Semantic Positive Pairs for Enhancing Visual Representation Learning of Instance Discrimination methods

Abstract

Self-supervised learning algorithms (SSL) based on instance discrimination have shown promising results, performing competitively or even outperforming supervised learning counterparts in some downstream tasks. Such approaches employ data augmentation to create two views of the same instance (i.e., positive pairs) and encourage the model to learn good representations by attracting these views closer in the embedding space without collapsing to the trivial solution. However, data augmentation is limited in representing positive pairs, and the repulsion process between the instances during contrastive learning may discard important features for instances that have similar categories. To address this issue, we propose an approach to identify those images with similar semantic content and treat them as positive instances, thereby reducing the chance of discarding important features during representation learning and increasing the richness of the latent representation. Our approach is generic and could work with any self-supervised instance discrimination frameworks such as MoCo and SimSiam. To evaluate our method, we run experiments on three benchmark datasets: ImageNet, STL-10 and CIFAR-10 with different instance discrimination SSL approaches. The experimental results show that our approach consistently outperforms the baseline methods across all three datasets; for instance, we improve upon the vanilla MoCo-v2 by 4.1% on ImageNet under a linear evaluation protocol over 800 epochs.

1 Introduction

In supervised learning, models are trained with input data X and their corresponding semantic labels or classes Y. It is rather common for each class to have several hundreds of instances available for training, which enables the model to extract the important features and create useful representations for the given samples (Van Gansbeke et al., 2020). This type of machine learning has been proven to perform well in various domains whenever data are available in abundance. In practice, that is often not the case, given that data annotation is laborious and expensive.

Recently, self-supervised learning (SSL) algorithms based on instance discrimination reduced the reliance on large annotated datasets for representation learning (He et al., 2020; Chen et al., 2020a;b; Misra & Maaten, 2020; Chen & He, 2021; Grill et al., 2020). These approaches treat each instance as a class on its own, so they employ random data augmentation for every single image in the dataset to prevent the model from learning trivial features and become invariant to all augmentations (Tian et al., 2020; Xiao et al., 2020; Chen et al., 2020a; Misra & Maaten, 2020). The model learns the image representation by attracting the positive pairs (i.e., two views of the same instance) closer in the embedding space without representation collapse. Contrastive and non-contrastive instance discrimination methods (Chen et al., 2020a; Caron et al., 2020; He et al., 2020; Grill et al., 2020; Bardes et al., 2021) have shown promising performance, often close to supervised learning or even better in some downstream tasks (Chen et al., 2020a; Chen & He, 2021; Chuang et al., 2020; Misra & Maaten, 2020; Huynh et al., 2022; Dwibedi et al., 2021). However, these approaches have two main limitations: 1) the data augmentation is limited in representing positive pairs (i.e., can not cover all variances in given class); 2) the repulsion process between the images in contrastive learning is implemented regardless of their semantic content, which may cause the loss of important features and slow model convergence (Huynh et al., 2022). For example, Figure 1 shows two images that have similar semantic

Figure 1: Example of an instance discrimination task where positive pairs are attracted together and negative pairs are pushed apart, even if they have similar semantic content.

content (aeroplanes). In contrastive instance discrimination, such images are repelled in the embedding space because the objective of such discrimination is to only attract the positive pairs and push apart all the other images even though they have similar semantic content. This is a major limitation that requires attention, as the performance of the downstream tasks depends on high-quality representations learnt by self-supervised pre-training (Donahue et al., 2014; Manová et al., 2023; Girshick et al., 2014; Zeiler & Fergus, 2014; Durrant & Leontidis, 2022; Kim & Walter, 2017; Durrant & Leontidis, 2023).

Two recent prominent approaches, which are Nearest-Neighbor Contrastive Learning of Visual Representations (NNCLR) (Dwibedi et al., 2021), and False Negative Cancellation (FNC) (Huynh et al., 2022) proposed to find semantic pairs in the dataset, treating them as positive pairs during representation learning, to improve the model performance on downstream tasks. NNCLR uses a support set Q to keep a representation of the dataset during model training. The model learns visual representations by creating a representation for the two views of the input instance (z_i, z_i^+), and then finds the nearest neighbours for the first view (i.e., z_i) from the support set Q, and so the nearest neighbour is $S = NN(z_i, Q)$. NNCLR then treats S as semantic positive pairs for the second view of the instance (i.e., z_i^+) regardless of the semantic content of S, which may belong to a category different to z_i^+. FNC creates more than two views for each instance which are $[z_i, z_i^+, z_s^1, z_s^2]$, where (z_i, z_i^+) are positive pairs and (z_s^1, z_s^2) are support views for the instance. They find the potential semantic pairs for the support views of each instance from negative examples in the batch by computing their similarity. Finally, they treat the identified semantic pairs as positive pairs during model training.

Finding images that have similar content (i.e., same category) and treating them as positive pairs increases the data diversity which could thus improve the power of representation learning (Tian et al., 2020; Dwibedi et al., 2021; Huynh et al., 2022; Khosla et al., 2020). Contrariwise, mapping wrong semantic pairs and encouraging the model to treat them as positive pairs causes reduced representation learning and slow model convergence. In this paper, we introduce an approach for enhancing the process of finding semantic pairs to improve visual representation learning. We name our method Semantic Positive Pairs for enhancing Instance Discrimination (SePP- ID) since our experiments indicate that accurate semantic positive pairs could significantly improve the performance of instance discrimination SLL. For identifying semantic positive pairs, we propose to use pre-trained models to firstly map the original images from the dataset (i.e., not augmented images) into latent representations and then the semantic positive pairs are matched by computing the similarity scores based on the latent representation vectors. Any self-supervised learning algorithms could be used as a pre-trained model for our purpose. For example, our experiments show that a model pre-trained by MoCo-v2 (Chen et al., 2020b) approach is good for identifying semantic positive pairs. These semantic positive pairs set (SPPS) along with the positive pairs (i.e., two views for the same instance) are used to train instance discrimination self-supervised model. The key difference to our approach is using pre-trained models and original images from the dataset to match semantic positive pairs, whereas the methods

