Unsupervised learning

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

Departamento de Automática

Universidad de Alcalá
ISG

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

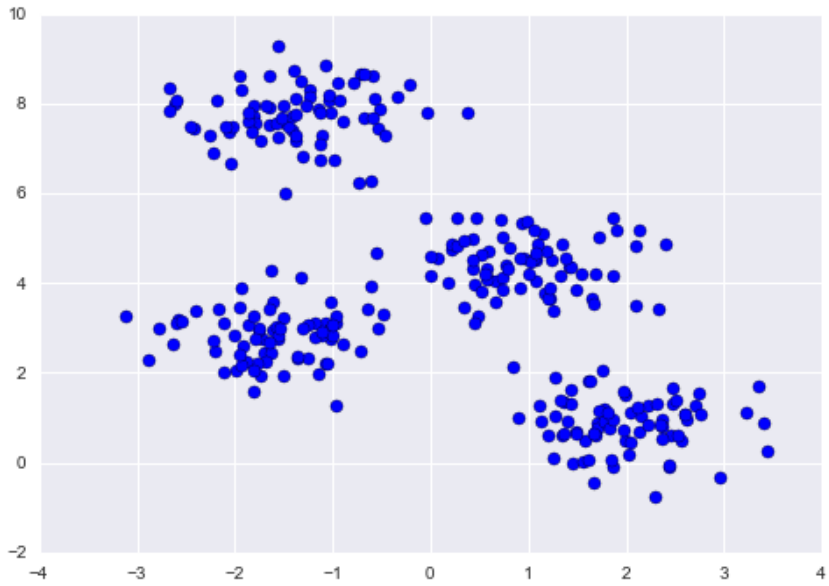
Main algorithms

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

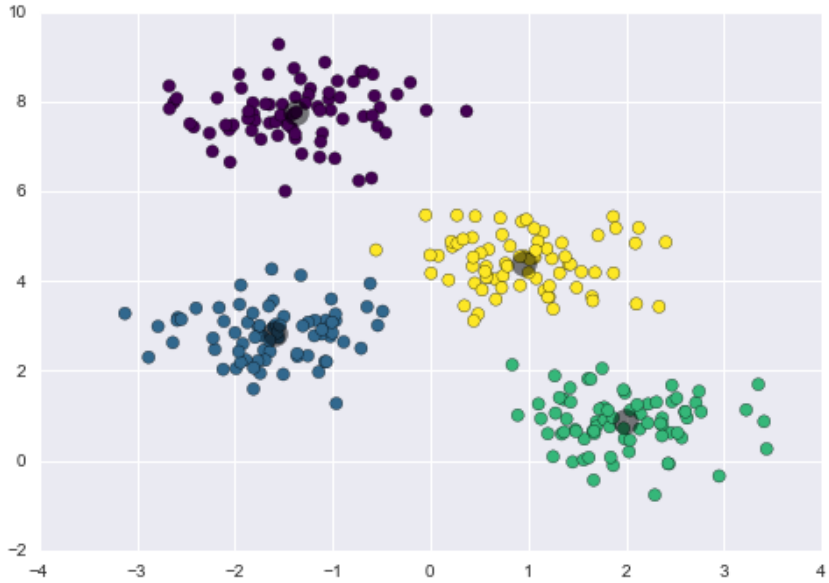
Algorithms

K-means (I)

Original data



Clustered data



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In k-means, clusters are identified by a centroid

