From PCA to Autoencoders

Unsupervised Representation Learning

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Do better than linear dimensionality techniques (PCA) Using neural networks. Handle very-high-dimensional data (i.e. d = 1k-1M) Scale linearly with the size of data. [4]

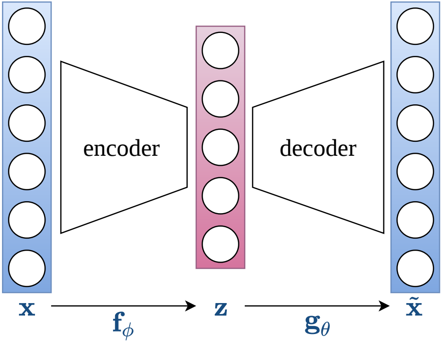
Introduction to autoencoders

Definition

Definition

An autoencoder is a neural network trained to reconstruct its inputs. It is composed of two parts:

1. an encoder, mapping the input to a latent representation ("code") $\mathbf{z} = \mathbf{f}_{\boldsymbol{\phi}}(\mathbf{x})$
2. a decoder, mapping the code back to the input space $\tilde{\mathbf{x}} = \mathbf{g}_{\boldsymbol{\theta}}(\mathbf{z})$



Definition

Challenge

We do not want the encoder to learn the identity function, but to learn a *good representation* of our data.

Regularization?

Reducing the size of the *hypothesis set* $\mathcal{H}$ by constraining the space of possible solutions to the optimization problem.

- L2 weight decay
- Sparsity, L1 weight decay
- ...

Introduction to autoencoders

Mathematical formulation

What is a good representation?

Let $q_{\boldsymbol{\phi}}(Z|X)$ be a (stochastic) parametric mapping from X to Z. A good representation Z of a random variable X maximizes mutual information between X and Z (*infomax principle*):

$$\begin{aligned}\mathbb{I}(X;Z) &= \mathbb{H}(X) - \mathbb{H}(X|Z)\\ &= C(X) + \mathbb{E}_{q_{\boldsymbol{\phi}}(X,Z)}\left[\log q_{\boldsymbol{\phi}}(X|Z)\right]\end{aligned}$$

For any parametric distribution $p_{\boldsymbol{\theta}}(X|Z)$ we have $\mathbb{E}_{q_{\boldsymbol{\phi}}(X,Z)}\left[\log p_{\boldsymbol{\theta}}(X|Z)\right] \leq \mathbb{E}_{q_{\boldsymbol{\phi}}(X,Z)}\left[\log q_{\boldsymbol{\phi}}(X|Z)\right]$ (using $D_{KL}(q||p) \geq 0$).

Task: maximize a lower bound on $\mathbb{I}(X;Z)$

$$\underset{\boldsymbol{\phi},\boldsymbol{\theta}}{\text{maximize}}\ \mathbb{E}_{q_{\boldsymbol{\phi}}(X,Z)}\left[\log p_{\boldsymbol{\theta}}(X|Z)\right]$$

Loss function for deterministic autoencoders

We consider deterministic mappings $Z = \mathbf{f}_{\boldsymbol{\phi}}(X)$ (or $q_{\boldsymbol{\phi}}(Z|X) = \delta(Z - \mathbf{f}_{\boldsymbol{\phi}}(X))$) and $\tilde{X} = \mathbf{g}_{\boldsymbol{\theta}}(\mathbf{f}_{\boldsymbol{\phi}}(X))$.

$$\underset{\boldsymbol{\phi},\boldsymbol{\theta}}{\text{maximize}}\ \mathbb{E}_{q_{\boldsymbol{\phi}}(X)}\left[\log p_{\boldsymbol{\theta}}(X|Z = \mathbf{f}_{\boldsymbol{\phi}}(X))\right]$$

