Clustering

Unsupervised classification / clustering

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- **Input**: $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n \in \mathbb{R}^d$, target cardinality $k \in \mathbb{N}$.
- **Output**: function $f \colon \mathbb{R}^d \to \{1, 2, \ldots, k\} =: [k]$.
- **Typical semantics**: hidden subpopulation structure.

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- Often done via unsupervised classification;
  $\Rightarrow$ "clustering" often synonymous with "unsupervised classification".
- Sometimes also have a "representative" $\boldsymbol{c}_j \in \mathbb{R}^d$ for each $j \in [k]$
  (e.g., average of the $\boldsymbol{x}_i$ in jth group) $\longrightarrow$ **quantization**.

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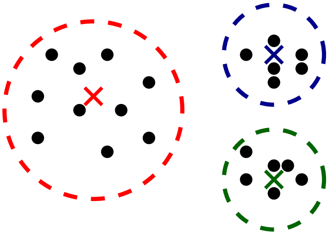

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Uses of clustering: feature representations

"One-hot" / "dummy variable" encoding of $f(\boldsymbol{x})$

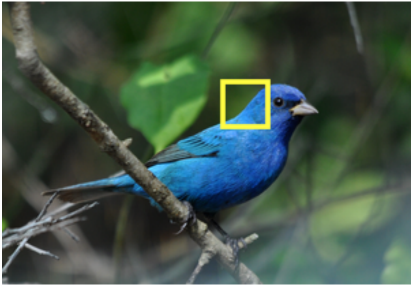
$$\boldsymbol{\phi}(\boldsymbol{x}) = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \begin{matrix} \\ \\ \\ \longleftarrow f(\boldsymbol{x}) \text{ position} \\ \\ \\ \\ \end{matrix}$$

(Often used together with other features.)

Uses of clustering: feature representations

Histogram representation

- Cut up each $\boldsymbol{x}_i \in \mathbb{R}^d$ into different parts $\boldsymbol{x}_{i,1}, \boldsymbol{x}_{i,2}, \ldots, \boldsymbol{x}_{i,m} \in \mathbb{R}^p$ (e.g., small patches of an image) .
- Cluster all the parts $\boldsymbol{x}_{i,j}$: get k representatives $\boldsymbol{c}_1, \boldsymbol{c}_2, \ldots, \boldsymbol{c}_k \in \mathbb{R}^p$.
- Represent $\boldsymbol{x}_i$ by a histogram over $\{1, 2, \ldots, k\}$ based on assignments of $\boldsymbol{x}_i$'s parts to representatives.



Uses of clustering: compression

Quantization

Replace each $\boldsymbol{x}_i$ with its representative

$$\boldsymbol{x}_i \;\mapsto\; \boldsymbol{c}_{f(\boldsymbol{x}_i)}\,.$$

Example: quantization at image patch level.

k-MEANS CLUSTERING

k-means clustering

Problem

- **Input**: $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n \in \mathbb{R}^d$, target cardinality $k \in \mathbb{N}$.
- **Output**: k representatives ("centers", "means") $\boldsymbol{c}_1, \boldsymbol{c}_2, \ldots, \boldsymbol{c}_k \in \mathbb{R}^d$.
- **Objective**: choose $\boldsymbol{c}_1, \boldsymbol{c}_2, \ldots, \boldsymbol{c}_k \in \mathbb{R}^d$ to minimize

$$\sum_{i=1}^{n} \min_{j \in [k]} \|\boldsymbol{x}_i - \boldsymbol{c}_j\|_2^2 .$$

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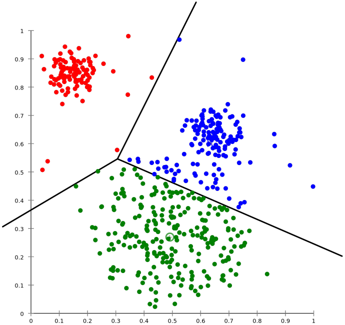

Natural assignment function

$$f(\boldsymbol{x}) \;:=\; \arg\min_{j \in [k]} \|\boldsymbol{x} - \boldsymbol{c}_j\|_2^2 .$$

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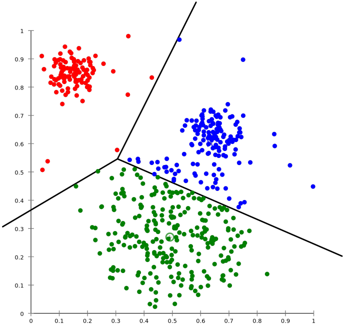

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NP-hard, even if $k = 2$ or $d = 2$.

The easy cases

k-means clustering for $k = 1$

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Solution: "bias/variance decomposition"

$$\frac{1}{n} \sum_{i=1}^{n} \|\boldsymbol{x}_i - \boldsymbol{c}\|_2^2 \;=\; \|\boldsymbol{\mu} - \boldsymbol{c}\|_2^2 + \frac{1}{n} \sum_{i=1}^{n} \|\boldsymbol{x}_i - \boldsymbol{\mu}\|_2^2$$

where $\boldsymbol{\mu} = \frac{1}{n} \sum_{i=1}^{n} \boldsymbol{x}_i$.

