Feature Spaces and Clustering

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Outline

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Outline

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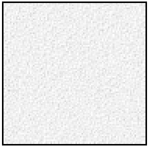
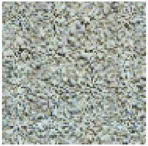
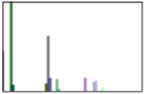
Categories of Feature Descriptors for Images

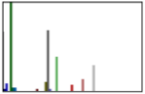
- distribution of colors
- texture
- shapes (contoures)



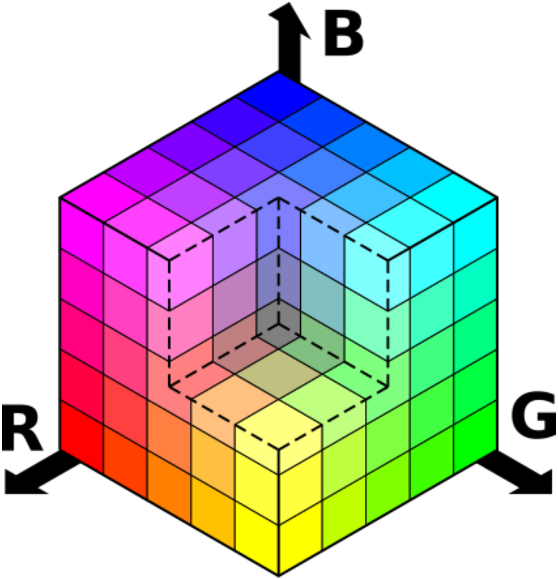
Color Histogram



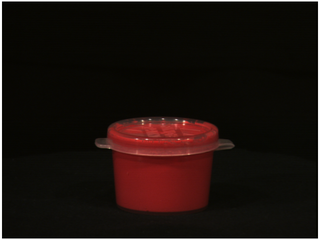
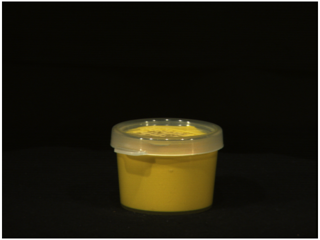
- a histogram represents the distribution of colors over the pixels of an image
- definition of an color histogram:
  - choose a color space (RGB, HSV, HLS, . . .)
  - choose number of representants (sample points) in the color space
  - possibly normalization (to account for different image sizes)

Color Space Example: RGB cube



Impact of Number of Representants

original images in full RGB space $(256^3 = 16,777,216)$


Impact of Number of Representants

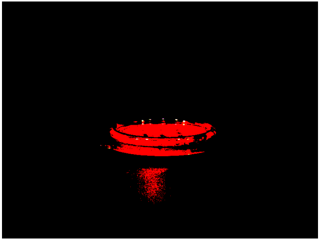
2^3

3^3

4^3

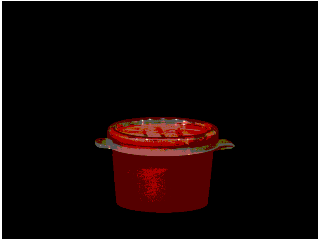
16^3

Impact of Number of Representants

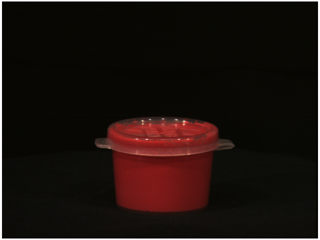


2^3

3^3



4^3



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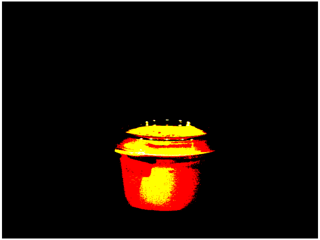
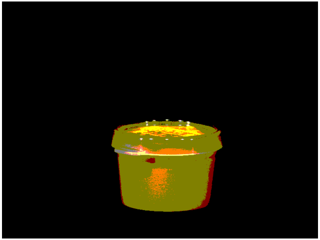
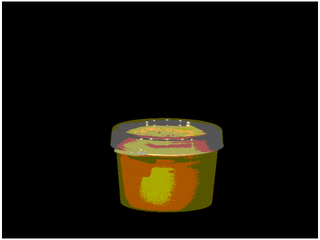


2^3



3^3



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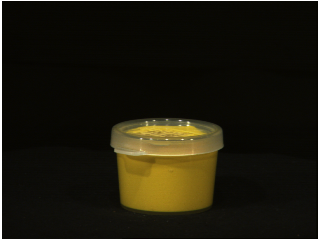

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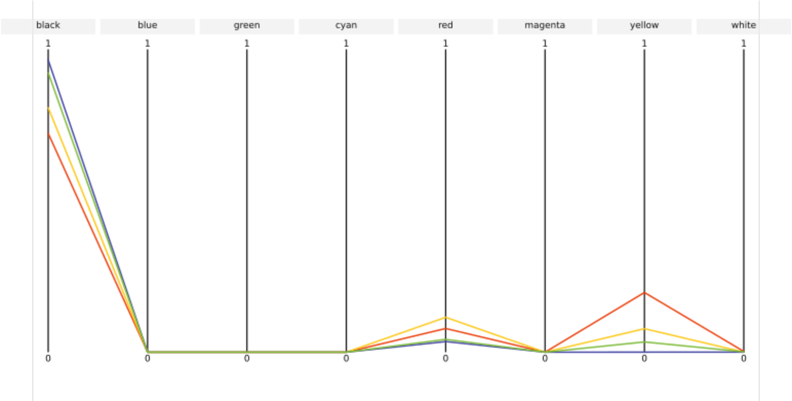
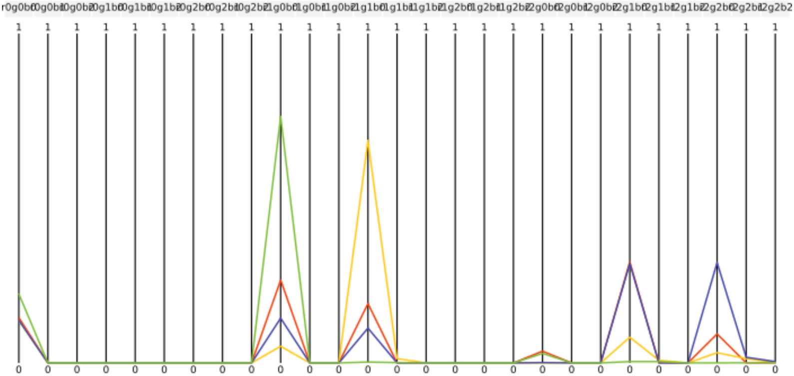


