technische universität
dortmund

Computational Intelligence

Winter Term 2021/22

Prof. Dr. Günter Rudolph

Lehrstuhl für Algorithm Engineering (LS 11)

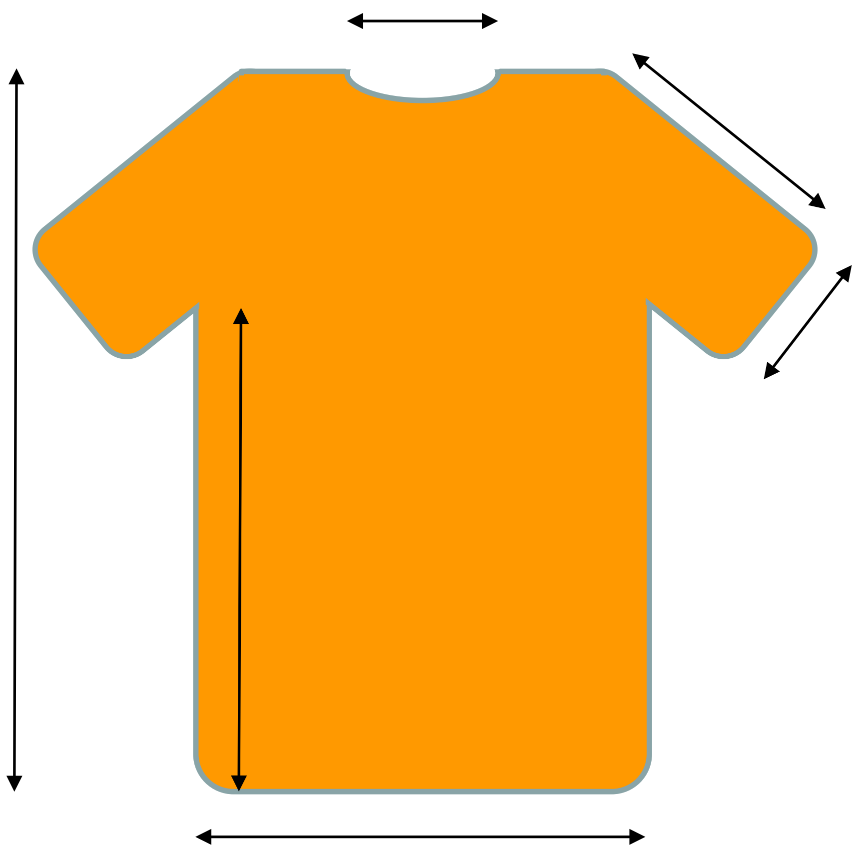
Fakultät für Informatik

TU Dortmund

- Fuzzy Clustering

Introductory Example: Textile Industry

→ production of T-shirts (for men)



best for producer : one size

vs.

best for consumer: made-to-measure

⇒ compromize: S, M, L, XL, 2XL

5 sizes

→ OK, but which lengths for which size?

idea:

- select, say, 2000 men at random and measure their “body lengths“
- arrange these 2000 men into five disjoint groups

  such that

  – deviations from mean of group as small as possible

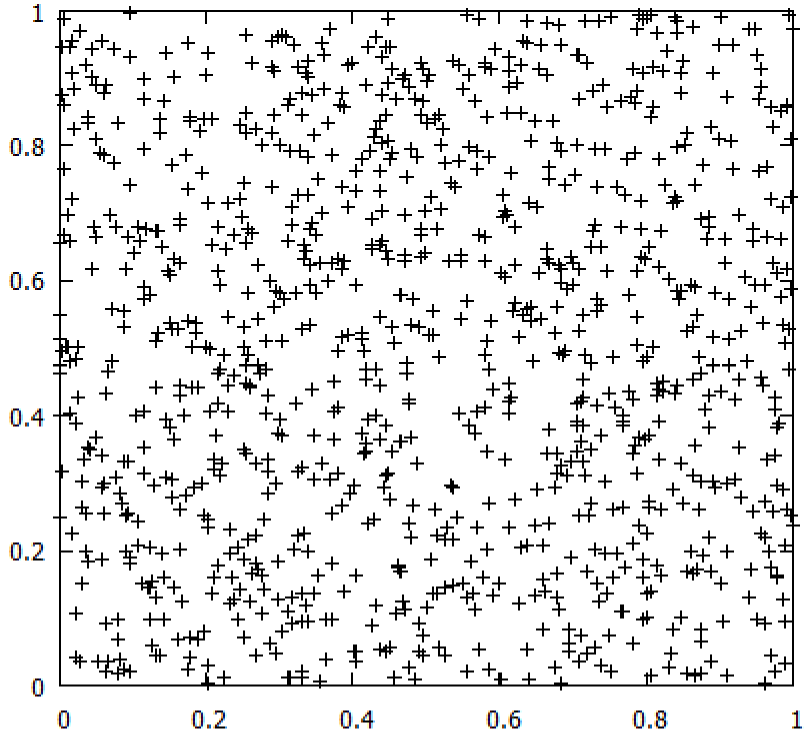
  – differences between group means as large as possible

