Unsupervised learning

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

Departamento de Automática

Objectives

1. Define Machine Learning (ML)
2. Delimite ML scope
3. Introduce the main ML tasks
4. Recognize problems as ML tasks

Bibliography

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

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Algorithms

K-means, DBSCAN and GMM

Clustering

Applications

Clustering is a set of unsupervised techniques that identify groups of data (named clusters)

- No universal definition of cluster
  - Centroid, meroid, dense regions, etc

Applications

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

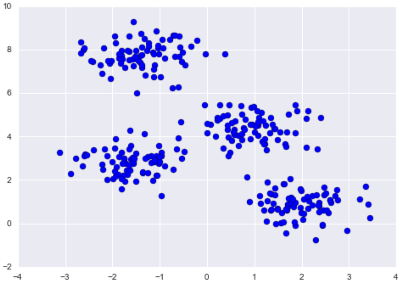
Main algorithms

- K-means, DBScan, Gaussian Mixture Models (GMM), Expectation Maximization (EM), ...

Algorithms

K-means (I)

Original data



Clustered data

(Source)

In k-means, clusters are identified by a centroid

Algorithms

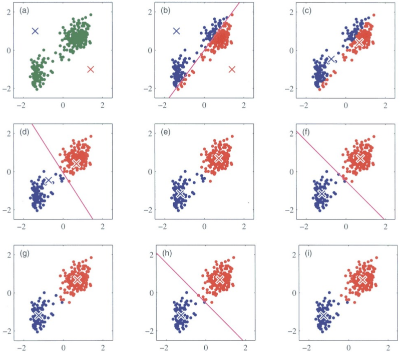
K-means (II)

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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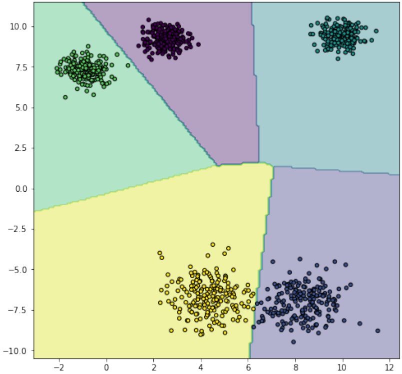
Algorithms

K-means (III)

New data points are assigned to its closest centroid

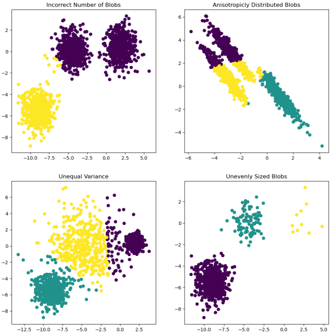


Algorithms

K-means (IV)

K-means can fail in several conditions

1. Incorrect number of clusters
2. Different clusters "diameter"
3. Non-spheric clusters



Algorithms

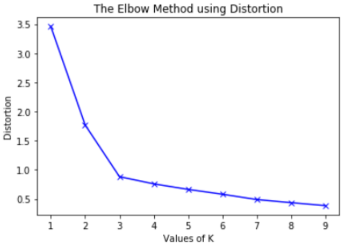
K-means (V)

K-means drawbacks

- Initial seed
- K election

Elbow method

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

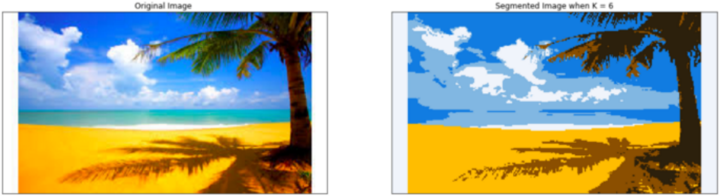


Performance measures

- 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

Algorithms

K-means: Image segmentation



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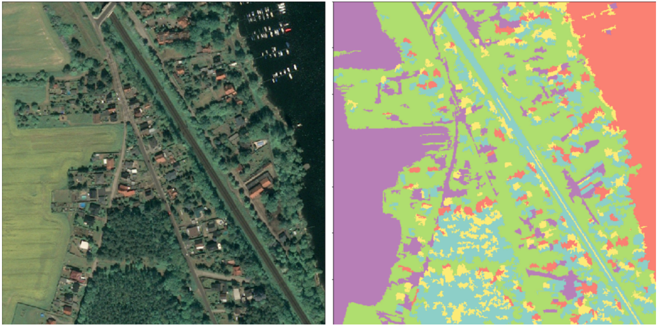

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Algorithms

K-means: 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

Algorithms

K-means: Summary

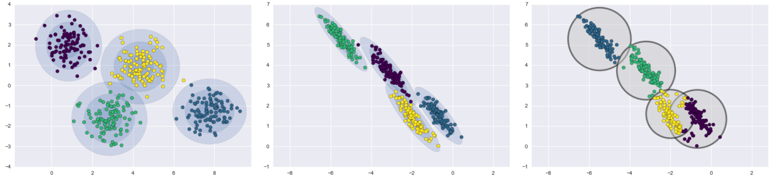
Hyperparameters	Advantages	Disadvantages
	Fast	Simple shapes
k	Few hyperparameters	Determine k
	Scalable	Random initialization

Algorithms

DBSCAN

GMM builds a probabilic model of our data

- GMM is a generative clustering algorithm
- Assumes data coming from a set of multidimensional gaussian distributions
  - GMM fits a set $\{(\mu_i, \sigma_i)\}_{i=1,\dots,K}$
  - μ is a vector
  - σ is a covariance matrix



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Algorithms

Gaussian Mixure Model (GMM)

GMM builds a probabilic model of our data

- GMM is a generative clustering algorithm
- Assumes data coming from a set of multidimensional gaussian distributions
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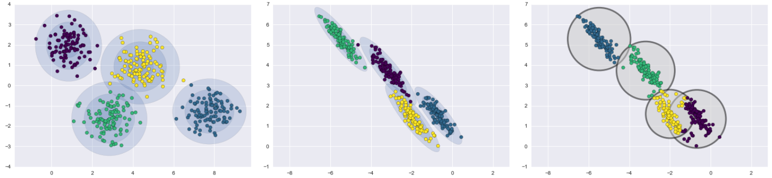

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Algorithms

PCA and manifold learning

Algorithms

Principal Components Analysis (I)

Dimensionality reduction transforms data into more convenient representations

- Reduce data dimensionality
- Visualize multidimensional data

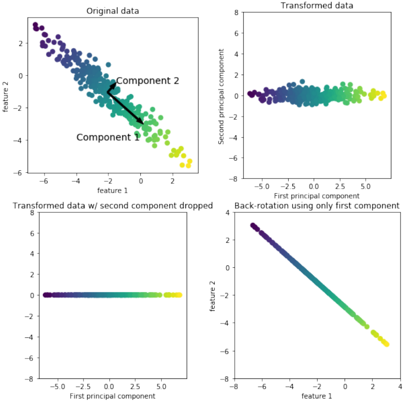
Main algorithms

- Isomap
- T-distributed Stochastic Neighbor Embedding (t-SNE)
- Principal Components Analysis (PCA)

Algorithms

Principal Components Analysis (II)

PCA maximizes data variance



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Algorithms

Principal Components Analysis (III)

Example: Hand-written digits recognition

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