

Machine Learning for Networking

ML4N

Luca Vassio
Gabriele Ciravegna
Zhihao Wang
Tailai Song

The three components of ML



- ...
- ...
- ...

ML for supervised



- Learn to predict the label y of a data point from its features \mathbf{x}
- ML model = learn a hypothesis $h \in \mathcal{H} \quad h : \mathcal{X} \rightarrow \mathcal{Y}$
such that $h(\mathbf{x}) \approx y$
- Loss function: how to quantify/weight error between y and $h(\mathbf{x})$

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**Still valid for unsupervised ML,
with minor modifications**



Clustering

Learning goals

- **Hard** clustering and **soft** clustering
- **k-Means** method for hard clustering
- **Gaussian Mixture Models** for soft clustering
- Other clustering techniques
- How to **compare** clustering techniques

What is a Cluster?

Noun [[edit](#)]

cluster (*plural* **clusters**)

1. A **group** or **bunch** of several discrete items that are **close** to each other. [[quotations ▼](#)]

*a **cluster** of islands*

*A **cluster** of flowers grew in the pot.*

*A **leukemia** cluster has developed in the town.*

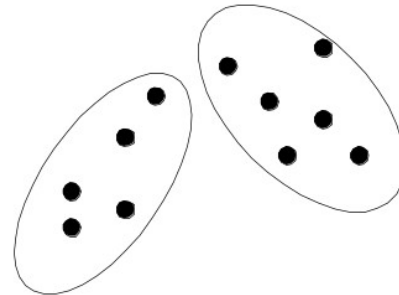
Unsupervised learning: Clustering

- Detecting **groups of similar data points**
- **Unsupervised**: no labelled data points, no ground truth to compare with, no y



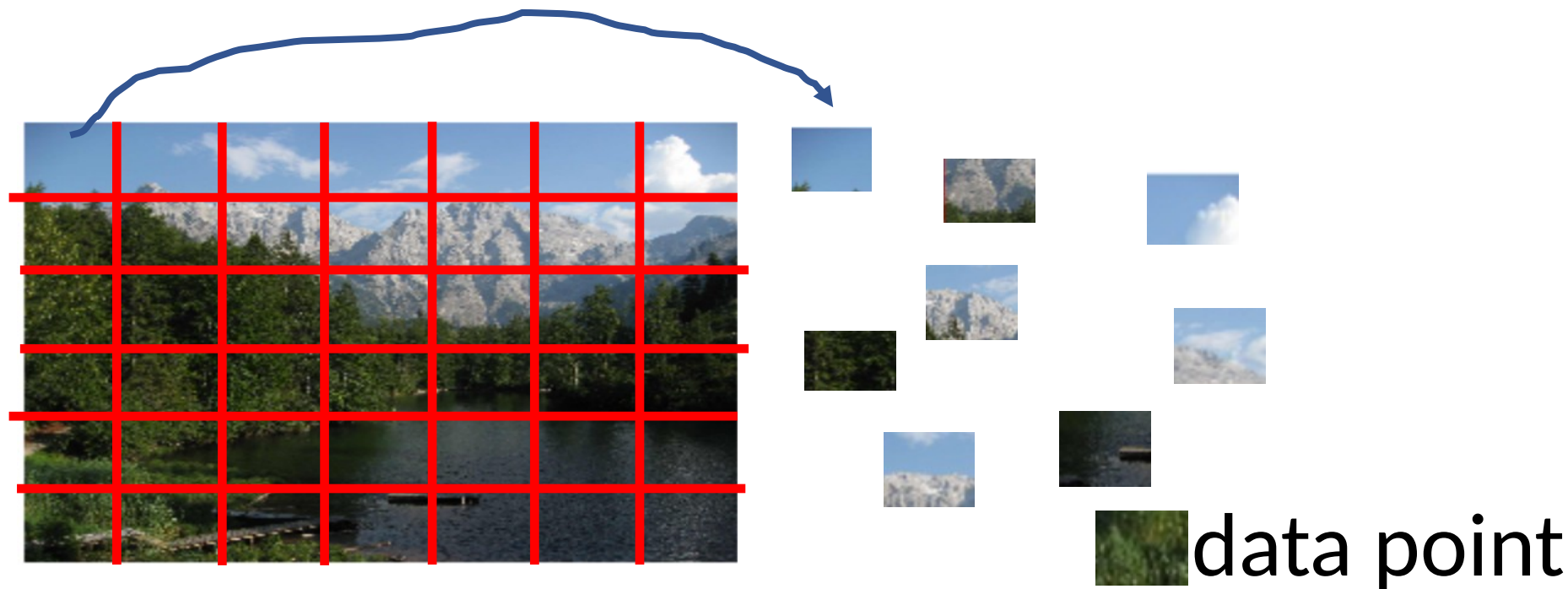
Unsupervised learning: Clustering

- A **cluster** corresponds to a **subset of data points** that are in some sense **homogeneous or similar**
- At the same time **different from** (or unrelated to) the data points in **other subsets**
- Plethora of different definitions for “homogeneous” and “similar/different”



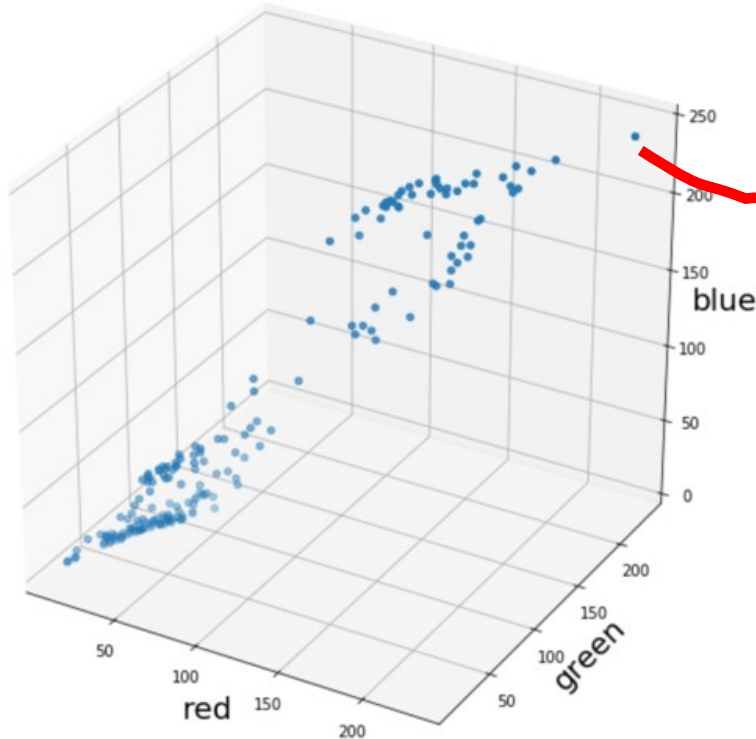
Clustering for image segmentation

- dataset=patches of an image



Clustering for image segmentation

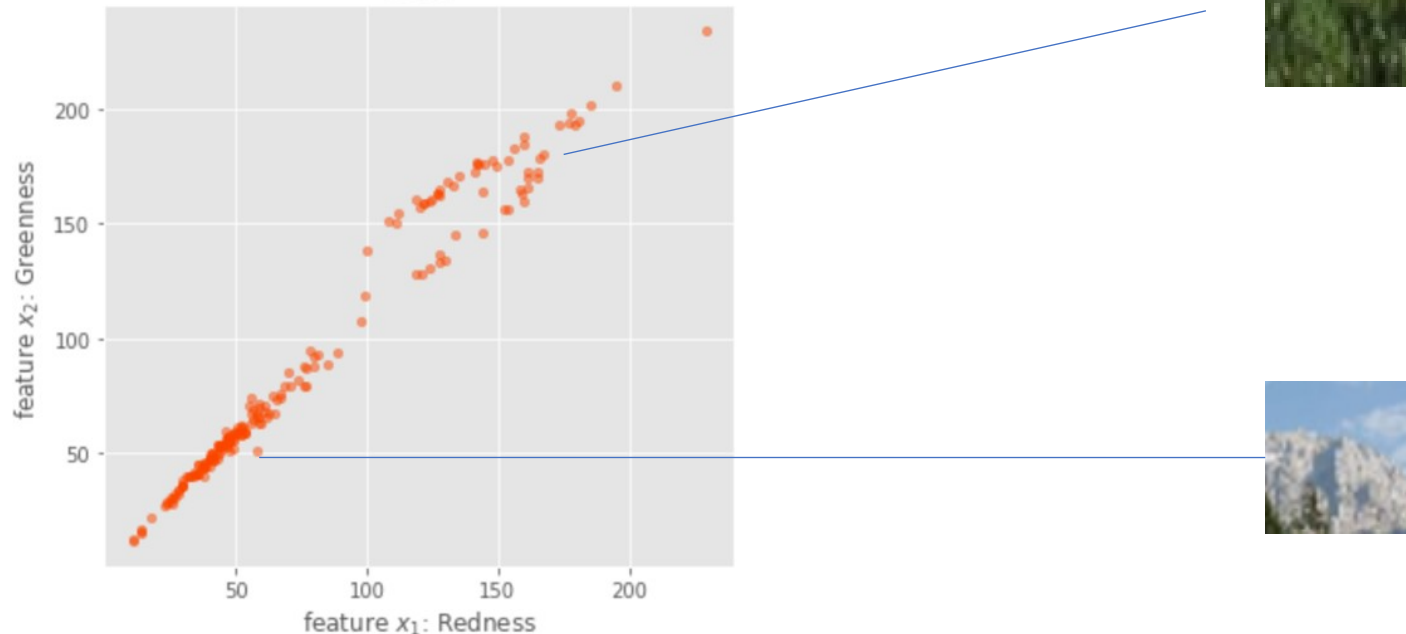
- Using three features



three features:
average red, green and blue
component

Clustering for image segmentation

- Using two features (Red+Green)

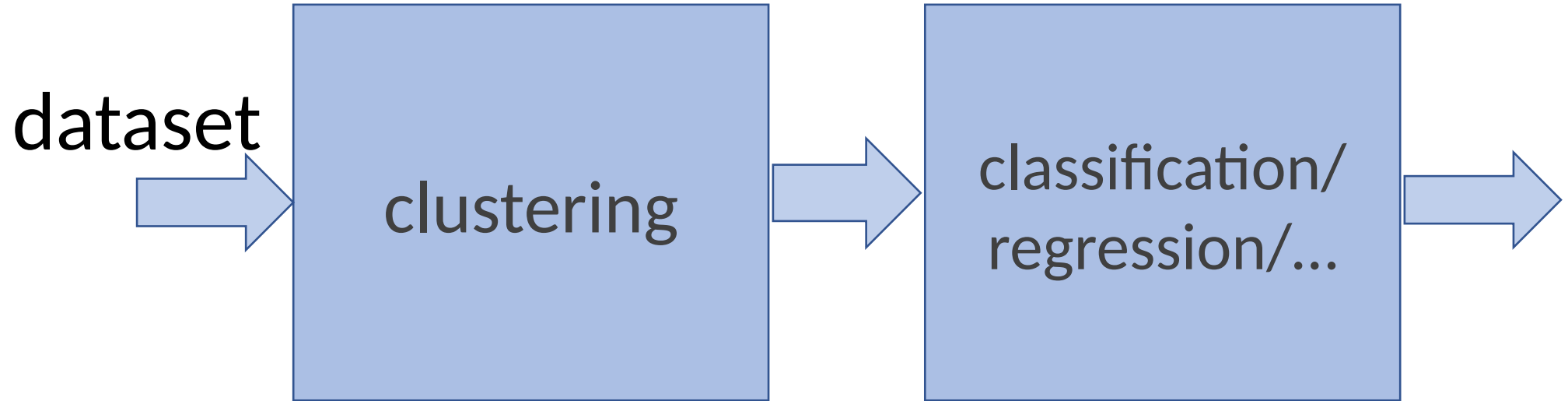


Clustering for image segmentation

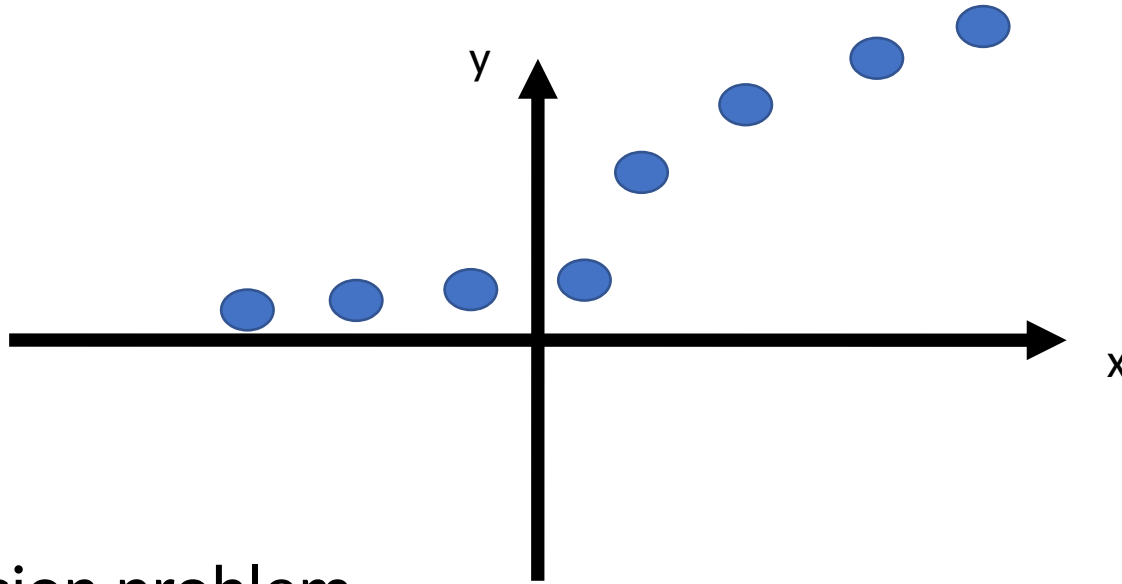
- The two clusters segment the image



Clustering as pre-processing

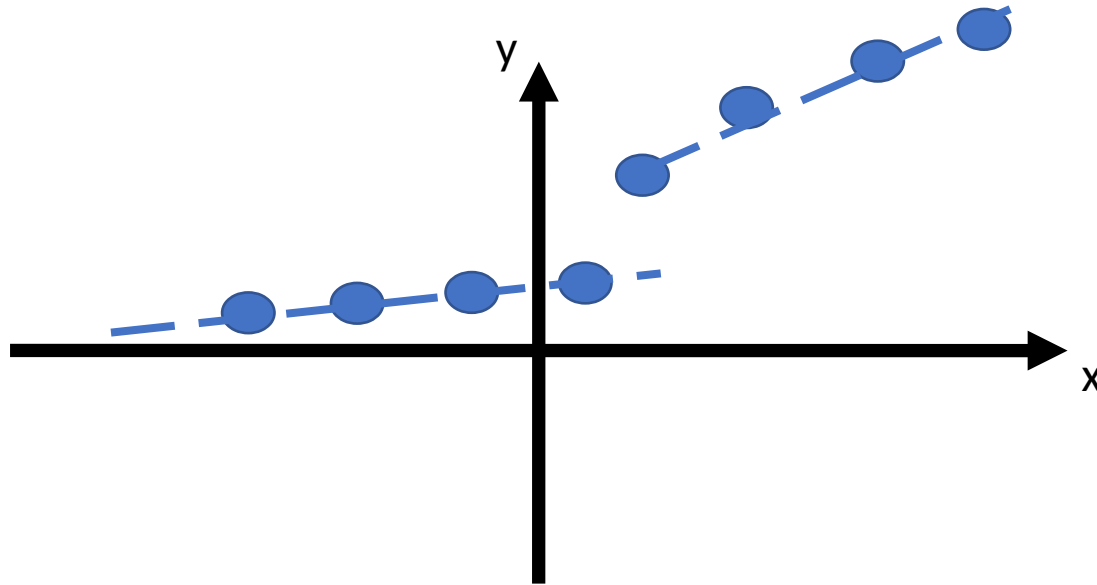


Clustering as pre-processing



- Regression problem
- Use linear regression

Clustering as pre-processing



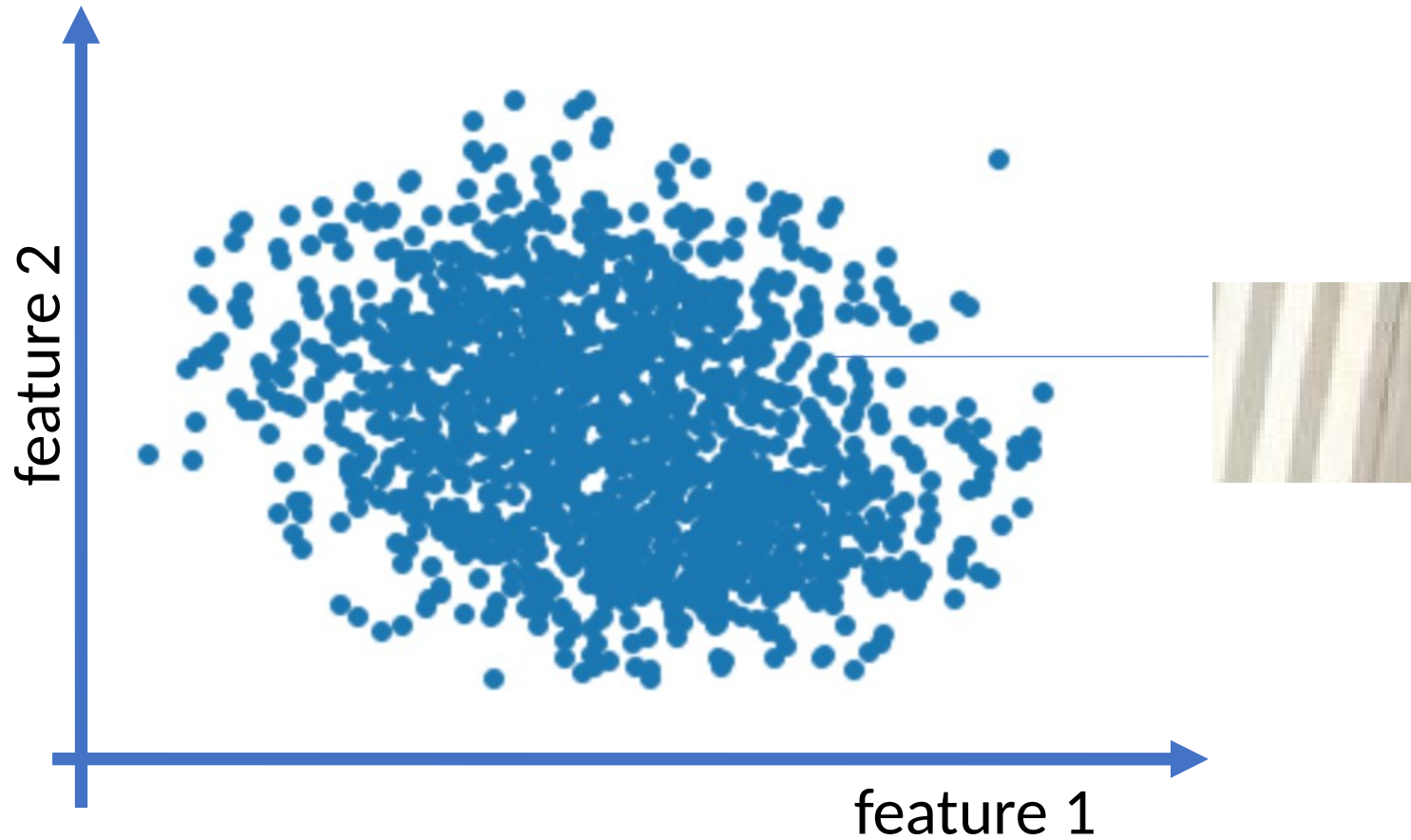
- First partition into two clusters
- Then apply linear regression separately to each cluster

