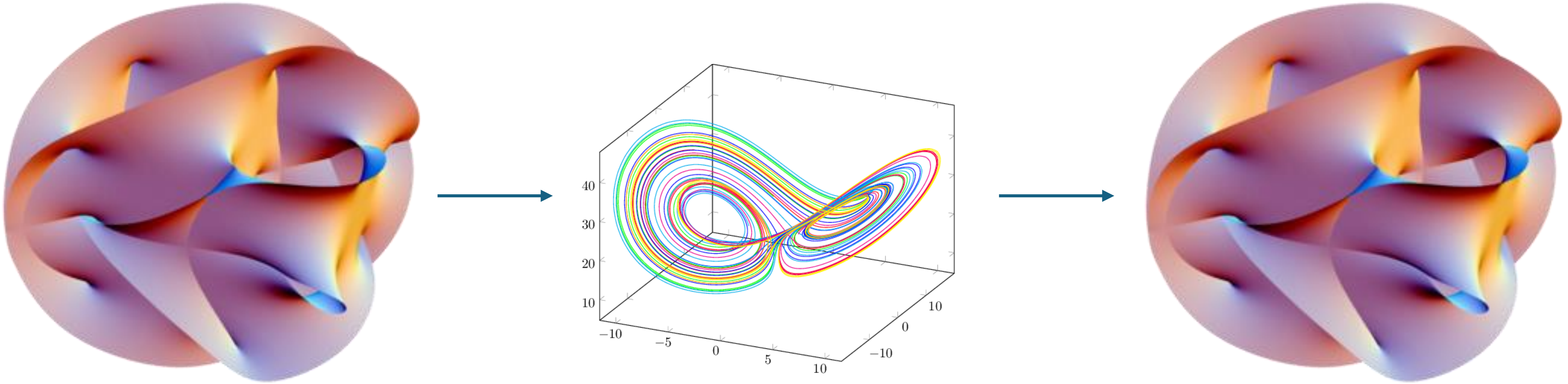
ML Enabled Representation and Visualization



Dr. Bryan Scott

LSST Discovery Alliance Data Science Fellowship Program Session 22

(partially) adapted from a tutorial on VAEs by Charles Kenneth Fisher and Raghav Kansal

Overview

Representations in Machine Learning:

Why representation learning? What is the connection between representation learning and visualization?

Specific Example: Autoencoders

Overview of autoencoder architectures and latent space representations

Revenge of the Bayesians: Variational Autoencoders (VAEs)

How can we make this probabilistic? Why would we want to?

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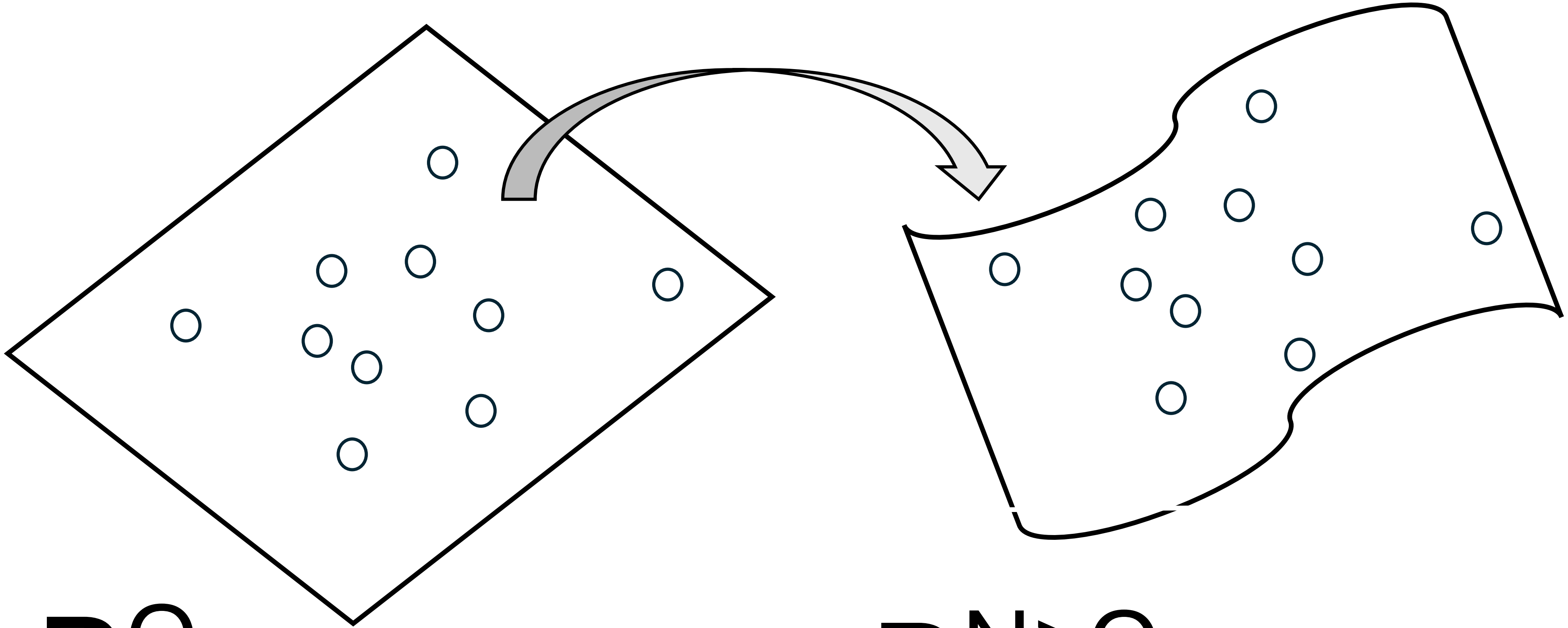


R^Q

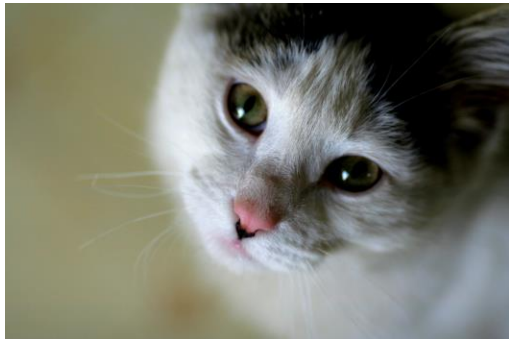
Data is “generated” in this space.