Using empirical mean over a set of i.i.d. data samples:

$$\underset{\boldsymbol{\phi},\boldsymbol{\theta}}{\text{maximize}}\ \sum_i \log p_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}|\mathbf{z}^{(i)} = \mathbf{f}_{\boldsymbol{\phi}}(\mathbf{x}^{(i)}))$$

equivalent to:

$$\underset{\boldsymbol{\phi},\boldsymbol{\theta}}{\text{maximize}}\ \sum_i \log p(\mathbf{x}^{(i)}|\tilde{\mathbf{x}}^{(i)} = \mathbf{g}_{\boldsymbol{\theta}}(\mathbf{f}_{\boldsymbol{\phi}}(\mathbf{x}^{(i)})))$$

Let us turn this into a minimization the negative sum of individual loss functions $\mathcal{L}(\mathbf{x}|\tilde{\mathbf{x}}) = -\log p(\mathbf{x}|\tilde{\mathbf{x}})$.

Loss function for deterministic autoencoders

The reconstruction $\tilde{\mathbf{x}}$ is the mean of a distribution that may have generated $\mathbf{x}$.

Continuous variables: $\mathbf{x} \in \mathbb{R}^d$

- Gaussian distribution: $X|\tilde{X} = \tilde{\mathbf{x}} \sim \mathcal{N}(\tilde{\mathbf{x}}, \sigma^2\mathbf{I})$
- Loss function: $\mathcal{L}(\mathbf{x}|\tilde{\mathbf{x}}) \propto ||\mathbf{x} - \tilde{\mathbf{x}}||_2^2$

$\rightarrow$ Mean Squared Error (MSE) loss

Binary variables: $\mathbf{x} \in \{0,1\}^d$, or $\mathbf{x} \in [0,1]^d$

- Bernoulli distribution: $X|\tilde{X} = \tilde{\mathbf{x}} \sim \mathcal{B}(\tilde{\mathbf{x}})$
- Loss function: $-\sum_{j=1}^{d} [\mathbf{x}_j \log \tilde{\mathbf{x}}_j + (1 - \mathbf{x}_j) \log(1 - \tilde{\mathbf{x}}_j)]$

$\rightarrow$ Cross-entropy loss

Neurons can learn principal components

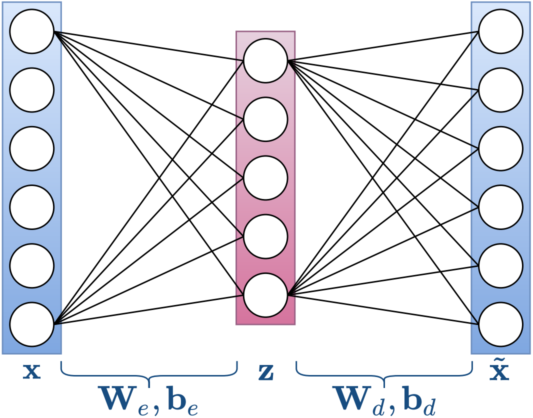
Hebb's Learning Rule

Learning PC with Oja's rule

[1], [7], [8]

Linear autoencoders

Definition



$\mathbf{x}$
$\mathbf{W}_e, \mathbf{b}_e$
$\mathbf{z}$
$\mathbf{W}_d, \mathbf{b}_d$
$\tilde{\mathbf{x}}$

Similarity with PCA

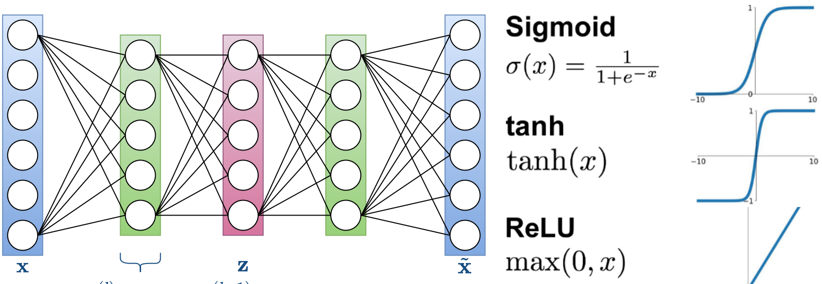
Show equivalence to PCA

[9]

Real-life autoencoders

Real-life autoencoders

Non-linear and deep autoencoders



$$\mathbf{h}^{(l)} = \sigma(\mathbf{W}\mathbf{h}^{(l-1)} + \mathbf{b})$$

Trained end-to-end with backprop. Layer-wise pretraining [4] is in fact not necessary (thanks to ReLU, better optimization and regularization).

