

# Unsupervised learning

Inteligencia Artificial en los Sistemas de Control Autónomo  
Máster en Ciencia y Tecnología desde el Espacio

Departamento de Automática

## Objectives

### i. TODO

## Bibliography

- TODO Bishop, Christopher M. *Pattern Recognition and Machine Learning*. 2nd edition. Springer-Verlag. 2011
- TODO Müller, Andreas C., Guido, Sarah. *Introduction to Machine Learning with Python*. O'Reilly. 2016

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# Clustering

K-means, agglomerative clustering, DBSCAN and GMM

# Clustering Applications

Set of unsupervised techniques that identify groups of data (named clusters)

- No universal definition of cluster: Centroid, medoid, dense regions, etc

## Applications

- Customer segmentation
- Data analysis
- Dimensionality reduction
- Anomaly detection
- Semi-supervised learning
- Search engines
- Image segmentation

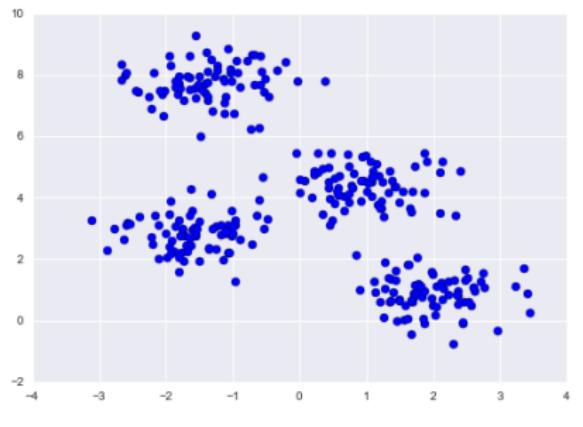
## Main algorithms

- K-means, DBScan, GMM, hierarchical clustering, EM, ...

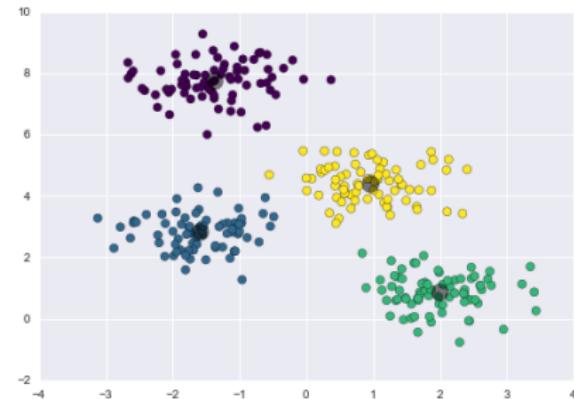
# K-means

## Overview

Original data



Clustered data



In k-means, clusters are identified by a **centroid**

# K-means

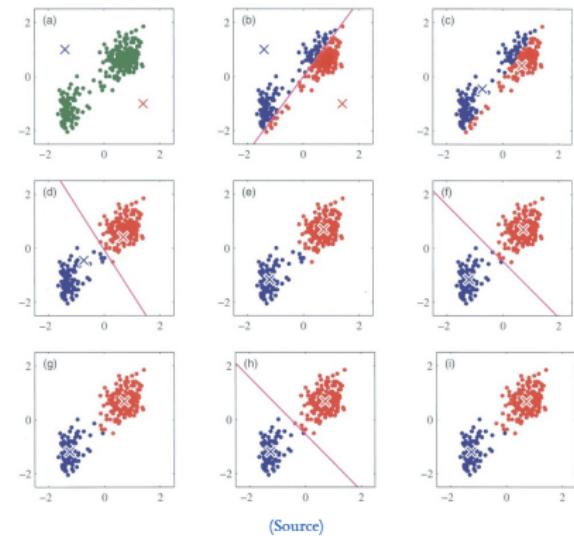
## K-means algorithm (I)

### K-means algorithm

1. Set  $k$  random centroids
2. Assign each data point to its closest centroid
3. Recompute centroids
4. Go to 2 until no point reassignment