The histogram for each image is essentially a visualization of a vector:

$(0.77, 0, 0, 0, 0.08, 0, 0.15, 0)$ $(0.8, 0, 0, 0, 0.11, 0, 0.09, 0)$

$(0.9, 0, 0, 0, 0.05, 0, 0.05, 0)$ $(0.955, 0, 0, 0, 0.045, 0, 0, 0)$

Impact of Number of Representants



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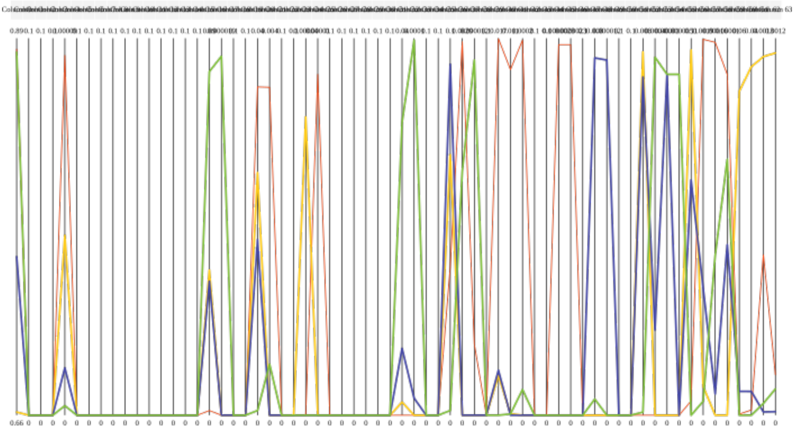
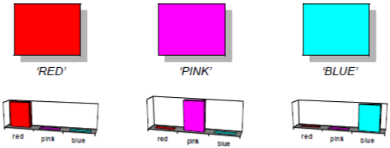


Outline

Distances for Color Histograms

Euclidean distance for images P and Q using the color histograms h_P and h_Q:

$$\mathrm{dist}(P, Q) = \sqrt{(h_P - h_Q) \cdot (h_P - h_Q)^\mathsf{T}}$$



$(1, 0, 0)$ $(0, 1, 0)$ $(0, 0, 1)$

$$\mathrm{dist}(\text{RED}, \text{PINK}) = \sqrt{2}$$
$$\mathrm{dist}(\text{RED}, \text{BLUE}) = \sqrt{2}$$
$$\mathrm{dist}(\text{BLUE}, \text{PINK}) = \sqrt{2}$$

A 'psychologic' distance would consider that red is (in our perception) more similar to pink than to blue.

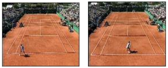
Example for the Distance Computation of Histograms

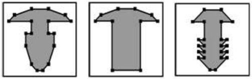
$$\mathrm{dist}(P, Q) = \sqrt{(h_P - h_Q) \cdot (h_P - h_Q)^{\mathsf{T}}}$$

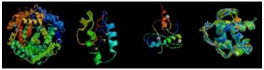
$$\begin{aligned}
\mathrm{dist}(\mathsf{RED}, \mathsf{PINK}) &= \sqrt{((1,0,0) - (0,1,0)) \cdot ((1,0,0) - (0,1,0))^{\mathsf{T}}} \\
&= \sqrt{(1,-1,0) \cdot (1,-1,0)^{\mathsf{T}}} \\
&= \sqrt{(1 \cdot 1 + (-1) \cdot (-1) + 0 \cdot 0)} \\
&= \sqrt{2}
\end{aligned}$$

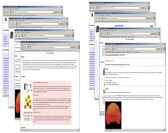
Similarity

- Similarity (as given by some distance measure) is a central concept in data mining, e.g.:
  - clustering: group similar objects in the same cluster, separate dissimilar objects to different clusters
  - outlier detection: identify objects that are dissimilar (by some characteristic) from most other objects
- definition of a suitable distance measure is often crucial for deriving a meaningful solution in the data mining task
  - images
  - CAD objects
  - proteins
  - texts
  - . . .







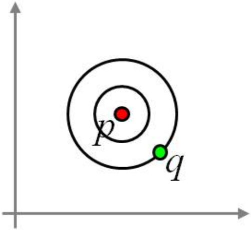


Spaces and Distance Functions

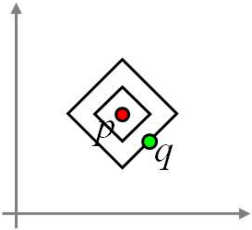
Common distance measure for (Euclidean) feature vectors: L_P-norm

$$\mathrm{dist}_P(p,q) = \left(|p_1 - q_1|^P + |p_2 - q_2|^P + \ldots + |p_n - q_n|^P\right)^{\frac{1}{P}}$$

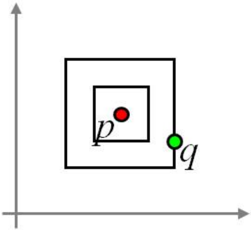
Euclidean norm (L_2):



Manhattan norm (L_1):



Maximum norm (L_∞, also: $L_{\max}$, supremum dist., Chebyshev dist.)



Spaces and Distance Functions

weighted Euclidean norm:

$$\operatorname{dist}(p,q) = \left(w_1|p_1 - q_1|^2 + w_2|p_2 - q_2|^2 + \ldots + w_n|p_n - q_n|^2\right)^{\frac{1}{2}}$$

*note that we assume vectors to be row vectors here

Outline

Your Choice of a Distance Measure

There are hundreds of distance functions [Deza and Deza, 2009].

- For time series: DTW, EDR, ERP, LCSS, ...
- For texts: Cosine and normalizations
- For sets – based on intersection, union, ... (Jaccard)
- For clusters (single-link, average-link, etc.)
- For histograms: histogram intersection, “Earth movers distance”, quadratic forms with color similarity
- With normalization: Canberra, ...
- Quadratic forms / bilinear forms: $d(x, y) := x^T M y$ for some positive (usually symmetric) definite matrix M.

Note that:

Choosing the appropriate distance function can be seen as a part of “preprocessing”.

