Departamento de Eletrónica, Telecomunicações e Informática

PRE-PROCESSING AND UNSUPERVISED LEARNING

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Outline

Unsupervised learning

1. **Pre Processing**

2. **Data dimensionality reduction**
   - data compression /data visualization

3. **Principal Component Analysis (PCA)**

4. **K-means clustering**

Pre- Processing and Data preparation

1. Feature Extraction

- Extracting the right features is often a skill that requires an understanding of the specific application domain at hand.

2. Data cleaning

- The extracted data may have erroneous or missing entries.

3. Feature Selection and Transformation

- A variety of methods are used to either remove irrelevant features or transform the current set of features to a new data space that is more amenable for analysis

Pre- Processing and Data preparation

1. Feature Extraction

- Extracting the right features is often a skill that requires an understanding of the specific application domain at hand.

Pre- Processing and Data preparation

2. Data cleaning

- The extracted data may have erroneous or missing entries.

Pre- Processing and Data preparation

2. Data cleaning

- Missing data
- Incorrect entries
- Scaling and normalization

Pre- Processing and Data preparation

2. Data cleaning

- Missing data
  - Are this missing values informative?
    - Yes. So, use it.
    - No.
      1. Eliminate the entry.
      2. Estimate the value, by find the model that describes the data.
      3. Use robust data mining methods that deal with missing values.

When working with time series, that has a temporal dependency, estimation is the usual process.

Pre- Processing and Data preparation

2. Data cleaning

- Incorrect entries
  - Inconsistency detection
    - If data is available from diferente sources, identify inconsistencies. (e.g. HR information from ECG and pletismography)
  - Domain knowledge
    - If data has requisites, evaluate them, e.g.: negative blood pressure value.
  - Outlier detection
    - Boxplot
    - Data distribution
    - Clustering
    - Distance base methods
    - Information theory models

Pre- Processing and Data preparation

2. Data cleaning

- Scaling and normalization
  - Data may present different scales, and therefore it is not comparable.
  - Also, some methods present inconsistencies when features have different scales. (e.g. distance base methods, results will be biased to the attribute with higher magnitude)
- Solution
  - Standardization
  - Min-Max scaler

$$y_i = \frac{x_i^j - \mu_j}{\sigma_j}$$

$$y_i = \frac{x_i^j - min_j}{max_j - min_j}$$

- Disadvantage
  - The physical meaning is lost.
  - When data present outliers, careful is needed in the application of min-max scaler.

Pre- Processing and Data preparation

3. Feature Selection and Transformation

Pre- Processing and Data preparation

3. Feature Selection and Transformation

- Usually implemented in the pre-processing step.
- Some analytical models, include the feature selection or a strategy to deal with high dimensional data.

- Goal:
  - Reduce the size of the data through:
    - feature subset selection;
    - data transformation.

- Consequence:
  - When the size of the data is reduced, the algorithms are generally more efficient.
  - Elimination of irrelevant features or irrelevant records improve the quality of the data mining process.

Pre- Processing and Data preparation

3. Feature Selection and Transformation

- Data sampling
  - The records from the underlying data are sampled to create a much smaller database.
- Feature selection
  - A subset of features is selected and used on the analytical process.
  - It depends on the problem and scientific question.
- Data reduction with axis rotation
  - Information between features (correlation, variance) is used to build a projection of the data in a new data space with smaller dimension.
- Data reduction with type transformation
  - Convert the data type to reduce its dimension.

Pre- Processing and Data preparation

3. Feature Selection and Transformation

- Data sampling
  - The main advantage of sampling is that it is simple, intuitive, and relatively easy to implement.
  - Select some data points from the entire sample.
- **Biased sampling:** If it is known that some parts of the data have more importance than others, sampling may intentionally select those subsets.
- **Stratified sampling:** When rare events are present on data, traditional sampling may neglect them. So sampling by strata, independently selecting samples based on a predefined proportion may solve that problem.

Pre- Processing and Data preparation

3. Feature Selection and Transformation

- Feature selection
  - Feature selection is primarily focused on removing non-informative or redundant predictors from the model.

Low information quantity, that may be evaluated for example by variance of the predictor.

Collinearity is the technical term for the situation where a pair of predictor variables have a substantial correlation with each other. It is also possible to have relationships between multiple predictors at once (called multicollinearity).

Pre- Processing and Data preparation

3. Feature Selection and Transformation

- **Wrapper methods:** Methods to find the optimal predictors combination to maximize model performance.
  - Computationally more heavy.
  - Risk of over-fitting.

- **Filter methods:** Evaluate the predictor relevance, and only the ones that pass a criteria will be included in the model.
  - Computationally more effective.
  - Selection criteria is not related to model effectiveness.
  - Most filter methods performs a univariable evaluation, missing predictors relations.

- **Unsupervised feature selection:** Removal of noisy or redundant predictors, by clustering.

Pre- Processing and Data preparation

3. Feature Selection and Transformation

- **Filter methods:**
  - Evaluate the ability of the features to significantly discriminate conditions. E.g.:
    - Hypothesis testing.

Pre- Processing and Data preparation

3. Feature Selection and Transformation

- Dimensionality reduction with axis rotation
  - Project the data in a new data space reducing the correlation between predictors.

Pre- Processing and Data preparation

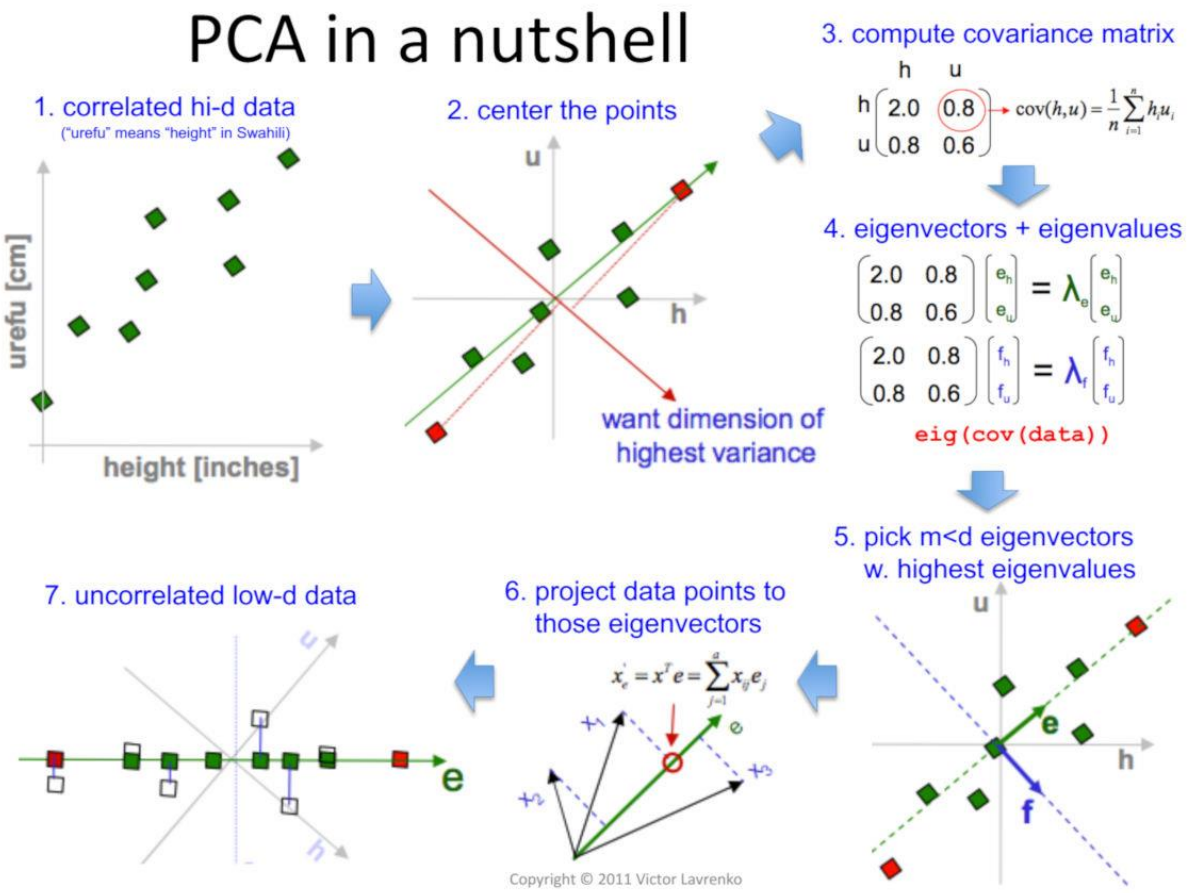
3. Feature Selection and Transformation

- **Principal component analysis (PCA):** The goal is to rotate the data into an axis-system where the greatest amount of variance is captured in a small number of dimensions.
  - Usually the method should be applied after mean centering of the data (subtracting the mean to each data point).
  - It is an orthogonal transformation of the data to convert a possibly correlated observations in a set of variables linearly non correlated called principal components.
  - The number of principal components is always smaller that the number of original variables.
  - The first PC is defined as the linear combination of the predictors that captures the most variability of all possible linear combinations. Then, subsequent PCs are derived such that these linear combinations capture the most remaining variability while also being uncorrelated with all previous PCs.
  - PCA is sensible to the scale of the original data.
  - PCA can be seen a trade-off between faster computation and less memory consumption versus information loss.

Pre- Processing and Data preparation

3. Feature Selection and Transformation

- **Principal component analysis (PCA):**



Pre- Processing and Data preparation

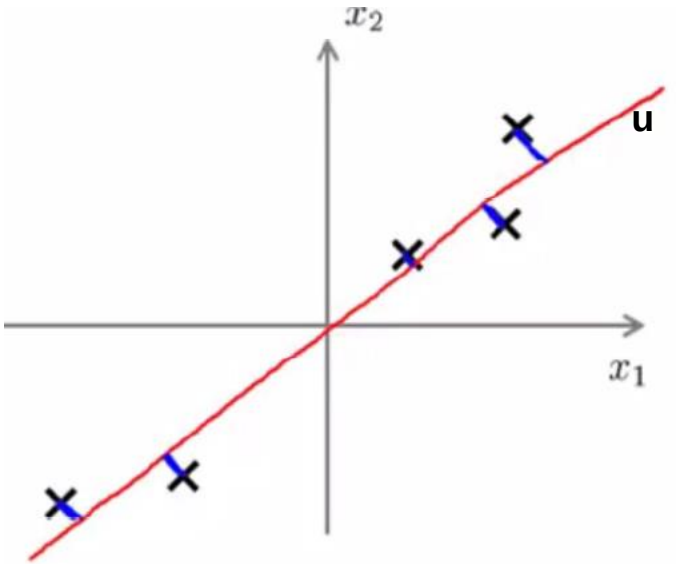
3. Feature Selection and Transformation

- **Principal component analysis (PCA):**
  - Drawbacks:
    - PCA works only if the observed variables are linearly correlated. If there's no correlation, PCA will fail to capture adequate variance with fewer components.
    - PCA is lossy. Information is lost when we discard insignificant components.
    - Scaling of variables can yield different results. Hence, scaling that you use should be documented. Scaling should not be adjusted to match prior knowledge of data.
    - Since each principal components is a linear combination of the original features, visualizations are not easy to interpret or relate to original features.

