Training Vision Transformers with Only 2040 Images

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Abstract

Vision Transformers (ViTs) is emerging as an alternative to convolutional neural networks (CNNs) for visual recognition. They achieve competitive results with CNNs but the lack of the typical convolutional inductive bias makes them more data-hungry than common CNNs. They are often pretrained on JFT-300M or at least ImageNet and few works study training ViTs with limited data. In this paper, we investigate how to train ViTs with limited data (e.g., 2040 images). We give theoretical analyses that our method (based on parametric instance discrimination) is superior to other methods in that it can capture both feature alignment and instance similarities. We achieve state-of-the-art results when training from scratch on 7 small datasets under various ViT backbones. We also investigate the transferring ability of small datasets and find that representations learned from small datasets can even improve large-scale ImageNet training.

1. Introduction

Transformers [31] have recently emerged as an alternative to convolutional neural networks (CNNs) for visual recognition [13, 28, 40]. The vision transformer (ViT) introduced by Dosovitskiy et al. [13] is an architecture directly inherited from natural language processing [12], but applied to image classification with raw image patches as input. ViT and variants achieve competitive results with CNNs but require significantly more training data. For instance, ViT performs worse than ResNets [16] with similar capacity when trained on ImageNet [26] (1.28 million images). One possible reason may be that ViT lacks certain desirable properties inherently built into the CNN architecture that make CNNs uniquely suited to solve vision tasks, e.g., locality, the translation invariance and the hierarchical structure [37]. As a result, ViTs need a lot of data for training, usually more data-hungry than CNNs.

In order to alleviate this problem, a lot of works try to introduce convolutions to ViTs [21, 35, 37, 40]. These architectures enjoy the advantages of both paradigms, with attention layers modeling long-range dependencies while convolutions emphasizing the local properties of images. Empirical results show that these ViTs trained on ImageNet outperform similar-size ResNets on this dataset. However, ImageNet is still a large-scale dataset and it is still not clear what is the behavior of these networks when trained on small datasets (e.g., 2040 images). As will be further analysed in Sec. 4.1, we cannot always rely on such large-scale datasets from the perspective of data, computing and flexibility.

In this paper, we investigate how to train ViTs from scratch with limited data. We first perform self-supervised pretraining and then supervised fine-tuning on the same target dataset, as done in [3]. We focus on the self-supervised pretraining stage and our method is based on parametric instance discrimination [14]. We theoretically analyze that parametric instance discrimination can not only capture feature alignment between positive pairs but also find potential similarities between instances thanks to the final learnable fully connected layer $W$. Experimental results further verify our analyses and our method achieves better performance than other non-parametric contrastive methods [7–10]. It is known that instance discrimination suffers from high GPU computation, high memory overload and slow convergence for high-dimensional $W$ on large-scale datasets. Since in this paper we focus on small datasets, we do not need complicated strategies for large-scale datasets as in [2, 19]. Instead, we adopt small resolution [3], multi-crop [6] and CutMix [41] for the small data setup and we also analyze them from both the theoretical and empirical perspectives.

We name our method as Instance Discrimination with Multi-crop and CutMix (IDMM) and achieve state-of-the-art results on 7 small datasets when training from scratch under various ViT backbones. For instance, we achieve 96.7% accuracy when training from scratch on flowers [23] (2040 images), which shows that training ViTs with small data is surprisingly viable. Moreover, we first analyze the transferring ability of small datasets. We find that ViTs also have good transferring ability even when pretrained on small datasets and can even facilitate training on large-scale datasets, e.g., ImageNet. Liu et al. [20] also investigate
training ViTs with small-size datasets but they focus on the fine-tuning stage while we focus on the pretraining stage. More importantly, we achieve much better results than [20], where the best reported accuracy on flowers was 56.3%.

In summary, our contributions are:

- We propose IDMM for self-supervised ViT training and achieve state-of-the-art results even when training from scratch for various ViT backbones on 7 small datasets.
- We give theoretical analyses on why we should prefer parametric instance discrimination when dealing with small data from the loss perspective. Moreover, we show how strategies like CutMix alleviate the infrequent updating problem from the gradient perspective.
- We empirically show that the projection MLP head is essential for non-parametric contrastive methods (e.g., SimCLR [8]) but not for parametric instance discrimination, thanks to the final learnable \( W \) in instance discrimination.
- We analyze the transferring ability of small datasets and find that ViTs also have good transferring ability even when pretrained on small datasets.

