A family of adaptive fuzzy clustering models

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Introduction

- There exist evergreen mathematical problems in AI as well
- I was in the kindergarten when we studied the new algorithm of Bezdek, the fuzzy c-means clustering
- I decided that I would try to find the best c-means clustering model
- Goals
  - Create the c-means clustering model that produces fine partitions on any data and any possibles circumstances. The fewer exceptions the better.
- Limitations
  - Stay within the bounds of alternating optimization of a quadratic objective function
  - Using zero gradient conditions and Lagrange multipliers only, no numerical approximations

Where are we now?

- The PFCM algorithm is one of the best existing models
- Uses a mixed partition, linear combination of probabilistic and possibilistic ones
- The possibilistic partition strongly depends on the constant penalty terms established at initialization
- Proposing a modification that would allow us to update the penalty terms in every optimization cycle
- This way our model could adapt the penalty terms to the data and circumstances
- Expecting better performances

$$\mathbb{N}_a = \{1, 2, \ldots, a\}$$

Fuzzy c-means (FCM)

- Bezdek (1981)
- Objective function

$$J_{\mathrm{FCM}} = \sum_{i=1}^{c}\sum_{k=1}^{n} u_{ik}^{m}\|\mathbf{x}_k - \mathbf{v}_i\|^2 = \sum_{i=1}^{c}\sum_{k=1}^{n} u_{ik}^{m} d_{ik}^2$$

- Probabilistic constraints

$$\begin{cases} 0 \le u_{ik} \le 1, & \forall i \in \mathbb{N}_c, \forall k \in \mathbb{N}_n \\ \sum_{i=1}^{c} u_{ik} = 1, & \forall k \in \mathbb{N}_n \end{cases}$$

- Alternating optimization
- Partition update formula

$$u_{ik} = \frac{d_{ik}^{-2/(m-1)}}{\sum_{j=1}^{c} d_{jk}^{-2/(m-1)}} \qquad \begin{matrix} \forall i \in \mathbb{N}_c \\ \forall k \in \mathbb{N}_n \end{matrix}$$

- Cluster prototype update formula

$$\mathbf{v}_i = \frac{\sum_{k=1}^{n} u_{ik}^{m}\mathbf{x}_k}{\sum_{k=1}^{n} u_{ik}^{m}} \qquad \forall i \in \mathbb{N}_c$$

FCM evaluation

- Simple, stable, very popular
- Sensitive to noise
  - A true outlier belongs to each class with 1/c probability, which can damage the partition

$$\mathbf{v}_i = \frac{\sum_{k=1}^{n} u_{ik}^{m} \mathbf{x}_k}{\sum_{k=1}^{n} u_{ik}^{m}} \qquad \forall i \in \mathbb{N}_c$$

- Reason:
  - The probabilistic constraint is too strong
  - Needs to be relaxed

Fuzzy (c+1)-means

- Davé (1991)
- Objective function

$$d_{0k} = d_0 \qquad \forall k \in \mathbb{N}_n$$

$$J_{\mathrm{F(C+1)M}} = \sum_{k=1}^{n} \left(u_{0k}^{m} \cdot d_0^2 + \sum_{i=1}^{c} u_{ik}^{m} \cdot d_{ik}^2 \right)$$

- Constraints

$$\begin{cases} 0 \le u_{ik} \le 1, & \forall i \in \mathbb{N}_c^0, \forall k \in \mathbb{N}_n \\ \sum_{i=0}^{c} u_{ik} = 1, & \forall k \in \mathbb{N}_n \end{cases}$$

- Alternating optimization
- Partition update formula

$$u_{ik} = \frac{d_{ik}^{-2/(m-1)}}{\sum_{j=0}^{c} d_{jk}^{-2/(m-1)}} \qquad \begin{matrix} \forall i \in \mathbb{N}_c^0 \\ \forall k \in \mathbb{N}_n \end{matrix}$$

- Cluster prototype update formula

$$\mathbf{v}_i = \frac{\sum_{k=1}^{n} u_{ik}^{m} \mathbf{x}_k}{\sum_{k=1}^{n} u_{ik}^{m}} \qquad \forall i \in \mathbb{N}_c$$

F(C+1)M evaluation

- Suppresses the noise
- Not very popular as standalone clustering model because it cannot handle clusters of different width

Possibilistic c-means

- Krishnapuram & Keller (1993)
- Objective function

$$J_{\mathrm{PCM}} = \sum_{i=1}^{c} \sum_{k=1}^{n} [t_{ik}^{p} \cdot d_{ik}^{2} + (1 - t_{ik})^{p} \eta_i]$$

- Constraints

$$\begin{cases} 0 \le t_{ik} \le 1, & \forall i \in \mathbb{N}_c, \forall k \in \mathbb{N}_n \\ 0 < \sum_{i=1}^{c} t_{ik} < c, & k \in \mathbb{N}_n \end{cases}$$

- Alternating optimization
- Partition update formula

$$t_{ik} = \left[1 + \left(\frac{d_{ik}^{2}}{\eta_i} \right)^{1/(p-1)} \right]^{-1} \qquad \begin{matrix} \forall i \in \mathbb{N}_c \\ \forall k \in \mathbb{N}_n \end{matrix}$$

- Cluster prototype update formula

$$\mathbf{v}_i = \frac{\sum_{k=1}^{n} t_{ik}^{p} \mathbf{x}_k}{\sum_{k=1}^{n} t_{ik}^{p}} \qquad \forall i \in \mathbb{N}_c$$

Recipe for the possibilistic penalty terms

- They are CONSTANT through the optimization of PCM
- Krishnapuram & Keller (1996)
- Run a few iterations of FCM, and use its outcome to set the penalty terms

$$\eta_i = \kappa \cdot \eta_{i0} = \kappa \cdot \frac{\sum_{k=1}^{n} u_{ik}^m d_{ik}^2}{\sum_{k=1}^{n} u_{ik}^m} \qquad \forall i \in \mathbb{N}_c$$

- The constant κ is recommended to be chosen between 1 and 2

PCM evaluation

- It can handle clusters of different size (width or radius)
- Not sensitive to noise
  - Successfully relaxed the probabilistic constraint
- Problem: frequently produces coincident clusters

- Reason:
  - The possibilistic constraint is too week
  - Clusters d do not depend on each other

$$u_{ik} = \frac{d_{ik}^{-2/(m-1)}}{\sum_{j=1}^{c} d_{jk}^{-2/(m-1)}} \qquad \forall i \in \mathbb{N}_c \quad \forall k \in \mathbb{N}_n$$

$$t_{ik} = \left[1 + \left(\frac{d_{ik}^2}{\eta_i}\right)^{1/(p-1)}\right]^{-1} \qquad \forall i \in \mathbb{N}_c \quad \forall k \in \mathbb{N}_n$$

Mixed clustering models

- Fuzzy-possibilistic c-means (Pal et al 1997) – not scalable
  - We fixed it in (Naghi, Szilágyi et al 2022)
- Possibilistic-fuzzy c-means (Pal et al 2005) – successful algorithm
  - Self-tuning version introduced in (Naghi, Szilágyi et al FUZZ-IEEE 2023), extended version presented here
- Fuzzy-possibilistic product partition c-means (Szilágyi 2011) – totally rejects outliers
  - Self-tuning version introduced in (Naghi, Szilágyi et al SMC 2024), extended version under construction

Possibilistic-fuzzy c-means (PFCM)

- Pal & Pal & Keller & Bezdek (2005)
- Objective function

$$J_{\mathrm{PFCM}} = \sum_{i=1}^{c}\sum_{k=1}^{n}[(au_{ik}^{m} + bt_{ik}^{p})d_{ik}^{2} + (1 - t_{ik})^{p}\eta_i]$$

- Constraints: probabilistic from FCM, possibilistic from PCM
  - a>0, b>0, m>1, p>1, κ =1

$$u_{ik} = \frac{d_{ik}^{-2/(m-1)}}{\sum_{j=0}^{c} d_{jk}^{-2/(m-1)}} \qquad \forall i \in \mathbb{N}_c^0 \quad \forall k \in \mathbb{N}_n$$

- Partition update formula

$$t_{ik} = \left[1 + \left(\frac{bd_{ik}^{2}}{\eta_i}\right)^{1/(p-1)}\right]^{-1} \qquad \forall i \in \mathbb{N}_c \quad \forall k \in \mathbb{N}_n$$

- Cluster prototype update formula

$$\mathbf{v}_i = \frac{\sum_{k=1}^{n}(au_{ik}^{m} + bt_{ik}^{p})\mathbf{x}_k}{\sum_{k=1}^{n}(au_{ik}^{m} + bt_{ik}^{p})} \qquad \forall i \in \mathbb{N}_c$$

PFCM evaluation

- It can handle clusters of different size
- FCM and PCM components compensate each other's drawback to a certain extent
- It is still possible to
  - Obtain coincident clusters
  - Make the algorithm crash with a single outlier

- Considered a successful algorithm
- It deserves further development

Let us make it adaptive

- Why is the penalty term treated as constant?
- Minimizing against penalty terms would reduce them to 0
  - Which would reduce the algorithm to FCM

