













Inspire...Educate...Transform.

Unsupervised models

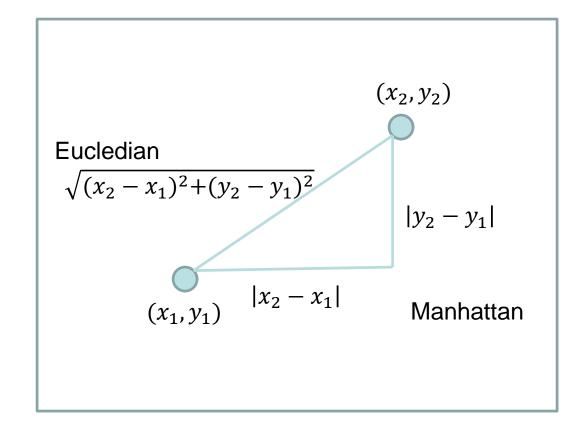
Clustering

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UNDERSTANDING DISTANCE



Numeric



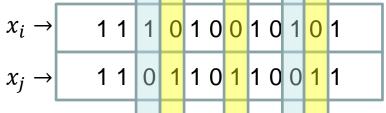


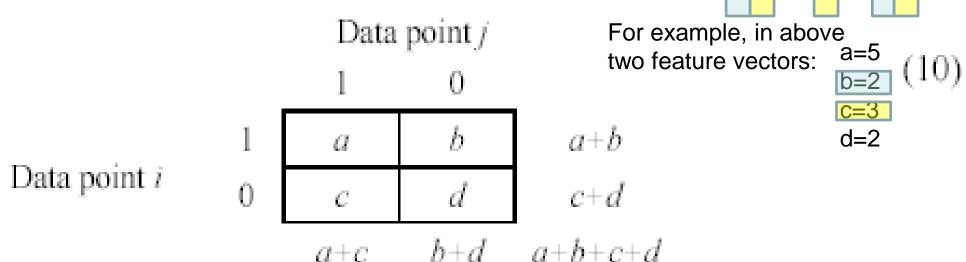
Distance between categorical attributes

- For each categorical variable
 - Distance is zero if two records have same value
 - -1 if different
 - Sum the total distance across all attributes



Categorical attributes





- a: the number of attributes with the value of 1 for both data points.
- b: the number of attributes for which $x_{if} = 1$ and $x_{jf} = 0$, where $x_{if}(x_{jf})$ is the value of the fth attribute of the data point $\mathbf{x}_i(\mathbf{x}_j)$.
- c: the number of attributes for which $x_{ij} = 0$ and $x_{jj} = 1$.
- d: the number of attributes with the value of 0 for both data points.



Symmetric binary attributes

 Hamming distance function: Simple Matching Coefficient, proportion of mismatches of their values

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \frac{b+c}{a+b+c+d}$$

 $Dist = \frac{number\ of\ dissimiar\ attributes\ between\ the\ records}{number\ of\ dissimilar\ attributes + number\ of\ similar\ attributes}$



Asymmetric binary attributes

- Asymmetric: if one of the states is more important or more valuable than the other.
 - By convention, state 1 represents the more important state, which
 is typically the rare or infrequent state.
 - Jaccard coefficient is a popular measure

 $Dist = \frac{number\ of\ dissimilar\ attributes\ between\ the\ records}{number\ of\ dissimilar\ attributes\ +\ number\ of\ similar\ attributes\ (excluding\ records\ with\ 0,0)}$

$$dist(\mathbf{x}_i, \mathbf{x}_j) = \frac{b+c}{a+b+c}$$

We can have some variations, adding weights



Dissimilarity between Binary Variables

Example

Name	Gender	Fever	Cough	Test-1	Test-2	Test-3	Test-4
Jack	M	Y	N	P	N	N	N
Mary	F	Y	N	P	N	P	N
Jim	M	Y	P	N	N	N	N

- gender is a symmetric attribute
- the remaining attributes are asymmetric binary
- let the values Y and P be set to 1, and the value N be set to 0

$$d(jack, mary) = \frac{0+1}{2+0+1} = 0.33$$

$$d(jack, jim) = \frac{1+1}{1+1+1} = 0.67$$

$$d(jim, mary) = \frac{1+2}{1+1+2} = 0.75$$



Another distance metric used in supervised learning

Value difference measure (VDM):d_{ij}

$$\sum_{h=1}^{|P(h|val_i) - P(h|val_j)|} |P(h|val_i) - P(h|val_j)|$$



Value Distance Measure

ID	Age	Income	Fa	mily	CCAvq	Personal* Loan
1	Young	Low			Low	0
	Old	Low			Low	0
3	Middle	Low		1	Low	0
4	Middle	Medium		1	Low	0
5	Middle	Low		4	Low	0
6	Middle	Low		4	Low	0
10	Middle	High		1	High	1
17	Middle	Medium	,	4	Medium	1
19	Old	High		2	High	1
30	Middle	Medium		1	Medium	1
39	Old	Medium		3	Medium	1
43	Young	Medium		4	Low	1
48	Middle	High		4	Low	1

 $VDM_{family1,family2}$

$$|P(0|f_1) - P(0|f_2)| + |P(1|f_1) - P(1|f_2)|$$

$$|0.5 - 0| + |0.5 - 1|$$

$$= 1$$

$$\begin{split} VDM_{family1,family3} &= |P(0|f_1) - P(0|f_3)| \\ &+ |P(1|f_1) - P(1|f_3)| \\ &= |0.5 - 0.5| + |0.5 - 0.5| \\ &= 0 \end{split}$$



Ordinal variables

Same as numeric

Look up is better than computation



Look up matrix for ordinal with 3 states

	1	2	3]	Γ	1	2	3]
1	0	1	2	1	0	1	3
2	1	0	1	2	1	0	2
L 3	2	1	$0 \rfloor$	L 3	3	2	0

Distance between different ordinals may not be same !!! On the right, distance between state 1 and state 2 is much less than distance between state 1 and state 3.

