

Autoencoders

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Outline

- Clustering
- Autoencoders
 - Variational autoencoders
 - Conditional variational autoencoders

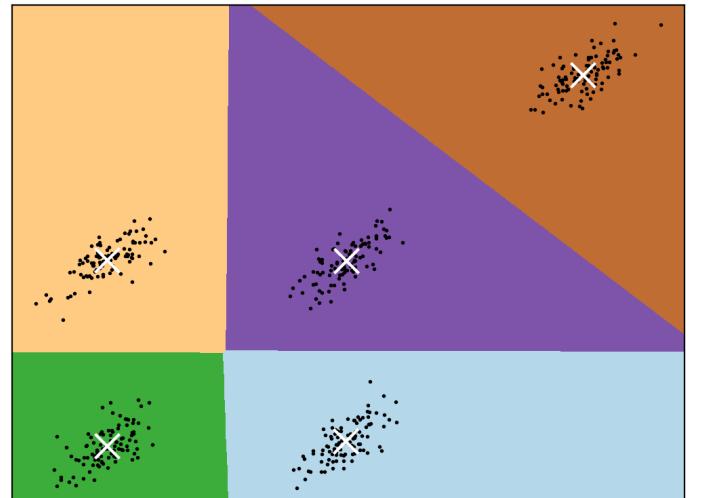
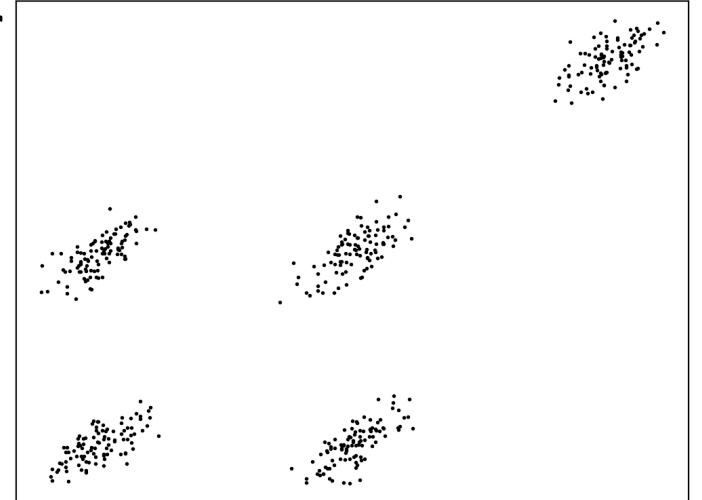
Motivating Example

- Imagine you are an alien species that comes across the MNIST dataset that only has images, but no corresponding labels
- You suspect that there is some structure to this data, and you hope to discover it
- Furthermore, you hope to generate data similar to it to imitate humans



Clustering

- Grouping objects into clusters where objects in a cluster are more similar than compared to those in other clusters
- Natural sciences
 - High-energy physics
 - Biology
 - Chemistry
- Medicine
 - Patients
 - Diseases
- Reinforcement learning
 - Cluster similar states for hierarchy
 - Cluster similar actions to create meta-actions



Curse of Dimensionality

- The phrase was coined by Richard Bellman in reference to solving problems with dynamic programming
- However, this is relevant to many other cases
- In high-dimensions, data has many possibly surprising properties
- In particular, data points tend to be sparse when the dimensionality is increased
 - Euclidean distance becomes less meaningful
 - This makes partitioning data into meaningful clusters difficult or impossible

Curse of Dimensionality: Examples

- Suppose we have a, relatively small, 28×28 images
 - There are $28 \times 28 = 784$ –dimensional data points
 - Running K-means on this data will most likely result in meaningless clusters

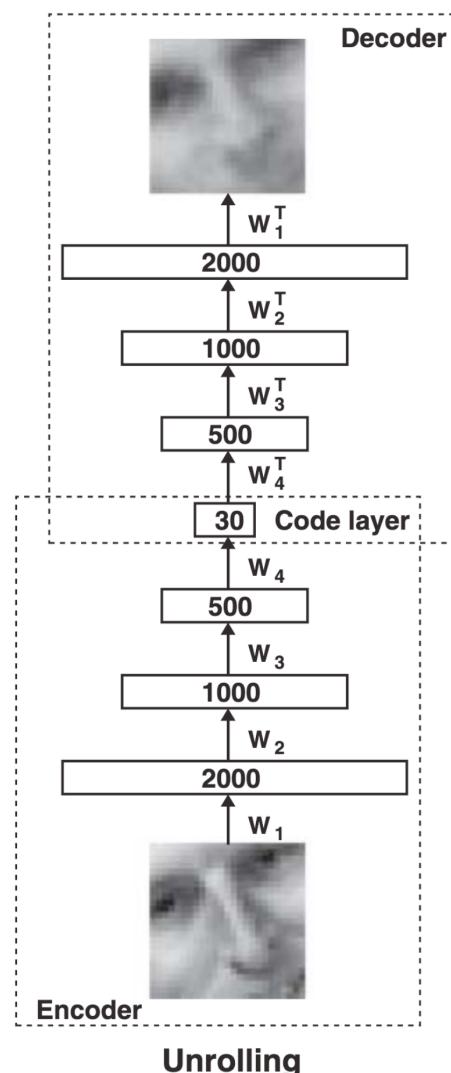


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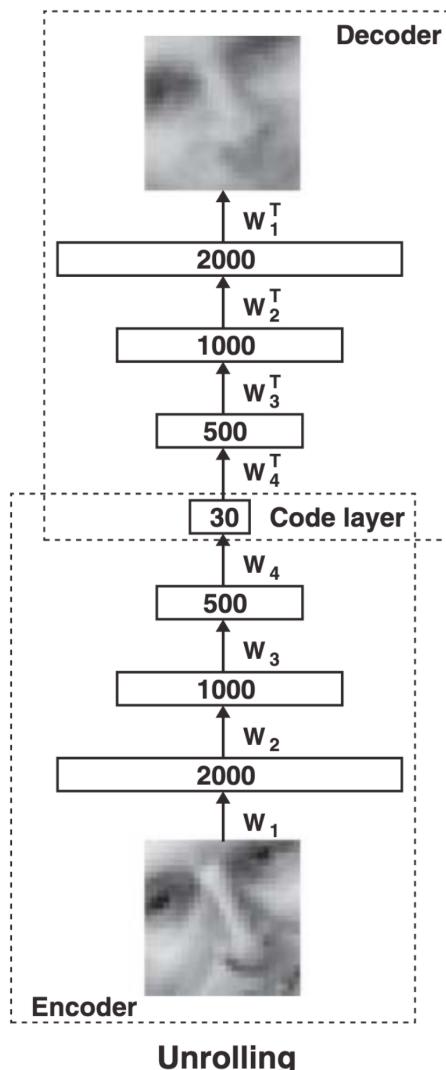
Autoencoders

- Neural networks that are trained without labels
- The input is passed through an **encoder**
 - The dimensionality of the output of the encoder is usually much less than the dimensionality of the input
 - Called code layer or bottleneck layer
- The output of the encoder is then passed to the **decoder** which is trained to mimic the input
- This is known as minimizing the **reconstruction error**



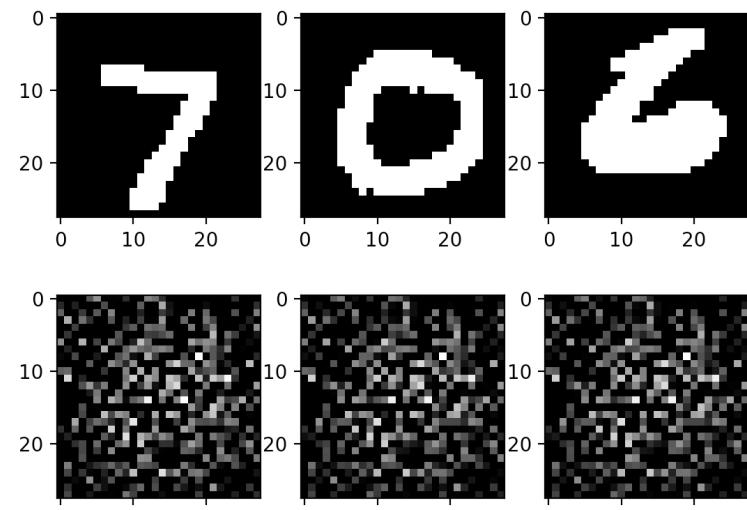
Autoencoders

- The larger the code layer, the better the reconstruction error tends to be
 - However, the autoencoder may then start capturing features that are irrelevant to the relevant structure of the data, such as background data
- We can use this autoencoder to dimensionally reduce the MNIST dataset and then do clustering on it

