Course 3: Unsupervised Learning

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Bretagne-Pays de la Loire
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Summary

Last session

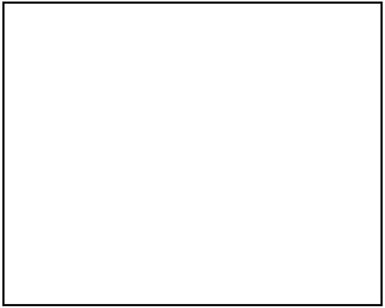
1. Supervised learning - learning from labeled examples
2. Bias/variance tradeoff
3. Overfitting and cross-validation
4. Curse of dimensionality
5. Computational requirements

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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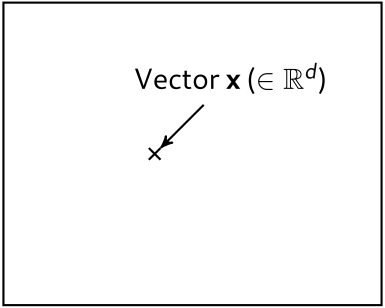

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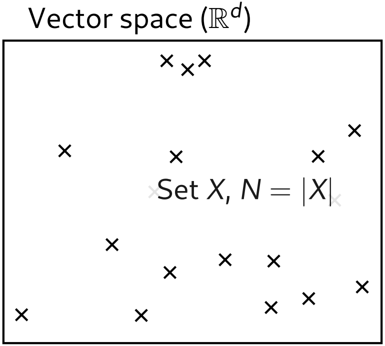

Unsupervised learning

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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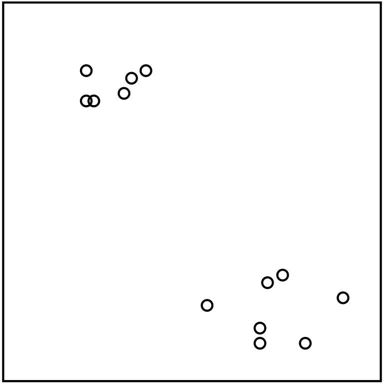

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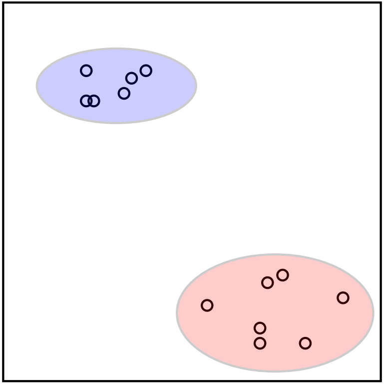

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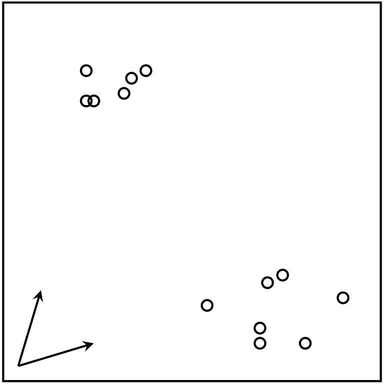

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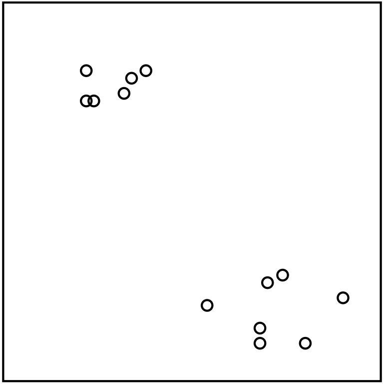