- Not equivalent to PCA! (see paper AA-PCA)

Real-life autoencoders

Different types of regularization

Undercomplete or overcomplete

Let's code! (1)

The danger of overfitting

Problem: even a single continuous latent variable can remember the entire training set (one real number per sample).

The latent space is not continuous.

Sparse autoencoders

Denoising autoencoders

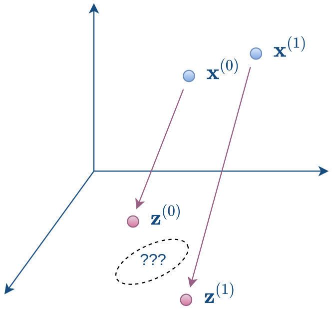
[10]

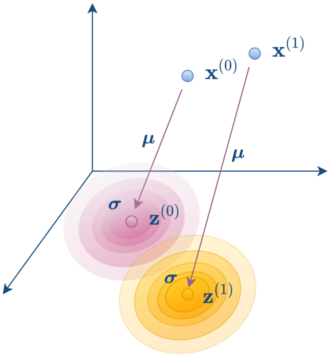
Real-life autoencoders

Variational autoencoders (VAE)

Motivations

Limitation of standard AE: the latent space has *no structure* and may not be continuous; we cannot explore it nor sample from it.





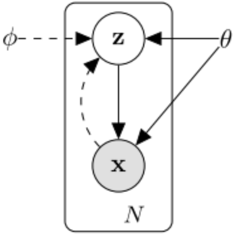
Example latent space figures, examples with MNIST, faces, music styles...

Variational autoencoders (VAE)

Probabilistic setting

Generative model $p_{\boldsymbol{\theta}}(\mathbf{x}, \mathbf{z})$:

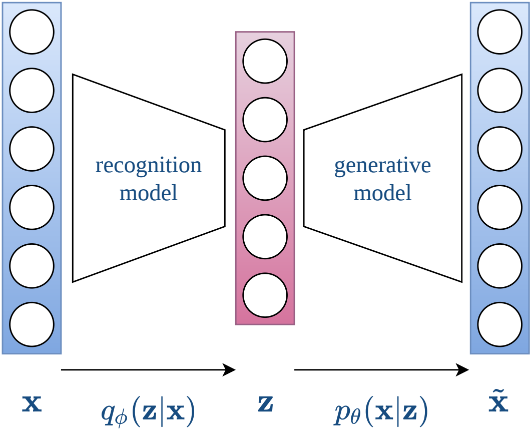
1. $\mathbf{z}$ is sampled from the prior $p_{\boldsymbol{\theta}}(\mathbf{z})$
2. $\mathbf{x}$ is generated with likelihood $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})$ (*probabilistic decoder*)



Problem: $\boldsymbol{\theta}$ is a NN, so $p_{\boldsymbol{\theta}}(\mathbf{x})$ and $p_{\boldsymbol{\theta}}(\mathbf{z}|\mathbf{x})$ are intractable.

▶ Stochastic Gradient Variational Bayes (SGVB) [5] is an efficient estimation method in case of intractable marginal likelihood/posterior and large datasets.

Variational autoencoders (VAE)



Recognition model $\rightarrow$ approximate posterior $q_\phi(\mathbf{z}|\mathbf{x})$ (*probabilistic encoder*)

VAE loss function

VAE ELBO (evidence lower bound)

$$\underset{\boldsymbol{\phi},\boldsymbol{\theta}}{\text{maximize}} \; - D_{KL}\left(q_{\boldsymbol{\phi}}(Z|X)||p_{\boldsymbol{\theta}}(Z)\right) + \mathbb{E}_{q_{\boldsymbol{\phi}}(Z|X)}\left[\log p_{\boldsymbol{\theta}}(X|Z)\right]$$

Key ideas

- The second term is a (negative) reconstruction error (e.g. MSE or cross-entropy) as in a deterministic AE.
- The first term, a Kullback-Leibler divergence between $q_{\boldsymbol{\phi}}(Z|X)$ and $p_{\boldsymbol{\theta}}(Z)$, acts as a regularizer pushing the encoder distribution closer to the prior distribution (typically a gaussian)

VAE loss function

Let's put gaussians everywhere!

