

# Unsupervised learning

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# Learning goals

During this lecture we will:

- ▶ Define the concept of unsupervised learning.
- ▶ Describe the concept of dimensionality reduction and explain two methods in this category: Principal Component Analysis (PCA) and t-SNE.
- ▶ Describe the concept clustering and explain two methods in this category: K-means and hierarchical clustering.
- ▶ Illustrate the application of these methods to a specific case study and interpret the results.
- ▶ Compare the different methods from a theoretical prospective and using the case study.

Materials:

- ▶ Chapters 14 from Friedman et al., *The Elements of Statistical Learning*.

# Overview

Topics of the lecture:

- ▶ What is unsupervised learning?
- ▶ Methods for dimensionality reduction
  - ▶ Principal components analysis
  - ▶ t-SNE
- ▶ Methods for clustering
  - ▶ K-means clustering
  - ▶ Hierarchical clustering

# Difference between supervised and unsupervised learning

With both supervised and unsupervised learning we have a set of features  $X_1, X_2, \dots, X_p$ .

- ▶ with **supervised learning** (or *learning with a teacher*) we also have a variable  $Y$  (a label).
- ▶ with **unsupervised learning** (or *learning without a teacher*) we don't have the label.

# Unsupervised learning

The goal of **unsupervised learning** is to find similarities among observations based on the set of features.

Two categories:

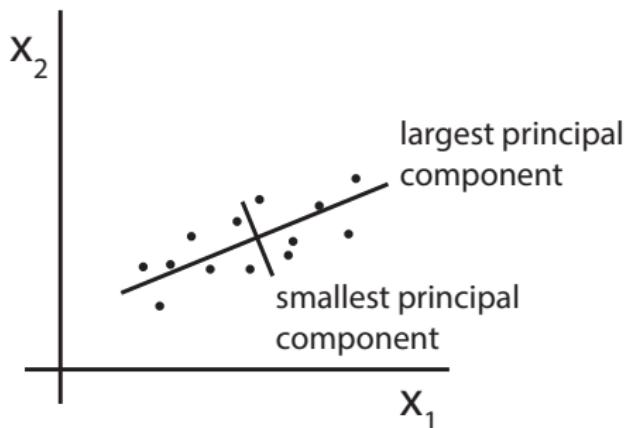
- ▶ **Dimensionality reduction:** reduce the dimensions of the input features to facilitate visualisation and identification of groups. Also used as preprocessing before applying supervised techniques.
- ▶ **Clustering:** techniques to discover unknown groups (clusters) in data.

Compared to supervised learning:

- ▶ No need for labels (often difficult to retrieve)
- ▶ No quantitative metrics to measure success; evaluation based on heuristic arguments.

# Principal Component Analysis (PCA)

Idea: From the  $p$  variables (often correlated), derive a smaller subset of variables that explain most of the variability of the original set.



# Principal Component Analysis (PCA)

Starting from a set of features  $X_1, X_2, \dots, X_p$ , the *first principal component* is the normalised linear combination of the features.

$$Z_1 = v_{11}X_1 + v_{21}X_2 + \cdots + v_{p1}X_p$$

where  $\sum_{j=1}^p v_{j1}^2 = 1$ , and  $v_{11}, v_{21}, \dots, v_{p1}$  are the *loadings* of the first principal component and  $v_1 = (v_{11}, v_{21}, \dots, v_{p1})$  is the *first principal component loading vector*.

## PCA computation - first principal component (PC1)

We have our  $N$  observations  $x_1, x_2, \dots, x_N$ , where each  $x_i = (x_{i1}, x_{i2}, \dots, x_{ip})^T$ , or in matrix form  $\mathbf{X}$  of size  $N \times p$ .

Since we are interested only in the variance we assume that each feature has 0 mean, i.e.  $\mathbf{X}$  has columns with mean zero.

We want to find the linear combination of the sample feature value:

$$z_{i1} = v_{11}x_{i1} + v_{21}x_{i2} + \cdots + v_{p1}x_{ip}$$

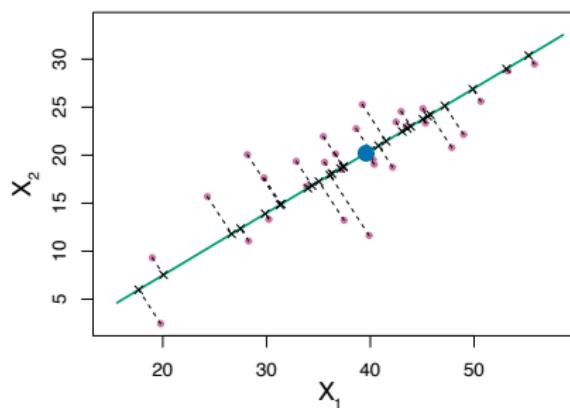
with the largest sample variance, i.e.

$$\max_{v_{11}, \dots, v_{p1}} \left\{ \frac{1}{N} \sum_{i=1}^N \left( \sum_{j=1}^p v_{j1} x_{ij} \right)^2 \right\} \text{ subject to } \sum_{j=1}^p v_{j1}^2 = 1$$

Since each  $x_{ij}$  has mean zero, also does  $z_{ij}$ . Hence we are maximising the sample variance of  $Z_1$  which is  $\frac{1}{N} \sum_{i=1}^N z_{i1}^2$ .

## PCA computation - PC1 geometrical interpretation

- ▶ The loading vector  $v_1$  with elements  $v_{11}, v_{21}, \dots, v_{p1}$  define the direction along which the data vary the most.
- ▶ The projections of the  $N$  points  $x_1, x_2, \dots, x_N$  onto this direction are the principal component scores  $z_{11}, z_{21}, \dots, z_{N1}$ .