- We need an optimal formula which allows the change of penalty terms η_i

FCMA to handle clusters of different width

- Miyamoto & Kurosawa (2004)
- Objective function
- Probabilistic constraints as in FCM
- Extra constraint

$$J_{\mathrm{FCMA}} = \sum_{i=1}^{c} \sum_{k=1}^{n} \alpha_i^{1-m} u_{ik}^m d_{ik}^2$$

$$\sum_{i=1}^{c} \alpha_i = 1.$$

- Partition update formula

$$u_{ik} = \frac{\alpha_i d_{ik}^{-2/(m-1)}}{\sum_{j=1}^{c} \alpha_j d_{jk}^{-2/(m-1)}} \qquad \forall i \in \mathbb{N}_c \quad \forall k \in \mathbb{N}_n$$

- Cluster prototype update formula

$$\mathbf{v}_i = \frac{\sum_{k=1}^{n} u_{ik}^m \mathbf{x}_k}{\sum_{k=1}^{n} u_{ik}^m} \qquad \forall i \in \mathbb{N}_c$$

- Update formula

$$\alpha_i = \frac{\left(\sum_{k=1}^{n} u_{ik}^m d_{ik}^2\right)^{1/m}}{\sum_{j=1}^{c} \left(\sum_{k=1}^{n} u_{jk}^m d_{jk}^2\right)^{1/m}} \qquad \forall i \in \mathbb{N}_c$$

Self-tuning PFCM

- Objective function

$$J_{\mathrm{ST-PFCM}} = \sum_{i=1}^{c}\sum_{k=1}^{n} \rho_i^{1-m}(au_{ik}^m + bt_{ik}^p)d_{ik}^2 + (1-t_{ik}^p)\eta$$

- Subject to

$$\begin{cases} u_{ik}, t_{ik} \in [0,1] & \forall i \in \mathbb{N}_c,\ \forall k \in \mathbb{N}_n \\ \sum_{i=1}^{c} u_{ik} = 1 & \forall k \in \mathbb{N}_n \\ 0 < \sum_{i=1}^{c} t_{ik} < c & \forall k \in \mathbb{N}_n \\ \rho_i \in [0,c] & \forall i \in \mathbb{N}_c \\ \sum_{i=1}^{c} \rho_i = c & \forall i \in \mathbb{N}_c \\ m > 1,\ p > 1, a > 0 & b > 0 \end{cases}$$

AO of ST-PFCM

$$u_{ik} = \frac{\rho_i d_{ik}^{-2/(m-1)}}{\sum_{j=1}^{c} \rho_j d_{jk}^{-2/(m-1)}} \qquad \forall i \in \mathbb{N}_c \quad \forall k \in \mathbb{N}_n$$

$$t_{ik} = \left[1 + \left(\frac{b d_{ik}^2}{\eta \rho_i^{m-1}} \right)^{1/(p-1)} \right]^{-1} \qquad \forall i \in \mathbb{N}_c \quad \forall k \in \mathbb{N}_n$$

$$\mathbf{v}_i = \frac{\sum_{k=1}^{n} (a u_{ik}^m + b t_{ik}^p) \mathbf{x}_k}{\sum_{k=1}^{n} (a u_{ik}^m + b t_{ik}^p)} \qquad \forall i \in \mathbb{N}_c$$

$$\rho_i = c \cdot \frac{\left(\sum_{k=1}^{n} (a u_{ik}^m + b t_{ik}^p) d_{ik}^2 \right)^{1/m}}{\sum_{j=1}^{c} \left(\sum_{k=1}^{n} (a u_{jk}^m + b t_{jk}^p) d_{jk}^2 \right)^{1/m}} \qquad \forall i \in \mathbb{N}_c$$

What makes it self-tuning?

- True penalty term for cluster i

$$\eta_i = \eta \rho_i^{m-1} / b$$

$$t_{ik} = \left[1 + \left(\frac{d_{ik}^2}{\eta_i} \right)^{1/(p-1)} \right]^{-1} \qquad \forall i \in \mathbb{N}_c \quad \forall k \in \mathbb{N}_n$$

$$t_{ik} = \left[1 + \left(\frac{b d_{ik}^2}{\eta \rho_i^{m-1}} \right)^{1/(p-1)} \right]^{-1} \qquad \forall i \in \mathbb{N}_c \quad \forall k \in \mathbb{N}_n$$

- ST-PFCM changes the values of ρ_i every cycle
- It updates the width of the clusters

Penalty terms contain a constant η

- It is only a component of the penalty terms
- Recommendation
- Use F(C+1)M, not FCM

$$\eta = \frac{1}{c} \cdot \sum_{i=1}^{c} \eta_{i0} = \frac{1}{c} \cdot \sum_{i=1}^{c} \frac{\sum_{k=1}^{n} u_{ik}^{m} \overline{d}_{ik}^{2}}{\sum_{k=1}^{n} u_{ik}^{m}}$$

$$\overline{d}_{ik} = \begin{cases} d_0 & \text{if} \quad \max\{u_{jk}, j \in \mathbb{N}_c\} < \varepsilon \\ d_{ik} & \text{otherwise} \end{cases}$$

Expectation

- Conditions of success
  - ST-PFCM should work fine wherever PFCM works fine
  - ST-PFCM should work fine also in some cases where PFCM fails

- ST-PFCM is still not expected to be the ideal c-means clustering algorithm

Evaluation criteria

- Main criterion is cluster validity
- There is no cluster validity index for such mixed partitions, so we invent some

- Modified Xie-Beni

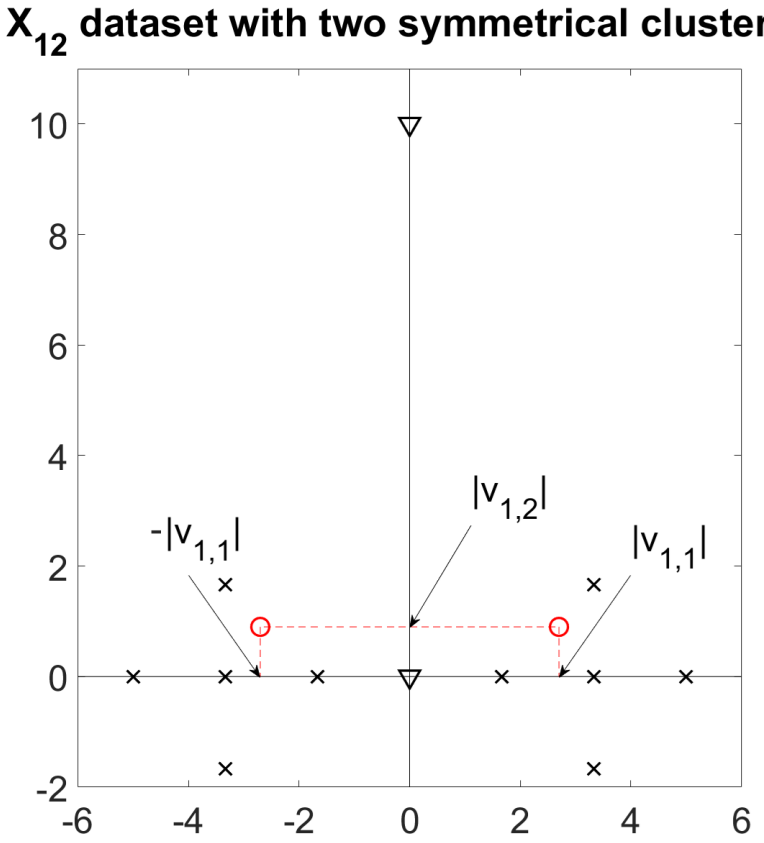
$$MXB = \frac{\sum_{i=1}^{c} \sum_{k=1}^{n} (au_{ik}^{m} + bt_{ik}^{p}) \|\mathbf{x}_k - \mathbf{v}_i\|^2}{n \cdot \min_{i \neq j} \|\mathbf{v}_i - \mathbf{v}_j\|^2}$$