PRINCIPAL COMPONENT ANALYSIS (PCA)

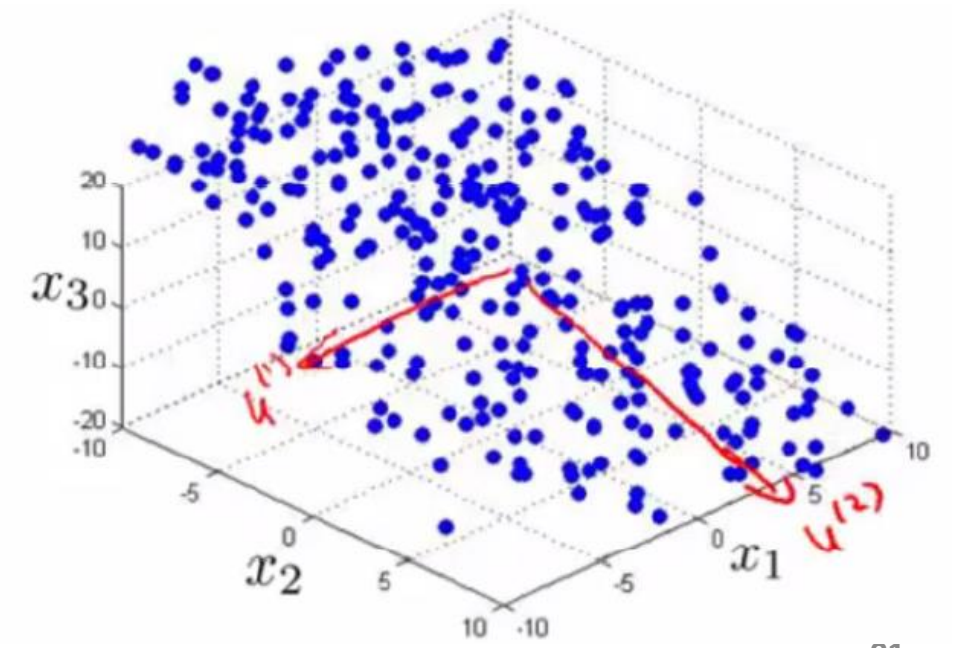
Reduce from 2D to 1D:

find the best direction (vector u) onto which to project data such that to minimize the projection error



Reduce from 3D to 2D:

find the orientation of the best plane (vectors u1, u2) onto which to project data such that to minimize the projection error



PCA – DATA PREPROCESSING (step 1)

Training set: $x^{(1)}, x^{(2)}, \ldots, x^{(m)}$

Preprocessing (feature scaling/mean normalization):

$$\mu_j = \frac{1}{m} \sum_{i=1}^{m} x_j^{(i)}$$

Replace each $x_j^{(i)}$ with $x_j - \mu_j$.

Thus, all features have zero mean !

If the features have significantly different range of values, normalize them., e.g. in the interval [0,1] or [-1,1] or mean=0 & std=1

matrix X (mxn)	feature x_1	feature x_2	.....	feature x_n
Example 1	$x_1^{(1)}$	$x_2^{(1)}$		$x_n^{(1)}$
Example 2	$x_1^{(2)}$	$x_2^{(2)}$		$x_n^{(2)}$
...				
Example i	$x_1^{(i)}$	$x_2^{(i)}$		$x_n^{(i)}$
...				
...				
Example m	$x_1^{(m)}$	$x_2^{(m)}$		$x_n^{(m)}$

DATA NORMALIZATION

from sklearn.preprocessing import MinMaxScaler

```
mms = MinMaxScaler()
mms.fit(data)
data_transformed = mms.transform(data)
```

MinMaxScaler?

MinMaxScaler(feature_range=(0, 1), copy=True)

Transforms features by scaling each feature to a given range.

from sklearn.preprocessing import StandardScaler

```
sc=StandardScaler()
sc.fit(data)
data_transformed =sc.transform(data)
```

Standardize features by removing the mean and scaling to unit variance.

PCA – Singular Value Decomposition (step 2)

- Compute Covariance matrix of the mean normalized data matrix *X* (dimension *mxn* - m examples, n features):

$$\mathbf{Cov = X^T * X \,/ m}$$

- Compute Singular Value Decomposition(SVD) of Covariance matrix:

$$\mathbf{Cov = U * S * V}$$

U (*nxn*) - matrix of eigenvectors:

$$U = \begin{bmatrix} | & | & & | \\ u^{(1)} & u^{(2)} & \dots & u^{(n)} \\ | & | & & | \end{bmatrix} \in \mathbb{R}^{n \times n}$$

S (*nxn*)– diagonal matrix of singular values in decreasing order:

$$S_{nxn} = \begin{bmatrix} S_{11} & 0 & \cdots & 0 \\ 0 & S_{22} & \vdots & \vdots \\ \vdots & \vdots & \ddots & 0 \\ 0 & \cdots & 0 & S_{nn} \end{bmatrix}$$

SVD is equivalent to eigen-values/eigen-vector decomposition.

PCA

The projection vectors are the first k columns of U (k<n): -***Task 1***

$$U = \begin{bmatrix} | & | & & | \\ u^{(1)} & u^{(2)} & \cdots & u^{(n)} \\ | & | & & | \end{bmatrix} \in \mathbb{R}^{n \times n} \qquad Ureduce_{nxk} = U(:, 1:k)$$

Step 3: Compute the new (projected) data matrix Z (m examples, k features): - ***Task 2***

$$Z_{mxk} = X_{mxn} * Ureduce_{nxk}$$

Step 4: Reconstruct data matrix X from the projected Z matrix :

$$X_{approx(mxn)} = Z_{mxk} * Ureduce^{T}_{kxn}$$

Choosing k (number of principal components)

Average squared approximation error:

$$\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)} - x_{approx}^{(i)}\|^2$$

Total data variation:

$$\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)}\|^2$$

Typically, choose k to be smallest value so that

$$\frac{\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)} - x_{approx}^{(i)}\|^2}{\frac{1}{m}\sum_{i=1}^{m}\|x^{(i)}\|^2} \leq 0.01 \qquad (1\%)$$

"99% of variance is retained"

(typically the desired retained variance is between 90-99%)

PCA – summary

PCA is used to reduce the dimensionality of the original feature space and, at the same time, to maximise the orthogonality between the features in the transformed feature space.

The new set of features obtained through the PCA process are the principal components, which are computed by applying a linear transform to the original features.

Such principal components correspond to largest eigenvalues of the co-variance matrix of features. Then a reduced set of principal components can be used to reconstruct most of the original data with maximum variance, thus keeping most of its information.

The orthogonality between components ensures decorrelation in the transformed feature space.

SUPERVISED vs. UNSUPERVISED LEARNING

Supervised Learning - (given DATA + LABELS):
ML method is trained with labeled data to predict the labels of new examples (learning by labeled examples)

Matrix X	feature x_0	feature x_1	.....	feature x_n	Vector y - output (label)
Example 1	1	$x^{(1)}$		$x_n^{(1)}$	$y^{(1)}$
Example 2	1	$x^{(2)}$		$x_n^{(2)}$	$y^{(2)}$
	1				
				$x_n^{(i)}$	
Example m	1	$x^{(m)}$		$x_n^{(m)}$	$y^{(m)}$

Unsupervised Learning - given UNLABELED DATA
ML method to discover the data internal (statistical) structure

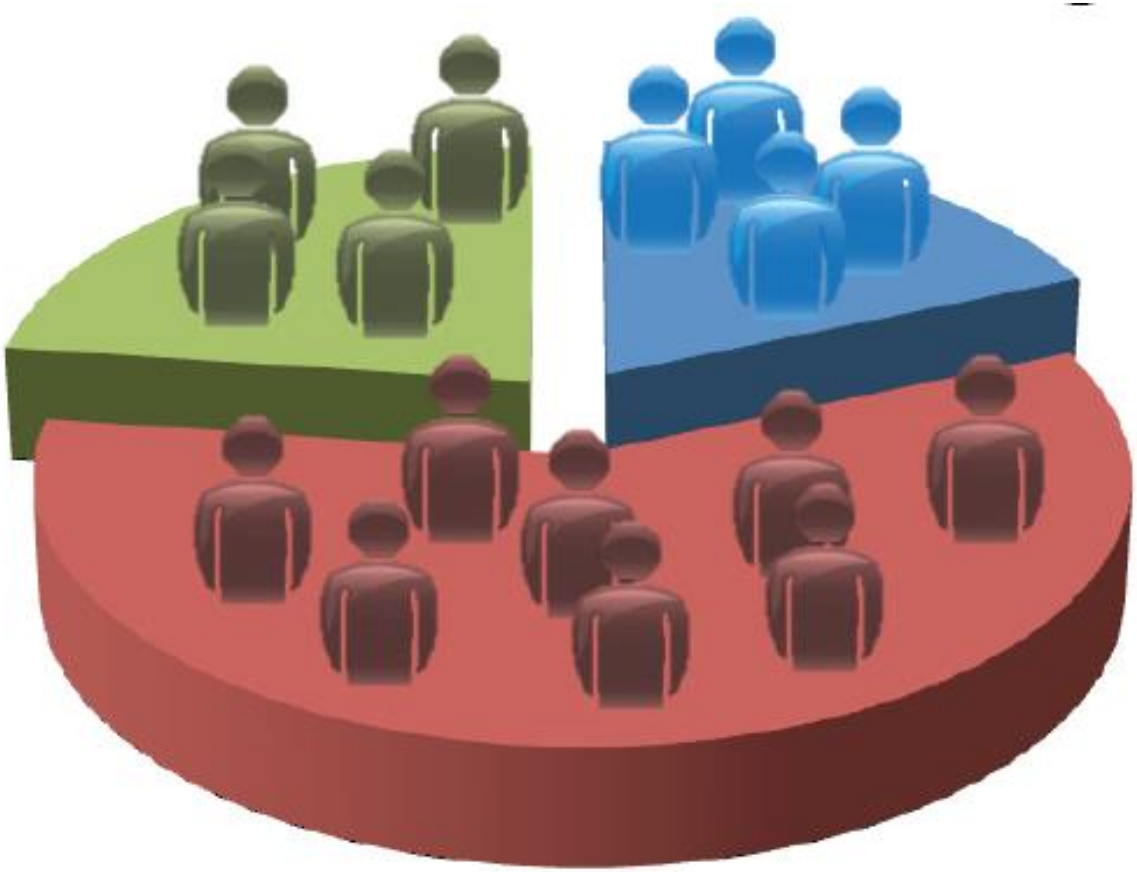
Matrix X	feature x_1	feature x_2	.....	feature x_n
Example 1	$x_1^{(1)}$	$x_2^{(1)}$		$x_n^{(1)}$
Example 2	$x_1^{(2)}$	$x_2^{(2)}$		$x_n^{(2)}$
...				
Example i	$x_1^{(i)}$	$x_2^{(i)}$		$x_n^{(i)}$
...				
...				
Example m	$x_1^{(m)}$	$x_2^{(m)}$		$x_n^{(m)}$