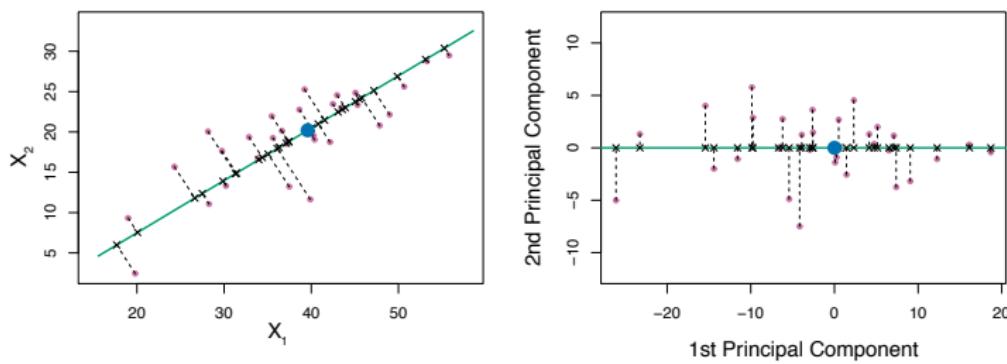


## PCA computation - further principal components

Now that we have the first principal component  $Z_1$  we want to find the *second principal component*.  $Z_2$ .

$Z_2$  needs to be uncorrelated with  $Z_1$ . This is equivalent to constrain the direction of the loading vector  $v_2$  is orthogonal to the direction of  $v_1$ .

Same for the following principal components.



# PCA computation using SVD

This optimisation problem can be solved via *singular value decomposition* of the matrix  $\mathbf{X}$ :

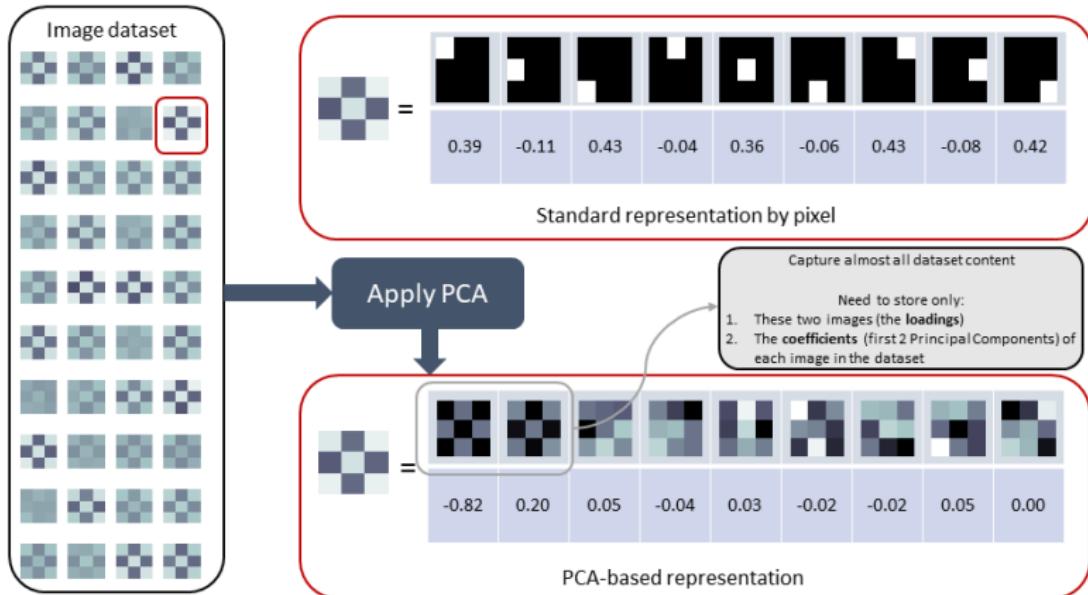
$$\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^T$$

which is a unique decomposition such that (for  $N \geq p$ ):

- ▶  $\mathbf{U}$  is a  $N \times p$  orthogonal matrix ( $\mathbf{U}^T\mathbf{U} = \mathbf{I}_p$ )
- ▶  $\mathbf{D}$  is a  $p \times p$  diagonal matrix with  $d_i \geq 0$  and  $d_i \geq d_{i+1}$  known as the *singular value*
- ▶  $\mathbf{V}$  is a  $p \times p$  orthogonal matrix ( $\mathbf{V}^T\mathbf{V} = \mathbf{I}_p$ )

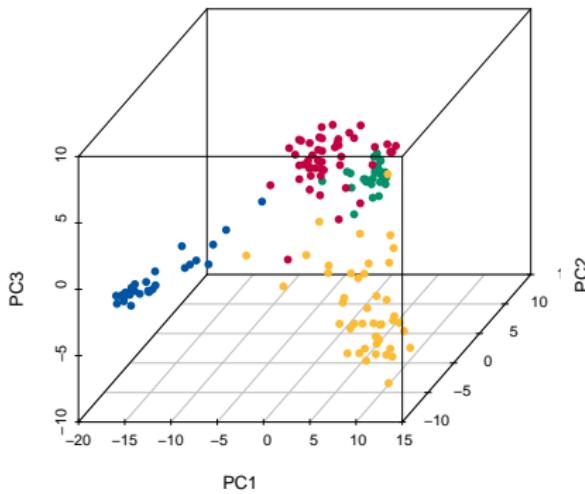
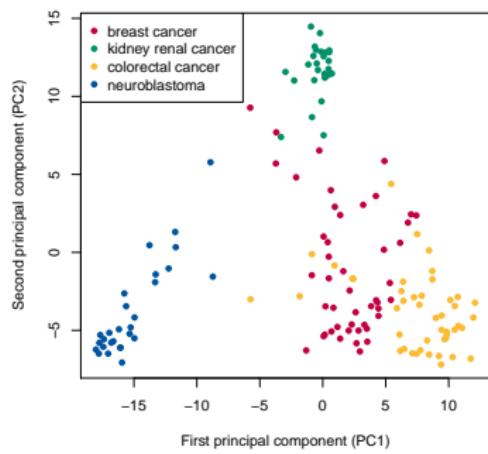
The columns of  $\mathbf{UD}$  are the *principal components* of  $\mathbf{X}$  ( $PC1 = u_{i1}d_1, PC2 = u_{i2}d_2, \dots$ ) and  $\frac{d_1^2}{N}, \frac{d_2^2}{N}, \dots$  is the variance explained by each principal component.

