

From Soft Clustering to Hard Clustering: A Collaborative Annealing Fuzzy c -Means Algorithm

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Abstract—The fuzzy c -means clustering algorithm is the most widely used soft clustering algorithm. In contrast to hard clustering, the cluster membership of data generated using the fuzzy c -means algorithm is ambiguous. Similar to hard clustering algorithms, the clustering results of the fuzzy c -means clustering algorithm are also suboptimal with varied performance depending on initial solutions. In this paper, a collaborative annealing fuzzy c -means algorithm is presented. To address the issue of ambiguity, the proposed algorithm leverages an annealing procedure to phase out the fuzzy cluster membership degree toward a crispy one by reducing the exponent gradually according to a cooling schedule. To address the issue of suboptimality, the proposed algorithm employs multiple fuzzy c -means modules to generate alternative clusters based on memberships repeatedly reinitialized using a metaheuristic rule. Experimental results on eight benchmark datasets are elaborated to demonstrate the superiority of the proposed algorithm to thirteen prevailing hard and soft algorithms in terms of internal and external cluster validity indices.

Index Terms—Annealing procedure, collaborative clustering, fuzzy c -means (FCM) clustering, k -means (KM) clustering.

I. INTRODUCTION

CLUSTERING is a popular unsupervised or semisupervised learning technique to explore the hidden structures of datasets. It is to group unlabeled data into multiple disjoint subsets with high intracluster similarity and low intercluster similarity. It arises in numerous applications, such as image segmentation [1], information retrieval [1], data mining [1], document clustering [2], video surveillance [2], feature selection [3], and pattern recognition [3].

Over the past decades, numerous clustering algorithms have been proposed, and they are mainly divided into two classes,

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including hard and soft clustering. Hard clustering is based on the assumption of mutually exclusive clusters, whereas soft clustering relaxes the assumption allowing overlapped clusters. In addition, hard clustering provides a simpler and more straightforward interpretation of the results, whereas soft clustering usually requires further interpretation and analysis to determine appropriate cutoff values for membership assignments.

Hard clustering assigns each datum to one and only one cluster. Hard clustering methods may be classified as full-space clustering algorithms, subspace clustering algorithms, feature-weighted clustering algorithms, and multiview clustering algorithms, depending on the feature spaces of their operations. Subspace clustering methods include the deep subspace clustering algorithm [4] and the robust possibilistic k -subspace clustering algorithm [5]. Feature-weighted clustering methods include the entropy weighting k -means (KM) clustering algorithm [6], the entropy-weighted power k -means (EWPKM) clustering algorithm [7], and the LASSO-weighted KM clustering algorithm [8]. Multiview clustering methods include the weighted multiview possibilistic c -means clustering algorithm with L2 regularization [9], and the multiview adjacency-constrained hierarchical clustering (HC) algorithm [10]. The hard clustering methods may be classified into hierarchical-based, center-based, distribution-based, and density-based clustering algorithms, according to the structure of the algorithms. HC-based methods cluster data based on the rule that closer data points exhibit more similarity to each other than the data points lying farther away, including divisive hierarchical algorithms [11] and agglomerative hierarchical algorithms [12]. The center-based clustering methods cluster data based on the rule that similarity is derived by the closeness of data to clusters, including KM [13], k -medoids algorithms [14], [15], k -harmonic means [16], and spectral clustering (SC) algorithms [17], [18], [19]. Distribution-based clustering methods cluster data based on the probability of data belonging to a specific distribution, including the expectation-maximization for Gaussian mixture model algorithms [20]. Density-based clustering methods cluster data based on the density of data points in the feature space, including the mean-shift algorithm [21], and the temporal streaming fuzzy density-based spatial clustering algorithm [22]. In addition, several collaborative clustering methods were proposed [23], including deep multiview collaborative clustering [24]. In spite of the progress, the clustering methods cannot guarantee the global optimality of clustering results. To mitigate the difficulty of discontinuity in the underlying objective function of KM, the power k -means

(PKM) algorithm clusters data by minimizing the majorization function of an annealed power-mean function [25]. Though the clustering performance using PKM is significantly improved, the clustering result is still suboptimal and dependent on initialization. To achieve optimal clustering results, the collaborative annealing power k -means++ (CAPKM++) algorithm clusters data by employing multiple PKM modules reinitialized using a particle swarm optimization rule [26]. CAPKM++ is demonstrated to outperform PKM and many other baselines [26]. As an upgraded version of CAPKM++, CAPKM++2.0 [27] is shown to be able to improve clustering efficiency via reinitialization during annealing [27].

As a relaxation of hard clustering, soft clustering allows each datum to belong to multiple clusters with membership degrees. Soft clustering methods include possibilistic clustering algorithms [28] and fuzzy clustering algorithms [29]. Possibilistic clustering methods include the robust automatic merging possibilistic clustering algorithm [30], the sparse possibilistic c -means algorithm [31], and the robust possibilistic k -subspace clustering algorithm [5]. Fuzzy clustering methods include the fuzzy c -means (FCM) algorithm [32], the centroid autofused hierarchical FCM clustering algorithm [33], fuzzy density peaks clustering [34], the robust jointly sparse fuzzy clustering algorithm [35], the fuzzy low-rank structural clustering algorithm [36], and the robust FCM algorithm [37]. Soft clustering introduces ambiguity in clustering results due to assigning each data point a membership value to each cluster. In addition, similar to existing hard clustering methods, the results of the soft clustering methods are also suboptimal.

FCM is one of the popular soft clustering methods due to its efficiency and simplicity [29]. However, it suffers the same drawback as other fuzzy clustering algorithms. To remedy the shortcoming of performance sensitivity to initialization, many alternative methods have been proposed, such as the FCM variants with improved objective function and initialization, and additional constraints. FCM-like algorithms with improved objective function include adaptive FCM algorithm [38], generalized FCM clustering [39], enhanced FCM [40], fast generalized FCM [41], fuzzy weighted c -means [42], [43], generalized FCM algorithm with improved fuzzy partition [44], fuzzy local information c -means [45], Bayesian fuzzy clustering (BFC) [46], and kernel fuzzy c -means clustering (KFCM) [47]. FCM with improved initialization includes multistage random sampling [48], the genetic algorithm [49], the Gustafson–Kessel algorithm [50], initialization schemes by utilizing color space in image segmentation [51], [52], the Markov random field [53], and the two-phase fuzzy c -means (2PFCM) [54]. Constrained FCM algorithms with additional constraints include the FCM method with spatial constraints [55], [56].

