Unsupervised Learning

COMP9417 Machine Learning and Data Mining

Term 2, 2022

Acknowledgements

Aims

This lecture will develop your understanding of unsupervised learning methods. Following it you should be able to:

- compare supervised with unsupervised learning
- describe k-means clustering
- describe hierarchical clustering
- discuss inductive bias in clustering
- describe methods of evaluation for unsupervised learning
- describe the problem of dimensionality reduction

Supervised vs. Unsupervised Learning

i.e labels　　　*model*

Supervised learning — classes are *known* and need a "definition", in terms of the data. Methods are known as: classification, discriminant analysis, class prediction, supervised pattern recognition.

Unsupervised learning — classes are initially *unknown* and need to be "discovered" with their definitions from the data. Methods are known as: cluster analysis, class discovery, unsupervised pattern recognition.

So: *unsupervised learning* methods, such as *clustering*, address the problem of assigning instances to classes *given only observations about the instances*, i.e., without being given class "labels" for instances by a "teacher".

Unsupervised learning

Why do we need unsupervised learning ?

- most of the world's data is *unlabelled*
- getting a human to label data is often
  - difficult (what are the classes ?)
  - time-consuming (labelling requires thinking)
  - expensive (see above)
  - error-prone (mistakes, ambiguity)
- in principle, can use any feature as the "label"
- unfortunately, often the class is not a known feature

Unsupervised learning

What is unsupervised learning good for ?

- simplifying a problem, e.g., by dimensionality reduction
- exploratory data analysis, e.g., with visualization   *EDA*
- data transformation to simplify a classification problem
- to group data instances into subsets   *"segmentation"*
- to discover structure, like hierarchies of subconcepts
- to learn new "features" for later use in classification
- to track "concept drift" over time   *reconstruct data*
- to learn generative models for images, text, video, speech, etc.

self-supervised
— language models (predict next word)

deep learning
— GANs (labelled)

Clustering

- is finding groups of items that are similar
- clustering is unsupervised
  - the class of any data instance is not known
- success of clustering often measured subjectively
  - OK for *exploratory data analysis* (EDA) . . .
  - but problematic if you need quantitive results . . .
  - some visual and statistical approaches
- a dataset for clustering is just like a dataset for classification, but without the class ! No labels!

Simple 2D representations of clustering

Clusters form a partition
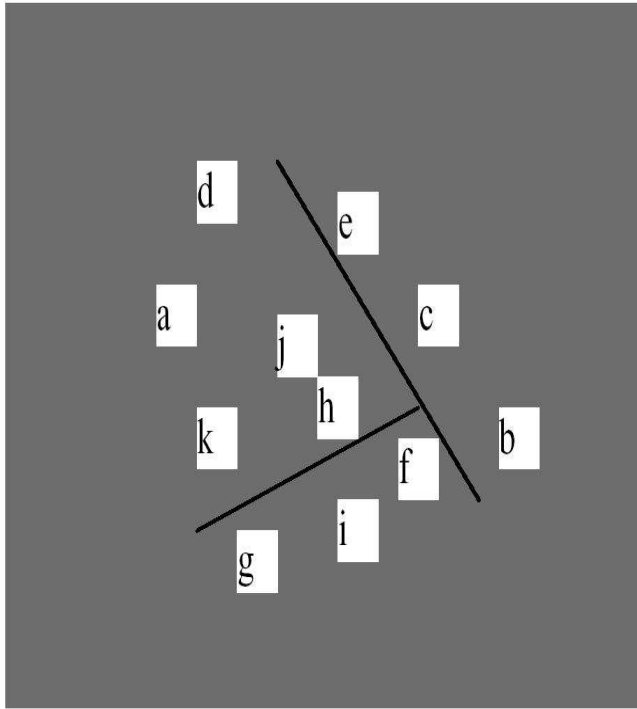
Venn diagram (overlapping clusters)
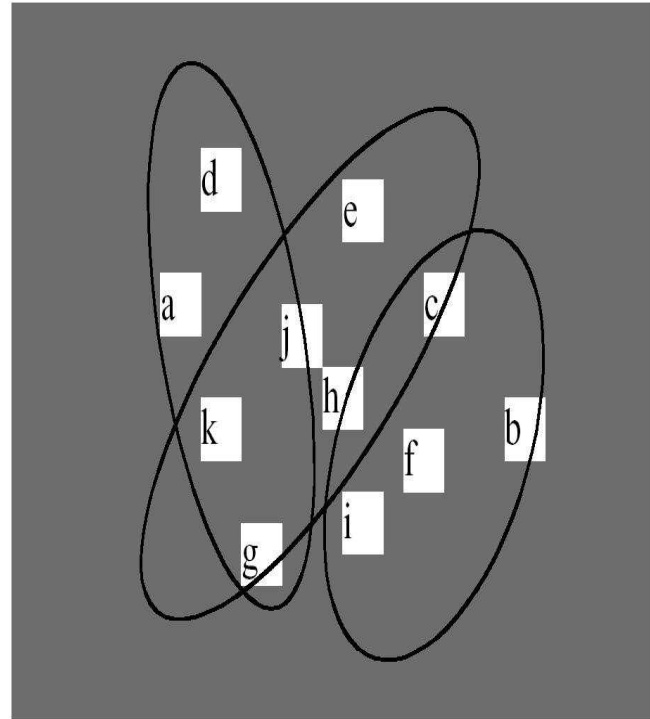
Other representations of clustering

recall
252lass2

Probabilistic assignment

	1	2	3
a	0.4	0.1	0.5
b	0.1	0.8	0.1
c	0.3	0.3	0.4
d	0.1	0.1	0.8
e	0.4	0.2	0.4
f	0.1	0.4	0.5
g	0.7	0.2	0.1
h	0.5	0.4	0.1
...			

Dendrogram

g a c i e d k b j f h

Clusters represented by mean, s.d.
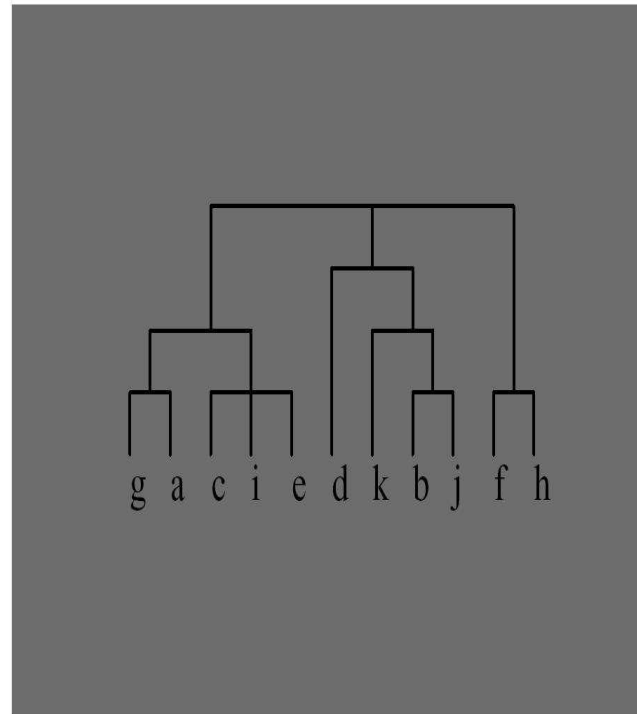
Cluster analysis

Clustering algorithms form two broad categories: **hierarchical methods** and **partitioning methods**.

Hierarchical algorithms are either **agglomerative** i.e. bottom-up or **divisive** i.e. top-down.

In practice, hierarchical agglomerative methods often used - efficient exact algorithms available, but more importantly to users the *dendrogram*, or tree, can be visualized.

Partitioning methods usually require specification of the number of clusters, then try to construct the clusters and fit objects to them.

Representation

Let $X = \{e_1, \ldots, e_n\}$ be a set of elements, i.e. instances.

Let $\mathcal{C} = (C_1, \ldots, C_l)$ be a *partition* of X into subsets.

Each subset is called a *cluster*, and $\mathcal{C}$ is called a *clustering*.

Input data can have two forms: *(for input to a clustering)*

1. each element is associated with a real-valued vector of p features e.g. measurement levels for different features

2. pairwise similarity data between elements, e.g. correlation, distance (dissimilarity)

Feature-vectors have more information, but similarity is generic (given the appropriate function). Feature-vector matrix: $n \times p$, similarity matrix $n \times n$. In general, often $n \gg p$.
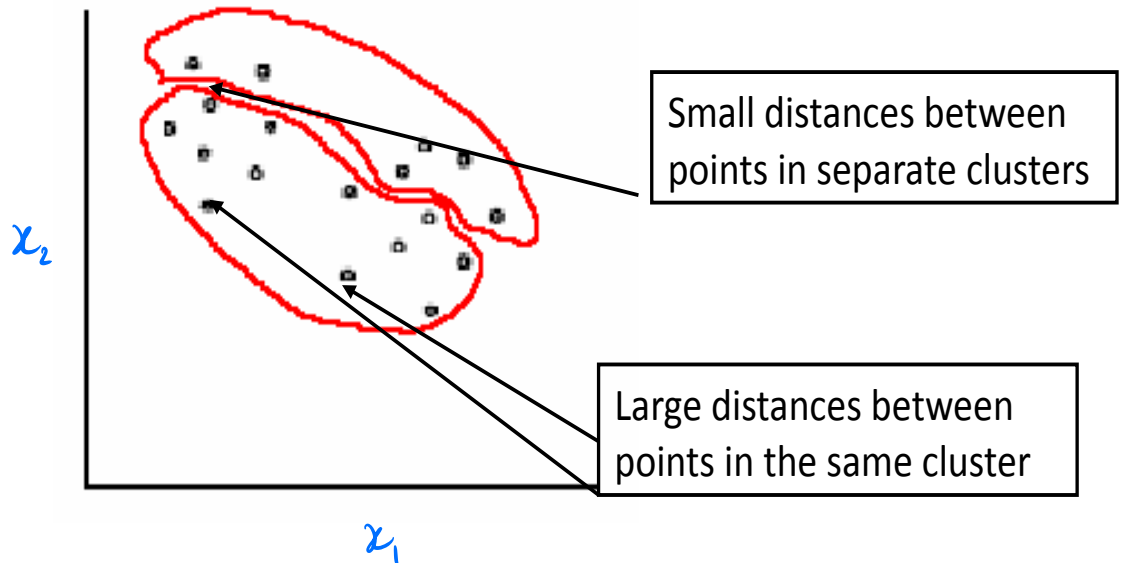
Clustering framework