Depends on what the ordinals represent.

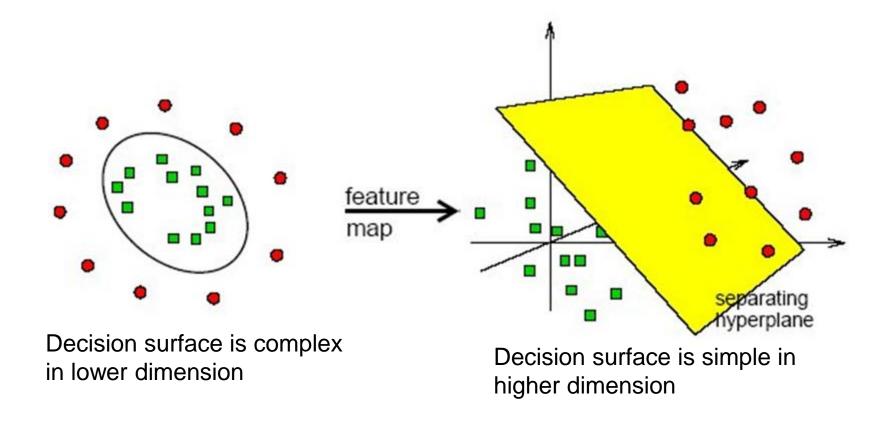
E.g.: If ordinals represent education: class 5, Class 10, Degree. Distance between class 5 and class 10 may be considered less than distance between class 10 and degree



KERNEL TRICK

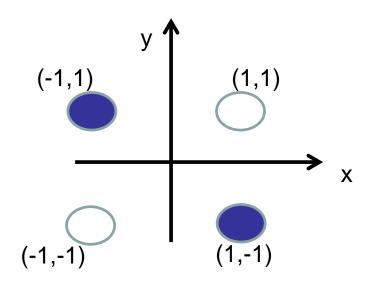


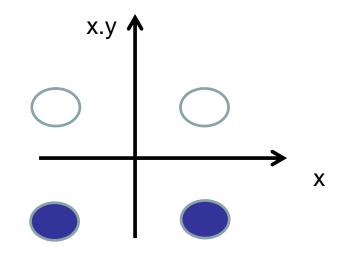
Moving into higher dimensions





Linear Separation of XOR





- XOR is not linearly separable in x,y space
- Linearly separable in x.y space
 - The kernel here is K(x,y) = x.y



Standard Kernels

Polynomial

$$-(\alpha x^T y + c)^d$$

Radial Basis

$$-\exp(-\gamma \|x-y\|^2)$$



Clustering

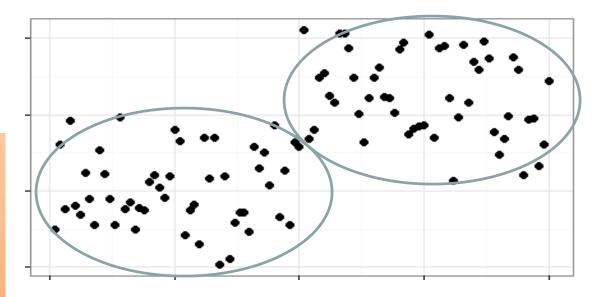


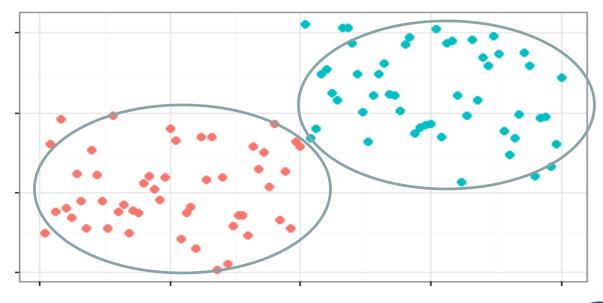
Unsupervised learning

Supervised: Data and target

Unsupervised: Just data









Clustering

- Finding similarity groups in data, called clusters. I.e.,
 - data instances that are similar to (near) each other are in the same cluster
 - data instances that are very different (far away) from each other fall in different clusters.



A few clustering applications

 In marketing, segment customers according to their similarities

- -To do targeted marketing.
- -It is not uncommon to have over 100,000 segments in insurance clustering



Google search

- Given a collection of text documents, organize them according to their content similarities,
 - -E.g., Google news
- Blind signal separation (separating two speakers)



Algorithms

- <u>Hierarchical approach</u>: Create a hierarchical decomposition of the set of data (or objects) using some criterion (Wald)
- <u>Partitioning approach</u>: Construct various partitions and then evaluate them by some criterion, e.g., minimizing the sum of square errors (K-means, Spectral clustering)
- Model-based methods: A model is hypothesized for each of the clusters and tries to find the best fit of that model to each other (Gaussian mixture model using EM)



HIERARCHICAL (AGGLOMERATIVE) CLUSTERING



Example of agglomerative clustering

	BOS	NY	DC	MIA	СНІ	SEA	SF	LA	DEN
BOS	0	206	429	1504	963	2976	3095	2979	1949
NY	206	0	233	1308	802	2815	2934	2786	1771
DC	429	233	0	1075	671	2684	2799	2631	1616
МІА	1504	1308	1075	0	1329	3273	3053	2687	2037
CHI	963	802	671	1329	0	2013	2142	2054	996
SEA	2976	2815	2684	3273	2013	0	808	1131	1307
SF	3095	2934	2799	3053	2142	808	0	379	1235
LA	2979	2786	2631	2687	2054	1131	379	0	1059
DEN	1949	1771	1616	2037	996	1307	1235	1059	0

At each iteration, pick two data points that have least distance between them. Add the points into a cluster.