# PCA example using images



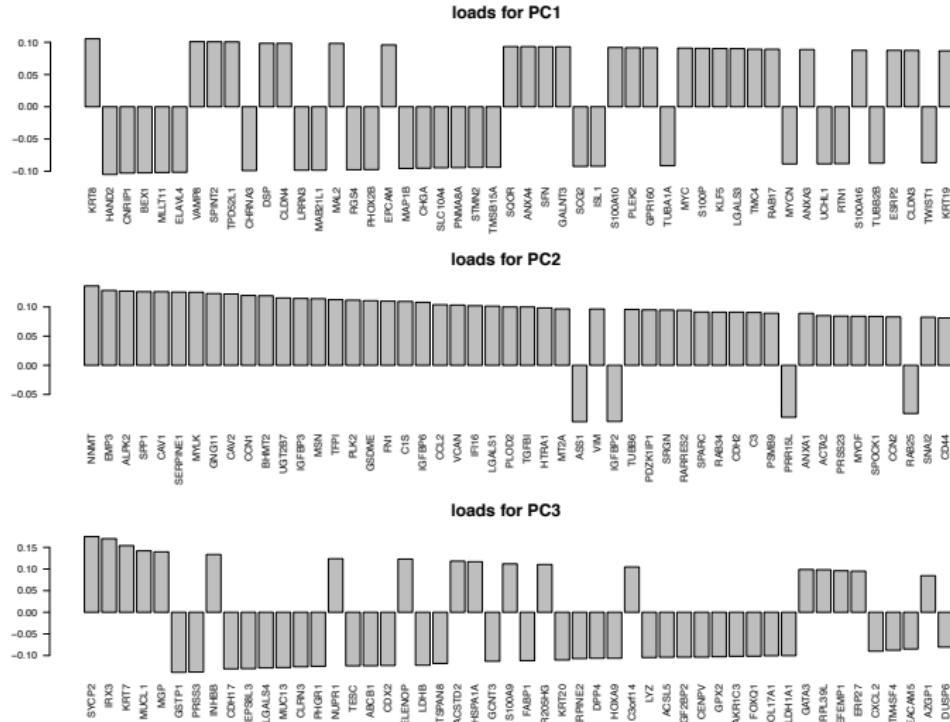
# PCA example using GDSC dataset

RNA expression data (244 genes) for 148 cell lines from four cancer types. Samples are *a posteriori* coloured by cancer type.



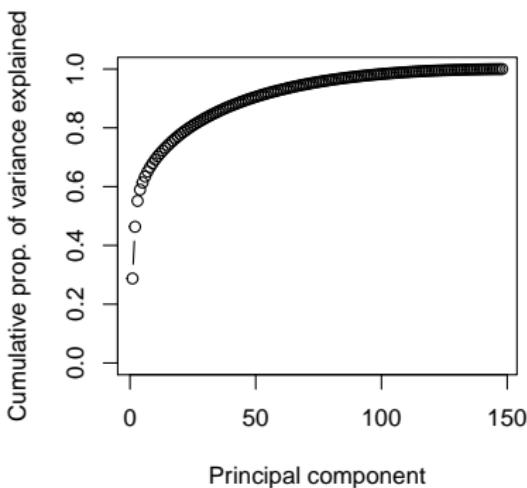
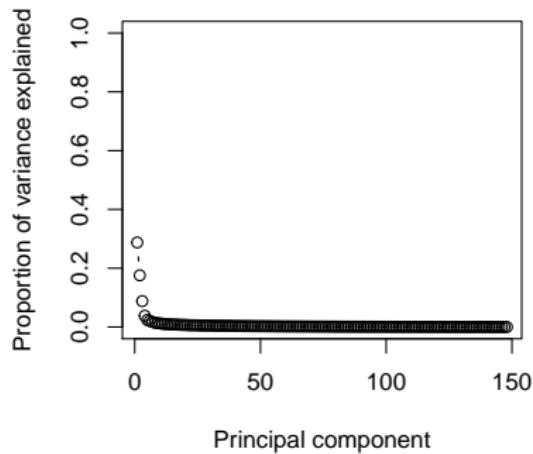
# PCA example using GDSC dataset - loads

Loads of the first 3 principal components (only top 50 genes)



# PCA example using GDSC dataset - variance explained

Variance explained by the principal components.



Elbow in the "proportion of variance explained" plot can be used as a criteria to decide how many principal components to use.

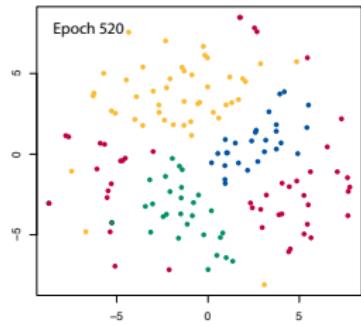
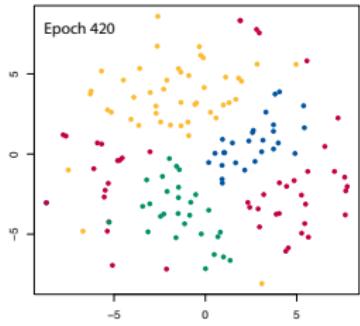
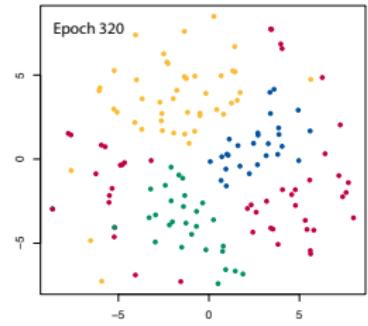
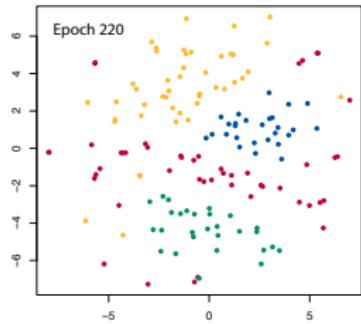
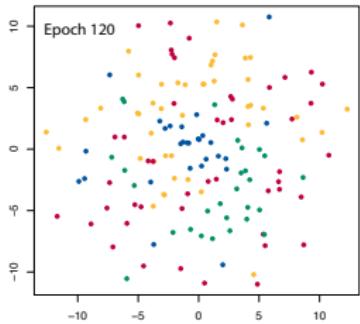
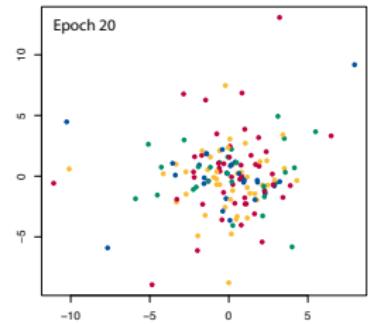
# t-SNE

- ▶ PCA is a linear algorithm, i.e. principal components are linear combinations of the features.
- ▶ t-Distributed Stochastic Neighbor Embedding (t-SNE) is a non-linear technique for dimensionality reduction.
- ▶ t-SNE works very well in high dimensional data.
- ▶ Cons: it is computationally demanding, it is stochastic and it is governed by hyperparameters.

