Learn by Challenging Yourself: Contrastive Visual Representation Learning with Hard Sample Generation

Yawen Wu  
University of Pittsburgh  
yawen.wu@pitt.edu

Zhepeng Wang  
George Mason University  
zwang48@gmu.edu

Dewen Zeng  
University of Notre Dame  
dzeng2@nd.edu

Yiyu Shi  
University of Notre Dame  
yshi4@nd.edu

Jingtong Hu  
University of Pittsburgh  
jthu@pitt.edu

Abstract

Contrastive learning (CL), a self-supervised learning approach, can effectively learn visual representations from unlabeled data. However, CL requires learning on vast quantities of diverse data to achieve good performance, without which the performance of CL will greatly degrade. To tackle this problem, we propose a framework with two approaches to improve the data efficiency of CL training by generating beneficial samples and joint learning. The first approach generates hard samples for the main model. The generator is jointly learned with the main model to dynamically customize hard samples based on the training state of the main model. With the progressively growing knowledge of the main model, the generated samples also become harder to constantly encourage the main model to learn better representations. Besides, a pair of data generators are proposed to generate similar but distinct samples as positive pairs. In joint learning, the hardness of a positive pair is progressively increased by decreasing their similarity. In this way, the main model learns to cluster hard positives by pulling the representations of similar yet distinct samples together, by which the representations of similar samples are well-clustered and better representations can be learned. Comprehensive experiments show superior accuracy and data efficiency of the proposed methods over the state-of-the-art on multiple datasets. For example, about 5% accuracy improvement on ImageNet-100 and CIFAR-10, and more than 6% accuracy improvement on CIFAR-100 are achieved for linear classification. Besides, up to $2 \times$ data efficiency for linear classification and up to $5 \times$ data efficiency for transfer learning are achieved.

1. Introduction

Contrastive learning (CL), a highly effective self-supervised learning approach [6, 12, 16], has recently shown great promise to learn visual representations from unlabeled data. CL performs a proxy task of instance discrimination to learn data representations without requiring labels, leading to well-clustered and transferable representations for downstream tasks. In the proxy task, the representations of two transformations of one image (a positive pair) are pulled close to each other and pushed away from the representations of other samples (negatives), by which high-quality representations are learned [16].

Most recent CL methods focus on designing variants of the proxy task [4, 8, 11, 32], while the underlying data availability for training CL has received less emphasis. Compared with supervised learning, CL relies more on large amounts of diverse data. This is because CL learns by comparing different samples while supervised learning learns from every single sample and its label. CL models are usually trained on large-scale datasets with millions of samples [4, 6, 12]. For example, the ImageNet dataset [24] widely used in CL has more than a million images with various object categories. Collecting such large-scale datasets require months or even years of considerable human efforts [35]. Besides, for many application domains, collecting a sufficiently large-scale dataset could be prohibitive and even infeasible due to imaging cost, privacy, and copyright constraints. Examples of such domains include medical images, images from scientific experiments, or images from rare natural phenomenons [5].

Training CL with scarce samples leads to drastic degradation in the quality of learned representations because of insufficient contrast between diverse samples. More specifically, CL is trained by performing a proxy task to discriminate two transformations of one image from other images [4]. Without diverse samples to discriminate from, the proxy task becomes relatively easy and the model can achieve high accuracy on this simple task without the need to learn high-quality discriminative representations [16]. The poor quality of learned representations will further degrade the perfor-
mance of downstream tasks. For example, when performing CL on the CIFAR-10 dataset without using labels and then fine-tuning the trained model on 1% labeled data (500 samples), the classification accuracy reaches 84.99%. However, training CL with only 10% of CIFAR-10, and then also fine-tuning with 500 labeled samples, the accuracy dramatically decreases to 68.77%, which is substantially lower than performing CL on the full dataset. Therefore, in the absence of large datasets, it is crucial to achieve data-efficient CL training to make CL applicable to more scenarios.

Towards this goal, we propose a framework to generate effective data for CL training based on given data. The data generation and CL model are jointly optimized by using the given data, and no additional training data is used. The framework consists of two approaches. The first approach generates hard samples for the main contrastive model. The generated samples dynamically adapt to the training state of the main model, rather than fixed throughout the whole training process. With the progressively growing knowledge of the main model, the generated samples also become harder to encourage the main model to learn better representations. The hard samples adversarially explore the weakness of the main model, which forces it to learn discriminative features and improves the generalization performance.

The second approach generates two similar but distinct images as hard positive pairs. Existing CL frameworks form a positive pair by applying two data transformations (e.g. cropping and color distortions) to one image to generate two transformed images. While the two transformed images look different, they still share the same identity since they originate from the same image. Only clustering these positive pairs will limit the quality of learned representation since other similar objects are not considered in clustering. We form hard positive pairs by generating two images of distinct identities but similar objects without using labels, which is achieved by using a generator and its slowly evolving version. In joint learning, the positive pair becomes harder by decreasing their similarity. The main model has to learn to cluster hard positives when minimizing the contrastive loss. By pulling the representations of similar but distinct (hard) objects together, better clustering of the representation space can be learned [17]. With better representations, the performance of downstream tasks will also be improved.

