Autoencoders

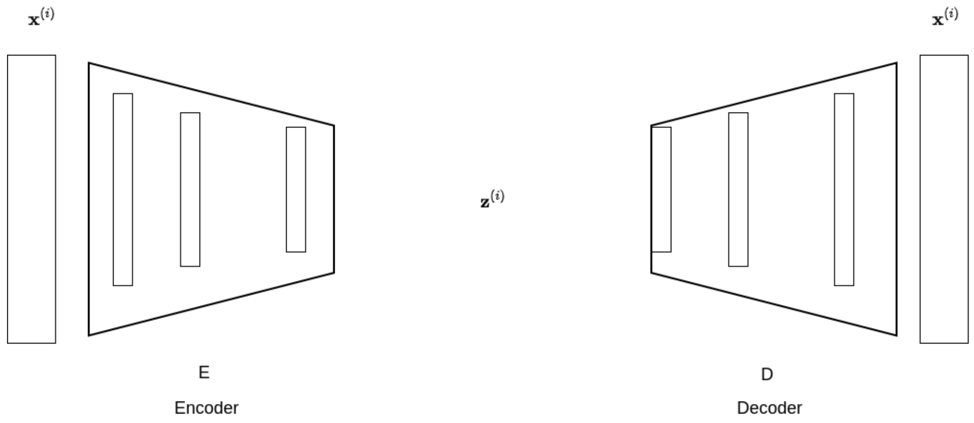
An *Autoencoder* (AE) is a Neural Network comprised of two parts:

- an *Encoder*, which takes the input $\mathbf{x}$ and produces an intermediate ("latent") representation $\mathbf{z}$ as output
- a *Decoder*, which takes $\mathbf{z}$ as input and attempts to reproduce $\mathbf{x}$ as output

Both the Encoder and Decoder are Neural Networks

- their weights are learned by training them in tandem
- on training set $\langle \mathbf{X}, \mathbf{y} \rangle = \langle \mathbf{X}, \mathbf{X} \rangle$

Autoencoder



A non-trivial Autoencoder (i.e., one in which the parts are not merely the Identity transformation)

- has latent representation $\mathbf{z}$ of dimension less than input $\mathbf{x}$
- $\mathbf{z}$ is a *bottle-neck*
- forcing dimensionality reduction, like PCA
- causing the inversion of the Decoder to be imperfect

Comparison of Autoencoders and PCA

Both the AE and PCA are methods to create representations of an input of length n via reduced dimensionality vectors of length $r \le n$

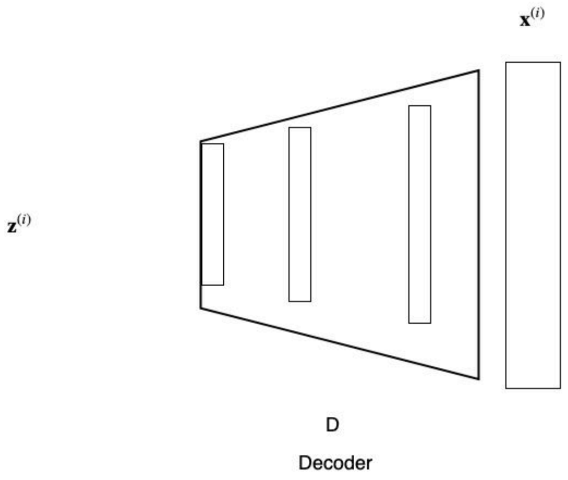
They are similar in *purpose* but different in *detail*

- PCA creates n vectors (of length n) called *components*
    - Each $\mathbf{x}^{(\mathbf{i})}$ of length n is represented as a linear combination of $r \le n$ components
        - The reduced dimensionality representation is a vector of length $r \le n$: the weights used in the linear combination
    - The components are common to all inputs $\mathbf{x}^{(\mathbf{i})}$
- Autoencoder
    - the reduced dimensionality representation is a vector of length $r \le n$
    - the representation is unique to $\mathbf{x}^{(\mathbf{i})}$: not shared "components"