$R^{N>Q}$

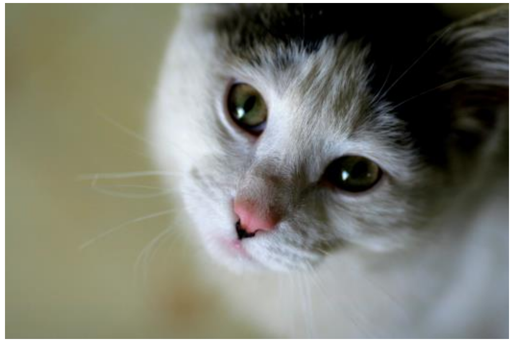
Observations are made in this space.

Supervised Learning

Unsupervised Learning

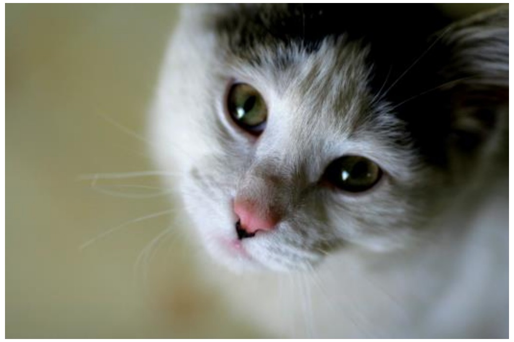


Unsupervised Learning



Representation Learning, a secret third thing?



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Representation Learning and Visualization

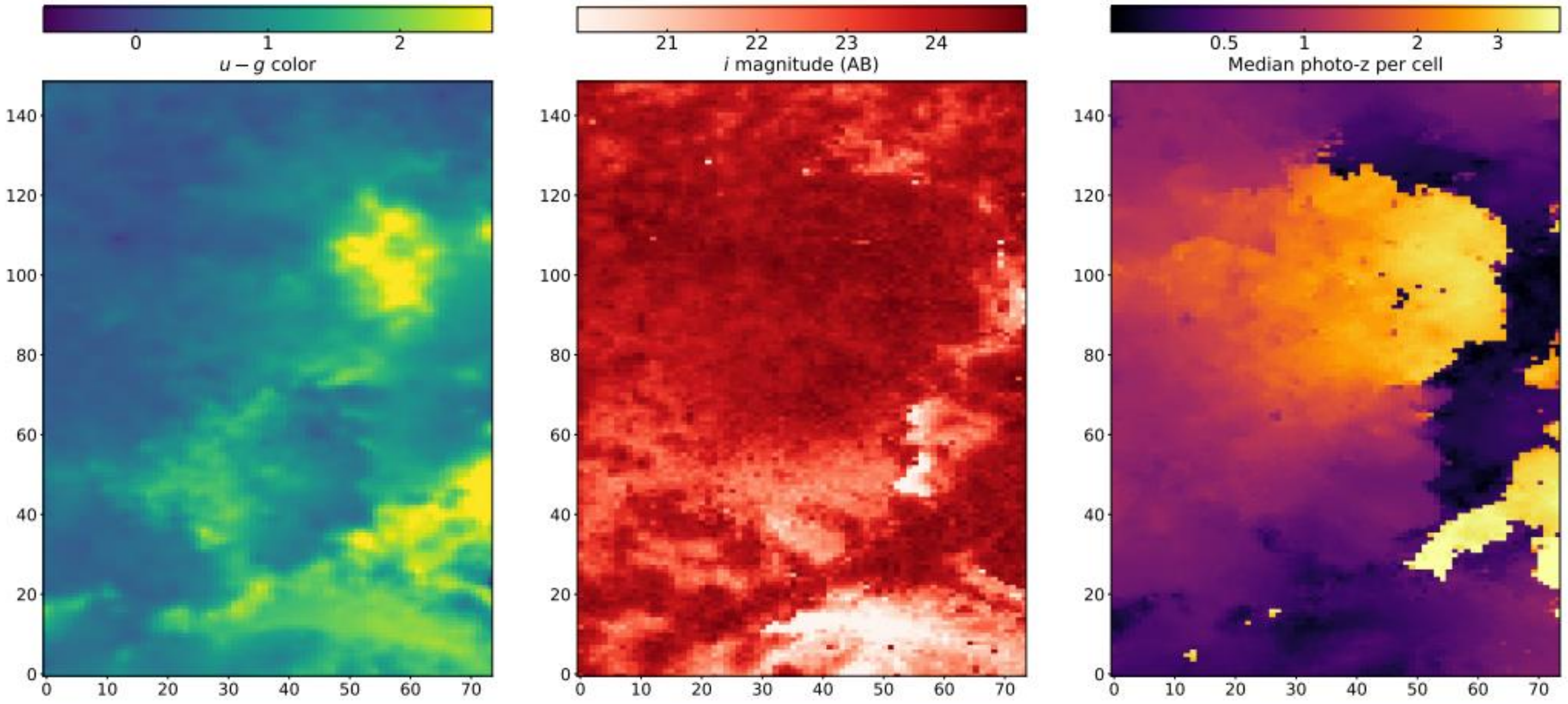

Figure 4. Illustration of the updated self-organized map (SOM) used for the C3R2 DR2 source selection and analysis. Each cell of the SOM represents a particular spectral energy distribution (SED) that shows up with regularity in the deep field data. The axes should be thought of as indices to parts of the high-dimensional galaxy color space. *Left:* The map colored according to one of the features it encodes, namely the u-g color. *Middle:* The map colored according to the median i band magnitude of galaxies occupying each cell. It is clear that the typical magnitude is strongly color dependent. *Right:* The SOM colored by the median photometric redshift of galaxies occupying each cell. Note the topological nature of the SOM: similar SEDs group together, producing relatively smooth variation of photo-z with position on the map.