In summary, the main contributions of the paper include:

- **Data-efficient contrastive learning framework.** We propose a framework with two approaches for data-efficient contrastive learning by jointly optimizing contrastive learning and hard samples generation. The first approach generates hard samples and the second approach generates hard positive pairs without using labels.

- **Dynamic hard samples generation.** We propose an approach to generate hard samples by dynamically tracking the training state of the main model. In the joint learning process, hard samples are customized on the fly to the progressive knowledge of the main model, which are fed into the main model to constantly encourage the main model to learn better representations.

- **Hard positive pair generation without using labels.** We propose an approach to further generate hard positive pairs without leveraging labels. The generator and its slowly evolving version generate a pair of similar but distinct objects as a positive pair. The hardness of a positive pair is further increased by decreasing their similarity in joint learning. By learning from hard positive pairs, similar objects are well-clustered for better representations.

### 2. Background and Related Work

#### Revisiting Contrastive Learning

Contrastive learning is a self-supervised approach to learning an encoder for extracting visual representations from unlabeled images by performing a proxy task of instance discrimination [6, 12, 30]. CL pre-trains a model and provides high generalization performance for downstream tasks such as classification and segmentation [7, 29, 33].

Our work in this paper is built upon SimCLR [6], which is a simple yet powerful contrastive learning approach for unsupervised representation learning. For an input image $x$, its representation vector $v$ is obtained by $v = f(x, \theta)$, $z \in \mathbb{R}^d$, where $f(\cdot, \theta)$ is the encoder with parameters $\theta$. In the training process of CL, a raw batch of $N$ samples $\{x_k\}_{k=1...N}$ are first randomly sampled from the dataset. Then for each raw sample $x_k$, two transformations ($t \sim \mathcal{T}$ and $t' \sim \mathcal{T}$) sampled from a family of augmentations $\mathcal{T}$ (e.g. cropping, color distortion, etc.) are applied to $x_k$ to generate two transformed samples (a.k.a. two views). $\tilde{x}_{2k-1} = t(x_k)$ and $\tilde{x}_{2k} = t'(x_k)$ are a positive pair, and all of the generated pairs form the batch for training $\{\tilde{x}_i\}_{i=1...2N}$, consisting of $2N$ samples [17]. In the remainder of this paper, we will refer to the set of $N$ samples as a **raw batch** and the set of $2N$ transformed samples as a **multiviewed batch**.

In the multiviewed batch, let $i \in I = \{1...2N\}$ be the index of a transformed sample, and let $j(i)$ be the index of the transformed sample originating from the same raw sample as $i$. The contrastive loss is as follows.

$$
\mathcal{L}_{CL} = \sum_{i \in I} \mathcal{L}_i = - \sum_{i \in I} \log \frac{\exp \left( \langle v_i, v_{j(i)} \rangle / \tau \right)}{\sum_{a \in A(i)} \exp (\langle v_i, v_a \rangle / \tau)}.
$$  

where $v_i = f(\tilde{x}_i, \theta)$, the operator $\cdot$ is the inner product to compute the cosine similarity of two vectors, $\tau$ is the temperature. The index $i$ is the anchor. $A(i) = I \setminus \{i\}$ is the set of indices excluding $i$. For each anchor $i$, there is one positive and $2N-2$ negatives. The index $j(i)$ is the positive to $i$ (i.e. a positive pair $(i, j(i))$, while other $2N-2$ indices $\{k \in A(i) \setminus \{j(i)\}\}$ are the negatives.
Existing works focus on developing contrastive learning methods while assuming vast quantities of training data are available, without which the performance will drastically degrade. Different from these works, we aim to achieve data-efficient CL on scarce samples by dynamically customizing hard samples based on the training state of the main model.

Adversarial Samples for Improving Accuracy and Robustness of CL. To improve the quality of learned representations, adversarial attacks can be used to create additional training samples by adding pixel-level perturbations to clean samples [14]. While adversarial samples are more challenging and can generate a higher loss than the original samples, the perturbed samples still have the same identities as the original ones, which provide limited additional information for learning. Besides, training with adversarial samples is originally designed for the robustness of models against attacks, instead of improving model performance on clean samples [10, 20, 21]. As a result, only marginal improvement [14] or even degraded performance [15, 18] of the learned CL model is observed. Different from these works, we generate image-level hard samples, instead of adding pixel-level noises to the existing images, which are more informative for improving the learned representations of CL.

GAN for Data Augmentation. [1, 2, 23, 34] employ supervised class-conditional GAN to augment the training data to improve classification performance. However, these works require fully labeled datasets for training GAN. Since labels are not available in CL, the quality of images from GAN will greatly degrade [22, 35] and the performance of trained CL model also degrades. Besides, either GAN and the main model are isolated and the generated data are not adapted to the training state of the main model [1, 2, 34], or both GAN and the classification model aim to minimize the classification loss [23]. Different from these works, our methods do not rely on labels. Besides, the generator and main model are jointly learned, in the way that the generator aims to maximize the CL loss while the CL model aims to minimize the CL loss. Also, we generate hard positive pairs for unsupervised representation learning by CL, which is unexplored in these works on conventional supervised learning.

