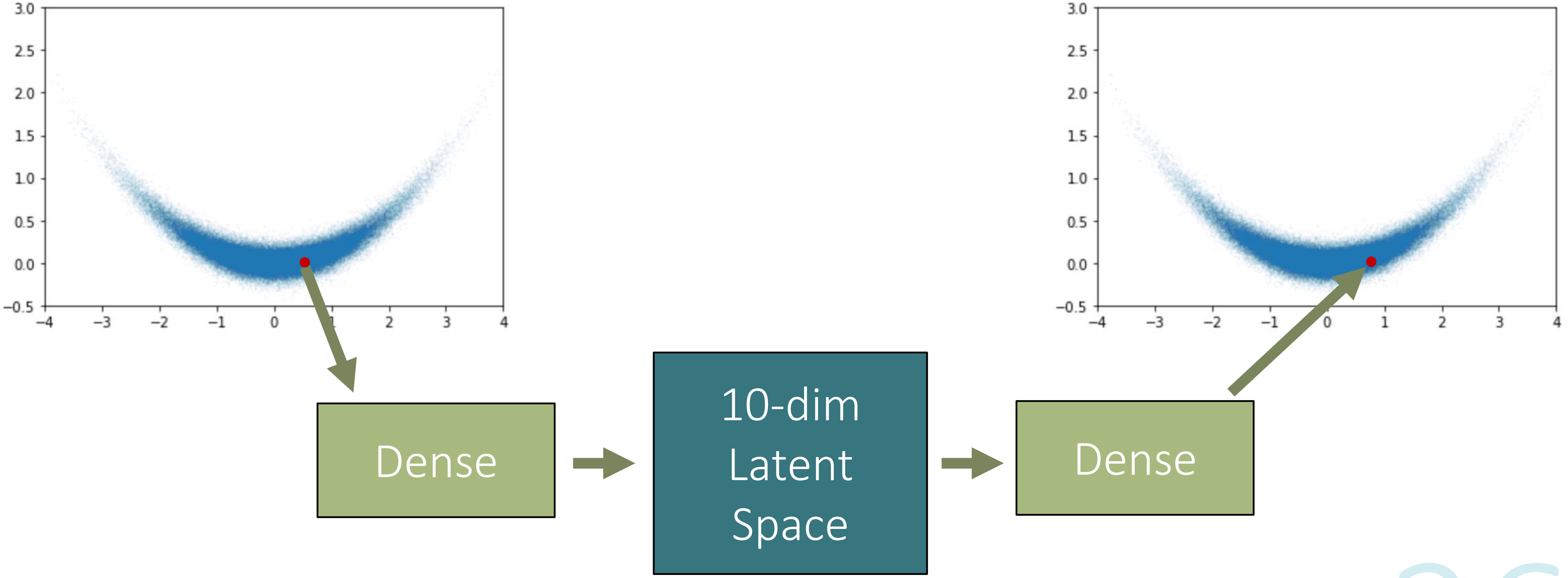
3) $\boldsymbol{\beta}$ is the distance resolution in reconstruction space

The stochasticity of the latent sampling will smear the reconstruction at scale $\sim \beta$



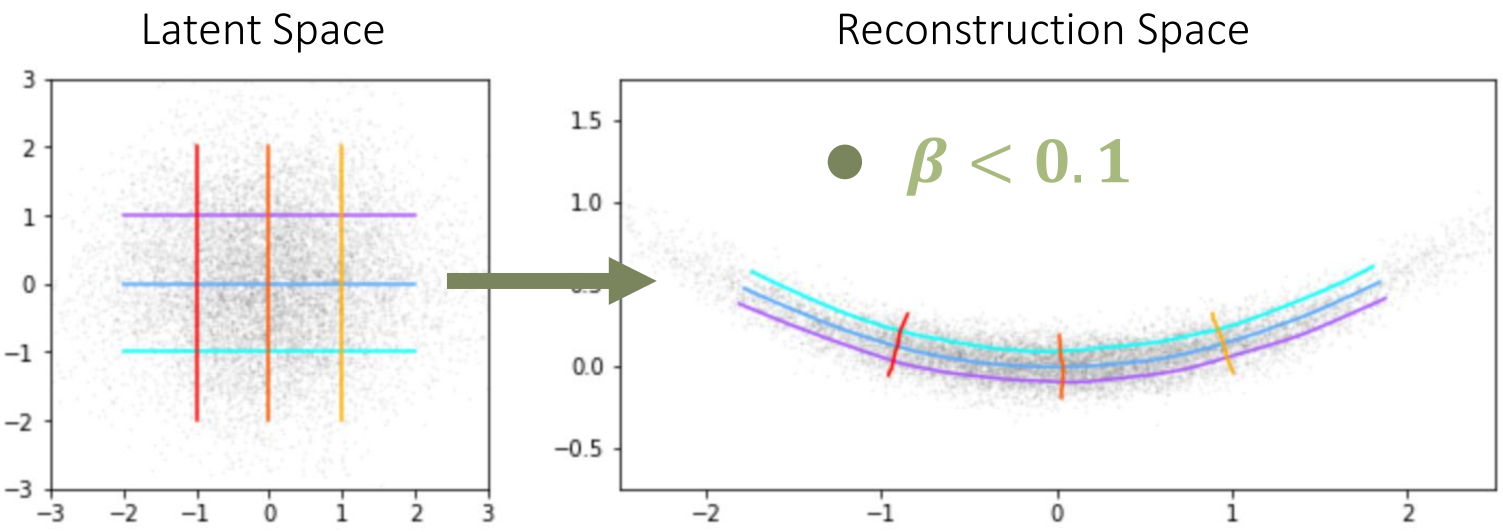
The Variational Autoencoder

Bananas



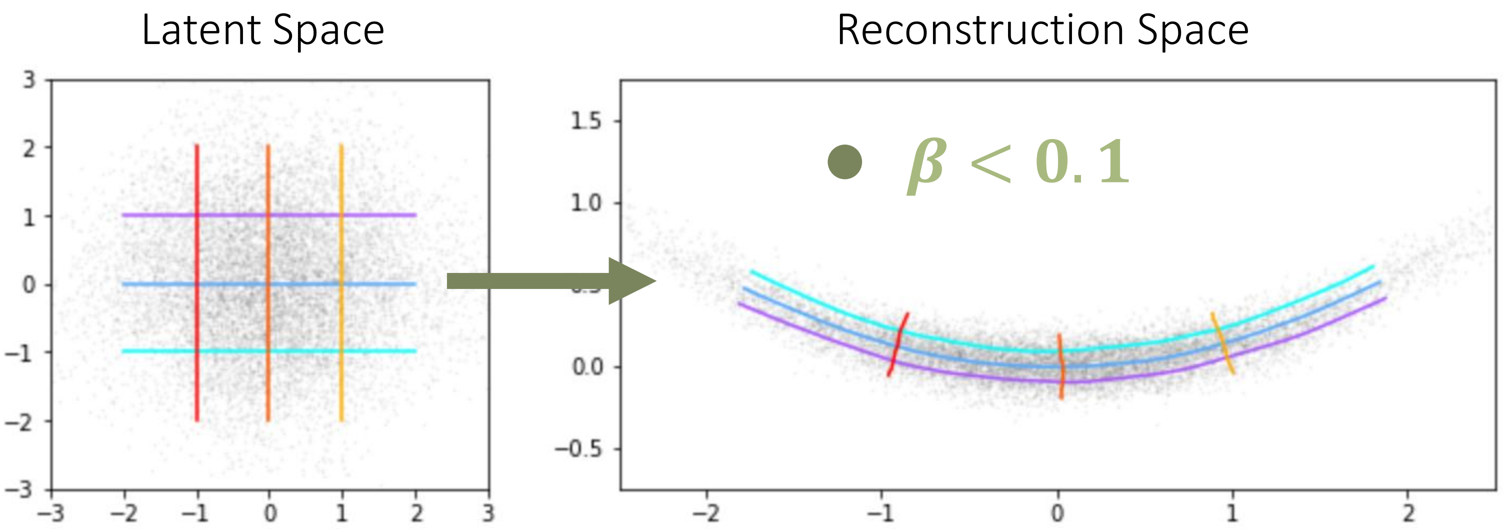
The Variational Autoencoder:

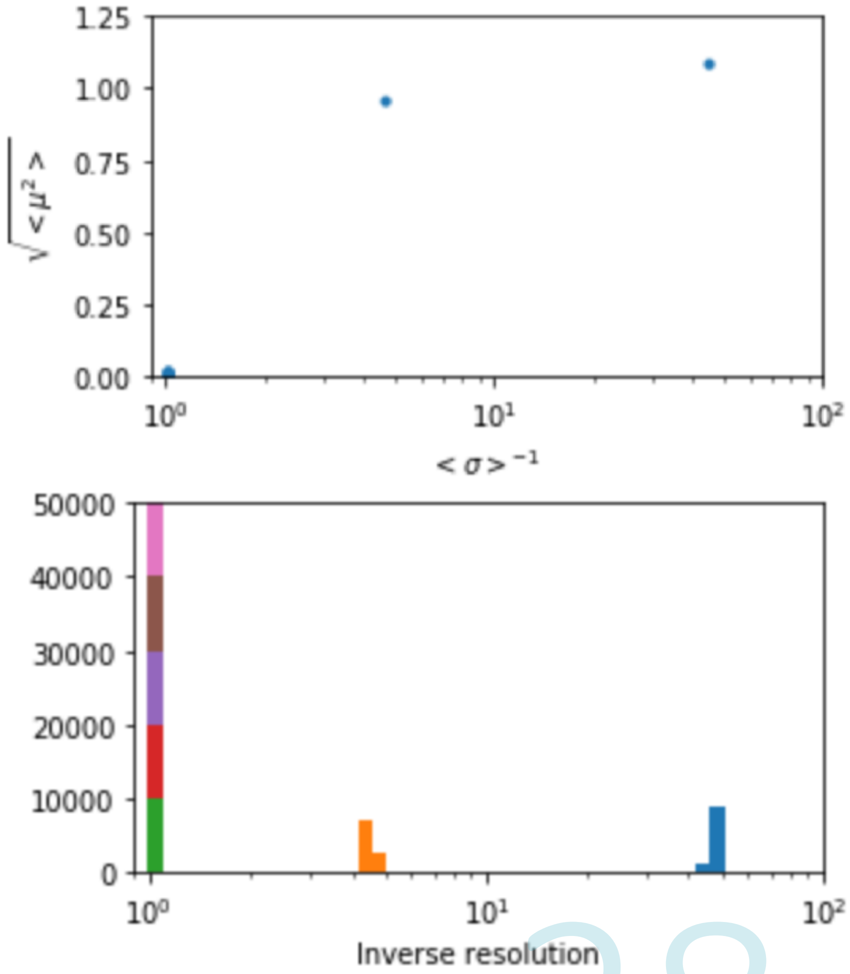
Bananas



The Variational Autoencoder:

Bananas

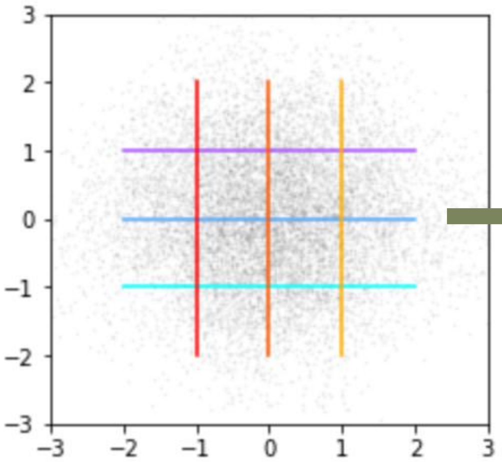




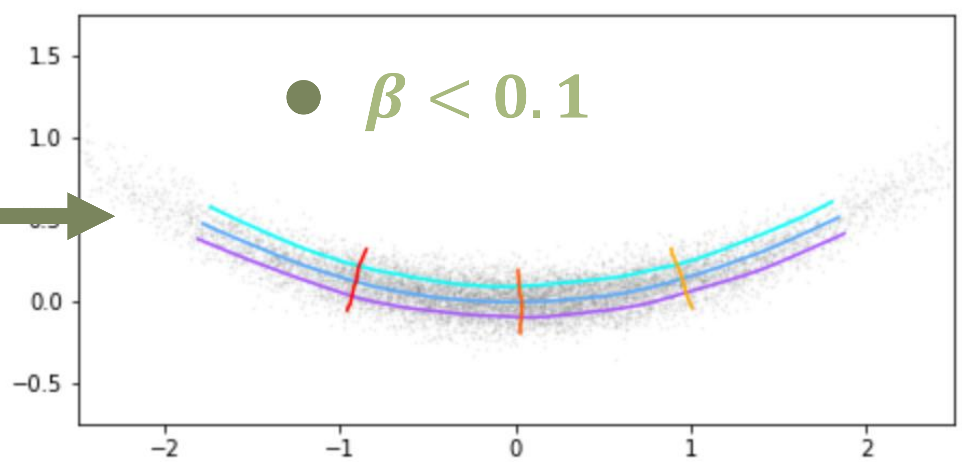
The Variational Autoencoder:

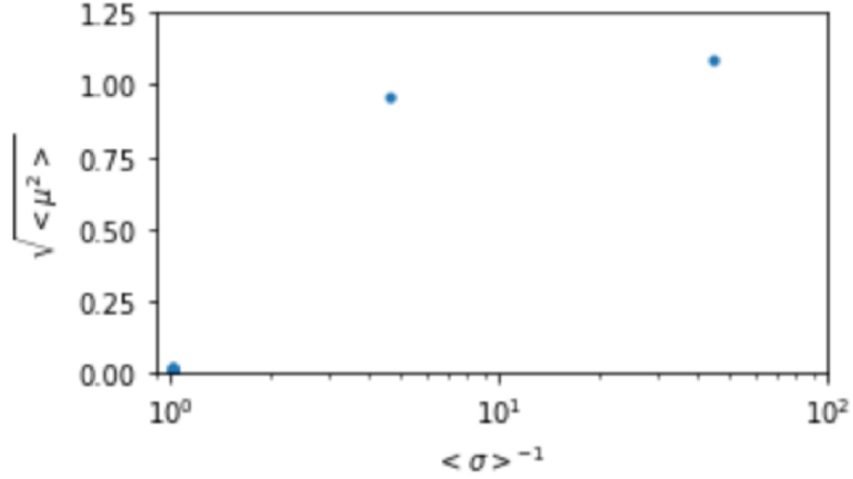
Bananas

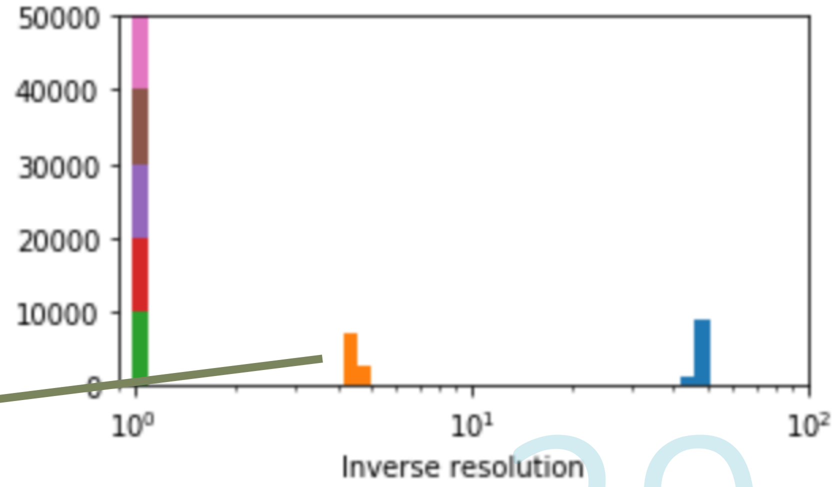
Latent Space



Reconstruction Space





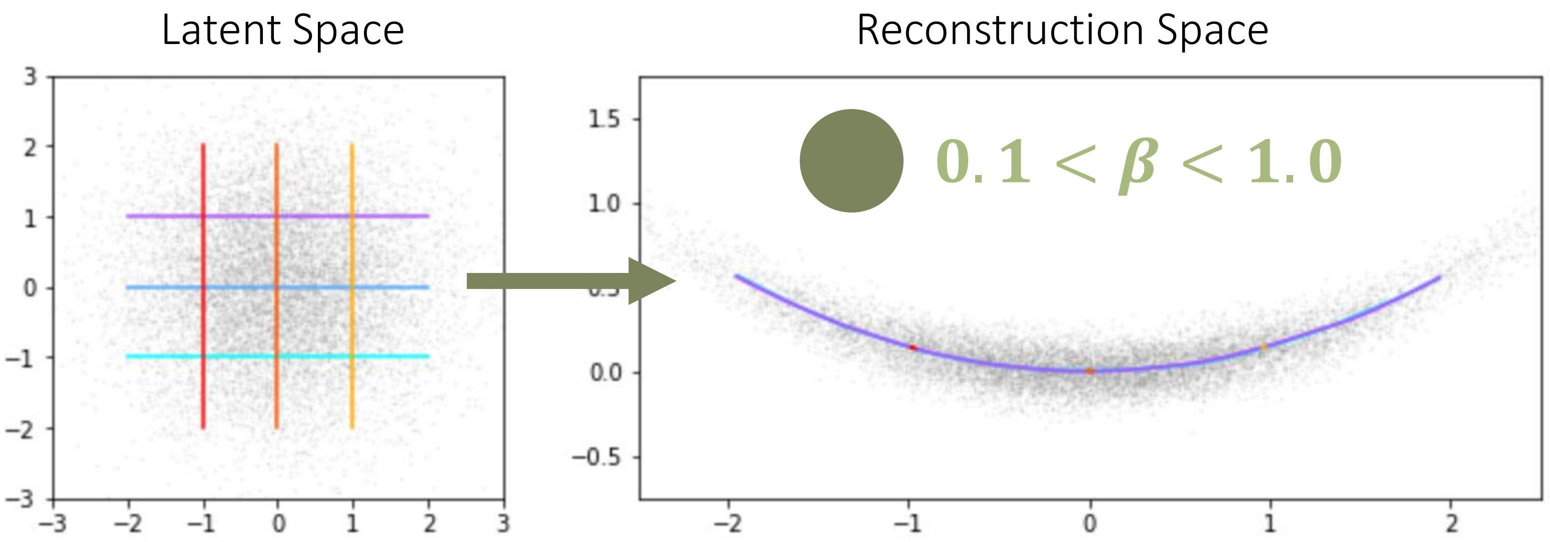


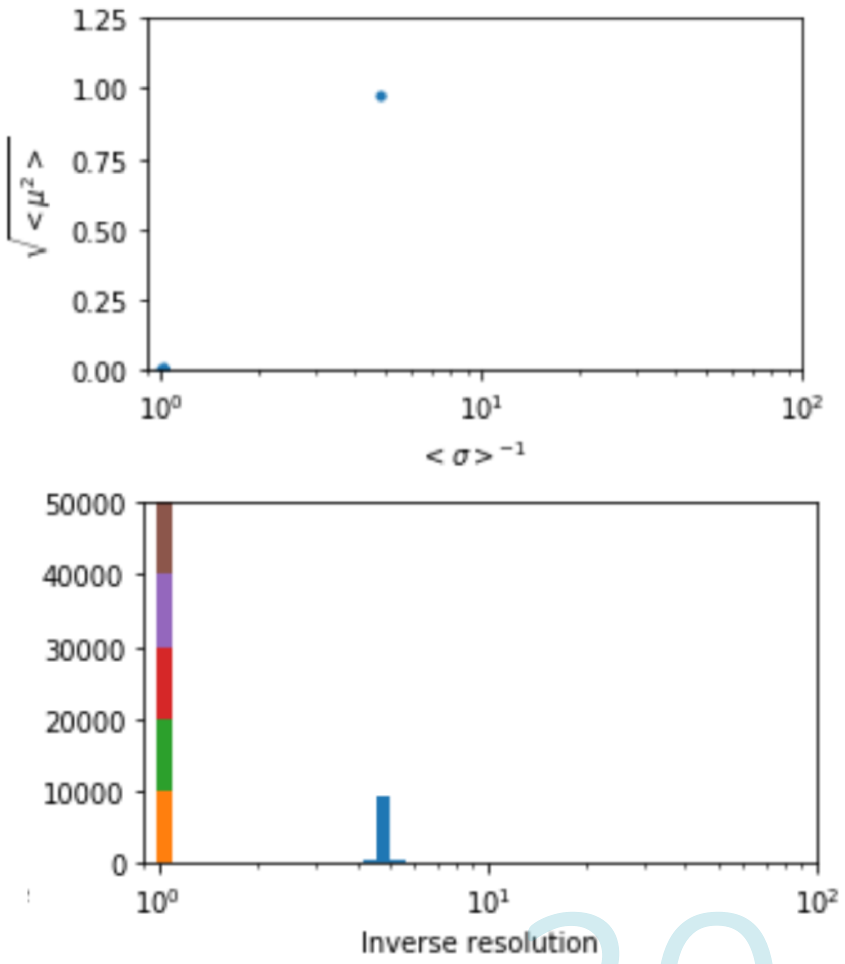
The VAE is doing non-linear PCA

Size = $^{\beta}/_{\sigma}$

The Variational Autoencoder:

Bananas

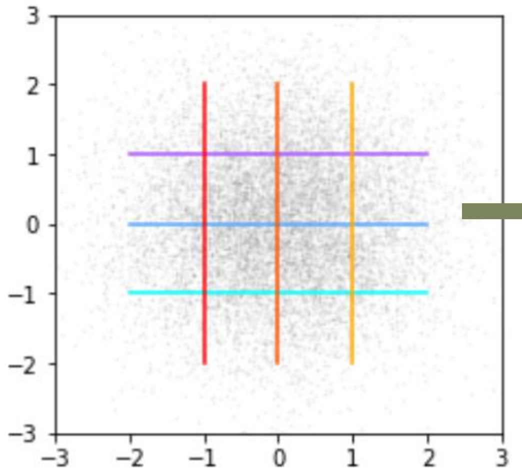




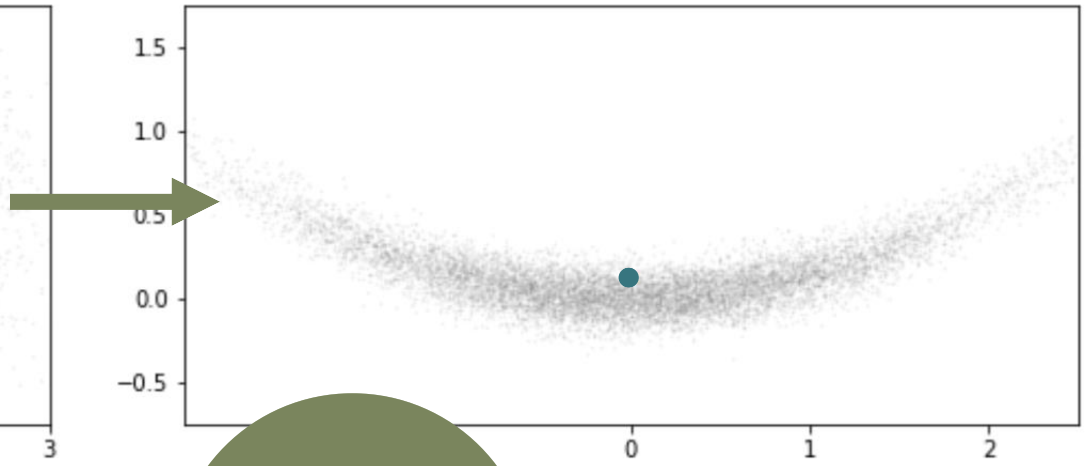
The Variational Autoencoder:

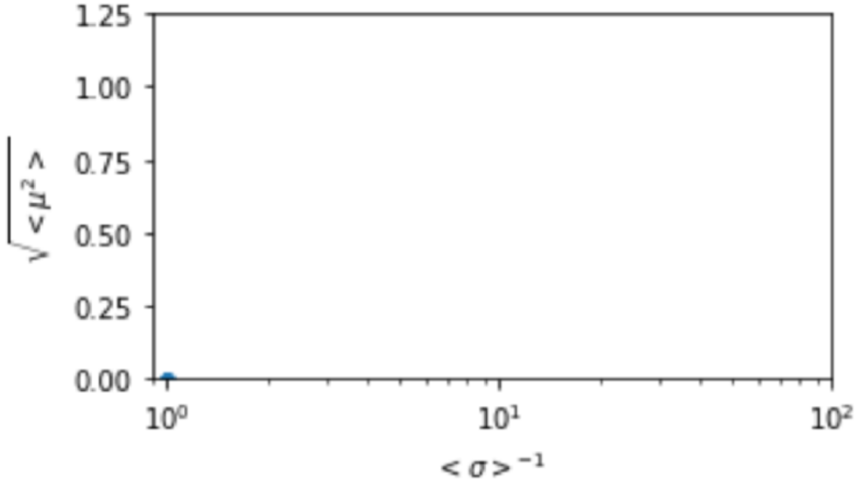
Bananas

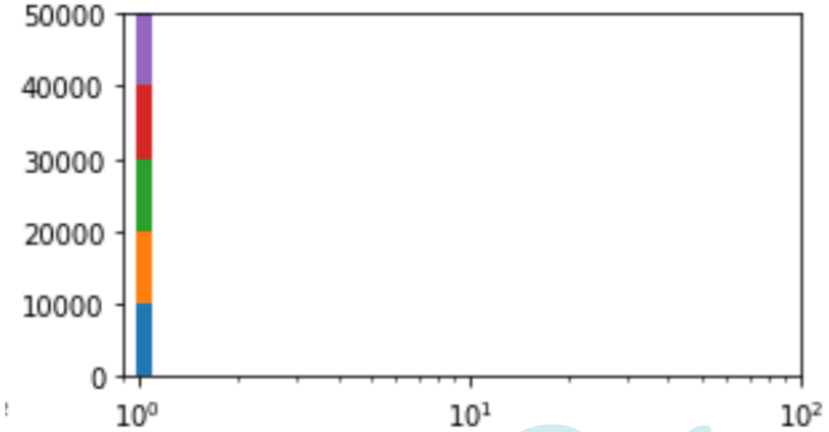
Latent Space



Reconstruction Space







$\beta \gg 1$

The Variational Autoencoder

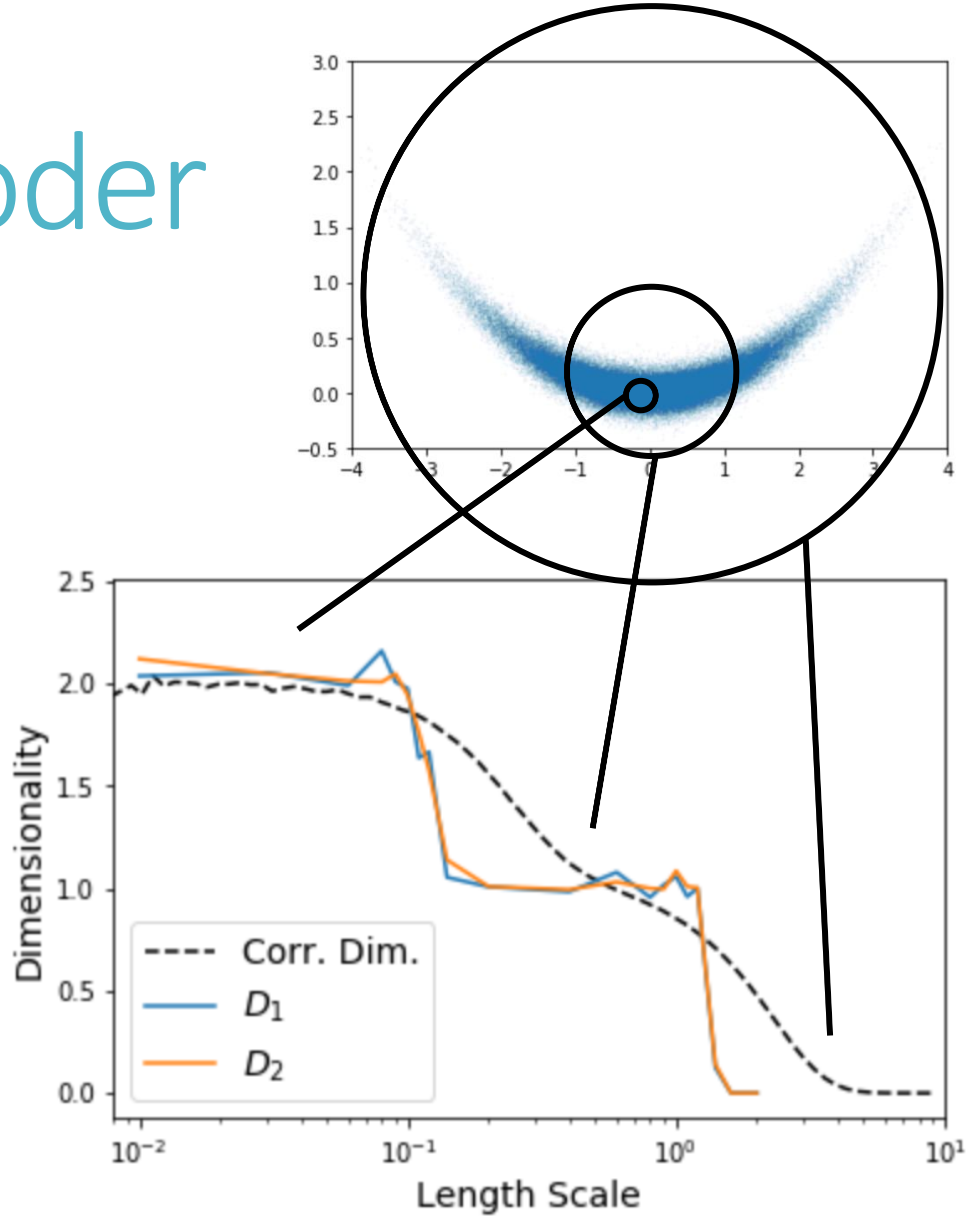
Dimensionality

$$D_1 \equiv 2\,\frac{d\langle|\Delta \boldsymbol{x}|^2\rangle}{d\,\beta^2}$$

Variation of resolution with scale (think $\langle r^2\rangle = D\,\sigma^2$ for D-dimensional Gaussian).

$$D_2 \equiv \frac{d\;KL}{d\log\beta}$$

Variation of information with scale.



I am still trying to work out formally the meaning of these expressions, but they have an air of truthiness about them and empirically give sensible results.

The Variational Autoencoder

What is new?

Dimensionality Analysis

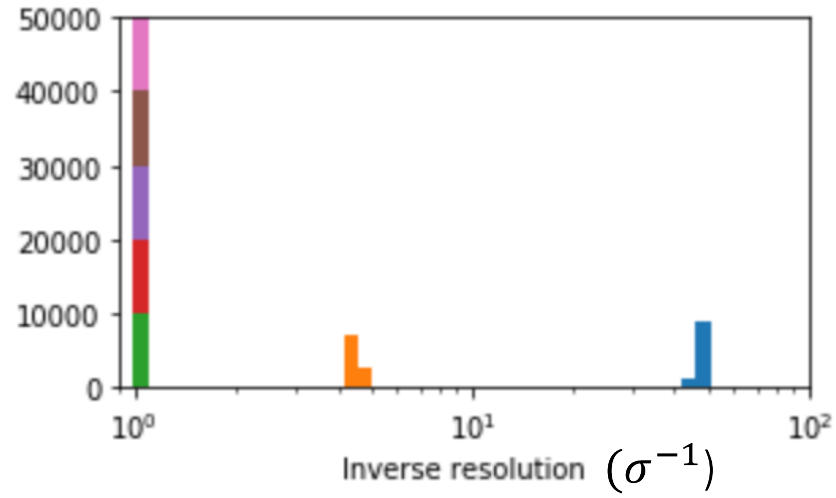
$$D_1 \equiv 2\frac{d\langle|\Delta \boldsymbol{x}|^2\rangle}{d\ \beta^2}$$

$$D_2 \equiv \frac{d\ KL}{d \log \beta}$$

Are these new?