Our interest in Autoencoders

- Study Functional architecture
    - [TensorFlow Tutorial on Autoencoders (https://www.tensorflow.org/tutorials/generative/autoencoder)](https://www.tensorflow.org/tutorials/generative/autoencoder)
- Generative
    - Create *synthetic* examples $\mathbf{x}'$
    - By sampling $\mathbf{z}'$ from the space of latent representations
    - And inverting them

Generator



Uses

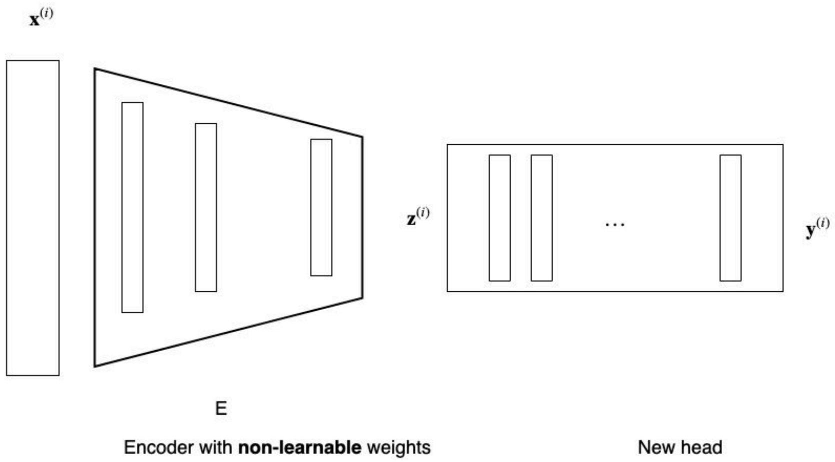
As an aside, we mention other use cases

Dimensionality reduction and Transfer learning

Once the Autoencoder has been trained, we can discard the Decoder

- Use the Encoder to create reduced dimension representations of large and high dimension inputs
    - Image search by replacing 3D megapixel images by shorter, 1D vectors
- Transfer to another task

Autoencoder: Encoder + New head



De-noising Autoencoder

Using an AE for dimensionality reduction is similar to using PCA

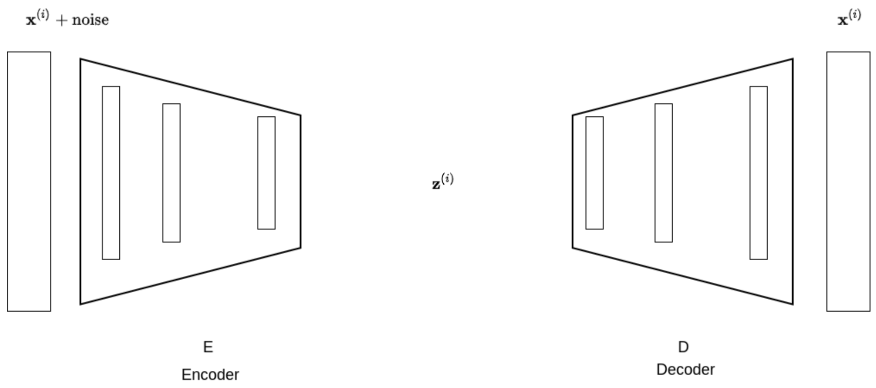
- **But** unlike PCA, there is no **explicit** "relative importance" associated with the retained dimensions

But we can *hope* that the information lost through the bottleneck process is less important.