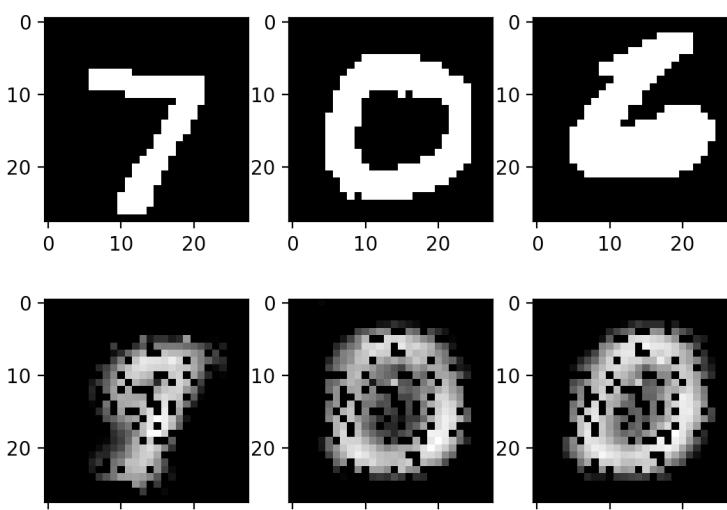


Autoencoders

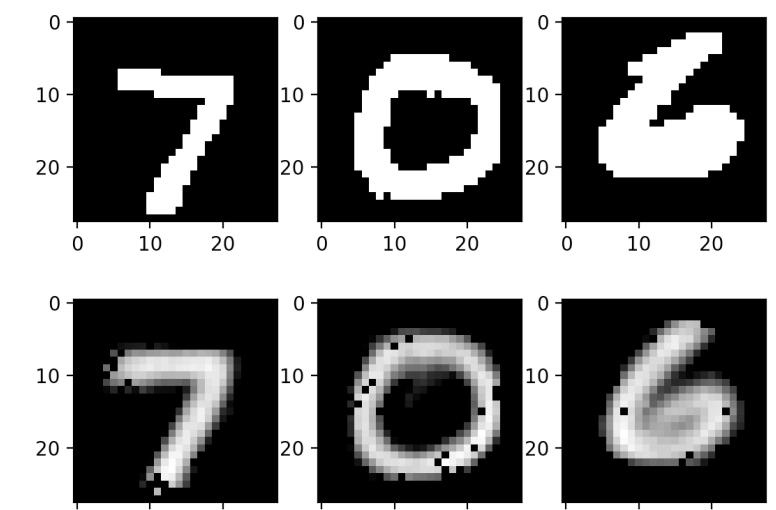
- The reconstructed input initially looks nothing like the input image
- However, after training, the output starts to match the input



Initialization



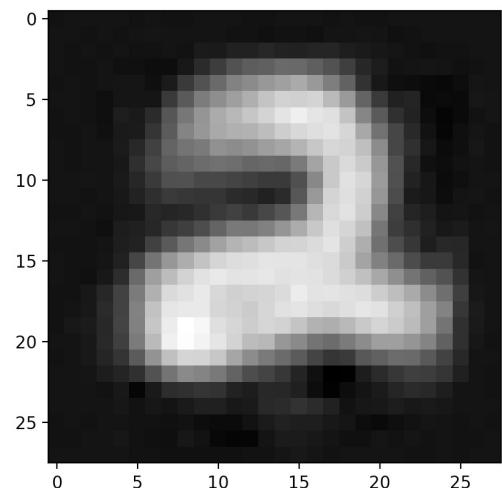
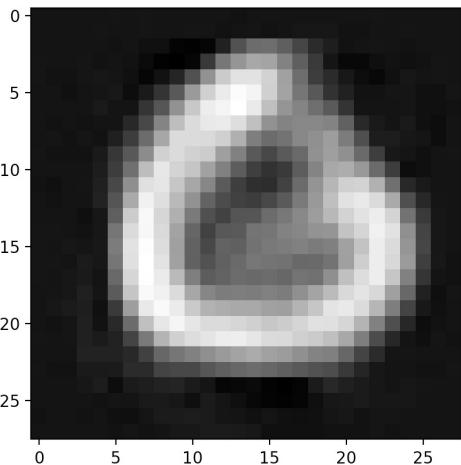
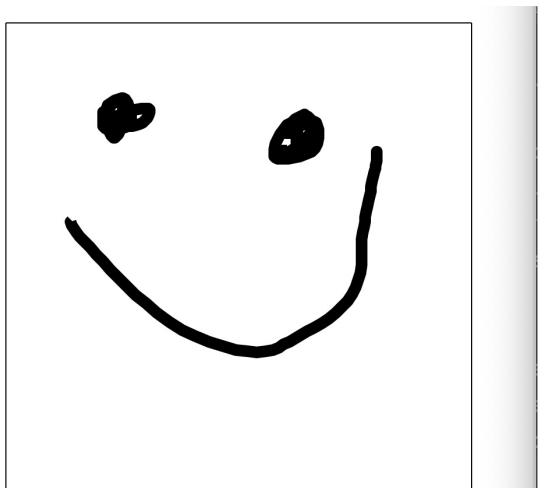
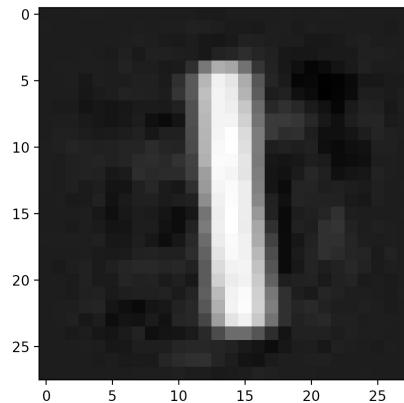
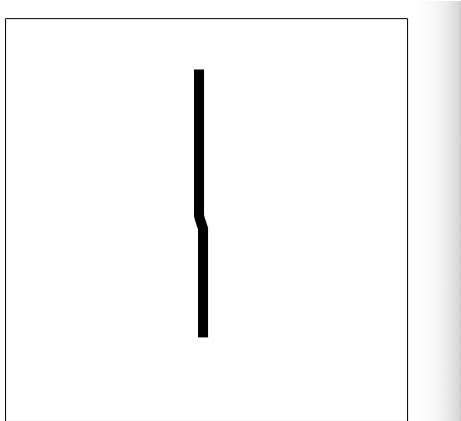
100 iterations



10,000 iterations

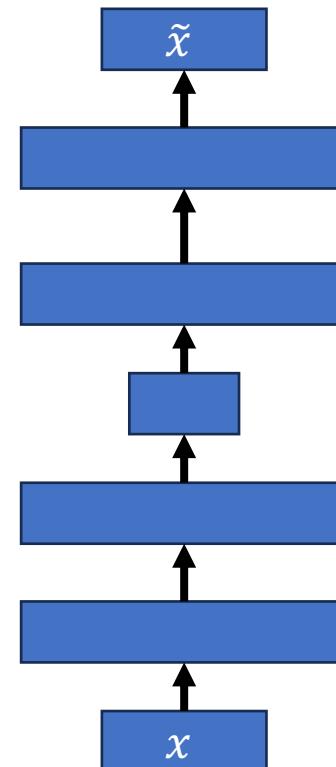
Out of Distribution Data

- As we saw in supervised learning, when testing on data that is significantly different than the training data, the performance of the neural network may be much worse

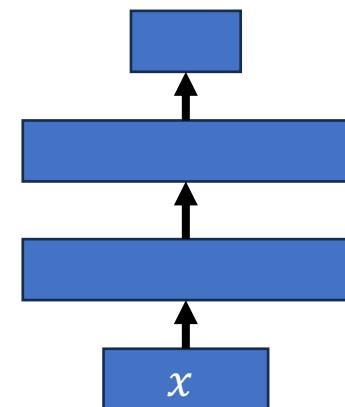


Dimensionality Reduction

- An autoencoder is composed of an encoder and decoder
- We can encoder inputs into a space of a smaller dimension by just putting data through the encoder and obtaining its output



