OUTLINE

- I. Introduction
- II. Background
- III. Fitting a Model
- IV. Supervised Learning
- V. Unsupervised Learning

VI. Convolutional Neural Networks





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OUTLINE

- **Introduction**
- II. Background
- III. Fitting a Model
- IV. Supervised Learning

V. Unsupervised Learning

- •
- Overview Clustering Dimensionality Reduction

VI. Convolutional Neural Networks





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► Overview

Supervised Learning



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Artificial Intelligence & Deep Learning

► Overview



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Unsupervised Learning

Artificial Intelligence & Deep Learning



Unsupervised Learning



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Applications of Unsupervised Learning



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Applications of Unsupervised Learning



« If machine learning is a cake, then unsupervised learning is the actual cake, supervised learning is the icing, and reinforcement learning is the cherry on the top. »

-Yann Lecun (Facebook AI) at NIPS 2016



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Applications of Unsupervised Learning



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-Yann Lecun (Facebook AI) at NIPS 2016



Potential to learn from massive amount of unlabeled data to generate even more

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efficiently learn from it



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- Desirable properties
 Can be used to reconstruct it / generalize it / efficiently learn from it
- A unifying view : Generative models



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- Desirable properties
 Can be used to reconstruct it / generalize it / efficiently learn from it
- A unifying view : Generative models

Find $\begin{cases} p_{\theta}(\boldsymbol{z}) \text{ (as simple as possible)} \\ p_{\theta}(\boldsymbol{x}|\boldsymbol{z}) \text{ (typically, transformation of } \boldsymbol{z}) \end{cases} \text{ so that } p_{\theta}(\boldsymbol{x}) = \int_{\boldsymbol{z}} p_{\theta}(\boldsymbol{x}|\boldsymbol{z}) p_{\theta}(\boldsymbol{z}) d\boldsymbol{z} \end{cases}$

fits the data (e.g., maximum likelihood).

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Desirable properties

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Preserve information from original data

Can be used to reconstruct it / generalize it / efficiently learn from it

• A unifying view : Generative models

Find $\begin{cases} p_{\theta}(\boldsymbol{z}) \text{ (as simple as possible)} \\ p_{\theta}(\boldsymbol{x}|\boldsymbol{z}) \text{ (typically, transformation of } \boldsymbol{z}) \end{cases} \text{ so that } p_{\theta}(\boldsymbol{x}) = \int_{\boldsymbol{z}} p_{\theta}(\boldsymbol{x}|\boldsymbol{z}) p_{\theta}(\boldsymbol{z}) d\boldsymbol{z} \end{cases}$

fits the data (e.g., maximum likelihood).

Generation	$p_{ heta}(oldsymbol{z}) ightarrow oldsymbol{z} ightarrow oldsymbol{x}$
Compression	$oldsymbol{x} ightarrow p_{ heta}(oldsymbol{z} oldsymbol{x}) ightarrow oldsymbol{z}$
Reconstruction / Completion / Denoising	$egin{array}{l} ilde{oldsymbol{x}} o p_{ heta}(oldsymbol{z} ilde{oldsymbol{x}}) o oldsymbol{z} \ o p_{ heta}(oldsymbol{x} oldsymbol{z}) o \hat{oldsymbol{x}} \end{array}$



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Artificial Intelligence & Deep Learning



1. Pick K = 4 points at random

• The centroids $\{c_k\}_{k=1}^K \subset \mathbb{R}^2$

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1. Pick K = 4 points at random

• The centroids $\{c_k\}_{k=1}^K \subset \mathbb{R}^2$

2. For each point x_n , find its nearest centroid c_k . Place n in cluster \mathcal{G}_k .

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2. For each point x_n , find its nearest centroid c_k . Place n in cluster \mathcal{G}_k .