$k$  is an hyperparameter

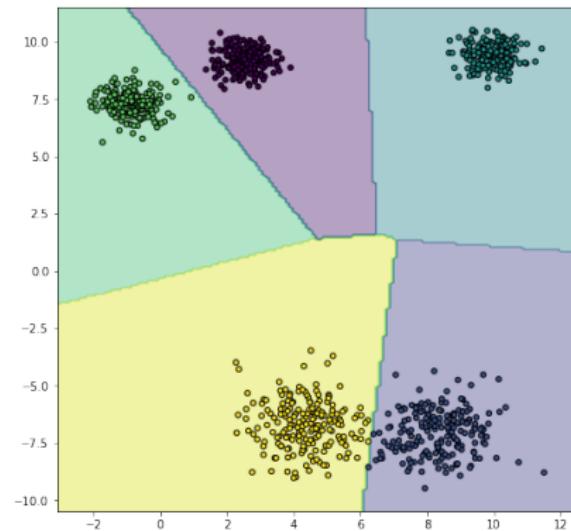
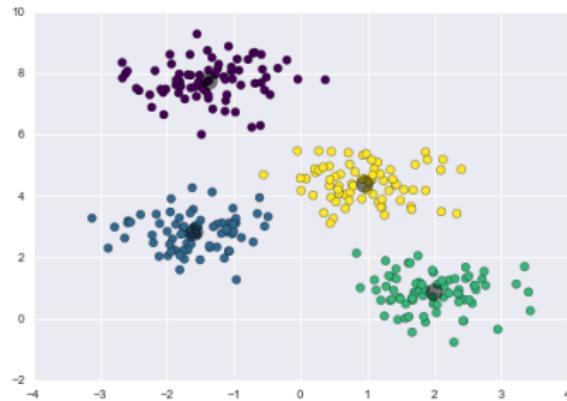
- Number of clusters



# K-means

## K-means algorithm (II)

New data points are assigned to its closest centroid

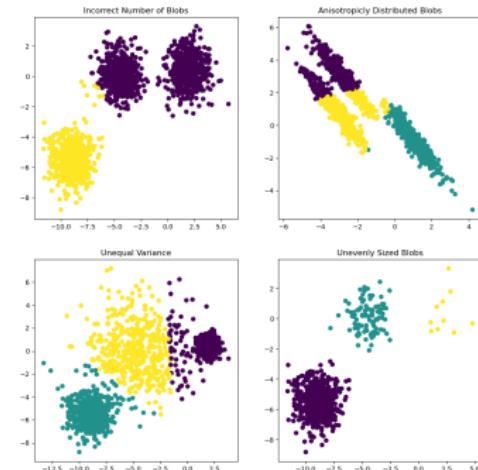


# K-means

## K-means limitations

K-means can fail in several conditions

- Incorrect number of clusters
- Different clusters variance
- Non-spheric clusters ⇒ normalization



(Source)

# K-means

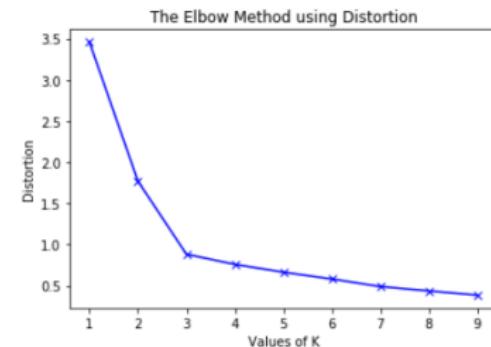
## Elbow's method

### Election of k

- Not a problem when domain information is available
- ... that is rarely the case

### Elbow's method

1. Select  $K = 1, \dots, n$
2. Visualize performance for each  $k$
3. Choose  $K$  where metric stabilizes



### Performance measures

- Inertia: mean squared error between each instance and its closest centroid
- Silhouette:  $(b - a)/\max(a, b)$ , where  $a$  mean intra-cluster distance, and  $b$  is the mean nearest-cluster distance

# K-means

## Application: Image segmentation



(Source)



