THE UNIVERSITY *of* EDINBURGH
informatics

Applied Machine Learning (AML)

Clustering

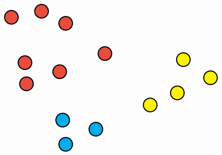
Oisin Mac Aodha • Siddharth N.

Outline

- What is clustering and why is it useful?
- What kinds are there and how are they characterised?
- Explore
  - K-Means
  - Hierarchical Clustering
- How do we evaluate clustering?

Clustering

- Discover the underlying structure of data



Clusters in 2D

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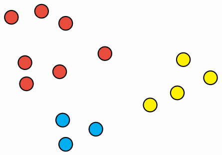
- Discover the underlying structure of data
- What sub-groups exist in the data
  - # clusters, size, …
  - common properties within sub-group
  - potential for further clustering



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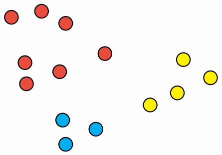

Clusters in 2D

Applications

- discover classes / structure in an unsupervised manner
  - clustering images of handwritten digits (K=10)
  - finding phylogenetic trees using DNA
- dimensionality reduction: clusters ↔ “latent factors”
  - use cluster id as representation
  - assume relevant characteristics reflected in cluster membership

Features of Clustering Algorithms

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Soft: objects have soft assignments—distribution over clusters

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Idea

Ensure points closest to some special point end up in the same cluster

- Top-down approach
- Produces a partition of the data
- Requires defining a distance metric over points

K-Means Algorithm

Require: $\mathcal{D}, K, \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ ▹ # clusters, points

$\{\boldsymbol{c}_1, \ldots, \boldsymbol{c}_K\} \leftarrow$ random initialisation ▹ centroids of clusters

repeat

  for $\boldsymbol{x}_n \in \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ **do**

    $\boldsymbol{c}_k^* = \arg\min_{\boldsymbol{c}_k} \mathcal{D}(\boldsymbol{x}_n, \boldsymbol{c}_k)$ ▹ find nearest centroid id

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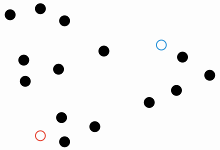

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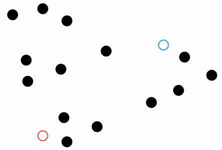

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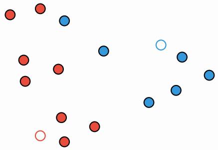

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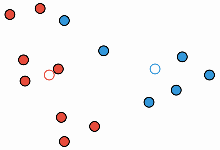

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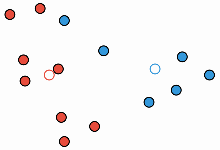

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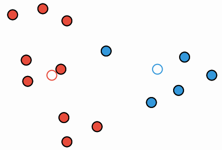

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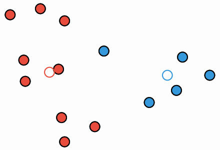

K-Means Properties

- Minimises aggregate intra-cluster distance: $V = \sum_{k} \sum_{\boldsymbol{x}_n \to \boldsymbol{c}_k} \mathcal{D}(\boldsymbol{x}_n, \boldsymbol{c}_k)$
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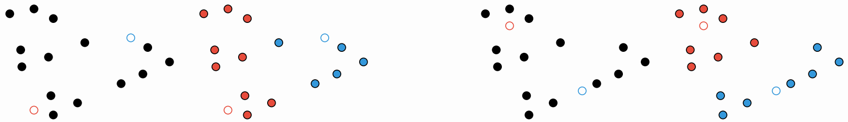

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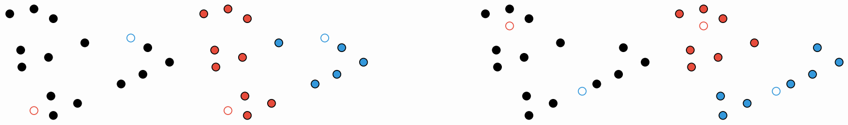
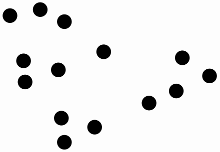


