Preservational Learning Improves Self-supervised Medical Image Models by Reconstructing Diverse Contexts

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Abstract

Preserving maximal information is one of principles of designing self-supervised learning methodologies. To reach this goal, contrastive learning adopts an implicit way which is contrasting image pairs. However, we believe it is not fully optimal to simply use the contrastive estimation for preservation. Moreover, it is necessary and complemental to introduce an explicit solution to preserve more information. From this perspective, we introduce Preservational Learning to reconstruct diverse image contexts in order to preserve more information in learned representations. Together with the contrastive loss, we present Preservational Contrastive Representation Learning (PCRL) for learning self-supervised medical representations. PCRL provides very competitive results under the pretraining-finetuning protocol, outperforming both self-supervised and supervised counterparts in 5 classification/segmentation tasks substantially. Codes are available at https://github.com/Luchixiang/PCRL.

1. Introduction

It is common practice that training deep neural networks often requires a large amount of manually labeled data. This requirement is easy to satisfy in natural images as both the cost of labor and the difficulty of labeling can be acceptable. However, in medical image analysis, reliable medical annotations usually come from domain experts’ diagnoses which are hard to access considering the scarcity of target disease, the protection of patient’s privacy and the limited medical resources. To address these problems, self-supervised learning has been widely adopted as a practical way to learn medical image representations without manual annotations.

Nowadays, contrastive representation learning has been widely applied and outstandingly successful in medical image analysis [51, 33, 6]. The goal of contrastive learning is to learn invariant representations via contrasting medical image pairs, which can be regarded as an implicit way to preserve maximal information. Nonetheless, we think it is still beneficial and complemental to explicitly preserve more information in addition to the contrastive loss. To achieve this goal, an intuitive solution is to reconstruct the original inputs using learned representations so that these representations can preserve the information closely related to the inputs. However, we discover that directly adding a plain reconstruction branch for restoring the original inputs would not significantly improve the learned representations. To address this problem, we introduce Preservational Contrastive Representation Learning to reconstruct diverse contexts using representations learned from the contrastive loss.
As shown in Fig.1, we attempt to incorporate the diverse image reconstruction, as a pretext task, into contrastive learning. The main motivation is to encode more information into the learned representations. Specifically, we introduce Transformation-conditioned Attention and Cross-model Mixup to enrich the information carried by representations. The first module embeds a transformation indicator vector \( e_{cc}(T) \) in Figure 1) to high-level feature maps following an attentional mechanism. Based on the embedded vector, the network is required to dynamically reconstruct different image targets while the input is fixed. Cross-model Mixup is developed to generate a hybrid encoder by mixing the feature maps of the ordinary and the momentum encoders, where the hybrid encoder is asked to reconstruct mixed image targets. We show that both modules can help to encode more information and produce stronger representations compared to using contrastive learning only.

Besides the learning algorithm, this paper also addresses another issue when using unlabeled medical images for pre-training, that is lacking a fair and thorough comparison of different self-supervised learning methodologies. In this paper, we design extensive experiments to analyze the performance of different algorithms across different datasets and data modalities. Generally speaking, the contributions of this paper can be summarized into three aspects:

- Preservational Contrastive Representation Learning is introduced to encode more information into the representations learned from the contrastive loss by reconstructing diverse contexts.

- In order to restore diverse images, we propose two modules: Transformation-conditioned Attention and Cross-model Mixup to build a triple encoder, single decoder architecture for self-supervised learning.

- Extensive experiments and analyses show that the proposed PCRL has observable advantages in 5 classification/segmentation tasks, outperforming both self-supervised and supervised counterparts by substantial and significant margins.

2. Related Work

In this section, we mainly review deep model based self-supervised learning approaches and mixup strategies. Note that for self-supervised learning, we only list the most related ones based on pretext tasks, ignoring clustering based approaches [4, 47] and video based representation learning [38, 39, 28, 40].