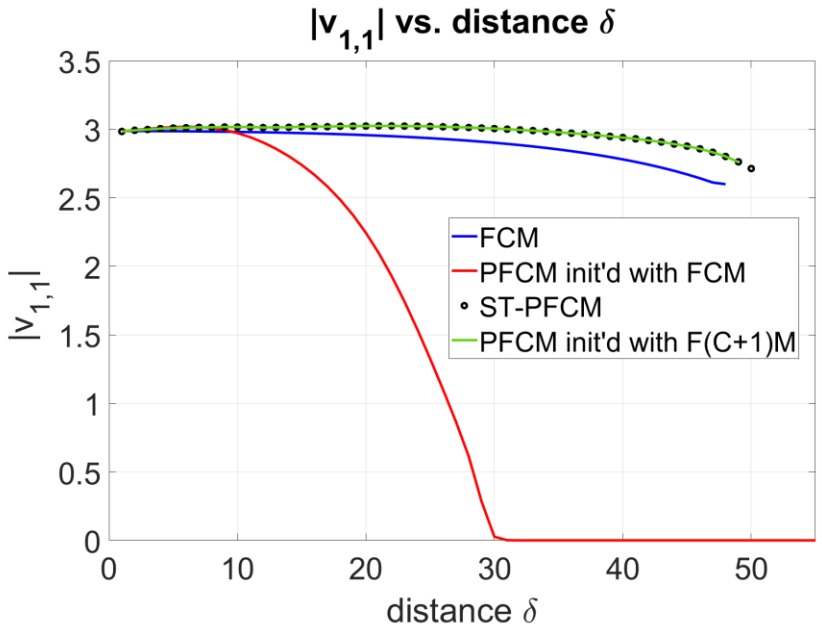
- Modified Fukuyama-Sugeno

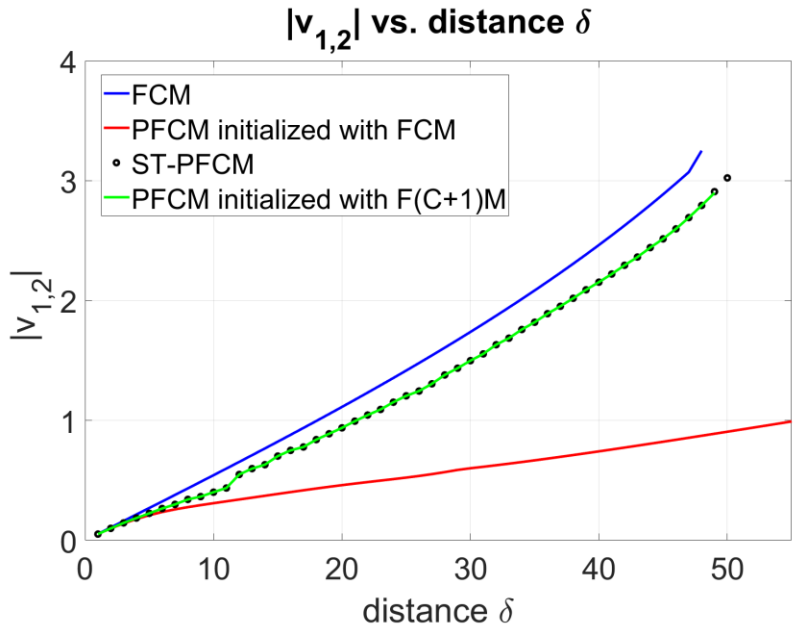
$$MFS = \sum_{i=1}^{c} \sum_{k=1}^{n} (au_{ik}^{m} + bt_{ik}^{p})(\|\mathbf{x}_k - \mathbf{v}_i\|^2 - \|\mathbf{v}_i - \overline{\mathbf{v}}\|^2),$$

- Valid partitions are represented by low values
- MFS can be negative

Initialization problem demonstrated





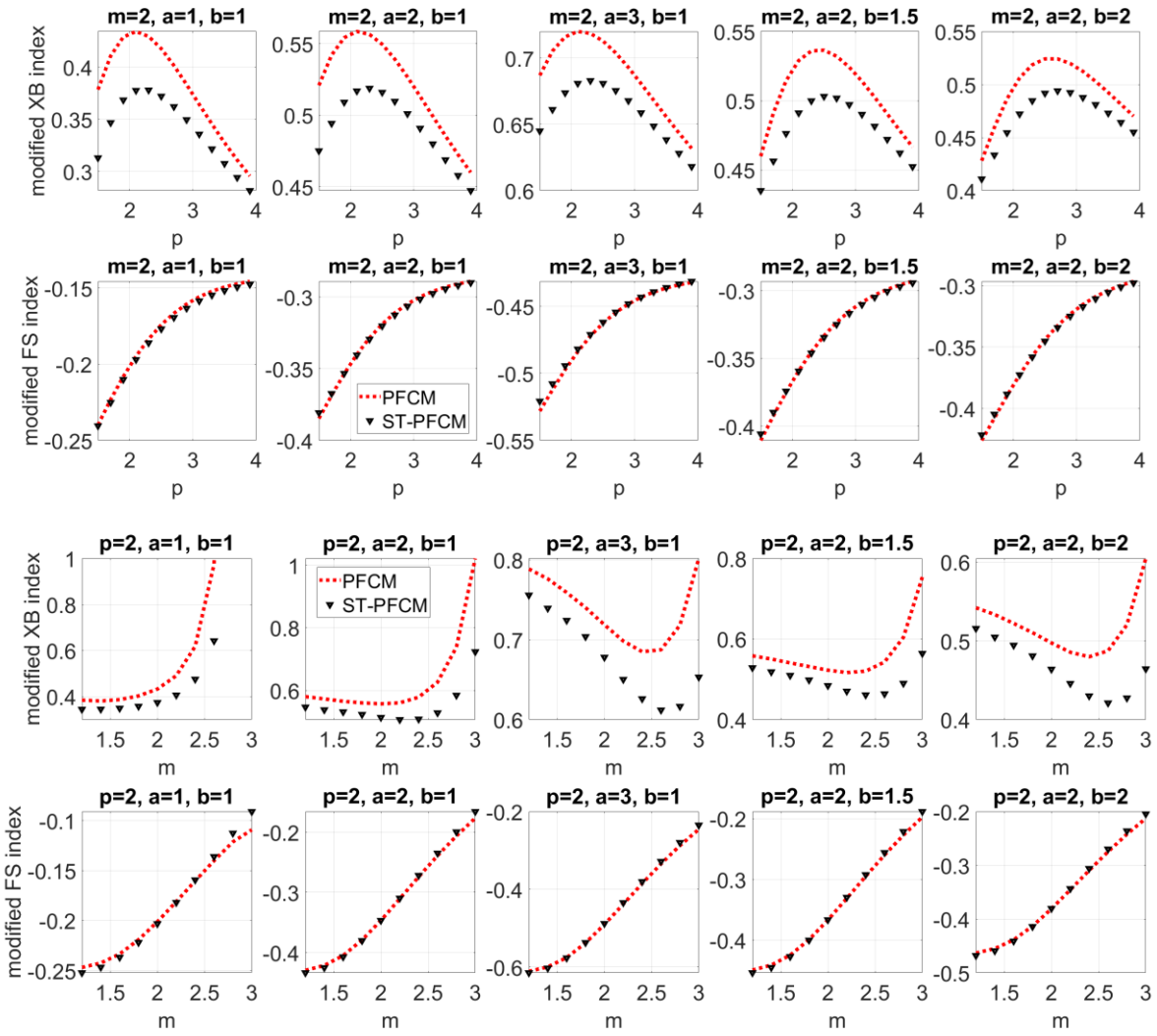


Data

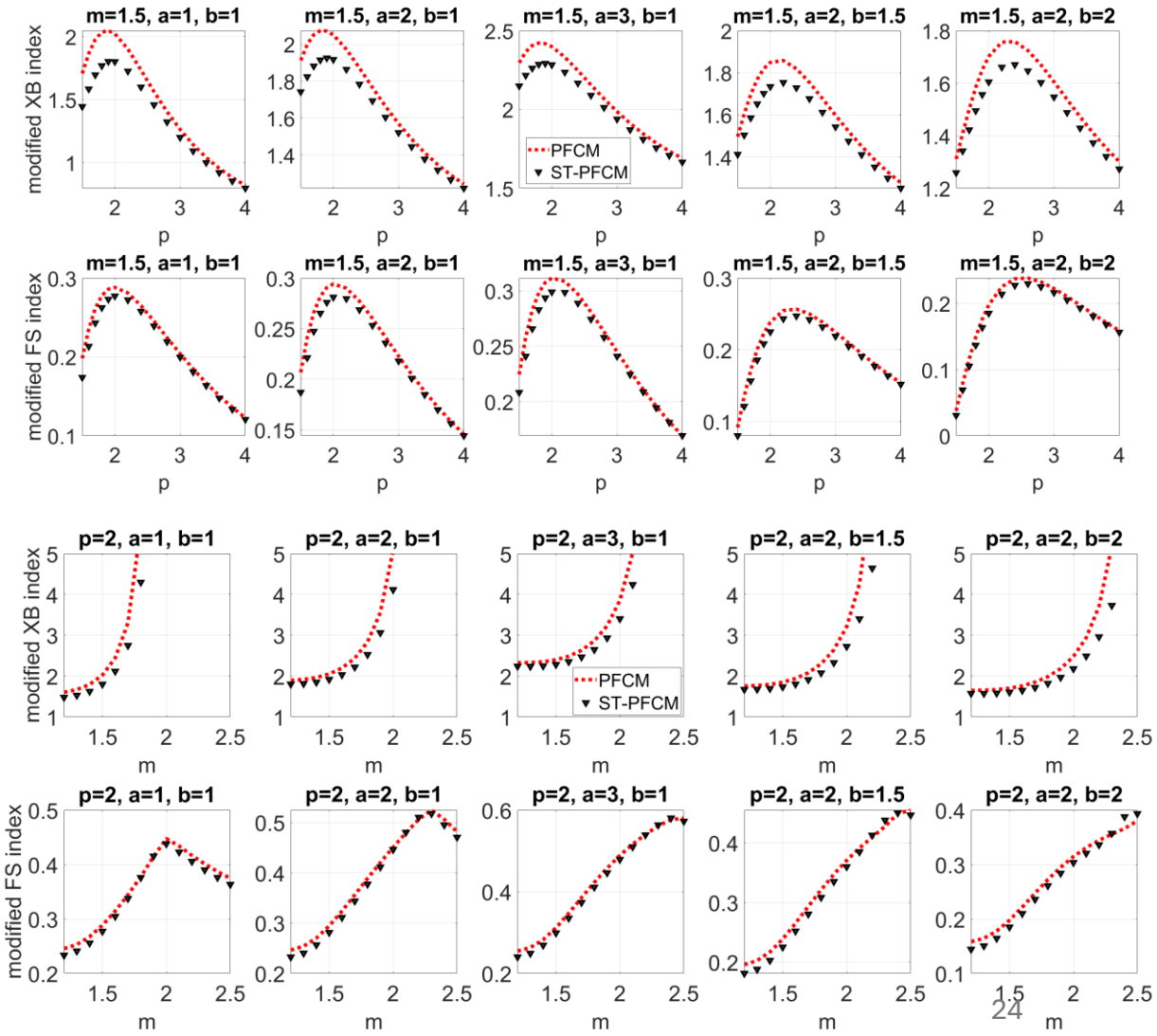
- Test datasets in Table below
- All data vectors normalized, sclaed to [0,1] interval in all dimensions
- Scenario 1: no added noise
- Scenario 2: single outlier at (δ,δ. δ,… δ), with δ>1
- Scenario 3: increasing number of random data points with coordinates in [-1,1] interval in all dimensions