Masters et al., 2019

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How can we make this probabilistic? Why would we want to?

What is an autoencoder?

An autoencoder is a type of algorithm with the primary purpose of learning an "informative" ***representation*** *of the data that can be used for different applications a by learning to* ***reconstruct*** *a set of input observations well enough*.

The **reconstruction** is the “*auto*” part

The **representation** is the “*encoding*” part.

Autoencoders are an ‘architecture’ for performing the representation learning task. The specific implementation can take many forms.

How to build an autoencoder?

Autoencoders are approximations to the identity function.

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Given a dataset x, what function x' = f(x) yields x = x'? Neural networks are universal function approximators, so a neural network should be a good choice for approximating the simplest possible function – the identity.

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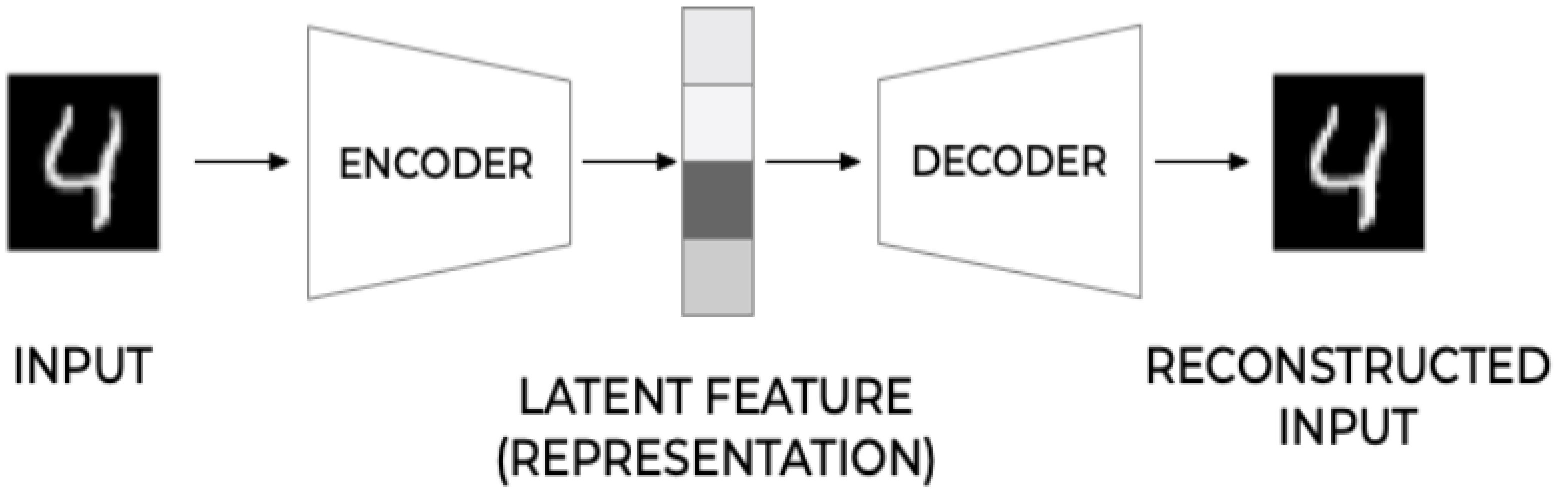
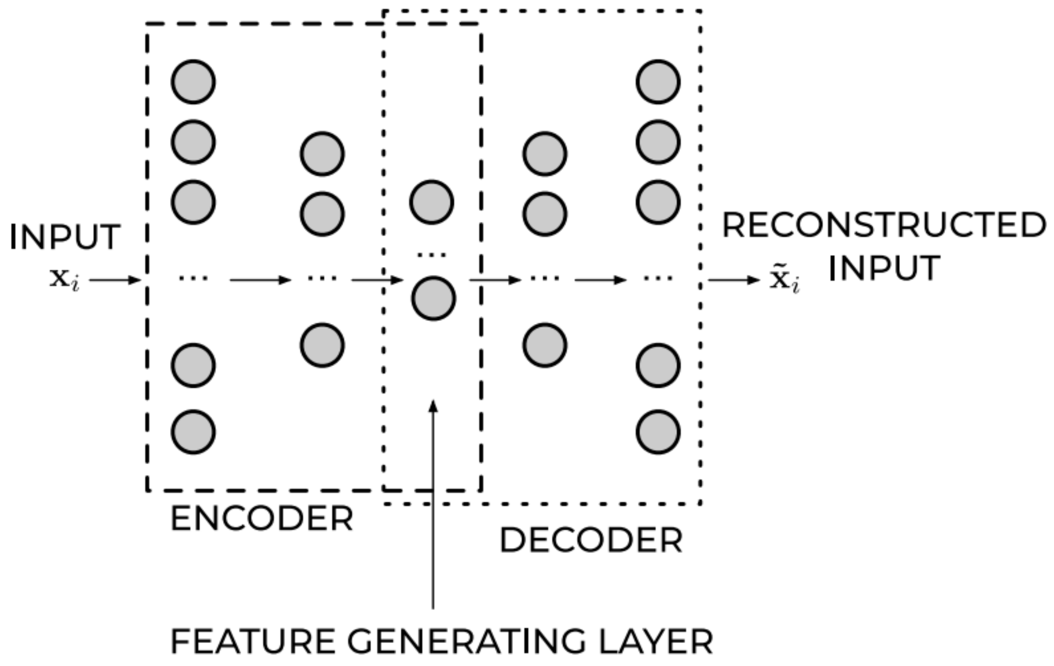
Given a dataset x, what function x’ = f(x) yields x = x’? Neural networks are universal function approximators, so a neural network should be a good choice for approximating the simplest possible function – the identity.