## t-SNE computation

- ▶ Computes a measure of pairwise similarity in the original (multi-dimensional) feature space;
- ▶ Tries to minimise the difference between the similarity in the high-dimensional space and the similarity in a lower-dimensional space (typically 2 or 3 dimensions);
- ▶ The measure of similarity in the high- and low- dimensional space is different and this allows to visualise the clusters as more homogeneous.

# t-SNE example using GDSC data



# Clustering

- ▶ Aim: Group observations into subsets or *clusters* or *segments* so that observations within a cluster are more similar to each other than observations assigned to different cluster.
- ▶ Requires a definition of *similarity* or *difference*.
- ▶ This is similar to the definition of the cost function for supervised learning, the most appropriate definition of *similarity* or *difference* depend on the type of data.

## K-means clustering

- ▶ Assign each observation  $i \in \{1, 2, \dots, N\}$  to one cluster  $k \in \{1, 2, \dots, K\}$ .
- ▶  $K$  need to be predefined, and  $K < N$
- ▶ This assignment correspond to a many-to-one mapping  $k = C(i)$ , which is an *encoder* that assigns the  $i$ th observation to the  $k$ th cluster.
- ▶ Each observation is assigned to one and only one cluster.

## K-means clustering

We want to define the clusters so that similar points are in the same cluster and dissimilar points are in different clusters.

Defining  $d_{i,i'} = d(x_i, x_{i'})$  as a measure of dissimilarity between a pair of observations  $x_i$  and  $x_{i'}$ , the total point scatter  $T$  is :

$$T = \frac{1}{2} \sum_{i=1}^N \sum_{i'=1}^N d_{i,i'} = \frac{1}{2} \sum_{k=1}^K \left( \sum_{C(i)=k} d_{i,i'} + \sum_{C(i')=k} d_{i,i'} \right)$$

Where:

- ▶  $W(C) = \frac{1}{2} \sum_{k=1}^K \sum_{C(i)=k} \sum_{C(i')=k} d_{i,i'}$  is the *within-cluster* point scatter that we want to minimise
- ▶  $B(C) = \frac{1}{2} \sum_{k=1}^K \sum_{C(i)=k} \sum_{C(i') \neq k} d_{i,i'}$  is the *between-cluster* point scatter that we want to maximise

Minimising  $W(C)$  or maximising  $B(C)$  is equivalent.

## K-means clustering

With K-means all variables has to be quantitative and we use the Euclidian distance as a measure of similarity:

$$d(x_i, x_{i'}) = \sum_{j=1}^p (x_{ij} - x_{i'j})^2 = \|x_i - x_{i'}\|^2$$

The within-point scatter can be written as:

$$W(C) = \frac{1}{2} \sum_{k=1}^K \sum_{C(i)=k} \sum_{C(i')=k} \|x_i - x_{i'}\|^2 = \sum_{k=1}^K N_k \sum_{C(i)=k} \|x_i - \bar{x}_k\|^2$$

where  $N_k$  is the number of points in the  $k$ th cluster and  $\bar{x}_k = (\bar{x}_{1k}, \dots, \bar{x}_{pk})$  is the mean vector associated with the  $k$ th cluster

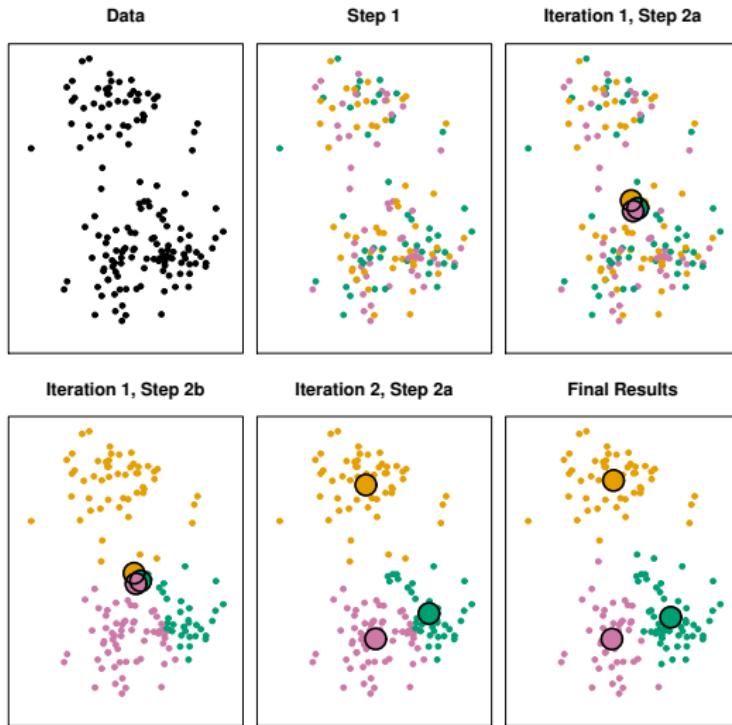
## K-means clustering algorithm

For high number of points  $N$  it is infeasible to test all possible clustering assignments.

We need *iterative greedy descent* strategies to iteratively improve clustering assignments:

1. Randomly assign each observation to one cluster.
2. Iterate the next two steps until cluster assignment stops changing
  - 2.1 For each cluster compute the mean vector  $x_k$  (i.e. *centroid*)
  - 2.2 Assign each observation to the cluster whose centroid is closest (based on Euclidian distance).