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k-means clustering for $d = 1$

Dynamic programming in time $O(n^2 k)$.

Alternating optimization algorithm

Assignment variables

For each data point $\boldsymbol{x}_i$, let $\boldsymbol{\phi}_i \in \{0,1\}^k$ denote its "one-hot" representation:

$$\phi_{i,j} \;=\; \mathbb{1}\{\boldsymbol{x}_i \text{ is assigned to cluster } j\}\,.$$

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Initialize $\boldsymbol{c}_1, \boldsymbol{c}_2, \ldots, \boldsymbol{c}_k \in \mathbb{R}^d$ somehow. Then repeat until convergence:

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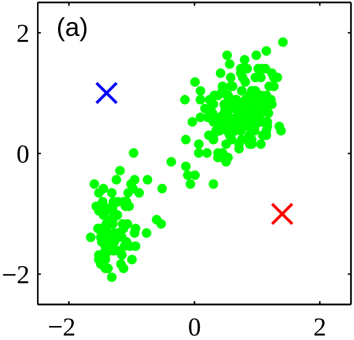
Sample run of Lloyd's algorithm



Arbitrary initialization of $\boldsymbol{c}_1$ and $\boldsymbol{c}_2$.

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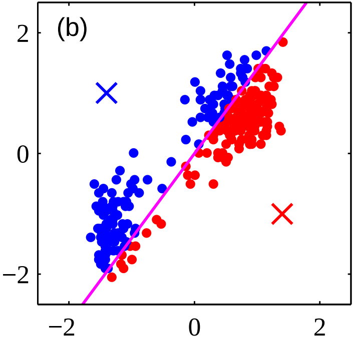

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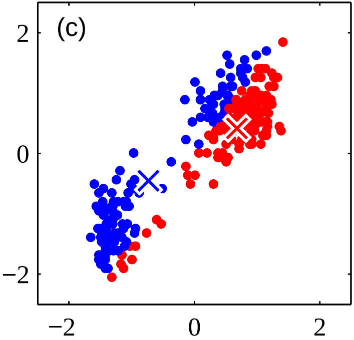

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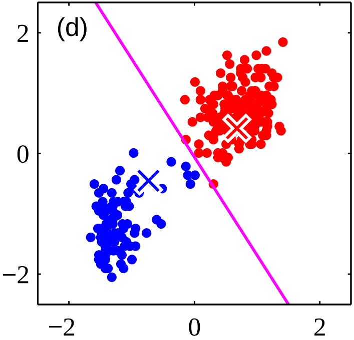

Iteration 2
Optimize assignments ϕ_i.

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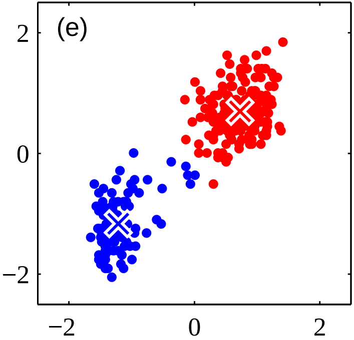

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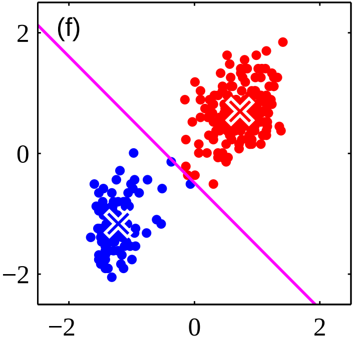

Iteration 3
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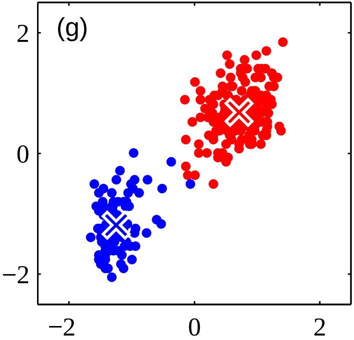

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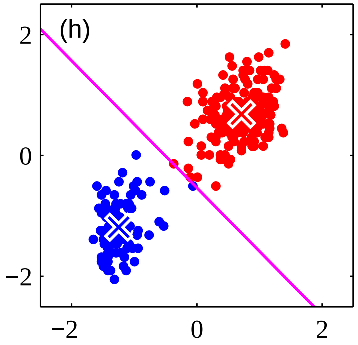

Iteration 4
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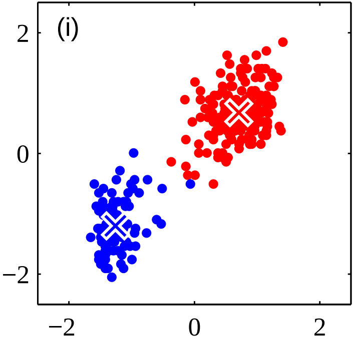

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Initializing Lloyd's algorithm

Basic idea: Choose initial centers to have good coverage of the data points.