By choosing a neural network architecture, we will introduce additional degrees of freedom that can yield *representative* or *interpretable* **compressions** of the data.

Schematic Representation



Dimensionality Reduction in Autoencoders:



The encoder can reduce the number of dimensions of the input observation (n) and create a learned representation (hi)of the input that has a smaller dimension q < n. This learned representation is enough for the decoder to reconstruct the input accurately (if the autoencoder training was successful as intended).

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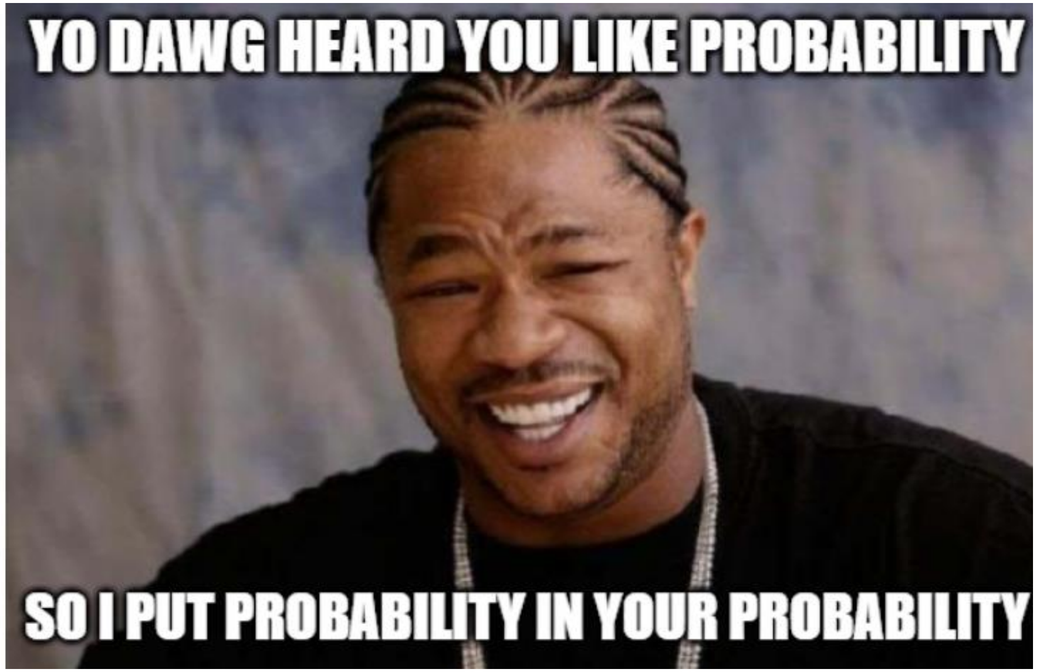

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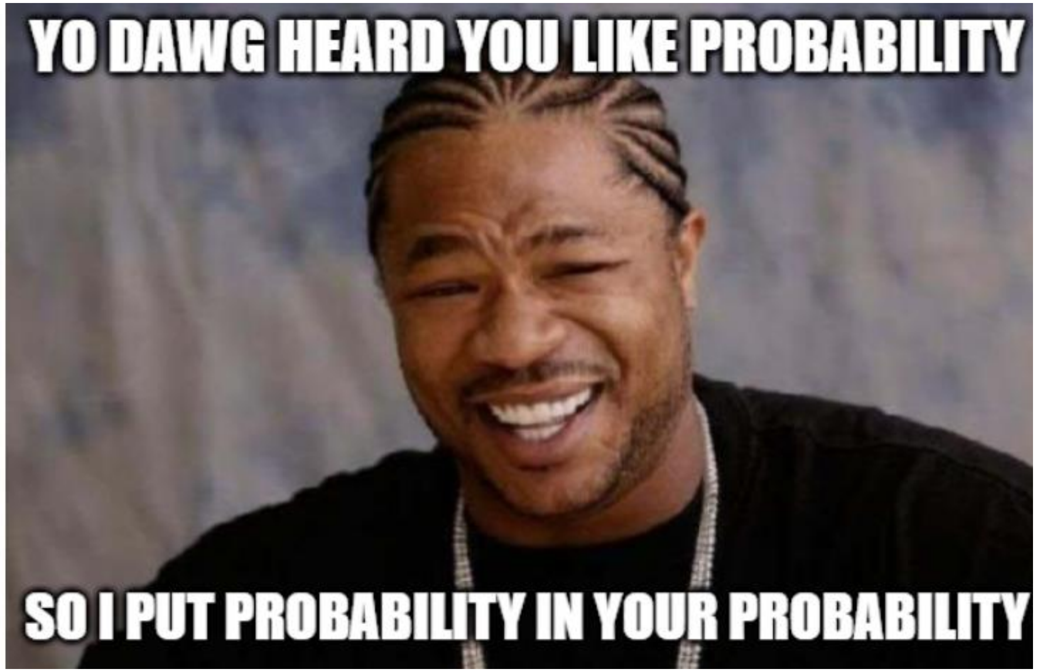
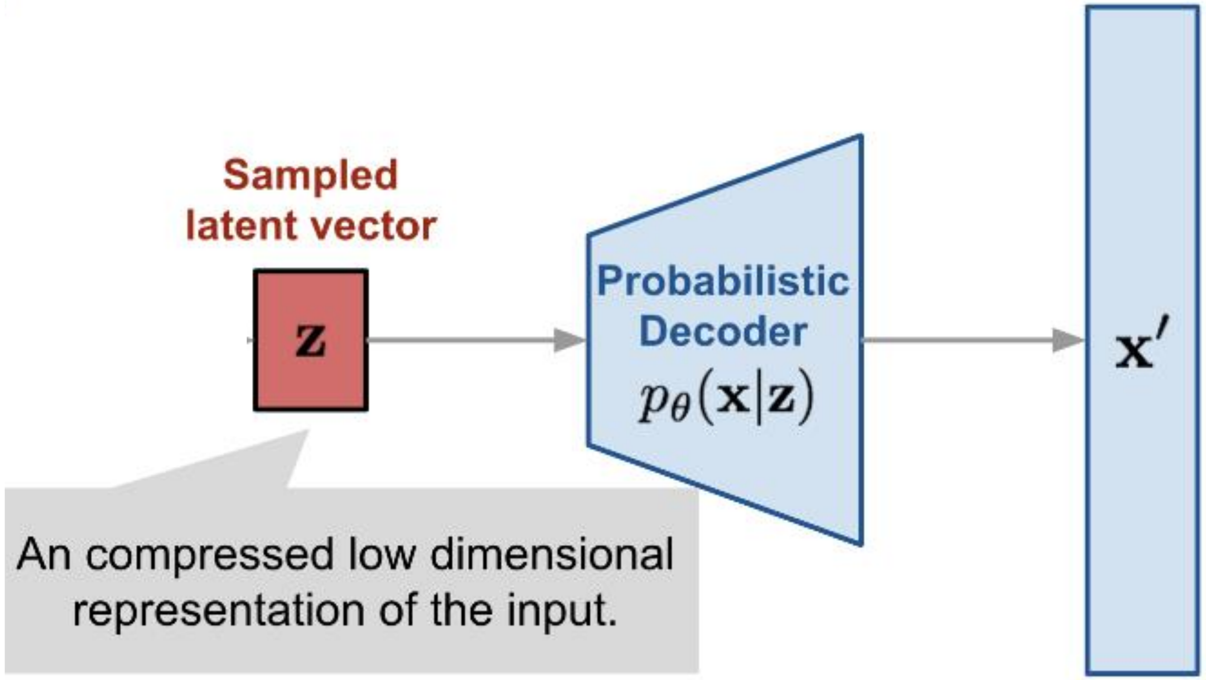