mentioned above, such as NNCLR and FNC are finding semantic positive pairs during the representation learning. Such approaches may have a lower chance of matching the right semantic positive pairs, leading to slow model convergence and degrading representation learning. One possible reason would be that the model requires the necessary number of epochs to converge to learn a similar representation for the images from the same category (i.e., at the beginning of model training the semantic pairs are mapped based on texture and color, later in training the model become better in recognize class); another reason would be that the similarity score was computed using the embedding vectors of the augmented images. For example, with 1000 epochs, NNCLR reached 57% accuracy in terms of true semantic pairs, while FNC achieved 40% accuracy (Dwibedi et al., 2021; Huynh et al., 2022). Also, we show an empirical example in Figure 2 that using augmented images and a non-pre-trained model to find semantic pairs may lead to mapping wrong semantic pairs. In contrast, the accuracy in terms of true semantic positive pairs was achieved over 92% when MoCo-v2 was used as the pre-trained model with the original dataset in our proposed approach. Our contributions are as follows:

- We propose to use the representations of the pre-trained models for the original images from the dataset to match semantic positive pairs, which achieved as high as 92% accuracy in terms of true semantic positive pairs, compared to 57% using NNCLR and 40% using FNC.

- We demonstrate that SePP-ID outperformed other state-of-the-art (SOTA) approaches. For example, SePP-ID achieved 76.3% accuracy on ImageNet, compared to 74.4% using FNC.

- We demonstrate that the SPPS found by using our scheme improve the performance of several instance discrimination approaches across various epoch scenarios and datasets which indicates that the SPPS could be adapted to improve visual representation learning of any other instance discrimination approach.

2 Related Work

There have been several SSL approaches proposed, all of which aim to improve representation learning and achieve better performance on a downstream task. In this section, we provide a brief overview of some of these approaches, but we would encourage the readers to read the respective papers for more details.

Clustering-Based Methods: The samples that have similar features are assigned to the same cluster. Therefore, discrimination is based on a group of images rather than on instance discrimination (Caron et al., 2020; Van Gansbeke et al., 2020; Caron et al., 2018; Asano et al., 2019). DeepCluster (Caron et al., 2018) obtains the pseudo-label from the previous iteration which makes it computationally expensive and hard to scale. SWAV (Caron et al., 2020) solved this issue by using online clustering, but it needs to determine the correct number of prototypes. Also, there has been a body of research in an area called Multi-view Clustering (MVC) (Yang et al., 2022a; Trosten et al., 2021; Lu et al., 2023; Li et al., 2022a) whereby contrastive learning is used with clustering to find semantic pairs and alleviate the false negative issue. However, our approach does not rely on a clustering method to identify semantic pairs, providing two main advantages over clustering approaches. Firstly, we avoid some drawbacks of clustering methods, such as predefining the number of prototypes (i.e. clusters), less separable clusters and resorting to labels or pseudo-labels. Secondly, our approach can be applied to both contractive and non-contrastive learning, as demonstrated in this work.

Distillation Methods: BYOL (Grill et al., 2020) and SimSiam (Chen & He, 2021) use techniques inspired by knowledge distillation where a Siamese network has an online encoder and a target encoder. The target network parameters are not updated during backpropagation. Instead, the online network parameters are updated while being encouraged to predict the representation of the target network. Although these methods have produced promising results, it is not fully understood how they avoid collapse. Self-distillation with no labels (DINO) (Caron et al., 2021) was inspired by BYOL but they use a different backbone (ViT) and loss function, which enables it to achieve better results than other self-supervised methods while being more computationally efficient. Bag of visual words (Gidaris et al., 2020; 2021) also uses a teacher-student scheme, and it is inspired by natural language processing (NLP) to avoid representation collapse. The student network

is encouraged to predict the features' histogram for the augmented images, similar to the teacher network's histogram.

Information Maximization: Barlow twins (Zbontar et al., 2021) and VICReg (Bardes et al., 2021) do not require negative examples, stop gradient or clustering. Instead, they use regularisation to avoid representation collapse. The objective function of these methods aims to reduce the redundant information in the embeddings by making the correlation of the embedding vectors closer to the identity matrix. Though these methods provide promising results, they have some limitations, such as the representation learning being sensitive to regularisation. The effectiveness of these methods is also reduced if certain statistical properties are not available in the data.

Contrastive Learning: Instance discrimination, such as SimCLR, MoCo, and PIRL (Chen et al., 2020a; He et al., 2020; Chen et al., 2020b; Misra & Maaten, 2020) employ a similar idea. They attract the positive pairs together and push the negative pairs apart in the embedding space albeit through a different mechanism. SimCLR (Chen et al., 2020a) uses an end-to-end approach where a large batch size is used for the negative examples and both encoders' parameters in the Siamese network are updated together. PIRL (Misra & Maaten, 2020) uses a memory bank for negative examples and both encoders' parameters are updated together. MoCo (Chen et al., 2020b; He et al., 2020) uses a moment contrastive approach whereby the query encoder is updated during backpropagation and the query encoder updates the key encoder. The negative examples are located in a dictionary separate from the mini-batch, which enables holding large batch sizes.

Enhanced Contrastive Learning: Such mechanisms focus on the importance of the negative examples and find different ways to sample negative examples regardless of their content, which may cause undesired behaviour between images with similar semantic content. Some studies have focused on improving the quality of the negative examples which in turn improves representation learning. (Kalantidis et al., 2020) and (Robinson et al., 2020) focused on the hard negative samples around the positive anchor, whereas (Wu et al., 2020) introduced the percentile range for negative sampling. Another approach introduced by Chuang et al.(Chuang et al., 2020) gives weights for positive and negative terms to reduce the effects of undesirable negatives. Other methods such as (Dwibedi et al., 2021), (Huynh et al., 2022), and (Auh et al., 2023) use similarity metrics to define the images that have similar semantic content and treat them as positive pairs during model training. Although these approaches provide a solution to determine variant instances for the same category and treat them as positive pairs, there are common drawbacks in these approaches that hinder them from mapping highly accurate semantic pairs, such as:

1. They use a non-pre-trained model to represent the images before measuring the similarity between them.

2. They compute the similarity between transformed images, not the original images in the original dataset.

Counting on non-pre-trained models with augmented images to find semantic positive pairs akin to (Dwibedi et al., 2021; Huynh et al., 2022; Auh et al., 2023) may lead to inaccurate results. To demonstrate such issue, Figure 2 shows an empirical example of the inaccurate similarity scores we obtained when we used a non-pre-trained model and random augmented images to determine the instances that belong to the same class in the dataset. The similarity scores show that the horse and deer are more similar to the anchor (i.e., car) than car 1 and car 2, and the train is more similar to the anchor than car 2, which is not correct either.

