Deep Probability Aggregation Clustering

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Abstract. Combining machine clustering with deep models has shown remarkable superiority in deep clustering. It modifies the data processing pipeline into two alternating phases: feature clustering and model training. However, such alternating schedule may lead to instability and computational burden issues. We propose a centerless clustering algorithm called Probability Aggregation Clustering (PAC) to proactively adapt deep learning technologies, enabling easy deployment in online deep clustering. PAC circumvents the cluster center and aligns the probability space and distribution space by formulating clustering as an optimization problem with a novel objective function. Based on the computation mechanism of the PAC, we propose a general online probability aggregation module to perform stable and flexible feature clustering over mini-batch data and further construct a deep visual clustering framework deep PAC (DPAC). Extensive experiments demonstrate that PAC has superior clustering robustness and performance and DPAC remarkably outperforms the state-of-the-art deep clustering methods.

Keywords: Deep Clustering · Fuzzy Clustering

1 Introduction

Clustering analysis [3] is a widely explored domain in the field of unsupervised learning, aiming to group the unlabeled samples into clusters that have common characteristics. Conventional machine clustering is favored by many researches due to its significant interpretability and stable optimization. In recent years, deep clustering has received more attention due to its powerful representation extraction capabilities. Previous deep clustering models [8, 22, 54, 55] directly combine deep network with machine clustering and utilize designed loss functions to guide both representation learning and clustering. Deepcluster [9] and PCL [32] decouple representation learning and clustering to leverage the offline pseudo labels of K-means (KM) to cluster images. Unfortunately, these offline methods typically require running multiple times of standard KM over the entire dataset, which brings much time and space complexity. Besides, simply grouping data in batches instead of whole dataset to obtain online clustering causes collapsing

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and degradation issues. To tackle these problems, researchers have given two dominant solutions; batch clustering and contrastive clustering.

Batch clustering [20, 28, 36, 56] focuses on modifying the conventional machine clustering algorithms [58] to adapt the data flow of deep models, which has high extensibility. The pseudo labels are generated online by machine clustering based on embedding space distribution. For example, Online Deep Clustering (ODC) [56] incorporates memory banks to online update pseudo labels and centroids of KM. ODC decomposes the standard KM process into batch clustering with memory banks and optimizes the clustering and network shoulderto-shoulder (online) to facilitate stable learning. CoKe [41] proposes the moving average strategy to reassignment pseudo labels and introduces Constrained Kmeans [7] into training to ensure minimal size of clusters to avoid collapsing. Most existing batch clustering approaches pay more attention to center-based machine clustering algorithms, such as KM and fuzzy c-means (FCM) [6], which require specially designed center update rules. Moreover, center-based machine clustering is easily susceptible to the influence of cluster center [4,21]. Random initialization of cluster centers introduces instability to subsequent training. And partitioning based on nearest centers cannot provide fine-gained discrimination hyperplanes for clusters, affecting clustering performance. In other words, the inherent complexity and instability of center-based machine clustering brings biases to batch clustering models.

Recently, contrastive clustering [34, 44, 47, 59] has achieved significant success in online deep clustering. Contrastive methods perform online clustering by exploring multi-view correlations of data. Compared with batch clustering, contrastive clustering is more stable, suitable for small batches of data, and can be easily compatible with deep learning technologies such as distributed training. Formally, instances are augmented by using random data augmentation to establish contrastive frameworks. IIC [27] maximizes mutual information between augmented pairs. CC [33] and PICA [26] proposes cluster-level contrastive loss to perform online deep clustering. SwAV [10] and SeLa [5] adopt a balanced cluster discrimination task and calculate assignments of instances via Sinkhorn-Knopp algorithm. However, the establishment of contrastive framework introduces a lot of artificial prior information, including data augmentation method, hyperparameter setting and model architecture. Contrastive models often need thousands of epochs to reach convergence. Besides, they make a balanced assumption for clustering (i.e. each cluster has exactly the same number of samples), which require additional regular terms to constrain optimization and avoid crashes problem (i.e. a few clusters have a majority of instances). The essence of contrastive clustering methods is to leverage the nearest-neighbor relationship of augmented instances in the semantic space to unsupervisedly train the classifier. Such semantic nearest-neighbor learning only uses a portion of data and its corresponding augmented version, failing to capture the global distribution [13] and encode spatial structure.

In this work, considering the adverse effect of the cluster center, we first introduce a novel objective function quantifying the intra-cluster distances without

cluster centers. Furthermore, inspired by fuzzy c-means, a concise optimization program is formulated via incorporating a fuzzy weighting exponent into objective function, resulting in a centerless machine clustering method called Probability Aggregation Clustering (PAC). In optimization program of PAC, the probability of one sample belonging to a cluster is aggregated across samples with distance information in an iterative way. Unlike KM that assigns instances by cluster centers, PAC directly outputs probabilities which is more stable and easy to deploy in deep model. Therefore, we extend the PAC to the online probability aggregation module (OPA), a simple plug-in component for online deep clustering tasks. OPA seamlessly combines calculation process of PAC with loss computation, which overcomes the disadvantages of both batch and contrastive clustering and implements efficient stable clustering. Besides, OPA does not impose any constraints on the size of clusters, mitigating the suboptimal solutions introduced by balanced clustering. It computes clustering codes with the batches of data and updates the network by KL divergence, which leaves out the complicated clustering steps and trains the model in a supervised manner. Furthermore, a deep image clustering model Deep PAC (DPAC) is established, which ensures stable learning, global clustering, and superior performance. The major contributions of this work include:

- A novel centerless partition clustering method PAC is proposed to implement clustering by exploring the potential relation between sample distribution and assignment probability.
- An online deep clustering module OPA is exploited based on PAC, which encodes spatial distances into online clustering without incorporating plenty hyper-parameters and components. OPA leaves out the cluster size constraint to perform flexible and stable clustering.
- A simple end-to-end unsupervised deep clustering framework DPAC is established for stable and efficient clustering. Both PAC and DPAC achieve significant performance on five challenging image benchmarks compared with the state-of-the-art approaches.

