Autoencoders

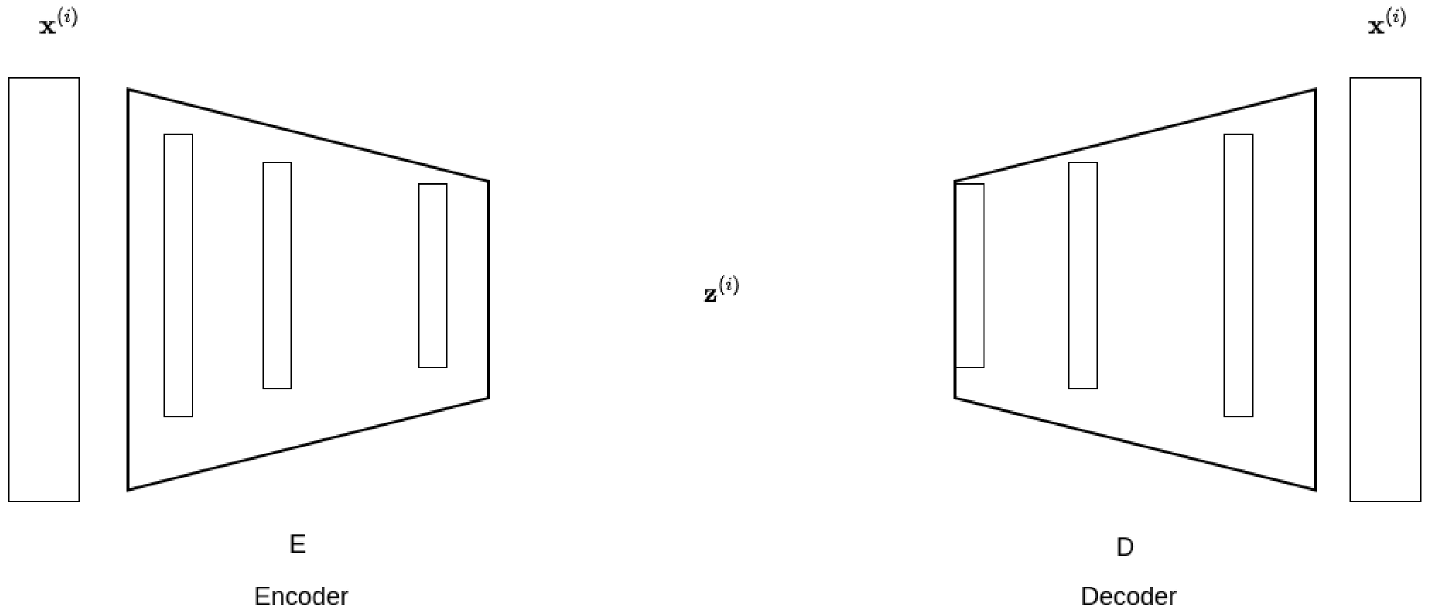
An *Autoencoder* (AE) is a Neural Network comprised of two parts:

- 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

Recall

We saw code (Functional_Models.ipynb#Example:-Nested-Models) for an Autoencoder as part of our introduction to the Functional API of Keras.

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 example $\mathbf{x^{(i)}}$ can be represented
        - *exactly* as a linear combination of n components
        - *approximately* as a linear combination of $r < n$ 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 example inputs $\mathbf{x^{(i)}}$
- Autoencoder
    - the reduced dimensionality representation is a vector of length $r \le n$
    - the representation is unique to $\mathbf{x^{(i)}}$: 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