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# K-means

## Application: Clustering for semi-supervised learning

Semi-supervised learning: Only a subset of the dataset is labeled

- Supervised and unsupervised learning
- Quite common in real-world applications (labels used to be expensive)

| $f_1$     | $f_2$     | $\dots$ | $f_n$     | $y$   |
|-----------|-----------|---------|-----------|-------|
| $a_{1,1}$ | $a_{2,1}$ | $\dots$ | $a_{n,1}$ | $y_1$ |
| $a_{1,2}$ | $a_{2,2}$ | $\dots$ | $a_{n,2}$ |       |
| $a_{1,3}$ | $a_{2,3}$ | $\dots$ | $a_{n,3}$ |       |
| $a_{1,4}$ | $a_{2,4}$ | $\dots$ | $a_{n,4}$ | $y_4$ |
| $a_{1,5}$ | $a_{2,5}$ | $\dots$ | $a_{n,5}$ |       |

## Label propagation

1. Obtain  $k$  clusters
2. Get a representative instance of each cluster (**medoid**) measuring the distance to the centroid
3. Label the members of each cluster with its medoid's label

# K-means

## K-means: Summary

| Hyperparameters | Advantages                              | Disadvantages   |
|-----------------|---|---|
| $k$             | Fast<br>Few hyperparameters<br>Scalable | Simple shapes<br>Determine $k$<br>Random initialization |

# Other clustering algorithms

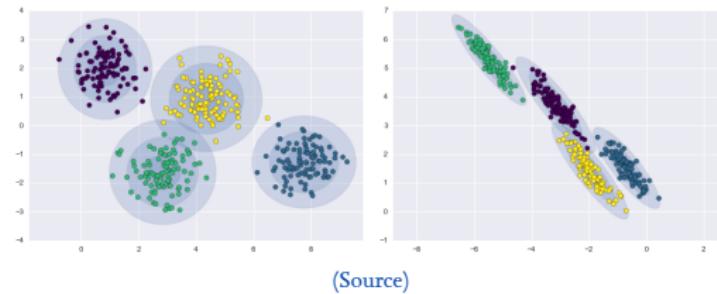
## Gaussian Mixure Model (GMM) (I)

GMM is a generative clustering algorithm

- Assumes data coming from a set of multidimensional gaussian distributions

GMM fits a set  $\{(\phi_i, \mu_i, \sigma_i)\}_{i=1,\dots,k}$

- $\phi$  is a weight
- $\mu$  is a multidimensional mean
- $\sigma$  is a covariance matrix
- $k$  is the number of clusters (hyperparameter)



Unsupervised learning

# Other clustering algorithms

## Gaussian Mixure Model (GMM) (II)

Gaussian parameters are fit with the Expectation-Maximization (E-M) algorithm

- E-M is a generalization of K-means

### Expectation-Maximization algorithm

1. Init parameters randomly
2. Expectation step: Assign each instance to a cluster
  - Assignment is probabilistic
3. Maximization step: Update cluster parameters
  - Each cluster is updated using all the data
  - Instances contribution to a cluster parameters is weighted by the probability that it belongs to it
4. Go to 2

GMM can be seen as a fuzzy clustering algorithm

# Other clustering algorithms

## Gaussian Mixure Model (GMM) (III)

Gaussian parameters are fit with the Expectation-Maximization (E-M) algorithm

- E-M is a generalization of K-means

### Expectation-Maximization algorithm

1. Init parameters randomly
2. Expectation step: Assign each instance to a cluster
  - Assignment is probabilistic
3. Maximization step: Update cluster parameters
  - Each cluster is updated using all the data
  - Instances contribution to a cluster parameters is weighted by the probability that it belongs to it
4. Go to 2

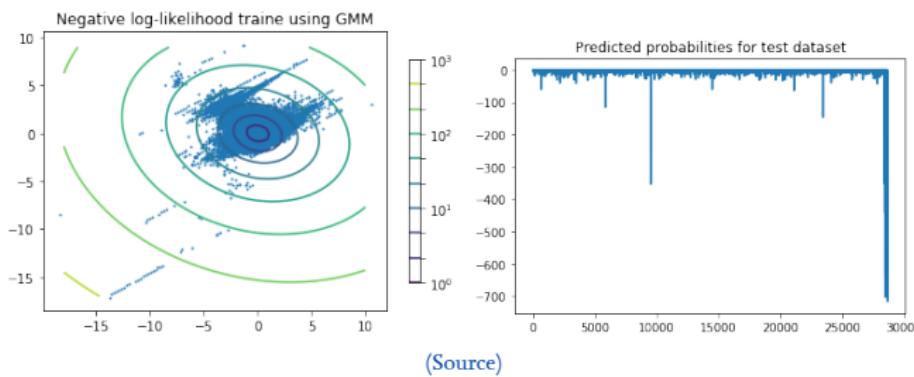
GMM can be seen as a fuzzy clustering algorithm