# K-means iterations

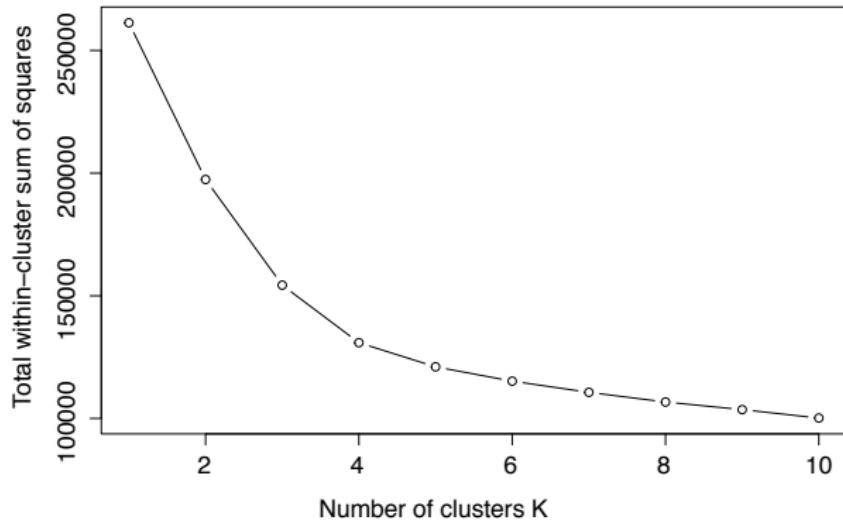


## K-means problems and solutions

- ▶ Problem: Does not guarantee the global minimum. Solution: we can check that no single switch of an observation to a different group decreases the objective function.
- ▶ Problem: Different random initialisation can provide different solutions. Solution: We can run it multiple times and select the solution with minimum objective function.
- ▶ We need to define the number of clusters.

## K-means example using GDSC data

Compute K-means for different number of clusters and look at total within-cluster sum of squares for each clustering.



Look at the elbow to define optimal number of cluster (not always possible).

## K-means example using GDSC data

Number of cases of each cancer type (columns) in each cluster (rows), when using  $K = 4$ .

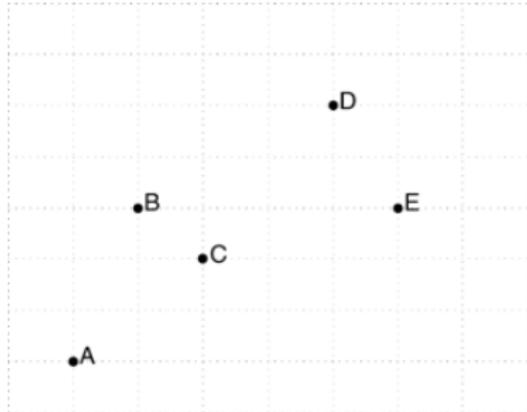
	breast	colorectal	kidney	neuroblastoma
1	6	0	28	1
2	41	7	0	0
3	0	37	0	0
4	0	1	0	27

# Hierarchical clustering

- ▶ Differently from K-means, *hierarchical clustering* does not require to specify a number of clusters.
- ▶ It organises observations in a hierarchy, where clusters at each level of the hierarchy are created merging clusters at the next lower level.
- ▶ The approach that we will see is *bottom-up*
  1. It starts from the lowest level, where each observation is a singleton cluster.
  2. For  $N - 1$  steps it merges a selected pairs of clusters (i.e. the most similar) in a single cluster.
- ▶ This process can be visualized as a *dendrogram*

