SPICE: Semantic Pseudo-Labeling for Image Clustering

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Abstract—The similarity among samples and the discrepancy among clusters are two crucial aspects of image clustering. However, current deep clustering methods suffer from inaccurate estimation of either feature similarity or semantic discrepancy. In this paper, we present a Semantic Pseudo-labeling-based Image ClustEring (SPICE) framework, which divides the clustering network into a feature model for measuring the instance-level similarity and a clustering head for identifying the cluster-level discrepancy. We design two semantics-aware pseudo-labeling algorithms, prototype pseudo-labeling and reliable pseudo-labeling, which enable accurate and reliable self-supervision over clustering. Without using any ground-truth label, we optimize the clustering network in three stages: 1) train the feature model through contrastive learning to measure the instance similarity; 2) train the clustering head with the prototype pseudo-labeling algorithm to identify cluster semantics; and 3) jointly train the feature model and clustering head with the reliable pseudo-labeling algorithm to improve the clustering performance. Extensive experimental results demonstrate that SPICE achieves significant improvements (∼10%) over existing methods and establishes the new state-of-the-art clustering results on six balanced benchmark datasets in terms of three popular metrics. Importantly, SPICE significantly reduces the gap between unsupervised and fully-supervised classification; e.g., there is only 2% (91.8% vs. 93.8%) accuracy difference on CIFAR-10. Our code is made publicly available at https://github.com/niuchuangnn/SPICE.

Index Terms—Deep clustering, self-supervised learning, semi-supervised learning, representation learning.

I. INTRODUCTION

I

mage clustering aims to group images into different meaningful clusters without human annotations, and is an essential task in unsupervised learning with applications in many areas. At the core of image clustering are the measurements of the similarity among samples (images) and the discrepancy among semantic clusters. Recently, deep learning-based clustering methods have achieved great progress thanks to the strong representation capability of deep neural networks.

Initially, by combining autoencoders with clustering algorithms, some deep clustering methods were proposed to learn representation features and perform clustering simultaneously and alternatively [2], [3], [4], [5], [6], [7], [8], [9], [10], achieving better results than the traditional methods. Due to the overestimation of low-level features, these autoencoder-based methods hardly capture discriminative features of complex images. Thus, a number of methods were proposed to learn discriminative label features under various constraints [11], [12], [13], [14], [15], [16]. However, these methods have limited performance when directly using the label features to measure the similarity among samples. This is because the category-level features lose too much instance-level information to accurately measure the instance similarity.

Very recently, Van Gansbeke et al. [1] proposed to leverage the embedding features of the unsupervised representation learning model to search for similar samples across the whole dataset, and then encourage a clustering model to output the same labels for similar instances, which further improved the clustering performance. Considering the imperfect embedding features, the local nearest samples in the embedding space do not always have the same semantics especially when the samples lie around the borderlines between different clusters as shown in Fig. 1(a), which may compromise the performance. Essentially, SCAN only utilizes the instance similarity for training the clustering model without explicitly exploring the semantic discrepancy between clusters, as shown in Fig. 1(b), so that it cannot identify the semantically inconsistent samples.

To this end, we propose a Semantic Pseudo-labeling-based Image ClustEring (SPICE) framework that synergizes the similarity among instances and semantic discrepancy between clusters to generate accurate and reliable self-supervision over clustering. In SPICE, the clustering network is divided into two parts: a feature model and a subsequent clustering head, which is exactly a traditional classification network. To effectively
measure the instance similarity and the cluster discrepancy, we split the training process into three stages: 1) training the feature model; 2) training the clustering head; and 3) jointly training the feature model and the clustering head. We highlight that there is no any annotations throughout the training process. More specifically, in the first stage we adopt the self-supervised contrastive learning paradigm to train the feature model, which can accurately measure the similarity among instance samples. In the second stage, we propose a prototype pseudo-labeling algorithm to train the clustering head in the expectation-maximization (EM) framework with the feature model fixed, which can take into account both the instance similarity and the semantic discrepancy for clustering. In the final stage, we propose a reliable pseudo-labeling algorithm to jointly optimize the feature model and the clustering head, which can boost both the clustering performance and the representation ability.

Compared with the instance similarity based method [1], the proposed prototype pseudo-labeling algorithm can leverage the predicted cluster labels, obtained from the clustering head, to identify cluster prototypes in the feature space, and then assign each prototype label to its neighbor samples for training the clustering head alternatively. Thus, the inconsistency among borderline samples can be avoided when the prototypes are well captured, as shown in Fig. 1(b). On the other hand, given the predicted labels, the reliable pseudo-labeling algorithm can identify unreliable samples in the embedding space, as the yellow circles in Fig. 1(c), which will be filtered out during joint training. Therefore, the proposed SPICE can generate more accurate and reliable supervision by synergizing the similarity and discrepancy.
representation features during training and as the one-hot encoded cluster indices during testing [1], [11], [12], [13] [14], [15], [16], [23], [24], [25], [26], as shown in Fig. 2(b). Actually, these methods aim to train the clustering model in the unsupervised setting while using multiple indirect loss functions, such as sample relations [11], invariant information [12], mutual information [13], partition confidence maximisation [25], attention [14], and entropy [1], [14], [15], [25]. Gupta et al. [27] proposed to train an ensemble of deep networks and select the predicted labels that a large number of models agree on as the high-quality labels, which are then used to train a ladder network [28] in a semi-supervised learning mode. However, the performance of these methods may be sub-optimal when using such label features to compute the similarity and discrepancy between samples, as the category-level label features can hardly reflect the relations of instance-level samples accurately.

To improve the representation learning ability, a two-stage unsupervised clustering method (TSUC) [29] was proposed. In the first stage, the unsupervised representation learning model was trained for initialization. In the second stage, a mutual information loss [13] based on the label features and a contrastive loss based on the embedding features were simultaneously optimized for training the whole model, as shown in Fig. 2(c). Although better initialization and contrastive loss can help learn representation features, the supervision based on the similarity and the discrepancy are computed independently, and the end-to-end training without accurate discriminative supervision will even harm the representation features as analyzed in Section IV-F.2.