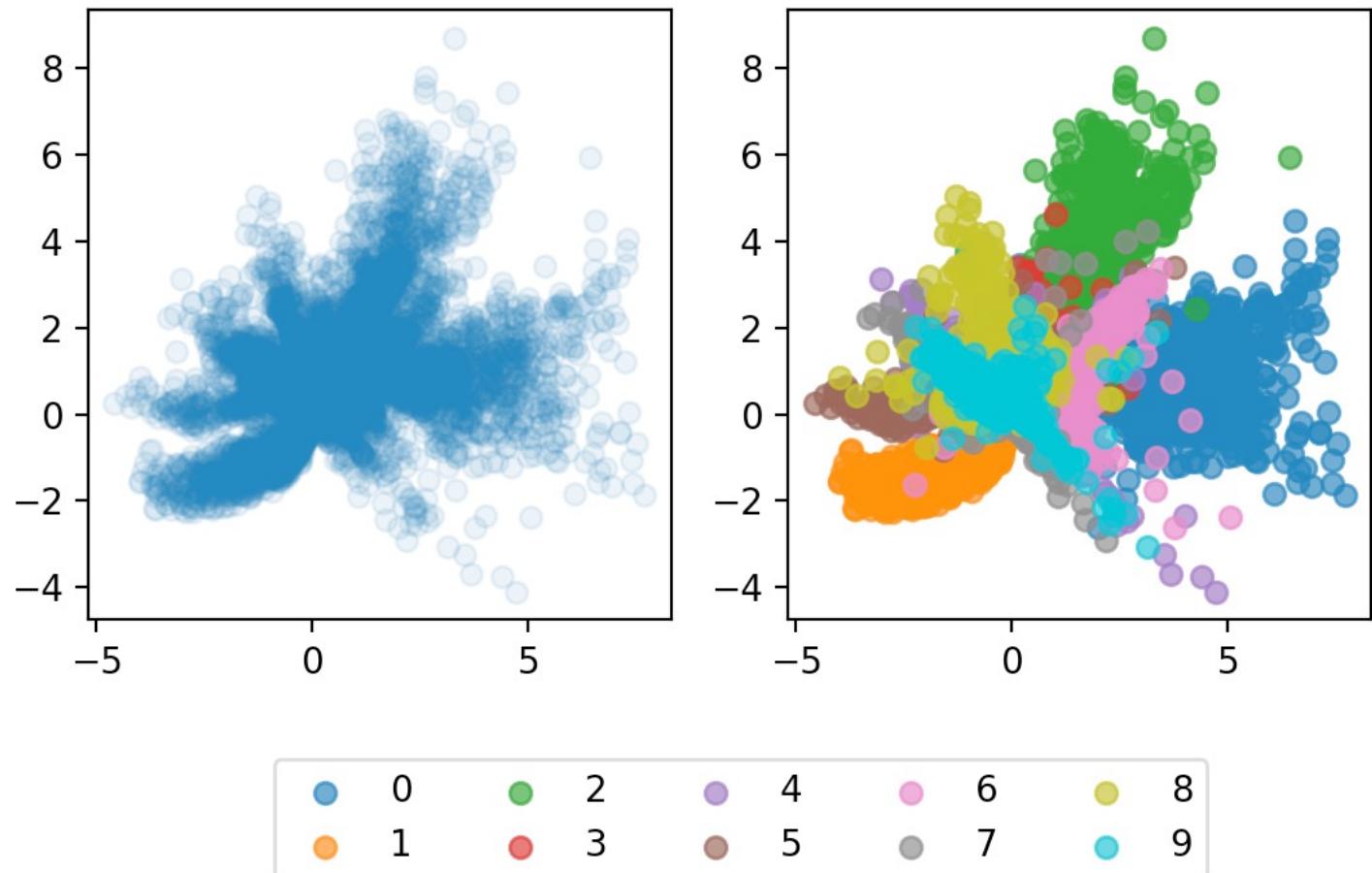
Autoencoder



Encoder

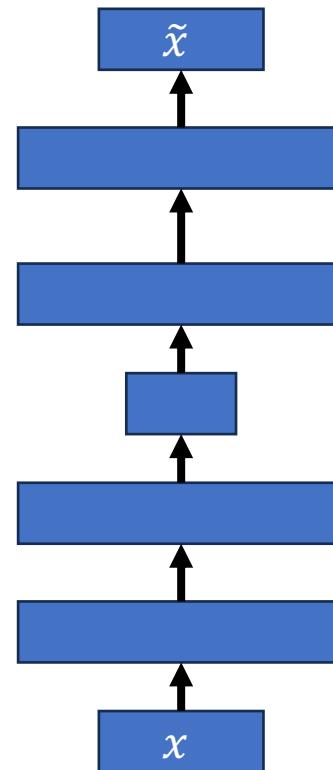
Dimensionality Reduction Results

- When visualizing our trained autoencoder with a bottleneck size of 2, we can see that there appear to be clusters
- When adding in label information, we see that similar digits do, indeed, cluster together
- How can we generate new data with an autoencoder?

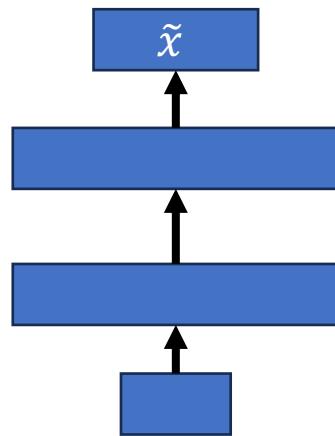


Generating New Data

- An autoencoder is composed of an encoder and decoder
- One can take data in the encoded space and put it through the decoder to generate new data



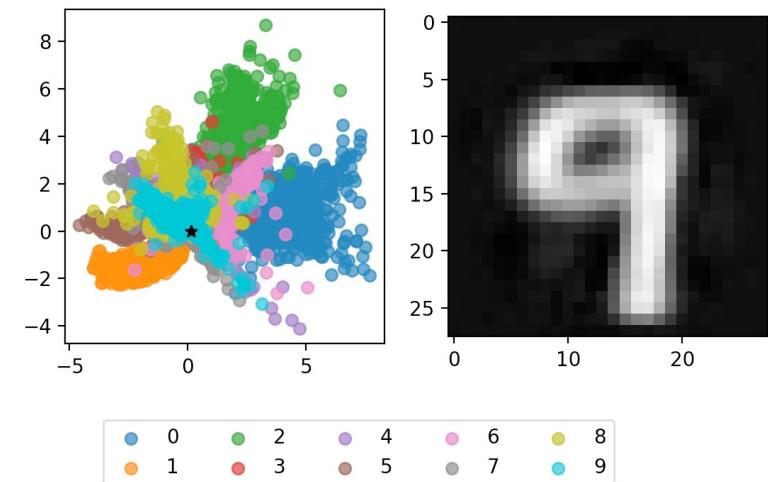
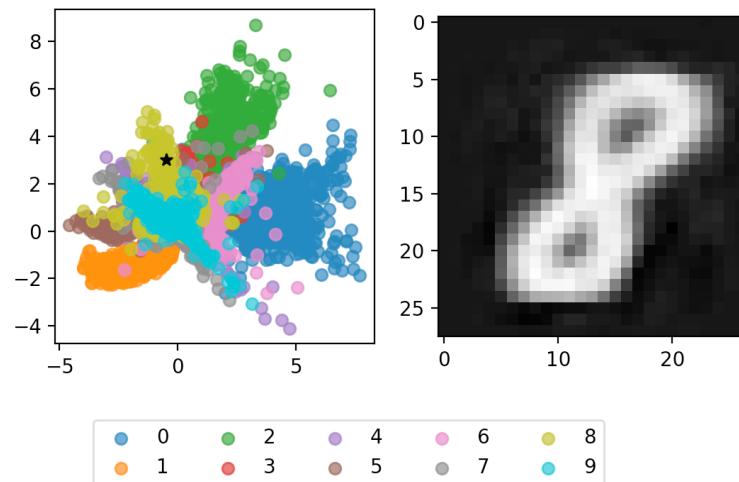
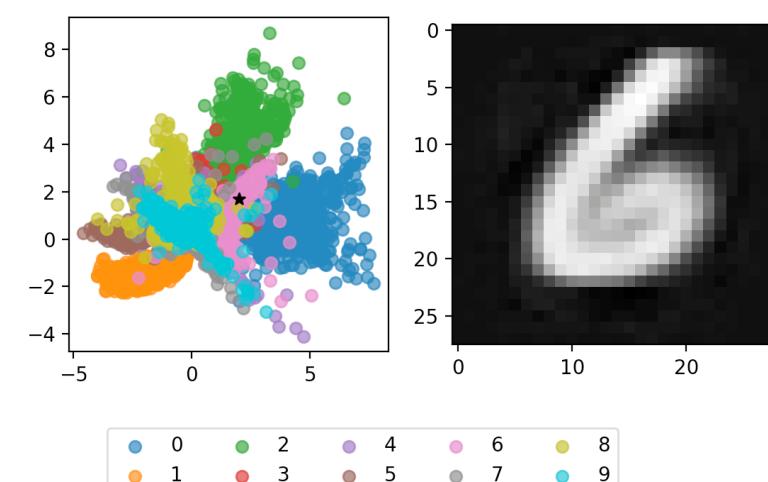
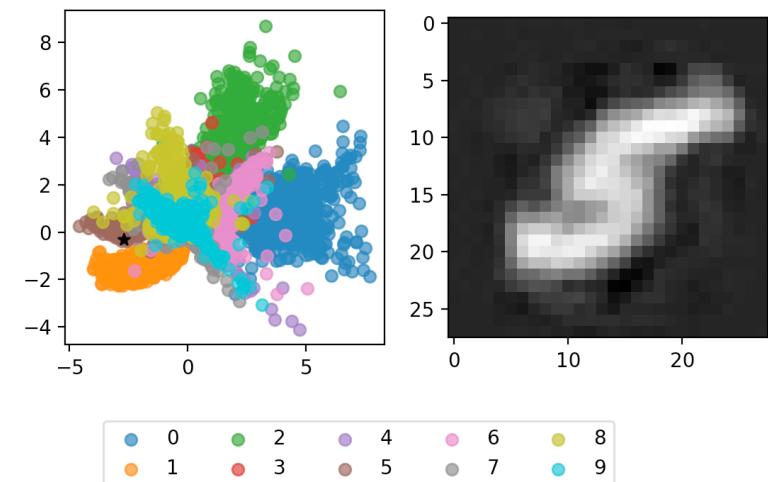
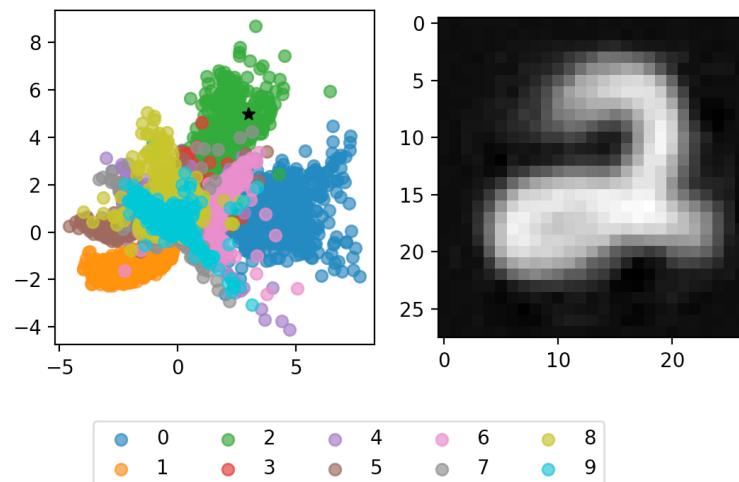
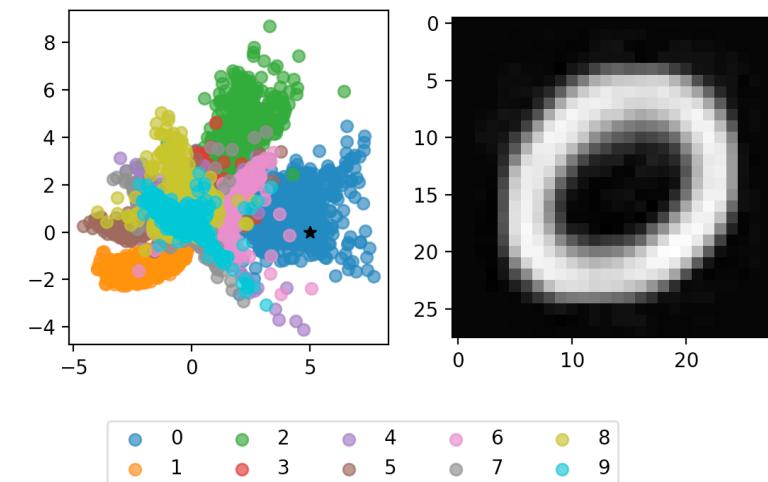
Autoencoder