	BOS/NY	DC	MIA	СНІ	SEA	SF	LA	DEN
BOS/NY	0	223	1308	802	2815	2934	2786	1771
DC	223	0	1075	671	2684	2799	2631	1616
MIA	1308	1075	0	1329	3273	3053	2687	2037
СНІ	802	671	1329	0	2013	2142	2054	996
SEA	2815	2684	3273	2013	0	808	1131	1307
SF	2934	2799	3053	2142	808	0	379	1235
LA	2786	2631	2687	2054	1131	379	0	1059
DEN	1771	1616	2037	996	1307	1235	1059	0

Note how we update distances between other clusters. The lower distance is picked. Distance between BOS to DC was 429, now set to 233. Distance from BOS to MIA was 1504, now set to 1308.

Averaging may also be used instead of taking distance to the closest point.



	BOS/NY/DC	МІА	СНІ	SEA	SF	LA	DEN
BOS/NY/DC	0	1075	671	2684	2799	2631	1616
MIA	1075	0	1329	3273	3053	2687	2037
СНІ	671	1329	0	2013	2142	2054	996
SEA	2684	3273	2013	0	808	1131	1307
SF	2799	3053	2142	808	0	379	1235
LA	2631	2687	2054	1131	379	0	1059
DEN	1616	2037	996	1307	1235	1059	0



	BOS/	MIA	СНІ	SEA	SF/LA	DEN
	NY/DC					
BOS/NY/DC	0	1075	671	2684	2631	1616
MIA	1075	0	1329	3273	2687	2037
СНІ	671	1329	0	2013	2054	996
SEA	2684	3273	2013	0	808	1307
SF/LA	2631	2687	2054	808	0	1059
DEN	1616	2037	996	1307	1059	0

Note how creation of SF/LA cluster has changed distances

	BOS/NY/DC	МІА	CHI	SEA	SF	LA	DEN
BOS/NY/DC	0	1075	671	2684	2799	2631	1616
MIA	1075	0	1329	3273	3053	2687	2037
CHI	671	1329	0	2013	2142	2054	996
SEA	2684	3273	2013	0	808	1131	1307
SF	2799	3053	2142	808	0	379	1235
LA	2631	2687	2054	1131	379	0	1059
DEN	1616	2037	996	1307	1235	1059	0



	BOS/NY/DC/	МІА	SEA	SF/LA	DEN
	сні				
BOS/NY/DC/CHI	0	1075	2013	2054	996
МІА	1075	0	3273	2687	2037
SEA	2013	3273	0	808	1307
SF/LA	2054	2687	808	0	1059
DEN	996	2037	1307	1059	0



	BOS/NY/DC/CHI	МІА	SF/LA/SEA	DEN
BOS/NY/DC/CHI	0	1075	2013	996
MIA	1075	0	2687	2037
SF/LA/SEA	2054	2687	0	1059
DEN	996	2037	1059	0

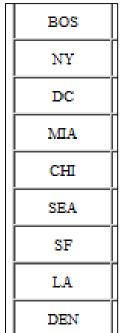


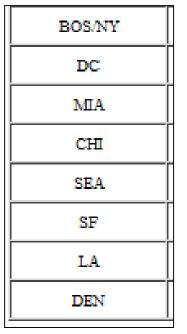
	BOS/NY /DC/CHI/DEN	МІА	SF/LA/SEA
BOS/NY/DC/CHI/DEN	0	1075	1059
МІА	1075	0	2687
SF/LA/SEA	1059	2687	0

	BOS/NY /DC/CHI /DEN/SF /LA/SEA	MIA
BOS/NY/DC/CHI/DEN/SF/LA/SEA	0	1075
MIA	1075	0



Agglomerative clustering (Hierarchical)

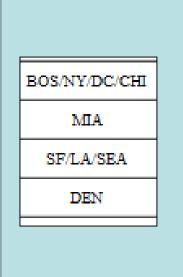




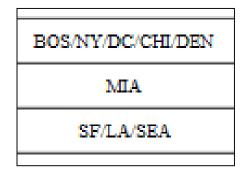








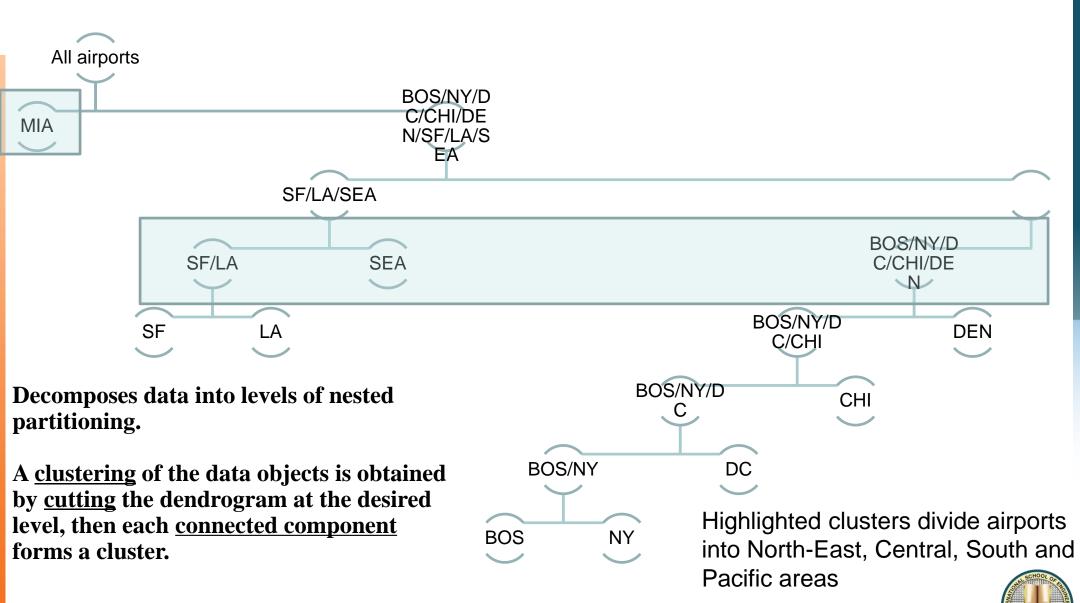
BOS/NY/DC/CHI/DEN/SF/LA/SEA
MIA



Typically, a particular "level" of the hierarchy is selected to be your clustering result