3. Joint Contrastive Learning with Hard Sample and Hard Positive Pair Generation

We propose a framework to generate individually hard samples and hard positive pairs for contrastive learning, such that better representations can be learned with limited data.

Figure 2. SimCLR’s performance degrades when additional training data is provided by GAN due to the low quality of the synthetic data. With the proposed hard sample generation, we are able to dramatically improve SimCLR’s performance by +2.6% and 3.5% top-1 accuracy on CIFAR-10 and CIFAR-100, respectively.

Challenge: Low quality of generated samples de-
When the dataset is unlabeled and the generator is trained where the generator maximizes the contrastive loss by generating hard samples, while the main model minimizes the contrastive loss by learning representations from both the generated and real samples. The sample generator consists of two components, the generator \( G \) and its slowly-evolving version \( G_{\text{ema}} \). \( G \) and \( G_{\text{ema}} \) are first pre-trained with a discriminator \( D \) on the given unlabeled data by using the GAN objective [3] to generate data following the real data distribution. Then the joint contrastive learning and hard sample generation starts, which has 3 steps. First, \( G \) generates individually hard samples, and \( G \) and \( G_{\text{ema}} \) collaboratively generate pairs of hard positives. The hard samples, hard positives, and real samples from the dataset form a batch and are fed into the main model to compute the contrastive loss. After that, main model \( f \) is updated to minimize the contrastive loss. Finally, \( G \) is updated to maximize the contrastive loss to generate harder samples for the main model based on the current training state of the main model. Momentum update is applied to \( G_{\text{ema}} \) to follow \( G \). Meanwhile, we are using \( D \) to force \( G \) to generate meaningful data following real data distributions. In this way, the generator and the main model are jointly optimized, such that we can generate progressively harder samples and adapt to the training progress of the main model as shown in Figure 1 (Right). The details of each step will be discussed in the following subsections.

### 3.1. Hard Sample Generation and Joint Learning

In this subsection, we first introduce the details of the hard sample generator. The generator \( G \) generates synthetic data to augment the training data and the contrastive loss is:

\[
L_{\text{gen+real}} = \sum_{i \in \{I_{\text{gen}} \cup I_{\text{real}}\}} L_i, \tag{2}
\]

where \( L_i \) is the contrastive loss of multiviewed sample \( i \) defined in Eq.(1). \( I_{\text{gen}} \) is the set of indices of generated and then transformed (multiviewed) samples \( \{x^k_{\text{gen}}\}_{i \in I_{\text{gen}}} \), and \( I_{\text{real}} \) is the set of indices of multiviewed real samples. The generated raw samples \( \{x^k_{\text{gen}}\} = \{G(z_k)\} \) are from the generator \( G \) by taking a set of vectors \( \{z_k\} \sim \mathcal{N}(0, I) \), as input. Two transformations are then applied to each \( x^k_{\text{gen}} \) to get two views \( \tilde{x}^{2k-1}_{\text{gen}} \) and \( \tilde{x}^{2k}_{\text{gen}} \) to form multiviewed samples \( \{\tilde{x}^{2k-1}_{\text{gen}}\}_{i \in I_{\text{gen}}} \).

As shown in Figure 2, simply using a generator to provide additional synthetic data cannot improve contrastive learning. To generate samples that benefit contrastive learning, we form a Min-Max game to jointly optimize the generator and the contrastive model. In this way, the generator dynamically adapts to the training state of the main model and generates hard samples (i.e. high-quality samples from the perspective of training the main model). The dynamically customized hard samples in each training state of the main model will explore its weakness and encourage it to learn better representations to compete with the generator. Formally, the joint learning objective is defined as follows.

\[
\min_{\theta} \max_{w} L_{\text{gen+real}}. \tag{3}
\]

where \( \theta \) and \( w \) are the parameters of the main model and the generator, respectively. To solve the Min-Max game, a pair of gradient descent and ascent are applied to the main model.
and the generator to update their parameters, respectively.

The details of the update are shown as follows.

\[
\frac{\partial L_{gen+real}}{\partial \theta} = \eta \theta \quad \text{and} \quad \frac{\partial L_{gen+real}}{\partial w} = \eta w
\]

where \( \eta \) is the learning rate.

Updating \( w \) requires gradients to be propagated from the
main model through the data transformations of generated samples to \( G \). Therefore, the transformations \( T \) must be differentiable as depicted by \( T(\cdot) \) in Figure 1, which is unexplored in existing CL frameworks [6, 12] since they only need gradient propagation within the main model to the generator for harder samples. In this way, \( G \) can be trained to customize hard samples for the main model in the joint learning process to improve the learning of the main model.

### 3.2. Hard Positive Generation without Using Labels

In addition to generating hard samples, we also propose a new method to generate hard positive pairs. The main idea is that we can use two similar yet different generators \( G \) and \( G_{ema} \) to generate two similar but distinct samples as a positive pair, when taking the same latent vector as input. In joint learning, the hardness of a positive pair is further increased by decreasing their similarity for better CL.