Property	IRIS	WINE	BC	SEEDS
Items	150	178	569	210
Dimensions	4	13	30	7
Clusters	3	3	2	3
Cluster sizes	50, 50, 50	59, 71, 48	357, 212	70, 70, 70

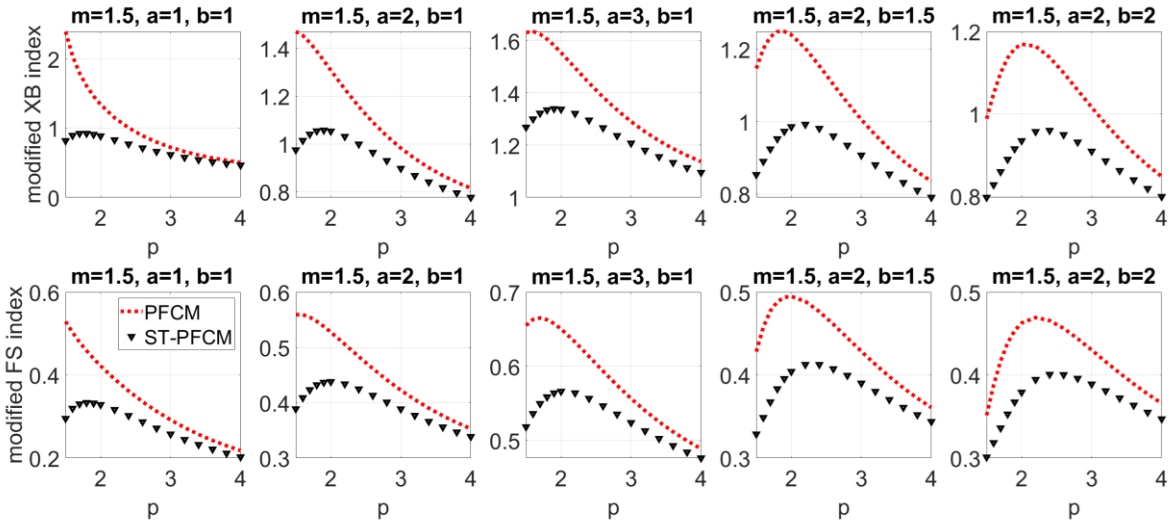
IRIS data

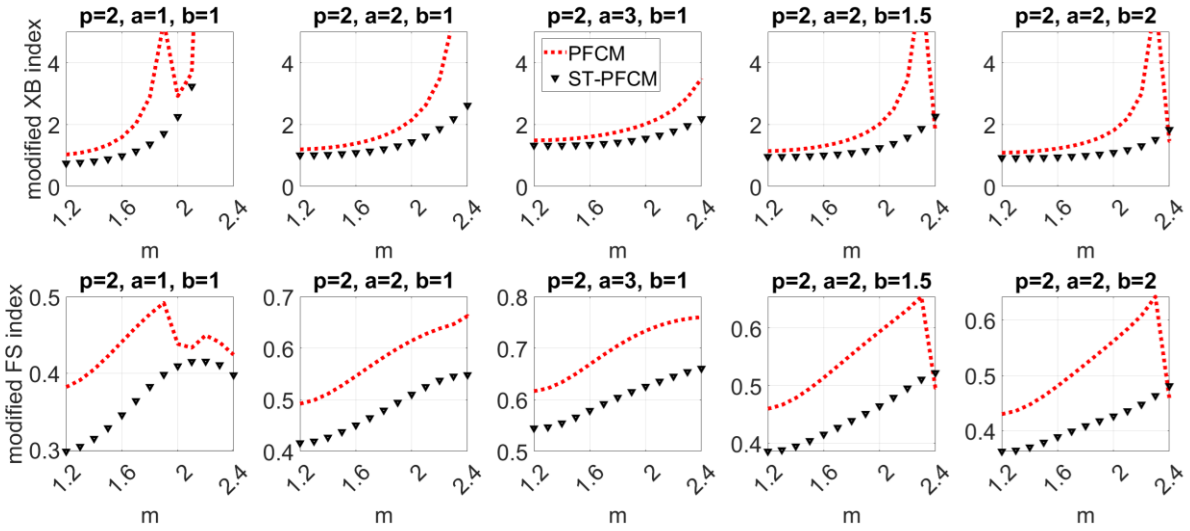