Algorithms

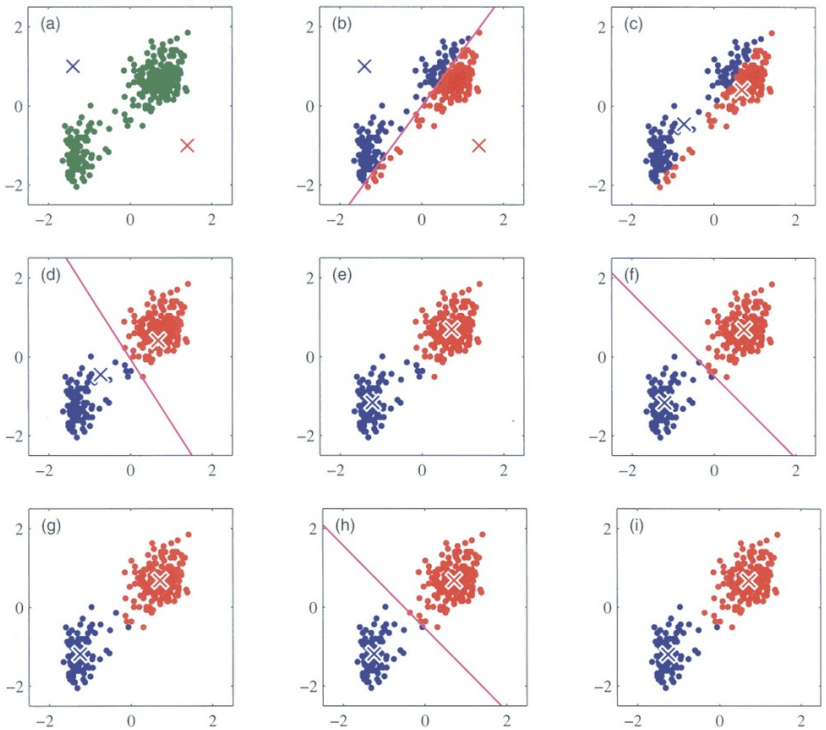
K-means (II)

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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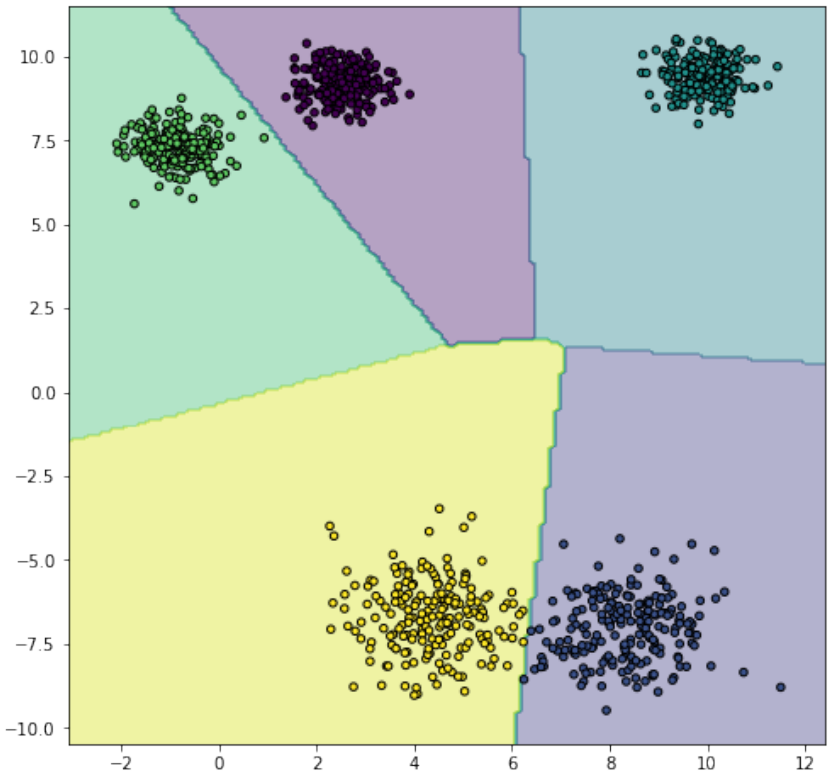
Algorithms

K-means (III)