**Positive pair generation.** To generate each positive pair, we use a generator \( G \) and its slowly-evolving version \( G_{ema} \), which are very similar but different. By feeding a latent vector \( z_i \) sampled from a Gaussian distribution to both \( G \) and \( G_{ema} \), a pair of raw samples \( (x_{i1}, x_{i2}) \), which are similar but distinctive, is generated as a positive pair. The process is described as follows.

\[
x_{i1} = G(z_i), \quad x_{i2} = G_{ema}(z_i), \quad z_i \sim p(z).
\]

To make the positives harder by increasing their difference, in joint learning \( G \) is updated with gradients from the main model by Eq.(4) while \( G_{ema} \) is not. On the other hand, to keep the similarity of generated positive pairs, we update \( G_{ema} \) by momentum update following \( G \). Denoting the parameters of \( G \) as \( w \) and the parameters of \( G_{ema} \) as \( w_{ema} \), \( w_{ema} \) is updated by:

\[
w_{ema} \leftarrow mw_{ema} + (1 - m)w.
\]

where \( m \in (0, 1) \) is a momentum parameter.

To generate \( N \) samples with \( \frac{N}{2} \) positive pairs, we sample \( \frac{N}{2} \) latent vectors \( \{z_i\}_{i=1}^{N} \) to generate a batch of \( N \) raw samples \( B_{gen} = \{x_k\}_{k=1}^{N} \) following Eq.(5). To leverage the diversity and hardness of generated samples, and the high quality of real samples, we further sample \( N \) real samples \( B_{real} = \{x_k\}_{k=N+1\ldots2N} \) from the dataset. Then a raw batch is formed as \( B = B_{gen} \cup B_{real} = \{x_k\}_{k=1\ldots2N} \) with \( N \) generated samples and \( N \) real samples. After that, two transformations are applied to each \( x_k \) to form a multiviewed batch \( B_{mv} = \{\tilde{x}_i\}_{i=1\ldots2N} \) for training as shown in Step 1 of Algorithm 1.

**Partially pseudo-labeled contrastive loss (PPCL).** The contrastive loss in Eq.(2) only uses two views of a raw sample as positive pairs. It does not leverage the fact that samples generated by \( G \) and \( G_{ema} \) are actually positive pairs to learn better representations. To better cluster the generated positive pairs, we define a partially pseudo-labeled contrastive loss by using the input latent vectors \( z_i \) as pseudo-labels. Each \( z_i \) \( (i = 1\ldots\frac{N}{2}) \) generates two positives \((x_{i1-1}, x_{i2})\) in the raw batch and four positives \((\tilde{x}_{4i-3}, \tilde{x}_{4i-2}, \tilde{x}_{4i-1}, \tilde{x}_{4i})\) in the multiviewed batch, which are assigned the same pseudo-label for clustering their representations.

Within the multiviewed batch \( B_{mv} \), let \( i \in I_{gen} = \{1\ldots2N\} \) be the indices of generated samples and \( i \in I_{real} = \{2N + 1\ldots4N\} \) be the indices of real samples. The PPCL loss is defined as follows.

\[
L_{ppcl} = \sum_{i \in I} \sum_{p \in P(i)} \log \exp \left( \frac{v_i \cdot v_p}{\tau} \right) \sum_{a \in A(i)} \exp \left( \frac{v_i \cdot v_a}{\tau} \right),
\]

where \( I = I_{gen} \cup I_{real} \), \( A(i) = I \setminus \{i\} \) is the set of indices of \( i \)'s positives and negatives, and \( P(i) \) is the set of indices of \( i \)'s positives in the multiviewed batch. For real samples \( i \in I_{real} \), the positive \( P(i) = j(i) \) is the index of the other view of \( i \) in the multiviewed batch. For generated samples \( i \in I_{gen} \), the positives \( P(i) \) are defined by the pseudo-labels from the input latent vector \( z_i \), which includes the indices of multiviewed samples originating from the same \( z_i \).

### 3.3. Effectiveness of Hard Sample and Hard Positive Pair Generation

By plugging the PPCL loss in Eq.(7) into the Min-Max problem in Eq.(3), in joint learning the main model will minimize the loss to learn effective representations from hard samples. Meanwhile, the generator will maximize the loss, which achieves three goals simultaneously: generating individually hard samples, generating hard positive pairs, and generating hard negatives following real data distribution.

For the multiviewed positives \((\tilde{x}_{4i-3}, \tilde{x}_{4i-2}, \tilde{x}_{4i-1}, \tilde{x}_{4i})\) originating from \( z_i \), taking \( \tilde{x}_{4i-3} \) as an example, its positives are \((\tilde{x}_{4i-2}, \tilde{x}_{4i-1}, \tilde{x}_{4i})\) and its PPCL loss can be rewritten
as:

\[ L_{4i-3} = \frac{-1}{3} \sum_{p \in \{4i-2,4i-1,4i\}} \log \frac{\exp(f(\bar{x}_{4i-3}) \cdot f(\bar{x}_{p})/\tau)}{Q}, \]

\[ Q = \sum_{k \in \{1\ldots2N\}, k \neq 4i-3} \exp(f(\bar{x}_{4i-3}) \cdot f(\bar{x}_k)/\tau). \]

When maximizing Eq. (8) by updating \( G \), the cosine similarity between positive pairs (in the numerator) will be minimized for each of the three positives \( p \), and the cosine similarity between negative pairs (in the denominator \( Q \)) will be maximized. Three goals are achieved in the optimization.