To achieve optimal clustering performance and eliminate the ambiguity in cluster membership and the dependency of performance on initial solutions, we propose the collaborative annealing fuzzy c -means based on FCM (CAFCEM). An annealing procedure is used in CAFCEM to phase out the fuzziness of cluster membership. In addition, multiple modules are employed

to engender alternative clusters and reinitialized repeatedly using a metaheuristic rule to maximize clustering quality and eliminate the influence of initialization on clustering performance. The innovative contributions of this work are summarized as follows.

- 1) We theoretically prove that the underlying objective function of FCM is equivalent to that of PKM without annealing.
- 2) We propose CAFCEM with a cooling schedule and experimentally demonstrate that the polynomial cooling schedule is the most cost-effective one.
- 3) We empirically estimate the computational complexity of CAFCEM based on many datasets.
- 4) We experimentally demonstrate that CAFCEM outperforms existing hard and soft clustering algorithms in terms of the mean values and standard deviations of many indices.

The rest of this paper is organized as follows. The related work on KM, FCM, PKM, CAPKM++, and CAPKM++2.0 is provided in Section II. The details of the CAFCEM algorithm are presented in Section III. Experimental results on eight datasets are reported in Section IV. The paper is concluded in Section V.

II. RELATED WORK

A. KM Algorithm

The KM algorithm is one of the most popular unsupervised learning algorithms. It groups the data into a preset number of clusters by minimizing the following objective function [13]:

$$f(\Theta) = \sum_{i=1}^n \min_{1 \leq j \leq k} \|x_i - \theta_j\|_2^2, \quad (1)$$

where $X = \{x_1, \dots, x_n\} \in \mathbb{R}^{n \times p}$ is an unlabeled dataset, n is the number of data points, k is the number of clusters, p is the number of features, $\Theta = [\theta_1, \dots, \theta_k]$, and $\theta_j \in \mathbb{R}^p$ is the j -th center.

B. FCM Algorithm

As an extension of KM, FCM was developed by Dunn [57], and improved by Bezdek [32]. Differing from KM that assigns each data point to exactly one cluster, FCM allows data points to belong to multiple clusters with different degrees of membership. It is based on the minimization of the following biconvex objective function [32]:

$$f_m(\mu, \Theta) = \sum_{i=1}^n \sum_{j=1}^k \mu_{ij}^m \|x_i - \theta_j\|^2, \quad (2)$$

where $\mu_{ij} \in [0, 1]$ is the degree of membership of the i -th datum in the j -th cluster, $m > 1$ is an exponent for controlling the degree of fuzzy overlap, and θ_j is the center of the j -th cluster. The fuzzy objective function is subject to a constraint $\sum_{j=1}^k \mu_{ij} = 1$ ($i = 1, \dots, n$); i.e., for each datum, the sum of the membership degrees over all clusters is one. For $j = 1, \dots, k$, the centers are updated as follows [32]:

$$\theta_j = \frac{\sum_{i=1}^n \mu_{ij}^m x_i}{\sum_{i=1}^n \mu_{ij}^m}. \quad (3)$$

For $i = 1, \dots, n$ and $j = 1, \dots, k$, the degrees are updated alternately as follows [32]:

$$\mu_{ij} = \frac{1}{\sum_{l=1}^k \left(\frac{\|x_i - \theta_j\|}{\|x_i - \theta_l\|} \right)^{\frac{2}{m-1}}}. \quad (4)$$

Similar to KM, FCM iterates over (3) and (4) until no degree changes. Due to the biconvexity of the fuzzy objective function in (2), the alternating method cannot guarantee to converge to the global optimal cluster.

Note that $\lim_{m \rightarrow 1} \mu_{ij} \in \{0, 1\}$; i.e., FCM degenerates to KM [29].

C. PKM Algorithm

PKM [25] is proposed to improve KM algorithms by minimizing the following annealed power function:

$$f_s(\Theta) := \sum_{i=1}^n \left(\frac{1}{k} \sum_{j=1}^k \|x_i - \theta_j\|_2^{2s} \right)^{\frac{1}{s}}, \quad (5)$$

where $s < 0$ denotes a power parameter.

Rather than minimizing the concave power-mean functions in (5), PKM minimizes the following convex majorization function [25]:

$$\hat{f}_s(\Theta) = \sum_{i=1}^n \sum_{j=1}^k w_{ij}(t) \|x_i - \theta_j(t+1)\|_2^2. \quad (6)$$

The weights are updated as follows [25]:

$$w_{ij}(t) = \frac{\|x_i - \theta_j(t)\|^{2(s-1)}}{\left(\sum_{l=1}^k \|x_i - \theta_l(t)\|^{2s} \right)^{1-\frac{1}{s}}}. \quad (7)$$

The clusters are updated as follows [25]:

$$\theta_j(t+1) = \frac{1}{\sum_{i=1}^n w_{ij}(t)} \sum_{i=1}^n w_{ij}(t) x_i.$$

The power parameter s is decreased at each step according to the following cooling schedule [25]:

$$s(t+1) = \eta s(t),$$

where $s(0) < 0$ and $\eta > 1$.

Let $s = -\frac{1}{m-1}$. The weight updating rule in (7) is rewritten as follows:

$$\begin{aligned} w_{ij} &= \frac{\|x_i - \theta_j\|^{2(s-1)}}{\left(\sum_{l=1}^k \|x_i - \theta_l\|^{2s} \right)^{1-\frac{1}{s}}} \\ &= \frac{\|x_i - \theta_j\|^{-2m/(m-1)}}{\left(\sum_{l=1}^k \|x_i - \theta_l\|^{-2/(m-1)} \right)^m}. \end{aligned} \quad (8)$$

Via substituting the weight updating rule in (8), the objective function in (5) is rewritten as follows:

$$\begin{aligned} \hat{f}_s(\Theta) &= \sum_{i=1}^n \sum_{j=1}^k w_{ij} \|x_i - \theta_j\|^2 \\ &= \sum_{i=1}^n \sum_{j=1}^k \frac{\|x_i - \theta_j\|^{-2m/(m-1)}}{\left(\sum_{l=1}^k \|x_i - \theta_l\|^{-2/(m-1)} \right)^m} \end{aligned}$$

$$\|x_i - \theta_j\|^2. \quad (9)$$

The degree updating rule of FCM in (4) is rewritten as follows:

$$\begin{aligned} \mu_{ij} &= \frac{1}{\sum_{l=1}^k \left(\frac{\|x_i - \theta_j\|}{\|x_i - \theta_l\|} \right)^{\frac{2}{m-1}}} \\ &= \frac{\|x_i - \theta_j\|^{-2/(m-1)}}{\sum_{l=1}^k \|x_i - \theta_l\|^{-2/(m-1)}}. \end{aligned} \quad (10)$$

Via substituting degree updating rule (10), the objective function of FCM in (2) is rewritten as follows:

$$\begin{aligned} f_m(\mu, \Theta) &= \sum_{i=1}^n \sum_{j=1}^k \mu_{ij}^m \|x_i - \theta_j\|^2 \\ &= \sum_{i=1}^n \sum_{j=1}^k \frac{\|x_i - \theta_j\|^{-2m/(m-1)}}{\left(\sum_{l=1}^k \|x_i - \theta_l\|^{-2/(m-1)} \right)^m} \|x_i - \theta_j\|^2. \end{aligned} \quad (11)$$

It indicates that the objective functions of FCM in (2) and PKM in (6) are equivalent.