In contrast, Van Gansbeke et al. [1] proposed a method called SCAN to use embedding features of the representation learning model for computing the instance similarity, based on which the label features are learned by encouraging similar samples to have the same label, as shown in Fig. 2(d). Sharing the same idea with SCAN, NNM [30] was proposed to enhance SCAN by searching similar samples on both the entire dataset and the sub-dataset. However, since the embedding features are not perfect, similar instances do not always have the same semantics especially when the samples lie near the borderlines of different clusters. Therefore, only using the instance similarity and ignoring the semantic discrepancy between clusters to guide model training may limit the clustering performance. Recently, Park et al. [31] proposed an add-on module for improving the off-the-shelf unsupervised clustering method based on the semi-supervised learning [32] and label smoothing techniques [33], [34].

Based on the comprehensive analysis of existing deep clustering methods, we present a new framework for image clustering, as shown in Fig. 2(e), which can accurately measure the similarity among samples and the discrepancy between clusters for the model training, and effectively reduce the semantic inconsistency for similar samples. On the other hand, our method is also related to the prototype-based traditional clustering algorithms [35], [36] and prototype-based learning for robust supervised classification [37]. Different from these methods, our proposed prototype pseudo-labeling algorithm alternatively estimates cluster labels and optimizes clustering heads to explicitly leverage the feature similarity among similar samples and the discrepancy between clusters in an unsupervised learning manner. In addition to the image clustering methods mentioned above, there are also promising deep learning-based clustering methods focusing on special [38], [39], multi-view clustering datasets [40], [41], and segmentation applications [42].

B. Unsupervised Representation Learning

Unsupervised representation learning aims to map samples/images into semantically meaningful features without human annotations, which facilitates various downstream tasks, such as object detection and classification. Previously, various pretext tasks were heuristically designed for this purpose, such as colorization [45], rotation [46], jigsaw [47], etc. Recently, contrastive learning methods combined with data augmentation strategies have achieved great success, such as SimCLR [48], MOCO [49], and BYOL [43], just to name a few. On the other hand, clustering based representation learning methods have also achieved great progress. Caron et al. [50] proposed to alternatively perform...
The k-means clustering algorithm on the entire dataset and train the classification network using the cluster labels. Without explicitly computing cluster centers, Asano et al. [51] proposed a self-labeling approach that directly infers the pseudo-labels from the predicted cluster labels of the full dataset based on the Sinkhorn-Knopp algorithm [52], and then uses the pseudo labels to train the clustering network. Taking the advantages of contrastive learning, SwAV [53] was proposed to simultaneously cluster the data while enforcing different transformations of the same image having the same cluster assignment. It is worth emphasizing that, different from the unsupervised deep clustering methods in Section II-A, these clustering based representation learning methods aim to learn the representation features by clustering a much larger number of clusters than the number of ground-truth classes. This is consistent with our observation that directly clustering the target number of classes without accurate supervision will harm the representation learning due to the over-compression of instance-level features. Usually, to evaluate the quality of learned features, a linear classifier is independently trained with ground truth labels by freezing the parameters of representation learning models.

In this work, we aim to achieve unsupervised clustering with the exact number of real classes. On the other hand, we not only train the feature model but also the clustering head without using any annotations. Actually, any unsupervised representation learning methods can be implemented as our feature model, which can be further improved via the joint training in SPICE.

C. Semi-Supervised Classification

Our method is also related to the semi-supervised classification methods as actually we reformulate the unsupervised clustering task into a semi-supervised learning paradigm in the joint training stage. Semi-supervised classification methods aim to reduce the requirement of labeled data for training a classification model by providing a means of leveraging unlabeled data. In this category, remarkable results were obtained with consistency regularization [54], [55] that constrains the model to output the same prediction for different transformations of the same image, pseudo-labeling [56] that uses confident predictions of the model as the labels to guide training processes, and entropy minimization [56], [57] that steers the model to output high-confidence predictions. MixMatch [32] algorithm combines these principles in a unified scheme and achieves an excellent performance, which is further improved by ReMixMatch [58] along this direction. Recently, FixMatch [59] proposed a simplified framework that uses the confident prediction of a weakly transformed image as
the pseudo label when the model is fed a strong transformation of the same image, delivering superior results.

In this work, we target a more challenging task of training the clustering network without using any annotations, sometimes achieving comparable or even better results than the state-of-the-art semi-supervised learning methods.

III. METHOD

We aim to cluster a set of $N$ images $\mathbf{x} = \{\mathbf{x}_i\}_{i=1}^N$ into $K$ classes by training a clustering network without using any annotations. The clustering network can be conceptually divided into two parts: a feature model that maps images to feature vectors, $f_{i} = \mathcal{F}(\mathbf{x}_i; \theta_{\mathcal{F}})$, and a clustering head that maps feature vectors to the probabilities over $K$ classes, $p_{i} = \mathcal{C}(f_{i}; \theta_{C})$, where $\theta_{\mathcal{F}}$ and $\theta_{C}$ represent the trainable parameters of the feature model $\mathcal{F}$ and the clustering head $\mathcal{C}$, respectively.

Different from the existing deep clustering methods, we use the outputs of the feature model to measure the similarity among samples and use the clustering head to identify the discrepancy between clusters for pseudo-labeling, as shown in Fig. 2. By effectively measuring both the similarity and discrepancy, we design two semantics-aware pseudo-labeling algorithms, prototype pseudo-labeling and reliable pseudo-labeling, to generate accurate and reliable self-supervision.

Specifically, we split the network training into three stages as shown in Fig. 3. First, we optimize the feature model $\mathcal{F}$ through the instance-level contrastive learning that enforces the features from different transformations of the same image being similar and the features from different images being discriminative from each other. Second, we optimize the clustering head $\mathcal{C}$ with the proposed prototype pseudo-labeling algorithm while freezing the feature model learned in the first stage. Third, we optimize the feature model and the clustering head jointly with the proposed reliable pseudo-labeling algorithm.

In the following subsections, we introduce each training stage in detail.

A. Feature Model Training With Contrastive Learning

To accurately measure the similarity of instance samples, here we adopt the instance discrimination based unsupervised representation learning method [49] for training the feature model. As shown in Fig. 3(a), there are two branches taking two random transformations of the same image as inputs, and each branch includes a feature model and a projection head that is a two-layer multilayer perceptron (MLP). During training, we only optimize the lower branch while the upper branch is updated as the moving average of the lower branch.

