Course 3: Unsupervised Learning

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Bretagne-Pays de la Loire
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Summary

Last session

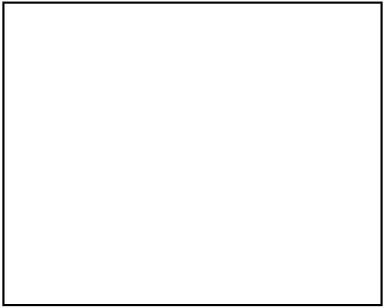
1. Supervised learning - learning from labeled examples
2. Bias/variance tradeoff
3. Overfitting
4. Curse of dimensionality
5. Computational requirements

Today's session

1. Learning from Unlabeled examples
2. Clustering
3. Decomposition
4. Manifold learning
5. Feature Selection and preprocessing

Notations

Vector space ($\mathbb{R}^d$)



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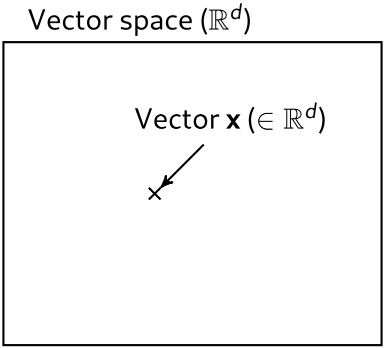

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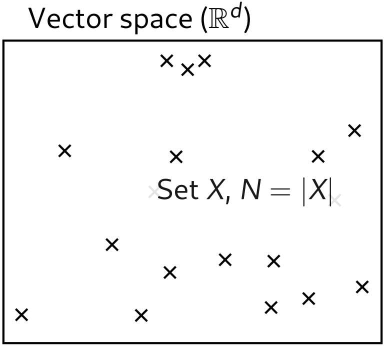
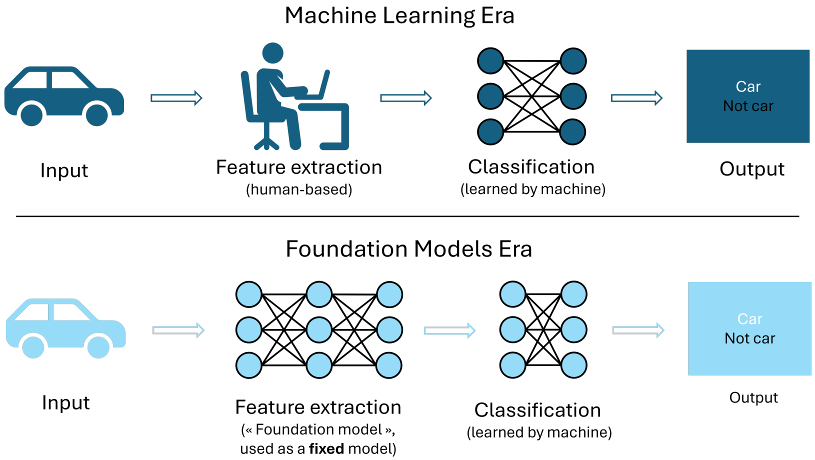


What is the vector x? (1/2)



(Similar to last session)

Unsupervised learning

Goal

Discover patterns/structure in X,

Unsupervised learning

- Unsupervised = no expert, no labels
- Main approaches:
  - Clustering = find a partition of X in K subsets,
  - Decomposition using K vectors.
  - Manifold Learning.
- Applications :
  - Dimensionality reduction, Quantization
  - Visualization...

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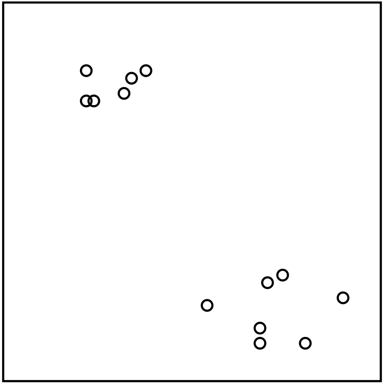

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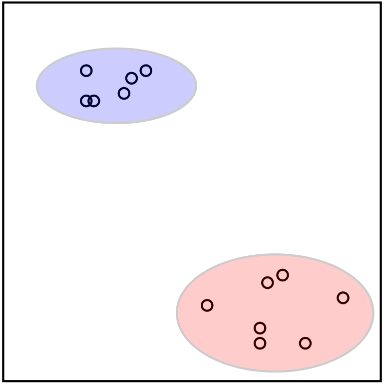