D. CAPKM++ and CAPKM++2.0 Algorithms

PKM is demonstrated in [25] to perform better than Lloyd's algorithm [13] and k -harmonic means [16]. Nevertheless, its clustering results are not globally optimal since its performance heavily depends on the anchor points where its majorization functions are located. To address the aforementioned issue, CAPKM++ [26] employs multiple PKM modules to generate centers for alternative clusters, and use a particle swarm optimization rule for repositioning the initial centers.

CAPKM++2.0 [27] is an upgraded version of CAPKM++. CAPKM++2.0 reinitializes the weights in the majorization function during annealing rather than reinitializing cluster centers after annealing. In addition, CAPKM++2.0 minimizes the power-mean functions directly instead of their majorization function as in PKM and CAPKM++. It is demonstrated in [27] that CAPKM++2.0 is more efficient than CAPKM++ in terms of algorithmic complexities.

III. ALGORITHM DESCRIPTION

The proposed CAFCM algorithm consists of triple loops: an FCM clustering loop, a reinitialization loop, and an annealing loop. In the FCM clustering loop, multiple FCM modules iterate until convergence. In the reinitialization loop, the FCM modules are reinitialized. In the annealing loop, an exponent $m(t)$ decreases iteratively. The fuzzy objective function in (2) is minimized during such an annealing process, similar to PKM [25], CAPKM++ [26], and CAPKM++2.0 [27]. As shown in Fig. 1, the following three types of cooling schedules may be used for the annealing of exponent $m(t)$. An exponential cooling schedule

$$m_e(t) = (m_e(0) - 1) \exp(-t) + 1. \quad (12)$$

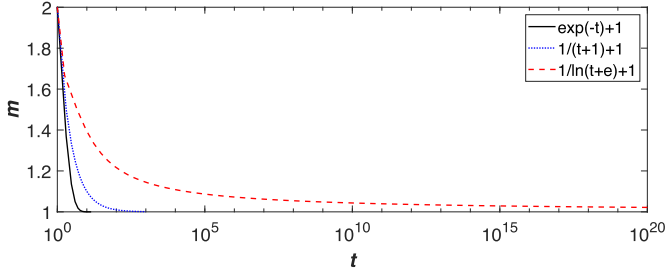


Fig. 1. Annealing curves of the three cooling schedules.

A polynomial cooling schedule

$$m_p(t) = \frac{m_p(0) - 1}{t + 1} + 1. \quad (13)$$

A logarithmic cooling schedule

$$m_l(t) = \frac{m_l(0) - 1}{\ln(t + e)} + 1. \quad (14)$$

Note that $\lim_{t \rightarrow \infty} m_e(t) = \lim_{t \rightarrow \infty} m_p(t) = \lim_{t \rightarrow \infty} m_l(t) = 1$. Each of the three cooling schedules has its pros and cons. As shown in Fig. 1, the exponential cooling schedule is the fastest, and it may cause prematurity in analogy to simulated annealing. The logarithmic cooling schedule is the slowest, and it takes a very long time to reduce to 1. The polynomial schedule is in-between.

In analogy to CAPKM++ [26] and CAPKM++2.0 [27], to overcome the biconvexity, $\mu(0)$ is repeatedly reinitialized according to the following particle swarm optimization rule in [58]:

$$v^{(i)}(t + 1) = c_0 v^{(i)}(t) + c_1 r_1 (\mu^{(i)*} - \mu^{(i)}(t)) \quad (15a)$$

$$+ c_2 r_2 (\mu^* - \mu^{(i)}(t)), \quad (15b)$$

$$\mu^{(i)}(t + 1) = \mu^{(i)}(t) + v^{(i)}(t + 1), \quad (15c)$$

where $v^{(i)}(t)$ is an incremental vector of the i -th module, $\mu^{(i)*}$ is the current best degree vector of the i -th module, $\mu^{(i)}(t)$ is the current degree vector of the i -th module, μ^* is the current best degree vector of the multiple modules, $c_0 \in [0, 1]$ is a constant, c_1, c_2 are two positive constants, and r_1, r_2 are two random numbers in $[0, 1]$.

The high diversity of solutions is essential for improving clustering performance. A diversity measure of solutions is defined as follows:

$$\delta(\mu) = \frac{1}{Nnk} \sum_{j=1}^N \|\mu^{(j)} - \mu^*\|_2, \quad (16)$$

where N is the population size (i.e., the number of alternative cluster sets).

Mutation operation is a commonly used method to maintain a certain level of diversity and prevent premature convergence. If the diversity measure is below a threshold (i.e., $\delta(\mu) < \delta_{\min}$),

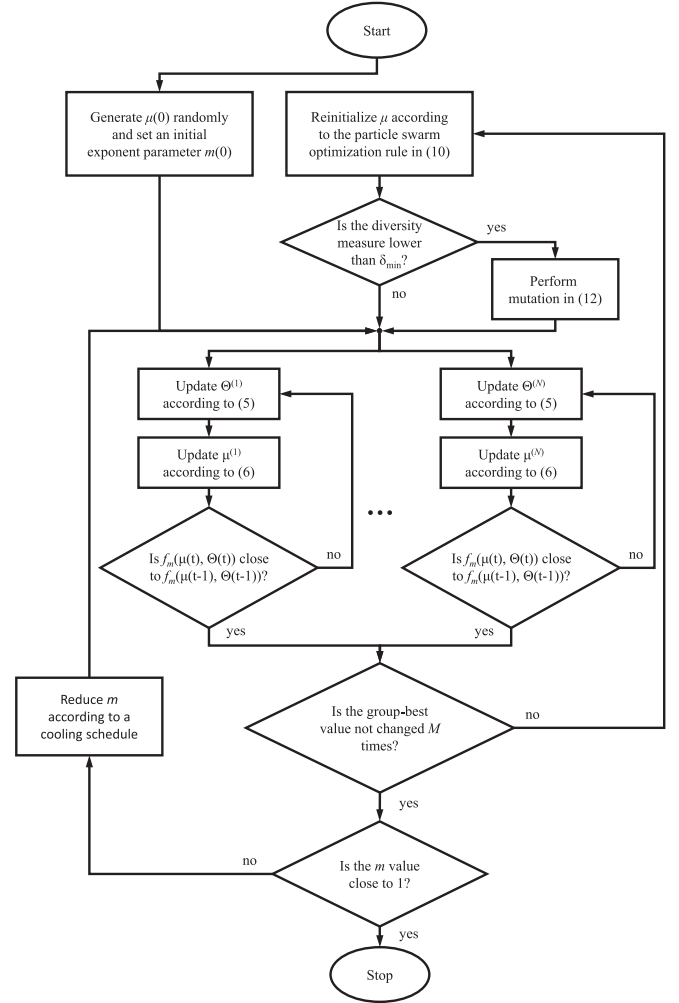


Fig. 2. Flowchart of CAFCM.