Decoder

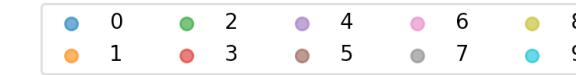
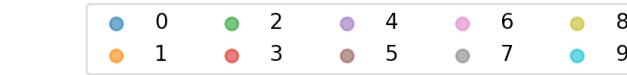
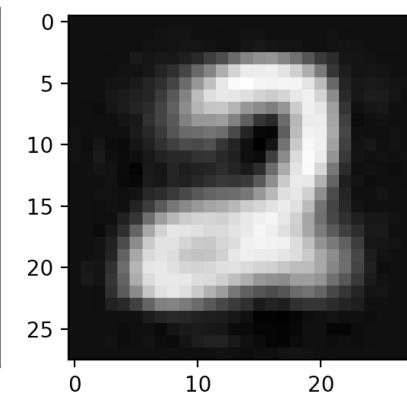
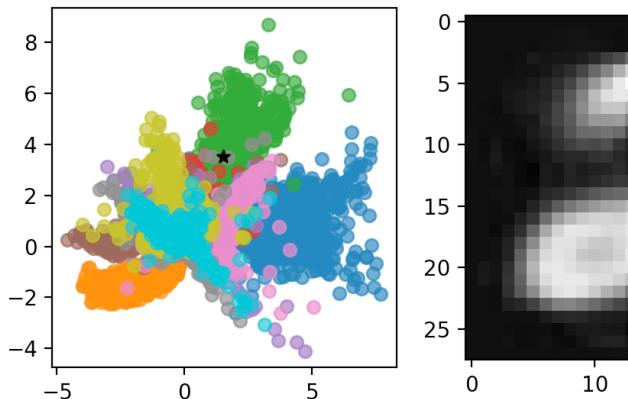
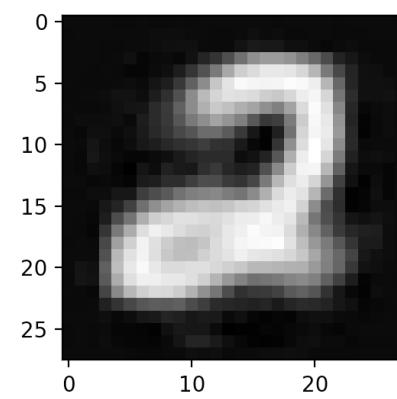
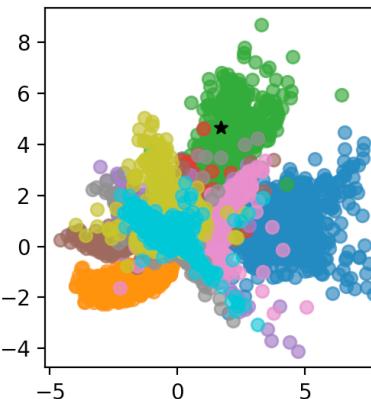
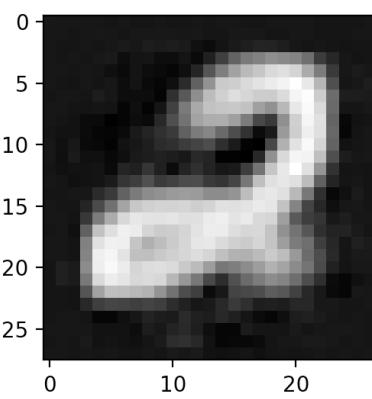
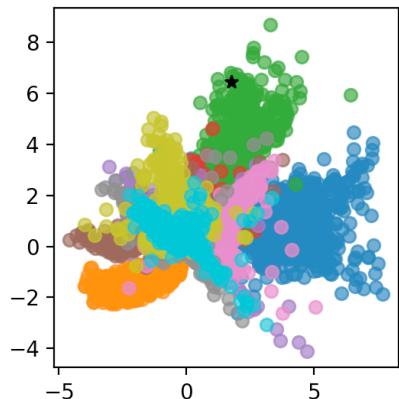
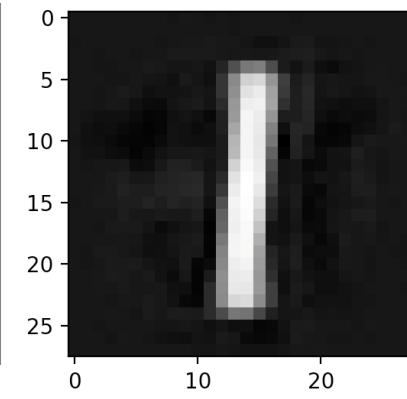
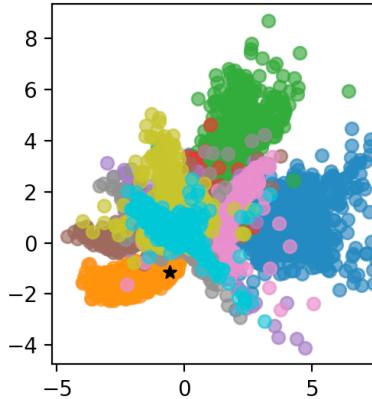
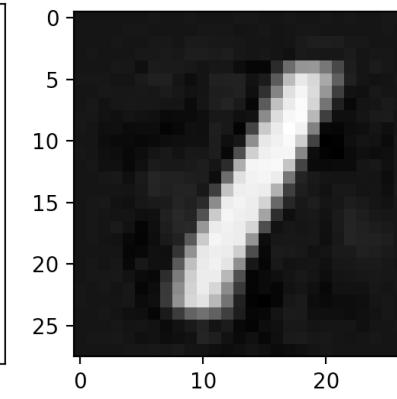
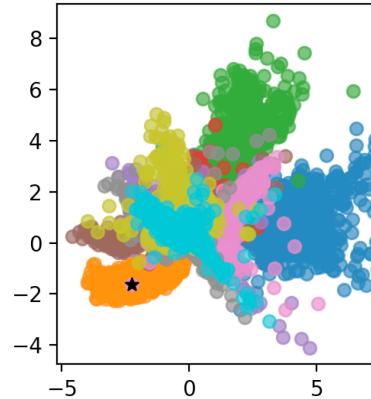
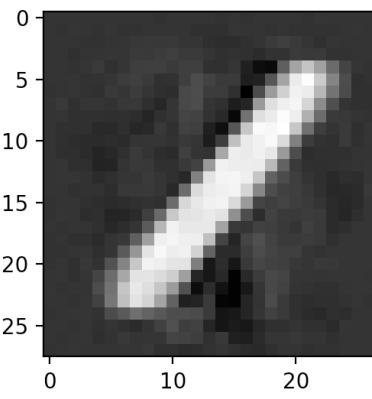
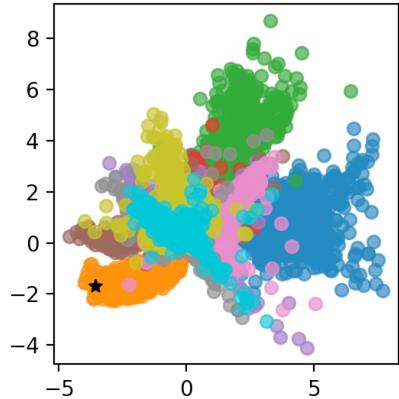
Generating New Data