2 Related Work

Deep Clustering: Deep clustering [12,18,44,53] combines representation learning with clustering through deep models. SCAN [48] conducts the KNN algorithm for the pre-trained model and leverages neighbor information to group samples. The clustering loss proposed by SCAN only maximizes the agreements of assignments among neighbors, which inevitably need a additional balanced cluster constraint to avoid trivial solutions. SeCu [40] proposes a hardness-aware clustering criterion to obtain more detailed cluster centers and stable contrastive cluster discrimination. SeCu also employs a additional global entropy constraint to relax the balanced constraint to a lower-bound size constraint that limits the minimal size of clusters. Compared with the SeCU and SCAN, DPAC encodes online spatial information into learning and obtains more flexible partitioning without any cluster size constraints.

Machine Clustering: Machine clustering [11, 25, 31] tries to decompose the data into a set of disjoint clusters by machine learning algorithms. FCM [6] obtains soft cluster assignment by alternately updating the fuzzy partition matrix and cluster center. Many modified methods [35,39,49] have been proposed to improve clustering and robustness of center-base clustering. K-medoids (PAM) [31] chooses actual samples as cluster centers to mitigate the impact of cluster centers in K-means. Spherical K-means (SPKM) [25] clustering employs cosine dissimilarities to perform prototype-based partitioning to improve solution quality and computational efficiency. Robust continuous clustering (RCC) [43] deconstructs heavily mixed clusters by optimizing a smooth continuous objective based on robust statistics. However, the complex clustering progresses involved in these algorithms prevent them from being deployed in neural networks.

3 Method

The following sections present the theoretical basis of our approach. We first derive a novel objective function and analyze how the proposed objective function relates to existing methods. Second, we present a scalable centerless clustering algorithm PAC based on FCM. Finally, we extend PAC to a novel online clustering module OPA, and construct a novel online deep clustering model DPAC to learn the semantic knowledge of unlabeled data.

3.1 Objective Function

Let $\boldsymbol{X} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \cdots, \boldsymbol{x}_N\}$ be an N-point dataset, where $\boldsymbol{x}_i \in \mathbb{R}^{D \times 1}$ is the ith D-dimensional instance. The clustering algorithm aims to divide \boldsymbol{X} into K mutually disjoint clusters, where $2 \leq K < N, K \in \mathbb{N}$. $\boldsymbol{P} = [p_{i,k}]_{N \times K}$ is the soft partition matrix, $p_{i,k}$ is the probability of one sample belonging to certain cluster indicating the relationship between sample \boldsymbol{x}_i and cluster k which satisfies $\boldsymbol{P} \in \{\Gamma^{N \times K} | \gamma_{i,k} \in [0,1], \forall i,k; \sum_{k=1}^K \gamma_{i,k} = 1, \forall i; 0 < \sum_{i=1}^N \gamma_{i,k} < N, \forall k\}$. And the cluster prediction of \boldsymbol{x}_i can be predicted by $\hat{p}_i = \arg\max_k p_{i,k}, 1 < k \leq K$.

Different from the existing classical nonparametric clustering methods [51], we utilize the inner product operation of probability vectors instead of cluster center to indicate cluster relations of samples. Formally, we multiply the inner product results with corresponding distance measurements to quantify the global intra-cluster distance of the data. The objective function J_{pac} is defined as:

$$J_{pac} = \sum_{i=1}^{N} \sum_{j=1}^{N} \mathbf{p}_{i}^{\mathsf{T}} \mathbf{p}_{j} \| \mathbf{x}_{i} - \mathbf{x}_{j} \|^{2},$$
 (1)

where $\boldsymbol{p}_i = [p_{i,1}, p_{i,2}, \dots, p_{i,K}]^\mathsf{T}$ is the probability vector. $\boldsymbol{p}_i^\mathsf{T} \boldsymbol{p}_j \in [0,1]$ can be regarded as the probability weight for $\|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2$. By minimizing Eq. (1), $\boldsymbol{p}_i^\mathsf{T} \boldsymbol{p}_j$ can be negatively related to $\|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2$, which denotes the probabilities of instances consistent with nearby samples, but not with distant samples.

3.2 Relation to Existing Algorithms

We provide a new perspective to further understand the proposed objective function. We summarize the difference between our method and Spectral Clustering (SC) [49] and SCAN [48]. The minimizing problem for J_{pac} can be rewritten as:

$$\min_{\boldsymbol{P} \in \Gamma^{N \times K}} Tr(\boldsymbol{P}^{\mathsf{T}} \widetilde{\boldsymbol{D}}_{x} \boldsymbol{P}), \tag{2}$$

where $\widetilde{\boldsymbol{D}}_x$ is the distances matrix, $\widetilde{d}_{i,j} = \|\boldsymbol{x}_i - \boldsymbol{x}_j\|^2$. Obviously, $\widetilde{d}_{i,j}$ can be replaced by many other distance measurement. We use L_2 distance as the default distance measure in the following experiments. The graph partitioning problem of SC is formulated as:

$$\min_{\boldsymbol{H} \in \mathbb{R}^{N \times K}} Tr(\boldsymbol{H}^{\mathsf{T}} \widetilde{\boldsymbol{L}}_{x} \boldsymbol{H}),$$
s.t. $\boldsymbol{H}^{\mathsf{T}} \boldsymbol{H} = \boldsymbol{I}$. (3)

where $\widetilde{\boldsymbol{L}}_x$ is the Laplacian matrix of graph. The indicator matrix \boldsymbol{H} contains arbitrary real values with orthogonality constraint. The semantic clustering loss in SCAN can be reformulated as:

$$\max_{\boldsymbol{P} \in \Gamma^{N \times K}} \sum_{i=1}^{N} \sum_{j \in \mathcal{N}_{i}} \log \boldsymbol{p}_{i}^{\mathsf{T}} \boldsymbol{p}_{j} - \lambda \mathcal{H}(\boldsymbol{P}) \Leftrightarrow \max_{\boldsymbol{P} \in \Gamma^{N \times K}} Tr(\boldsymbol{P}^{\mathsf{T}} \widetilde{\boldsymbol{A}}_{x} \boldsymbol{P}) - \lambda \mathcal{H}(\boldsymbol{P}), \quad (4)$$

where $\mathcal{H}(\boldsymbol{P}) = \sum_{k=1}^K \frac{\sum_{i=1}^N p_{i,k}}{N} \log \frac{\sum_{i=1}^N p_{i,k}}{N}$, \mathcal{N}_i is the K nearest neighbor set of instance i, $\widetilde{\boldsymbol{A}}_x$ is the adjacent matrix, $\widetilde{\boldsymbol{a}}_{i,j} = 1$ when $j \in \mathcal{N}_i$, otherwise $\widetilde{\boldsymbol{a}}_{i,j} = 0$. λ is the hyper-parameter. The second term $\mathcal{H}(\boldsymbol{P})$ in Eq.(4) denotes balanced constrain of cluster. Compared with Eq.(3), Eq.(2) transforms the partitioning problem in Euclidean space into the graph-cut problem. And different from balanced partitioning in Eq.(4), we convert maximum problem to minimum problem to efficiently avoids trivial solution. The intrinsical constraints of probability matrix \boldsymbol{P} enable J_{pac} directly clustering without using orthogonality and balanced constraints. Therefore, DPAC dose not require additional clustering regular terms [33, 44, 48] to avoid collapse and performs more flexible cluster assignment. Moreover, unlike only using neighbors to group, J_{pac} introduces the distance information into optimization to obtain an global clustering.

3.3 Probability Aggregation Clustering

The proposed Eq. (2) is a constrained optimization problem. Inspired by FCM, we incorporate the fuzzy weighting exponent m into objective function and obtain an scalable machine clustering algorithm based on Lagrange method. The new objective function with m can be formulated as:

$$\tilde{J}_{pac} = \sum_{i=1}^{N} \sum_{j=1}^{N} \varphi(i,j) \tilde{d}_{i,j}, \text{ with } \varphi(i,j) = \sum_{k=1}^{K} p_{i,k}^{m} p_{j,k},$$
 (5)

where $m \in (1, +\infty)$. The corresponding Lagrange function is:

$$\tilde{L}_{pac} = \sum_{i=1}^{N} \sum_{j \neq i} \varphi(i, j) \tilde{d}_{i, j} + \sum_{i=1}^{N} \lambda_{i} (1 - \sum_{k=1}^{K} p_{i, k}) - \sum_{i=1}^{N} \sum_{k=1}^{K} \gamma_{i, k} p_{i, k},$$
 (6)

where λ and $\gamma_{\cdot,\cdot}$ are the Lagrange multipliers respectively for the sum constraint and the non-negativity constraint on P. The partial derivative of \widetilde{L}_{pac} with respect to $p_{i,k}$ should be equal to zero at the minimum as:

$$\frac{\partial \tilde{L}_{pac}}{\partial p_{i,k}} = 2\sum_{j \neq i} m p_{i,k}^{m-1} p_{j,k} \tilde{d}_{i,j} - \lambda_i - \gamma_{i,k} = 0.$$
 (7)

And according to the Karush-Kuhn-Tucker conditions we have: $1 - \sum_{k=1}^{K} p_{i,k} = 0$, $\gamma_{i,k}p_{i,k} = 0$, $\gamma_{i,k} \geq 0$, $\forall i,k$. For soft clustering, endpoints are generally unreachable during optimization. Therefore, we only consider the case when $p_{i,k} \in (0,1)$, $\gamma_{i,k} = 0$. Let $\alpha = 1/(m-1)$, it can be obtained from Eq. (7) that $p_{i,k} = \lambda_i^{\alpha} (2m \sum_{j \neq i} p_{j,k} \tilde{d}_{i,j})^{-\alpha}$. Considering the sum constraint, the equation becomes $\lambda_i^{\alpha} \sum_{k=1}^{K} (2m \sum_{j \neq i} p_{j,k} \tilde{d}_{i,j})^{-\alpha} = \sum_{k=1}^{K} p_{i,k} = 1$. By solving λ_i and taking it into Eq. (7), we can finally obtain:

$$p_{i,k} = \frac{s_{i,k}^{-\alpha}}{\sum_{r=1}^{K} s_{i,r}^{-\alpha}}, \quad \text{with } s_{i,k} = \sum_{j \neq i} p_{j,k} \tilde{d}_{i,j}.$$
 (8)

Take one element $p_{i,k}$ as a variable and all the rest elements as constant, \mathbf{P} can be iteratively updated with Eq. (8). $s_{i,k}$ aggregates the probabilities and distances to compute a score that \mathbf{x}_i belongs to cluster k. In the other word, PAC solves $p_{i,k}$ through all other instances instead of cluster centers. PAC only needs to initialize the \mathbf{P} following approximately uniform distribution, that is $p_{i,k} \approx 1/K$. Therefore, PAC circumvents the delicate cluster center initialization problem caused by disparate data distributions in the feature space [4]. The detailed steps of PAC are summarized in Algorithm 1.

