Abstract

We propose a novel framework for image clustering that incorporates joint representation learning and clustering. Our method consists of two heads that share the same backbone network - a “representation learning” head and a “clustering” head. The “representation learning” head captures fine-grained patterns of objects at the instance level which serve as clues for the “clustering” head to extract coarse-grain information that separates objects into clusters. The whole model is trained in an end-to-end manner by minimizing the weighted sum of two sample-oriented contrastive losses applied to the outputs of the two heads. To ensure that the contrastive loss corresponding to the “clustering” head is optimal, we introduce a novel critic function called “log-of-dot-product”. Extensive experimental results demonstrate that our method significantly outperforms state-of-the-art single-stage clustering methods across a variety of image datasets, improving over the best baseline by about 5-7% in accuracy on CIFAR10/20, STL10, and ImageNet-Dogs. Further, the “two-stage” variant of our method also achieves better results than baselines on three challenging ImageNet subsets.

1. Introduction

The explosion of unlabeled data, especially visual content in recent years has led to the growing demand for effective organization of these data into semantically distinct groups in an unsupervised manner. Such data clustering facilitates downstream machine learning and reasoning tasks. Since labels are unavailable, clustering algorithms are mainly based on the similarity between samples to predict the cluster assignment. However, common similarity metrics such as cosine similarity or (negative) Euclidean distance are ineffective when applied to high-dimensional data like images. Modern image clustering methods [7, 19, 20, 43, 46, 47], therefore, leverage deep neural networks (e.g., CNNs, RNNs) to transform high-dimensional data into low-dimensional representation vectors in the latent space and perform clustering in that space. Ideally, a good clustering model assigns data to clusters to keep inter-group similarity low while maintaining high intra-group similarity. Most existing deep clustering methods do not satisfy both of these properties. For example, autoencoder-based clustering methods [21, 46, 48] often learn representations that capture too much information including distracting information like background or texture. This prevents them from computing proper similarity scores between samples at the cluster-level. Autoencoder-based methods have only been tested on simple image datasets like MNIST. Another class of methods [7, 19, 20] directly use cluster-assignment probabilities rather than representation vectors to compute the similarity between samples. These methods can only differentiate objects belonging to different clusters but not in the same cluster, hence, may incorrectly group distinct objects into the same cluster. This leads to low intra-group similarity.

To address the limitations of existing methods, we propose a novel framework for image clustering called Contrastive Representation Learning and Clustering (CRLC). CRLC consists of two heads sharing the same backbone network: a “representation learning” head (RL-head) that outputs a continuous feature vector, and a “clustering” head (C-head) that outputs a cluster-assignment probability vector. The RL-head computes the similarity between objects at the instance level while the C-head separates objects into different clusters. The backbone network serves as a medium for information transfer between the two heads, allowing the C-head to leverage discriminative fine-grained patterns captured by the RL-head to extract correct coarse-grained cluster-level patterns. Via the two heads, CRLC can effectively modulate the inter-cluster and intra-cluster similarities between samples. CRLC is trained in an end-to-end manner by minimizing a weighted sum of two sample-oriented contrastive losses w.r.t. the two heads. To ensure that the contrastive loss corresponding to the C-head leads to the tightest InfoNCE lower bound [35], we propose a novel critic called “log-of-dot-product” to be used in place of the conventional “dot-product” critic.

In our experiments, we show that CRLC significantly outperforms a wide range of state-of-the-art single-
As the “contrastive loss” in other works [8, 39], $f(x, x_i)$ and $(\tilde{x}, x_i)$ are called “negative” pairs.

In summary, our main contributions are:

1. A novel framework for joint representation learning and clustering trained via two sample-oriented contrastive losses on feature and probability vectors;
2. An optimal critic for the contrastive loss on probability vectors; and,
3. Extensive experiments and ablation studies to validate our proposed method against baselines.

2. Preliminaries

2.1. Representation learning by maximizing mutual information across different views

Maximizing mutual information across different views (or ViewInfoMax for short) allows us to learn view-invariant representations that capture the semantic information of data important for downstream tasks (e.g., classification). This learning strategy is also the key factor behind recent successes in representation learning [18, 33, 39, 42].

Since direct computation of mutual information is difficult [29, 37], people usually maximize the variational lower bounds of mutual information instead. The most common lower bound is InfoNCE [35] whose formula is given by:

$$I(X, \tilde{X}) \geq I_{\text{InfoNCE}}(X, \tilde{X}) \triangleq \sum_{i=1}^{M} \log \frac{e^{f(\tilde{x}, x_i)}}{\sum_{j=1}^{M} e^{f(\tilde{x}, x_j)}} + \log M$$

where $X$, $\tilde{X}$ denote random variables from different views. $x_{1:M}$ are $M$ samples from $p_X$, $\tilde{x}$ is a sample from $p_{\tilde{X}}$ associated with $x_1$. $(\tilde{x}, x_i)$ is called a “positive” pair and $(\tilde{x}, x_i)$ (i = 2, ..., $M$) are called “negative” pairs. $f(x, y)$ is a real value function called “critic” that characterizes the similarity between $x$ and $y$. $L_{\text{contrast}}$ is often known as the “contrastive loss” in other works [8, 39].

Since $\log \sum_{i=1}^{M} e^{f(\tilde{x}, x_i)} \leq 0$, $I_{\text{InfoNCE}}(X, \tilde{X})$ is upper-bounded by $\log M$. It means that: i) the InfoNCE bound is very loose if $I(X, \tilde{X}) \gg \log M$, and ii) by increasing $M$, we can achieve a better bound. Despite being biased, $I_{\text{InfoNCE}}(X, \tilde{X})$ has much lower variance than other unbiased lower bounds of $I(X, \tilde{X})$ [35], which allows stable training of models.

Implementing the critic

In practice, $f(\tilde{x}, x_i)$ is implemented as the scaled cosine similarity between the representation of $\tilde{x}$ and $x_i$ as follows:

$$f(\tilde{x}, x_i) = \tilde{z}^T z_i / \tau$$

where $\tilde{z}$ and $z_i$ are unit-normed representation vectors of $\tilde{x}$ and $x_i$, respectively; $\|\tilde{z}\|_2 = \|z_i\|_2 = 1$. $\tau > 0$ is the “temperature” hyperparameter. Interestingly, $f$ in Eq. 4 matches the theoretically optimal critic that leads to the tightest InfoNCE bound for unit-normed representation vectors (detailed explanation in Appdx. A.4).

In Eq. 4, we use $f(\tilde{z}, z_i)$ instead of $f(\tilde{x}, x_i)$ to emphasize that the critic $f$ in this context is a function of representations. In regard to this, we rewrite the contrastive loss in Eq. 3 as follows:

$$L_{\text{FC}} = \mathbb{E}_{p(x, x_i)} \left[ -\log \frac{e^{f(\tilde{z}, z_i)}}{\sum_{i=1}^{M} e^{f(\tilde{z}, z_i)}} \right]$$

$$= \mathbb{E}_{p(x, x_i)} \left[ \tilde{z}^T z_i / \tau - \log \sum_{i=1}^{M} \exp(\tilde{z}^T z_i / \tau) \right]$$

where FC stands for “feature contrastive”.

3. Method

3.1. Clustering by maximizing mutual information across different views

In the clustering problem, we want to learn a parametric classifier $s_0$ that maps each unlabeled sample $x_i$ to a cluster-assignment probability vector $q_i = (q_{i1}, ..., q_{iC})$ ($C$ is the number of clusters) whose component $q_{ic}$ characterizes how likely $x_i$ belongs to the cluster $c$ ($c \in \{1, ..., C\}$). Intuitively, we can consider $q_i$ as a representation of $x_i$ and use this vector to capture the cluster-level information in $x_i$ by leveraging the “ViewInfoMax” idea discussed in Section 2.1. It leads to the following loss for clustering:

$$L_{\text{cluster}} = \mathbb{E}_{p(x, x_i)} \left[ -\log \frac{e^{f(q, q_i)}}{\sum_{i=1}^{M} e^{f(q, q_i)}} \right] - \lambda H(\hat{Q}_{\text{avg}})$$

$$= L_{\text{PC}} - \lambda H(\hat{Q}_{\text{avg}})$$

where $\lambda \geq 0$ is a coefficient; $\hat{q}, q_i$ are probability vectors associated with $\tilde{x}$ and $x_i$, respectively. $L_{\text{PC}}$ is the proba-
Thus, the most suitable critic is $$f(q_{\text{avg}}) = \log(q_{\text{avg}}^T q_i)$$ which we refer to as the “log-of-dot-product” critic. This critic achieves its maximum value when $$\hat{q}$$ and $$q_i$$ are the same one-hot vectors and its minimum value when $$\hat{q}$$ and $$q_i$$ are different one-hot vectors. Apart from this critic, we also list other nonoptimal critics in Appdx. A.1. Empirical comparison of the “log-of-dot-product” critic with other critics is provided in Section 5.3.