then a wavelet mutation operator is used to assure the diversity [59]

$$\mu^{(i)}(t + 1) = \begin{cases} \mu^{(i)}(t) + \zeta(\bar{\mu}^{(i)} - \mu^{(i)}(t)) & \zeta > 0 \\ \mu^{(i)}(t) + \zeta(\underline{\mu}^{(i)} - \mu^{(i)}(t)) & \zeta < 0, \end{cases} \quad (17)$$

where $\bar{\mu}^{(i)} = 1$ and $\underline{\mu}^{(i)} = 0$ are the upper bound and lower bound of the membership degree of the i -th module, and ζ is defined by a wavelet function

$$\zeta = \frac{1}{\sqrt{a}} \exp\left(-\frac{1}{2} \left(\frac{\psi}{a}\right)^2\right) \cos\left(\frac{5\psi}{a}\right),$$

where $a = \exp(10(\ell/\ell_{\max}))$ is the amplitude of the wavelet function, ℓ_{\max} is the maximum iterative number, and ψ is the frequency of the wavelet function to be randomly generated from the interval $[-2.5a, 2.5a]$.

Fig. 2 portrays a flowchart of the CAFCM algorithm, and Algorithm 1 details its procedure. In Steps 6–10, centers Θ and degrees μ are updated alternately until convergence, where ϵ in Step 10 is to determine whether $f_m(\mu^{(i)}(\hat{t}), \Theta^{(i)}(\hat{t}))$ and $f_m(\mu^{(i)}(\hat{t} - 1), \Theta^{(i)}(\hat{t} - 1))$ are close enough. In Steps 11–13, the individual best degrees $\tilde{\mu}^{(i)}$ are determined. In Steps 15–21,

Algorithm 1: CAFCM.

Input: $M, N, m(0), c_0, c_1$ and $c_2, X \in \mathbb{R}^{n \times p}$.
particle/group best degrees $\tilde{\mu}^{(p)}/\mu^*$,
 $f(\tilde{\mu}^{(p)}) = f(\mu^*) = \infty$, initial degrees
 $[\mu^{(1)}(0), \dots, \mu^{(N)}(0)]$, initial incremental vector
 $[v^{(1)}(0), \dots, v^{(N)}(0)]$,

Output: μ^* .

```

1  $t \leftarrow 0$ ;
2 repeat
3   while  $l \leq M$  do
4     for  $i = 1$  to  $N$  do
5        $\hat{t} \leftarrow 1$ ;
6       repeat
7         Update  $\Theta^{(i)}(\hat{t})$  according to Eqn. (3);
8         Update  $\mu^{(i)}(\hat{t})$  according to Eqn. (4);
9          $\hat{t} \leftarrow \hat{t} + 1$ ;
10        until  $|f_m(\mu^{(i)}(\hat{t}), \Theta^{(i)}(\hat{t})) - f_m(\mu^{(i)}(\hat{t} - 1), \Theta^{(i)}(\hat{t} - 1))| < \epsilon$ ;
11        if  $f(\mu^{(i)}) < f(\tilde{\mu}^{(i)})$  then
12           $\tilde{\mu}^{(i)} \leftarrow \mu^{(i)}$ ;
13        end
14      end
15       $i^* = \arg \min_i \{f(\mu^{(1)}), \dots, f(\mu^{(i)}), \dots, f(\mu^{(N)})\}$ ;
16      if  $f(\mu^{(i^*)}) < f(\mu^*)$  then
17         $\mu^* \leftarrow \mu^{(i^*)}$ ;
18         $l \leftarrow 0$ ;
19      else
20         $l \leftarrow l + 1$ ;
21      end
22      for  $i = 1$  to  $N$  do
23        Update  $v^{(i)}$  according to Eqn. (15a);
24        Update  $\mu^{(i)}$  according to Eqn. (15c);
25      end
26      Compute  $\delta(\mu)$  according to Eqn. (16);
27      if  $\delta(\mu) < \delta_{\min}$  then
28        Perform mutation according to Eqn. (17);
29      end
30    end
31     $t \leftarrow t + 1$ ;
32    Reduce  $m(t)$  according to Eqn. (12), Eqn. (13), or
    Eqn. (14);
33  until  $m(t) - 1 < \epsilon$ ;
34  return  $\mu^*$ .
```

the group best degrees μ^* are determined and the termination counter is updated. In Steps 22–25, the degrees are reinitialized according to (15). In Step 26, the diversity of the N sets of degrees is measured according to (16). In Steps 27–29, the wavelet mutation operator in (17) is performed if the diversity measure is below the preset threshold δ_{\min} . In Step 32, the exponent m is reduced according to one of the three cooling schedules. In Step 10, the termination condition whether m is close to 1 is determined. The code of CAFCM is available in Github.¹

¹[Online]. Available: <https://github.com/HongzongLI-CS/CAFCM-Github>

TABLE I
INFORMATION ABOUT THE EIGHT BENCHMARK DATASETS AND THE
CORRESPONDING HYPER-PARAMETER VALUES USED IN CAFCM

Datasets	n	p	k	N	M
NCI9 ² [60]	60	9712	9	2	10
WarpPIE10P ³ [60]	210	2420	10	2	5
WQ-White ⁴ [61]	4898	11	11	2	15
PageBlocks ⁵ [61]	5472	10	5	2	5
Texture ⁶ [61]	5500	40	11	3	15
Optdigits ⁷ [61]	5620	65	10	2	5
EGS ⁸ [62]	10000	13	2	2	5
LR ⁹ [63]	20000	16	26	3	15

² [Online]. Available: <https://jundongli.github.io/scikit-feature/files/datasets/nci9.mat>

³ [Online]. Available: <https://jundongli.github.io/scikit-feature/files/datasets/warpPIE10P.mat>

