# MATH60026/MATH70026
# **Methods for Data Science**
# Lecture 7

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Department of Mathematics, Academic year 2024-2025

IMPERIAL

# Supervised vs Unsupervised

Data available:

$$\{\mathbf{x}^{(i)}, y^{(i)}\}_{i=1}^{N}$$

Multiple-feature data + **labels**

$$\mathbf{x}^{(i)} \in \mathbb{R}^p \quad \text{or} \quad \mathbf{x}^{(i)} \in A_1 \times A_2 \cdots \times A_p$$

Continuous or categorical

$$\begin{cases} y^{(i)} \in \mathbb{R} & \text{(regression)} \\ \text{or} & \\ y^{(i)} \in \{c_1, \ldots, c_Q\} & \text{(classification)} \end{cases}$$

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We are interested in: making a prediction

$$\text{Given } \mathbf{x}^{\text{in}}, \quad \text{predict } \widehat{y} = \begin{cases} f_{\boldsymbol{\theta}}(\mathbf{x}^{\text{in}}) \in \mathbb{R} & \text{(regression)} \\ \text{or} & \\ f_{\boldsymbol{\theta}}(\mathbf{x}^{\text{in}}) \in \{c_1, \ldots, c_Q\} & \text{(classification)} \end{cases}$$

learning the optimal parameters for the prediction task

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How?

Finding **informative similarities** between data points,

Finding **convenient representations** for inspection, etc.

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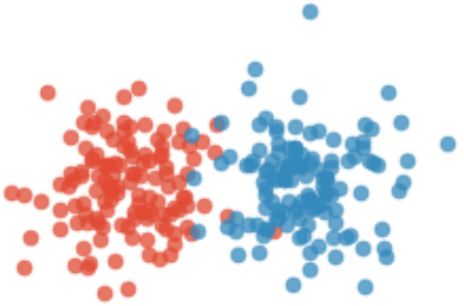
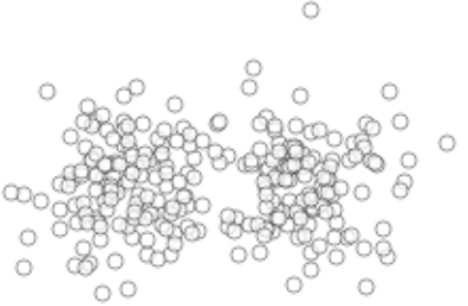
We are interested in: learning intrinsic data properties
How?
Finding **informative similarities** between data points,
Finding **convenient representations** for inspection, etc.

Key: a posteriori step of **interpretation & inspection**

# Learning paradigms

| | Supervised | Unsupervised |
|---|---|---|
| Data | $\mathbf{X}, \boldsymbol{y}$  | $\mathbf{X}$  |
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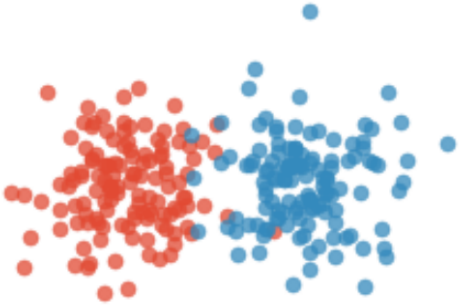
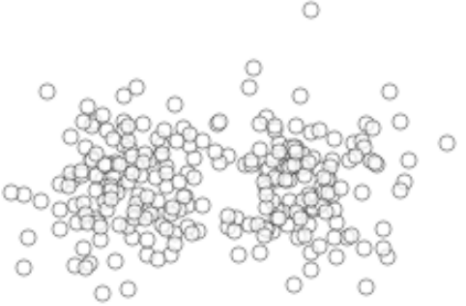
| Data | $\mathbf{X}, \boldsymbol{y}$  | $\mathbf{X}$  |
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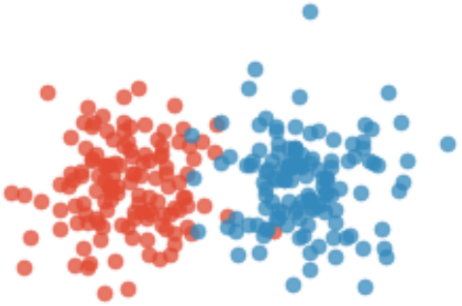
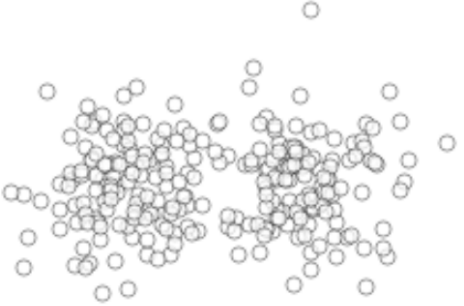
| Data | $\mathbf{X}, \boldsymbol{y}$  | $\mathbf{X}$  |
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*Graph-based techniques helping further!*

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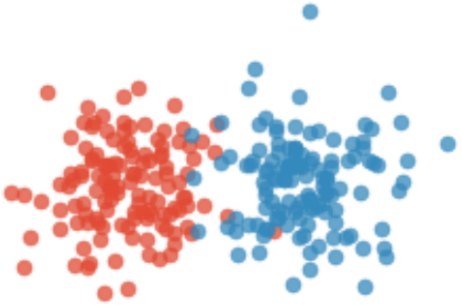
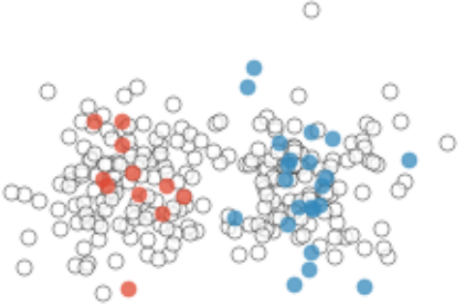
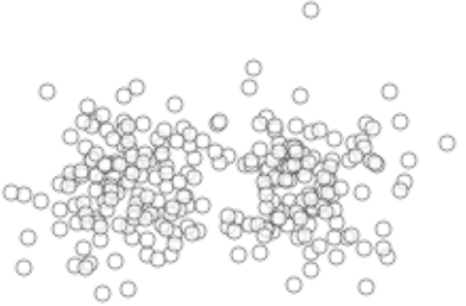
| |  |  |  |
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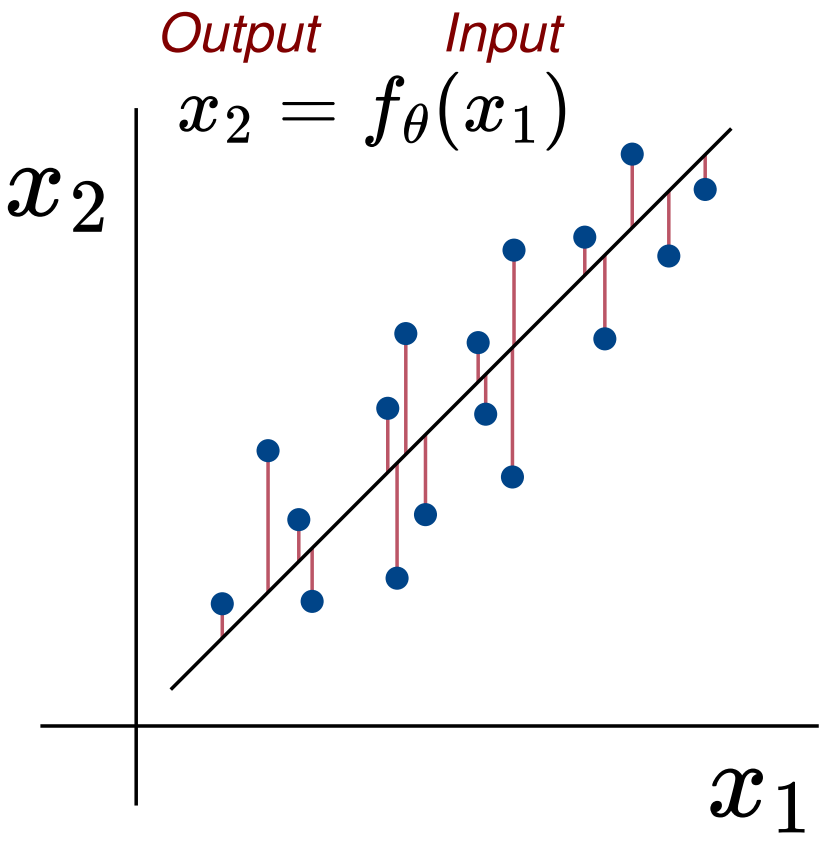
# Regression vs Dimensionality Reduction

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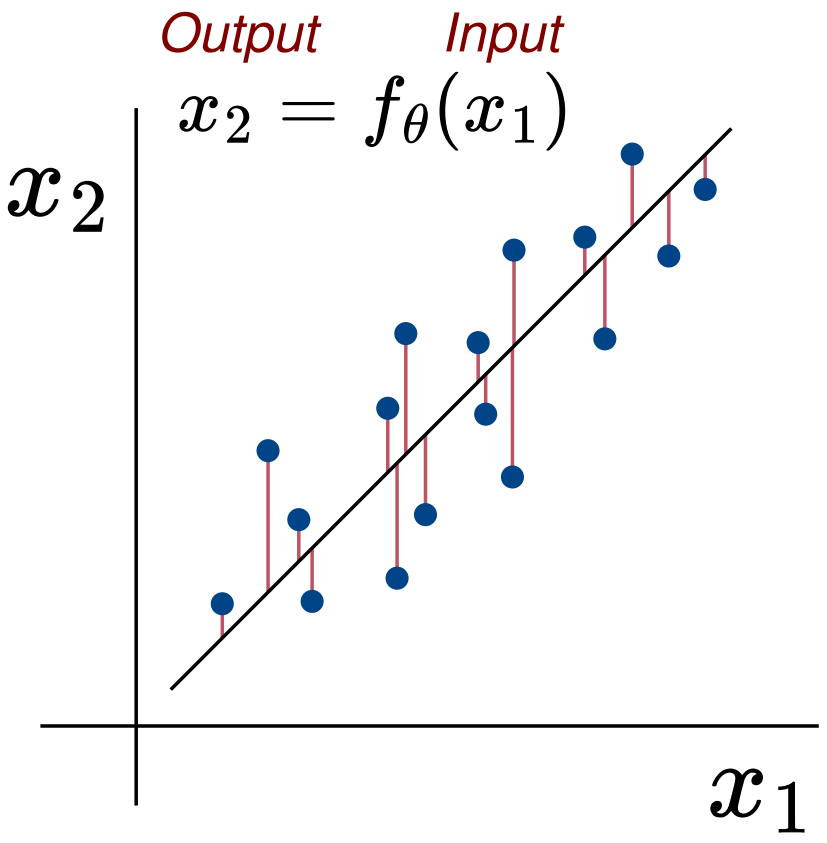


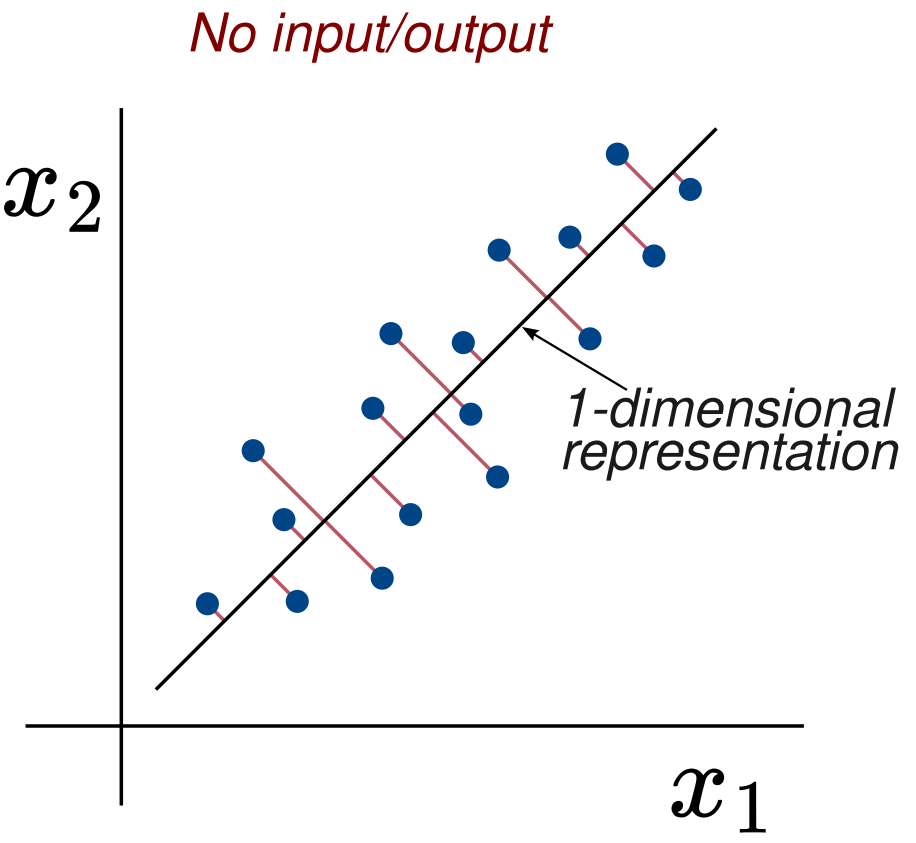


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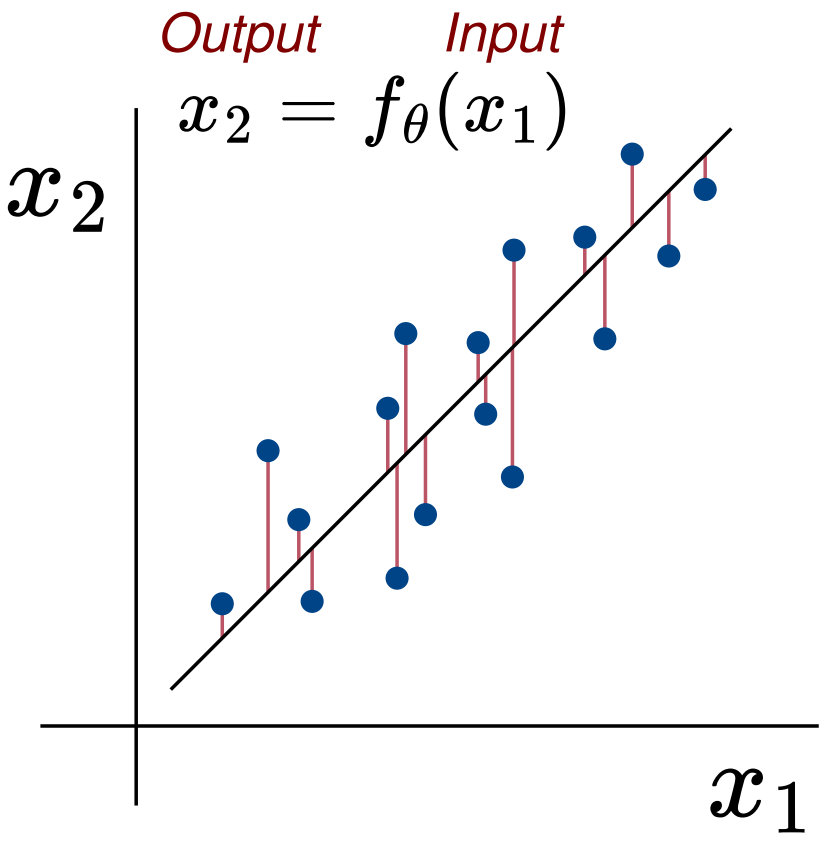


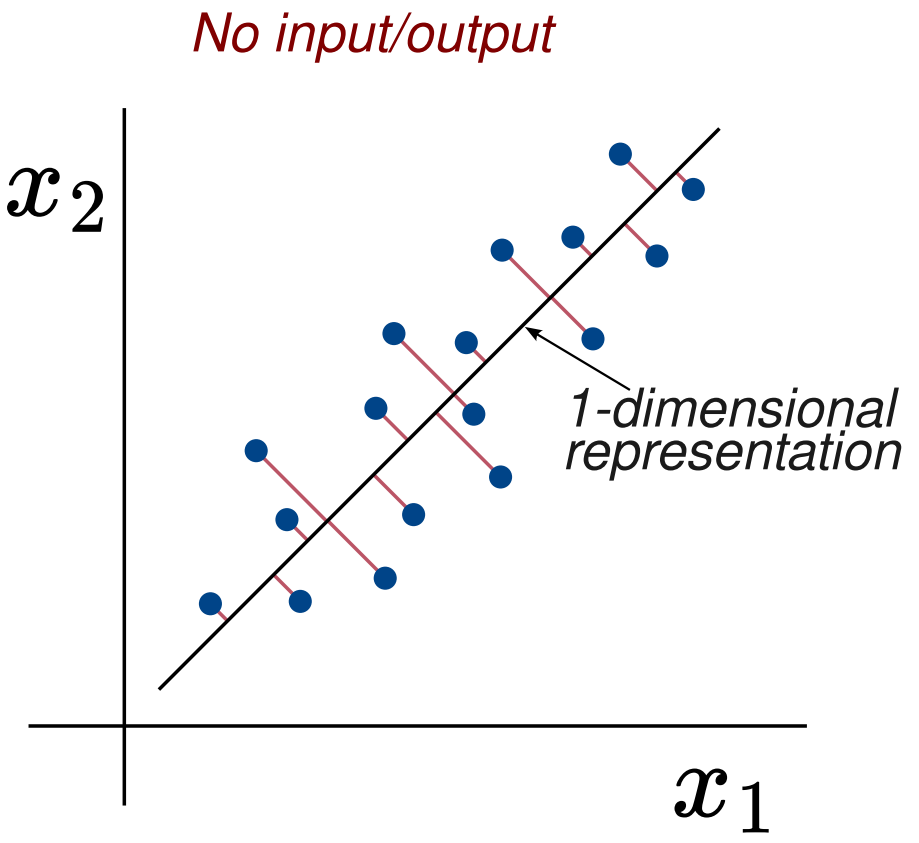


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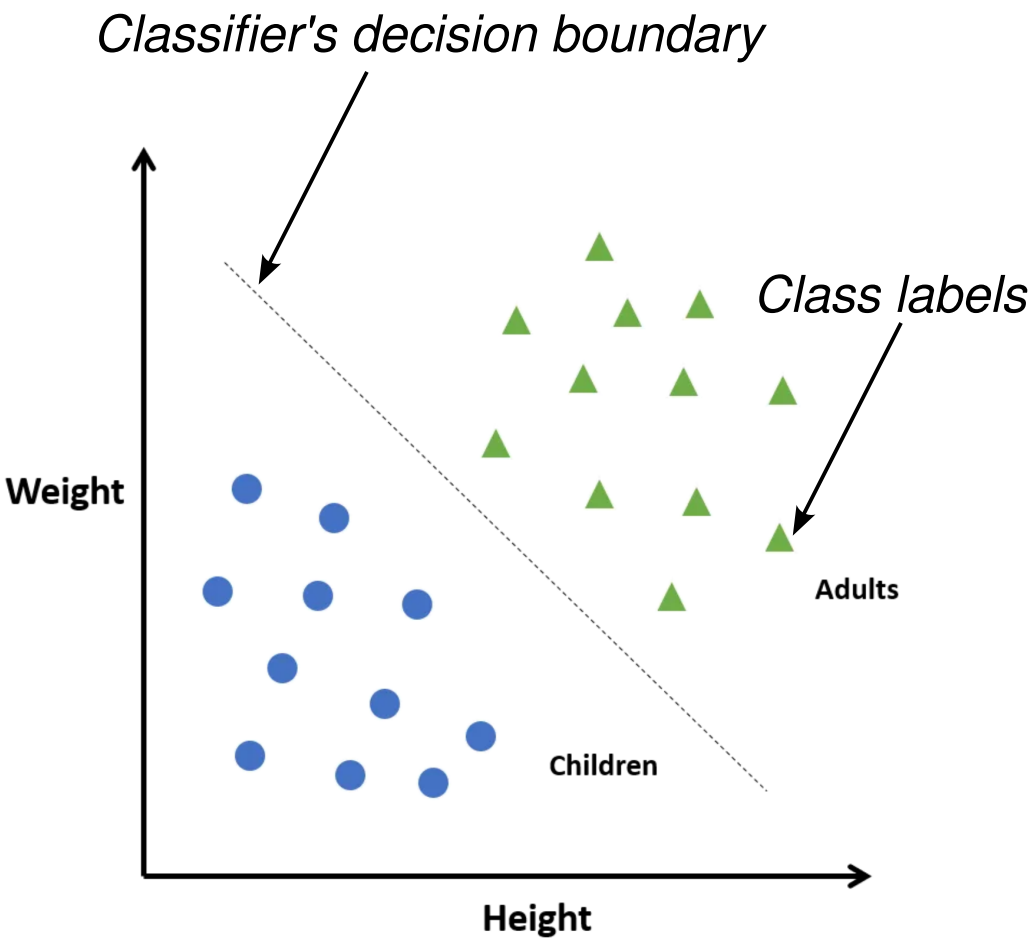
**Optimisation remains crucial!**