Summary

You learned in this section:

- *distances (L_p-norms, weighted, quadratic form)*
- *color histograms as feature (vector) descriptors for images*
- *impact of the granularity of color histograms on similarity measures*

Outline

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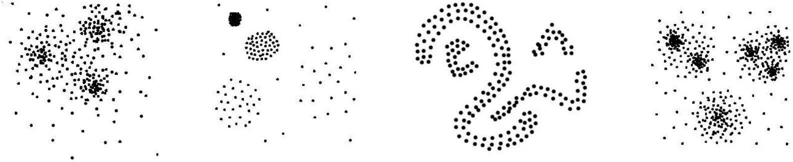
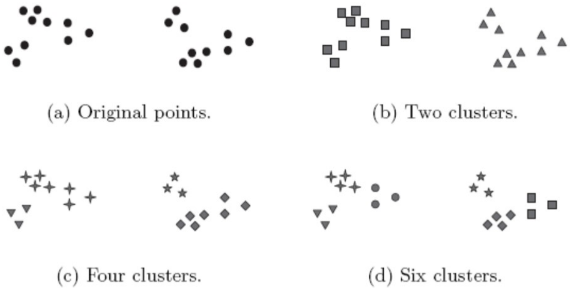
Purpose of Clustering

- identify a finite number of categories (classes, groups: clusters) in a given dataset
- *similar* objects shall be grouped in the same cluster, *dissimilar* objects in different clusters
- “similarity” is highly subjective, depending on the application scenario



A Dataset can be Clustered in Different Meaningful Ways



(a) Original points.

(b) Two clusters.

(c) Four clusters.

(d) Six clusters.

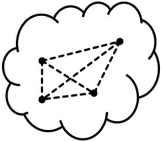
Figure 8.1. Different ways of clustering the same set of points.

(Figure from Tan et al. [2006].)

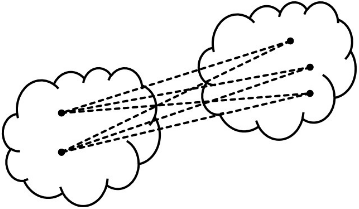
Outline

Criteria of Quality: Cohesion and Separation

- cohesion: how strong are the cluster objects connected (how similar, pairwise, to each other)?
- separation: how well is a cluster separated from other clusters?



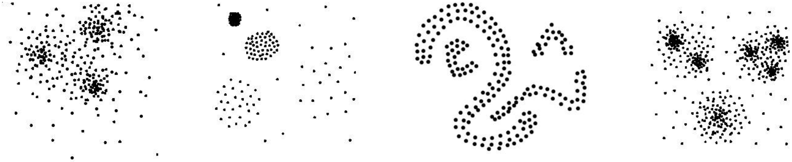
small within cluster distances



large between cluster distances

Optimization of Cohesion

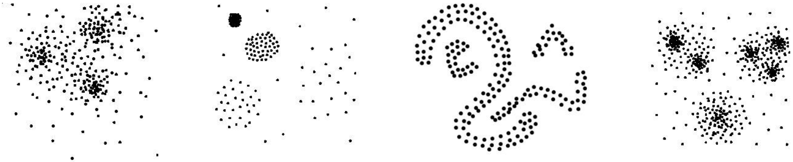
Partitional clustering algorithms partition a dataset into k clusters, typically minimizing some cost function (compactness criterion), i.e., optimizing cohesion.



Assumptions for Partitioning Clustering

Central assumptions for approaches in this family are typically:

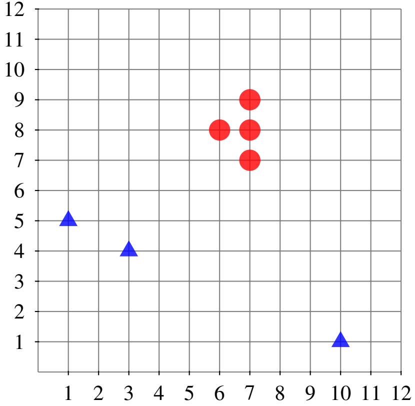
- number k of clusters known (i.e., given as input)
- clusters are characterized by their compactness
- compactness measured by some distance function (e.g., distance of all objects in a cluster from some cluster representative is minimal)
- criterion of compactness typically leads to convex or even spherically shaped clusters



Outline

Construction of Central Points: Basics

- objects are points $x = (x_1, \ldots, x_d)$ in Euclidean vector space $\mathbb{R}^d$, dist = Euclidean distance (L_2)
- centroid μ_C: mean vector of all points in cluster C



$$\mu_{C_i} = \frac{1}{|C_i|} \cdot \sum_{o \in C_i} o$$

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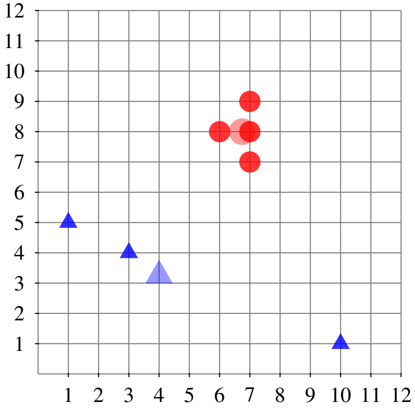


$$\mu_{C_i} = \frac{1}{|C_i|} \cdot \sum_{o \in C_i} o$$

Construction of Central Points: Basics

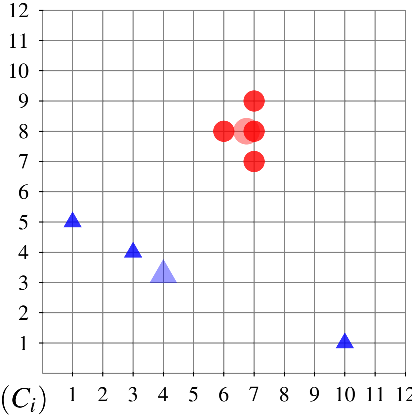
- measure of compactness for a cluster C:

$$TD^2(C) = \sum_{p \in C} \text{dist}(p, \mu_C)^2$$

(a.k.a. SSQ: sum of squares)

