

Improving Contrastive Learning by Visualizing Feature Transformation

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Abstract

Contrastive learning, which aims at minimizing the distance between positive pairs while maximizing that of negative ones, has been widely and successfully applied in unsupervised feature learning, where the design of positive and negative (pos/neg) pairs is one of its keys. In this paper, we attempt to devise a feature-level data manipulation, differing from data augmentation, to enhance the generic contrastive self-supervised learning. To this end, we first design a visualization scheme for pos/neg score¹ distribution, which enables us to analyze, interpret and understand the learning process. To our knowledge, this is the first attempt of its kind. More importantly, leveraging this tool, we gain some significant observations, which inspire our novel Feature Transformation proposals including the extrapolation of positives. This operation creates harder positives to boost the learning because hard positives enable the model to be more view-invariant. Besides, we propose the interpolation among negatives, which provides diversified negatives and makes the model more discriminative. It is the first attempt to deal with both challenges simultaneously. Experiment results show that our proposed Feature Transformation can improve at least 6.0% accuracy on ImageNet-100 over MoCo baseline, and about 2.0% accuracy on ImageNet-1K over the MoCoV2 baseline. Transferring to the downstream tasks successfully demonstrate our model is less task-bias. Visualization tools and codes: <https://github.com/DTennant/CL-Visualizing-Feature-Transformation>.

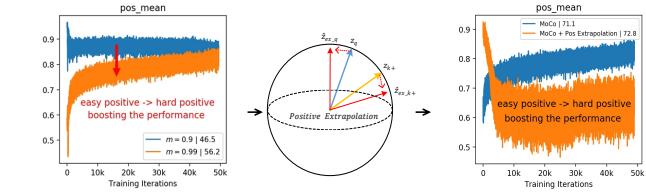
1. Introduction

Finetuning from ImageNet [34] supervised pre-train networks [16, 37, 19] for down-stream tasks, such as object detection [27, 31, 32] and semantic segmentation [28, 5], is a de facto dominant approach in computer vision community. But recently self-supervised contrastive learn-

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¹Pos/neg score indicates cosine similarity of pos/neg pair.



(a) Observation

(b) Proposed Method

(c) Performance Gain

Figure 1. The motivation of visualizing the score distribution. (a) It draws the score distribution of positive pairs for m (the momentum in MoCo[14]) being 0.99 and 0.9, showing that smaller positive scores generally need longer time to converge and obtain better accuracy. (b) Inspired by (a), we apply extrapolation on positive pairs to slightly decrease the scores, generating harder positives. (c) Leveraging the extrapolation of positives, we improve the performance from 71.1% (the blue) to 72.8% (the orange). The performance increase is consistent with the change of distribution. The mean score of positive pairs changes from blue plot (before extrapolation) to orange plot (after extrapolation).

ing achieves comparable transfer performance without the human-provided annotations. One of the key issues of contrastive learning is to design positive and negative (pos/neg) pairs to learn an embedding space such that the positives stay closer in the space while the negatives are pushed away.

Most existing approaches [4, 6, 40, 7] acquire pos/neg pairs by data augmentation, which exploits various views of the same image to form positive pairs. For example, CMC[39] uses the luminance and chrominance color channel of an image as two views. InfoMin [40] demonstrates that incremental data augmentations indeed lead to decreasing mutual information between views and thus improve transfer performance. In other words, an effective positive pair prefers to convey more variance of one instance. With a series of promotions, the contrastive learning methods based on data augmentations [4, 6, 40, 7] are achieving closer to the fully supervised performance on ImageNet[6].

Most previous data augmentations (*e.g.*, cropping, color distortion) are directly sourced from human intuitions, which may lack much interpretability, thus they can not guarantee their effectiveness. We argue, however, that the feature-level data manipulation (*i.e.*, feature transformation) can provide more explainable or effective pos/neg pairs to

enhance the feature embedding. To this end, we first design a scheme to visualize the pos/neg pair score distributions during the training. We believe that, from these score distributions, we can reveal and explain how the model parameter values affect its performance. The visualization can help us trace back the training process. Moreover, it enables us to observe the characteristics of the pos/neg pairs, and then invent more effective feature transformations (**FT**).

Figure 1 demonstrates the motivation of score visualization. By plotting the score distributions under different momentum values of MoCo [14], we can clearly observe that the case of $m = 0.99$ has smaller positive scores while achieves better performance. A small positive score indicates less similarity between the pair, which means this positive pair actually carrying large view variance of one example. Actually, this is consistent with the goal of feature learning, which targets at a more view-invariant visual representation. Therefore, we conjecture that “hard positives” are the ones conveying large view variance of a sample. Inspired by this observation, we introduce an extrapolation operation on positive pairs to increase view variance and thus acquire hard positives. Figure 1(c) shows that the extrapolation of positives can boost the model performance from the “blue” one to the “orange” one.

Besides, to make full use of negative features, we propose the random interpolation among negatives, which intuitively provides diversified negatives for each training step and makes the model more discriminative.