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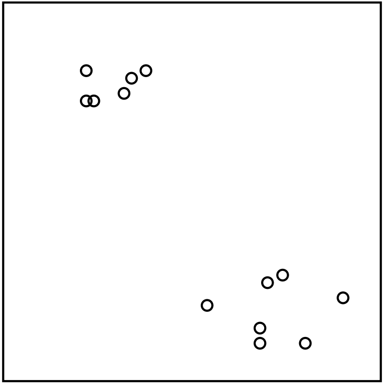
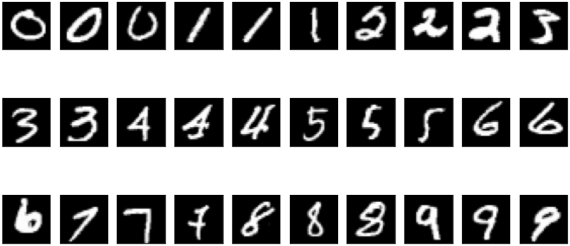
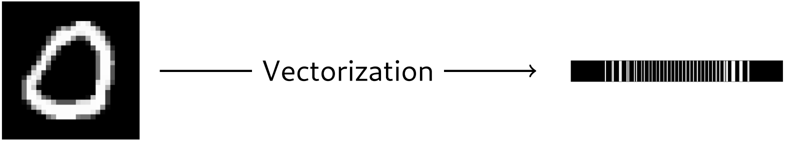


A classical dataset: MNIST dataset (1/2)

MNIST Dataset

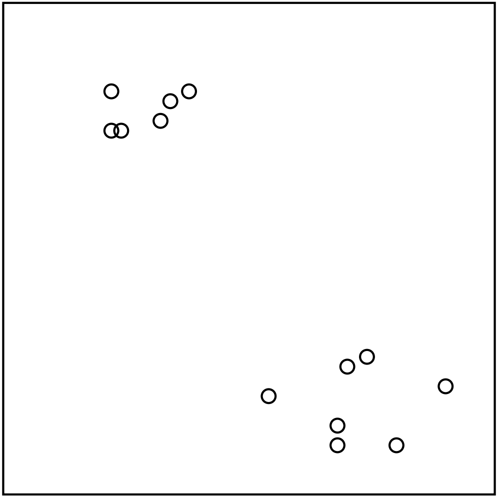
- "Toy" dataset (=small and easy)
- 60000 + 10000 handwritten digits





Hence, all images are interpreted as 1D vectors!

Example: clustering using L_2 norm (1/8)



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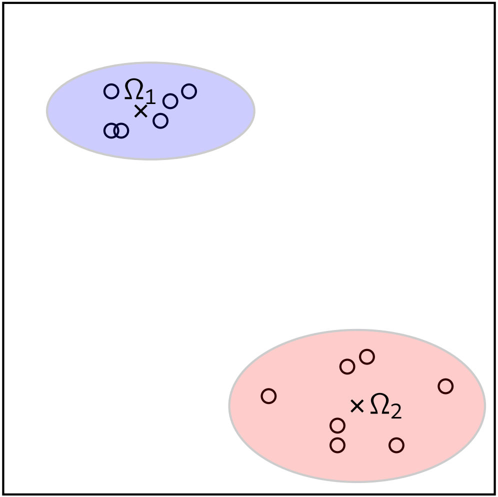


Example: clustering using L_2 norm (2/8)

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

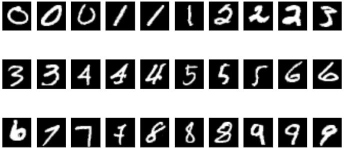
We denote $q : \mathbb{R}^d \to [1..K]$ a function that associates a vector $\mathbf{x}$ with the index of (one of) its closest centroid $q(\mathbf{x})$. Formally:

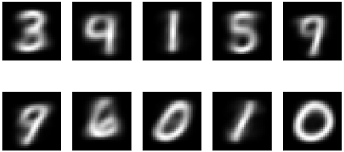
- $\forall k \in [1..K], \Omega_k \in \mathbb{R}^d$
- $\forall \mathbf{x} \in X, \forall j \in [1..K], \|\mathbf{x} - \Omega_{q(\mathbf{x})}\|_2 \leq \|\mathbf{x} - \Omega_j\|_2$
- Error $E(q) \triangleq \sum_{\mathbf{x} \in X} \|\mathbf{x} - \Omega_{q(\mathbf{x})}\|_2$
- $X = \bigcup_k \underbrace{\{\mathbf{x}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

Clustering using L_2 norm (3/8)