Semi-Supervised Learning: The advantage of training a model on instance variants of the same category to improve the representation learning is used in semi-supervised approaches (Bošnjak et al., 2023; Yang et al., 2022b). (Bošnjak et al., 2023) present an approach to train the model on semantic positive pairs by leveraging a few labelled data. In their approach, they use labelled data and k-nearest neighbour to provide pseudo-labels for unlabelled points based on the most frequent class near the unlabelled data. Following that, they treat the data points that have similar pseudo-labels as semantic positive pairs in a contrastive learning setting. Such methods still require labelled data during training to provide semantic positive pairs. Our proposed pre-processing method provides a different way of approaching this, as we will demonstrate below across several datasets and ablation studies. We used a model pre-trained with SSL approaches and worked with the original dataset rather than augmented images to determine semantic positive pairs. In

Figure 2: Similarity scores are shown for anchor (car) with instances from other classes using non-pre-trained models and random augmented images.

addition, our method does not require labelled data, specialised architecture or support set to hold the semantic positive pairs, which makes it easier to be integrated with any self-supervised learning methods.

3 Methodology

This section proposes an approach to enhancing the visual representation learning of instance discrimination SSL methods by using semantic positive pairs (i.e., two different instances belong to the same category). To achieve that, we introduce the Semantic Sampler whose purpose is to find semantic positive pairs from the training data. The main idea of our approach is to find semantic positive pairs set (SPPS) from the original dataset (i.e., not distorted images by augmentation) by using the Semantic Sampler which consists of a pre-trained model and similarity metric. As shown in Figure 3 for finding the SPPS, the pre-trained model in the Semantic Sampler firstly maps K images from the original dataset into latent representations and then the semantic positive pairs are matched by computing the similarity scores based on the latent representation vectors. Note that K is a constant number that defines the number of images involved in the process of finding semantic pairs. These SPPS are used along with positive pairs from the dataset for training instance discrimination SSL models. In the literature, as noted previously, there are methods using semantic pairs to improve the performance of instance discrimination SSL, such as the FNC (Huynh et al., 2022), the NNCLR and (Dwibedi et al., 2021). In this section, we propose a different scheme for searching SPPS, inducing a modified loss function for training contrastive instance discrimination model. Our experiments show that our approach improves the performance of instance discrimination methods significantly and outperforms the STOA approaches including both FNC and NNCLR. In the following, we will introduce how the SPPS is obtained as well as our SSL algorithm using SPPS. Algorithm 1 shows how the proposed method is implemented.

3.1 Semantic Positive Pairs

We use a pre-trained SSL model with similarity metrics in the Semantic Sampler to search for semantic positive pairs in the original dataset. Figure 4 shows the whole process for creating SPPS.

As shown in Figure 4, K images are randomly chosen from the training data set, and then they are encoded by using the pre-trained SSL model. The embedding vectors generated by the pre-trained model are duplicated in two lists: one list contains anchors and another list contains semantic candidate embedding vectors. In our approach, the cosine similarity function is used to find semantic positive pairs for each anchor (i.e., the list B in Figure 4) from those semantic candidates embedding vectors (i.e., the list A in the figure). The anchors may have more than one positive sample chosen from the candidates. This allows the model to go beyond a single positive instance and capture divergence feature information from different instances

Figure 3: The proposed methodology: Firstly, k images are chosen from the dataset and encoded by the pre-trained model; Secondly, a similarity metric is used to find the semantic positive pairs for each anchor, followed by data transformations applied to both the original dataset and the semantic positive pairs set. Eventually, all the images are combined in one dataset which will be used to train the instance discrimination model.

Figure 4: Illustrate the process of Semantic Sampler in identifying the semantic positive pairs.

belonging to the same category. Eventually, a Semantic positive pairs set (SPPS) is created containing pairs of the semantic positive samples. The semantic positive samples were paired when the similarity score lies in the range [0.97, 0.99] and our experiments show that the accuracy of mapping semantic pairs as well as model performance increased on downstream tasks when choosing such threshold values (see Section 4 for computing the accuracy of finding SPPS). Note that the maximum threshold, i.e., 0.99, was chosen to avoid identical image samples. Compared to the previous approaches such as FNC and NNCLR, the semantic positive pairs are found by the Semantic Sampler before training the instance discrimination model, therefore the model is trained on accurately identified semantic pairs from the beginning and this leads to faster convergence and improves the representation learning. On the contrary, FNC and NNCLR search the semantic positive samples in the batch during the training by using augmented images (i.e., distorted images) and a non-pre-trained model which slows model convergence and degrades representation learning because of inaccurate semantic pairs.

Figure 5 shows examples of SPPS obtained from the STL10 dataset. It shows that our approach finds the true semantic positive pairs very well for those anchors, despite the anchor image having different properties (e.g. colour, direction, background, and size).

Figure 5: Example of semantic positive pairs found by our approach for different anchors in the STL10-unlabelled dataset.

Algorithm 1 Combining SPPS with original data

Input: Dataset samples, constant k, and structure *f*.