- goal of clustering: find a partition of n X elements (instances) *in X* into *homogeneous* and *well-separated* clusters
- elements from same cluster should have high similarity, i.e, form a homogeneous cluster, while elements from different clusters should have low similarity, i.e., be well-separated
- note: homogeneity and separation need to be defined
- in practice, use a distance measure appropriate to the problem
- also note: typically there are interactions between homogeneity and separation – usually, high homogeneity is linked with low separation, and vice versa, unless there is clear *structure* in the data
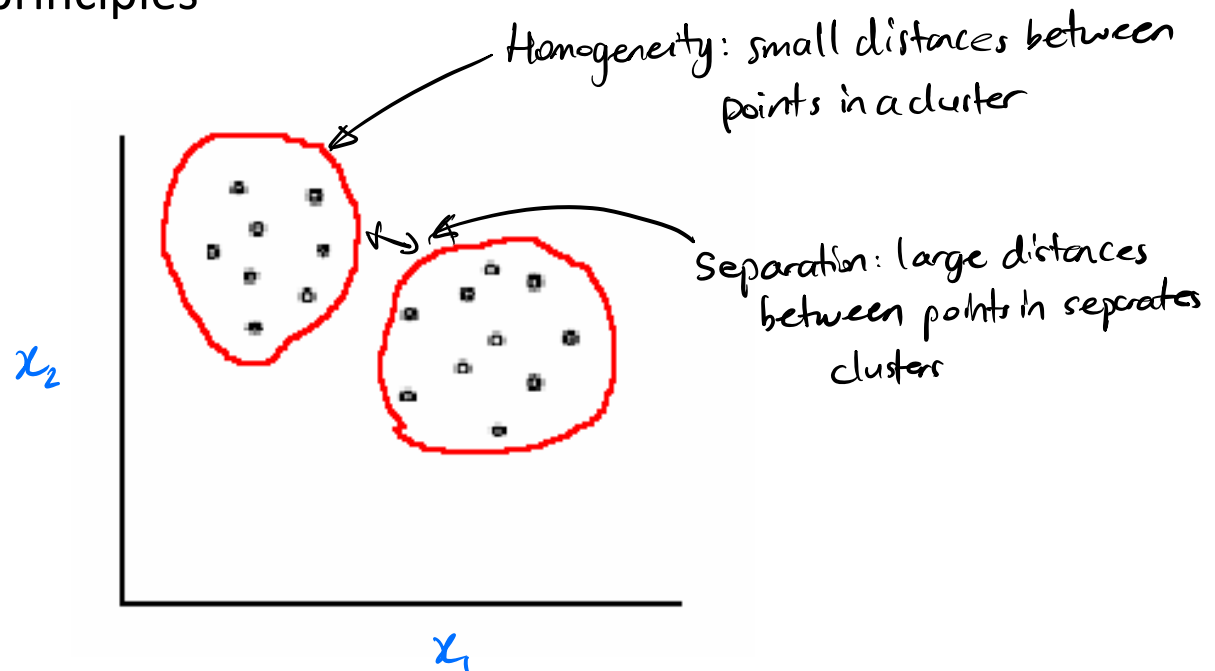
A bad clustering

This clustering violates both Homogeneity and Separation principles

$x_i \in \mathbb{R}^2$

x_2

Small distances between points in separate clusters

Large distances between points in the same cluster

x_1

A good clustering

This clustering satisfies both Homogeneity and Separation principles

Homogeneity: small distances between points in a cluster

Separation: large distances between points in separate clusters

k-means Clustering *not kNN!! supervised*

— unsupervised
— partitioning

k-means: k is number of clusters

Simple, but often effective, algorithm to cluster numerical data around k centroids, i.e., *means*. *typically, mean vector for all items in the cluster*

Need to choose value for k, and initialise the centroids.

Procedure:

Find a "good" clustering by iteratively assigning each data point to the nearest of the k centroids, then updating each centroid to reflect any points that have been re-assigned

Example: one variable 2-means (& standard deviations)

A	51	B	62	B	64	A	48	A	39	A	51
A	43	A	47	A	51	B	64	B	62	A	48
B	62	A	52	A	52	A	51	B	64	B	64
B	64	B	64	B	62	B	63	A	52	A	42
A	45	A	51	A	49	A	43	B	63	A	48
A	42	B	65	A	48	B	65	B	64	A	41
A	46	A	48	B	62	B	66	A	48		
A	45	A	49	A	43	B	65	B	64		
A	45	A	46	A	40	A	46	A	48		

model
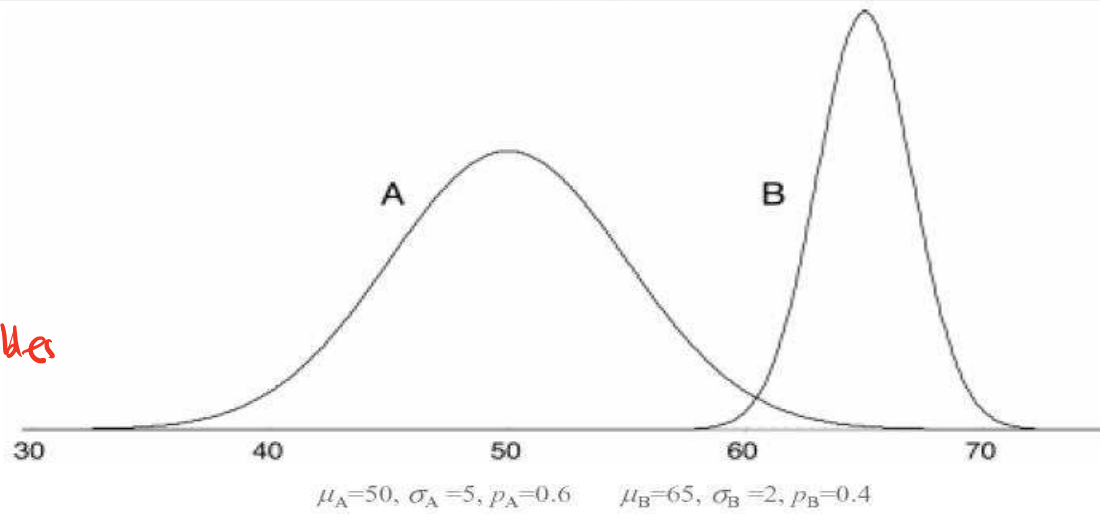
"Hidden" cluster variables A, B [Gaussian Dist]

$\mu_A=50$, $\sigma_A=5$, $p_A=0.6$ $\mu_B=65$, $\sigma_B=2$, $p_B=0.4$

k-means Clustering

$P(i)$ is the cluster assigned to element i, $c(j)$ is the centroid of cluster j, $d(v_1, v_2)$ the Euclidean distance *between feature vectors v_1 and v_2.

The goal is to find a partition P for which the error (distance) function $E_P = \sum_{i=1}^{n} d(i, c(P(i))$ is minimum.   *"dispersion"*

$$E_P^{ij} = \sum_{i=n}^{n} d(i, c(P(j))) \text{ where } i \neq j$$

Centroid is the mean or weighted average of the points in the cluster.

k-means is an important clustering method, widely-used in many different areas, that can be viewed in terms of the EM (Expectation-Maximization) algorithm.

* as long as data dimensionality is not "too high"
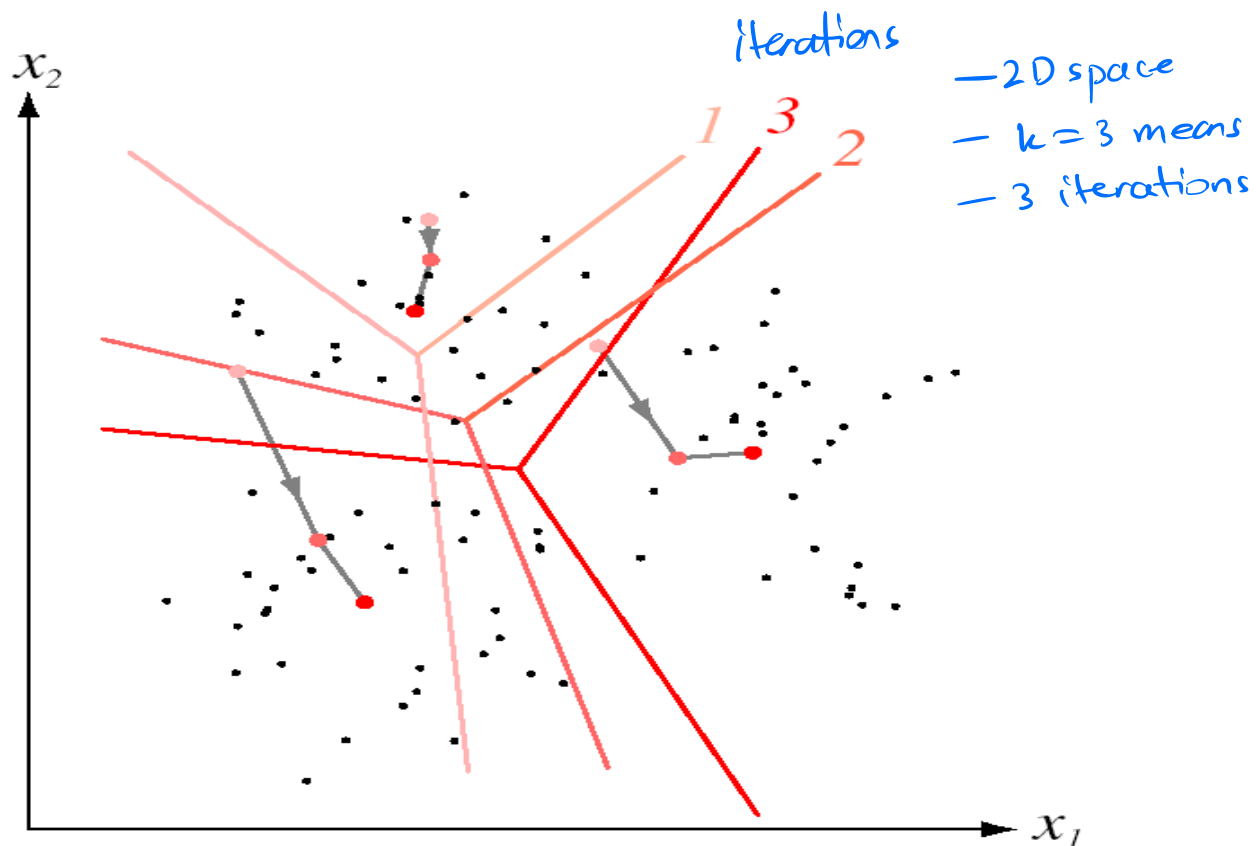
k-means Clustering algorithm

Algorithm k-means

$X^{n \times p}$

/* feature-vector matrix ~~(X)~~ is given */

① Start with an arbitrary partition P of X into k clusters

② for each element i and cluster $j \neq P(i)$ let E_P^{ij} be the cost of a solution in which i is moved to j:

     ① if $E_P^{i^* j^*} = min_{ij} E_P^{ij} < E_P$ then move i^* to cluster j^* and repeat step 2 else halt.
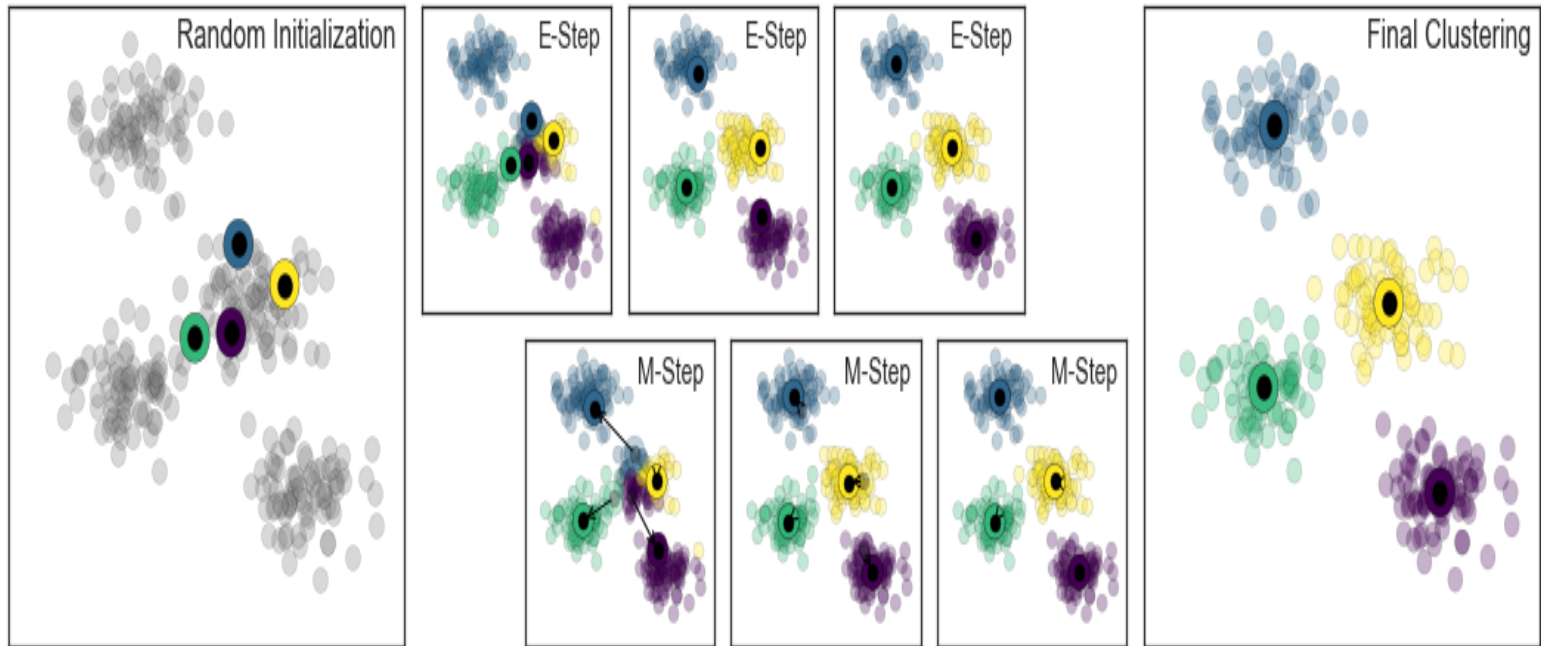
k-means Clustering

k-means Clustering

Previous diagram shows three steps to convergence in k-means with $k = 3$

- means move to minimize squared-error criterion
- approximate method of obtaining maximum-likelihood estimates for means
- each point assumed to be in exactly one cluster
- if clusters "blend", fuzzy k-means (i.e., overlapping clusters)

k-Means Clustering – steps in EM algorithm

k-means clustering: initialisation

$X = n = 1, \; p = 2$

X_1	X_2	Centroid
1	4	-
1	6	-
2	5	-
3	4	-
3	6	-
5	1	-
5	2	-
6	1	-
6	2	-
6	3	-
7	2	-

Centroid locations
centroid 1: $(3.2, 9.8)$
centroid 2: $(9.3, 7.1)$

Initial dataset and centroids before clustering starts
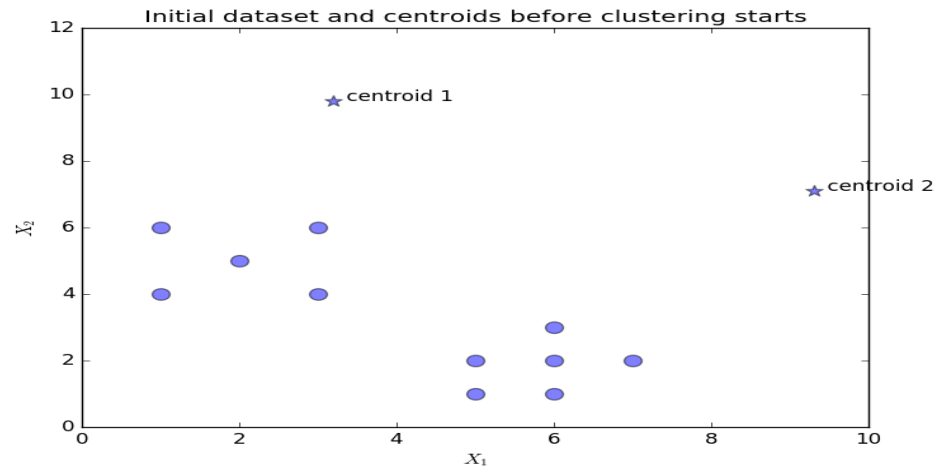
k-means clustering: assign to centroids

X_1	X_2	Centroid
1	4	1
1	6	1
2	5	1
3	4	1
3	6	1
5	1	2
5	2	2
6	1	2
6	2	2
6	3	2
7	2	2

Centroid locations
centroid 1: $(3.2, 9.8)$
centroid 2: $(9.3, 7.1)$

Clustering after assignment of points to centroids
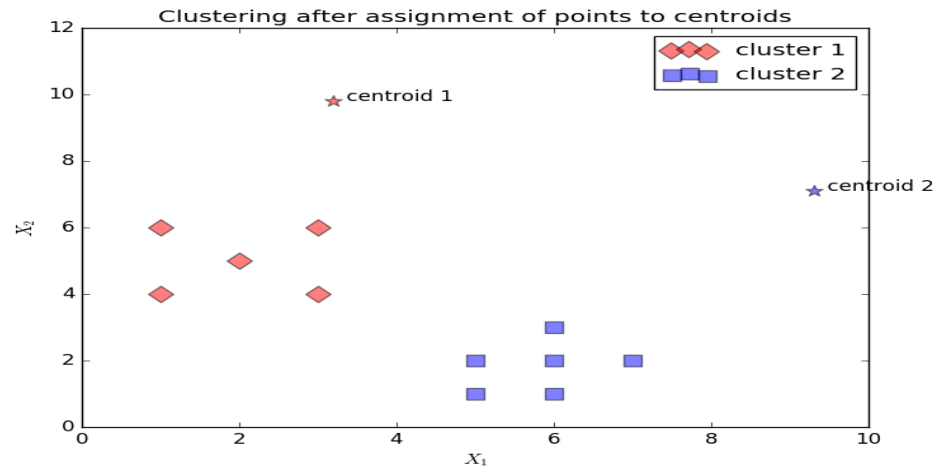
k-means clustering: recompute centroids

X_1	X_2	Centroid
1	4	1
1	6	1
2	5	1
3	4	1
3	6	1
5	1	2
5	2	2
6	1	2
6	2	2
6	3	2
7	2	2

Centroid locations
centroid 1: $(2.0, 5.0)$
centroid 2: $(5.8, 1.8)$
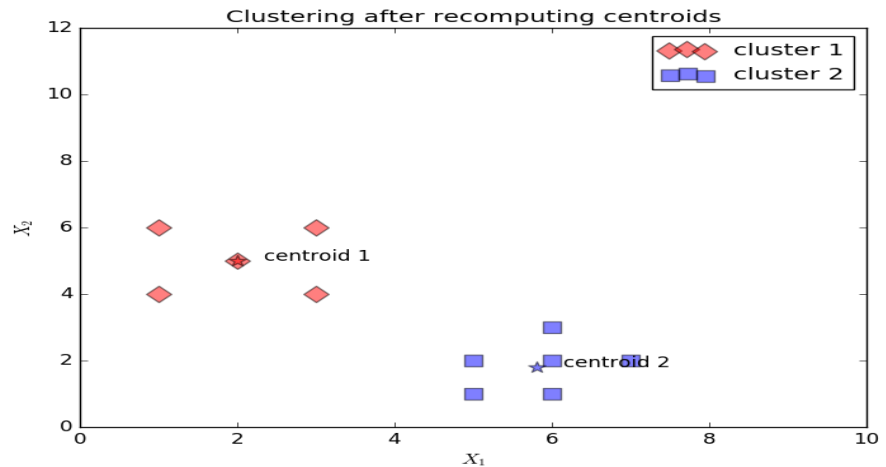
k-means clustering: solution found

Shown on the 3 previous slides are the initialization and the two main steps of the k-means algorithm on the given dataset.

In this simple example k-means clustering has found a solution (the two centroids) after a single iteration, and the algorithm will not change it on further iterations.

By inspection, we can see the solution is a "good clustering", in the sense that the two "natural" clusters in the dataset have been identified.

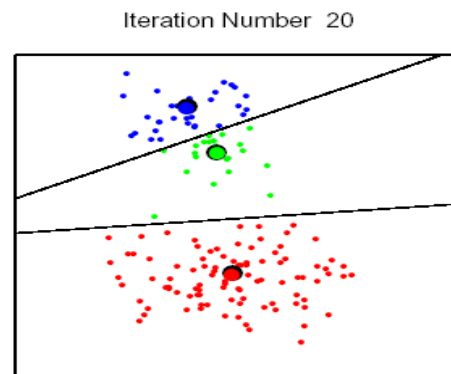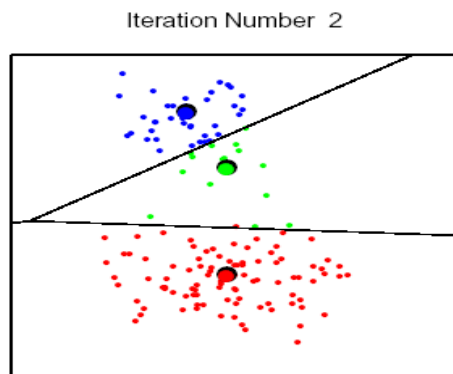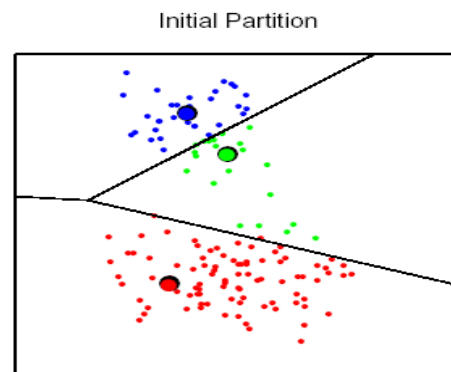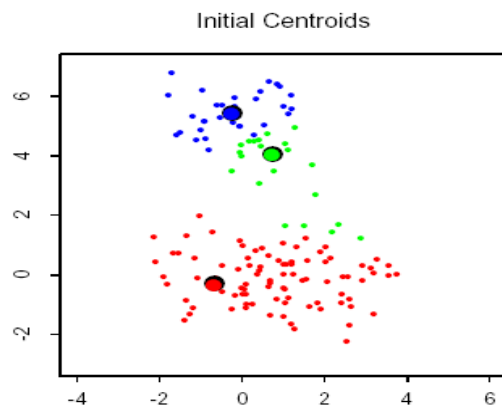In general, the quality of the solution will depend on
- the distribution of the points in the dataset
- the choice of k
- the choice of the location to initialise the centroids.

k-means Clustering

What about the number of clusters k ?