# Other clustering algorithms

## Gaussian Mixure Model (GMM) (IV)

GMM provides a probability of an instance to belong to a cluster

- This can be used to detect anomalies
- Just assign a probability threshold



# Other clustering algorithms

## GMM: Summary

| Hyperparameters        | Advantages               | Disadvantages         |
|------------------------|--------------------------|-----------------------|
| Number of clusters     | Probabilistic clustering | Number of clusters    |
| Covariance matrix type | Generative model         | Gaussian data         |
|                        | Anomaly detection        | Sensitive to outliers |

# Other clustering algorithms

## DBSCAN (I)

DBSCAN: Density-Based Spatial Clustering of Applications with Noise

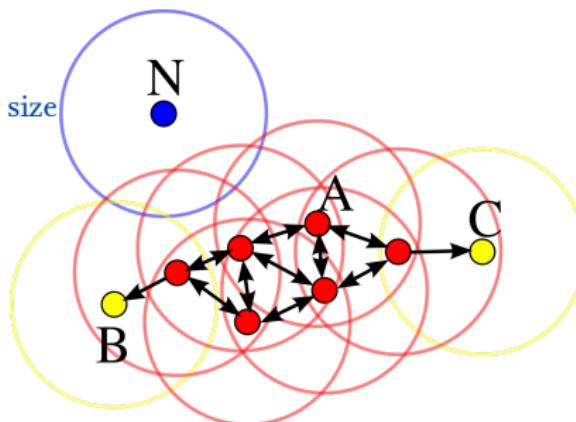
- Identifies high density regions (dense regions) in feature space
- Asumtion: Clusters form dense regions separated by empty areas

Hyperparameters

- $\epsilon$ : Radius of a neighborhood
- min\_samples: Minumun cluster size

Type of points

- Core instance
- Outliers



(Source)

# Other clustering algorithms

## DBSCAN (II)

$\epsilon=0.05, \text{min\_samples} = 5$



$\epsilon=0.2, \text{min\_samples} = 5$



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# Other clustering algorithms

## DBSCAN: Summary

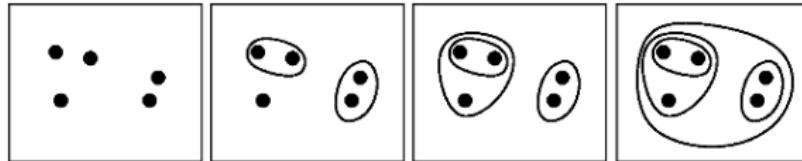
| Hyperparameters | Advantages  | Disadvantages                     |
|-----------------|---|-----------------------------------|
| $\epsilon$      | No explicit number of clusters  | Slower than K-means               |
| min_samples     | Scales relatively well<br><br>Almost deterministic<br><br>Robust to outliers<br><br>Anomaly detection | Clusters with different densities |

# Other clustering algorithms

## Agglomerative clustering (I)

### Agglomerative clustering

1. Initially, each instance forms a cluster
2. Merge the two most similar clusters according to a metric
3. Repeat 2 until a stop criterion is satisfied