WINE data

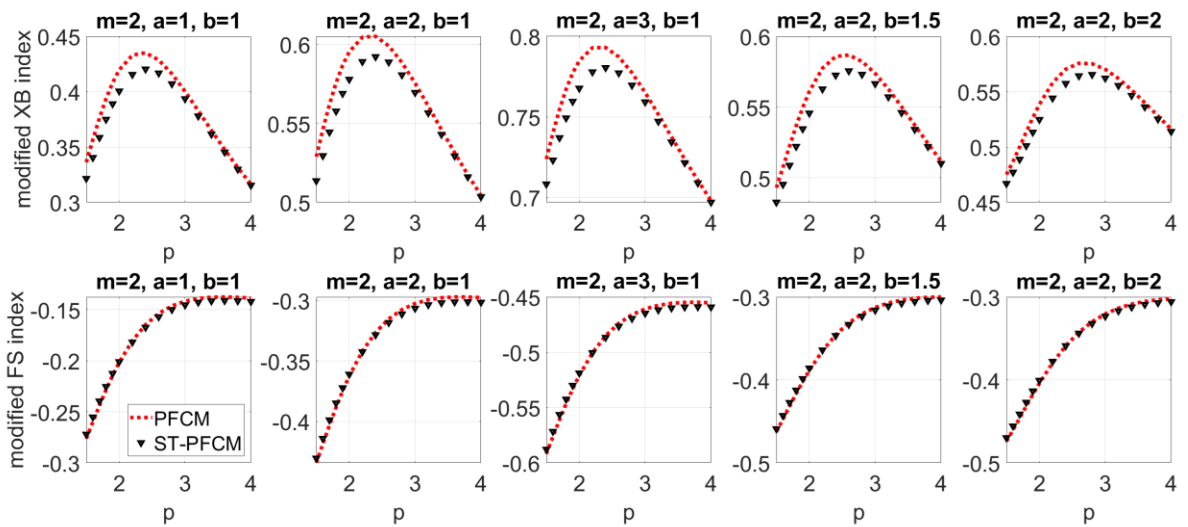


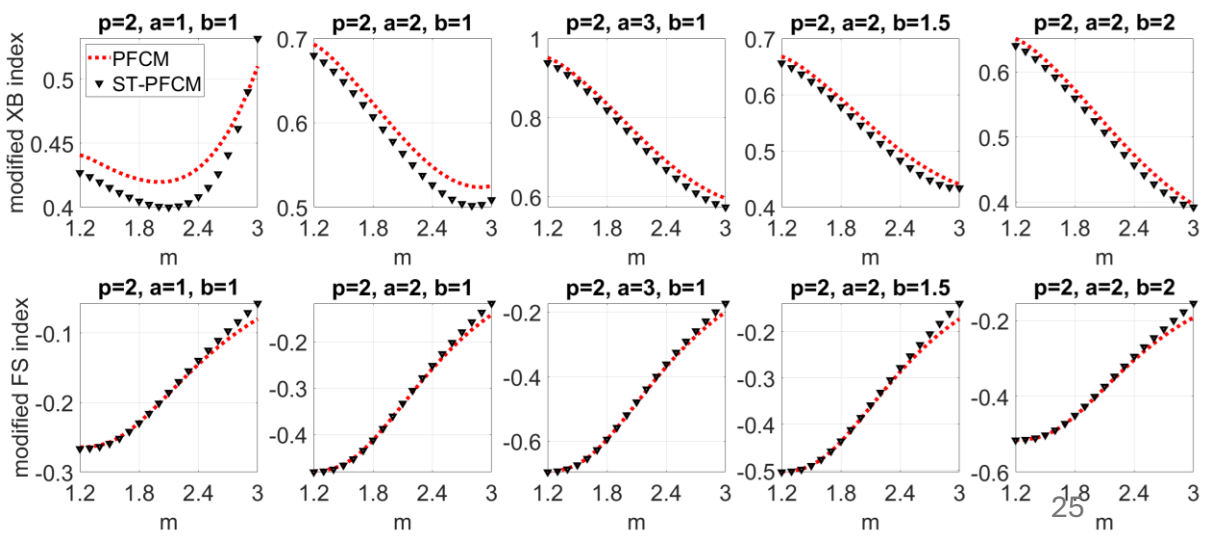
BC data



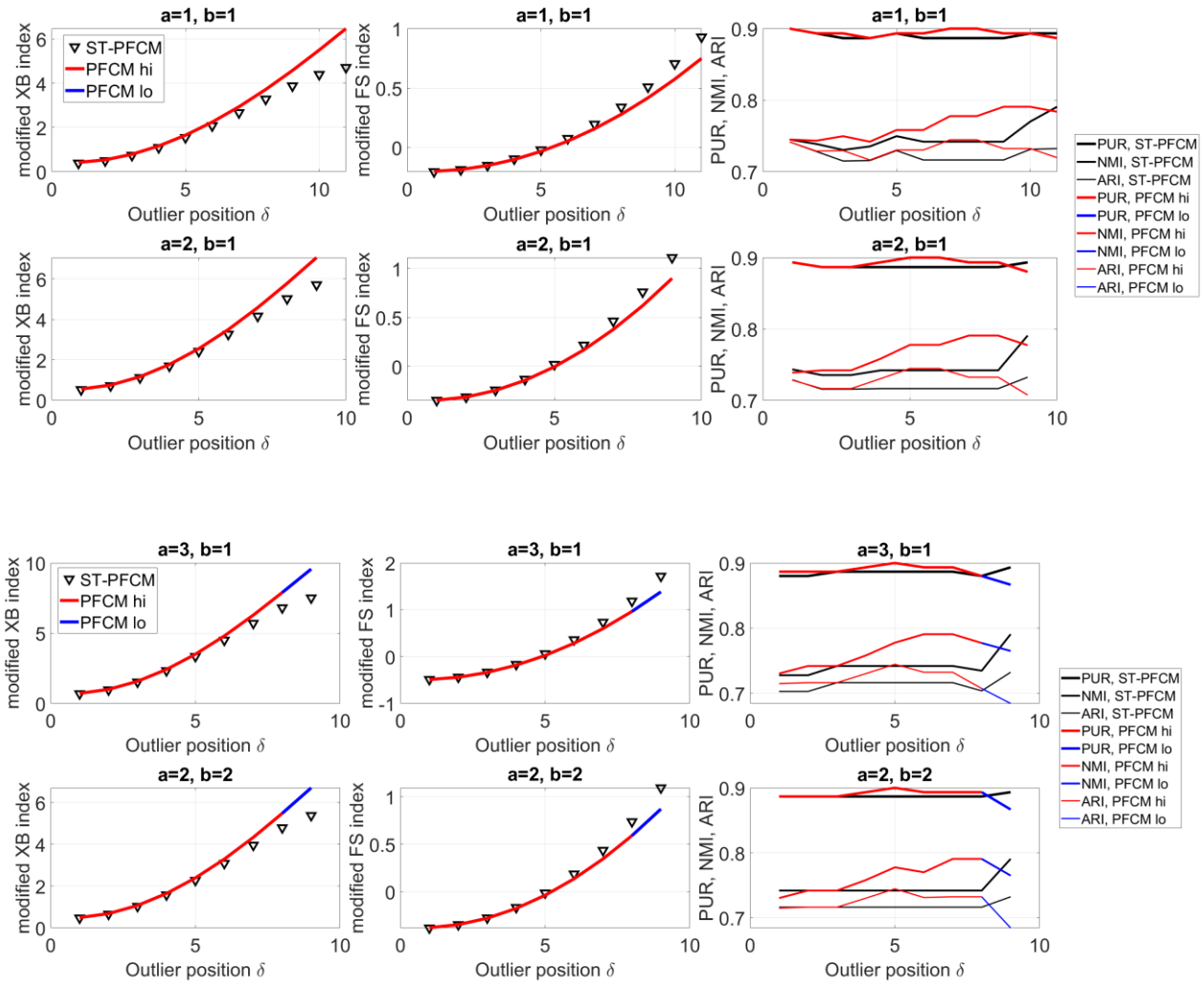


SEEDS data

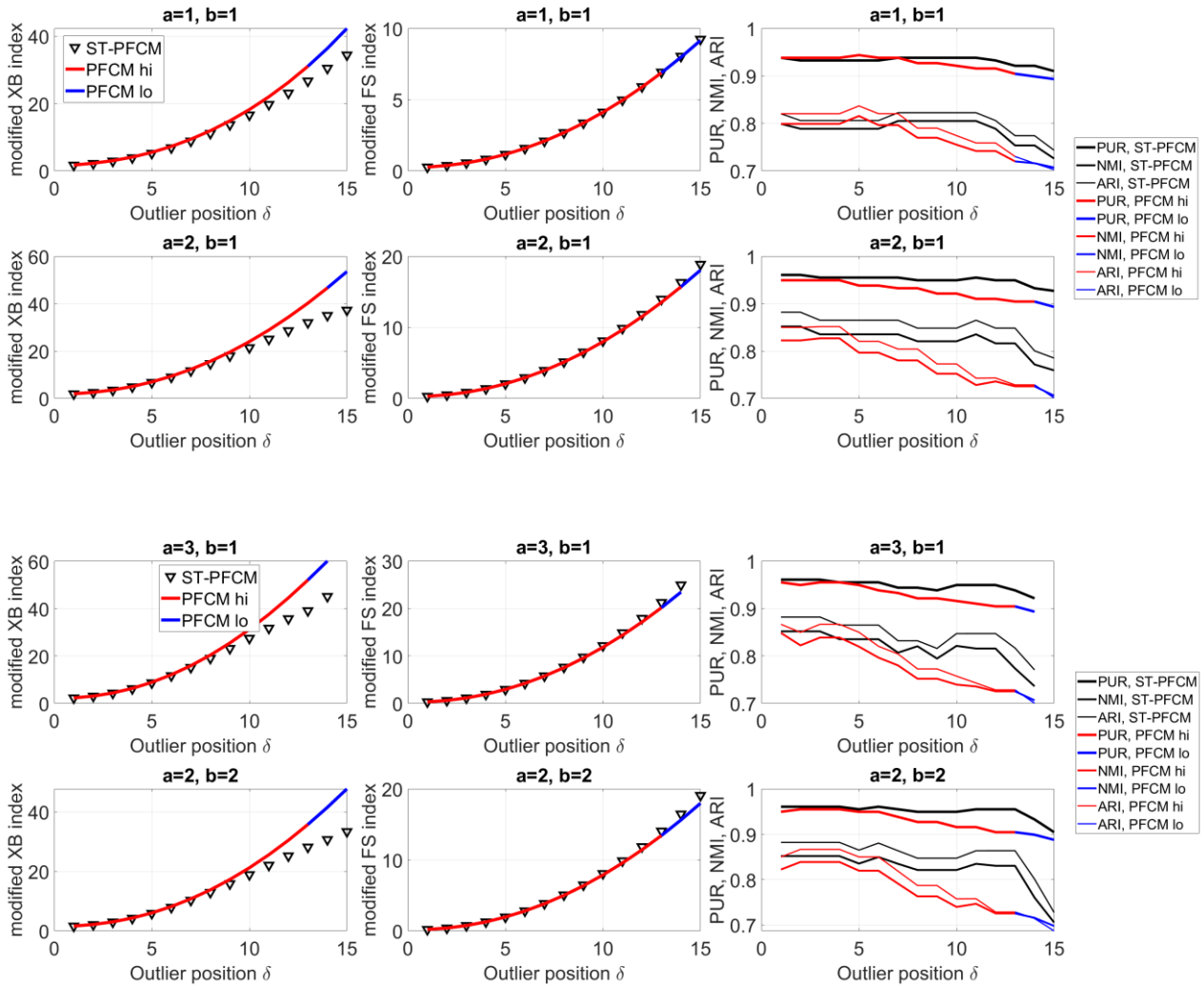




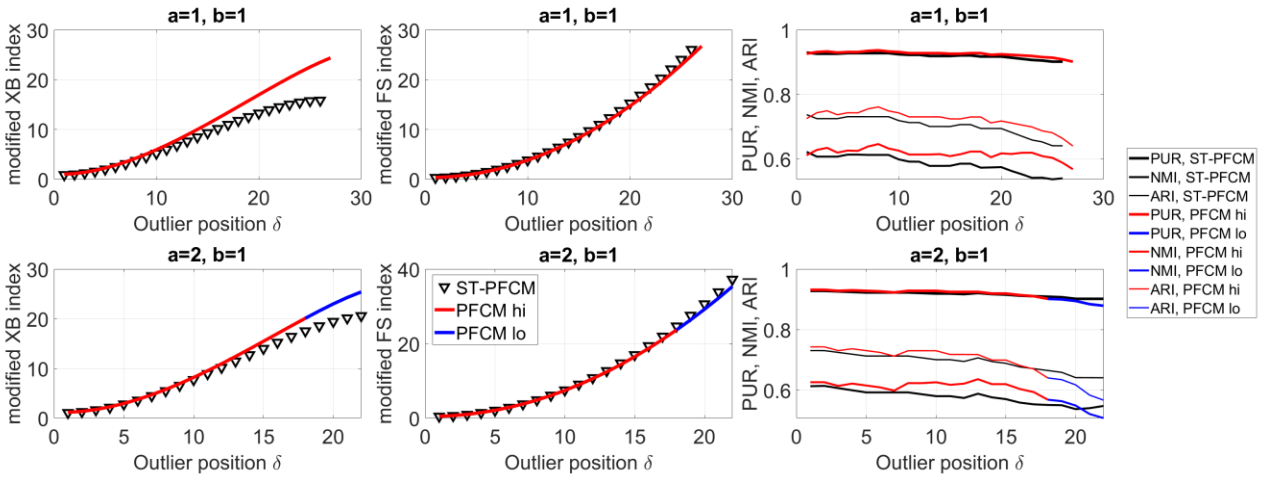