1: ImageList1=[ ]
2: ImageList2=[ ]
3: **for** $k \leftarrow 1$ to N **do**
4:     $image \leftarrow tensor(x_k)$ ▷ convert k images from dataset to tensor
5:     $emb\_vector \leftarrow f(image)$ ▷ encode images by pre-trained model
6:     $norm\_vector \leftarrow Normalize(emb\_vector)$ ▷ $l2$ norm
7:     ImageList1.append($norm\_vector$)
8: **end for**
9:
10: ImageList2 $\leftarrow$ ImageList1   ▷ both lists have similar embedding vectors
11: Max= 0.99 and Min= 0.97   ▷ define threshold
12: sim= torch.mm(ImageList1, ImageList2.T)   ▷ compute similarity

13: semantic_pairs_list=[ ]
14: **for** $i \leftarrow 1$ to $sim.size()[0]$ **do**
15:     **for** $j \leftarrow 1$ to $sim.size()[1]$ **do**
16:         **if** $Sim[i, j] \geq Min$ and $Sim[i, j] \leq Max$ **then**
17:             $Positive\_pair \leftarrow tuple(Dataset[i], Dataset[j])$
18:             semantic_pairs_list.append($Positive\_pair$)
19:         **end if**
20:     **end for**
21: **end for**
22: applies a random transformation to semantic_pairs_list.
23: combines the semantic_pairs_list with the original dataset.
Output: combine dataset

3.2 Learning with Semantic Positive Pairs

This subsection describes how our approach SePP-ID (i.e., Semantic Positive Pairs for enhancing Instance Discrimination) uses SPPS to train instance discrimination SSL models. As demonstrated in Figure 6 a copy for each instance in the original dataset is created and random augmentations are applied for each copy to generate positive pairs. For those semantic positive pairs described in Section 3.1, we do not need to create copy for the instances because we already have pairs so we only need to apply random transformations to each instance in the pairs. After that, the SPPS is merged with the original training dataset and so the training dataset is slightly larger than the original one.

After combining the SPPS with the original dataset, we train the contrastive instance discrimination model on the new *combined* dataset with a momentum encoder approach (similar to MoCo-v2 Chen et al. (2020b)). The contrastive loss function attracts the two views of the same instance (i.e., positive pairs) closer in the

Figure 6: The second step of the methodology: the instances of the original dataset and the SPPS are transformed and combined into one dataset.

embedding space while pushing apart all the other instances (i.e., negative samples):

$$\ell(u,v) = -\log \frac{\exp(\mathrm{sim}(u,v)/\tau)}{\sum_{k=1}^{2N} \mathbb{1}_{[k \neq i]} \exp(\mathrm{sim}(u,w_k)/\tau)} \tag{1}$$

As shown in Equation 1, our approach encourages the model to increase the similarity between the two views $\mathrm{sim}(u,v)$ and reduce the similarity with all other images in the batch w_k where v and u could be either semantic positive pairs (i.e., two images belong to the same category) or positive pair (i.e., two views for the same instance). Note that the number of semantic positive samples of instance x may vary. For example, some instances may not have any semantic positive pair, while others may have more than one semantic positive sample. Thus, the overall loss of our contrastive instance discrimination approach is given by the following equation:

$$loss = \frac{1}{N} \sum_{i=1}^{N} \left[\ell(u,v) + \sum_{m=1}^{M} \lambda_{im}\ell(u,v_m) \right], \tag{2}$$

where $0 \leq \lambda \leq 1$ represents regularization. In the overall loss function (Equation 2), the contrastive loss for the positive pairs is defined by the first term $\ell(u,v)$ where the second term $\ell(u,v_m)$ defines the semantic positive pairs for the instance that has semantic pairs. In the case of $\lambda_{im} = 0$, there are no semantic positive pairs and the model will be trained only on the positive pairs $\ell(u,v)$, thus the overall loss is equal to the loss of the positive pairs. Under this scenario, the model training is reduced to the original approach such as vanilla MoCo-V2 (Chen et al., 2020b). On the other hand, if $\lambda_{im} = 1$ that means we have semantic pairs so the term for semantic positive pairs $\ell(u,v_m)$ is added to the overall loss and is computed in the same manner that is being used to compute positive pairs. This approach would increase the richness of the latent space during visual representation learning. Our experiments show that this scheme improves model performance on the downstream tasks.

4 Experiments and Results

Datasets: We evaluated SePP-ID approach on three datasets, i.e. STL-10 "unlabelled" with 100K training images (Coates & Ng, 2011), CIFAR-10 with 50K training images (Krizhevsky, 2009), and ImageNet-1K with 1.28M training images (Russakovsky et al., 2015).

Pre-trained model: Many candidate approaches can be used to train the pre-trained model of the Semantic Sampler for finding SPPS from the original dataset. As a pre-trained model is only used for finding SPPS, we prefer choosing models with relatively low computational overhead. The following are the intuitions on how the approach was chosen to train the Semantic Sampler's pre-trained model: 1) The model backbone

was chosen to be ResNet50 because it is used in most instance discrimination approaches so that we can easily compare them; 2) The approach should provide reasonable performance when they are trained on a small batch size (e.g., 256) and a small number of epochs (e.g., 100) to use low computational overhead; 3) The approach uses a small projection head (e.g., 256) while training the model because we want to keep the projection head in the process of creating SPPS. If the projection head has a large output dimension such as VICReg (i.e., 8192 dimensions), it will add a large computational overhead for finding SPPS.

Based on the above intuition, SimSiam (Chen & He, 2021), MoCo-V2 (Chen et al., 2020b) and SimCLR (Chen et al., 2020a) were chosen as the candidate to train the Semantic Sampler's pre-trained model. To choose the best approach for training the pre-trained model across these three approaches, we trained three models on ImageNet-1K for 100 epochs with batch size 256. After model training, we froze the model parameters and kept the projection head (256D). we evaluate the three pre-trained models (i.e., model pre-trained by SimSiam, MoCo-v2, and SimCLR) by creating SPPS and computing the accuracy of selected semantic pairs by leveraging the ImageNet labels. Table 1 demonstrates the performance of the three candidate Semantic Samplers' pre-trained model, showing that MoCo-v2 was the best-performing model for finding SPPS in terms of accuracy. Thus we use the model which pre-trained by the MoCo-v2 approach in the Semantic Sampler for all the following experiments.