Next diagrams show convergence in k-means with $k = 3$ for data with two clusters not well separated

k-means Clustering
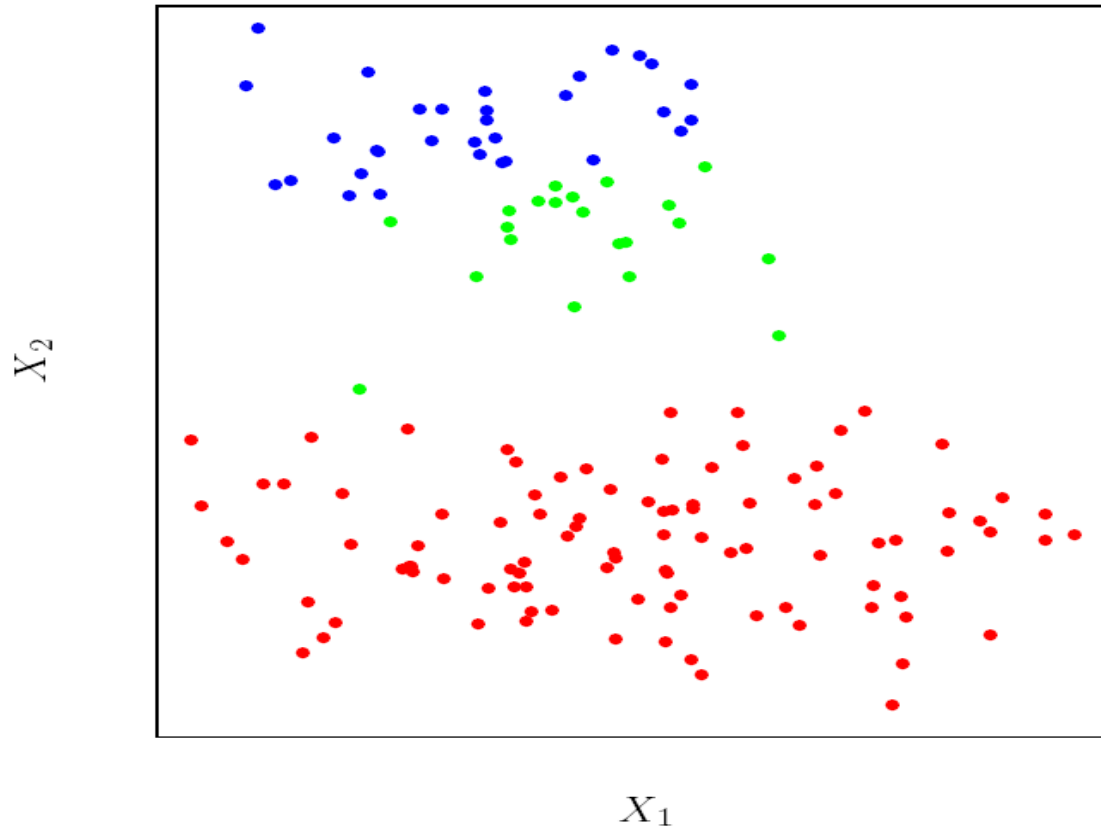
k-means Clustering

Practical k-means

- Algorithm can get trapped in a local minimum
  - For example:
    - place four instances at the vertices of a two-dimensional rectangle
    - local minimum: two cluster centers at the midpoints of the rectangle's long sides
- Result can vary significantly based on initial choice of seeds
- Simple way to increase chance of finding a global optimum: restart with different random seeds
  - can be time-consuming
- Or use the k-means++ algorithm, which initialises k centroids to be maximally distant from each other

Hierarchical clustering

- Bottom up: at each step join the two closest clusters (starting with single-instance clusters)
  - Design decision: distance between clusters
    — *i.e, sets of points*
    - E.g. two closest instances in clusters vs. distance between means
- Top down: find two clusters and then proceed recursively for the two subsets
  - Can be very fast
- Both methods produce a dendrogram (tree of "clusters")

Hierarchical clustering

Distances

$D \in \mathbb{R}^{n \times n}$

Data

$X \in \mathbb{R}^{n \times p}$

$\Downarrow$

distancematrix

all pairwise distances

Algorithm   Hierarchical agglomerative

/* Distance matrix $D(ij)$ is given */

❶ Find minimal entry d_{ij} in D and merge clusters i and j

❷ Update D by deleting column i and row j, and adding new row and column $i \cup j$

❸ Revise entries in D by recalculating distances between new cluster and existing clusters

❹ If there is more than one cluster then go to step 1.

Hierarchical clustering
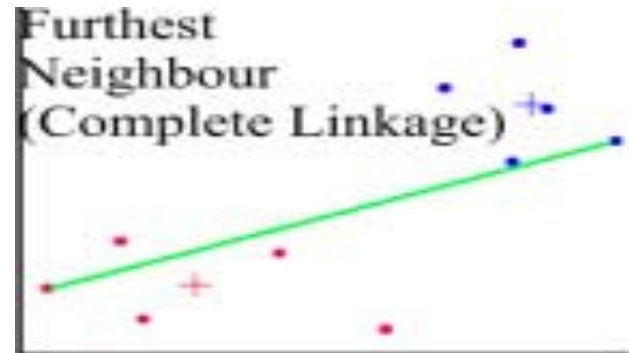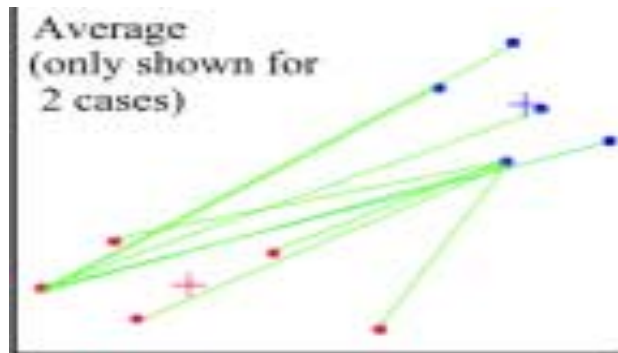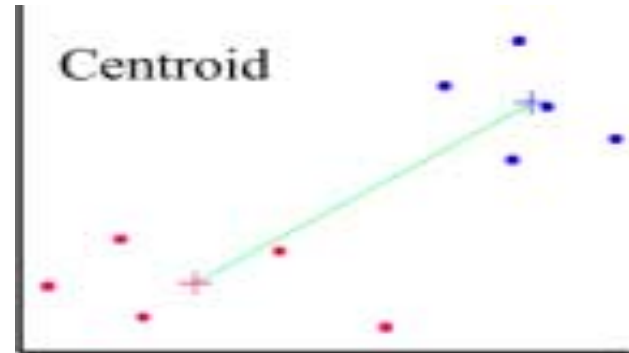
Average Linkage

Average-linkage distance computation is a common method in hierarchical agglomerative clustering.

One version known as "Unweighted pair-group method using arithmetic mean" (UPGMA).

Any data instances with a well-defined distance measure can be clustered.

The distance matrix contains all pair-wise distances between objects.

In output dendrogram edges can be labelled with distances between clusters.

Example using average linkage

"Protein Bioinformatics" (2004) Eidhammer, Jonassen & Taylor

We need a method to compute distance between a new node w formed by combining two clusters (root nodes of sub-trees in the dendrogram) u and v, and all other clusters x:

$$D_{w,x} = \frac{m_u D_{u,x} + m_v D_{v,x}}{m_u + m_v}$$

where m_u is the number of objects in the sub-tree with root node u.

We need a method to calculate the distances on the new edges (v, w) and (u, w) in the dendrogram:

$$L_{v,w} = \frac{1}{2}D_{u,v} - L_{v,y_v}$$

where y_v is a leaf of the sub-tree with root v.

Example using average linkage

A distance matrix for 5 objects:

	B	C	D	E
A	3	7	8	10
B		6	8	7
C			4	5
D				6

Exercise: apply algorithm using average linkage to this distance matrix and construct tree

Distance $X = \{A, B, C, D, E\}$. Distance matrix: all pairwise distances

	A	B	C	D
A	3	7	8	10
B		6	8	7
C			4	5
D				6

$$D_{(A,B),D} = \frac{1 \times 8 + 1 \times 8}{1+1} = 8$$

$$D_{(A,B),E} = \frac{1 \times 10 + 1 \times 7}{1+1}$$
$$= 8.5$$

Find the min. dist. pair = (A,B)

$w = (A,B)$, $u = A$, $v = B$

$$D_{w,x} = \frac{m_u * D_{u,x} + m_v * D_{v,x}}{m_u + m_v}$$

$$D_{(A,B),C} = \frac{1 * 7 + 1 * 6}{1+1} = 6.5$$

Find closest pair: (C,D)

$w = (C,D)$ $u = C$ $v = D$

	(A,B)	C	D	E
C	6.5		8	6.5
D			4	5
E				6

Rest of the working out is on the last page!