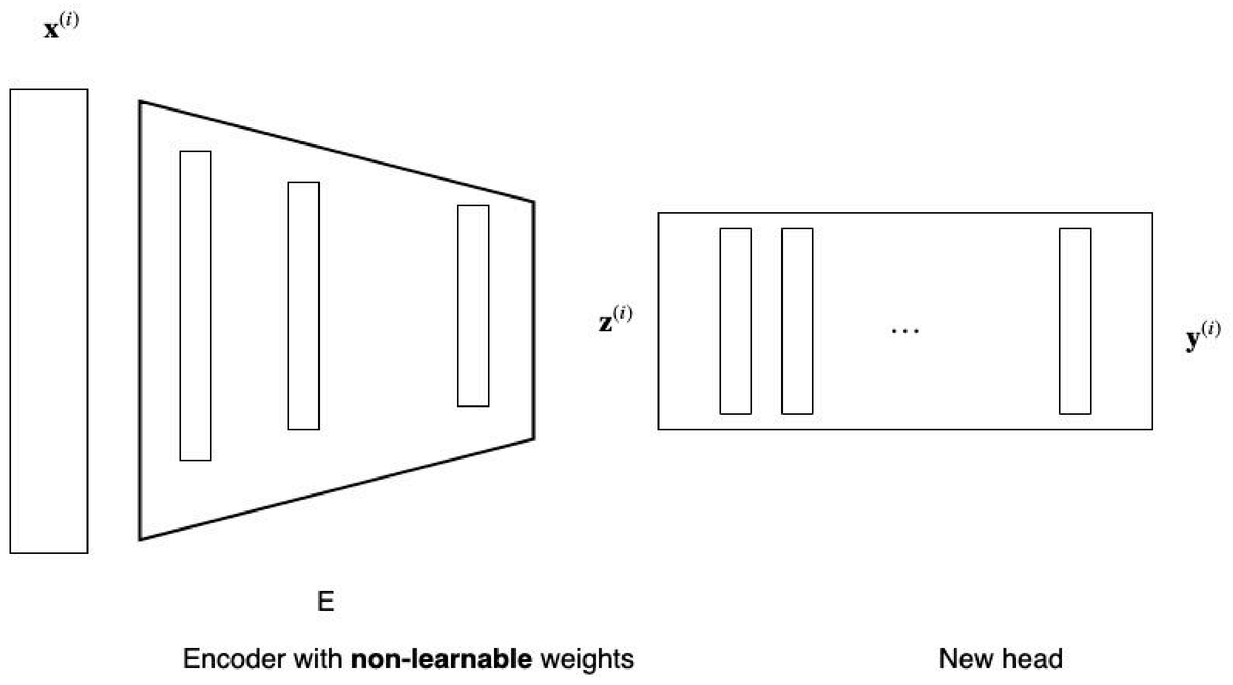
As an aside, we mention other use cases

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



For example, we can solve a Classification task

- by encoding an input that has many features
- into a shorter set of synthetic features
- an appending as the New Head: implementing Logistic Regression

De-noising Autoencoder

Using an AE for dimensionality reduction is similar to using PCA

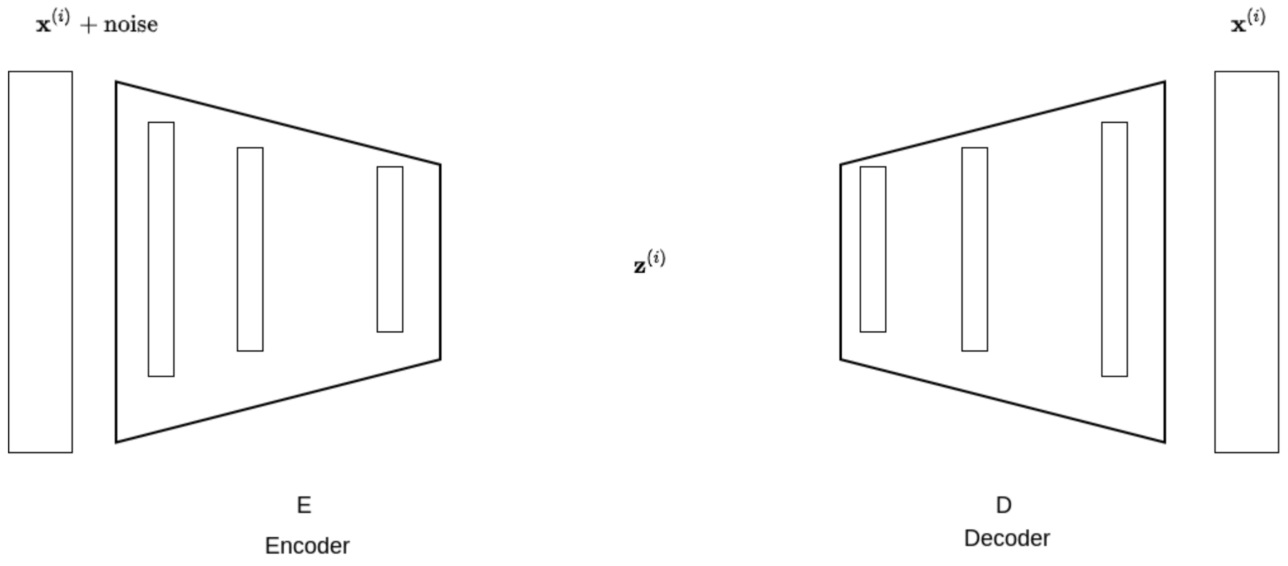
- **But** unlike PCA, there is no **explicit** "relative importance" associated with the retained dimensions