2. Related Works

Self-supervised learning. Self-supervised learning (SSL) has emerged as a powerful method to learn visual representations without labels. Many recent works follow the contrastive learning paradigm [29], which is also known as non-parametric instance discrimination [38]. For instance, SimCLR [8] and MoCo [15] trained networks to identify a pair of views originating from the same image when contrasted with many views from other images. Unlike the two-branch structure in contrastive methods, some approaches [2,14,19] employ a parametric, one-branch structure for instance discrimination. Exemplar-CNN [14] learned to discriminate between a set of surrogate classes, where each class represents different transformed patches of a single image. [2] and [19] proposed different methods to alleviate the infrequent instance visiting problem or reduce the GPU memory consumption for large-scale datasets, but rely on complicated engineering techniques for CNNs and lack theoretical analyses. In this paper, we not only apply parametric instance discrimination to ViTs, but also focus on small datasets. In addition, we give theoretical analyses of why should we prefer parametric method, at least for small datasets.

Recently, there have also been self-supervised methods designed for ViTs. [10] found that instability is a major issue that impacts self-supervised ViT training and proposed a simple contrastive baseline MoCov3. DINO [7] designed a simple self-supervised approach that can be interpreted as a form of knowledge distillation with no labels. However, they focused on large-scale datasets while we focus on small data. Our method is more stable for various networks and more effective for small data.

Vision Transformers. Vision Transformer (ViT) [13] treated an image as patches/tokens and employed a pure transformer structure. With sufficient training data, ViT outperforms CNNs on various image classification benchmarks, and many ViT variants have been proposed since then. Touvron et al. [28] introduced a teacher-student distillation token strategy into ViT, namely DeiT. Beyond classification, Transformer has been adopted in diverse vision tasks, including detection [4], segmentation [36], etc. Many ViT variants were proposed in recent months. Swin Transformer [21] applied the shifted window approach to compute self-attention matrix. Wang et al. proposed PVT-based model (PVTv1 & v2) [34, 35], which built a progressive shrinking pyramid and a spatial-reduction attention layer to generate multi-resolution feature maps. T2T-ViT [40] introduced a tokens-to-token (T2T) module to aggregate neighboring tokens into one recursively. However, ViTs are known to be data-hungry [20] and how to train ViTs with limited data is an important but not fully investigated question. [20] proposed a self-supervised task for ViTs, which can extract additional information from images and make training much more robust when training data are scarce. In contrast, we focus on the self-supervised pretraining stage while [20] focuses on the supervised fine-tuning stage. Moreover, we achieve much higher accuracy when training from scratch and we investigate the transferring ability when training on small datasets.

3. Method

We first explain why we use parametric instance discrimination (Sec. 3.1), then analyze how our strategies help weight updating (Sec. 3.2), and describe the complete method.

3.1. Analyses on instance discrimination

As shown in Figure 1, an input image \( x_i \) \((i = 1, \cdots, N)\) is sent to a network \( f(\cdot) \) and get output representation \( z_i = f(x_i) \in \mathbb{R}^d \), where \( N \) denotes the total number of instances. Then, a fully connected (fc) layer \( W \) is used for classification and the number of classes equals the total number of training instances \( N \) for parametric instance discrimination. We denote \( w_j \in \mathbb{R}^d \) as the weights for the \( j \)-th
There are typically 2 views (i.e., positive pairs) for each input also give a theoretical interpretation of the contrastive prior the contrastive loss when we set \(w\) couranging the features to be roughly uniformly distributed on more aligned positive features and the uniformity term en-

\[
L_{\text{InsDis}} = - \sum_{i=1}^{N} \sum_{j=1}^{N} y^{(i)}_{c} \log P^{(i)}_{c} = - \sum_{i=1}^{N} \log P^{(i)}_{i} \tag{1}
\]

\[
= - \sum_{i=1}^{N} \log \frac{\exp(w^{T}_{i} z_{i})}{\sum_{i=1}^{N} \exp(w^{T}_{i} z_{i})} \tag{2}
\]

\[
= - \sum_{i=1}^{N} w^{T}_{i} z_{i} + \sum_{i=1}^{N} \log \sum_{j=1}^{N} e^{w^{T}_{i} z_{j}} , \tag{3}
\]

where the superscript \(i\) sums over instances while the sub-
script \(c\) sums over classes. For instance discrimination, the class label corresponds to the instance ID: \(y^{(i)}_{c} = 1\) iff \(c = i\).