⁴ [Online]. Available: <https://sci2s.ugr.es/keel/dataset.php?cod=209>

⁵ [Online]. Available: <https://sci2s.ugr.es/keel/dataset.php?cod=104>

⁶ [Online]. Available: <https://sci2s.ugr.es/keel/dataset.php?cod=72>

⁷ [Online]. Available: <https://sci2s.ugr.es/keel/dataset.php?cod=199>

⁸ [Online]. Available: <https://archive.ics.uci.edu/ml/datasets/Electrical+Grid+Stability+Simulated+Data+>

⁹ [Online]. Available: <https://archive.ics.uci.edu/ml/datasets/Letter+Recognition>

IV. EXPERIMENTAL RESULTS

In the experiments, the CAFCM parameters are set as follows. The value of the initial exponent $m(0)$ is set to 2, as in most of the existing references. The diversity threshold δ_{\min} is set to a sufficiently small value (i.e., 10^{-3}). In the FCM clustering loop of CAFCM, the parameter ϵ is also set to a sufficiently small value (i.e., 10^{-3}) as a stopping criterion of cluster membership updating. In the particle swarm optimization rule in (15), c_0, c_1 , and c_2 are set to 1, as typically in many references, e.g., in [26] and [27].

A. Cooling Schedules

In this section, we compare the performances of CAFCM with the three cooling schedules. To make a fair comparison, the three cooling schedules are set to the same number of iterations. Since the logarithmic cooling schedule takes a long time for $m(t)$ to reduce to 1, instead of iterating over every t , sampling time $\tau(t)$ is used under the condition that the value of $m_l(\tau)$ is larger than that of the polynomial cooling schedule at every sampling time (i.e., $m_l(\tau(t)) > m_p(t)$) to keep its annealing process slower than the polynomial one. Since $\frac{m_p(0)}{t+2} > \frac{m_p(0)-1}{t+1}$ for $t > m_p(0) - 1$, letting $\frac{m_l(0)-1}{\ln(\tau(t)+e)} + 1 = \frac{m_p(0)}{t+2} + 1$ enables $m_l(\tau(t)) > m_p(t)$. The solution to the equation is $\tau(t) = \exp\left(\frac{(m_l(0)-1)(t+2)}{m_l(0)}\right) - e$, assuming that $m_l(0) = m_p(0)$.

The experimental results are based on eight commonly used datasets summarized in Table I. In addition, to show the superiority of CAFCM with the logarithmic cooling schedule on the dataset that is difficult to cluster, a dataset under uniform distribution (UDD) is generated, where $n = 5000$ and $p = 2$.

Fig. 3 shows 20-run Monte Carlo test results of CAFCM ($N = 2$ and $M = 5$) with the three cooling schedules on the six datasets in Table I and the UDD. As shown in Fig. 3, CAFCM with the polynomial cooling schedule or the logarithmic cooling

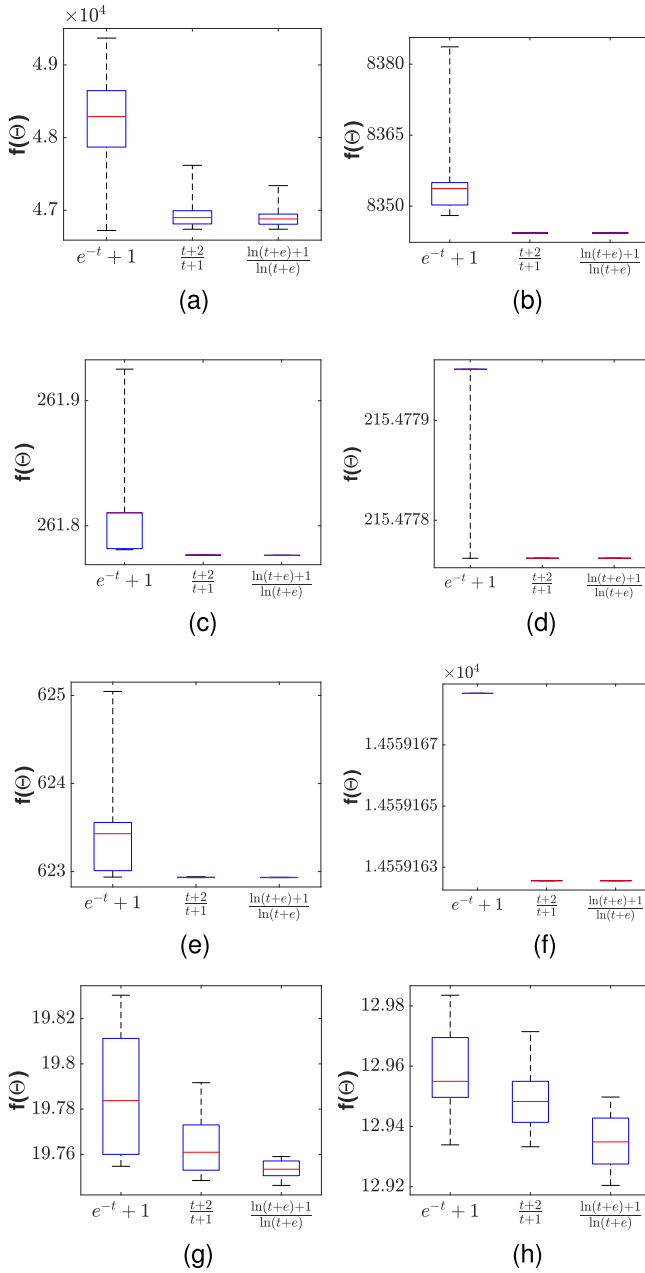


Fig. 3. Monte Carlo test results of CAFCM ($N = 2$ and $M = 5$) with the three cooling schedules on the six datasets and the UDD with two different k values. (a) NCI9. (b) WarpPIE10P. (c) WQ-White. (d) PageBlock. (e) Texture. (f) Optdigits. (g) UDD ($k = 40$). (h) UDD ($k = 60$).

schedule outperforms that with the exponential cooling schedule. It is also shown in Fig. 3 that CAFCM with the logarithmic cooling schedule outperforms that with the polynomial cooling schedule on NCI9, Texture, and UDD, especially on the UDD, and the superiority is more evident for a larger k value on the UDD.

Although the performance of CAFCM with the logarithmic cooling schedule is better than that with the polynomial cooling schedule, it takes too long time to reach 1, or it is difficult to set a reasonable sampling time to achieve high performance. In view of the fact that CAFCM with the polynomial cooling schedule

performs well on the six datasets in Table I, the polynomial cooling schedule $m_p(t)$ is used in all the other experiments.