- $p_{\boldsymbol{\theta}}(\mathbf{z}) = \mathcal{N}(\mathbf{z}; \mathbf{0}, \mathbf{I})$
- $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x}) = \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}, \boldsymbol{\sigma}^2\mathbf{I})$

The reparameterization trick

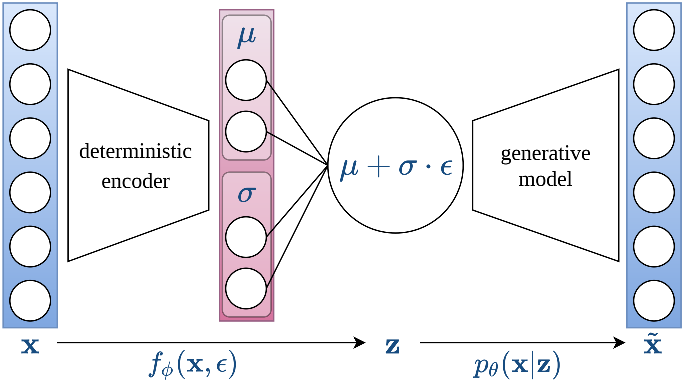
To sample from $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$, we use the reparameterization $\mathbf{z} = f_{\boldsymbol{\phi}}(\mathbf{x}, \epsilon) = \boldsymbol{\mu} + \boldsymbol{\sigma} \cdot \boldsymbol{\epsilon}$ where $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

For a given $\mathbf{x}^{(i)}$, and using 1-sample Monte-Carlo estimation, the ELBO becomes:

$$\frac{1}{2}\sum_j \left(1 + \log(\boldsymbol{\sigma}_j^{(i)})^2 - \boldsymbol{\mu}_j^{(i)} - (\boldsymbol{\sigma}_j^{(i)})^2\right) + \log p_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}|\mathbf{z}^{(i)})$$

where $\mathbf{z}^{(i)} = \boldsymbol{\mu}^{(i)} + \boldsymbol{\sigma}^{(i)} \cdot \boldsymbol{\epsilon}$

VAE: the reparameterization trick



Let’s code! (2)

Applications

Autoencoders can extract useful low-dimensional representations from high-dimensional data. They can be used as:

- a pre-processing step for any other ML algorithm (clustering, supervised classification or regression)
- an unsupervised pre-training prodecure for supervised deep neural networks (e.g. layer-wise pre-training) $\rightarrow$ See [4], [3], [10].

Data compression

Autoencoders can be used as a compression algorithm, but it is:

- lossy
- data-specific

Not commonly used in practice...

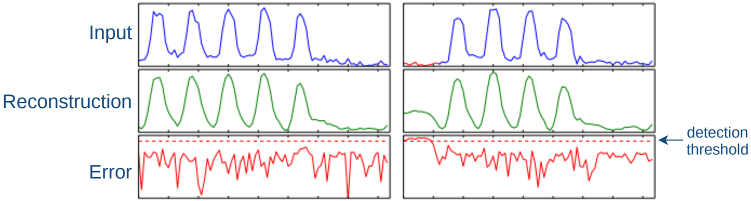
Data augmentation

The decoder model can be used to generate new data samples:

- Deterministic AEs: adding noise, interpolating or extrapolating in latent space [2]
- Generative models (VAE, GAN)

Anomaly detection

When the input differs from the training data distribution (e.g. an outlier), the autoencoder will produce a large reconstruction error. This error can be used to score anomalies [6].



(Malhotra et al, 2016)

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