Highlighted clusters divide airports into North-East, Central, South and Pacific areas

Agglomerative clustering (Hierarchical)



Agglomerative clustering (Hierarchical)

- Assign each item to its own cluster, so that if you have N items, you now have N clusters, each containing just one item.
- Merge most similar clusters into a single cluster, so that now you have one less cluster.
- Compute distances (similarities) between the new cluster and each of the old clusters.
- Repeat steps 2 and 3 until all items are clustered into a single cluster of size N.



Partitioning algorithms

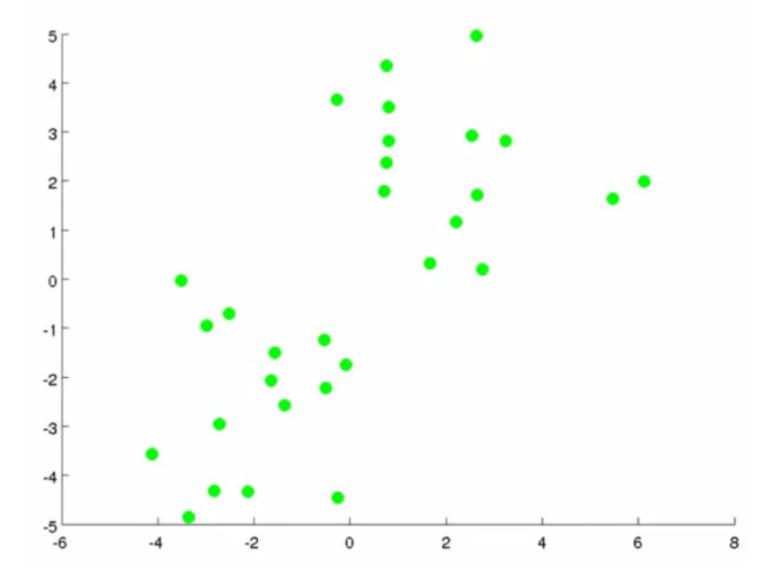
K-MEANS AND K-MEDOIDS



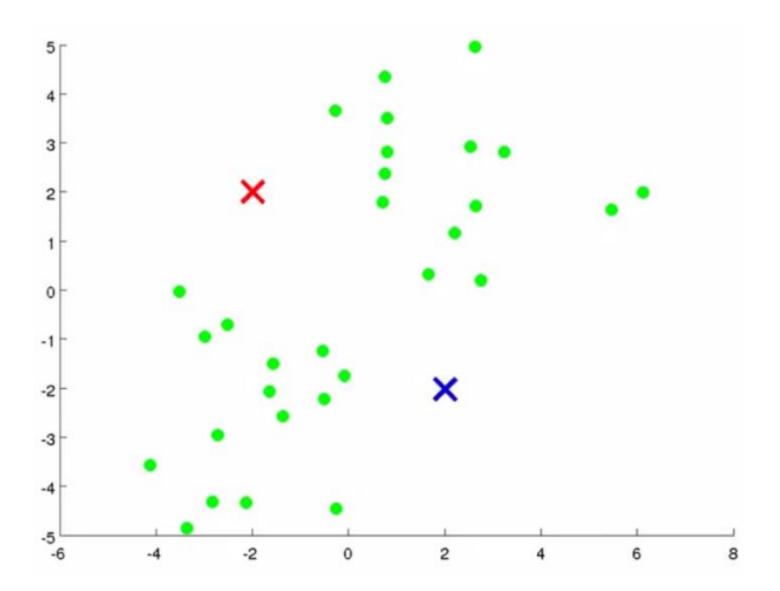
K-means clustering

- K-means is a partitional clustering algorithm as it partitions the given data into *k* clusters.
 - Each cluster has a cluster center, called centroid.
 - k is specified by the user