**Generating individually hard samples.** For the first positive pair \((\bar{x}_{4i-3}, \bar{x}_{4i-2})\), both of them originate from raw sample \( x_{2i-1} = G(z_i) \). To minimize \( P_1 = f(\bar{x}_{4i-3}) \cdot f(\bar{x}_{4i-2}) = f(t_{2i-1}(x_{2i-1})) \cdot f(t_{2i-1}(x_{2i-1})) \), where \( t_{2i-1}, t_{2i-1}' \sim \mathcal{T} \) are sampled transformations, \( x_{2i-1} = G(z_i) \) will become individually harder such that the main model \( f(\cdot) \) cannot perfectly generate similar representations for this positive pair originating from \( x_{2i-1} \).

**Generating hard positive pairs.** For the second positive pair \((\bar{x}_{4i-3}, \bar{x}_{4i-1})\) and the third positive pair \((\bar{x}_{4i-3}, \bar{x}_{4i})\), the first multi-viewed sample in each pair \( \bar{x}_{4i-3} \) is from raw sample \( x_{2i-1} = G(z_i) \) by \( G \), and the second multi-viewed sample in each pair \( \bar{x}_{4i-1}, \bar{x}_{4i} \) are from raw sample \( x_{2i} = G_{ema}(z_i) \) by \( G_{ema} \). To minimize \( P_2 = f(\bar{x}_{4i-3}) \cdot f(\bar{x}_{4i-1}) = f(t_{2i-1}(x_{2i-1})) \cdot f(t_{2i}(x_{2i})) \) and \( P_3 = f(\bar{x}_{4i-3}) \cdot f(\bar{x}_{4i}) = f(t_{2i-1}(x_{2i-1})) \cdot f(t_{2i}(x_{2i})) \), both of which take \( x_{2i-1} \) and \( x_{2i} \) as input, the difference between \( x_{2i-1} \) and \( x_{2i} \) will be increased. To achieve this, since no gradients are propagated to \( G_{ema} \), it will be fixed when optimizing Eq. (8) and \( G \) will be pushed apart from \( G_{ema} \). In this way, distinct samples will be generated as positive pairs by \( G \) and \( G_{ema} \). On the other hand, \( G_{ema} \) is slowly updated following \( G \) by Eq. (6), which encourages them to generate similar samples when taking the same latent vector \( z_i \) as input. As a result, by updating \( G \) and \( G_{ema} \) by Eq. (7) and Eq. (6), distinct yet similar samples can be generated as a positive pair as shown in Figure 1 (Right).

**Generating hard negatives while following real distributions.** For the negative pairs, when maximizing Eq. (8), \( Q \) will be maximized. For the first set \( k \in \{1\ldots2N\}, k \neq 4i-3 \), the term \( N_k = f(\bar{x}_{4i-3}) \cdot f(\bar{x}_k) = f(t_{2i-1}(x_{2i-1})) \cdot f(t(x|_{\frac{x}{x}})), t \in \{t_{2i-1}, t'_{2i-1}\} \) is the cosine similarity of two samples generated by \( G \) or \( G_{ema} \). When maximizing \( N_k \) by optimizing \( G \), \( G \) will generate challenging samples that the main model cannot effectively discriminate. As a result, the main model will learn to discriminate these hard negatives.

For the second set \( k \in \{2N + 1\ldots4N\} \), \( N_k \) is the cosine similarity between features of one generated (and transformed) sample \( t_{2i-1}(x_{2i-1}) \) and one transformed real sample \( t(x|_{\frac{x}{x}}), t \in \{t_{2i-1}, t'_{2i-1}\} \). When maximizing \( N_k \), \( G \) will generate samples that have larger similarities to real samples. Therefore, \( G \) will be optimized to generate samples following real data distributions.

### 4. Experimental Results

**Datasets and model architecture.** We evaluate the proposed approaches on five datasets, including ImageNet-100, CIFAR-10 [19], CIFAR-100 [19], Fashion-MNIST [31] and ImageNet-10. ImageNet-100 is widely used in contrastive learning [16,26–28] and is a subset of ImageNet [24]. ImageNet-10 is a smaller subset of ImageNet. We use ResNet-18 as the main model and use a 2-layer MLP to project the output to 128-dimensional representation space [6, 12]. We use the generator and discriminator architectures from [3]. The batch size is 256 and the main model is trained for 100 epochs on ImageNet-100 for efficient evaluation, 300 epochs on CIFAR-10, CIFAR-100 and ImageNet-10, and 200 epochs on Fashion-MNIST. The details of training and model architectures can be found in the Appendix.