As contrastive learning methods benefit from a large training batch, a memory bank [60] is used to maintain a queue of encoded negative samples for reducing the requirement of GPU memory size, which is denoted as $[z^-_1, z^-_2, \ldots, z^-_{N_q}]$, where $N_q$ is the queue size.

Formally, given two transformations $\mathbf{x}'$ and $\mathbf{x}''$ of an image $\mathbf{x}$, the output of the upper branch is $z^{+} = \mathcal{P}(\mathcal{F}(\mathbf{x}'; \theta_{\mathcal{F}'}) ; \theta_{\mathcal{P}})$, and the output of the lower branch is $z = \mathcal{P}(\mathcal{F}(\mathbf{x}'' ; \theta_{\mathcal{F}}) ; \theta_{\mathcal{P}})$, where $\mathcal{P}$ denotes the projection head with the parameters $\theta_{\mathcal{P}}$, and $\theta_{\mathcal{F}'}$ and $\theta_{\mathcal{P}}$ are the moving averaging versions of $\theta_{\mathcal{F}}$ and $\theta_{\mathcal{P}}$. The parameters $\theta_{\mathcal{F}}$ and $\theta_{\mathcal{P}}$ are optimized with the following loss function:

$$
\mathcal{L}_{fe} = -\log \left( \frac{\exp(z^+ T z^+ / \tau)}{\sum_{i=1}^{N_q} \exp(z_i T z^+ / \tau) + \exp(z^+ T z_i / \tau)} \right),
$$

where the negative sample $z_i^-$ may be computed from any images other than the current image $\mathbf{x}$, and $\tau$ is the temperature. Therefore, minimizing Eq. (1) is to make the representation features of different transformations from the same instance similar and the representation features of different instances dissimilar, which has been demonstrated as an effective pretext task to learn visual representations in the self-supervised learning setting [48], [49]. Then, the parameters of the upper branch is updated as $\theta_{\mathcal{F}'} \leftarrow \mu \theta_{\mathcal{F}'} + (1 - \mu) \theta_{\mathcal{F}}$, and $\theta_{\mathcal{P}} \leftarrow \mu \theta_{\mathcal{P}} + (1 - \mu) \theta_{\mathcal{P}}$, where $\mu \in [0, 1)$ is a momentum coefficient. The queue is updated by adding $z^+$ to the end and removing the first item. All hyperparameters including $\tau = 0.2$ and $\mu = 0.999$ are the same as those in [49]. The finally optimized feature model parameters are denoted as $\theta_{\mathcal{F}'}$, which will be used in the next stage.

Remark: In practice, any unsupervised representation learning methods and network architectures can be applied in the SPICE framework.

B. Clustering Head Training With Prototype Pseudo-Labeling

Based on the trained feature model, here we train the clustering head by explicitly exploring both the similarity among samples and the discrepancy between clusters. Formally, given the image dataset $\mathbf{x}$ and the feature model parameters $\theta_{\mathcal{F}'}$ obtained in Section III-A, we aim to train the clustering head only for predicting the cluster labels $\{\gamma_i\}_{i=1}^N$. The clustering head $\mathcal{C}$ is a two-layer MLP mapping the features to the probabilities, $p_{i} = \mathcal{C}(f_{i}; \theta_{\mathcal{C}})$, where $f_{i} = \mathcal{F}(\mathbf{x}_i; \theta_{\mathcal{F}'})$. However, in the unsupervised setting we do not have the ground truth for training. To address this issue, we propose a prototype pseudo-labeling algorithm that alternatively estimates the pseudo labels of batch-wise samples and optimizes the parameters of the clustering head in an EM framework.

Generally, this training stage is to solve two sets of variables, i.e., the parameters of the clustering head $\theta_{\mathcal{C}}$, and the cluster labels $\{\gamma_i\}$ of $\mathbf{x}$ over $K$ clusters. Analogous to $k$-means clustering algorithm [61], we solve two underlying sub-problems alternatively in an EM framework: the expectation (E) step is solving $\{\gamma_i\}$ given $\theta_{\mathcal{C}}$, and the maximization (M) step is solving $\theta_{\mathcal{C}}$ given $\{\gamma_i\}$. Taking the advantages of contrastive learning, we clone the feature model into three branches as shown in Fig. 3(b):

- The top branch takes original images as inputs and outputs the embedding features $f_{i}$;
- The middle branch takes the weakly transformed images as inputs and estimates the probabilities $p_{i}$ over $K$ clusters, which is then combined with $f_{i}$ to generate the pseudo labels $\gamma_i'$ through the proposed prototype pseudo-labeling algorithm;
The bottom branch takes strongly transformed images as inputs and optimizes $\theta_C$ with the pseudo-labels.

The EM process for the clustering head training is detailed as follows.

1) Prototype Pseudo-Labeling (E-Step): The top branch computes the embedding features, $F = [f_1, f_2, \ldots, f_M]^T \in \mathbb{R}^{M \times D}$, of a mini-batch of samples $X_b$, and the middle branch computes the corresponding probabilities, $P = [P_1, P_2, \ldots, P_M]^T \in \mathbb{R}^{M \times K}$, for the weakly transformed samples, $\alpha(X_b)$; here, $M$ is mini-batch size, $D$ is the dimension of the feature vector, and $\alpha$ denotes the weak transformation over the input image.

