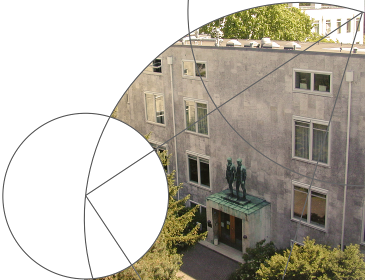
Faculty of Science

# $k$-means Clustering

## Machine Learning

Christian Igel
Department of Computer Science



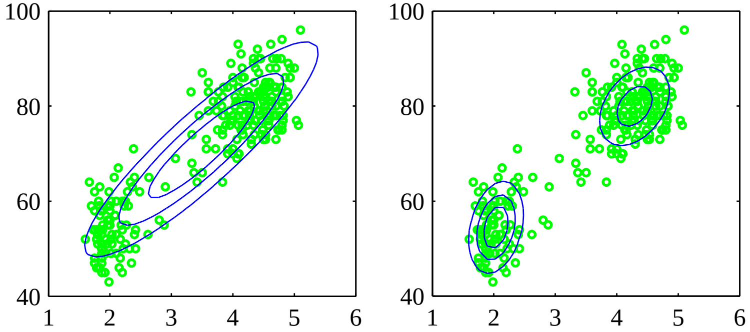
# Outline

# Outline

# Unsupervised learning

Unsupervised learning means

- learning (important aspects of) a data distribution $p$,
- finding new *representations* of data that foster learning, generalisation, and communication.

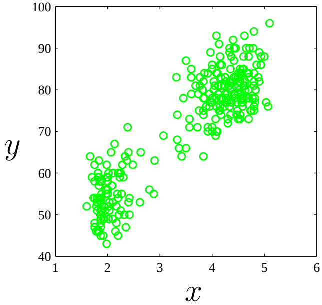


# Unsupervised learning tasks

- Density estimation
  - Creating “closed-form” compact representation of data
  - Generative modeling
  - Classification/regression
  - Outlier detection
- Clustering
  - Unsupervised classification
  - Summarization by prototypes
- Feature extraction/visualization
  - Finding sub-space with highest variance and enabling best reconstruction
  - Finding regions with high density ($k$-means).

# Example: Old Faithful

- Hydrothermal geyser in Yellowstone National Park, Wyoming, USA.




- $x$-axis duration of eruption in minutes
- $y$-axis time to next eruption in minutes

# Outline

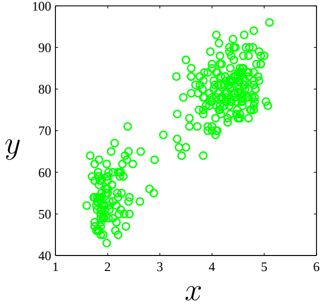
1. Unsupervised Learning
2. Clustering
3. $k$-means Clustering
4. Deriving $k$-means
5. $k$-means Clustering for Image Segmentation
6. Summary

# Clustering

- Clustering/segmentation assigns data records to clusters/groups
- Similar points should be in same cluster, dissimilar points in different clusters
- Hard clustering: every data point belongs to a single group; soft clustering: a data point can belong to more than one cluster

# Example: Old Faithful

- Hydrothermal geyser in Yellowstone National Park, Wyoming, USA.




- $x$-axis duration of eruption in minutes
- $y$-axis time to next eruption in minutes

# Outline

# $\boldsymbol{k}$-means clustering

- Data set $S = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$, $\boldsymbol{x}_i \in \mathbb{R}^n, 1 \le i \le N$
- A priori chosen number $k$ of groups
- Each group $i$ is identified by a prototype/mean vector/cluster centroid $\boldsymbol{\mu}_i \in \mathbb{R}^n$
- All records assigned to group $i$ are collected in $S_i$
- Similarity is measured by the Euclidean distance
- Objective function (distortion measure) to be minimized by finding optimal partitions $S_i$ and cluster centroids $\boldsymbol{\mu}_i$ $(i = 1, \dots, k)$:

$$J = \sum_{i=1}^{k} \sum_{\boldsymbol{x} \in S_i} \|\boldsymbol{x} - \boldsymbol{\mu}_i\|^2$$

# $k$-means outline

Goal:

$$\min_{\substack{\boldsymbol{\mu}_1,\dots,\boldsymbol{\mu}_k\\ S_1,\dots,S_k : S = \\ S_1\cup\dots\cup S_k}} \sum_{i=1}^{k}\sum_{\boldsymbol{x}\in S_i} \|\boldsymbol{x}-\boldsymbol{\mu}_i\|^2$$

Iterate:

**Data assignment:** Assign each data point to cluster represented by the most similar prototype. This leads to a new partitioning of the data.