Pretext-based self-supervised learning in natural images. Pretext-based methods rely on predicting input images’ properties that are covariant to the transformations, such as recognizing image patches’ content [29], relative position [14, 24], rotation degree [17, 14], object color [23, 46], the number of objects [25] and the applied transformation function [30]. Contrastive-estimation based approaches also utilize pretext tasks to learn invariant representations by contrasting image pairs [43, 26, 10, 5, 20, 48]. Recently, there are some works trying to remove the negative pairs in contrastive learning [18, 12]. By comparison, our method follows a different principle which is making representations able to fully describe their sources (i.e., corresponding input images).

Self-supervised learning in medical image analysis. Before contrastive learning, solving the jigsaw problem [54, 53, 35] and reconstructing corrupted images [9, 52] are two major topics for pretext-based approaches in medical images. Besides them, Xie et al. [44] introduced a triplet loss for self-supervised learning in nuclei images. Haghighi et al. [19] improved [52] by appending a classification branch to classify the high-level features into different anatomical patterns. For contrastive learning, Zhou et al. [51] applied contrastive loss to 2D radiographs. Similar ideas have also appeared in few-shot [49] and semi-supervised learning [50]. Taleb et al. [34] proposed 3D Contrastive Predictive Coding from utilizing 3D medical images. There are two works [16, 8] most related to ours. Feng et al. [16] showed that the process of reconstructing part images displays similar effects with those of employing a contrastive loss. Chakraborty et al. [8] introduced a denoising autoencoder to capture a latent space representation. However, both methods failed to improve contrastive learning with context reconstruction while our methodology succeeds in this aspect.

Mixup in medical imaging. Mixup [45], as an augmentation strategy, has been widely adopted in medical imaging [27, 7, 22, 15, 2, 37]. The proposed Cross-model Mixup is most related to Manifold mixup [36, 22, 2]. However, as far as we know, there is no previous method applying manifold mixup to cross-model representations, which is exactly the core contribution of our CROSS-MODEL Mixup.

3. Methodology

An overview of Preservational Contrastive Representation Learning (PCRL) is provided in Figure 2. Generally, PCRL contains three different encoders and one shared decoder. The encoder and the decoder are connected via a U-Net like architecture. We first apply exponential moving average to the parameters of the ordinary encoder to produce the momentum encoder. Then, for each input, we apply Cross-model mixup to both encoders’ representations (feature maps) to build a hybrid encoder. Given a batch of images \( X' \), we first apply random crop, random flip and random rotation to generate three batches of images.
the number of transformations decreases to 6 where \( F(z) \) strategies (cf. Figure 3). For 2D inputs (such as X-rays), the vector has 7 components denoting different transformation mechanisms. Such process can force the encoder to preserve information into the high-level representations following an attentional mechanism where we suppose that different channels of feature maps may have different impacts on the reconstructed results. Note that TransAtt is only applied to the last convolutional layer (before FC layers) of each encoder.

As shown in Figure 3, for each input, the indicator vector consists of mixed feature maps from both the ordinary encoder and the momentum encoder. \( \{ \text{C., F., R., I., O., B.} \} \) are abbreviations for random crop, random flip, random rotation, inpainting, outpainting and gaussian blur, respectively. NCE is short for noise-contrastive estimation. GO represents global operations which include global average pooling and fully-connected layers. \( \text{vec}(\cdot) \) represents the indicator vector. \( T_{o,m,h}(\cdot) \) denote a set of transformation functions for different encoders. \( \odot \) represents channel-wise multiplication.

### 3.1. Transformation-conditioned Attention

In this section, we propose Transformation-conditioned Attention (TransAtt) to enable the reconstruction of diverse contexts. This module encodes the transformation vector into the high-level representations following an attentional mechanism. Such process can force the encoder to preserve more information in learned representations.

As shown in Figure 3, for each input, the indicator vector contains a combination of different transformations. Specifically, given 3D inputs (CT and MRI scans), the indicator vector has 7 components denoting different transformation strategies (cf. Figure 3). For 2D inputs (such as X-rays), the number of transformations decreases to 6 where \( F(z) \) does not exist. Each component contains an indicator function (1 or 0) representing whether the specific transformation is applied or not. To encode the indicator vector into high-level feature maps, we propose an attentional mechanism where we suppose that different channels of feature maps may have different impacts on the reconstructed results. Note that TransAtt is only applied to the last convolutional layer (before FC layers) of each encoder.