We need a similarity measure between two clusters

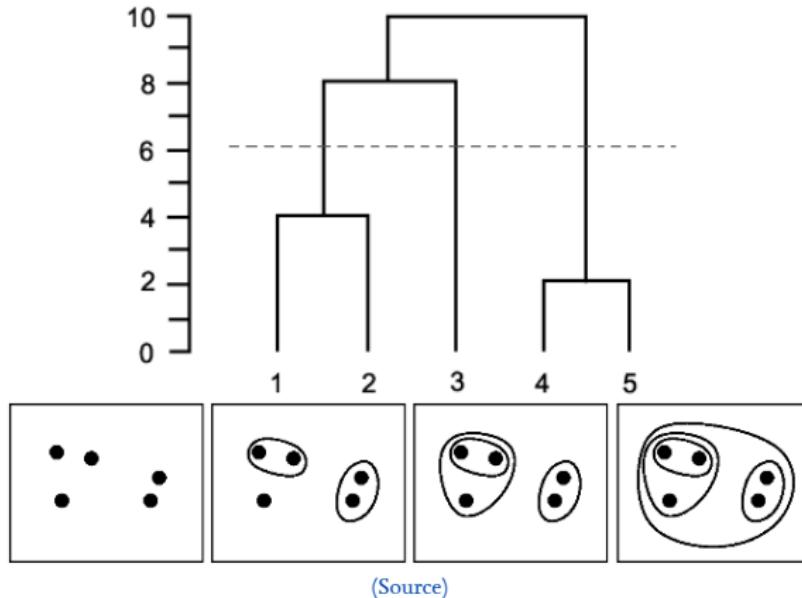
- **Ward:** Minimizes variance within merged clusters. Leads to equally sized clusters
- **Average:** Minimizes average distances between their points
- **Complete:** Minimizes maximum distance between their points

# Other clustering algorithms

## Agglomerative clustering (II)

Agglomerative clustering is a special case of hierarchical clustering

Dendrogram



# Other clustering algorithms

## Agglomerative clustering: Summary

| Hyperparameters | Advantages                                | Disadvantages |
|-----------------|---|---------------|
|                 | Complex shapes<br>Hierarchical clustering |               |

# Anomaly detection

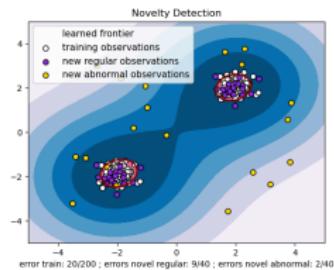
Two related concepts

- Outlayer detection and novelty detection

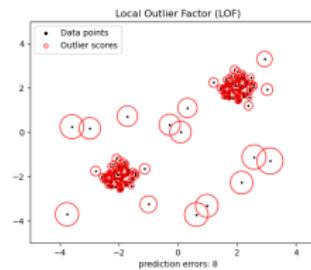
Adaptation of clustering and classification algorithms

- PCA, GMM, autoencoders, etc

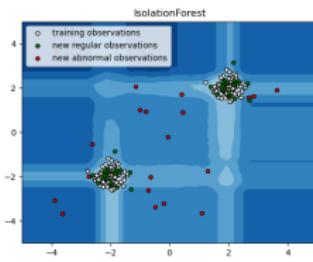
One-Class SVM



LOF



Isolation Forest



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# Dimensionality reduction

## PCA and manifold learning

# Dimensionality reduction

## Main approaches for dimensionality reduction (I)

Two main approaches to dimensionality reduction: Projection and manifold learning