Semi-Supervised Learning – mixture of labeled and unlabeled data

Unsupervised learning -

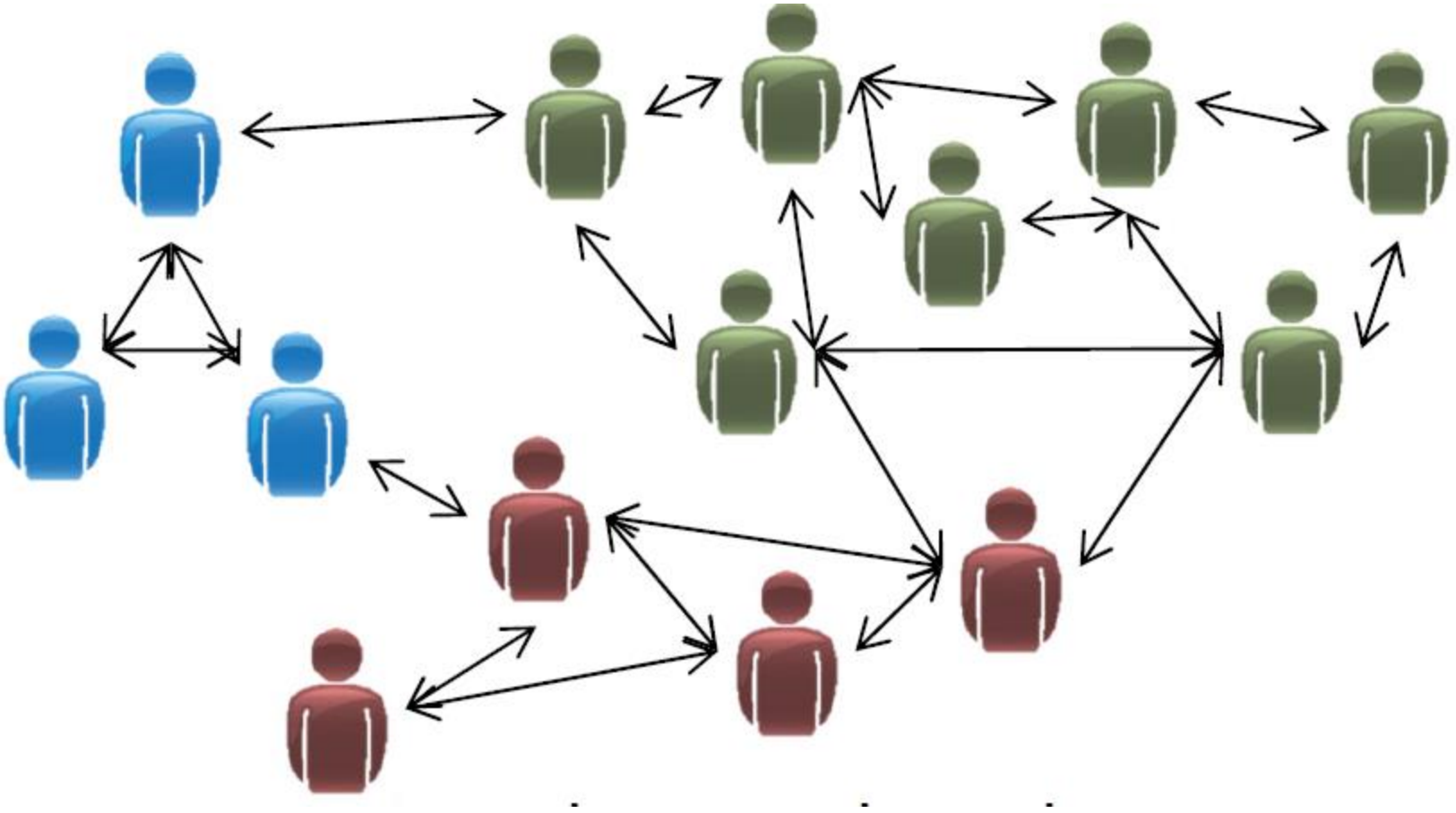
Market segmentation: data base of customers => division in target groups

Features: education, job, age, marital status, etc.

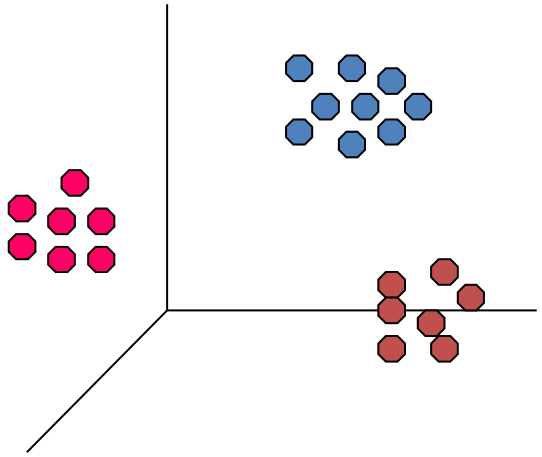


Unsupervised learning

Social network analysis: user grouping, group-specific advertising



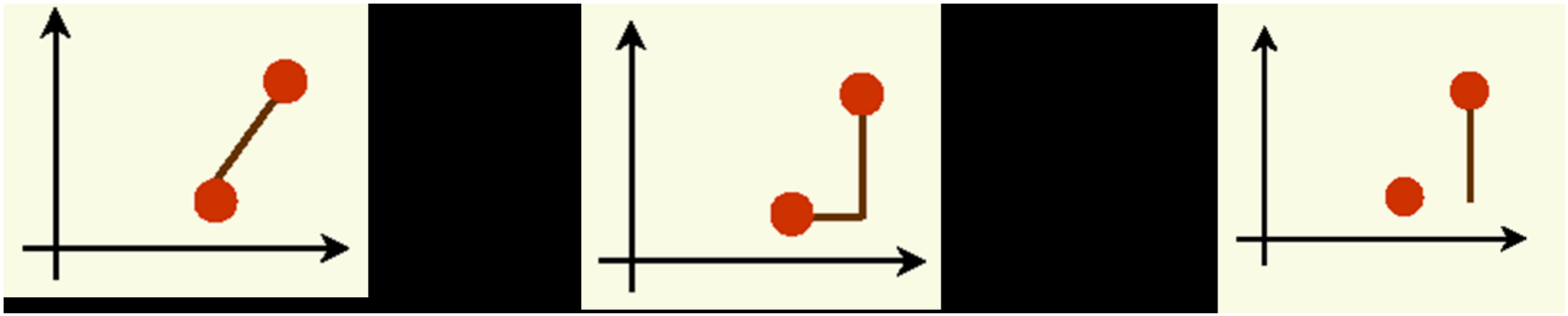
Clustering intuition



- Given a set of not labeled examples
- Find a relevant grouping of the examples into clusters such that:
  - Examples in the same cluster have **high similarity**
  - Examples from different clusters have **high dissimilarity**

Similarity measures –
Euclidian distance; Chebyshev distance; Manhattan distance

Distance (similarity) measures



Euclidian Distance (L2 norm)

$$d(p,q) = \sqrt{(x_p - x_q)^2 + (y_p - y_q)^2}$$

Manhattan Distance (L1 norm)

$$d(p,q) = |x_p - x_q| + |y_p - y_q|$$

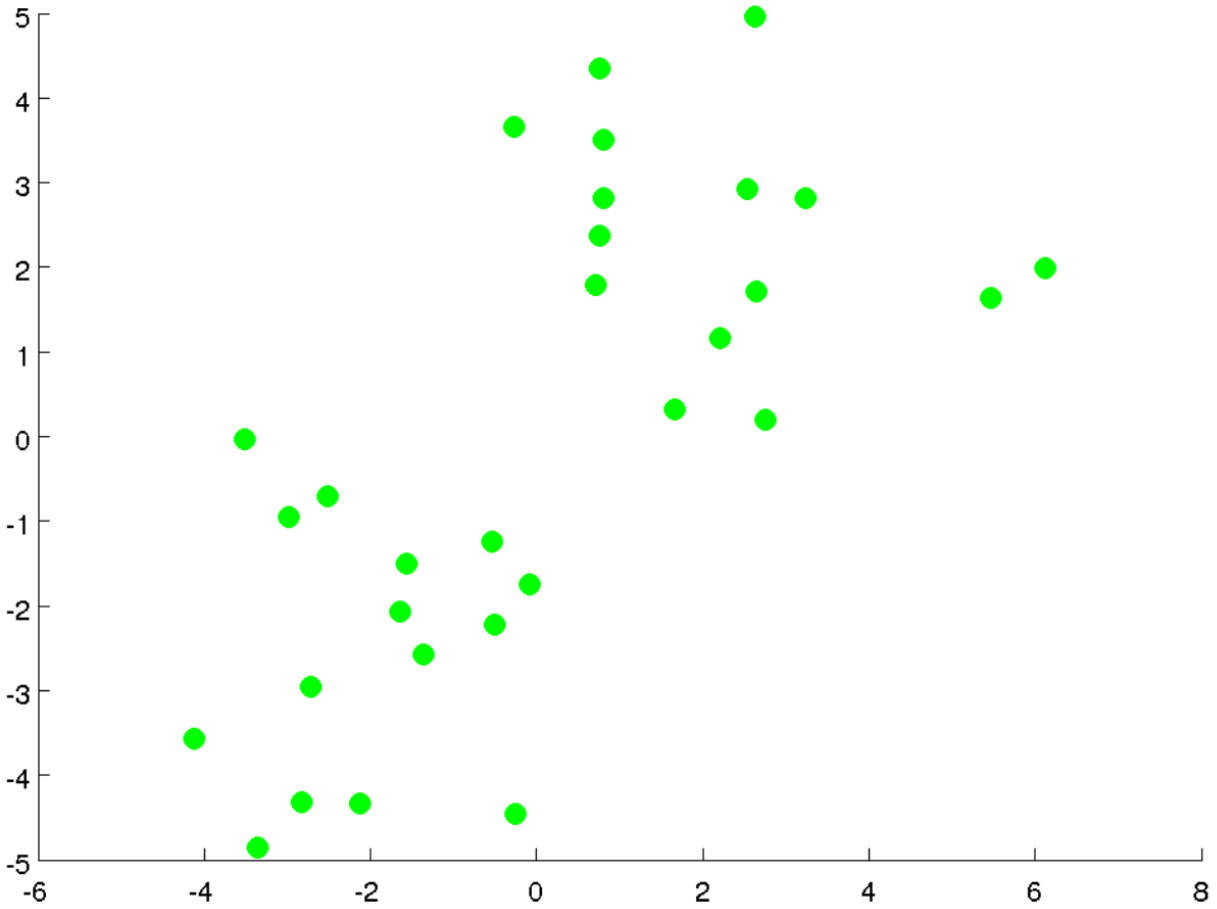
Chebyshev distance

$$d(p,q) = \max|(x_p - x_q), (y_p - y_q)|$$

K-means algorithm

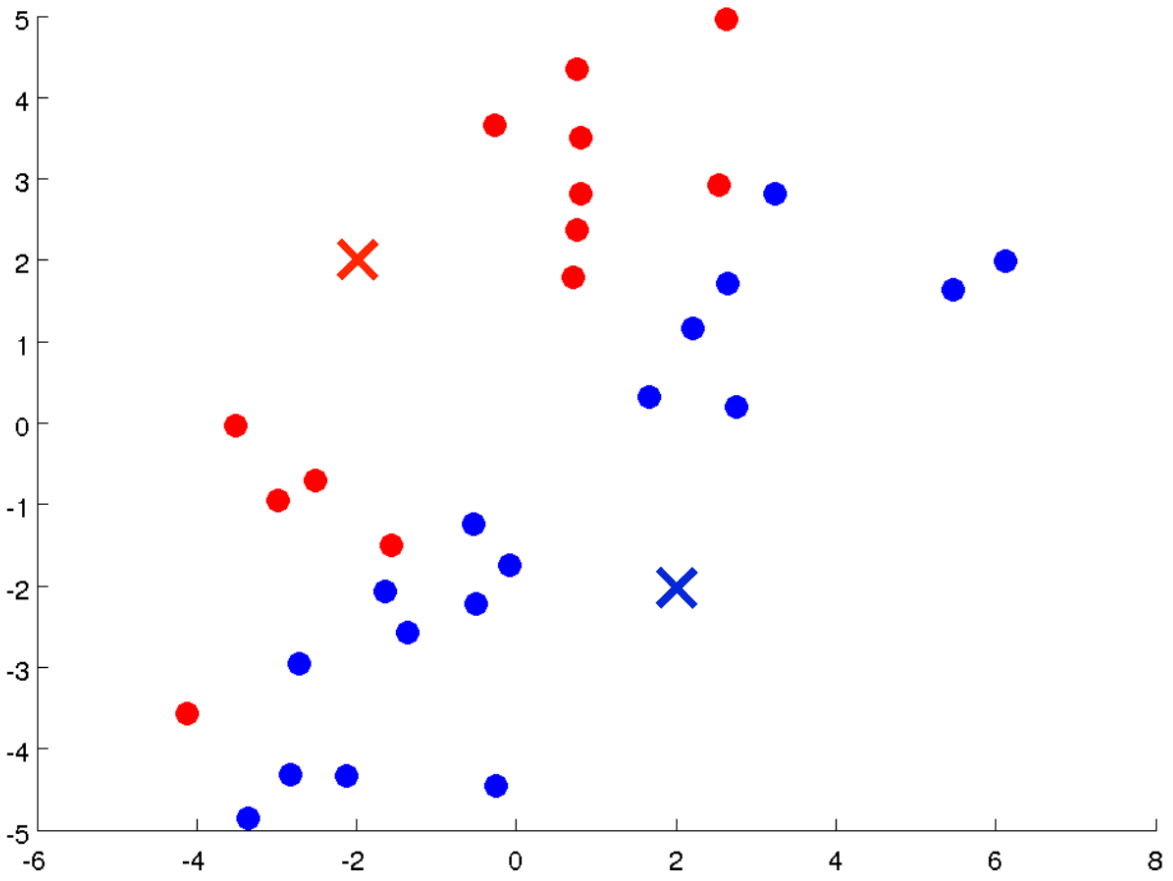
Given:

- **K – the number of clusters**
- **Training set - no labels**



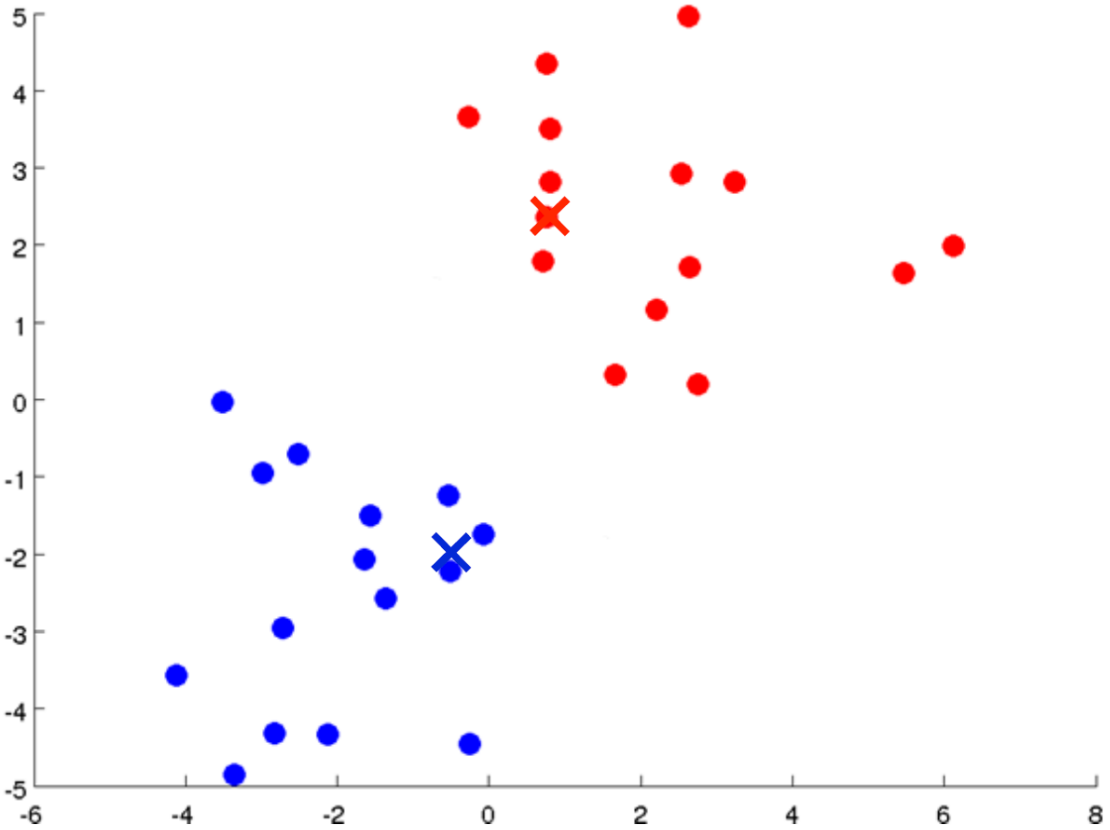
K-means algorithm

Randomly initialize K cluster centroids (e.g. K=2)
Assign data points to their closest centroid (Euclidian distance)



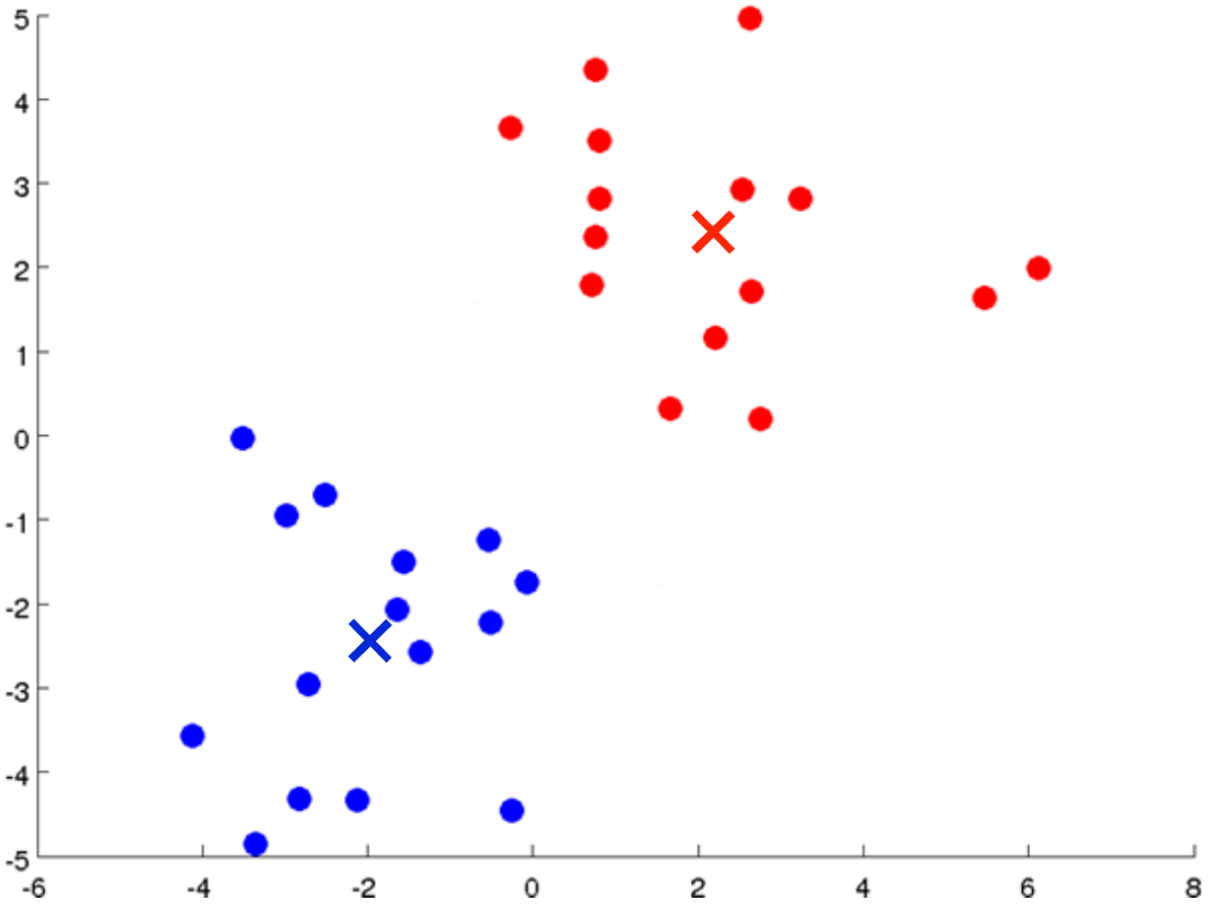
K-means algorithm

Compute new centroids = mean of the points assigned to that cluster.
Assign data points to the new closest centroid.



K-means algorithm

Repeat until convergence



K-means algorithms

Input:
- K (number of clusters)
- Training set (no labels)

Cluster assignment => step

Move centroid => step

Randomly initialize K cluster centroids $\mu_1, \mu_2, \ldots, \mu_K \in \mathbb{R}^n$

Repeat {

for i = 1 to m

$c^{(i)}$:= index (from 1 to K) of cluster centroid closest to $x^{(i)}$

for k = 1 to K

μ_k := average (mean) of points assigned to cluster k

}

K-means optimization objective (distortion = average distance)

$$J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K) = \frac{1}{m} \sum_{i=1}^{m} ||x^{(i)} - \mu_{c^{(i)}}||^2$$

$$\min_{\substack{c^{(1)}, \ldots, c^{(m)}, \\ \mu_1, \ldots, \mu_K}} J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K)$$

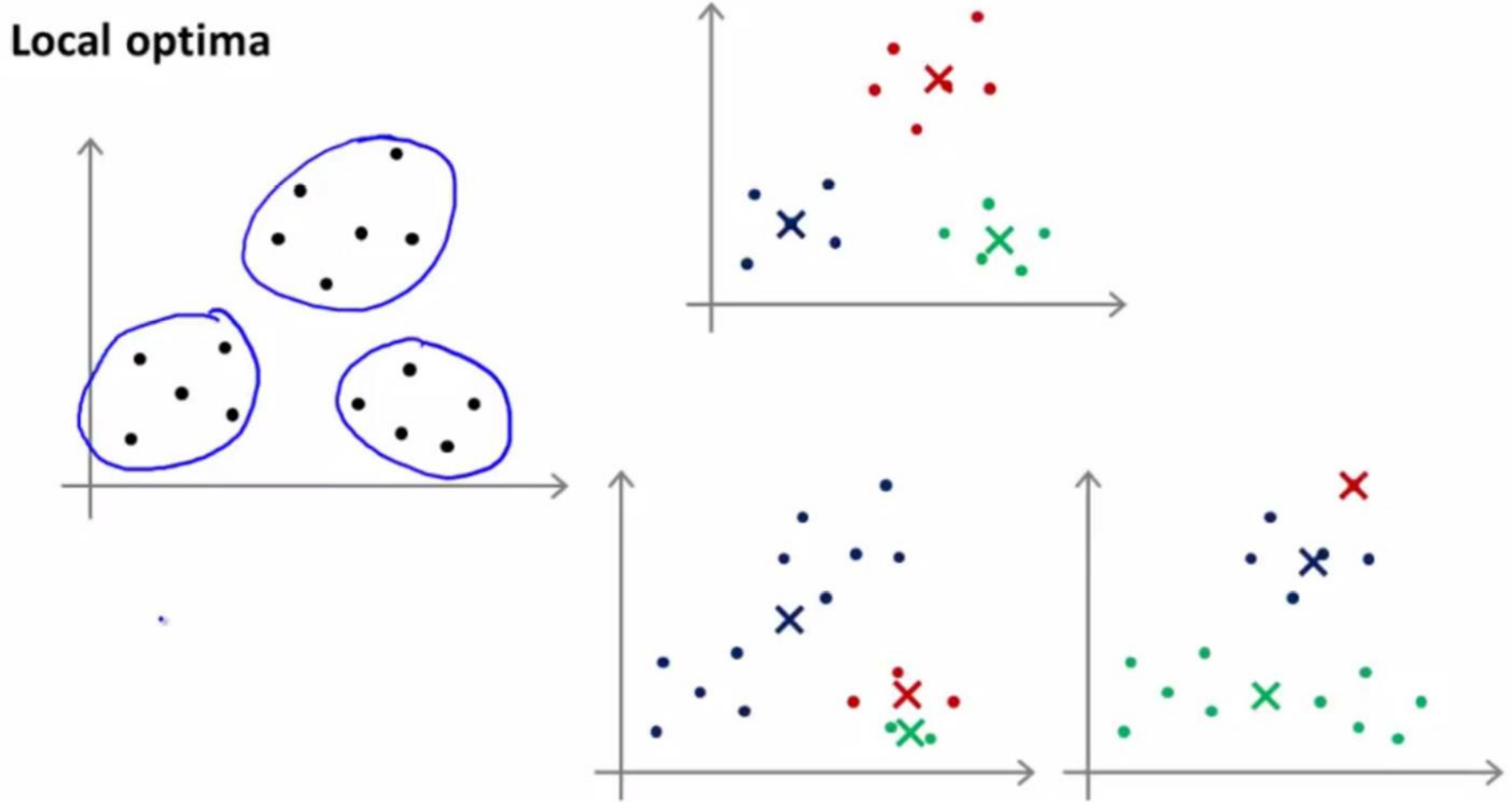
Stop K-means learning (different criteria):

- Achieved Max number of iterations
- J < some threshold
- No improvement of *J* between subsequent iterations

Single (Random) Initialization

Choose number of clusters K

Inicialize K cluster centroids = randomly picked K training examples



Repeat Random Initializations

For i = 1 to 100 {

Randomly initialize K-means.