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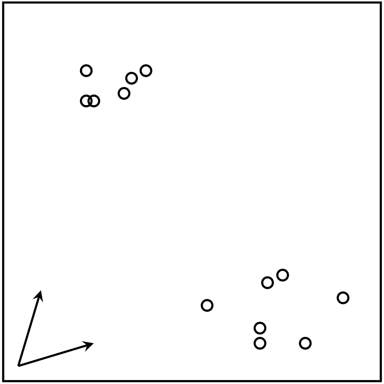

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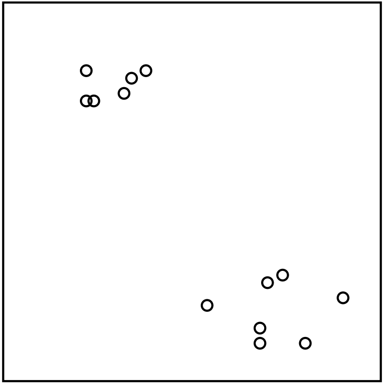

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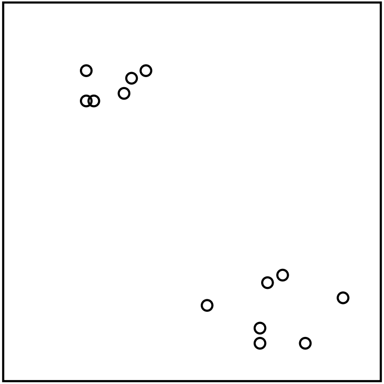
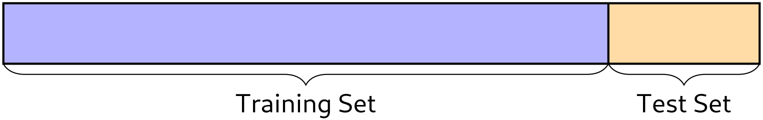


Training and Test sets?

Full Dataset in train/test sets (as for supervised):



...Or actually:

The same training and test sets??

Because unsupervised learning does not rely on external annotations, the “training” and “test” settings are not relevant **(there is no “correct answer” to learn and generalize!)**.

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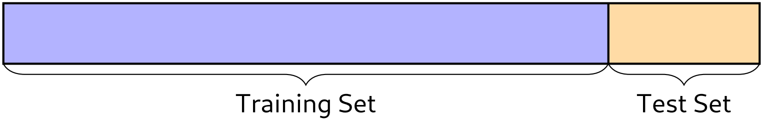


...Or actually:

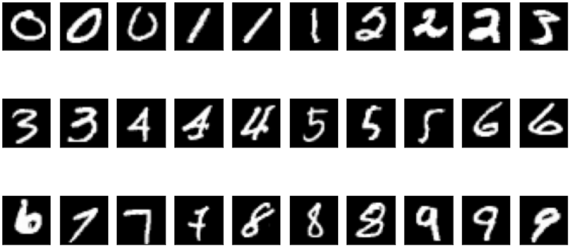
The same training and test sets??

Because unsupervised learning does not rely on external annotations, the “training” and “test” settings are not relevant **(there is no “correct answer” to learn and generalize!)**.

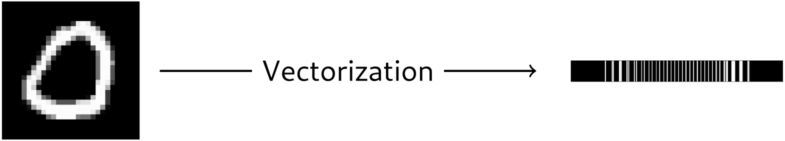
A classical dataset: MNIST dataset (1/2)

MNIST Dataset

- "Toy" dataset (=small and easy)
- 60000 + 10000 handwritten digits

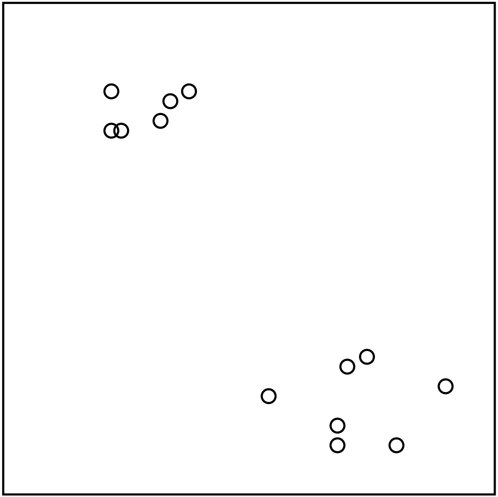


A classical dataset: MNIST dataset (2/2)



Hence, all images are interpreted as 1D vectors!

