Computational Intelligence

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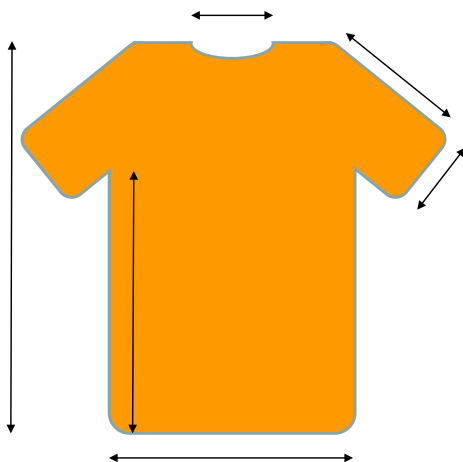
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- Fuzzy Clustering

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?

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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,
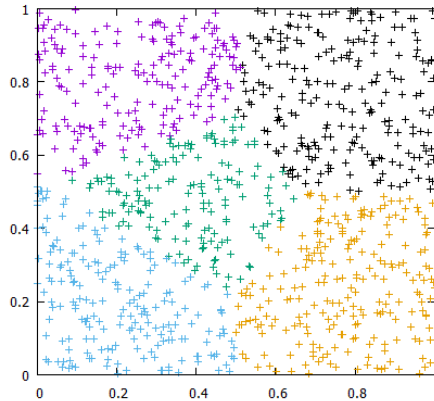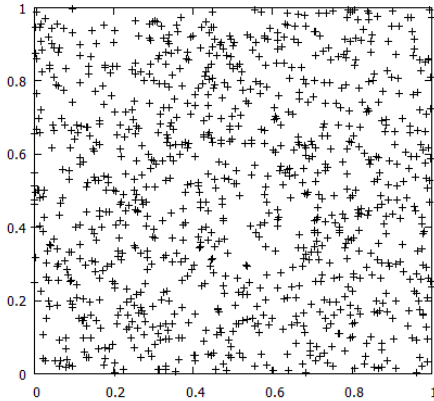collar size,
chest girth, …

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] → form 5 cluster

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

objective: 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 $\{ x_1, x_2, ..., x_N \}$, i.e.,

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

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 / labelled

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

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

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!

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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, $\quad d(x_i, y) = \|x_i - y\| = \sqrt{(x_i - y)'(x_i - y)} \quad$ (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

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

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

$\forall k = 1, \ldots, K$: 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 $D(C) = \sum_{j=1}^{K} \sum_{i \in C_j} d(x_i, \bar{x}_j)^2 \to \min!$

→ rewrite objective:

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

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

objective for **fuzzy** clustering:

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

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

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 $C_1, \ldots, C_K$ → 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

two questions:

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

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

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

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

$$\Leftrightarrow \sum_{i=1}^{N} u_{ij}^m x_i \overset{!}{=} \sum_{i=1}^{N} u_{ij}^m \bar{x}_j \qquad \Leftrightarrow \qquad \boxed{\bar{x}_j = \frac{\sum_{i=1}^{N} u_{ij}^m x_i}{\sum_{i=1}^{N} u_{ij}^m}} \qquad \rightarrow \text{ weighted mean!}$$

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

*apply **Lagrange multiplier** method:*

$$\frac{\partial}{\partial u_{ij}} \sum_{j=1}^{K} \sum_{i=1}^{N} u_{ij}^m \cdot d_{ij}^2 - \sum_{i=1}^{N} \lambda_i \left(\sum_{j=1}^{K} u_{ij} - 1 \right) = m\, u_{ij}^{m-1} \cdot d_{ij}^2 - \lambda_i \overset{!}{=} 0$$

without constraints $\rightarrow u_{ij}^* = 0$

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

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

set $q = m - 1$

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

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after insertion:

$$u_{ij}^* = \left(\frac{1}{m \cdot d_{ij}^2} \left[\frac{1}{\sum_{k=1}^{K} \left(\frac{1}{m \cdot d_{ik}^2} \right)^{\frac{1}{m-1}}} \right]^{m-1} \right)^{\frac{1}{m-1}} = \boxed{\left[\sum_{k=1}^{K} \left(\frac{d_{ij}}{d_{ik}} \right)^{\frac{2}{m-1}} \right]^{-1}}$$

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 $J_i = \{ j : x_i = \bar{x}_j \}$
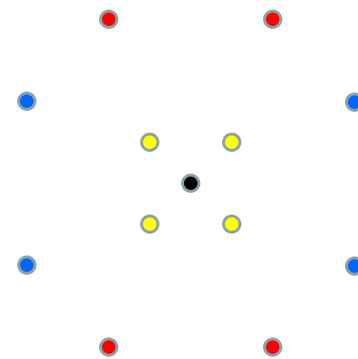　　　　if $J_i = \emptyset$ determine memberships u_{ij}
　　　　else
　　　　　　choose u_{ij} such that $\sum_{j \in J_i} u_{ij} = 1$
　　　　　　and $u_{ij} = 0$ for $j \notin J_i$
until $D(C^{(t)}) - D(C^{(t+1)}) < \varepsilon$ or $t = t_{max}$

problems:

- choice of *K*
  calculate quality measure
  for each #cluster;
  then choose best

- choice of *m*
  try some values;
  typical: *m*=2;
  use interval → fuzzy type-2

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black dot is center of

- red cluster
- blue cluster
- yellow cluster

in case of equal weights

u_{ij} = 1 / |J_i| for j ∈ J_i appears plausible

but: different values algorithmically better

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

- **Partition Coefficient**

$$\mathsf{PC}(C_1, \ldots, C_K) \;=\; \frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{K} u_{ij}^2 \qquad\qquad (\text{``larger is better''})$$

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

minimum if $u_{ij} = \dfrac{1}{K}$ $\rightarrow$ entirely fuzzy

$$\left.\rule{0pt}{40pt}\right\} \qquad \frac{1}{K} \leq \mathsf{PC}(C_1, \ldots, C_K) \leq 1$$

- **Partition Entropy**

$$\mathsf{PE}(C_1, \ldots, C_K) \;=\; -\frac{1}{N} \sum_{i=1}^{N} \sum_{j=1}^{K} u_{ij} \cdot \log_2(u_{ij}) \qquad (\text{``smaller is better''})$$

maximum if $u_{ij} = \dfrac{1}{K}$ $\rightarrow$ entirely fuzzy

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

$$\left.\rule{0pt}{40pt}\right\} \qquad 0 \leq \mathsf{PE}(C_1, \ldots, C_K) \leq \log_2(K)$$