- If we sample from data in distribution, we usually generate reasonable images



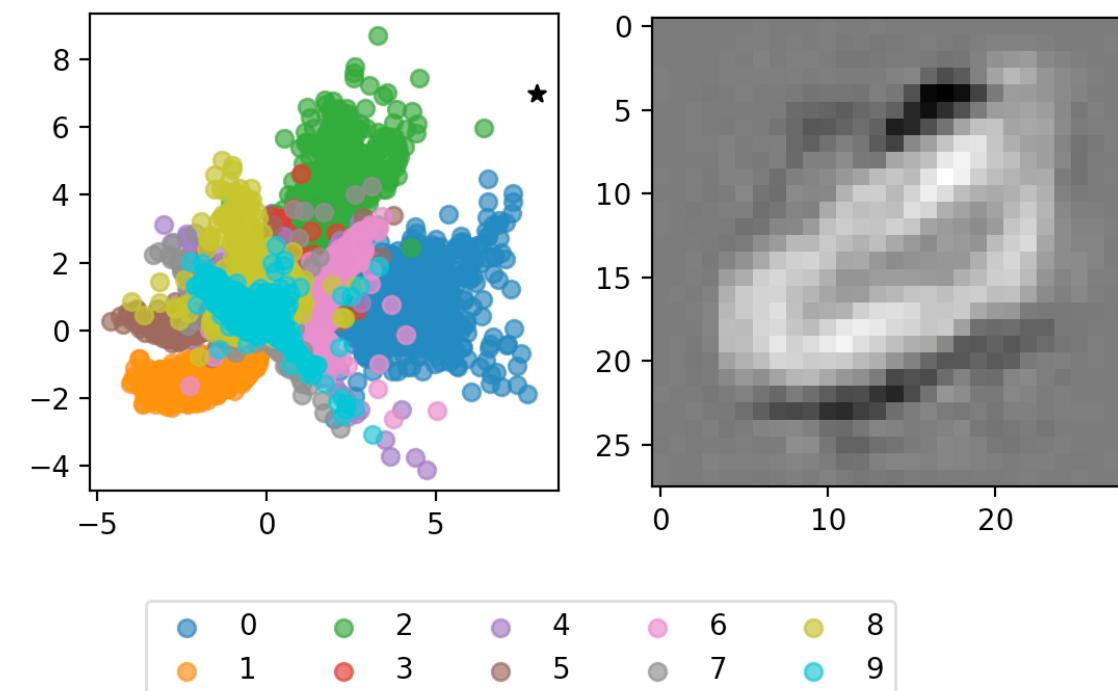
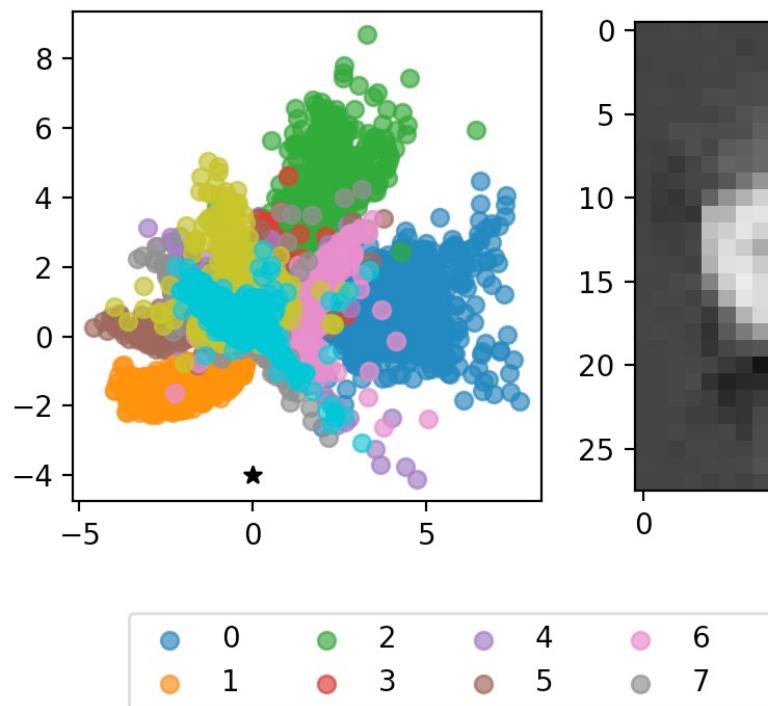
Traversing the Latent Manifold

- We can see how digits change by sampling different points in the latent space that are related to that digit



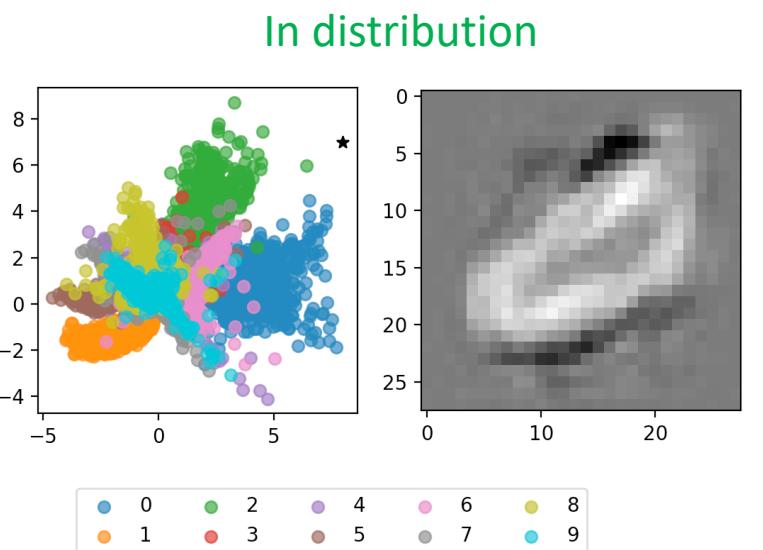
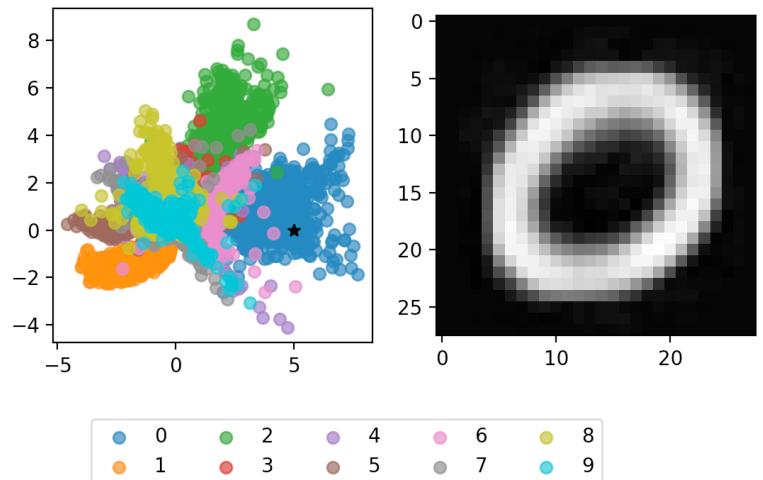
Generating Data: Out of Distribution Data

- Sampling from a point in the encoded space that the decoder has not observed during training can generate data that does not look like it comes from the original data distribution
 - Compare to silly ChatGPT outputs
 - How can we ensure that we are only sampling data that is in distribution?



Distributions

- To generate data, we sample data from the latent space and put it through the decoder
- One of the difficulties of generating data is characterizing the **distribution** of the latent space
 - Gets much harder in higher dimensional spaces
- If we could accurately characterize the distribution, then we could more reliably sample realistic data



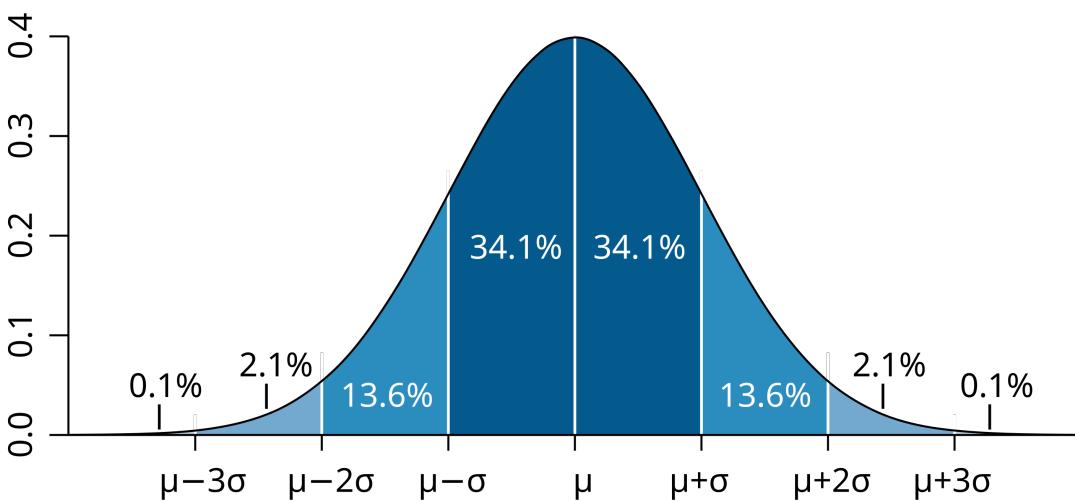
Out of distribution

Outline

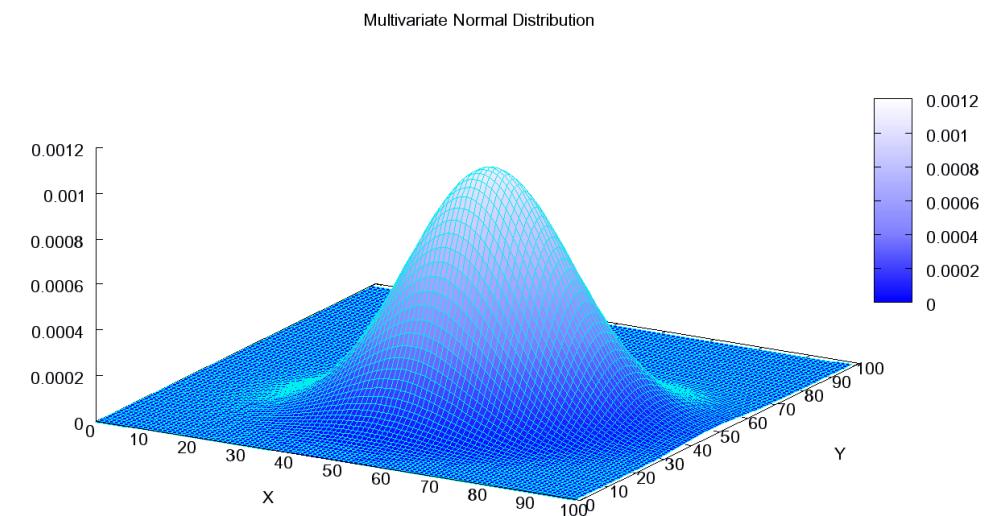
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Distribution

