COMS 4771 Lecture 18

1. k-means clustering
2. Dictionary learning

Clustering

Unsupervised classification

- **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.

Unsupervised classification / clustering

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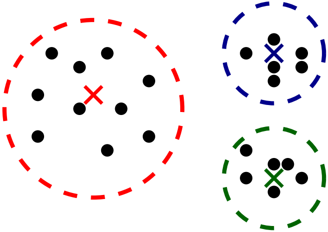
- **Output**: partitioning of $\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \dots, \boldsymbol{x}^{(n)}$ into k groups.
- Often done via unsupervised classification;
  $\Rightarrow$ "clustering" often synonymous with "unsupervised classification".
- Sometimes also have a "representative" $\boldsymbol{c}_j \in \mathbb{R}^d$ for each $j \in [k]$
  (e.g., average of the $\boldsymbol{x}^{(i)}$ in jth group) $\longrightarrow$ **quantization**.

UNSUPERVISED CLASSIFICATION / CLUSTERING



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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.)

Histogram representation

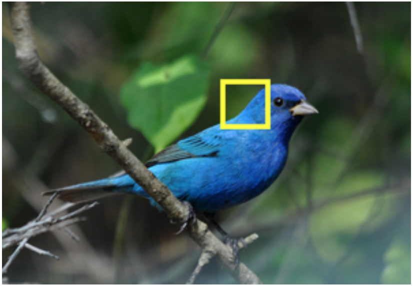
- Cut up each $\boldsymbol{x}^{(i)} \in \mathbb{R}^d$ into different parts $\boldsymbol{x}^{(i,1)}, \boldsymbol{x}^{(i,2)}, \ldots, \boldsymbol{x}^{(i,m)} \in \mathbb{R}^p$ (e.g., small patches of an image) .

cluster over all pathes

- Cluster all the $\boxed{\text{parts } \boldsymbol{x}^{(i,j)}\text{:}}$ 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 $\boxed{\boldsymbol{x}^{(i)}\text{'s parts to representatives.}}$

choose the right representative(k representatives in total) at each path!!!

replace each path with a representative from k



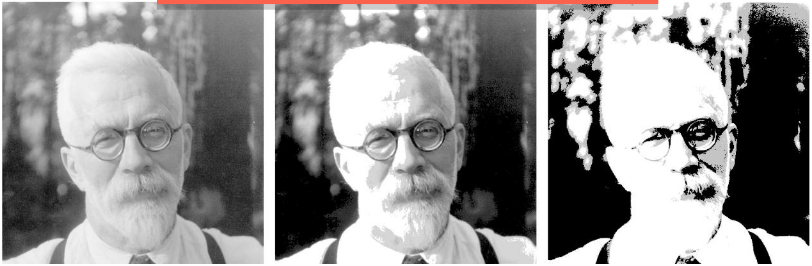
Uses of clustering: compression

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

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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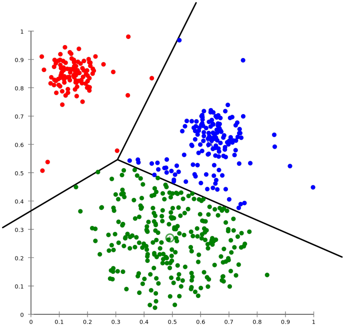

Natural assignment function

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

Problem

the input could be pathes

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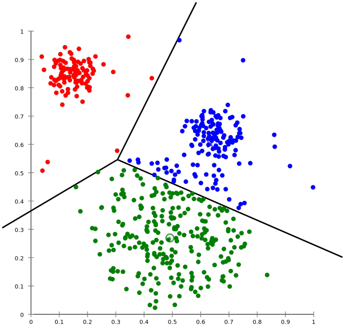

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NP-hard, even if $k = 2$ or $d = 2$.

k-means clustering for $k = 1$

Problem: Pick $\boldsymbol{c} \in \mathbb{R}^d$ to minimize

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

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Therefore, optimal choice for $\boldsymbol{c}$ is $\boldsymbol{\mu}$.