- 'Adjacent' points can end up in different clusters

Estimating Number of Clusters



data

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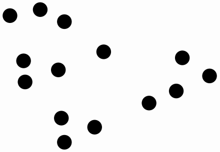

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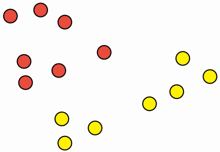

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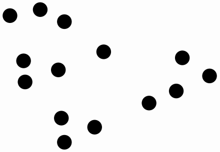

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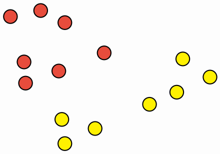

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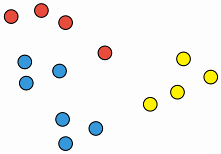

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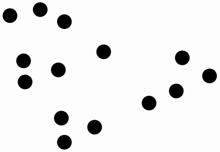

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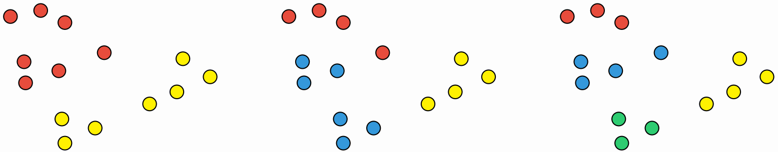

2 clusters 3 clusters 4 clusters

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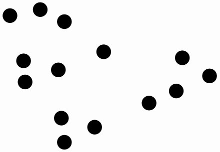

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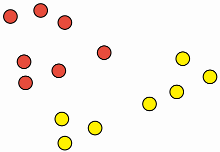

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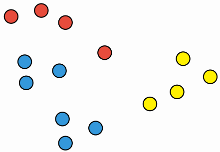

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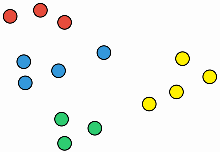

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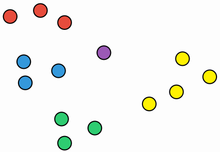

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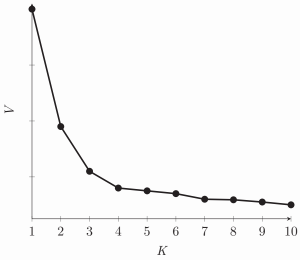
  - Choose visually from a ***elbow*** plot
    – point that maximises the 2nd derivative of V



K-Means: Example

Colour Quantisation

- Original Image: 96,615 colours

Original

Figures: Scikit Learn: Colour Quantization using K-Means

K-Means: Example

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- Quantised Image: 64 colours (K-Means)
    - Replace pixel value $\boldsymbol{x}_i$ with cluster centroid $\boldsymbol{c}_k$ value

$$\boldsymbol{x}_i \in \mathbb{R}^3 \qquad \text{(pixel values in RGB)}$$

$$\mathcal{D}(\boldsymbol{x}_i, \boldsymbol{x}_j) = \|\boldsymbol{x}_i - \boldsymbol{x}_j\|_2^2$$

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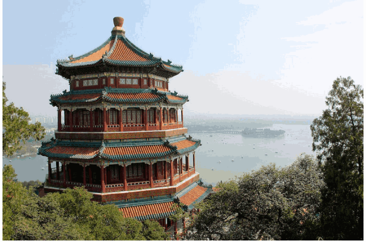
K-Means Quantised



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K-Means: Example

Colour Quantisation

- Original Image: 96,615 colours
- Quantised Image: 64 colours (K-Means)
  - Replace pixel value $\boldsymbol{x}_i$ with cluster centroid $\boldsymbol{c}_k$ value
- Quantised Image: 64 colours (Random)
  - Select random set of K pixels as "centroids"
  - Replace pixel value $\boldsymbol{x}_i$ with nearest "centroid" value