$$D_{(C,D),(A,B)} = \frac{1 \times D_{C,(A,B)} + 1 \times D_{D,(A,B)}}{1+1}$$

$$= \frac{1 + 6.5 + 1 \times 8}{2} = \frac{14.5}{2} \approx 7.25$$

$$D_{(C,D),E} = \frac{1 \times 5 + 1 \times 6}{2} = 5.5$$

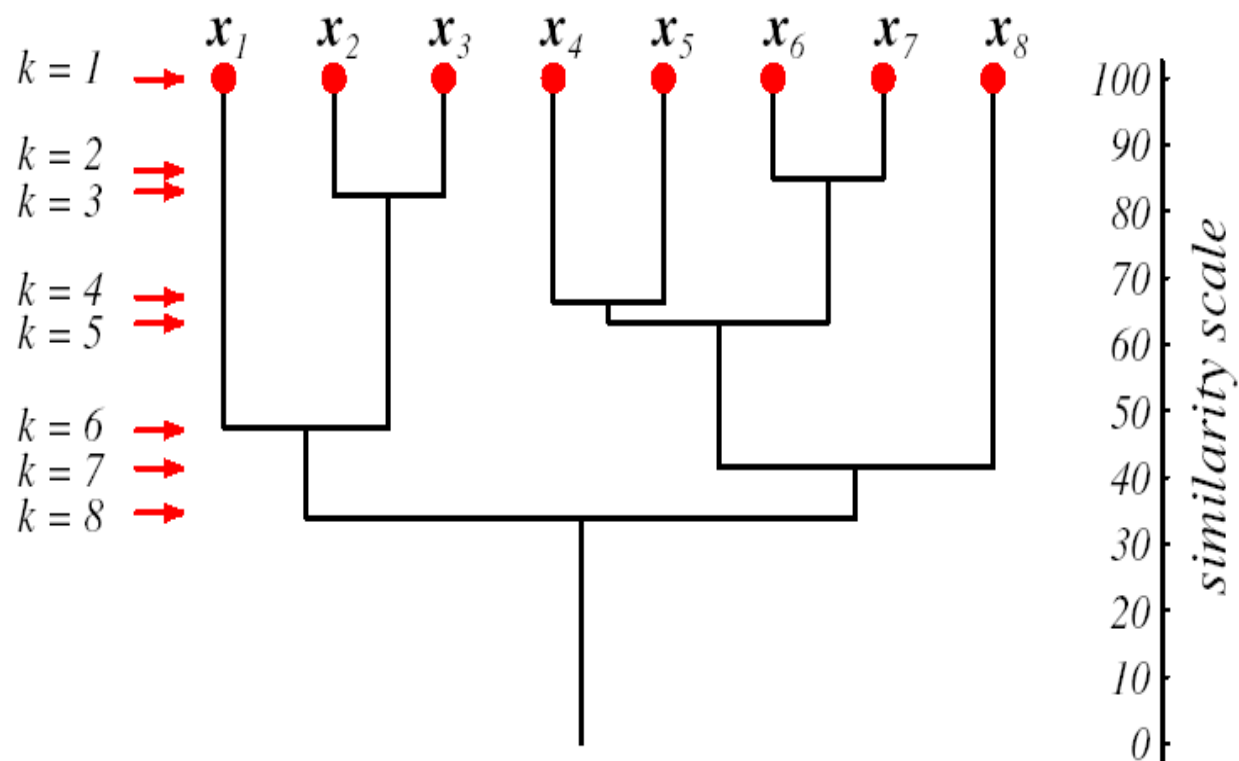|	(C,D)	E
(A,B)	7.25	8.5
(C,D)		5.5

Hierarchical clustering

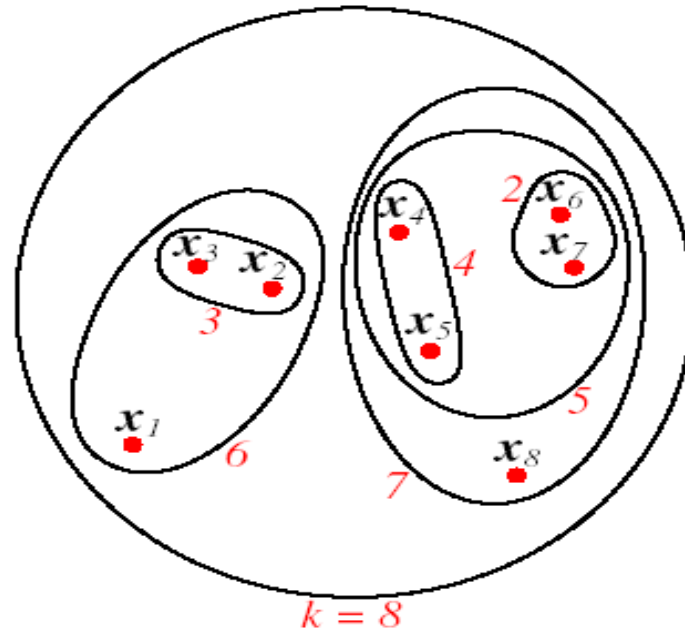Represent results of hierarchical clustering with a *dendrogram*
See next diagram

- at level 1 all points in individual clusters
- x_6 and x_7 are most similar and are merged at level 2
- dendrogram drawn to scale to show similarity between grouped clusters

Hierarchical clustering

Hierarchical clustering

An alternative representation of hierarchical clustering based on sets shows hierarchy (by set inclusion), but not distance.

Dendrograms

Two things to beware of:

1. tree structure is not unique for given clustering - for each bottom-up merge the sub-tree to the right or left must be specified - 2^{n-1} ways to permute the n leaves in a dendrogram

2. hierarchical clustering imposes a bias - the clustering forms a dendrogram despite the possible lack of a implicit hierarchical structuring in the data
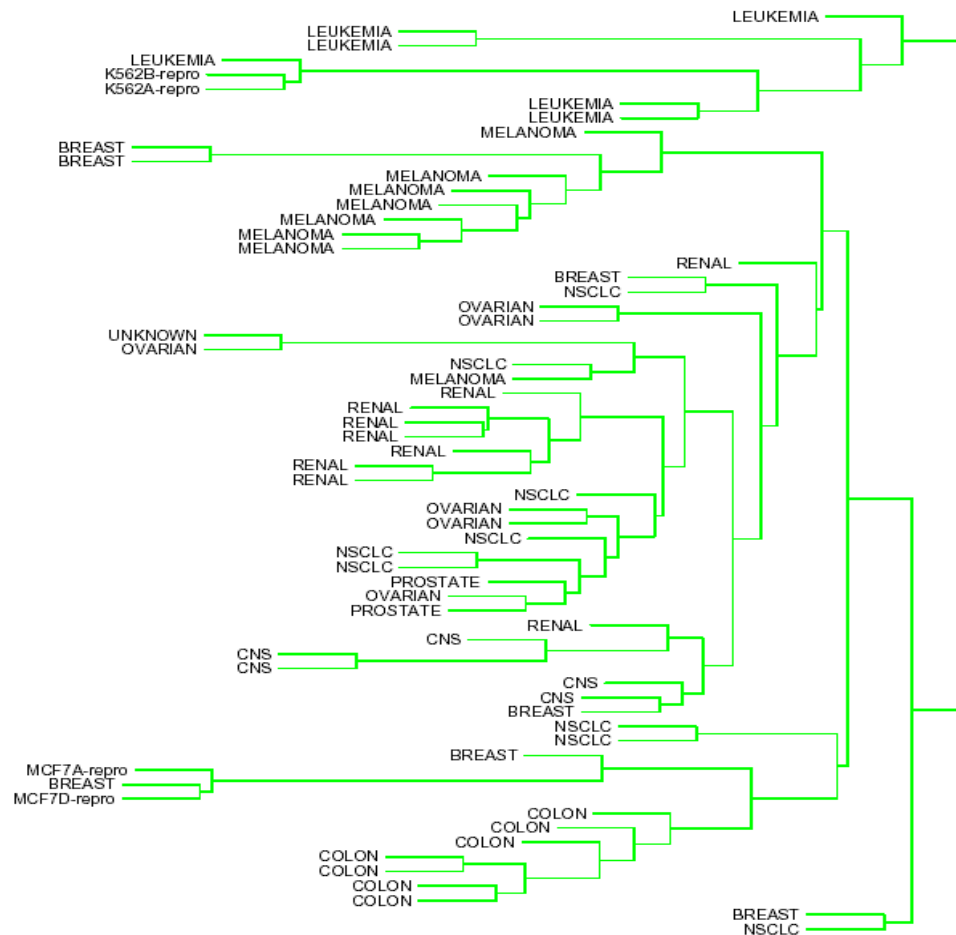
Dendrograms

Next diagram: average-linkage hierarchical clustering of microarray data. For this dataset the class of each instance is shown in each leaf of dendrogram to illustrate how clustering has grouped similar tissue samples coincides with the labelling of samples by cancer subtype.
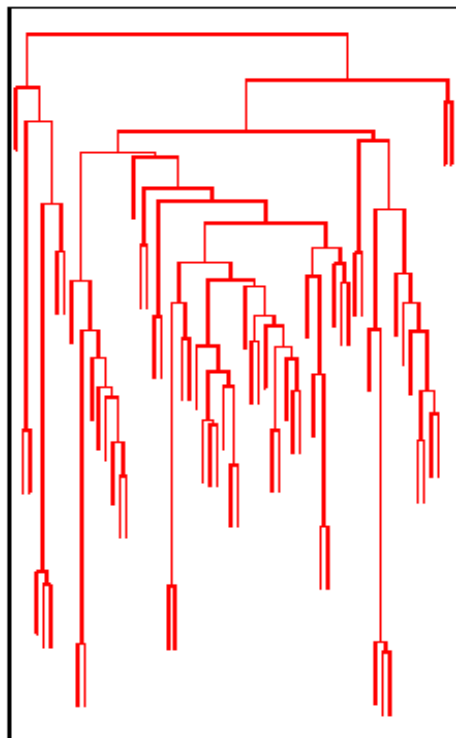
Followed on next slide by diagram showing:

- average-linkage based on average dissimilarity between groups
- complete-linkage based on dissimilarity of furthest pair between groups
- single-linkage based on dissimilarity of closest pair between groups
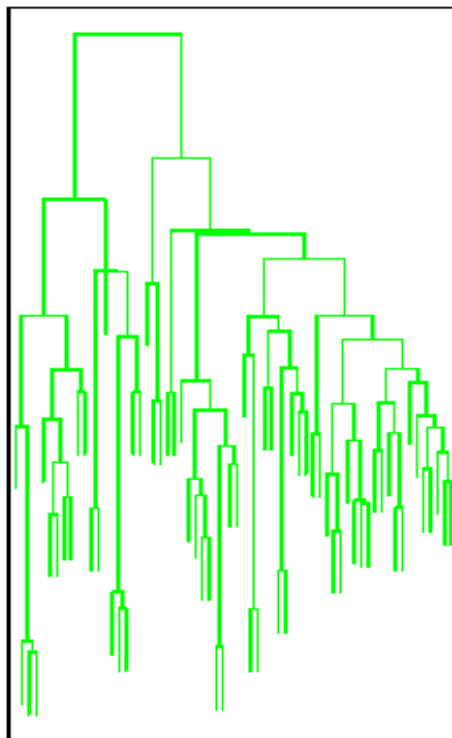
Dendrograms
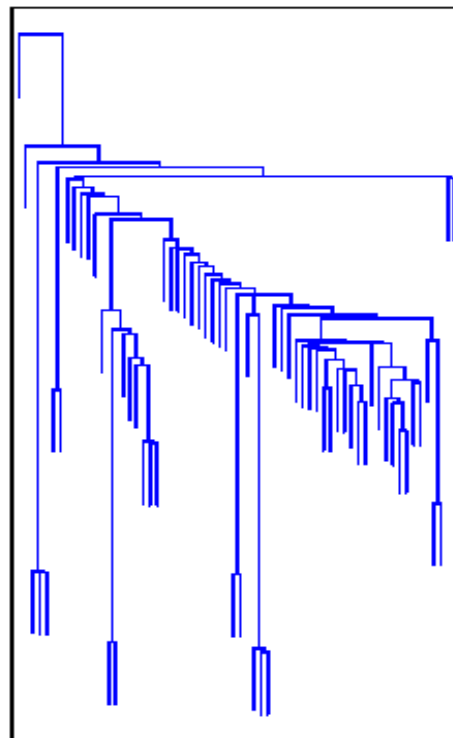
Dendrograms