Clustering for outlier detection

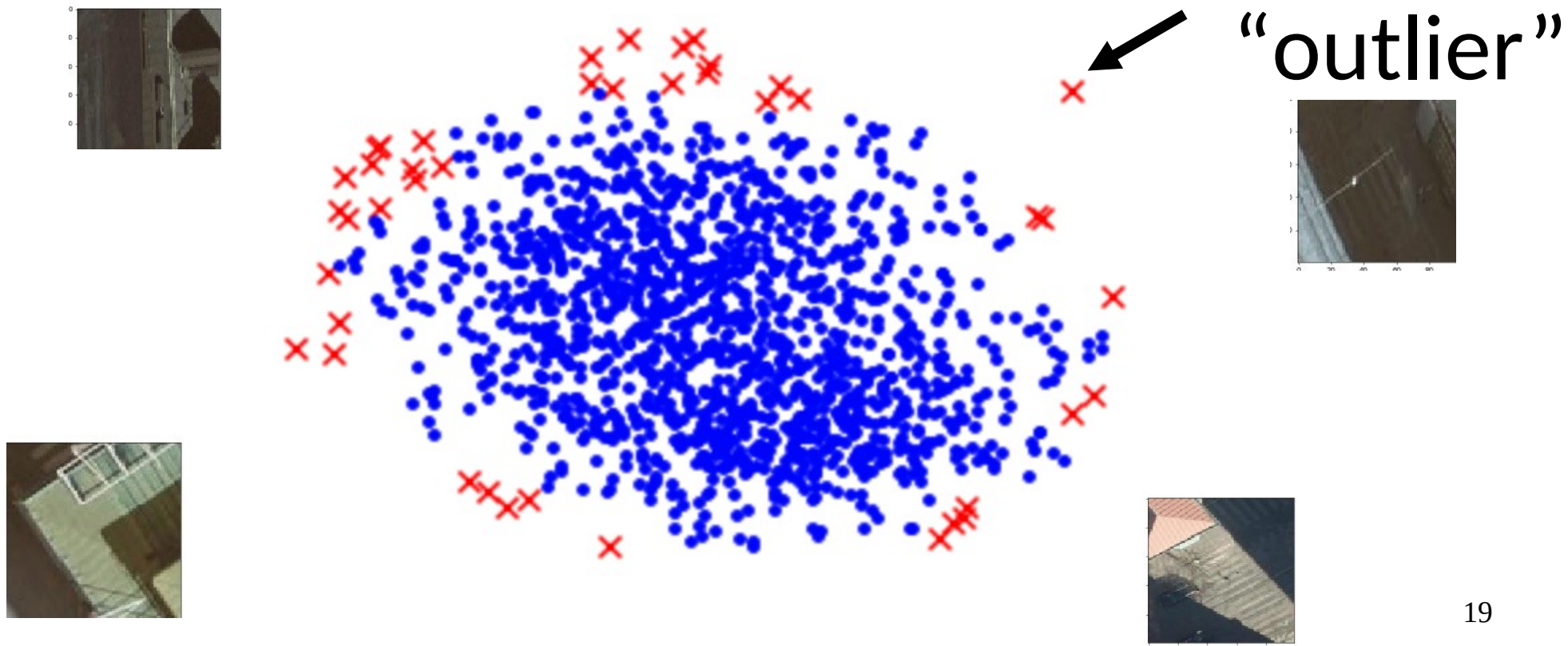
- Dataset="some images"



Clustering for outlier detection



Clustering for outlier detection



Clustering: ambiguity

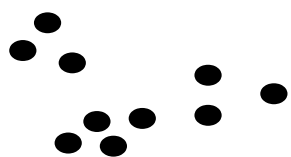
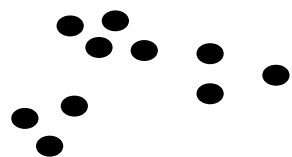
- Notion of a cluster can be ambiguous



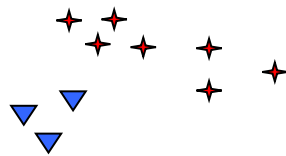
How many clusters?

Clustering: ambiguity

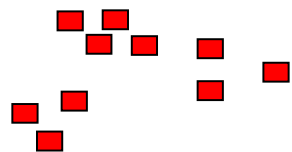
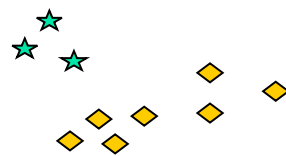
- Notion of a cluster can be ambiguous



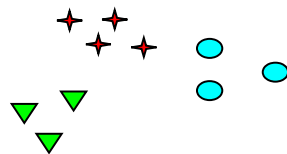
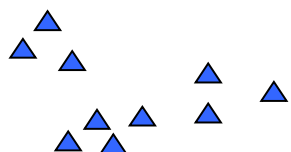
How many clusters?



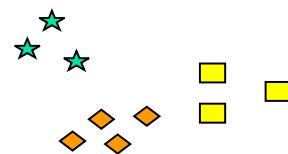
Four Clusters



Two Clusters



Six Clusters



Hard Clustering

Hard clustering

$$\mathcal{D} = \{(\mathbf{x}^{(1)}, y^{(1)}), \dots, (\mathbf{x}^{(m)}, y^{(m)})\}.$$

Data points characterized by n features

- Features of i-th data

$$\mathbf{x}^{(i)} = (x_1^{(i)}, \dots, x_n^{(i)})$$

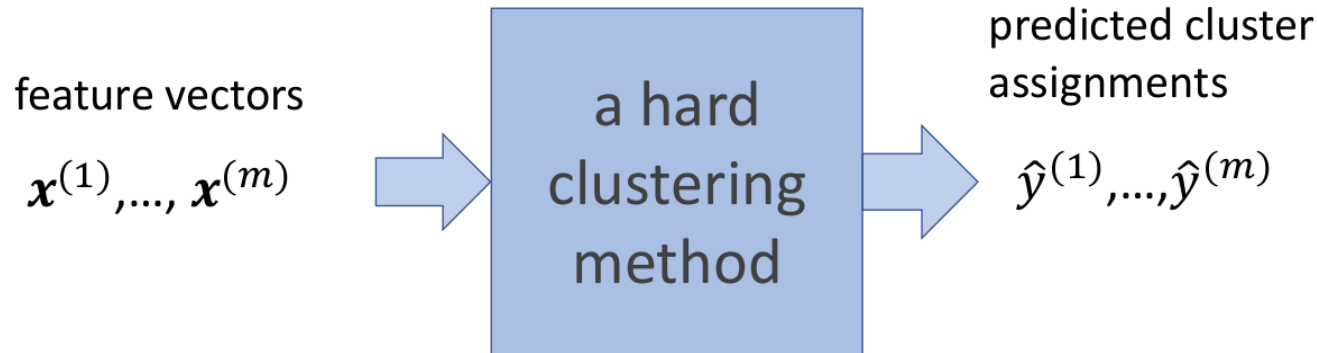
- i-th data point belongs to one of k clusters
- Cluster index of i-th datapoint is $y^{(i)} \in \{1, \dots, k\}$

Hard clustering

- Cluster index of i-th datapoint is $y^{(i)} \in \{1, \dots, k\}$
- Hard clustering methods compute predicted cluster indices $\hat{y}^{(i)}$ based solely on features $\mathbf{x}^{(i)} = (x_1^{(i)}, \dots, x_n^{(i)})$
- Does not require true cluster index $y^{(i)}$ of any data point

Hard clustering

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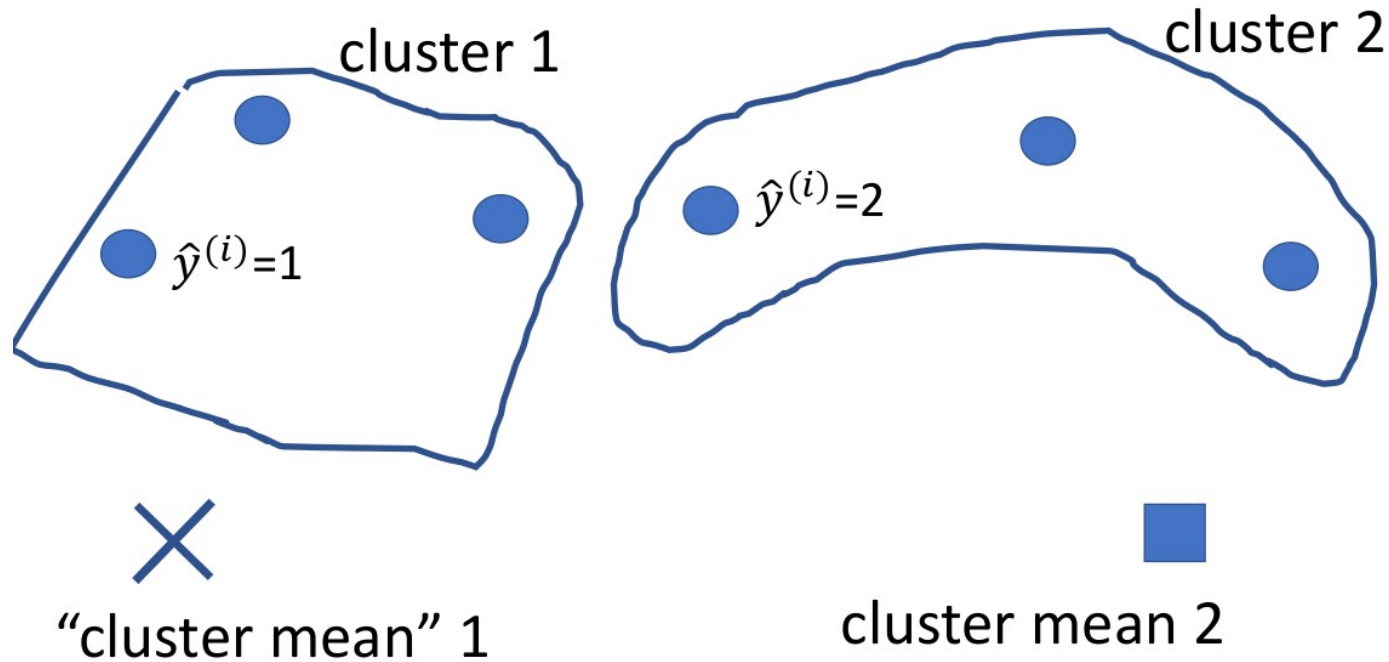


Hard Clustering with k-Means

k-Means clustering algorithm

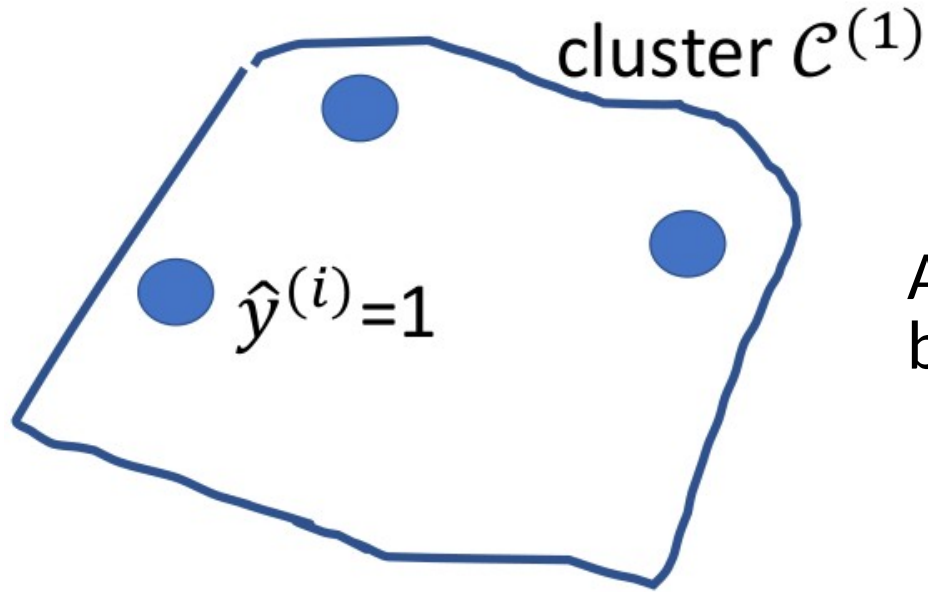
- It is characterized by one important hyperparameter: the number of clusters k
- Each cluster is associated with a point (mean or centroid)

Representing a cluster by a point



Representative point: prototype feature vector for the cluster
Let's call it "mean"

Cluster spread



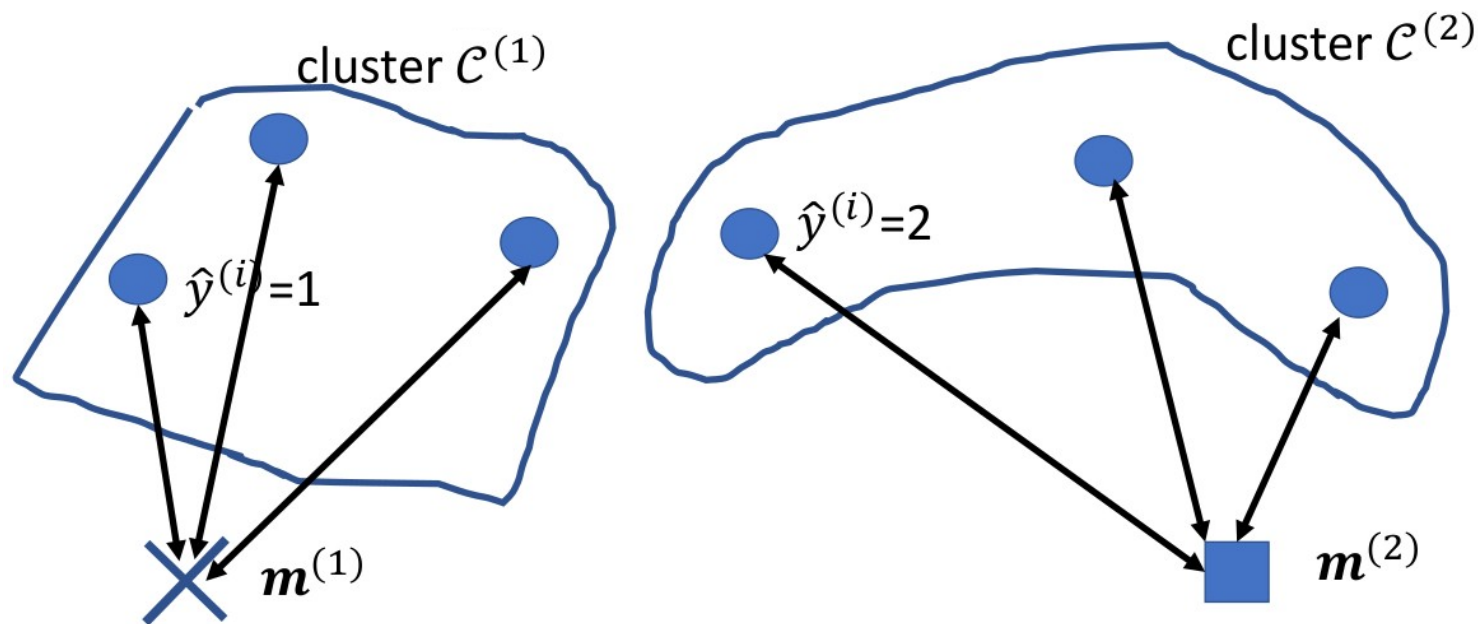
Average squared Euclidean distance between points and mean of cluster:

$$(1/|\mathcal{C}^{(1)}|) \sum_{i \in \mathcal{C}^{(1)}} \|\mathbf{m}^{(1)} - \mathbf{x}^{(i)}\|^2$$