Unlike the traditional data augmentation, our feature transformation does not bring additional training examples. Instead, it aims at reshaping the feature distribution by manipulating both positive and negative pairs. Basically, our feature transformation will create hard positives and diversified negatives to learn a more view-invariant (hard positive) and a more discriminative (diversified negatives) representation. It is directly driven by the performance of the learned representation, while data augmentation is kind of blind to the performance. Furthermore, our feature transformation makes the model less “task-bias”, which means we can achieve performance improvement for various downstream tasks. It has been verified by our experiments on object detection, instance segmentation, and long-tailed classification with significant improvement.

Both our visualization tool and feature transformation are generic, and can be applied to various self-supervised contrastive learning including MoCo[14], SimCLR[6], InfoMin[40], SwAv[4], SimSiam[8]. In the following sections, we employ the classic model MoCo to demonstrate our framework. To summarize, our contributions include:

- We are the first to design a visualization tool to analyze and interpret how the score distribution of pos/neg pairs affects the model’s capability. The visualization also helps us come into some significant observations.

- Inspired by the observations on the model visualization, we propose a simple yet effective feature transformation, which creates both “hard positives” and “diversified negatives” to enhance the training. The feature transformations enable to learn more “view-invariant” and discriminative representations.
- We conduct thorough experiments and our model achieves the state-of-the-art performance. In addition, the experiments on the downstream tasks successfully demonstrate our model is less task biased.

2. Related Work

Contrastive Learning: Contrastive losses have been widely used in self-supervised learning and brought significant improvements on classification [13, 1, 14, 39, 40, 6, 7, 12, 4, 18, 2, 57, 47, 50, 9, 3, 39, 43, 49, 54, 45, 44, 23] and detection [46, 51, 52, 53]. InfoMin [40] uses the lower bound of NCE to demonstrate that incremental data augmentations lead to decreasing mutual information between views and thus improve transfer performance. In other words, relatively harder data augmentation for contrastive learning boosts the transfer performance[20, 6]. We show that our proposed feature transformation can be easily adopted on current state-of-the-art models.

MixUp for contrastive learning Mixup [56] and its numerous variants [42, 55, 21] provide highly effective data augmentation strategies when paired with a cross-entropy loss for supervised and semi-supervised learning. Manifold mixup [42] is a feature-level regularization for supervised learning while Un-mix [36] proposes using mixup in the image/pixel space for self-supervised learning; And in MoChi [20] the authors propose mixing the negative sample in the embedding space for hard negatives augmentation but hurt the classification accuracy. i-Mix [24] proposed a strategy mixing instances in both input and virtual label spaces to regularize contrastive training. In this paper, we proposed to use feature transformation rather than data augmentation. Positive features are extrapolated to increase the hardness of positives, and negative features in the memory queue are interpolated to increase the diversity. Our FT provides more efficacy compared with augmentations.

Generating examples for metric learning: The idea of generating new examples for metric learning has been explored by [26, 10, 22]. The Embedding Expansion [22] work uses uniform interpolation between two positive and negative points, creates a set of synthetic points, and then selects the hardest pair as negative. [26, 10] generate new hard examples by generators and improve performance for metric learning. Different from the approaches [26, 10] for supervised metric learning, our pos/neg FTs are aiming at self-supervised learning and doesn’t require labels, extra parameters and loss terms to be optimized.

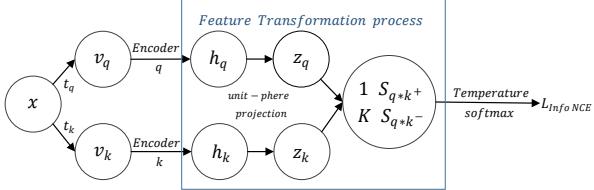


Figure 2. Feature Transformation Contrastive learning pipeline.

3. Visualization of Contrastive Learning

3.1. Preliminaries

Let us start from the basic procedures of contrastive learning, as shown in Figure 2. Each data sample x passes through two separate data augmentation pipeline t_q and t_k , which are randomly sampled from the same data augmentation pool, and two views v_q and v_k will be acquired to construct positive pairs [6, 12]. The encoder q and k ² will respectively map two views into feature embedding space. An ℓ_2 normalization is applied on feature vector h_q and h_k to project the corresponding vector h_q and h_k (*i.e.*, $z_q = h_q / \|h_q\|_2$) onto the unit sphere and obtain z_q and z_k . Their inner product will produce the cos similarity score, namely one positive pair score $S_{q,k+}$ and K negative pair scores $S_{q,k-}$. These pair scores are input to InfoNCE loss 1 for contrastive learning:

$$\mathcal{L} = -\log \left[\frac{\exp(S_{q,k+}/\tau)}{\exp(S_{q,k+}/\tau) + \sum_K \exp(S_{q,k-}/\tau)} \right] \quad (1)$$

Here we roughly defined Feature Transformation process as certain manipulations on encoder embeddings h_q and h_k , in order to reshape the distribution of the output pos/neg pair score ($S_{q,k+}$ and $S_{q,k-}$), for better contrastive learning in the follow-up InfoNCE loss. The most common FT applied in current SOTA is the [4, 6, 40, 7, 14] unit-sphere projection of ℓ_2 normalization. We provide empirical studies of this regular FT and illustrate its importance for significant constriction of feature length (ℓ_2) in Supp F.