In addition, to avoid the gradient saturation problem of minimizing $$L_{\text{PC}}$$ when probabilities are close to one-hot (explanation in Appdx. A.5), we smooth out the probabilities as follows:

$$q = (1 - \gamma)q + \gamma r$$

where $$r = \left(\frac{1}{C}, \ldots, \frac{1}{C}\right)$$ is the uniform probability vector over $$C$$ classes; $$0 \leq \gamma \leq 1$$ is the smoothing coefficient set to 0.01 if not otherwise specified.

### Choosing a suitable critic

It is possible to use the conventional “dot-product” critic for $$L_{\text{PC}}$$ as for $$L_{\text{FC}}$$ (Eq. 4). However, this will lead to suboptimal results (Section 5.3) since $$L_{\text{FC}}$$ is applied to categorical probability vectors rather than continuous feature vectors. Therefore, we need to choose a suitable critic for $$L_{\text{FC}}$$ so that the InfoNCE bound associated with $$L_{\text{PC}}$$ is tightest. Ideally, $$f(x, x_i)$$ should match the theoretically optimal critic $$f^*(x, x_i)$$ which is proportional to $$\log p(\tilde{x}|x_i)$$ (detailed explanation in Appdx. A.3). Denoted by $$\tilde{y}$$ and $$y_i$$ the cluster label of $$\tilde{x}$$ and $$x_i$$ respectively, we then have:

$$\log p(\tilde{x}|x_i) \approx \log \sum_{c=1}^{C} p(\tilde{y} = c|y_i = c)$$

$$\propto \log \sum_{c=1}^{C} \tilde{q}_c q_{i,c} = \log(\tilde{q}^T q_i) \quad (9)$$

Thus, the most suitable critic is $$f(\tilde{q}, q_i) = \log(\tilde{q}^T q_i)$$ which we refer to as the “log-of-dot-product” critic. This critic achieves its maximum value when $$\tilde{q}$$ and $$q_i$$ are the same one-hot vectors and its minimum value when $$\tilde{q}$$ and $$q_i$$ are different one-hot vectors.

### Implementing the contrastive probability loss

To implement $$L_{\text{PC}}$$, we can use either the SimCLR framework [8] or the MemoryBank framework [42]. If the SimCLR framework is chosen, both $$\tilde{q}$$ and $$q_i$$ ($$i \in \{1, \ldots, M\}$$) are computed directly from $$\tilde{x}$$ and $$x_t$$ respectively via the parametric classifier $$s_0$$. On the other hand, if the MemoryBank framework is chosen, we maintain a nonparametric memory bank $$M$$ - a matrix of size $$N \times C$$ containing the cluster-assignment probabilities of all $$N$$ training samples, and update its rows once a new probability is computed as follows:

$$q_{n,t+1} = \alpha q_{n,t} + (1 - \alpha)\hat{q}_n \quad (10)$$

where $$\alpha$$ is the momentum, which is set to 0.5 in our work if not otherwise specified; $$q_{n,t}$$ is the probability vector of the training sample $$x_n$$ at step $$t$$ corresponding to the $$n$$-th row of $$M$$; $$\hat{q}_n = s_0(x_n)$$ is the new probability vector. Then, except $$\hat{q}$$ computed via $$s_0$$ as normal, all $$\tilde{q}_i$$ in Eq. 7 are sampled uniformly from $$M$$. At step 0, all the rows of $$M$$ are
3.2. Incorporating representation learning

Due to the limited representation capability of categorical probability vectors, models trained by minimizing the loss \( L_{\text{cluster}} \) in Eq.7 are not able to discriminate objects in the same cluster. Thus, they may capture suboptimal cluster-level patterns, which leads to unsatisfactory results.

To overcome this problem, we propose to combine clustering with contrastive representation learning into a unified framework called CRLC\(^2\). As illustrated in Fig. 1, CRLC consists of a “clustering” head (C-head) and a “representation learning” head (RL-head) sharing the same backbone network. The backbone network is usually a convolutional neural network which maps an input image \( x \) into a hidden vector \( h \). Then, \( h \) is fed to the C-head and the RL-head to produce a cluster-assignment probability vector \( q \) and a continuous feature vector \( z \), respectively. We simultaneously apply the clustering loss \( L_{\text{cluster}} \) (Eq. 8) and the feature contrastive loss \( L_{\text{FC}} \) (Eq. 6) on \( q \) and \( z \) respectively and train the whole model with the weighted sum of \( L_{\text{cluster}} \) and \( L_{\text{FC}} \) as follows:

\[
L_{\text{CRLC}} = L_{\text{cluster}} + \lambda L_{\text{FC}} = L_{\text{FC}} - \lambda_1 H(\tilde{Q}_{\text{avg}}) + \lambda_2 L_{\text{FC}} \tag{11}
\]

where \( \lambda_1, \lambda_2 \geq 0 \) are coefficients.

3.3. A simple extension to semi-supervised learning

Although CRLC is originally proposed for unsupervised clustering, it can be easily extended to semi-supervised learning (SSL). There are numerous ways to adjust CRLC so that it can incorporate labeled data during training. However, within the scope of this work, we only consider a simple approach which is adding a cross-entropy loss on labeled data to \( L_{\text{CRLC}} \). The new loss is given by:

\[
L_{\text{CRLC-semi}} = L_{\text{CRLC}} + \lambda \mathbb{E}_{(x_i,y_i) \sim D_1} [-\log p(y_i|x_i)] = L_{\text{PC}} - \lambda_1 H(\tilde{Q}_{\text{avg}}) + \lambda_2 L_{\text{FC}} + \lambda_3 L_{\text{cons}} \tag{12}
\]

We call this variant of CRLC “CRLC-semi”. Despite its simplicity, we will empirically show that CRLC-semi outperforms many state-of-the-art SSL methods when only few labeled samples are available. We conjecture that the clustering objective arranges the data into disjoint clusters, making classification easier.

\(^2\)CRLC stands for Contrastive Representation Learning and Clustering.

4. Related Work

There are a large number of clustering and representation learning methods in literature. However, within the scope of this paper, we only discuss works in two related topics, namely, contrastive learning and deep clustering.

4.1. Contrastive Learning

Despite many recent successes in learning representations, the idea of contrastive learning appeared long time ago. In 2006, Hadsell et. al. [15] proposed a max-margin contrastive loss and linked it to a mechanical spring system. In fact, from a probabilistic view, contrastive learning arises naturally when working with energy-based models. For example, in many problems, we want to maximize \( \log p(y|x) = \log \frac{e^{f(y,x)}}{\sum_{y' \in \mathcal{Y}} e^{f(y',x)}} \), where \( y \) is the output associated with a context \( x \) and \( \mathcal{Y} \) is the set of all possible outputs or vocab. This is roughly equivalent to maximizing \( f(y,x) \) and minimizing \( f(y',x) \) for all \( y' \neq y \) but in a normalized setting. However, in practice, the size of \( \mathcal{Y} \) is usually very large, making the computation of \( p(y|x) \) expensive. This problem was addressed in [32, 42] by using Noise Contrastive Estimation (NCE) [14] to approximate \( p(y|x) \). The basic idea of NCE is to transform the density estimation problem into a binary classification problem: “Whether samples are drawn from the data distribution or from a known noise distribution?”. Based on NCE, Mikolov et. al. [30] and Oord et. al. [33] derived a simpler contrastive loss which later was referred to as the InfoNCE loss [35] and was adopted by many subsequent works [8, 12, 16, 31, 39, 49] for learning representations.

Recently, there have been several attempts to leverage inter-sample statistics obtained from clustering to improve representation learning on a large scale [1, 4, 54]. PCL [26] alternates between clustering data via K-means and contrasting samples based on their views and their assigned cluster centroids (or prototypes). SwAV [5] does not contrast two sample views directly but uses one view to predict the code of assigning the other view to a set of learnable prototypes. InterCLR [44] and ODC [51] avoid offline clustering on the entire training dataset after each epoch by storing a pseudo-label for every sample in the memory bank (along with the feature vector) and maintaining a set of cluster centroids. These pseudo-labels and cluster centroids are updated on-the-fly at each step via mini-batch K-means.