Algorithm 1: PAC Program

```
1 Input: dataset X; weighting exponent m; cluster number K.
2 Initialize P and calculate \widetilde{D}_x;
3 while not converage do
4 | for i \leftarrow 1 to N do
5 | for k \leftarrow 1 to K do
6 | p_{i,k} \leftarrow \text{Eq.}(8)
7 | end
8 | end
9 end
10 Output: Clustering result P
```

3.4 Online Probability Aggregation

A deep neural network $\hat{x}_i = f(I_i)$ maps data I_i to feature vector \hat{x}_i . And a classifier h maps x_i to K-dimensional class probabilities \hat{p}_i . We proposed an simple online clustering module OPA, which combines the optimization process of PAC with loss computation to generate pseudo labels step by step. Specifically, B denotes the size of mini-batch in the current epoch, OPA has two steps:

Target Computation: Sec. 3.3 demonstrates the optimization program for single variable, we extend it to the matrix for multivariables to adopt batch clustering. Given the current model $h \circ f$, the clustering score $\mathbf{S} \in \mathbb{R}^{+B \times K}$ is calculated by:

$$S = \widetilde{D}_{\hat{x}} \hat{P}. \tag{9}$$

The target clustering code $Q \in \Gamma^{B \times K}$ can be obtained by normalizing S, i.e., $q_{i,k} = s_{i,k}^{-\alpha} / \sum_{r=1}^K s_{i,r}^{-\alpha}$. We call the operation in Eq. (9) as online probability aggregation. The probability outputs form classifier are aggregated by matrix multiplication to compute corresponding scores, which not only incorporates historical partitioning knowledge but also encodes distance information.

Self-labeling: Given the current target clustering code Q, the whole model $h \circ f$ is updated by minimizing the following KL divergence:

$$KL(\mathbf{Q} \parallel \hat{\mathbf{P}}) = \langle \mathbf{Q}, \log \mathbf{Q} \rangle - \langle \mathbf{Q}, \log \hat{\mathbf{P}} \rangle$$
 (10)

where $\langle \cdot \rangle$ is the frobenius inner product, $\log \mathbf{Q} = [\log(q_{i,k})]_{N \times K}$ and $\log \hat{\mathbf{P}} = [\log(\hat{p}_{i,k})]_{N \times K}$. Different from directly leveraging J_{pac} in Eq.(1) as clustering loss, OPA trains model in a supervised way rather than solving the clustering problem in Eq.(2) exactly. The pseudo code of OPA is illustrated in Alg. 2, which demonstrates OPA involves a mini-batch matrix multiplication and power, so the computation cost of OPA equals to general loss.

Algorithm 2: Pseudo code for OPA in pytorch-style

```
Input: distance matrix P; probability matrix P; weighting exponent m.

S = torch.matmul(D.detach(), P) // Probability Aggregation

S = torch.pow(S, -1/(m-1)) // Scale Up

Q = S/S.sum(1).view(-1,1) // Normalize to 1

Output: (Q * \log Q - Q * \log P).sum(1).mean() // KL divergence loss
```

3.5 Deep Probability Aggregation Clustering

With the proposed loss function, we construct an online deep clustering framework DPAC, which has two heads: contrastive learning and online clustering. Let $\hat{\boldsymbol{X}}^1$ and $\hat{\boldsymbol{X}}^2$ denote two-view features of $\hat{\boldsymbol{X}}$ generated by image augmentation. We reformulate the standard contrastive loss in SimCLR [13] as weight

contrastive loss (WCL) to mitigate the semantic distortion caused by negative samples. The weight contrastive loss $\ell(\hat{X}_1, \hat{X}_2, \hat{P})$ is defined as:

$$-\sum_{i=1}^{N} \log \frac{\exp(\hat{\boldsymbol{z}}_{i}^{\mathsf{TT}} \hat{\boldsymbol{z}}_{i}^{2} / \tau)}{\sum_{j \neq i} (1 - \hat{\boldsymbol{p}}_{i}^{\mathsf{T}} \hat{\boldsymbol{p}}_{j}) \exp(\hat{\boldsymbol{z}}_{i}^{\mathsf{TT}} \hat{\boldsymbol{z}}_{j}^{1} / \tau) + \sum_{j=1}^{N} (1 - \hat{\boldsymbol{p}}_{i}^{\mathsf{T}} \hat{\boldsymbol{p}}_{j}) \exp(\hat{\boldsymbol{z}}_{i}^{\mathsf{TT}} \hat{\boldsymbol{z}}_{j}^{2} / \tau)},$$
(11)

where τ is the temperature hyper-parameter, $\hat{\boldsymbol{z}}_i$ is the normalized feature projected by projector g, where $\hat{\boldsymbol{z}}_i = g(\hat{\boldsymbol{x}}_i)/\|g(\hat{\boldsymbol{x}}_i)\|$. $(1-\hat{\boldsymbol{p}}_i^\mathsf{T}\hat{\boldsymbol{p}}_j)$ is a coefficient masking the negative samples that may have the same class as $\hat{\boldsymbol{x}}_i$.