Table 1: The accuracy of finding semantic positive pairs in ImageNet across the three candidate approaches.

Approach	Accuracy
MoCo-v2	92.03%
SimSiam	91,44%
SimCLR	90.72%

Training Setup: We use ResNet50 as a backbone and the model is trained with SGD optimizer, weight decay 0.0001, momentum 0.9 and initial learning rate 0.03. The mini-batch size is 256 and the model is trained up to 800 epochs. We set the K-value = 10% of the ImageNet dataset (i.e., 128K random images are picked from the Imagenet dataset for finding semantic pairs). In our ablation study, we compared the performance of our models when various proportions (i.e., various K-value) of data were used for choosing SPPS.

Evaluation: We evaluated SePP-ID approach by using linear evaluation and semi-supervised setting against leading SOTA approaches on the ImageNet-1K. In linear evaluation, we followed standard evaluation protocol (Chen et al., 2020a; He et al., 2020; Huynh et al., 2022; Dwibedi et al., 2021). We trained a linear classifier for 100 epochs on top of a frozen backbone pre-trained by SePP-ID. We used an ImageNet training set with random cropping and random left-to-right flipping augmentations to train the linear classifier from scratch. The results are reported on the ImageNet evaluation set with centre crop (224×224). In a semi-supervised setting, we fine-tune the network with 60 epochs using 1% labelled data and 30 epochs using 10% labelled data.

Comparing with SOTA Approaches: We use linear evaluation to compare our approach (i.e., SePP-ID), which is momentum contrastive with semantic positive pairs, against vanilla MoCo-v2 on different epochs on the ImageNet-1k dataset. In addition, we compare our approach after 800 epochs with the performance of other SOTA on the ImageNet-1k.

Table 2: Comparisons between vanilla MoCo-v2 and SePP-ID on the ImageNet dataset with different epochs.

Approach\Epochs	100	200	400	800
MoCo-v2 (Chen et al., 2020b)	67.4 %	69.9%	71.0%	72.2%
SePP-ID (*ours*)	69.2%	72.3%	75.2%	76.3 %

Table 2 shows that our approach consistently improved the performance of the instance discrimination approach across various numbers of epochs. Our approach SePP-ID significantly outperforms the vanilla MoCo-v2 by 4.1% on 800 epochs. The results substantiate the importance of semantic pairs in instance

discrimination representation learning. For example, our approach with 400 epochs surpasses the vanilla MoCo-v2 with 800 epochs by 3%.

Table 3: Comparisons between SePP-ID and SOTA approaches on ImageNet.

Approach	Epochs	Accuracy
MoCo-v2 (Chen et al., 2020b)	800	72.2%
BYOL (Grill et al., 2020)	1000	74.4%
SimCLR (Chen et al., 2020a)	1000	69.3%
SimSiam (Chen & He, 2021)	800	71.3%
VICReg (Bardes et al., 2021)	1000	73.2%
SWAV (Caron et al., 2020)	800	75.4%
OBoW(Gidaris et al., 2021)	200	73.8 %
DINO (Caron et al., 2021)	800	75.3%
Barlow Twins (Zbontar et al., 2021)	1000	73.2%
CLSA (Wang & Qi, 2022)	200	73.3%
HCSC (Guo et al., 2022)	200	73.3%
SNCLR (Ge et al., 2023)	800	75.3%
SCFS (Song et al., 2023)	800	75.7%
UniVIP (Li et al., 2022b)	300	74.2%
IFND (Chen et al., 2021)	200	69.7%
CLFN (Auh et al., 2023)	100	59.6%
NNCLR (Dwibedi et al., 2021)	1000	75.5%
FNC (Huynh et al., 2022)	1000	74.4%
SePP-ID(*ours*)	800	**76.3 %**

Table 3 highlights the advantage of using our approach to enhance the contrastive instance discrimination SSL approaches, clearly outperforming all baselines. This supports our hypothesis that we can obtain more accurate semantic positive pairs by using Semantic Sampler and the original dataset. Consequently, we can train the instance discrimination models on correct semantic pairs, thereby enhancing representation learning and improving model performance on the downstream task. Also, the result shows that using a non-pre-trained model with augmented images to determine the semantic pairs may slow the model convergence because the model needs several epochs to be able to pick the correct semantic positive pairs. Therefore, our approach achieves 76.3% after 800 epochs, which is better than NNCLR and FNC by 0.8% and 1.9%, respectively (after 1000 epochs).

NNCLR, FNC and CLFN are attracting the nearest neighbour of the anchor in the embedding space because they assume that they have similar content (same category). However, using a non-pre-trained model and augmented images (distortion images) to find images that have similar content may cause obtaining wrong semantic pairs during model training which leads to slow model convergence and reduced model performance as shown in Table 3. On the contrary, our approach acquires more accurate semantic pairs by using the Semantic Sampler with the original dataset. Therefore, the instance discrimination model is trained on the right semantic pairs from the beginning of the training which leads to improved model performance and fast convergence.

Semi-Supervised Learning on ImageNet: In this part, we evaluate the performance of SePP-ID under the semi-supervised setting. Specifically, we use 1% and 10% of the labelled training data from ImageNet-1k for fine-tuning, which follows the semi-supervised protocol in SimCLR (Chen et al., 2020a). The top-1 accuracy is reported in Table 4 after fine-tuning using 1% and 10% training data. SePP-ID outperforms all the compared methods. The results demonstrate that SePP-ID achieves the best feature representation quality.