Run K-means. Get $c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K$.

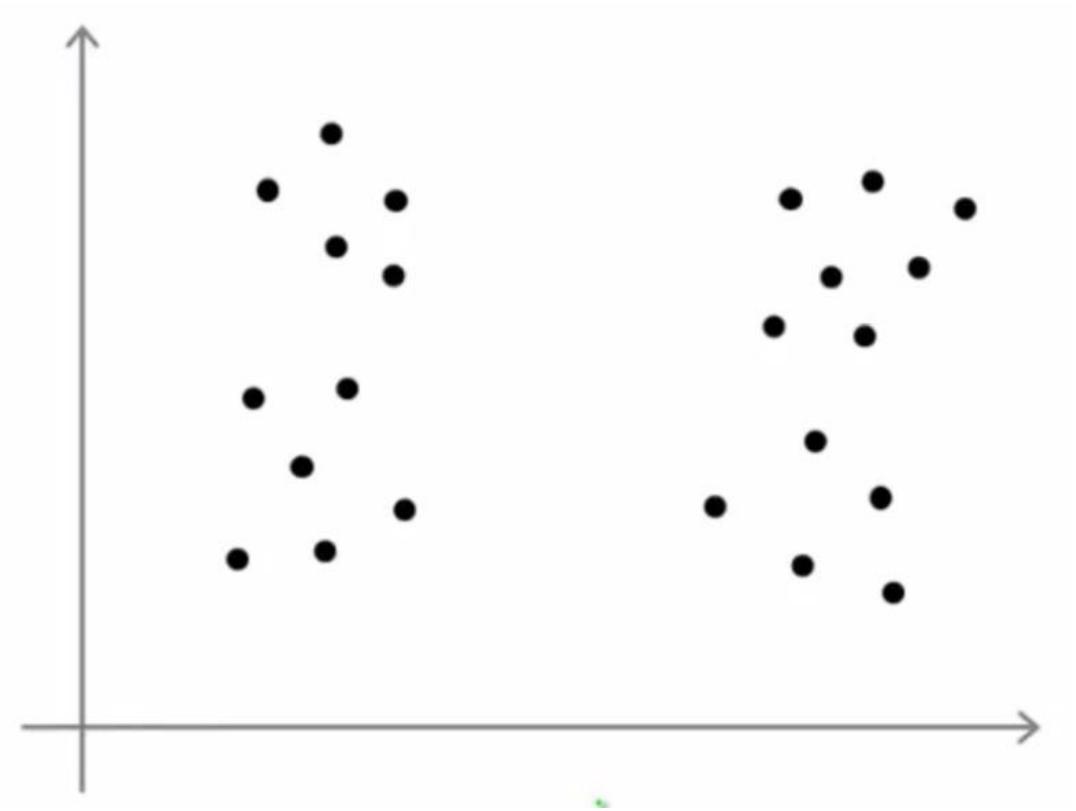
Compute cost function (distortion)

$J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K)$

}

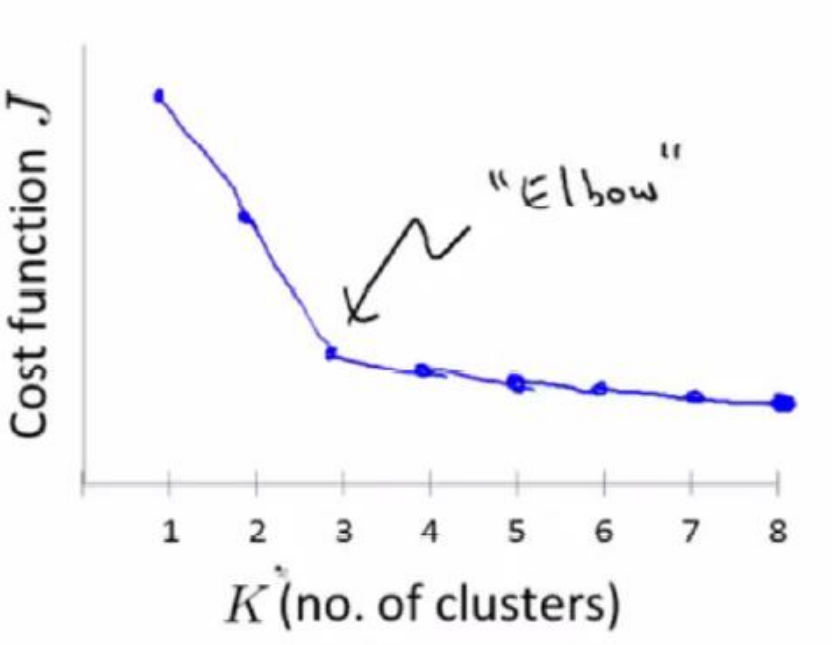
Pick clustering that gave lowest cost $J(c^{(1)}, \ldots, c^{(m)}, \mu_1, \ldots, \mu_K)$

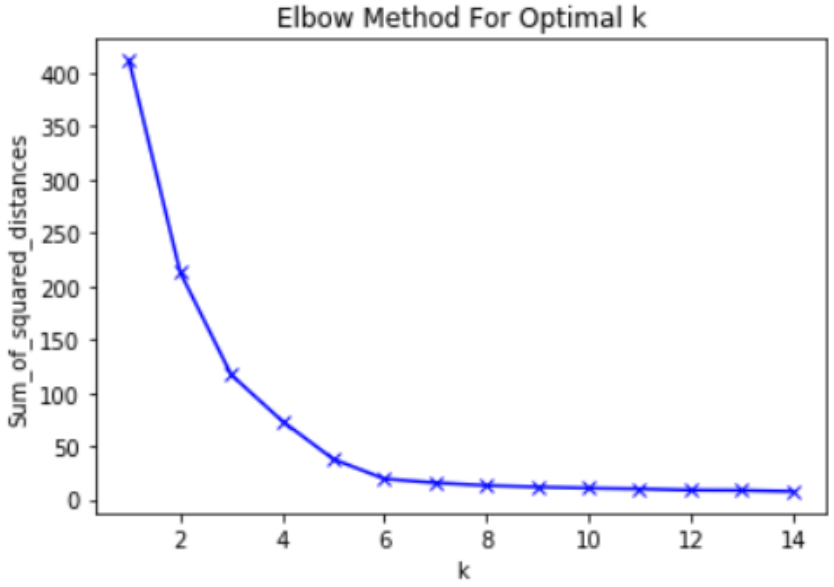
How to Choose # of clusters



- Choose K by data visualisation (if possible)
- Ask domain experts (highly recommendable) , e.g. anomaly detection (experts should know how many types of anomalies are expected)
- Choose K automatically (e.g. Elbow method)

Choosing the number of clusters (Elbow method)

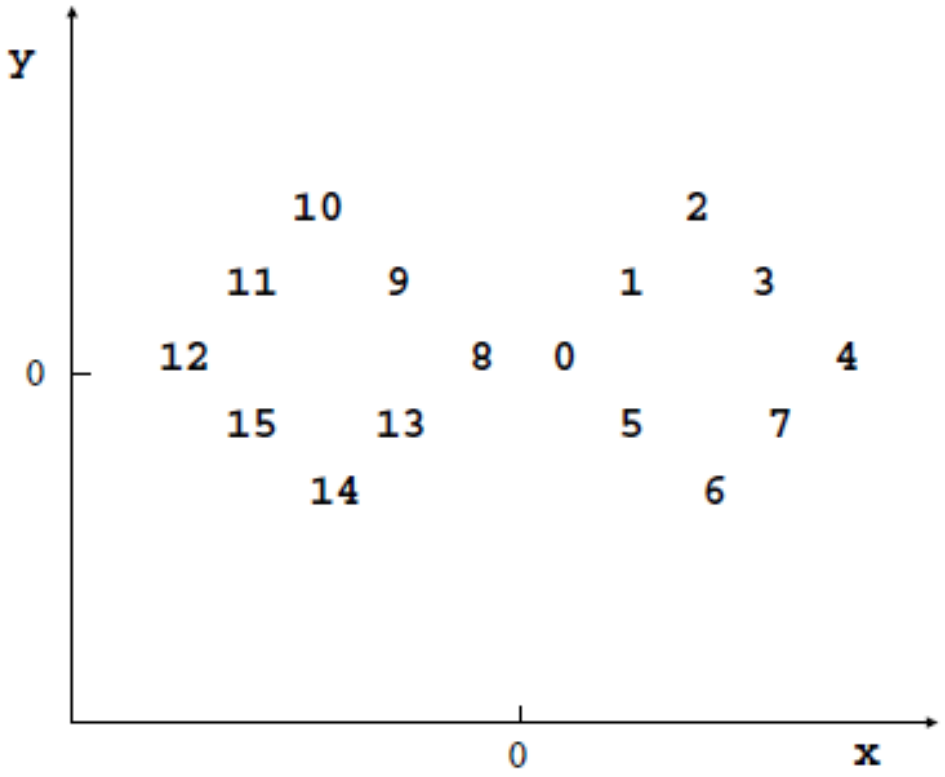




Tutorial: How to determine the optimal number of clusters for k-means clustering | by Tola Alade | Cambridge Spark
https://blog.cambridgespark.com/how-to-determine-the-optimal-number-of-clusters-for-k-means-clustering-14f27070048f

K-MEANS CLUSTERING – Example

Id	x	y
0:	1.0	0.0
1:	3.0	2.0
2:	5.0	4.0
3:	7.0	2.0
4:	9.0	0.0
5:	3.0	-2.0
6:	5.0	-4.0
7:	7.0	-2.0
8:	-1.0	0.0
9:	-3.0	2.0
10:	-5.0	4.0
11:	-7.0	2.0
12:	-9.0	0.0
13:	-3.0	-2.0
14:	-5.0	-4.0
15:	-7.0	-2.0