To imitate such process, we first forward the indicator vector \( \text{vec}(T) \) to two fully-connected (FC) layers which produces a vector \( f^p \in \mathbb{R}^{C \times 1} \). Meanwhile, we apply global average pooling to each encoder’s high-level feature maps.
where $$f \in \mathbb{R}^{C \times D \times H \times W}$$ resulting in a vector $$f^l \in \mathbb{R}^{C \times 1}$$, where $$l$$ denotes the layer index. Then, we compute the outer product of $$f^p$$ and $$f^l$$:

$$M = f^p \otimes f^l,$$

where $$M \in \mathbb{R}^{C \times C}$$. Next, we flatten $$M$$ and forward it to another fully-connected layer:

$$f^q = \text{ReLU}(W_{\theta} \text{flat}(M)),$$

where $$W_{\theta} \in \mathbb{R}^{C \times C^2}$$ stands for the weight parameters of the FC layer. To perform rescaling, we further append a sigmoid function to $$f^q$$:

$$f^w = \text{sigmoid}(f^q),$$

where $$f^w \in \mathbb{R}^{C \times 1 \times 1 \times 1}$$. Finally, we apply channel-wise multiplication between $$F^l$$ and $$f^w$$ and append a convolutional layer whose kernel size is 3:

$$F^{l+1} = \text{conv}(F^l \odot f^w),$$

where $$F^{l+1} \in \mathbb{R}^{C \times D \times H \times W}$$.

### 3.2. Cross-model Mixup

Apart from TransAtt, we introduce Cross-model Mixup (CrossMix) for shuffling these feature representations in order to enable more diverse restoration. Different from traditional mixup [45] which applies to network inputs, we propose to mix the feature maps from two different models to build a new hybrid encoder.

Accordingly, the reconstruction target of the hybrid encoder is a mixed input $$X_h^1$$. In practice, for each training iteration,

$$X_h^1 = \lambda X_o^1 + (1 - \lambda)X_m^1,$$

where $$\lambda \sim \text{Beta}(\alpha, \alpha)$$, $$\alpha$$ is a hyperparameter\(^2\). For network feature maps, we use $$F^l_o$$ to denote the feature maps at layer $$i$$ of the ordinary encoder, $$i \in \{1, ..., l\}$$. Similarly, $$F^l_m$$ and $$F^l_h$$ stand for the features maps at the same location in the momentum encoder and the hybrid encoder, respectively. Thus, the process of cross-model representation mixup can be formulated as:

$$F_h^l = \lambda F_o^l + (1 - \lambda)F_m^l.$$

Together with the one shared decoder, we can directly use $$F_h^{l (1, ..., l)}$$ to reconstruct $$T_h(X_h^l)$$.

### 3.3. Loss Functions and Model Update

To store past features for contrasting, we employ a queue $$\mathcal{K} = \{k_1, ..., k_N\}$$ to store them following [20]. The length of $$\mathcal{K}$$ is $$N$$. In contrastive learning, we treat all features in queue $$\mathcal{K}$$ as negative samples. Here we use $$g_o(\cdot)$$ and $$g_m(\cdot)$$ to denote the projectors of the ordinary encoder and the momentum encoder, respectively. The contrastive loss $$\mathcal{L}_c$$ can be formulated as:

$$\mathcal{L}_c = -\log \frac{\exp((g_o(F_o^{l+1})^T g_m(F_m^{l+1})/\tau)}{\sum_{j=1}^{N} \exp((g_o(F_o^{l+1})^T k_j/\tau))},$$

where $$\tau$$ is a temperature hyperparameter. $$g_o(\cdot)$$ and $$g_m(\cdot)$$ contains global average pooling and two FC layers, independently. After each training iteration, we push $$g_o(F_o^{l+1})$$, $$g_m(F_m^{l+1})$$, and $$g_h(F_h^{l+1})$$ to $$\mathcal{K}$$ as negative samples for further contrasting.

