Unsupervised learning

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

Departamento de Automática

Objectives

1. Extend unsupervised learning algorithms
2. Apply unsupervised learning to real-world problems

Bibliography

- Géron, Aurélien. *Hands-On Machine Learning with Scikit-Learn, Keras & TensorFlow*. O'Reilly. 2020
- Müller, Andreas C., Guido, Sarah. *Introduction to Machine Learning with Python*. O'Reilly. 2016

Table of Contents

Clustering

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

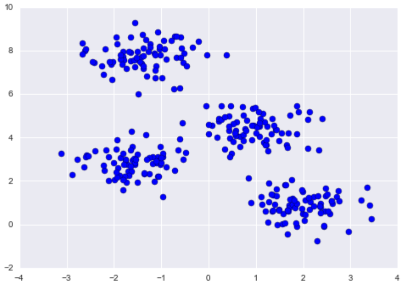
Main algorithms

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

K-means

Overview

Original data



Clustered data

(Source)

In k-means, clusters are identified by a centroid

K-means

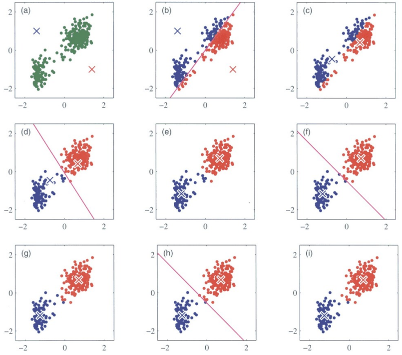
K-means algorithm (I)

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



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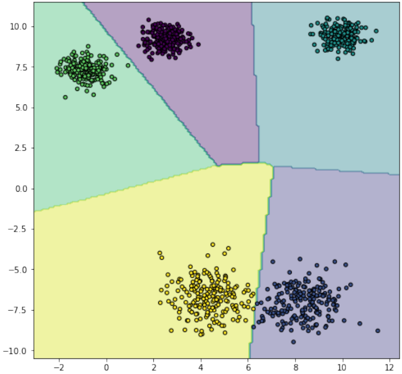
K-means

K-means algorithm (II)

New data points are assigned to its closest centroid

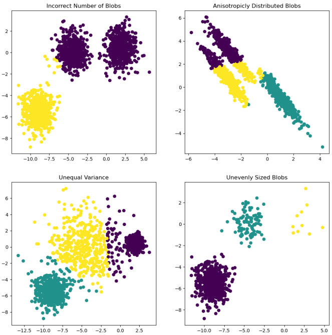


K-means

K-means limitations

K-means can fail in several conditions

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



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K-means

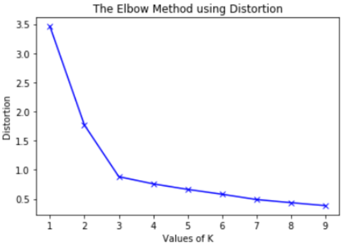
Elbow's method

Election of k

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

Elbow's method

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

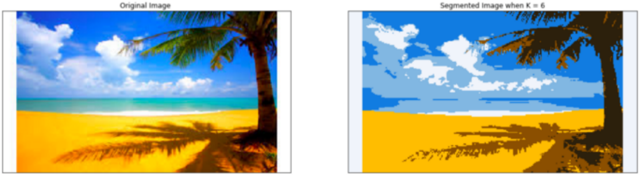


Performance measures

- 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



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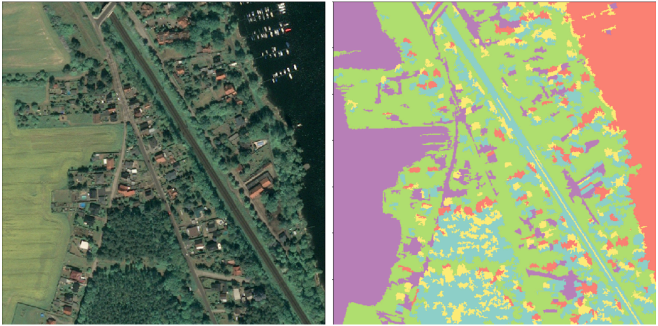