Goal of a VAE: Learn the Joint Distribution

Estimate

$$p_\theta(\mathbf{x}, \mathbf{z}) = p_\theta(\mathbf{x}|\mathbf{z})p(\mathbf{z}).$$

VAE Latent Space and Decoder



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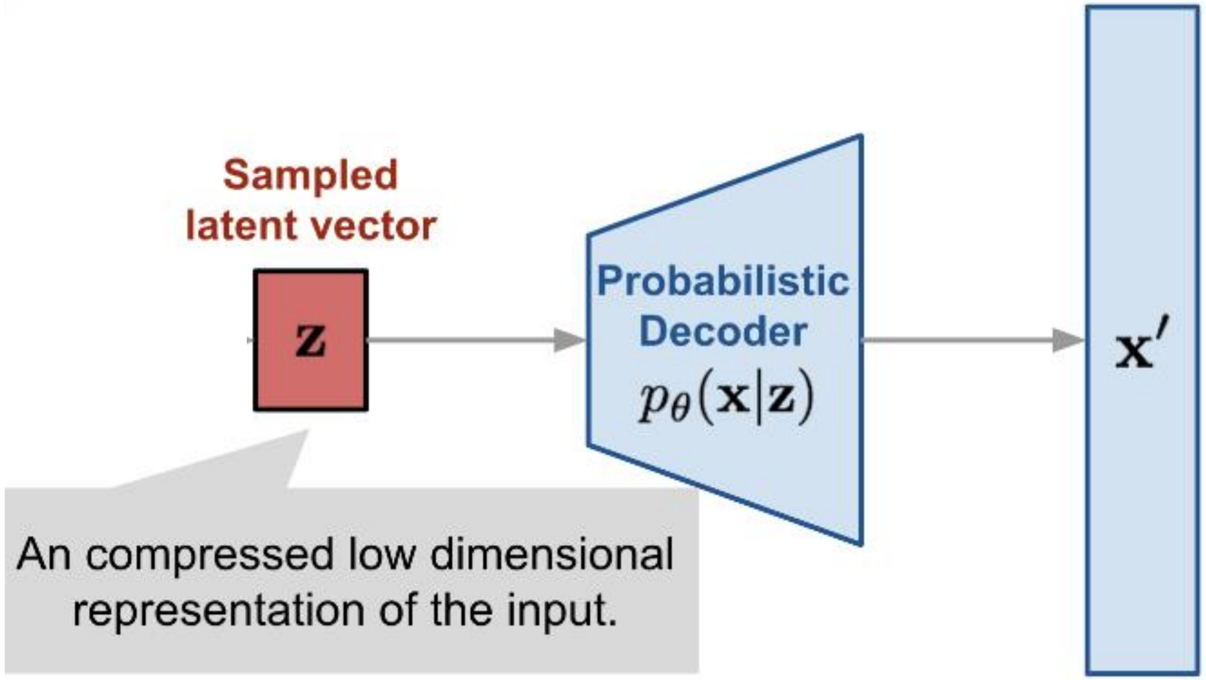


"Generative Model"