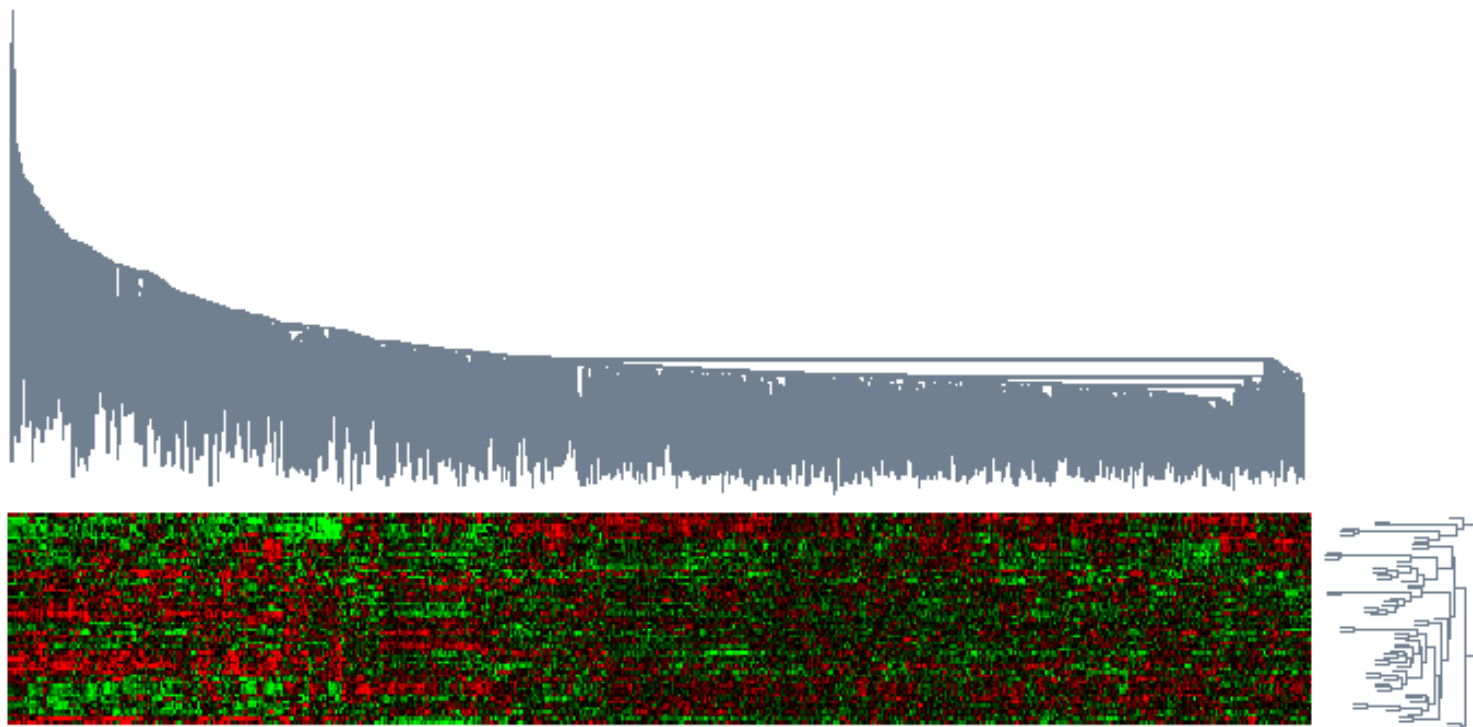Average Linkage   Complete Linkage   Single Linkage
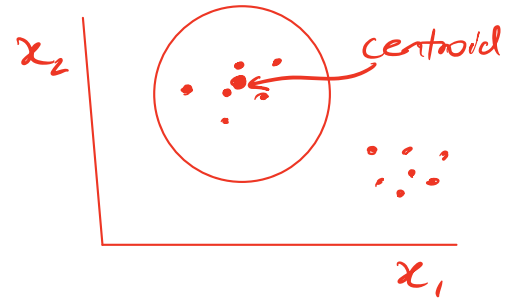
Dendrograms – hierarchical clustering of data by rows or columns

Inductive bias of clustering

- k-means: clusters spherical around centroid
- hierarchical agglomerative: clusters form a tree (dendrogram)

These assumptions may not be justified, and can be relaxed, e.g., kernel k-means.

Many other clustering algorithms are available . . .

Cluster quality visualisation - Silhouette plot

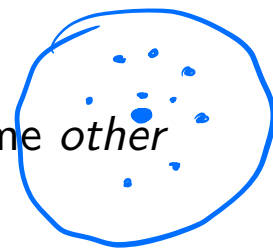Key idea: compare each object's *separation* from other clusters relative to the *homogeneity* of its cluster.

For each object i, define its silhouette width $s(i) \in [-1, 1]$:
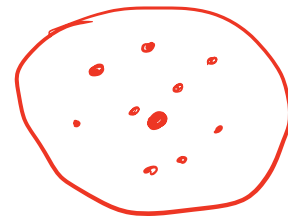
Let $a(i)$ be the average dissimilarity between i and elements of $P(i)$, i.e., cluster to which i belongs,

Let $d(i, C)$ be the average dissimilarity of i to elements of some *other* cluster C.
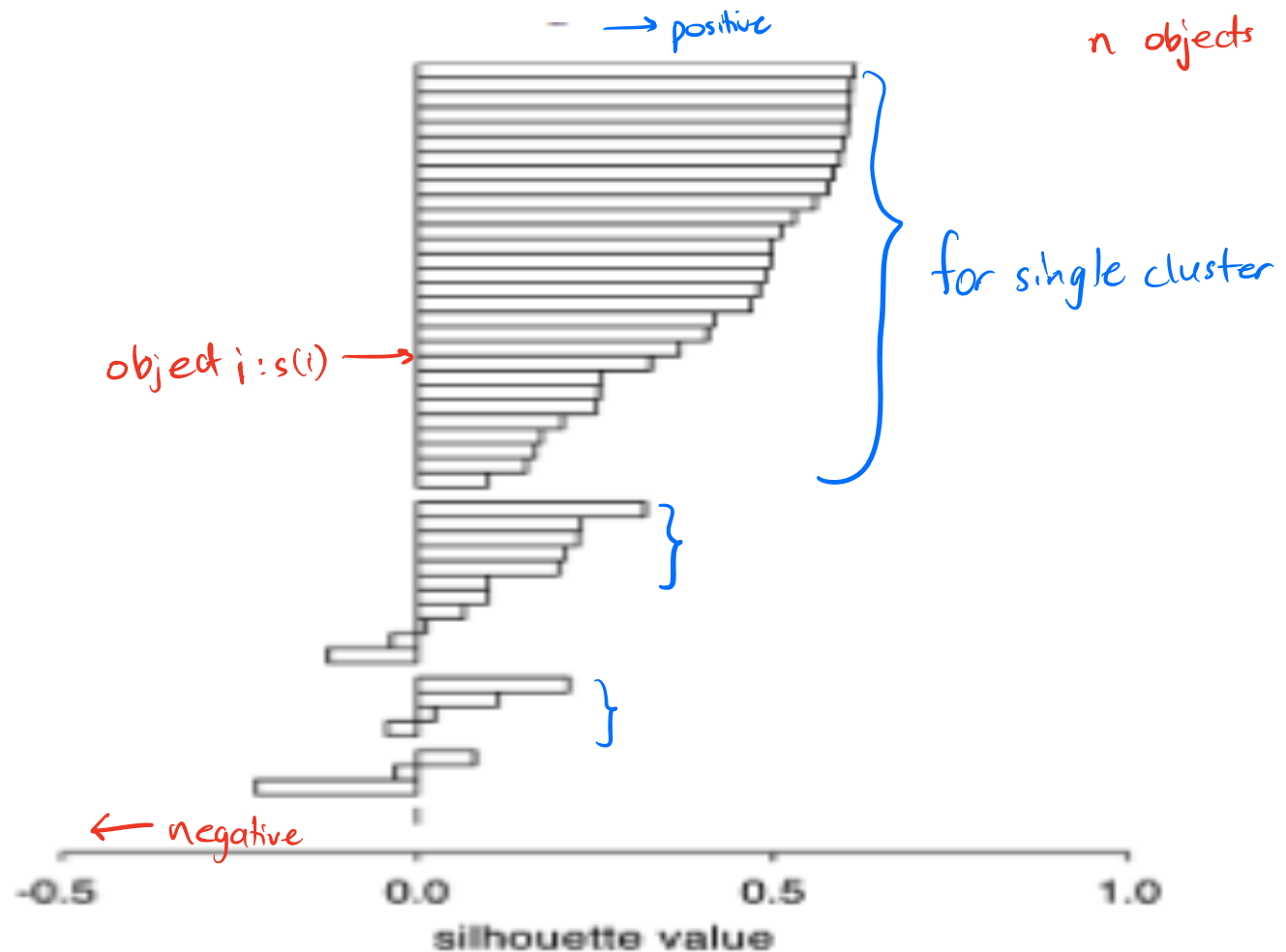
Let $b(i) = \min_C d(i, C)$. The *silhouette width* is

$$\frac{b(i) - a(i)}{\max(a(i), b(i))}$$

good
clustering $s(i)$ ↑

bad
clustering $s(i)$ ↓

Cluster quality visualisation - Silhouette plot

Cluster quality visualisation - Silhouette plot

How can we intepret a Silhouette plot ?

- say for some object i we have $b(i) \gg a(i)$
- then it will be well-separated from all the other clusters, and its cluster will probably be homogeneous
- in such cases $s(i)$ will tend to be close to 1 for object i, and we can take it to be "well-classified" by its cluster
- conversely, if $s(i)$ is close to -1 we can view it as "misclassified" by its cluster
- can see which clusters are "good" or otherwise, and estimate number of clusters
- can take average $s(i)$ over different clusterings for comparison

Silhouette plots available in R.
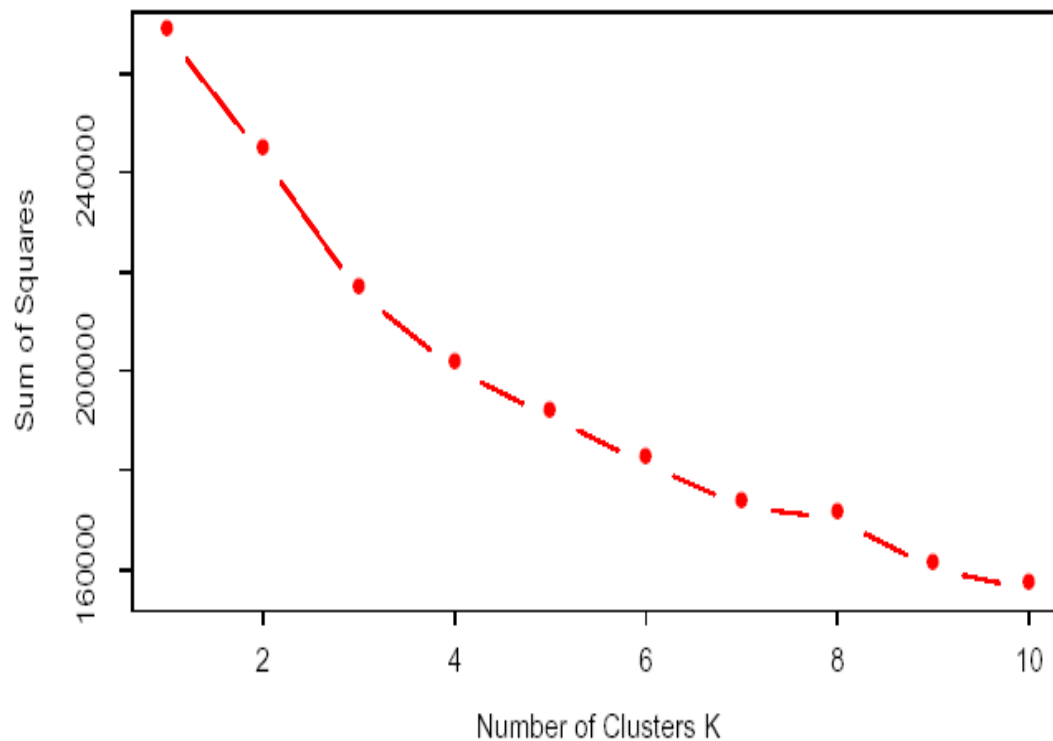
How many clusters ?

Example: in k-means clustering, trying to *minimize* a loss function in which the goal of clustering is *not* met:

- running on microarray data of 6830×64 matrix
- total within-cluster "dispersion" (i.e., sum of squared distances from each point to the cluster centroid) is reduced for $k = 1$ to 10
- look for "elbow", but no obvious "correct" k

How many clusters ?

$$\longrightarrow 0$$
$$as$$
$$k \longrightarrow n$$

How many clusters ?