$\times \mathbf{m}^{(1)}$

mean for $\mathcal{C}^{(1)}$

Clustering Error



$$\frac{1}{m} \sum_{c=1}^2 \sum_{i \in \mathcal{C}^{(c)}} \|\mathbf{m}^{(c)} - \mathbf{x}^{(i)}\|^2$$

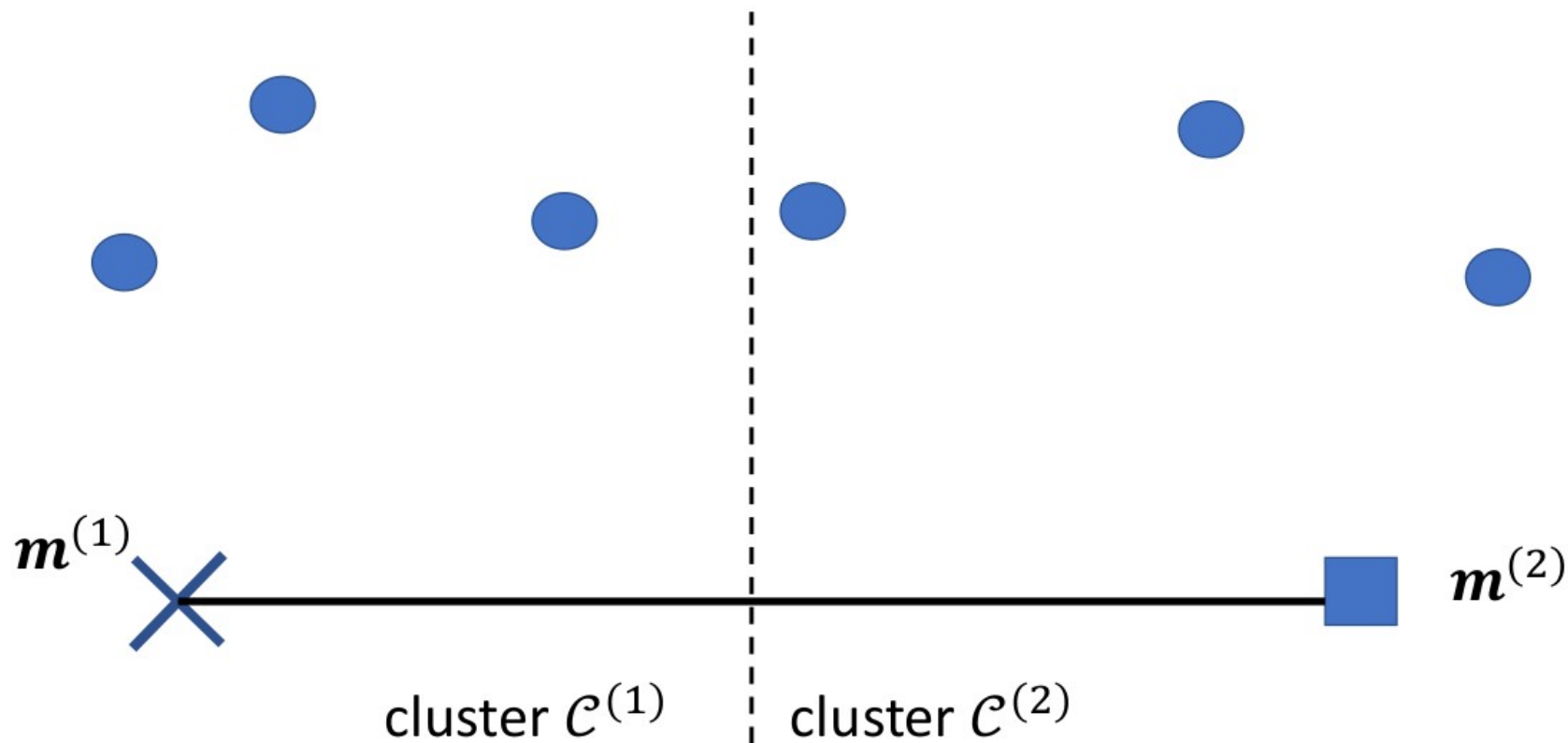
Update cluster assignments

- For given cluster means, clustering error is minimized by assigning i-th data point to cluster with **nearest cluster mean**

$$\hat{y}^{(i)} := c$$

$$\text{with } \|\mathbf{m}^{(c)} - \mathbf{x}^{(i)}\|^2 = \min_{c'=1,\dots,k} \|\mathbf{m}^{(c')} - \mathbf{x}^{(i)}\|^2$$

Update cluster assignment



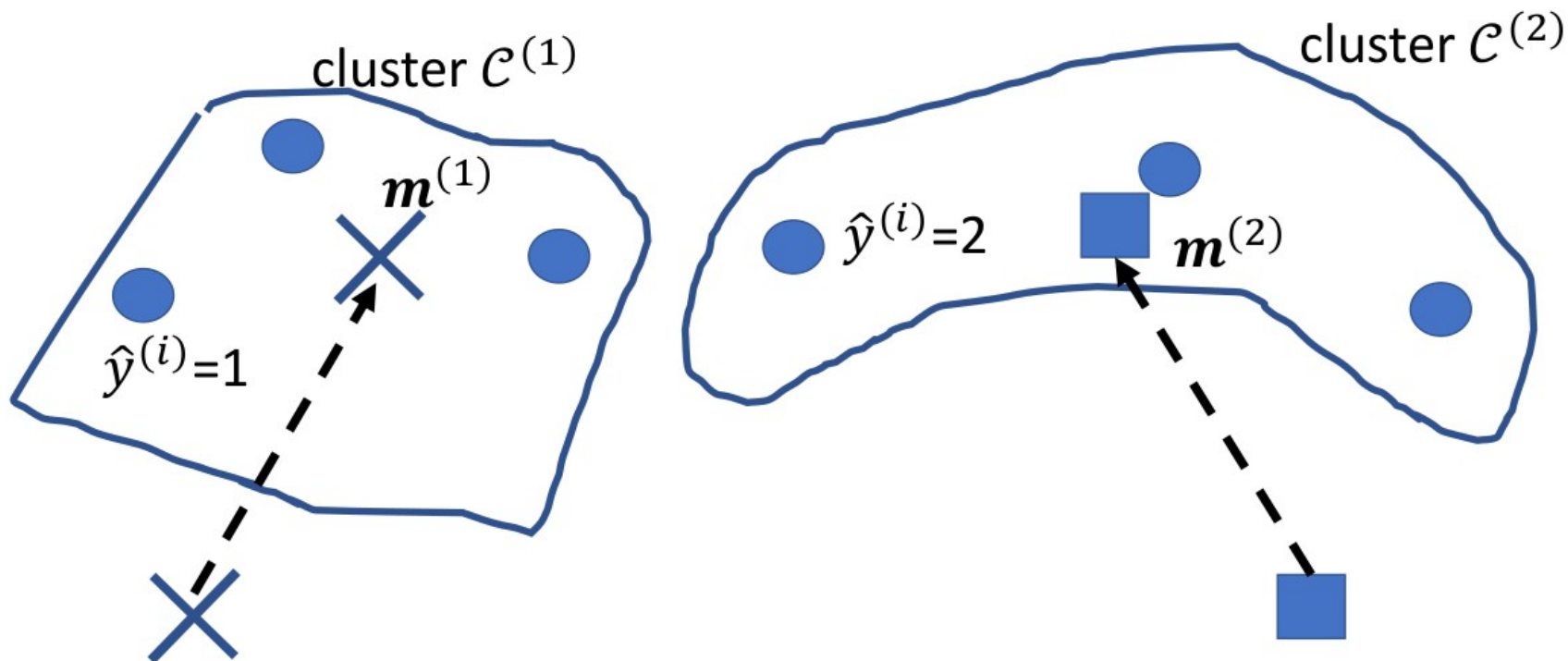
Update cluster means

- For given cluster assignments, clustering error is minimized by representing c-th cluster by the cluster mean of feature vectors of its data points

$$m^{(c)} := \frac{1}{|\mathcal{C}^{(c)}|} \sum_{i \in \mathcal{C}^{(c)}} \mathbf{x}^{(i)}$$

with cluster $\mathcal{C}^{(c)} = \{i: \hat{y}^{(i)} = c\}$

Update cluster means



Minimizing the clustering error

- Clustering error, to be minimized

$$\mathcal{E}(\{m^{(c)}\}, \{\hat{y}^{(i)}\}) := \frac{1}{m} \sum_{i=1}^m \left\| \mathbf{m}^{(\hat{y}^{(i)})} - \mathbf{x}^{(i)} \right\|^2$$

Minimizing the clustering error

- Clustering error, to be minimized

$$\varepsilon(\{m^{(c)}\}, \{\hat{y}^{(i)}\}) := \frac{1}{m} \sum_{i=1}^m \left\| \mathbf{m}^{(\hat{y}^{(i)})} - \mathbf{x}^{(i)} \right\|^2$$

- This is basically an empirical risk minimization problem

$$\hat{L}(h|\mathcal{D}) = (1/m) \sum_{i=1}^m \left\| \mathbf{x}^{(i)} - \frac{\sum_{i' \in \mathcal{D}^{(i)}} \mathbf{x}^{(i')}}{|\mathcal{D}^{(i)}|} \right\|^2 \quad \text{with } \mathcal{D}^{(i)} := \{i' : h(\mathbf{x}^{(i)}) = h(\mathbf{x}^{(i')})\}$$

Minimizing the clustering error

- Clustering error, to be minimized

$$\mathcal{E}(\{\mathbf{m}^{(c)}\}, \{\hat{\mathbf{y}}^{(i)}\}) := \frac{1}{m} \sum_{i=1}^m \left\| \mathbf{m}^{(\hat{\mathbf{y}}^{(i)})} - \mathbf{x}^{(i)} \right\|^2$$

- Simultaneously finding cluster means $\mathbf{m}^{(c)}$ and assignments $\hat{\mathbf{y}}^{(i)}$ that minimize clustering error is difficult (“NP-hard”)

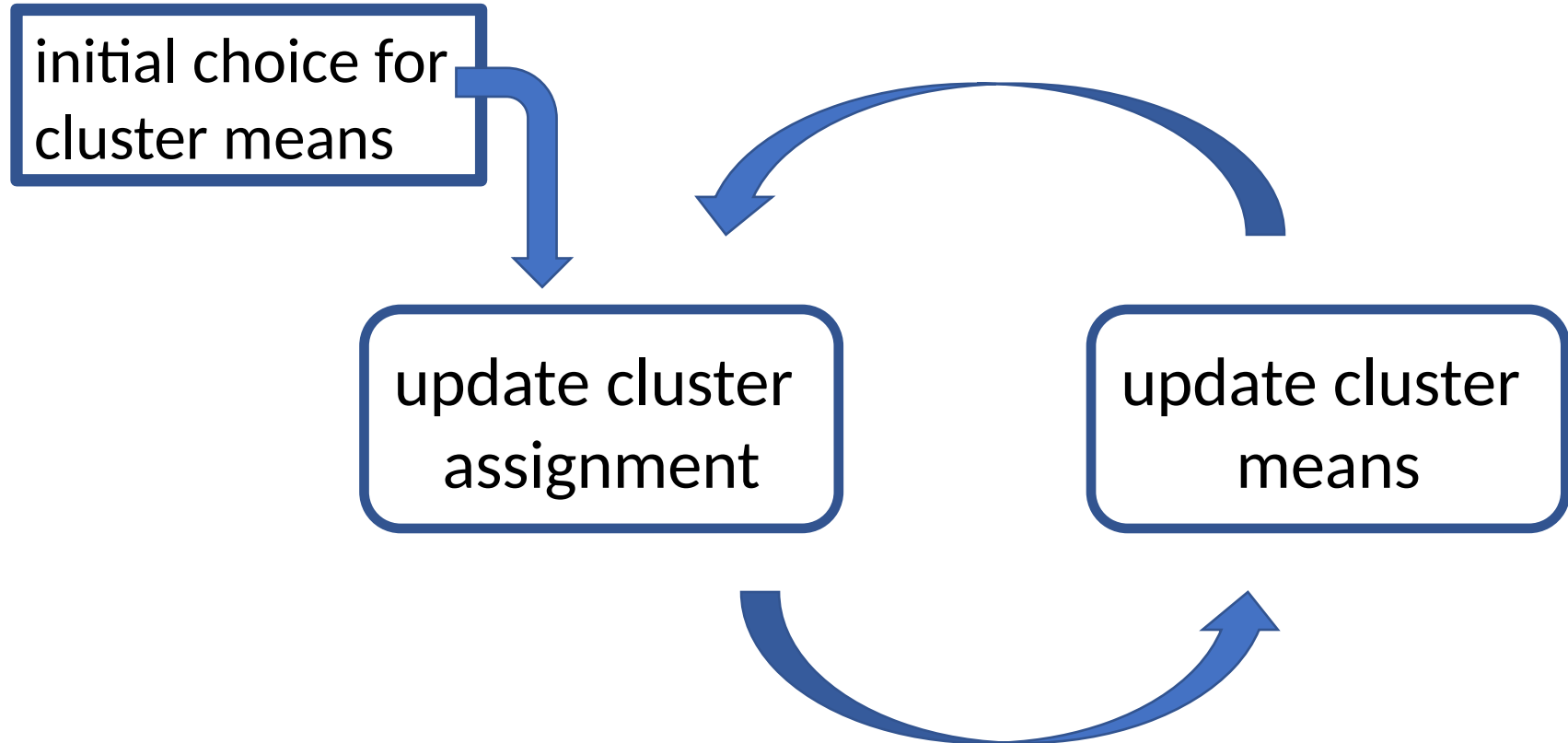
Alternating minimization

- Clustering error, to be minimized

$$\varepsilon(\{m^{(c)}\}, \{\hat{y}^{(i)}\}) := \frac{1}{m} \sum_{i=1}^m \left\| \mathbf{m}^{(\hat{y}^{(i)})} - \mathbf{x}^{(i)} \right\|^2$$

- For **given assignments**, finding cluster means that **minimize clustering error is easy**
- For **given cluster means**, finding assignments that **minimize clustering error is easy**

k-Means

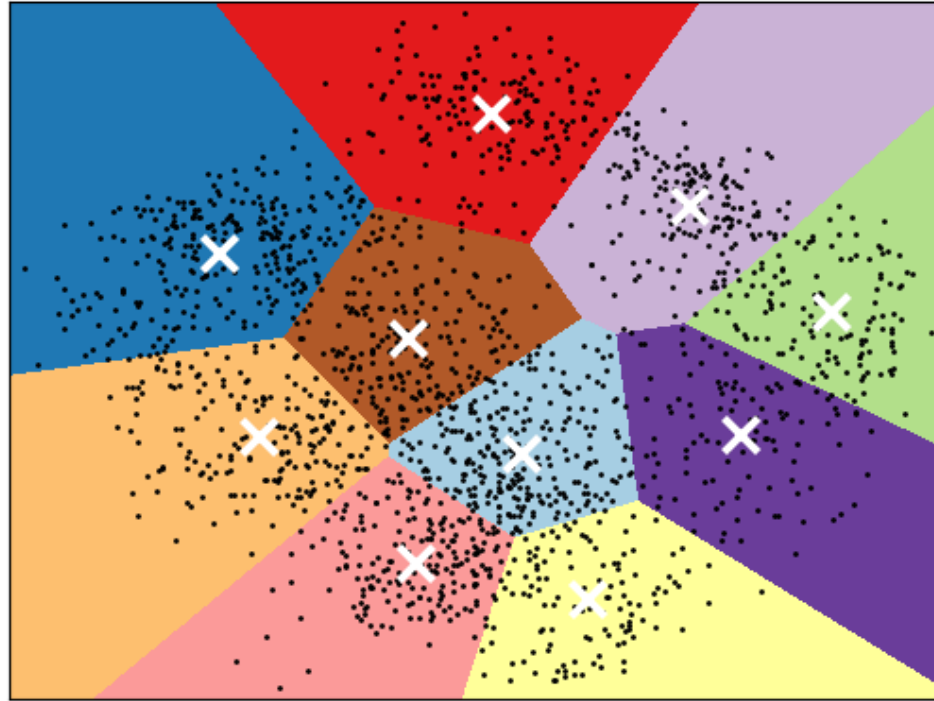


k-Means

- **Input:** number k of clusters, initial cluster means
- Step 1: update cluster assignments
- Step 2: update cluster means
- Go to Step 1 unless “Finished”
- **Output:** final cluster means

Cluster shape of k-means

K-means clustering on the digits dataset (PCA-reduced data)
Centroids are marked with white cross