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- High-dimensional data

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Clustering Handwritten Digits

- High-dimensional data
- Dimensionality reduction (e.g. PCA)
- K-Means on embeddings

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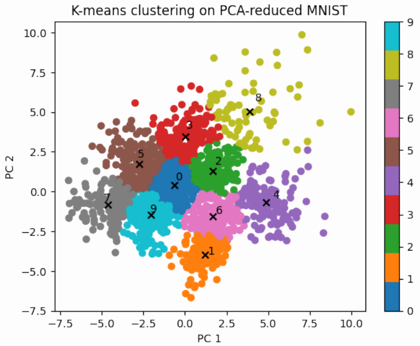
$$K = 10$$



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Find a hierarchy of structure

- **Upper levels:** coarse groups (e.g. collection of objects; bedroom, kitchen, etc.)
- **Lower levels:** fine-grained (e.g. object parts; chair leg, table top, etc.)
- Stategies
  - Top-Down: start with everything in one cluster, then split recursively
  - Bottom-up: start with each item separately, then merge recursively

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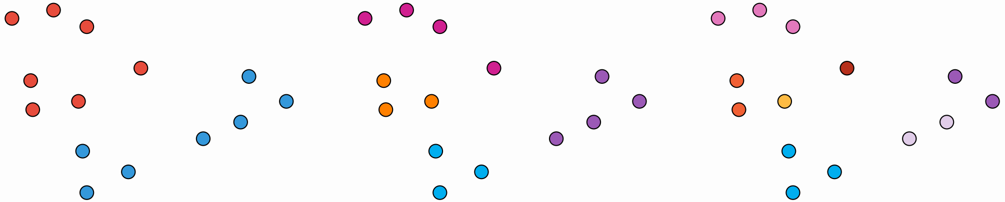
- **Fast:** recursive calls on successively smaller datasets
- **Greedy:** once cluster has been determined at top level; cannot change



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Idea

Ensure “nearby” points end up in the same cluster

- Bottom-up approach
- Generates a dendrogram: hierarchical tree of clusters
- Requires defining a distance metric over *clusters*

Agglomerative Clustering: Sketch

$\mathcal{D}(\boldsymbol{x}_l, \boldsymbol{x}_m)$ —distance between *points*

$\mathcal{G}_{\mathcal{D}}(\boldsymbol{c}_i, \boldsymbol{c}_j)$ —distance between *clusters* of points

Require: $\mathcal{G}_{\mathcal{D}}, \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$ ▹ points

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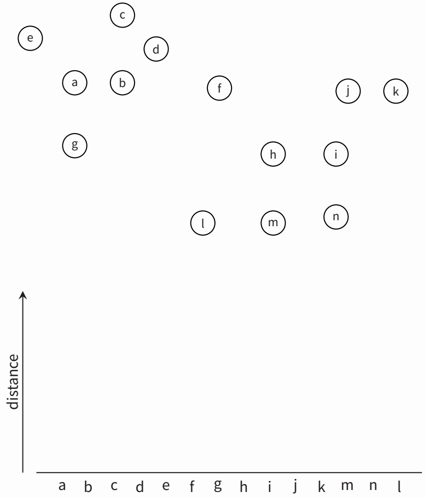
until only one cluster remaining



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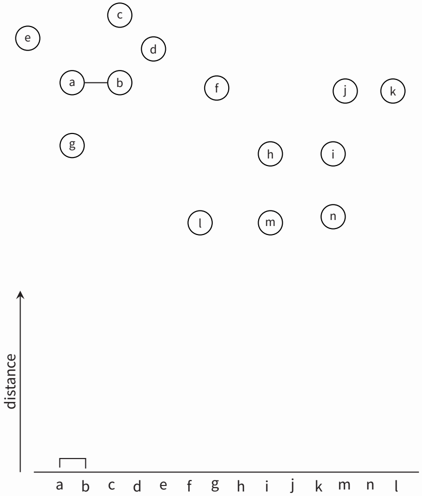