A *De-noising Autoencoder* is an Autoencoder trained on a slightly corrupted "noisy" input

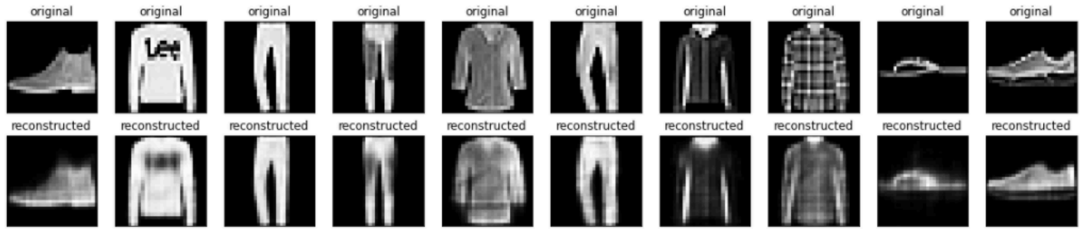
- $\langle \mathbf{X}, \mathbf{y} \rangle = \langle \mathbf{X} + \epsilon, \mathbf{X} \rangle$

Autoencoder: Denoising



De-noising may be useful as a pre-processing step for cleaning noisy data.

De-noising autoencoder: noisy inputs, de-noised outputs



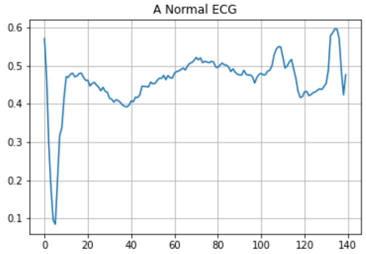
Autoencoder as Anomaly Detector

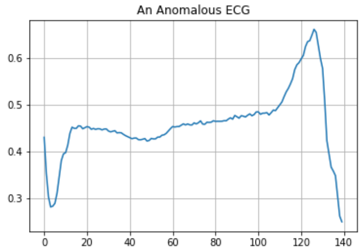
By forcing the input $\mathbf{x}$ through a bottleneck, the reconstructed input hopefully has "less important" information stripped away.

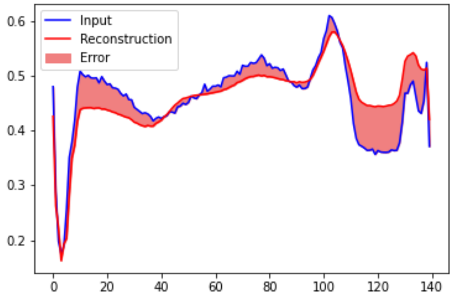
We may choose to characterize this lost information as an *anomaly* if the magnitude of the reconstruction error is larger than some threshold.

- Error: noise to be removed
- Signal: something unusual to be flagged for attention
- Signal: a source of alpha
    - Reconstructed input is our model's prediction
    - The noise is divergence from our model
        - trading opportunity ?

Anomaly Detector







Details

Notation summary

term	dimension	meaning
$\mathbf{x}$	n	Input
$\tilde{\mathbf{x}}$	n	Output: reconstructed $\mathbf{x}$
$\mathbf{z}$	$n' << n$	Latent representation
E	$\mathbb{R}^n \to \mathbb{R}^{n'}$	Encoder
		$E(\mathbf{x}) = \mathbf{z}$
D	$\mathbb{R}^{n'} \to \mathbb{R}^n$	Decoder
		$\tilde{\mathbf{x}} = D(\mathbf{z})$
		$\tilde{\mathbf{x}} = D(E(\mathbf{x}))$
		$\tilde{\mathbf{x}} \approx \mathbf{x}$

Loss function

The obvious loss functions compare the original $\mathbf{x}^{(\mathbf{i})}$ and reconstructed $\tilde{\mathbf{x}}^{(\mathbf{i})}$ feature by feature:

Mean Squared Error (MSE)

$$\mathcal{L}^{(\mathbf{i})} = \sum_{j=1}^{|\mathbf{x}|} (\mathbf{x}_j^{(\mathbf{i})} - \tilde{\mathbf{x}}_j^{(\mathbf{i})})^2$$

Binary Cross Entropy

For the special case where *each* original feature is in the range $[0, 1]$ (e.g., an image)

$$\mathcal{L}^{(\mathbf{i})} = \sum_{j=1}^{|\mathbf{x}|} \left(\mathbf{x}_j^{(\mathbf{i})} \log(\tilde{\mathbf{x}}_j^{(\mathbf{i})}) + (1 - \mathbf{x}_j^{(\mathbf{i})}) \log(1 - \tilde{\mathbf{x}}_j^{(\mathbf{i})}) \right)$$

Generative Limitations

We propose to create synthetic examples $\mathbf{x}'$ by sampling $\mathbf{z}$.