Clustering MNIST

Using K-means algorithm with $K = 10$





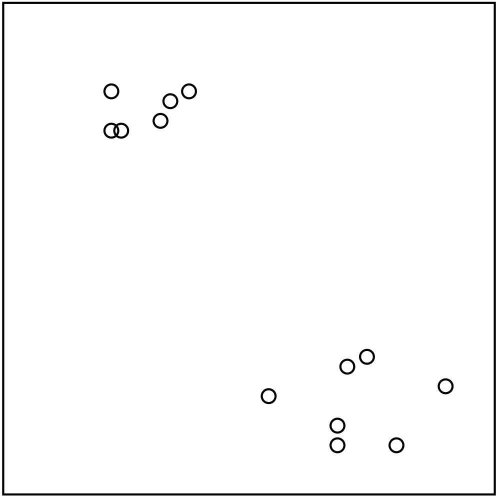
Note: we recall that images are vectorized for the clustering to make sense!
They are only displayed in 2D to be interpretable.

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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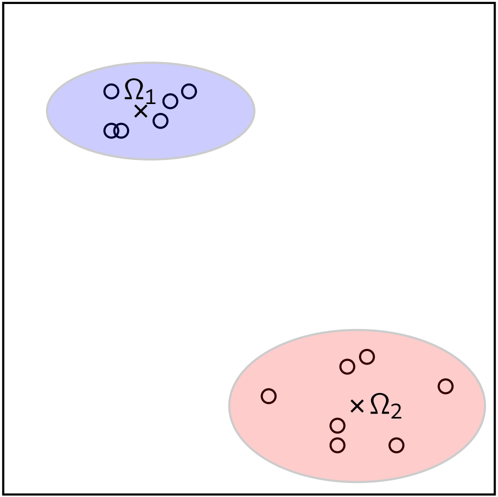
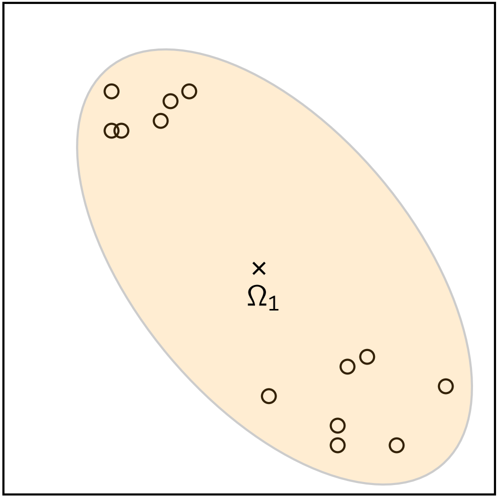