**Centroid relocation:** Recompute cluster centroids as mean of data points assigned to respective cluster.

# $k$-means clustering algorithm

**Algorithm 1:** $k$-means clustering

**Input:** $S = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$, number of clusters $k$

**Output:** cluster centers $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_k$, partitioning of the data $S_1, \dots, S_k$

initialize class centroids $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_k$

**repeat**

$\forall i = 1, \dots, k : S'_i \leftarrow S_i$

`/* data assignment; ties are broken at random or by deterministic rule */`

$\forall i = 1, \dots, k : S_i \leftarrow \{\boldsymbol{x} \,|\, \boldsymbol{x} \in S \wedge i = \operatorname{argmin}_j \|\boldsymbol{\mu}_j - \boldsymbol{x}\|\}$

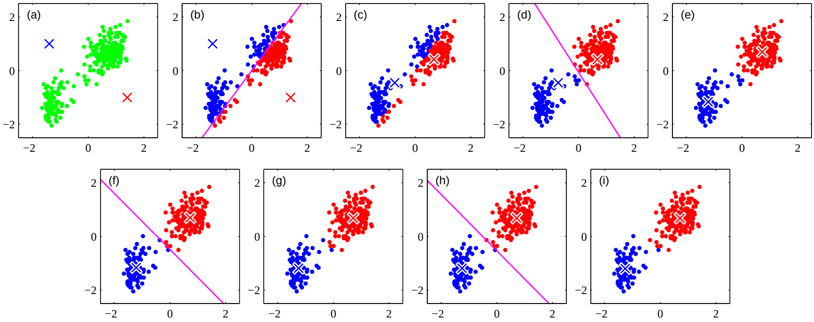
`/* centroid relocation */`

$\forall i = 1, \dots, k : \boldsymbol{\mu}_i \leftarrow \frac{1}{|S_i|} \sum_{\boldsymbol{x} \in S_i} \boldsymbol{x}$

**until** $\forall i = 1, \dots, k : S'_i = S_i$

**Result:** $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_k; S_1, \dots, S_k$

# $k$-means for Old Faithful




What are good initializations?

Noticed anything remarkable with the axes?

# Outline

# Minimization of distortion measure

Data assignment: For fixed cluster centroids, $\boldsymbol{x}$ should be assigned to nearest cluster $i$, because $\|\boldsymbol{\mu}_j - \boldsymbol{x}\| \geq \|\boldsymbol{\mu}_i - \boldsymbol{x}\|$ and thus assigning to $j$ could only increase $J$.

Centroid relocation: Let $\mu_{ij}$ and $x_j$ be the $j$th component of $\boldsymbol{\mu}_i$ and $\boldsymbol{x}$, respectively. Setting

$$\frac{\partial J}{\partial \mu_{ij}} = -2 \sum_{\boldsymbol{x} \in S_i} (x_j - \mu_{ij})$$

to zero gives

$$\boldsymbol{\mu}_i = \frac{1}{|S_i|} \sum_{\boldsymbol{x} \in S_i} \boldsymbol{x} \ .$$

Thus, cluster means minimize $J$ with fixed partitioning.

# Stopping criterion

For simplicity, let us assume deterministic breaking of ties.

Termination: Each partitioning uniquely defines cluster means. Each set of cluster means implies a particular partitioning. Thus, once the partitioning does not change after a relocation step the algorithm has converged.

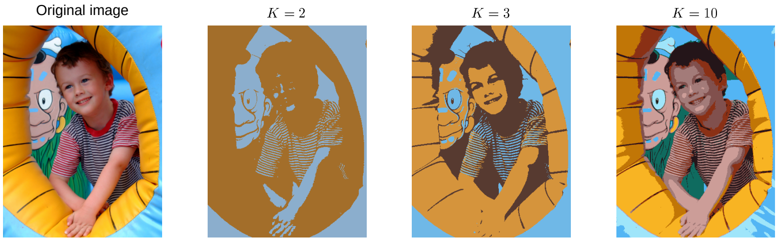
# Outline

# *k*-means for image segmentation

- Images are quite redundant.
- Many small patches are very similar.
- In the example we treat each RGB pixel as a 3D vector.
- Compression strategy: Cluster with $k$-means and transmit cluster centers (code vectors) and assignments.

Original image

# Image segmentation results



# Compression

- Compression for 8 bit accuracy and $N$ pixel image
- Original image: $3 \cdot 8 \cdot N$ bits
- Cluster means (code vectors): $3 \cdot 8 \cdot k$ bits
- Assignments: $N \cdot \log_2 k$ bits
- Ratio, $k = 2, 3, 10$: $4.2\%, 8.3\%, 16.3\%$

# Outline

# Summary and references

Clustering/segmentation:

- Clustering automatically groups data according to task-specific similarity measure
- There is neither a single "best" cluster algorithm nor a single "best" segmentation

$k$-means:

$\oplus$ Simple, still gives good results

$\oplus$ Just a single hyperparameter

$\ominus$ $k$ has to be chosen beforehand

$\ominus$ Result heavily depends on initialization

- Random data points are usually chosen as initial cluster means
- Algorithm is usually run several times in practice

Pictures from C. M. Bishop. *Pattern Recognition and Machine Learning*, Springer, 2006, sections 9.1 & 9.3.2; slides inspired by Ole Winther.