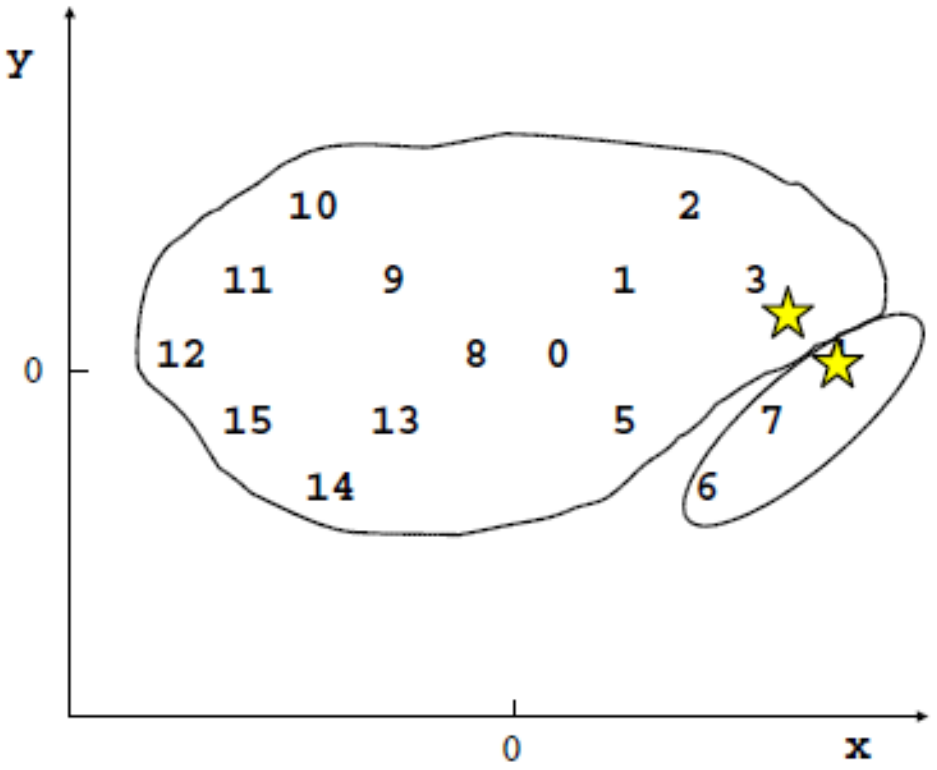


- find the best 2 clusters

K-MEANS CLUSTERING – Example

Seed: (9 0) (8 1)

Clustering: (4 6 7) (0 1 2 3 5 8 9 10 11 12 13 14 15)
Cluster Centers: (7.0 -2.0) (-1.61538 0.46153)
Average Distance: 4.35887



K-MEANS CLUSTERING – Example

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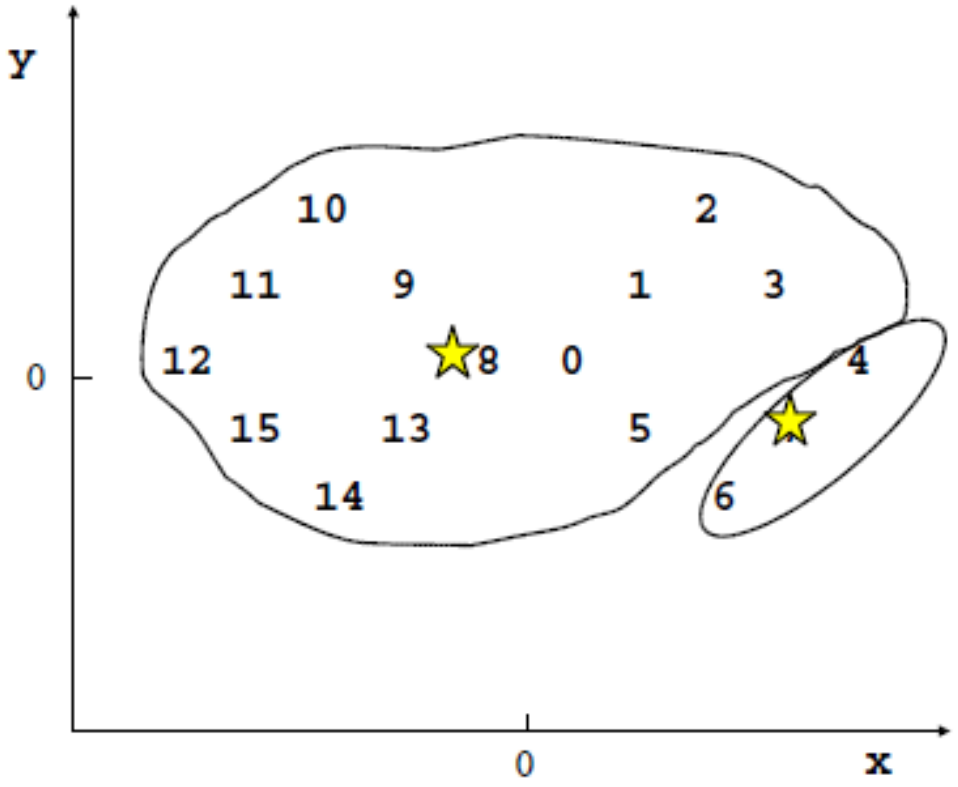
Clustering: (2 3 4 5 6 7) (0 1 8 9 10 11 12 13 14 15)



K-MEANS CLUSTERING – Example

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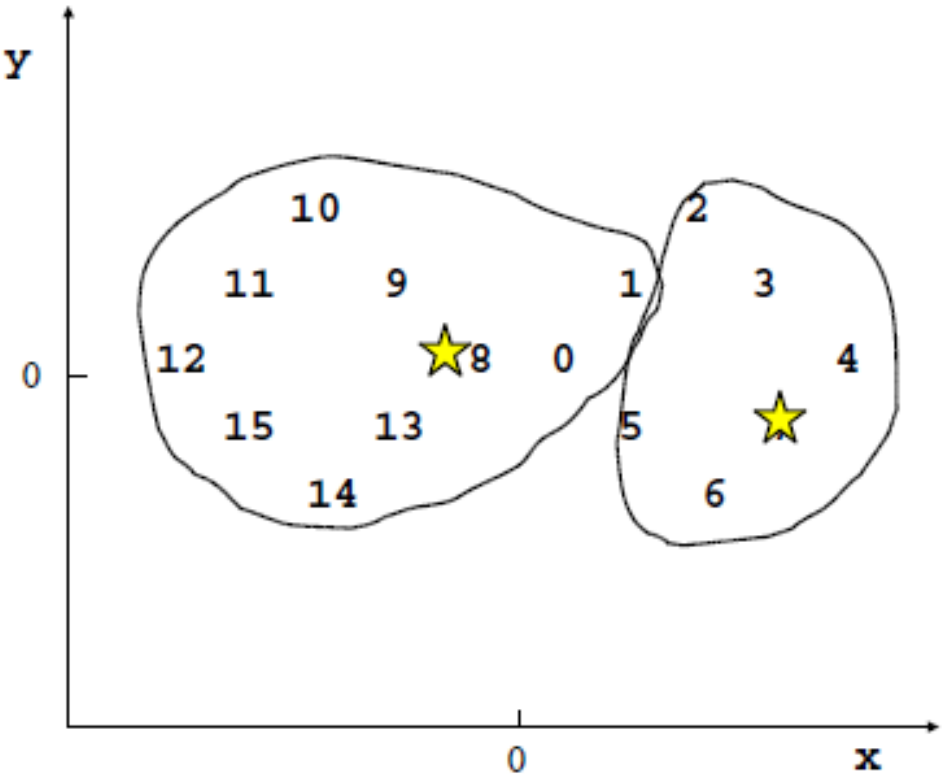
Average Distance: 4.35887

Clustering: (2 3 4 5 6 7) (0 1 8 9 10 11 12 13 14 15)
Cluster Centers: (6.0 -0.33334) (-3.6 0.2)
Average Distance: 3.6928



K-MEANS CLUSTERING – Example

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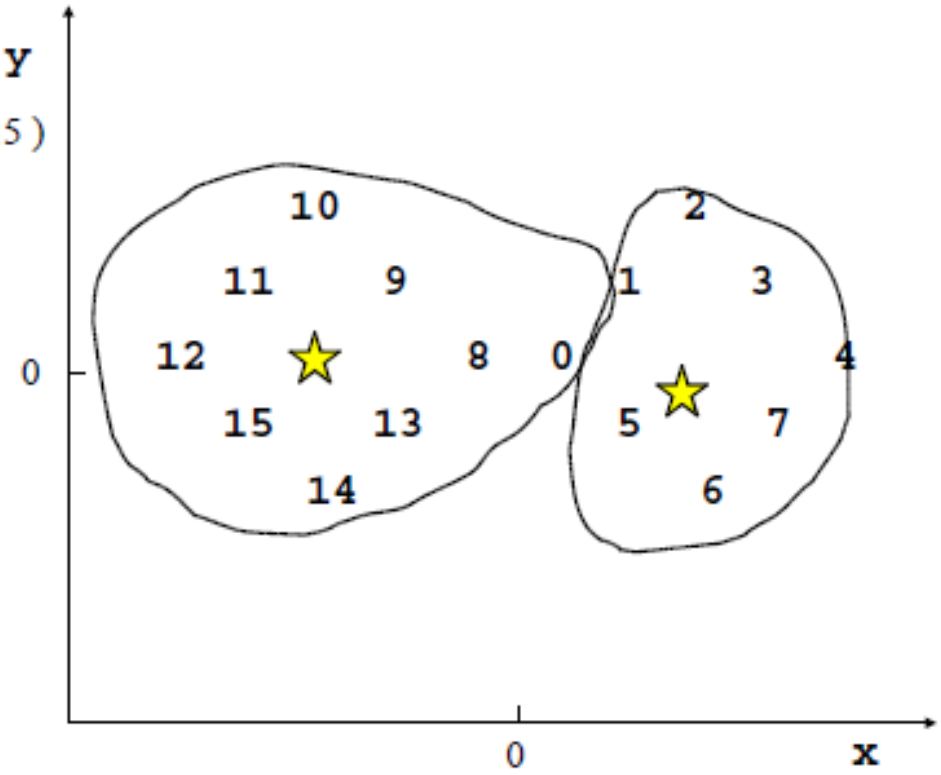
Clustering: (2 3 4 5 6 7) (0 1 8 9 10 11 12 13 14 15)
Cluster Centers: (6.0 -0.33334) (-3.6 0.2)
Average Distance: 3.6928

Clustering: (1 2 3 4 5 6 7) (0 8 9 10 11 12 13 14 15)



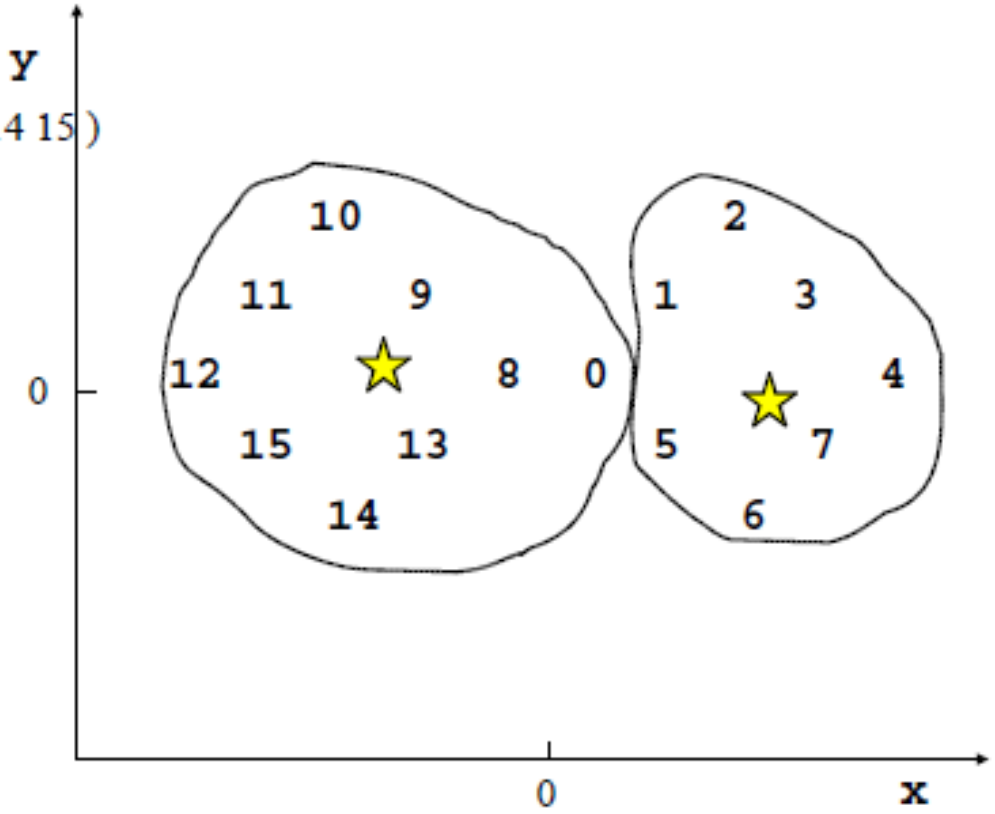
K-MEANS CLUSTERING – Example

Seed: (9 0) (8 1)