3. Update each c_k as the mean of all points in \mathcal{G}_k :

$$lacksim egin{aligned} lacksim egin{aligned} lacksim egin{aligned} & lacksim egin{align$$

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1. Pick K = 4 points at random • The *centroids* $\{c_k\}_{k=1}^K \subset \mathbb{R}^2$ **2.** For each point x_n , find its nearest centroid c_k . Place $n \not$

3. Update each c_k as the mean of all points in \mathcal{G}_k : • $c_k = \frac{1}{|\mathcal{G}_k|} \sum_{n \in \mathcal{G}_k} x_n$

in cluster \mathcal{G}_k .

4. Repeat **2.** and **3.** until convergence

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The K-means Algorithm

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 \mathcal{L}

• It decreases this **total loss** at each iteration:

$$\mathcal{C}(\mathbf{X},\mathcal{G}, heta) = \sum_{k=1}^{K} \sum_{n \in \mathcal{G}_k} \|oldsymbol{x}_n - oldsymbol{c}_k\|^2, \quad heta = \{oldsymbol{c}_1,\ldots,oldsymbol{c}_K\}$$





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Non-Convex
 (Depends on init.)

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- « Compression » interpretation: ${f X}$ is « summarized » by heta



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- Probabilistic / Generative interpretation (where is z)?





 \mathcal{K}

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$$\begin{cases} p(z_{n,k} = 1) = \frac{1}{K} & \text{where } \boldsymbol{z}_n = \begin{bmatrix} 0 \\ 0 \\ k \end{bmatrix} \in \{0,1\}^K \\ k \to 1 \\ p_{\theta}(\boldsymbol{x}_n | \boldsymbol{z}_n \equiv k) = \mathcal{N}(\boldsymbol{x}_n; \boldsymbol{c}_k, \mathbf{I}) & \text{(Gaussian centered on } \boldsymbol{c}_k) \end{cases}$$



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Artificial Intelligence & Deep Learning
K-means: What does it do?

 \mathcal{L}

• It decreases this **total loss** at each iteration:

$$C(\mathbf{X}, \mathcal{G}, \theta) = \sum_{k=1}^{K} \sum_{n \in \mathcal{G}_{k}} \| \boldsymbol{x}_{n} - \boldsymbol{c}_{k} \|^{2}, \quad \theta = \{ \boldsymbol{c}_{1}, \dots, \boldsymbol{c}_{K} \} \quad \stackrel{\bullet}{\to} \begin{array}{l} \text{Non-Convex} \\ \text{(Depends on init.)} \end{array}$$

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K-means: What does it do?

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K-means can be seen as a maximum a posteriori (MAP) approach!

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V. Unsupervised Learning Clustering

Gaussian mixture models: a generalization

$$\begin{cases} p(z_{n,k} = 1) = \pi_k, \quad \sum_{k=1}^{K} \pi_k = 1 \\ p_{\theta}(\boldsymbol{x}_n | \boldsymbol{z}_n \equiv k) = \mathcal{N}(\boldsymbol{x}; \boldsymbol{c}_k, \Sigma_k) \\ \Rightarrow p_{\theta}(\boldsymbol{x}_n) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\boldsymbol{x}_n; \boldsymbol{c}_k, \Sigma_k) \end{cases}$$

$$egin{aligned} heta &= \{\pi_1, \dots, \pi_K, \ oldsymbol{c}_1, \dots, oldsymbol{c}_K, \ \Sigma_1, \dots, \Sigma_K \end{aligned}$$

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• Find θ that maximizes the observed data log-likelihood:

$$\mathcal{L}_{\theta}(\mathbf{X}) = \log p_{\theta}(\mathbf{X}) = \sum_{n} \log p_{\theta}(\boldsymbol{x}_{n})$$

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...very hard to solve directly.