I have never seen them before.

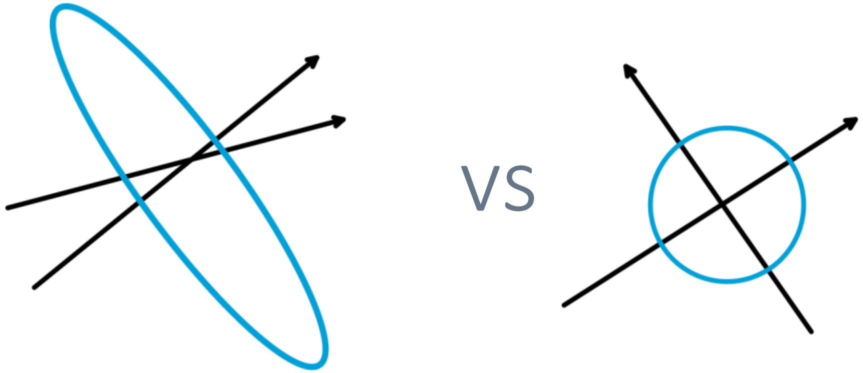
Spectral Analysis



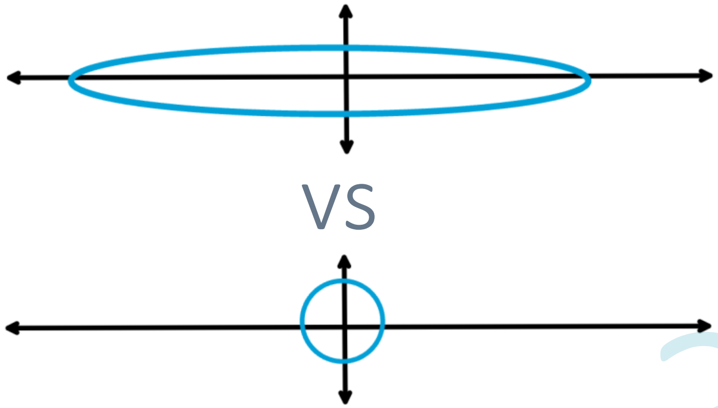
The Variational Autoencoder

Orthogonalization and Organization is Information-Efficient

Orthogonalization:



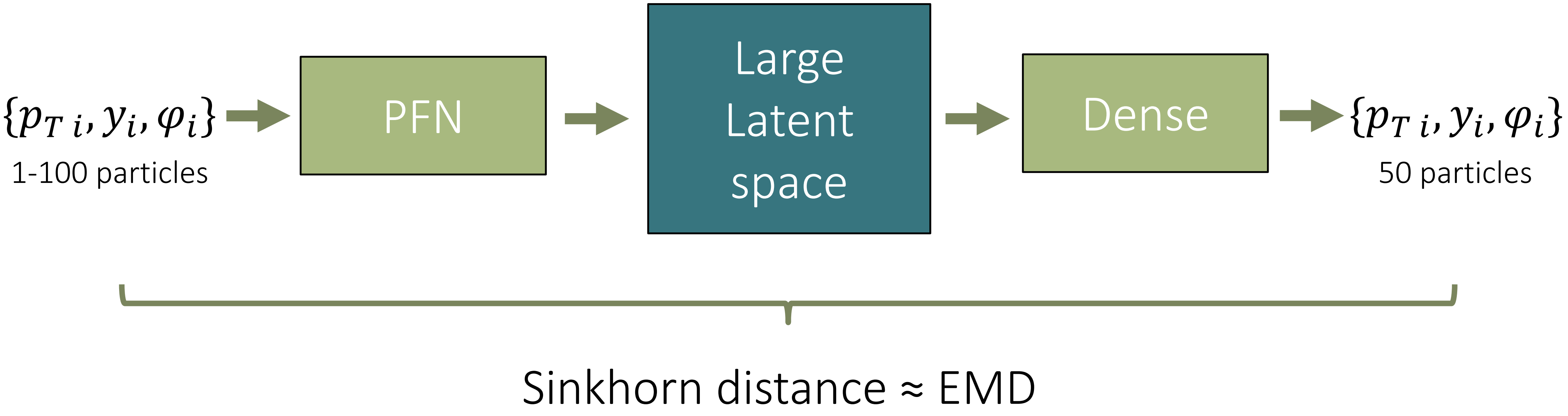
Organization:



Cheese Course

Application to Top Jets

Jet VAE

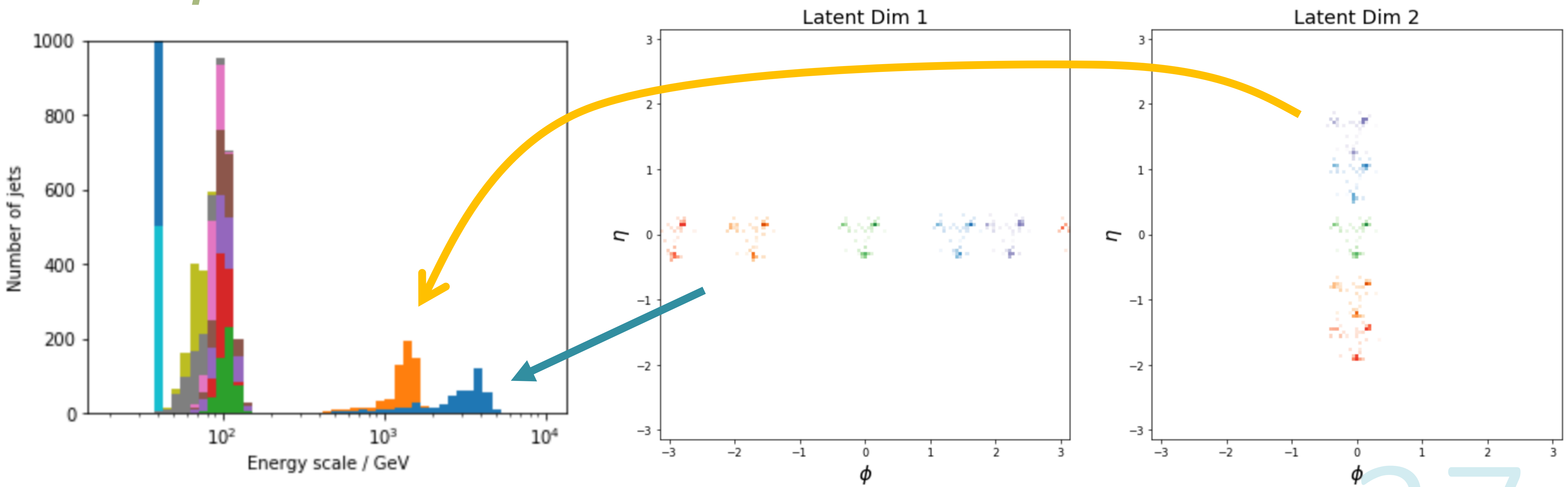


$\{p_{T\,i}, y_i, \varphi_i\}$
1-100 particles
PFN
Large Latent space
Dense
$\{p_{T\,i}, y_i, \varphi_i\}$
50 particles
Sinkhorn distance ≈ EMD

Exploring the Learnt Representation:

Top Jets

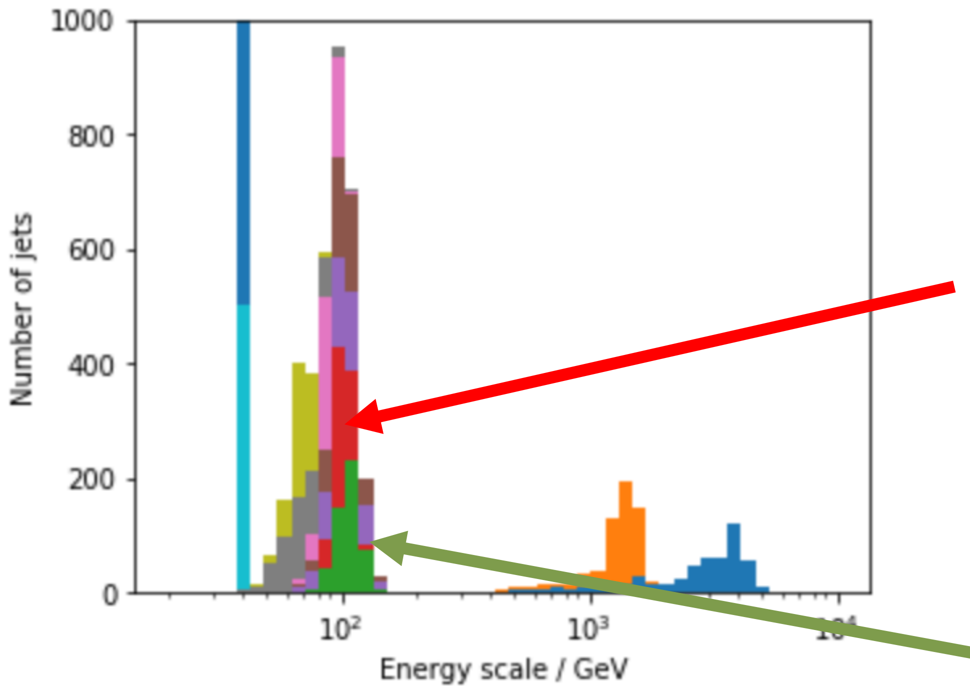
$$\beta = 40\ GeV$$

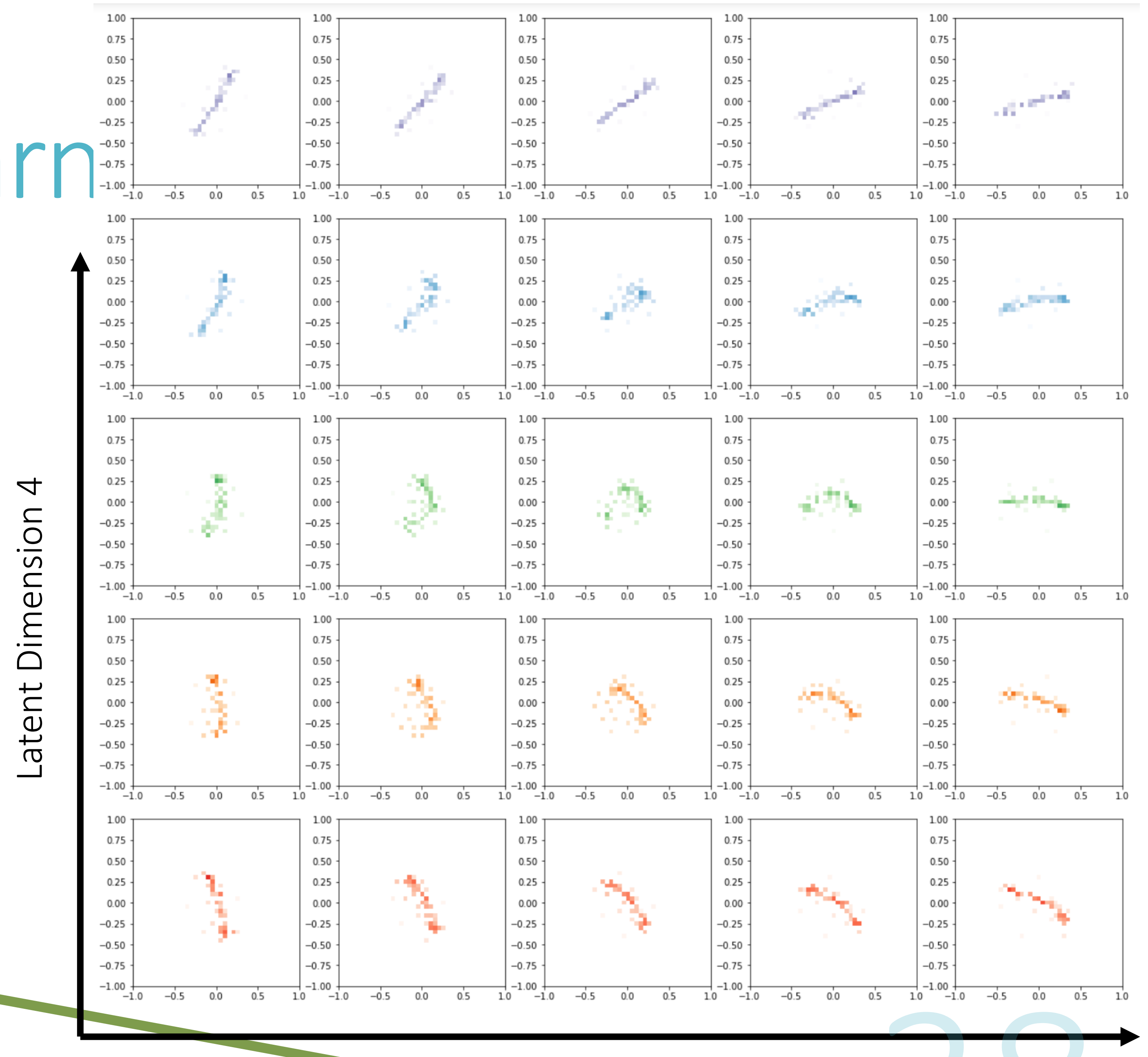


Exploring the Learn

Top Jets

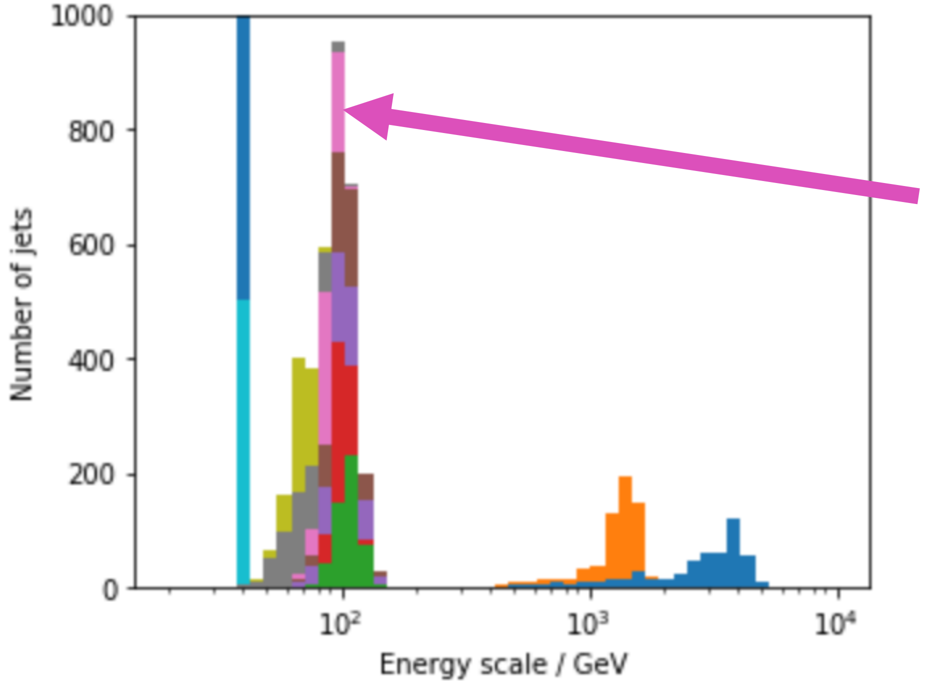
$\beta = 40\ GeV$

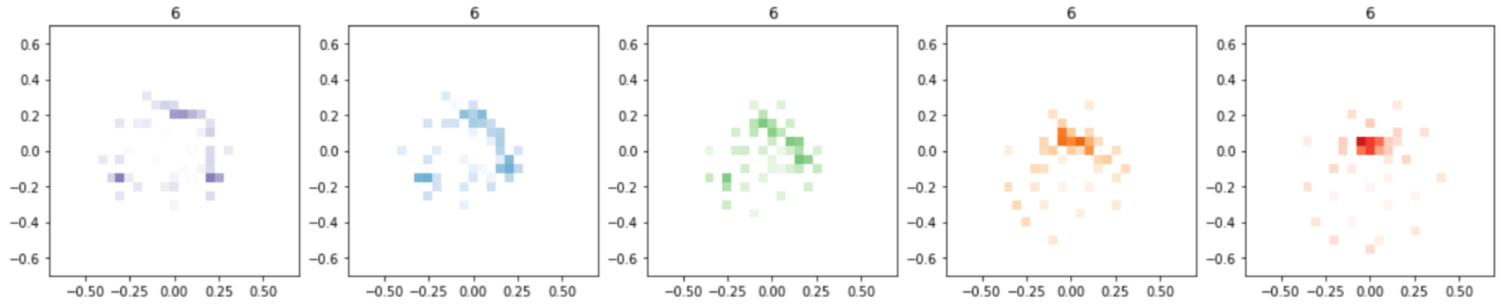




Exploring the Learnt Representation:
Top Jets

$\beta = 40\ GeV$

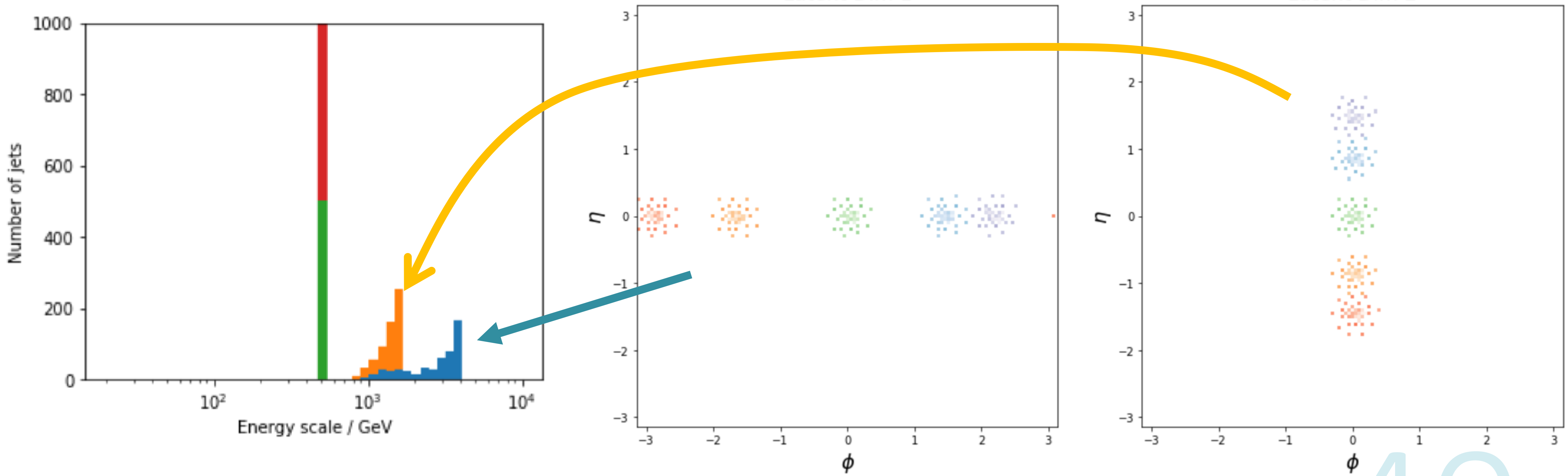




Exploring the Learnt Representation:

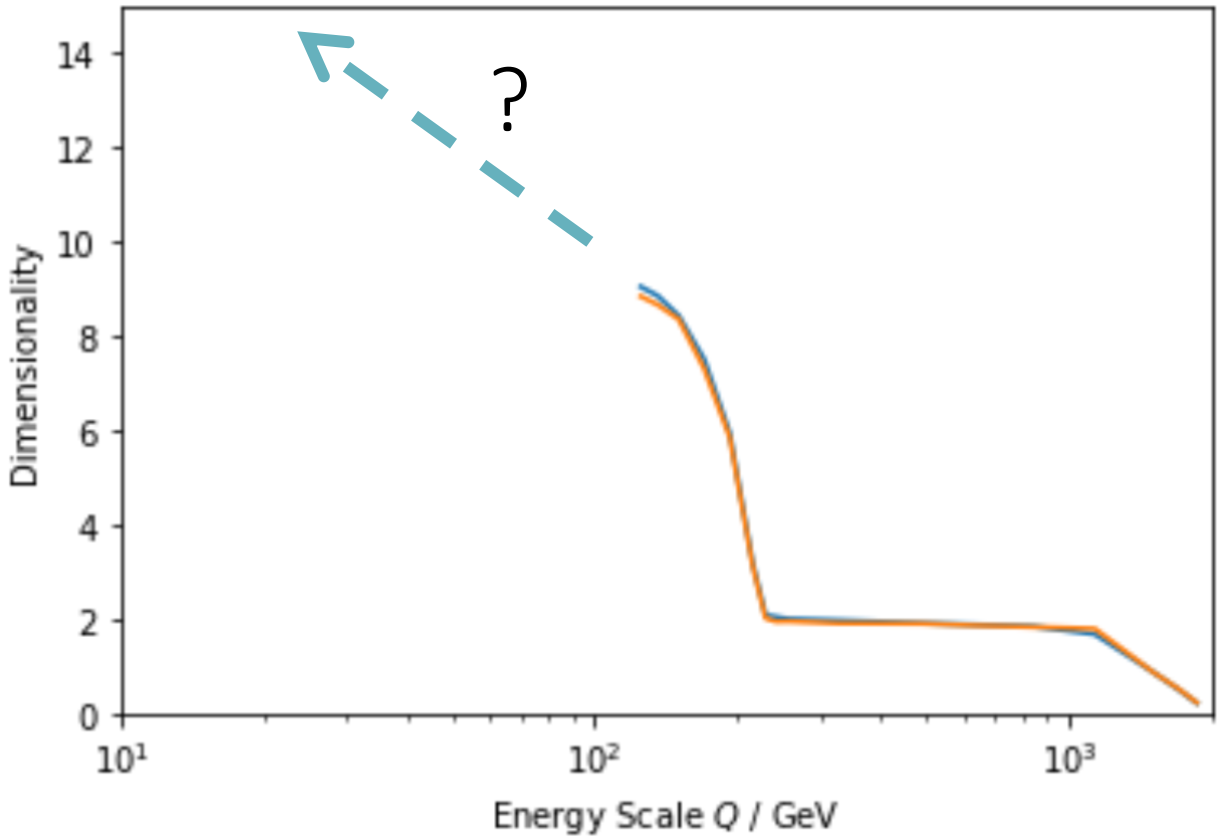
Top Jets

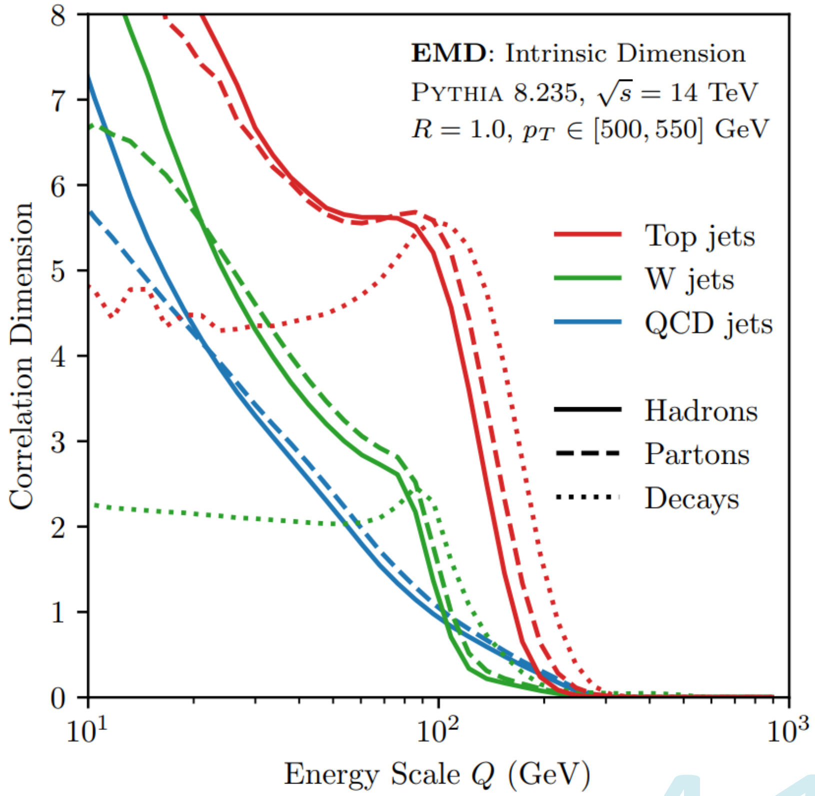
$\boldsymbol{\beta = 400\ GeV}$



Exploring the Learnt Representation:

Dimensionality





What is the point?

“Can we learn something new from dimensionality and geometry? Maybe something in the nonperturbative regime?”

Anonymous Professor A

“Once you have understood the geometry of the data manifold you have understood everything about the problem”

Anonymous Professor B

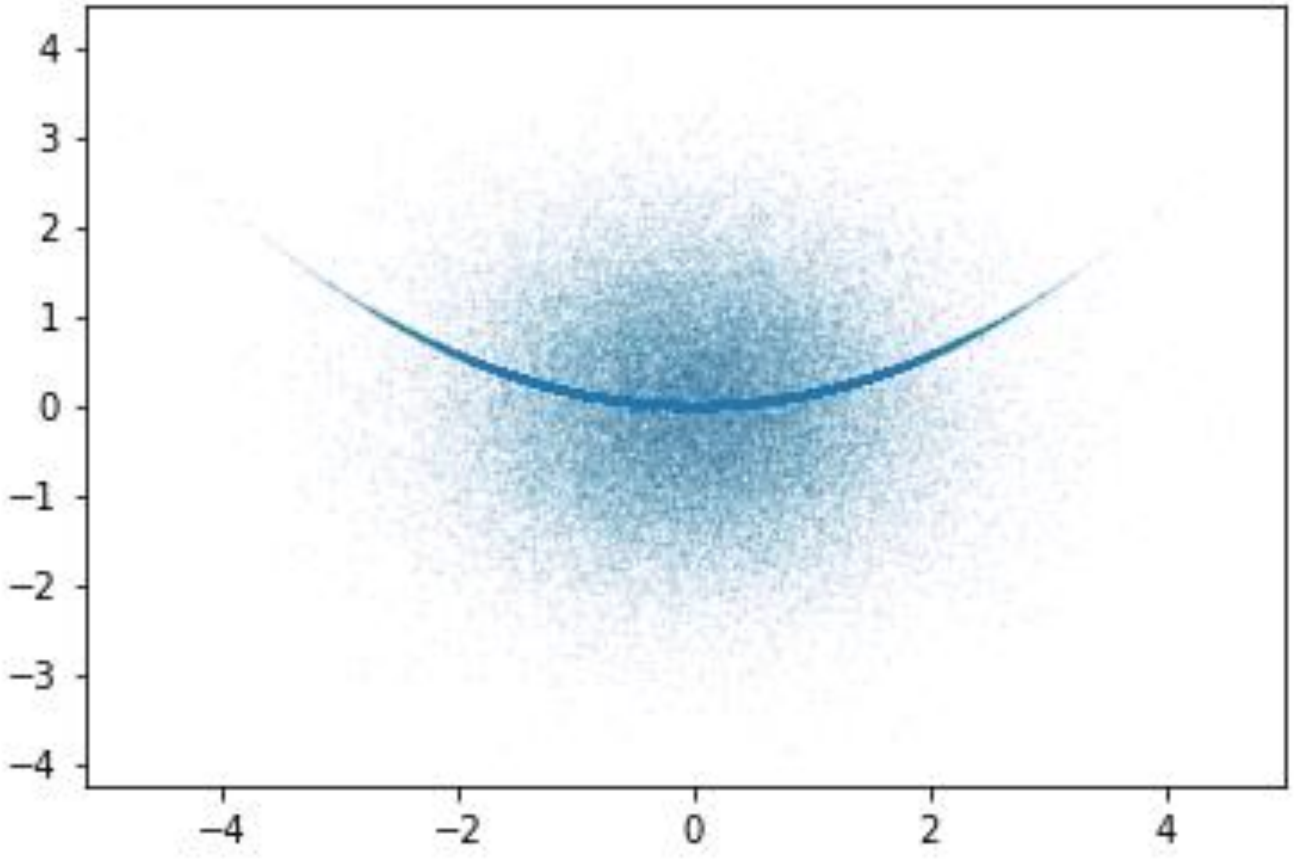
“Ehhhh, I don’t know, probably not.”

These are not exact quotes, just based on recollection, please don’t take them too seriously!