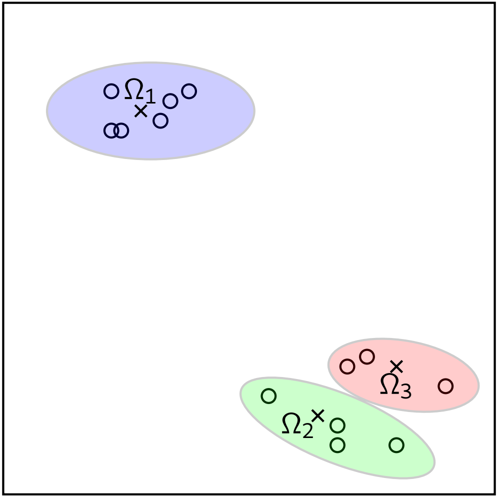
$K = 2$

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



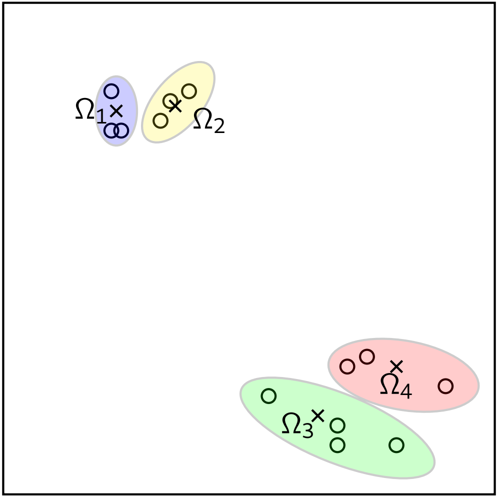
$$K = 1$$

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



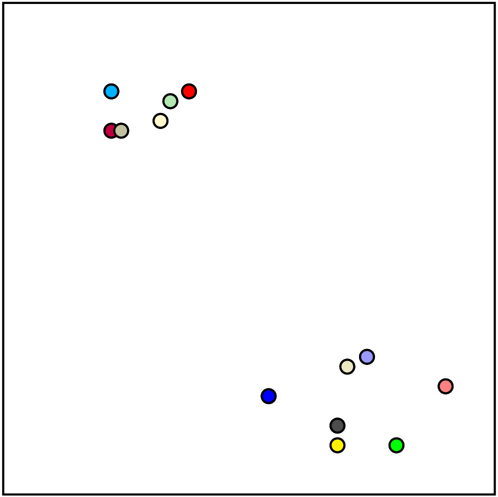
$K = 3$

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



$K = 4$

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



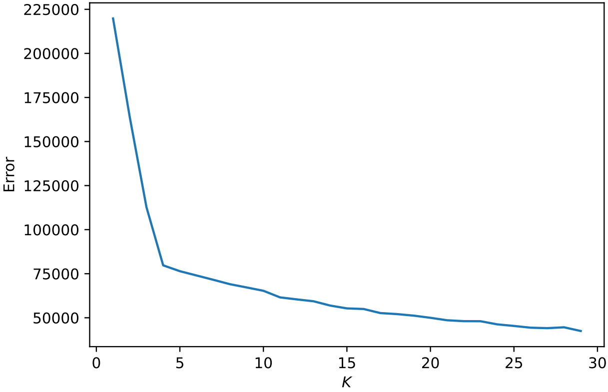
$K = N$

(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

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

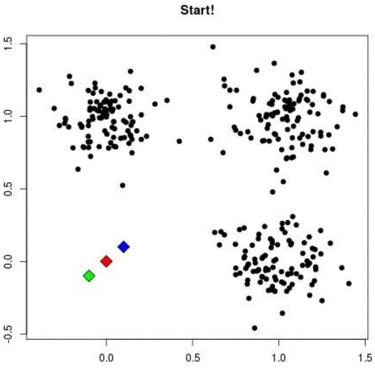
Changing the number of centroids changes the clustering... And the signification of clusters.

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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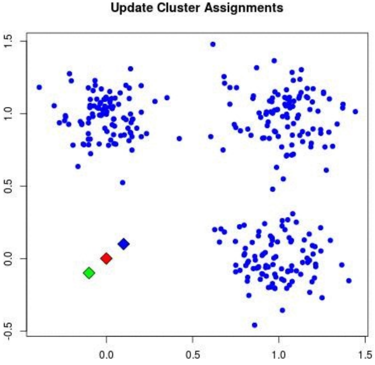

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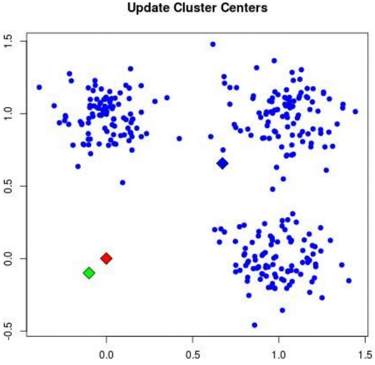

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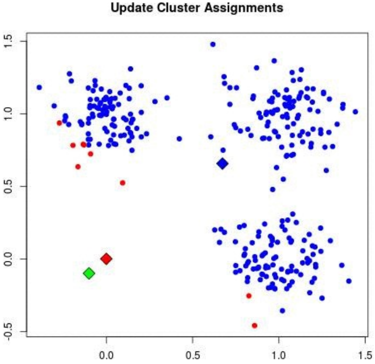

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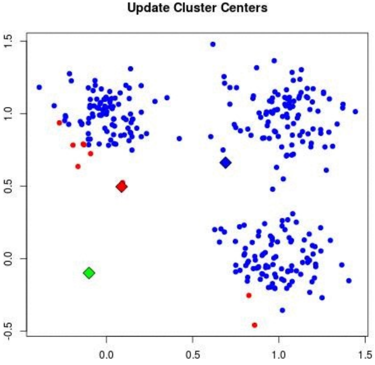