3.2. Score Distribution Visualization

We choose to visualize the score distribution of pos/neg pairs instead of the loss curves and transfer accuracy, as the inside training dynamics can unearth the learning capability of the model. Specifically, there are two practical reasons: (1) The basic idea of InfoNCE loss is to compare the pos/neg scores in a log-softmax manner, so visualizing the input score pairs can help study the contrastive learning process. (2) The normalized feature vectors z_q and z_k are high-dimensional, which is challenging for storage and visualization; The exponential amplification of scores is too large to observe the details of characteristics of pos/neg scores.

²Encoder q and k might be the same [6] or different network [14, 12].

m	≤ 0.5	0.6	0.7	0.8	0.9	0.99	0.999	1
acc (%) collapse	21.2	32.8	39.3	46.5	56.2	53.1	31.2	

Table 1. The parameter experiments of m on MoCo ($\tau = 0.07$).

However, $S_{q,k}$ is one-dimensional and limited to $[-1, 1]$, which is suitable to observe inside the contrastive process.

Notice that this practical visualization tool is offline and doesn't affect training speed with negligible computation. Even with larger datasets and batch size, it's still feasible. The details of the visualization tool are present in Supp A.

3.3. Visualization Examples with MoCo

We choose the computationally-efficient model, MoCo [14] as an example to demonstrate our visualization design. **Momentum Update Mechanism:** Memory queue [49] is an initial approach for solving the large batch computational burden which stores K negative features in the memory that will be updated using the output of the encoder at each training step. However, the rapid change of the encoder (f_q and f_k) could bring inconsistency into the memory queue which usually contains outdated features. MoCo solves the inconsistency issue by leveraging a momentum update mechanism [38] where only f_q is updated by back-propagation and the f_k is updated by momentum mechanism:

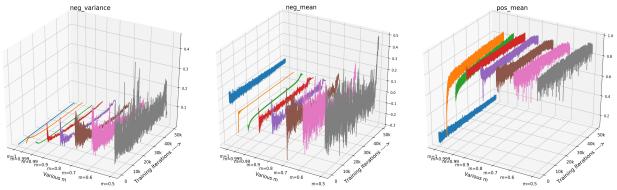
$$\theta_{f_k} \leftarrow m\theta_{f_k} + (1-m)\theta_{f_q} \quad (2)$$

where $m \in [0, 1]$ is the momentum coefficient and has a huge influence to the final transfer accuracy. The memory queue is then updated using the features from f_k because the momentum update of f_k brings a smoother change of features that could reduce the inconsistency in memory queue.

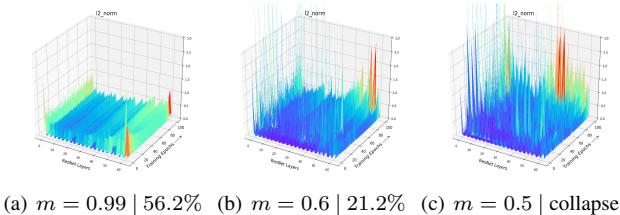
In the following sections, we provide thorough experiments and visualization analysis to show how the parameter m affects the contrastive learning process. We attempt various m for MoCo on ImageNet-100 (denoted as IN-100) [39] with linear readout protocol for evaluation (details in Supp B). As the Tab 1 shown, with the decrease of m (increasing the update speed of encoder f_k), the accuracy presents an inverse U-shape and the max 56.24% locates at $m = 0.99$ and the model collapse³ when $m \leq 0.5$. The trend of these results is similar with BYOL [12].

We choose three non-trivial statistics to visualize the score distribution: the mean of pos/neg scores (indicating the approximate average of the pos/neg pair distance) and the variance of negative scores (indicating the fluctuation degree of the negative samples in the memory queue). As shown in Fig 3(a), when m becomes smaller, the update speed of encoder k is increasing, leading to incremental differences of features among training steps, which is reflected as the growing variance of negative scores of the queue,

³Model collapse means that the transfer accuracy with linear readout protocol can not achieve the accuracy of training from random initialization, *i.e.*, 15.90%, indicating the negative effect brought by pre-train.

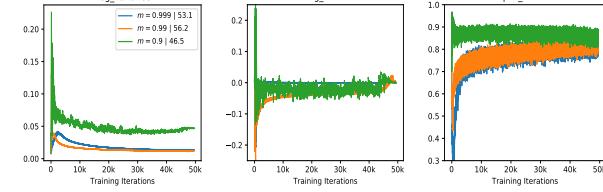


(a) Var of neg scores (b) Mean of neg scores (c) Mean of pos scores
Figure 3. Pos/neg score statistics of various m in MoCo training



(a) $m = 0.99 | 56.2\%$ (b) $m = 0.6 | 21.2\%$ (c) $m = 0.5 | \text{collapse}$

Figure 4. Gradient (ℓ_2 norm) landscape of various m



(a) Var of neg scores (b) Mean of neg scores (c) Mean of pos scores

Figure 5. 2D view of pos/neg score statistics of various m

namely the inconsistency. Specifically, when $m = 1$ (no update of f_k during training), the variance is closed to zero (blue line) while the variance of $m = 0.9$ (red) is larger but relatively unstable. $m = 0.5$ (grey) brings more violent fluctuations/inconsistency in the memory queue, leading to a poor transfer accuracy even model collapse.