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K-means

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 use to be expensive)

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

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
	Fast	Simple shapes
k	Few hyperparameters	Determine k
	Scalable	Random initialization

Other clustering algorithms

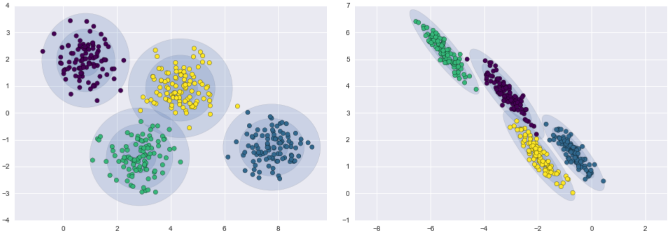
Gaussian Mixure Model (GMM) (I)

GMM is a generative clustering algorithm

- Assumes data coming from a set of multidimensional gaussian distributions

GMM fits a set $\{(\phi_i, \mu_i, \sigma_i)\}_{i=1,\ldots,k}$, where k is the number of clusters and

- ϕ is a weight
- μ is a multidimensional mean
- σ is a covariance matrix



(Source)

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

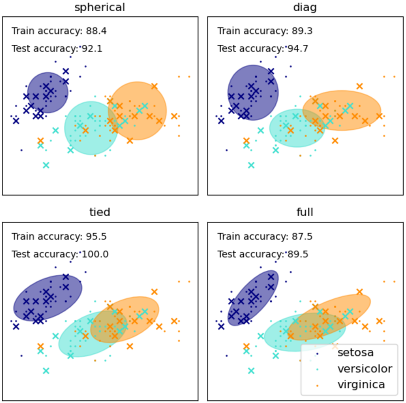
GMM can be seen as a fuzzy clustering algorithm

Other clustering algorithms

Gaussian Mixure Model (GMM) (III)

Covariance matrices can be constrained

- Full: No restriction
- Spherical: Sheprical shapes, different diameters
- Diag: Ellipsoidal shapes, axes parallel to the coordinate system
- Tied: Same ellipsoidal shapes, size and orientation

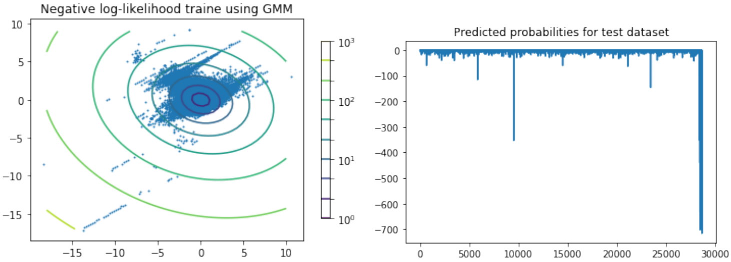


Other clustering algorithms

GMM for anomaly detection

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

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



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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

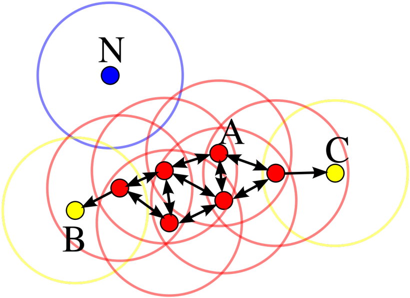
- Identifies high density regions (dense regions) in feature space
- Asumtion: Clusters form dense regions separated by empty areas

Hyperparameters

- *min_samples*: Minimun cluster size
- ϵ: Radius of a neighborhood

Type of points

- Core instance
- Frontier instance
- Outliers



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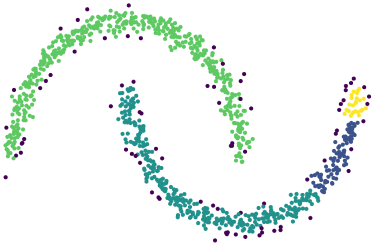
Other clustering algorithms