In pre-training step, DPAC is trained by contrastive loss: $\frac{1}{2}[\ell(\hat{\boldsymbol{X}}^1, \hat{\boldsymbol{X}}^2, \hat{\boldsymbol{P}}) + \ell(\hat{\boldsymbol{X}}^2, \hat{\boldsymbol{X}}^1, \hat{\boldsymbol{P}})]$, where $\hat{p}_{i,j} = 1/K, \forall i,j$ due to lack of cluster information. Then in clustering step, self-supervised loss is also employed to learn the local structure of the data in feature space [22]. The whole model in clustering step is updated by minimizing the sum of contrastive and clustering loss:

$$\min_{\boldsymbol{\theta}_{f,g,h}} \frac{1}{2} [\ell(\hat{\boldsymbol{X}}^{1}, \hat{\boldsymbol{X}}^{2}, \hat{\boldsymbol{P}}) + \ell(\hat{\boldsymbol{X}}^{2}, \hat{\boldsymbol{X}}^{1}, \hat{\boldsymbol{P}})] + KL(\boldsymbol{Q} \parallel \hat{\boldsymbol{P}}^{1}), \tag{12}$$

$$\min_{\boldsymbol{\theta}_{f,q,h}} \frac{1}{2} [\ell(\hat{\boldsymbol{X}}^{1}, \hat{\boldsymbol{X}}^{2}, \hat{\boldsymbol{P}}) + \ell(\hat{\boldsymbol{X}}^{2}, \hat{\boldsymbol{X}}^{1}, \hat{\boldsymbol{P}})] + Tr(\hat{\boldsymbol{P}}^{1\mathsf{T}} \widetilde{\boldsymbol{D}}_{\hat{x}} \hat{\boldsymbol{P}}^{1}), \tag{13}$$

where $\theta_{f,g,h}$ are the parameters of neural network, classifier, and projector. The optimization goal in Eq. (12) is the deep clustering method based on OPA mentioned in Sec. 3.4. And Eq. (13) is the deep clustering method that directly minimizes J_{pac} . The proposed methods are easy to implement and the overall training procedure is shown in Alg. 3. Besides, for fair comparison in subsequent experiments, we also implement a self-labeling boosting as [34, 45] to further improve the clustering performance.

Algorithm 3: Training algorithm for DPAC

```
1 Input: image set I; clustering epochs E; batch size B; weighting exponent m.
 2 for epoch \leftarrow 1 to E do
            Sample a mini-batch \{I_i\}_{i=1}^B and conduct augmentations \{I_i^1, I_i^2\}_{i=1}^B;
  3
            Get \{\hat{\boldsymbol{x}}_i, \hat{\boldsymbol{x}}_i^1, \hat{\boldsymbol{x}}_i^2, \hat{\boldsymbol{p}}_i, \hat{\boldsymbol{p}}_i^1\}_{i=1}^B through forward propagation;
  5
            if choose OPA as optimal object then
                   Compute clustering codes \{q_i\}_{i=1}^B by Alg. (2) with \{\hat{\boldsymbol{x}}_i, \hat{\boldsymbol{p}}_i\}_{i=1}^B;
  6
                   Compute overall loss \mathcal{L} by Eq. (12) with \{\hat{\boldsymbol{x}}_i^1, \hat{\boldsymbol{x}}_i^2, \hat{\boldsymbol{p}}_i, \hat{\boldsymbol{p}}_i^1, \boldsymbol{q}_i\}_{i=1}^B;
  7
            end
  8
            if choose J_{pac} as optimal object then
  9
                   Compute overall loss \mathcal{L} by Eq. (13) with \{\hat{\boldsymbol{x}}_i^1, \hat{\boldsymbol{x}}_i^2, \hat{\boldsymbol{p}}_i, \hat{\boldsymbol{p}}_i^1\}_{i=1}^B;
10
11
            Update \theta_f, \theta_g, \theta_h through gradient descent to minimize \mathcal{L};
12
13 end
14 Output: Deep clustering model h \circ f
```

Dataset Sample Class Image Size Sample Class Dimension Dataset CIFAR-10 [30] Coil-100 [37] 100 60,000 10 32×32 7,200 49.152 CIFAR-100 [30] 32×32 Isolet [16] 7,796 26 617 60,000 20 Pendigits [2] STL-10 [15] 13,000 10 224×224 10,992 10 16 ImageNet-10 [12] 13,000 10 224×224 MNIST [19] 10,000 10 784 ImageNet-Dogs [12] | 19,500 224×224

Table 1: Dataset settings for our experiments.

4 Experiment

Dataset: Four real-world datasets and five widely used natural image datasets are involved to evaluate the clustering ability of PAC and DPAC. The details of the datasets are summarized in the Table 1.For CIFAR-100, we used its 20 superclasses rather than 100 classes as the ground truth. ImageNet-10 and ImageNet-Dogs are subsets of ImageNet-1k. For STL-10, its 100,000 unlabeled images are additionally employed in the pre-training step. Clustering accuracy (ACC), normalized mutual information (NMI), and adjusted random index (ARI) are adopted to compare the clustering results.

4.1 Probability Aggregation Clustering

Hyperparameter and Method Setting The effectiveness of the proposed PAC was verified by comparing it with multiple clustering methods on nine datasets. We predefine m of PAC to 1.03 for all datasets. KNN graph is selected for SC [49]. The threshold value of RCC [43] is set to 1. The weighting exponent m of FCM is set to 1.1 for real-world datasets and 1.05 for natural image datasets. All algorithms are initialized randomly. The mean and standard deviation of 10 run experiments is reported in the following comparison.