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

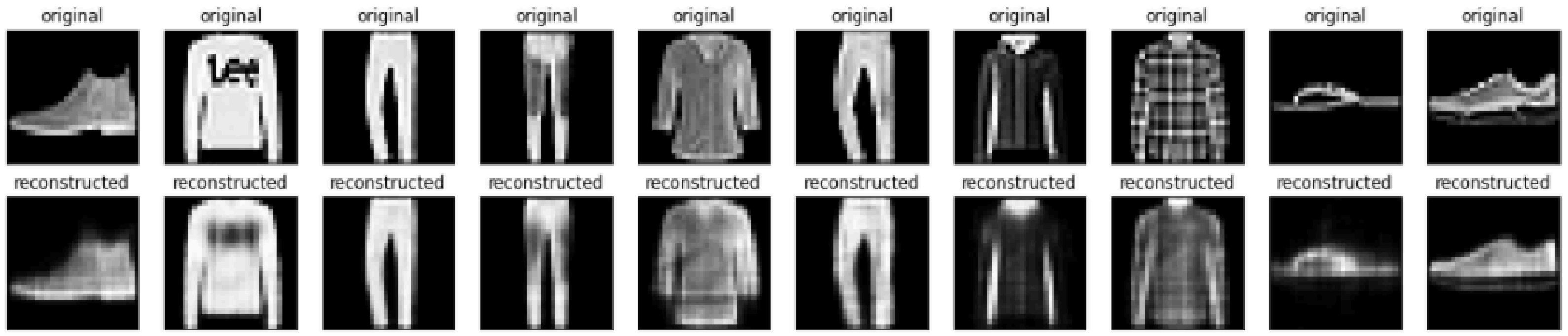
- $\langle \mathbf{X}, \mathbf{y} \rangle = \langle \mathbf{X} + \epsilon, \mathbf{X} \rangle$

Autoencoder: Denoising



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

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



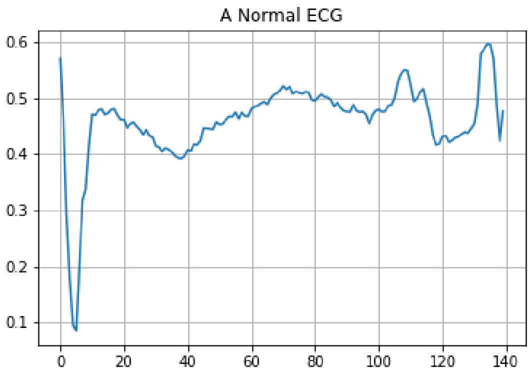
Autoencoder as Anomaly Detector

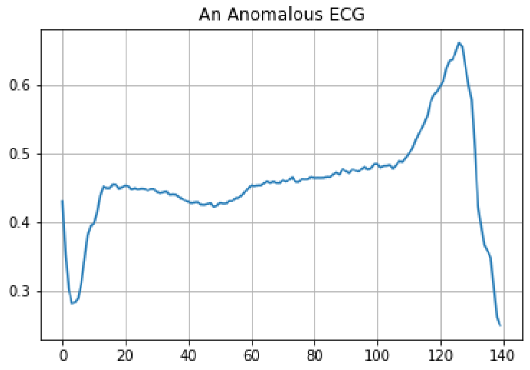
By forcing the input $\mathbf{x}$ through a bottleneck, the reconstructed input hopefully has "less important" information stripped away.