Example: clustering using L_2 norm (1/8)



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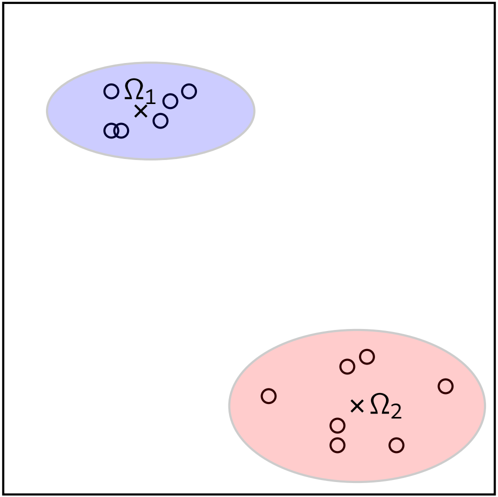


Example: clustering using L_2 norm (2/8)

An example to perform clustering is to rely on distances to centroids.
We define K *cluster centroids* $\Omega_k, \forall k \in [1..K]$.
Here, each vector is associated with the cluster whose centroid is of minimal distance.

Definitions

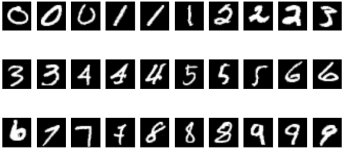
We denote $q : \mathbb{R}^d \rightarrow [1..K]$ a function that associates a vector $\mathbf{x}$ with the index of (one of) its closest centroid $\Omega_{q(\mathbf{x})}$. Formally:

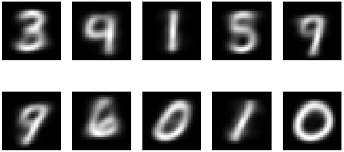
- $\forall k \in [1..K], \Omega_k \in \mathbb{R}^d$
- $\forall \mathbf{x} \in X, \forall j \in [1..K], \|\mathbf{x} - \Omega_{q(\mathbf{x})}\|_2 \leq \|\mathbf{x} - \Omega_j\|_2$
- Error $E(q) \triangleq \sum_{\mathbf{x} \in X} \|\mathbf{x} - \Omega_{q(\mathbf{x})}\|_2$
- $X = \bigcup_k \underbrace{\{\mathbf{x} \in X, q(\mathbf{x}) = k\}}_{\text{cluster } k}$

Clustering using L_2 norm (3/8)

Clustering MNIST

Using K-means algorithm with $K = 10$





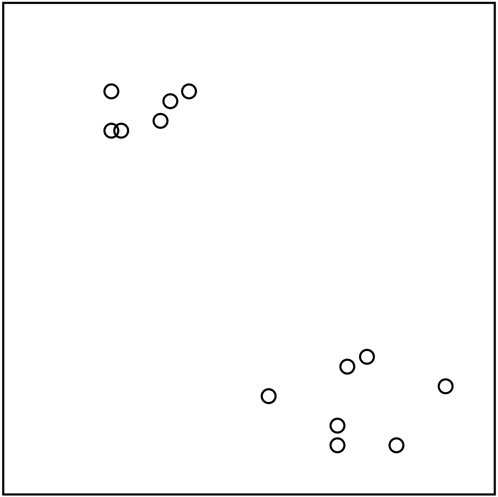
Note: we recall that images are vectorized for the clustering to make sense!
They are only displayed in 2D to be interpretable.

Clustering using L_2 norm (4/8)

Quantizing MNIST

- Replace $\mathbf{x}$ by $\Omega_{k(\mathbf{x})}$
- Compression factor $\kappa = 1 - K/N$

Clustering using L_2 norm (5/8): Choosing K



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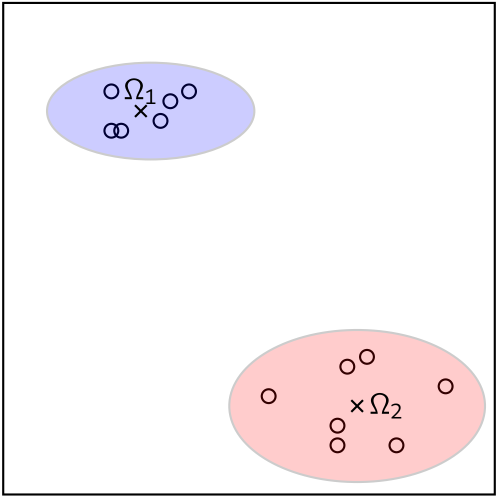
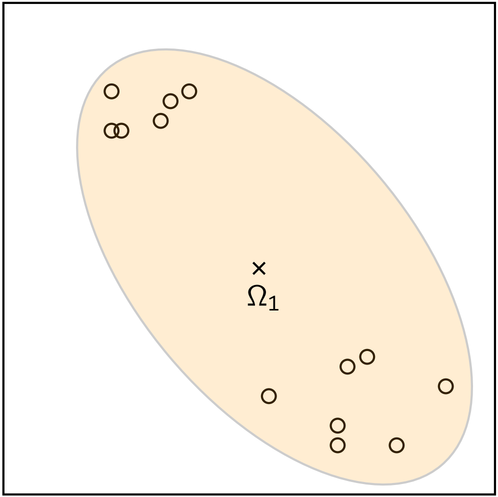