4.2. Deep Clustering

Traditional clustering algorithms such as K-means or Gaussian Mixture Model (GMM) are mainly designed for low-dimensional vector-like data, hence, do not perform well on high-dimensional structural data like images. Deep clustering methods address this limitation by leveraging the representation power of deep neural networks (e.g., CNNs,
RNNs) to effectively transform data into low-dimensional feature vectors which are then used as inputs for a clustering objective. For example, DCN [46] applies K-means to the latent representations produced by an auto-encoder. The reconstruction loss and the K-means clustering loss are minimized simultaneously. DEC [43], by contrast, uses only an encoder rather than a full autoencoder like DCN to compute latent representations. This encoder and the cluster centroids are learned together via a clustering loss proposed by the authors. JULE [47] uses a RNN to implement agglomerative clustering on top of the representations outputted by a CNN and trains the two networks in an end-to-end manner. VaDE [21] regards clustering as an inference problem and learns the cluster-assignment probabilities of data using a variational framework [22]. Meanwhile, DAC [7] treats clustering as a binary classification problem: “Whether a pair of samples belong to the same cluster or not?” To obtain a pseudo label for a pair, the cosine similarity between the cluster-assignment probabilities of the two samples in that pair is compared with an adaptive threshold. IIC [20] learns cluster assignments via maximizing the mutual information between clusters under two different data augmentations. PICA [19], instead, minimizes the contrastive loss derived from the the mutual information in IIC. While the cluster contrastive loss in PICA is cluster-oriented and can have at most \( C \) negative pairs (\( C \) is the number of clusters). Our probability contrastive loss, by contrast, is sample-oriented and can have as many negative pairs as the number of training data. Thus, in theory, our proposed model can capture more information than PICA. In real implementation, in order to gain more information from data, PICA has to make use of the “over-clustering” trick [20]. It alternates between minimizing \( L_{\text{PICA}} \) for \( C \) clusters and minimizing \( L_{\text{PICA}} \) for \( kC \) clusters (\( k > 1 \) denotes the “over-clustering” coefficient). DRC [53] and CC [27] enhances PICA by combining clustering with contrastive representation learning, which follows the same paradigm as our proposed CRLC. However, like PICA, DRC and CC uses cluster-oriented representations rather than sample-oriented representations.

In addition to end-to-end deep clustering methods, some multi-stage clustering methods have been proposed recently [34, 40]. The most notable one is SCAN [40]. This method uses representations learned via contrastive learning during the first stage to find nearest neighbors for every sample in the training set. In the second stage, neighboring samples are forced to have similar cluster-assignment probabilities. Our probability contrastive loss can easily be extended to handle neighboring samples (see Section 5.1.2).

5. Experiments

Dataset We evaluate our proposed method on 5 standard datasets for image clustering which are CIFAR10/20 [23], STL10 [9], ImageNet10 [11, 7], and ImageNet-Dogs [11, 7], and on 3 big ImageNet subsets namely ImageNet50/100/200 with 50/100/200 classes, respectively [11, 40]. A description of these datasets is given in Appdx. A.6. Our data augmentation setting follows [16, 42]. We first randomly crop images to a desirable size (32×32 for CIFAR, 96×96 for STL10, and 224×224 for ImageNet subsets). Then, we perform random horizontal flip, random color jittering, and random grayscale conversion. For datasets which are ImageNet subsets, we further apply Gaussian blurring at the last step [8]. Similar to previous works [7, 20, 19], both the training and test sets are used for CIFAR10, CIFAR20 and STL10 while only the training set is used for other datasets. We also provide results where only the training set is used for CIFAR10, CIFAR20 and STL10 in Appdx. A.8. For STL10, 100,000 auxiliary unlabeled samples are additionally used to train the “representation learning” head. However, when training the “clustering” head, these auxiliary samples are not used since their classes may not appear in the training set.

Model architecture and training setups Following previous works [19, 20, 40, 53], we adopt ResNet34 and ResNet50 [17] as the backbone network when working on the 5 standard datasets and on the 3 big ImageNet subsets, respectively. The “representation learning” head (RL-head) and the “clustering” head (C-head) are two-layer neural networks with ReLU activations. The length of the output vector of the RL-head is 128. The temperature \( \tau \) (Eq. 5) is fixed at 0.1. To reduce variance in learning, we train our model with 10 C-subheads\(^3\) similar to [20]. This only adds little extra computation to our model. However, unlike [19, 20, 53], we do not use an auxiliary “over-clustering” head to exploit additional information from data since we think our RL-head can do that effectively.

Training setups for end-to-end and two-stage clustering are provided in Appdx. A.7.

Evaluation metrics We use three popular clustering metrics namely Accuracy (ACC), Normalized Mutual Information (NMI), Adjusted Rand Index (ARI) for evaluation. For unlabeled data, ACC is computed via the Kuhn-Munkres algorithm. All of these metrics scale from 0 to 1 and higher values indicate better performance. In this work, we convert the \([0, 1]\) range into percentage.

5.1. Clustering

5.1.1 End-to-end training

Table 1 compares the performance of our proposed CRLC with a wide range of state-of-the-art deep clustering methods. CRLC clearly outperforms all baselines by a large

\(^3\)The final \( L_{\text{cluster}} \) in Eq. 8 is the average of \( L_{\text{cluster}} \) of these C-subheads.
Table 1: End-to-end clustering results on 5 standard image datasets. Due to space limit, we only show the means of the results. For the standard deviations, please refer to Appdx. A.8.

| Dataset | CIFAR10 | CIFAR20 | STL10 | ImageNet10 | ImageNet-Dogs |
|---------|---------|---------|--------|------------|---------------|
| Metric  | ACC NMI ARI | ACC NMI ARI | ACC NMI ARI | ACC NMI ARI | ACC NMI ARI |
| JULE [47] | 27.2 19.2 13.8 | 13.7 10.3 3.3 | 27.7 18.2 16.4 | 30.0 17.5 13.8 | 13.8 5.4 2.8 |
| DEC [43] | 30.1 25.7 16.1 | 18.5 13.6 5.0 | 35.9 27.6 18.6 | 38.1 28.2 20.3 | 19.5 12.2 7.9 |
| DAC [7] | 52.2 39.6 30.6 | 23.8 18.5 8.8 | 47.0 36.6 25.7 | 52.7 39.4 30.2 | 27.5 21.9 11.1 |
| DDC [6] | 52.4 42.4 32.9 | - - - | 48.9 37.1 26.7 | 57.7 43.3 34.5 | - - - |
| DACCM [41] | 62.3 49.6 40.8 | 32.7 28.5 17.3 | 48.2 37.6 26.2 | 70.1 60.8 55.5 | 38.3 32.1 18.2 |
| IIC [20] | 61.7 - - | 25.7 - - | 61.0 - - | - - - | - - - |
| MCR2 [50] | 68.4 63.0 50.8 | 34.7 36.2 16.7 | 49.1 44.6 29.0 | - - - | - - - |
| PICA [19] | 69.6 59.1 51.2 | 33.7 31.0 17.1 | 71.3 61.1 53.1 | 87.0 80.2 76.1 | 35.2 35.2 20.1 |
| DRC [53] | 72.7 62.1 54.7 | 36.7 35.6 20.8 | 74.7 64.4 56.9 | 88.4 | 83.0 | 79.8 |
| C-head only | 66.9 56.9 47.5 | 37.7 35.7 21.6 | 61.2 52.7 43.4 | 80.0 75.2 67.6 | 36.3 37.5 19.8 |
| CRLC | 79.9 67.9 63.4 | 42.5 41.6 26.3 | 81.8 72.9 68.2 | 85.4 | 83.1 | 75.9 |

Table 2: Two-stage clustering results on ImageNet50/100/200.

| ImageNet | 50 classes | 100 classes | 200 classes |
|----------|------------|-------------|-------------|
| Metric   | ACC ACC5 NMI ARI | ACC ACC5 NMI ARI | ACC ACC5 NMI ARI |
| K-means [40] | 65.9 - 77.5 57.9 | 59.7 - 76.1 50.8 | 52.5 - 75.5 43.2 |
| SCAN [40] | 75.1 91.9 80.5 63.5 | 66.2 88.1 78.7 54.4 | 56.3 80.3 75.7 44.1 |
| Two-stage CRLC | 75.4 93.3 80.6 63.4 | 66.7 88.3 79.2 55.0 | 57.9 80.6 76.4 45.9 |

margin on most datasets. For example, in term of clustering accuracy (ACC), our method improves over the best baseline (DRC [53]) by 5-7% on CIFAR10/20, STL10, and ImageNet-Dogs. Gains are even larger if we compare with methods that do not explicitly learn representations such as PICA [19] and IIC [20]. CRLC only performs worse than DRC on ImageNet10, which we attribute to our selection of hyperparameters. In addition, even when only the “clustering” head is used, our method still surpasses most of the baselines (e.g., DCCM, IIC). These results suggest that: i) we can learn semantic clusters from data just by minimizing the probability contrastive loss, and ii) combining with contrastive representation learning improves the quality of the cluster assignment.

