

The non-linear impact of the scaling factor α on the outcomes of Semi-Supervised Fuzzy C-Means

Kamil Kmita Katarzyna Kaczmarek-Majer Olgierd Hryniewicz

Systems Research Institute Polish Academy of Sciences, Warsaw, Poland

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Fuzzy clustering - finding good c -partitions

Clustering: partitioning data set X into c clusters that contain observations **similar** to each other and dissimilar to the rest of the data,

Fuzzy clustering: uses a soft assignment of each observation to each cluster (a **membership degree** u_{jk}) that is grounded in fuzzy set theory.

Fuzzy c -partition space¹

Let X be any finite set, c a number of clusters $2 \leq c < N$, W_{Nc} a set of real matrices of $N \times c$ dimension. Then a **fuzzy c -partition space** for X is the set

$$M_{fc} = \left\{ U \in W_{Nc} \mid u_{jk} \in [0, 1]; \sum_{k=1}^c u_{jk} = 1 \forall j; \quad 0 < \sum_{j=1}^N u_{jk} < n \forall k \right\} \quad (1)$$

¹James C. Bezdek. *Pattern Recognition with Fuzzy Objective Function Algorithms*.

Springer US, Boston, MA, 1981



An illustrative example of a fuzzy 2-partition

$$X = \{x_1, x_2, x_3\}, x_j \in R^p.$$

$$j = 1, \dots, 3; N = 3.$$

$$k \in \{1, 2\}; c = 2.$$

A possible fuzzy 2-partition:

$$U = \begin{array}{cc} & k = 1 & k = 2 \\ \begin{array}{c} x_1 \\ x_2 \\ x_3 \end{array} & \left(\begin{array}{cc} 0.98 & 0.02 \\ 0.6 & 0.4 \\ 0.06 & 0.94 \end{array} \right) \end{array}$$

Observation x_1 belongs strongly to cluster 1, observation x_3 belongs strongly to cluster 2, while observation x_2 seems to be a “hybrid”: it belongs to both clusters to similar degree.



Struggling with imagining a “hybrid”?

A classical example from [Bez81]:

- x_1 : a peach,
- x_3 : a plum,
- x_2 : a nectarine, **supposedly** a hybrid of a peach and a plum.

Supposedly...

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Supposedly... because it turns out to be a controversial topic, e.g.

<http://www.bctreefruits.com/fruits/other-fruits/detail/0/Nectarines/> state
“There is some misconception that nectarines are a cross between a peach and a plum, **but this is not the case. They’re simply a fuzzless peach.**”

Unreal (?), but proper hybrid



- x_1 : a butterfly,
- x_3 : an elephant,
- x_2 : a butterphant,
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Figure: A butterphant. Source: https://www.boredpanda.com/animals-hybrids-photoshop/?media_id=321587

Semi-supervised fuzzy clustering

- Semi-Supervised Learning (SSL)²: labels $y_j \in Y$ are available for a part of observations M out of all N observations ($M < N$),
- an arbitrary 1-1 mapping must be established between clusters (columns of U) and classes (columns of F).

$$U = \begin{matrix} & k=1 & k=2 \\ \begin{matrix} x_1 \\ x_2 \\ x_3 \end{matrix} & \begin{bmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \\ u_{31} & u_{32} \end{bmatrix} \end{matrix} \quad F = \begin{matrix} & k=1 & k=2 & s(i) \\ \begin{matrix} x_1 \\ x_2 \\ x_3 \end{matrix} & \begin{bmatrix} 1 & 0 \\ 0 & 0 \\ 0 & 1 \end{bmatrix} & \begin{matrix} s(1) = 1 \\ \\ s(3) = 2 \end{matrix} \end{matrix}$$

Function $s(i)$ retrieves the index of the class (a column in F) associated with i -th supervised observation.

²Olivier Chapelle, Bernhard Schölkopf, and Alexander Zien, editors. *Semi-Supervised Learning*.

Adaptive Computation and Machine Learning. MIT Press, Cambridge, Mass, 2006

Semi-Supervised Fuzzy C-Means (SSFCMeans) model

Objective function J based on [PW97]³ introducing *partial supervision*

$$J = \sum_{k=1}^c \sum_{j=1}^N u_{jk}^2 \cdot d^2(x_j, v_k) + \alpha \sum_{k=1}^c \sum_{j=1}^N \underbrace{(u_{jk} - b_j f_{jk})^2}_{\text{penalization}} \cdot d^2(x_j, v_k).$$

- $u_{jk} \in [0, 1]$ is a membership degree
- $d_{jk} = d(x_j, v_k)$ is a Euclidean distance between j th observation and k th prototype v_k ,
- $F = [f_{jk}]$ is a matrix introducing partial supervision with binary entries $f_{jk} \in \{0, 1\}$,
- $b_j \in \{0, 1\}$ is an indicator variable equal to 1 iff x_j is labeled,
- $\alpha \geq 0$ is a scaling factor that weighs the strength of partial supervision.