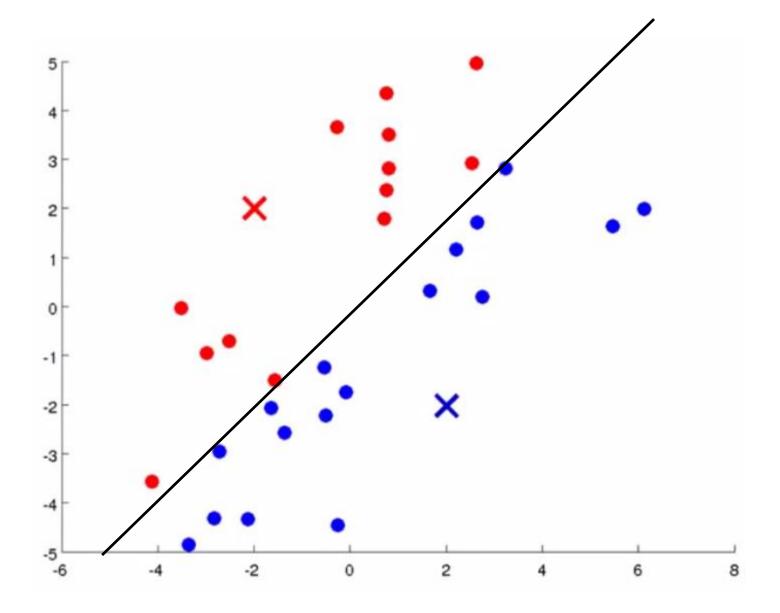




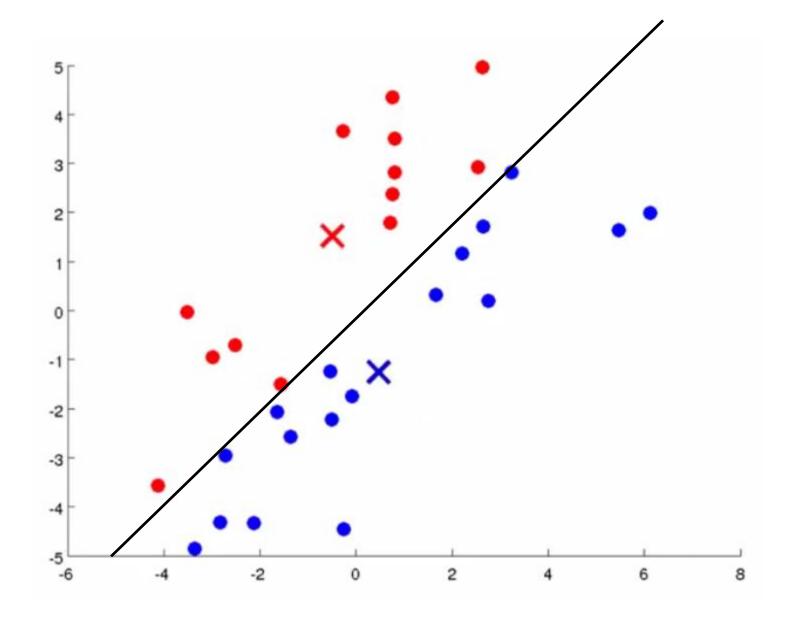




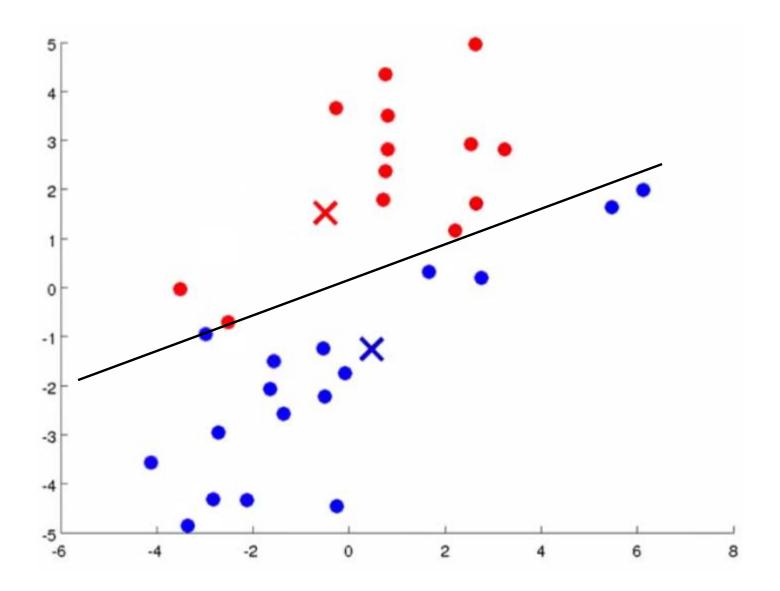




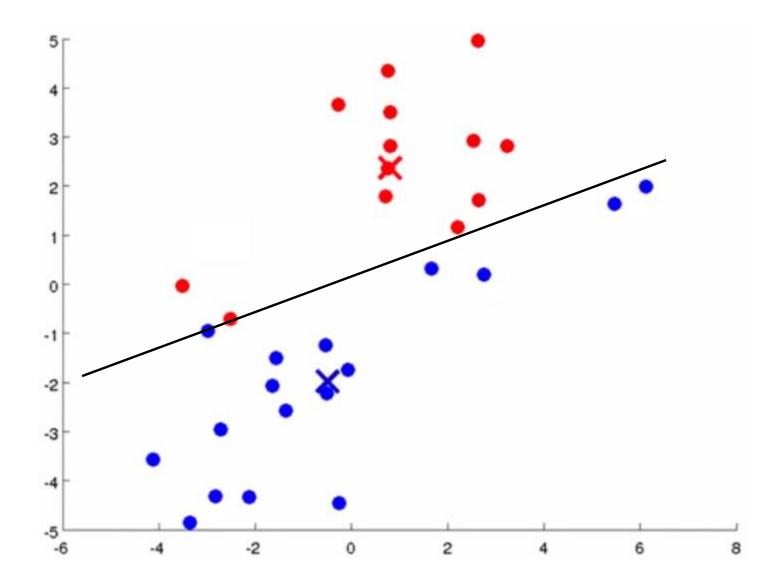




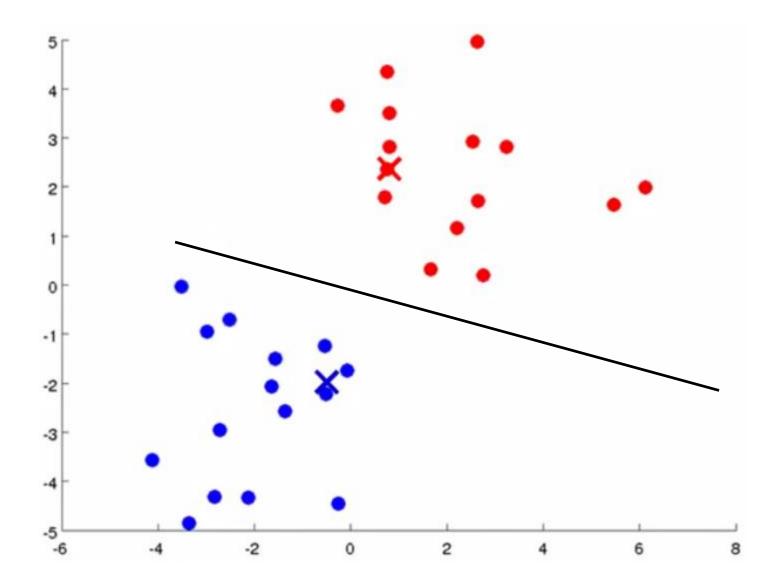




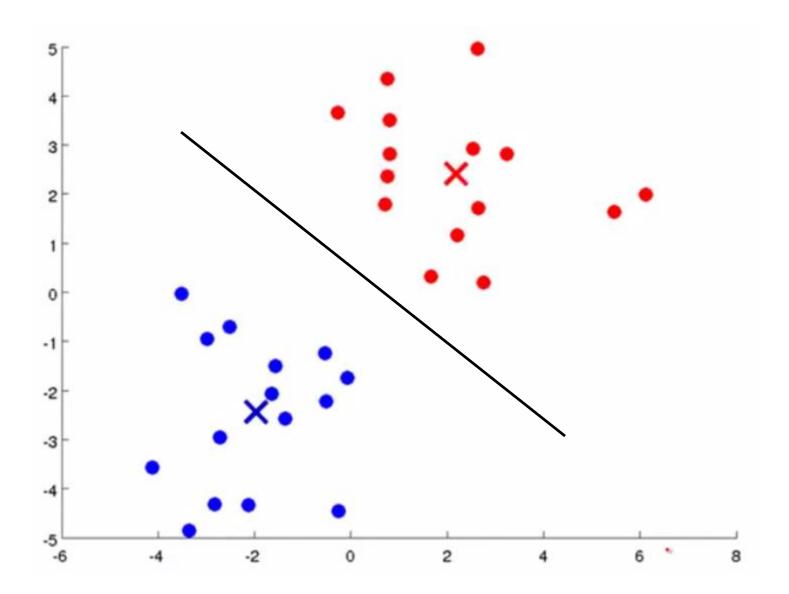














K-means algorithm

 Given k, the k-means algorithm works as follows:

- 1. Randomly choose *k* data points (seeds) to be the initial centroids, cluster centers
- Assign each data point to the closest centroid
- Re-compute the centroids using the current cluster memberships.
- 4. If a convergence criterion is not met, go to 2.



Stopping/convergence criterion

- 1. no (or minimum) re-assignments of data points to different clusters,
- 2. no (or minimum) change of centroids, or
- 3. minimum decrease in the sum of squared error (SSE),

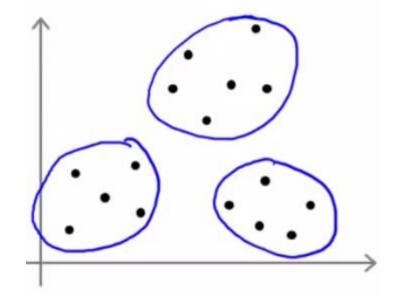
$$SSE = \sum_{j=1...k} \sum_{x \in C_j} dist(x, m_j)^2$$
(1)

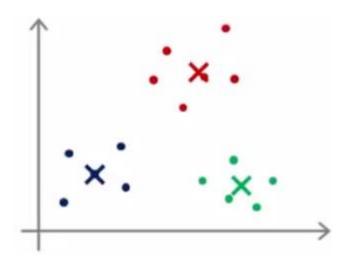
- C_j is the jth cluster, \mathbf{m}_j is the centroid (mean) of cluster C_j

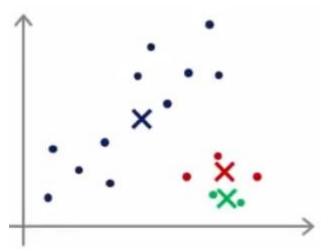
Check SCREE plots.

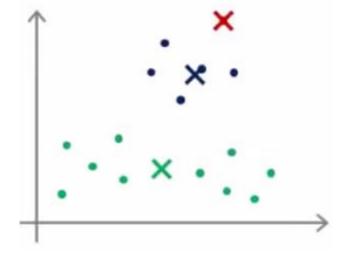


Local optima











What Is the Problem With K-Means?

- The k-means algorithm is sensitive to outliers!
- K-Medoids: Instead of taking the mean value of the object in a cluster as
 a reference point, medoids can be used, which is the most centrally
 located object in a cluster.



What Is the Problem with Medoids?

- More robust than k-means in the presence of noise and outliers because a medoid is less influenced by outliers or other extreme values than a mean
- Works efficiently for small data sets but does not scale well for large data sets.
 - In regular K-Means, the new mean is merely average of values O(nkt)
 - In K-Medoid, if a particular cluster has n_c data points, you will need $(n_c)^2$ computations
 to determine the medoid for that cluster
 - While the cost of the configuration decreases:
 - For each medoid m, for each non-medoid data point o:
 - » Swap m and o, recompute the cost (sum of distances of points to their medoid)
 - » If the total cost of the configuration increased in the previous step, undo the swap
 - $O(k(n-k)^2)$ for each iteration, where n is # of data, k is # of clusters, t: # of iterations



K-means versus Hierarchical

- K-means produces a single partitioning
- K-means needs the number of clusters to be specified
- K-means is usually more efficient run-time wise