Farthest-first traversal

For $j = 1, 2, \ldots, k$:

- Pick $\boldsymbol{c}_j \in \mathbb{R}^d$ from among $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n$ farthest from previously chosen $\boldsymbol{c}_1, \boldsymbol{c}_2, \ldots, \boldsymbol{c}_{j-1}$.

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But this can be thrown off by outliers...

A better idea:

D^2 sampling (a.k.a. "k-means++")

For $j = 1, 2, \ldots, k$:

- Randomly pick $\boldsymbol{c}_j \in \mathbb{R}^d$ from among $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_n$ according to distribution

$$P(\boldsymbol{x}_i) \propto \min_{\ell=1,2,\ldots,j-1} \|\boldsymbol{x}_i - \boldsymbol{c}_\ell\|_2^2 .$$

  (Uniform distribution when $j = 1$.)

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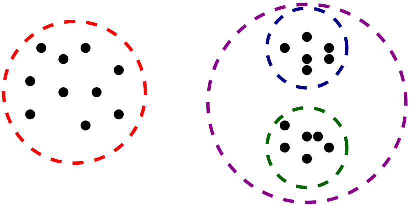
- *Heuristic*: Find large gap between $(k-1)$-means cost and k-means cost.

Clustering at multiple scales



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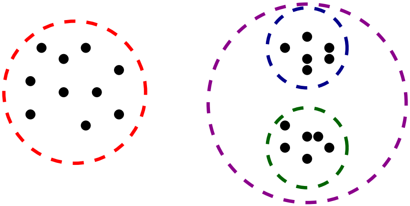

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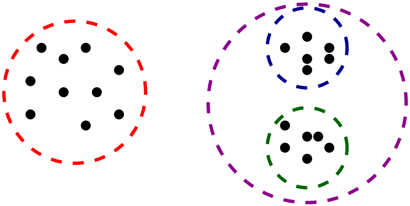

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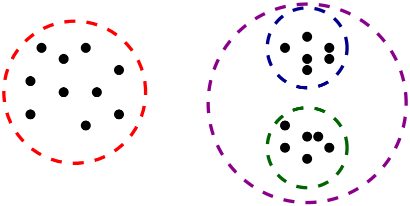

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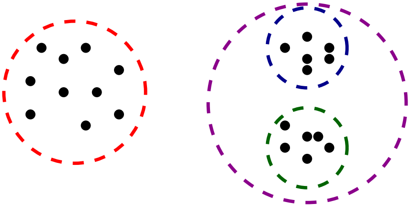

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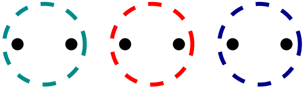
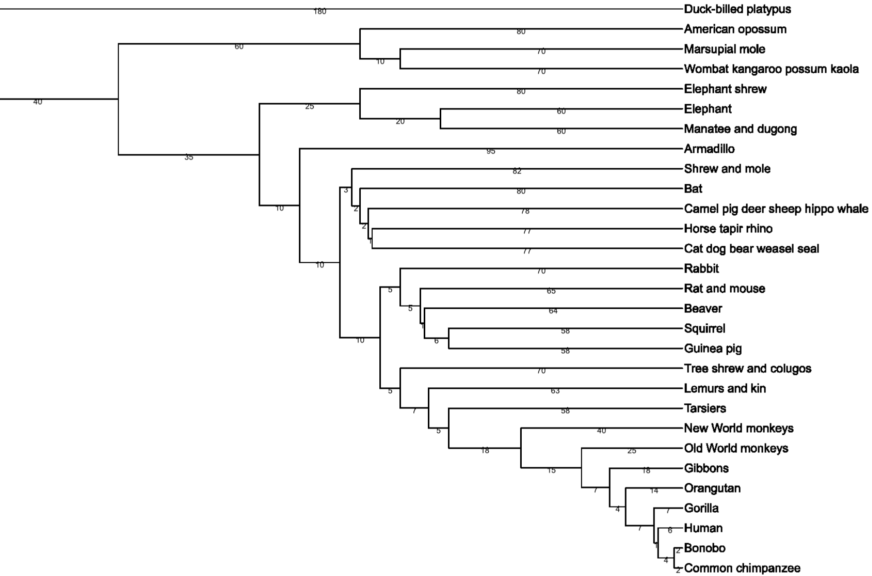


Example: phylogenetic tree



Hierarchical clustering

Divisive (top-down) clustering

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- Recurse on each part.

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  Example: *Ward's average linkage method*

$$\operatorname{dist}(C, \tilde{C}) \ := \ \frac{|C| \cdot |\tilde{C}|}{|C| + |\tilde{C}|} \| \operatorname{mean}(C) - \operatorname{mean}(\tilde{C}) \|_2^2$$

  (the increase in k-means cost caused by merging C and $\tilde{C}$).

Recap

- Uses of clustering:
  - Unsupervised classification ("hidden subpopulations").
  - Quantization
  - ...
- k-means clustering: popular objective for clustering and quantization.
- Lloyd's algorithm: alternating optimization, needs good initialization.
- Hierarchical clustering: clustering at multiple levels of granularity.