Goal of a VAE: Learn the Joint Distribution

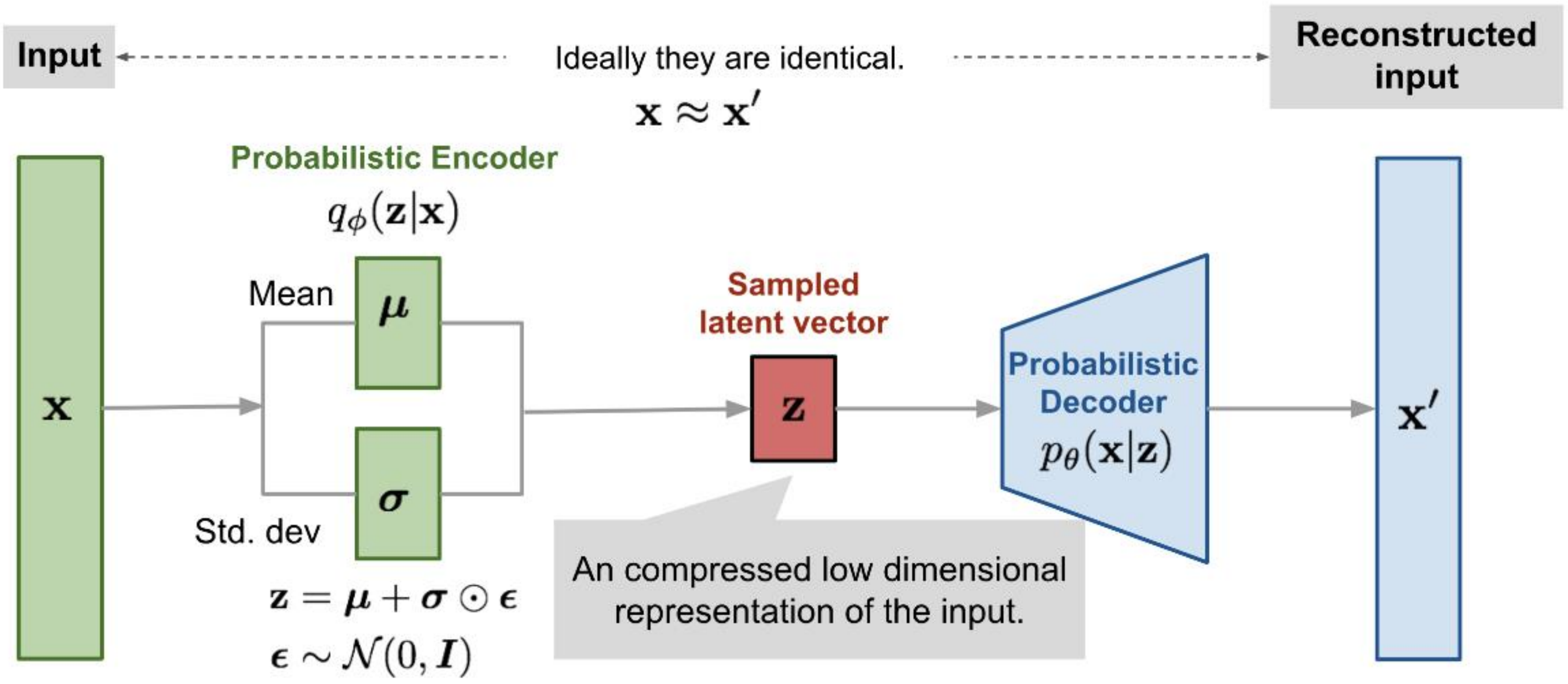
Estimate

$$p_\theta(\mathbf{x}, \mathbf{z}) = p_\theta(\mathbf{x}|\mathbf{z})p(\mathbf{z}).$$

Assuming,

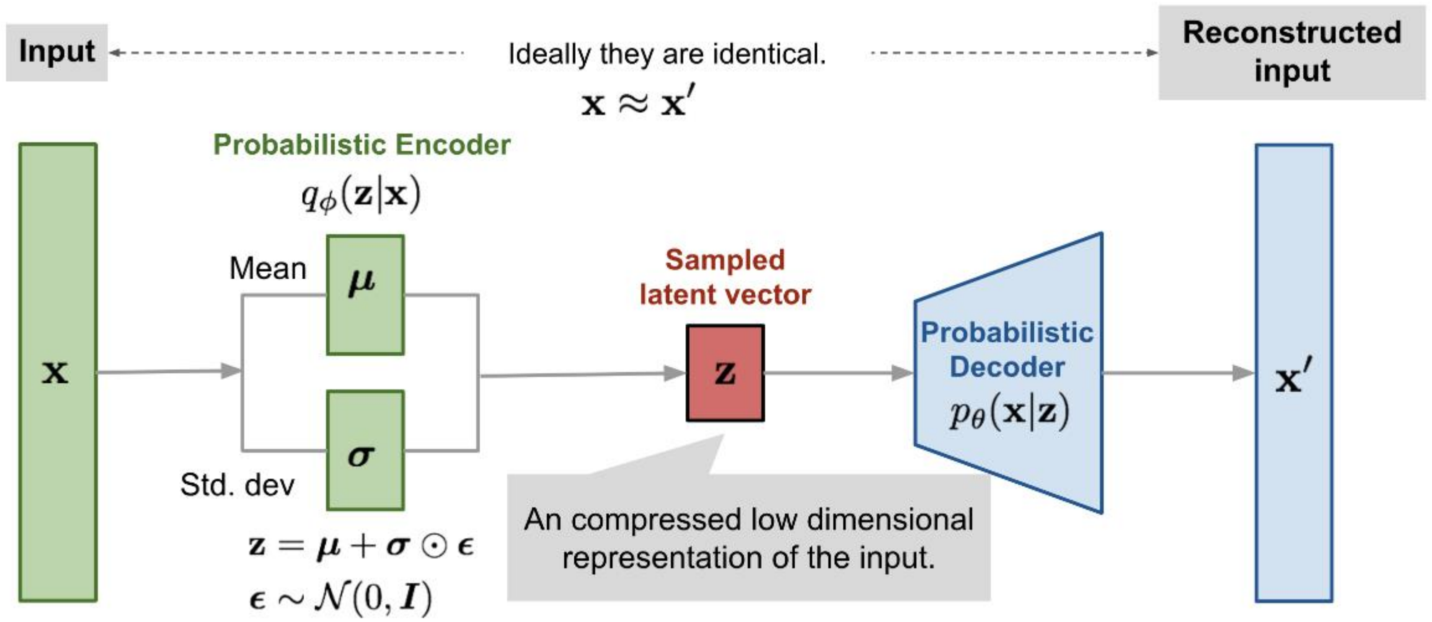
$$p(\mathbf{z}) = \mathcal{N}(\mathbf{0}, \mathbf{I}).$$