- measure of compactness for a clustering

$$TD^2(C_1, C_2, \ldots, C_k) = \sum_{i=1}^{k} TD^2(C_i)$$



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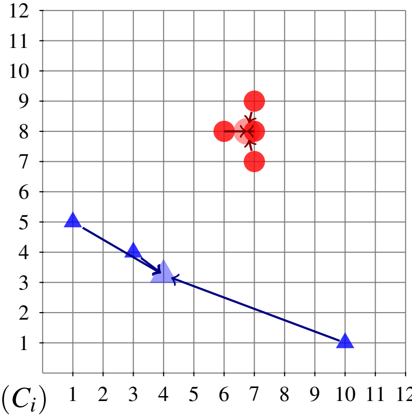
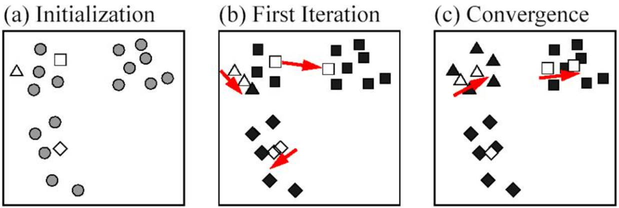


Basic Algorithm [Forgy, 1965, Lloyd, 1982]

Algorithm 2.1 (Clustering by Minimization of Variance)

- *start with k (e.g., randomly selected) points as cluster representatives (or with a random partition into k "clusters")*
- *repeat:*
  - *assign each point to the closest representative*
  - *compute new representatives based on the given partitions (centroid of the assigned points)*
- *until there is no change in assignment*



k-means

k-means [MacQueen, 1967] is a variant of the basic algorithm:

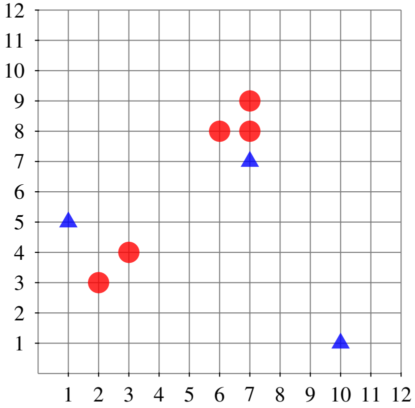
- a centroid is immediately updated when some point changes its assignment
- k-means has very similar properties, but the result now depends on the order of data points in the input file

Note that:

The name "k-means" is often used indifferently for any variant of the basic algorithm, in particular also for Algorithm 2.1 [Forgy, 1965, Lloyd, 1982].

Outline

k-means Clustering – Lloyd/Forgy Algorithm



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k-means Clustering – Lloyd/Forgy Algorithm

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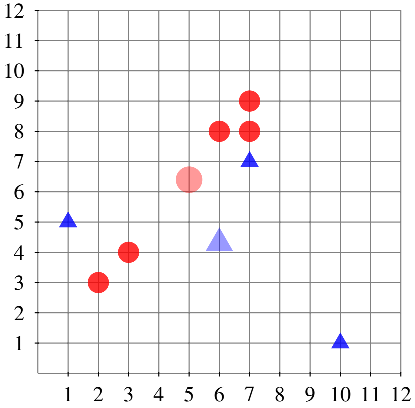
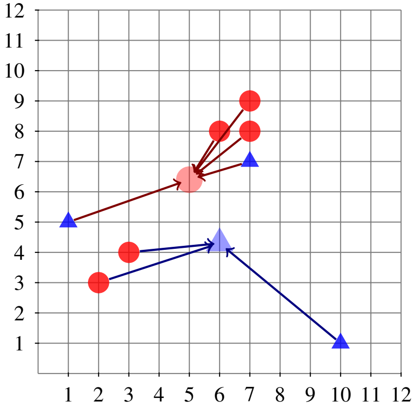


recompute centroids:

$$\mu \approx (6.0, 4.3)$$

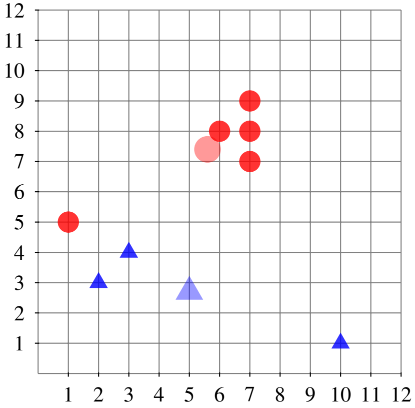
$$\mu \approx (5.0, 6.4)$$

k-means Clustering – Lloyd/Forgy Algorithm



reassign points

k-means Clustering – Lloyd/Forgy Algorithm

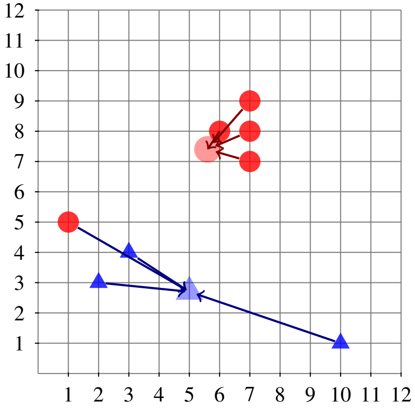


recompute centroids:

$$\mu \approx (5.0, 2.7)$$

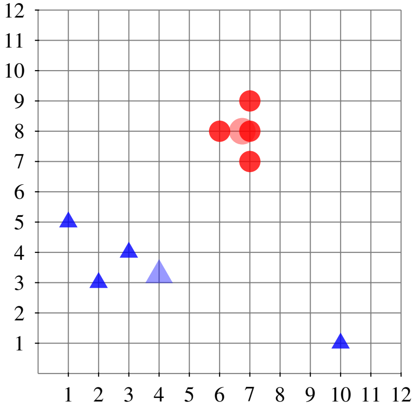
$$\mu \approx (5.6, 7.4)$$

k-means Clustering – Lloyd/Forgy Algorithm



reassign points

k-means Clustering – Lloyd/Forgy Algorithm

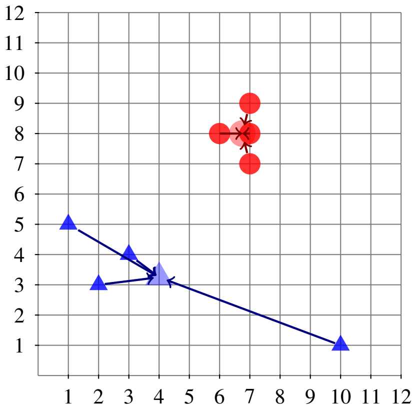


recompute centroids:

$$\mu \approx (4.0, 3.25)$$

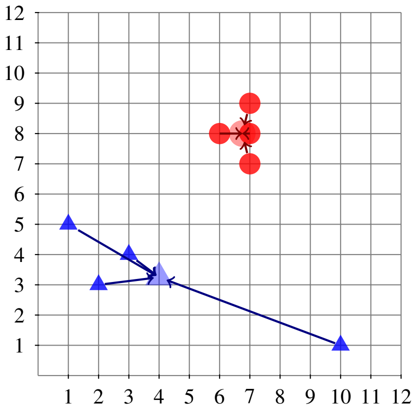
$$\mu \approx (6.75, 8.0)$$

k-means Clustering – Lloyd/Forgy Algorithm



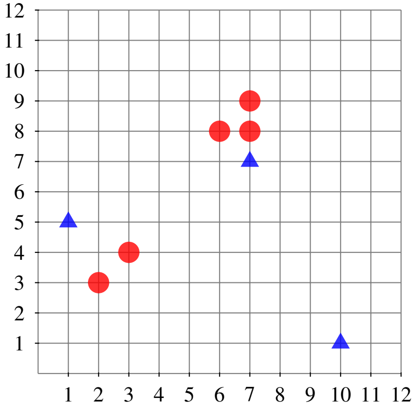
reassign points

k-means Clustering – Lloyd/Forgy Algorithm

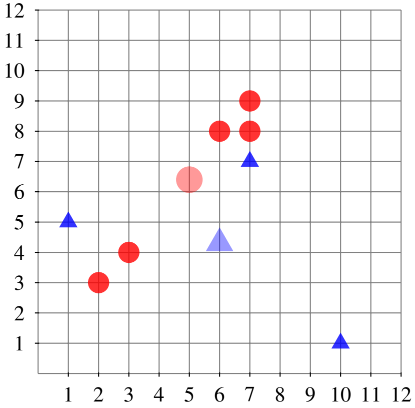


reassign points
no change
convergence!

k-means Clustering – MacQueen Algorithm



k-means Clustering – MacQueen Algorithm

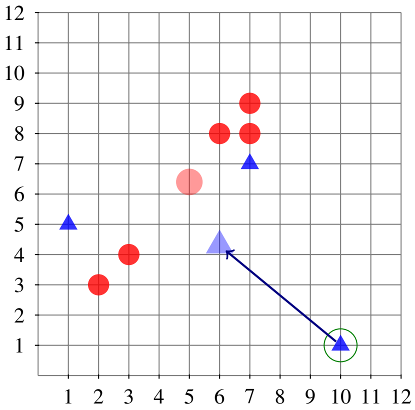


Centroids (e.g.: from previous iteration):

$$\mu \approx (6.0, 4.3)$$

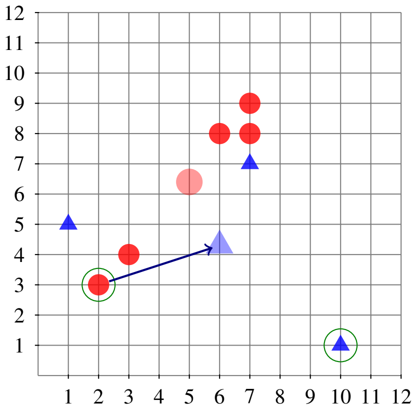
$$\mu \approx (5.0, 6.4)$$

k-means Clustering – MacQueen Algorithm



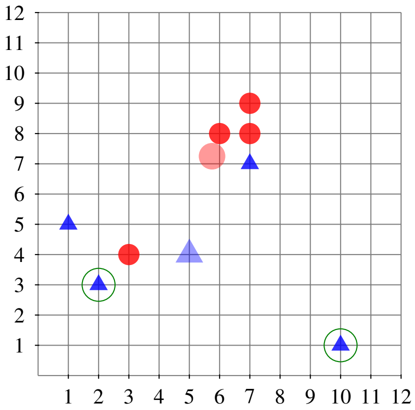
assign first point

k-means Clustering – MacQueen Algorithm



assign second point

k-means Clustering – MacQueen Algorithm



recompute centroids:

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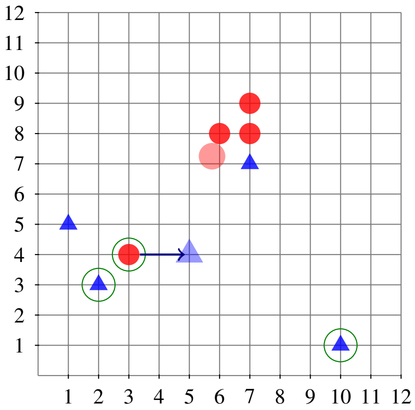
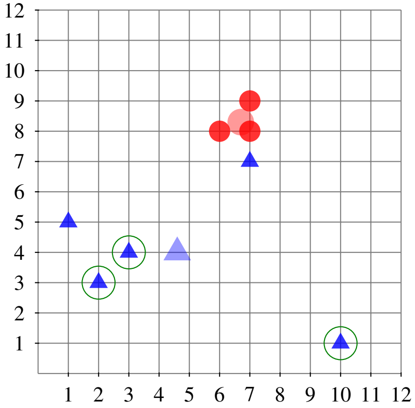
k-means Clustering – MacQueen Algorithm



assign third point

k-means Clustering – MacQueen Algorithm

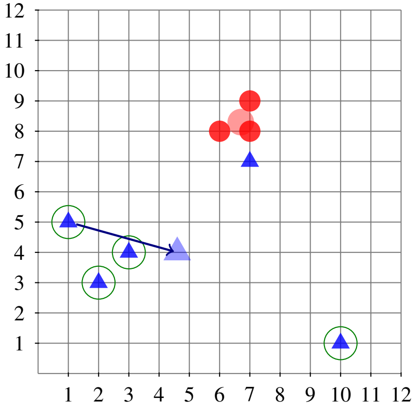


recompute centroids:

$$\mu \approx (4.6, 4.0)$$

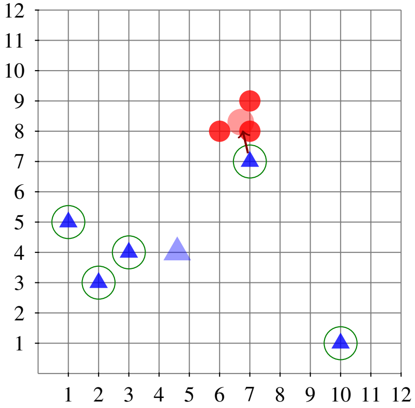
$$\mu \approx (6.7, 8.3)$$

k-means Clustering – MacQueen Algorithm



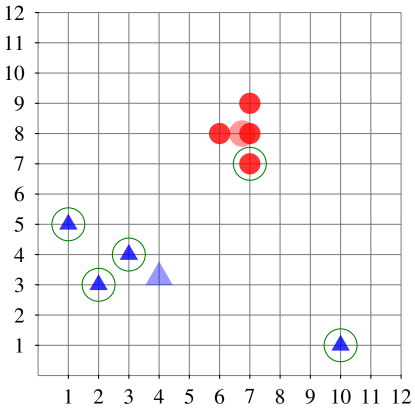
assign fourth point

k-means Clustering – MacQueen Algorithm



assing fifth point

k-means Clustering – MacQueen Algorithm

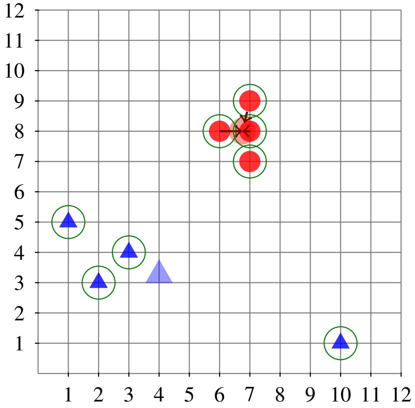


recompute centroids:

$$\mu \approx (4.0, 3.25)$$

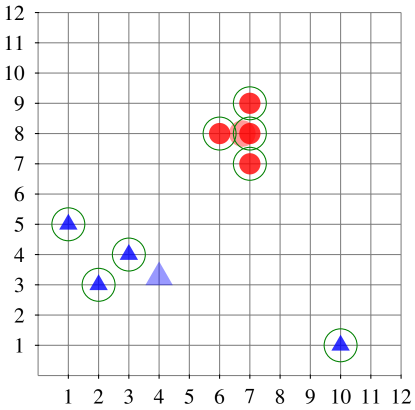
$$\mu \approx (6.75, 8.0)$$

k-means Clustering – MacQueen Algorithm



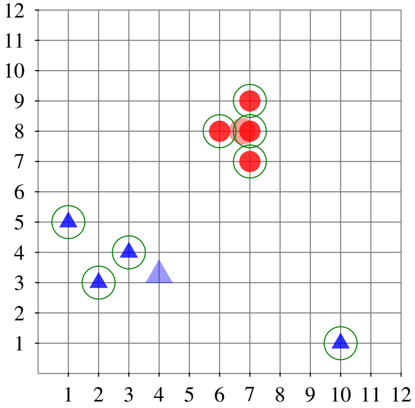
reassign more points

k-means Clustering – MacQueen Algorithm



reassign more points
possibly more iterations

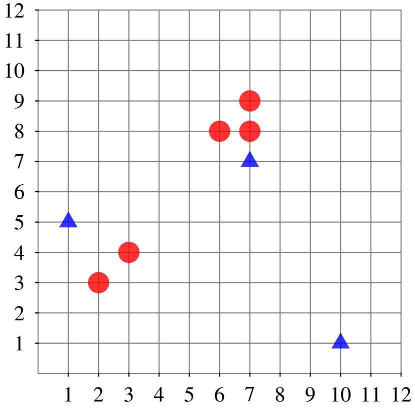
k-means Clustering – MacQueen Algorithm



reassign more points
possibly more iterations
convergence

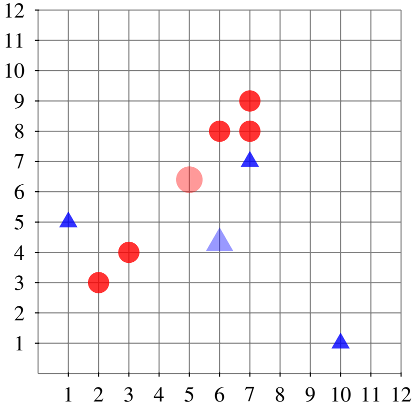
k-means Clustering – MacQueen Algorithm

Alternative Run – Different Order



k-means Clustering – MacQueen Algorithm

Alternative Run – Different Order



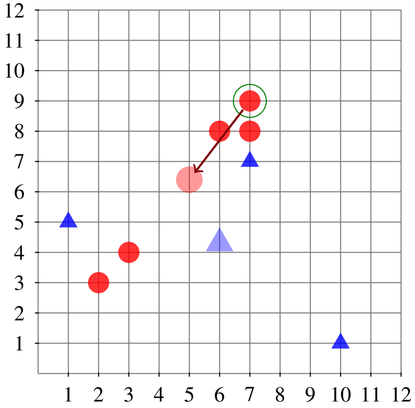
Centroids (e.g.: from previous iteration):

$$\mu \approx (6.0, 4.3)$$

$$\mu \approx (5.0, 6.4)$$

k-means Clustering – MacQueen Algorithm

Alternative Run – Different Order



assign first point

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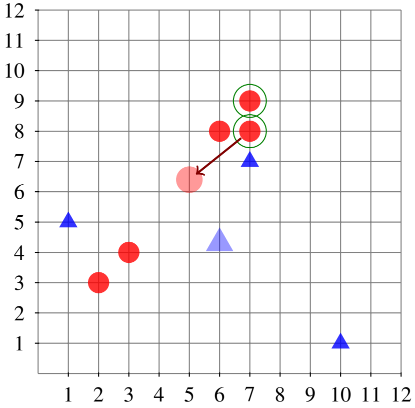
k-means Clustering – MacQueen Algorithm