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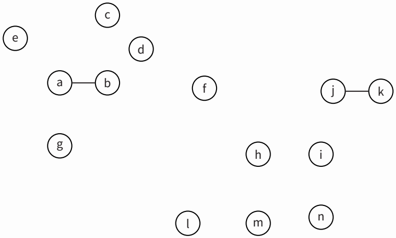

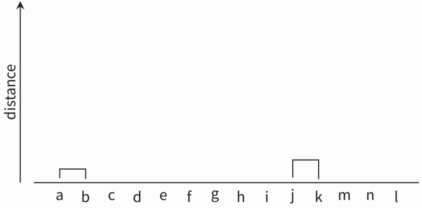

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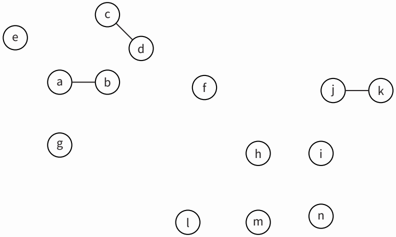

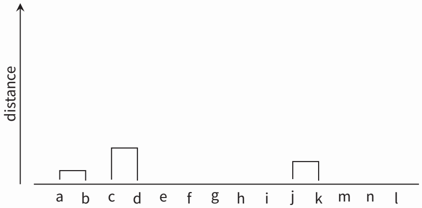

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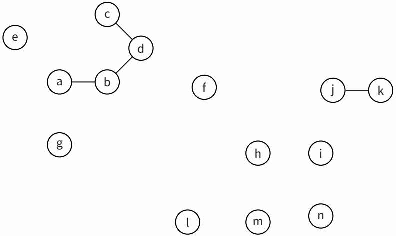

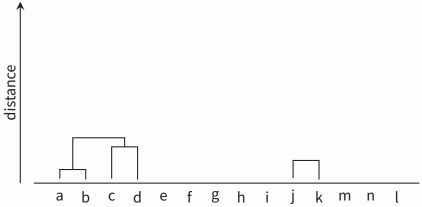

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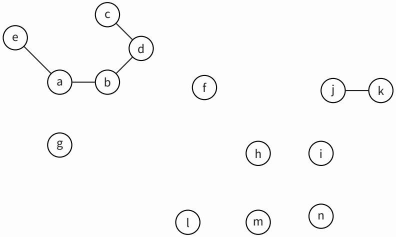

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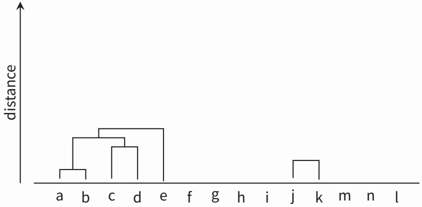

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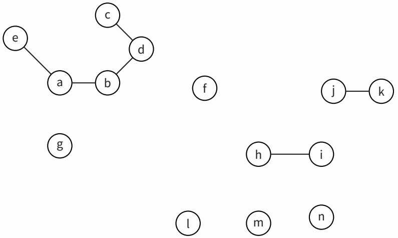

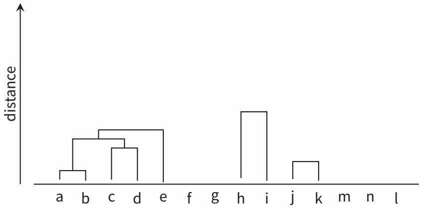

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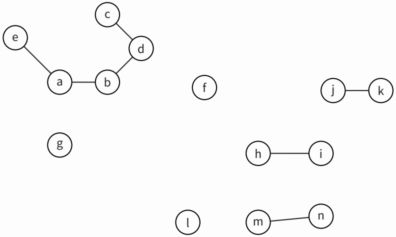