³W. Pedrycz and J. Waletzky. [Fuzzy clustering with partial supervision](#).

IEEE Transactions on Systems, Man, and Cybernetics, Part B (Cybernetics), 27(5):787–795, October 1997

Finding optimal c -partitions

Notation:

- $X = [x_j]$, $x_j \in R^p$
- $U \in W_{Nc}$: a memberships matrix,
- $V \in W_{cp}$: a prototypes matrix (k -th cluster is associated with its prototype $v_k \in R^p$),
- Θ : a set of hyper-parameters.

Task:

$$(U^*, V^*) = \arg \min_{U, V} J(U, V; X, \Theta), \quad (2)$$

where objective function J quantifies a notion of similarity between observations and prototypes (*typically, using a distance function such as e.g. Euclidean distance*).

Optimal \hat{U} 

An iterative optimization algorithm is frequently performed. Optimal $\hat{U} = [\hat{u}_{jk}]$ matrix is obtained by considering first-order necessary conditions of a global minimizer, leading to

$$\hat{u}_{jk} = \frac{1}{1 + \alpha} \cdot \left(\frac{1 + \alpha \cdot (1 - b_j \sum_{s=1}^c f_{js})}{\sum_{s=1}^c (d_{jk}^2 / d_{js}^2)} + \alpha f_{jk} b_j \right). \quad (3)$$

In a case of a supervised observation i and its membership degree to the supervised cluster $s(i)$

$$\hat{u}_{i,s(i)} = \frac{1}{1 + \alpha} \cdot \frac{1}{\sum_{s=1}^c (d_{ik}^2 / d_{is}^2)} + \frac{\alpha}{1 + \alpha}. \quad (4)$$

Interpretations of the scaling factor α

objective function	$\sum_{k=1}^c \sum_{j=1}^N u_{jk}^2 d_{jk}^2 + \alpha \sum_{k=1}^c \sum_{j=1}^N \underbrace{(u_{jk} - b_j f_{jk})^2}_{\text{penalization}} d_{jk}^2.$
optimal membership $\hat{u}_{i,s(i)}$	$\frac{1}{1+\alpha} \cdot \frac{1}{\sum_{s=1}^c \left(d_{ik}^2 / d_{is}^2 \right)} + \underbrace{\frac{\alpha}{1+\alpha}}_{\text{ALB}}$

- [PW97, p. 788] “a scaling factor whose role is **to maintain a balance** between the supervised and unsupervised component”,
- “The scaling factor α quantifies the **impact of partial supervision** as $\text{IPS}(\alpha) = \frac{\alpha}{1+\alpha}$, and establishes an Absolute Lower Bound for a membership of a supervised observation to the supervised cluster $u_{i,s(i)} > \text{IPS}(\alpha)$ ”⁴.

⁴K. Kmita, K. Kaczmarek-Majer, O. Hryniewicz, [Explainable Impact of Partial Supervision in Semi-Supervised Fuzzy Clustering](#), *manuscript under review*

Experiments on real-life data

Data for this work were collected from patients diagnosed with bipolar disorder within a prospective observational study⁵ carried out by the Institute for Psychiatry and Neurology and Systems Research Institute, Polish Academy of Sciences in Warsaw, Poland in years 2017-2018.

- $N = 1295$ summaries of phone calls (indexed by $j = 1, \dots, N$),
- each phone call's summary $x_j \in R^5$. The 5 selected variables include physical descriptors of speech (e.g. jitter),
- $M = 261$ phone calls are treated as supervised (indexed by $i = 1, \dots, M$),
- $Y = \{\text{depression, mixed, euthymia, dysfunction}\}$,

class	depression	mixed	euthymia	dysfunction
#	58	55	85	63

⁵The study obtained the consent of the Bioethical Commission at the District Medical Chamber in Warsaw (agreement no. KB/1094/17)