# Classification vs clustering




If class labels are given,
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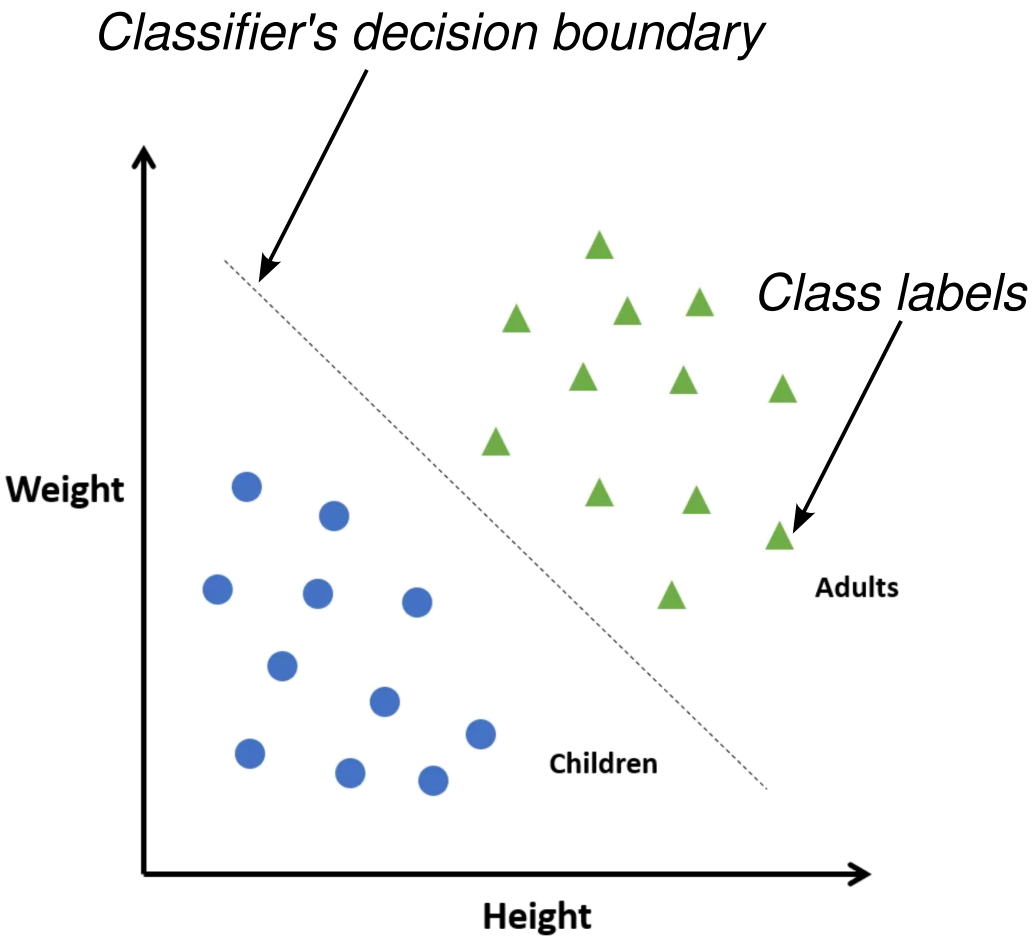


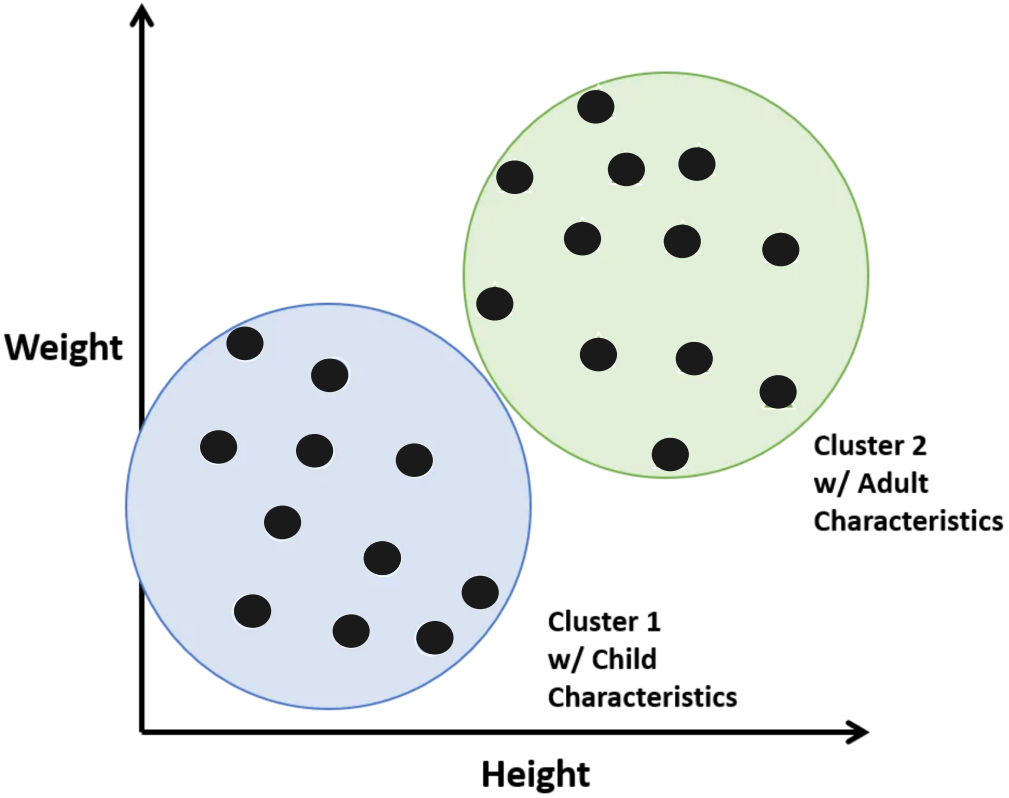


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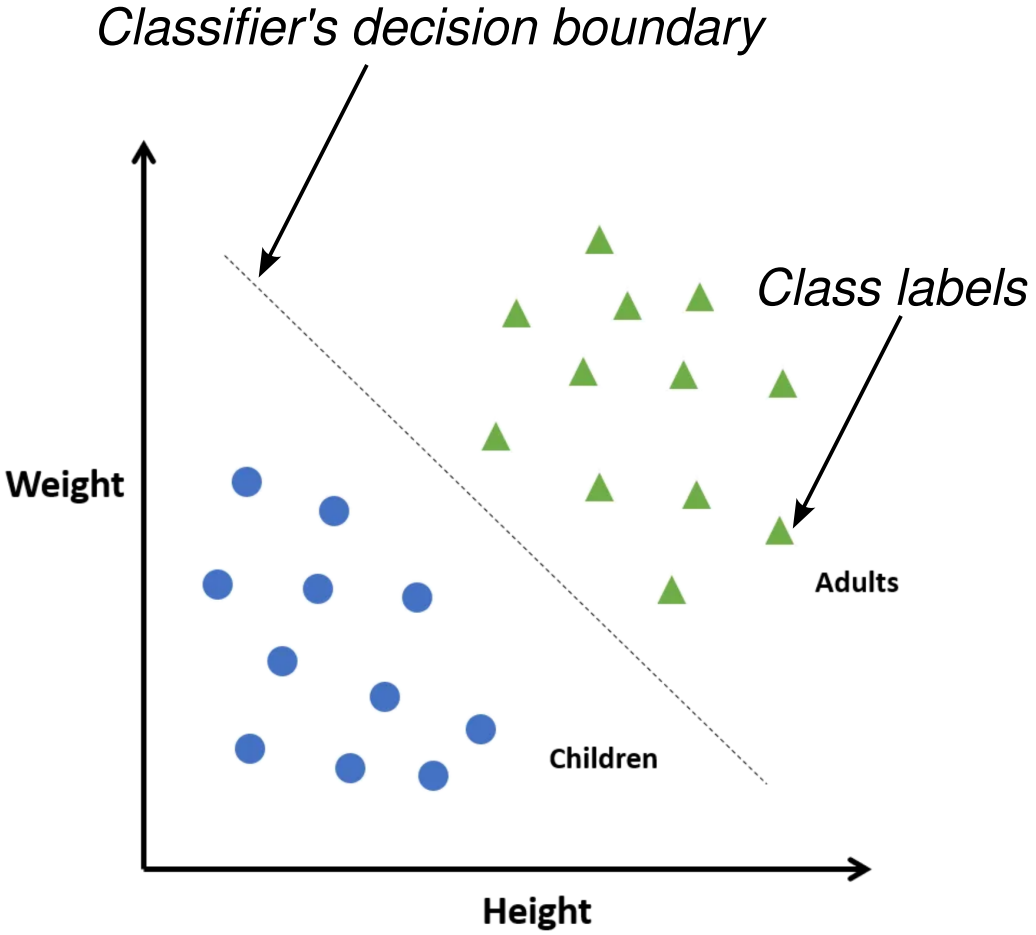


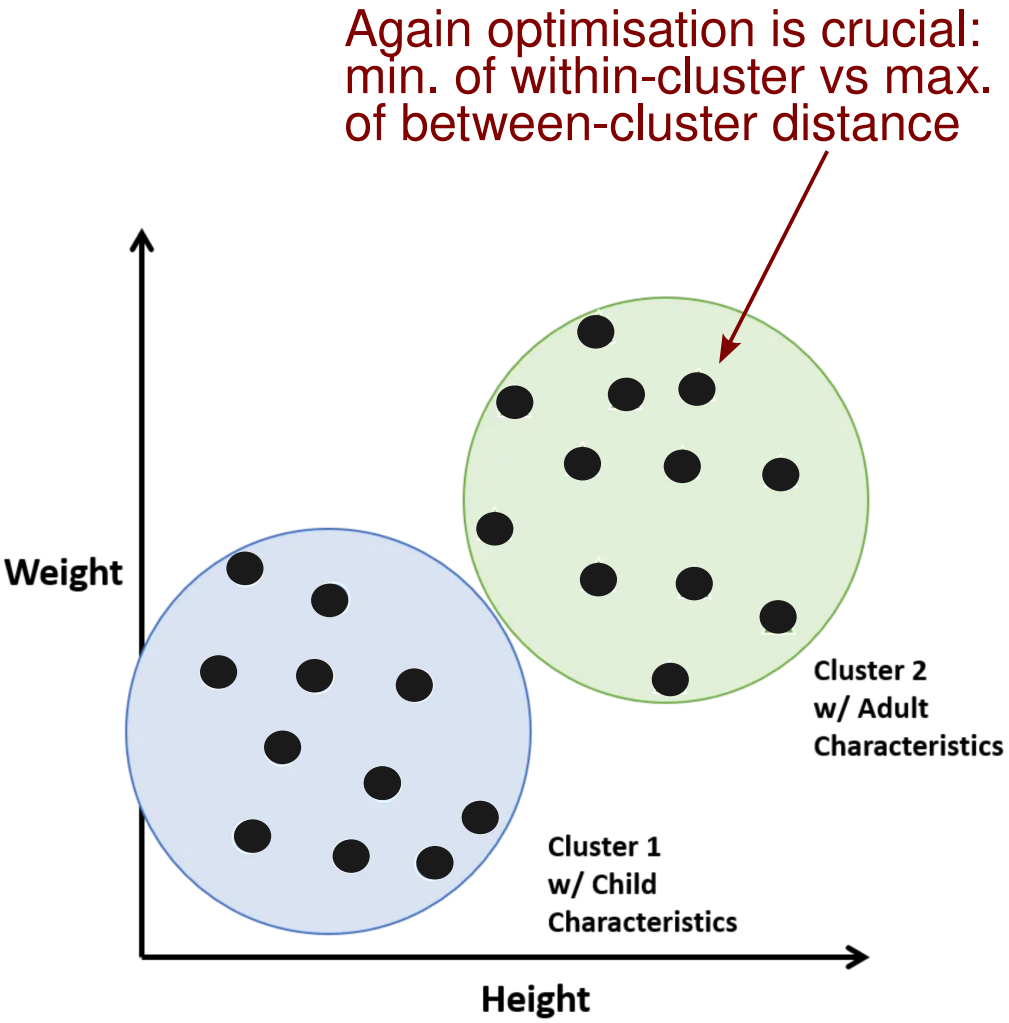


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# Clustering:

**Hard clustering** = each data point is assigned to a single cluster

**Soft clustering** = each data point is assigned to different clusters with a certain probability

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*K*-means & Hierarchical Clustering

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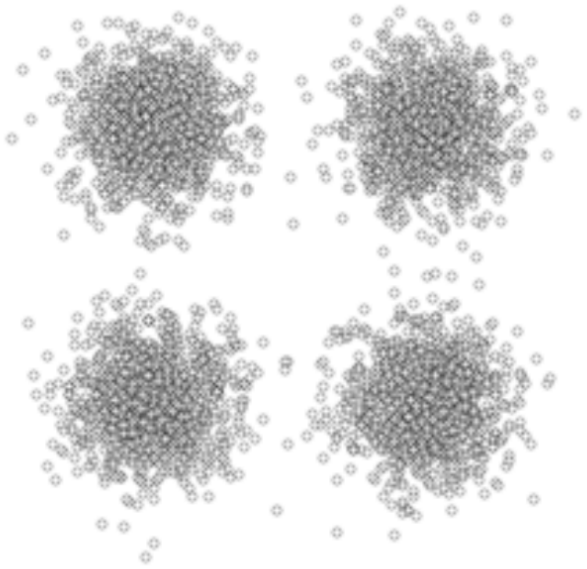
Gaussian Mixture Models

# What is a *cluster*?

Dataset 1



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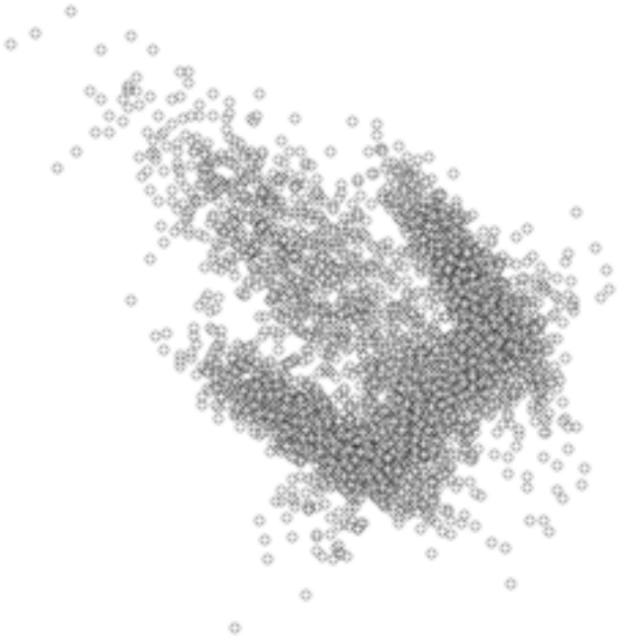