To have a better insight into the performance of CRLC, we visualize some success and failure cases in Fig. 2 (and also in Appdx. A.11). We see that samples predicted correctly with high confidence are usually representative for the cluster they belong to. It suggests that CRLC has learned coarse-grained patterns that separate objects at the cluster level. Besides, CRLC has also captured fine-grained instance-level information, thus, is able to find nearest neighbors with great similarities in shape, color and texture to the original image. Another interesting thing from Fig. 2 is that the predicted label of a sample is often strongly correlated with that of the majority of its neighbors. It means that: i) CRLC has learned a smooth mapping from images to cluster assignments, and ii) CRLC tends to make “collective” errors (the first and third rows in Fig. 2c). Other kinds of errors may come from the closeness between classes (e.g., horse vs. dog), or from some adversarial signals in the input (e.g., the second row in Fig. 2b). Solutions for fixing these errors are out of scope of this paper and will be left for future work.

5.1.2 Two-stage training

Although CRLC is originally proposed as an end-to-end clustering algorithm, it can be easily extended to a two-stage clustering algorithm similar to SCAN [40]. To do that, we first pretrain the RL-head and the backbone network with $L_{FC}$ (Eq. 6). Next, for every sample in the training data, we find a set of $K$ nearest neighbors based on the cosine similarity between feature vectors produced by the pretrained network. In the second stage, we train the C-head by minimizing $L_{cluster}$ (Eq. 8) with the positive pair consisting of a sample and its neighbor drawn from a set of $K$ nearest neighbors. We call this variant of CRLC “two-stage” CRLC. In fact, we did try training both the C-head and the RL-head in the second stage by minimizing $L_{CRLC}$ but could not achieve good results compared to training only the C-head. We hypothesize that finetuning the RL-head causes the model to capture too much fine-grained informa-
Table 3: Classification errors on CIFAR10. Lower values are better. Results of baselines are taken from [36]. Results obtained from external implementations of models.

| Dataset          | CIFAR10          |
|------------------|------------------|
|                  |                  |
| **MixMatch [3]** | -                |
| **UDA [45]**     | -                |
| **ReMixMatch**   | -                |
| **ReMixMatch†**  | 59.86±9.34       |
|                  | 41.68±8.15       |
|                  | 28.31±6.72       |
| **CRLC-semi**    | 46.75±8.01       |
|                  | 29.81±1.18       |
|                  | 19.87±0.82       |

5.2. Semi-supervised Learning

Given the good performance of CRLC on clustering, it is natural to ask whether this model also performs well on semi-supervised learning (SSL) or not. To adapt for this new task, we simply train CRLC with the new objective $L_{CRLC-semi}$ (Eq. 12). The model architecture and training setups remain almost the same (changes in Appdx. A.13).

From Table 3, we see that CRLC-semi, though is not designed especially for SSL, significantly outperforms many state-of-the-art SSL methods (brief discussion in Appdx. A.12). For example, CRLC-semi achieves about 30% and 10% lower error than MixMatch [3] and UDA [45] respectively on CIFAR10 with 4 labeled samples per class. Interestingly, the power of CRLC-semi becomes obvious when the number of labeled data is pushed to the limit. While most baselines cannot work with 1 or 2 labeled samples per class, CRLC-semi still performs consistently well with very low standard deviations. We hypothesize the reason is that CRLC-semi, via minimizing $L_{FC}$, models the “smoothness” of data better than the SSL baselines. For more results on SSL, please check Appdx. A.14.

5.3. Ablation Study

Comparison of different critics in the probability contrastive loss

In Fig. 3 left, we show the performance of CRLC on CIFAR10 and CIFAR20 w.r.t. different critic functions. Apparently, the theoretically sound “log-of-dot-product” critic (Eq. 9) gives the best results. The “negative-L2-distance” critic is slightly worse than the “log-of-dot-
product” critic while the “dot-product” and the “negative-JS-divergence” critics are the worst.

**Contribution of the feature contrastive loss** We investigate by how much our model’s performance will be affected if we change the coefficient of \( \mathcal{L}_{FC} (\lambda_2 \text{ in Eq. 11}) \) to different values. Results on CIFAR20 are shown in Fig. 3 middle, right. Interestingly, minimizing both \( \mathcal{L}_{PC} \) and \( \mathcal{L}_{FC} \) simultaneously results in lower values of \( \mathcal{L}_{PC} \) than minimizing only \( \mathcal{L}_{PC} (\lambda_2 = 0) \). It implies that \( \mathcal{L}_{FC} \) provides the model with more information to form better clusters. In order to achieve good clustering results, \( \lambda_2 \) should be large enough relative to the coefficient of \( \mathcal{L}_{PC} \) which is 1. However, too large \( \lambda_2 \) results in a high value of \( \mathcal{L}_{PC} \), which may hurts the model’s performance. For most datasets including CIFAR20, the optimal value of \( \lambda_2 \) is 10.

**Nonparametric implementation of CRLC** Besides using SimCLR [8], we can also implement the two contrastive losses in CRLC using MemoryBank [42] (Section 3.1). This reduces the memory storage by about 30% and the training time by half (on CIFAR10 with ResNet34 as the backbone and the minibatch size of 512). However, MemoryBank-based CRLC usually takes longer time to converge and is poorer than the SimCRL-based counterpart as shown in Fig. 4 left. The contributions of the number of negative samples and the momentum coefficient to the performance of MemoryBank-based CRLC are analyzed in Appdx. A.10.2.

**Mainfold visualization** We visualize the manifold of the continuous features learned by CRLC in Fig. 4 middle. We observe that CRLC usually groups features into well-separate clusters. This is because the information captured by the C-head has affected the RL-head. However, if the RL-head is learned independently (e.g., in SimCLR), the clusters also emerge but are usually close together (Fig. 4 right). Through both cases, we see the importance of contrastive representation learning for clustering.

6. **Conclusion**

We proposed a novel clustering method named CRLC that exploits both the fine-grained instance-level information and the coarse-grained cluster-level information from data via a unified sample-oriented contrastive learning framework. CRLC showed promising results not only in clustering but also in semi-supervised learning. In the future, we plan to enhance CRLC so that it can handle neighboring samples in a principled way rather than just views. We also want to extend CRLC to other domains (e.g., videos, graphs) and problems (e.g., object detection).
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A. Appendix

A.1. Possible critics for the probability contrastive loss

We list here several possible critics that could be used in $L_{PC}$. If we simply consider a critic $f$ as a similarity measure of two probabilities $p$ and $q$, $f$ could be the negative Jensen Shannon (JS) divergence\(^5\) between $p$ and $q$:

$$ f(p, q) = -D_{JS}(p||q) = - \frac{1}{2} \left( D_{KL} \left( p \left\| \frac{p+q}{2} \right\| \right) + D_{KL} \left( q \left\| \frac{p+q}{2} \right\| \right) \right) $$

(13)

or the negative L2 distance between $p$ and $q$:

$$ f(p, q) = - \|p - q\|_2^2 = - \sum_{c=1}^{C} (p_c - q_c)^2 $$

(14)

In both cases, $f$ achieves its maximum value when $p = q$ and its minimum value when $p$ and $q$ are different one-hot vectors.

We can also define $f$ as the dot product of $p$ and $q$ as follows:

$$ f(p, q) = p^\top q = \sum_{c=1}^{C} p_c q_c $$

(15)

However, the maximum value of this critic is no longer obtained when $p = q$ but when $p$ and $q$ are the same one-hot vector (check Appdx. A.2 for details). It means that maximizing this critic encourages not only the consistency between $p$ and $q$ but also the confidence of $p$ and $q$.