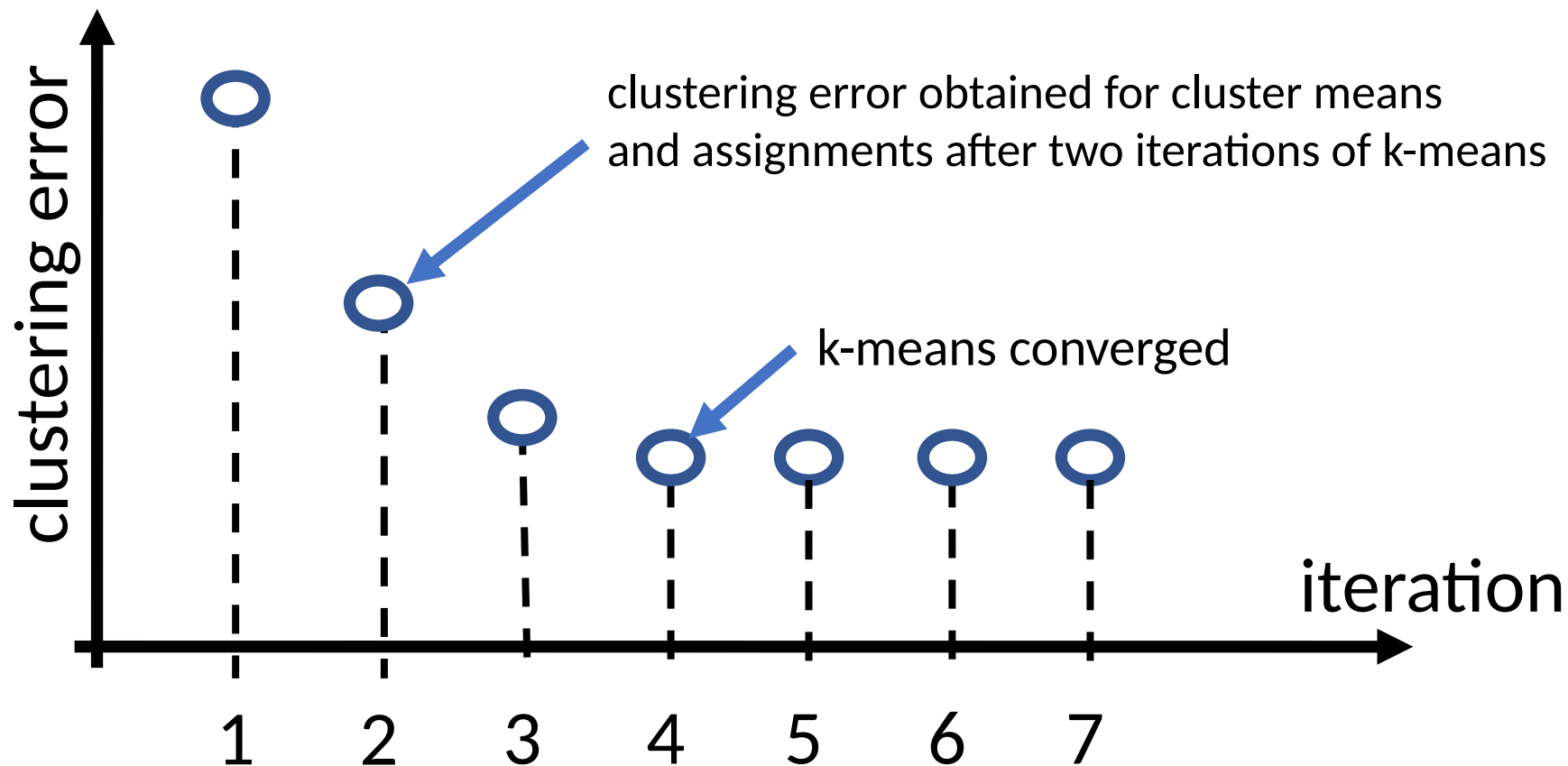


k-Means never increases clustering error

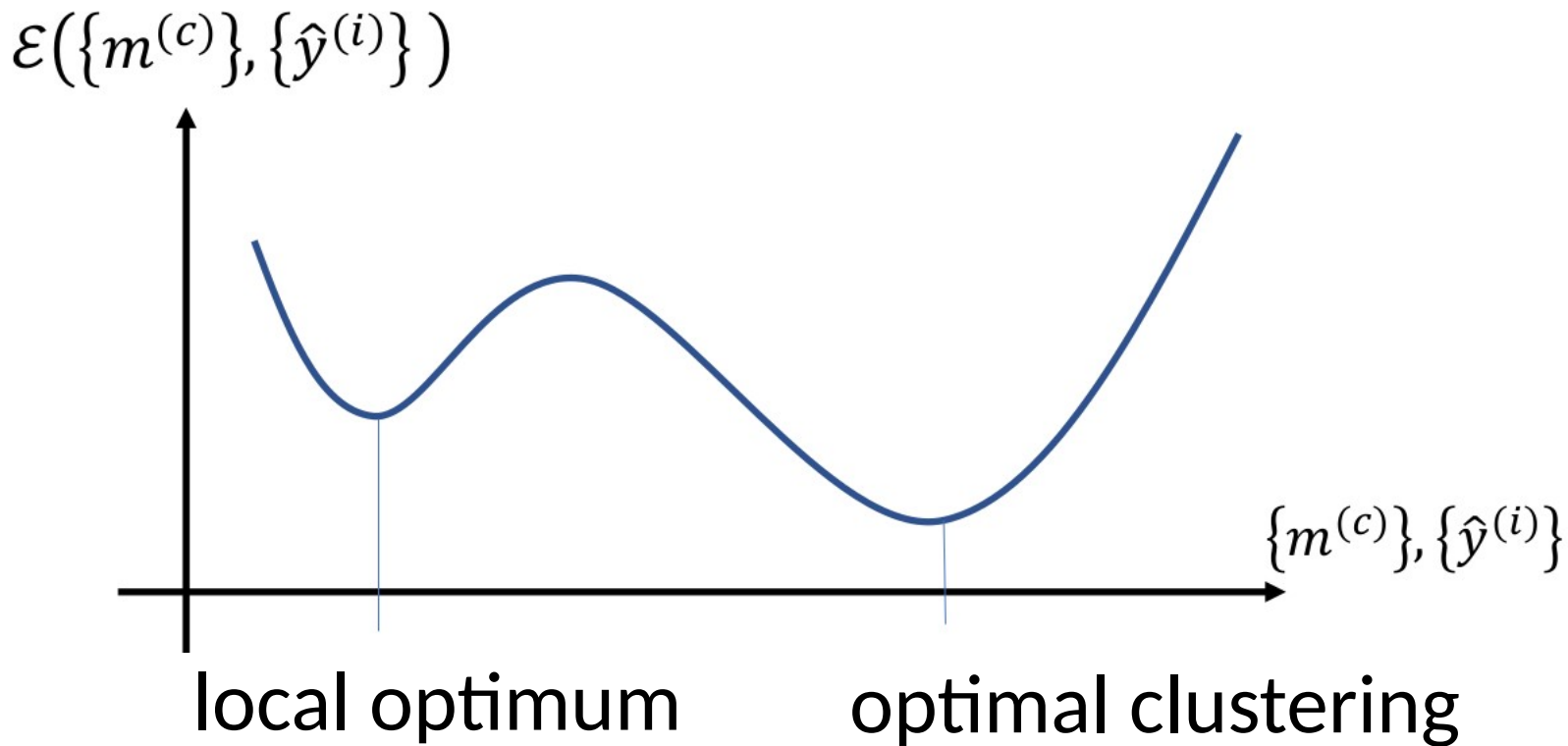
- Consider cluster means $m^{(c)}$ and assignments $\hat{y}^{(i)}$
- Run one iteration of k-Means
- Results in new cluster means $\tilde{m}^{(c)}$ and assignments $\tilde{y}^{(i)}$

$$\mathcal{E}(\{\tilde{m}^{(c)}\}, \{\tilde{y}^{(i)}\}) \leq \mathcal{E}(\{m^{(c)}\}, \{\hat{y}^{(i)}\})$$

k-Means as iterative optimization method



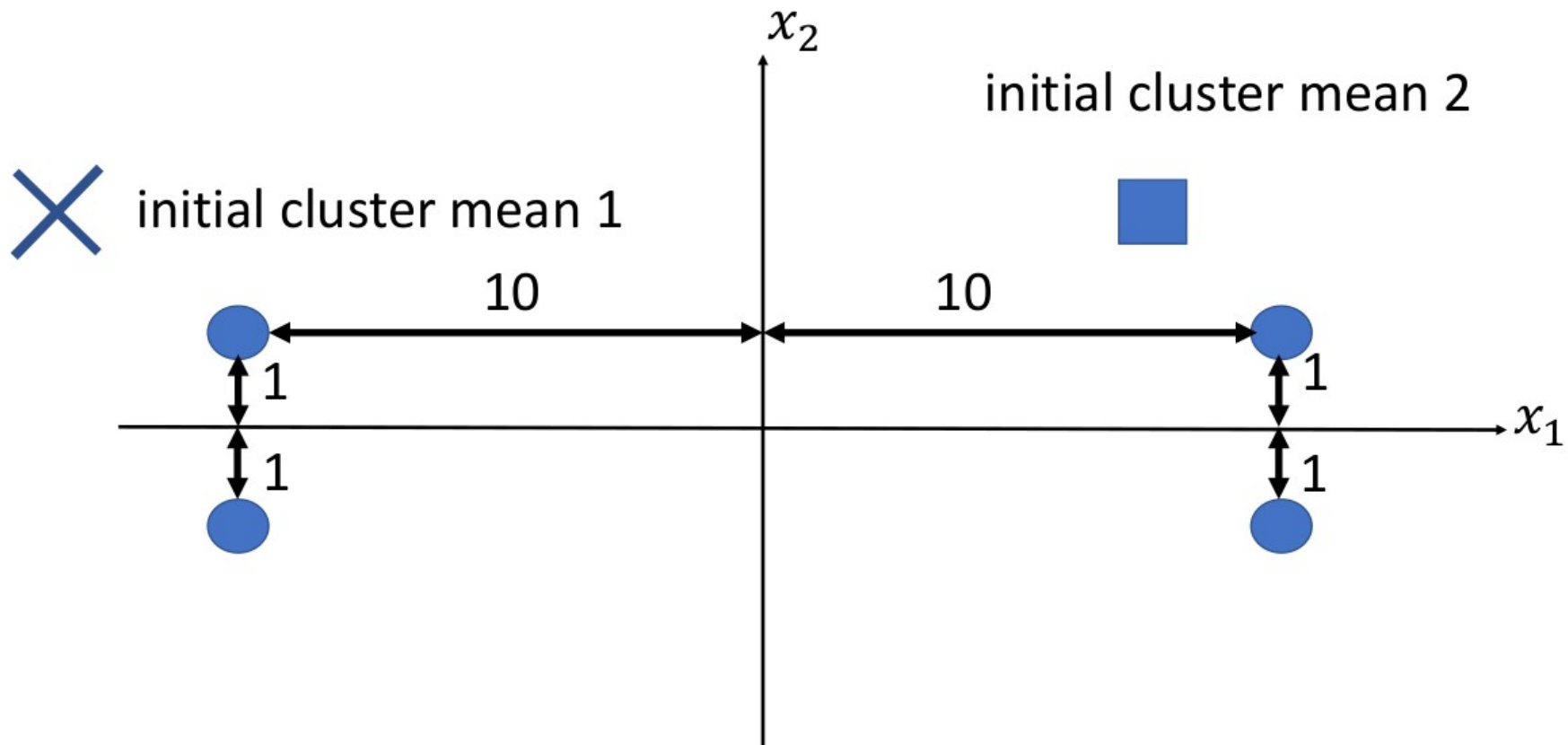
Non-convexity of clustering error



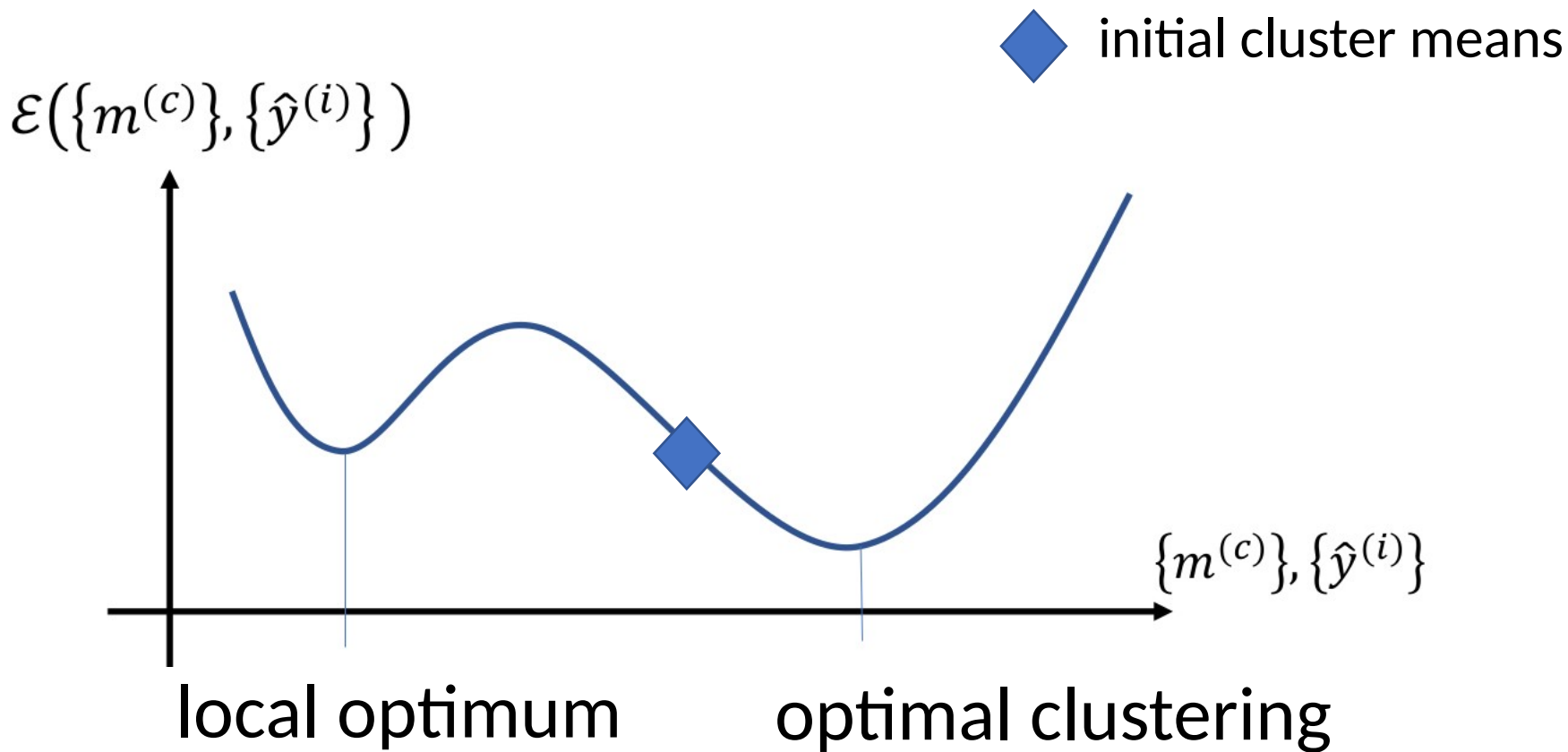
Initialization is crucial

- k-Means requires initial cluster means as inputs
- k-Means result depends crucially on initial means
- **Repeat k-Means several times with different initializations**