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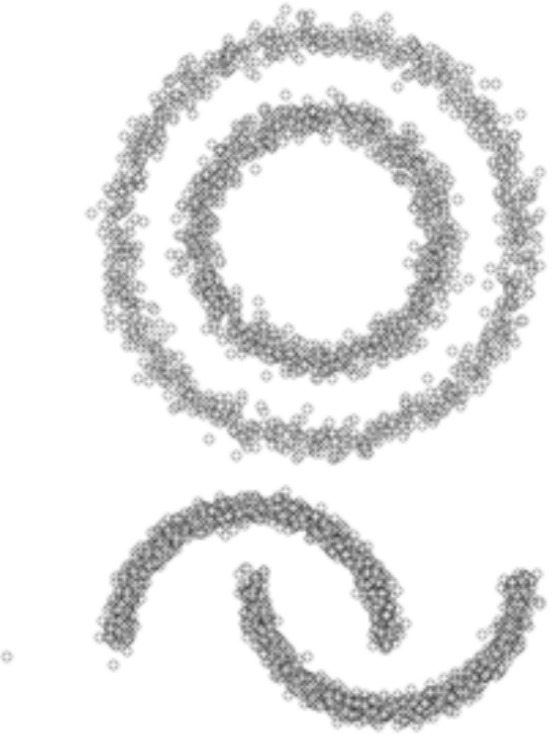
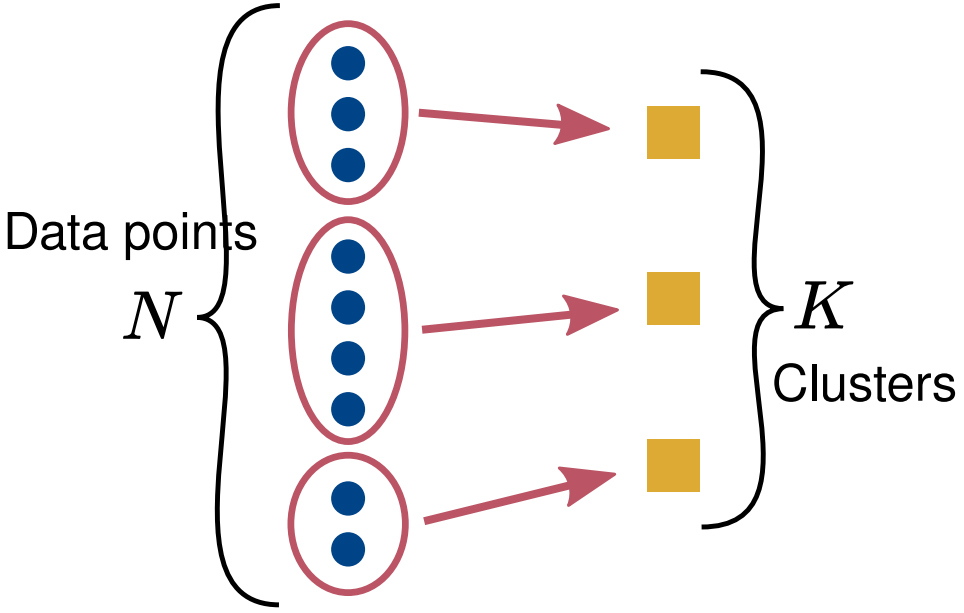


We require a notion of **distance** or **distribution**

# The clustering problem, mathematically



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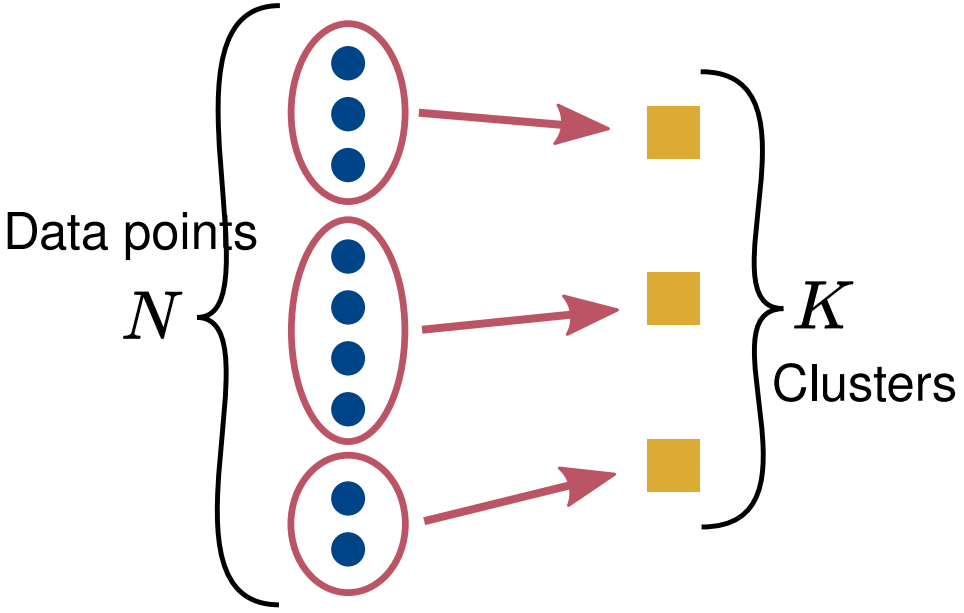


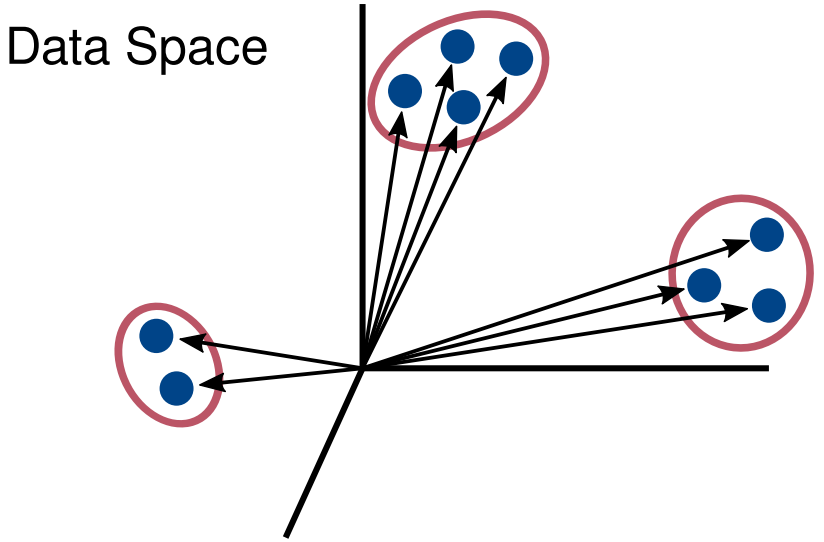


**Desiderata:** low distance within-cluster
high distance between-cluster

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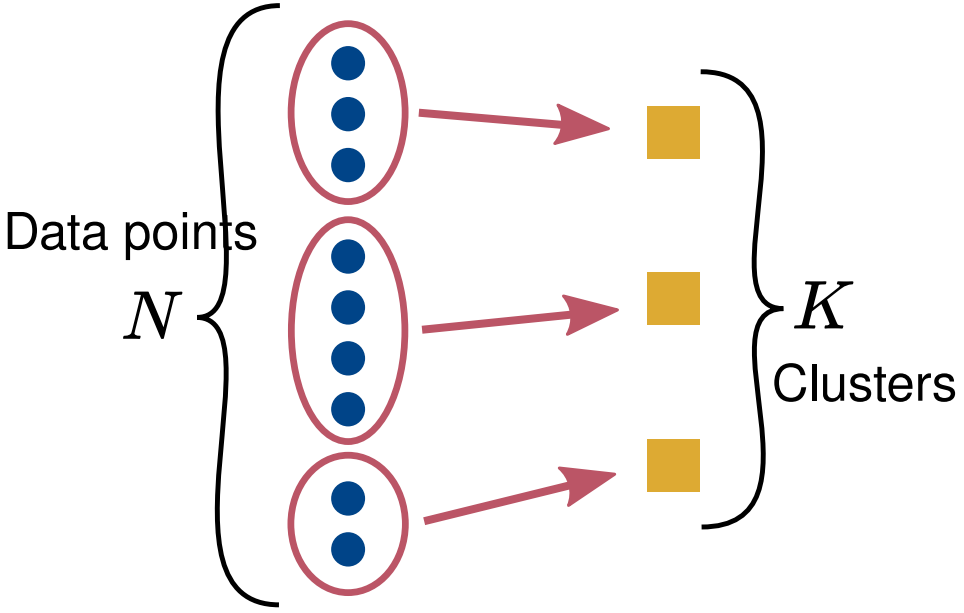


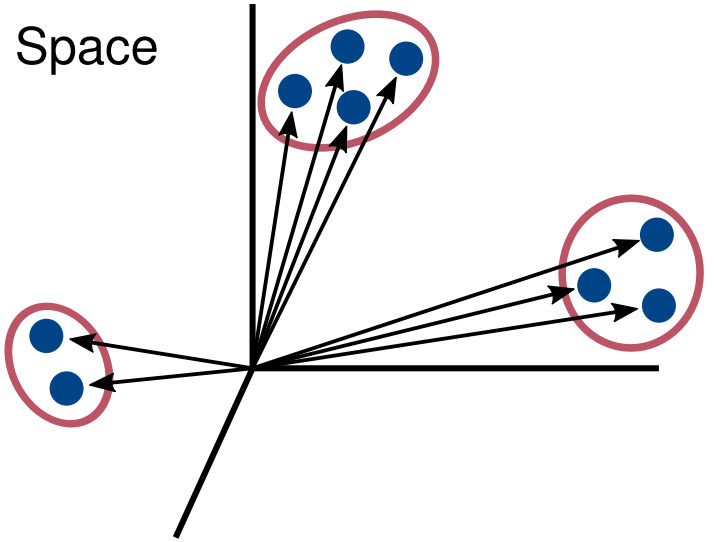


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Key notion 1: **Distance**, for example:

**squared Euclidean dist.** (continuous)

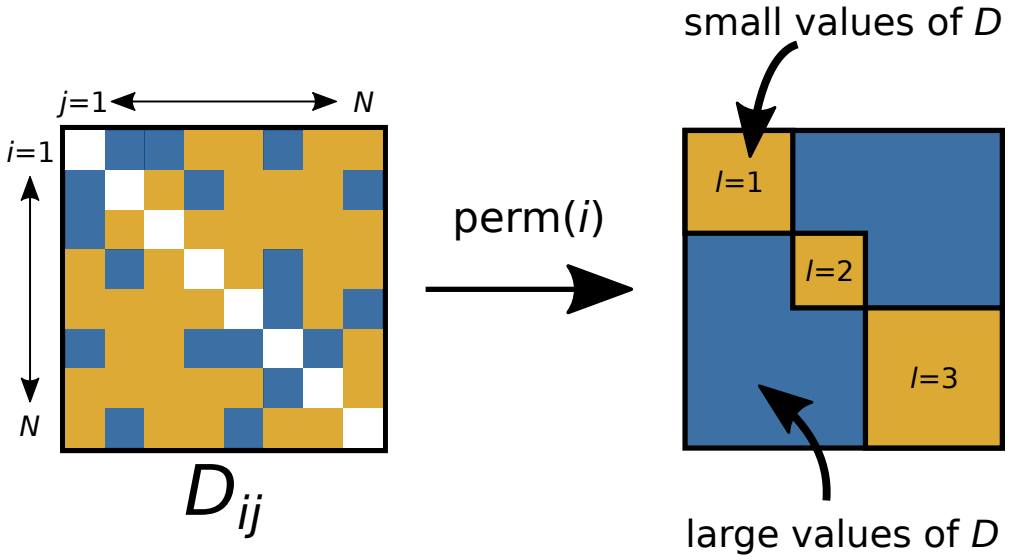
$$D(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}\|^2$$

**Hamming distance** (discrete)

$$D_H(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \sum_{m=1}^{p} I(x_m^{(i)} \neq x_m^{(j)})$$

# The clustering problem, mathematically

In other words, clustering = producing a rearrangement of the matrix of distances that is **maximally block-diagonal** (1 block = 1 cluster)



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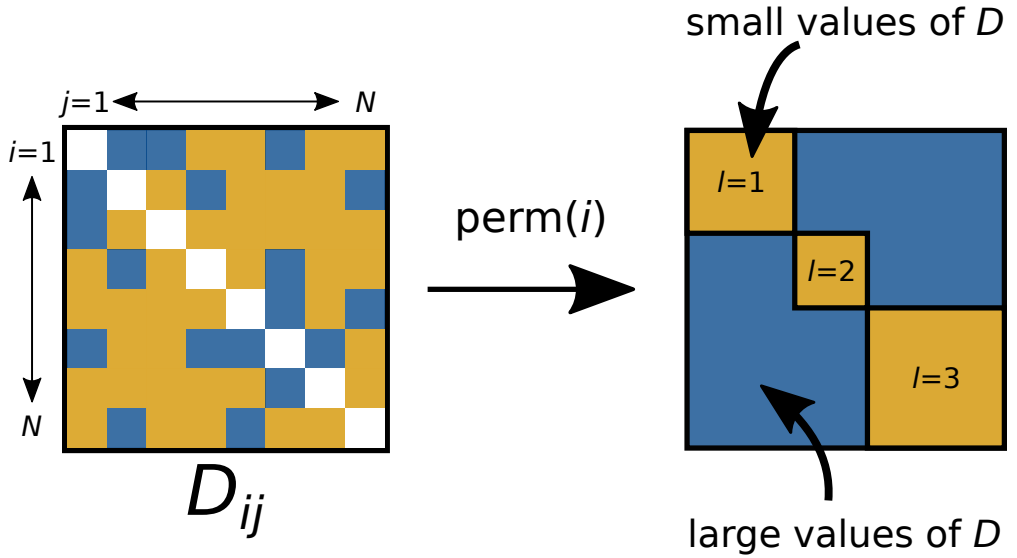


We look for a *i,j* permutation that solves a *combinatorial optimisation*:

$$W(\mathcal{C}) = \frac{1}{2}\sum_{k=1}^{K}\sum_{i,j\in c_k} D(\mathbf{x}^{(i)},\mathbf{x}^{(j)})$$

minimise within-cluster distance,

$$B(\mathcal{C}) = \frac{1}{2}\sum_{k=1}^{K}\sum_{i\in c_k}\sum_{j\notin c_k} D(\mathbf{x}^{(i)},\mathbf{x}^{(j)})$$

or maximise between-cluster one.

# *K*-means: hard, flat clustering

Continuous data, squared Euclidean distance $D(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \|\mathbf{x}^{(i)} - \mathbf{x}^{(j)}\|^2$

Find the clustering $\mathcal{C} = \{c_k\}_{k=1}^{K}$ minimising the normalised within-cluster distance:

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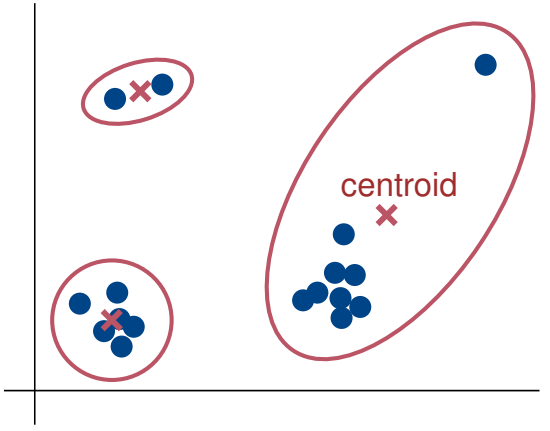

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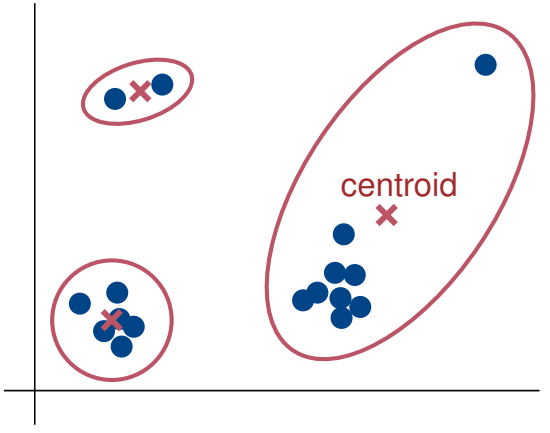
*K*-means algorithm:

Iterative algorithm that leads to a decreasing $W(\mathcal{C})$

Guarantees convergence only to a **local minimum**
(repeat for a few initialisations and take the best)

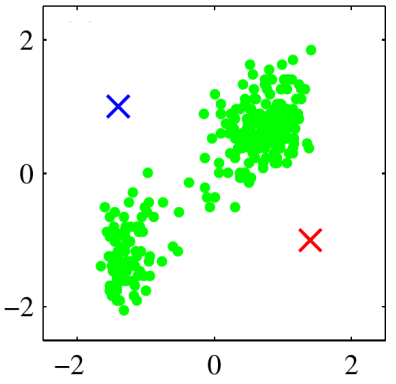


# Running the *K*-means algorithm:

**Step 0:** Given a number of clusters $K$, assign every sample to one of the $K$ clusters at random.

**Step 1:** Compute the *centroid* of each of the $K$ clusters:

$$\mathbf{m}_k = \frac{1}{|c_k|} \sum_{i \in c_k} \mathbf{x}^{(i)}, \quad k = 1, \ldots, K$$




Figures adapted from Bishop, *Pattern Recognition and Machine Learning,* chap. 9

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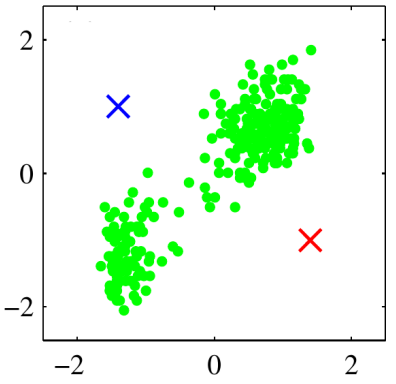
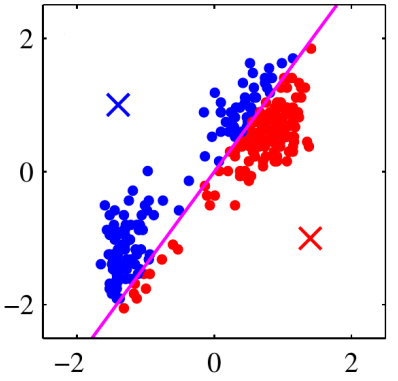



**Step 2:** Reassign each $\mathbf{x}^{(i)}$ to the closest centroid. Mathematically speaking, we consider the cluster assigned to $\mathbf{x}^{(i)}$ at iteration $t$, which is denoted by $k_i^{(t)}$, and evaluate the following:

$$k_i^{(t+1)} = \underset{k}{\operatorname{argmin}} \|\mathbf{x}^{(i)} - \mathbf{m}_k\|^2$$




Figures adapted from Bishop, *Pattern Recognition and Machine Learning*, chap. 9

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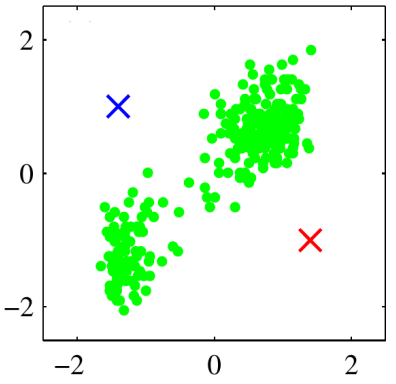