Inside Analysis of Model Collapse: The model collapse is caused by various reasons. Small m (fast update speed of f_k) brings not only the inconsistency, but also the confusion of negative scores. For the mean of neg scores (lines in Fig 3(b)), the volatility degree of $m = 0.6$ (pink) and $m = 0.5$ (grey) is much sharper than the best model $m = 0.99$ (green). The mean of neg scores reflects the approximate score for all the negative pairs in the memory queue. If it becomes drastically volatile with the training process, the corresponding loss value and gradient will fluctuate violently, resulting in bad convergence. As shown in Fig 4, the smooth and stable gradient landscape of $m = 0.99$ (Fig 4(a)) becomes sharp and messy with the decrease of m (Fig 4(b) for $m = 0.6$ and Fig 4(c) for $m = 0.5$). Details of gradient landscape are put in Supp C. *Basically, to learn a better pre-trained model, we need to prepare negative pairs that can maintain the stability and smoothness of score distribution and gradient for the training process, which is similar to supervised learning [35].*

α_{ex}	-	0.2	0.4	0.6	1.4	1.6	2.0
acc (%)	71.1	71.6	71.8	71.9	72.7	72.4	72.8

Table 2. Various α_{ex} for positive extrapolation, the best result is marked in bold. We employ ResNet-50 [16] for the results. '-' indicates MoCo baseline without using extrapolation.

Hard Positive Boosts Performance: Small m not only indicates the faster update speed, but also more similarity between encoder f_k and f_q , i.e., in an extreme case, when $m = 0$, the parameters θ_k is completely the same with θ_q in each training step. The increasing similarity of encoder f_q and f_k will reduce the dissimilarity between z_q and z_{k+} , and only the view variance brought by data augmentations remains, leading to a higher positive score. Fig 3(c) shows that high positive scores of $m \leq 0.9$ will produce easy positive pairs with the close distance and little view variance in feature space.

However, in Fig 5(c), when we increase m from 0.9 (green) to 0.99 (orange), the easy pos pair becomes hard pos pair (from very similar 0.9 to less similar 0.7), leading to a higher transfer accuracy (46.5% v.s 56.2%, 9.7% increased). Note that this observation (converting easy positive to hard one) could be explained by InfoMin principle [40]: Raising the view variance between z_q and z_{k+} corresponds to increasing the mutual information for contrastive learning, which forces the encoder learns a more robust embedding and thus improves the transfer accuracy.

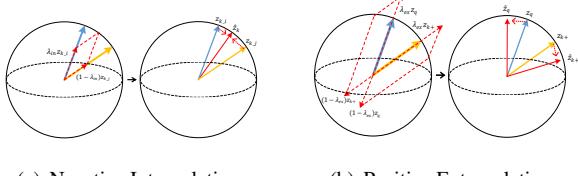
In the guarantee of stable and smooth score distribution and gradient, we can adopt some feature transformation methods which create hard ones by decreasing easy positive scores. Thus, we propose a positive feature extrapolation method to improve transfer accuracy in section 4.1.

4. Proposed Feature Transformation Method

The learning objective of Info-NCE is to draw the positive pair (z_q and z_{k+}) closer while pushing away negative pairs (z_q and all the z_{k-} in memory queue) in the embedding space. Therefore, we could directly apply feature transformation on the pos/neg features, in order to provide appropriate regularization [42] or make the learning harder [40]. Specifically, we develop positive extrapolation to transform the original positive pair to be further to increase the hardness and negative interpolation of memory queue to increase the diversity of negative samples, as Fig 6 shown. Notably, our method does not change the loss terms because it only replaces original pair scores with the new transformed pos/neg scores for calculating loss term.

4.1. Positive Extrapolation

Following the discussion in Sec 3.3 which indicates that lowering the easy positive pair scores to create hard positive pairs during training could be beneficial for the final transfer performance. Thus we would like to explore a way to



(a) Negative Interpolation (b) Positive Extrapolation

Figure 6. The process of our proposed negative interpolation and positive extrapolation. For the negative interpolation, we randomly interpolate two features in memory queue to produce a new negative. For positive extrapolation, the two positive features are pushed away from each other using extrapolation, changing easy positives to hard positives, which is better for contrastive learning.

manipulate the positive features z_q and z_{k+} to increase the view variance between them during training.