**Metrics.** To evaluate the quality of learned representations, we use two metrics linear classification and transfer learning widely used for self-supervised learning [6]. In linear classification, a linear classifier is trained on top of the frozen encoder, and the test accuracy represents the quality of learned representations. We first perform CL by the proposed approaches without labels to learn representations. Then we fix the encoder and train a linear classifier on 100% labeled data on top of the encoder. The classifier is trained for 500 epochs with Adam optimizer and learning rate 3e-4. Transfer learning evaluates the generalization of learned features. The encoder is first learned on the source dataset, then evaluated on the target task. Following [3], we train a linear classifier on top of the frozen encoder on the target task, using the same hyper-parameters as linear classification.

**Method**

| Method     | Same data                                      | Different data formed by each method |
|------------|-----------------------------------------------|-------------------------------------|
| SimCLR     | Real data                                     | Real data 2                         |
| SimCLR-DD  | Real data                                     | Real data                           |
| CLAE       | Data from GAN                                 | Hard data                           |
| BigGAN     | Data from GAN                                 | Data from GAN                       |
| Proposed   | Data from GAN                                 | Hard data                           |

Figure 3. Mini-batch data organization. In each mini-batch, the first half of data is the same for different methods, while the second half are formed by each method and are different across methods.

**Baselines.** We compare the proposed approaches with multiple approaches, which use different strategies to form each mini-batch for contrastive learning. As shown in Figure 3, for each mini-batch, the first half of data are the same in different methods and are sampled directly from the available training set. The second half of the data are different and are
formed by each method as follows. SimCLR is the original contrastive learning approach by using only real data [6] and does not use the second half of data. SimCLR-DD is a variant of SimCLR by sampling additional real data from the dataset as the second half of mini-batch (i.e. Double Data), serving as a strong baseline. By comparing our approaches with SimCLR-DD, we evaluate if the samples generated by our approaches have a higher quality than additional real data from the perspective of CL training. CLAE is the SOTA data generation approach for CL by using pixel-level adversarial perturbations of the real data as the additional data [14]. BigGAN uses a generator from BigGAN [3] to generate synthetic training data for SimCLR [6] without joint learning. By comparing with BigGAN, we evaluate if the hard samples generated by our approaches benefit CL training more than synthetic data generated by a standalone BigGAN.

4.1. Linear Classification

Linear classification on ImageNet-100 with different amount of training data. We evaluate the proposed approaches by linear classification when different amounts of training data are available for contrastive representation learning. Linear classification evaluates the linear separability (clustering) of learned representations [6], and higher accuracy indicates more discriminative and desirable features. As shown in Table 2, with different amounts of training data to perform CL, the proposed approaches consistently outperform the baselines. First, with 100%, 20%, and 10% training data, the proposed methods substantially outperform SimCLR by 3.95%, 5.24%, and 5.81%, respectively. Second, surprisingly, the proposed methods even outperform SimCLR-DD by 0.68%, 1.92%, and 2.66% with different amounts of training data, which shows that the generated hard samples are even better than the additionally sampled real data. Third, the proposed methods outperform the BigGAN based data generation method by 2.70%, 2.84%, 3.87% with different amounts of training data, respectively, showing that the generated hard data benefit contrastive learning much more than the synthetic data from a standalone GAN. These results show the proposed approaches can effectively leverage available data to learn high-quality representations.

Linear classification on various datasets. We further evaluate the proposed methods on more datasets. As shown in Table 1, the proposed approaches consistently outperform the SOTA approaches by a large margin. With 20% training data, 6.11% and 4.92% improvements over SimCLR are observed on CIFAR-100 and CIFAR-10, respectively. Notably, the proposed approaches outperform or perform on par with the best-performing baselines trained with 2× data, achieving 2× data efficiency. For example, with 10% training data on CIFAR-10, the best-performing baseline with 20% training data achieves 81.04% accuracy, while the proposed approaches achieve a similar accuracy of 80.94% by using only 10% training data. Besides, the proposed approaches even largely outperform SimCLR-DD, which samples 2× real data in each training batch. This result shows that the customized hard data by the proposed approaches benefit the CL training more than the real data.

When full training data (i.e. 100%) is available for CL, the proposed approaches still significantly outperform the baselines. As shown in Table 1, substantial improvements of 2.57%, 3.48%, 1.59%, 4.27%, and 4.00% over the original CL framework SimCLR are observed on five datasets, respectively. This result shows that the proposed methods can effectively leverage given data for CL.

4.2. Transfer Learning

Transfer learning by using ImageNet-100 as the source dataset. We evaluate the generalization performance of learned representations by transfer learning to downstream vision tasks. The encoder is trained on the source dataset ImageNet-100 and transferred to target tasks, and we report the linear classification performance on the target task. First, with different amounts of training data to perform CL, the proposed approaches consistently outperform the baselines as shown in Table 3. For example, 2.55%, 5.08%, and 5.50% improvements over SimCLR are observed on the CIFAR-10 target task. Second, the proposed approaches outperform or perform on par with the best-performing baselines trained with 2× data on the source dataset, achieving about 2× data efficiency. For example, with 20% training data on the source dataset ImageNet-100 and transferring to CIFAR-10, the best-performing baseline achieves 77.79% accuracy, while the proposed approaches achieve a higher accuracy of 78.16% by using only 10% training data on the source dataset. Similar results of 2× data efficiency are also observed when transfer learning to CIFAR-100.