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• The Expectation-Maximization (EM) algorithm iteratively maximizes the *expected complete-data log-likelihood* instead:

$$\theta^{(i+1)} = \underset{\theta}{\operatorname{argmax}} \ \mathbb{E}_{p_{\theta}(i)(Z|X)}\{\log p_{\theta}(\mathbf{X}, \mathbf{Z})\}$$

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 $\left\{ \begin{array}{l} \textbf{Repeat until convergence:} \\ \bullet \ r_{n,k}^{(i)} = p_{\theta^{(i-1)}}(z_{n,k} = 1 | \boldsymbol{x}_n) \\ \bullet \ \pi_k^{(i)} = \frac{1}{N} \sum_n r_{n,k}^{(i)} = \frac{\overline{r}_k}{N} \\ \bullet \ \boldsymbol{c}_k^{(i)} = \frac{1}{\overline{r}_k} \sum_n r_{n,k}^{(i)} \boldsymbol{x}_n \\ \bullet \ \Sigma_k^{(i)} = \frac{1}{\overline{r}_k} \sum_n r_{n,k}^{(i)}(\boldsymbol{x}_n - \boldsymbol{c}_k^{(i)}) \\ & \cdot (\boldsymbol{x}_n - \boldsymbol{c}_k^{(i)})^\top \end{array} \right.$



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And in the Deep Learning Era ...

 Deep clustering: trains a DNN to project data to a feature space where K-means can be optimally used

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V. Unsupervised Learning Clustering

And in the Deep Learning Era ...

- Deep clustering: trains a DNN to project data to a feature space where K-means can be optimally used
- Application to blind speech source separation:

John R. Hershey, Zhuo Chen, Jonathan Le Roux, and Shinji Watanabe. "Deep clustering: Discriminative embeddings for segmentation and separation." In 2016 IEEE International Conference on Acoustics, Speech and Signal Processing (ICASSP), pp. 31-35. IEEE, 2016.



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V. Unsupervised Learning Clustering

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• Application to feature learning from images:

Mathilde Caron, Piotr Bojanowski, Armand Joulin, and Matthijs Douze. **"Deep clustering for unsupervised learning of visual features."** In *Proceedings of the European Conference on Computer Vision (ECCV)*, pp. 132-149. 2018.





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Typical applications of clustering



Image segmentation ($\{x_n\}_{n=1}^N$ are local descriptors)



Audio segmentation ($\{x_n\}_{n=1}^N$ are sound segment)

Anti-spam filters

Data Quantification

DNA sequence analysis

Medical imaging

Speech diarization

Social network analysis

Ínría



Species classificaton (biology)

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Dimensionality Reduction



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Artificial Intelligence & Deep Learning



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Artificial Intelligence & Deep Learning





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Artificial Intelligence & Deep Learning



1. Find $v_1 \in \mathbb{R}^3$ such that $\operatorname{Var}(\mathbf{X}v_1) = \operatorname{Var}([v_1^\top x_1, \dots, v_1^\top x_n]^\top) = \frac{1}{N} \sum_{n=1}^N |v_1^\top x_n|^2$ is largest



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Artificial Intelligence & Deep Learning

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- **3.** Find $v_3 \perp [v_1, v_2] \dots$ etc.

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 \blacktriangleright The Principal Axes of ${\bf X}$ are the P dominant eigenvectors of ${\bf C}$.



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• The **Principal Axes** of \mathbf{X} are the P dominant eigenvectors of \mathbf{C} .

Principal Component Anaysis

• Probabilistic / Generative interpretation:

$$\begin{cases} p_{\theta}(\boldsymbol{z}_n) = \mathcal{N}(\boldsymbol{z}_n; \boldsymbol{0}_P, \boldsymbol{\Lambda} - \sigma^2 \mathbf{I}_P), & \boldsymbol{\Lambda} = \operatorname{diag}(\lambda_1, \dots, \lambda_P), & \sigma^2 \leq \lambda_P \\ p_{\theta}(\boldsymbol{x}_n | \boldsymbol{z}_n) = \mathcal{N}(\boldsymbol{x}_n; \mathbf{V} \boldsymbol{z}_n + \boldsymbol{\mu}, \sigma^2 \mathbf{I}_D), & \mathbf{V} = [\boldsymbol{v}_1, \dots, \boldsymbol{v}_P] \in \mathbb{R}^{D \times P}, \\ \theta = \{\boldsymbol{\Lambda}, \sigma^2, \mathbf{V}\} \end{cases}$$



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PCA is equivalent to:

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- $\hat{m{z}}_n = \operatorname*{argmax}_{m{z}_n} p_{\hat{m{ heta}}}(m{z}_n | m{x}_n)$ (Maximum a posteriori)

M.E. Tipping and C.M. Bishop. **"Probabilistic PCA."** *Journal of the Royal Statistical Society: Series B*, 61, no. 3 (1999): 611-622.