### Projection

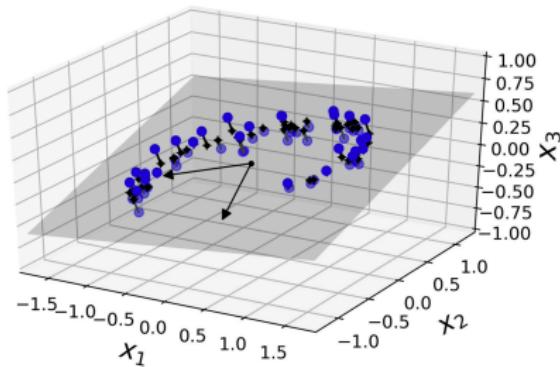


Figure 8-2. A 3D dataset lying close to a 2D subspace

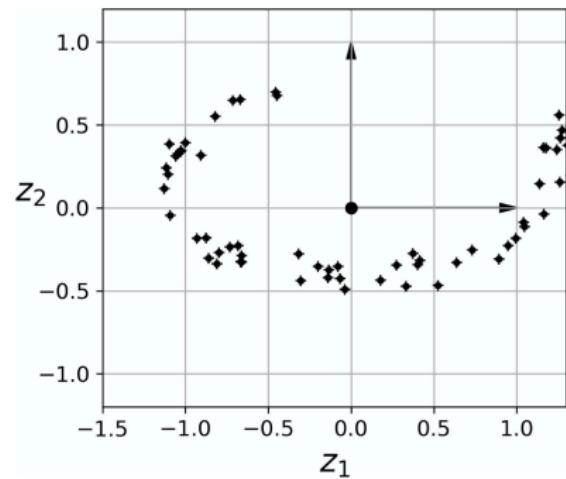


Figure 8-3. The new 2D dataset after projection

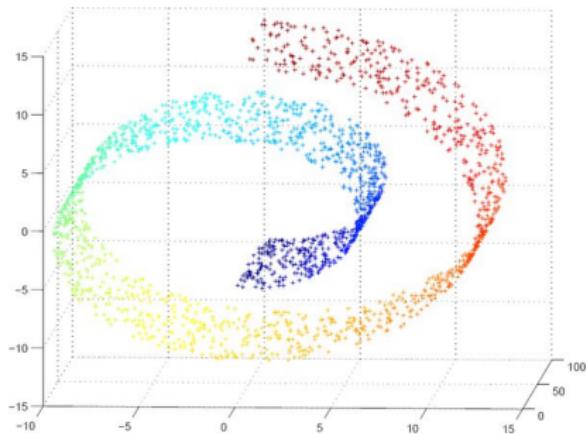
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## Algorithms

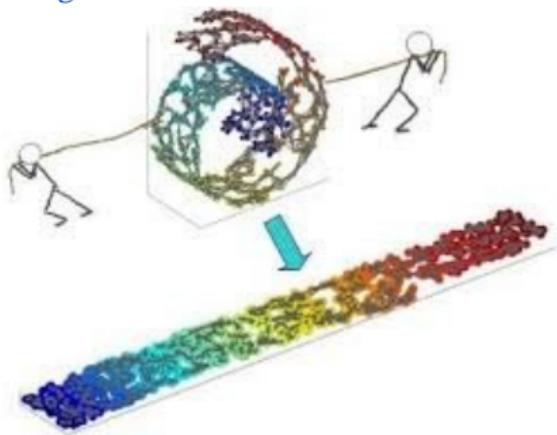
# Dimensionality reduction

## Main approaches for dimensionality reduction (II)

### Manifold learning



(Source)



### Manifold learning algorithms

- Isomap, T-distributed Stochastic Neighbor Embedding (t-SNE), Multi-dimensional Scaling (MDS), Locally Linear Embedding (LLE), ...

# Dimensionality reduction

## Principal Components Analysis (I)

Dimensionality reduction transforms data into more convenient representations

- Reduce data dimensionality
- Visualize multidimensional data

Main algorithms

# Dimensionality reduction

## Principal Components Analysis (I)

PCA create a new coordinate system

- New axes capture maximum variance and are orthogonal
  - They are named **principal components**
- The amount of variance captured by each principal component is captured
- PCA does not change the original dimensionality

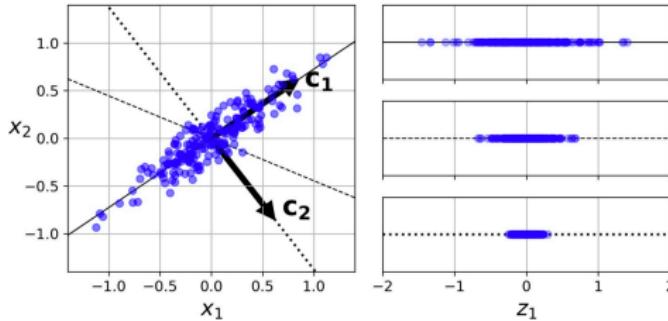
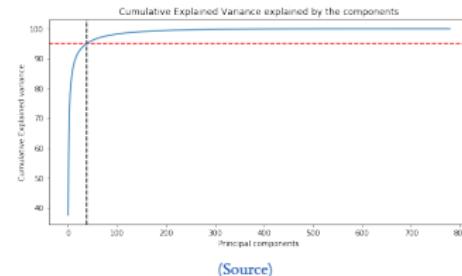