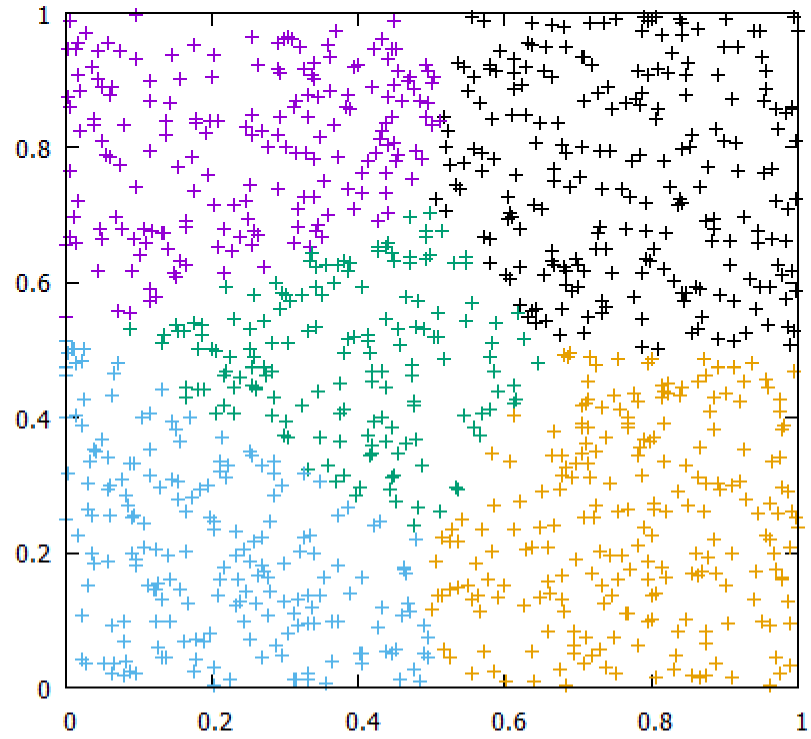
arm‘s length, collar size, chest girth, …

in general:

arrange objects into groups / clusters
such that
– elements within a cluster are as homogeneous as possible
– elements across clusters are as heterogeneous as possible

numerical example: 1000 points uniformly sampled in [0,1] x [0,1] $\rightarrow$ form 5 cluster





given data points $x_1, x_2, \ldots, x_N \in \mathbb{R}^n$

<u>objective:</u> group data points into cluster such that
- *points within cluster* are as *homogeneous* as possible
- *points across clusters* are as *heterogeneous* as possible

⇒ crisp clustering is just a partitioning of data set $\{ x_1, x_2, \ldots, x_N \}$, i.e.,

$$\bigcup_{k=1}^{K} C_k = \{ x_1, x_2, \ldots, x_N \} \quad \text{and} \quad \forall j \neq k : C_j \cap C_k = \emptyset$$

where C_k is Cluster k and K denotes the number of clusters.