Given $P$ and $F$, the top confident samples are selected to estimate the prototypes for each cluster, and then the indices of the cluster prototypes are assigned to their nearest neighbors as the pseudo labels. Formally, the top confident samples for each cluster, taking the $k$-th cluster as an example, are selected as:

$$3_k = \{ f_i | i \in \text{argtop}_k(P_{:,k}, M) \}, \forall \; i = 1, 2, \ldots, M, \quad (2)$$

where $P_{:,k}$ denotes the $k$-th column of matrix $P$ and $\text{argtop}_k(P_{:,k}, M)$ returns the top $M$ confident sample indices from $P_{:,k}$. Naturally, the cluster centers $\{3_k\}_{k=1}^K$ in the embedding space are computed as

$$y_k = \frac{K}{M} \sum_{f_i \in 3_k} f_i, \; \forall \; k = 1, 2, \ldots, K. \quad (3)$$

By computing the cosine similarity between embedding features $f_i$ and the center cluster $y_k$, we select $M$ nearest samples to $y_k$, denoted by $X^k$, to have the same cluster label, $y_i^k = k, \forall x_i \in X^k$. Thus, a mini-batch of images with semantic pseudo-labels, $X^s$, is constructed as

$$X^s = \{(x_i, y_i^s)|\forall x_i \in X^k, k = 1, 2, \ldots, K\}. \quad (4)$$

A toy example of the prototype pseudo-labeling process is shown in Fig. 4, where there is a batch of 10 samples and 3 clusters, 3 confident samples for each cluster are selected according to the predicted probabilities to calculate the prototypes in the feature space, and 3 nearest samples to each cluster are selected and labeled. Note that there may exist overlapped samples between different clusters, so there are two options to handle these labels: one is the overlap assignment that one sample may have more than one cluster labels as indicated by the blue and red circles in Fig. 4, and the other is the non-overlap assignment that all samples have only one cluster label as indicated by the dashed red circle. We found that the overlap assignment is better as analyzed in Section IV-F.2.

2) Training Clustering Head (M-Step): Given the labeled samples $X^s$, the clustering head parameters are optimized in a supervised learning manner. Specifically, we compute the probabilities of strong transformations $\beta(X^s)$ in the forward pass, where $\beta$ denotes the strong augmentation operator. Then, the clustering head $C$ can be optimized in the backward pass by minimizing the following cross-entropy (CE) loss:

$$L_{\text{ce}} = \frac{1}{M} \sum_{i=1}^{M} L_{\text{ce}}(y_i^s, p_i^s), \quad (5)$$

where $p_i^s = \text{softmax}(p_i)$ and $p_i = A(F(\beta(x_i); \theta_\beta); \theta_A)$. $L_{\text{ce}}$ is the cross-entropy loss function.

In Eq. (5), we use double softmax functions before computing CE loss, as $p_i$ is already the output of a softmax function. Considering that the pseudo-labels are not as accurate as the ground truth labels, the basic idea behind the double softmax implementation is to reduce the learning speed especially when the predictions are of low probabilities, which can benefit the dynamically clustering process during training (please see Appendix A for the detailed analysis of the double softmax implementation). The above process for training the clustering head is summarized in Algorithm 1.

![Fig. 4. A toy example for prototype pseudo-labeling. First, given the predicted probabilities of 10 samples over 3 clusters, top 3 confident samples are selected for each cluster, marked as green, blue, and red colors respectively. Then, the selected samples are mapped into the corresponding features (denoted by dots) to estimate the prototypes (denoted by stars) for each cluster, where stars are estimated with connected dots. Finally, the top 3 nearest samples to each cluster prototype (the dots within the same ellipse) are selected and assigned with the index of the corresponding prototype. Other unselected samples are signed with -1 and will not be used for training. The dashed ellipse denotes the non-overlap assignment.](image-url)
selected for the minimum loss value of $\mathcal{L}_{clu}$ over the whole dataset; i.e., we set $M = N$ and follow E-step and M-step in Algorithm 1 to compute the loss value. During testing, the best clustering head is used to cluster the input images into different clusters.

C. Joint Training With Reliable Pseudo-Labeling

The feature model and the clustering head are optimized separately so far, which tends to be a sub-optimal solution. On the one hand, the imperfect feature model may lead to some similar features corresponding to really different clusters; thus, assigning neighbor samples with the same pseudo-label is not always reliable. On the other hand, the imperfect clustering head may assign really dissimilar samples with the same cluster label, such that only using the predicted labels for fine-tuning is also not always reliable. To overcome these problems, we design a reliable pseudo-labeling algorithm to train the feature model and clustering head jointly for further improving the clustering performance.

1) Reliable Pseudo-Labeling: Given the embedding features and the predicted labels $\{(x_j, f_j, y_j^p)\}_{j=1}^N$ obtained in Section III-B, we select $N_i$ nearest samples for each sample $x_i$ according to the cosine similarity between embedding features. The corresponding labels of these nearest samples are denoted by $\mathcal{L}_i$. Then, the semantically consistent ratio $r_i$ of the sample $x_i$ is defined as

$$r_i = \frac{1}{N_i} \sum_{y \in \mathcal{L}_i} \mathbb{1}(y = y_i^p).$$

Given a predefined threshold $\lambda$, if $r_i > \lambda$, the sample $(x_i, y_i^p)$ is identified as the reliably labeled for joint training, and otherwise the corresponding label is ignored. Through the reliable pseudo-labeling, a subset of reliable samples $\mathcal{X}'$ are selected as:

$$\mathcal{X}' = \{(x_i, y_i^p)|r_i > \lambda, \ \forall \ i = 1, 2, \ldots, N\}.$$  

2) Joint Training: Given the above partially labeled samples, the clustering problem can be converted into a semi-supervised learning paradigm to train the clustering network jointly. Here we adapt a simple semi-supervised learning method [59]. During training, the subset of reliably labeled samples keep fixed. On the other hand, all training samples should be consistently clustered, i.e., different transformations of the same image are constrained to have the consistent prediction. To this end, as shown in Fig. 3(c), the confidently predicted label of weak transformations is used as the pseudo-label for strong transformations of the same image. Formally, the consistency pseudo label $y_j^c$ of the sample $x_j$ is calculated as in Eq. (8):

$$y_j^c = \arg \max \{p_j \} \ \text{if} \ \max \{p_j \} \geq \eta,$$

$$\text{otherwise}$$

where $p_j = \mathcal{C}(\mathcal{F}(\alpha(x_j); \theta_{\mathcal{F}}; \theta_{\mathcal{C}}))$, and $\eta$ is the confidence threshold.