Now we move on to the contrastive learning (CL) loss. There are typically 2 views (i.e., positive pairs) for each input \(x_{i}\) and we call them \(x_{iA}, x_{iB}\) (corresponding representations are \(z_{iA}, z_{iB}\)). The contrastive loss can be represented as follows (we omit hyper-parameter \(\tau\) for simplicity):

\[
L_{\text{CL}} = - \sum_{i=1}^{N} \log \frac{e^{z^{T}_{iA} z_{B}}}{\sum_{i=1}^{N} e^{z^{T}_{iA} z_{B}}} = - \sum_{i=1}^{N} z^{T}_{iA} z_{B} + \sum_{i=1}^{N} \log \left( e^{z^{T}_{iA} z_{B}} + \sum_{i=1}^{N} e^{z^{T}_{iA} z_{B}} \right) , \tag{4}
\]

where \(z_{B}^{-}\) enumerates all negative pairs for \(z_{i}\), i.e., \(z_{jA}\) and \(z_{jB}\) for all \(j \neq i\). Consider the loss term for the \(i\)-th instance:

\[
L^{(i)}_{\text{CL}} = - z^{T}_{iA} z_{iB} + \log \left( e^{z^{T}_{iA} z_{B}} + \sum_{j \neq i} e^{z^{T}_{iA} z_{j}} \right) \tag{5}
\]

If we set \(w_{i} = z_{i}\) in instance discrimination, then from Eq. 3 we have (also consider the \(i\)-th term):

\[
L^{(i)}_{\text{InsDis}} = - z^{T}_{iA} z_{i} + \log \left( e^{z^{T}_{iA} z_{i}} + \sum_{j \neq i} e^{z^{T}_{iA} z_{j}} \right) \tag{6}
\]

Moreover, we can also use multiple views in instance discrimination. If we set \(w_{j} = z_{jA}\), we have (see the appendix for detailed derivation):

\[
L^{(i)}_{\text{InsDis}} = - z^{T}_{iA} z_{iB} + \log \left( e^{z^{T}_{iA} z_{B}} + \sum_{j \neq i} e^{z^{T}_{iA} z_{j}} \right) \tag{7}
\]

In other words, the contrastive loss is a special case of instance discrimination, with each \(w_{j}\) set to the representation of \(x_{i}\) in the current batch (i.e., non-parametric instance discrimination). In contrast, the learnable fc \(W\) in instance discrimination has at least two advantages:

(i) Separate representation learning from learning specific properties of the loss. As known in many contrastive learning methods (e.g., SimCLR [8]), using extra projection head (MLPs) after representation is essential to learn good representations. However, we find that this projection head is not necessary for instance discrimination, thanks to the learnable weights \(W\) of this fc, as will be shown in Section 4.4.

(ii) Find potential similarities between instances (classes). Now we consider DeepClustering [5], whose clustering loss can be reformulated as follows using our notation:

\[
L_{\text{DC}} = - \sum_{i=1}^{N} \sum_{k=1}^{K} y^{(i)}_{k} \log P^{(i)}_{k} , \tag{8}
\]

where \(K\) denotes the number of clusters, \(y^{(i)}_{k}\) indicates whether the \(i\)-th instance belongs to the \(k\)-th cluster, and \(P^{(i)}_{k}\) denotes the probability that the \(i\)-th instance belongs to the \(k\)-th cluster. Let \(C_{k}\) denotes the index of instances in cluster \(k\), then if we set all \(\{w_{j} \mid j \in C_{k}\}\) to the same, i.e., \(w_{j} = \bar{w}_{k}\) for all \(j \in C_{k}\), we have:

\[
L_{\text{InsDis}} = - \sum_{i=1}^{N} \log P^{(i)}_{i} = - \sum_{k=1}^{K} \sum_{j \in C_{k}} \log P^{(j)}_{j} \tag{9}
\]

\[
= - \sum_{k=1}^{K} \sum_{j \in C_{k}} \log \sigma(w^{T}_{j} z_{j}) \tag{10}
\]

\[
= - \sum_{k=1}^{K} \sum_{j \in C_{k}} \log \sigma(\bar{w}^{T}_{k} z_{j}) , \tag{11}
\]