Table 4: Semi-supervised learning results on ImageNet. Top-1 performances are reported on fine-tuning a pre-trained ResNet-50 with ImageNet 1% and 10% datasets.

	top-1	
Approach\Fraction	ImageNet 1%	ImageNet 10%
simCLR (Chen et al., 2020a)	48.3%	65.6%
BYOL(Grill et al., 2020)	53.2%	68.8%
SWAV (Caron et al., 2020)	53.9%	70.2%
DINO (Dwibedi et al., 2021)	50.2%	69.3%
SCFS (Song et al., 2023)	54.3%	70.5%
NNCLR (Dwibedi et al., 2021)	56.4%	69.8%
FNC (Huynh et al., 2022)	63.7%	71.1%
SePP-ID(*ours*)	64.2%	71.8%

4.1 Ablation Study

In this section, we provide a more in-depth analysis of our approach by conducting four different studies as follows: 1) We apply our method to different datasets to show that our approach performs consistently across different datasets; 2) We experimentally explore the impact of the parameter k on model performance; 3) We also randomly selected images from the original dataset, and then add them into the original data after augmentation to ensure that the improvement of performance was due to the SPPS rather than simply increasing data size; and 4) Conduct experiments on different instance discrimination approaches.

4.1.1 Comparisons on Different Datasets

we aim to verify that our method maintains its performance across various datasets when using different backbones (e.g. ResNet18). To achieve this, we compare vanilla MoCo-v2 with our approach, i.e. SePP-ID on two datasets (STL-10 and CIFAR-10) with k-value = 10% of the dataset. Note the K-value with ImageNet dataset is 10%, fix the proportion (10%) with the other datasets (STL-10 and CIFAR-10) to see if we can obtain the same improvement in representation learning with the same proportion on smaller datasets. Table 5 illustrates that our method outperforms the vanilla approach by 4.55% after 200 epochs on STL-10 and achieved 80.36% after 400 epochs which is better than Vanilla MoCo-v2 at 800 epochs. On CIFAR-10, SePP-ID outperforms MoCo-v2 across all the different epochs and achieved 77.46% after 800 epochs which is higher than the vanilla MoCo-v2 by 3.58%. These results show that our approach is working properly even with smaller datasets and different backbones.

Table 5: MoCo-v2 versus SePP-ID on CIFAR-10 and STL-10 with ResNet18

	STL-10			CIFAR-10		
Approach\Epoch	200	400	800	200	400	800
MoCo-v2	69.46%	77.37%	80.08 %	65.27%	69.50 %	73.88%
SePP-ID(*ours*)	74.01%	80.36%	82.29 %	72.05 %	73.87 %	77.46%

4.1.2 Impact of the k Value

In this subsection, we experimentally analysed the impact of the k parameter on the performance of our model. To obtain the effect of the (k-value), we trained models for 100 epochs on the ImageNet dataset and we fixed all the parameters except the k parameter. Then we linearly evaluate the models to see the effect of k on downstream tasks.

It is obvious in Table 6 that when increasing k, the number of semantic positive pairs is increased (i.e., Number of SPPS), and so is the model performance. This suggests that semantic positive pairs affect positively the performance of instance discrimination models. On the other hand, a larger k needs more

Table 6: SePP-ID performance with varying k-value.

$k\%$	0%	5%	10%	25%	50%	80%	100%
Number of SPPS	0	12,752	18,109	23,968	48,308	54,710	61,200
Hours for training	≈ 30	≈ 37	≈ 45	≈ 66	≈ 103	≈ 148	≈ 172
Accuracy	67.40%	68.63%	69.20%	69.56%	69.70%	69.82%	69.85%

training hours as expected. Therefore, we decided to choose k equal to (10%) for all of our experiments. Note that we used two A100 80GB to train the models in our experiments.

To ensure that the enhancement in the performance was attributed to the semantic positive pairs rather than increasing the size of the dataset, we randomly picked 18,109 images from ImageNet (which is similar to the number of semantic positive samples found with 10% of the ImageNet dataset) and created two copies of them (x_i and x_i') each of which is randomly augmented. We added these samples to the original ImageNet dataset. This allows us to test whether the improvement came from the semantic positive pairs or from increasing the size of the dataset. The results shown in Table 7 indicate that simply adding random augmented images to the original dataset has negligible improvement (i.e., 0.2%) to MoCo-v2's performance, while the performance improved by 4.1% when adding semantic positive samples.

Table 7: Compare the performance of MoCo-V2 with random add augmented images against SePP-ID (k=10%) after 800 epochs on ImageNet.

Dataset pre-process	Number of added pairs	Accuracy
MoCo-V2	0	72.2%
MoCo-V2 (added random augmented images)	18,109	72.4%
SePP-ID($k = 10\%$)	18,109	76.3%

4.1.3 Non-contrastive Learning With our Approach

In these experiments, we want to study the effect of our approach on non-contrastive learning. To do so, we used the framework of three SOTA approaches, SimSiam(Chen & He, 2021), DINO (Dwibedi et al., 2021), and VICReg(Bardes et al., 2021).

Table 8: Compare our approach (SePP-ID) with SimSiam framework versus vanilla Simsiam .

Approach\Epochs	100	200	400	800
SimSiam (Chen et al., 2020a)	68.1%	70.0%	70.8%	71.3%
SePP-ID (*ours*)	68.9%	71.1%	71.9 %	72.5 %

Table 8 shows that semantic positive pairs found by our approach consistently improve the representation learning of the non-contrastive instance discrimination method (knowledge distillation). our approach surpasses vanilla SimSiam by 1.2% on 800 epochs. Also, our approach with 400 epochs achieved better than the vanilla approach with 800 epochs.

Furthermore, our approach also significantly improves the performance of an information maximisation instance discrimination method, i.e. VICReg. Table 9 indicates that using the VICReg framework with semantic positive pairs found by our approach increases the performance by 2.35% on 100 epochs and 2.9% on 1000 epochs.

Finally, we used DINO (Caron et al., 2021) frameworks, which use centring and sharping to avoid representation collapse. We used the publicised implementation of DINO to train two models: Vanilla DINO and DINO with semantic positive pairs found by our approach for 200 epochs on the ImageNet dataset.

Table 9: Comparisons between VICReg and SePP-ID on ImageNet.

Approach\Epochs	100	1000
VICReg (Bardes et al., 2021)	68.6 %	73.2%
SePP-ID (*ours*)	70.95%	76.1%

Table 10: Compare the performance accuracy between vanilla DINO and SePP-ID on ImageNet.