- Hierarchical Clustering can give different partitions depending on the level-of-resolution we are looking at
- Hierarchical clustering doesn't need the number of clusters to be specified
- Hierarchical clustering can be slow (has to make several merge/Split decisions)



HOW DO WE EMPLOY DISTANCE IN A CLUSTER



What do we mean by distance between Clusters

- Single link: smallest distance between an element in one cluster and an element in the other, i.e., $dis(K_i, K_j) = min(t_{ip}, t_{jq})$
- Complete link: largest distance between an element in one cluster and an element in the other, i.e., $dis(K_i, K_i) = max(t_{ip}, t_{iq})$
- Average: average distance between an element in one cluster and an element in the other, i.e., $dis(K_i, K_i) = avg(t_{ip}, t_{iq})$
- Centroid: distance between the centroids of two clusters, i.e., dis(K_i, K_j) = dis(C_i, C_i)
- Medoid: distance between the medoids of two clusters, i.e., dis(K_i , K_j) = dis(M_i , M_j)
 - Medoid: one chosen, centrally located object in the cluster



Centroid, Radius & Diameter of a Cluster (for numerical data sets)

• Centroid: the "middle" of a cluster

$$C_{m} = \frac{\sum_{i=1}^{N} (t_{ip})}{N}$$

Radius: square root of average distance from any point of the cluster to its centroid

$$R_m = \sqrt{\frac{\sum_{i=1}^{N} (t_{ip} - c_m)^2}{N}}$$

 Diameter: square root of average mean squared distance between all pairs of points in the cluster

$$D_{m} = \sqrt{\frac{\sum_{i=1}^{N} \sum_{i=1}^{N} (t_{ip} - t_{iq})^{2}}{N(N-1)}}$$



ENGINEERING

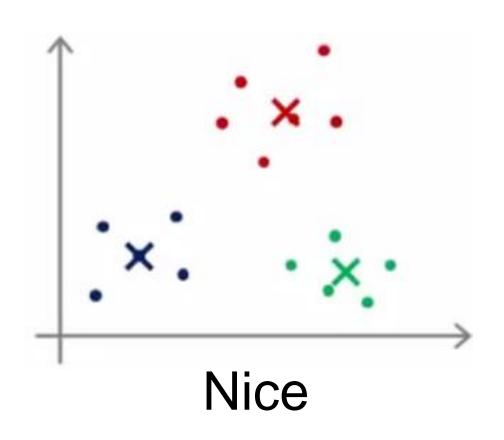


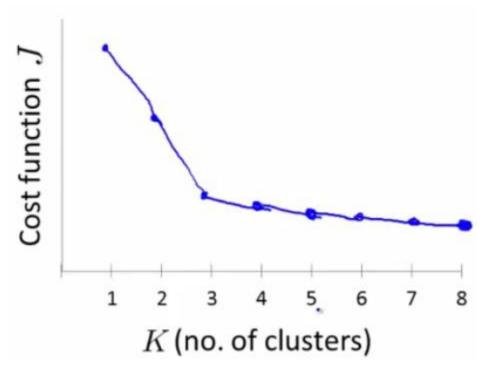
Stability Check of the Clusters

• To check the stability of the clusters take a random sample of 95% of records. Compute the clusters. If the clusters formed are very similar to the original, then the clusters are fine.



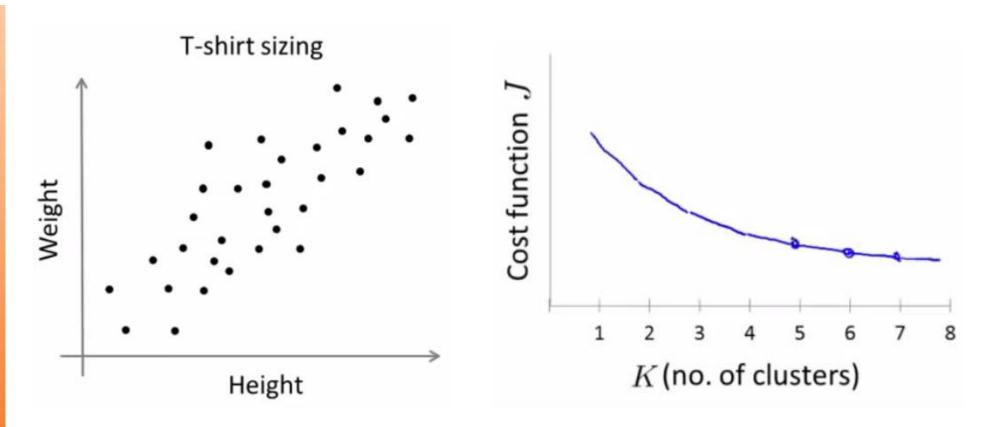
Linearly clustered data







Linearly separable but merged

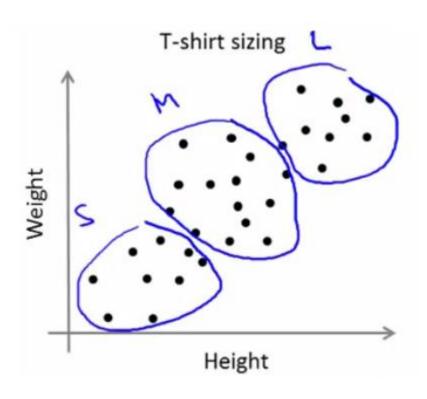


Data points of individuals of a particular height and weight

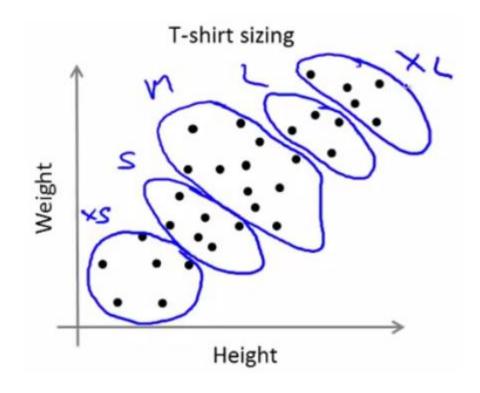


58

Linearly separable but merged



Clustering the data points into T-shirt sizes. Top: Three sizes, Right: Five sizes