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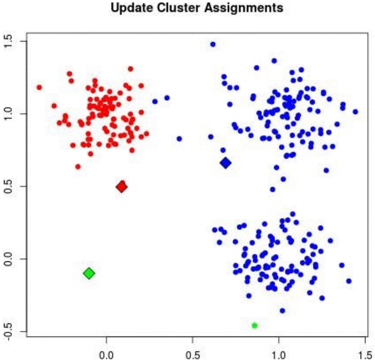

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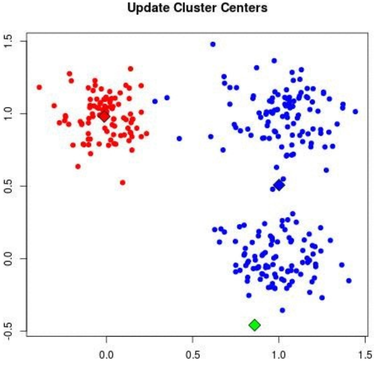

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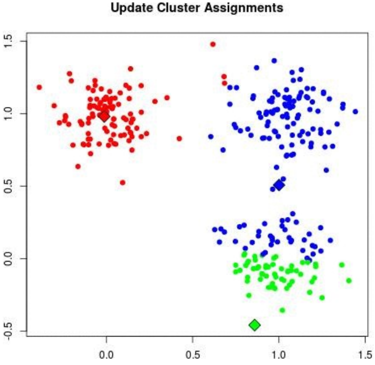

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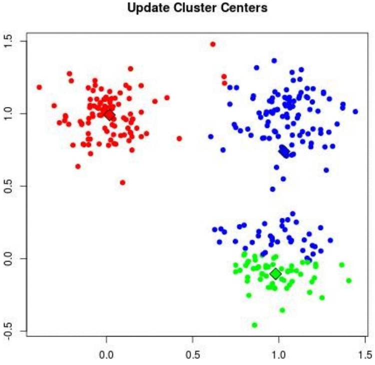

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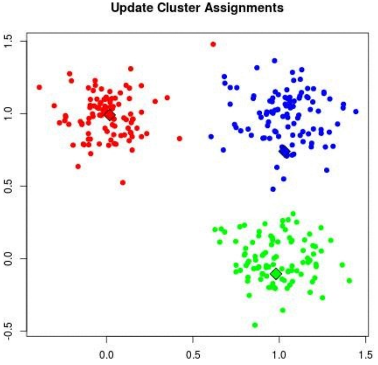

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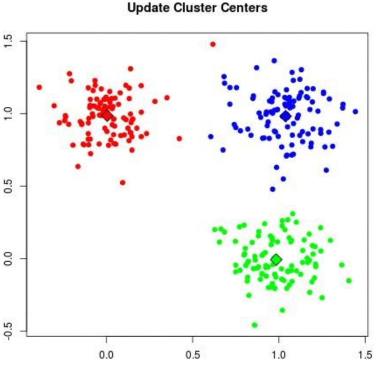

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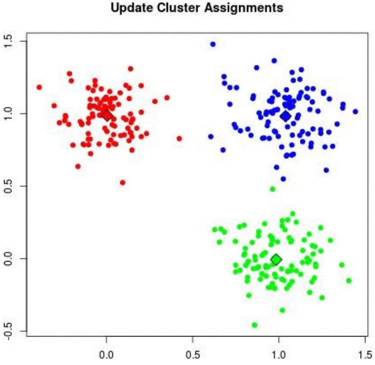

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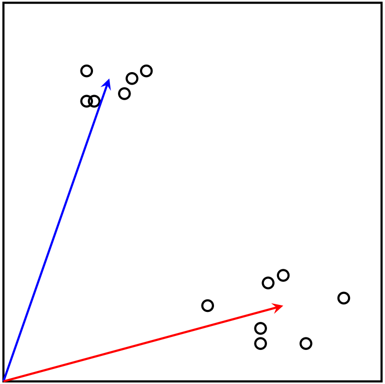
Decomposition