Clustering: (4 6 7) (0 1 2 3 5 8 9 10 11 12 13 14 15)
Cluster Centers: (7.0 -2.0) (-1.61538 0.46153)
Average Distance: 4.35887

Clustering: (2 3 4 5 6 7) (0 1 8 9 10 11 12 13 14 15)
Cluster Centers: (6.0 -0.33334) (-3.6 0.2)
Average Distance: 3.6928

Clustering: (1 2 3 4 5 6 7) (0 8 9 10 11 12 13 14 15)
Cluster Centers: (5.57143 0.0) (-4.33334 0.0)
Average Distance: 3.49115



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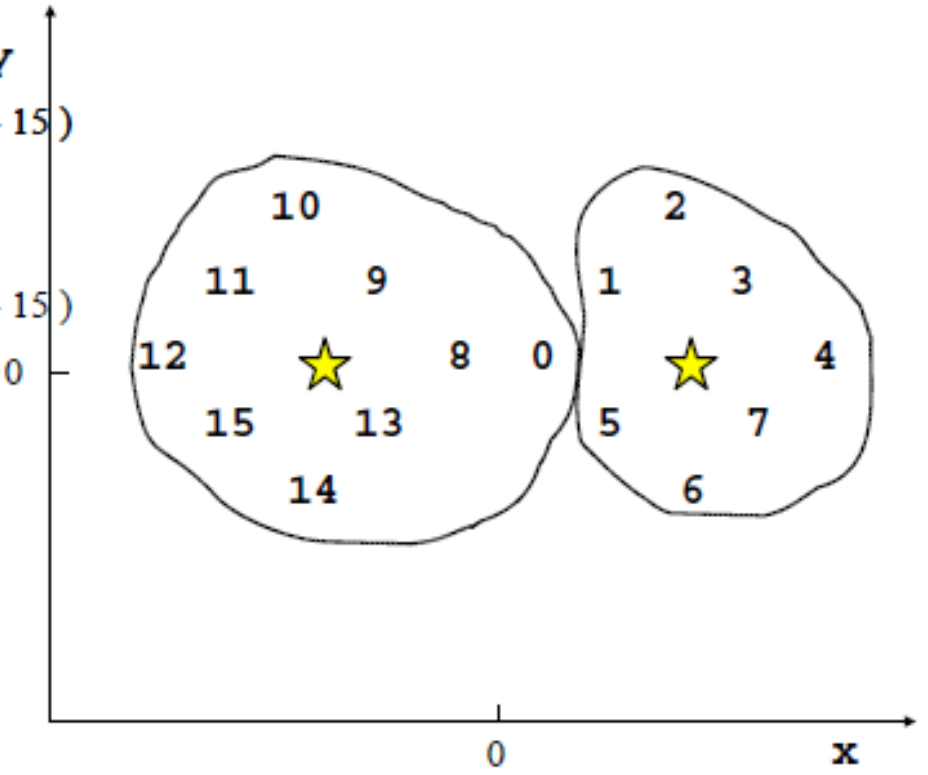

K-MEANS CLUSTERING – Example

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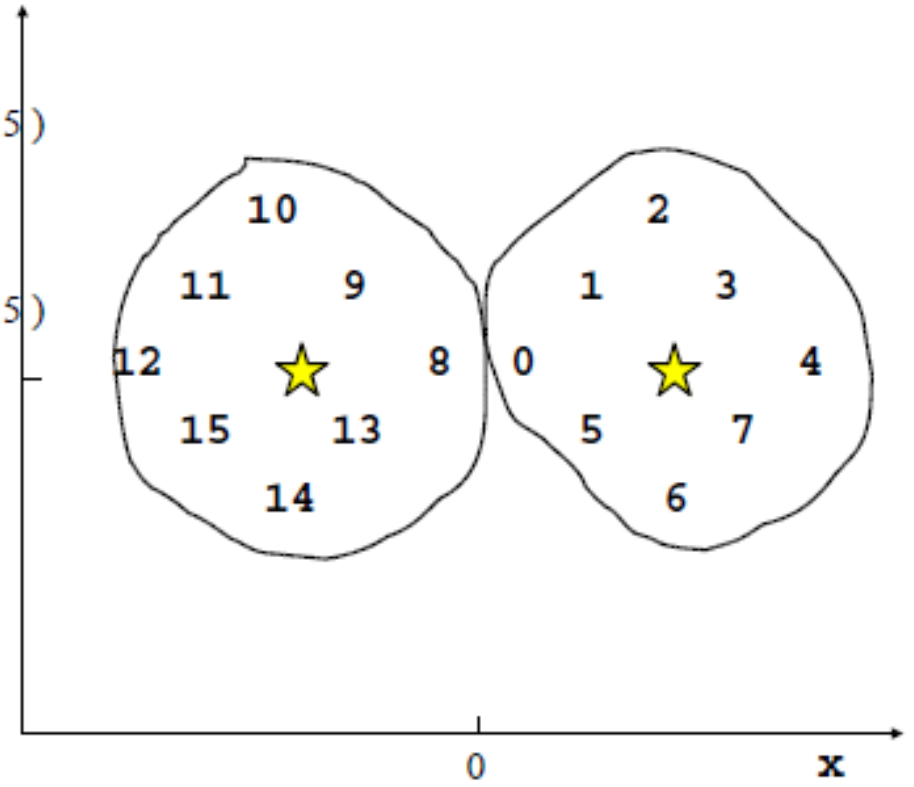
Average Distance: 3.49115

Clustering: (0 1 2 3 4 5 6 7) (8 9 10 11 12 13 14 15)
Cluster Centers: (5.0 0.0) (-5.0 0.0)
Average Distance: 3.41421



K-MEANS CLUSTERING – Example

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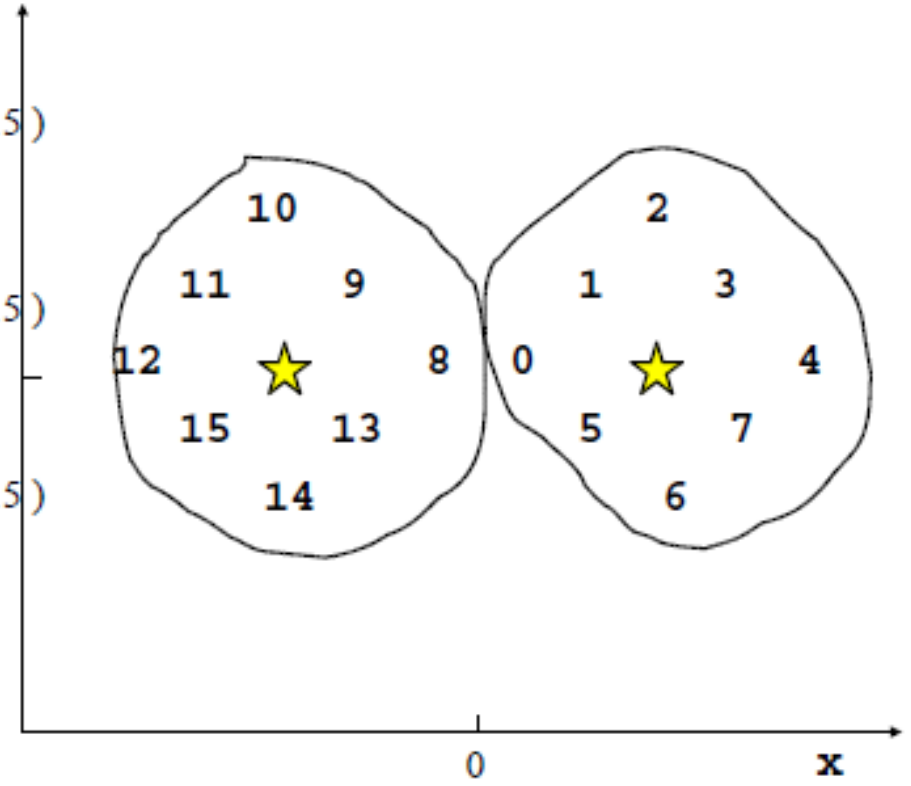
Average Distance: 3.49115

Clustering: (0 1 2 3 4 5 6 7) (8 9 10 11 12 13 14 15)
Cluster Centers: (5.0 0.0) (-5.0 0.0)
Average Distance: 3.41421

Clustering: (0 1 2 3 4 5 6 7) (8 9 10 11 12 13 14 15)
No improvement.



K-MEANS -summary

- The most popular clustering method.
- Need to know K.
- May converge to a Local Minimum .
- High number of computations.

K-means for dimensionality reduction

dimensionality reduction is useful for:

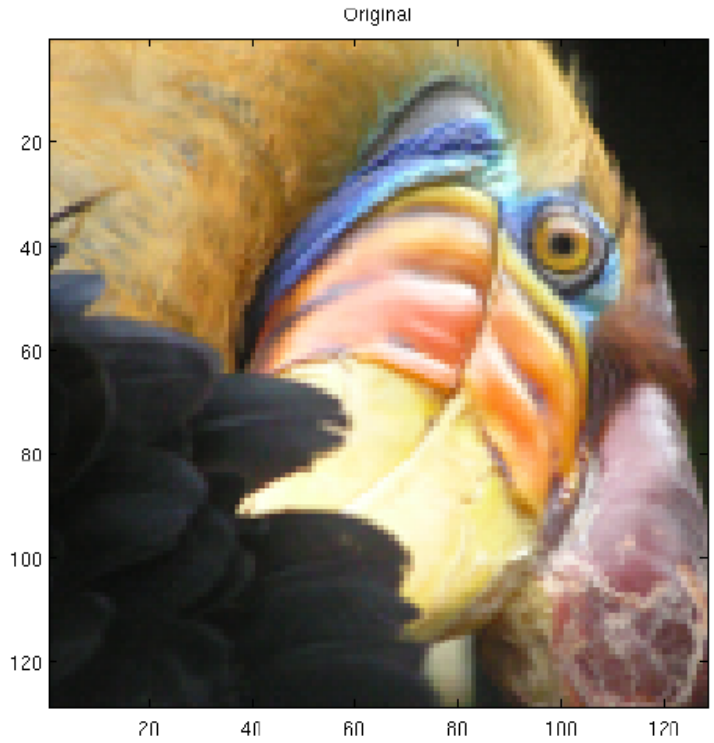
Data compression (from 10000-1000 D to) 100 D