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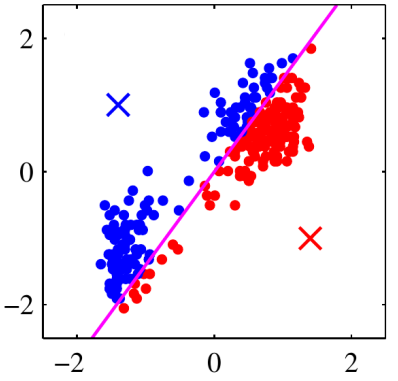


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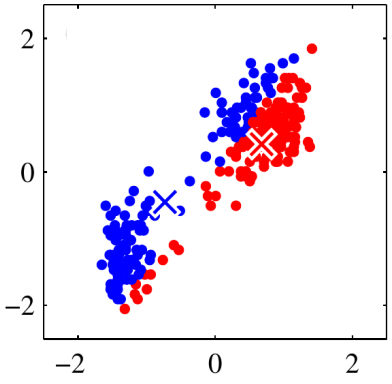


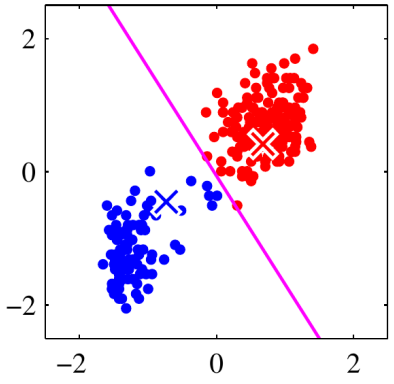


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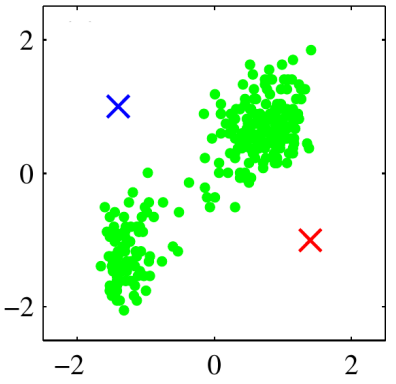


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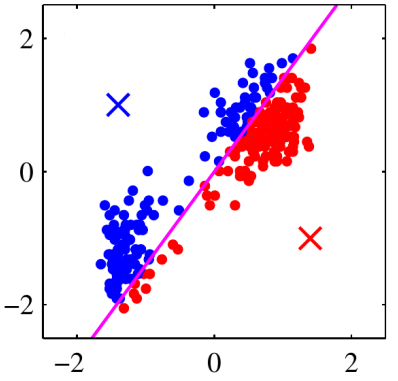


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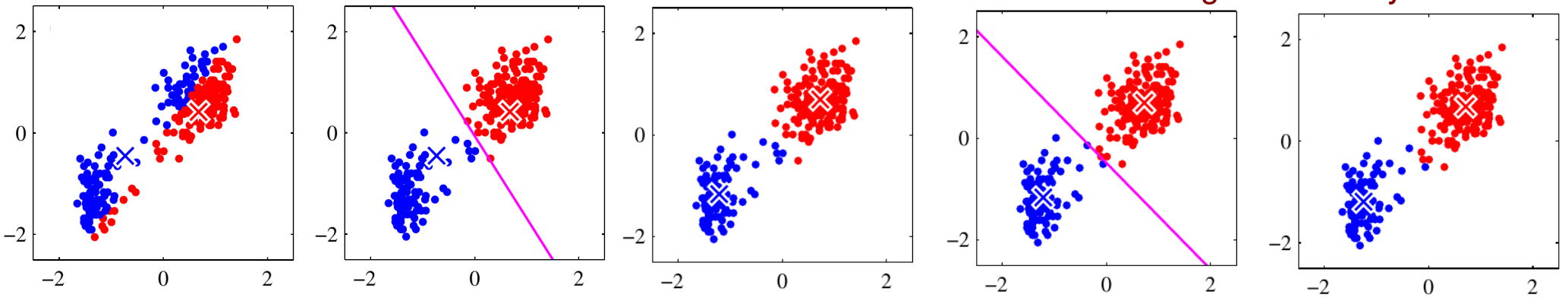
Cluster Assignments stay stable




Figures adapted from Bishop, *Pattern Recognition and Machine Learning*, chap. 9

# Example: segment and compress images


**Image segmentation:** breaking up the image into meaningful or perceptually similar regions

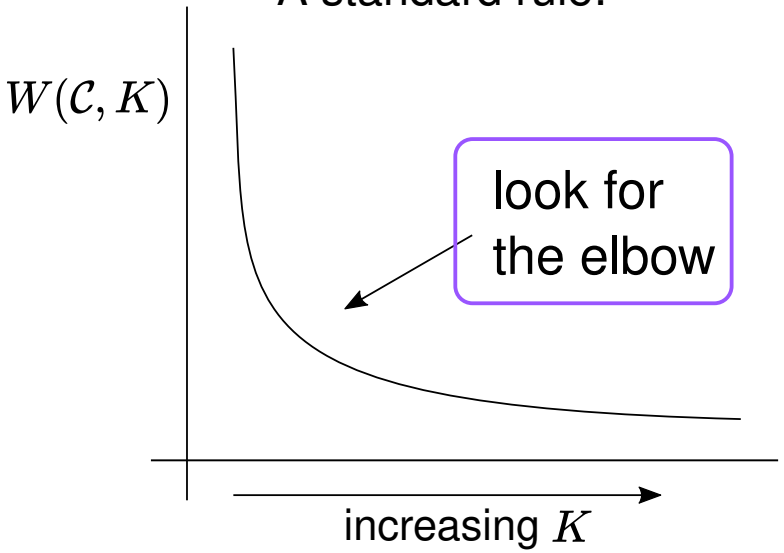
**(Lossy) data compression:** for each pixel, we store only its cluster and the cluster center

Figure from Bishop, *Pattern Recognition and Machine Learning,* chap. 9

# *K*-means: a few considerations

**1. Number of clusters K? Key, but hard choice.**

A standard rule:

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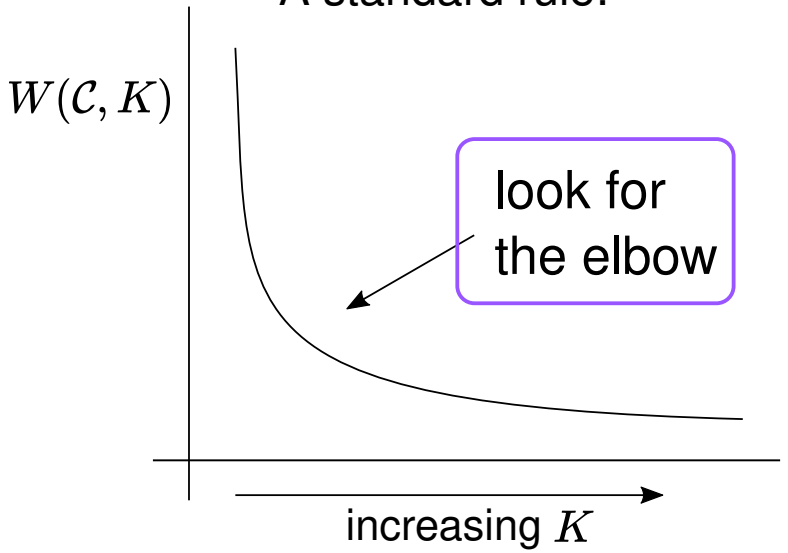


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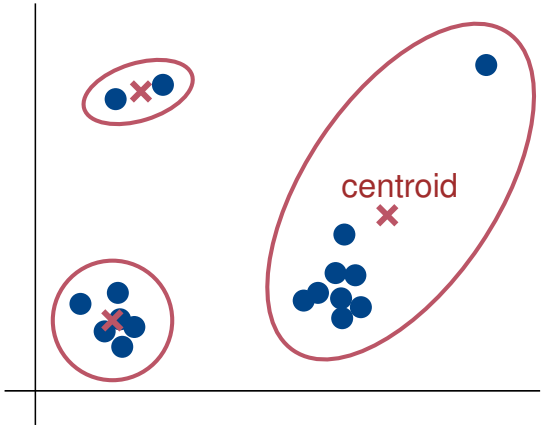


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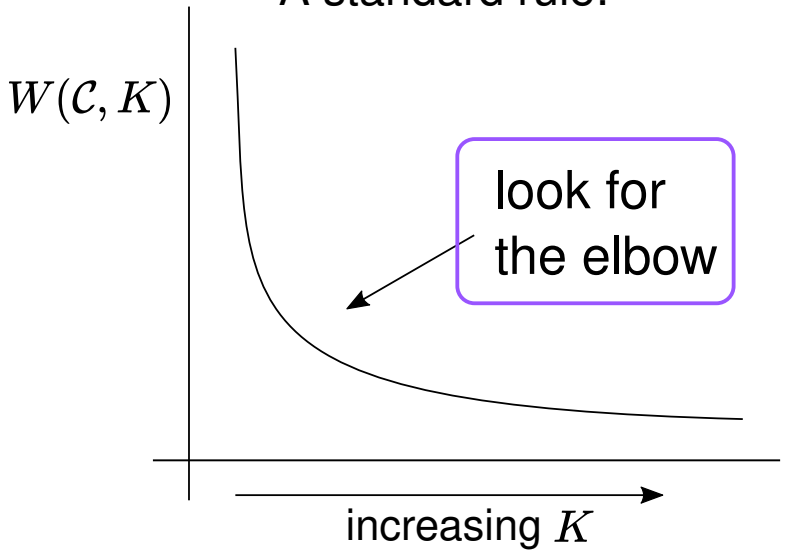


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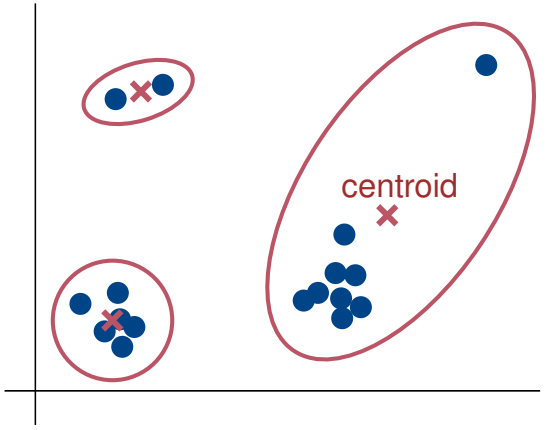


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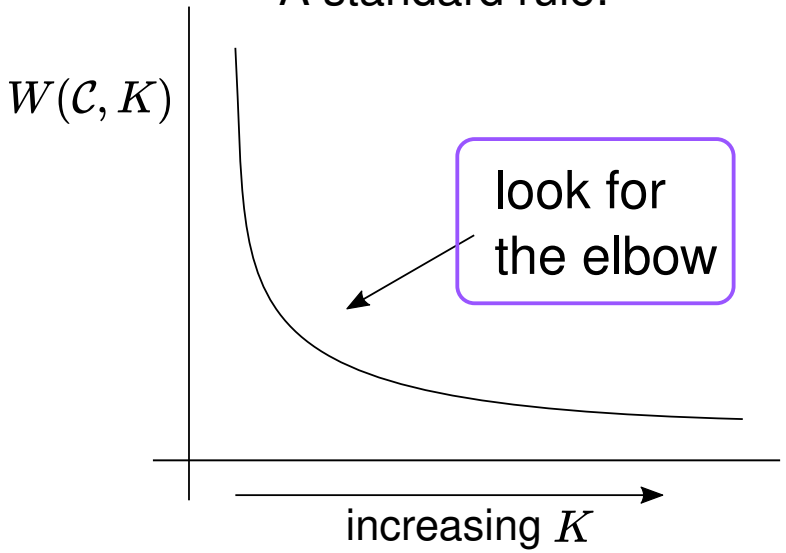


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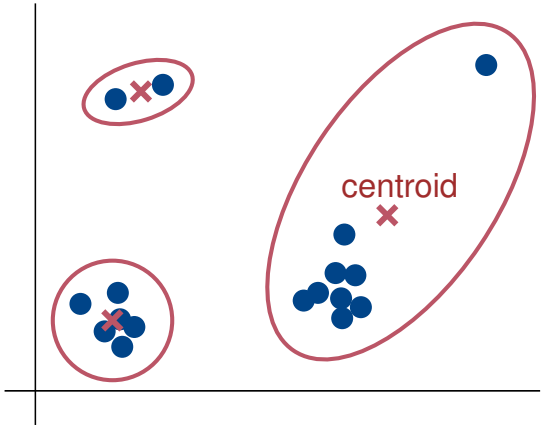


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**4. Hard clustering:** ambigous samples in borderline regions?

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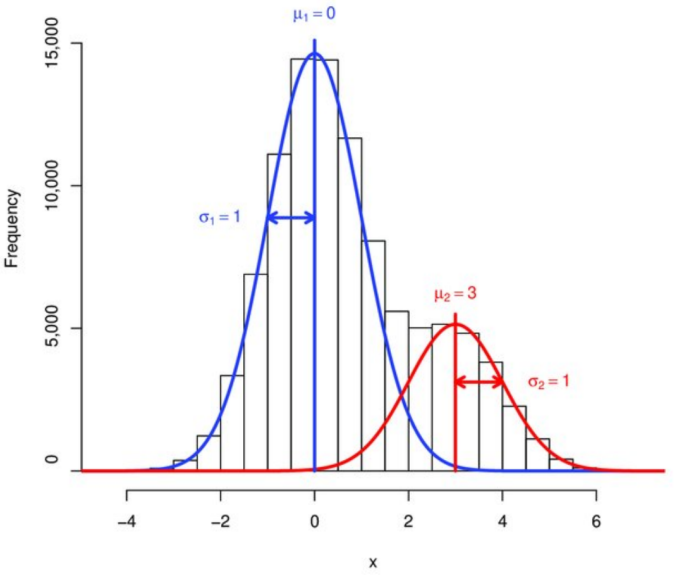
**Here: Gaussian Mixture Model (GMM)**



# GMMs as latent variable models

We introduce a latent variable $z$
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We model the joint probability:

$$P(\boldsymbol{x}, z)$$

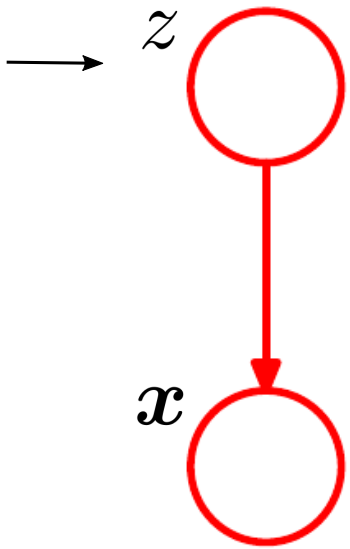


Figure from Bishop, *Pattern Recognition and Machine Learning,* chap. 9

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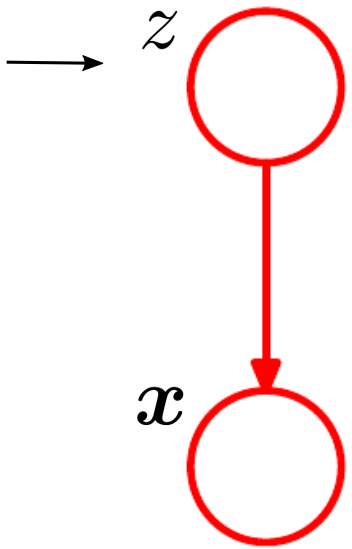


**Mixture components**

Marginal data probability

$$P(\boldsymbol{x} = \mathbf{x}^{(i)}) = \sum_{k=1}^{K} P(z = k) P(\boldsymbol{x} = \mathbf{x}^{(i)} | z = k) = \sum_{k=1}^{K} \pi_k p_k(\mathbf{x}^{(i)} | \boldsymbol{\theta})$$

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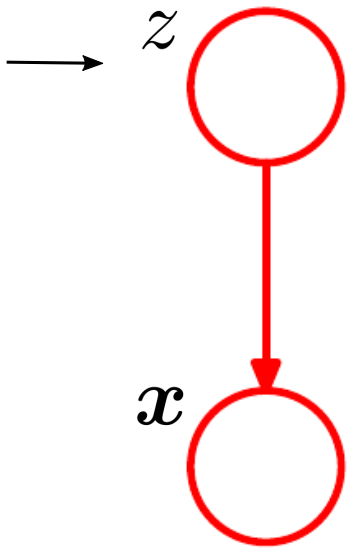


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**The cluster probability:**

$$r_{ik}(\boldsymbol{\theta}) = P(z = k | \boldsymbol{x} = \mathbf{x}^{(i)}, \boldsymbol{\theta}) = \frac{P(z = k, \boldsymbol{x} = \mathbf{x}^{(i)}, \boldsymbol{\theta})}{P(\boldsymbol{x} = \mathbf{x}^{(i)}, \boldsymbol{\theta})} = \frac{\pi_k p_k(\mathbf{x}^{(i)} | \boldsymbol{\theta})}{\sum_{k'=1}^{K} \pi_{k'} p_{k'}(\mathbf{x}^{(i)} | \boldsymbol{\theta})}$$