- A distribution (a [probability distribution](#), in specific) is a function that maps outcomes to the probability that they occur
- One of the most common examples of this is the normal distribution (also known as the Gaussian distribution)



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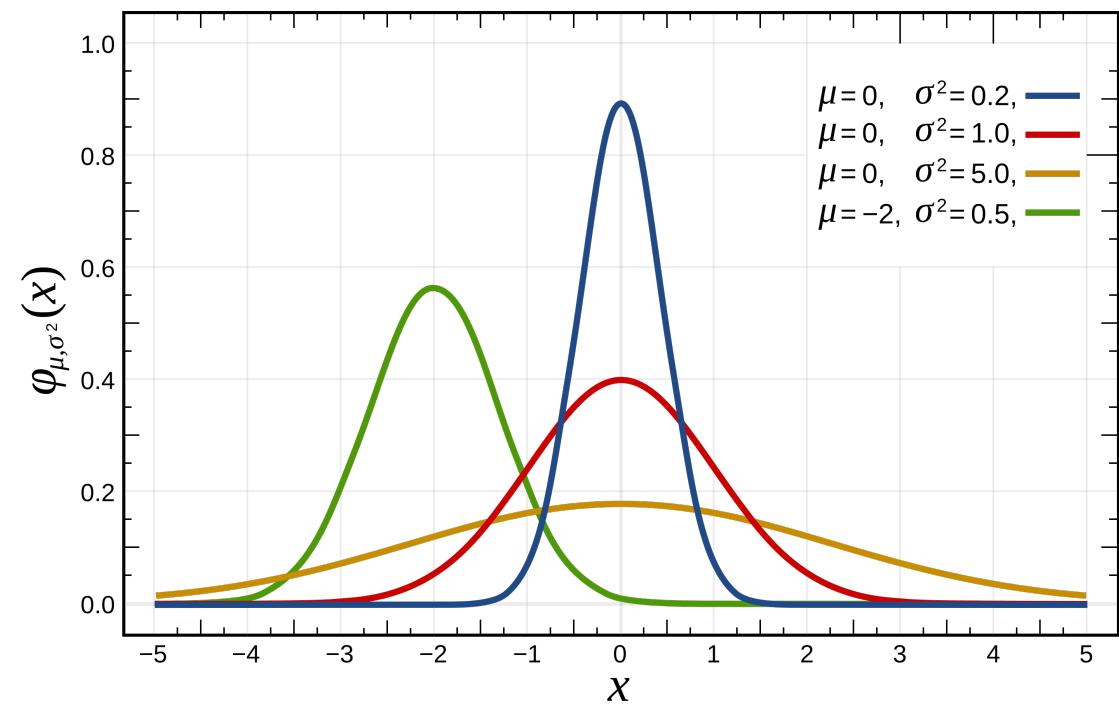
https://en.wikipedia.org/wiki/Probability_distribution

https://en.wikipedia.org/wiki/Normal_distribution

https://en.wikipedia.org/wiki/Multivariate_normal_distribution

Normal Distribution

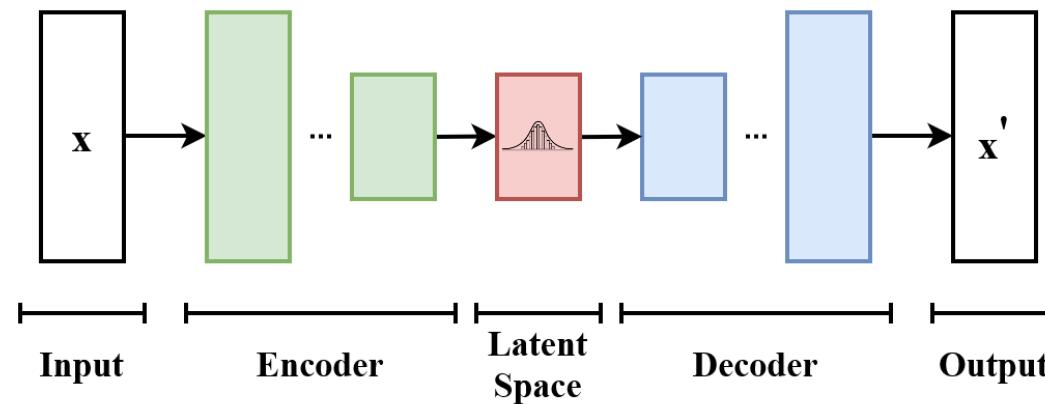
- The normal distribution is characterized by a mean (denoted μ) and standard deviation (denoted σ)
- A standard normal distribution is one with mean zero and standard deviation 1
- If we know the latent space follows a standard normal distribution, sampling from such a distribution becomes easy
- How can we ensure the latent space follows such a distribution?



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Variational Autoencoders

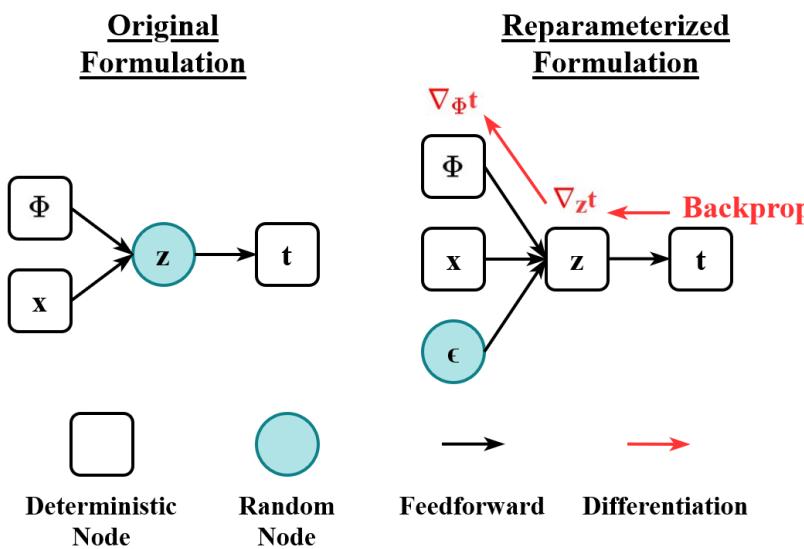
- Instead of mapping inputs to a point in a latent space, variational autoencoders map inputs to a distribution in the latent space
- They enforce a particular distribution on this latent space, which is usually a standard normal distribution



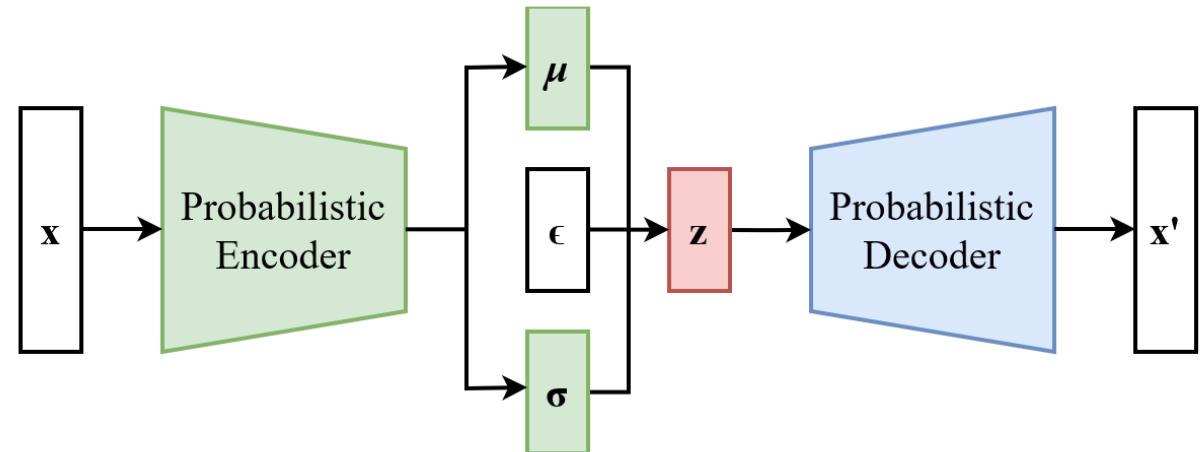
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Reparameterization Trick

- We cannot directly map inputs to a distribution since we cannot backpropagate through randomness
- Therefore, we map inputs to the mean and variance, and combine these parameters with randomness to encode the input to a distribution