First, we simply adopt weighted addition for the two positive features to generate new feature:

$$\begin{aligned}\hat{z}_q &= \lambda_{ex} z_q + (1 - \lambda_{ex}) z_{k+} \\ \hat{z}_{k+} &= \lambda_{ex} z_{k+} + (1 - \lambda_{ex}) z_q\end{aligned}\quad (3)$$

where \hat{z}_q and \hat{z}_{k+} are the transformed new features. Meanwhile, considering the design principle of mixup [42, 56], we make sure that the summation of weights equals to 1. More importantly, we should guarantee than the transformed pos score $\hat{S}_{q \cdot k+}$ is smaller than the original pos score $S_{q \cdot k+}$, namely $\hat{z}_q \hat{z}_{k+} \leq z_q z_{k+}$. Take Equation 3 into the transformed score:

$$\hat{S}_{q \cdot k+} = 2\lambda_{ex}(1 - \lambda_{ex})(1 - S_{q \cdot k+}) + S_{q \cdot k+} \leq S_{q \cdot k+} \quad (4)$$

Because $S_{q \cdot k+} \in [-1, 1]$ and thus $(1 - S_{q \cdot k+}) \geq 0$. To make sure the lower score $\hat{S}_{q \cdot k+} \leq S_{q \cdot k+}$, we need to set $\lambda_{ex} \geq 1$ to let $2 \cdot \lambda_{ex}(1 - \lambda_{ex}) \leq 0$. So we choose $\lambda_{ex} \sim Beta(\alpha_{ex}, \alpha_{ex}) + 1$ ⁴ is sampled from a beta distribution and then adding 1 results in a range of $(1, 2)$. And the range of transformed pos score will be $\hat{S}_{q \cdot k+} \in [-4 + 5S_{q \cdot k+}, S_{q \cdot k+}]$.

Intuitively, it can be seemed as a simple approach to push away z_q and z_{k+} in feature space. After extrapolation, the distance between the extrapolated feature vector is enlarged. Therefore the extrapolation can serve as a feature transformation to create hard positives from easy ones. As shown in Fig 6(b), it brings a minor direction change for two positive vectors and meanwhile conveying a larger view variance of a sample for better contrastive learning. The visualization of lowering pos score by extrapolation is shown in Fig 1(c).

We evaluate the efficacy of positive extrapolation on IN-100 and attempt various α_{ex} in Tab 2. The positive extrapolation with various α_{ex} consistently improves the accuracy from the baseline MoCo (71.1%), which clearly

⁴We choose to set the two parameter α_{ex} of the beta distribution to be the same, because the two mixed features are symmetrical. And the same applies to the negative feature interpolation.

Method	α_{ex}	pos interpolation/extrapolation
MoCo	0.2	69.1 / 71.6
(baseline: 71.1)	2.0	67.4 / 72.8

Table 3. Positive extrapolation v.s. interpolation. Interpolation hurts the performance while extrapolation improves.

demonstrates the efficacy of positive extrapolation. It is interesting that $\alpha_{ex} > 1$ will get better results than those of $\alpha_{ex} < 1$. Because the beta distribution with $\alpha_{ex} < 1$ provides extreme large or small λ_{ex} with high probability, e.g., 1.1 or 1.9, while the beta distribution with $\alpha_{ex} > 1$ gives neutral $\lambda_{ex} = 1.5$ with high probability⁵. According to Equation 4, extreme λ_{ex} will bring too much/little hardness, so the corresponding performance is not robust as the neutral one.

What if Positive Interpolation? To further verify our conjecture that extrapolation can create hard positives while interpolation won't, we also conduct experiments for the interpolation of positive features, shown in Tab 3. We can observe a clear performance drop (5.4% drop for neutral $\alpha_{ex} = 2$) for this experiment. The reason is that the interpolation between positive features pulls the positive pairs together thus reducing the hardness in the training process. In other words, the view variance of positive pairs is decreasing, and thus easy to cause non-robust features.

4.2. Negative Interpolation

Previous contrastive models [6, 14] do not make full use of negative samples. e.g., In MoCo, there are many repetitive negative features stores in the memory queue iteration by iteration. Thus we could design a new strategy to fully utilize negative features and increase the diversity of the memory queue. With sufficient randomness, we propose the negative interpolation in memory queue, which intuitively provides diversified negatives for each training step.

Specifically, we denote the negative memory queue of MoCo as $Z_{neg} = \{z_1, z_2, \dots, z_K\}$ where K is the size of the memory queue, and Z_{perm} as the random permutation of Z_{neg} . We propose to use a simple interpolation between two memory queue to create a new queue $\hat{Z}_{neg} = \{\hat{z}_1, \hat{z}_2, \dots, \hat{z}_K\}$:

$$\hat{Z}_{neg} = \lambda_{in} \cdot Z_{neg} + (1 - \lambda_{in}) \cdot Z_{perm} \quad (5)$$

where $\lambda_{in} \sim Beta(\alpha_{in}, \alpha_{in})$ is in the range of $(0, 1)$, as Fig 6(a) shown. The transformed memory queue \hat{Z}_{neg} provides fresh interpolated negatives for contrastive loss iteration by iteration, where the random permutation and λ_{in} ensure the diversity of \hat{Z}_{neg} of each training step. The diversity makes the model to compare with much more linear combinations

⁵The beta distribution with $\alpha_{ex} > 1$ shows an inverted U shape which samples 0.5 with a greater probability and thus making λ_{ex} to have a greater chance to be 1.5.