Then, the whole network parameters $\theta_{\mathcal{F}}$ and $\theta_{\mathcal{C}}$ are optimized with the following loss function:

$$\mathcal{L}_{joint} = \frac{1}{L} \sum_{i=1}^{L} \mathcal{L}_{ce}(y_i^p, \mathcal{C}(\mathcal{F}(\alpha(x_i); \theta_{\mathcal{F}}; \theta_{\mathcal{C}})))$$

$$+ \frac{1}{U} \sum_{j=1}^{U} \mathbb{1}(y_j^c \geq 0) \mathcal{L}_{ce}(y_j^c, \mathcal{C}(\mathcal{F}(\beta(x_j); \theta_{\mathcal{F}}; \theta_{\mathcal{C}}))),$$

where the first term is computed with reliably labeled samples $(x_i, y_i^p)$ drawn from $\mathcal{X}'$, and the second term is computed with pseudo-labeled samples $(x_i, y_i^c)$ drawn from the whole dataset $\mathcal{X}$, which is dynamically labeled by thresholding the confident predictions as in Eq. (8). $L$ and $U$ denote the numbers of labeled and unlabeled images in a mini-batch.

Remark: Although we adapt the FixMatch [59] semi-supervised classification method for image clustering in this work, we highlight that other semi-supervised algorithms can also be used here with reliable samples generated by the proposed reliable pseudo-labeling algorithm.

Note that SPICE sheds light on the importance of utilizing both instance-level similarity and semantic-level discrepancy for clustering. With this key idea in mind, this study focuses on developing the semantic pseudo-labeling algorithms that can actually estimate the instance similarity and semantic discrepancy for better clustering results. Actually, SPICE presents a general unsupervised clustering framework that gradually trains the feature model, clustering head, and whole model end-to-end. This framework is able to organically unify advanced unsupervised representation learning and semi-supervised learning methods for clustering through the proposed semantic pseudo-labeling method.

IV. EXPERIMENTS AND RESULTS

A. Benchmark Datasets and Evaluation Metrics

We evaluated the performance of SPICE on six commonly used image clustering datasets, including STL10, CIFAR-10, CIFAR-100-20, ImageNet-10, ImageNet-Dog, and Tiny-ImageNet. The key details of each dataset are summarized in Table I, where the datasets reflect a diversity of image sizes, the number of images, and the number of clusters. Different existing methods used different image sizes for training and testing; for example, CC [15] resizes all images of these six datasets into $224 \times 224$, and GATCluster [14] studies the effectiveness of different image sizes on ImageNet-10 and

| Dataset         | Image size | # Training | # Testing | # Classes (K) |
|-----------------|------------|------------|-----------|---------------|
| STL10           | 96 × 96    | 5,000      | 8,000     | 10            |
| CIFAR-10        | 32 × 32    | 50,000     | 10,000    | 10            |
| CIFAR-100-20    | 32 × 32    | 50,000     | 10,000    | 20            |
| ImageNet-10     | 224 × 224  | 13,000     | N/A       | 10            |
| ImageNet-Dog    | 224 × 224  | 19,500     | N/A       | 15            |
| Tiny-ImageNet   | 64 × 64    | 100,000    | 10,000    | 200           |
ImageNet-Dog, showing that too large or too small may harm the clustering performance. In this work, we naturally use the original size of images without resizing to a larger size of images. For the ImageNet, we adopt the commonly used image size of 224 × 224.

Three popular metrics are used to evaluate clustering results, including Adjusted Rand Index (ARI) [62], Normalized Mutual Information (NMI) [63], and clustering Accuracy (ACC) [64].

B. Implementation Details

For a fair comparison, we mainly adopted two backbone networks, i.e. ResNet18 and ResNet34 [73], for representation learning. The clustering head in SPICE consists of two fully-connected layers, where the dimensions of the input and intermediate layer are the same and denoted as $D$, and the dimension of the output is the number of clusters and denoted as $K$. Specifically, $D = 512$ for both ResNet18 and ResNet34 backbone networks, and the cluster number $K$ is predefined as the number of classes on the target dataset as shown in Table I. To show how the joint training (third stage) improves the clustering performance, we refer to SPICE without joint training as SPICE$_s$, where the subscript $s$ indicates the separate training.

For representation learning, we use MoCo-v2 [49] in all our experiments, which was also used in SCAN [1]. For weak augmentation, a standard flip-and-shift augmentation strategy is implemented as in FixMatch [59]. For strong augmentation, we adopt the same strategies used in SCAN [1]. Specifically, the images were strongly augmented by composing Cutout [74] and four randomly selected transformations from RandAugment [75].

In the first training stage, we duplicated the optimization settings in [49] that the stochastic gradient descent (SGD) optimizer was used with weight decay of 0.0001, momentum of 0.9 and the cosine learning rate schedule, batch size was set to 128, and the initial learning rate to 0.015. Note that the memory bank size in [49] was set to 65,536 by default. However, the datasets CIFAR-10, CIFAR-100-20, ImageNet-10, and ImageNet-Dog contain less than 65,536 images, and thus the memory back size for these datasets was empirically set to 10,240. In the second training stage, the Adam optimizer was used with the constant learning rate of 0.005, and the batch size $M$ was set to 1,000. Here 10 clustering heads were simultaneously trained, and the best head with the minimum loss was selected as the final head in each trial. In the third training stage, we used the same optimization settings in [59] that the SGD optimizer was used with weight decay of 0.0005, momentum of 0.9 and the cosine learning rate schedule, batch size was set to 128 (16 reliable labeled samples and 112 unlabeled samples), the initial learning rate to 0.03, and the threshold $\eta$ to 0.95. To select the reliably labeled images for SPICE through reliable pseudo-labeling, we empirically selected $N_t = 100$ and $\lambda = 0.95$.

In all our experiments, feature model training and joint training were distributed across 4 GPUs, and clustering heads were trained on a single GPU. The training time depends on various factors, such as the number of images, image size, model size, training epochs, etc. By default, we set the number of training epochs for the feature model and the clustering head to 1,000 and 100 epochs respectively in our experiments, which are the same as those used for training the competing models [1], and the number of training iterations for joint learning to 1,048,576, the same as that in [59]. As an example, clustering STL10 images with SPICE took about 18 hours (800 epochs for feature learning, 30 epochs for training clustering heads, and 500,000 iterations for joint learning) to achieve state-of-the-art results.