DBSCAN (II)

ϵ=0.05, $min\_samples = 5$



ϵ=0.2, $min\_samples = 5$

(Source)

Other clustering algorithms

DBSCAN: Summary

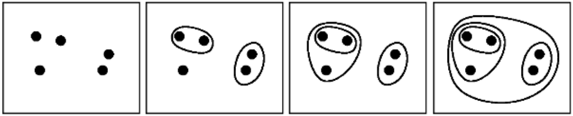
Hyperparameters	Advantages	Disadvantages
ϵ	Unknown number of clusters	Slower than K-means
min_samples	Scales relatively well	No model
	Almost deterministic	Clusters with different densities
	Robust to outliers	
	Anomaly detection	

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

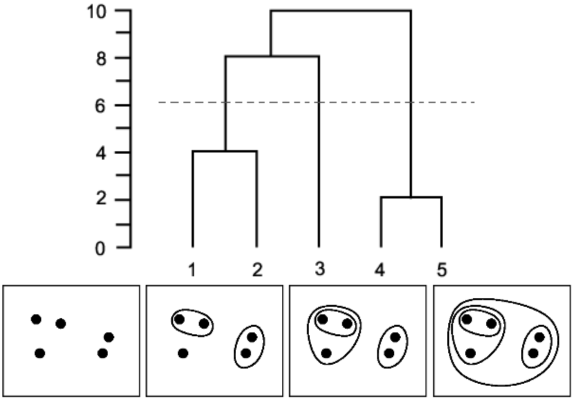
- *Ward*: Variance within merged clusters. Leads to equally sized clusters
- *Average*: Average distances
- *Complete*: Maximun distance
- *Single*: Minimum distance

Other clustering algorithms

Agglomerative clustering (II)

Agglomerative clustering is a special case of hierarchical clustering

Dendrogram



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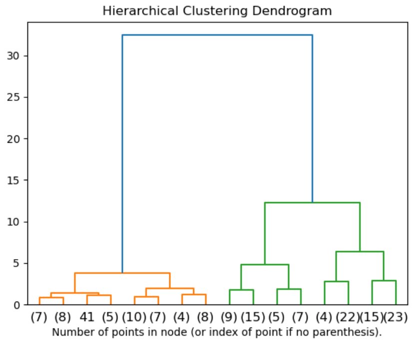
Other clustering algorithms

Agglomerative clustering (III)

Iris dataset dendrogram



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Other clustering algorithms

Agglomerative clustering: Summary

Hyperparameters	Advantages	Disadvantages
Similarity	Complex shapes Hierarchical clustering	Slow No model

Anomaly detection

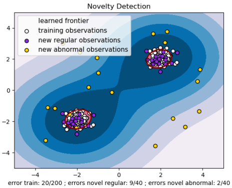
Two related concepts

- Outlayer detection and novelty detection

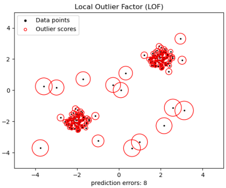
Adaptation of clustering and classification algorithms

- PCA, GMM, autoencoders, etc

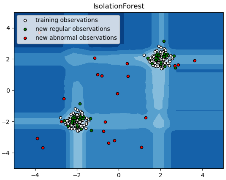
One-Class SVM



LOF



Isolation Forest



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Dimensionality reduction

Main approaches (I)

Two main approaches to dimensionality reduction: Projection and manifold learning