For reconstructing diverse contexts, we use mean square error (MSE) as the default reconstruction loss. Formally, if we denote the shared decoder network as $$D_\theta$$, considering the whole network has a U-Net like architecture, the decoder’s inputs should be multi-layer feature maps $$F_{\{o,m,h\}}^3$$. The computation of the reconstruction loss can be summarized as follows:

$$\mathcal{L}_p = \text{MSE}(D_\theta(F_o), T_h(X_h^1)) + \text{MSE}(D_\theta(F_m), T_h(X_m^1))$$

+ $$\text{MSE}(D_\theta(F_h), T_h(X_h^1)).$$

We finally sum up $$\mathcal{L}_c$$ and $$\mathcal{L}_p$$ as the complete loss function with equal weight (0.5 to 0.5). For network parameters, we denote the parameters of the ordinary encoder and the momentum encoder as $$\theta_o$$ and $$\theta_m$$, respectively. We update $$\theta_m$$ by using an exponential moving average (EMA) factor $$\beta$$:

$$\theta_m = \beta \theta_m + (1 - \beta)\theta_o.$$\(^3\)

Note that the hybrid encoder has no encoder parameters as it directly takes a combination of the feature maps from the ordinary and the momentum encoders. The mixed feature maps are then treated as the inputs to the shared decoder as shown in Equation 8.

### 4. Experiments

In this section, we first make ablation studies to demonstrate the advantages of TransAtt and CrossMix. Then, we introduce a thorough analysis of different self-supervised algorithms from different aspects. For all tasks, we employ the notation of source dataset $\rightarrow$ target dataset. The source dataset is used for self-supervised pretraining while the target dataset is used for supervised finetuning.

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1. Here we omit the subscript $$\{o, m, h\}$$ which means $$F^l$$ can represent feature maps from different encoders.

2. Beta distribution is employed in the original mixup paper.

3. We omit the superscript which is $$\{1, ..., l+1\}$$.
4.1. Baselines

For medical pretraining approaches, we divide them into two categories: 2D and 3D, simply based on their input dimension (e.g., X-ray is 2D while CT scan is 3D). For 2D image pretraining, our baselines include train from scratch (TS), ImageNet pretraining (IN), Model Genesis (MG) [52], Semantic Genesis (SG) [19] and Comparing to Learn (C2L) [51]. Here we ignore the method proposed in [44] which made prior assumptions on the number of nuclei and is not be suitable for other datasets. For 3D volume pretraining, we also include train from scratch (TS), Model Genesis (MG), Semantic Genesis (SG) and 3D-CPC [34]. Additionally, Cube++ [5] is included as it is an improved version of Rubik’s Cube [54] and Rubik’s Cube+ [53].

4.2. Datasets

In 2D tasks, we make experiments on two X-ray datasets: Chest14 [41] and CheXpert [21]. We use Chest14 for both 2D pretraining and 2D finetuning while CheXpert is only used for pretraining considering CheXpert contains a number of uncertain labels. The evaluation metric in 2D tasks is AUC. In order to evaluate the performance of algorithms on 3D volumes, we make experiments on CT and MRI datasets, including LUNA [32], BraTS [1] and LiTS [3]. We use LUNA for both 3D pretraining and 3D finetuning. The evaluation metric of finetuning on LUNA is AUC. BraTS is mainly used for 3D finetuning on liver segmentation. The evaluation metric for segmentation is mean dice score. In practice, we divide each dataset into the training set, the validation set and the test set. The pretraining data always come from the training set (without labels). Please refer to the supplementary material for more details.

4.3. Implementation Details

We use 2D U-Net [31] and 3D U-Net [13] as the backbone networks for 2D and 3D tasks, where we replace the encoder in 2D U-Net with ResNet-18. The EMA factor $\beta$ of updating momentum encoder is set to 0.99. For self-supervised pretraining, we employ momentum SGD as the default optimizer whose initial learning rate is set to 1e-3 while the momentum value is set to 0.9. We employ the cosine annealing strategy for decreasing learning rate and stop the training when the validation loss does not change for 30 epochs. The checkpoints with lowest validation loss values are saved for finetuning. For supervised finetuning, we use Adam as the optimizer with 1e-4 as the initial learning rate. Similar to pretraining, we rely on validation loss to determine when to end the training stage, and we save the checkpoints with lowest validation loss values for testing. Dice loss is used for segmentation tasks while cross entropy is employed for classification tasks. For other hyperparameters in baselines, we simply follow the choices in their official papers. $\alpha$ is set to 1 (for $\lambda$) in both Equation 5 and 6. We set the temperature factor $\tau$ of softmax function in Equation 7 to 0.2 in practice. For each experiment, we repeat it for three times and report their average results. More details can be found in attached supplementary material.