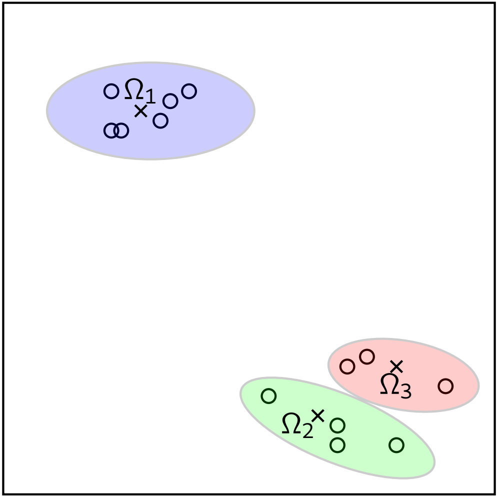
$K = 2$

Clustering using L_2 norm (5/8): Choosing K



$K = 1$

Clustering using L_2 norm (5/8): Choosing K



$K = 3$

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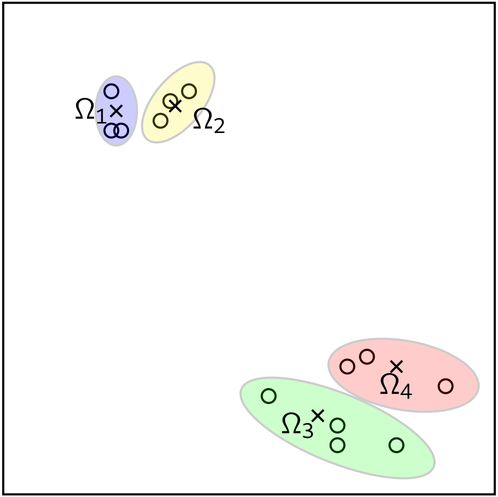
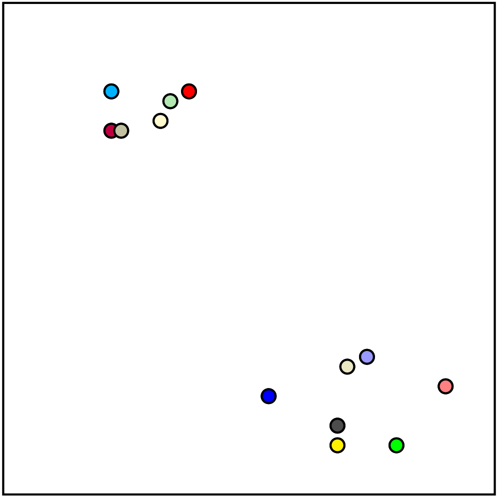


$K = 4$

Clustering using L_2 norm (5/8): Choosing K



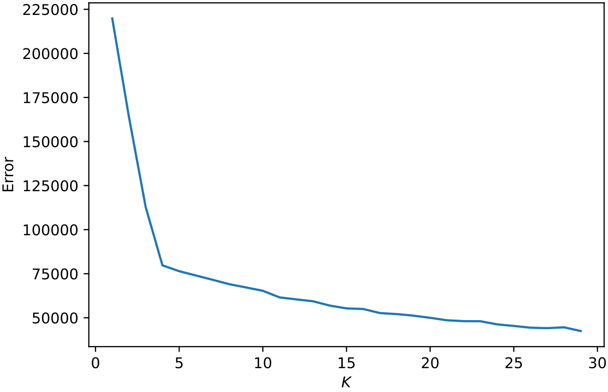
$K = N$

(each data point is its own centroid)

Clustering using L_2 norm (6/8)

Choosing K

- Finding a compromise between error and compression,
- Simple practical method : "elbow".



Clustering using L_2 norm (7/8)

Optimal clustering

- Define $E_{opt_K}(q^*) \triangleq \arg \min_{q:\mathbb{R}^d \to [1..K]} E(q)$,
- Finding an optimal clustering is an NP-hard problem.

Properties

- $0 = E_{opt_N}(q^*) \leq E_{opt_{N-1}}(q^*) \leq \cdots \leq E_{opt_1}(q^*) = var(X)$,
  - Proof: monotonicity by particularization, extremes with identity function (left) and variance (right).
- $0 \leq K \leq \frac{N-1}{N}$.