IRIS data

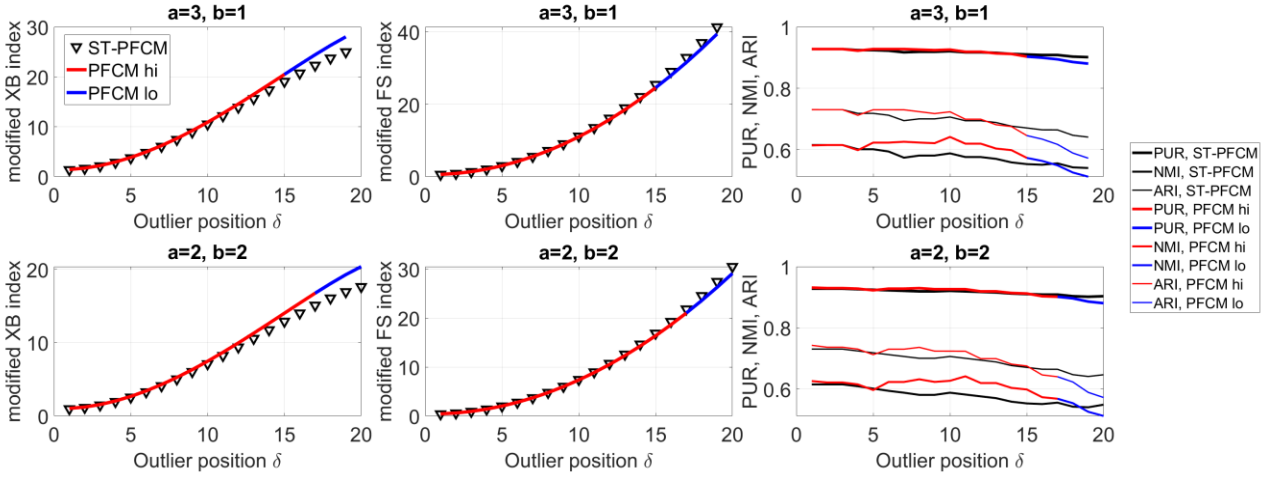


WINE data



BC data





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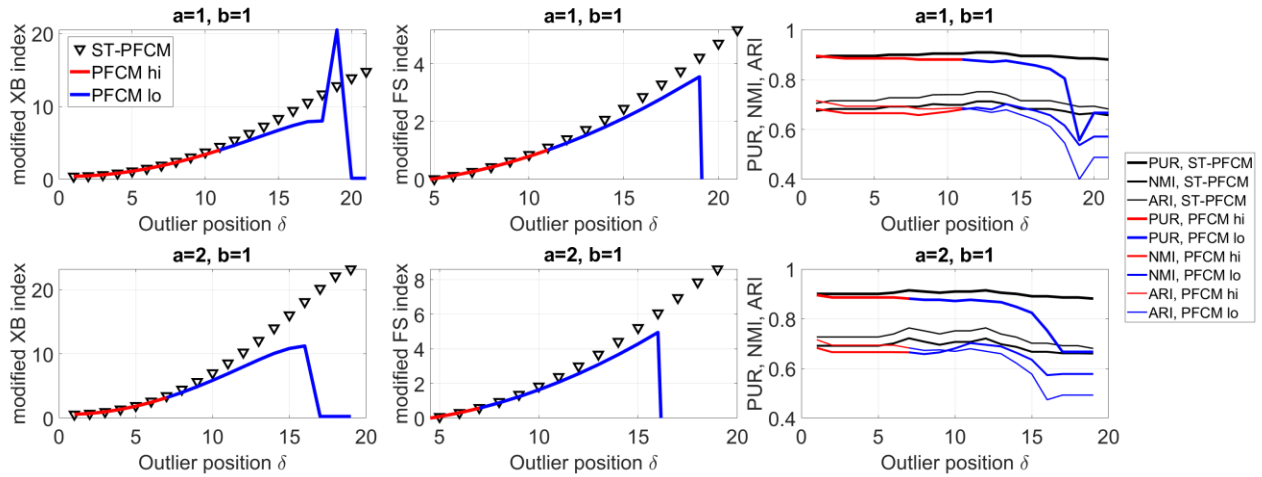
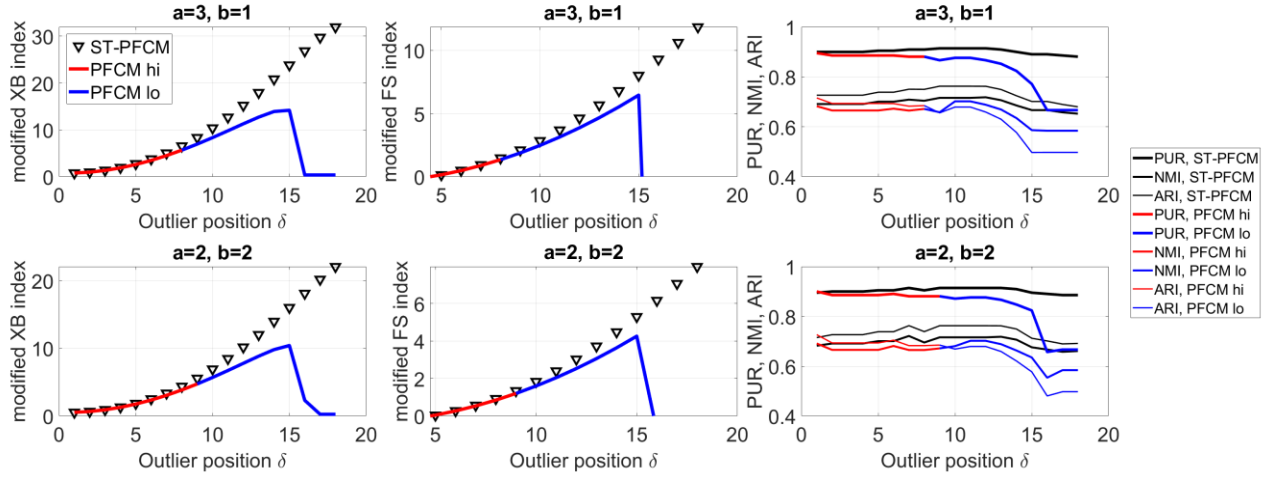