\(\sigma(\cdot)\) is the softmax function. Similarly, Eq. (8) becomes

\[
L_{\text{DC}} = - \sum_{k=1}^{K} \sum_{j \in C_{k}} \log P^{(j)}_{j} = - \sum_{k=1}^{K} \sum_{j \in C_{k}} \log \sigma(\bar{w}^{T}_{k} z_{j}) . \tag{12}
\]

Hence, when the weights \(W\) are appropriately set, instance discrimination is equivalent to the deep clustering
loss, which can observe potential instance similarities. As can be seen from Figure 2, instance discrimination learns more distributed representations and captures better intra-class similarities when compared to other methods.

Since in this paper we focus on ViTs, there is another important reason why we choose parametric instance discrimination: the simplicity and stability. As noted in [10], instability is a major issue that impacts self-supervised ViT training. Hence, the form of instance discrimination (cross entropy) is more stable and easier to optimize. It will be further demonstrated in Sec. 4.3 and Sec. 4.4 that our method can better adapt to various emerging ViT networks and does not rely on specific designs (e.g., projection MLP head).

3.2. Gradient Analysis

Consider the loss term for the $i$-th instance in Eq. (3):

$$L_{\text{InsDis}}^{(i)} = -w_i^T z_i + \log \sum_{j=1}^{N} e^{w_j^T z_i}. \quad (13)$$

Then, the gradient w.r.t. $z_i$ can be calculated as follows:

$$\frac{\partial L}{\partial z_i} = -w_i + \sum_{j=1}^{N} \frac{e^{w_j^T z_i}}{\sum_{k=1}^{N} e^{w_k^T z_i}} w_j \approx -w_i + \sum_{j=1}^{N} \frac{P_{j}^{(i)} w_j}{}, \quad (14)$$

and similarly the gradient w.r.t. $w_k$ is:

$$\frac{\partial L}{\partial w_k} = (P_k^{(i)} - \delta_{(k=i)}) z_i, \quad (15)$$

where $\delta$ is an indicator function, equals 1 iff $k = i$.

Notice that for instance discrimination the number of classes $N$ can easily go very large and there exists extremely infrequent visiting of instance samples [2, 19]. Hence for infrequent instances $k \neq i$, we can expect $P_k^{(i)} \approx 0$ and hence $\frac{\partial L}{\partial w_k} \approx 0$, which means extremely infrequent update of $w_k$. [2] and [19] introduced different strategies to alleviate the problems for large datasets, such as the high GPU computation and memory overhead. Since in this paper we focus on small datasets, such strategies are not necessary. Instead, we use CutMix [41] and label smoothing [27] to update the weight matrix more frequently by directly modifying the one-hot label, which are also commonly used in supervised training of ViTs. If we use label smoothing, then

$$y_c^{(i)} = \begin{cases} 1 - \epsilon & \text{if } c = i, \\ \frac{\epsilon}{N-1} & \text{otherwise} \end{cases}, \quad (17)$$

where $\epsilon$ is the smoothing factor and we set it to 0.1 through-out this paper. Then the loss becomes:

$$L_{\text{InsDis}}^{(i)} = -(1 - \epsilon) w_i^T z_i + (1 - \epsilon) \log \sum_{j=1}^{N} e^{w_j^T z_i} - \frac{\epsilon}{N-1} \sum_{k \neq i} w_k^T z_i + \epsilon \log \sum_{j=1}^{N} e^{w_j^T z_i} \approx -(1 - \epsilon) w_i^T z_i - \frac{\epsilon}{N-1} \sum_{k \neq i} w_k^T z_i + \log \sum_{j=1}^{N} e^{w_j^T z_i}. \quad (18)$$

If we continue to use CutMix, Eq. (18) becomes:

$$L_{\text{InsDis}}^{(i)} = -C_i w_i^T z_{i'k'} - C_{i'} w_{i'}^T z_{i'i'} + \log \sum_{j=1}^{N} e^{w_j^T z_{i'i'}},$$

where $\lambda$ is the mixed coefficient, $i'$ is the index of the other instance in CutMix, $z_{i'i'}$ is the output of the mixed input and

$$\begin{cases} C_i = \lambda (1 - \epsilon) + (1 - \lambda) \frac{1}{N-1} \\ C_{i'} = (1 - \lambda) (1 - \epsilon) + \lambda \frac{1}{N-1} \\ C = \lambda \frac{1}{N-1} \end{cases}. \quad (19)$$