New data points are assigned to its closest centroid

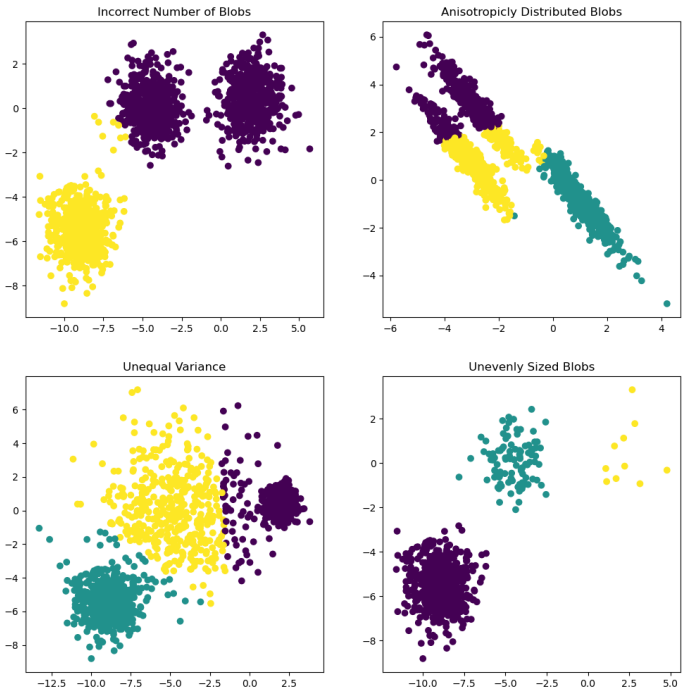


Algorithms

K-means (IV)

K-means can fail in several conditions

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



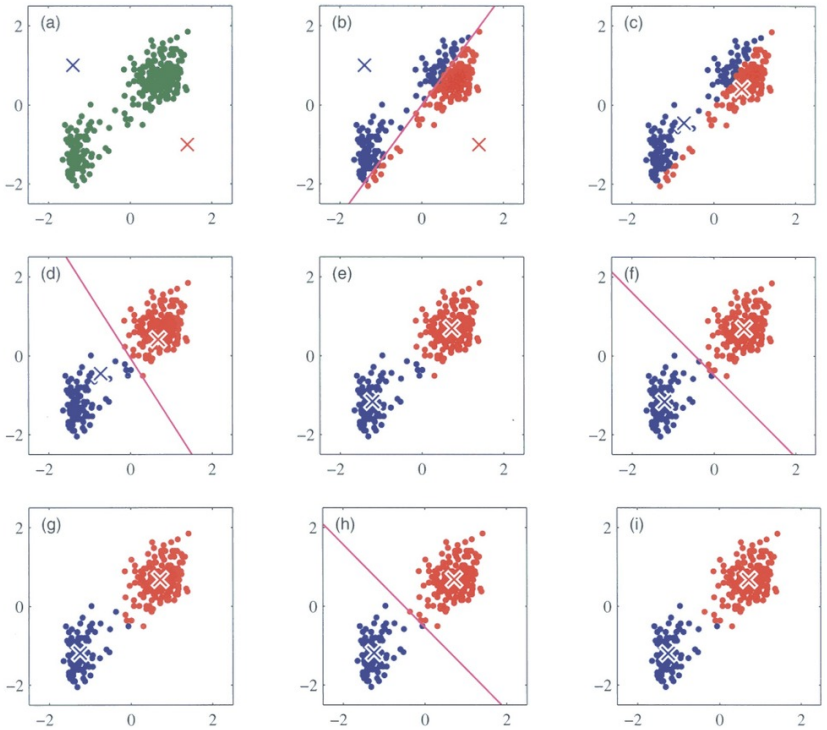
Algorithms

K-means (V)

New data points are assigned to its closest centroid

K-means algorithm

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



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Algorithms

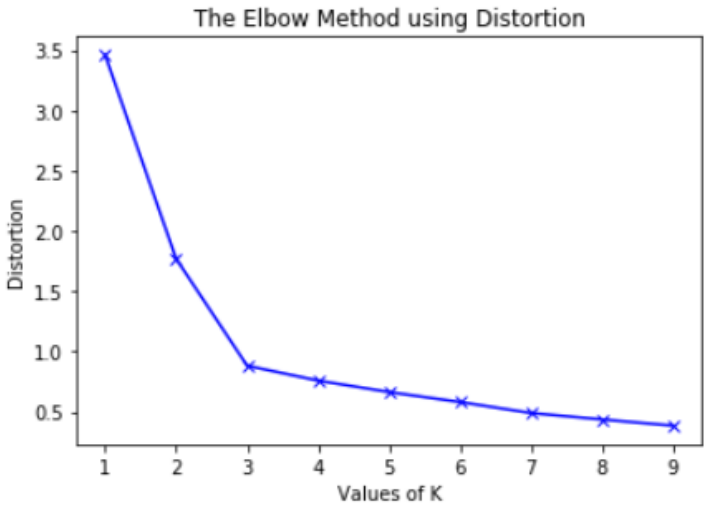
K-means (VI)