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Variational Autoencoders

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Variational Autoencoders

• Generalize PCA by replacing this by a DNN (the decoder)

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- Generalize PCA by replacing this by a **DNN** (the *decoder*)
- Optimized using a variational approximation of $p_{\theta}(\boldsymbol{z}|\boldsymbol{x})$ by another neural network (the *encoder*)

Diederik P. Kingma and Max Welling. "Auto-encoding variational bayes.", ICLR 2014.

• A neural network trained to predict its input: a pretext task

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- A neural network trained to predict its input: a pretext task
- Consists of two parts:
 - An encoder function $\boldsymbol{h} = \operatorname{enc}(\boldsymbol{x})$
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The task is non-trivial if the encoder is dimensionality-reducing



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 h is called an *embedding* of x, i.e., a nonlinear representation of the input.





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The encoder and decoder parameters can be *tied* together

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Local Tangent Space Alignment (LTSA)



Zhang, Zhenyue, and Hongyuan Zha. "Principal manifolds and nonlinear dimensionality reduction via tangent space alignment." *SIAM journal on scientific computing* 26, no. 1 (2004): 313-338.



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Local Tangent Space Alignment (LTSA)



1. Builds local k-nearest neighborhoods on the data

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- **1.** Builds local k-nearest neighborhoods on the data
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• Graph-Based Methods: Isomap, LLE, Laplacian Eigenmap, ...

Ghodsi, Ali. "Dimensionality reduction a short tutorial." Department of Statistics and Actuarial Science, Univ. of Waterloo, Ontario, Canada 37, no. 38 (2006): 2006.

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- Graph-Based Methods: Isomap, LLE, Laplacian Eigenmap, ...
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 Stochastic neighbor embedding (SNE): match neighborhood probabilities in the high- and low-dim. spaces

Hinton, Geoffrey E., and Sam Roweis. "Stochastic neighbor embedding." Advances in neural information processing systems 15 (2002).

Ghodsi, Ali. "Dimensionality reduction a short tutorial." Department of Statistics and Actuarial Science, Univ. of Waterloo, Ontario, Canada 37, no. 38 (2006): 2006.

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 Ex: t-SNE: uses a Gaussian model for similarity between data points and a Student's t (Cauchy) model for similarity in the latent space (2D or 3D)





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- The variances of the Gaussians are fixed to attain a given *entropy* value.
- The latent representation is found by minimizing the *Kullback-Leibler* divergence wrt. these distributions using gradient descent.
- Easy to use thanks to the Scikit Learn implementation

sklearn.manifold.TSNE

class sklearn.manifold.TSNE(n_components=2, *, perplexity=30.0, early_exaggeration=12.0, learning_rate='auto', n_iter=1000, n_iter_without_progress=300, min_grad_norm=1e-07, metric='euclidean', metric_params=None, init='pca', verbose=0, random_state=None, method='barnes_hut', angle=0.5, n_jobs=None, square_distances='deprecated') [source]

Documentation:

https://scikit-learn.org/stable/modules/generated/sklearn.manifold.TSNE.html

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Manifold Learning

Examples of t-SNE visualizations

MNIST dataset



Examples of t-SNE visualizations

Speech recognition (Wall Street Journal Dataset)



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Diederik P. Kingma and Max Welling. "Auto-encoding variational bayes.", arXiv:1312.6114 (2013).

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Typical applications:

Dataset Visualization



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Data generation (Glow)



Pre-processing to speed up learning

Compression

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+ extensions (Normalizing Flows, Glow...)

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