4.4. Ablation Study

In this section, we mainly investigate two problems: (1) whether the proposed method preserves more information than contrastive learning (Table 1) and (2) if the preserved information lead to the improved performance (Table 2). In Table 2, we make experiments on Chest14 to investigate the effectiveness of different module combinations, where we treat different ratios of the dataset as labeled data for supervised finetuning while the rest are used as unlabeled data for self-supervised pretraining.

Preservational learning brings more information to representations. In Table 1, we show that reconstructing
demonstrates that TransAtt is able to preserve much more information than using ContraLoss only by preserving more information than using ContraLoss + Self-Recons. that ContraLoss + Self-Recons. can already perform better than RotNet shows that image reconstruction branch only brings marginal improvements than the others, again verifying reconstructing diverse contexts do help preserve more information in learned features.

Preserved information lead to better performance. We report the performance of different module combinations in Table 2, where we can observe similar trends as those in Table 1. It is obvious that the results on pretext tasks are closely correlated with the performance on Chest14. In other words, given a method, we can rely on its performance on two pretext tasks to roughly predict its performance in Chest14. Considering the performance on two pretext tasks can reflect the amount of information in learned representations, we can easily draw a conclusion: reconstructing diverse contexts introduce more information which help improve the overall performance of algorithms.

From Table 2, we can easily find that adding a self-reconstruction branch only brings marginal improvements over the baseline model. Similar phenomena can also be observed when applying CrossMix. Finally, PCRL achieves much higher accuracy than the others, again verifying reconstructing diverse contexts do help preserve more information in learned features.
Figure 5: Visual analysis of segmentation results when finetuning on LiTS and BraTS. For each dataset, we provide 2 cases where we report the dice scores using different self-supervised pretraining methodologies. Specifically, in LiTS, the goal is to segment liver. In BraTS, we only display the results of WT. We ignore MG because SG is built on top of MG.

find that adding the rotation transformations can obviously improve the overall performance. This is consistent with the results in Table 1, where TransAtt also performs better than TransAtt (Flip) on two pretext tasks. We also investigate the influence of the hyperparameter $\alpha$ in CrossMix. The observation is that by decreasing its value by half, the overall performance slightly drops. Equipped with TransAtt and CrossMix, PCRL can surpass the baseline model ContraLoss by approximate 4 points in different labeled ratios. Moreover, we find that the improvement is most significant at 10%. This phenomenon implies that the reconstructing diverse contexts is more useful when the amount of labeled data is small.

4.5. Comparison with State-of-the-Arts in 2D Tasks

In this part, we evaluate the performance of various self-supervised pretraining approaches on 2 different 2D tasks: Chest14→Chest14 and CheXpert→Chest14. All results are displayed in Table 4a.

If we look at the results in Chest14→Chest14, it is obvious that all pretraining methods (including IN) can boost the performance apparently when compared to TS. We can see that MG and SG achieve similar performance in different ratios. Such comparison is easy to explain as SG is built upon MG. However, both MG and SG still cannot surpass IN especially when the amount of labeled data is limited, which demonstrates that being pretrained on a large-scale natural image dataset can benefit medical image analysis a lot. As for C2L, we find that C2L is the only baseline method which is able to surpass IN in different ratios. When we compare PCRL with other baseline algorithms, it is easy to find that PCRL has the ability to outperform different baselines in various ratios significantly. Particularly, PCRL seems to have more advantages in small labeled ratios. The underlying reason may be that TransAtt and CrossMix may help to learn more diversified representations and alleviate the overfitting problem of training deep neural networks with limited supervision.