Projection

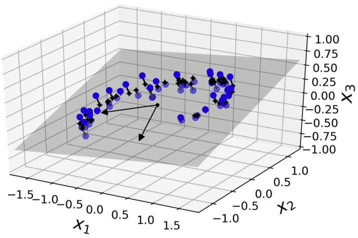


Figure 8-2. A 3D dataset lying close to a 2D subspace

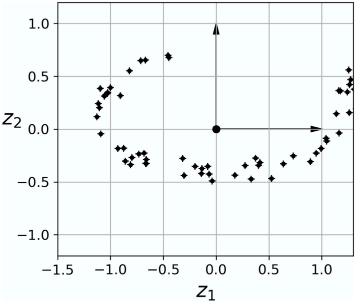


Figure 8-3. The new 2D dataset after projection

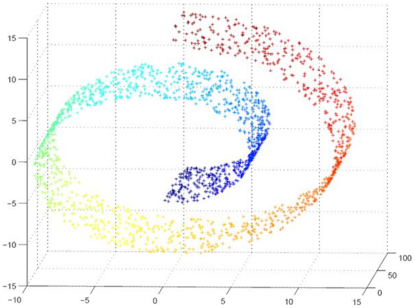
(Source)

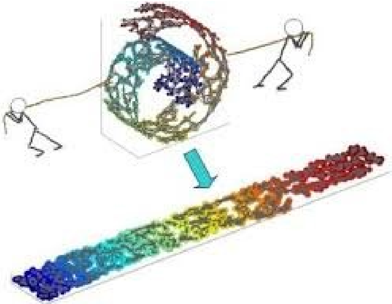
Algorithms: Principal Components Analysis (PCA), kernelized PCA, ...

Dimensionality reduction

Main approaches (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

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

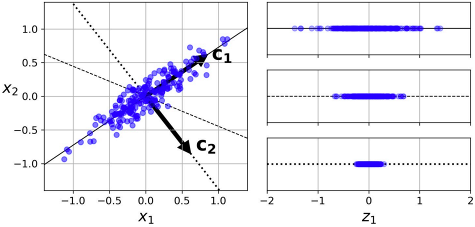


Figure 8-7. Selecting the subspace to project on

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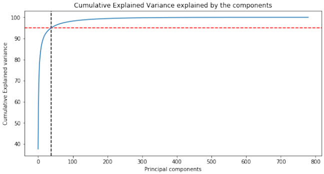


(Source)

Dimensionality reduction

Principal Components Analysis: Applications (I)

PCA application: Image compression

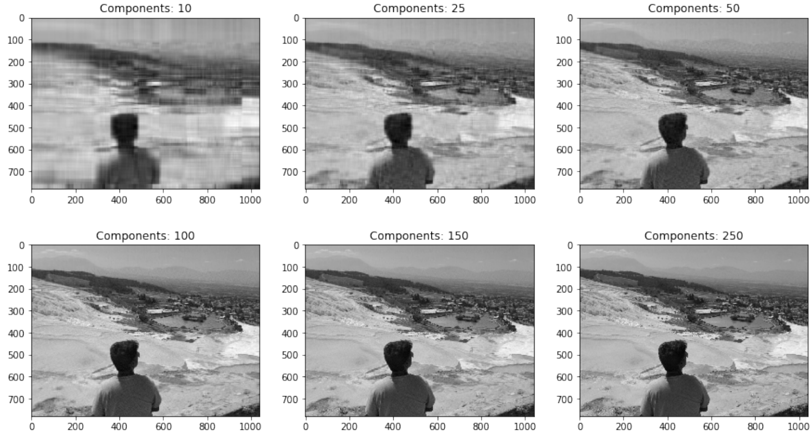
Original image

Compressed image (38 dimensions)

(Source)

Dimensionality reduction

Principal Components Analysis: Applications (II)



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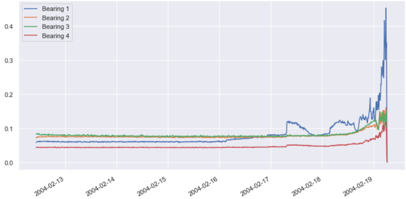
Dimensionality reduction

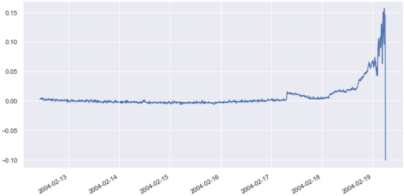
Principal Components Analysis: Applications (III)