Approach\Epochs	200
DINO (Dwibedi et al., 2021)	66.8%
SePP-ID (*ours*)	68.6%

We employed the same hyperparameters used in the original paper. The reported results in Table10 are for training without multi-crop. It is apparent that semantic positive pairs found by our approach play an important role in improving the representation learning for the DINO framework. Our approach with the DINO framework outperforms the Vanilla DINO by 1.8% in linear evaluation.

5 Conclusion

In this paper, we have proposed to use a Semantic Sampler (pre-trained model and similarity metric) with the original dataset to find semantic positive pairs. We demonstrated that these semantic positive samples can significantly improve the visual representation learning of the SSL instance discrimination methods on three datasets which are ImageNet, STL-10, and CIFAR-10. Our experiments also indicate that our approach outperformed other methods, including NNCLR, FNC and CLFN, which are using semantic positive samples. This suggests that the true semantic positive samples are important for learning visual representations with instance discrimination approaches.

References

Yuki Markus Asano, Christian Rupprecht, and Andrea Vedaldi. Self-labelling via simultaneous clustering and representation learning. *arXiv preprint arXiv:1911.05371*, 2019.

Joonsun Auh, Changsik Cho, and Seon-Tae Kim. Contrastive learning for reducing false negatives with global and local views in augmented data. In *2023 Innovations in Intelligent Systems and Applications Conference (ASYU)*, pp. 1–5, 2023. doi: 10.1109/ASYU58738.2023.10296635.

Adrien Bardes, Jean Ponce, and Yann LeCun. Vicreg: Variance-invariance-covariance regularization for self-supervised learning. *arXiv preprint arXiv:2105.04906*, 2021.

Matko Bošnjak, Pierre H Richemond, Nenad Tomasev, Florian Strub, Jacob C Walker, Felix Hill, Lars Holger Buesing, Razvan Pascanu, Charles Blundell, and Jovana Mitrovic. Semppl: Predicting pseudo-labels for better contrastive representations. *arXiv preprint arXiv:2301.05158*, 2023.

Mathilde Caron, Piotr Bojanowski, Armand Joulin, and Matthijs Douze. Deep clustering for unsupervised learning of visual features. In *Proceedings of the European conference on computer vision (ECCV)*, pp. 132–149, 2018.

Mathilde Caron, Ishan Misra, Julien Mairal, Priya Goyal, Piotr Bojanowski, and Armand Joulin. Unsupervised learning of visual features by contrasting cluster assignments. *Advances in neural information processing systems*, 33:9912–9924, 2020.

Mathilde Caron, Hugo Touvron, Ishan Misra, Hervé Jégou, Julien Mairal, Piotr Bojanowski, and Armand Joulin. Emerging properties in self-supervised vision transformers. In *Proceedings of the IEEE/CVF international conference on computer vision*, pp. 9650–9660, 2021.

Ting Chen, Simon Kornblith, Mohammad Norouzi, and Geoffrey Hinton. A simple framework for contrastive learning of visual representations. In *International conference on machine learning*, pp. 1597–1607. PMLR, 2020a.

Tsai-Shien Chen, Wei-Chih Hung, Hung-Yu Tseng, Shao-Yi Chien, and Ming-Hsuan Yang. Incremental false negative detection for contrastive learning. *arXiv preprint arXiv:2106.03719*, 2021.

Xinlei Chen and Kaiming He. Exploring simple siamese representation learning. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pp. 15750–15758, 2021.

Xinlei Chen, Haoqi Fan, Ross Girshick, and Kaiming He. Improved baselines with momentum contrastive learning. *arXiv preprint arXiv:2003.04297*, 2020b.

Ching-Yao Chuang, Joshua Robinson, Yen-Chen Lin, Antonio Torralba, and Stefanie Jegelka. Debiased contrastive learning. *Advances in neural information processing systems*, 33:8765–8775, 2020.

Adam Coates and Andrew Y Ng. Analysis of large-scale visual recognition. In *Advances in neural information processing systems*, pp. 284–292, 2011.

Jeff Donahue, Yangqing Jia, Oriol Vinyals, Judy Hoffman, Ning Zhang, Eric Tzeng, and Trevor Darrell. Decaf: A deep convolutional activation feature for generic visual recognition. In *International conference on machine learning*, pp. 647–655. PMLR, 2014.

Aiden Durrant and Georgios Leontidis. Hyperspherically regularized networks for self-supervision. *Image and Vision Computing*, 124:104494, 2022.

Aiden Durrant and Georgios Leontidis. Hmsn: Hyperbolic self-supervised learning by clustering with ideal prototypes. *arXiv preprint arXiv:2305.10926*, 2023.

Debidatta Dwibedi, Yusuf Aytar, Jonathan Tompson, Pierre Sermanet, and Andrew Zisserman. With a little help from my friends: Nearest-neighbor contrastive learning of visual representations. In *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pp. 9588–9597, 2021.

Chongjian Ge, Jiangliu Wang, Zhan Tong, Shoufa Chen, Yibing Song, and Ping Luo. Soft neighbors are positive supporters in contrastive visual representation learning. *arXiv preprint arXiv:2303.17142*, 2023.

Spyros Gidaris, Andrei Bursuc, Nikos Komodakis, Patrick Pérez, and Matthieu Cord. Learning representations by predicting bags of visual words. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 6928–6938, 2020.

Spyros Gidaris, Andrei Bursuc, Gilles Puy, Nikos Komodakis, Matthieu Cord, and Patrick Perez. Obow: Online bag-of-visual-words generation for self-supervised learning. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 6830–6840, 2021.

Ross Girshick, Jeff Donahue, Trevor Darrell, and Jitendra Malik. Rich feature hierarchies for accurate object detection and semantic segmentation. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pp. 580–587, 2014.

Jean-Bastien Grill, Florian Strub, Florent Altché, Corentin Tallec, Pierre Richemond, Elena Buchatskaya, Carl Doersch, Bernardo Avila Pires, Zhaohan Guo, Mohammad Gheshlaghi Azar, et al. Bootstrap your own latent-a new approach to self-supervised learning. *Advances in neural information processing systems*, 33:21271–21284, 2020.