VAE Encoder



Input
Ideally they are identical.
$\mathbf{x} \approx \mathbf{x}'$
Reconstructed input
Probabilistic Encoder
$q_\phi(\mathbf{z}|\mathbf{x})$
$\mathbf{x}$
Mean
$\boldsymbol{\mu}$
Std. dev
$\boldsymbol{\sigma}$
$\mathbf{z} = \boldsymbol{\mu} + \boldsymbol{\sigma} \odot \boldsymbol{\epsilon}$
$\boldsymbol{\epsilon} \sim \mathcal{N}(0, \boldsymbol{I})$
Sampled latent vector
$\mathbf{z}$
An compressed low dimensional representation of the input.
Probabilistic Decoder
$p_\theta(\mathbf{x}|\mathbf{z})$
$\mathbf{x}'$

Loss Function Terms



$$-D_{KL}(q_\phi(\mathbf{z}|\mathbf{x})|p(\mathbf{z})) = \frac{1}{2}\sum_{j=1}^{J}\left(1 + \log \sigma_j^2(\mathbf{x}) - \mu_j^2(\mathbf{x}) - \sigma_j^2(\mathbf{x})\right.$$

What have we done? Variational Posterior Estimation (A preview of Session 23)

Dealing with Intractable Posteriors: Evidence Lower Bound

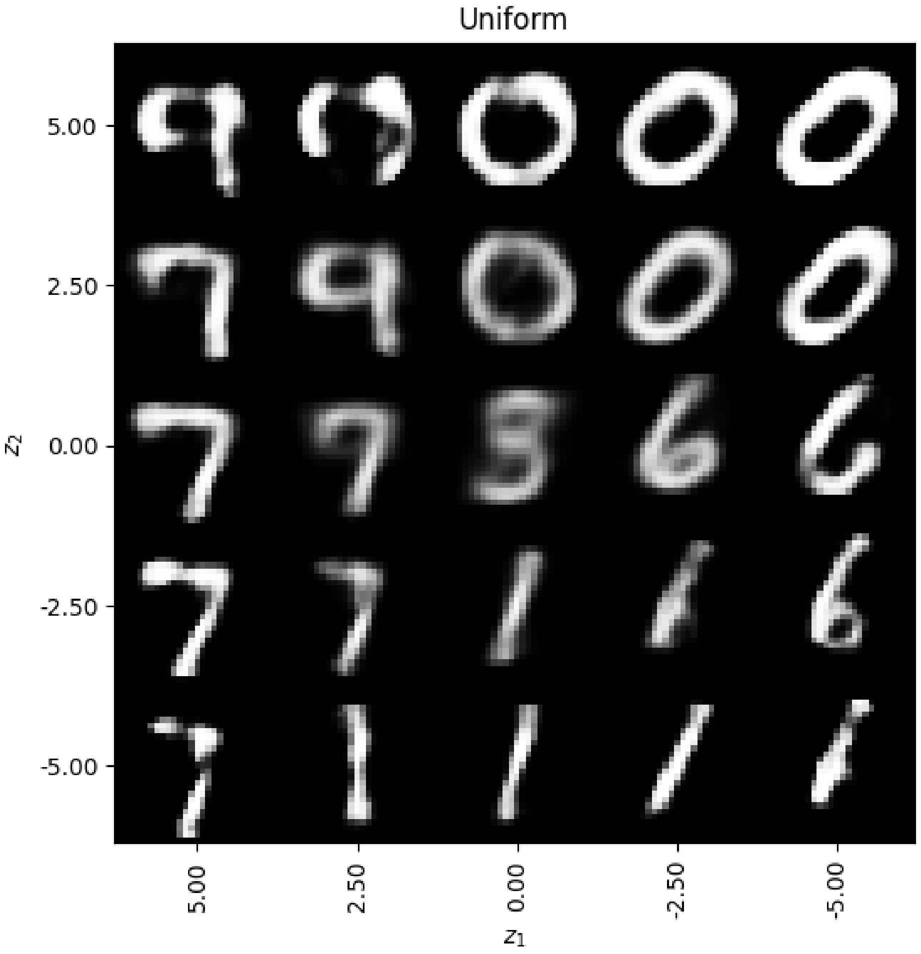
$$\begin{aligned}\mathrm{ELBO}(q) &= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}|\mathbf{z}) + \log p(\mathbf{z}) - \log q_\phi(\mathbf{z}|\mathbf{x})] \\ &= \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[\log p_\theta(\mathbf{x}|\mathbf{z})] - \mathrm{KL}[q_\phi(\mathbf{z}|\mathbf{x})||p(\mathbf{z})].\end{aligned}$$