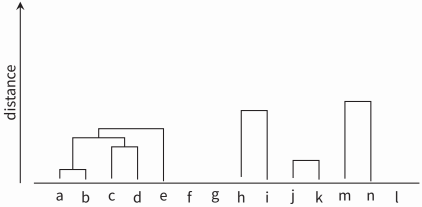

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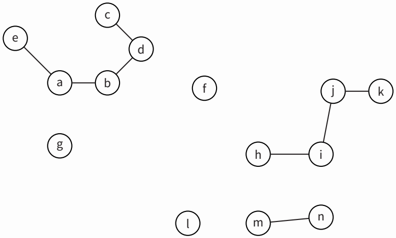

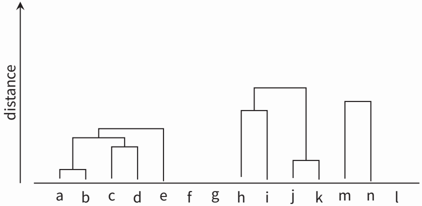

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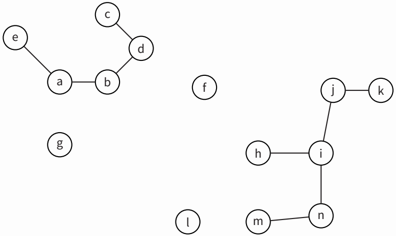

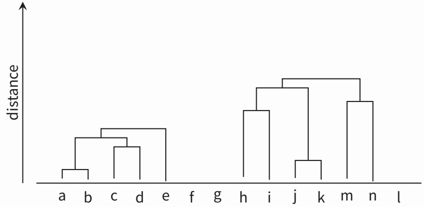

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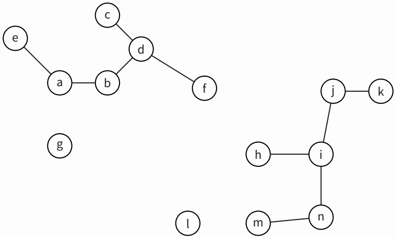

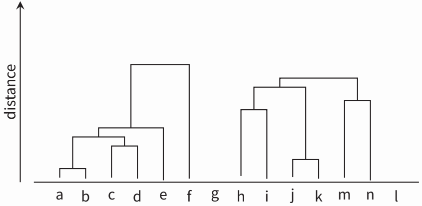

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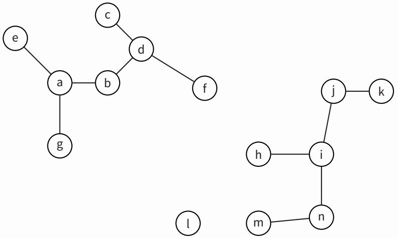

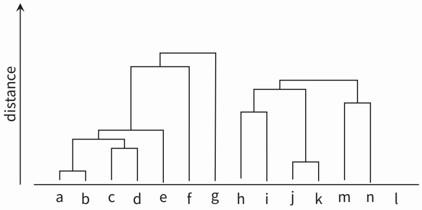

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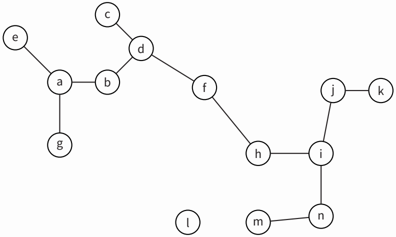

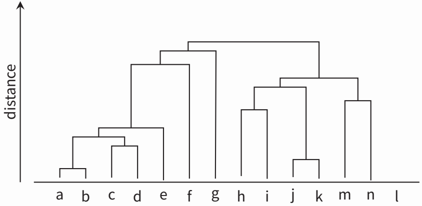

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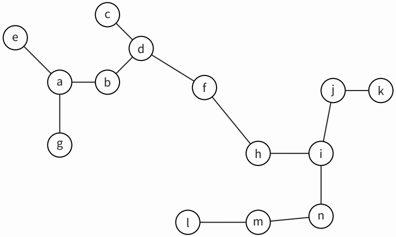