α_{in}	-	0.2	0.4	0.6	1.4	1.6	2.0
acc (%)	71.1	73.3	74.1	74.2	73.5	74.6	74.1

Table 4. Various α_{in} for negative interpolation, the best result is marked in bold. We employ ResNet-50 [16] for the results. ‘-’ indicates MoCo baseline without using negative interpolation.

Method	α_{in}	Z_n	queue size	Acc
moco+ original queue	-	Z_{neg}	K	71.10
moco+ original queue	-	Z_{neg}	$2K$	71.40
moco+ Neg FT queue	1.6	\tilde{Z}_{neg}	K	74.64
moco+ Neg FT+original	1.6	\tilde{Z}_{neg}	$2K$	74.73

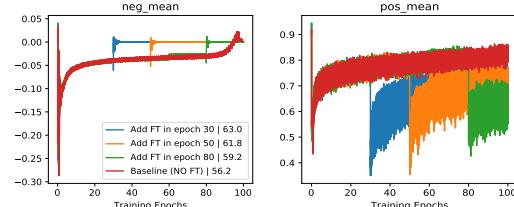
Table 5. Ablation results for using different queue of negative features (Res50). The transformed queue \tilde{Z}_{neg} can completely replace the extended queue \tilde{Z}_{neg} with small computations.

of previous negatives in each training step. Positive extrapolation increases the view variance between two pos features while the negative interpolation similarly boosts the “sample variance” (diversity) of the memory queue. We conjecture that original queue Z_{neg} provides discrete distribution of negative samples but our method can fill in the incomplete sample points of the distribution by random interpolation, leading to a more discriminative model. We evaluate the efficacy of negative interpolation on IN-100 and attempt various α_{in} in Tab 4. The neg interpolation is fairly robust with various α_{in} , with the improvement of 2.2%-3.5% from the baseline (71.1%). More interesting discussions about negative feature transformation (hard negatives & negative extrapolation) are shown in Supp G.

Previous works have explored the method leveraging image-level [36] and feature-level [20] mixing in contrastive learning. Our method differs from the previous works in three ways, first is the motivation, we are motivated by our observation in Sec 3.2 to propose the feature transformation strategies. Second, the way we extrapolate between two positive features is novel and outperforms the other two methods on several experiments in Tab 8 and 9. Third, the negative interpolation aims at fully utilizing negative samples in each training step. Both FT methods focus on exploring an effective way to perform feature transformation, not simply extending hard negatives to memory queue [20], neither the image-level mixup [36]. In the following sections, we provide inside discussions for the proposed FT, including (1) What if extending memory queue instead of FT? (2) When to add FT? (3) Dimension-level mixing rather than linear mixup. (4) Could the gains brought by FT vanish if training longer?

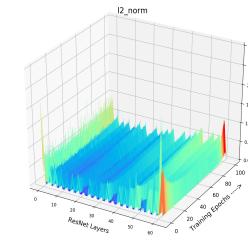
4.3. Discussions

Extending memory queue instead of FT: Previous works [14, 6] show that increasing the number of negative example (K) in contrastive learning could be beneficial for the final performance, thus they either uses a memory

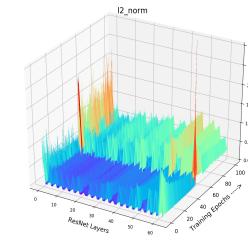


(a) Mean of neg scores

(b) Mean of pos scores



(c) Baseline MoCo landscape



(d) Adding FT in 50th epoch

Figure 7. Visualization of when to add FT, including score distribution and Gradient (ℓ_2 norm) landscape.

FT begin epoch	0	2	30	50	80	-
Res18 acc (%)	62.6	63.3	62.9	61.8	59.2	56.2
Res50 acc (%)	76.9	76.4	75.9	74.0	72.2	71.1

Table 6. When to add feature transformation. We employ Res-18 (total 100 epochs) and Res-50 (total 200 epochs) on IN-100 for the results. ‘-’ indicates MoCo baseline without using any FT.

queue [14] or a large batchsize [6] to obtain more negative examples. Specifically, [30, 17, 40] shows that increasing K will improve the lower bound of the mutual information. The negative interpolation method could also be leveraged to enlarge the number of negative examples: We use the union queue of original negatives and interpolated queue, $\tilde{Z}_{neg} = \hat{Z}_{neg} \cup Z_{neg}$, which contains twice the number of negative examples ($2K$) than \hat{Z}_{neg} .

We compare the performance of using only the interpolated queue \hat{Z}_{neg} , original Z_{neg} with $K/2K$ negative samples, and their combination \tilde{Z}_{neg} , in Tab 5. We found that using the combination queue shows negligible improvement over the performance (74.73%) of using the interpolated queue alone (74.64%). We consider that the interpolated negative features contain sufficient diversified negatives compared with the original queue. So even the double negative samples (more mutual information) of the extended queue (\tilde{Z}_{neg}) cannot boost the performance. Notably, the extended queue requires double times computation for each contrastive loss. Thus we recommend feature transformations with less computation but more efficiency rather than feature augmentation.