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: summary

Hyperparameters

- k

Advantages

- Fast
- Few hyperparameters
- Scalable

Disadvantages

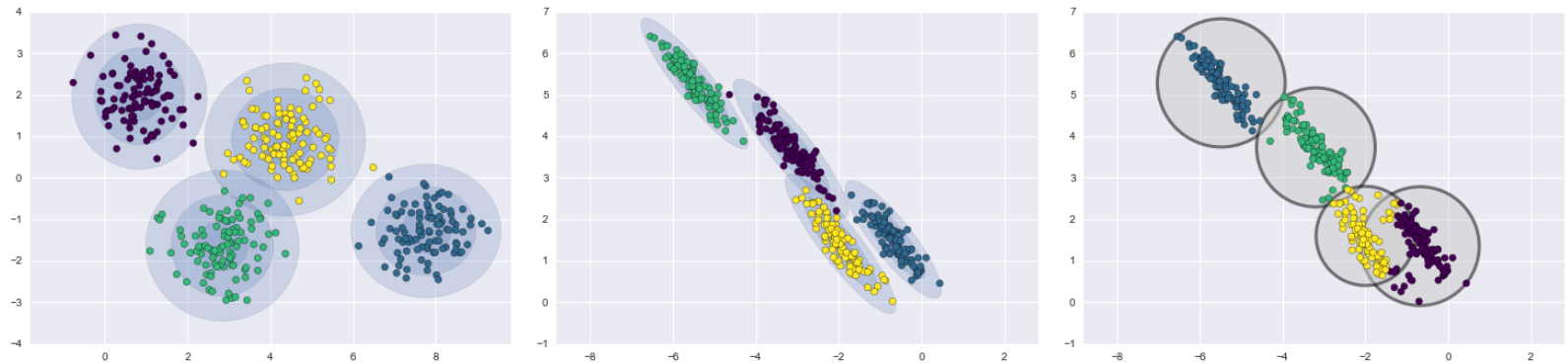
- Spherical shapes
- Dependence on k

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
  - 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

PCA and manifold learning

Algorithms

Principal Components Analysis (I)

Dimensionality reduction transforms data into more convenient representations

- Reduce data dimensionality
- Visualize multidimensional data

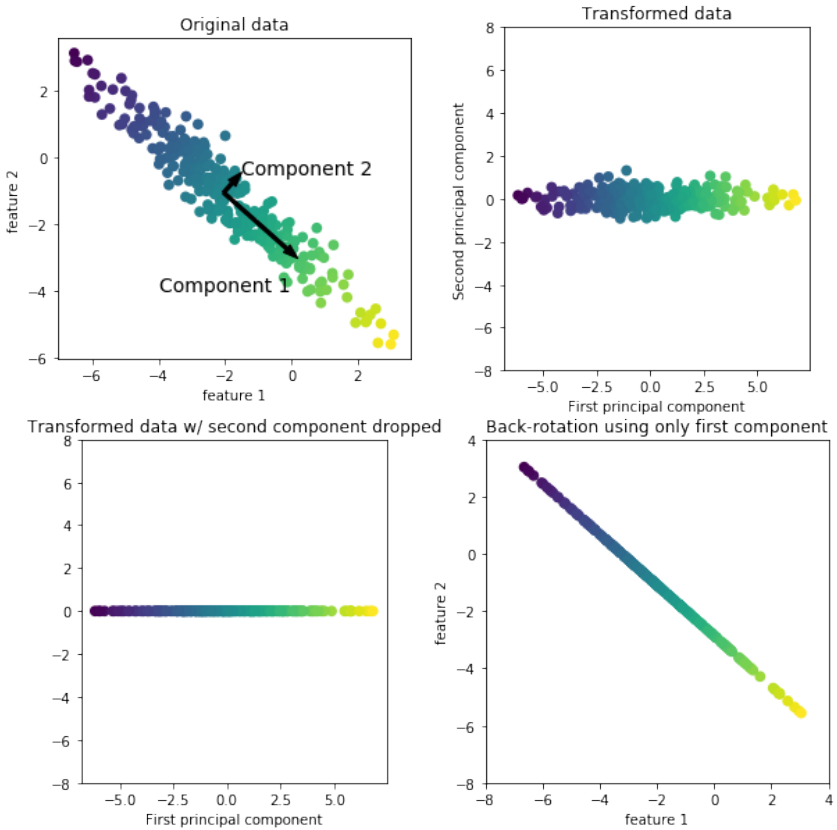
Main algorithms

- 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