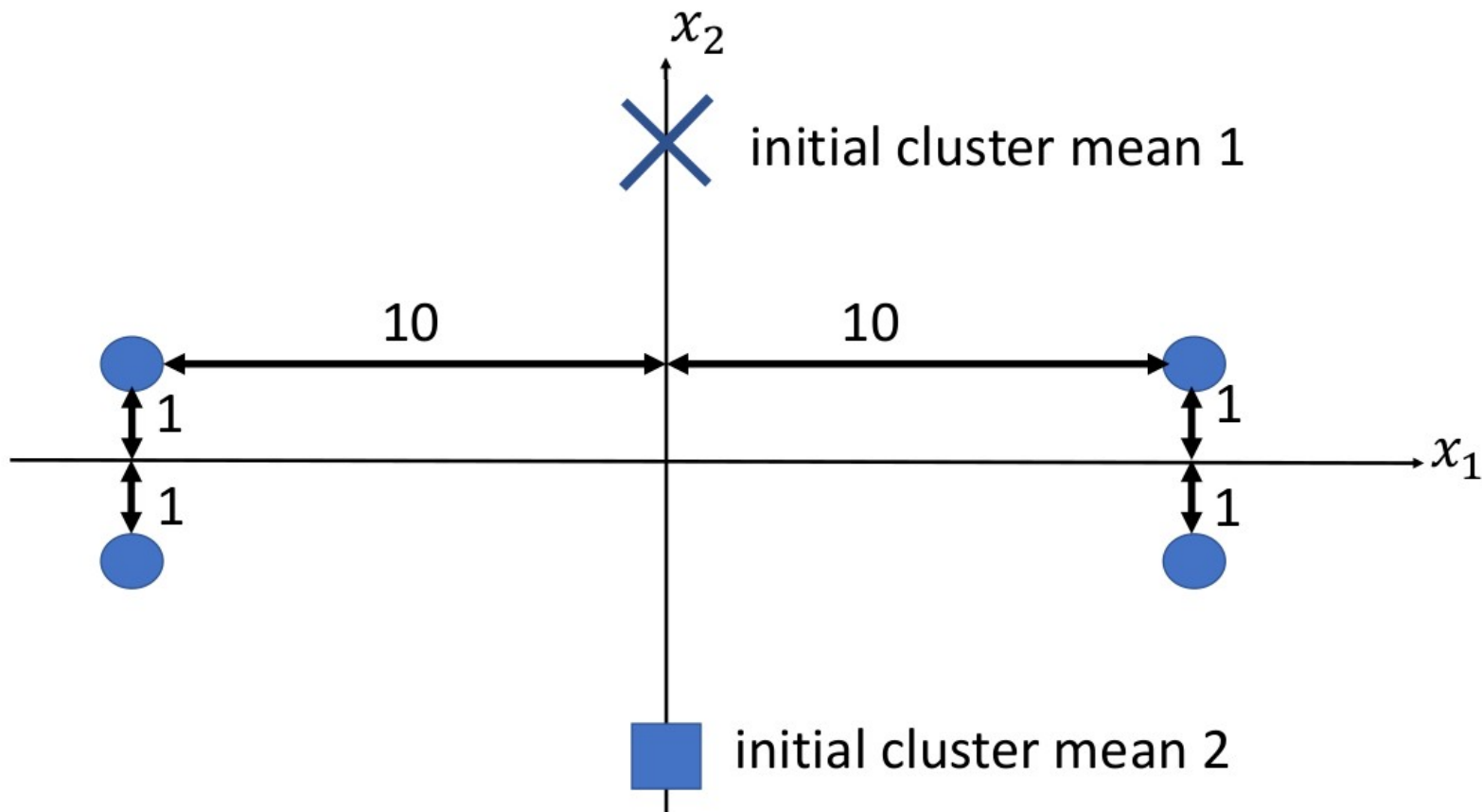
Good initialization



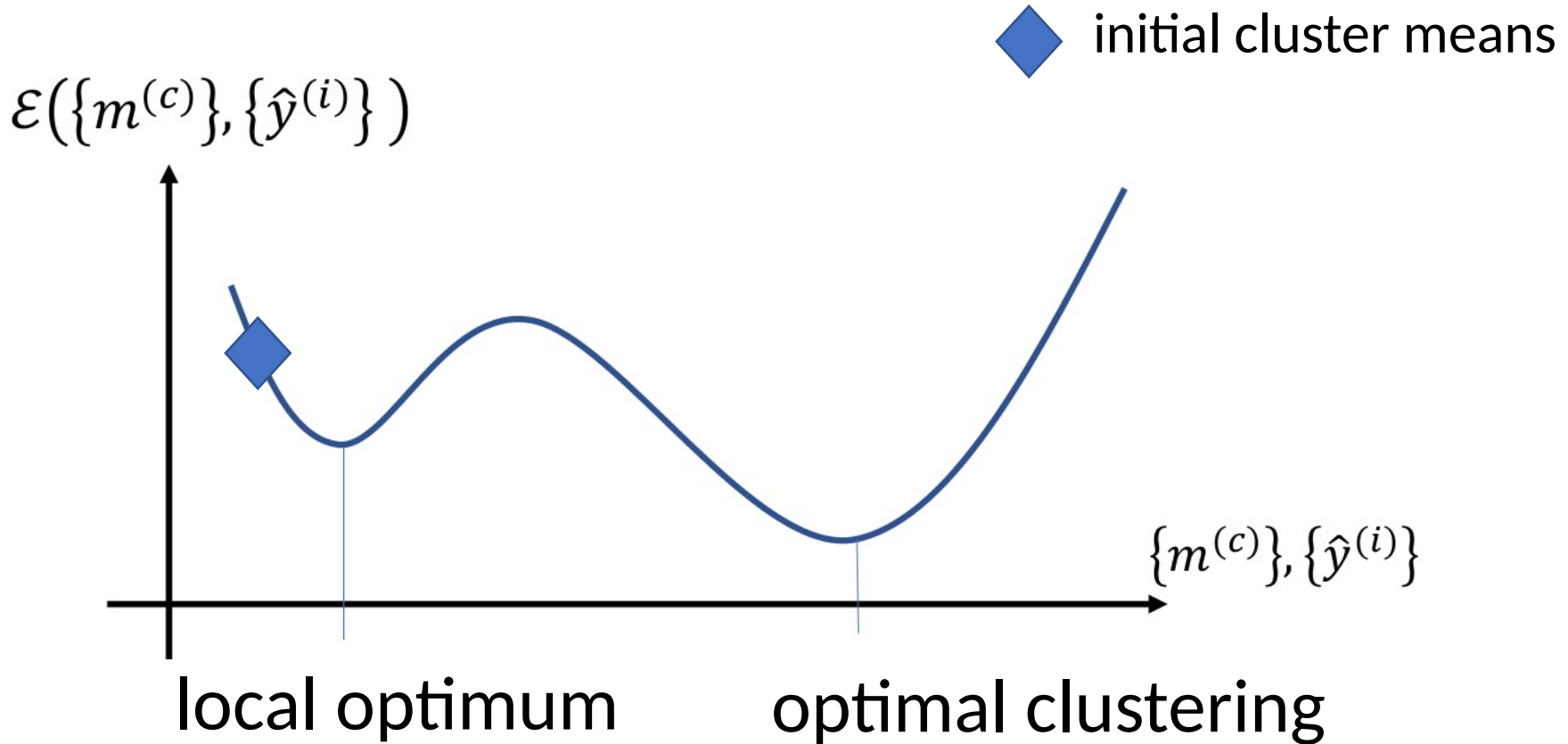
Good initialization



Bad initialization

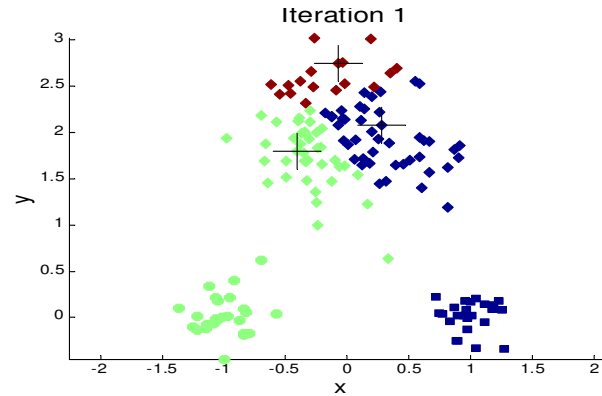


Bad initialization

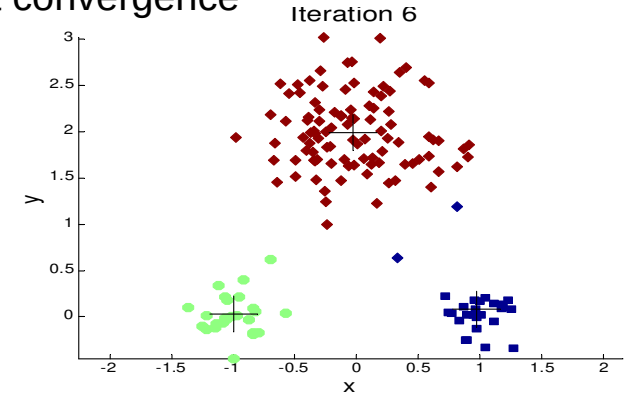


Good vs. bad initializations

- Case 1:

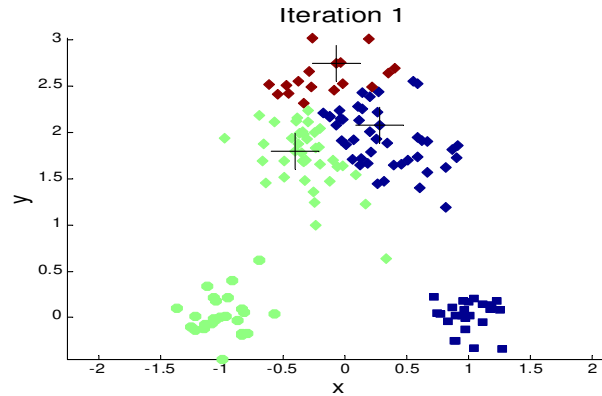


At convergence

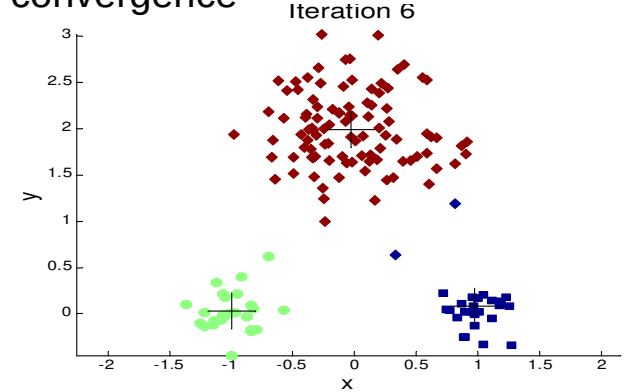


Good vs. bad initializations

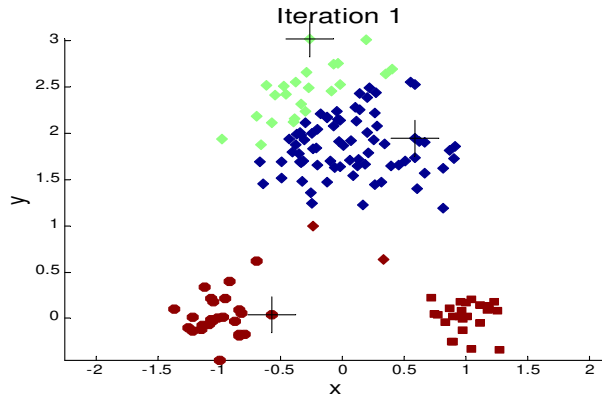
- Case 1:



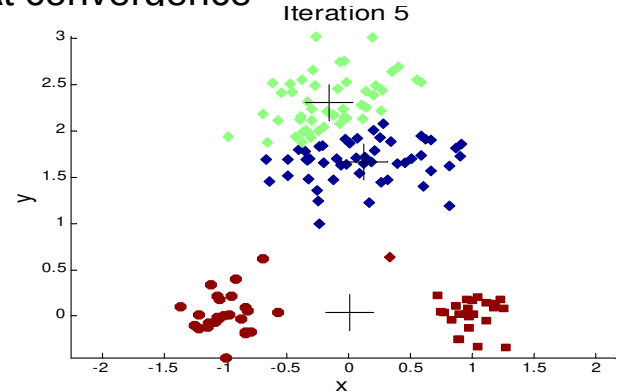
At convergence



- Case 2:



At convergence



How to choose number k of clusters?

- Increasing k will decrease error (up to 0 when $k=m$)
- Hence:
 - Defined by application (as in image segmentation)
 - Desired compression rate
 - Elbow (or knee) method
 - Validation error

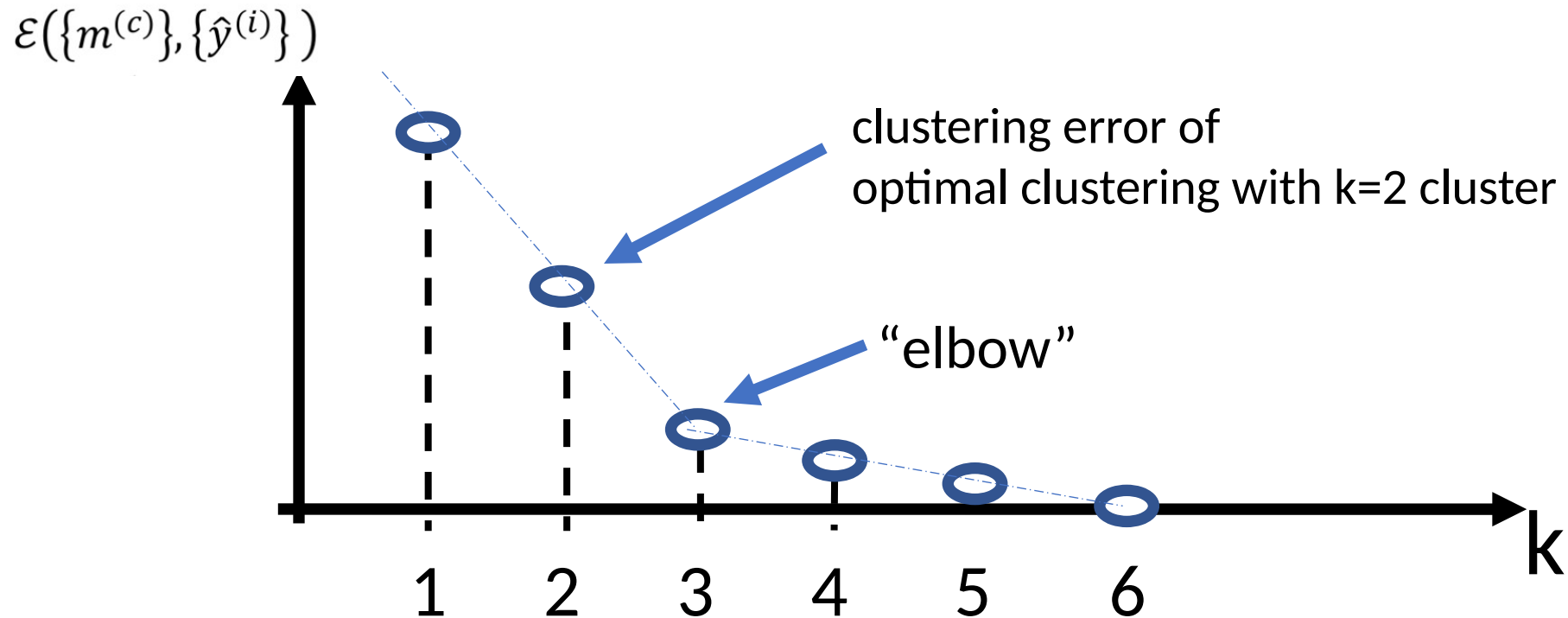
How to choose number k of clusters?

- For background segmentation $k=2$
- Cluster 1 = Background, Cluster 2=Foreground



Elbow method

- The gain from adding a cluster becomes negligible

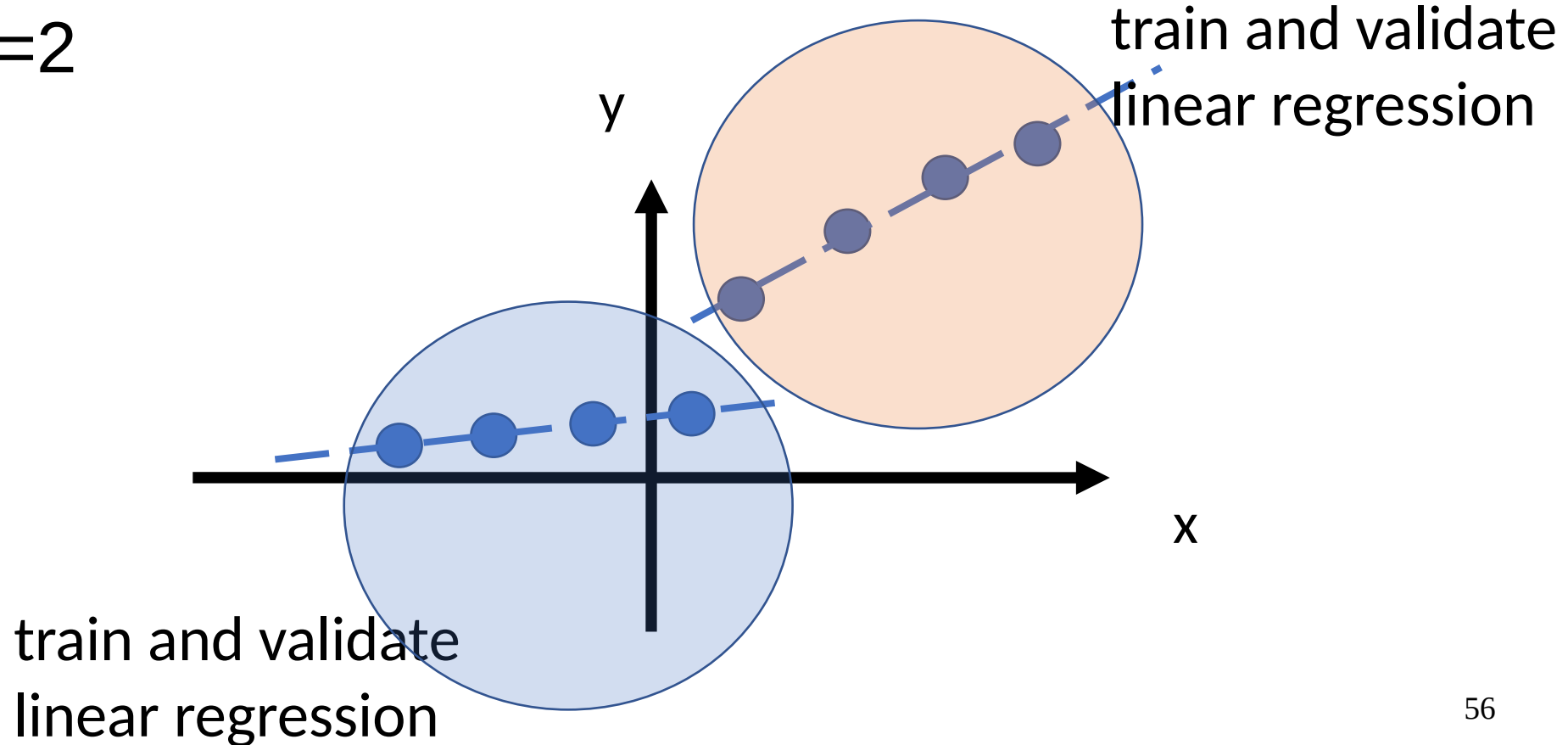


Choose k by validation error

- Clustering can be used as pre-processing for follow-up supervised (regression or classification) problem
- Try different values of k and pick the one resulting in smallest validation error in the supervised problem