The easy cases

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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 $\boldsymbol{\phi}^{(i)} \in \{0,1\}^d$ denote its "one-hot" representation:

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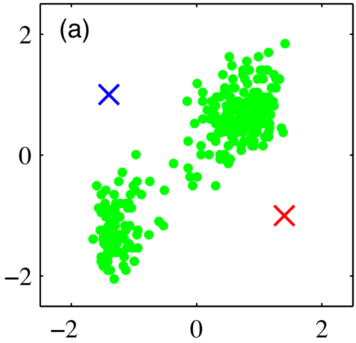
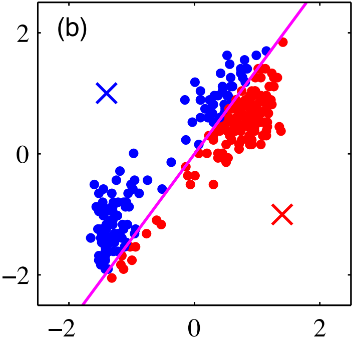
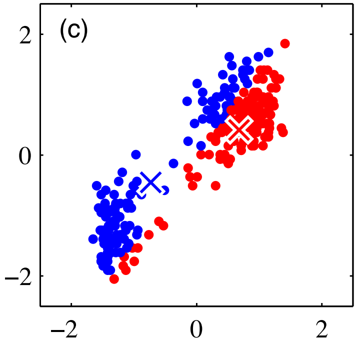
Sample run of Lloyd's algorithm



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



Iteration 1
Optimize assignments $\phi^{(i)}$.



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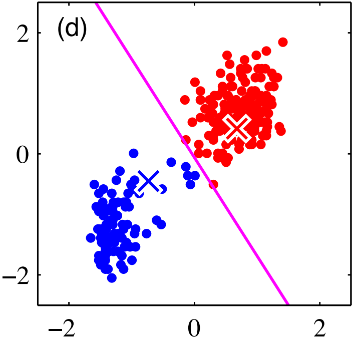
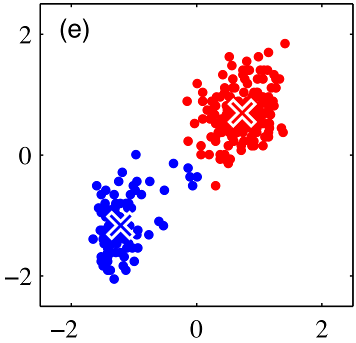


Iteration 2

Optimize assignments $\phi^{(i)}$.



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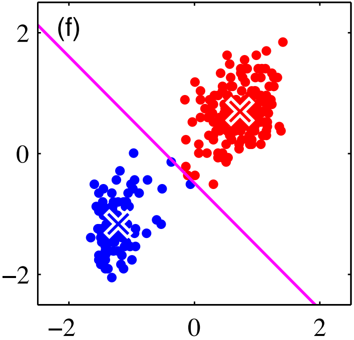
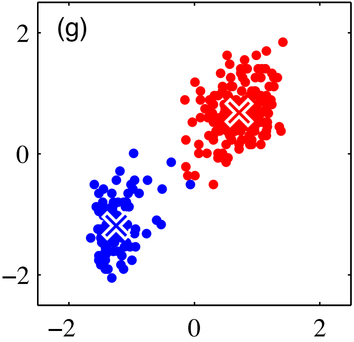


Iteration 3
Optimize assignments $\phi^{(i)}$.



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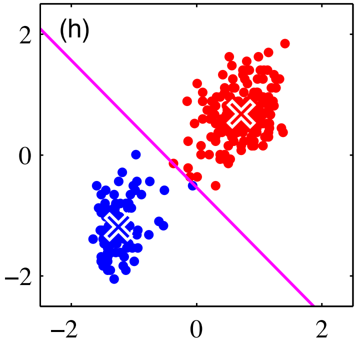

Iteration 4
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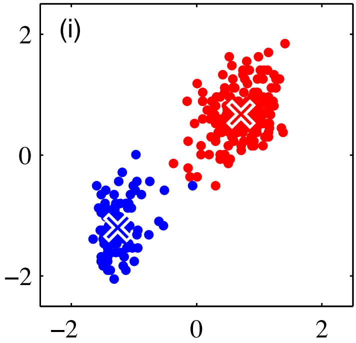

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Initializing Lloyd's algorithm

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

Farthest-first traversal

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

- Pick $\boldsymbol{c}_j \in \mathbb{R}^d$ from among $\boldsymbol{x}^{(1)}, \boldsymbol{x}^{(2)}, \dots, \boldsymbol{x}^{(n)}$ farthest from previously chosen $\boldsymbol{c}_1, \boldsymbol{c}_2, \dots, \boldsymbol{c}_{j-1}$.

  ($\boldsymbol{c}_1$ chosen arbitrarily.)

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But this can be thrown off by outliers. . .

A better idea:

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

x(i)'s distance to all previous cj (choose the minimal one!)