In CheXpert→Chest14, we can see that MG and SG achieve comparable results with TS when the labeled ratio
Table 3: Results in natural images. We transfer the self-supervised pretrained models on ImageNet-1k to downstream tasks, including segmentation (Cityscapes) and detection (COCO). On Cityscapes, we use ResNet-50 as backbone to build a FCN segmentation model where the evaluation metric is mIoU. On COCO, we use the ResNet-50-FPN model from Detectron2 [42] and the evaluation metric is mAP (0.5:0.05:0.95).

| Method         | #. Epoch | Cityscapes | COCO  |
|----------------|----------|------------|-------|
| SimCLR [9]     | 1000     | 75.6       | 39.6  |
| SwAV [4]       | 400      | 76.0       | -     |
| MoCov2 [11]    | 800      | 76.3       | 40.5  |
| PCRL           | 800      | 77.3       | 41.3  |

is equal or greater than 50%, demonstrating purely pretext-based approaches may have unstable performance under varying labeled ratios. If we look at C2L, we find that C2L consistently outperforms IN and other pretraining methods in almost all ratios. Somewhat surprisingly, we find that PCRL can still outperform C2L and IN by a significant margin even if the labeled ratio is 100%. Such comparison further demonstrates the robustness of PCRL.

### 4.6. Comparison with State-of-the-Arts in 3D Tasks

Besides 2D tasks, we also analyze the results of 3D self-supervised learning approaches in 3 different 3D tasks: LUNA→LUNA, LUNA→LiTS and LUNA→BraTS, where all experimental results are shown in Table 4b.

In LUNA→LUNA, it is interesting to find that the performance gaps between TS and self-supervised pretraining are smaller than those in Chest14. One explanation is that the nodule classification task is less sensitive to the amount of labeled data. Among MG, SG, Cube++ and 3D-CPC, 3D-CPC gives the best results in large labeled ratios while Cube++ performs better in small ones. Interestingly, as the labeled ratio increases, SG quickly catches up with MG and Cube++, showing its ability to utilize a large number of labeled images. Again, we can see that PCRL is able to outperform other baselines significantly in different ratios. Particularly, when the baseline approaches show similar results as the labeled ratio becomes larger, PCRL can still display impressive improvements over previous self-supervised pretraining approaches and outperforms TS substantially. In LUNA→LiTS, Cube++ performs slightly better than MG and SG while 3D-CPC outperforms Cube++ in almost all ratios. By comparison, PCRL has apparent advantages over other baselines especially when the labeled ratio is smaller or equal to 50%.

When we transfer knowledge from LUNA to BraTS, MG, SG and Cube++ display similar performance, all surpassing TS significantly in different labeled ratios. Due to advantages of contrastive learning, 3D-CPC again outperforms other baselines. Meanwhile, PCRL once again surpasses previous baselines consistently and remarkably. We think that such significant improvements can be attributed to the incorporation of the reconstruction of diverse contexts.

### 4.7. Visual Analysis

In Figure 5, we provide comparative visual analysis results of segmentation tasks in LiTS and BraTS, where the samples are randomly selected. We can obviously observe that PCRL handles the details much better than those of other baselines. For instance, in the first example of LiTS, PCRL delineates the corners accurately. In the second example of BraTS, PCRL can detect the isolated tumor regions while other methods cannot well handle these difficult cases.

### 4.8. Comparison with State-of-the-Arts in Natural Image Segmentation and Detection Tasks

To investigate the performance of PCRL in natural images, we conduct pretraining tasks on ImageNet-1k and transfer the pretrained models to downstream segmentation and detection tasks. The results are displayed in Table 3. We can see that PCRL is able to outperform MoCov2 and other popular self-supervised learning methods substantially in both Cityscapes and COCO, which are two widely adopted datasets in segmentation and detection. The superior performance on Cityscapes and COCO again verify the advantages of incorporating diverse context reconstruction.

### 5. Discussion and Conclusion

We show that by reconstructing diverse contexts, the learned representations using the contrastive loss can be greatly improved in medical image analysis. Our approach has shown positive results of self-supervised learning in a variety of medical tasks and datasets. There are some questions worth further discussing and verifying. For example, is preserving more information the only reason leading to the improvements over the contrastive loss? We hope the proposed PCRL can lay the foundations for real-world medical imaging tasks.

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