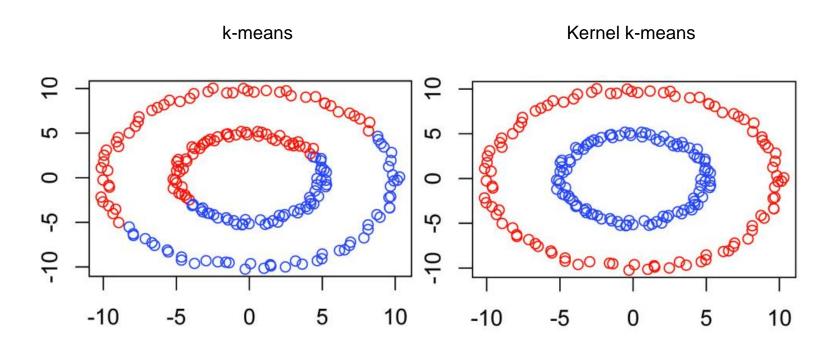


Linearly separable

- Run 50-500 simulations for small k (2-10). For large k (100 or so), we can do 1-5 simulations
- Pick the one that gives the best SSE



k-means Vs. Kernel k-means





Performance of Kernel K-means

Clustering accuracy (%) achieved by each clustering algorithm for 10 data sets

Data set	Conventional k-means	Kernel k-means
DUNN	70.00	71.11
IRIS	89.33	96.00
ECOLI	42.86	68.75
CIRCLE	50.76	100.0
BLE-3	65.67	76.33
BLE-2	88.50	100.0
UE-4	77.25	100.0
UE-3	95.83	98.83
ULE-4	76.25	98.00
Avg. (%)	73.60	89.27

Evaluation of the performance of clustering algorithms in kernel-induced feature space, Pattern Recognition, 2005



Kernel Trick

- The original way is to transform each data point into a high dimensional space and then do computation
 - -This can be computationally complex
- Note that we need to compute distances in Euclidian space, or sometimes scalar product



Kernel Trick

- Take two points: $X_1 = (x_{11}, x_{12}) X_2 = (x_{21}, x_{22})$
 - Euclidian distance: $d(X_1, X_2) = \sqrt{(x_{11} x_{21})^2 + (x_{12} x_{22})^2}$
 - Dot product: $X_1.X_2 = (x_{11}.x_{21}) + (x_{12}.x_{22})$
- Take to a higher dimensional space

$$\check{X}_1 = (x_{11}, x_{12}, x_{11}^2, x_{12}^2, \sqrt{2}x_{11}x_{12})$$

$$\check{X}_2 = (x_{21}, x_{22}, x_{21}^2, x_{22}^2, \sqrt{2}x_{21}x_{22})$$



$$\Phi(\mathbf{a}) \bullet \Phi(\mathbf{b}) = \begin{pmatrix} 1 \\ \sqrt{2}a_1 \\ \sqrt{2}a_2 \\ \vdots \\ \sqrt{2}a_m \\ a_1^2 \\ a_2^2 \\ \vdots \\ \sqrt{2}a_1a_2 \\ \sqrt{2}a_1a_3 \\ \vdots \\ \sqrt{2}a_1a_m \\ \sqrt{2}a_2a_3 \\ \vdots \\ \sqrt{2}a_1a_m \\ \vdots \\ \sqrt{2}a_1a_m \\ \vdots \\ \sqrt{2}b_1b_m \\ \vdots \\ \sqrt{2}b_1b_m \\ \vdots \\ \sqrt{2}b_1b_m \\ \vdots \\ \sqrt{2}b_1b_m \\ \vdots \\ \vdots \\ \end{bmatrix}$$

Define K(**a**,**b**) =
$$(\mathbf{a}.\mathbf{b}+1)^2$$

= $(\mathbf{a}.\mathbf{b})^2 + 2\mathbf{a}.\mathbf{b} + 1$
= $\left(\sum_{i=1}^m a_i b_i\right)^2 + 2\sum_{i=1}^m a_i b_i + 1$
= $\sum_{i=1}^m \sum_{j=1}^m a_i b_i a_j b_j + 2\sum_{i=1}^m a_i b_i + 1$
= $\sum_{i=1}^m (a_i b_i)^2 + 2\sum_{i=1}^m \sum_{j=1}^m a_i b_i a_j b_j + 2\sum_{i=1}^m a_i b_i + 1$

Both are same!

And K(a,b) is only O(m) to compute!

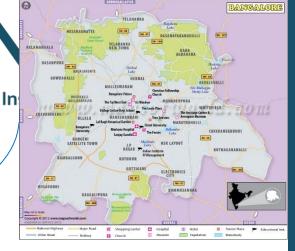


Other Topics

- Clustering large datasets
 - Select a small % of data, run K-means or K-medoids
 - CLARA and CLARANS (Ng and Han 1994, 2002)
- Parallel and Efficient implementations of K-means / K-medoids

http://www.math.unipd.it/~dulli/corso04/ng94efficient.pdf
https://anuradhasrinivas.files.wordpress.com/2013/04/lesson8-clustering.pdf
http://www.vlfeat.org/overview/kmeans.html
http://repository.cmu.edu/cgi/viewcontent.cgi?article=2397&context=compsci
http://www.cs.ucsb.edu/~veronika/MAE/Global_Kernel_K-Means.pdf





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