Algorithm Scalability The clustering results of the real-world datasets, which consist of samples with varying numbers, classes, and dimensions, are summarized in Table 2. PAM and RCC time out due to the high dimensionality of Coil. From Table 2 we can see that PAC outperforms all the compared clustering algorithms on Coil and Isolet but is not as effective as RCC on Mnist and Pendigit, which is specially designed for entangled data. The robustness and performance of PAC surpass those of center-based clustering.

Moreover, we also provide the clustering results on neural network feature data in Table 3 to explore the ability of algorithms to handle data extracted by neural networks. RCC experienced extreme performance degradation failing to cluster on neural network extracted data, so we exclude it from the comparison. PAC also performs well in processing neural network data. The improvement is not significant in CIFAR-100 and ImageNet-Dogs. A possible explanation is that these datasets give subtle differences in object classes causing the pretrained representations to be indistinguishable.

Table 2: Clustering results (Avg \pm Std) and average time (s) of PAC on real-world datasets. The best and second-best results are shown in bold and underlined, respectively. Metric: ACC (%).

Method	Coil-10	Isolet	Pendigits	MNIST	A	verage	Time	9
KM [51]	56.4±1.7	52.7±4.5	67.0±4.7	53.0 ± 3.6	98.1	0.2	0.05	0.07
PAM [31]	N/A	55.5±0.0	75.6 ± 2.5	47.2 ± 1.7	N/A	341.9	141.6	124.0
FCM [6]	61.6 ± 1.2	55.8 ± 2.3	70.5 ± 2.1	56.6 ± 2.6	2001.5	8.6	0.9	0.6
SC [49]	58.2 ± 0.7	53.5 ± 2.5	62.4 ± 4.2	54.6 ± 2.2	11.7	3.4	5.8	6.2
SPKF [25]	59.7 ± 1.3	55.2 ± 2.0	71.4 ± 4.4	53.9 ± 2.7	101.6	0.6	0.07	0.2
RCC [43]	N/A	15.3 ± 0.0	79.6 ± 0.0	65.7 \pm 0.0	N/A	122.8	6.9	6.9
FINCH [42]	56.4 ± 0.0	47.5 ± 0.0	62.7 ± 0.0	57.9 ± 0.0	15.1	0.5	0.05	0.05
PAC	$ $ 65.1 ± 1.5	61.8 ±0.0	$ \underline{78.0}\pm0.0 $	59.7 ± 3.6	5179.0	249.6	153.6	423.4

Table 3: Clustering results (Avg±Std) of PAC on deep features. Metric: ACC (%).

Method	CIFAR-10	CIFAR-100	STL-10	ImageNet-10	ImageNet-Dogs
KM [51]	76.8±6.8	41.8 ± 1.7	66.8 ± 4.3	76.8 ± 6.8	41.8±1.7
PAM [31]	77.8 ± 2.5	41.0 ± 1.1	64.3 ± 4.8	79.9 ± 4.6	52.6 ±3.1
FCM [6]	75.9 ± 2.1	$42.3 {\pm} 0.7$	66.6 ± 4.7	75.9 ± 2.1	42.3 ± 0.7
SC [49]	83.5±0.0	40.0 ± 1.1	63.8 ± 2.9	82.9 ± 1.3	47.6 ± 1.4
SPKF [25]	75.9 ± 5.7	42.9 ± 1.9	65.8 ± 5.5	80.6 ± 7.6	49.1 ± 3.8
FINCH [42]	49.2±0.0	32.0 ± 0.0	42.9 ± 0.0	52.6 ± 0.0	43.8±0.0
PAC	87.1±0.0	43.8 ±0.7	74.9 ±2.6	95.8 ±0.0	47.3±3.9

Time Complexity Analysis The average calculation time for each dataset is listed in Table 2. The computational complexity of PAC is analyzed in this section. It takes $\mathcal{O}(N)$ time to calculate $\sum_{j\neq i} p_{j,k} \tilde{d}_{i,j}$ in Eq. (8). And PAC updates entire \boldsymbol{P} by NK iterations. So the time complexity PAC is $\mathcal{O}(N^2K)$, which is the square complexity.

Parameter Sensibility Analysis We evaluated the parameter sensitivity of m for both FCM and PAC on Pendigits. Fig. 1 reports the average ACC for different m. It was indicated that in comparison to FCM, PAC has a narrower optimal range of m and smaller results variance, which is not sensitive to parameter m.

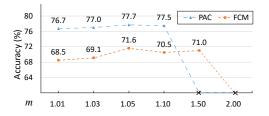


Fig. 1: The effect of weighting exponent m in PAC and FCM.

Table 4: Performance comparison of deep clustering methods on five benchmarks. Metrics: NMI / ACC / ARI (%). Temu* incorporates extra ImageNet-1k data to pretrain the model, so we exclude it in comparison. 1 denotes online deep clustering methods, while 2 denotes offline deep clustering methods.