And the gradient w.r.t. $w_k$ becomes:

$$\frac{\partial L}{\partial w_k} = \left( P_k^{(i')^'} - C_i \delta_{(k=i)} - C_{i'} \delta_{(k=i')} \right) z_{i'i'} + \left( C (1 - \delta_{(k=i)} - \delta_{(k=i')}) \right) z_{i'i'}. \quad (20)$$

If we set $\lambda = 0.5$ and $N = 2040$, then $C_i = C_{i'} \approx 0.45$ and $C \approx 2.5 \epsilon - 5$. Hence, we are able to update $w_k$ even for instances $k \neq i$ (with relative large gradients for $w_i$ and $w_{i'}$ and small gradients for others), which alleviates the infrequent updating problem. Moreover, we can also alleviate the overfitting problem by using CutMix as our regularization with limited data, as revealed in [41,42].

In conclusion, we use the following strategies to enhance instance discrimination on small datasets:

1. Small resolution. It has been shown in [3] that small resolution during pretraining is useful for small datasets.

2. Multi-crop. As analyzed before, instance discrimination generalizes the contrastive loss to capture both feature alignment and uniformity when using multiple crops.

3. CutMix and label smoothing. As analyzed above, it helps us alleviate the overfitting and infrequent accessing problem when applying instance discrimination.

We name our method as instance discrimination with multi-crop and CutMix (IDMM) and we conduct ablation studies on these strategies in Sec. 4.4.

4. Experiments

We used 7 small datasets for our experiments, as shown in Table 1. First, we explain the reasons why do we need
training from scratch in Sec. 4.1 and training from scratch results in Sec. 4.2. Then, we study the transferring ability of ViTs pretrained on small datasets (even facilitate large-scale datasets training) in Sec. 4.3. Finally, we conduct ablation studies on different components in Sec. 4.4. All our experiments were conducted using PyTorch, and we used Titan Xp GPUs for ImageNet experiments and Tesla K80 for small datasets. Codes will be made publicly available.

4.1. Why training from scratch?

We explain the reasons why do we need training from scratch directly on target datasets from 3 aspects:

- **Data.** Current ViT models are often pretrained on a large-scale dataset (such as ImageNet or even larger ones), and then fine-tuned in various downstream tasks. Moreover, the lack of the typical convolutional inductive bias makes these models more data-hungry than common CNNs. Hence, it is critical to investigate whether we can train ViTs from scratch for a task where the total amount of available images is limited (e.g., 100 categories with roughly 20 images per category).

- **Computing.** The combination of a large-scale dataset, a large number of epochs and a complex backbone network means that ViT training are extremely computationally expensive. This phenomenon makes ViT a privilege for researchers at few institutions.

- **Flexibility.** The pretraining followed by downstream fine-tuning paradigm will sometimes become cumbersome. For instance, we may need to train 10 different models for the same task, and deploy them to different hardware platforms [1], but it is impractical to pretrain 10 models on a large-scale dataset.

As shown in Fig. 3, it is obvious that ImageNet pretrained models need much more data and computational cost when compared to training from scratch. Moreover, when we need to deploy models of different sizes on terminal devices, training from scratch provides better parameter-accuracy trade-offs. For instance, the smallest ImageNet pretrained model of PVTv2 (i.e., B0) has 3.4M parameters, which may still be too big for some devices. In contrast, we can train
We use 112x112 resolution during pretraining and 224x224 methods are pretrained for 800 epochs and then fine-tuned for both CNNs and ViTs in Table 2. For fair comparisons, all our IDMM. We follow the settings in the original papers for $\alpha$ as in the fine-tuning stage. We set $\alpha = 0.5$ and $\gamma$ for CutMix in all methods are pretrained for 800 epochs and our IDMM follows the same training settings as in the fine-tuning stage. We set $\alpha = 0.5$ for CutMix in our IDMM. We follow the settings in the original papers for other methods and more details are included in the appendix. We use 112x112 resolution during pretraining and 224x224 during fine-tuning for all methods, as suggested in [3].