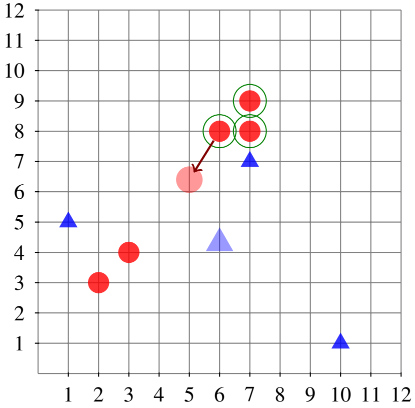
Alternative Run – Different Order



assign second point

k-means Clustering – MacQueen Algorithm

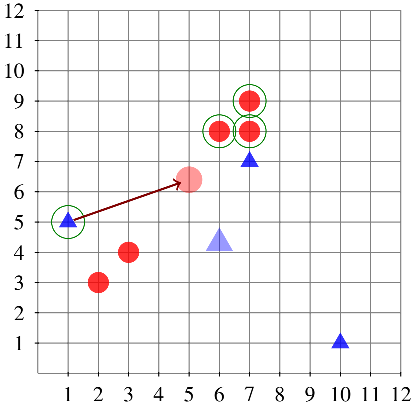
Alternative Run – Different Order



assign third point

k-means Clustering – MacQueen Algorithm

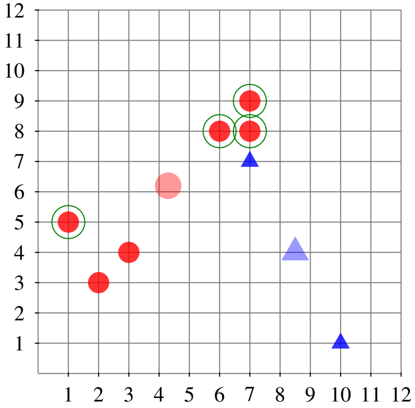
Alternative Run – Different Order



assign fourth point

k-means Clustering – MacQueen Algorithm

Alternative Run – Different Order



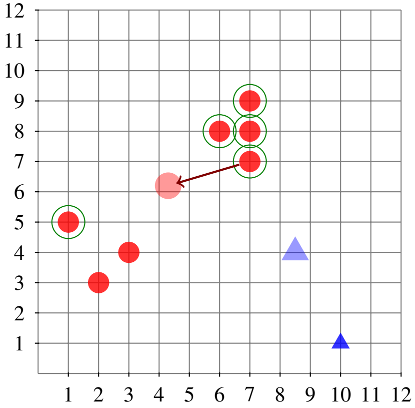
recompute centroids:

$$\mu \approx (4.0, 8.5)$$

$$\mu \approx (4.3, 6.2)$$

k-means Clustering – MacQueen Algorithm

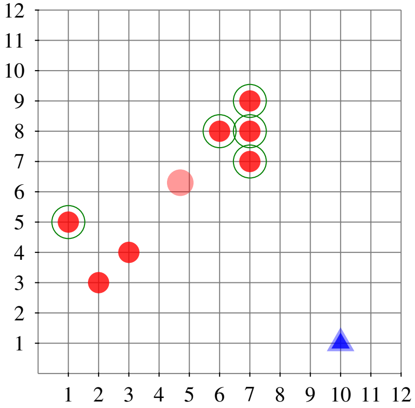
Alternative Run – Different Order



assign fifth point

k-means Clustering – MacQueen Algorithm

Alternative Run – Different Order



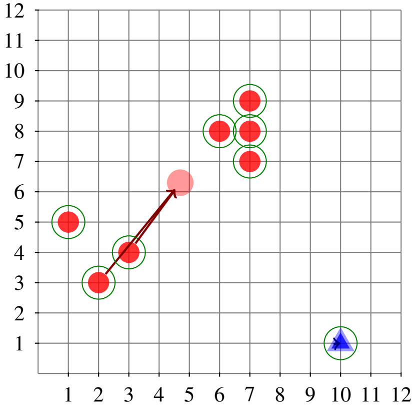
recompute centroids:

$\mu \approx (10.0, 1.0)$

$\mu \approx (4.7, 6.3)$

k-means Clustering – MacQueen Algorithm

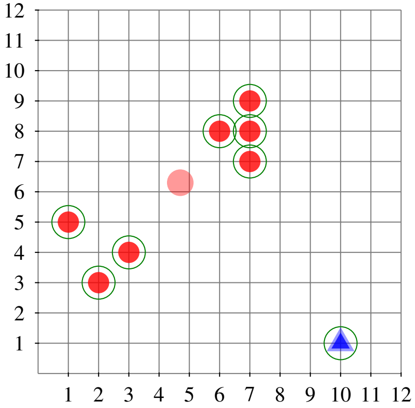
Alternative Run – Different Order



reasign more points

k-means Clustering – MacQueen Algorithm

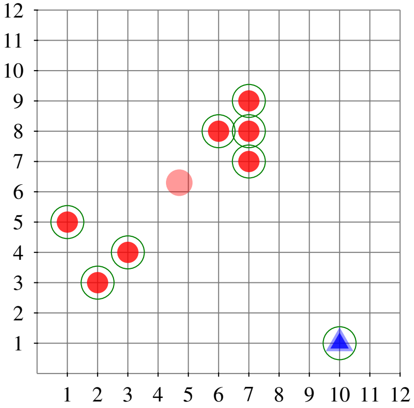
Alternative Run – Different Order



reasign more points
possibly more iterations

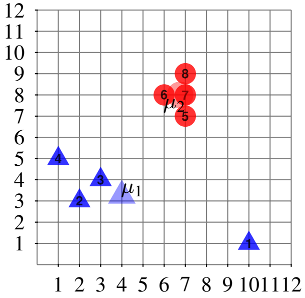
k-means Clustering – MacQueen Algorithm

Alternative Run – Different Order



reasign more points
possibly more iterations
convergence

k-means Clustering – Quality



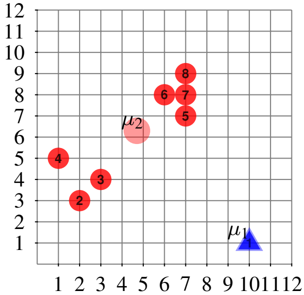
$$SSQ(\mu_1, p_1) = |4-10|^2 + |3.25-1|^2 = 36 + 5\tfrac{1}{16} = 41\tfrac{1}{16}$$
$$SSQ(\mu_1, p_2) = |4-2|^2 + |3.25-3|^2 = 4 + \tfrac{1}{16} = 4\tfrac{1}{16}$$
$$SSQ(\mu_1, p_3) = |4-3|^2 + |3.25-4|^2 = 1 + \tfrac{9}{16} = 1\tfrac{9}{16}$$
$$SSQ(\mu_1, p_4) = |4-1|^2 + |3.25-5|^2 = 9 + 3\tfrac{1}{16} = 12\tfrac{1}{16}$$
$$TD^2(C_1) = 58\tfrac{3}{4}$$