Transfer learning on various datasets. We further evaluate the proposed approaches by transfer learning on various source datasets. First, with different amounts of data available for learning the encoder on the source datasets, the proposed approaches consistently outperform the baselines as shown in Table 4. For instance, when transferring from the source dataset CIFAR-10 to the target dataset CIFAR-100, 4.75%, 5.63%, and 5.10% improvements over SimCLR are observed with 100%, 20%, and 10% training data, respectively. Second, notably, with only 20% training data of the source dataset CIFAR-10 and transferring to CIFAR-100, the proposed approaches outperform the best-performing baseline with 100% training data of CIFAR-10 (52.51% vs. 52.47%), which achieves 5× data efficiency. Third, when more training data (100%) is available for the source datasets, our approaches still consistently outperform the baselines on four source datasets with various target tasks.
### Table 1. Linear classification on various datasets with different amounts of training data for CL. Available data are labeled and used for learning the classifier on the fixed encoder learned by CL and top-1 accuracy is reported.

| Method          | CIFAR-10         | CIFAR-100        | FMNIST        | ImageNet-100 |
|-----------------|------------------|------------------|---------------|--------------|
|                 | 100% data | 20% data | 10% data | 100% data | 20% data | 10% data | 100% data | 20% data | 10% data |
| SimCLR [6]      | 90.37    | 80.19    | 76.05    | 63.93   | 44.13   | 37.46   | 92.35   | 87.92   | 87.26   | 83.20  | 62.60  | 49.60  |
| SimCLR-DD [6]   | 91.37    | 81.04    | 76.06    | 64.88   | 44.75   | 37.10   | 92.50   | 89.60   | 87.49   | 82.20  | 65.00  | 53.00  |
| CLAE [14]       | 90.13    | 79.84    | 74.38    | 63.25   | 45.17   | 37.28   | 92.36   | 88.48   | 87.38   | 81.20  | 59.60  | 52.00  |
| BigGAN [3]      | 89.90    | 80.81    | 78.36    | 63.82   | 46.94   | 40.03   | 92.64   | 88.85   | 87.68   | 83.40  | 64.20  | 52.40  |
| Proposed        | 92.94    | 85.11    | 80.94    | 67.41   | 50.24   | 43.74   | 93.94   | 91.77   | 89.79   | 87.40  | 68.40  | 56.40  |

### Table 2. Linear classification on ImageNet-100. Available data are labeled and used for learning the classifier on the fixed encoder learned by CL and top-1 accuracy is reported.

| Method          | ImageNet-100 |
|-----------------|--------------|
|                 | 100% tr. data | 20% tr. data | 10% tr. data |
| SimCLR [6]      | 67.45        | 50.09        | 40.63        |
| SimCLR-DD [6]   | 70.72        | 53.38        | 43.78        |
| CLAE [14]       | 66.40        | 49.55        | 40.16        |
| BigGAN [3]      | 68.70        | 52.49        | 42.57        |
| Proposed        | 71.40        | 55.33        | 46.44        |

### Table 3. Transfer learning to downstream tasks by using ImageNet-100 as the source dataset. Top-1 accuracy of linear classification on top of a fixed encoder is reported.

| Source ImageNet-100 | CIFAR-10 100% tr. data | CIFAR-10 20% tr. data | CIFAR-10 10% tr. data | CIFAR-100 100% tr. data | CIFAR-100 20% tr. data | CIFAR-100 10% tr. data |
|---------------------|------------------------|-----------------------|-----------------------|-------------------------|------------------------|-----------------------|
| SimCLR              | 80.84                  | 56.06                 | 76.97                 | 50.68                   | 73.91                  | 46.73                 |
| SimCLR-DD           | 81.10                  | 56.03                 | 77.13                 | 52.46                   | 76.63                  | 49.29                 |
| CLAE                | 80.80                  | 57.08                 | 77.79                 | 52.63                   | 74.77                  | 48.61                 |
| BigGAN              | 81.13                  | 56.59                 | 77.54                 | 52.28                   | 74.98                  | 48.70                 |
| Proposed            | 83.25                  | 58.61                 | 80.10                 | 55.76                   | 78.16                  | 52.23                 |

Figure 4. Effectiveness of hard samples, positive pairs, and hard positive pairs. Enabling the components in the proposed approaches one by one accumulatively improves the performance. \( G \) is using a standalone generator, \( G+\text{Hard} \) is jointly optimizing \( G \) and the main model to generate hard samples, \( G+\text{Pos.} \) is \( G \) with positive pair generation, and \( G+\text{P.+Hard} \) is the proposed approach with all the components enabled. Top-1 accuracy of linear classification is reported. Error bars are the standard deviations across three independent runs.

### 4.3. Ablations

Effectiveness of hard samples, positive pairs, and hard positive pairs. We perform ablation studies to evaluate the effectiveness of hard samples (\( G+\text{Hard} \)), positive pairs (\( G+\text{Pos.} \)), and hard positive pairs (\( G+\text{Pos.}+\text{Hard} \)). The results of linear classification are shown in Figure 4. On CIFAR-10, using a simple generator degrades the performance of CL compared with the original SimCLR due to the low-quality samples from the generator. Using the proposed hard samples and positive pairs recover the accuracy by 0.39% and 0.62%, respectively, while using hard positive pairs outperforms SimCLR by 2.57% (92.94% vs. 90.37%). Similar results are observed on CIFAR-10 with 20% training data, where using a separate generator can slightly improve the accuracy by 0.15%, while enabling all the proposed components significantly improves the accuracy by 4.92%.