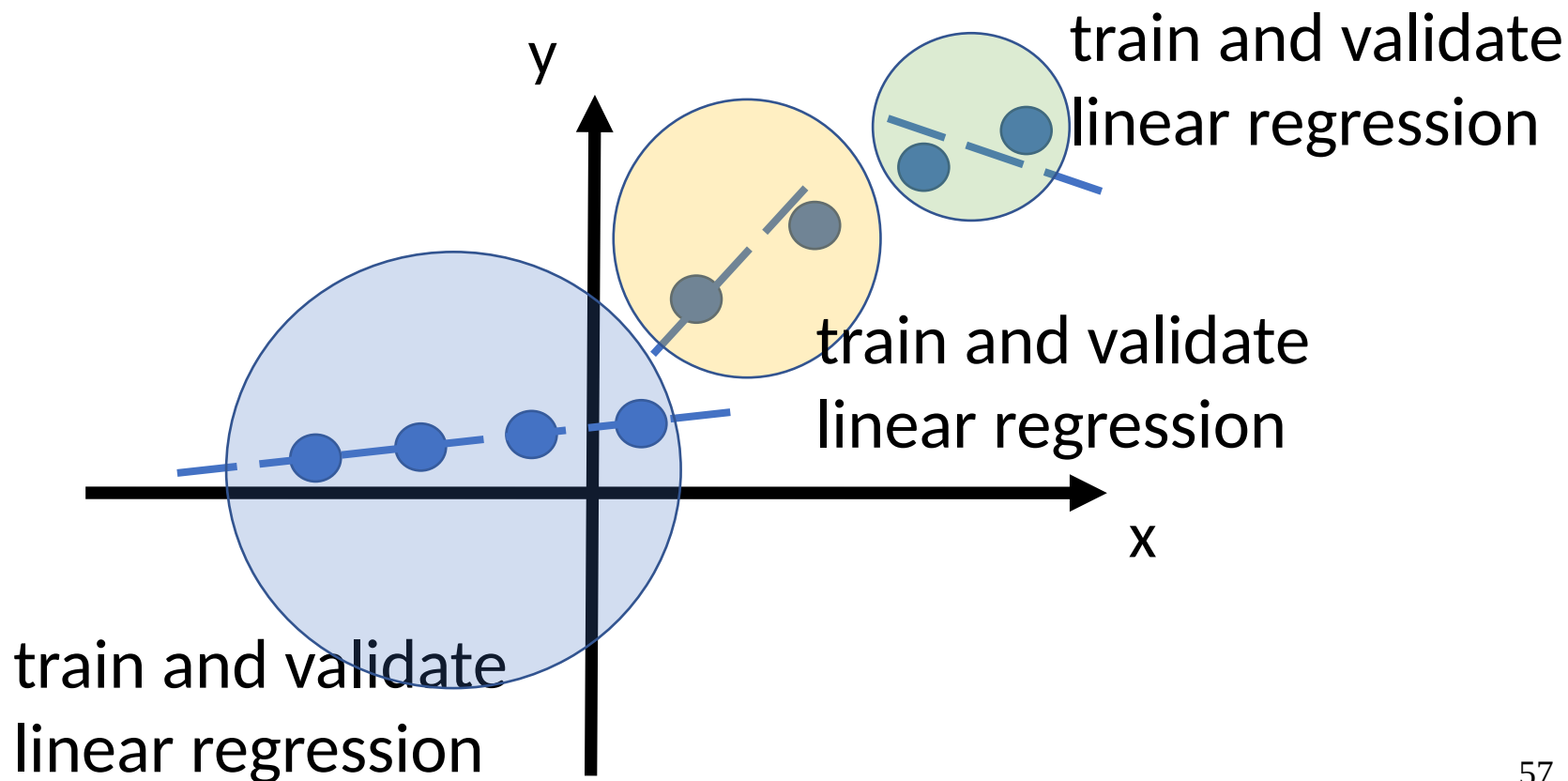
Choose k by validation error

- $k=2$



Choose k by validation Error

- $k=3$



k-Means in Python

sklearn.cluster.KMeans

```
class sklearn.cluster.KMeans(n_clusters=8, *, init='k-means++', n_init='warn', max_iter=300, tol=0.0001, verbose=0, random_state=None, copy_x=True, algorithm='lloyd')
```

[\[source\]](#)

K-Means – recap

- k-Means partitions dataset into k clusters
- Number k of clusters needs to be given
- k-Means iteratively minimizes clustering error
- k-Means might deliver sub-optimal clustering:
repeat it with different initial cluster means

Soft Clustering

Soft clustering

$$\mathcal{D} = \{(\mathbf{x}^{(1)}, y^{(1)}), \dots, (\mathbf{x}^{(m)}, y^{(m)})\}.$$

Data points characterized by n features

- Features of i-th data

$$\mathbf{x}^{(i)} = (x_1^{(i)}, \dots, x_n^{(i)})$$

- i-th data point **characterized by k numerical label values**

$$\mathbf{y}^{(i)} = (y_1^{(i)}, \dots, y_k^{(i)})$$

Degree of belonging

- i-th data point **characterized by k numerical label values**

$$\mathbf{y}^{(i)} = (y_1^{(i)}, \dots, y_k^{(i)})$$

- $y_1^{(i)}$ degree of i-th datapoint belonging to cluster 1
- $y_2^{(i)}$ degree of i-th datapoint belonging to cluster 2
- ...
- $y_k^{(i)}$ degree of i-th datapoint belonging to cluster k

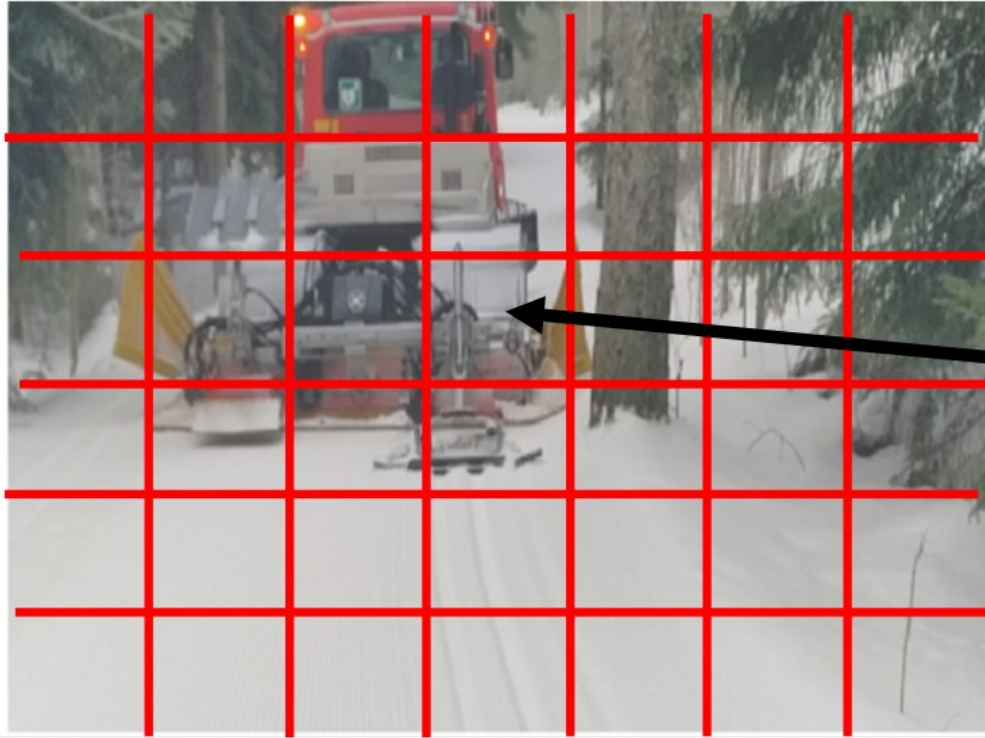
Probabilistic interpretation

- $y_c^{(i)}$ degree of i-th datapoint belonging to cluster c
- Interpret $y_c^{(i)}$ as **probability**:
p(“i-th datapoint belongs to cluster c”)
- $y_c^{(i)}$ can be any number between 0 and 1
- i-th datapoint must belong to some cluster $\sum_{c=1}^k y_c^{(i)} = 1$
- Hard clustering requires $y_c^{(i)}$ is either 0 or 1

Soft clustering methods



Dataset = Set of image patches



data point



Output of Hard Clustering (k-Means)

k=2



Output of Soft Clustering (GMM)

k=2



Soft Clustering with GMM

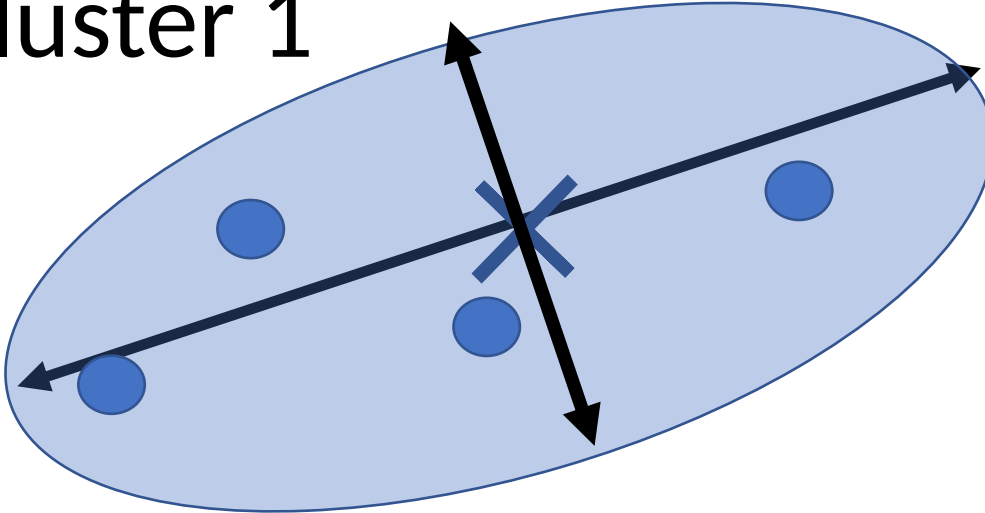
Gaussian mixture model

- Each cluster produces data based upon random draws from a (multi-dimensional) Gaussian distribution
- Clusters should be less likely to have data at the edge
- Each Gaussian cluster has its own mean and standard deviation

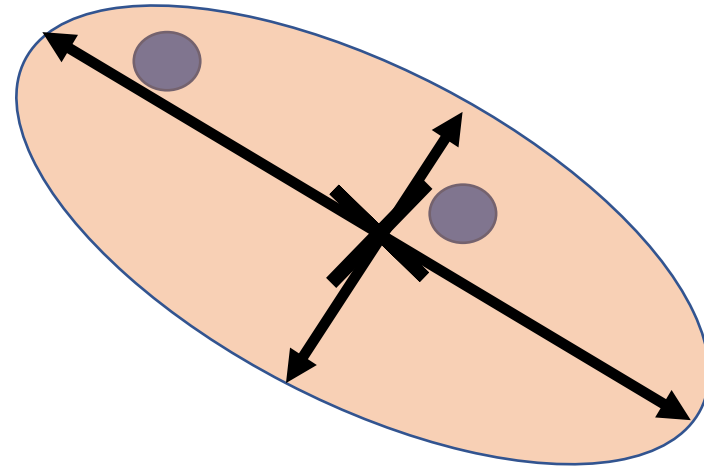
Represent clusters by Gaussians

- Gaussian mixture model (GMM)

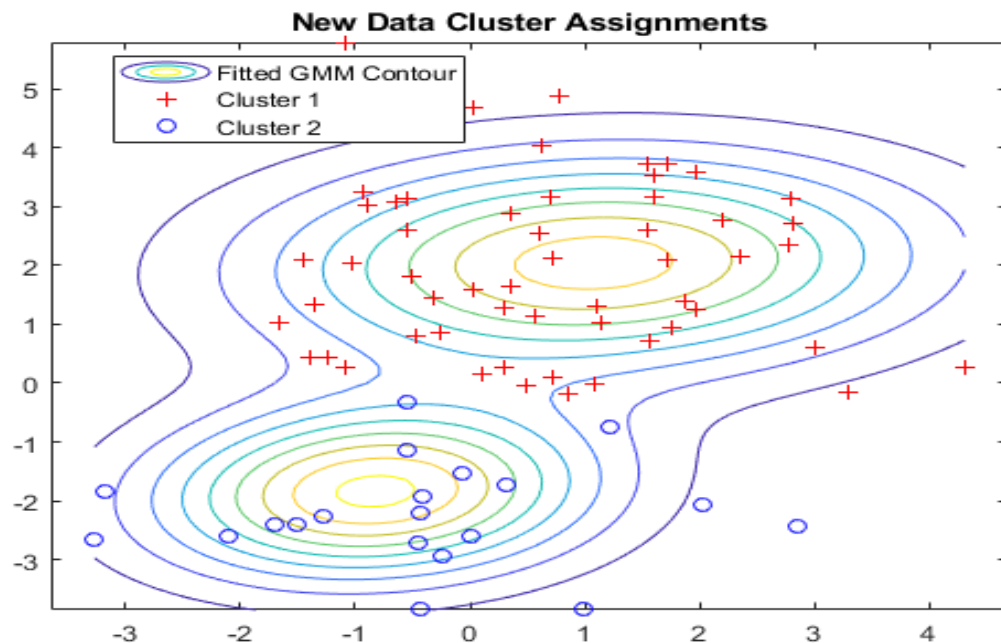
cluster 1



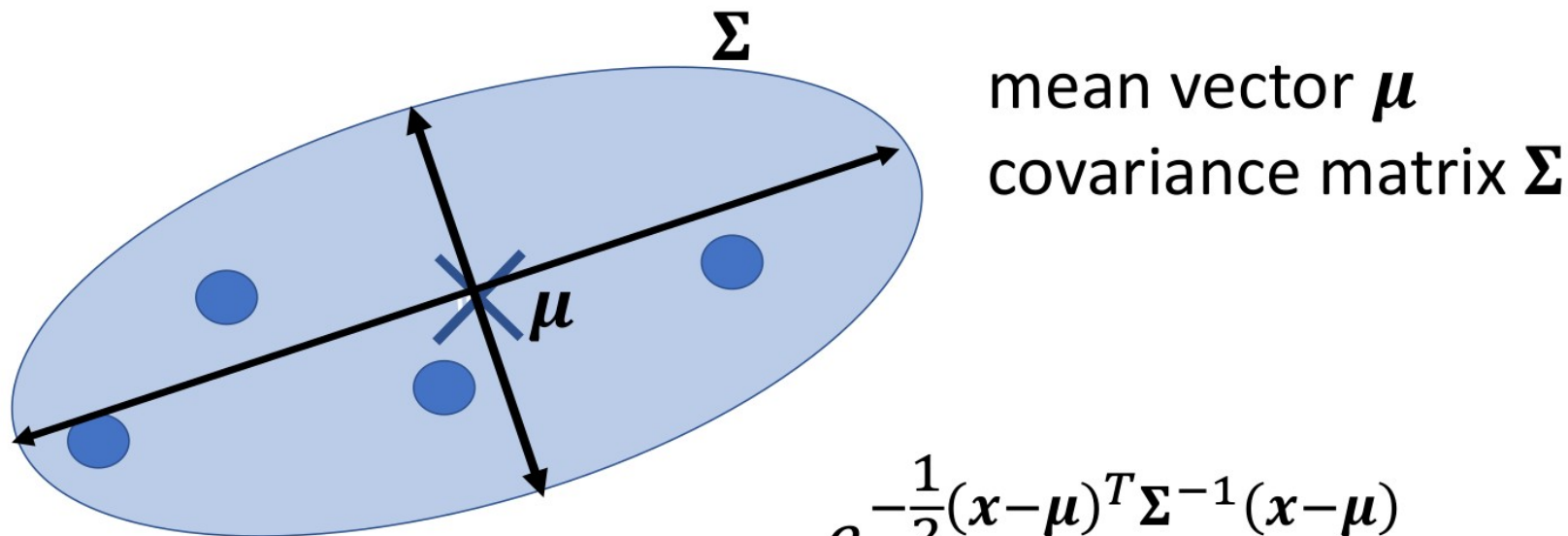
cluster 2



Sum of the Gaussians: GMM

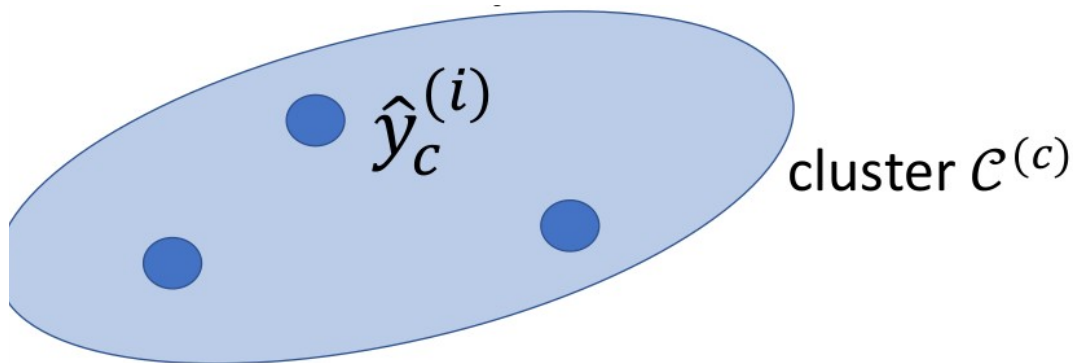


Gaussian distribution



$$p(\mathbf{x}; \mu, \Sigma) = \frac{e^{-\frac{1}{2}(\mathbf{x}-\mu)^T \Sigma^{-1}(\mathbf{x}-\mu)}}{\sqrt{(2\pi)^n \det(\Sigma)}}$$

Cluster spread



$$\frac{1}{m^{(c)}} \sum_{i=1}^m \hat{y}_c^{(i)} (\mathbf{x}^{(i)} - \boldsymbol{\mu}^{(c)})^T (\boldsymbol{\Sigma}^{(1)})^{-1} (\mathbf{x}^{(i)} - \boldsymbol{\mu}^{(c)})$$