B. Hyperparameters Selection

Similar to CAPKM++ [26] and CAPKM++2.0 [27], the values of two hyperparameters N and M in Algorithm 1 are selected based on 50-run Monte Carlo tests on the six datasets. Fig. 4 depicts the boxplots of the Monte Carlo test results obtained using the CAFCM algorithm over 20 runs on the six datasets. As shown in Fig. 4, the results of the objective function values reaching zero standard deviation with $N = 2$ and $M = 10$ on NCI9, $N = 2$ and $M = 5$ on WQ-White, $N = 2$ and $M = 15$ on WarpPIE10P, $N = 2$ and $M = 5$ on PageBlocks, $N = 3$ and $M = 15$ on Texture, and $N = 2$ and $M = 5$ on Optdigits. Table I tabulates the values of the two hyperparameters (i.e., N and M) used in CAFCM on the eight datasets.

C. Convergent Behaviors

Fig. 5 depicts twelve snapshots of the convergent centers Θ and the convergent degrees μ values in the FCM clustering loop (Steps 6–10) of CAFCM on the six datasets. Fig. 6 depicts the monotonically decreasing values of $f_m(\mu, \Theta)$ in (2) corresponding to Θ and μ in Fig. 5. They show that the centers and the degrees reach their equilibria and the fuzzy objective function values reach their minima with a range of 40–400 iterations in the FCM clustering loop of CAFCM.

Fig. 7 depicts the monotonically decreasing values of $f(\Theta)$ in the annealing loop (Steps 2–33) of CAFCM on the six datasets. It shows that CAFCM converges within 120 iterations on NCI9, 80 iterations on WarpPIE10P, 1 000 iterations on WineQuality-White, 30 iterations on PageBlocks, 160 iterations on Texture, and 1 500 iterations on Optdigits.

D. Performance Comparison

The clustering performance of CAFCM is compared with the following six fuzzy clustering algorithms and seven crisp clustering algorithm: KM,¹⁰ k -mean++ (KM++),¹¹ PKM [25], EWPKM,¹² (SC,¹³ HC,¹⁴ CAPKM++2.0 [27], BFC [46], fuzzy subspace clustering (FSC) [64], maximum entropy clustering (MEC) [65], FCM,¹⁵ KFCM [47], and 2PFCM [54]. The clustering results of the fuzzy clustering algorithms (i.e., BFC, FSC, MEC, FCM, KFCM, and 2PFCM) are determined by the maximum fuzzy membership degrees. The code of PKM is provided by the authors of [25]. The agglomerative HC algorithm is used. The code of BFC is obtained from a link in [46]. As BFC involves the Cholesky factorization of the covariance matrices of data, and the covariance matrices of some data are not positive

¹⁰[Online]. Available: https://www.mathworks.com/help/stats/kmeans.html?s_tid=srchtitle_kmean_1

¹¹[Online]. Available: <https://github.com/xuyxu/Clustering>

¹²[Online]. Available: <https://github.com/DebolinaPaul/EWP>

¹³[Online]. Available: <https://www.mathworks.com/help/stats/spectralcluster.html>

¹⁴[Online]. Available: https://www.mathworks.com/help/stats/hierarchical-clustering.html?s_tid=srchtitle_hierarchical%20clustering_1

¹⁵[Online]. Available: <https://www.mathworks.com/help/fuzzy/fcm.html>

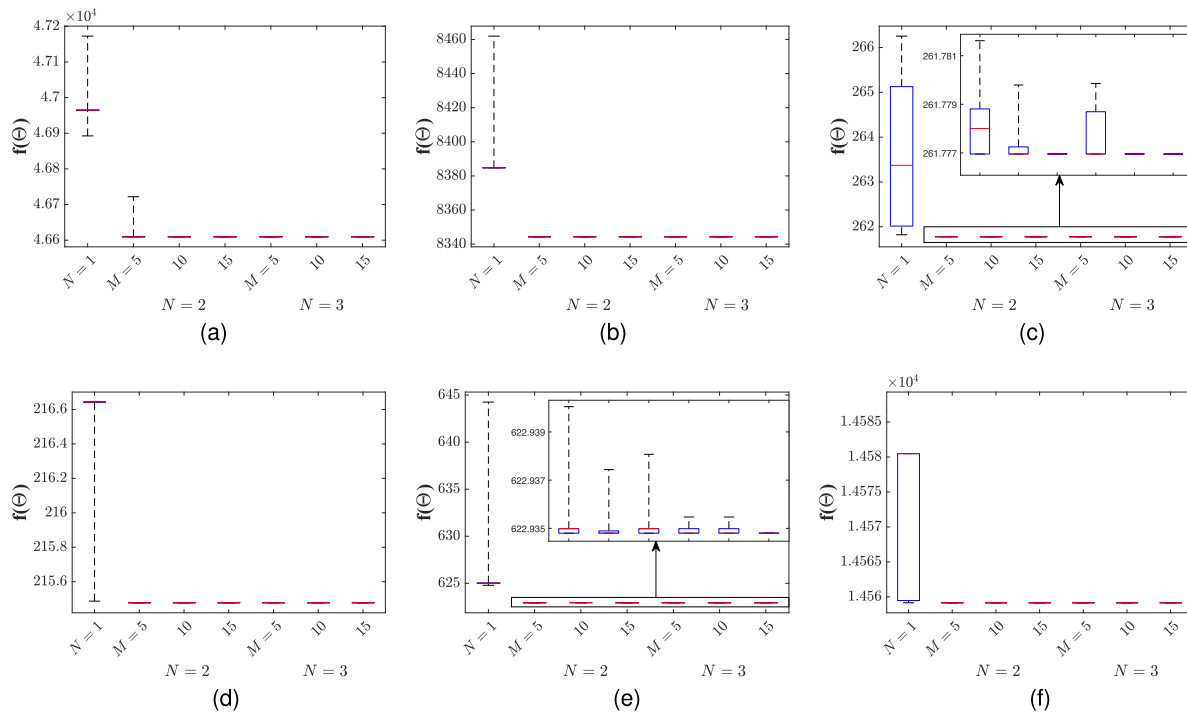


Fig. 4. Monte Carlo test results using CAFCM with several values of N and M on the six datasets. (a) NCI9. (b) WarpPIE10P. (c) WineQuality-White. (d) PageBlock. (e) Texture. (f) Optdigits.