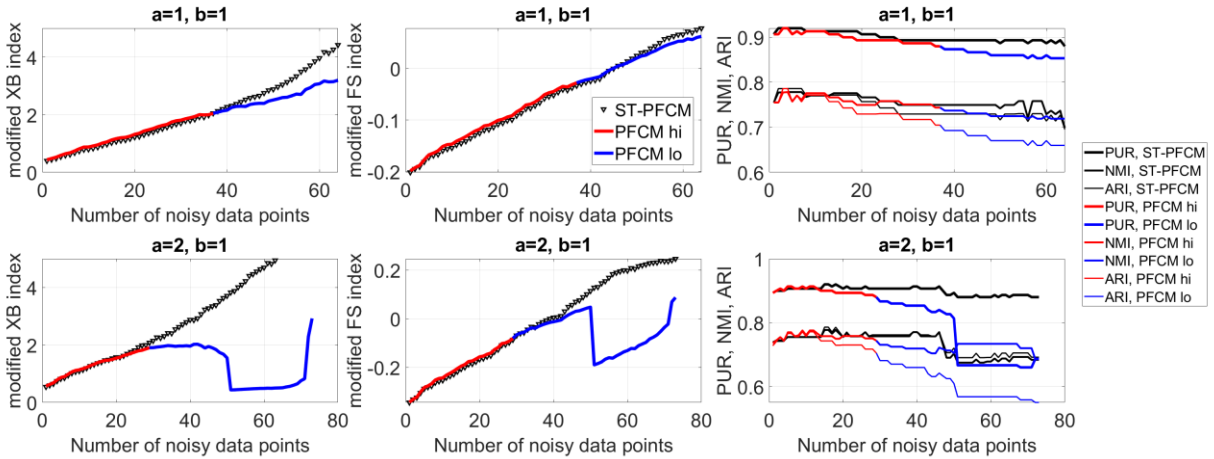


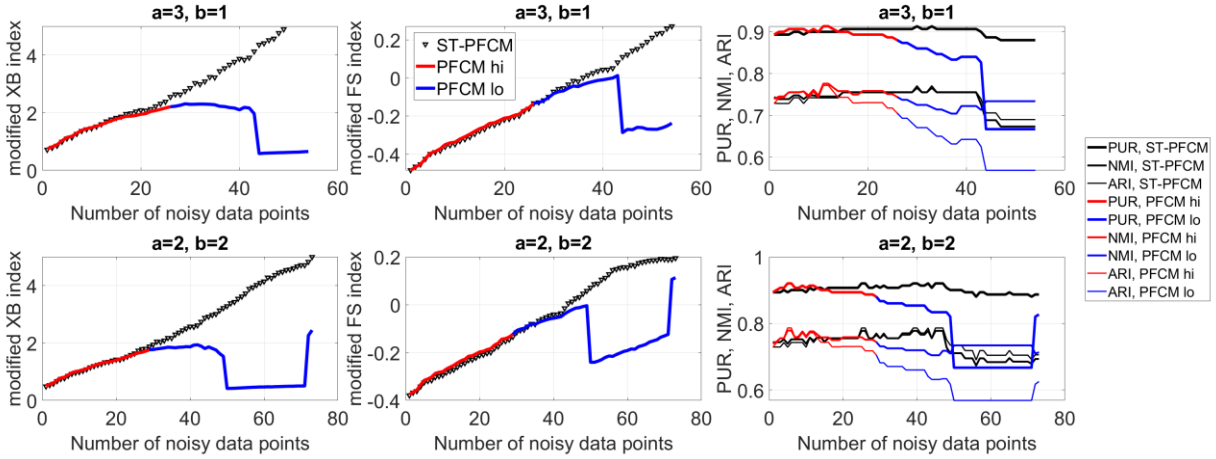
Limit value of δ, PFCM vs. ST-PFCM

Table 3: Comparison PFCM vs ST-PFCM in case of a single outlier: the limit value of parameter δ tolerated by the algorithms while providing acceptable partition

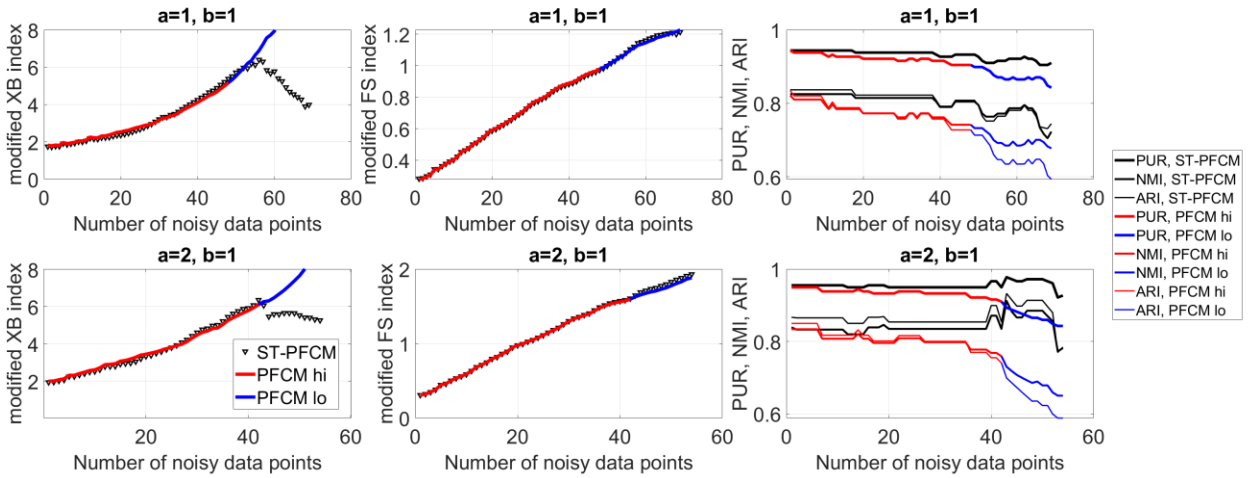
Trade-off		IRIS data				WINE data				BC data				SEEDS data			
		$m = 2.0$				$m = 1.5$				$m = 1.5$				$m = 2.0$			
a	b	$p = 1.5$	$p = 2$	$p = 2.5$	$p = 3$	$p = 1.5$	$p = 2$	$p = 2.5$	$p = 3$	$p = 1.5$	$p = 2$	$p = 2.5$	$p = 3$	$p = 1.5$	$p = 2$	$p = 2.5$	$p = 3$
1	1	11:11	11:11	11:11	10:11	14:16	13:15	14:16	13:16	25:24	22:26	25:25	21:22	12:21	12:21	11:21	10:19
2	1	9:9	9:9	9:9	8:9	14:15	14:15	13:14	13:14	18:20	18:22	17:21	15:21	9:19	7:19	9:18	9:18
3	1	8:9	8:9	8:9	7:9	13:14	13:14	12:13	12:13	15:19	15:19	15:19	13:19	8:18	8:18	6:18	8:17
2	2	8:9	8:9	8:9	8:9	14:15	13:15	13:14	13:14	14:18	17:20	17:20	15:21	9:18	9:18	9:18	9:17