Effective cluster size:

$$m^{(c)} := \sum_{i=1}^m \hat{y}_c^{(i)}$$

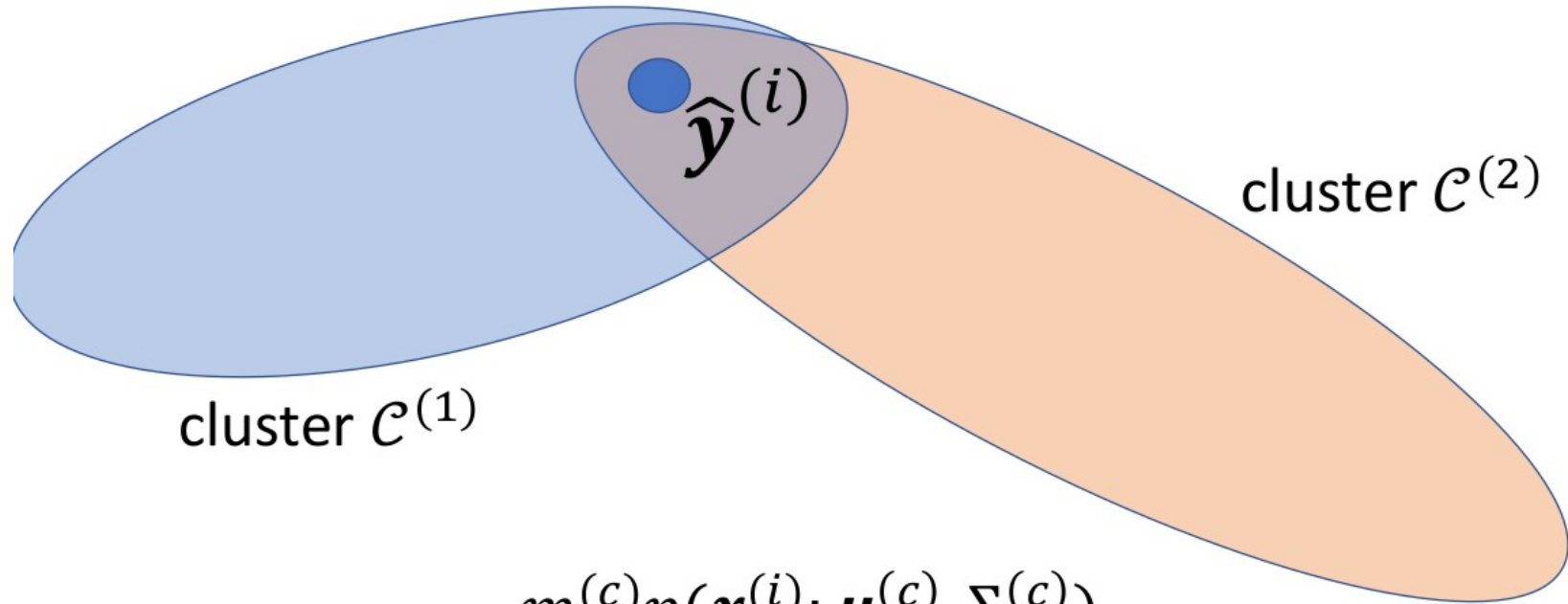
Update cluster mean and covariance

- For given (soft) cluster assignments chose cluster **means and covariance to minimize cluster spreads**

$$\boldsymbol{\mu}^{(c)} := \frac{1}{m^{(c)}} \sum_{i=1}^m \hat{y}_c^{(i)} \mathbf{x}^{(i)} \quad \text{for all } c = 1, \dots, k$$

$$\boldsymbol{\Sigma}^{(c)} := \frac{1}{m^{(c)}} \sum_{i=1}^m \hat{y}_c^{(i)} (\mathbf{x}^{(i)} - \boldsymbol{\mu}^{(c)}) (\mathbf{x}^{(i)} - \boldsymbol{\mu}^{(c)})^T$$

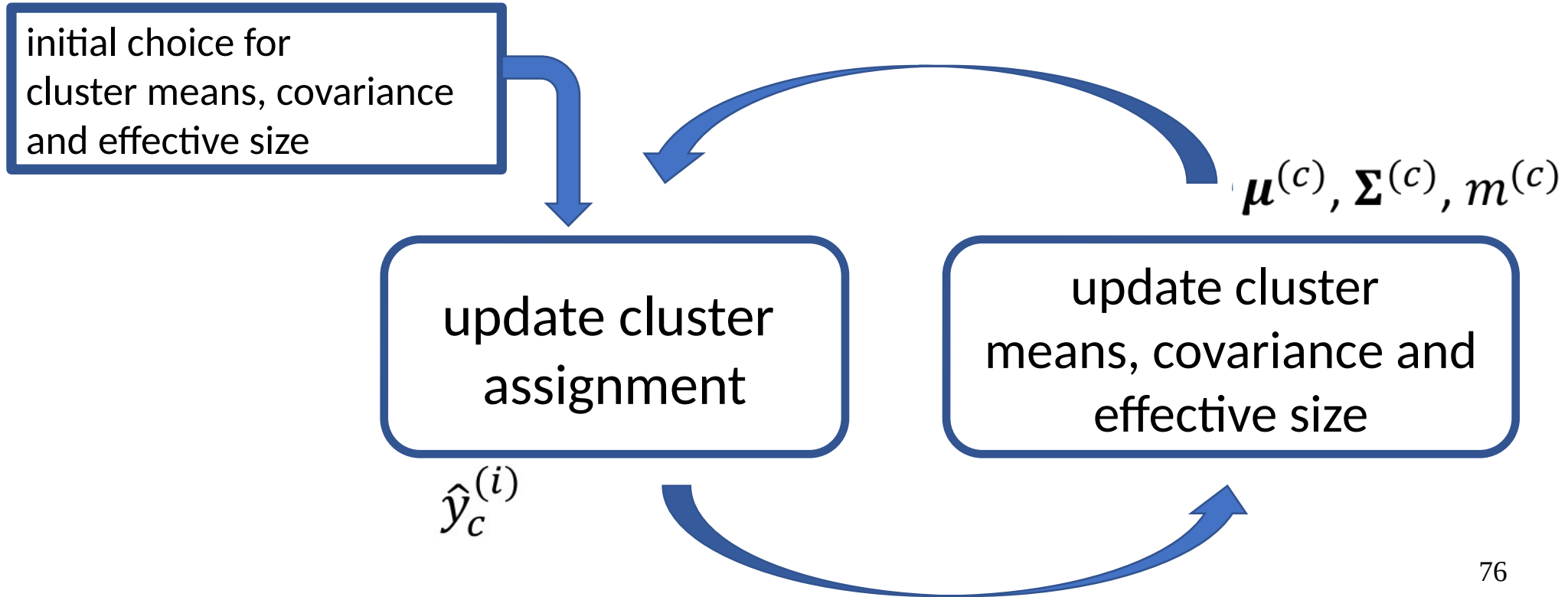
Cluster assignment update



$$\hat{\mathbf{y}}_c^{(i)} := \frac{m^{(c)} p(\mathbf{x}^{(i)}; \boldsymbol{\mu}^{(c)}, \Sigma^{(c)})}{\sum_{c'=1}^k m^{(c')} p(\mathbf{x}^{(i)}; \boldsymbol{\mu}^{(c')}, \Sigma^{(c')})}$$

GMM Algorithm

$$\boldsymbol{\mu}^{(c)}, \boldsymbol{\Sigma}^{(c)}, m^{(c)}$$



GMM Algorithm

- **Input:** $\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}, k, \{\boldsymbol{\mu}^{(c)}, \boldsymbol{\Sigma}^{(c)}, m^{(c)}\}$
 1. Update soft cluster assignments $\hat{y}_c^{(i)}$
 2. Update cluster params $\boldsymbol{\mu}^{(c)}, \boldsymbol{\Sigma}^{(c)}, m^{(c)}$
 3. Go to 1. unless “finished”
- **Output:** $\hat{y}_c^{(i)}, \boldsymbol{\mu}^{(c)}, \boldsymbol{\Sigma}^{(c)}, m^{(c)}$

Falls in the category of expectation–maximization (EM) algorithms (as k-means)

Soft-Clustering Error

$$\mathcal{E}(\{\boldsymbol{\mu}^{(c)}\}, \{\boldsymbol{\Sigma}^{(c)}\}, \{m^{(c)}\}) :=$$
$$-\sum_{i=1}^m \log \sum_{c=1}^k \frac{m^{(c)}}{m} p(\mathbf{x}^{(i)}; \boldsymbol{\mu}^{(c)}, \boldsymbol{\Sigma}^{(c)})$$

- This is negative logarithm of probability to sample data points under Gaussian mixture model
- Minimize error equal to maximize (log) likelihood

Soft-Clustering Error

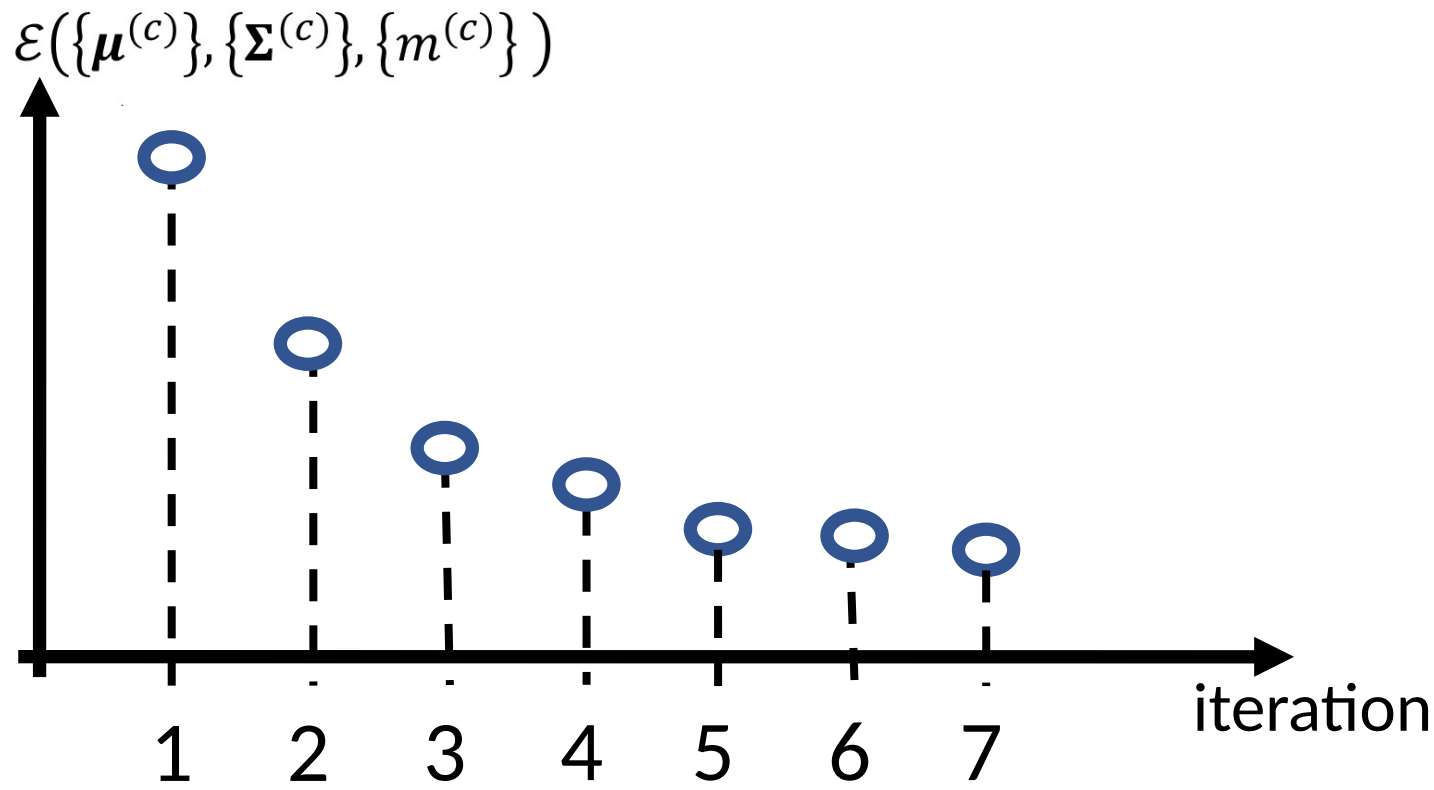
$$\mathcal{E}(\{\boldsymbol{\mu}^{(c)}\}, \{\boldsymbol{\Sigma}^{(c)}\}, \{m^{(c)}\}) := \\ -\sum_{i=1}^m \log \sum_{c=1}^k \frac{m^{(c)}}{m} p(\mathbf{x}^{(i)}; \boldsymbol{\mu}^{(c)}, \boldsymbol{\Sigma}^{(c)})$$

- Again, this is an Empirical Risk Minimization problem:

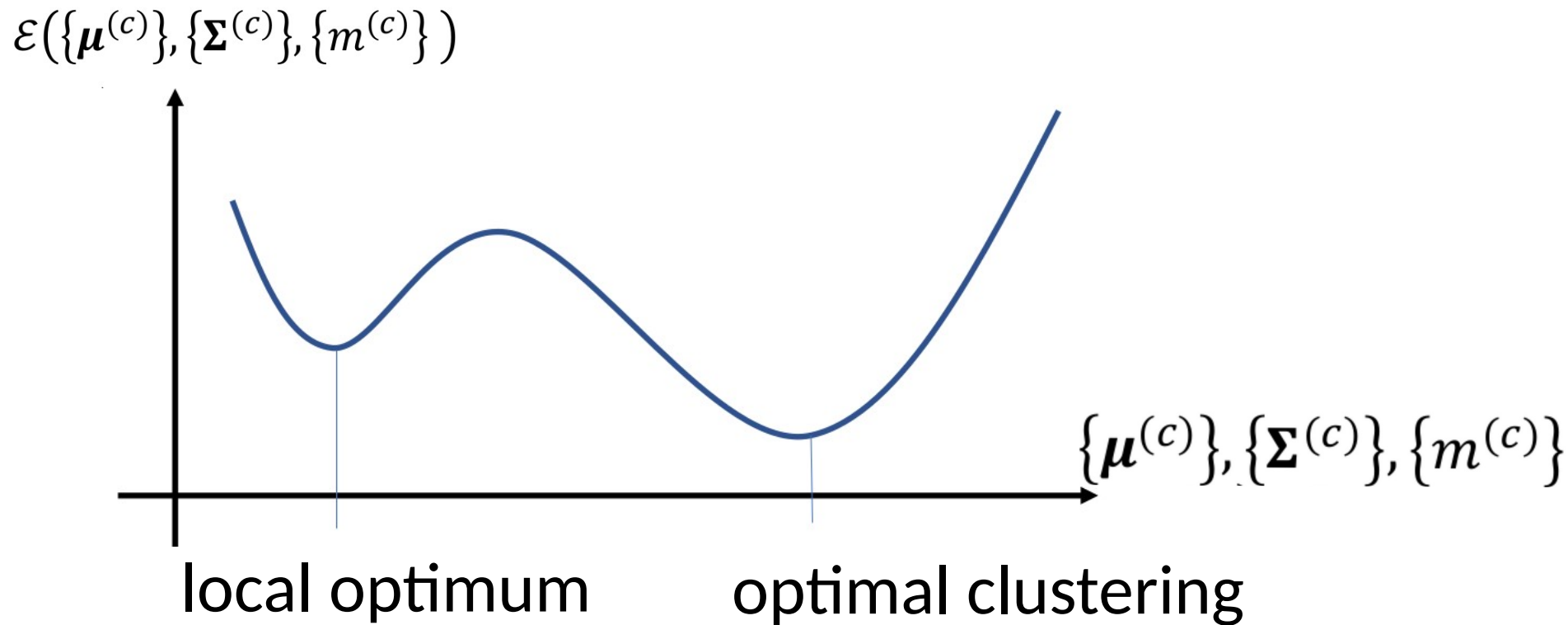
$$\hat{L}(\boldsymbol{\theta} \mid \mathcal{D}) := -\log p(\mathcal{D}; \boldsymbol{\theta}) \text{ with GMM parameters } \boldsymbol{\theta} := \{\boldsymbol{\mu}^{(c)}, \boldsymbol{\Sigma}^{(c)}, p_c\}_{c=1}^k$$

When to stop?

- Stop when decrease too small
- After fixed number of iteration



Non-convexity of soft-clustering error



Initialization is crucial

- Soft clustering depends crucially on initialization means
- Repeat several times with different initializations

How to choose number k of clusters?

- As in k-Means:
 - Defined by application
 - Desired compression rate
 - Elbow (knee) method
 - Validation error

GMM in Python

2.1. Gaussian mixture models

`sklearn.mixture` is a package which enables one to learn Gaussian Mixture Models (diagonal, spherical, tied and full covariance matrices supported), sample them, and estimate them from data. Facilities to help determine the appropriate number of components are also provided.

