From PCA to Autoencoders

Unsupervised Representation Learning

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Table of contents

Introduction to autoencoders

Motivations

[4]

Introduction to autoencoders

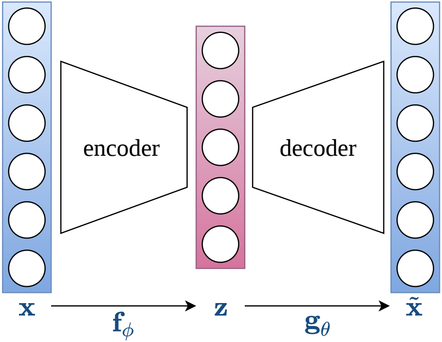
Definition

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

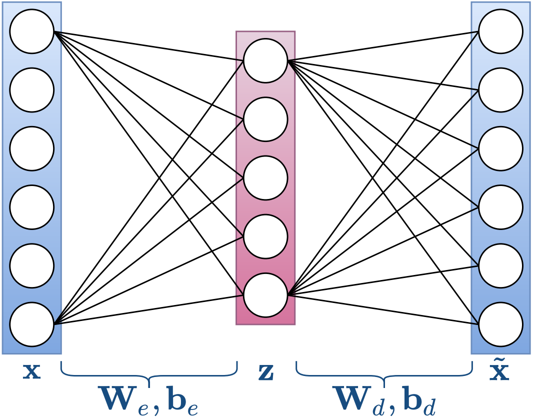
Hebb's Learning Rule

Learning PC with Oja's rule

[1], [6], [7]

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

[8]

Non-linear autoencoders

Non-linear autoencoders

Non-linear and deep autoencoders

Non-linear autoencoders

Non-linearity: sigmoid, tanh, ReLU...

Several layers

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

Deep autoencoders

Layer-wise pretraining: [4] In fact, not necessary (source?).

Non-linear 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

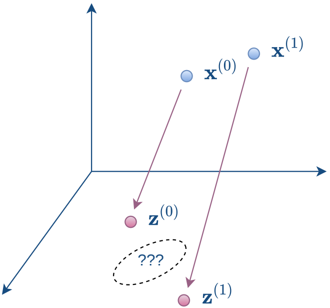
[9]

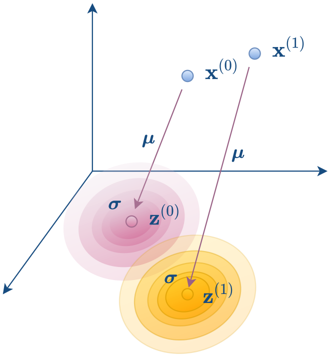
Non-linear autoencoders

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.



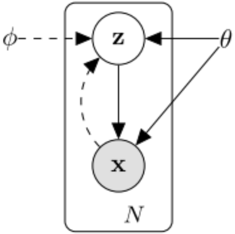


Example latent space figures, examples with MNIST, faces, music styles…

Probabilistic setting

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

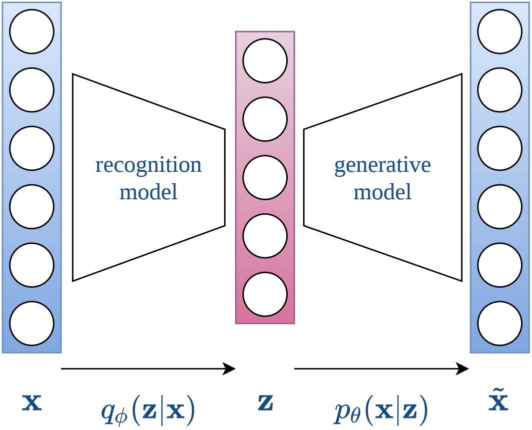
1. $\mathbf{z}$ sampled from $p_{\boldsymbol{\theta}}(\mathbf{z})$ (prior)
2. $p_{\boldsymbol{\theta}}(\mathbf{x}|\mathbf{z})$ (likelihood/*probabilistic decoder*)



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

Stochastic gradient variational Bayes (SGVB) [5] is an efficient method to estimate the parameters in case of intractable likelihood/posterior and large datasets (as in DL).