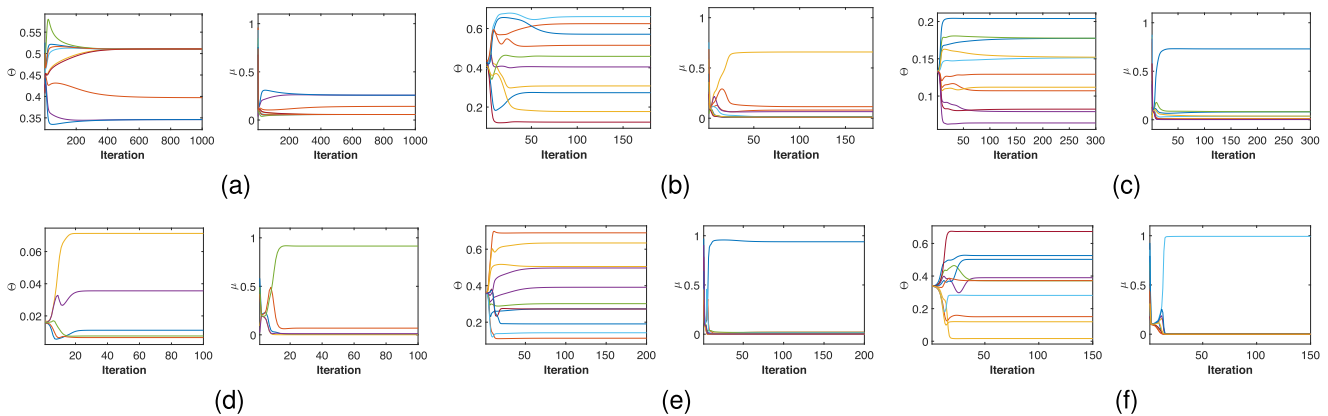


Fig. 5. Snapshots of the convergent centers Θ and the membership degrees μ values in the FCM clustering loop of CAFCM (Steps 6–10) on the six datasets, where the lines in the left-hand side subplots portray the first feature values of k centers, and the lines in the right-hand side subplots portray the k membership degrees. (a) NCI9. (b) WarpPIE10P. (c) WineQuality-White. (d) PageBlock. (e) Texture. (f) Optdigits.

definite, BFC may not be applicable to some datasets. The codes of FSC and MEC are obtained from Github.¹⁶ The codes of KFCM and 2PFCM are shared by the authors of [47] and [54], respectively. The Euclidean distance is used as the dissimilarity measure in all algorithms.

The performance evaluation for the experimental results is based on nineteen internal criteria listed in Table S-I in the Supplementary Materials, and three external criteria described in Section S-I in the Supplementary Materials. Due to the wide range of values of WGSS, CHI, XBI, and TWI, they are

¹⁶[Online]. Available: https://github.com/kailugaji/Fuzzy_Clustering_Algorithms

normalized by p , $(n - k)/(k - 1)$, n , and pk , respectively, to facilitate the later tabular presentation.

Tables II–V tabulate the means and standard deviations of the internal and external cluster validity indices values over 50 runs by using CAFCM and thirteen prevailing algorithms with random initialization on the eight datasets, where \times indicates “not applicable”, and the best and second-best results are boldfaced and underlined, respectively. Specifically, CAFCM achieves 81 best and 20 second-best means out of 168 entries (i.e., 48.21% and 60.12% for the best and the best plus the second-best), and CAPKM++2.0 ranks in second place, achieving 40 best and 55 second-best means (i.e., 23.81% and 56.55%), and SC ranks in third place, achieving 23 best and

TABLE II
MEAN VALUES AND STANDARD DEVIATIONS OF INTERNAL AND EXTERNAL CLUSTER VALIDITY INDICES RESULTING FROM CAFCM, AND THIRTEEN BASELINES ON NCI9 AND WARPPIE10P, WHERE N = 2 AND M = 10 IN CAPKM++2.0 AND CAFCM ON NCI9, AND N = 2 AND M = 5 IN CAPKM++2.0 AND CAFCM ON WARPPIE10P

Table with multiple sections for NCI9 and WarpPIE10P, each containing sub-sections for different clustering methods (KM, PKM, EWP, SC, HC, CAPKM++2.0) and validation indices (WGSS, MRI, GPI, BHGI, CI, TI, DGI, RLI, CHI, RTI, WGI, DI, BHI, PBMI, XBI, DBL, LSSRI, TWI, ACC, NMI, ARI). Values are presented as mean ± standard deviation.

The best ones are boldfaced and second best ones are underlined.

TABLE IV
MEAN VALUES AND STANDARD DEVIATIONS OF INTERNAL AND EXTERNAL CLUSTER VALIDITY INDICES RESULTING FROM CAFCM, AND THIRTEEN BASELINES ON TEXTURE AND OPTDIGITS, WHERE N = 3 AND M = 15 IN CAPKM++2.0 AND CAFCM ON TEXTURE, AND N = 2 AND M = 5 IN CAPKM++2.0 AND CAFCM ON OPTDIGITS

Table with 8 columns: Metric, Method, KM, KM++, PKM, EWPKM, SC, HC, CAPKM++2.0. Rows are categorized by Texture and Optdigits, each with sub-headers for different methods (FCM, MEC, FSC, 2PFCM, BFC, KFCM, CAFCM).

The best ones are boldfaced and second best ones are underlined.

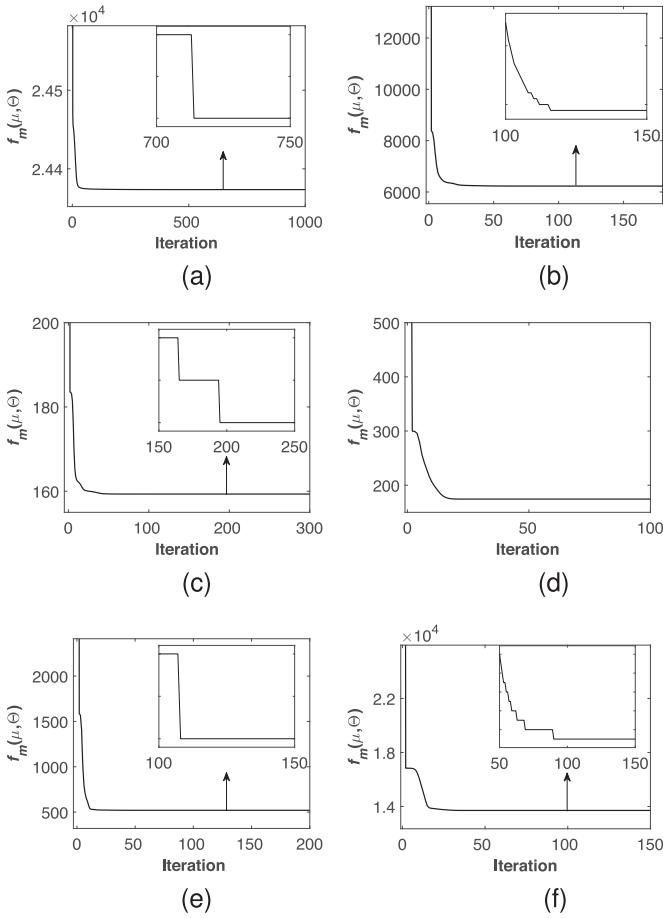


Fig. 6. Snapshots of the fuzzy objective function values of $f_m(\mu, \Theta)$ in (2) with $m = 1.5$ in the FCM clustering loop of CAFCM (Steps 6–10) on the six datasets. (a) NCI9. (b) WarpPIE10P. (c) WineQuality-White. (d) PageBlock. (e) Texture. (f) Opltdigits.