Method	Cluster size	CI	FAR-	-10	CII	FAR-	100	S	TL-1	.0	Ima	geNe	t-10	Imag	geNet	-Dogs
- Incomod	constraint	NMI	ACC	ARI	NMI	ACC	ARI									
PICA ₁ [26]	✓	59.1	69.6	51.2	31.0	33.7	17.1	61.1	71.3	53.1	80.2	87.0	76.1	35.2	35.2	20.1
PCL_2 [32]		80.2	87.4	76.6	52.8	52.6	36.3	41.0	71.8	67.0	84.1	90.7	82.2	44.0	41.2	29.9
$IDFD_2$ [46]		71.1	81.5	66.3	42.6	42.5	26.4	64.3	75.6	57.5	89.8	95.4	90.1	54.6	59.1	41.3
NNM_1 [18]	✓		84.3		-							-	-	-	-	-
CC_1 [33]	✓	1	79.0													27.4
GCC_1 [57]	✓	1	85.6													36.2
TCC_1 [44]	✓	1	90.6													41.7
$SPICE_1$ [38]	✓		83.8									92.1	83.6	<u>57.2</u>	64.6	47.9
$SeCu_1$ [40]	✓		88.5									-	-	-	-	-
Temi ₂ * [1]	✓	82.9	90.0	80.7	59.8	57.8	42.5	93.6	96.7	93.0	-	-	-	-	-	
$DPAC_1^{J_{pac}}(Eq. (13))$		81.2	89.0	79.1	48.3	50.2	34.4	81.8	89.7	80.0	90.1	96.0	91.1	51.9	53.9	38.9
$\mathrm{DPAC}_{1}^{opa}(\mathrm{Eq.}\ (12))$		82.7	90.7	81.2	52.9	51.6	36.2	84.5	92.6	84.7	90.8	96.2	91.8	60.2	65.5	50.0
With self-labeling fir	ne-tuning (†)	:														
SCAN ₂ † [48]	√	79.7	88.3	77.2	48.6	50.7	33.3	69.8	80.9	64.6	-	-	-	-	-	-
$SPICE_1\dagger$ [38]	✓	86.5	92.6	85.2	56.7	53.8	38.7	87.2	93.8	87.0	90.2	95.9	91.2	62.7	67.5	52.6
$TCL_1\dagger$ [34]	✓	81.9	88.7	78.0	52.9	53.1	35.7	79.9	86.8	75.7	87.5	89.5	83.7	62.3	64.4	51.6
$SeCu_1\dagger$ [40]	✓	86.1	93.0	85.7	55.2	55.1	39.7	73.3	83.6	69.3	-	-	-	-	-	-
$\overline{\mathrm{DPAC}_{1}^{opa}}$ †		87.0	93.4	86.6	54.2	55.5	39.3	86.3	93.4	86.1	92.5	97.0	93.5	66.7	72.6	59.8

4.2 Deep Probability Aggregation Clustering

Implementation Details ResNet-34 [24] was used as the backbone network in DPAC to ensure a fair comparison. We employed the architecture of SimCLR [14] with a MLP clustering classifier as model architecture. DPAC incorporates the image transformation of SimCLR as one view of augmentation and randomly selects four transformations from Rand Augment [17] as another view of augmentation. We maintained a consistent set of hyperparameters ($m=1.03, \tau=0.5$) across all amounts of benchmarks. The model is trained for 1,000 epochs in the pre-training step and 200 epochs in the clustering step. As for self-labeling boosting, we utilize a linear classifier and train the model as [45]. The thresholds are set to 0.95 for each datasets to select sufficient pseudo labels from clustering classifier outputs. Adam [29] with a constant learning rate of 1×10^{-4} and a weight decay of 1×10^{-4} was employed. The batch size is set as 240 and the experiments are implemented on single NVIDIA 4090 24G GPU.

Comparison with State of the Arts The comparison of DPAC with a wide range of state-of-the-art deep clustering methods is presented in Table 4, where methods with additional cluster size constraint are marked. We have the following observations: (1) DPAC significantly surpasses the performance of Sim-CLR+PAC across all benchmarks. DPAC achieves an accuracy exceeding PAC by more than 10% on CIFAR-100, STL-10, and ImageNet-Dogs benchmarks, which demonstrates the semantic learning ability of DPAC. (2) Compared with directly minimizing objection function J_{pac} , DPAC^{opa} has better performance.

Table 5: Ablation studies of DPAC.

CIFAR-10.

(a) Comparison of differ- (b) Clustering performance com- (c) Effect of balanced clusterent contrastive framework on pared with AE based clustering ing regularization (CR) term on approaches on MNIST.

CIFAR-10. Metric: ACC (%).

Method	ACC
SimCLR+KM SimCLR+OPA MoCo+KM MoCo+OPA	80.7 89.7 77.6 86.5
DPAC^{opa}	90.8

Method	NMI	ACC
IDEC [22]	86.7 86.7 86.2 95.0	88.1
AE+OPA	90.3	95.4

Method	w/ CR	w/o~CR
SCAN CC GCC	85.7 79.2 85.6	0.1 68.7 68.0
$\begin{array}{c} \mathrm{DPAC}^{J_{pac}} \\ \mathrm{DPAC}^{opa} \end{array}$	88.0 0.1	89.0 90.7

Table 6: Hyperparameter analysis of exponent m in OPA. Metrics:ACC (%).