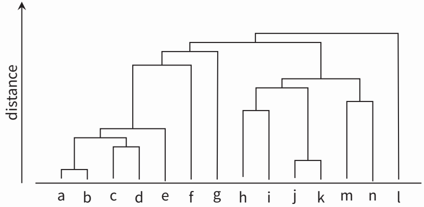

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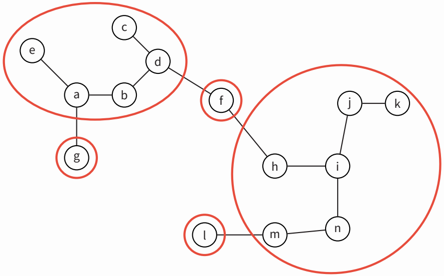

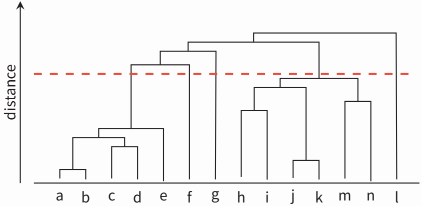

Cluster Distance Measures

Single Link

$$\mathcal{G}_{\mathcal{D}}(\boldsymbol{c}_i, \boldsymbol{c}_j) = \min_{\substack{\boldsymbol{x}_{i,l} \in \boldsymbol{c}_i \\ \boldsymbol{x}_{j,m} \in \boldsymbol{c}_j}} \mathcal{D}(\boldsymbol{x}_{i,l}, \boldsymbol{x}_{j,m})$$

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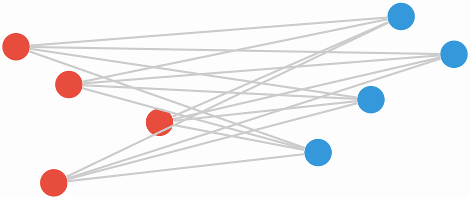

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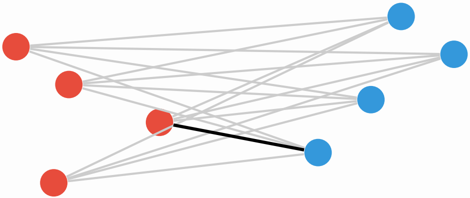

Cluster Distance Measures

Complete Link

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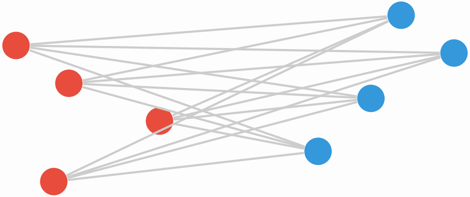

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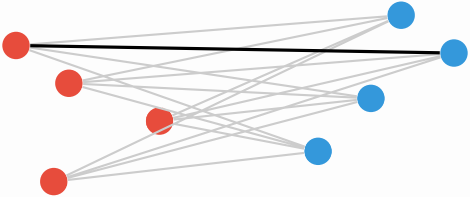

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Average Link

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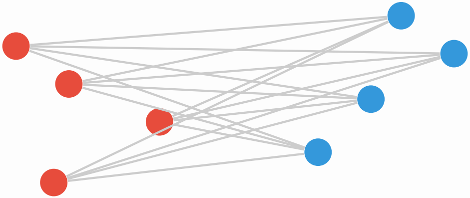

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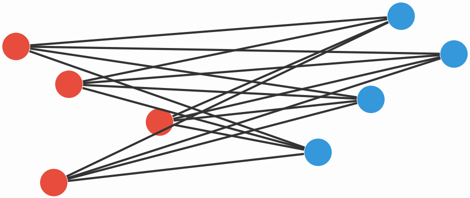

Cluster Distance Measures

Ward's Method

$$\bar{\boldsymbol{x}}_{ij} = \frac{1}{|\boldsymbol{c}_{ij}|} \sum_{\boldsymbol{x}_l \in \boldsymbol{c}_{ij}} \boldsymbol{x}_l \qquad (\boldsymbol{c}_{ij} = \boldsymbol{c}_i \cup \boldsymbol{c}_j)$$