A.2. Global maxima and minima of the dot product critic for probabilities

**Proposition 1.** The dot product critic $f(p, q) = \sum_{c=1}^{C} p_c q_c$ achieves its global maximum value at 1 when $p_c$ and $q_c$ are the same one-hot vector, and its global minimum value at 0 when $p_c$ and $q_c$ are different one-hot vectors.

**Proof.** Since $0 \leq p_c, q_c \leq 1$, we have $\sum_{c=1}^{C} p_c q_c \geq 0$. This minimum value is achieved when $p_c q_c = 0$ for all $c \in \{1, ..., C\}$. And because $\sum_{c=1}^{C} p_c = \sum_{c=1}^{C} q_c = 1$, $p_c$ and $q_c$ must be different one-hot vectors.

In addition, we also have $\sum_{c=1}^{C} p_c q_c \leq \sum_{c=1}^{C} p_c = 1$. This maximum value is achieved when $p_c q_c = p_c$ or $p_c (q_c - 1) = 0$ for all $c \in \{1, ..., C\}$, which means $p_c$ and $q_c$ must be the same one-hot vectors. \qed

Since the gradient of $\sum_{c=1}^{C} p_c q_c$ w.r.t. $q_c$ is proportional to $p_c$, if we fix $p$ and only optimize $q$, maximizing $\sum_{c=1}^{C} p_c q_c$ via gradient ascent will encourage $q$ to be one-hot at the component $k$ at which $p_k$ is the largest. Similarly, minimizing $\sum_{c=1}^{C} p_c q_c$ via gradient descent will encourage $q$ to be one-hot at the component $k$ at which $p_k$ is the smallest.

In case $p_1 = ... = p_C = \frac{1}{C}$, all the components of $q$ have similar gradients. Although it does not change the relative order between the components of $q$ after update, it still push $q$ towards the saddle point $(\frac{1}{C}, ..., \frac{1}{C})$. However, chance that models get stuck at this saddle point is tiny unless we explicitly force it to happen (e.g., maximizing $H(q)$).

For better understanding of the optimization dynamics, we visualize the surface of $\sum_{c=1}^{C} p_c q_c$ with $C = 2$ in Fig. 5a. $\log \left( \sum_{c=1}^{C} p_c q_c \right)$ has the same global optimal values and surface as $\sum_{c=1}^{C} p_c q_c$.

A.3. Derivation of the InfoNCE lower bound

The variational lower bound of $I(X;Y)$ can be computed as follows:

$$ I(X;Y) = \mathbb{E}_{p(x,y)} \left[ \log \frac{p(x,y)}{p(x)p(y)} \right] = \mathbb{E}_{p(x,y)} \left[ \log \frac{q_0(x,y)}{p(x)p(y)} + D_{KL}(p(x,y)\|q_0(x,y)) \right] \geq \mathbb{E}_{p(x,y)} \left[ \log \frac{q_0(x,y)}{p(x)p(y)} \right] $$

(17)

where $q_0(x,y)$ is the variational approximation of $p(x,y)$. Following [35], we assume that $q_0(x,y)$ belongs to the energy-based variational family that uses a critic $f_\theta(x,y)$ and is scaled by the data density $p(x)p(y)$:

$$ q_0(x,y) = \frac{p(x)p(y)e^{f_\theta(x,y)}}{\sum_{x,y} p(x)p(y)e^{f_\theta(x,y)}} = \frac{p(x)p(y)e^{f_\theta(x,y)}}{Z_\theta} $$

(18)

where $Z_\theta = \sum_{x,y} p(x)p(y)e^{f_\theta(x,y)}$, $\mathbb{E}_{p(x)p(y)}[e^{f_\theta(x,y)}]$ is the partition function which does not depend on $x, y$.

Since the optimal value of $q_0(x,y)$ is $q^*_\theta(x,y) = p(x,y)$, we have:

$$ \frac{p(x)p(y)e^{f_\theta(x,y)}}{Z_\theta} = p(x,y) \Leftrightarrow f_\theta^*(x,y) = \log Z_\theta + \log \frac{p(x,y)}{p(x)p(y)}, $$

(19)

which means the optimal value of $f_\theta(x,y)$ is proportional to $\log \frac{p(x,y)}{p(x)p(y)}$.

Next, we will show that $f_\theta$ is the critic in the InfoNCE lower bound. We start by rewriting the lower bound in Eq. 17 using the formula of $q_0(x)$ in Eq. 18 as follows:

$$ I(X;Y) \geq \mathbb{E}_{p(x,y)} \left[ \log \frac{e^{f_\theta(x,y)}}{Z_\theta} \right] = \mathbb{E}_{p(x,y)} \left[ f_\theta(x,y) \right] - \log Z_\theta $$

(20)
Here, we encounter the intractable \( \log Z_\theta \). To form a tractable lower bound of \( I(X; Y) \), we continue replacing \( \log Z_\theta \) with its variational upper bound:

\[
\log Z_\theta \leq \frac{Z_\theta}{a_\theta} + \log a_\theta - 1 \quad (21)
\]

where \( a_\theta \) is the variational approximation of \( Z_\theta \). We should choose \( a_\theta \) close to \( Z_\theta \) so that the variance of the bound in Eq. 21 is small. Recalling that \( Z_\theta = \mathbb{E}_{p(x)p(y)} \left[ e^{f_\theta(x,y)} \right] \), we define \( a_\theta \) as follows:

\[
a_\theta = \frac{1}{M} \sum_{i=1}^{M} e^{f_\theta(x_i,y)} \quad (22)
\]

where \( x_1, \ldots, x_M \) are \( M \) samples from \( p(x) \). \( a_\theta \) in Eq. 22 can be seen as a stochastic estimation of \( Z_\theta \) with \( x \) sampled \( M \) times more than \( y \). Thus, \( \frac{Z_\theta}{a_\theta} \approx 1 \) and from Eq. 21, we have \( \log Z_\theta \leq \log a_\theta \). Apply this result to Eq. 20, we have:

\[
I(X; Y) \geq \mathbb{E}_{p(x,y)} \left[ f_\theta(x,y) \right] - \log a_\theta \quad (23)
\]

\[
= \mathbb{E}_{p(x_2,M)} \mathbb{E}_{p(y|x_1)} \left[ f_\theta(x_1,y) - \log \frac{1}{M} \sum_{i=1}^{M} e^{f_\theta(x_i,y)} \right] \quad (24)
\]

\[
= \mathbb{E}_{p(x_1,M)} p(y|x_1) \left[ \log \sum_{i=1}^{M} e^{f_\theta(x_i,y)} \right] + \log M \quad (25)
\]

\[
\triangleq I_{\text{InfoNCE}}(X; Y) \quad (26)
\]

where Eq. 24 is obtained from Eq. 23 by using the fact that \( \mathbb{E}_{p(x,y)} \left[ f_\theta(x,y) \right] = \mathbb{E}_{p(x_2,M)} \mathbb{E}_{p(y|x_1)} \left[ f_\theta(x_1,y) \right] \) and the assumption that the samples \( x_1, \ldots, x_M \) and \( y \) in \( a_\theta \) (Eq. 22) are drawn from \( p(x_2,M) \).

Combining with the result in Eq. 19, we have the optimal critic \( f_\theta^*(x,y) \) in the InfoNCE lower bound is proportional to \( \log p(x,y) - \log p(y|x) \). Since \( p(y) \) does not depend on \( x \) and will be cancelled by both the nominator and denominator in Eq. 25, \( f_\theta^*(x,y) \) is, in fact, proportional to \( \log p(y|x) \).

### A.4. Derivation of the scaled dot product critic in representation learning

Recalling that in contrastive representation learning, the critic \( f \) is defined as the scaled dot product between two unit-normed feature vectors \( \tilde{x}, z_1 \):

\[
f(\tilde{x}, x_i) = \tilde{x}^T z_i / \tau
\]

Interestingly, this formula of \( f \) is accordant with the formula of \( f^* \) and is proportional to \( \log p(\tilde{x}|x_i) \). To see why, let’s assume that the distribution of \( \tilde{x} \) given \( z_1 \) is modeled by an isotropic Gaussian distribution with \( z_1 \) as the mean vector and \( \tau I \) as the covariance matrix. Then, we have:

\[
f^* \propto \log p(\tilde{x}|x_i)
\]

\[
\approx \log p(\tilde{x}|z_1)
\]

\[
\approx \log \frac{e^{-\frac{1}{2 \tau^2} \| \tilde{x} - z_1 \|^2}}{\sqrt{2\pi \tau}}
\]

\[
= -\frac{1}{\tau} \left( \| \tilde{x} \|^2_2 - 2 \tilde{x}^T z_1 + \| z_1 \|^2_2 \right)
\]

\[
= \tilde{x}^T z_1 / \tau - 1 / \tau
\]

\[
\approx \tilde{x}^T z_1 / \tau
\]

where \( \| \tilde{x} \|^2_2 = \| z_1 \|^2_2 = 1 \) due to the fact that \( \tilde{x} \) and \( z_1 \) are unit-normed vectors.