# Hierarchical clustering - Bottom-up approach

Data set

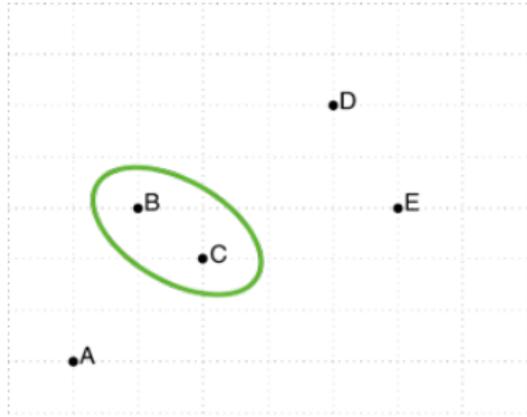


Dendrogram

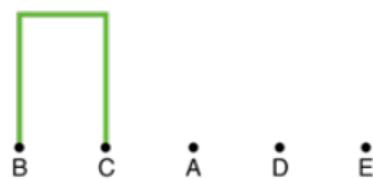


# Hierarchical clustering - Bottom-up approach - step 1

Data set

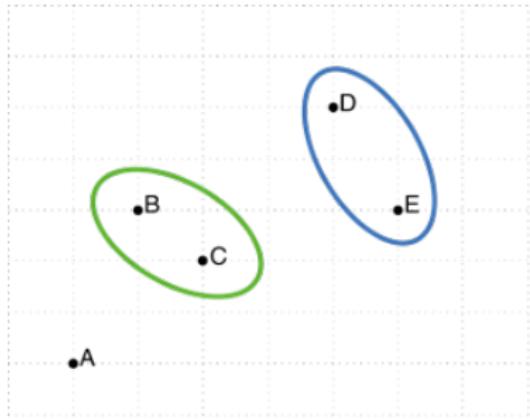


Dendrogram

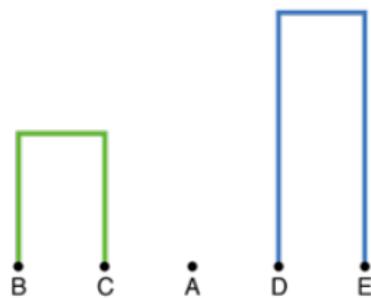


## Hierarchical clustering - Bottom-up approach - step 2

Data set

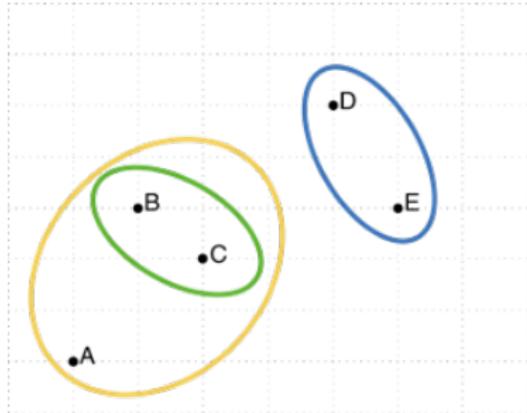


Dendrogram

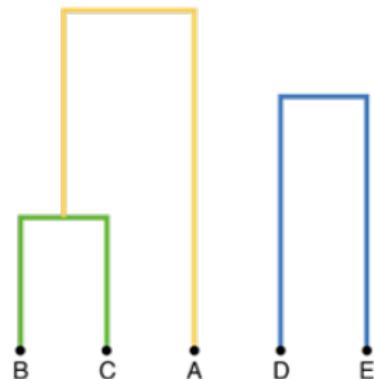


## Hierarchical clustering - Bottom-up approach - step 3

Data set

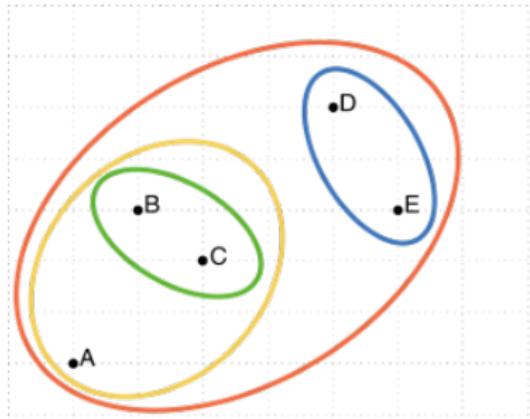


Dendrogram

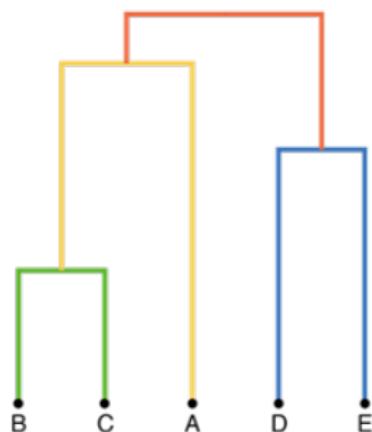


## Hierarchical clustering - Bottom-up approach - step 4

Data set



Dendrogram



## Hierarchical clustering - Linkage

How do we measure dissimilarity between two clusters (i.e. groups of observations)? Consider two clusters  $G$  and  $H$ , most used approaches are:

- ▶ *Single linkage*

$$d_{SL}(G, H) = \min_{i \in G, i' \in H} d_{ii'}$$

- ▶ *Complete linkage*

$$d_{CL}(G, H) = \max_{i \in G, i' \in H} d_{ii'}$$

- ▶ *Average linkage*

$$d_{CL}(G, H) = \frac{1}{N_G N_H} \sum_{i \in G} \sum_{i' \in H} d_{ii'}$$

## Hierarchical clustering - Dissimilarity measure

How do we measure dissimilarity between two points?

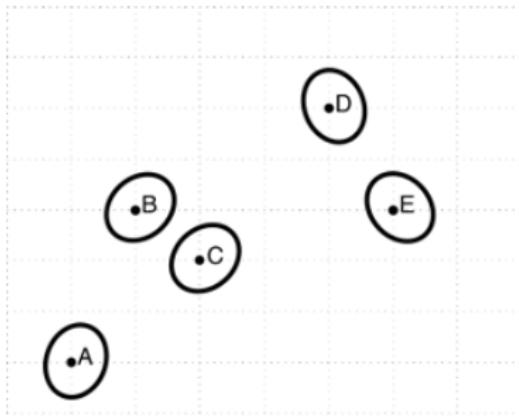
- ▶ Most commonly used is Euclidean distance.
- ▶ Another used metric is correlation (of observations across features).

## Hierarchical clustering - How to interpret a dendrogram

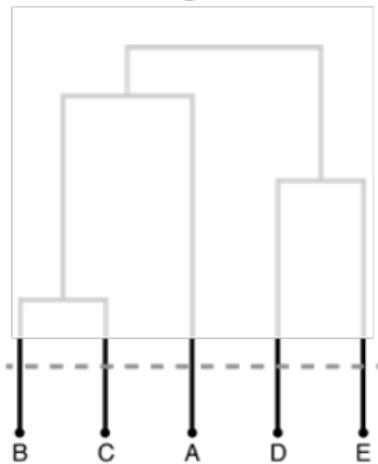
- ▶ Branches' height is proportional to the similarity between nodes.
  - ▶ Observations that fuse at the bottom of the dendrogram are similar to each other.
  - ▶ Observations that fuse at the top of the dendrogram are different from each other.
- ▶ We can cut the dendrogram at a certain height to obtain clusters.