Probability of belonging to a cluster *k*

Figure from Bishop, *Pattern Recognition and Machine Learning*, chap. 9

# GMMs as latent variable models

**Mixture weights**

To be a valid probability:

$$0 \leq \pi_k \leq 1$$

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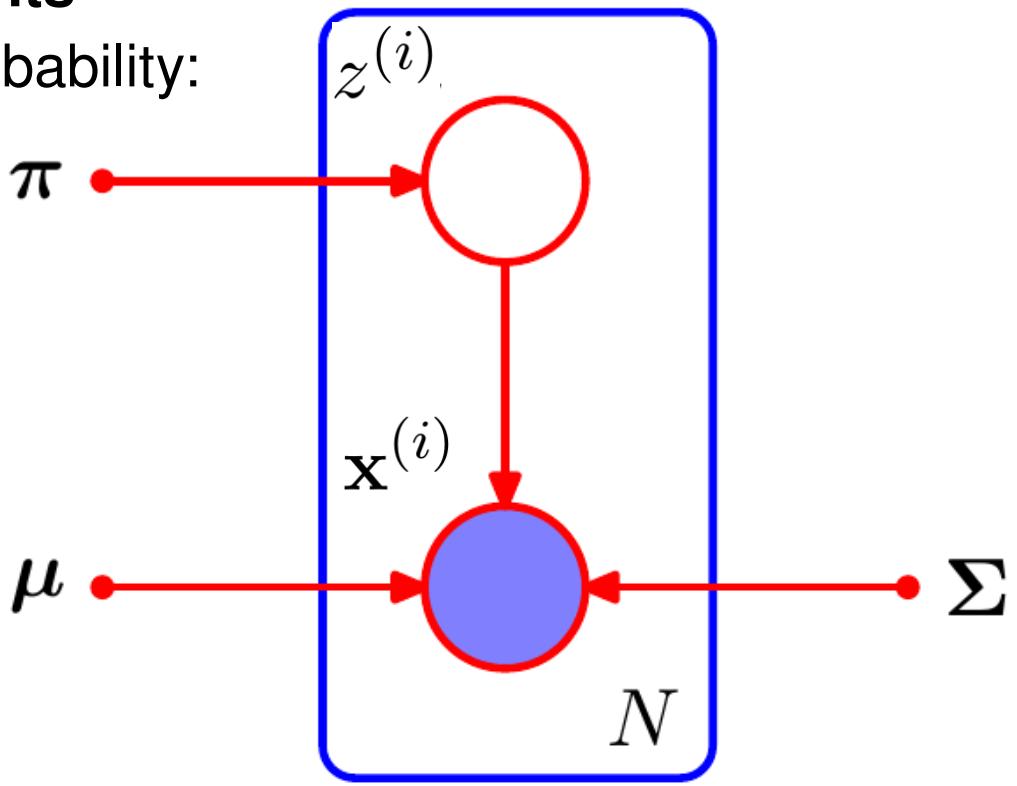


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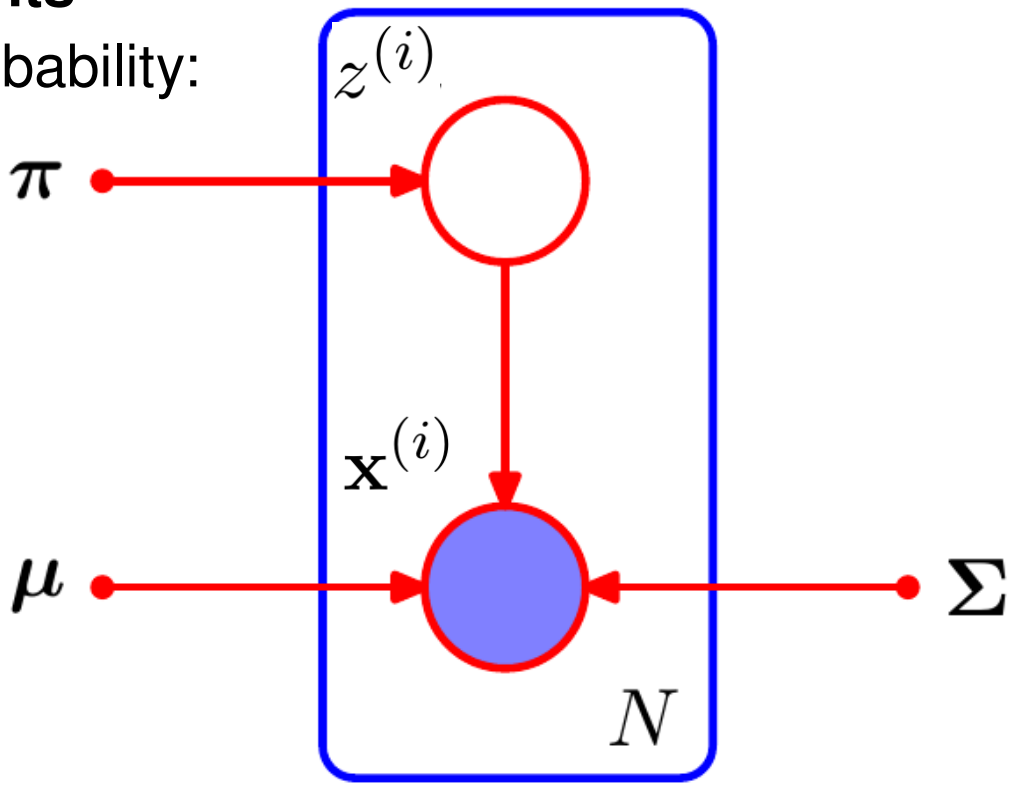


Each mixture component is a **Gaussian distribution**:

$$p_k(\boldsymbol{x}|\boldsymbol{\theta}) = (2\pi)^{-p/2} \det(\boldsymbol{\Sigma}_k)^{-1/2} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_k)^T \boldsymbol{\Sigma}_k{}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_k)\right)$$

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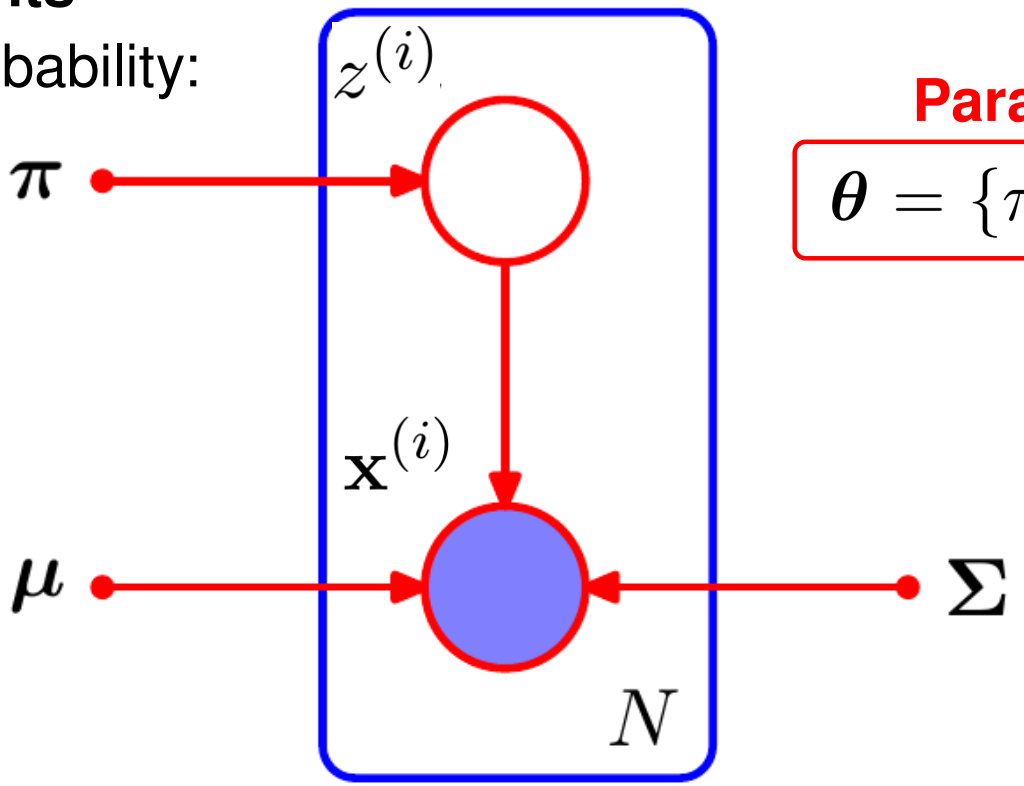


**Parameters to learn:**

$$\boldsymbol{\theta} = \{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1,..,K}$$

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# Expectation Maximisation Algorithm

Since we work with a distribution, we can apply **Maximum Likelihood**:

$$\boldsymbol{\theta}_{\text{MLE}} = \underset{\boldsymbol{\theta}}{\text{argmax}} \log \mathcal{L}(\boldsymbol{\theta}) = \underset{\boldsymbol{\theta}}{\text{argmax}} \sum_{i=1}^{N} \log P(\boldsymbol{x} = \mathbf{x}^{(i)} | \boldsymbol{\theta})$$

$\boldsymbol{\theta} = \{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1,..,K}$

**Expectation - Maximisation:** iterative algorithm to find a *local* maximum

Initialise $\boldsymbol{\theta}$

For iterations *t = 1,..., T*:

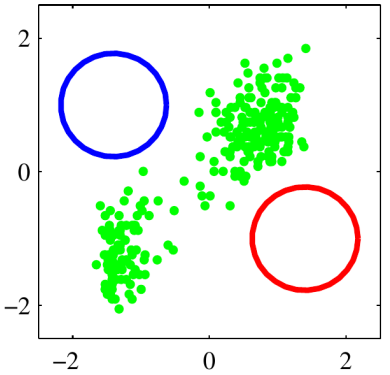
**Expectation Step:** estimate cluster probability

**Maximisation Step:** take the parameters maximising the log-likelihood

until convergence (log-likelihood stops changing)

## The Expectation-Maximisation (EM) algorithm:

Initialise at random the parameters $\boldsymbol{\theta} = \{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1,..,K}$

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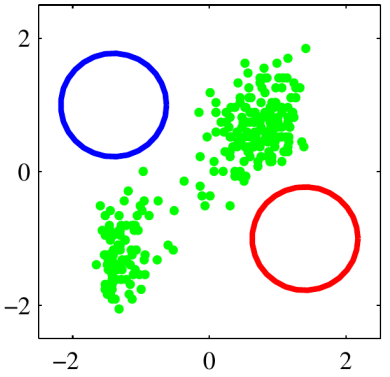
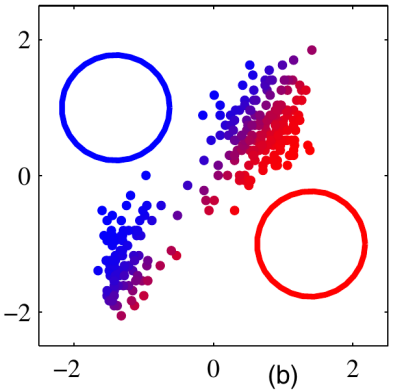



**Expectation step (E-step):** uses current parameter values $\boldsymbol{\theta}^t = \{\pi_k^t, \boldsymbol{\mu}_k^t, \boldsymbol{\Sigma}_k^t\}_{k=1,..,K}$ to compute cluster probabilities $r_{ik}(\boldsymbol{\theta}^t)$ and a set of weights:

$$w_{ik}(\boldsymbol{\theta}^t) = \frac{r_{ik}(\boldsymbol{\theta}^t)}{\sum_{i'=1}^{N} r_{i'k}(\boldsymbol{\theta}^t)} \tag{9.18}$$

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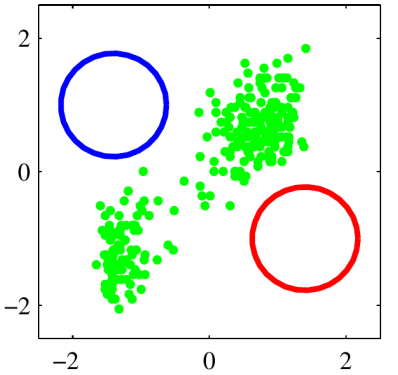


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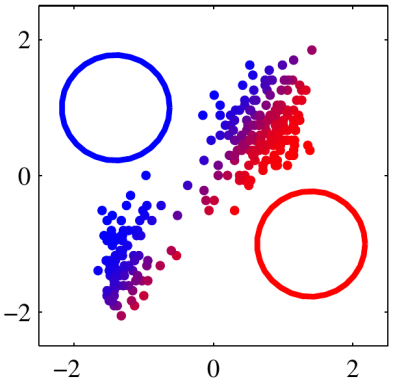
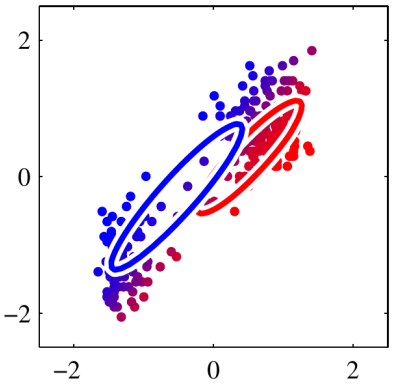



**Maximisation step (M-step):** updates the model's parameters for the next iteration $t+1$ maximising of the log-likelihood. One updates the mixture weight for the $k$-th component via the corresponding data-averaged cluster probability:

$$\pi_k^{t+1} = \frac{1}{N}\sum_{i=1}^{N} \mathbb{E}_{z^{(i)}|\mathbf{x}^{(i)},\boldsymbol{\theta}^t}[\delta_{z^{(i)},k}] = \frac{1}{N}\sum_{i=1}^{N} r_{ik}(\boldsymbol{\theta}^t) = \frac{N_k}{N} \tag{9.19}$$

Mixture weights




One updates the parameters of the Gaussian mixture components using $w_{ik}(\boldsymbol{\theta}^t)$:

$$\boldsymbol{\mu}_k^{t+1} = \sum_{i=1}^{N} w_{ik}(\boldsymbol{\theta}^t)\mathbf{x}^{(i)} \tag{9.20}$$

Gaussian means

$$\boldsymbol{\Sigma}_k^{t+1} = \sum_{i=1}^{N} w_{ik}(\boldsymbol{\theta}^t)(\mathbf{x}^{(i)} - \boldsymbol{\mu}_k^{t+1})(\mathbf{x}^{(i)} - \boldsymbol{\mu}_k^{t+1})^T \tag{9.21}$$

Gaussian covariances

Figures from Bishop, *Pattern Recognition and Machine Learning*, chap. 9

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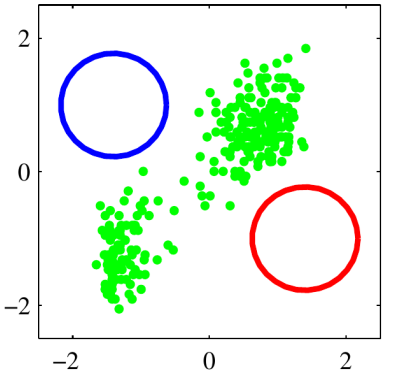

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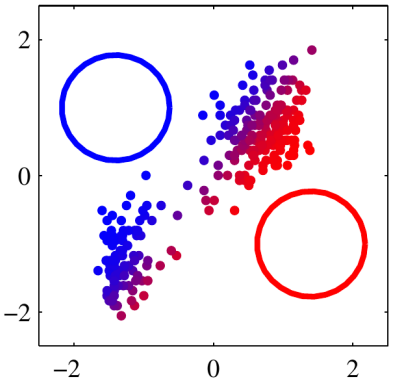

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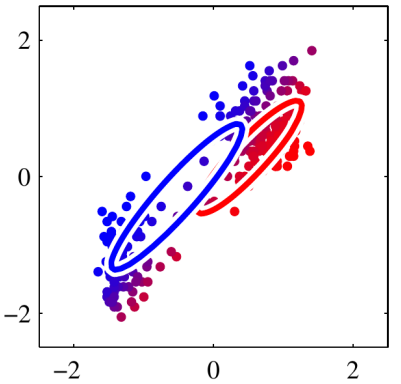
$$\pi_k^{t+1} = \frac{1}{N}\sum_{i=1}^{N} \mathbb{E}_{z^{(i)}|\mathbf{x}^{(i)},\boldsymbol{\theta}^t}[\delta_{z^{(i)},k}] = \frac{1}{N}\sum_{i=1}^{N} r_{ik}(\boldsymbol{\theta}^t) = \frac{N_k}{N} \tag{9.19}$$

Mixture weights



One updates the parameters of the Gaussian mixture components using $w_{ik}(\boldsymbol{\theta}^t)$:

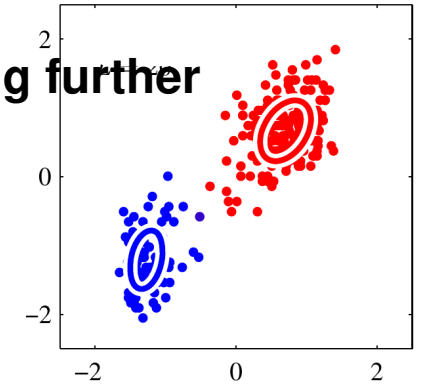
$$\boldsymbol{\mu}_k^{t+1} = \sum_{i=1}^{N} w_{ik}(\boldsymbol{\theta}^t)\mathbf{x}^{(i)} \tag{9.20}$$

Gaussian means

**Iterating further**

$$\boldsymbol{\Sigma}_k^{t+1} = \sum_{i=1}^{N} w_{ik}(\boldsymbol{\theta}^t)(\mathbf{x}^{(i)} - \boldsymbol{\mu}_k^{t+1})(\mathbf{x}^{(i)} - \boldsymbol{\mu}_k^{t+1})^T \tag{9.21}$$

Gaussian covariances



Figures from Bishop, *Pattern Recognition and Machine Learning*, chap. 9

# GMMs vs *K*-means

**Key differences:**

1. GMM: soft clustering,
   K-means: hard clustering

2. K-means: symmetrical and uniform clusters,
   GMM: ellipsoids to model each cluster

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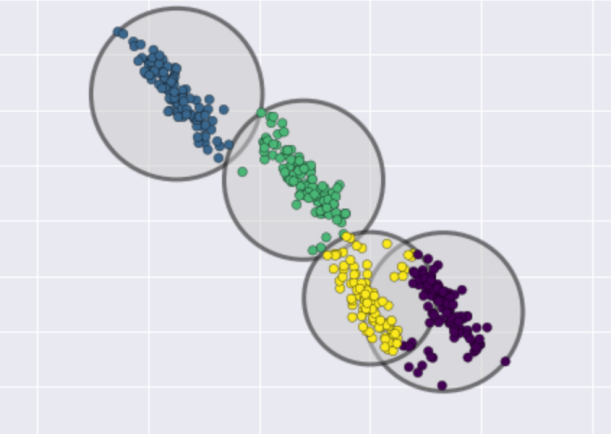
2. K-means: symmetrical and uniform clusters,
   GMM: ellipsoids to model each cluster

**GMM can be seen as a generalisation of *K*-means to soft clustering!**

If we look at the special GMM case:

$$\boldsymbol{\Sigma} = \text{diag}(1) \quad \pi_k = 1/K$$




and if we enforce hard clustering via argmax:

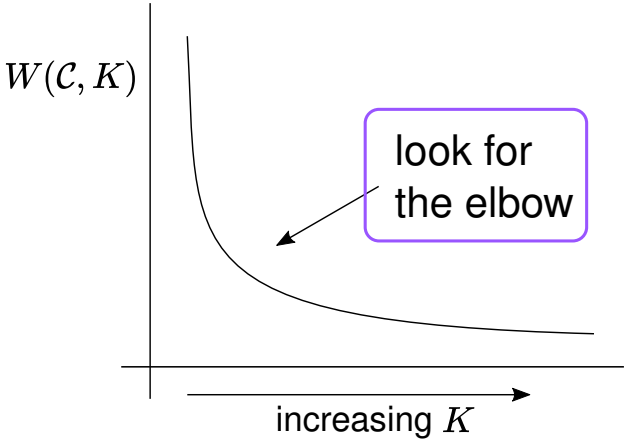
$$r_{ik}(\boldsymbol{\theta}) = \begin{cases} 1 & \text{if } k = \text{argmax}_j \, r_{ij}(\boldsymbol{\theta}) = \text{argmin}_j \, ||\mathbf{x}^{(i)} - \boldsymbol{\mu}_j||^2 \\ 0 & \text{otherwise} \end{cases}$$

We retrieve an assignment based on centroids, i.e., *K*-means!