### A.5. Analysis of the gradient of \( \mathcal{L}_{PC} \)

Recalling that the probability contrastive loss \( \mathcal{L}_{PC} \) for a sample \( \tilde{x} \) with the “log-of-dot-product” critic \( f(p,q) = \log (p^T q) \) is computed as follows:

\[
\mathcal{L}_{PC} = -\log \frac{e^{f(\tilde{x},q_1)}}{\sum_{i=1}^{M} e^{f(\tilde{x},q_i)}}
\]

\[
= -\log (\tilde{q}^T q_1) + \log \sum_{i=1}^{M} q_i^T q_i
\]

Because \( \tilde{q} \) is always parametric while \( q_i (i \in \{1, \ldots, M\}) \) can be either parametric (if \( \mathcal{L}_{PC} \) is implemented via the SimCLR framework [8]) or non-parametric (if \( \mathcal{L}_{PC} \) is implemented via the MemoryBank framework [42]), we focus
on the gradient of $L_{PC}$ back-propagating through $\hat{q}$. In practice, $\hat{q}$ is usually implemented by applying softmax to the logit vector $\hat{u} \in \mathbb{R}^{C}$:

$$
\hat{q}_c = \frac{\exp(\hat{u}_c)}{\sum_{k=1}^{C} \exp(\hat{u}_k)}
$$

where $\hat{q}_c$ denotes the $c$-th component of $\hat{q}$. Similarly, $q_{i,c}$ is the $c$-th component of $q$. Thus, the gradient of $L_{PC}$ w.r.t. $\hat{u}_c$ is given by:

$$
\frac{\partial L_{PC}}{\partial \hat{u}_c} = -\frac{\partial}{\partial \hat{u}_c} \log(\hat{q}^\top q_1) + \frac{\partial}{\partial \hat{u}_c} \log \sum_{i=1}^{M} \hat{q}_i^\top q_i
$$

(27)

The first term in Eq. 27 is equivalent to:

$$
-\frac{\partial}{\partial \hat{u}_c} \log(\hat{q}^\top q_1)
\Leftrightarrow \frac{-1}{\hat{q}^\top q_1} \left( \frac{\partial}{\partial \hat{u}_c} (\hat{q}_c q_1, c) + \sum_{k \neq c} \frac{\partial}{\partial \hat{u}_c} (\hat{q}_k q_{1,k}) \right)
\Leftrightarrow \frac{-1}{\hat{q}^\top q_1} \left( \hat{q}_c (1 - \hat{q}_c) q_{1,c} - \sum_{k \neq c} \hat{q}_k q_{1,k} \right)
\Leftrightarrow \frac{-1}{\hat{q}^\top q_1} \left( \hat{q}_c q_{1,c} - \hat{q}_c \sum_{k=1}^{C} \hat{q}_k q_{1,k} \right)
\Leftrightarrow \hat{q}_c - \sum_{k=1}^{C} \frac{\hat{q}_c q_{1,c}}{\hat{q}_k q_{1,k}}
$$

(28)

And the second term in Eq. 27 is equivalent to:

$$
\frac{\partial}{\partial \hat{u}_c} \log \sum_{i=1}^{M} \hat{q}_i^\top q_i
\Leftrightarrow \frac{1}{\sum_{i=1}^{M} \hat{q}_i^\top q_i} \left( \sum_{i=1}^{M} \frac{\partial}{\partial \hat{u}_c} (\hat{q}_i^\top q_i) \right)
\Leftrightarrow \frac{1}{\sum_{i=1}^{M} \hat{q}_i^\top q_i} \left( \sum_{i=1}^{M} \left( \hat{q}_c q_{i,c} - \hat{q}_c \sum_{k=1}^{C} \hat{q}_k q_{i,k} \right) \right)
\Leftrightarrow \frac{1}{\sum_{i=1}^{M} \sum_{k=1}^{C} \hat{q}_k q_{i,k}} \left( \sum_{i=1}^{M} \sum_{k=1}^{C} \frac{\hat{q}_c q_{i,c}}{\hat{q}_k q_{i,k}} - \hat{q}_c \sum_{k=1}^{C} \hat{q}_k q_{1,k} \right)
\Leftrightarrow \frac{\sum_{i=1}^{M} \sum_{k=1}^{C} \hat{q}_c q_{i,c}}{\sum_{i=1}^{M} \sum_{k=1}^{C} \hat{q}_k q_{1,k}} - \hat{q}_c.
$$

Thus, we have:

$$
\frac{\partial L_{PC}}{\partial \hat{u}_c} = \frac{\sum_{i=1}^{M} \hat{q}_c q_{i,c}}{\sum_{i=1}^{M} \sum_{k=1}^{C} \hat{q}_k q_{i,k}} - \hat{q}_c q_{1,c}
$$

(29)

We care about the second term in Eq. 29 which is derived from the gradient of the critic $f(\hat{q}, q_1)$ w.r.t. $\hat{u}_c$ (the negative of the term in Eq. 28). We rewrite this gradient with simplified notations as follows:

$$
\frac{\partial f(q_p, p)}{\partial u_c} = \frac{q_c p_c}{\sum_{k=1}^{C} \hat{q}_k p_k} - q_c
$$

where $u_c$ is the $c$-th logit of $q$. Since during training, $q$ is encouraged to be one-hot (see Appdx. A.2), the denominator may not be defined if we do not prevent $p$ from being a different one-hot vector. However, even when the denominator is defined, the update still does not happen as expected when $q$ is one-hot. To see why, let’s consider a simple scenario in which $q = [0, 1, 0]$ and $p = [0.998, 0.001, 0.001]$. Apparently, the denominator is $0.001 \neq 0$. By maximizing $f(q, p)$, we want to push $q$ toward $p$. Thus, we expect that $\frac{\partial f}{\partial u_1} > 0$ and $\frac{\partial f}{\partial u_2} < 0$. However, the gradients w.r.t. $u_c$ are $0$s for all $c \in \{1, 2, 3\}$:

$$
\frac{\partial f}{\partial u_1} = 0 \times 0.998 = 0
\frac{\partial f}{\partial u_2} = 1 \times 0.001 = 0
\frac{\partial f}{\partial u_3} = 0 \times 0.001 = 0
$$

The reason is that $q = [0, 1, 0]$ is a stationary point (minimum in this case). This means once the model has set $q$ to be one-hot, it tends to get stuck there and cannot escape regardless of the value of $p$. This problem is known in literature as the “saturating gradient” problem. To alleviate this problem, we propose to smooth out the values of $q$ and $p$ before computing the critic $f$:

$$
q = (1 - \gamma) q + \gamma r
$$

$$
p = (1 - \gamma) p + \gamma r
$$

where $0 \leq \gamma \leq 1$ is the smoothing coefficient, which is set to $0.01$ if not otherwise specified; $r = \left(\frac{1}{C}, \ldots, \frac{1}{C}\right)$ is the uniform probability vector over classes. We also regularize the value of $u_c$ to be within $[-25, 25]$.

| Dataset        | #Train | #Test | #Extra | #Classes | Image size |
|----------------|--------|-------|--------|----------|------------|
| CIFAR10        | 50,000 | 10,000| x      | 10       | 32 x 32 x 3|
| CIFAR20        | 50,000 | 10,000| x      | 20       | 32 x 32 x 3|
| STL10          | 5,000  | 8,000 | 100,000| 10       | 96 x 96 x 3|
| ImageNet10     | 13,000 | 500   | x      | 10       | 224 x 224 x 3|
| ImageNet-Dogs  | 19,500 | 750   | x      | 15       | 224 x 224 x 3|
| ImageNet-50    | 64,274 | 2,500 | x      | 50       | 224 x 224 x 3|
| ImageNet-100   | 128,545| 5,000 | x      | 100      | 224 x 224 x 3|
| ImageNet-200   | 256,558| 10,000| x      | 200      | 224 x 224 x 3|

Table 4: Details of the datasets used in this work.
Table 5: Clustering results of our proposed methods on CIFAR10, CIFAR20 and STL10 with only the training set used and with both the training and test sets used.