# Hierarchical clustering - How to obtain clusters

Data set

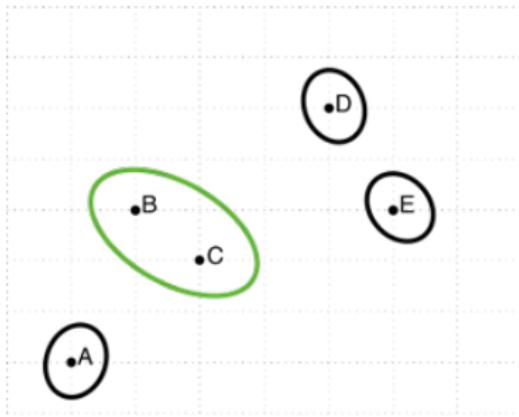


Dendrogram

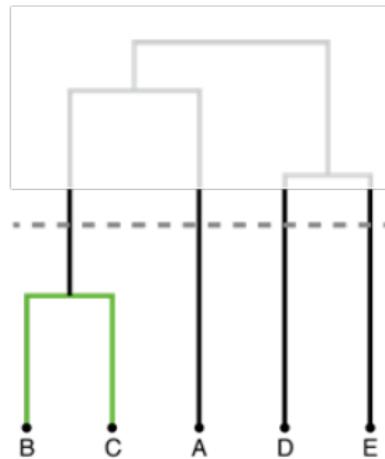


# Hierarchical clustering - How to obtain clusters

Data set

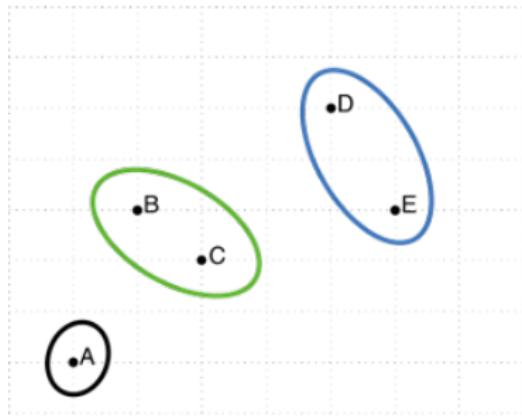


Dendrogram

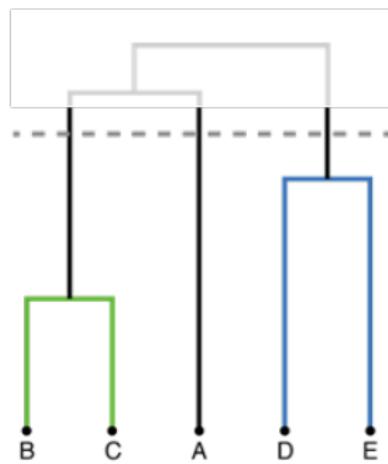


# Hierarchical clustering - How to obtain clusters

Data set

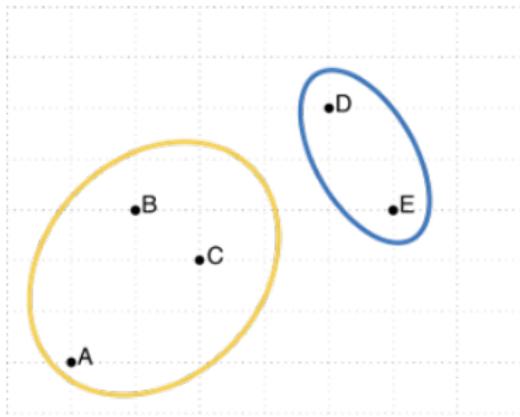


Dendrogram

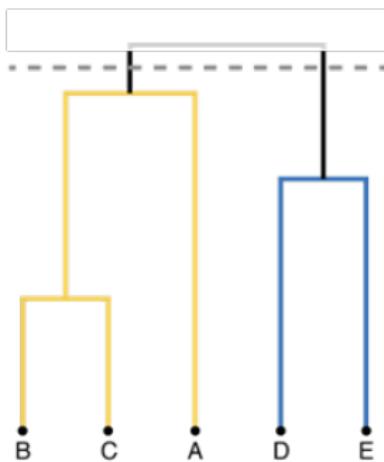


# Hierarchical clustering - How to obtain clusters

Data set

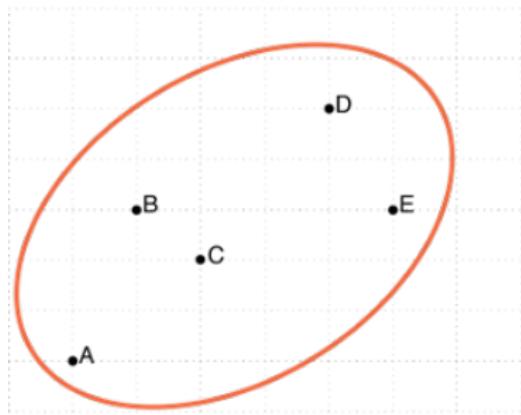


Dendrogram

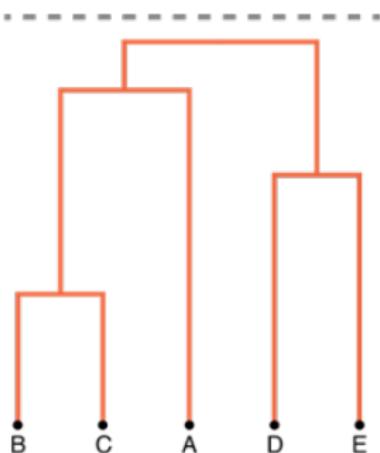


# Hierarchical clustering - How to obtain clusters

Data set

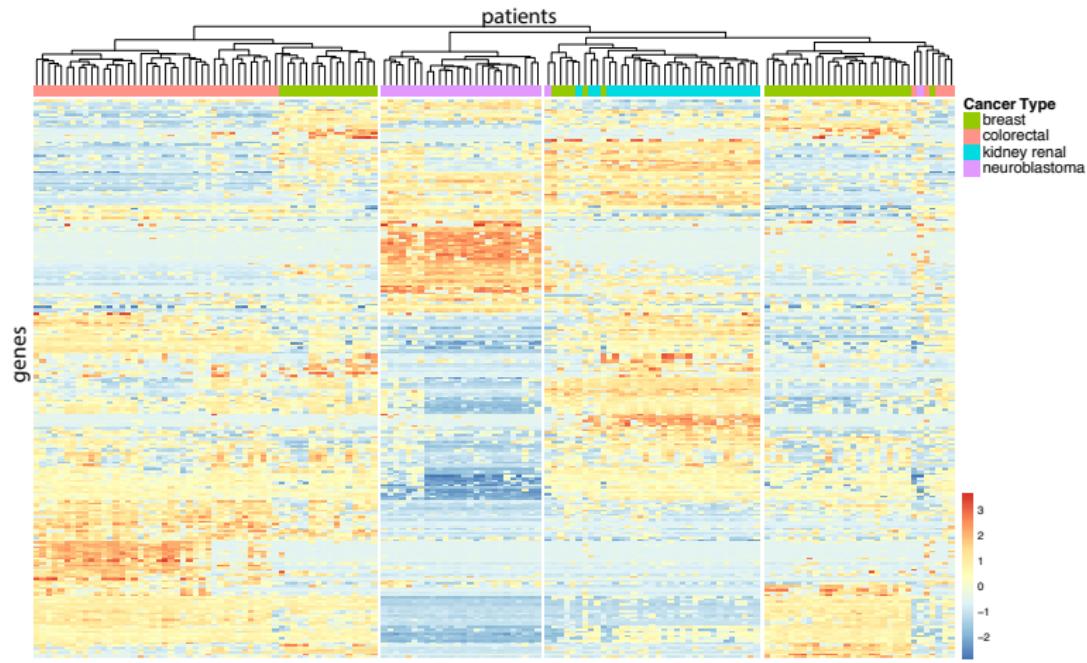


Dendrogram



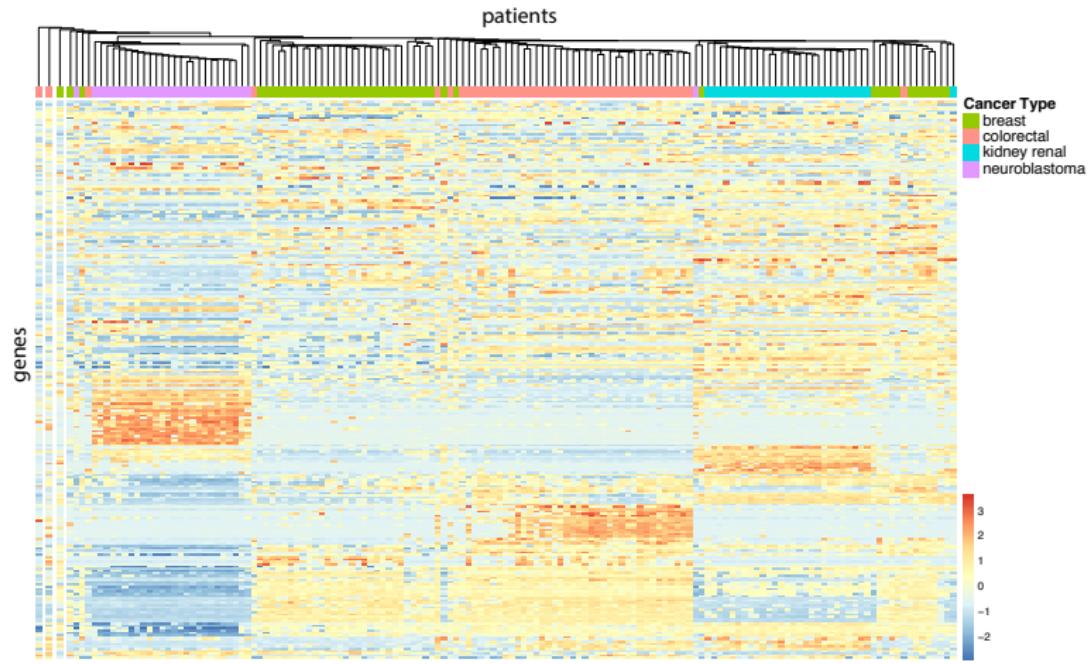
# Hierarchical clustering - examples with GDSC data

Clustering using complete linkage for cluster similarity and Euclidian distance as observations similarity metric.



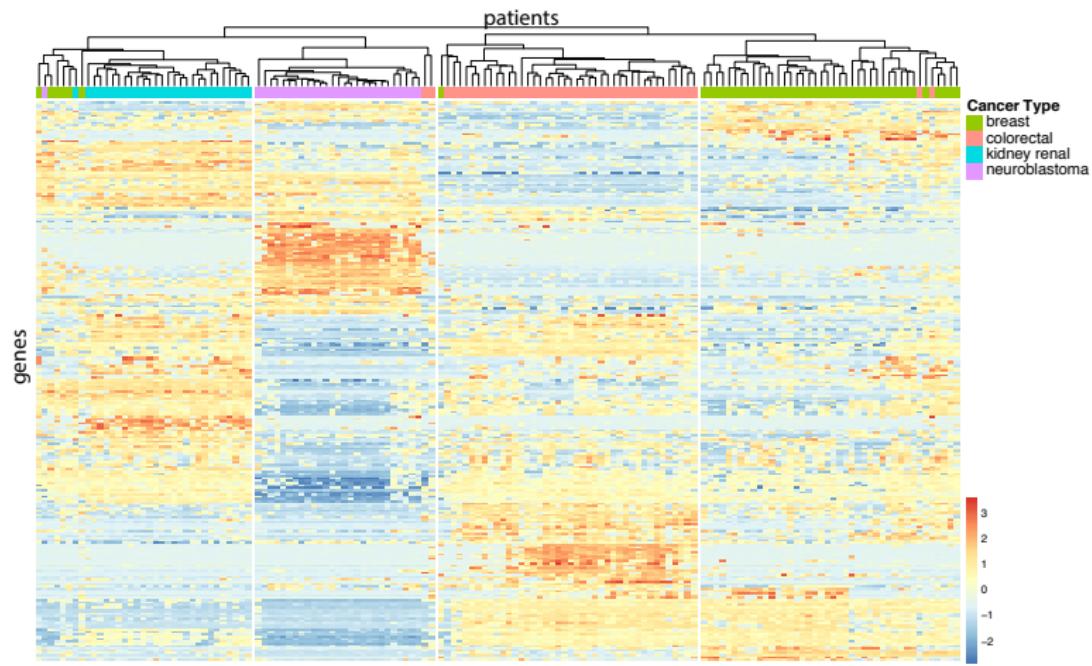
# Hierarchical clustering - examples with GDSC data

Clustering using single linkage for cluster similarity and Euclidian distance as observations similarity metric.



# Hierarchical clustering - examples with GDSC data

Clustering using complete linkage for cluster similarity for genes and correlation as observations similarity metric for patients.



# Conclusions

- ▶ Unsupervised learning is useful to find inherent patterns in data.
- ▶ It does not use/require labels on data.
- ▶ No gold standard to assess performances.
- ▶ Used a lot for data exploration and/or as first step to then apply supervised learning.
- ▶ Active field of research, essential to explore increasingly available high-dimensional data.

## References

- ▶ The figures showing geometrical interpretation of PCA and iterations of K-means are taken from "An Introduction to Statistical Learning, with applications in R" (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani



Friedman, J., T. Hastie, and R. Tibshirani. *The Elements of Statistical Learning*. Springer series in statistics New York, 2001.