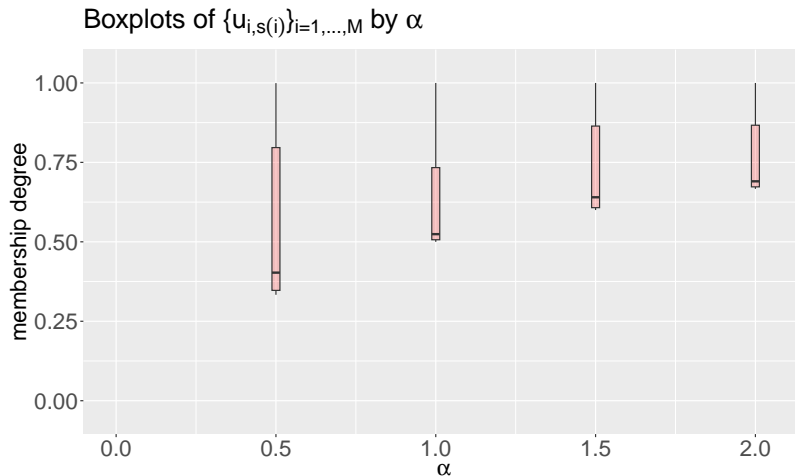
Results of SSFCMeans models by α - single observation

Results for a given observation $x_{i=3}$ for 4 SSFCMeans(α) models, $\alpha \in \{0.5, 1., 1.5, 2.\}$.

i	alpha	IPS	y_i	depression	mixed	euthymia	dysfunction
3	0.50	0.33	depression	0.95	0.01	0.03	0.01
3	1.00	0.50	depression	0.90	0.05	0.02	0.03
3	1.50	0.60	depression	0.90	0.03	0.05	0.02
3	2.00	0.67	depression	0.91	0.05	0.03	0.02

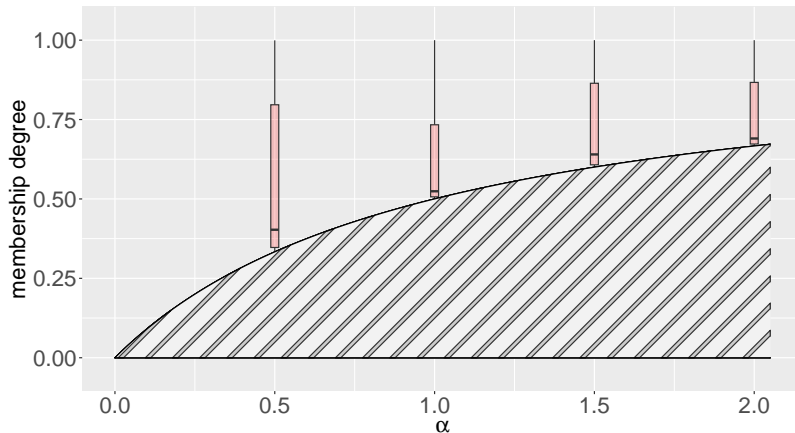
The blue color marks $u_{i,s(i)}$: a membership of a supervised observation $i = 3$ to the supervised cluster $s(i) = 1$.

Results of SSFCMeans models by α - a summary



Results of SSFCMeans models by α - a summary

Boxplots of $\{u_{i,s(i)}\}_{i=1,\dots,M}$ by α with $\text{IPS}(\alpha)$





The non-linear impact of α on outcomes of SSFCmeans

What if we are unhappy with the functional form $\text{IPS}(\alpha) = \frac{\alpha}{1+\alpha}$?

The form of IPS function is a result of⁶:

- the iterative optimization algorithm,
- the Lagrange multipliers technique,
- functional form of the objective function J ,
- the constraint $\sum_{k=1}^c u_{jk} = 1 \forall j$.

⁶K. Kmita, K. Kaczmarek-Majer, O. Hryniewicz, [Explainable Impact of Partial Supervision in Semi-Supervised Fuzzy Clustering](#), *manuscript under review*