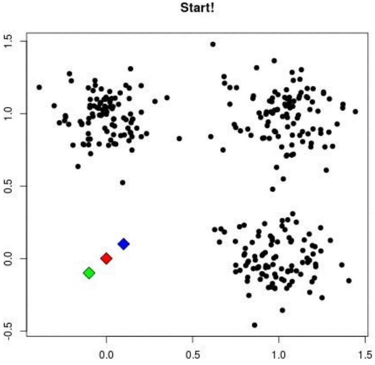
Changing the number of centroids changes the clustering... And the signification of clusters.

Clustering using L_2 norm (8/8)

K-means algorithm

First: initialize K cluster centroids.

1. Assign each data point to the cluster of closest centroid.
2. Compute the new centroids as the average of the data points in each cluster.
3. Repeat .



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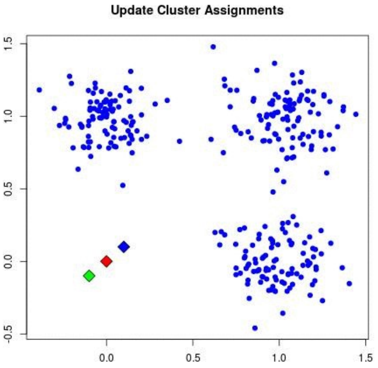

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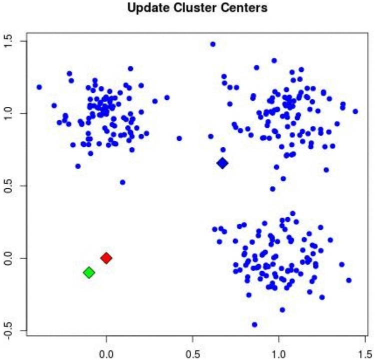

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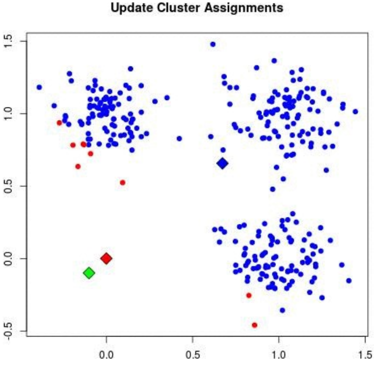

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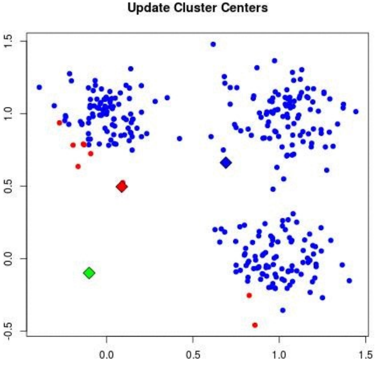

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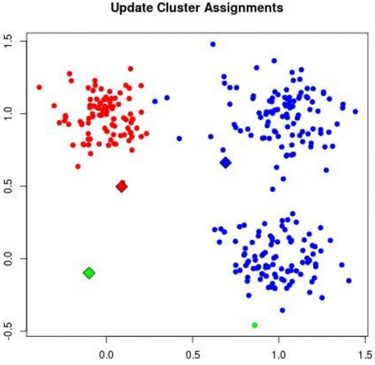

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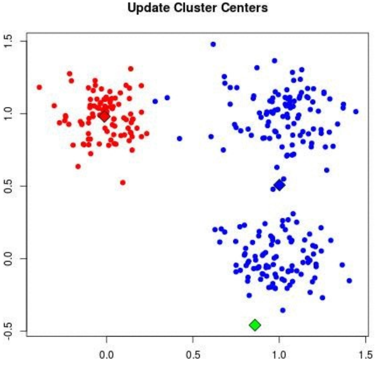

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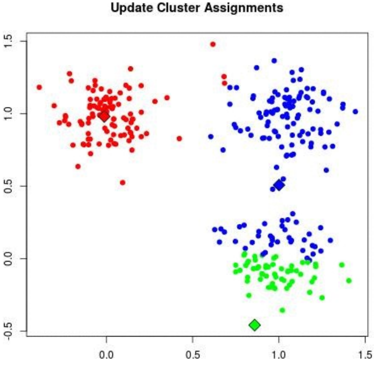