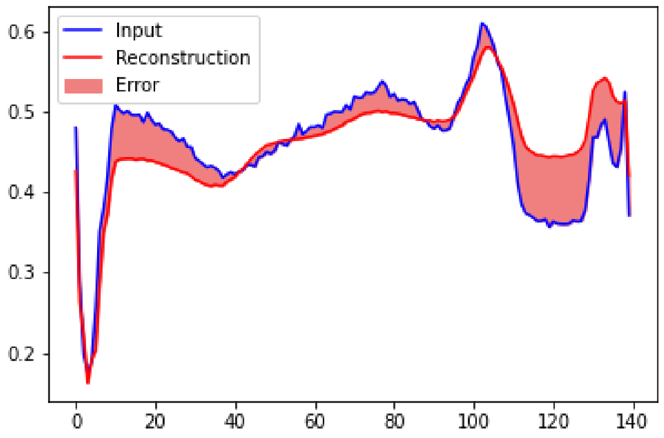
We may choose to characterize this lost information as an *anomaly* if the magnitude of the reconstruction error is larger than some threshold.

- 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

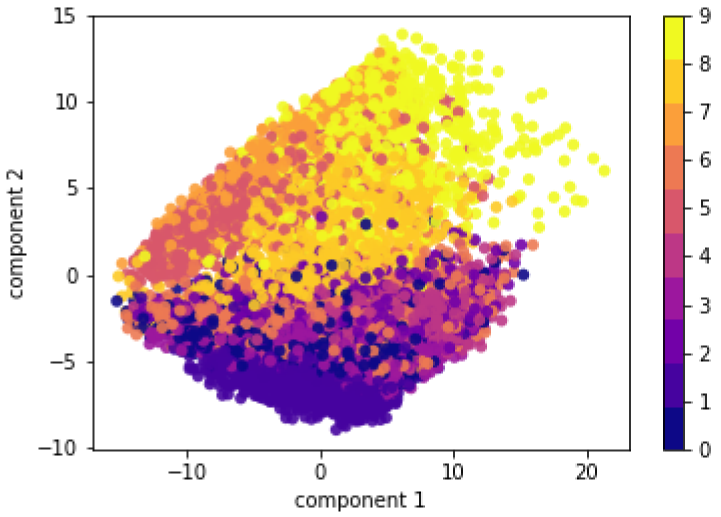
- Assuming we need labeled examples $\langle \mathbf{x}, \mathbf{y} \rangle$
    - we have no control as to the class $\mathbf{y}'$ of the synthetic $\mathbf{x}'$
- Our method of sampling $\mathbf{z}$ is not dependent on the distribution of $\mathbf{z}$
    - In general, the distribution is unknown
    - 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

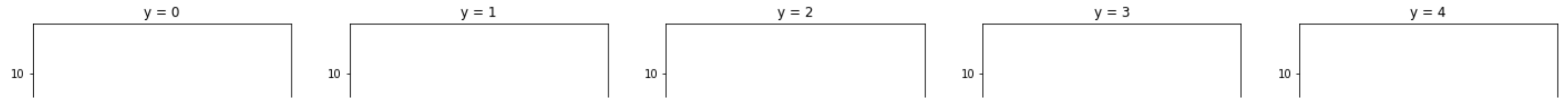
- create an [autoencoder (autoencoder.ipynb)]() for MNIST fashion
    - 10 classes
    - Latent representation are vectors of length 64
- obtain the latent representations for a set of test inputs
- create a scatter plot of the latents
    - using PCA to project the high dimensionality latents to 2D



As you can see

- the latents are not uniformly distributed in the two-dimensional space of the first two PCA components
- 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


y = 0
10
y = 1
10
y = 2
10
y = 3
10
y = 4
10

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)

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In [3]: print("Done")
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Done
```