VAE: the reparameterization trick



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

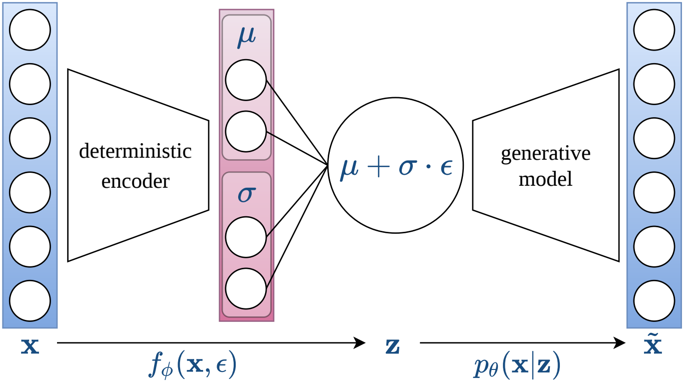
To sample from $q_{\boldsymbol{\phi}}(\mathbf{z}|\mathbf{x})$, we use the reparameterization $\mathbf{z} = f_{\boldsymbol{\phi}}(\mathbf{x}, \epsilon) = \boldsymbol{\mu} + \boldsymbol{\sigma} \cdot \boldsymbol{\epsilon}$ where $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$

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

Feature extraction

Dimensionality reduction, useful features

Pre-processing pour d'autres algos (regress, classif, clustering)

Unsupervised pretraining for supervised learning

Unsupervised pretraining -> supervised finetuning

[3]

Visualization

Data compression

Dimensionality reduction Data-specific, lossy compression.

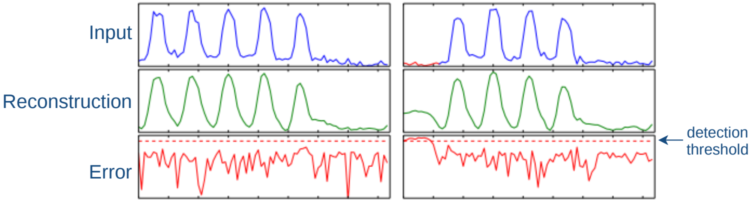
Data augmentation

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 is different 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 [?].



(Malhotra et al, 2016)

S. Becker.
Unsupervised Learning Procedures for Neural Networks.
The International Journal of Neural Systems, 1:17–33, 1991.

T. Devries and G. W. Taylor.
Dataset Augmentation in Feature Space.
In *ICLR 2017 Workshop*, pages 1–12, 2017.

D. Erhan, A. Courville, and P. Vincent.
Why Does Unsupervised Pre-training Help Deep Learning ?
Journal of Machine Learning Research, 11:625–660, 2010.

G. E. Hinton and R. Salakhutdinov.
Reducing the Dimensionality of Data with Neural Networks.
Science, 313(July):504–507, 2006.

D. P. Kingma and M. Welling.
Stochastic Gradient VB and the Variational Auto-Encoder.
2nd International Conference on Learning Representations (ICLR), pages 1–14, 2014.

E. Oja.
A Simplified Neuron Model as a Principal Component Analyzer.
Journal of Mathematical Biology, 15(3):267–273, 1982.

E. Oja.
Principal Components, Minor Components, and Linear Neural Networks, 1992.

E. Plaut.
From Principal Subspaces to Principal Components with Linear Autoencoders.
pages 1–6, 2018.

P. Vincent, H. Larochelle, I. Lajoie, Y. Bengio, and P.-A. Manzagol.
Stacked Denoising Autoencoders: Learning Useful Representations in a Deep Network with a Local Denoising Criterion.
Journal of Machine Learning Research, 11:3371–3408, 2010.