3 second-best means (i.e., 13.69% and 15.48%). Fig. 8 depicts the counts of the best and best plus second-best index mean values by using CAFCM and the thirteen baselines. As shown in Fig. 8, CAFCM, CAPKM+++2.0, and SC rank in the first three places in terms of the counts of the best index mean values. CAFCM, CAPKM+++2.0, and PKM rank in the first three places in terms of the counts of best plus second-best index mean values. In addition, the standard deviations of the results using CAFCM are zero, indicating the highest consistency of the algorithm.

E. Complexity Analysis

As shown in Tables I and Table S-II in the Supplementary Materials, the suitable number of modules N is 2 or 3, for 18 datasets with various values of n , p , and k . As N is a small constant, the spatial complexity of CAFCM is the same as FCM (i.e., $O((n+p)k)$ [66]).

The time complexity is empirically estimated via non-negative least-squares regression using the numbers of iterations on the 18 datasets

$$\begin{aligned} \min_w \|Cw - T\|_2^2 \\ \text{s.t. } w \geq 0, \end{aligned}$$

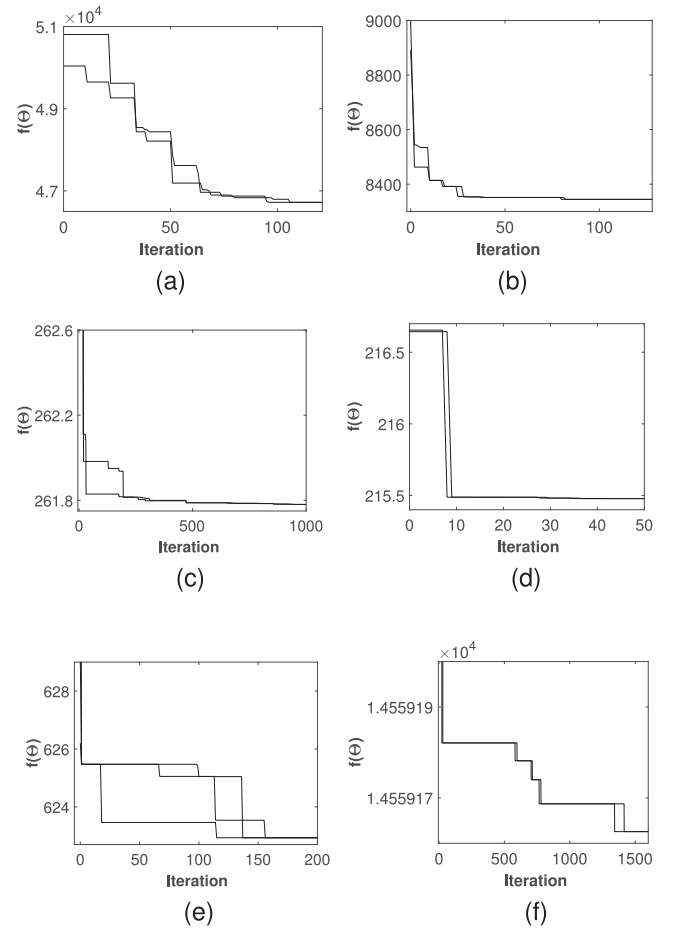


Fig. 7. Descending objective function values of $f(\Theta)$ in the annealing loop of CAFCM (Steps 2–33) on the six datasets. (a) NCI9 ($N = 2$ and $M = 10$). (b) WarpPIE10P ($N = 2$ and $M = 5$). (c) WineQuality-White ($N = 2$ and $M = 15$). (d) PageBlocks ($N = 2$ and $M = 5$). (e) Texture ($N = 3$ and $M = 15$). (f) Opltdigits ($N = 2$ and $M = 5$).

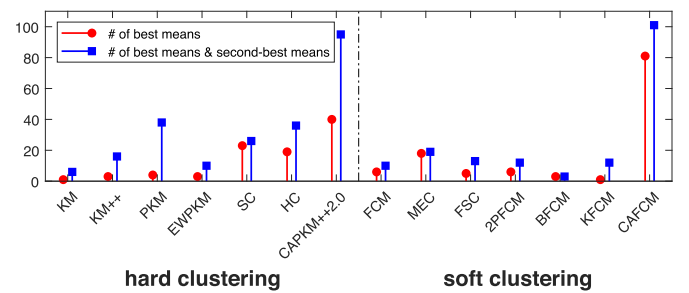


Fig. 8. Counts of the best and best plus second-best index mean values using CAFCM and the thirteen baselines.

where $w \in \mathbb{R}^{38}$ is the weight vector of the terms, $T \in \mathbb{R}^{18}$ is the vector of iteration counts, and $C \in \mathbb{R}^{18 \times 38}$ is the matrix of 38 combinations of polynomials and logarithms of n , m , and p . Table S-VIII in the Supplementary Materials lists the 38 combinations of polynomials and logarithms of n , m , and p , and their estimated coefficients. By neglecting the terms with their coefficients w smaller than 0.0001, the resulting estimate is $2\,288\,239\,k^2np + 351\,783\,k^2np \log(p)$. As the second term is of higher order, the estimated time complexity of CAFCM is

$O(k^2np \log(p))$. As the time complexity of FCM is $O(k^2np)$ per iteration [66], it is $\log(p)$ times that of FCM.

V. CONCLUSION

In this paper, a collaborative annealing fuzzy c -means clustering algorithm is proposed. The experimental results on eight datasets demonstrate that the proposed algorithm with only two or three modules statistically outperforms thirteen competing algorithms in terms of many cluster validity indices. The proposed method achieves superior performance, owing to the adoption of the annealing procedure to phase out fuzziness, as well as collaborative modules to maximize clustering quality and eliminate the influence of initial solutions on clustering performance. Further research may include improving the efficiency of the proposed method, extending it for robust clustering to cluster data in the presence of noises or outliers, extending it for semisupervised clustering to leverage information from labeled and unlabeled data, extending it for multiview clustering to take into account multiple perspectives or representations of data, and applying it to specific problems in science and engineering.

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