Impact of longer training. We evaluate the impact of training epochs. We increase the number of training epochs from the default 300 epochs to 600 epochs on CIFAR-10, and evaluate the learned representations by linear classification. As shown in Figure 5, with longer training, the advantage of the proposed approaches over the best-performing baseline becomes larger. This is because with longer training, more and harder samples are customised for the main model to improve its performance.

Evolution of positive pairs. The dynamically harder positive pairs in the training progress are shown in Figure 6. Every two adjacent rows show the evolution of positive pairs on ImageNet-10. With growing knowledge of the main model, positive pairs become progressively harder, while being similar objects. Learning from harder positive pairs improves the quality of learned representations.

5. Conclusion

This paper presents joint contrastive learning and hard sample generation for data-efficient unsupervised represen-
Table 4. Transfer learning to downstream tasks on various datasets with different amounts of training data for CL on the source datasets. Top-1 accuracy of linear classification on top of a fixed encoder is reported.

| Source       | Target CIFAR-10 | Target CIFAR-10 | Target CIFAR-10 | Target CIFAR-10 | Target CIFAR-10 | Target CIFAR-10 | Target CIFAR-10 | Target CIFAR-10 | Target CIFAR-10 | Target CIFAR-10 | Target CIFAR-10 |
|--------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Source       | 100% tr. data   | 20% tr. data    | 10% tr. data    | 100% tr. data   | 20% tr. data    | 10% tr. data    | 100% tr. data   | 20% tr. data    | 10% tr. data    | 100% tr. data   | 20% tr. data    |
| CIFAR-10     | 51.63           | 46.88           | 44.98           | 78.87           | 74.33           | 71.79           | 73.91           | 44.88           | 69.86           | 42.56           |
| CIFAR-10     | 52.22           | 48.45           | 46.74           | 78.53           | 73.94           | 72.49           | 73.77           | 46.53           | 71.20           | 43.82           |
| CIFAR-10     | 53.67           | 49.53           | 47.11           | 78.98           | 74.33           | 73.43           | 74.07           | 47.11           | 71.20           | 43.82           |
| CIFAR-10     | 56.38           | 52.51           | 50.08           | 82.24           | 77.26           | 75.10           | 75.38           | 49.03           | 73.08           | 46.46           |
| CIFAR-100    | 51.63           | 46.88           | 44.98           | 78.87           | 74.33           | 71.79           | 73.91           | 44.88           | 69.86           | 42.56           |
| CIFAR-100    | 52.22           | 48.45           | 46.74           | 78.53           | 73.94           | 72.49           | 73.77           | 46.53           | 71.20           | 43.82           |
| CIFAR-100    | 53.67           | 49.53           | 47.11           | 78.98           | 74.33           | 73.43           | 74.07           | 47.11           | 71.20           | 43.82           |
| CIFAR-100    | 56.38           | 52.51           | 50.08           | 82.24           | 77.26           | 75.10           | 75.38           | 49.03           | 73.08           | 46.46           |
| ImageNet-10  | 51.63           | 46.88           | 44.98           | 78.87           | 74.33           | 71.79           | 73.91           | 44.88           | 69.86           | 42.56           |
| ImageNet-10  | 52.22           | 48.45           | 46.74           | 78.53           | 73.94           | 72.49           | 73.77           | 46.53           | 71.20           | 43.82           |
| ImageNet-10  | 53.67           | 49.53           | 47.11           | 78.98           | 74.33           | 73.43           | 74.07           | 47.11           | 71.20           | 43.82           |
| ImageNet-10  | 56.38           | 52.51           | 50.08           | 82.24           | 77.26           | 75.10           | 75.38           | 49.03           | 73.08           | 46.46           |
| ImageNet-10  | 51.63           | 46.88           | 44.98           | 78.87           | 74.33           | 71.79           | 73.91           | 44.88           | 69.86           | 42.56           |
| ImageNet-10  | 52.22           | 48.45           | 46.74           | 78.53           | 73.94           | 72.49           | 73.77           | 46.53           | 71.20           | 43.82           |
| ImageNet-10  | 53.67           | 49.53           | 47.11           | 78.98           | 74.33           | 73.43           | 74.07           | 47.11           | 71.20           | 43.82           |
| ImageNet-10  | 56.38           | 52.51           | 50.08           | 82.24           | 77.26           | 75.10           | 75.38           | 49.03           | 73.08           | 46.46           |

Figure 6. Progressively harder positive pairs during training.

tation learning. A hard data generator is jointly optimized with the main model to customize hard samples for better contrastive learning. To further generate hard positive pairs without using labels, a pair of generators is proposed to generate similar but distinct samples. Experimental results show superior accuracy and data efficiency of the proposed approaches in visual representation learning.

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