| Dataset | CIFAR10 | CIFAR20 | STL10 |
|---------|---------|---------|-------|
| Metric  | ACC     | NMI     | ARI   | ACC     | NMI     | ARI   | ACC     | NMI     | ARI   |
| C-head only | 67.2±0.7 | 56.8±1.3 | 47.8±1.0 | 36.0±1.6 | 23.0±0.9 | 21.0±0.3 | 47.0±2.2 | 39.0±1.5 | 27.0±1.8 |
| Train + Test | 66.9±0.8 | 56.9±0.7 | 47.5±0.5 | 37.7±0.4 | 35.7±0.5 | 21.6±0.3 | 61.2±1.2 | 52.7±0.8 | 43.4±1.3 |
| CRLC | 79.4±0.3 | 66.7±0.6 | 62.3±0.4 | 43.4±0.8 | 43.1±0.5 | 27.7±0.3 | 57.6±1.6 | 50.8±1.5 | 41.9±1.2 |
| Train + Test | 79.9±0.6 | 67.9±0.6 | 63.4±0.4 | 42.5±0.7 | 41.6±0.8 | 26.3±0.5 | 81.8±0.3 | 72.9±0.4 | 68.2±0.3 |

Table 6: Clustering results of our proposed methods on ImageNet10 and ImageNet-Dogs.

| Dataset | ImageNet10 | ImageNet-Dogs |
|---------|------------|---------------|
| Metric  | ACC     | NMI    | ARI  | ACC    | NMI   | ARI   |
| C-head only | 80.0±1.4 | 75.2±1.9 | 67.6±2.2 | 36.3±0.9 | 37.5±0.7 | 19.8±0.4 |
| CRLC | 85.4±0.3 | 83.1±0.5 | 75.9±0.4 | 46.1±0.6 | 48.4±0.6 | 29.7±0.4 |

Figure 6: NMI curve of CRLC on ImageNet-Dogs w.r.t. different coefficients of $L_{FC}$.

A.6. Dataset description

In Table 4, we provide details of the datasets used in this work. CIFAR20 is CIFAR10 with 100 classes replaced by 20 super-classes. STL10 is different from other datasets in the sense that it has an auxiliary set of 100,000 unlabeled samples of unknown classes. Similar to previous works, we use samples from this auxiliary set and the training set to train the “representation learning” head.

A.7. Training setups for clustering

End-to-end clustering For end-to-end clustering, we use a SGD optimizer with a constant learning rate = 0.1, momentum = 0.9, Nesterov = False, and weight decay = 5e-4 based on the settings in [13, 16, 39]. We set the batch size to 512 and the number of epochs to 2000. In fact, on some datasets like ImageNet10 or ImageNet-Dogs, CRLC only needs 500 epochs to converge. The coefficients of the negative entropy and $L_{FC}$ ($\lambda_1$ and $\lambda_2$ in Eq. 11 in the main text) are fixed at 1 and 10, respectively. Each experiment is repeated 3 times with random initializations.

Two-stage clustering For two-stage clustering, we use the same settings as in [40]. Specifically, the backbone network is ResNet18 for CIFAR10/20, STL10 and is ResNet50 for ImageNet50/100/200. In the first (pretraining) stage, for CIFAR10/20 and STL10, we pretrain the backbone network and the RL-head via SimCLR [8] for 500 epochs. The optimizer is SGD with an initial learning rate = 0.4 decayed with a cosine decay schedule [28], momentum = 0.9, Nesterov = False, and weight decay = 1e-4. Meanwhile, for ImageNet50/100/200, we directly copy the pretrained weights of MoCo [16] to the backbone network and the RL-head. After the pretraining stage, we find for each sample in the training set 50 nearest neighbors based on the cosine similarity measure. Positive samples for contrastive learning in the second stage are drawn uniformly from these sets of nearest neighbors. In the second stage, for CIFAR10/20 and STL10, we train both the backbone network and the C-head for 200 epochs by minimizing $L_{cluster}$ (Eq. 8 in the main text) using an Adam optimizer with a constant learning rate = 1e-4 and weight decay = 1e-4. For ImageNet50/100/200, we freeze the backbone network and only train the C-head for 200 epochs by minimizing $L_{cluster}$ using an SGD optimizer with a constant learning rate = 5.0, momentum = 0.9, Nesterov = False, and weight decay = 0.0.

A.8. Complete end-to-end clustering results

Complete results with standard deviations on the five standard clustering datasets are shown in Tables 5 and 6. From Table 5, we see that for CIFAR10 using both the training and test sets does not cause much difference in performance compared to using only the training set. For CIFAR20, using only the training set even leads to slightly better results. By contrast, for STL10, models trained with both the training and test sets significantly outperform those trained with the training set only. We believe the reason
Table 7: Two-stage clustering results on CIFAR10/20 and STL10.

| Dataset   | CIFAR10 | CIFAR20 | STL10 |
|-----------|---------|---------|-------|
| Metric    | ACC     | NMI     | ARI   | ACC     | NMI     | ARI   | ACC     | NMI     | ARI   |
| K-means [40] | 65.9±5.7 | 59.8±2.0 | 50.9±3.7 | 39.5±1.9  | 40.2±1.1  | 23.9±1.1  | 65.8±5.1  | 60.4±2.5  | 50.6±4.1  |
| SCAN [40]   | 81.8±0.3  | 71.2±0.4  | 66.5±0.4  | 42.2±3.0  | 44.1±1.0  | 26.7±1.3  | 75.5±2.0  | 65.4±1.2  | 59.0±1.6  |
| two-stage CRLC | 84.2±0.1  | 74.7±0.3  | 70.6±0.5  | 45.0±0.7  | 44.8±0.8  | 28.7±0.9  | 78.7±1.1  | 68.4±1.6  | 62.7±1.8  |

Figure 7: Learning curves of MemoryBank-based CRLC on CIFAR20 w.r.t. different numbers of negative samples. The momentum is \( \alpha = 0.5 \). The InfoNCE w.r.t. a contrastive loss is computed by using Eq. 2 in the main text.

A.9. Additional two-stage clustering results

Table 7 compares the clustering results of “two-stage” CRLC and SCAN on CIFAR10/20, STL10. “Two-stage” CRLC clearly outperforms SCAN on all datasets.

A.10. Additional ablation study results

A.10.1 Contribution of the feature contrastive loss

In Fig. 6, we show the performance of CRLC on ImageNet-Dogs w.r.t. different coefficients of \( \mathcal{L}_FC \) (\( \lambda_2 \) in Eq. 11 in the main text). We observe that CRLC achieves the best clustering accuracy when \( \lambda_2 = 3 \). However, in Table 1 in the main text, we still report the result when \( \lambda_2 = 10 \).

A.10.2 Nonparametric implementation of CRLC

In this section, we empirically investigate the contributions of the number of negative samples and the momentum coefficient (\( \alpha \) in Eq. 10 in the main text) to the performance of MemoryBank-based CRLC.

Contribution of the number of negative samples From Fig. 7a, we do not see any correlation between the number of negative samples and the clustering performance of MemoryBank-based CRLC despite the fact that increasing the number of negative samples allows the RL-head and the C-head to gain more information from data (Figs. 7b and 7c). It suggests that for clustering (and possibly other classification tasks), getting more information may not lead to good results. Instead, we need to extract the right information related to clusters.

Contribution of the momentum coefficient From Fig. 8b, we see that changing the momentum value for updating probability vectors stored in the memory bank does not affects amount of information captured by the RL-head much. By contrast, in Fig. 8c, we see that larger values of the momentum cause the C-head to capture more information. This is reasonable because the accumulated probability vector \( \hat{q}_{n,t} \) is usually more stochastic (contains more information) than the probability vector \( q_{n,t} \) of a particular view (Eq. 10 in the main text). Larger values of the momentum also cause the model to converge slower but do not affect the performance much (Fig. 8a).

A.11. Qualitative evaluation

In Fig. 9, we show the top correctly predicted samples according to their confidence score for each of 5 classes from the training set of STL10. It is clear that these samples are representative of the cluster they belong to.