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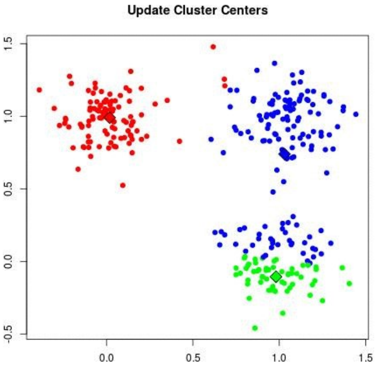

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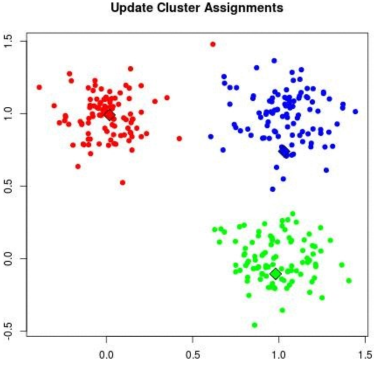

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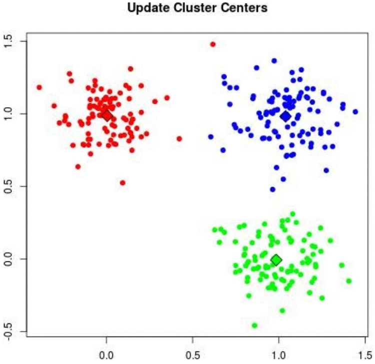

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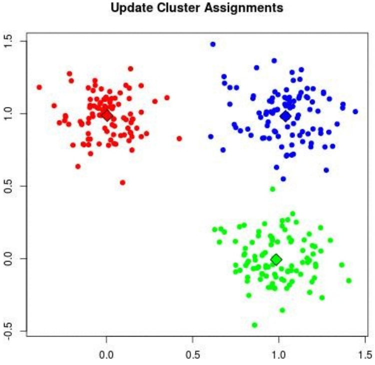

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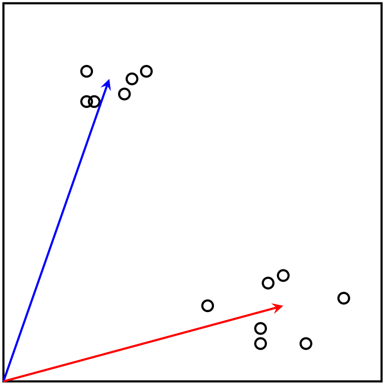
Decomposition



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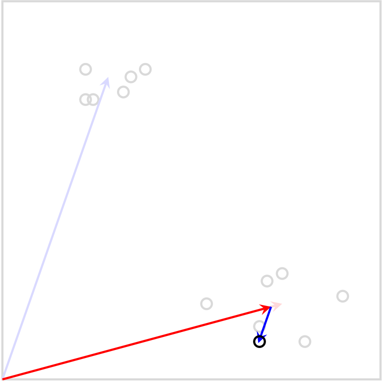
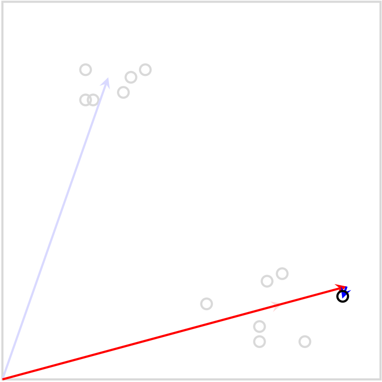


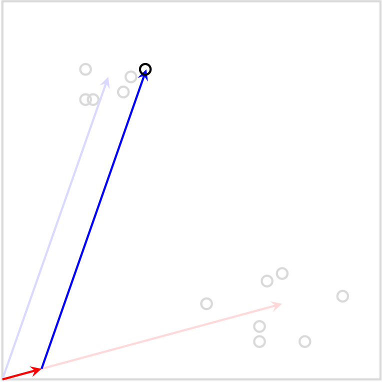
x = 0.96 × 
+ -0.12 × 

Decomposition



x = 1.23 × 
+ -0.04 × 

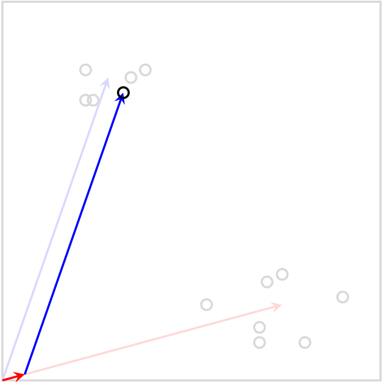
Decomposition



$x = \color{red}{0.14} \times$ 

$+ \color{blue}{0.99} \times$ 

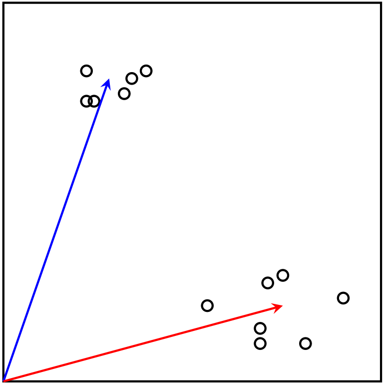
Decomposition



$x = 0.08 \times \longrightarrow$

$+ 0.93 \times \longrightarrow$

Decomposition



$\approx$

U

"weights"