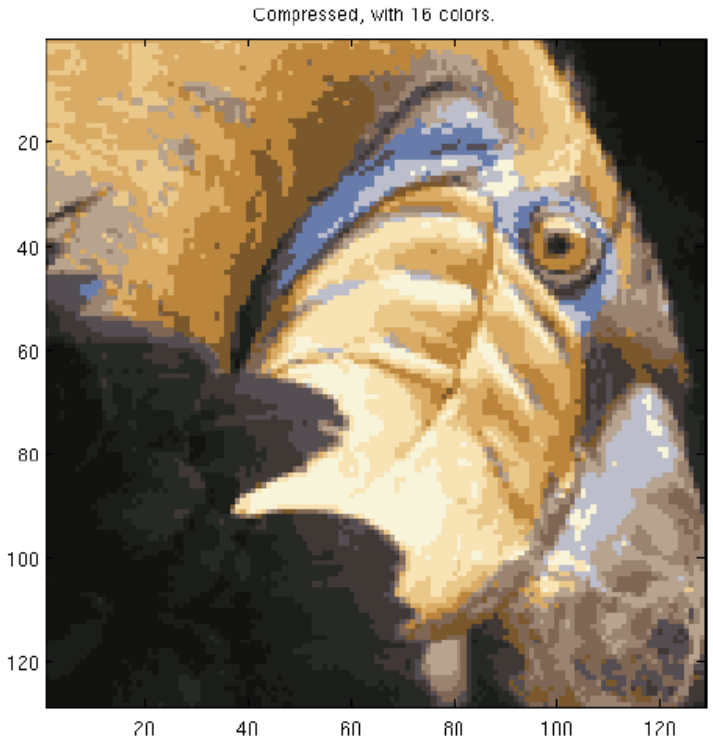
Reduce memory/ disk needed to store data
Speed up learning algorithm

Data visualization (from 100-50D to 2-3D)

Image compression with K-means

RGB image: 3*8 bits/pixel Compressed image:16 colors(clusters) => 4 bits

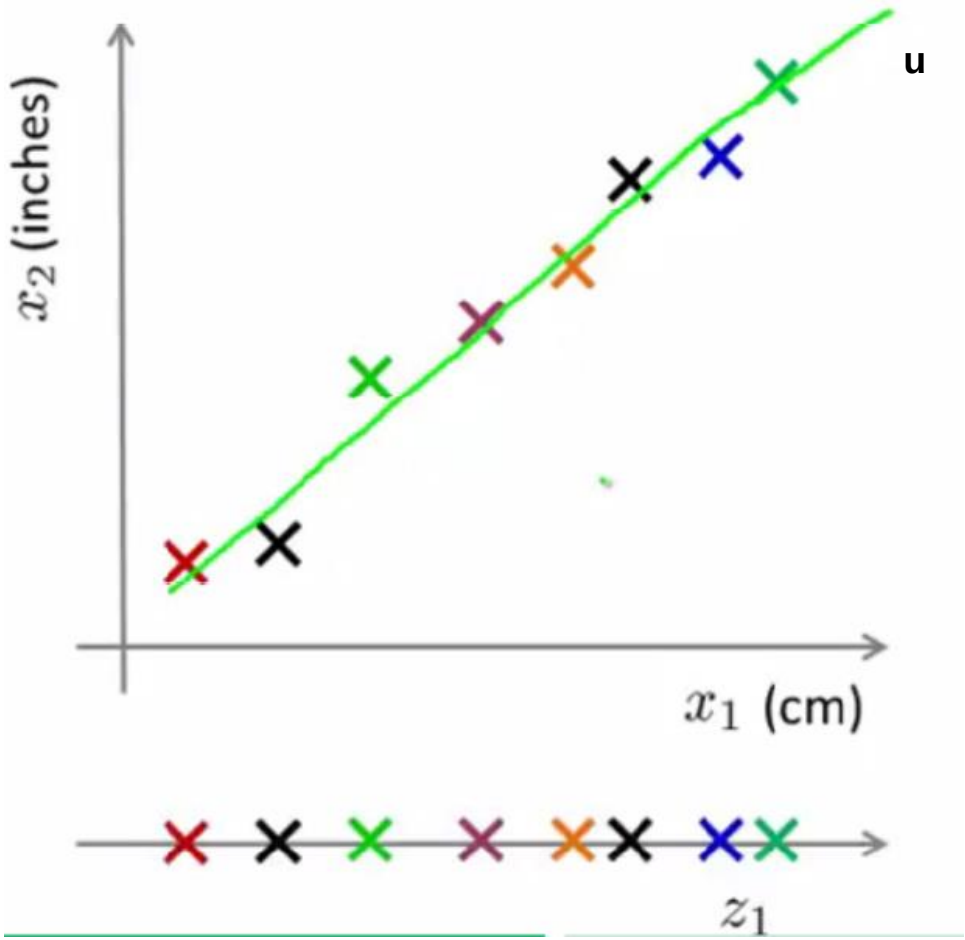




DATA COMPRESSION

Example: reduce data from 2D to 1D

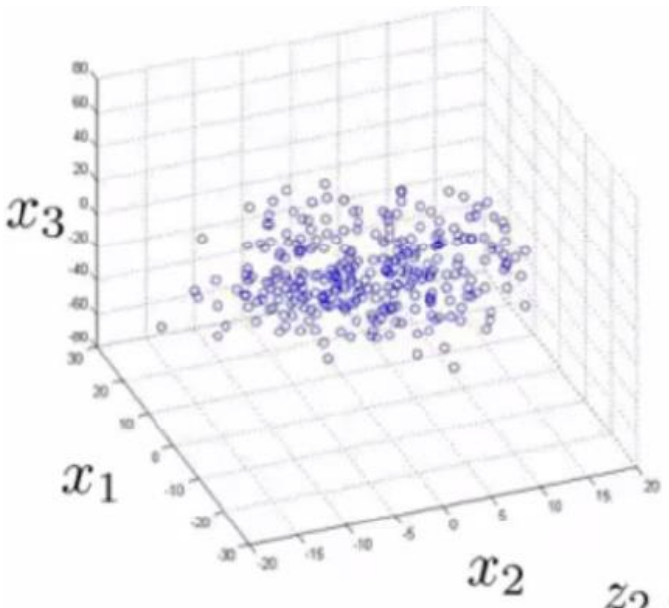
If 2D data is located along a line, the second dimension is redundant

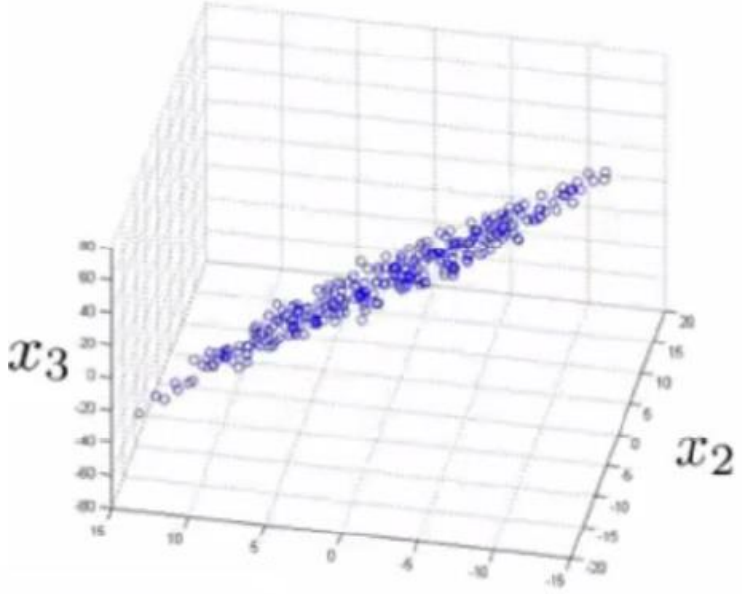


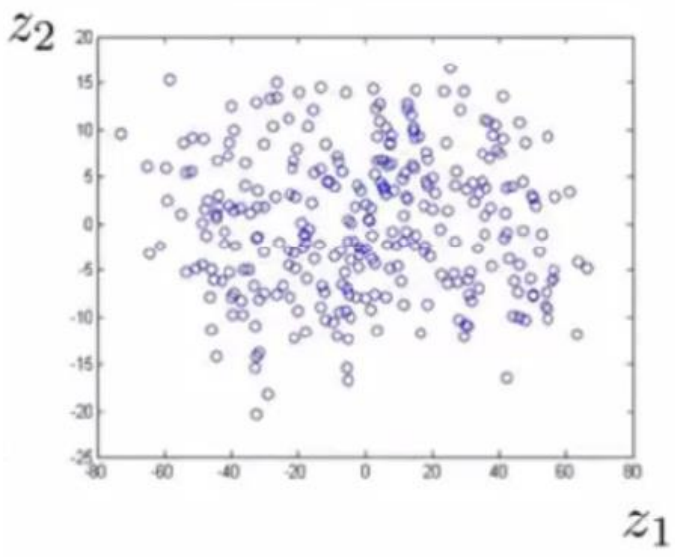
DATA COMPRESSION

Example: reduce data from 3D to 2D

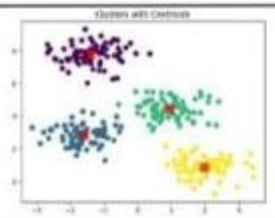
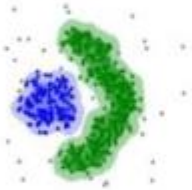
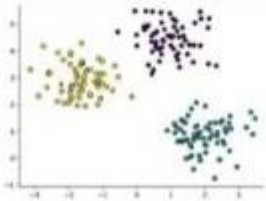
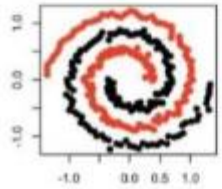
If 3D data is located along a plane, the 3rd dimension is redundant







Other Clustering Techniques

Representation	Algorithm Name	Hyperparameter
	K-Means Clustering	Partitions data into K clusters by minimizing variance within each cluster.
	Hierarchical Clustering	Builds a hierarchy of clusters by iteratively merging or splitting existing groups.
	DBSCAN	Forms clusters based on density; groups densely packed points and marks outliers.
	Mean Shift	Finds clusters by locating and adapting to the centroids of data points.
	Spectral Clustering	Uses eigenvalues of similarity matrix to reduce dimensions before clustering.

6 Types of Clustering Algorithms in Machine Learning

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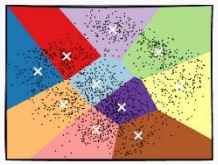
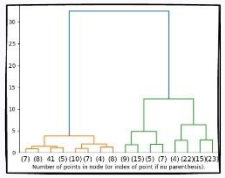
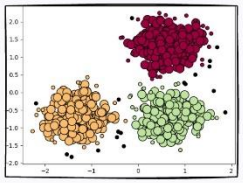
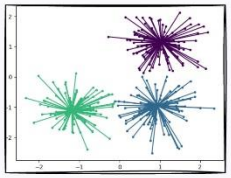
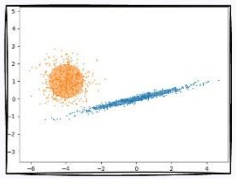
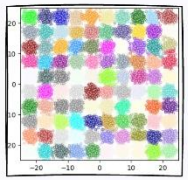
Clustering Algorithm Type		Clustering Methodology	Algorithm(s)
	Centroid-based	Cluster points based on proximity to centroid	KMeans KMeans++ KMedoids
	Connectivity-based	Cluster points based on proximity between clusters	Hierarchical Clustering (Agglomerative and Divisive)
	Density-based	Cluster points based on their density instead of proximity	DBSCAN OPTICS HDBSCAN
	Graph-based	Cluster points based on graph distance	Affinitiy Propagation Spectral Clustering
	Distribution-based	Cluster points based on their likelihood of belonging to the same distribution.	Gaussian Mixture Models (GMMs)
	Compression-based	Transform data to a lower dimensional space and then perform clustering	BIRCH