Figure 8-7. Selecting the subspace to project on

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# Dimensionality reduction

## Principal Components Analysis (II)

PCA application: Image compression

Original image



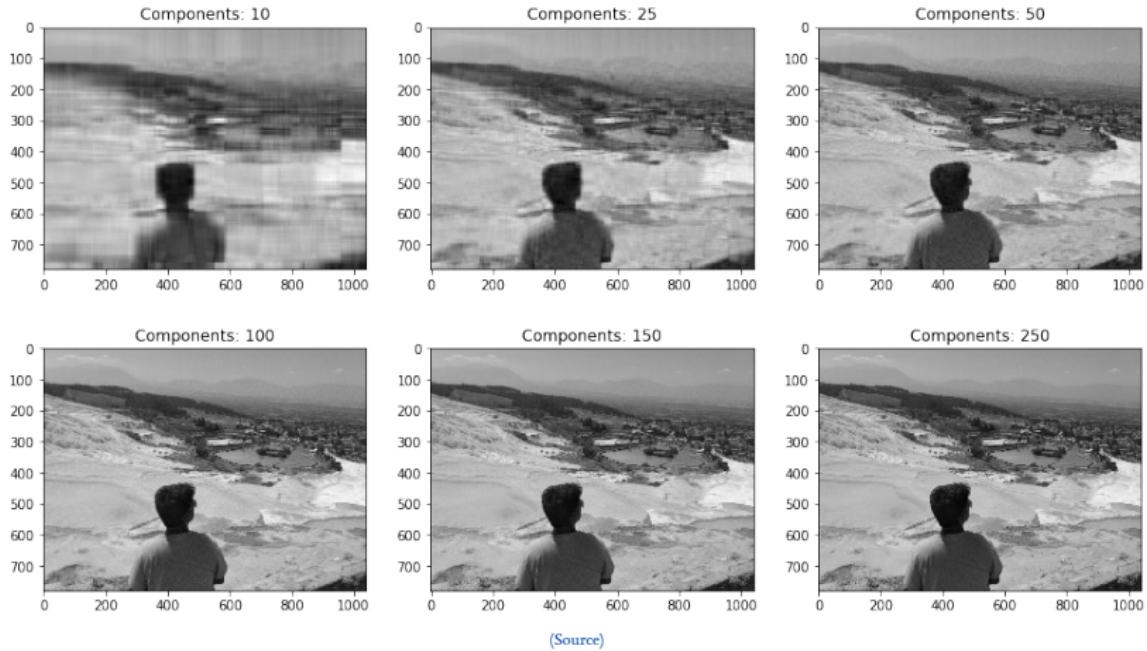
(Source)

Compressed image (38 dimensions)



# Dimensionality reduction

## Principal Components Analysis (III)



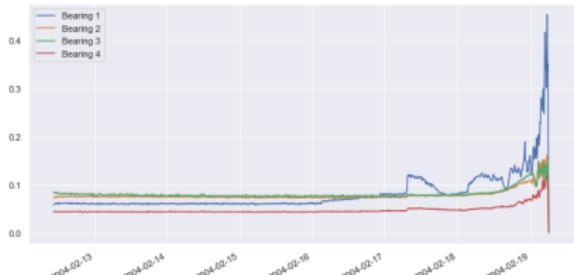
# Dimensionality reduction

## Principal Components Analysis (IV)

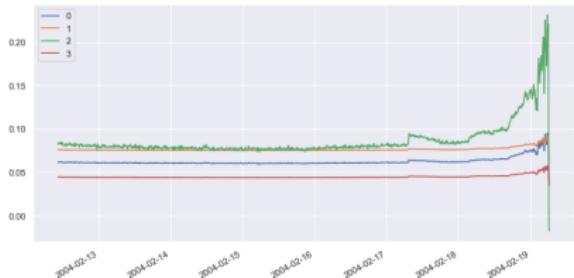
PCA application: Anomaly detection to predict bearing failure