C. Clustering Performance Comparison

The existing methods can be divided into two groups according to their training and testing settings. One is to train and test the clustering model on the whole dataset combining the train and test splits as one. The other is to train and test the clustering model on the separate train and test datasets. For a fair comparison, the proposed SPICE is evaluated under both two settings and compared with the existing methods accordingly.

Table II shows the comparison results of clustering on the whole dataset. The results obtained using classic clustering algorithms (i.e., k-means, spectral clustering, agglomerative clustering, NMF) and the unsupervised deep feature models (i.e., AE, SDAE, DCGAN, DeCNN, VAE) were originally reported in [11] and [25]. In reference to the recently developed methods [12], [14], [15], the same backbone, i.e. ResNet34, was used during learning the feature model and clustering head. Duplicating the original settings in FixMatch [59], we used WideResNet-28-2 for CIFAR-10, WideResNet-28-8 for CIFAR-100-20, and WideResNet-37-2 for STL-10. For ImageNet-10, ImageNet-Dog, and Tiny-ImageNet datasets that were not used in FixMatch, we simply used the same ResNet34 during joint learning. The results show that SPICE improves ACC, NMI, and ARI by 8.8%, 12.6%, and 14.4% respectively over the previous best results that were recently reported by CC [15] on STL10. On average, our proposed method also improves ACC, NMI, and ARI by about 10% on ImageNet-Dog-15, CIFAR-10, CIFAR-100-20, and Tiny-ImageNet-200. It is worth emphasizing that, without the joint training stage, SPICE$_s$ still performs better than the existing deep clustering methods using the same network architecture on most of the datasets. These results convincingly show the superior performance of the proposed method using exactly the same backbone networks and datasets. The final joint training results are obviously better than those from the separate training on all datasets, especially on CIFAR-10 (improved by 8.8% for ACC) and CIFAR-100-20 (improved by 7.0% for ACC). In clustering the images on Tiny-ImageNet-200, our results are significantly better than the existing results. These results are, however, still relatively low. This is mainly due to the class hierarchies, i.e., some classes share the same supper class, as analyzed in [1]. Due to this issue, some clusters cannot be reliably labeled based on the reliable pseudo-labeling algorithm so that end-to-end training cannot further boost clustering performance when directly using the...
produced labels in the second stage. Thus, it is still an open problem for clustering images which form a large number of hierarchical clusters.

Table III shows the comparison results of clustering on the split train and test datasets. For a fair comparison, we reimplement SCAN with MoCo [49] for representation learning, denoted as SCANMoCo. It can be seen that the results of SCANMoCo on STL10 are obviously better than SCAN, while the performance on CIFAR-10 and CIFAR-100-20 drops slightly. Compared with the baseline method SCANMoCo, SPICE improves ACC, NMI, and ARI by 6.5%, 9.4%, and 11.5% on STL10, by 4.4%, 6.4%, and 8.0% on CIFAR-10, and by 8.0%, 9.3%, and 9.4% on CIFAR-100-20, under the exactly the same setting. Without joint learning, SPICE already performs better than SCANMoCo that contains the pretraining, clustering, and finetuning stages on STL10 and CIFAR-100-20. Moreover, we evaluate the SPICE using larger backbone networks as used in the whole dataset setting, the results on STL10 and CIFAR-10 are very similar while the results on CIFAR-100-20 are significantly improved. Remarkably, SPICE significantly reduces the gap between unsupervised and supervised classification. On the STL10 that includes both labeled and unlabeled images, the results of unsupervised methods are better than the supervised as the unsupervised methods can leverage the unlabeled images for representation learning while the supervised cannot. On CIFAR-10 and CIFAR-100-20, all methods used the same images for training and the proposed SPICE further reduces the performance gap compared with the supervised counterpart, particularly, only 2% for ACC gap on CIFAR-10.
Table IV provides more detailed comparison results on STL10, where all these three methods use MoCo [49] for representation learning and were conducted five times for computing the mean and standard deviation of the results. Compared with SCAN$_{MoCo}^*$ that explores the instance similarity only without fine-tuning, SPICE$_s$ explicitly leverages both the instance similarity and semantic discrepancy for learning clusters. On the other hand, different from $k$-means that infers the cluster labels with cluster centers, SPICE$_s$ uses the non-linear clustering head to predict the cluster labels. It can be seen that SPICE$_s$ is significantly better than MoCo+$k$-means and SCAN$_{MoCo}^*$ in terms of both the mean and standard deviation metrics, demonstrating the superiority of the proposed prototype pseudo-labeling algorithm. The final results of SPICE is significantly better than those of SCAN$_{MoCo}^*$ in terms of mean performance and the stability.

Overall, our comparative results systematically demonstrate the superiority of the proposed SPICE method on both the whole and split dataset settings.

### E. Unsupervised Representation Learning

Here we aim to study the effects of the reliable pseudo-labeling-based joint training in SPICE on representation features. As in all unsupervised representation learning methods [49], the quality of representation features is evaluated by training a linear classifier while freezing the learned feature model using the ground-truth labels. The results in Table VI show that the quality of representation features on CIFAR-10 and STL10 is clearly improved after joint training, while keeping similar performance on CIFAR-100-20. The interpretation is that the feature improvement with joint learning requires very accurate pseudo-labels (the ACC of reliable labels on STL10 and CIFAR-10 are 97.7% and 96.5%), so that the improvement is not observed on CIFAR-100-20 (the ACC of reliable labels on CIFAR-100-20 is 67.7%). In comparison with SCAN, SPICE also achieved better results in the unsupervised representation learning. Thus, given more prior of the target dataset, e.g., the number of different semantic clusters with a roughly balanced distribution, the proposed framework has the potential to improve the unsupervised representation learning by generating accurate and reliable pseudo-labels.

### F. Empirical Analysis

In this subsection, we empirically analyze the effectiveness of different components and options in the proposed SPICE framework.