When to add feature transformation? Here we present the efficacy of FT by analysis of starting FT in various training stages. As shown in Tab 6, starting FT (pos extrapolation + neg interpolation) from various epoch can consis-

tently boost the accuracy of baseline, and starting from earlier can improve more (7.1%/5.8% boosts with Res-18/Res-50). With the visualizations of score distribution and gradient landscape in Fig 7, we can see that our FT brings hard positives (lowering pos scores in Fig 7(b)) and hard negatives (rising neg scores in Fig 7(a)) simultaneously when the combined FT is inserted in various stages. Besides, with the comparison of the gradient (ℓ_2 norm) landscape, we can observe that our FT brings a greater gradient for the training, which makes the model escape from the local minima and avoid over-fitting. These analyses indicate our FT is a plug-and-play method and brings persistent view-invariance and discrimination for the training of contrastive models. More detailed discussions and visualizations are put in Supp D.

How about Dimension-level mixing: Besides the proposed linear feature interpolation and extrapolation on the feature-level (128-d vector), we also extend the transformation to a dimension-level where the parameter λ is a vector rather than a scalar number, this dimension-level mixing can be described as follows:

$$\hat{z}_{new} = \lambda \odot z_i + (1 - \lambda) \odot z_j \quad (6)$$

where \odot stands for Hadamard product, and $\lambda \in [0, 1]^n$ is a vector with the same dimension as the feature vector. The value of each dimension of λ is randomly sampled from a beta distribution $\lambda_i \sim Beta(\alpha, \alpha)$. This formulation is used for negative interpolation; For positive, λ is added 1 to perform extrapolation. For neg/pos features, the dimension-level mixing could introduce more diversity/more view variance (hardness) because every dimension is performed with transformation. Experiments of dimension-level mixing on IN-100 shows improvement over the feature-level mixing (the 5th row in Tab 7).

Could the gains brought by FT vanish if training longer? Simply training longer leads to significant performance boost for contrastive pre-train. So here we provide the results of MoCov2/MoCov2+FT (500 epoch) on IN-100: 80.7%->81.5%. Compared with 200 epoch results (75.6%->78.3% in Tab 7), longer training actually minimizes the improvement over the baseline. More training epochs can lead to comparing much more pos/neg pairs to increase the diversity. However, our proposed FT accelerates this process by providing diversity and results in fast convergence, which responds to the motivation of learning diversified and discriminative representations.

5. Experiments

In this section, we evaluate our Feature Transformation methods from four perspectives: (1) Ablation studies (2) FT on various contrastive models. (3) Evaluating the representation on ImageNet-1k. (4) Finetuning on various downstream tasks. We keep the fairness of the experiments, especially when compared with other methods. Notice that the

Method	MoCov1	MoCov2	simCLR	Infomin	swav	SimSiam
baseline*	71.10	75.61	74.32	81.9	82.1	77.1
+pos FT	72.80	76.22	75.80	-	-	77.8
+neg FT	74.64	77.12	76.71	-	-	-
+both	76.87	78.33	78.25	83.2	83.2	-
+both _{dim}	77.21	79.21	78.81	-	-	-

Table 7. Ablation studies of proposed methods on various contrastive models. The models are pre-trained for 200 epochs with Res50 on IN-100. * indicates reproduced baseline results.

pre-train	IN-1k	inat-18	CUB200	FGVC-aircraft
supervised	76.1	66.1	81.9*	82.6*
mocov1[14]	60.6	65.6	82.8*	83.5*
mocov1+ours	61.9	67.3	83.2	84.0
mocov2[7]	67.5	66.8*	82.9*	83.6*
mocov2+ours	69.6	67.7	83.1	84.1
mocov2+MoCHi[20]	68.0	-	-	-
mocov2+UnMix[36]	68.6	-	-	-

Table 8. Classification results. * indicates our reproduced results.

data augmentations are followed with the baseline methods. Details of experiments and datasets are put in Supp B.

5.1. Ablation study

We adopt the linear readout protocol [14] to compare performance for image classification on IN-100, where we freeze the features and train a supervised linear classifier using softmax. Tab 7 summarizes the results of ablation studies. We observe that the positive extrapolation and negative interpolation components are complementary which can improve the top-1 accuracy by 5.77%/2.72% when combined on MoCoV1/MoCoV2. The dimension-level mix also shows improvement based on the already high performance of both components. The performance-boosting of ablation studies over MoCo shows the efficacy of our FT. Notice that the transformed features are not necessarily on the unit sphere (*i.e.*, has a norm of 1), we did not need to re-perform ℓ_2 norm for transformed features, because the performance difference is negligible (76.87% *v.s* post-norm 76.68%). More discussions about ℓ_2 for vector length are put in Supp F. Here we strongly recommend to re-perform ℓ_2 norm for the transformed features on all the datasets, for the sake of contrasting all the scores on the unit-sphere.