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

$$\Pr(\boldsymbol{c}_j = \boldsymbol{x}^{(i)}) \propto \min_{j' < j} \|\boldsymbol{x}^{(i)} - \boldsymbol{c}_{j'}\|_2^2.$$

  (Uniform distribution when $j = 1$.)

the prob of choosing xi for cj

Choosing k

- Usually by hold-out validation / cross-validation on auxiliary task (e.g., supervised learning task).

CHOOSING k

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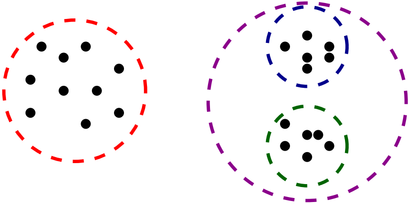
- *Heuristic*: Find large gap between $k-1$-means cost and k-means cost.

Clustering at multiple scales



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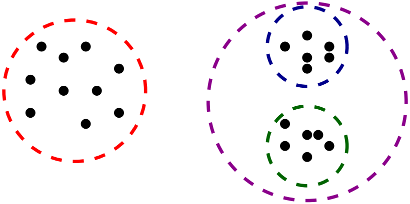

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Hierarchical clustering: encode clusterings for all values of k in a tree.

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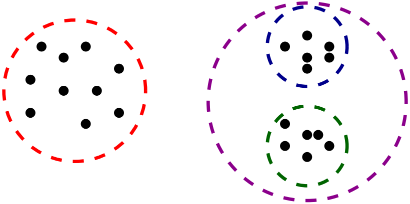

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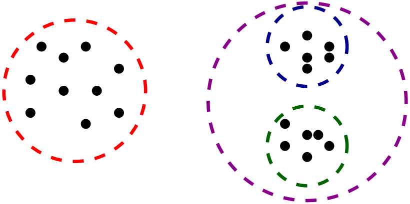

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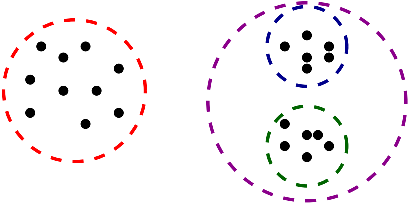

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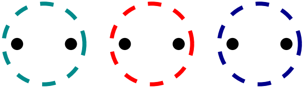
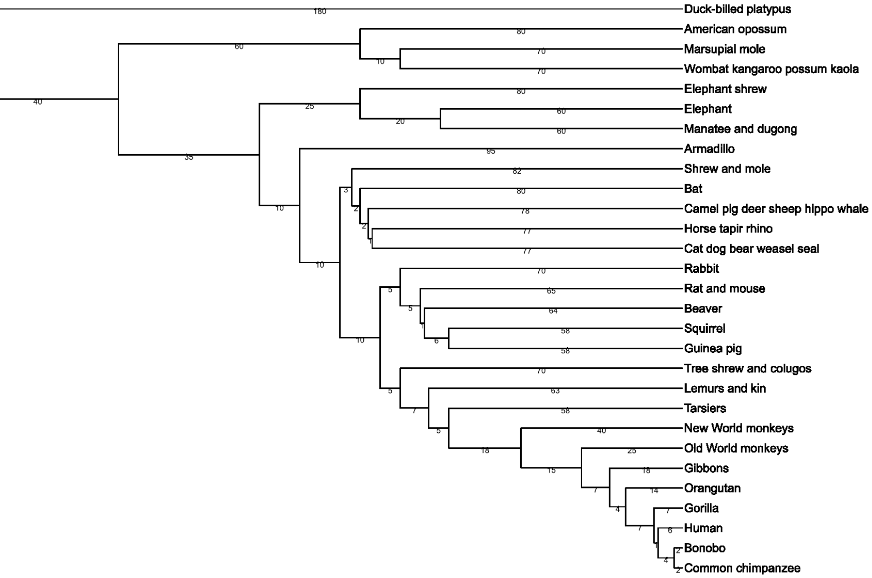


Example: phylogenetic tree



Divisive (top-down) clustering

- Partition data into two groups (e.g., via k-means clustering with $k = 2$).
- Recurse on each part.

Hierarchical clustering

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Agglomerative (bottom-up) clustering

- Start with every point $\boldsymbol{x}^{(i)}$ in its own cluster.
- Repeatedly merge "closest" pair of clusters.

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aggregate!!!

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 $\tilde{C}$).