$$\begin{bmatrix} 0.96 & -0.12 \\ 1.23 & -0.04 \\ \multicolumn{2}{c}{\cdots} \\ 0.14 & 0.99 \\ 0.08 & 0.93 \\ \multicolumn{2}{c}{\cdots} \end{bmatrix}$$

V

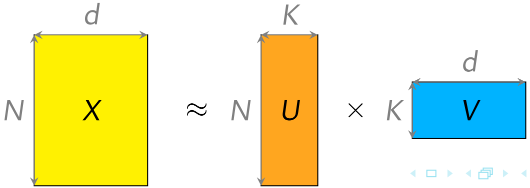
"Components"

Principal Components Analysis

Definitions

Principal components analysis solves the following matrix factorization problem:

- The set X is considered as a matrix $X \in \mathcal{M}_{N\times d}(\mathbb{R})$,
- We consider decompositions using components $V \in \mathcal{M}_{K\times d}(\mathbb{R})$ and weights $U \in \mathcal{M}_{N\times k}(\mathbb{R})$,
- PCA estimates K components that are orthogonal and ordered by importance (variance explained)
- It is based on the Singular Value Decomposition (SVD) of the covariance matrix $XX^\top$



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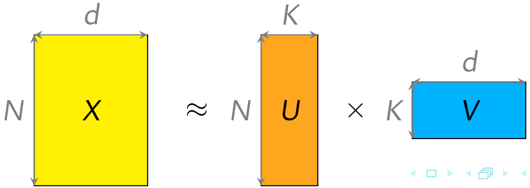

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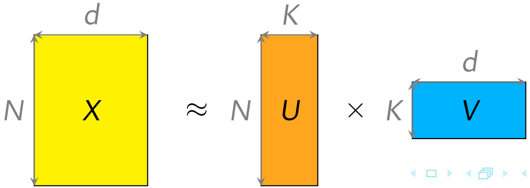
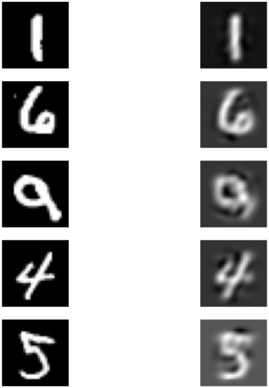
- PCA estimates K components that are orthogonal and ordered by importance (variance explained)
- It is based on the Singular Value Decomposition (SVD) of the covariance matrix $XX^\top$



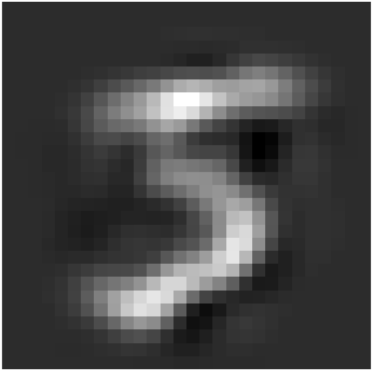
Example of reconstructions on MNIST with $K = 32$



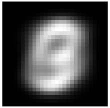
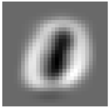
Recall that each image is vectorized, hence each of these images correspond to a row in V.

Principal Components Analysis

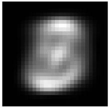
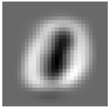
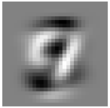
Detailed example of a reconstruction



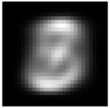
Principal Components Analysis

 $= 122.3\times$ 

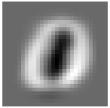
Principal Components Analysis

 $= 122.3\times$  $-316.2\times$ 

Principal Components Analysis



$= 122.3\times$



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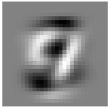
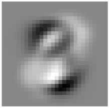


$-51.13\times$



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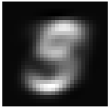
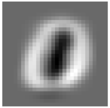
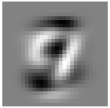
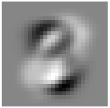
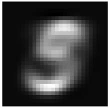
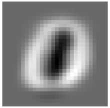
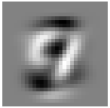
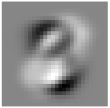
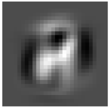
 $= 122.3\times$  $-316.2\times$ 