Many methods of estimating the "correct" number of clusters have been proposed. Here we mention two using some clustering criterion (such as "dispersion" i.e., sum of squared distances from each point to the cluster centroid).

- compare value for single cluster to sum of values for breaking cluster into two
- if there is a "significant" reduction then keep two clusters[1]
- formalise "elbow" detection
- Gap statistic[2]
- compares graph of within-cluster dispersion against k to a random reference value

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[1] "Pattern Recognition" Duda & Hart (1973).
[2] "Estimating the number of clusters in a data set via the gap statistic" R. Tibshirani *et al.* J. R. Statist. Soc. B (2001) 63, Part 2, 411–423.

Clustering Summary

- many techniques available – may not be single "magic bullet" rather different techniques useful for different aspects of data

- hierarchical clustering gives a view of the complete structure found, without restricting the no. of clusters, but can be computationally expensive

- different linkage methods can produce very different dendrograms

- higher nodes can be very heterogeneous

- problem may not have a "real" hierarchical structure

Clustering summary

- k-means avoids some of these problems, but also has drawbacks
- cannot extract "intermediate features" e.g., a subset of features in which a subset of objects is co-expressed
- for all of these methods, can cluster objects or features, but not both together (coupled two-way clustering)
- should all the points be clustered ? modify algorithms to allow points to be discarded
- visualization is important: dendrograms and alternatives like Self-Organizing Maps (SOMs) are good but further improvements would help; see also T-SNE for visualization
- algorithms like DBSCAN make fewer assumptions

Clustering summary

- how can the quality of clustering be estimated ?
  - if clusters known, measure proportion of disagreements to agreements
  - if unknown, measure homogeneity (average similarity between feature vectors in a cluster and the centroid) and separation (weighted average similarity between cluster centroids) with aim of increasing homogeneity and decreasing separation
  - sihouette method, etc.

- clustering is only the first step - mainly exploratory; classification, modelling, hypothesis formation, etc.

Dimensionality Reduction

What is this and why would we need it ?

- each numeric feature in a dataset is a dimension
- in general, no restrictions on the number of dimensions
- however, many features could be related
- do we need them all in our dataset ?
  - including them is all unlikely to improve models
  - feature selection may return arbitrary features
- so, what to do ?
- one solution would be to find set of *new* features
  - should be fewer than the original set
  - should preserve information in original set (as far as possible)

Principal Component Analysis (PCA)

*"factor analysis"*

"matrix factorisation"

Key idea: look for features in a transformed space *(feature)* so that each dimension in the new space captures the most variation in the original data when it is projected onto that dimension.

Any new features should be highly correlated with (some of) the original features, but not with any of the other new features.

This suggests an approach: consider using the variance-covariance matrix we recall from correlation and regression
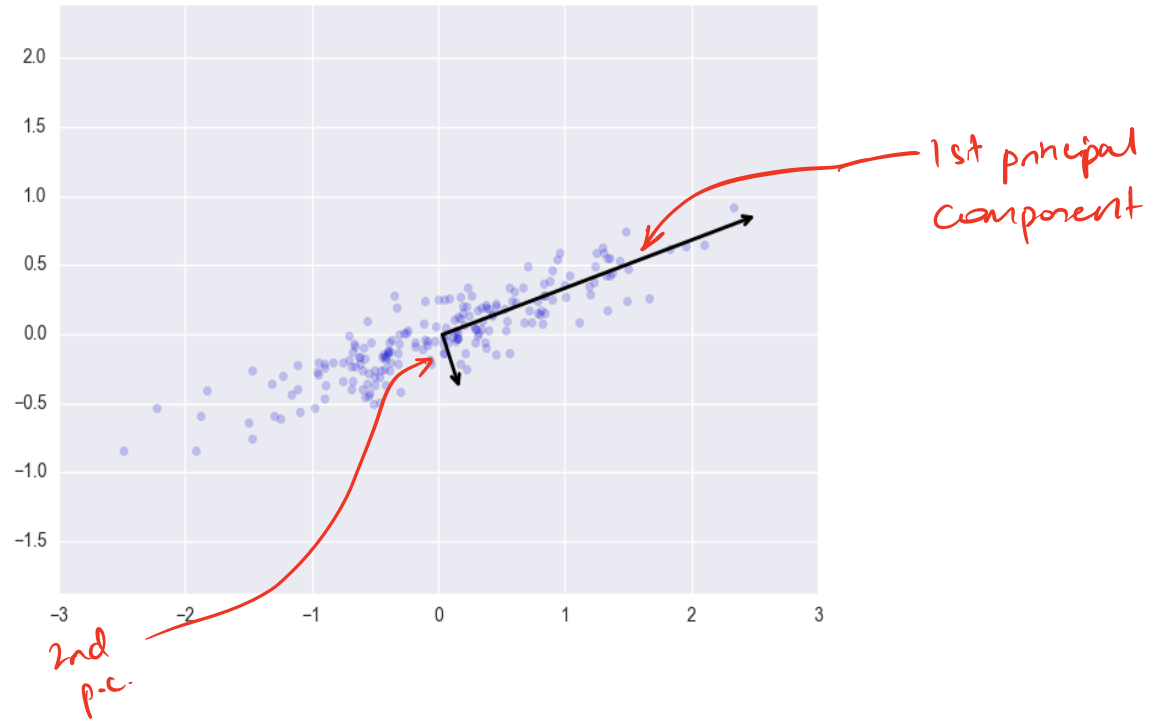
PCA Example
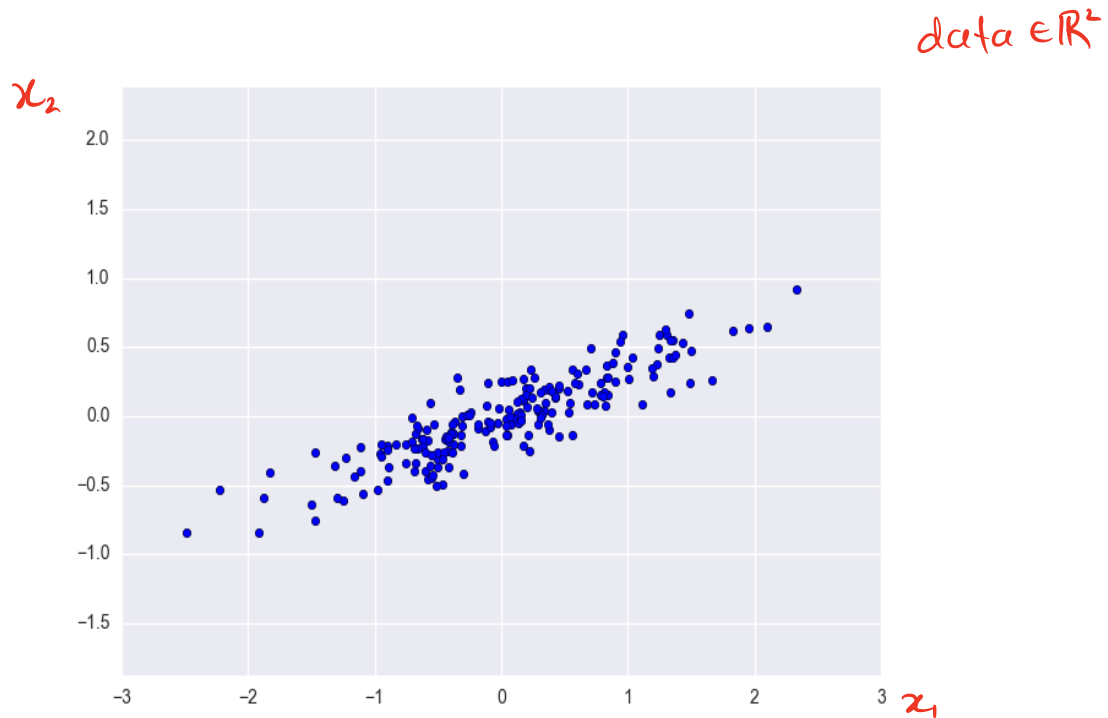
PCA looks for linear combinations of the original features. This dataset of 200 points seems to show such a relationship between two feature dimensions.

PCA Example

PCA finds two new features on which the original data can be projected, rotated and scaled. These explain respectively 0.75 and 0.02 of the variance.

PCA Algorithm

This algorithm can be presented in several ways.

Here we approach it using the Singular Value Decomposition (SVD).

Data matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ can be written as the product of three matrices:
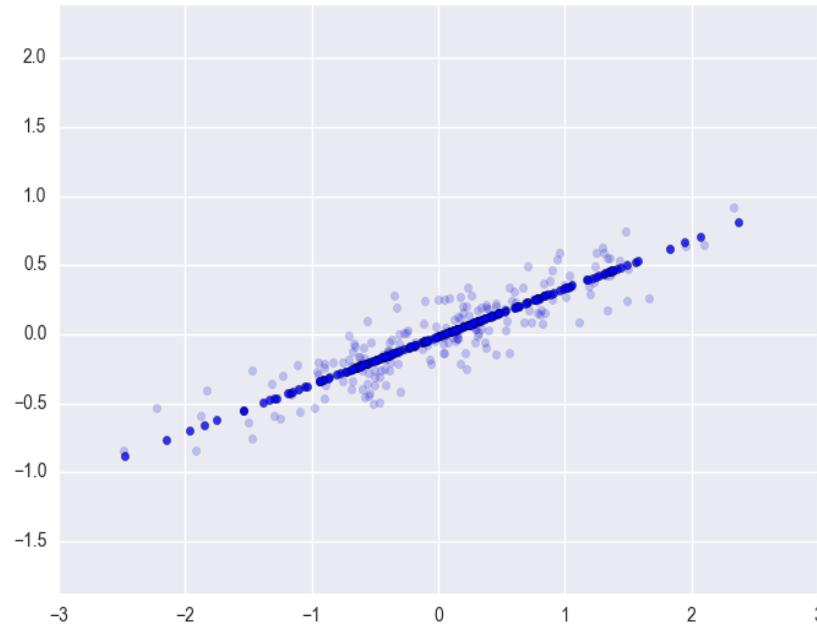
$$\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^{\top}$$

(explanation on last page!)

There is an extensive literature on SVD !

Here we will just give a simplified introduction.

PCA Example

By rejecting the second component we reduce the dimensionality by 50% while preserving much of the original variance, seen by plotting the inverse transform of this component along with the original data.

PCA and friends

- PCA typically computed using the Singular Value Decomposition (SVD)
- complexity is cubic in number of original features
- this is not feasible for high-dimensional datasets
- alternatively, approximate the sort of projection found by PCA
- for example, can use Random Projections
- more scalable, but what about quality of components ?
- can be shown to preserve distance relations from the original data
- many other methods use essentially the same *matrix decomposition* idea, such as finding "topics" in text using Latent Semantic Analysis, finding hidden "sub-groups" for recommender systems, and so on

Latent Factor Representations for Recommendation

Recommender systems typically based on a large sparse *ratings matrix*.

Every item is rated (or purchased) by a user

Ratings are often on a scale of 1 to 5

Matrix is m users $\times$ n items

Elements contain rating $r_{u,i}$ of user u for item i

Since most values $r_{u,i}$ are missing, apply *matrix decomposition*[3].

---

[3]See, e.g., Koren and Bell (2011).