# GMMs vs *K*-means

**One still needs to choose the number of mixture components *K***

*K*-Means, being distance-based:



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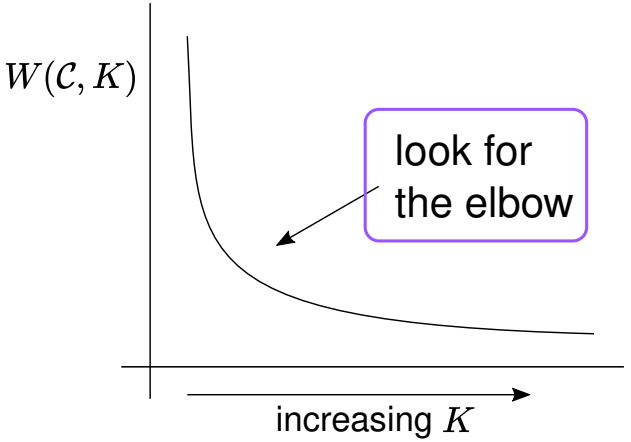



In GMMs (distribution-based) one uses criteria with the log-likelihood:

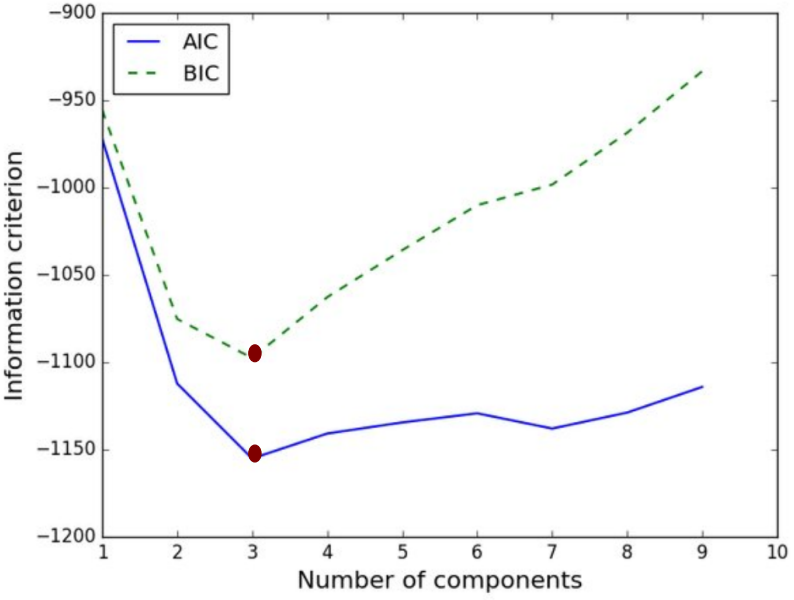
AIC: Akaike Information Criterion

$$AIC = 2N_{\boldsymbol{\theta}} - 2\ln(\mathcal{L}(\boldsymbol{\theta}))$$

BIC: Bayesian Information Criterion

$$BIC = N_{\boldsymbol{\theta}} lnN - 2\ln(\mathcal{L}(\boldsymbol{\theta}))$$

Balance fitting - model complexity, discouraging overfitting



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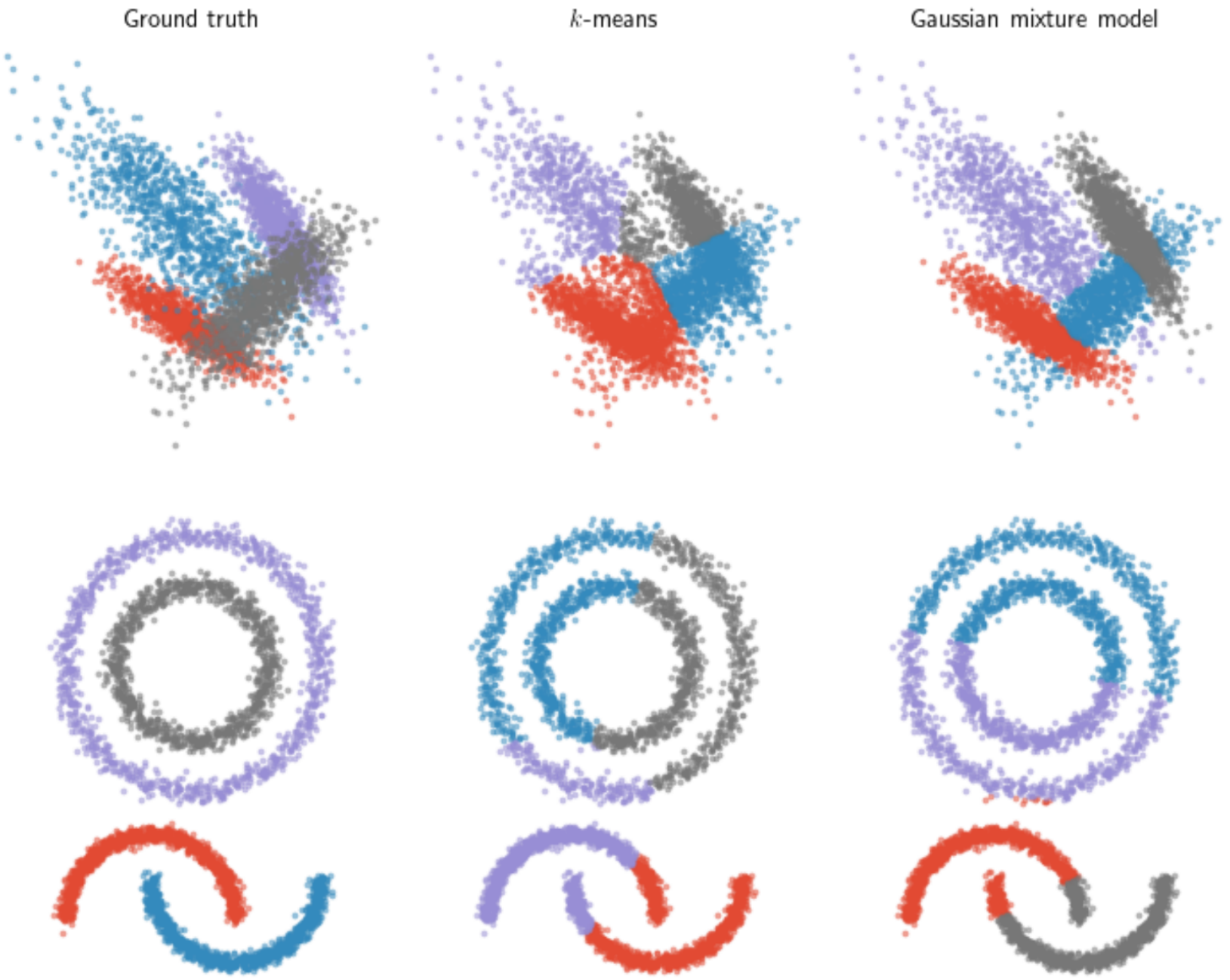

# Hierarchical Clustering (HC)

*K*-Means leads to *flat* clustering: i.e., it groups similar objects into a pre-defined number of clusters, without information on the overall data similarity structure.

HC goes beyond this, while still being: for *hard clustering* and *distance-based*

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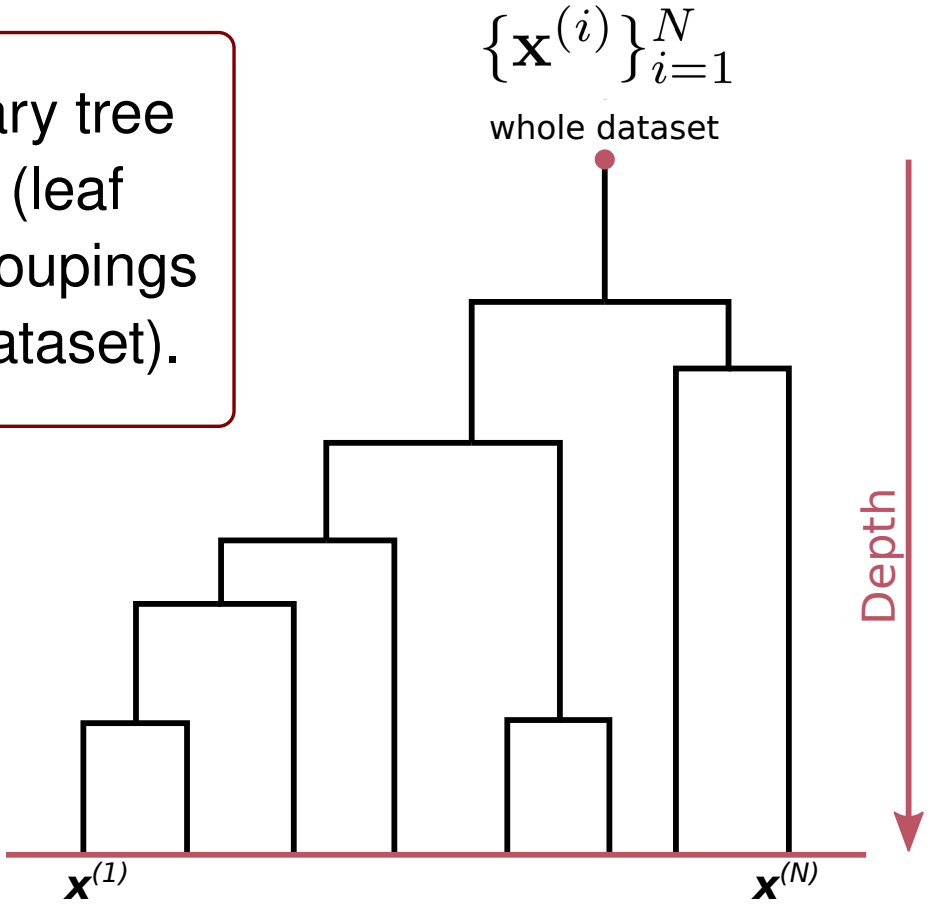
HC goes beyond this, while still being: for *hard clustering* and *distance-based*

HC represents whole dataset as a binary tree - **dendrogram** - tracking how samples (leaf nodes) get agglomerated into larger groupings going up to the root node (the whole dataset).

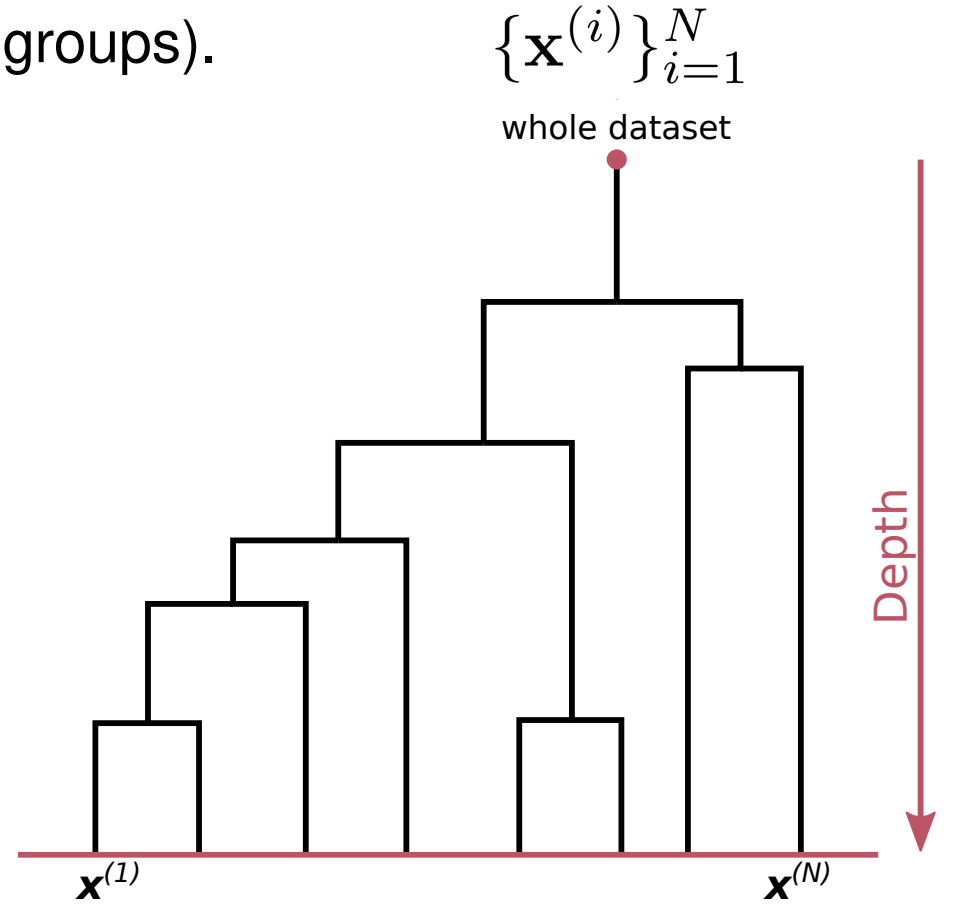
## Dendrogram



# Hierarchical Clustering (HC)

One starts from a matrix of *distances* between samples $D_{ij} := D(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$

Distances are used for the dendrogram's *repeated merges* of samples' groups:
1 merge = 1 binary split on the dendrogram;
every merge occurs at a specific depth;
strict hierarchy (no cross-over between groups).



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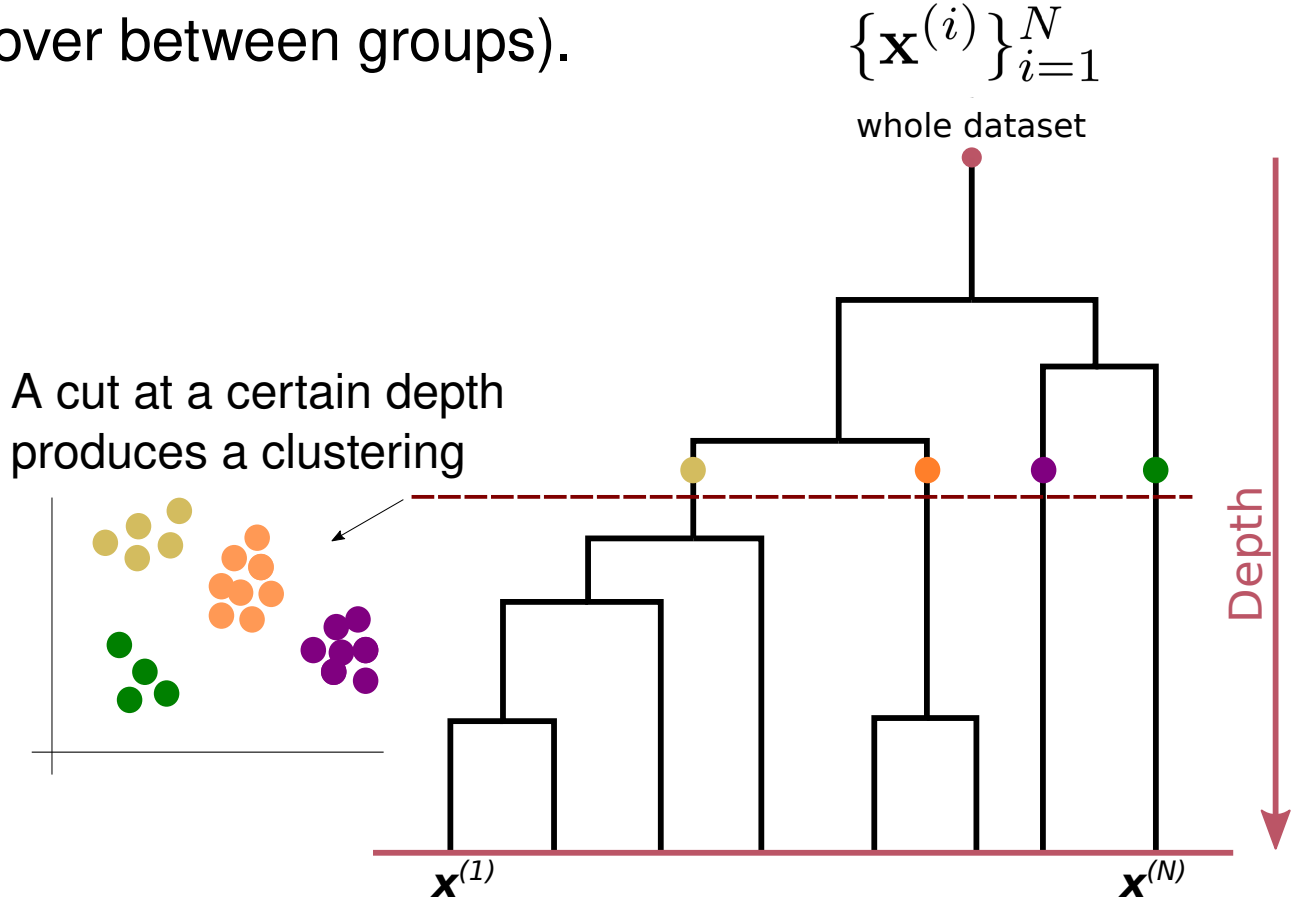