Constraint: $\forall k = 1, \ldots, K : |C_k| \geq 1$ hence $1 \leq K \leq N$

Complexity: How many choices to assign N objects into K clusters?

more precisely:

→ objects are distinguishable / labeled

→ clusters are nondistinguishable / unlabeled **and** nonempty

⇒ Stirling number of 2nd kind $S(\mathrm{N}, K) = \frac{1}{K!} \sum_{i=1}^{K} (-1)^{K-i} \binom{K}{i} \cdot i^{\mathrm{N}} \sim \frac{K^{\mathrm{N}}}{K!}$

N/K	1	2	3	4	5
10	1	511	9,330	34,105	42,525
11	1	1,023	28,501	145,750	246,730
12	1	2,047	86,526	611,501	1,379,400
13	1	4,095	261,625	2,532,530	7,508,501
14	1	8,191	788,970	10,391,745	40,075,035
15	1	16,383	2,375,101	42,355,950	210,766,920

$S(100, 5) = 6.6 \times 10^{67}$

$S(1000, 5) = 7.8 \times 10^{696}$

$S(2000, 5) = 7.3 \times 10^{1395}$

⇒ enumeration hopeless! ⇒ iterative improvement procedure required!

idea: define objective function

that measures compactness of clusters *and* quality of partition

→ elements in cluster C_j should be as homogeneous as possible!

→ sum of squared distances to unknown center y should be as small as possible

→ find y with $\sum_{i \in C_j} d(x_i, y)^2 \to \min!$

typically, $d(x_i, y) = \|x_i - y\| = \sqrt{(x_i - y)'(x_i - y)}$ (Euclidean norm)

$$\frac{d}{dy} \sum_{i \in C_j} (x_i - y)'(x_i - y) \;=\; -2 \sum_{i \in C_j} (x_i - y) \;\stackrel{!}{=}\; 0$$

$$\Rightarrow \sum_{i \in C_j} x_i \stackrel{!}{=} \sum_{i \in C_j} y = |C_j| \cdot y \qquad \Rightarrow y = \frac{1}{|C_j|} \sum_{i \in C_j} x_i \;=: \bar{x}_j$$

→ elements in <u>each</u> cluster C_j should be as homogeneous as possible!

→ find partition $C = (C_1, \ldots, C_K)$ with $D(C) = \sum_{j=1}^{K} \sum_{i \in C_j} d(x_i, \bar{x}_j)^2 \to \min!$

Definition

A partition C^* is optimal if

$$D(C^*) = \min\{\, D(C) \,:\, C \in P(\mathsf{N}, K) \,\}$$

where $P(\mathsf{N}, K)$ denotes all partitions of N elements in K clusters.

Theorem

$$\min_{C \in P(\mathsf{N},K)} D(C) \;=\; \max_{C \in P(\mathsf{N},K)} \sum_{j=1}^{K} |C_j| \cdot \|\bar{x}_j - \bar{x}\|$$

where $\bar{x}$ is the mean of all x.

Crisp K-Means Clustering

$\forall k = 1, \ldots, K$: set $C_k = \emptyset$

$\forall x \in \{x_1, \ldots, x_N\}$: assign x to some cluster C_k

set $t = 0$ and $D^{(t)} = \infty$

```
repeat
```

$t = t + 1$

$\forall k = 1, \ldots, K$: $\bar{x}_k = \dfrac{1}{|C_k|} \sum_{x \in C_k} x$

$\forall i = 1, \ldots, N$: $d_{ik} = d(x_i, \bar{x}_k)$ distance to center of cluster k

let k^* be such that $d_{ik^*} = \min\{d_{ik} : k = 1, \ldots, K\}$

assign x_i to C_{k^*}

$$D^{(t)} = \sum_{k=1}^{K} \sum_{x \in C_k} d(x, \bar{x}_k)$$

`until` $D^{(t-1)} - D^{(t)} < \varepsilon$

objective for **crisp** clustering:

find partition $C = (C_1, \ldots, C_K)$ with $D(C) = \sum_{j=1}^{K} \sum_{i \in C_j} d(x_i, \bar{x}_j)^2 \rightarrow \min!$