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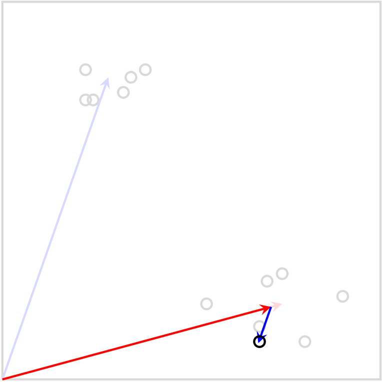
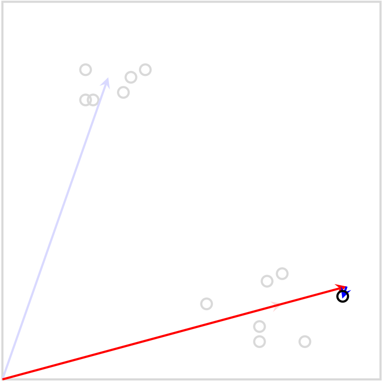


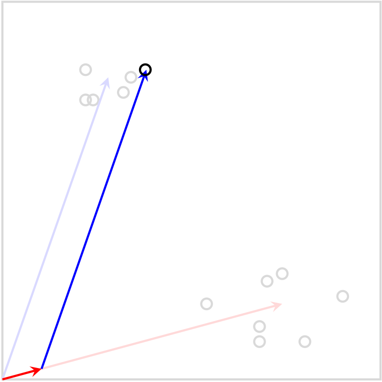
x = 0.96 × →
+ -0.12 × →

Decomposition



x = 1.23 × ⟶
+ -0.04 × ⟶

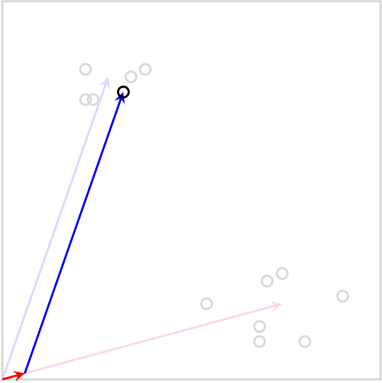
Decomposition



x = 0.14 × ⟶

+ 0.99 × ⟶

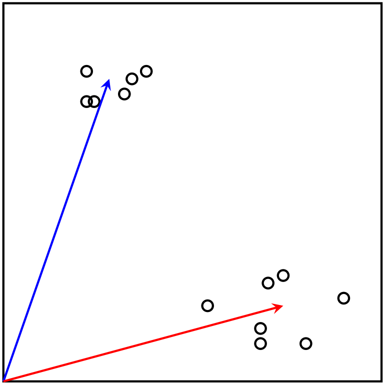
Decomposition



$x = 0.08 \times \longrightarrow$

$+\ 0.93 \times \longrightarrow$

Decomposition



$\approx$

$$U \quad \text{“weights”} \qquad \begin{array}{cc} 0.96 & -0.12 \\ 1.23 & -0.04 \\ \multicolumn{2}{c}{\dots} \\ 0.14 & 0.99 \\ 0.08 & 0.93 \\ \multicolumn{2}{c}{\dots} \end{array}$$

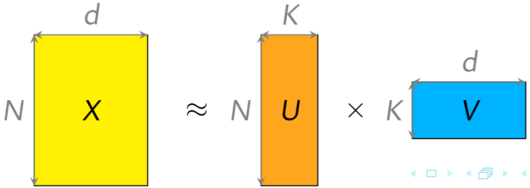
V “Components”

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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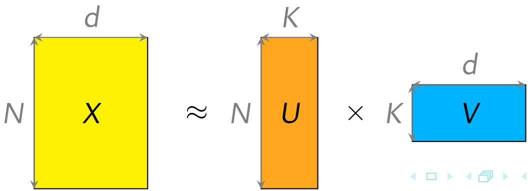

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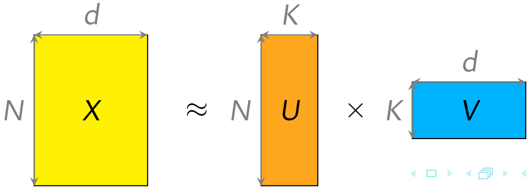
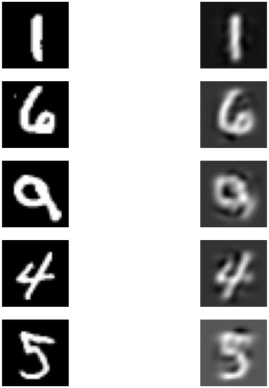
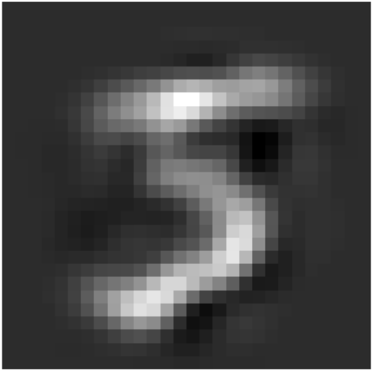


Example of reconstructions on MNIST with $K = 32$

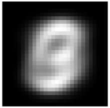


Recall that each image is vectorized, hence each of these images correspond to a row in V.