$$SSQ(\mu_2, p_5) = |6.75-7|^2 + |8-7|^2 = \tfrac{1}{16} + 1 = 1\tfrac{1}{16}$$
$$SSQ(\mu_2, p_6) = |6.75-6|^2 + |8-8|^2 = \tfrac{9}{16} + 0 = \tfrac{9}{16}$$
$$SSQ(\mu_2, p_7) = |6.75-7|^2 + |8-8|^2 = \tfrac{1}{16} + 0 = \tfrac{1}{16}$$
$$SSQ(\mu_2, p_8) = |6.75-7|^2 + |8-9|^2 = \tfrac{1}{16} + 1 = 1\tfrac{1}{16}$$
$$TD^2(C_2) = 2\tfrac{3}{4}$$

First solution: $TD^2 = 61\tfrac{1}{2}$

Note: $SSQ(\mu, p) = \mathit{Euclidean}(\mu, p)^2 = L_2^2(\mu, p)$.

k-means Clustering – Quality



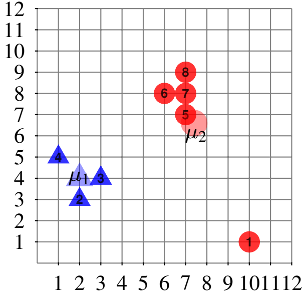
$SSQ(\mu_1, p_1) = |10 - 10|^2 + |1 - 1|^2 = 0$
$TD^2(C_1) = 0$

$SSQ(\mu_2, p_2) \approx |4.7 - 2|^2 + |6.3 - 3|^2 \approx 18.2$
$SSQ(\mu_2, p_3) \approx |4.7 - 3|^2 + |6.3 - 4|^2 \approx 8.2$
$SSQ(\mu_2, p_4) \approx |4.7 - 1|^2 + |6.3 - 5|^2 \approx 15.4$
$SSQ(\mu_2, p_5) \approx |4.7 - 7|^2 + |6.3 - 7|^2 \approx 5.7$
$SSQ(\mu_2, p_6) \approx |4.7 - 6|^2 + |6.3 - 8|^2 \approx 4.6$
$SSQ(\mu_2, p_7) \approx |4.7 - 7|^2 + |6.3 - 8|^2 \approx 8.2$
$SSQ(\mu_2, p_7) \approx |4.7 - 7|^2 + |6.3 - 9|^2 \approx 12.6$
$TD^2(C_2) \approx 72.86$

First solution: $TD^2 = 61\frac{1}{2}$
Second solution: $TD^2 \approx 72.68$

Note: $SSQ(\mu, p) = \textit{Euclidean}(\mu, p)^2 = L_2^2(\mu, p)$.

k-means Clustering – Quality



$$SSQ(\mu_1, p_2) = |2-2|^2 + |4-3|^2 = 0 + 1 = 1$$
$$SSQ(\mu_1, p_3) = |2-3|^2 + |4-4|^2 = 1 + 0 = 1$$
$$SSQ(\mu_1, p_4) = |2-1|^2 + |4-5|^2 = 1 + 1 = 2$$
$$TD^2(C_1) = 4$$

$$SSQ(\mu_2, p_1) = |7.4-10|^2 + |6.6-1|^2 = 6\tfrac{19}{25} + 31\tfrac{9}{25} = 38\tfrac{3}{25}$$
$$SSQ(\mu_2, p_5) = |7.4-7|^2 + |6.6-7|^2 = \tfrac{4}{25} + \tfrac{4}{25} = \tfrac{8}{25}$$
$$SSQ(\mu_2, p_6) = |7.4-6|^2 + |6.6-8|^2 = 1\tfrac{24}{25} + 1\tfrac{24}{25} = 3\tfrac{23}{25}$$
$$SSQ(\mu_2, p_7) = |7.4-7|^2 + |6.6-8|^2 = \tfrac{4}{25} + 1\tfrac{24}{25} = 2\tfrac{3}{25}$$
$$SSQ(\mu_2, p_8) = |7.4-7|^2 + |6.6-9|^2 = \tfrac{4}{25} + 5\tfrac{19}{25} = 5\tfrac{23}{25}$$
$$TD^2(C_2) = 50\tfrac{2}{5}$$

First solution: $TD^2 = 61\frac{1}{2}$
Second solution: $TD^2 \approx 72.68$
Optimal solution: $TD^2 = 54\frac{2}{5}$

Note: $SSQ(\mu, p) = \textit{Euclidean}(\mu, p)^2 = L_2^2(\mu, p)$.

Outline

Discussion

pros

- efficient: $\mathcal{O}(k \cdot n)$ per iteration, number of iterations is usually in the order of 10.
- easy to implement, thus very popular

cons

- k-means converges towards a *local* minimum
- k-means (MacQueen-variant) is order-dependent
- deteriorates with noise and outliers (all points are used to compute centroids)
- clusters need to be convex and of (more or less) equal extension
- number k of clusters is hard to determine
- strong dependency on initial partition (in result quality as well as runtime)

Summary

You learned in this section:

- *What is Clustering?*
- *Basic idea for identifying "good" partitions into k clusters*
- *selection of representative points*
- *iterative refinement*
- *local optimum*
- k*-means variants [Forgy, 1965, Lloyd, 1982, MacQueen, 1967]*

References I

M. M. Deza and E. Deza. *Encyclopedia of Distances*. Springer, 3rd edition, 2009. ISBN 9783662443415.

E. W. Forgy. Cluster analysis of multivariate data: efficiency versus interpretability of classifications. *Biometrics*, 21:768–769, 1965.

S. P. Lloyd. Least squares quantization in PCM. *IEEE Transactions on Information Theory*, 28(2):129–136, 1982. doi: 10.1109/TIT.1982.1056489.

J. MacQueen. Some methods for classification and analysis of multivariate observations. In *5th Berkeley Symposium on Mathematics, Statistics, and Probabilistics*, volume 1, pages 281–297, 1967.

P.-N. Tan, M. Steinbach, and V. Kumar. *Introduction to Data Mining*. Addison Wesley, 2006.