Although the synthetic $\mathbf{x}'$ created by this inversion seems appealing, there are some issues

- Assuming we need labeled examples $\langle \mathbf{x}, \mathbf{y} \rangle$
    - we have no control as to the class $\mathbf{y}'$ of the synthetic $\mathbf{x}'$

- Our method of sampling $\mathbf{z}$ is not dependent on the distribution of $\mathbf{z}$

    - In general, the distribution is unknown
    - In particular, the sample may not be representative of any known (e.g., training) true example

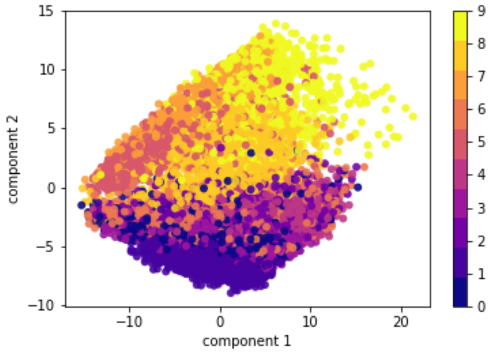
    - Even if we obtain $\mathbf{z}$ by slight modification of a particular $\mathbf{x}^{(\mathbf{i})}$

$$\boldsymbol{z} = E(\boldsymbol{x}^{(i)}) + \epsilon$$

there is no guarantee as to to the label or fidelity of $\mathbf{x}' = D(\mathbf{z})$

To illustrate, we

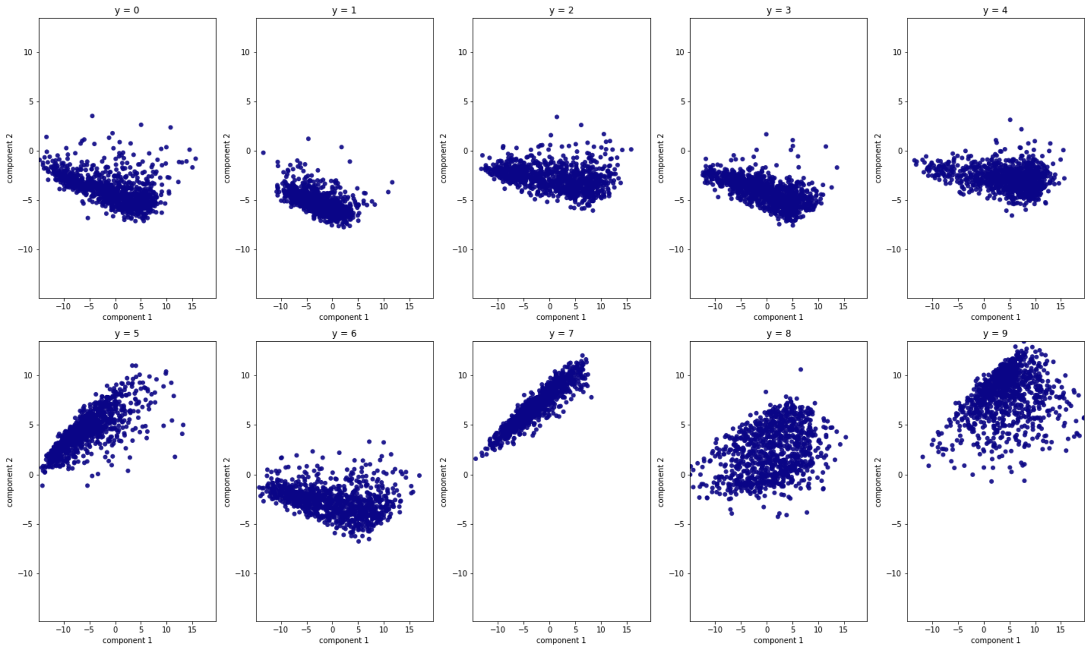
- create an [autoencoder (autoencoder.ipynb)](autoencoder.ipynb) for MNIST fashion
    - 10 classes
    - Latent representation are vectors of length 64
- obtain the latent representations for a set of test inputs
- create a scatter plot of the latents
    - using PCA to project the high dimensionality latents to 2D