First, we compare our method with popular SSL methods for both CNNs and ViTs in Table 2. For fair comparisons, all methods are pretrained for 800 epochs and then fine-tuned for 200 epochs. As can be seen in Table 2 and Figure 4, SSL pretraining is useful even when training from scratch and all SSL methods perform better than random initialization. Our method achieves the highest accuracy on all these datasets, except for aircraft. When the number of images is small (e.g., flowers and pets), the advantage of our method is more obvious, which is consistent to our analyses before.
Then, following [3], we fine-tune the models for longer epochs to get better results. Specifically, with the IDMM initialized weights, we first fine-tune for 800 epochs under 224x224 resolution and then continue fine-tuning for 100 epochs under 448x448 resolution. As shown in Table 3, we achieve the state-of-the-art results when training from scratch on these 7 datasets for all these ViT models, to the best of our knowledge. Moreover, the gap between training from scratch and using ImageNet pretrained models (colored in gray) has been greatly reduced using our method, which indicates that training from scratch is promising even for ViT models. Notice that PVTv2 models achieve better performance than DeiT and T2T by introducing convolutions to ViTs. The introduction of the typical convolutional inductive bias makes it less data-hungry than common ViTs and hence achieving better performance on these small datasets.

Further, we also investigate the randomness during both the pretraining and fine-tuning stage because the number of training images is small. For the pretraining stage, we pretrained 3 different models (using our method) and fine-tune these models separately. For the fine-tuning stage, we fine-tune 3 times with one pre-trained model. As shown in Table 4, the standard deviation is small in both stages on the two smallest datasets and hence we only report single run results in Table 2 and 3.

### 4.3. Transfer ability of small datasets

Having investigated training from scratch on small datasets for ViT models, we now study the transfer ability of the representations learned on these small datasets. The transfer ability of representations pretrained on large-scale datasets has been well studied, but few works studied the transfer ability of small datasets.

In Table 5 we evaluate the transferring accuracy of models pretrained on different datasets. As in Sec. 4.2, we train 800 epochs for pretraining and fine-tuning 200 epochs. The on-diagonal cells (colored gray) perform pretraining and fine-tuning on the same dataset. The off-diagonal cells evaluate transfer performance across these small datasets. From Table 5 we can have the following observations:

- ViTs have good transferring ability even when pretrained on small datasets. This means that we can use pretrained models from small datasets to transfer to other datasets in different domains to improve performance.
- Our method also has higher transferring accuracy on all these datasets when compared to SimCLR and SupCon. As analyzed before, we think that it is due to the learnable fully connected layer $W$, which can capture both feature alignment and instance similarity. Also, the learnable fc better protects features from learning specific properties of the loss, as will be shown in Sec. 4.4.
- We can obtain surprisingly good results even if the pretrained dataset and the target dataset are not in the same domain. For instance, models pretrained on Indoor67 achieve the highest accuracy when transfer to Aircraft. It is obvious that the number of images in the pretrained dataset matters, because Cars performs best in all. However, we want to argue that it is not the only reason because we can see that Indoor67 and CUB perform better than Cars in some cases despite having fewer training images. We leave it to future work to study what properties matter for pretraining datasets when transferring.

After observing that models pretrained on small datasets have surprisingly good transferring ability, we can further ex-
plore the potential of small datasets. We sample the original ImageNet to smaller subsets with 10,000 images (SIN-10k), motivated by [3]. By pretraining models on SIN-10k, we evaluate the performance when transferring to small datasets in Table 6 as well as the large-scale dataset ImageNet in Table 7. In Table 6 we compare our method with various SSL methods as well as the supervised baseline under different backbones. It can be seen that our method has a large edge over these comparison methods and representations learned on SIN-10k can serve as a good initialization when transferring to other datasets. It is worth noting that MoCov3 and DINO fail to converge under T2T-ViT-7 after trying various hyper-parameters so we don’t report the results for them in Table 6. It indicates our method can be easily applied to emerging ViTs without the need of special design or tuning.

Furthermore, we investigate whether we can benefit from pretraining on 10,000 images when training on ImageNet. As can be seen in Table 7, using the representation learned from 10,000 images as initialization can greatly accelerate the training process and finally achieve higher accuracy (about 1 point) on ImageNet. Notice that we sampled a balanced subset before (10 images per class) and we also compare with the setting where we randomly sample 10,000 images without using label information (SIN-total 10k). As can be seen, whether to use labels when sampling (balanced or not) has no effect on the result, as noted in [39].