**Result**: a sequence
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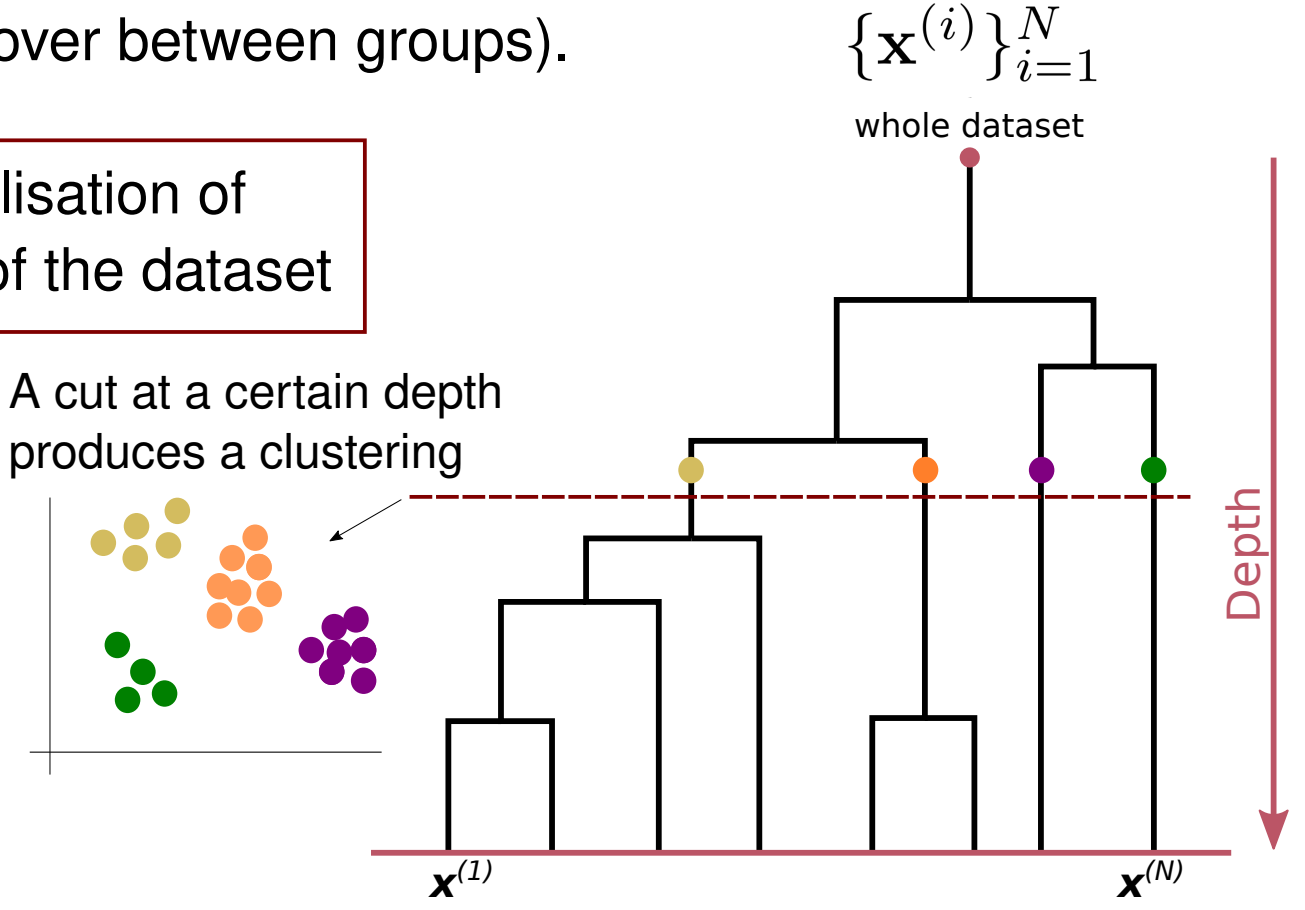
Dendrogram: global visualisation of the *intrinsic organisation* of the dataset




**Result**: a sequence of clustering assignments

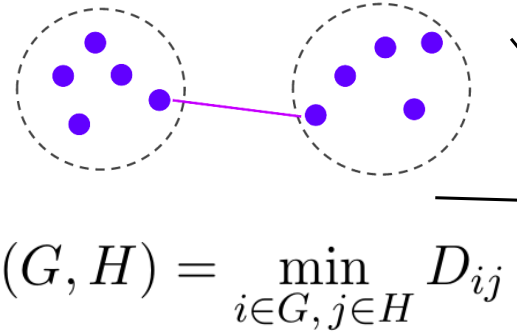
# Hierarchical Clustering (HC)

Distances are used for merges via *agglomerative* or *divisive* schemes.

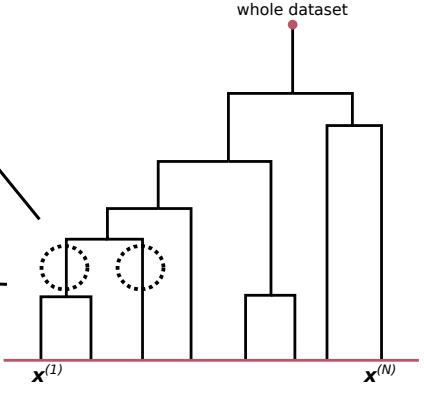
The most established are **agglomerative (bottom-up)** schemes: they proceed from leaves to root by merging groups.

At a given depth, the cluster merge is decided by taking the pair at minimal distance, defined by different linkage criteria:

**1. Single Linkage**



$$d_{\mathrm{SL}}(G, H) = \min_{i \in G,\, j \in H} D_{ij}$$



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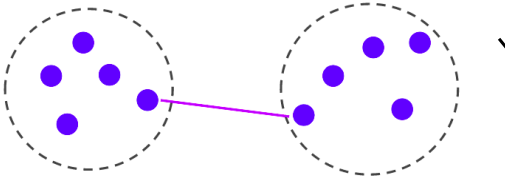
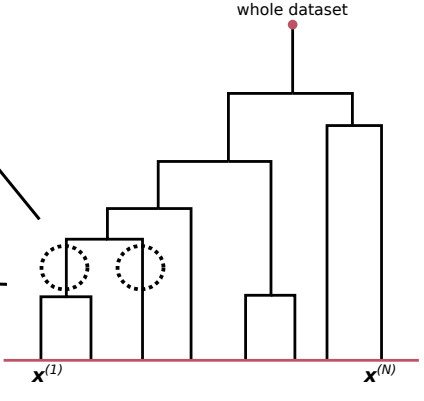
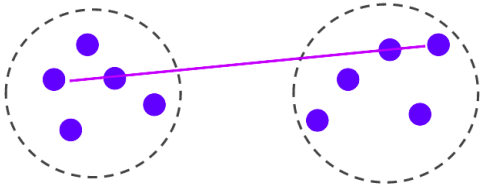





$$d_{\mathrm{SL}}(G, H) = \min_{i \in G,\, j \in H} D_{ij}$$

## 2. Complete Linkage



$$d_{\mathrm{CL}}(G, H) = \max_{i \in G,\, j \in H} D_{ij}$$

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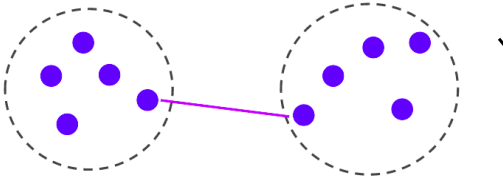

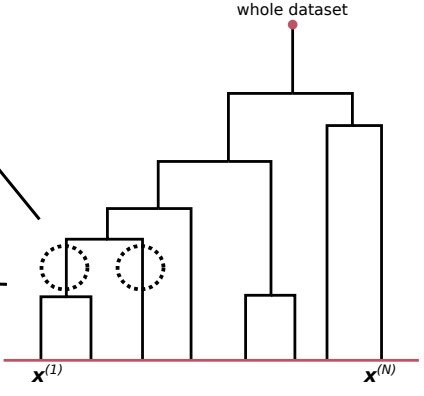


$$d_{\mathrm{SL}}(G, H) = \min_{i \in G,\, j \in H} D_{ij}$$

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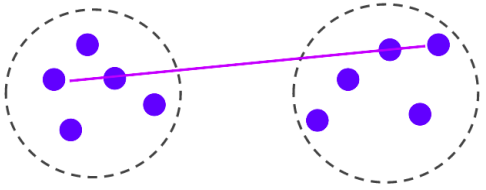
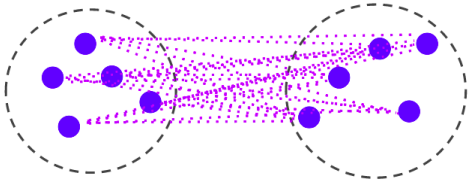


$$d_{\mathrm{CL}}(G, H) = \max_{i \in G,\, j \in H} D_{ij}$$

## 3. Average Linkage

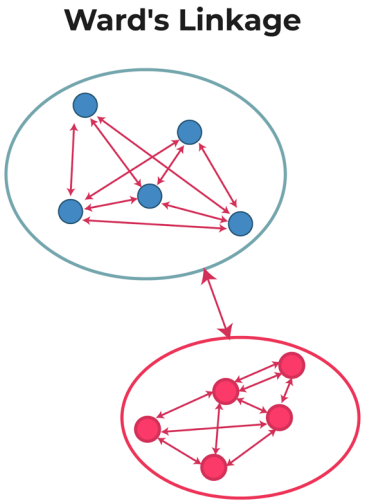


$$d_{\mathrm{GA}}(G, H) = \frac{1}{N_G N_H} \sum_{i \in G, j \in H} D_{ij}$$

Figures from https://stackabuse.com/hierarchical-clustering-with-python-and-scikit-learn/

# Hierarchical Clustering (HC)

And other linkage criteria, e.g. *variance*-based: take the merge minimising the within-cluster variance: this is the **Ward's criterion**



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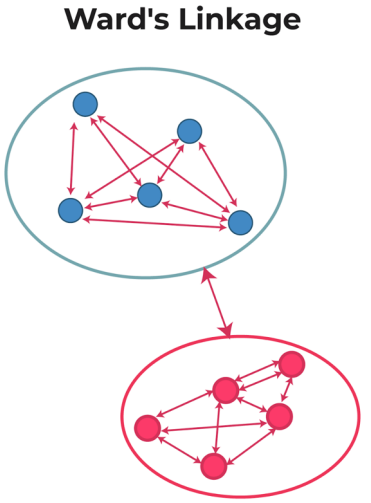
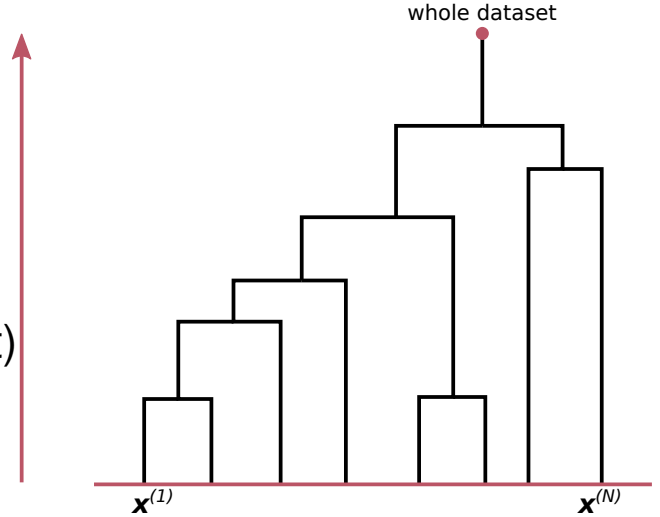



**Agglomerative**

(distance minimised at each merge monotonically increases towards the root)




**Divisive**

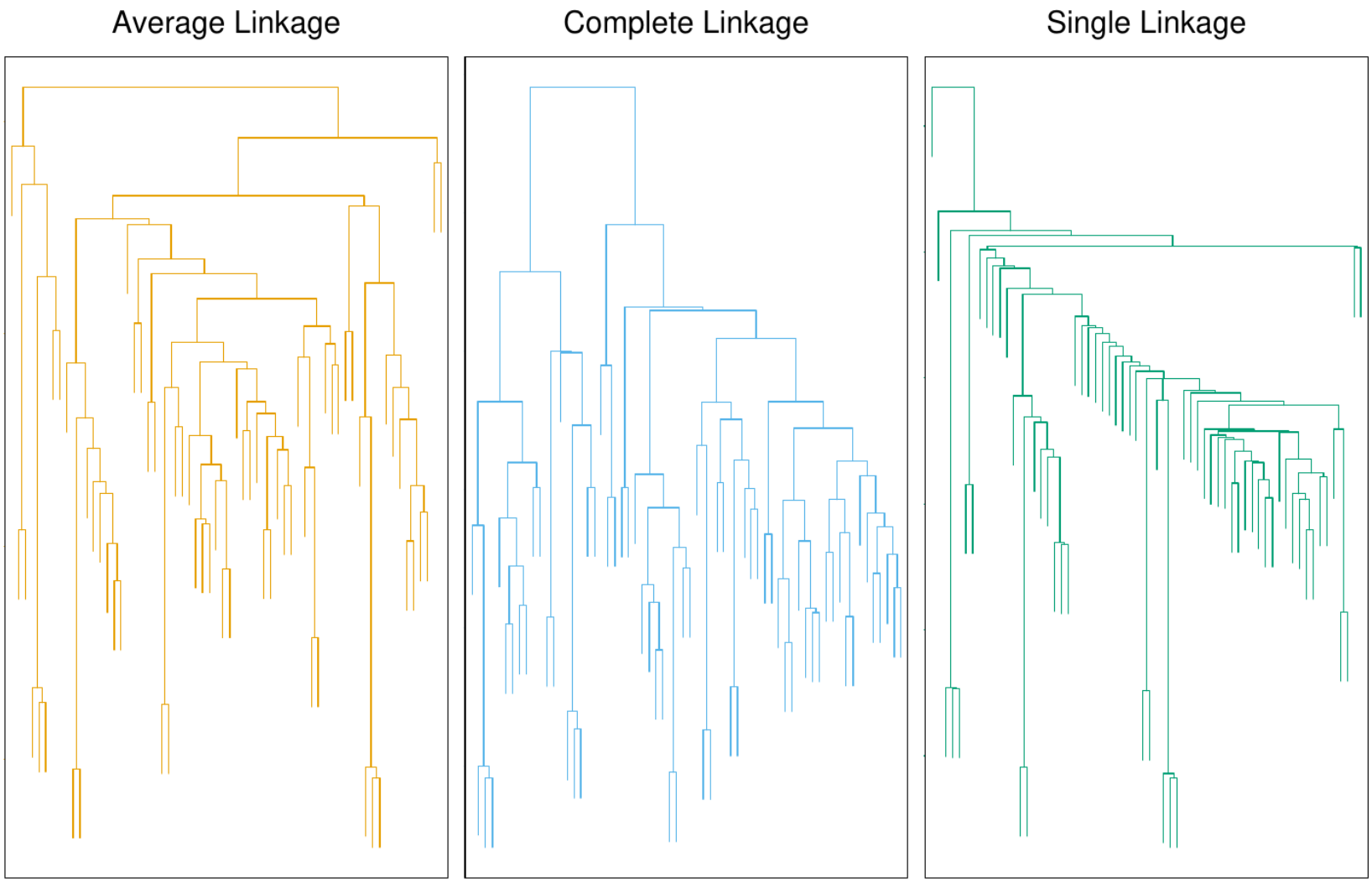
no monotonicity

**Divisive (top-down)** schemes:

by applying recursively *K*-means with (*K*=2), yielding a binary tree.

# Hierarchical Clustering (HC)

HC is sensitive to outliers and the linkage choice:



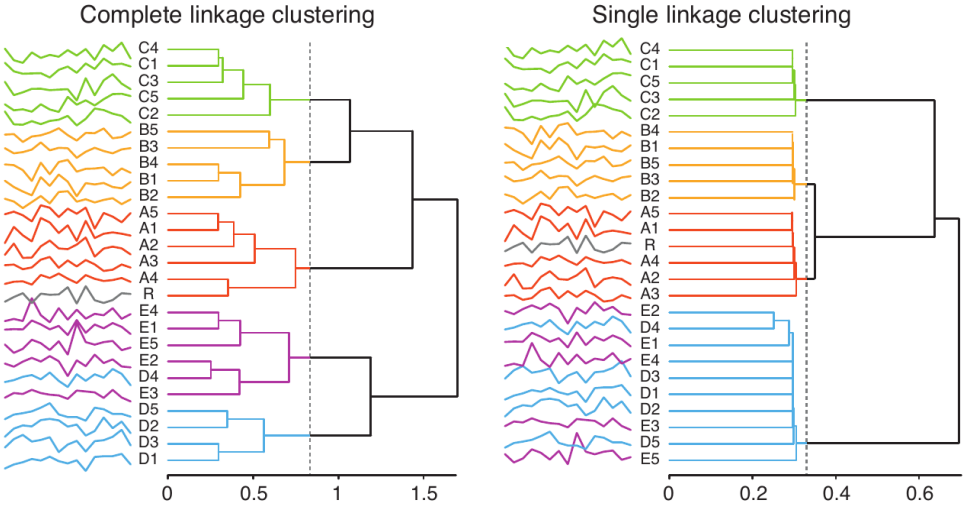

HC Dendrograms for Tumour Microarray Data, Hastie, Tibshirani, Friedman, The Elements of Statistical Learning, Chap. 14

# Hierarchical Clustering (HC)

HC allows for a visualisation of internal substructures of the data across different levels of resolution.