1) **Visualization of Cluster Semantics:** We visualize the semantic clusters learned by SPICE$_s$ in terms of the prototype samples and the discriminative regions, as shown in Fig. 5. Specifically, Fig. 5(a) shows the top three nearest samples of the cluster centers representing the cluster prototypes, and in Fig. 5(b), each cluster includes three samples and each sample is visualized with an original image and an attention map to highlight the discriminative regions. The attention maps of each cluster is computed by computing the cosine similarity between the cluster center (with Eqs. (2) and (3)) of the whole dataset and the convolutional feature maps of individual images, and then resized and normalized into $[0, 1]$. It shows that the prototype samples exactly match the human annotations, and the discriminative regions focus on the semantic objects. For example, the cluster with label ‘1’ captures the ‘dog’ class, and its most discriminative regions exactly capture the dogs at different locations, and similar results can be observed for all other clusters. The visual results indicate that semantically meaningful clusters are learned, and the cluster center vectors can extract the discriminative features.

2) **Ablation Study:** We evaluate the effectiveness of different components of SPICE$_s$ in an ablation study, as shown in Table VII. In each experiment, we replaced one component of SPICE$_s$ with another option, and five trials were conducted to report the mean and standard deviation for each metric.

We first evaluated the effectiveness of the overlap assignment and non-overlap assignment as described in Section III-B and Fig. 4. The results show that the overlap assignment is preferred over the non-overlap assignment.
TABLE V

Comparison Results with Semi-Supervised Learning on STL10 and CIFAR-10. Top-1 Classification Accuracy and Standard Deviation for Different Methods Are Reported. The Best Three Results Are in Bold.

| Method     | II-Model | Pseudo-Labeling | Mean Teacher | MixMatch | UDA | ReMixMatch | FixMatch | SCAN | SPICE |
|------------|----------|-----------------|--------------|----------|-----|------------|----------|------|-------|
| STL10      | 0.748±0.008 | 0.720±0.008     | 0.766±0.024  | 0.896±0.006 | 0.923±0.006 | 0.948±0.005 | 0.920±0.015 | 0.767±0.019 | 0.929±0.001 |
| CIFAR-10   | 0.457±0.040 | 0.502±0.004     | 0.677±0.009  | 0.890±0.009 | 0.912±0.011 | 0.947±0.001 | 0.949±0.003 | 0.876±0.004 | 0.917±0.002 |

Fig. 5. Visualization of learned semantic clusters on STL10. (a) The top three nearest samples to the cluster centers. (b) The attention maps of cluster center on individual images.

which may be explained by the fact that the non-overlap assignment may introduce extra local inconsistency when assigning the label to a sample far away from the cluster center, as shown in Fig. 4 (dashed red circle).

During training SPICE, we only optimize the clustering head while freezing the parameters of the feature model. To demonstrate the effectiveness of this separate training strategy, we compared it with two variants, i.e., jointly training the feature model and a single clustering head (Joint-SH) and jointly training the feature model and multiple clustering heads (Joint-MH). Note that the feature model in the first branch in

Table VI

Feature Quality Before and After Joint Training. The Format of Results for Before Joint Training Means the ACC of supervised / unsupervised / reliable labels, for After Joint Training Means the ACC of supervised / unsupervised. The Supervised Results Were Obtained by Training a Linear Classifier While Fixing the Feature Model.

| Method     | STL-10 | CIFAR-10 | CIFAR-100-20 |
|------------|--------|----------|--------------|
| Before     | 0.908/0.862/0.977 | 0.893/0.845/0.965 | 0.729/0.468/0.677 |
| After (SPICE) | 0.938/0.920 | 0.922/0.918 | 0.723/0.535 |
| After (SCAN) | 0.877/0.855 | 0.901/0.874 | 0.693/0.455 |

Table VII

Ablation Studies of SPICE on the Whole STL10 Dataset

| Variants | ACC      | NMI      | ARI      |
|----------|----------|----------|----------|
| Non-overlap | 0.885±0.002 | 0.788±0.003 | 0.771±0.003 |
| Joint-SH     | 0.622±0.061 | 0.513±0.037 | 0.437±0.053 |
| Joint-MH     | 0.687±0.037 | 0.577±0.029 | 0.512±0.033 |
| Entropy     | 0.907±0.001 | 0.817±0.003 | 0.810±0.003 |
| CE         | 0.875±0.031 | 0.784±0.017 | 0.764±0.033 |
| TCE        | 0.895±0.005 | 0.794±0.010 | 0.787±0.010 |
| SPICE_e    | 0.908±0.001 | 0.817±0.002 | 0.812±0.002 |

Fig. 3(b) is still fixed for accurately measuring the similarity. The results show that the clustering performance for these two variants became significantly worse. On the one hand, the quality of pseudo labels not only depends on the similarity measurement but also the predictions of the clustering head. On the other hand, the performance of the clustering head is also determined by the quality of representation features. When tuning all parameters during training, the feature model tends to be degraded without accurate labels and the clustering head tends to output incorrect predictions in the initial stage, which will harm the pseudo-labeling quality and get trapped in a bad cycle.
Usually, maximizing the entropy over different clusters is the necessary to avoid assign all samples into a single or a few clusters, as demonstrated in GATCluster [14]. Thus, we added another entropy loss during training, and the results were not changed. It indicates that our pseudo-labeling process with balance assignment has the ability to prevent trivial solutions. However, when clustering a large number of hierarchical clusters, e.g. 200 clusters in Tiny-ImageNet, the entropy loss was found necessary to avoid the empty clusters.

To evaluate the effectiveness of applying double softmax before CE, we replaced it with the plain CE or the CE with a temperature parameter (TCE) [80]. For TCE, we evaluated different temperature values including 0.01, 0.05, 0.07, 0.1, 0.2, 0.5, 0.8, 2, and found 0.2 achieve the best results that were included for comparison. The results show that TCE is better than CE, which is consistent with the literature [49]. On the other hand, the results of TCE are inferior to that with the double softmax CE. These experimental results are consistent with the detailed analysis in terms of the derivatives in Appendix A.

3) Clustering Head Selection: In unsupervised learning, the training process is hard to converge to the best state without the ground truth supervision, such that usually there is a large standard deviation among different trials. Thus, how to estimate the performance of models in the unsupervised training process to select the potential best model is very important. As introduced in Subsection III-B, we use the clustering loss defined in Eq. (5) on the whole test dataset to approximate the clustering performance; i.e., the smaller loss, the better clustering performance. The model selection process is shown in Fig. 6, it can be seen that the performance of the selected clustering head is very close to that of the ground truth selection, proving the effectiveness of this loss metric. In this way, the bad performance clustering heads can be filtered out. The results in Table IV show that SPICE has a lower standard deviation compared with the competing methods. Importantly, the lightweight clustering heads can be independently and simultaneously trained without affecting each other and without extra training time.