### 4.4. Ablation studies

In this section, we first investigate the effect of different components in our method in Table 8. Then, we investigate the effect of the projection MLP head in Table 9.

As can be seen in Table 8, all the 4 strategies are useful and combining all these strategies achieves the best results. The experimental results further confirm the analyses in Sec. 3.1 that using multiple views and CutMix is helpful.

In Table 9, all methods are pretrained for 800 epochs on SIN-10k and then fine-tuned for 200 epochs when transferring to target datasets. The projection MLP head is essential for contrastive methods like SimCLR while it is not the case for instance discrimination. It further confirms the analyses in Sec. 3.1 that the learnable fc $W$ protects features from learning specific properties of the loss and hence achieving better transferring ability. In contrast, the $W$ in contrastive loss is not learnable and they need extra projection head.

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### 5. Conclusions

In this paper, we proposed a method called IDMM for (pre)training ViTs with small data and the effectiveness of the proposed approach is well validated by both theoretical analyses and experimental studies. We achieved state-of-the-art results on 7 small datasets under various ViT backbones when training from scratch. Moreover, we studied the transferring ability of small datasets and found that ViTs also have good transferring ability even when pre-trained on small datasets. However, there is still room for improvement when training from scratch on these small datasets for architectures like DeiT. Furthermore, it is still unknown what properties matter for pretraining on small datasets when transferring and we leave them to future work.

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**Table 6. Transferring ability when pretrained on 10,000 images from ImageNet. All elements are obtained by finetuning for 200 epochs.**

| Backbone | Pretraining | Transferring Accuracy |
|----------|-------------|-----------------------|
|          | Datasets    | Flowers | Pets | Dtd | CUB | aircraft | Cars |
| PVTv2-B0 | SIN-10k     | IDMM    | 93.8 | 83.6 | 66.8 | 69.4     | 76.7 | 81.3 | 87.5 |
|          |             | MoCov3  | 91.0 | 81.4 | 62.3 | 66.3     | 63.7 | 74.5 | 86.2 |
|          |             | DINO    | 92.3 | 83.6 | 65.9 | 68.5     | 65.8 | 76.9 | 86.4 |
|          |             | supervised | 92.9 | 81.7 | 66.1 | 65.9     | 66.6 | 78.7 | 86.0 |
| PVTv2-B3 | SIN-10k     | IDMM    | 95.9 | 88.4 | 70.1 | 73.6     | 76.8 | 87.5 | 92.9 |
|          |             | MoCov3  | 95.7 | 87.1 | 66.0 | 70.5     | 65.7 | 82.2 | 89.3 |
|          |             | DINO    | 95.0 | 87.8 | 68.5 | 73.4     | 72.4 | 86.1 | 92.5 |
|          |             | supervised | 90.9 | 80.9 | 62.9 | 63.3     | 65.6 | 81.8 | 89.7 |
| T2T-ViT-7| SIN-10k     | IDMM    | 89.8 | 74.1 | 63.5 | 62.6     | 55.2 | 72.7 | 82.4 |
|          |             | supervised | 80.8 | 57.8 | 57.5 | 50.7     | 55.6 | 56.8 | 59.9 |

**Table 7. Top-1 accuracy (%) on ImageNet.**

| Backbone | Method              | Epochs | Acc. (%) |
|----------|---------------------|--------|----------|
| PVTv2-B0 | random init.        |        | 68.6     |
|          | MoCov3 (SIN-10k)    | 100    | 68.8     |
|          | IDMM (SIN-10k)      |        | 69.5     |
|          | random init.        | 300    | 70.0     |
|          | IDMM (SIN-total 10k)|        | 70.9     |
| DeiT-Tiny| random init.        | 100    | 66.8     |
|          | IDMM (SIN-10k)      |        | 67.8     |
|          | random init.        | 300    | 72.2     |

**Table 8. Ablation studies when training from scratch on flowers.**

| method | LS | small res. | multi-crop | CutMix | Acc. (%) |
|--------|----|------------|------------|--------|----------|
| InsDis | ✓  | ✓          | ✓          | ✓      | 70.4     |
| ✓      | ✓  | ✓          | ✓          | ✓      | 73.1     |
| ✓      | ✓  | ✓          | ✓          | ✓      | 76.9     |
| ✓      | ✓  | ✓          | ✓          | ✓      | 79.9     |