Yuanfan Guo, Minghao Xu, Jiawen Li, Bingbing Ni, Xuanyu Zhu, Zhenbang Sun, and Yi Xu. Hcsc: Hierarchical contrastive selective coding. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, pp. 9706–9715, June 2022.

Kaiming He, Haoqi Fan, Yuxin Wu, Saining Xie, and Ross Girshick. Momentum contrast for unsupervised visual representation learning. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pp. 9729–9738, 2020.

Tri Huynh, Simon Kornblith, Matthew R Walter, Michael Maire, and Maryam Khademi. Boosting contrastive self-supervised learning with false negative cancellation. In *Proceedings of the IEEE/CVF winter conference on applications of computer vision*, pp. 2785–2795, 2022.

Yannis Kalantidis, Mert Bulent Sariyildiz, Noe Pion, Philippe Weinzaepfel, and Diane Larlus. Hard negative mixing for contrastive learning. *Advances in Neural Information Processing Systems*, 33:21798–21809, 2020.

Prannay Khosla, Piotr Teterwak, Chen Wang, Aaron Sarna, Yonglong Tian, Phillip Isola, Aaron Maschinot, Ce Liu, and Dilip Krishnan. Supervised contrastive learning. *Advances in neural information processing systems*, 33:18661–18673, 2020.

Dong-Ki Kim and Matthew R Walter. Satellite image-based localization via learned embeddings. In *2017 IEEE International Conference on Robotics and Automation (ICRA)*, pp. 2073–2080. IEEE, 2017.

Alex Krizhevsky. Learning multiple layers of features from tiny images. Technical report, Citeseer, 2009.

Yunfan Li, Mouxing Yang, Dezhong Peng, Taihao Li, Jiantao Huang, and Xi Peng. Twin contrastive learning for online clustering. *International Journal of Computer Vision*, 130(9):2205–2221, 2022a.

Zhaowen Li, Yousong Zhu, Fan Yang, Wei Li, Chaoyang Zhao, Yingying Chen, Zhiyang Chen, Jiahao Xie, Liwei Wu, Rui Zhao, et al. Univip: A unified framework for self-supervised visual pre-training. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pp. 14627–14636, 2022b.

Yiding Lu, Yijie Lin, Mouxing Yang, Dezhong Peng, Peng Hu, and Xi Peng. Decoupled contrastive multi-view clustering with high-order random walks. *arXiv preprint arXiv:2308.11164*, 2023.

Alžběta Manová, Aiden Durrant, and Georgios Leontidis. S-jea: Stacked joint embedding architectures for self-supervised visual representation learning. *arXiv preprint arXiv:2305.11701*, 2023.

Ishan Misra and Laurens van der Maaten. Self-supervised learning of pretext-invariant representations. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pp. 6707–6717, 2020.

Joshua Robinson, Ching-Yao Chuang, Suvrit Sra, and Stefanie Jegelka. Contrastive learning with hard negative samples. *arXiv preprint arXiv:2010.04592*, 2020.

Olga Russakovsky, Jia Deng, Hao Su, Jonathan Krause, Sanjeev Satheesh, Sean Ma, Zhiheng Huang, Andrej Karpathy, Aditya Khosla, Michael Bernstein, Alexander C. Berg, and Li Fei-Fei. ImageNet Large Scale Visual Recognition Challenge. *International Journal of Computer Vision (IJCV)*, 115(3):211–252, 2015. doi: 10.1007/s11263-015-0816-y.

Kaiyou Song, Shan Zhang, Zimeng Luo, Tong Wang, and Jin Xie. Semantics-consistent feature search for self-supervised visual representation learning. In *Proceedings of the IEEE/CVF International Conference on Computer Vision (ICCV)*, pp. 16099–16108, October 2023.

Yonglong Tian, Chen Sun, Ben Poole, Dilip Krishnan, Cordelia Schmid, and Phillip Isola. What makes for good views for contrastive learning? *Advances in Neural Information Processing Systems*, 33:6827–6839, 2020.

Daniel J Trosten, Sigurd Lokse, Robert Jenssen, and Michael Kampffmeyer. Reconsidering representation alignment for multi-view clustering. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pp. 1255–1265, 2021.

Wouter Van Gansbeke, Simon Vandenhende, Stamatios Georgoulis, Marc Proesmans, and Luc Van Gool. Scan: Learning to classify images without labels. In *European conference on computer vision*, pp. 268–285. Springer, 2020.

Xiao Wang and Guo-Jun Qi. Contrastive learning with stronger augmentations. *IEEE transactions on pattern analysis and machine intelligence*, 45(5):5549–5560, 2022.

Mike Wu, Milan Mosse, Chengxu Zhuang, Daniel Yamins, and Noah Goodman. Conditional negative sampling for contrastive learning of visual representations. *arXiv preprint arXiv:2010.02037*, 2020.

Tete Xiao, Xiaolong Wang, Alexei A Efros, and Trevor Darrell. What should not be contrastive in contrastive learning. *arXiv preprint arXiv:2008.05659*, 2020.

Mouxing Yang, Yunfan Li, Peng Hu, Jinfeng Bai, Jiancheng Lv, and Xi Peng. Robust multi-view clustering with incomplete information. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 45(1): 1055–1069, 2022a.

Xihong Yang, Xiaochang Hu, Sihang Zhou, Xinwang Liu, and En Zhu. Interpolation-based contrastive learning for few-label semi-supervised learning. *IEEE Transactions on Neural Networks and Learning Systems*, 2022b.

Jure Zbontar, Li Jing, Ishan Misra, Yann LeCun, and Stéphane Deny. Barlow twins: Self-supervised learning via redundancy reduction. In *International Conference on Machine Learning*, pp. 12310–12320. PMLR, 2021.

Matthew D Zeiler and Rob Fergus. Visualizing and understanding convolutional networks. In *Computer Vision–ECCV 2014: 13th European Conference, Zurich, Switzerland, September 6-12, 2014, Proceedings, Part I 13*, pp. 818–833. Springer, 2014.