4) Effect of Reliable Labeling: In Section III-C, we introduced a reliable pseudo-labeling algorithm to select the reliably labeled images. Here we show the effectiveness of this algorithm in Fig. 7, where t-SNE was used to map the representation features of images in CIFAR-10 to 2D vectors for visualization. In Fig. 7(a), some obvious semantically inconsistent samples are evident, and the predicted ACC of SPICE is also 0.838. Using these samples directly for joint training, the ACC is not boosted. Fig. 7(b) shows the selected reliable samples, where the ratio of local inconsistency samples is significantly decreased, and the ACC is increased to 95.9% correspondingly. Using the reliable samples for joint training, the ACC of SPICE after joint training is significantly boosted (92.6% v.s. 83.8%) compared with that of SPICE.

5) Effect of Data Augmentation: We evaluated the effects of different data augmentations on SPICE, as shown in Table VIII, where Aug1 and Aug2 correspond to data augmentations of the second and the third branches in Fig. 3(b). The results show that when the second branch used the weak augmentation and the third branch used the strong augmentation, the model achieved the best performance. Moreover, the model had relatively worse performance when the second branch in labeling process uses the strong augmentation, which is due to that the labeling process aims to generate reliable pseudo labels that will be compromised by the strong augmentation. The model performs better when
the third branch used the strong augmentation, as it will drive the model to output consistent predictions of different transformations. Overall, the data augmentation has a small impact on the results, because the pre-trained feature model had been already equipped with the transformation invariance ability.

**G. Performance on Imbalanced Dataset**

This study assumes that the target image dataset can be clustered into a set of balanced groups, and thus the pseudo-labels in Eq. (2) are generated in a balanced manner. Here we aim to evaluate the performance and robustness of SPICE on imbalanced datasets. To this end, we simulated imbalanced datasets from the training set of CIFAR-10. Specifically, we randomly selected a subset of images for each class $k$ according to a predefined ratio $\xi_k$. Then a set of ratios for different classes are calculated in a linear way; i.e., $\xi_k = \xi + k \times (1 - \xi)/K$, where $k = 1, 2, \ldots, K$, the number of clusters $K = 10$ on the CIFAR-10 dataset, and the minimum ratio $\xi$ defines the imbalanced level. We generated five levels of imbalanced datasets with $\xi = 1.0, 0.8, 0.6, 0.4, 0.2$ respectively, where 1.0 means a balanced dataset and the smaller $\xi$ the more imbalanced. The cluster distributions for $\xi = 0.4$ and 0.2 are shown in Fig. 8. Both SPICE and SCAN methods using MoCo representations were evaluated and the results are reported in Table IX. Similar to the results on balanced datasets, SPICE achieved consistently better performance on different levels of imbalanced datasets than SCAN. Although using a balanced assignment, SPICE performs relatively well for $\xi \geq 0.4$ and shows robustness to some degree. However, the clustering performance is degraded on the highly imbalanced dataset $\xi = 0.2$. The clustering distributions shown in Fig. 8 further illustrate the numerical results. Therefore, SPICE still needs to be improved further in the case of the imbalanced dataset.

**V. DISCUSSIONS**

In this study, the SPICE network significantly improves the image clustering performance over the competing methods and reduces the performance gap between unsupervised and fully-supervised classification. However, there are opportunities for further refinements. First, existing deep clustering methods assume the clustering number $K$ is known. In real applications, we do not always have such a prior. Therefore, how to automatically determine the number of semantically meaningful clusters is an open problem for deep clustering research. Second, to avoid trivial solutions, almost all existing clustering methods assume that the target dataset contains a similar number of samples in each and every cluster, which may or may not be the case in a real-world application. Usually, there are at least two constraints that can be applied to implement this prior, including maximizing the entropy [14] and balancing assignment [77] (and SPICE) that is an optimal solution for maximizing entropy. On the other hand, if we do have a prior distribution of samples as a function of the cluster index, the constraints for these methods can be adapted from the uniform distribution to a specific one. The ideal clustering method should work well when neither the number of clusters nor the prior distribution of samples per cluster is known, which is a holy grail in this field. Finally, although the SPICE method achieved the superior results over the existing methods, the progressive training process through the three stages is computationally complicated based on multiple algorithmic ingredients. We recognize new opportunities to reduce the complexity and improve the performance of SPICE in a unified framework. For example, we could simultaneously train the feature model and clustering head in a single stage by combining the proposed semantic pseudo-labeling and the recently proposed representation learning methods [44], [81] that do not require any specific network architecture or particular optimization algorithm, being compatible with the current pseudo-labeling algorithm. Also, the single prototype pseudo-labeling could be extended to multiple prototypes as studied in [36] and [37] for further improvement. Nevertheless, our method is both effective and efficient, and easy to optimize and apply, because each training stage only has a single cross-entropy function and is fairly straightforward. Importantly, SPICE is an exemplary workflow to synergize both the instance similarity and semantic discrepancy for superior image clustering.

**VI. CONCLUSION**

We have presented a semantic pseudo-labeling framework for image clustering, with the acronym “SPICE”. To accurately
measure both the similarity among samples and the discrepancy between clusters for clustering, we divide the clustering network into a feature model and a clustering head, which are first trained separately with the unsupervised representation learning algorithm and the prototype pseudo-labeling algorithm, and then jointly trained with the reliable pseudo-labeling algorithm. Extensive experiments have demonstrated the superiority of SPICE over the competing methods on balanced close-set benchmarks with an average performance boost of 10% in terms of adjusted rand index, normalized mutual information, and clustering accuracy. The SPICE is comparable to or even better than the state-of-the-art semi-supervised learning methods and has the ability to improve the representation features. Remarkably, SPICE significantly reduces the gap between unsupervised and fully-supervised classification; e.g., only 2% gap on CIFAR-10. We believe the basic idea behind SPICE has the potential to help cluster other domain datasets, and apply to other learning tasks.

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