Advanced Institute for Artificial Intelligence

Autoencoders

Advanced Institute for Artificial Intelligence – AI2

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Variational Autoencoders

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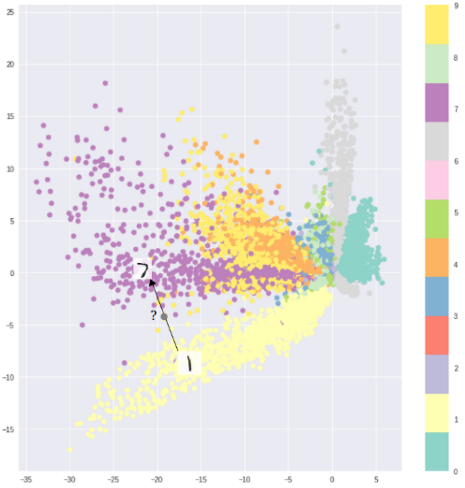
Recap: The problem with standard autoencoders

- Asides from a few applications like denoising autoencoders, they are fairly limited;
- The latent space they convert their inputs to and where their encoded vectors lie, may not be continuous, or allow easy interpolation.
- For example, training an autoencoder on the MNIST dataset, and visualizing the encodings from a 2D latent space reveals the formation of distinct clusters:



Recap: The problem with standard autoencoders

- When building a generative model, you don't want to prepare to replicate the same image you put in:
  - Randomly sample from the latent space, or
  - Generate variations on an input image, from a continuous latent space;
- If the space has discontinuities and you sample/generate a variation from there, the decoder will simply generate an unrealistic output;
  - The decoder has no idea how to deal with that region of the latent space;
  - During training, it never saw encoded vectors coming from that region of latent space;

Variational Autoencoders

Definitions

- Variational Autoencoders (VAEs) have one fundamentally unique property that separates them from regular autoencoders:
  - Their latent spaces are, by design, continuous;
  - The continuity of the latent space allows for easy random sampling and interpolation.
- Its encoder not output an encoding vector of size n;
- Instead, it outputs two vectors of size n:
  - a vector of means, μ, and
  - another vector of standard deviations, σ.
  - The mean and standard deviation of the i-th random variable, X_i from which we sample, to obtain the sampled encoding which we pass onward to the decoder;

Definitions

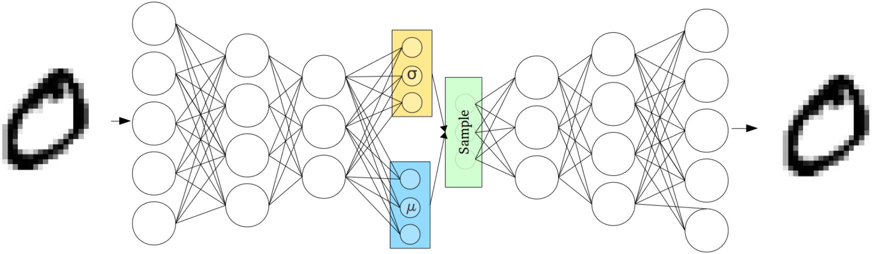


Figure: Variational Autoencoder with the μ and σ vectors

Image from Variational Autoencoder architecture by I

Example

In the scenario where we have an input signal with 500 features and we aim to reduce this signal to just 30, we could think of building a VAE just like this:

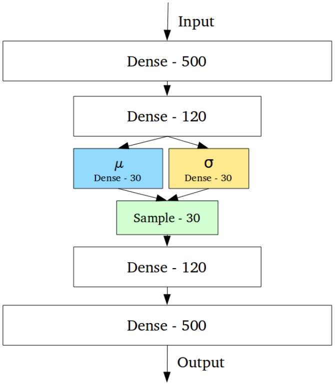


Figure: VAE that reduces a 500 dimensional input to a 30 dimensions latent space

Definitions

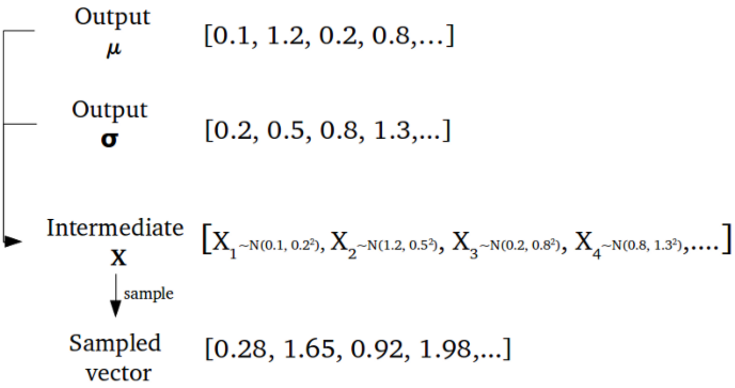


Figure: How the forward pass works

Definitions

- Stochastic generation of encoding vectors
  - For the same input, keeping the mean and standard deviation the same the actual encoding will vary on every single pass due to sampling.
- The mean vector controls where the encoding of an input should be centered;
- the standard deviation controls how much from the mean the encoding can vary (the area)