Weight exponent m	1.01	1.04	1.07	1.1	1.13	1.16	1.2
$\alpha = 1/(m-1)$	100.0	25.0	14.3	10.0	7.7	6.3	5.0
CIFAR-10	90.8 92.4 50.2	90.3	90.1	89.3	89.3	89.3	10.0
STL-10	92.4	92.1	92.0	91.8	90.7	10.0	10.0
CIFAR-100	50.2	51.1	51.0	5.0	5.0	5.0	5.0

We attribute this to the fact that the self-labeling manner of OPA alleviates the intrinsic bias brought by the objective function of feature clustering. (3) Compared with deep clustering with offline K-means IDFD [46] and PCL [32], DPAC has superior performance on most benchmarks due to the superior clustering capability offered by the online clustering module. (4) Compared with online contrastive clustering methods CC [33], TCC [44], and TCL [34], DPAC incorporates global spatial information to achieve a finer partitioning of cluster boundaries. (5) Compared with balanced clustering methods and minimal cluster size constraint SeCU [34], DPAC omits clustering regular term, is more concise, and outputs a flexible cluster distribution. (6) The DPAC with self-labeling finetuning demonstrates its remarkable extensibility, showcasing its potential for integration with diverse deep modules.

Ablation Study The ablation studies of DPAC are evaluated to illustrate the behavior of our method. First, we study the effect of proposed contrastive learning. We replace the weighted contrastive loss in Eq. (11) by standard contrastive loss, which involves all instances in batches as negative samples. Besides, we perform DPAC based on MoCo [23] to explore the universality of our method. Conventional contrastive loss treats corresponding augmented samples as positive pairs and others as negative pairs, which ignores the latent semantic structure between negative pairs, leading to the class collision issue [52]. Table 5a illustrates our weighted contrastive loss mitigates the semantic distortion caused by negative samples and encodes cluster knowledge into representation learning.

Second, we study the effect of different pretext tasks combined with DPAC. The autoencoder (AE) is used as backbone to prove the universality of our module. The clustering results on MNIST are shown in Table 5b, which demonstrate OPA can combine with other self-supervised approaches. And compared with center-based IDEC [54], our OPA does not require K-means to initialize cluster layer and has higher scalability.

Finally, we study the effect of balanced constraint in different online clustering methods. Most existing online clustering methods [48] introduce an average entropy as clustering regularization (CR) term to balance the cluster distribution. The clustering regularization experiments are shown in Table 5c, where DPAC avoids crashes without using the CR term. SCAN classifies all samples into single cluster, and CC, GCC descends into a suboptimal solution without the CR term. Besides, if the CR term is too large in the total loss, it will affect the clustering performance in these methods. DPAC^{opa} with (w/) CR term yields a uniform distribution with no predictive effect. We speculate that the constraint of the regularization term is too strong, so that the classifier cannot accumulate optimization enough information for OPA. And the performance of DPAC^J_{Pac} with CR term becomes worse under balanced constraint. It demonstrate the superiority of unconstrained clustering, that is, no trade-off between trivial solution and performance.

Hyperparameter Analysis As list in Alg. 2, weight exponent m is the key hyperparameter for OPA, $\alpha = 1/(m-1)$ is the power of $s_{i,k}$ that amplifies clustering score in Eq. 9 to become sharper to obtain distinguishable cluster assignments. The larger m becomes, the smaller the sharpening effect is, so the model tends to uniform assignments and clustering may fail due to insufficient scaling. The performance of OPA with different m settings has been evaluated in Table 6. Evidently, as features become more and more inseparable, he optimal range of m narrows. Therefore, we suggest setting m close to 1 to obtain a universal hyperparameter setting (m = 1.03 for all dataset).

Superiority of Online Clustering To facilitate a comparative analysis between online and offline clustering strategies, the offline clustering version of DPAC was performed on STL-10. We adopted KM, FCM and PAC to compute offline codes of all samples for Eq. (10) every 1, 10, and 200 epochs. The performance and training duration are reported in Table 7. It can be observed that the performance of KM and FCM gradually deteriorates as the update frequency decreases, whereas DPAC^{opa} exhibits superior performance and lower time complexity.

We recorded accumulated errors during DPAC + offline PAC training to observe the performance degeneration and error accumulation issues. Offline PAC was conducted every 10 epochs. As depicted in Fig. 2, errors (network classifies correctly while offline clustering classifies incorrectly when generating pseudo labels) are introduced every 10 epochs during offline clustering and continue to accumulate through the training process, ultimately resulting in a decline in performance. It demonstrates that OPA effectively mitigates performance degeneration and error accumulation issues to perform stable clustering.

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Table 7: The comparison of online and offline DPAC on STL-10. Metrics: Hour/ACC (%).

	Number of Offline Clustering Runs							
Method	200	20	1					
DPAC + offline KM DPAC + offline FCM DPAC + offline PAC	6.3 / 73.7	3.0 / 72.0	2.0 / 69.3					
DPAC + offline FCM	8.5 / 78.7	$\begin{vmatrix} 3.3 & 77.5 \\ 6.7 & 87.5 \end{vmatrix}$	2.0 / 68.4					
	1 02.2 / 03.1							
$DPAC^{opa}$		2.0 / 92.6						

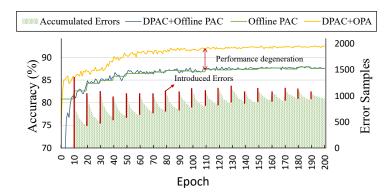


Fig. 2: Training process and error accumulation of online and offline DPAC on STL-10.

5 Conclusion

A novel machine clustering method PAC without cluster center was proposed from a very new perspective, which addresses the shortcomings of center-based clustering approaches and is well-suited for integration with deep models. Theoretical model and an elegant iterative optimization solution for PAC have been developed. PAC implements clustering through sample probability aggregation, which makes part samples based calculation possible. Therefore, a online deep clustering framework DPAC has been developed, which has no constraints on cluster size and can perform more flexible clustering. Experiments on several benchmarks verified the effectiveness of our proposal.

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