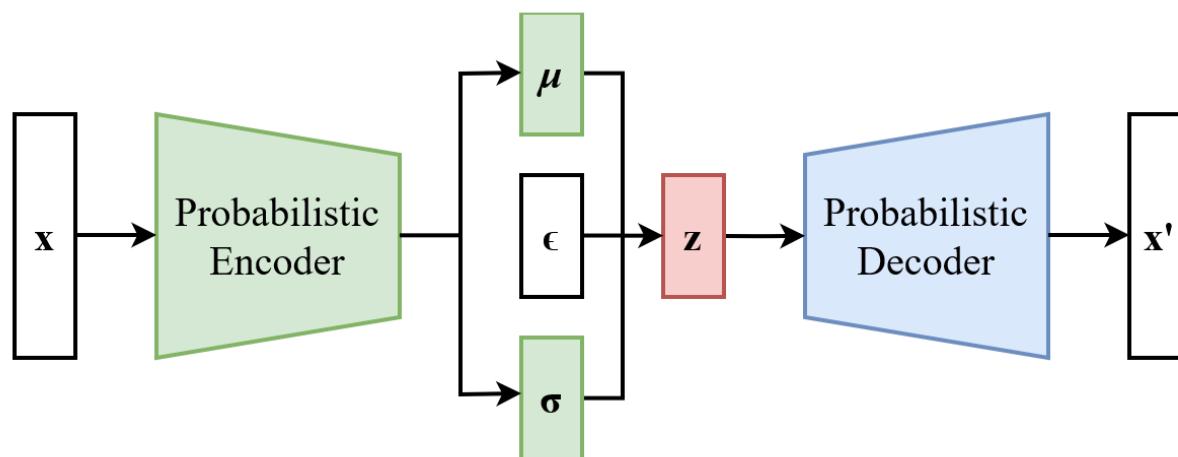
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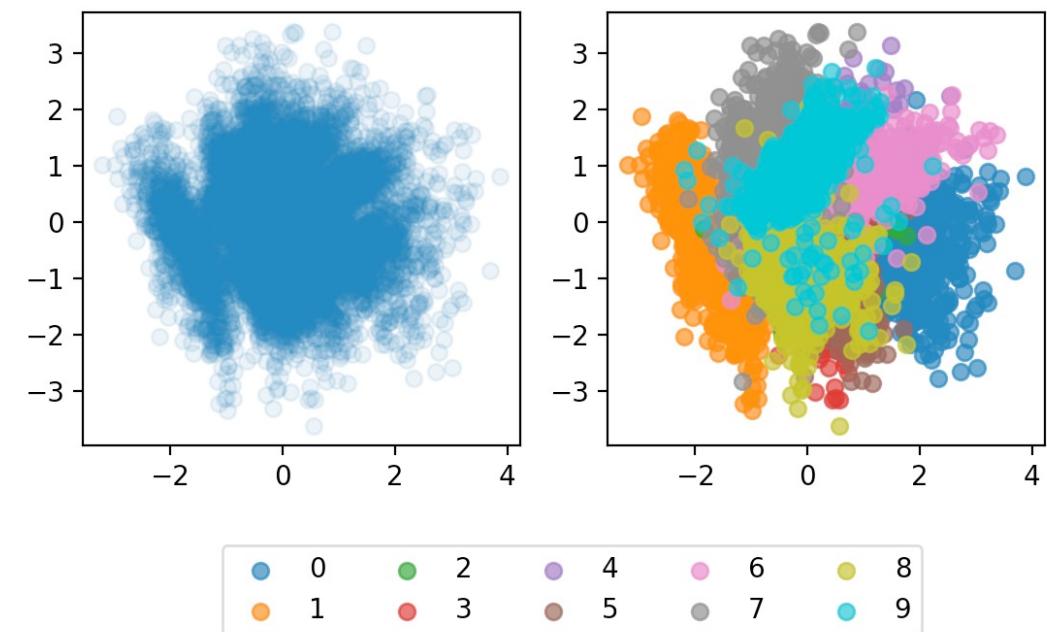
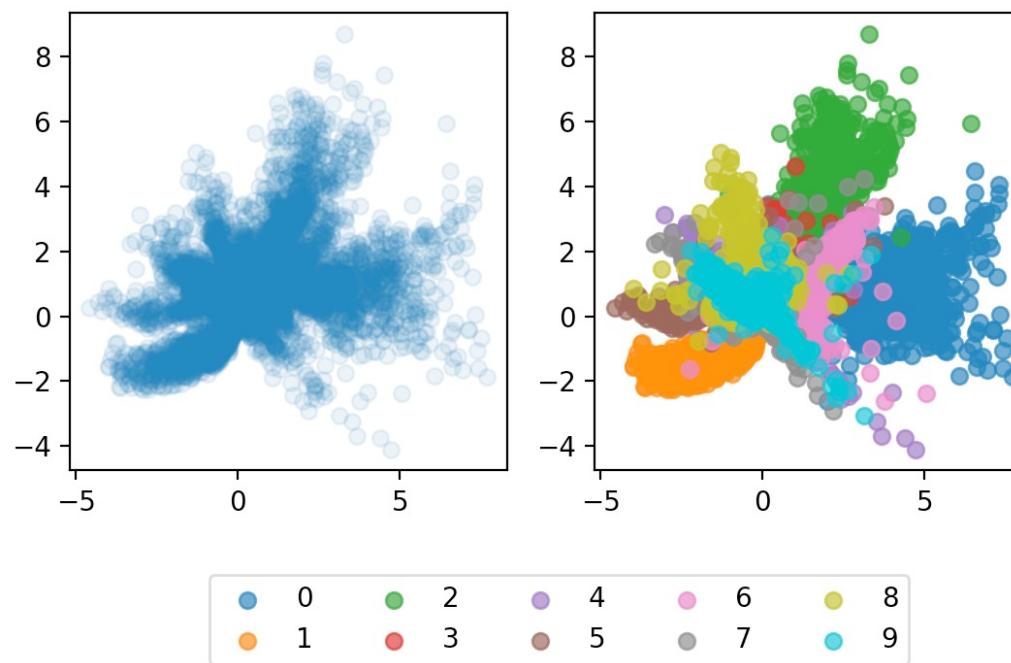
KL Divergence

- The Kullback-Leibler (KL) divergence is a measure of similarity between two different distributions
- We can add the KL divergence to the loss function to encourage the latent space to follow a standard normal distribution



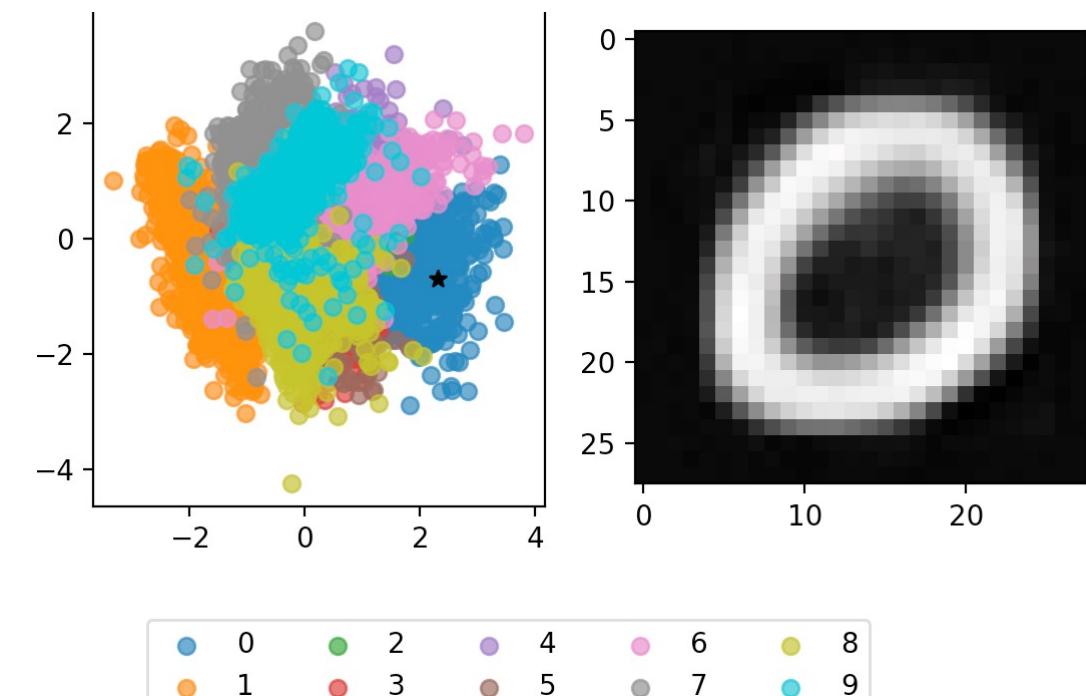
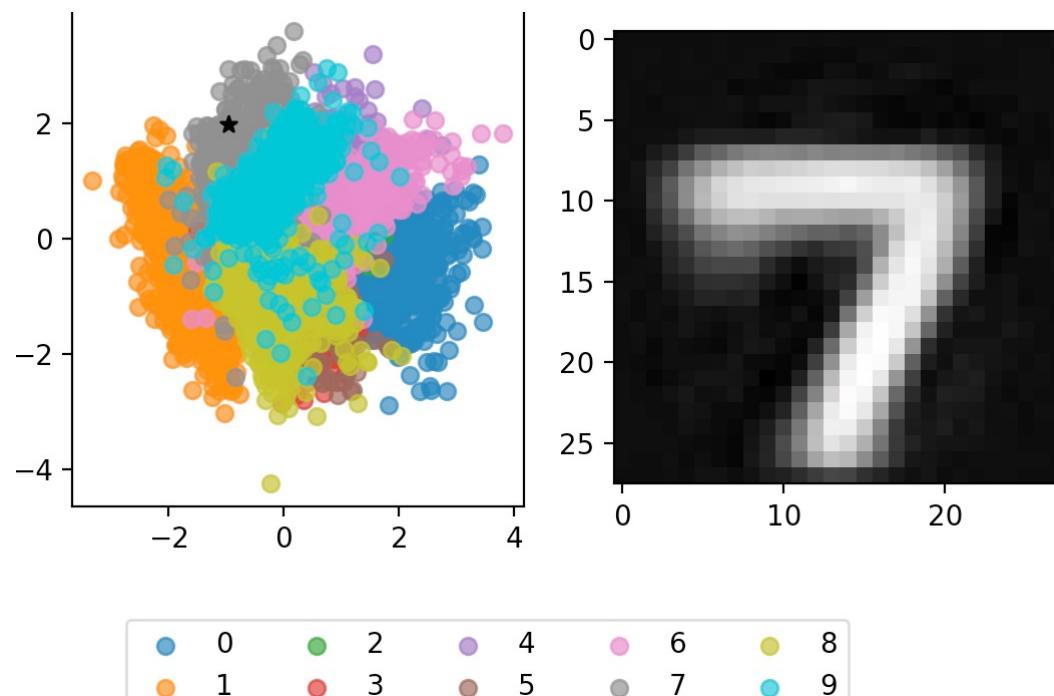
VAE Dimensionality Reduction Results