**Table 9. The effect of MLP head. All pretrained on SIN-10k.**

| backbone | method | proj. | MLP | flowers | pets | dtd | cub |
|----------|--------|-------|-----|--------|------|-----|-----|
| DeiT-Tiny| IDMM   |      |     |        |      |     |     |
|          |        |      |     |        | 86.6 | 65.3 | 59.1 |
|          |        |      |     |        | 51.2 | 57.8 | 47.6 |
| SimCLR   |      |      |     |        | 83.3 | 62.1 | 58.9 |
|          |        |      |     |        | 48.0 |     | 45.8 |
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A. Detailed Derivations of Eq. 6&7

From the main paper we know that

$$L^{(i)}_{\text{InsDis}} = -\mathbf{w}_i^T \mathbf{z}_i + \log \sum_{j=1}^{N} e^{\mathbf{w}_j^T \mathbf{z}_i}$$  \hspace{1cm} (21)

Now if we use 2 views ($\mathbf{x}_{iA}$ and $\mathbf{x}_{iB}$) for each instance in instance discrimination, then from Eq. (21) we have:

$$L^{(i)}_{\text{InsDis}} = -\mathbf{w}_i^T \mathbf{z}_{iA} + \log \sum_{j=1}^{N} e^{\mathbf{w}_j^T \mathbf{z}_{iA}} - \mathbf{w}_i^T \mathbf{z}_{iB} + \log \sum_{j=1}^{N} e^{\mathbf{w}_j^T \mathbf{z}_{iB}},$$  \hspace{1cm} (22)

where $\mathbf{z}_{iA}$ and $\mathbf{z}_{iB}$ are corresponding representations of $\mathbf{x}_{iA}$ and $\mathbf{x}_{iB}$. If we set $\mathbf{w}_j = \mathbf{z}_{jA}$ for $\forall j$, we have:

$$L^{(i)}_{\text{InsDis}} = -\mathbf{z}_i^T \mathbf{z}_{iA} + \log \left( e^{\mathbf{z}_i^T \mathbf{z}_{iA}} + \sum_{j \neq i} e^{\mathbf{z}_j^T \mathbf{z}_{iA}} \right)$$

$$- \mathbf{z}_i^T \mathbf{z}_{iB} + \log \left( e^{\mathbf{z}_i^T \mathbf{z}_{iB}} + \sum_{j \neq i} e^{\mathbf{z}_j^T \mathbf{z}_{iB}} \right)$$

$$= -\mathbf{z}_i^T \mathbf{z}_{iA} + \text{alignment}$$

$$- \mathbf{z}_i^T \mathbf{z}_{iB} + \text{uniformity}$$

$$= -\mathbf{z}_i^T \mathbf{z}_{iA} + \text{constant}$$

$$+ \log \left( e^{\mathbf{z}_i^T \mathbf{z}_{iB}} + \sum_{j \neq i} e^{\mathbf{z}_j^T \mathbf{z}_{iA}} \right)$$

$$= -\mathbf{z}_i^T \mathbf{z}_{iA} + \text{uniformity}$$

$$- \mathbf{z}_i^T \mathbf{z}_{iB} + \text{constant}$$

B. Training details

The training details for MoCov2, MoCov3, SimCLR, SupCon and DINO in Table 2 in the paper are shown in Table 10.

| Method   | opt    | bs   | lr       | wd     | dim | schedule | $\tau$ | k    |
|----------|--------|------|----------|--------|-----|----------|--------|------|
| MoCov2   | SGD    | 256  | 5e-4     | 0.001  | 256 | cosine   | 0.2    | 2048 |
| MoCov3   | adamW  | 256  | 1.5e-4   | 0.1    | 256 | cosine   | 0.2    | -    |
| SimCLR   | SGD    | 512  | 5e-4     | 0.001  | 256 | cosine   | 0.1    | -    |
| Supcon   | SGD    | 512  | 5e-4     | 0.001  | 256 | cosine   | 0.1    | -    |
| DINO     | adamW  | 512  | 5e-4     | 0.04   | 256 | cosine   | 0.1    | -    |