As you can see

- the latents are not uniformly distributed
- latents of particular classes (each class depicted with a unique color) form clusters

We can illustrate the latter point via a separate plot of the latents for each class



Thus, sampling latents uniformly will not necessarily find a latent "in the neighborhood"

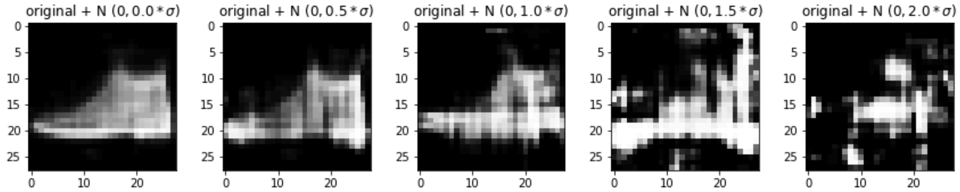
- of any of the classes
- of any particular class

We can emphasize the latter point.

Let's explore the neighborhood around a the latent representation of a single input

- add random normal noise with varying increments of standard deviation

We might expect to obtain images similar to the original.

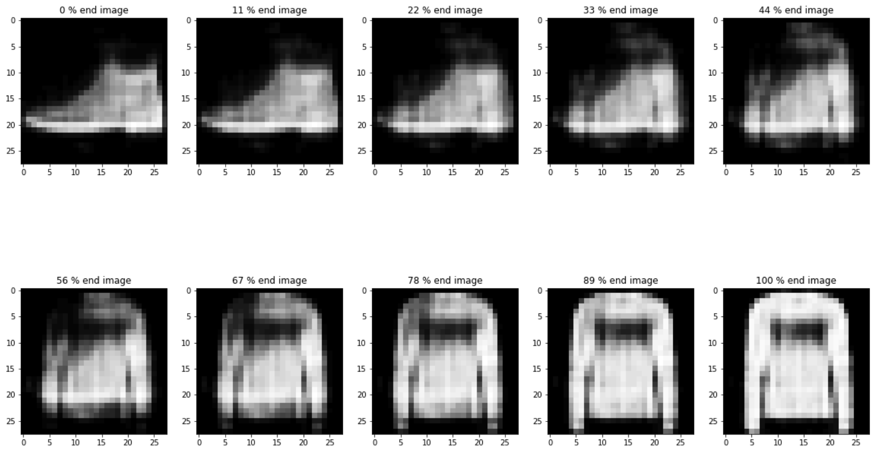


As you can see from the above, even moving in a small radius from the latent of the original does not guarantee a realistic decoded output.

- So we can't generate a synthetic example of a particular class by a small perturbation of the latent from a genuine image of the class

Next, we conduct an experiment in interpolating between the latents associated with 2 inputs.

- interpolate between the latents and decode
- first plot: 0% second "end" image; 100% first image
- last plot: 100% second image; 0% first image



As you can see from the intermediate outputs

- not all latents correspond to recognizable classes

Thus, we see issues associated with generating synthetic examples by simple-minded sampling of the latent space.

Experiments with Autoencoders

The plots in this notebook were generated by this notebook (Autoencoder_practice.ipynb)

- derived from the TensorFlow tutorial on Autoencoders (https://www.tensorflow.org/tutorials/generative/autoencoder)
- illustrates Latent representation, Denoising, Anomaly Detection
- (secondary objective: study the code)

In [3]:

```
print("Done")
```

```
Done
```