- The distribution of the encoder now approximately follows a normal distribution



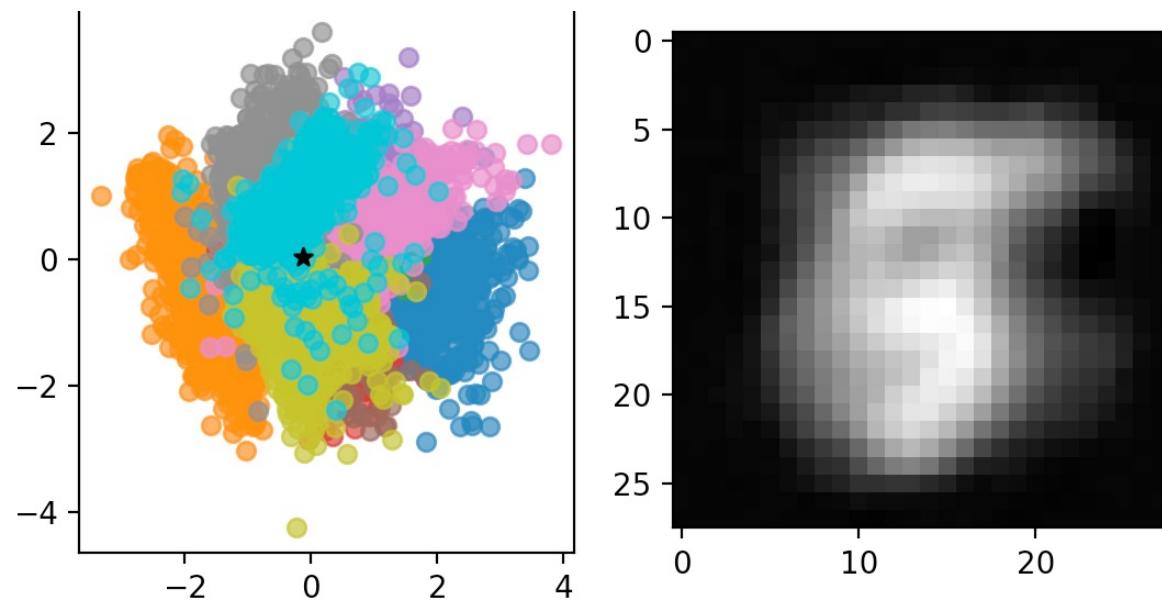
Generating Data with a VAE

- Now, we can simply sample from a normal distribution with mean zero and standard deviation one
- We can also easily detect out of distribution data
- Does this mean we can always prevent generating undesirable data?

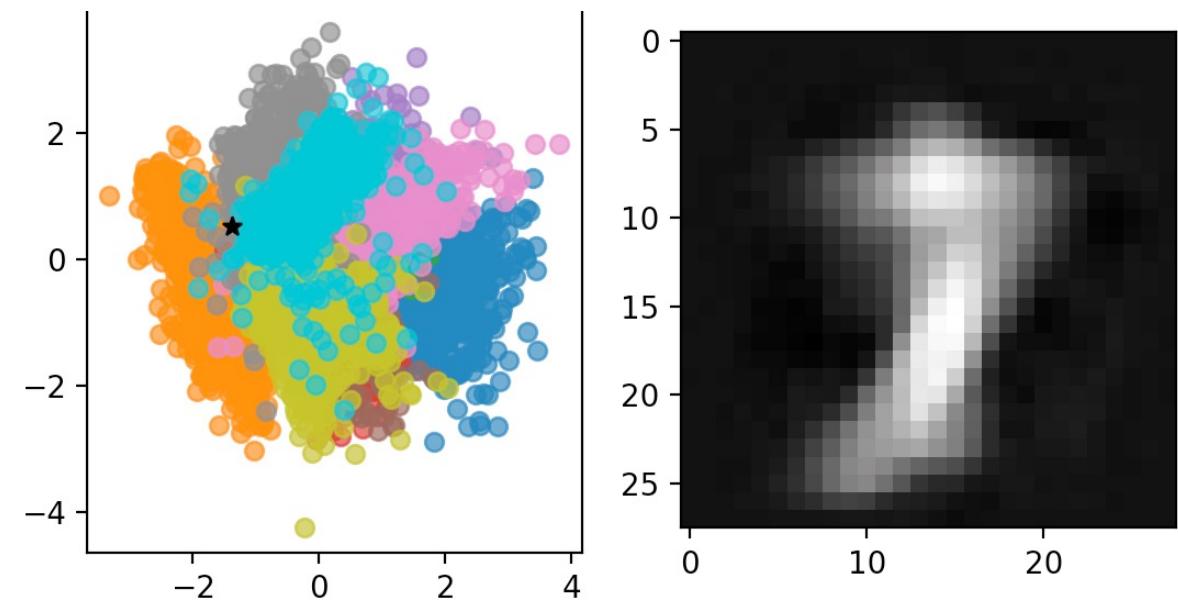


Generating Data with a VAE

- The same phenomena that caused adversarial examples to be such a problem is also present in VAEs
- Therefore, even if we stick to sampling samples that are highly likely for a normal distribution, we can still get undesirable outputs



| | | | | |
|---|---|---|---|---|
| 0 | 2 | 4 | 6 | 8 |
| 1 | 3 | 5 | 7 | 9 |



| | | | | |
|---|---|---|---|---|
| 0 | 2 | 4 | 6 | 8 |
| 1 | 3 | 5 | 7 | 9 |

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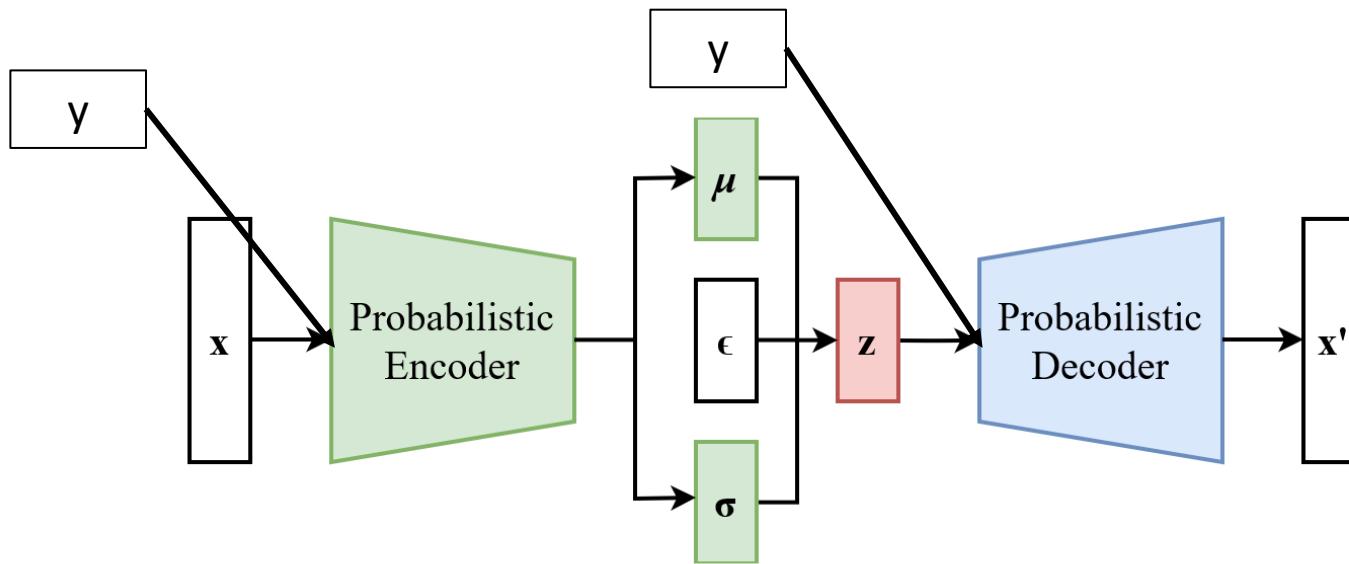
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Conditioning Data Generation on Properties

- Imagine we knew certain properties of the data, how can we train a generative model that can generate data with those specific properties?
- For example, digit class, size, angle, writing style, etc.

Conditional Variational Autoencoders

- We can add property information to the encoder and decoder
- This then encourages the inputs with each particular property to follow a normal distribution
- Then, to generate data, we sample from a normal distribution and give the desired properties to the decoder



Conditional Variational Autoencoders

- We can then explore the latent space for each property to better generate more fine-grained variations