Dictionary learning (a.k.a. sparse coding)

Dictionary learning

Goal: Find representatives $\boldsymbol{c}_1, \boldsymbol{c}_2, \ldots, \boldsymbol{c}_k \in \mathbb{R}^d$ such that each $\boldsymbol{x}^{(i)}$ is "well-represented" by a linear combination of $\leq s$ such representatives $\boldsymbol{c}_j$.

Special case: $s = 1 \implies$ clustering/quantization.

Generalizing k-means

k-means objective

$$\min_{\boldsymbol{C},\boldsymbol{\Phi}} \sum_{i=1}^{n} \left\| \boldsymbol{x}^{(i)} - \boldsymbol{C}\boldsymbol{\phi}^{(i)} \right\|_2^2$$

- $\boldsymbol{\Phi} = [\boldsymbol{\phi}^{(1)}|\boldsymbol{\phi}^{(2)}|\cdots|\boldsymbol{\phi}^{(n)}] \in \{0,1\}^{k\times n}$ are the cluster assignments.
- $\boldsymbol{C} = [\boldsymbol{c}_1|\boldsymbol{c}_2|\cdots|\boldsymbol{c}_k] \in \mathbb{R}^{d\times k}$ are the cluster representatives.

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Lloyd's algorithm:
Initialize $\boldsymbol{C}$ somehow. Then repeat:

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Generalization

Permit each $\boldsymbol{\phi}^{(i)}$ to have up to s non-zero entries (not necessarily equal to 1)

Common dictionary learning objective

$$\min_{\boldsymbol{C},\boldsymbol{\Phi}} \sum_{i=1}^{n} \left\| \boldsymbol{x}^{(i)} - \boldsymbol{C}\boldsymbol{\phi}^{(i)} \right\|_2^2.$$

Generalization of Lloyd's algorithm:
Initialize $\boldsymbol{C}$ somehow. Then repeat:

- Holding $\boldsymbol{C}$ fixed, pick (near) optimal $\boldsymbol{\Phi}$.

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Dictionary learning

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  Ordinary least squares solution:

  $$\boldsymbol{C}^\top := (\boldsymbol{\Phi}\boldsymbol{\Phi}^\top)^{-1}\boldsymbol{\Phi}\boldsymbol{X}$$

  where i-th row of $\boldsymbol{X}$ is $\boldsymbol{x}^{(i)\top}$.

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  where i-th row of $\boldsymbol{X}$ is $\boldsymbol{x}^{(i)\top}$.

Typical initialization: random (e.g., i.i.d. $\mathcal{N}(0,1)$ entries), or D^2 sampling.

Example: mixed-membership model

Represent corpus of documents by counts of words they contain:

	doc. 1	doc. 2	doc. 3	$\cdots$
aardvark	3	7	2	$\cdots$
abacus	0	0	4	$\cdots$
abalone	0	4	0	$\cdots$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	

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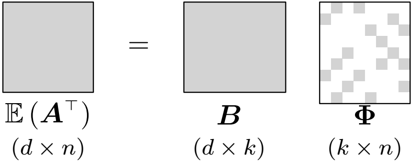
Modeling assumption:

- k "topics", each represented by a distributions over vocabulary words $\boldsymbol{\beta}_1, \boldsymbol{\beta}_2, \ldots, \boldsymbol{\beta}_k \in \mathbb{R}^d$.
- Each document i is associated with $\leq s$ topics.

  Document i's count vector is drawn from a multinomial distribution with probabilities given by $\sum_{t=1}^{k} w_t^{(i)} \boldsymbol{\beta}_t$ where $\boldsymbol{w}^{(i)}$ is a probability vector with $\leq s$ non-zero entries.

Example: mixed-membership model

In expectation:



- $\boldsymbol{\phi}_t^{(i)} = w_t^{(i)} \times$ length of document i.
- $\boldsymbol{\beta}_t = t$-th column of $\boldsymbol{B}$

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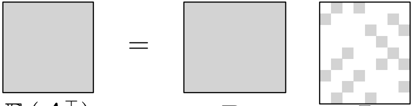

$\mathbb{E}(\boldsymbol{A}^\top)$ $(d \times n)$ $=$ $\boldsymbol{B}$ $(d \times k)$ $\boldsymbol{\Phi}$ $(k \times n)$

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Applying dictionary learning:

Identify $\boldsymbol{\beta}_1, \boldsymbol{\beta}_2, \ldots, \boldsymbol{\beta}_k$ as "representatives" $\boldsymbol{c}_1, \boldsymbol{c}_2, \ldots, \boldsymbol{c}_k \in \mathbb{R}^d$ ...

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.
- Dictionary learning/sparse coding: generalization of clustering.