Dessert

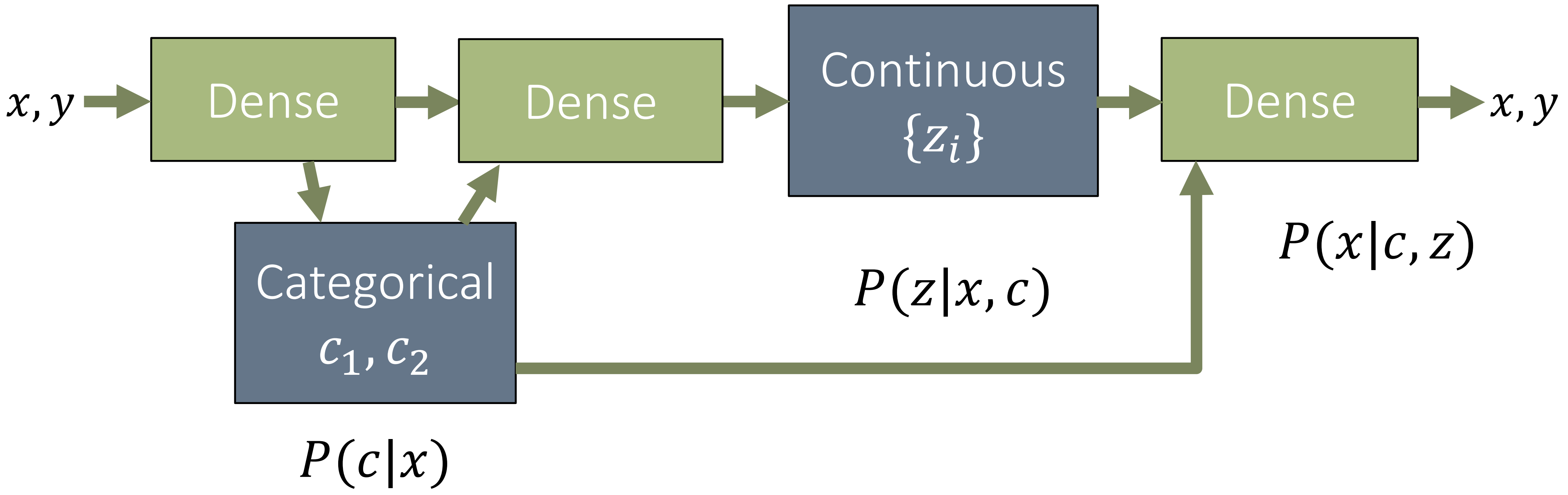
Unsupervised Classification

A Mixed Sample



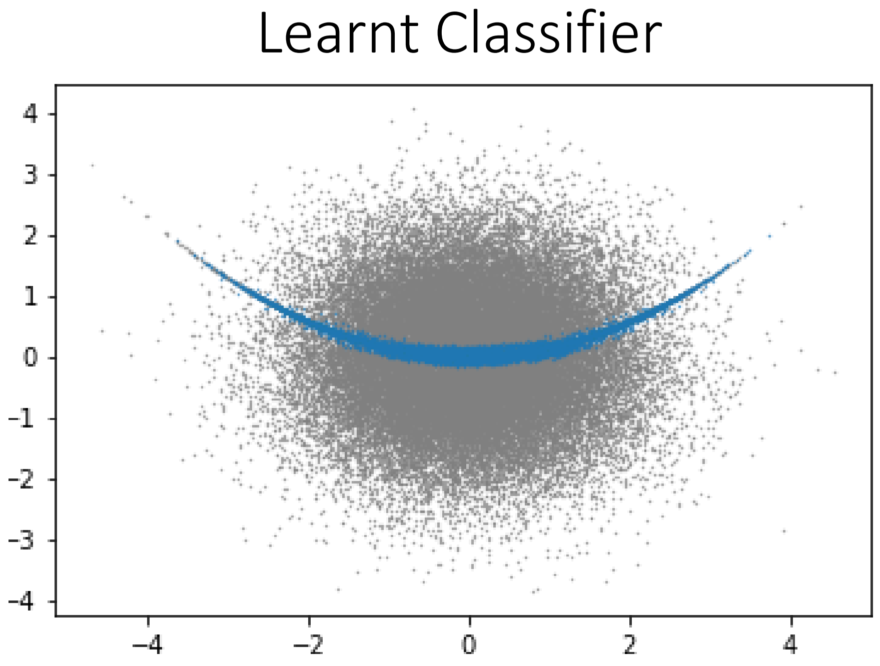
A Mixed Sample

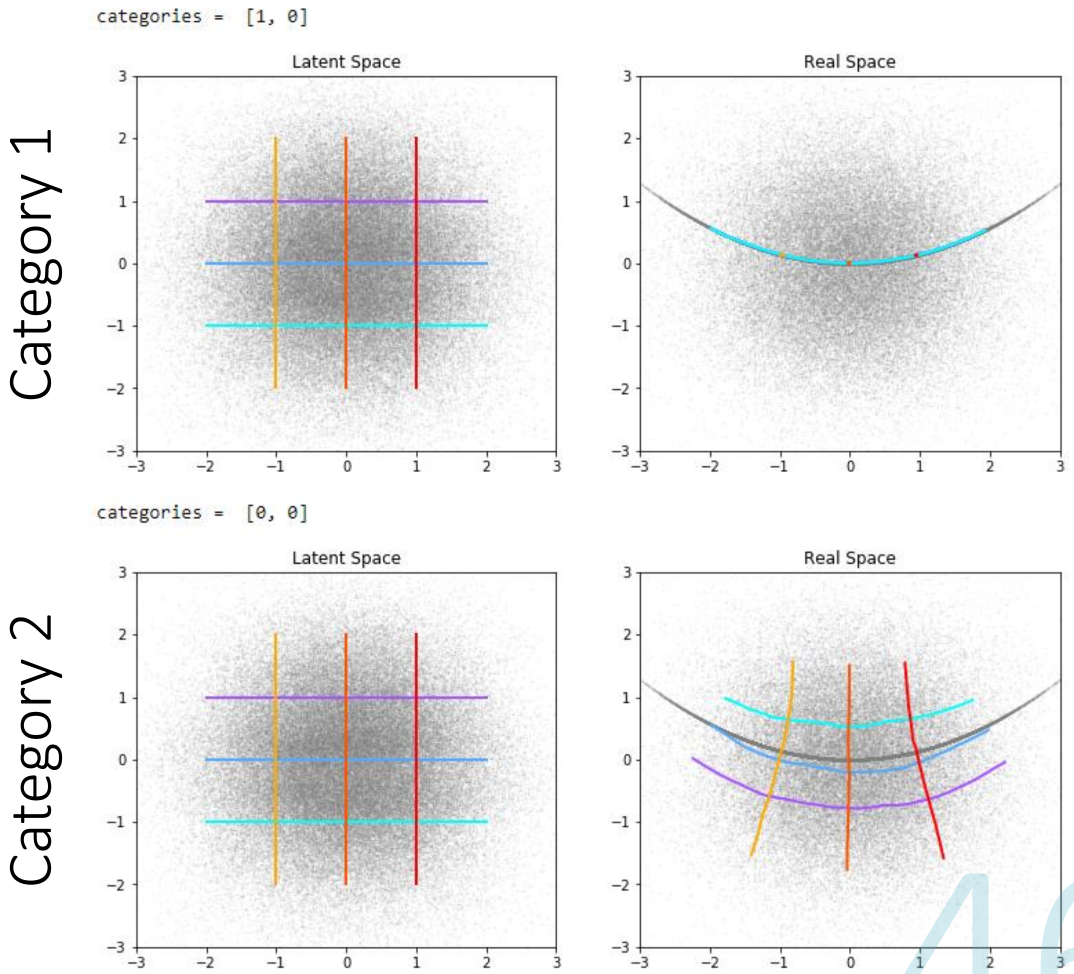
VAE structure



A Mixed Sample

VAE structure





A Note on Topology

The regular Gaussian VAE is trying to learn a mapping from the real data manifold M to the latent space R^N, because that is the structure imposed on the latent space.

The real data manifold might not be topologically equivalent to R^N. E.g. the φ coordinate of the jet is on S^1. In this case the plain VAE learns to cut the circle at an arbitrary position, which is not ideal. If I give it a latent space in $R^N \times (S^1)^M$, it should optimally learn to put periodic coordinates on S^1's… What about S^k?

A mixed sample is a superposition of manifolds $M_1 \times M_2 \times$…. This can be modelled using a categorical variable before the continuous ones.

My philosophy: give the VAE as many options for latent category and topology as I can think of and practically implement, and then attempt to learn the structure of the dataset by studying how it chooses to use them.

Is this new?

Digestif

Conclusions

VAE latent spaces learn concrete representations of the manifolds on which they are trained.

A meaningful distance metric which encodes interesting physics at different scales leads to a meaningful learnt representation which encodes interesting physics at different scales.

For a sufficiently simple manifold, the VAE learnt representation is:

- *Orthogonalized*
- *Hierarchically organized*
- *Has a scale-dependent fractal dimension which directly relates to that of the true data manifold*

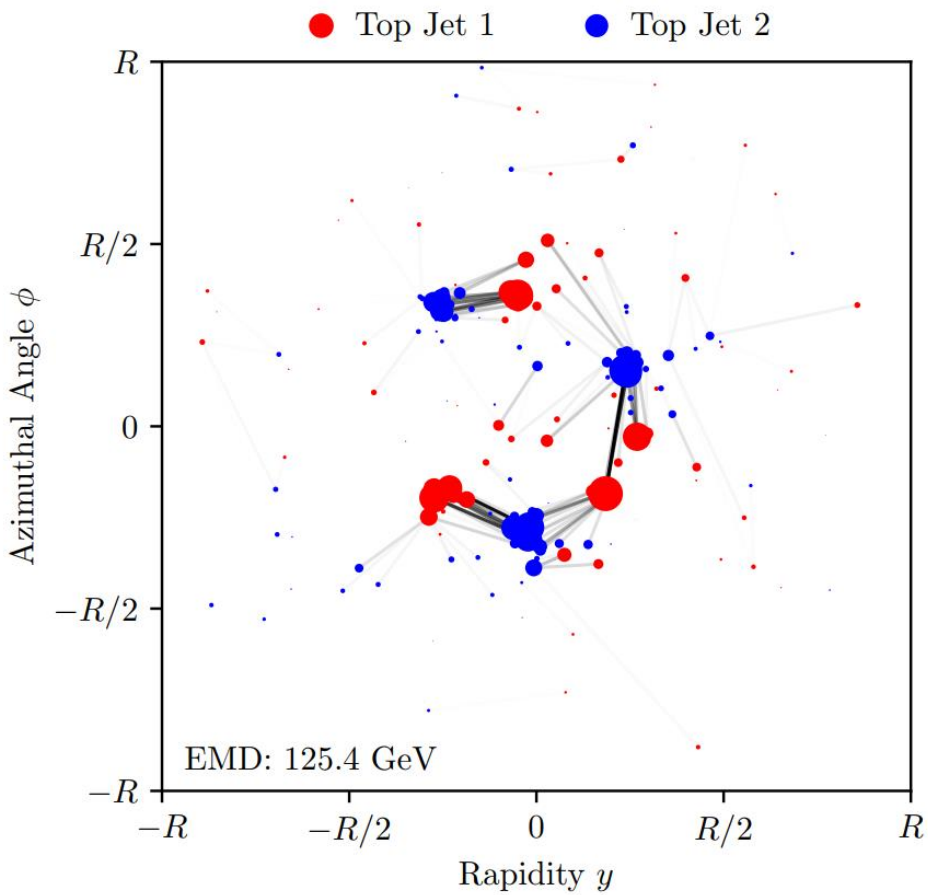
These properties are due to the demand to be ***parsimonious*** with information.

Special thanks to

Reconstruction Error

Sinkhorn Distance ≈ EMD



arXiv:1902.02346

Sinkhorn's algorithm; start with $\Delta R_{ij}, p_{Ti}, p_{Tj}$ then:

$$K_{ij} = \exp(\Delta R_{ij}/\tau)$$
$$u_i = \mathbf{1}_i$$
$$v_i = \mathbf{1}_j$$

Repeat N times:

$$u_i = p_{Ti}/(K.v)_i$$
$$v_i = p_{Tj}/\left(K^T.u\right)_j$$

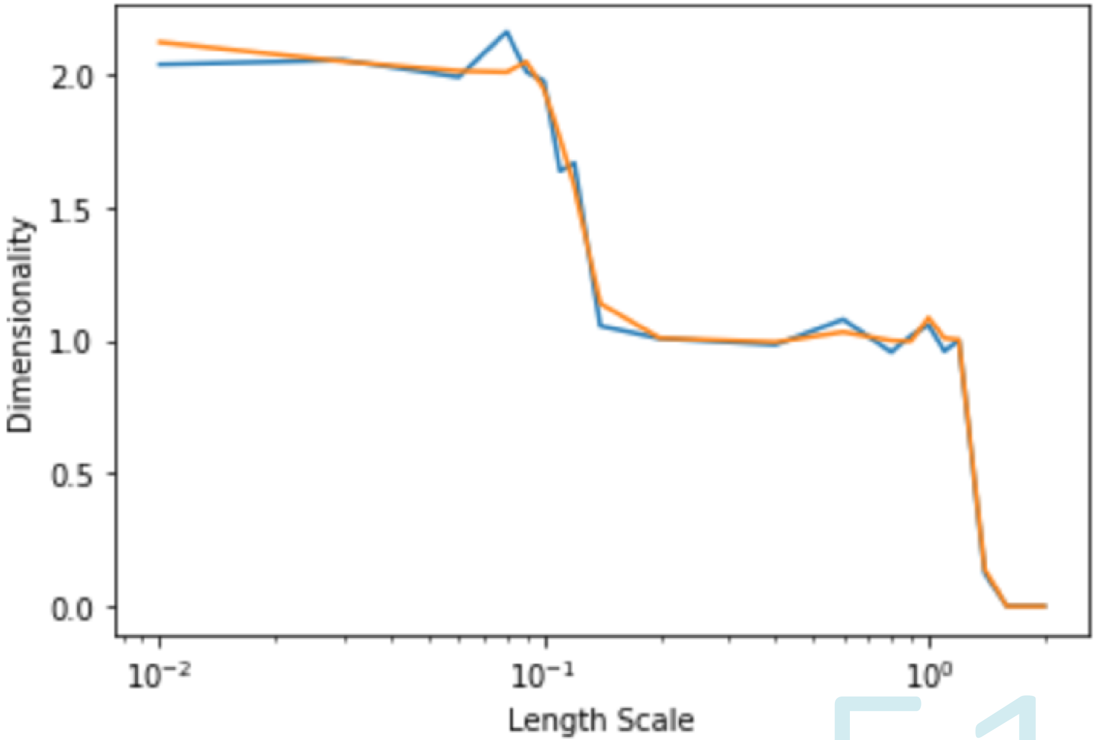
Return $T_{ij} = u_i K_{ij} v_j$

The Variational Autoencoder:

Dimensionality

$$\langle|\Delta \boldsymbol{x}|^2\rangle = \sum\langle|\Delta x_i|^2\rangle = D\rho^2 + \sum_{i>D} S_i^2$$

$$D = \frac{d\langle|\Delta \boldsymbol{x}|^2\rangle}{d\rho^2}$$



Setting $\frac{dL}{d\sigma} = 0$ implies:

1. $\rho = \beta$
2. $D = \frac{d\ KL}{d \log \beta}$

The Variational Autoencoder

Doesn't suffer from curse of dimensionality

Toy data generated from:

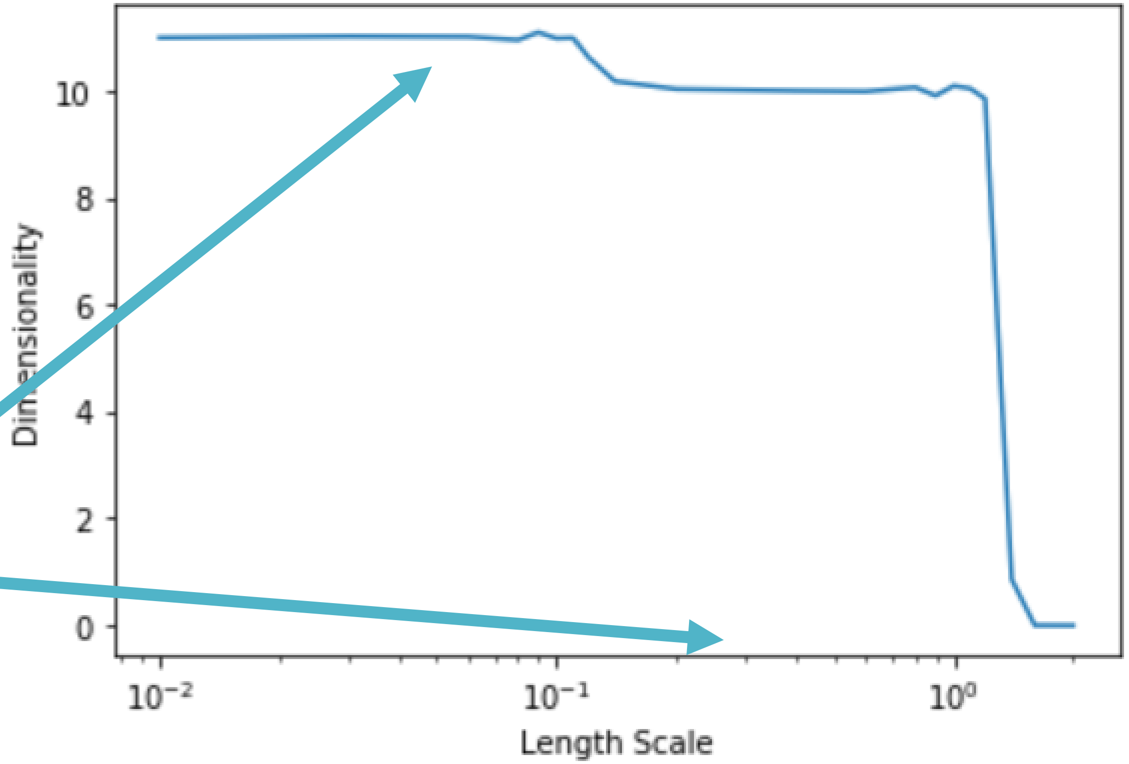
$$P(\vec{x}) = \left[\prod_{i=1}^{10} N_i(\mu = 0, \sigma = 1)\right] N_{11}\,(\mu = 0, \sigma = 0.1)$$

With $N_{tot} = 5 * 10^5$ points

Typical distance to neighbour $\sim N_{tot}^{-1/10} \sim 0.3$

Correlation dimension runs into sparsity limit before the small dimension is even discovered!

The VAE finds the small dimension.



The Plain Autoencoder

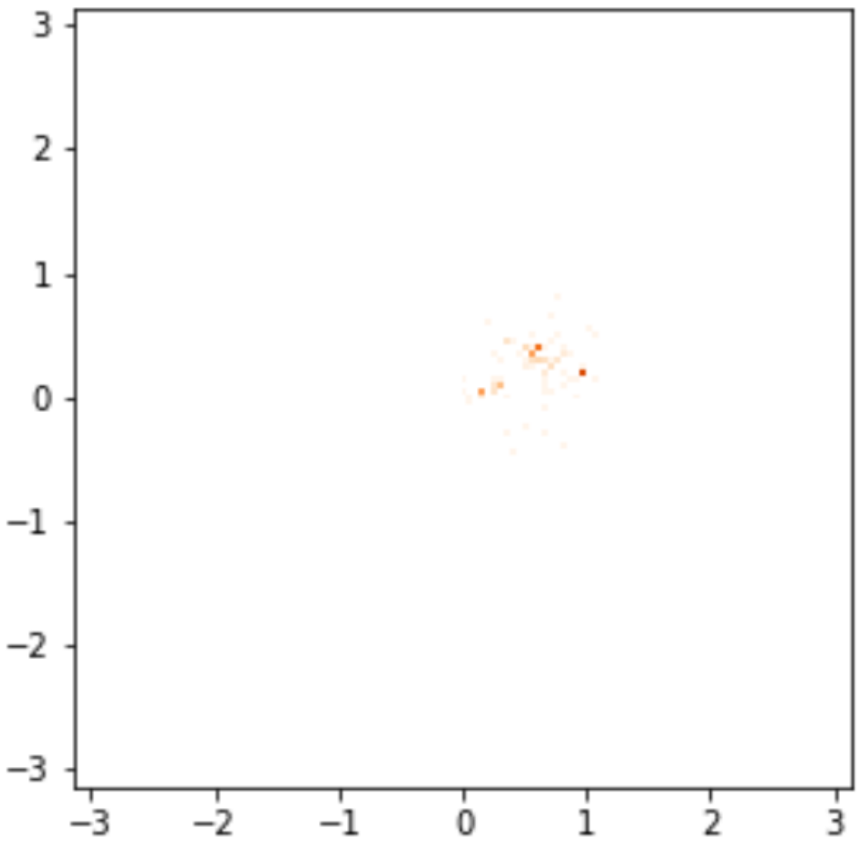
Garbage

My old plan:

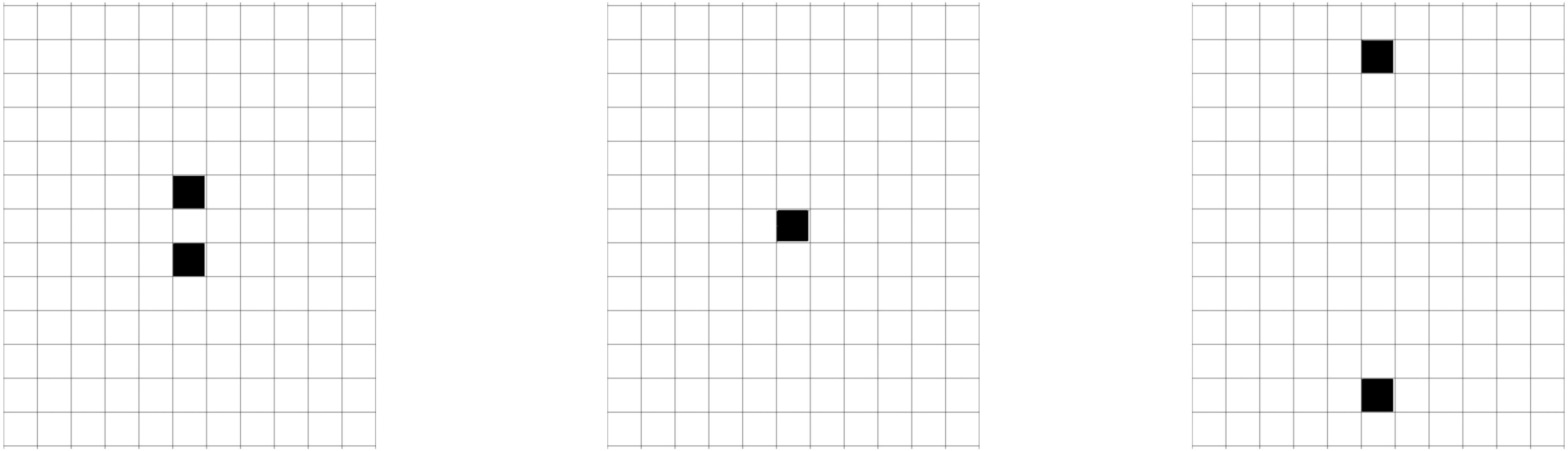
- Train AE on jet images using different latent space sizes N
- Study reconstruction quality as a function of N
- … Learn something about ‘jet information’?

Flaws:

1) Jet images are garbage
2) Autoencoders are garbage



“Jet Images are Garbage”



(a) (b) (c)

All three of these jet images are maximally different from eachother according to summed pixel intensity difference, but (a) and (b) are more physically similar than are (b) and (c).

Future Directions

1. What is the point?

2. Alternative latent priors?

3. Alternative metrics?

The Variational Autoencoder

ML Engineer:

"A VAE is a fancy AE with regulated stochastic latent space sampling"

Bayesian statistician:

*"A VAE is a probability model trained to extremize the **E**vidence **L**ower **BO**und on the posterior distribution p(x)"*