$-51.13\times$  $-556.9\times$ 

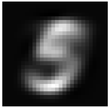
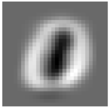
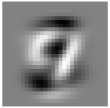
Principal Components Analysis

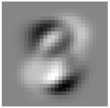
 $= 122.3\times$  $-316.2\times$ 

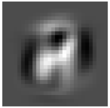
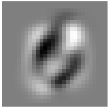
$-51.13\times$  $-556.9\times$ 

$-49.2\times$ 

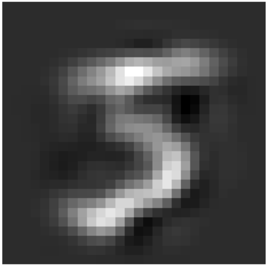
Principal Components Analysis

 $= 122.3\times$  $-316.2\times$ 

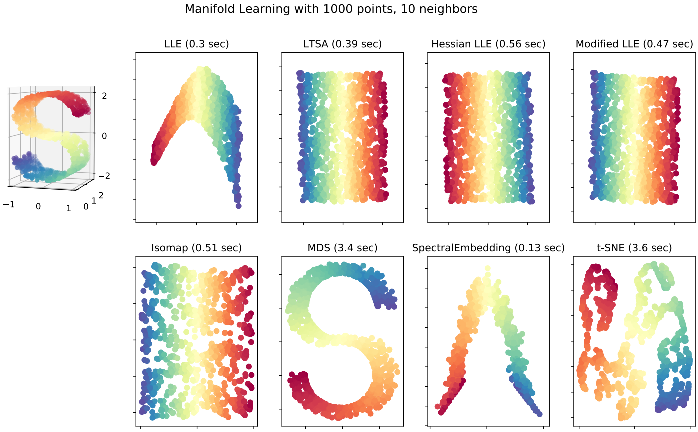
$-51.13\times$  $-556.9\times$ 

$-49.2\times$  $-217.1\times$  $\cdots$

Reconstruction with all 32 components:



Example 3: Manifold Learning



Approaches to uncover lower dimensional structure of high dimensional data. Source : Manifold module, sklearn website

Working with features

N.b. : valid in unsupervised and supervised settings.

Feature preprocessing

Objective : change the statistical distribution of the features

- Scaling / Normalization
- Power transform
- Encode, discretization
- Manual feature engineering
- See more `https://scikit-learn.org/stable/modules/preprocessing.html`

Many techniques need or are greatly helped when features are on the unit sphere.

Working with features

N.b. : valid in unsupervised and supervised settings.

Feature selection

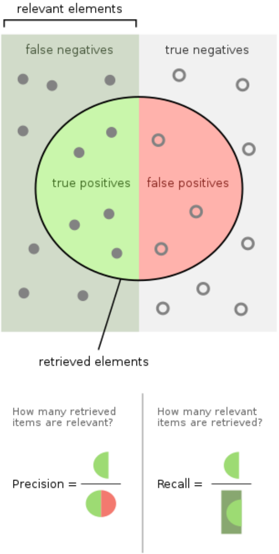
Objective : remove features

- Remove features with low variance
- Select features according to their explained variance towards labels (e.g. SelectKBest)
- See more `https://scikit-learn.org/stable/modules/feature_selection.html`

Helps to adress the dimensionality curse.

Metrics

In supervised learning : per class metric



Metrics

Clustering Metrics :

- Error defined slide 10 : similar to inertia (sum of squared distances)
- The Silhouette score (per sample) is $(b - a)/max(a, b)$, with mean intra-cluster distance (a) and the mean nearest-cluster distance (b).

Clustering metrics using labels :

- Random Index : measures the similarity of two assignments, ignoring permutations
- Homogeneity : each cluster contains only members of a single class.
- Completeness : all members of a given class are assigned to the same cluster.

See more on sklearn website and in the lab session

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Lab Session 3 and assignment (1/2)

Lab Unsupervised Learning

- Feature selection and preprocessing
- K-means clustering
- Principal Component Analysis (PCA)
- Tests on the modality chosen in Lab 1 (text, vision or audio).

Project 2 (P2)

You will choose one unsupervised learning method from the available options (see Lab 3). You will present

- A brief description of the theory behind the method,
- Basic tests on this technique for your modality.

During Session 4, even binome numbers will have 7 minutes to present.

Lab Session 3 and assignment (2/2)

List of Unsupervised Learning Methods

- Non-Negative Matrix Factorization
- DBSCAN
- Spectral Clustering
- Gaussian Mixture Models
- Agglomerative Clustering
- UMAP