$\rightarrow$ rewrite objective:

find partition $C = (C_1, \ldots, C_K)$ with $D(C) = \sum_{j=1}^{K} \sum_{i=1}^{N} u_{ij} \cdot d(x_i, \bar{x}_j)^2 \rightarrow \min!$

expresses membership $\longrightarrow$ $u_{ij} = \begin{cases} 1 & \text{if } x_i \in C_j \\ 0 & \text{otherwise} \end{cases}$

objective for **fuzzy** clustering:

find partition $C = (C_1, \ldots, C_K)$ with $D(C) = \sum_{j=1}^{K} \sum_{i=1}^{N} u_{ij}^m \cdot d(x_i, \bar{x}_j)^2 \rightarrow \min!$

$u_{ij} \in [0, 1] \subset \mathbb{R}, m > 1$

find partition $C = (C_1, \ldots, C_K)$ with $D(C) = \sum_{j=1}^{K} \sum_{i=1}^{N} u_{ij}^m \cdot d(x_i, \bar{x}_j)^2 \to \min!$

where

$u_{ij} \in [0,1] \subset \mathbb{R}$ denotes membership of x_i to cluster C_j

$m > 1$ denotes a fixed *fuzzifier* (controls / affects membership function)

subject to

$$\sum_{j=1}^{K} u_{ij} = 1 \qquad \forall i = 1, \ldots, N$$

each x_i distributes membership completely over clusters $C_1, \ldots, C_K$
$\to$ normalization

$$0 < \sum_{i=1}^{N} u_{ij} < N \qquad \forall j = 1, \ldots, K$$

at least one element belongs to some extent to a certain cluster, but not all elements to a single cluster

<u>two questions:</u>

(a) how to define and calculate centers $\bar{x}_j$?

(b) how to obtain optimal memberships u_{ij}?

ad a) let $d(x_i, \bar{x}_j) = \| x_i - \bar{x}_j \|_2$

$$\frac{d}{d\bar{x}_j} \sum_{i=1}^{N} u_{ij}^m \cdot (x_i - \bar{x}_j)'(x_i - \bar{x}_j) = -2 \sum_{i=1}^{N} u_{ij}^m \cdot (x_i - \bar{x}_j) \stackrel{!}{=} 0$$

$$\Leftrightarrow \sum_{i=1}^{N} u_{ij}^m \, x_i \stackrel{!}{=} \sum_{i=1}^{N} u_{ij}^m \, \bar{x}_j \quad \Leftrightarrow \quad \boxed{\bar{x}_j = \frac{\sum_{i=1}^{N} u_{ij}^m \, x_i}{\sum_{i=1}^{N} u_{ij}^m}}$$

→ weighted mean!

ad b) let $d_{ij} := d(x_i, \bar{x}_j) = \| x_i - \bar{x}_j \|_2$

*apply **Lagrange multiplier** method:*

$$\frac{\partial}{\partial u_{ij}} \sum_{j=1}^{K} \sum_{i=1}^{N} u_{ij}^m \cdot d_{ij}^2 - \underbrace{\sum_{i=1}^{N} \lambda_i \left(\sum_{j=1}^{K} u_{ij} - 1 \right)}_{\text{without constraints} \rightarrow u_{ij}^* = 0} = m\, u_{ij}^{m-1} \cdot d_{ij}^2 - \lambda_i \stackrel{!}{=} 0$$

$$\Updownarrow$$

$$u_{ij}^* = \left(\frac{\lambda_i}{m \cdot d_{ij}^2} \right)^{\frac{1}{m-1}}$$

$$\sum_{j=1}^{K} u_{ij} = \sum_{j=1}^{K} \left(\frac{\lambda_i}{m \cdot d_{ij}^2} \right)^{\frac{1}{m-1}} = \sum_{j=1}^{K} \frac{\lambda_i^{\frac{1}{q}}}{(m \cdot d_{ij}^2)^{\frac{1}{q}}} = \lambda_i^{\frac{1}{q}} \sum_{j=1}^{K} \frac{1}{(m \cdot d_{ij}^2)^{\frac{1}{q}}} \stackrel{!}{=} 1$$

set $q = m - 1$

$$\Rightarrow \quad \lambda_i^* = \left[\sum_{k=1}^{K} \frac{1}{(m \cdot d_{ik}^2)^{\frac{1}{q}}} \right]^{-q}$$

after insertion:

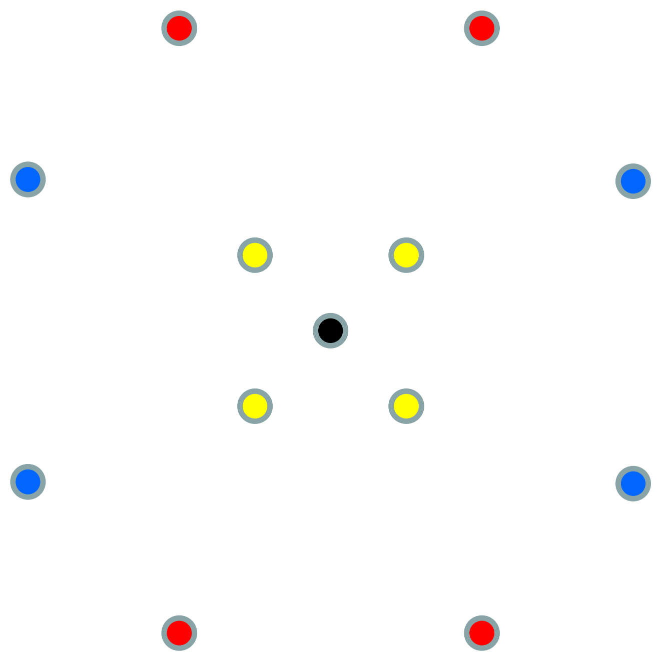
$$u^*_{ij} = \left(\frac{1}{m \cdot d^2_{ij}} \left[\frac{1}{\sum\limits_{k=1}^{K} \left(\frac{1}{m \cdot d^2_{ik}} \right)^{\frac{1}{m-1}}} \right]^{m-1} \right)^{\frac{1}{m-1}} = \left[\sum_{k=1}^{K} \left(\frac{d_{ij}}{d_{ik}} \right)^{\frac{2}{m-1}} \right]^{-1}$$

choose $K \in \mathbb{N}$ and $m > 1$
choose u_{ij} at random (obeying constraints)
repeat
  $\forall j = 1, \ldots, K$: calculate centers $\bar{x}_j$
  $\forall i = 1, \ldots, N$:
    let $J_i = \{ j : x_i = \bar{x}_j \}$
    if $J_i = \emptyset$ determine memberships u_{ij}
    else
      choose u_{ij} such that $\sum_{j \in J_i} u_{ij} = 1$
      and $u_{ij} = 0$ for $j \notin J_i$
until $D(C^{(t)}) - D(C^{(t+1)}) < \varepsilon$ or $t = t_{max}$

problems:

- <u>choice of K</u>
  calculate quality measure for each #cluster; then choose best
- <u>choice of *m*</u>
  try some values; typical: *m*=2; use interval → fuzzy type-2

Example: Special Case $|J_i| > 1$



black dot is center of

- red cluster
- blue cluster
- yellow cluster

in case of equal weights

$u_{ij} = 1 / |J_i|$ for $j \in J_i$ appears plausible

but: different values algorithmically better

→ cluster centers more likely to separate again (→ tiny randomization?)

- **Partition Coefficient**

$$\text{PC}(C_1, \ldots, C_K) = \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{K} u_{ij}^2$$

("larger is better")

maximum if $u_{ij} \in \{0, 1\}$ → crisp partition

minimum if $u_{ij} = \frac{1}{K}$ → entirely fuzzy

$$\frac{1}{K} \leq \text{PC}(C_1, \ldots, C_K) \leq 1$$

- **Partition Entropy**

$$\text{PE}(C_1, \ldots, C_K) = -\frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{K} u_{ij} \cdot \log_2(u_{ij})$$

("smaller is better")

maximum if $u_{ij} = \frac{1}{K}$ → entirely fuzzy

minimum if $u_{ij} \in \{0, 1\}$ → crisp partition

$$0 \leq \text{PE}(C_1, \ldots, C_K) \leq \log_2(K)$$