A.12. Consistency-regularization-based semi-supervised learning methods

When some labeled data are given, the clustering problem naturally becomes semi-supervised learning (SSL).
The core idea behind recent state-of-the-art SSL methods such as UDA [45], MixMatch [3], ReMixMatch [2], FixMatch [36] is consistency regularization (CR) which is about forcing an input sample under different perturbations/augmentations to have similar class predictions. In this sense, CR can be seen as an unnormalized version of the probability contrastive loss without the denominator. Different SSL methods extend CR in different ways. For example, UDA uses strong data augmentation to generate positive pairs. MixMatch and ReMixMatch combines CR with MixUp [52]. However, none of the above methods achieve consistent performance with extremely few labeled data (Section 5.2 in the main text). By contrast, clustering methods like CRLC perform consistently well even when no label is available. Thus, we believe designing a method that enjoys the strength of both fields is possible and CRLC-semi can be one step towards that goal.

A.13. Training setups for semi-supervised learning

To train CRLC-semi, we use a SGD optimizer with an initial learning rate = 0.1, momentum = 0.9, Nesterov = False, and weight decay = 5e-4. Similar to [36], we adjust the learning rate at each epoch using a cosine decay schedule [28] computed as follows:

\[\text{lr}_t = \text{lr}_{\text{init}} + (\text{lr}_{\text{init}} - \text{lr}_{\text{min}}) \times \frac{1 + \cos \left(\frac{t}{T}\right)}{2}\]

where \(\text{lr}_{\text{init}} = 0.1, \text{lr}_{\text{min}} = 0.001, \text{lr}_t\) is the learning rate at epoch \(t\) over \(T\) epochs in total. \(T\) is 2000 and 1000 for CIFAR10 and CIFAR100, respectively. The number of labeled and unlabeled samples in each batch is 64 and 512, respectively. In \(L_{\text{CRLC-semi}}\) (Eq. 12 in the main text), \(\lambda_1 = 1, \lambda_2 = 5, \) and \(\lambda_3 = 1\).

We reimplement FixMatch using sample code from Github\(^6\) with the default settings unchanged. In this code, the number of labeled and unlabeled data in a batch is 64 and 448, respectively. However, the number of steps in one epoch does not depend on the batch size but is fixed at 1024. Thus, FixMatch is trained in 1024 epochs \(\approx\) 1 million steps for both CIFAR10 and CIFAR100. Meanwhile, CRLC-semi is trained in only 194,000 steps for CIFAR10 and 97,000 steps for CIFAR100.

A.14. More results on semi-supervised learning

In Table 8, we show additional semi-supervised learning results of CRLC-semi on CIFAR10 and CIFAR100 in comparison with more baselines. CRLC-semi clearly outperforms all standard baselines like Π-model, Pseudo Labeling or Mean Teacher. However, CRLC-semi looses its advantage over holistic methods like MixMatch [3] and methods that use strong data augmentation like UDA [45] or ReMixMatch [2] when the number of labeled data is big.

---

\(^6\)https://github.com/CoinCheung/fixmatch-pytorch
Table 8: Full classification errors on CIFAR10 and CIFAR100. Lower values are better. Results of baselines are taken from [36]. †: Results obtained from external implementations of models.

| Dataset | CIFAR10 | CIFAR100 |
|---------|---------|----------|
|         | 10 | 20 | 40 | 250 | 100 | 200 | 400 | 2500 |
| II-model [24] | - | - | - | 54.26±3.97 | - | - | - | 57.25±0.48 |
| Pseudo Labeling [25] | - | - | - | 49.78±0.43 | - | - | - | 57.38±0.46 |
| Mean Teacher [38] | - | - | - | 32.32±2.30 | - | - | - | 53.91±0.57 |
| MixMatch [3] | - | - | - | 47.54±11.50 | 11.05±0.86 | - | - | 67.61±1.52 |
| UDA [45] | - | - | - | 29.05±5.93 | 8.82±1.08 | - | - | 59.28±0.88 |
| ReMixMatch [2] | - | - | - | 19.10±9.64 | 5.44±0.05 | - | - | 44.28±2.06 |
| FixMatch (RA) [36] | - | - | - | 13.81±3.37 | 5.07±0.65 | - | - | 48.85±1.75 |
| ReMixMatch† | 59.86±9.34 | 41.68±8.15 | 28.31±6.72 | - | 76.32±4.30 | 66.51±2.86 | 52.23±1.71 | - |
| FixMatch (RA)† | 25.49±7.74 | 21.15±8.96 | 8.87±4.29 | - | 79.27±2.65 | 68.58±0.70 | 57.52±1.50 | - |
| CRLC-semi | 46.75±8.01 | 29.81±1.18 | 19.87±0.82 | 13.53±0.21 | 82.20±1.15 | 73.04±1.15 | 60.87±0.17 | 41.10±0.12 |

Figure 10: Test accuracy and crossentropy curves of CRLC-semi (CRLC) and FixMatch (FM) on CIFAR10 and CIFAR100 with 1, 2, 4 labeled samples per class. It is clear that CRLC-semi performs consistently in all cases except for the case of CIFAR10 with 1 labeled sample per class. However, even in that case, the CRLC-semi still gives consistent performance for each run (Fig. 11). FixMatch, by contrast, is very inconsistent in its performance for each run, especially on CIFAR10.

Figure 11: Test accuracy curves of CRLC-semi (CRLC) and FixMatch (FM) on CIFAR10 with 1 labeled sample per class w.r.t. 3 different runs.

enough. Currently, we are not sure whether the problem comes from the feature contrastive loss $L_{FC}$ (when we have enough labels, representation learning may act as a regularization term and reduce the classification result), or from the negative entropy term in $L_{cluster}$ (causing too much regularization), or even from the probability contrastive loss (contrasting probabilities of two related views is not suit-
about the advantages of our proposed CRLC-semi, we provide detailed comparison between this method and the best SSL baseline - FixMatch [36] in the next section.

**Direct comparison between CRLC-semi and FixMatch**

FixMatch [36] is a powerful SSL method that makes use of pseudo-labeling [25] and strong data augmentation [10] to generate quality pseudo-labels for training. FixMatch has been shown to work reasonably well with only 1 labeled sample per class. In our experiment, we observe that FixMatch outperforms CRLC-semi on both CIFAR10 and CIFAR100. However, FixMatch must be trained in much more steps than CRLC-semi to achieve good results and its performance is very inconsistent (like other SSL baselines) compared to that of CRLC-semi (Figs. 10, 11).

**Details of the labeled samples** For the purpose of comparison and reproducing the results in Table 8, we provide the indices of 40 labeled CIFAR10 samples and 400 labeled CIFAR100 samples used in our experiments in Fig. 13 and Fig. 15, respectively. We also visualize these samples in Fig. 12 and 14. We note that we do not cherry-pick these samples but randomly draw them from the training set.
Figure 14: 400 labeled CIFAR100 samples organized into 4 image blocks where each image block is a set of 100 images corresponding to 100 classes. For 100 and 200 labeled samples, the first block and the first two blocks are considered, respectively.

```
[[11188 12218  6223 32575 15073 31887 46913 24978 26529 14442]
[29329 38925 42143  9627 17117 26223 49586 15463 14283 21116]
[14139  9544 25304 44940 23202 49718  3328  1538 42066 19066]
[35592 39911 26534 47536  5884 28737 31867 10818  2363 24205]]
```

```
[[39404 41352 37487 21791 24545 33045 39512 35960 33548 35465]
[32244 22764 42462 11395 10836 14064 20797 15878 37129 49852]
[11884 21483 27313 15139 31718 15536 38534 37706 10927 24588]]
```

```
[[36391 42934 35048 13579  8292 45480 42748 45984 11381 46018]
[25513 26523 7341 26116 10648 16563 20562 9467 42004 35726]
[46746 21177 42454 15881 26383 24142 43736 8800 34485 33238]
[12220 1216 34677 15429 35645 34202 43344 14024 1178 34224]]
```

```
[[30442 39988 32270  6709 7017 20662 47575 20284 20982 31699]
[29045 14242 36386 18365 35688 19535 39851 35734 15969 35477]
[12653 44887 37250 45939 27313 5377 7564 35108 38461 28811]
[24036 19749 16007 30737 2324 21277 38917 40713 25945 33506]]
```

```
[[45776 48496 34381 44941 8407 47812 11034 43694 47371 21209]
[13998 43513 39228 3563 44723 16640 38753 18465 38529 40484]
[26708 39133 36219 31865 40277 46837 19415 17068 26761 14293]]
```

```
[[30442 39988 32270  6709 7017 20662 47575 20284 20982 31699]
[29045 14242 36386 18365 35688 19535 39851 35734 15969 35477]
[12653 44887 37250 45939 27313 5377 7564 35108 38461 28811]
[24036 19749 16007 30737 2324 21277 38917 40713 25945 33506]
```

Figure 15: Indices in the training set of the images in Fig. 14