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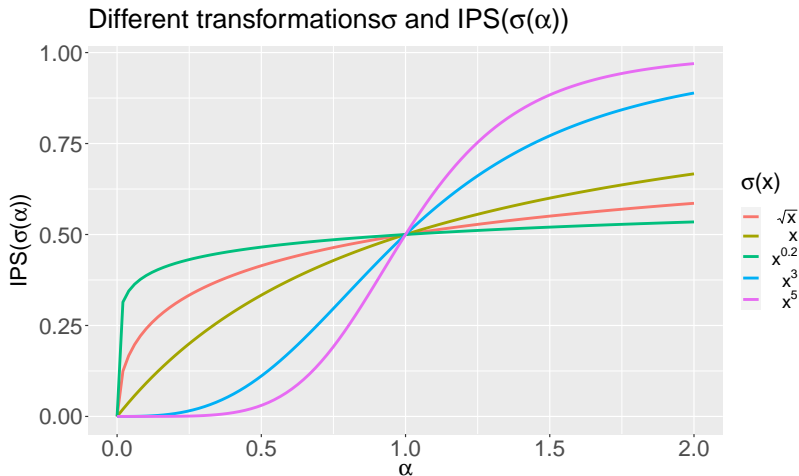
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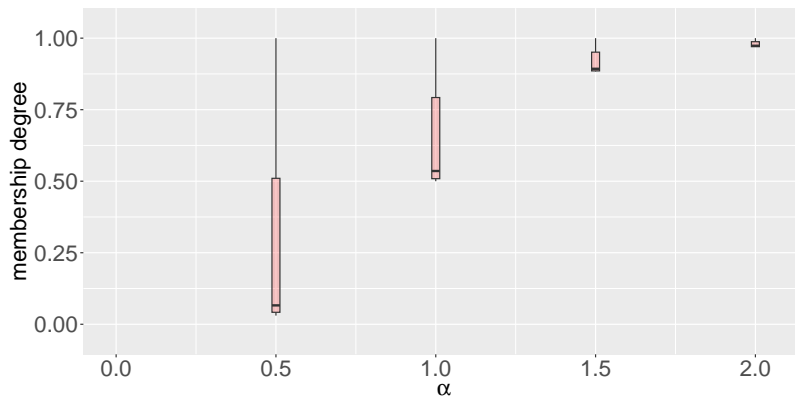
- the iterative optimization algorithm,
- the Langrange multipliers technique,
- functional form of the objective function J ,
- the constraint $\sum_{k=1}^c u_{jk} = 1 \forall j$.

But we could simply consider transformations $\sigma(\alpha)$, sustaining all of the above!

⁶K. Kmita, K. Kaczmarek-Majer, O. Hryniewicz, [Explainable Impact of Partial Supervision in Semi-Supervised Fuzzy Clustering](#), *manuscript under review*

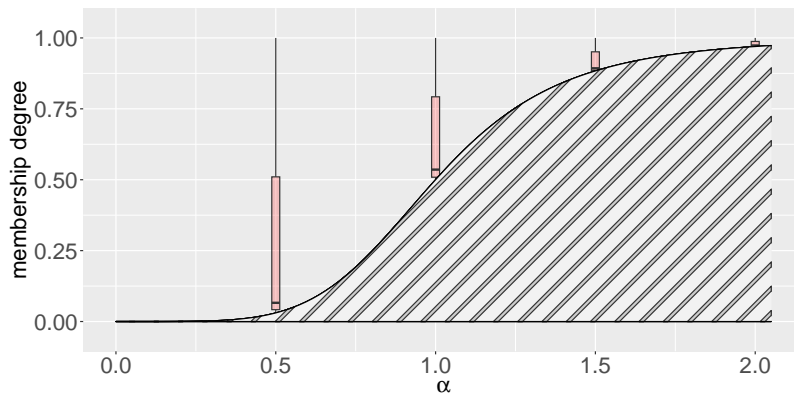
Simulations



Results for SSFCMeans models by α : $\sigma(\alpha) = \alpha^5$ Boxplots of $\{u_{i,s(i)}\}_{i=1,\dots,M}$ by α $\sigma(\alpha) = \alpha^5$ 

Results for SSFCMeans models by α : $\sigma(\alpha) = \alpha^5$ Boxplots of $\{u_{i,s(i)}\}_{i=1,\dots,M}$ by α with $\text{IPS}(\sigma(\alpha))$

$$\sigma(\alpha) = \alpha^5$$



Conclusions



- We have shown the differences in interpretation of the scaling factor α in SSCMeans;
- the impact of α on the estimated $\hat{u}_{i,s(i)}$ is non-linear and scales as $\text{IPS}(\alpha) = \frac{\alpha}{1+\alpha}$;
- it is hard to change the functional form of IPS, but one can adjust it by considering transformations $\sigma(\alpha)$.

Why it matters?

- 1 explainability, using $\hat{u}_{i,s(i)}$ in advanced procedures building on SSFCMeans,
- 2 the way α enters the objective function matters for the optimal prototypes as well (further research directions).

Thank you for your attention!

kmita@ibspan.waw.pl

<https://kamilkmita.com>

<http://bipolar.ibspan.waw.pl>

<https://github.com/ITPsychoiatry/bipolar>

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