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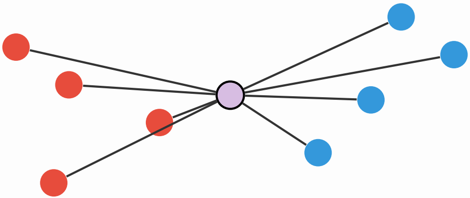

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Lance-Williams Algorithm

- When merging two clusters to get $\boldsymbol{c}_{i \cdot j}$
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For each remaining cluster $\boldsymbol{c}_k$, denoting $G_{i,j} = \mathcal{G}_{\mathcal{D}}(\boldsymbol{c}_i, \boldsymbol{c}_j)$

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Method	α_i	α_j	β	γ
Single Link	0.5	0.5	0	-0.5
Complete Link	0.5	0.5	0	0.5
Average Link	$\frac{\|\boldsymbol{c}_i\|}{\|\boldsymbol{c}_i\|+\|\boldsymbol{c}_j\|}$	$\frac{\|\boldsymbol{c}_j\|}{\|\boldsymbol{c}_i\|+\|\boldsymbol{c}_j\|}$	0	0
Ward's Method	$\frac{\|\boldsymbol{c}_i\|+\|\boldsymbol{c}_k\|}{\|\boldsymbol{c}_i\|+\|\boldsymbol{c}_j\|+\|\boldsymbol{c}_k\|}$	$\frac{\|\boldsymbol{c}_j\|+\|\boldsymbol{c}_k\|}{\|\boldsymbol{c}_i\|+\|\boldsymbol{c}_j\|+\|\boldsymbol{c}_k\|}$	$\frac{-\|\boldsymbol{c}_k\|}{\|\boldsymbol{c}_i\|+\|\boldsymbol{c}_j\|+\|\boldsymbol{c}_k\|}$	0

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Helps solve downstream task

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- **Key:** Does it help perform task better?

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Helps understand qualitative makeup of data

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- **Human:** compare judgements to humans on exemplars
  - ask human if pair $\boldsymbol{x}_i, \boldsymbol{x}_j$ belong together
  - compute match between human judgements and predictions: F1-score, κ, etc.

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In the absence of labels, or any other external measure of utility, can compute a generic measure of how well-clustered the data is.

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$$s = \frac{1}{N} \sum_{l=1}^{N} s_l \qquad -1 \leq s \leq 1$$

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Key Idea: Evaluate relationship between *pairs* of data points $\boldsymbol{x}_l, \boldsymbol{x}_m$

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True ($\mathcal{R}$) \ Predicted (C)	+	−
+	TP	FN
−	FP	TN

$$\mathrm{RI} = \frac{TP + TN}{TP + TN + FP + FN}$$

$=$ Accuracy!

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$\vdots$	$\vdots$	$\vdots$	$\ddots$	$\vdots$	$\vdots$
$\boldsymbol{r}_V$	N_{V1}	N_{V2}	$\cdots$	N_{VU}	a_V
sum	b_1	b_2	$\cdots$	b_U	N

$N_{ij} = |\boldsymbol{r}_i \cap \boldsymbol{c}_j|$ $\quad \binom{N}{2} = \frac{N(N-1)}{2}$

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$$\text{TP} = \sum_{ij} \binom{N_{ij}}{2}$$

$$\text{Expected RI} = \frac{1}{\binom{N}{2}} \left[\sum_v \binom{a_v}{2} \cdot \sum_u \binom{b_u}{2} \right]$$

$$\text{Max RI} = \frac{1}{2} \left[\sum_v \binom{a_v}{2} + \sum_u \binom{b_u}{2} \right]$$

$$\text{ARI} = \frac{\text{TP} - \text{Expected RI}}{\text{Max RI} - \text{Expected RI}}$$

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