Example: Latent Factors for Recommendation I

Consider the following matrix:

movies

users
$$\begin{pmatrix} 1 & 0 & 1 & 0 \\ 0 & 2 & 2 & 2 \\ 0 & 0 & 0 & 1 \\ 1 & 2 & 3 & 2 \\ 1 & 0 & 1 & 1 \\ 0 & 2 & 2 & 3 \end{pmatrix}$$

Imagine these represent ratings by six different people (in rows), on a scale of 0 to 3, of four different films – say *The Shawshank Redemption*, *The Usual Suspects*, *The Godfather*, and *The Big Lebowski*, (in columns, from left to right). *The Godfather* seems to be the most popular of the four with an average rating of 1.5, and *The Shawshank Redemption* is the least appreciated with an average rating of 0.5.

Can you see any structure in this matrix?

Example: Latent Factors for Recommendation II

Ratings

$$
\begin{pmatrix}
1 & 0 & 1 & 0 \\
0 & 2 & 2 & 2 \\
0 & 0 & 0 & 1 \\
1 & 2 & 3 & 2 \\
1 & 0 & 1 & 1 \\
0 & 2 & 2 & 3
\end{pmatrix}
=
\begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \\
1 & 1 & 0 \\
1 & 0 & 1 \\
0 & 1 & 1
\end{pmatrix}
\times
\begin{pmatrix}
1 & 0 & 0 \\
0 & 2 & 0 \\
0 & 0 & 1
\end{pmatrix}
\times
\begin{pmatrix}
1 & 0 & 1 & 0 \\
0 & 1 & 1 & 1 \\
0 & 0 & 0 & 1
\end{pmatrix}
$$

drama crime comedy — "weightings" — *drama crime comedy* — SR US GF BL

- The right-most matrix associates films (in columns) with genres (in rows): *The Shawshank Redemption* and *The Usual Suspects* belong to two different genres, say drama and crime, *The Godfather* belongs to both, and *The Big Lebowski* is a crime film and also introduces a new genre (say comedy).

- The tall, 6-by-3 matrix then expresses people's preferences in terms of genres.

Example: Latent Factors for Recommendation III

- Finally, the middle matrix states that the crime genre is twice as important as the other two genres in terms of determining people's preferences.

Dimensionality Reduction Summary

- PCA will transform original features to new space
- every new feature is a linear combination of original features
- aim for new dimensions to maximise variance
- order by decreasing variance and remove those below a threshold
- this reduces dimensionality
- algorithm applies matrix operations to translate, rotate and scale
- based on covariance matrix
  - can be "kernelised" (KernelPCA)
  - new feature space with non-linear axes
- many alternatives, e.g., Random Projections, Independent Component Analysis, Multi-dimensional Scaling, Word2Vec, etc.

Unsupervised Learning Summary

Unsupervised and supervised learning are at different ends of a continuum of "degrees of supervision". Between these extremes many other approaches are possible.

- semi-supervised learning, e.g.,
    - train with small labelled sample then improve with large unlabelled sample
    - train with large unlabelled sample then learn classes with small labelled sample
- reinforcement learning can be viewed as unsupervised
    - "reward" is a signal from the "environment"
    - learning is designed to optimize function of reward
- active learning
    - learning system acts to generate its own examples

Note: unsupervised learing an increasingly active research area, particularly in neural nets, such as Autoencoders. For more see, e.g., Yann LeCun: "How Could Machines Learn as Efficiently as Animals and Humans?"
`http://www.youtube.com/watch?v=uYwH4TSdVYs`

Koren, Y. and Bell, R. (2011). Advances in Collaborative Filtering. In Ricci, F., Rokach, L., Shapira, B., and Kantor, P., editors, *Recommender Systems Handbook*. Springer.

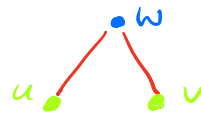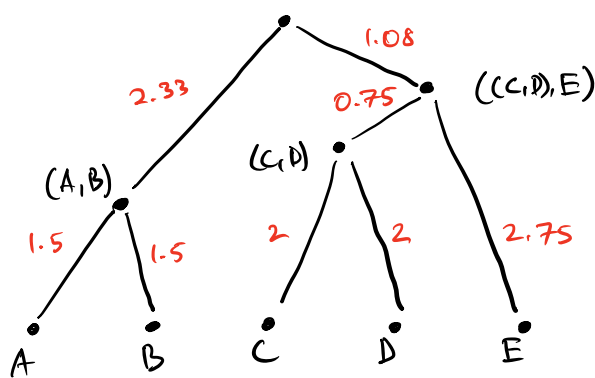Find closest pair: $((C,D),E)$

$w = (C,D), E$ $v = (C,D)$ $v = E$

$$D_{(C,D),E),(A,B)} = \frac{2 * D_{(C \times D),(A \times B)} + 1 * D_{E,(A,B)}}{2+7}$$

$$= \frac{2 * 7.25 + 1 * 5.5}{3}$$

$$\simeq 7.67$$

$((C,D),E)$

(A,B) 7.67

Dendrogram ((A,B), ((C,D), E))

$L_{A,(A,B)} = \frac{1}{2} 3 - 0 = 1.5$

$L_{B,(A,B)} = 1.5$

$L_{E,((C,D),E)} = \frac{1}{2} 5.5 = 2.75$

$L_{(A,B),((A,B),(C,D),E)} \cong 2.33$

$L_{(C,D),((C,D),E)} = \frac{1}{2} 5.5 - L_{(C,D),C}$

$= 2.75 - 2 = 0.75$

$$L_{v,w} = \frac{1}{2} D_{u,v} - L_{v,yv}$$

Assume: additive — distance between any 2 nodes is sum of edge distances connecting them; ultrametric — dist. to common ancestor is the same for any 2 nodes.

Note: tree * imposes a new set of distances between elements:

	B	C	D	E
A	3	7.66	7.66	7.66
B		7.66	7.66	7.66
C			4	5.5
D				5.5

* approximate due to rounding

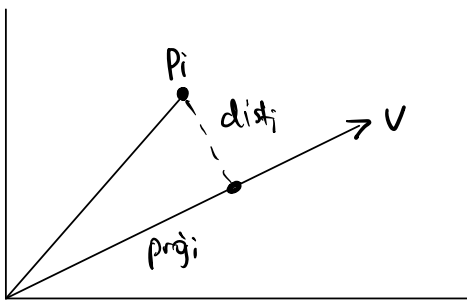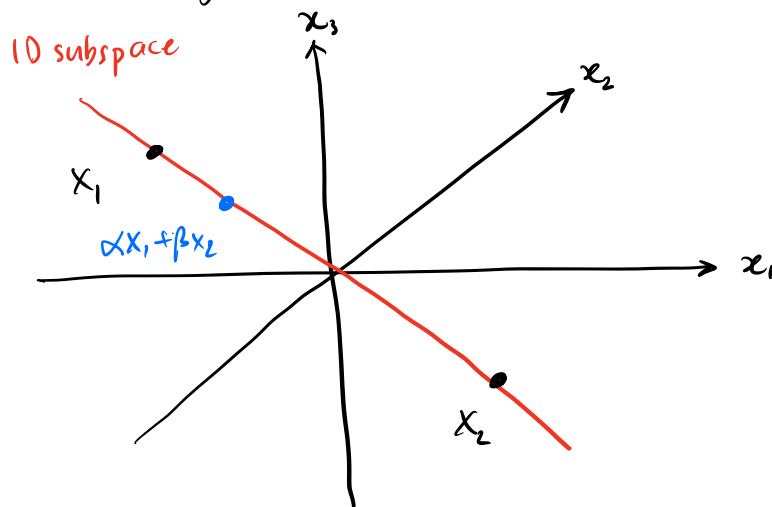Projection of data point Y onto a set (e.g., a subspace) is the closest point to Y in that set.
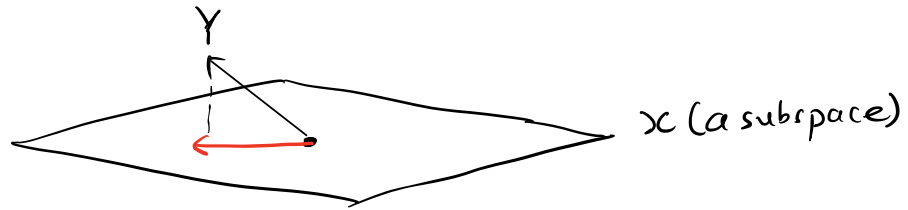
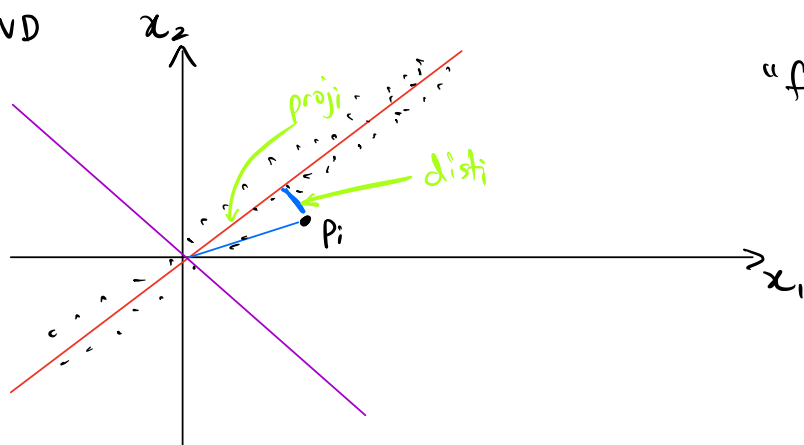Projection of Y on $\mathcal{X}$:= $\underset{x \in \mathcal{X}}{\arg\min} \|X - Y\|_2^2$

$\Rightarrow$ least squares approximation!

Consider 1D space: finding "best" projection of points in $\mathbb{R}^3$

x_3
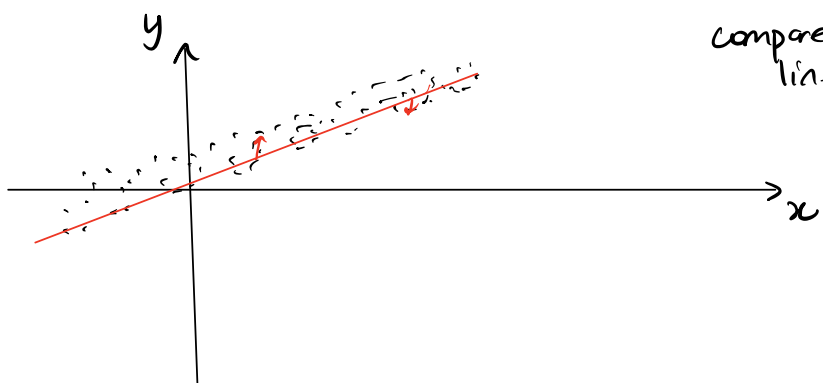
x_2

1D subspace

X_1

$\alpha x_1 + \beta x_2$

x_1

X_2

P_i

$dist_i$

V

$proj_i$

Minimising $\sum_i dist_i^2 \equiv$

Maximising $\sum_i proj_i^2$

SVD

"finding best 10 subspace for a set of points"

Simple algo for SVD:
repeatedly find best
10 subspace to data.

compared to
linear