5.2. FT on various contrastive models

We apply our FT to various contrastive models in Tab 7. It presents that our FT brings 5.77%, 3.93%, 1.3%, 1.1%, and 0.7% improvement over MoCo [14], SimCLR [6], InfoMin [40], SWAV [4] and SimSiam [8], respectively on IN-100 dataset (200 epoch). It is worthy to point out that the series of ablation studies of our FT can boosts the Sim-

pre-train	IN-1k Top-1	Faster [33] R50-C4 VOC			Mask R-CNN [15] R50-C4 COCO					
		AP	AP ₅₀	AP ₇₅	AP ^{bb}	AP ₅₀ ^{bb}	AP ₇₅ ^{bb}	AP ^{mk}	AP ₅₀ ^{mk}	AP ₇₅ ^{mk}
random init*	-	33.8	60.2	33.1	26.4	44.0	27.8	29.3	46.9	30.8
supervised*	76.1	53.5	81.3	58.8	38.2	58.2	41.2	33.3	54.7	35.2
infomin*	70.1	57.6	82.7	64.6	39.0	58.5	42.0	34.1	55.2	36.3
mocoV1[14]	60.6	55.9	81.5	62.6	38.5	58.3	41.6	33.6	54.8	35.6
mocoV1+ours	61.9	56.1	82.0	62.0	39.0	58.7	42.1	34.1	55.1	36.0
mocoV2[7]	67.5	57.0	82.4	63.6	39.0	58.6	41.9	34.2	55.4	36.2
mocoV2+ours	69.6	58.1	83.3	65.1	39.5	59.2	42.1	34.6	55.6	36.5
mocoV2+mochi[20]	68.0	57.1	82.7	64.1	39.4	59.0	42.7	34.5	55.7	36.7
DetCo[51]	68.6	57.8	82.6	64.2	39.4	59.2	42.3	34.4	55.7	36.6
InsLoc[53]	-	57.9	82.9	65.3	39.5	59.1	42.7	34.5	56.0	36.8

Table 9. Object detection. All model are pre-trained for 200 epochs on ImageNet-1k. * means that the results are followed from respective papers [14, 40]. The COCO results of mocoV2 is from [20]. Our results are reported using the average of 5 runs.

CLR model. The experiments shows our FT is generic and robust for various contrastive models.

5.3. Evaluating the representation on ImageNet-1k

After ablations on IN-100 dataset, we use the best settings of α_{in} and α_{ex} to train a model on ImageNet-1k (IN-1K). Note that the dimension-level mix is not used for the experiments on IN-1K due to computational constraints. We apply our method on the baseline MoCo [14] and MoCoV2 [7], which are both trained on IN-1K with 200 epochs. The results and comparison are summarized in Tab 8. Our method improves MoCoV1 and MoCoV2 by 1.3% and 2.1% on Top-1 accuracy respectively which are significant on a large dataset like IN-1K. UnMix [36] and MoCHi [20] are the methods that also leverage mixup to better aid the contrastive learning process. Notably, we can observe that our method with MoCoV2 can provide larger performance gain than UnMix and MoCHi respectively.

5.4. Downstream Tasks

Fine-grained image classification We evaluate the efficacy on real world fine-grained classification datasets, *e.g.*, large scale long-tail iNaturalist2018 [41], CUB-200 [48] and FGVC-aircraft [29]. As shown in Tab 8, our FT significantly boosts the transfer performance on iNat-18, with 1.7% and 0.9% improvement based on MoCo and MoCoV2. Besides, our FT brings consistent improvement on CUB-200 and FGVC-aircraft.

Object Detection Recent works [46, 51, 52, 53, 57] have shown that the transfer accuracy of state-of-the-arts (SOTAs) models [4, 6, 40, 7, 14] on classification and detection are inconsistent and have low correlation, denoted as “task-bias”. One important reason is that pre-tasks of SOTA are specifically designed and optimized for classification, such as instance discrimination [49, 14] and clustering [4], leading to substantial enhancement on classification but slight

gain for detection. Therefore we evaluate our FT on detection/instance segmentation tasks. As summarized in Tab 9, our FT can boosts the baseline model MoCo-V2 on various datasets and metrics respectively. Our FT strongly improves the transfer accuracy] on VOC [11] and MSCOCO [25]. Besides, our FT with MoCo-V2 can get slightly better accuracy than those contrastive models specifically designed for detection tasks, *e.g.*, DetCo[51] and InsLoc [53]. Moreover, our FT can get much better classification results than DetCo. Notice that our FT is not aiming at the local information during pre-task design, but more invariance from feature transformation. These experiments indicate that our FT is less task-bias than the pre-task-based contrastive models. The performance boosts suggest the efficacy and robustness of our proposed FT, and enable us to learn more “view-invariant” and discriminative representations.

6. Conclusions

In this work, we have developed a visualization tool to visualize the score distributions of positive and negative pairs. Leveraging this visualization tool, we can understand the inside of the contrastive learning process. More specifically, we discover significant observations inspiring our novel Feature Transformation, including positive extrapolation such that more hard positives are created for the training. Besides, we propose the interpolation among negatives, which makes full use of negatives and provides diversified negatives. The feature transformations enable to learn more view-invariant and discriminative representations. Experiments show that our proposed Feature Transformation can improve at least 6.0% accuracy on ImageNet-100 over MoCo, and about 2.0% accuracy on ImageNet-1K over the MoCoV2 baseline. Transferring to the downstream tasks successfully demonstrate our model is less task-bias. In our future work, we will explore more feature manipulation strategies with the help of our visualization tool.

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