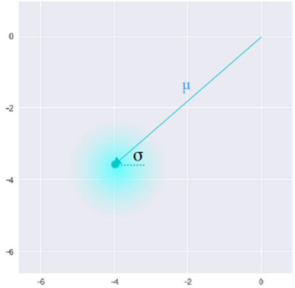


Figure: μ and σ to control the sampling

Definitions

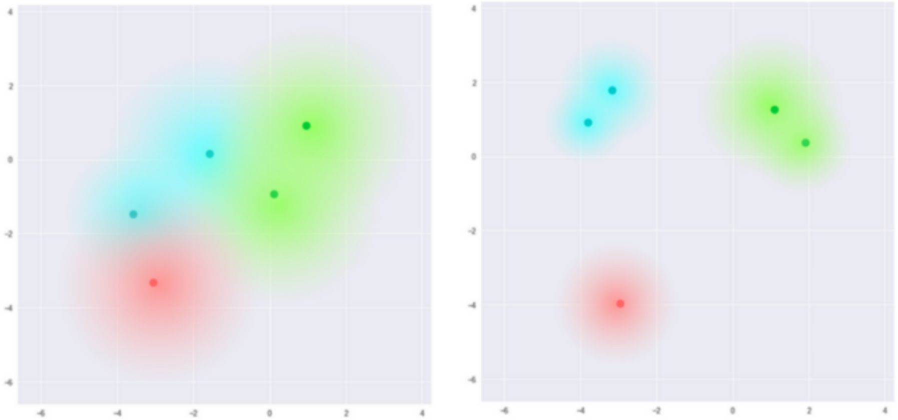
- Not only is a single point in latent space refers to a sample of that class.
- All nearby points refer to the same as well in a $sigma$-radius;
- The goal here is to try to create more homogeneous latent space, getting rid of the discontinuity;
  - The model is now exposed to a certain degree of local variation by varying the encoding of one sample;
  - We want overlap between samples that are not very similar too;
    - Interpolation between classes;

Definitions

- There are no limits on what values vectors μ and σ can take on:
  - Encoder can learn to generate very different μ for different classes, clustering them apart, and minimizing σ
  - Can come to a point that it looks like a single dot.
- Desirable: Encodings that are as close as possible while still being distinct, allowing smooth interpolation, and enabling the construction of new samples

Definitions

What we want, and what we may get:



Definitions - The KL Divergence

- Kullback–Leibler divergence [1]
- Measures how much they diverge from each other;
- For VAEs, the KL loss is equivalent to the sum of all the KL divergences between the component $X_i \sim \mathcal{N}(\mu_i, \sigma_i^2)$ and the standard normal.
  - This measure is minimized when $\mu_i = 0$ and $\sigma_i = 0$
- When the divergence is calculated between univariate distributions it can be simplified to:

$$\sum_{i=1}^{n} \sigma_i^2 + \mu_i^2 - log(\sigma_i^2) - 1$$

[1] Kullback-Leibler Divergence Explained

Definitions - The KL Divergence

- This loss forces the encoder to distribute all encodings evenly around the center of the latent space;
- Using purely KL loss results in a latent space results in encodings densely placed randomly, near the center of the latent space
- The decoder finds it impossible to decode anything meaningful from this space;

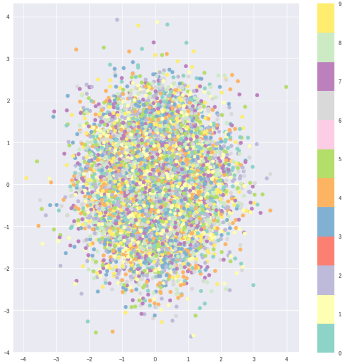


Figure: Latent space produced by VAE trained only with KL Loss

Putting it all together

- Use the KL divergence as a penalization mechanism;
- Optimizing the two together (reconstruction - e.g., crossentropy) and the KL divergence;
  - Generation of a latent space which maintains the similarity of nearby encodings;
  - Globally, is very densely packed near the latent space origin
  - Equilibrium reached by the cluster-forming nature of the reconstruction loss and the dense packing nature of the KL loss;

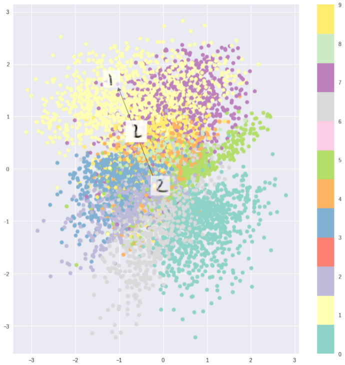


Figure: Using the composed loss