<https://scikit-learn.org/stable/modules/mixture.html#gmm>

`sklearn.mixture.GaussianMixture`

```
class sklearn.mixture.GaussianMixture(n_components=1, *, covariance_type='full', tol=0.001, reg_covar=1e-06,
max_iter=100, n_init=1, init_params='kmeans', weights_init=None, means_init=None, precisions_init=None, random_state=None,
warm_start=False, verbose=0, verbose_interval=10)
```

[\[source\]](#)

<https://scikit-learn.org/stable/modules/generated/sklearn.mixture.GaussianMixture.html#sklearn.mixture.GaussianMixture>

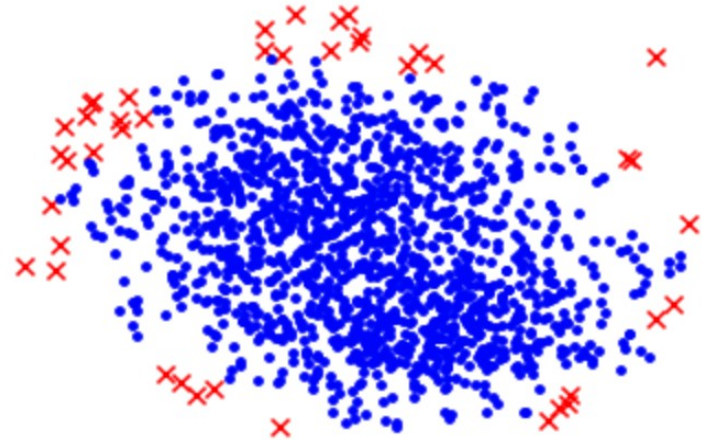
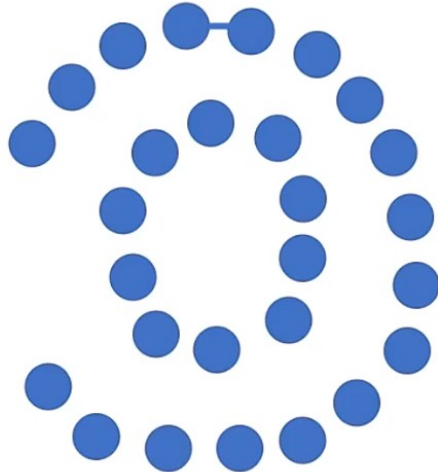
GMM – recap

- Represent clusters by Gaussian distributions
- Soft clustering algorithm fits GMM
- Iterative optimization of soft-clustering error
- Trapped in local minimum for bad initialization

Other clustering approaches

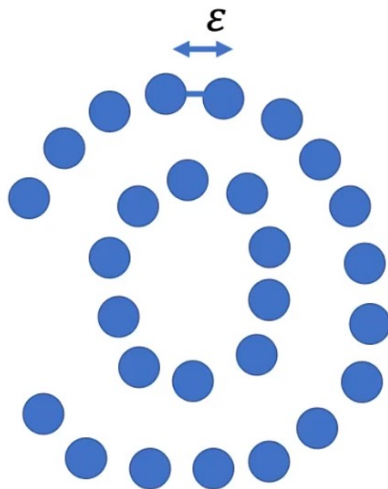
Connectivity based clustering

- k-Means and GMM fails on non-Euclidean cluster structure
- k-Means and GMM cannot recognize outliers/noise



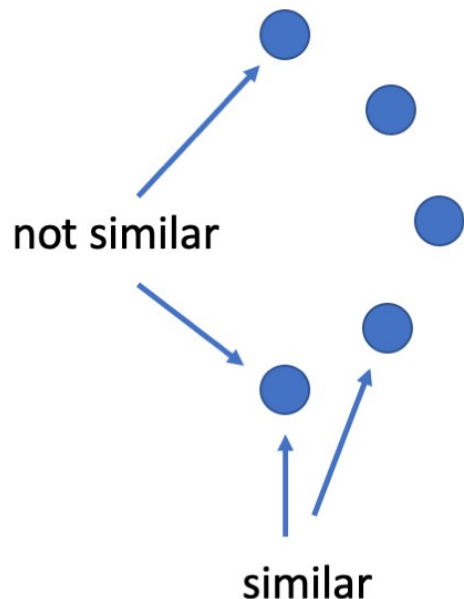
Connectivity based clustering

- Notions of connectivity between nodes
- Connect close-by data points obtaining an **empirical graph**
- Cluster \approx **connected graph component**



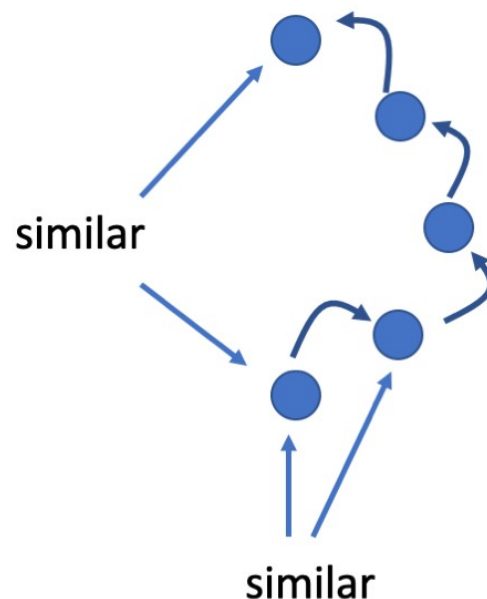
Connectivity based clustering

similarity based on
Euclidean distance



E.g.: K-means,
Gaussian mixture models,...

similarity based
on connectivity



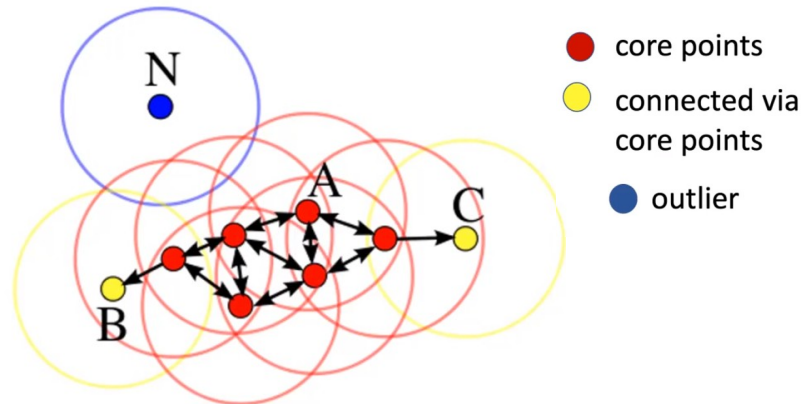
E.g.: DBSCAN

Connectivity based clustering

- Hard clustering
 - Spectral clustering
 - Eigenvectors of graph Laplacian matrix to measure connectivity between nodes
 - DBSCAN
 - Density based spatial clustering with noise

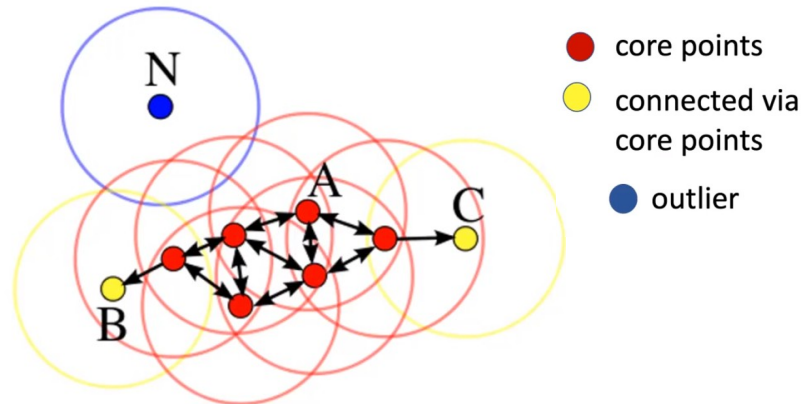
DBSCAN

- Data points need to be connected via **core points**
- Core points are the ones with a minimum number of neighbors
- Automatically determines number of k clusters



DBSCAN

- Parameters:
 - Epsilon: Maximum distance to be connected
 - MinPts: Minimum number of points to be a core point

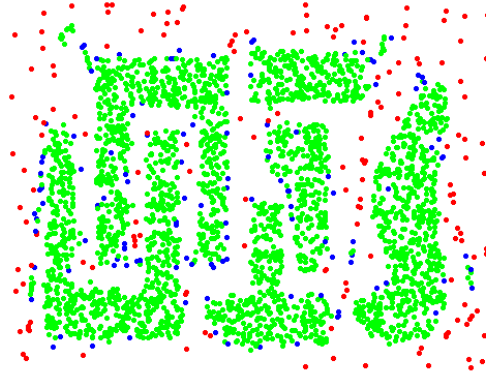


DBSCAN

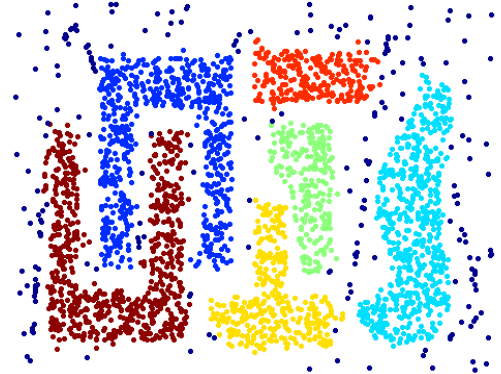
Eps = 10, MinPts = 4



Original points



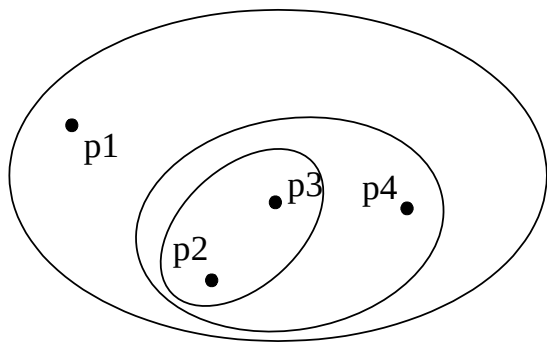
Core, border and
outlier/noise



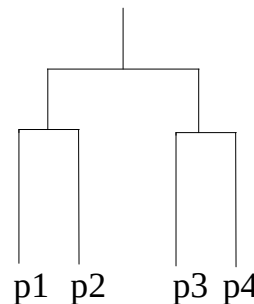
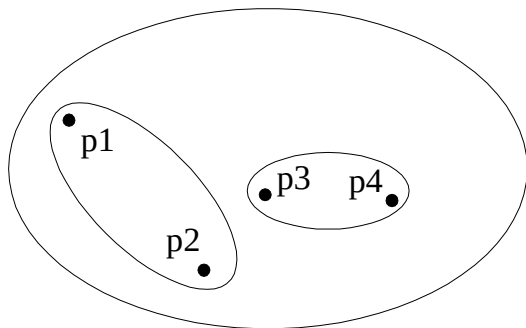
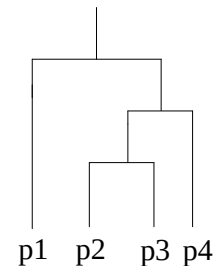
Clusters

Hierarchical clustering

- A set of nested clusters organized as a hierarchical tree (dendrogram)

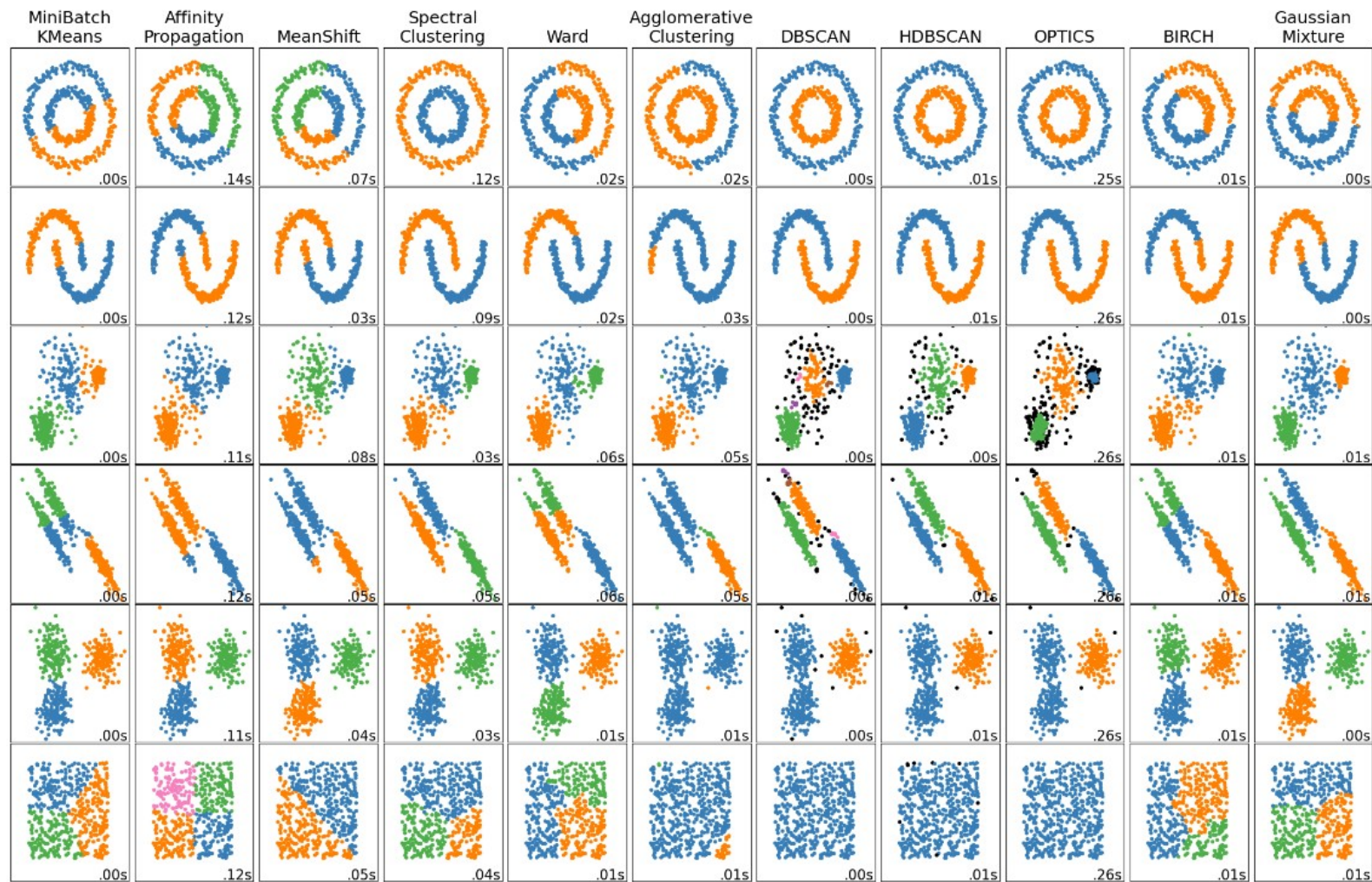


Dendrogram



Hierarchical clustering

- A set of nested clusters organized as a hierarchical tree (dendogram)
- Any desired number of clusters can be obtained by 'cutting' the dendogram at the proper level
- Different levels may correspond to meaningful taxonomies
- Key operation is the computation of the proximity of two clusters



A comparison of the clustering algorithms in scikit-learn

Evaluating/Comparing clustering

Measures of cluster validity

- **Internal Index:** goodness of a clustering structure without external information
 - e.g., Silhouette index, sum of squared error (k-Means), log-likelihood (GMM).
- **External or Relative Index:** extent to which cluster labels match externally supplied class labels or labels from another clustering
 - e.g., entropy, purity, rand-index, adjusted rand-index, mutual information, adjusted mutual information.

Silhouette

- Silhouette measures consistency within clusters of data: how similar a data point is to its own cluster (cohesion) compared to other clusters (separation)
- The Silhouette score is defined for each sample and is composed of two scores:
 - The mean distance between a sample and all other points in the same cluster (a)
 - The mean distance between a sample and all other points in the next nearest cluster (b)

$$s = \frac{b - a}{\max(a, b)}$$

- The Silhouette for a set of samples is given as the mean of the Silhouette for each sample

Silhouette

$$s = \frac{b - a}{\max(a, b)}$$

- It ranges from -1 to $+1$, where a high value indicates that the object is well matched to its own cluster and poorly matched to neighboring clusters
- Scores around zero indicate overlapping clusters
- If most objects have a high value, then the clustering configuration is appropriate
- The silhouette can be calculated with any distance metric
- The **average silhouette over all data of a cluster** measures how tightly grouped all the data in the cluster are
- The **average silhouette over all data of the dataset** measures how appropriately the data has been clustered

Rand Index

- Rand Index (RI) measures the similarity of two assignments
- Given a dataset D and two partitions S and R

$$RI(S, R) = \frac{a + b}{\binom{m}{2}}$$

- a is the number of pairs of elements in D that are in the same subset in S and in the same subset in R
- b is the number of pairs of elements in D that are in a different subset in S and in a different subset in R
- All possible pairs or element if D is the binomial coefficient $\binom{m}{2} = \frac{m(m-1)}{2}$

Adjusted Rand Index

- Rand Index can be interpreted as accuracy
- The Rand index does not ensure to obtain a value close to 0.0 for a random labelling
- The adjusted Rand index corrects for chance and will give such a baseline

$$ARI(S, R) = \frac{RI(S, R) - E[RI]}{\max(RI) - E[RI]}$$

- Max and expectation of RI are computed considering the number and size of clusters as in S and R, and all random clusterings are generated by shuffling the elements

Adjusted Rand Index

- Two example clusterings for a dataset. The calculated Adjusted Rand index for these two clusterings is 0.94



Final considerations: ML for clustering

- Learn to assign the cluster y of a data point from its features \mathbf{x}
- ML model = learn a hypothesis $h \in \mathcal{H} \quad h : \mathcal{X} \rightarrow \mathcal{Y}$
such that $h(\mathbf{x})$ minimize an empirical risk over data points
- Loss function: how to quantify how good is $h(\mathbf{x})$ with respect to the whole data $D \rightarrow$ clustering error
- Notice: even if not common, it is still possible to use a validation/test set for assessing how data generalize, stability of the clusters and tune hyper-parameters

Any questions?



Self-assessment quiz



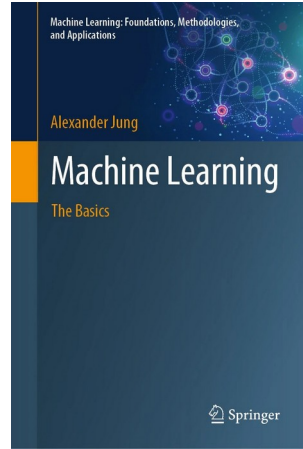
- Given the following dataset with 9 samples and 1 feature, provide the possible outputs for a hard-clustering method and for a soft-clustering method, both with 3 clusters
- Perform up to 5 iterations of k-Means, with $k=2$, on the same dataset
- Compute the Rand Index of the previous clustering with respect to the following clustering assignment: $[0, 0, 0, 0, 0, 0, 0, 1, 1]$

Feature 1
10
7
7
5
-1
10
2
-3
0



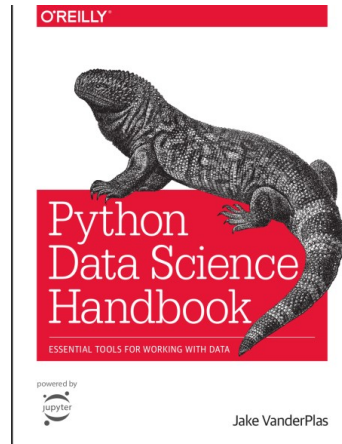
References: readings

- Chapter 8

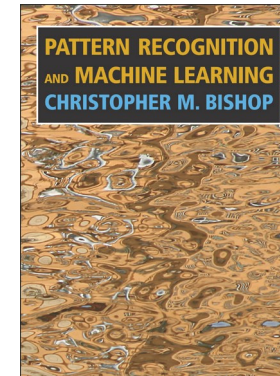


<https://scikit-learn.org/stable/modules/clustering.html>

- Chapter 5



- Chapter 9



Slide acknowledgments



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