Often used in **bioinformatics**, e.g. genomics

HC dendrograms for gene expression data, from Altman and Krzywinski, Nature Methods 2017 (see 'additional reading')



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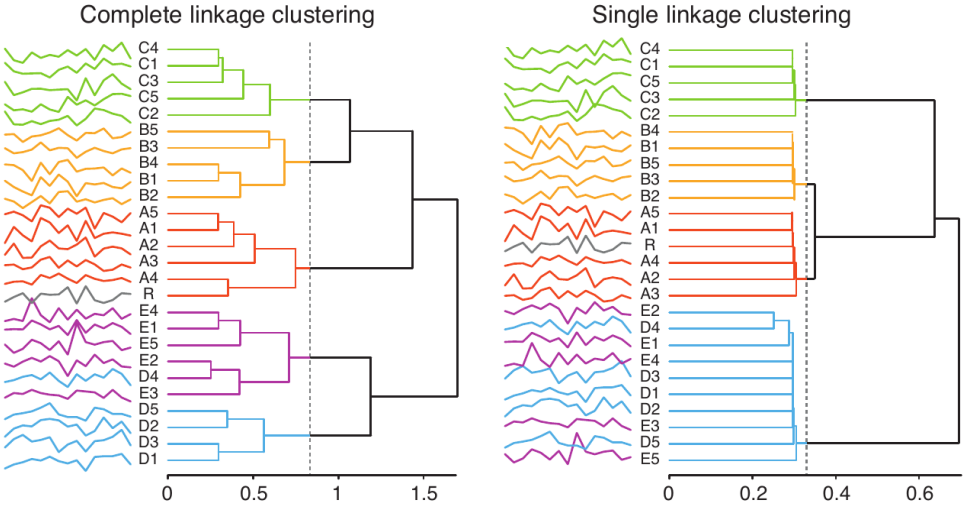
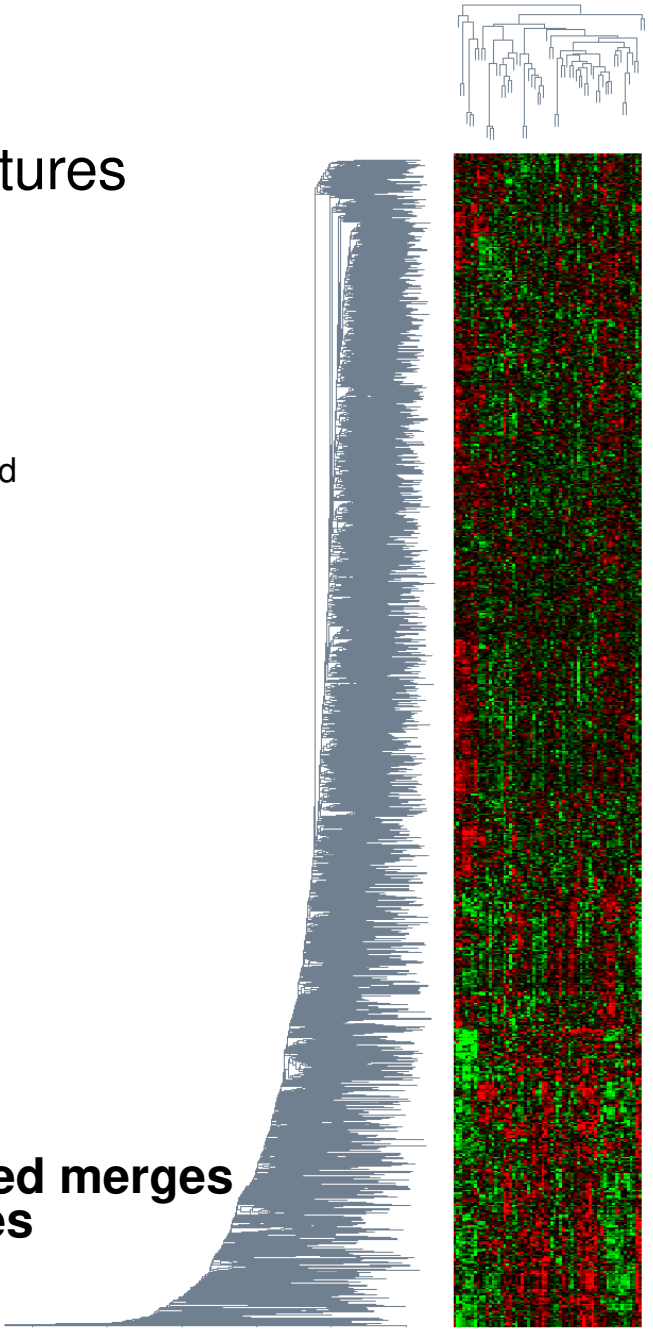



**Distance-based merges between samples**

**Distance-based merges between genes**



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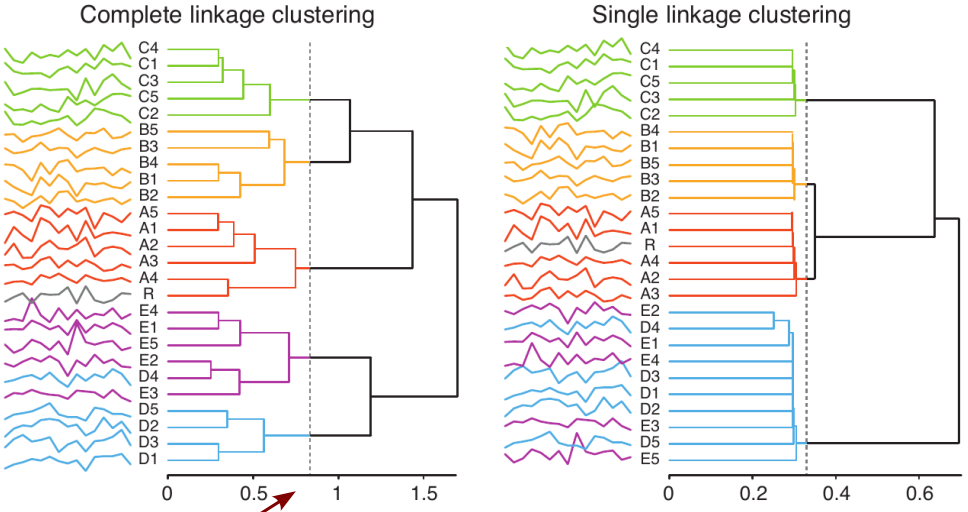


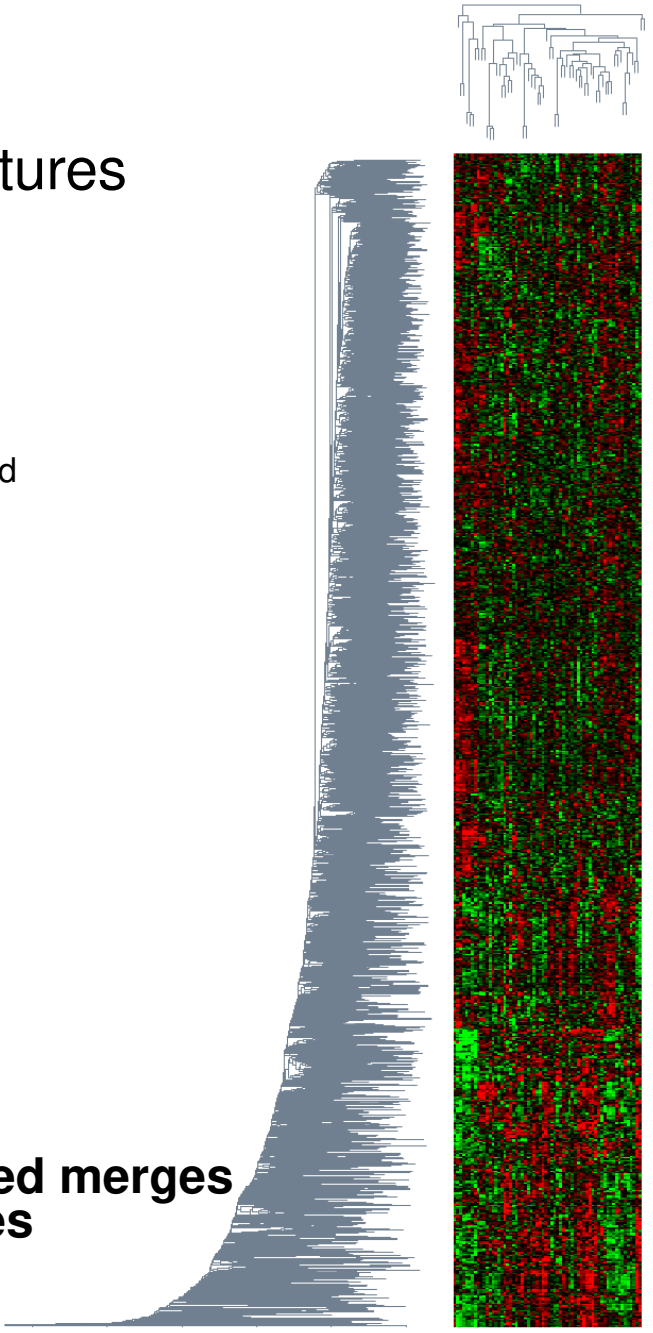

**What level of resolution to pick?**

Stable levels signalled by large jumps in depth

(as depth = function of the between-cluster distance)

**Distance-based merges between samples**

**Distance-based merges between genes**



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# Evaluating clustering performance

**External validity:** ground truth grouping well reproduced;
**Internal validity:** intra-cluster cohesion, inter-cluster separation

Let's recall:

$$W(\mathcal{C}) = \frac{1}{2}\sum_{k=1}^{K}\sum_{i,j\in c_k} D(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$$

within-cluster distance

$$B(\mathcal{C}) = \frac{1}{2}\sum_{k=1}^{K}\sum_{i\in c_k}\sum_{j\notin c_k} D(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$$

between-cluster distance

They, and their combinations, are measures of **clustering quality**

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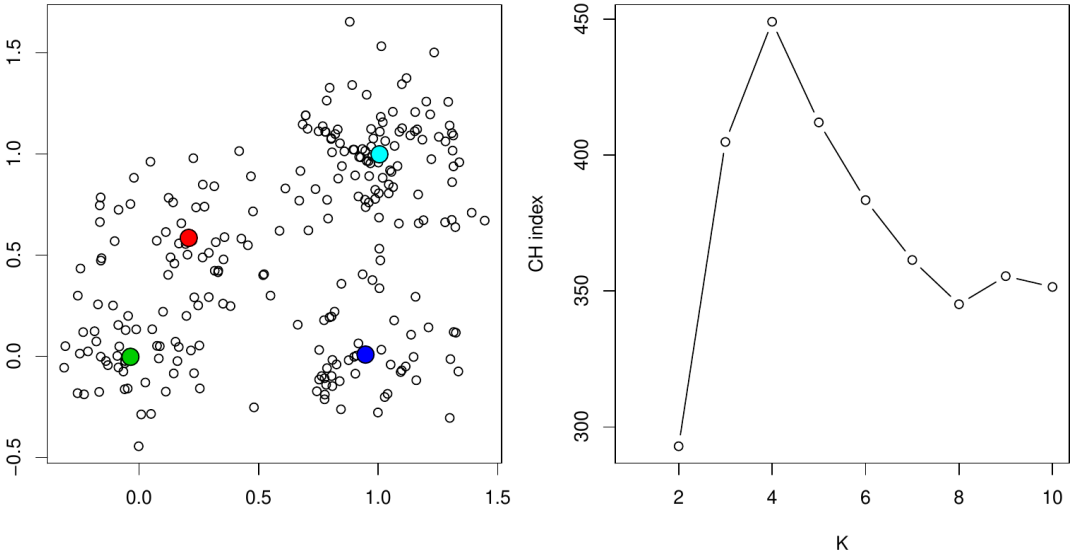


e.g. Calinski-Harabasz (CH) index

$$CH = \frac{B(\mathcal{C})/(K-1)}{W(\mathcal{C})/(N-K)}$$

its maximum helps set optimal *K*

# Comparing clusterings

**Count matrix:** of coincidences in each cluster of 2 clusterings

Clustering 2

| | $Y_1$ | $Y_2$ | $\cdots$ | $Y_{K'}$ |
|---|---|---|---|---|
| $X_1$ | $n_{11}$ | $n_{12}$ | $\cdots$ | $n_{1K'}$ |
| $X_2$ | $n_{21}$ | $n_{22}$ | $\cdots$ | $n_{2K'}$ |
| $\vdots$ | $\vdots$ | $\vdots$ | $\ddots$ | $\vdots$ |
| $X_K$ | $n_{K1}$ | $n_{K2}$ | $\cdots$ | $n_{KK'}$ |

Clustering 1

$$n_{ij} = |X_i \cap Y_j|$$

Frequency of coincidences:

$$P_{XY}(i,j) = \frac{|X_i \cap Y_i|}{N}$$

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| $\vdots$ | $\vdots$ | $\vdots$ | $\ddots$ | $\vdots$ |
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Clustering 1

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Frequency of coincidences:

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We can define **information-theoretic comparison metrics:**

**Mutual Information:**

$$MI(X,Y) = \sum_{i=1}^{K}\sum_{j=1}^{K'} P_{XY}(i,j)\log\frac{P_{XY}(i,j)}{P_X(i)P_Y(j)}$$

Clustering entropy

$$H(X) = -\sum_{i=1}^{K} P_X(i)\log P_X(i)$$

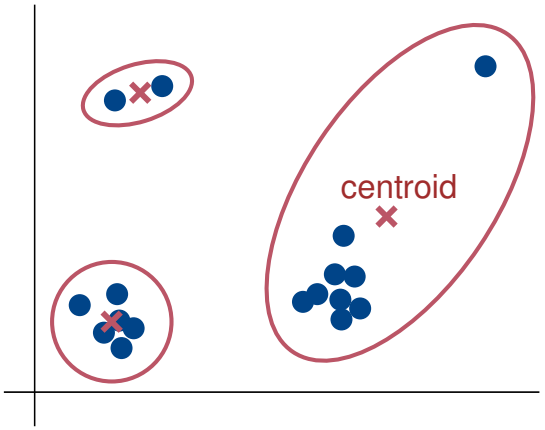
**Normalised Variation of Information:**

$$NVI(X,Y) = \frac{H(X)+H(Y)-2MI(X,Y)}{H(X)+H(Y)-MI(X,Y)}$$

and others, see lecture notes

# Summary: 3 clustering methods

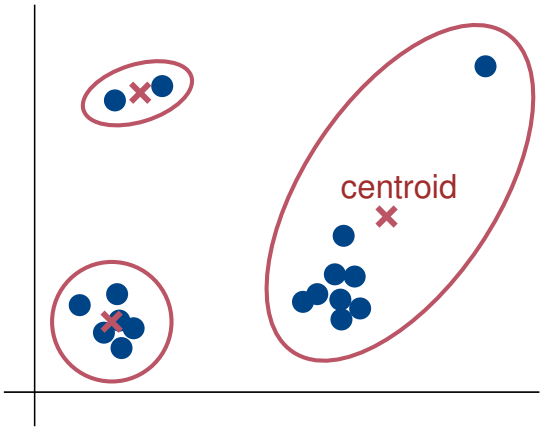
**_K_-Means**



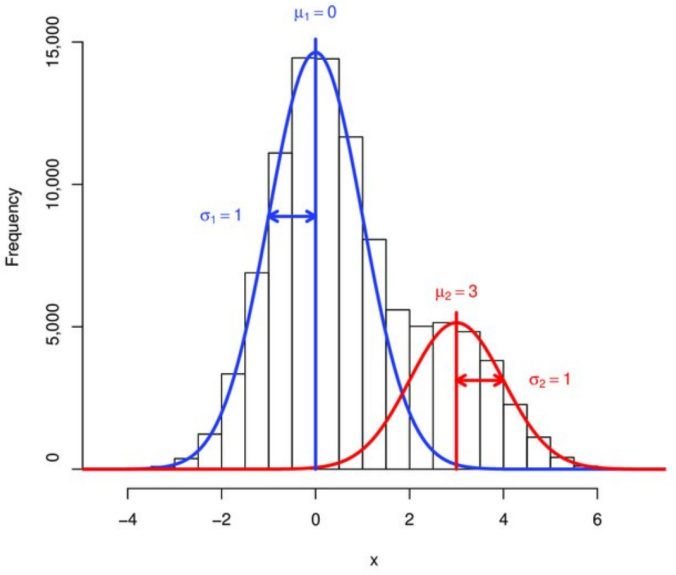

Hard clustering
Distance-based
Easy iterative algorithm
(sensitive to initialisation)

# Summary: 3 clustering methods

## *K*-Means




## GMM

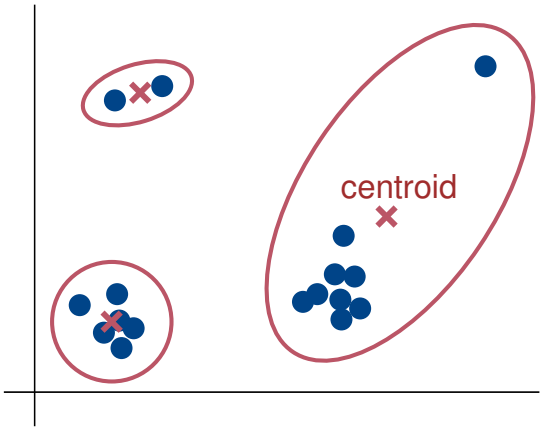



Hard clustering
Distance-based
Easy iterative algorithm
(sensitive to initialisation)

Soft clustering
Distribution-based
EM iterative algorithm
(more costly but flexible)

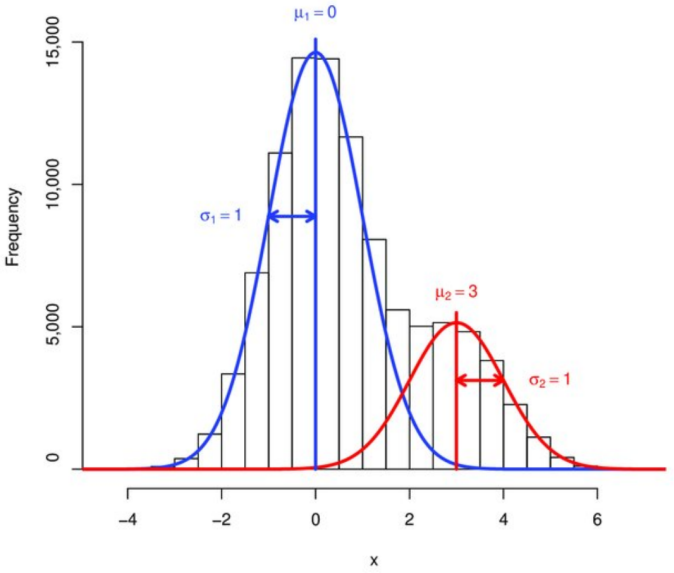
# Summary: 3 clustering methods

## *K*-Means



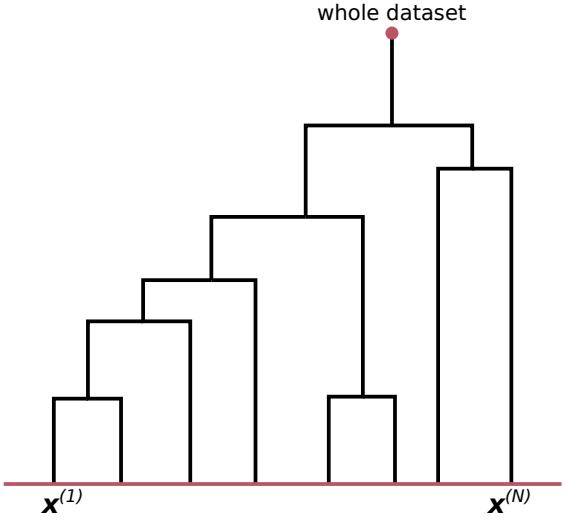

Hard clustering
Distance-based
Easy iterative algorithm
(sensitive to initialisation)

## GMM




Soft clustering
Distribution-based
EM iterative algorithm
(more costly but flexible)

## Hierarchical




Hard clustering
Distance-based
**Multi-resolution**
similarity structure

**Need to choose *K***