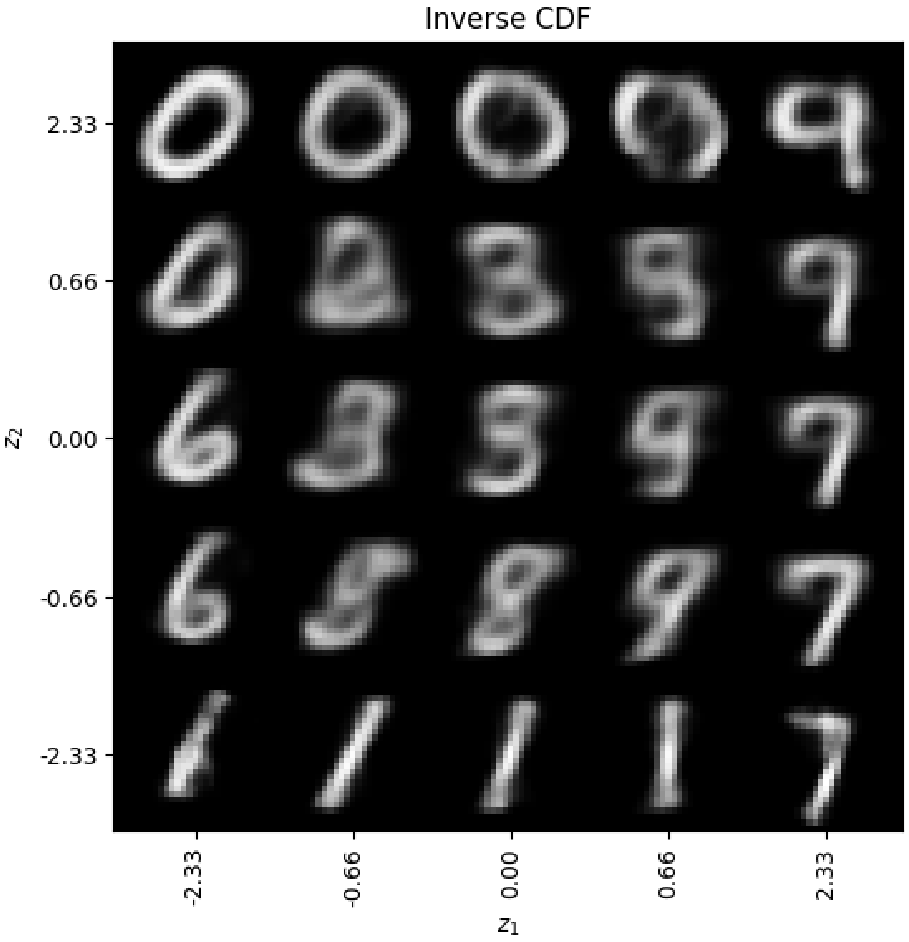
"Reparameterization Trick"

$$\begin{aligned}\nabla_\phi \mathbb{E}_{q_\phi(\mathbf{z}|\mathbf{x})}[f(\mathbf{x},\mathbf{z})] &= \nabla_\phi \mathbb{E}_{p(\epsilon)}[f(\mathbf{x}, g_\phi(\mathbf{x},\boldsymbol{\epsilon}))] \\ &= \mathbb{E}_{p(\epsilon)}[\nabla_\phi f(\mathbf{x}, g_\phi(\mathbf{x},\boldsymbol{\epsilon}))].\end{aligned}$$

Worked Example: MNIST Dataset

Latent Space Visualizations





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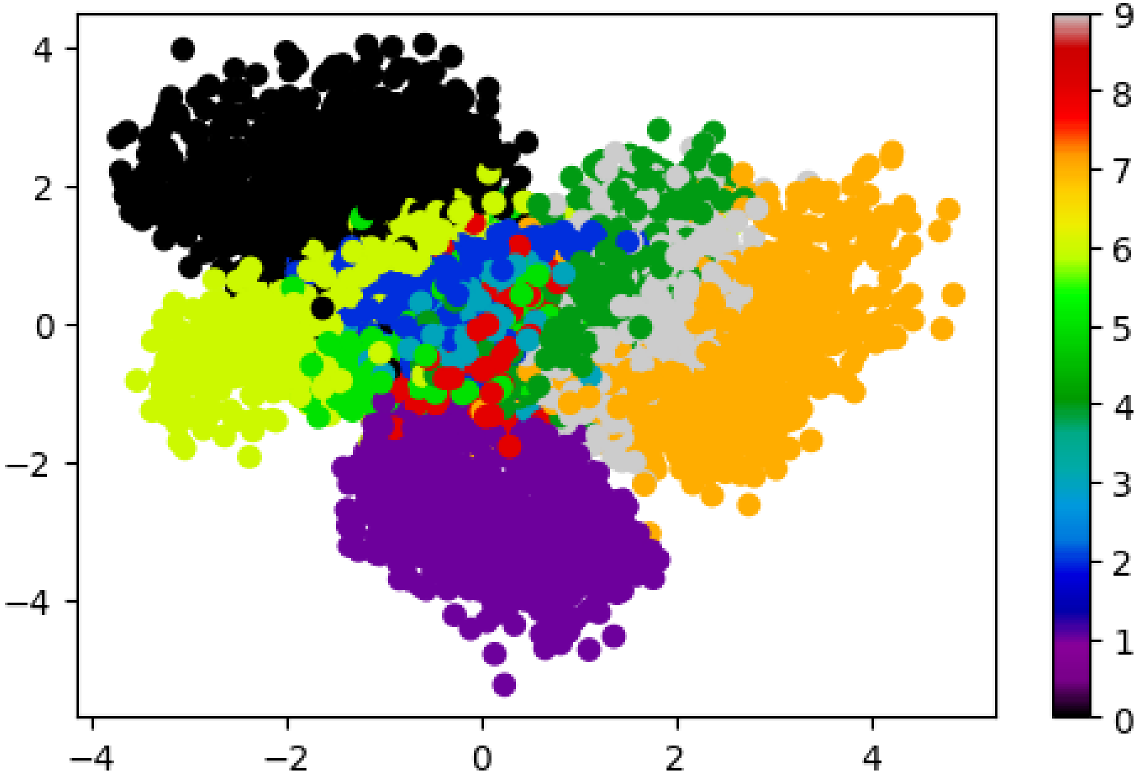

Problem Notebook

Using a Galaxy Zoo Hubble Space Telescope Image set, train a VAE for HST galaxy images.

Then, generate some examples from the latent space.

Use these to draw some conclusions about the learned representation of the image data. Does the two-dimensional latent space have a clear structure? What do the axes correspond to?