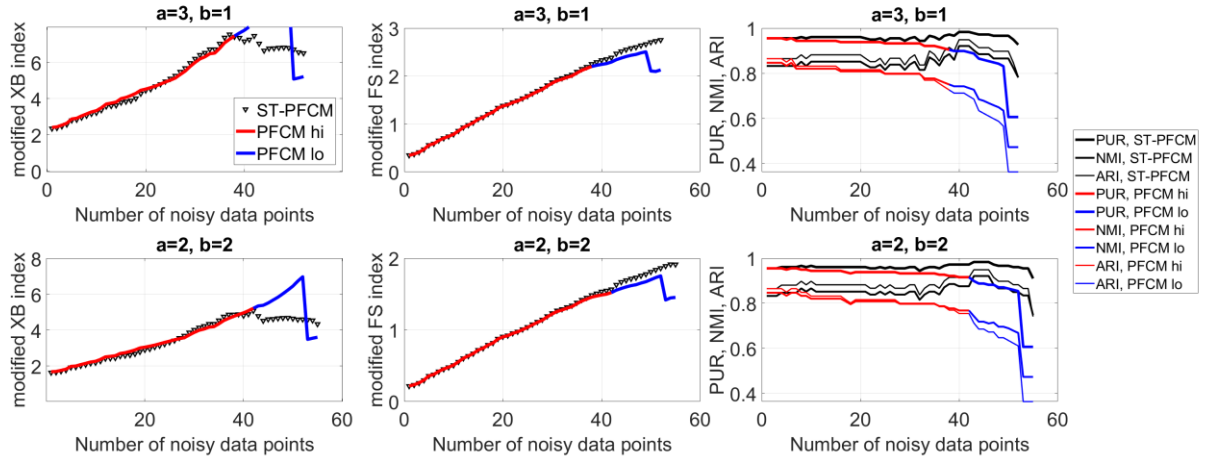
IRIS data



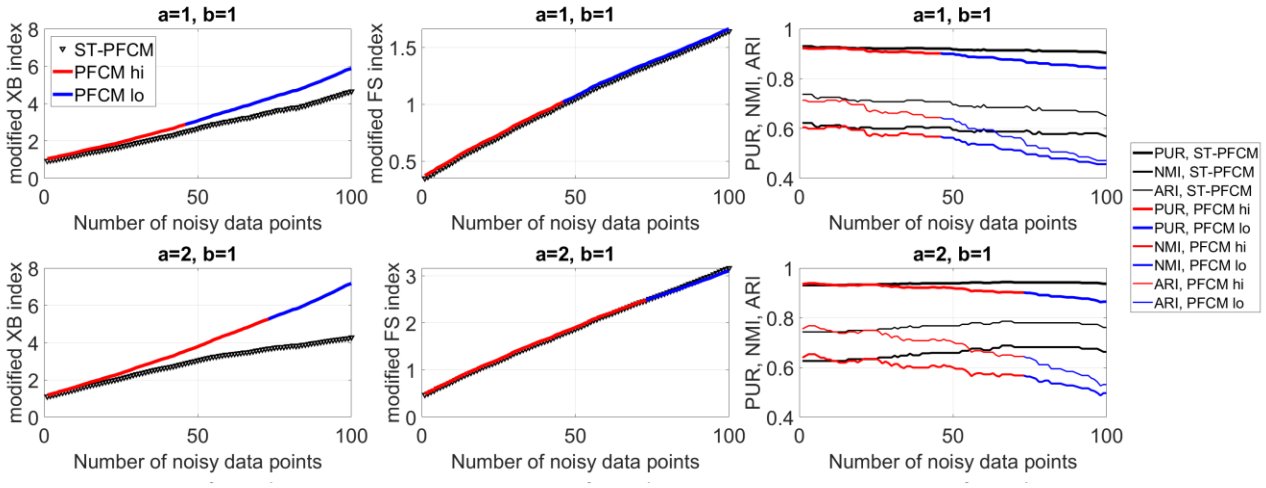


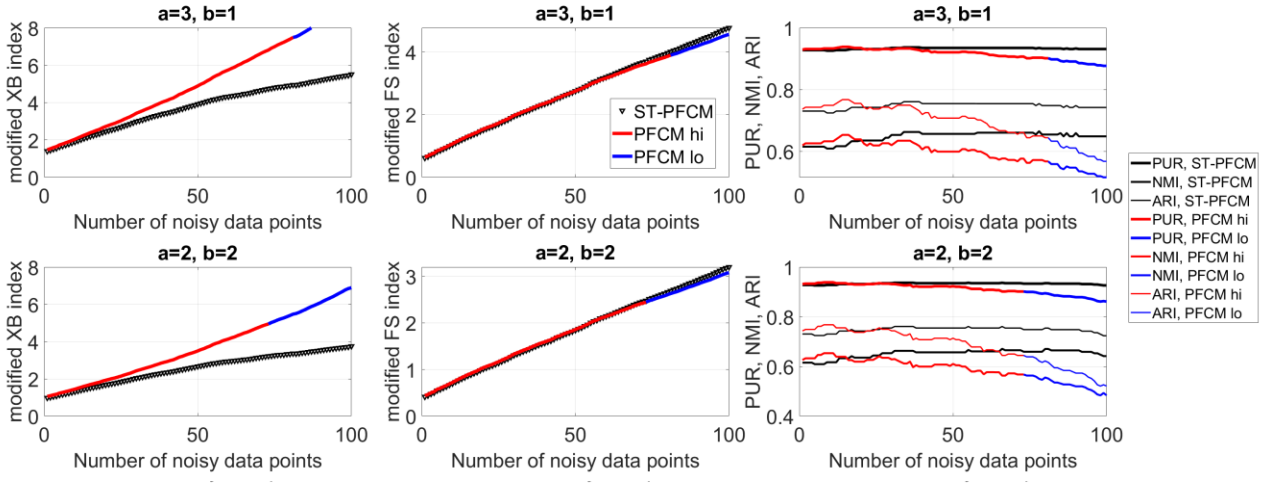
WINE data



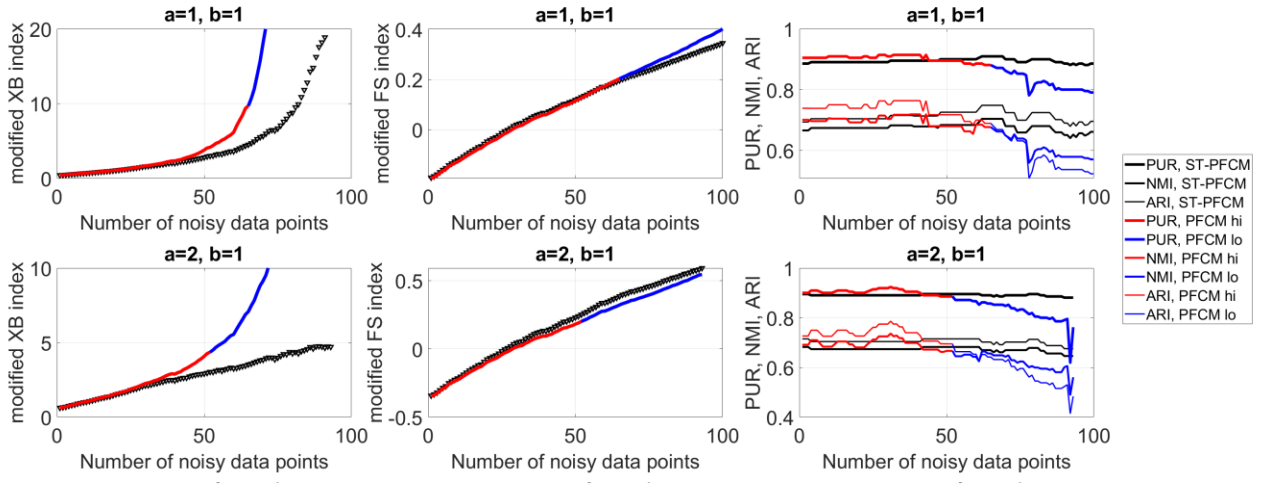


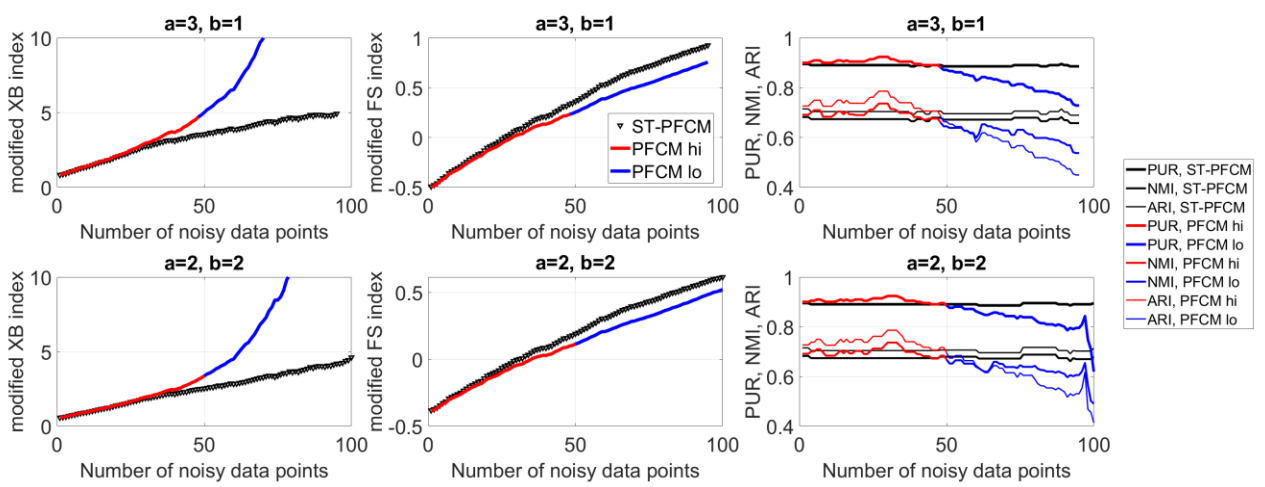
BC data





SEEDS data





Noisy data points tolerated, PFCM vs. ST-PFCM

Table 4: Comparison PFCM vs ST-PFCM in case of noisy data: the limit number of noisy vectors tolerated by the algorithms while providing acceptable partition

Trade-off		IRIS data				WINE data				BC data				SEEDS data			
		$m = 2.0$				$m = 1.5$				$m = 1.5$				$m = 2.0$			
a	b	$p = 1.5$	$p = 2$	$p = 2.5$	$p = 3$	$p = 1.5$	$p = 2$	$p = 2.5$	$p = 3$	$p = 1.5$	$p = 2$	$p = 2.5$	$p = 3$	$p = 1.5$	$p = 2$	$p = 2.5$	$p = 3$
1	1	43:67	33:60	29:76	26:51	65:65	47:67	41:55	38:59	21:53	62:116	75:200	75:200	62:47	47:112	55:92	52:83
2	1	29:47	28:73	25:56	25:50	49:59	47:54	37:50	35:49	44:200	73:200	80:200	73:200	52:93	47:122	46:92	45:89
3	1	27:43	25:46	25:52	23:45	42:55	37:52	35:50	35:49	63:200	81:200	85:200	79:200	49:50	43:48	43:95	43:89
2	2	27:48	27:54	25:56	25:53	43:55	42:54	39:52	36:50	75:97	85:200	89:200	83:200	55:45	47:48	46:106	45:89

Remarks

- If we are not sure that our data is noise-free, F(c+1)M should be used for initialization
- In most of the noise-free cases, PFCM and ST-PFCM perform equally well
- In few noise-free cases and in more noisy cases, ST-PFCM works better
- In a noisy environment, ST-PFCM is likely to perform better than PFCM
- It is hard to define cases where PFCM is definitely better than ST-PFCM

- Further needs: e.g. complexity analysis

Conclusions

- We proposed an alternative initialization scheme to avoid the mistaken start
- We have created a self-tuning version of the PFCM algorithm
- Adaptively changes the possibilistic penalty terms
- It has the chance to create finer partitions than PFCM
- In several test cases it really performed better than PFCM

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