- Vibrations of four bearings

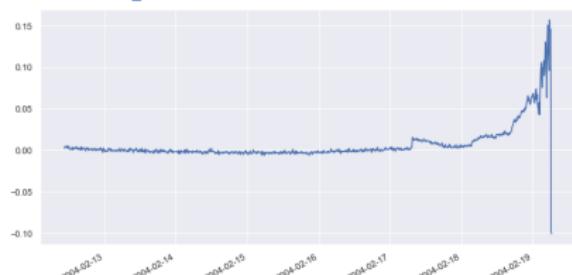
Vibration time series



Reconstructed time series



First component



Reconstruction error



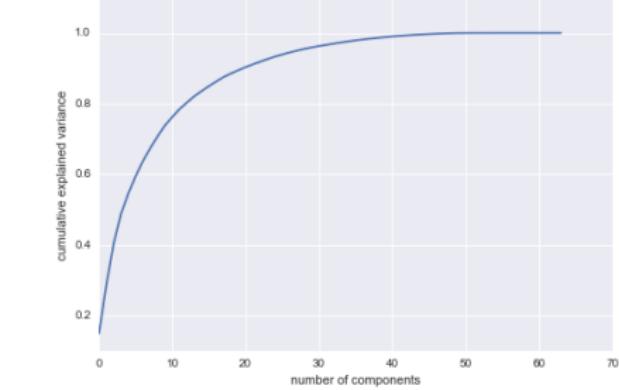
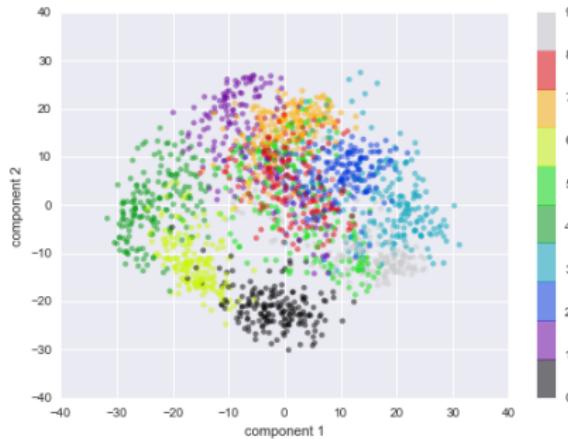
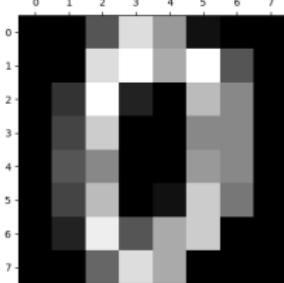
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# Dimensionality reduction

## Principal Components Analysis (III)

Example: Hand-written digits recognition

- Images of hand-written digits
- 8x8 images (64 dimensions)
- 10 digits
- Classification problem



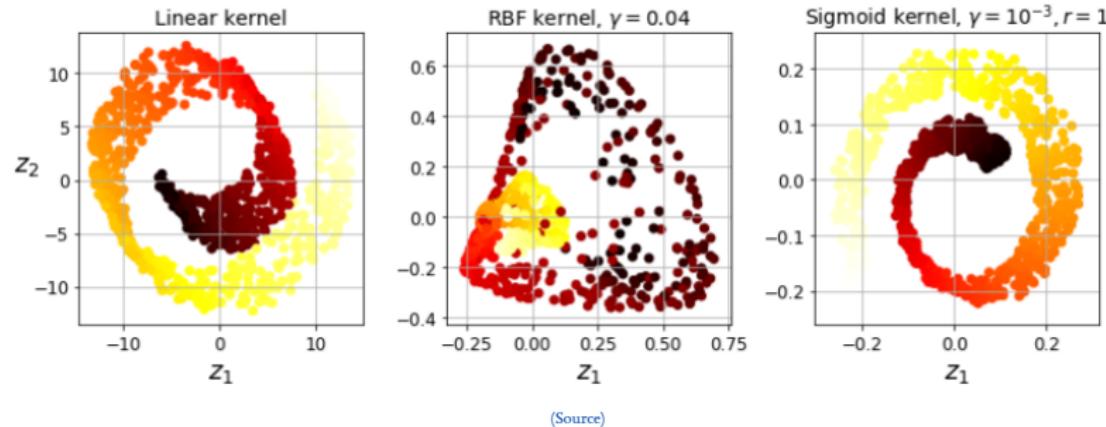
Unsupervised learning

# Dimensionality reduction

## Kernel PCA

The kernel trick applies to PCA

- kPCA captures non-linear structures



# Dimensionality reduction

## Manifold learning

The kernel trick applies to PCA

- kPCA captures non-linear structures