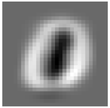
Detailed example of a reconstruction



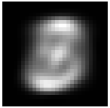
Principal Components Analysis



$= 122.3 \times$



Principal Components Analysis



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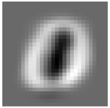
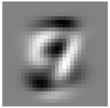


$-316.2\times$



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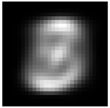
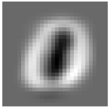
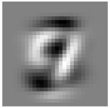
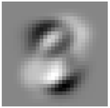
 $= 122.3\times$  $-316.2\times$ 

$-51.13\times$ 

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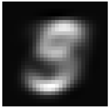
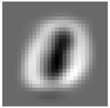
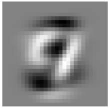
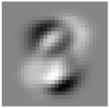
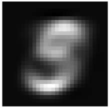
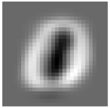
 $= 122.3\times$  $-316.2\times$ 

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

Principal Components Analysis



$= 122.3\times$



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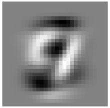

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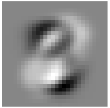

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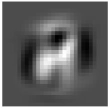
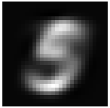
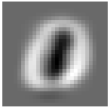
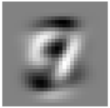
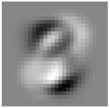
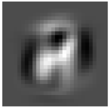
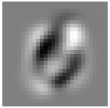


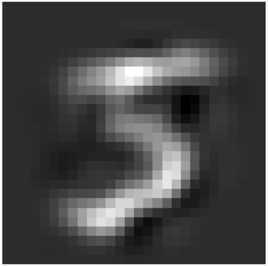
Principal Components Analysis

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

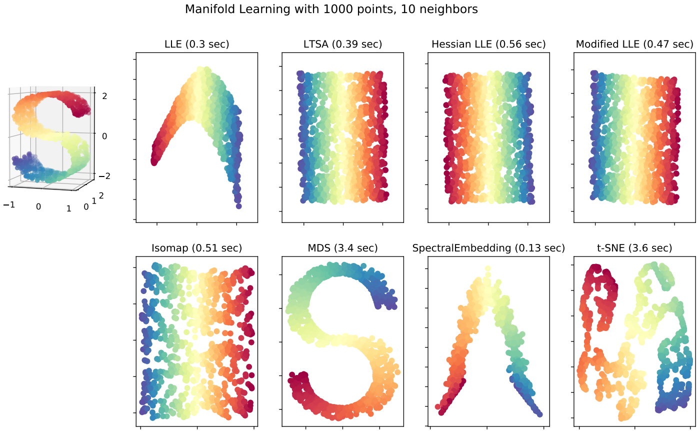
$-51.13\times$  $-556.9\times$ 

$-49.2\times$  $-217.1\times$  $\dots$

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

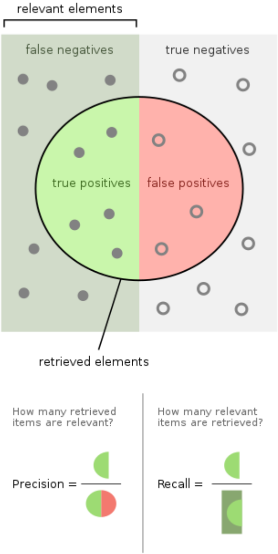
Objective : remove features

- 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 8 : 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), based on the same foundation model than in Lab 1.

Project 2 (P2)

You will choose a couple of unsupervised learning methods among those available (see Lab 3). You will present

- A brief description of the theory behind these methods,
- Basic tests on these techniques for your modality.

During Session 3 you will have 15 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