Application: Anomaly detection to predict bearing failure, vibrations of four bearings

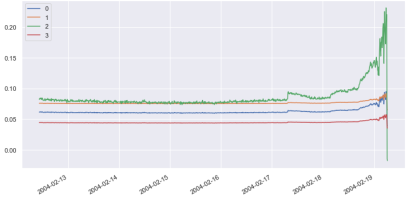
Vibration time series



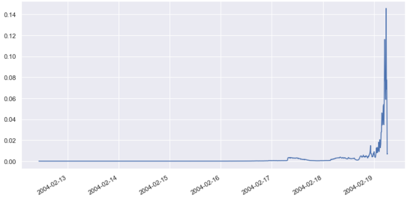
First component



Reconstructed time series



Reconstruction error



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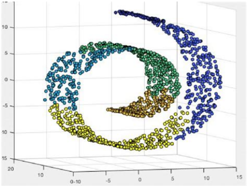
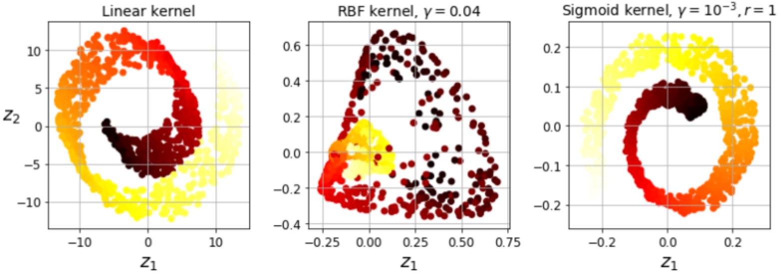
Dimensionality reduction

Kernel PCA

The kernel trick applies to PCA

- kPCA captures non-linear structures





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Dimensionality reduction

Manifold learning

Locally Linear Embedding (LLE)

- Measures how mach each training instance linearly relates to its closest neighbors preserving local relations

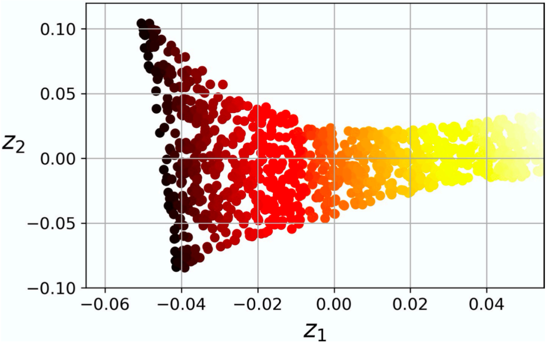


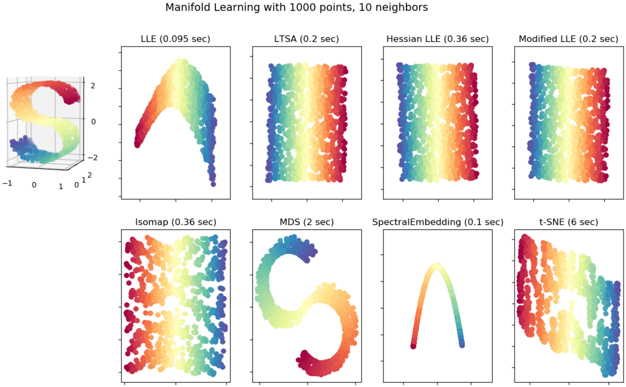
Figure 8-12. Unrolled Swiss roll using LLE

(Source)

Dimensionality reduction

Other manifold learning techniques

- Multidimensional Scaling (MDS): Preserves distances
- Isomap: Preserves geodesic distance
- t-Distributed Stochastic Neighbor Embedding (t-SNE): Preserves local distances and keep dissimilar instances apart



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Dimensionality reduction

Manifold learning demo

(Interactive demo)