Polycentric Clustering and Structural Regularization for Source-free Unsupervised Domain Adaptation

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Abstract

Source-Free Domain Adaptation (SFDA) aims to solve the domain adaptation problem by transferring the knowledge learned from a pre-trained source model to an unseen target domain. Most existing methods assign pseudo-labels to the target data by generating feature prototypes. However, due to the discrepancy in the data distribution between the source domain and the target domain and category imbalance in the target domain, there are severe class biases in the generated feature prototypes and noisy pseudo-labels. Besides, the data structure of the target domain is often ignored, which is crucial for clustering. In this paper, a novel framework named PCSR is proposed to tackle SFDA via a novel intra-class Polycentric Clustering and Structural Regularization strategy. Firstly, an inter-class balanced sampling strategy is proposed to generate representative feature prototypes for each class. Furthermore, k-means clustering is introduced to generate multiple clustering centers for each class in the target domain to obtain robust pseudo-labels. Finally, to enhance the model’s generalization, structural regularization is introduced for the target domain. Extensive experiments on three UDA benchmark datasets show that our method performs better or similarly against the other state of the art methods, demonstrating our approach’s superiority for visual domain adaptation problems.

1 Introduction

In recent years, unsupervised domain adaptation\cite{9} has been developed to reduce the domain shift by transferring knowledge from a labeled source domain to a target domain, and has achieved promising results in object detection\cite{3, 35}, semantic segmentation\cite{39, 52} and person re-identification\cite{7, 42}. The main research directions of the existing UDA methods include (i) minimizing the distribution discrepancy by matching the statistical distribution moments\cite{24, 30}; (ii) applying adversarial training to learn domain-invariant feature
representations [45, 51]; and (iii) bridging the domain gap by using clustering [8] or pseudo-labeling [1]. It is worth noting that all of them assume that both well-trained source models and labeled source data are available. However, with the increasing concerns about data privacy and intellectual property of users, the accessibility of well-labeled source data cannot be guaranteed for many real-world tasks.

To overcome the above problem, some recent works [14, 15, 18, 19, 33, 47] explored domain adaptation without source data. Source-free domain adaptation (SFDA) is a new unsupervised learning setup for the domain adaptation task. Recently, image generation [18], class prototypes [19, 47], and pseudo labeling [19] are widely utilized in the existing SFDA approaches. However, generative models require a large computational capacity for generating target-style images. Class prototypes and pseudo labeling methods have shown competitive results but noisy labels are introduced due to category biases in the source and target domains. We argue that only one clustering center for each category is insufficient to avoid negative transfer caused by hard transfer data in the target domain. Furthermore, the structural information of the target data in the feature space is often ignored, which is very helpful to reduce the noisy labels though.

Based on the ideas presented above, a simple yet effective structured clustering strategy for polycentric clustering is proposed in this paper. Specifically, due to class imbalance in the target domain, to avoid the easy data dominating the target model, an inter-class-balanced sampling strategy is designed to aggregate representative samples of each class. To assign more accurate pseudo-labels, polycentric clustering is proposed to generate multiple feature clustering centers within a class of the target data. In addition, to alleviate the noisy labels, a mixup structural regularization term is introduced into our framework, encouraging the interpolation samples to be consistent with the interpolation predictions. Under the guidance of structural regularization, the model is enforced to maintain consistency, thus the robustness against noisy labels is improved.

To evaluate the effectiveness of our model, we conduct extensive experiments on three benchmark datasets, and the experimental results show significant superiority of our method in SFDA. The main contributions of our work are summarized as follows:

- We propose a novel framework, Polycentric Clustering and Structure Regularization (PCSR) for SFDA tasks, which aims to protect data privacy and maintain the model performance without access to the source data.

- To avoid easy-transfer data dominating the target model, an inter-class-balanced sampling strategy is designed to address the challenge of class imbalance. And a polycentric clustering approach is proposed for each class to reduce the noisy labels for those hard data.

- To reduce the noisy labels, the mixup regularization module is introduced to interpolate the target data for consistent training, leading to more robust pseudo labels.

- Extensive experiments on three benchmark datasets validate the superiority of our PCSR strategy. The results show that our strategy is comparable to or significantly outperform existing methods.
2 Related Work

2.1 Unsupervised Domain Adaptation

As a classic example of transfer learning [28], in recent years, UDA methods for image classification tasks have aimed to align the source and target distributions in an attempt to minimize the domain gap in knowledge transfer. There are currently three main classes of UDA methods: discrepancy-, adversarial learning-, and reconstruction-based. The feature distributions of the source and target domains are aligned by minimizing Maximum Mean Discrepancy (MMD) [21, 22, 23] in the discrepancy-based methods. In the adversarial learning-based approaches, the network is trained to learn domain invariant features by adding a feature discriminator [10, 25, 34]. Different from the previous two methods, the network is guided to extract domain-invariant features by an auxiliary image reconstruction module in the reconstruction-based approaches [2, 27]. Although these UDA methods are effective, they require access to both the source and target data. In the real world, this is impractical due to data privacy or security concerns. In contrast, our method proposed in this paper does not require source data when performing adaptation, making it more suitable for real-world applications.

2.2 Unsupervised Source-Free Domain Adaptation

In most realistic scenarios, only source models and unlabeled target data are available. As a result, some recent work on source-free domain adaptation has emerged [15, 18, 19, 20, 31, 38, 44, 49]. Specifically, SHOT [19] proposed freezing the source classifier to maximize mutual information and minimize entropy, while using a pseudo-labeling strategy to obtain extra supervision. In 3C-GAN [18], labeled target-style training images were generated based on a conditional GAN to improve model performance on the target domain. In G-SFDA [49], the neighborhood structure of the target data for clustering enhanced the predictive consistency of local neighborhood features effectively. In CPGA [31], the source avatar prototypes were generated via contrastive learning to mine the hidden knowledge in the source model. Many methods described above freeze the source classifier during adaptation to preserve class information and assign pseudo-labels based on the classifier’s output. They mainly focus on a single feature prototype to align two domains, which often causes negative transfer and noisy labels. Instead, we here introduce polycentric clustering for each class to reduce noisy labels. In addition, a consistent training strategy is introduced to enhance the target domain for source-free domain adaptation.

3 Method

In this section, we first formally define the problem and the notation used for source-free domain adaptation followed by an overview of our framework. Later, a detailed description of our proposed strategy to solve the SFDA problem is presented.

3.1 Preliminaries and notations

We denote that the source domain with $n_s$ labeled samples as $D_s = \{x_{i}^{s}, y_{i}^{s}\}_{i=1}^{n_s}$, where $x_{i}^{s} \in X_s$, $y_{i}^{s} \in Y_s \subseteq \mathbb{R}^K$ is the one-hot ground-truth label and $K$ is the total number of classes of label
set $C = \{1, 2, ..., K\}$. Target domain dataset $\mathcal{D}_t$ has $n_t$ unlabeled samples $\{x^i_t\}_{i=1}^{n_t}$, where $x^i_t \in \mathcal{X}_t$, it has the same label set $C$ as that of $\mathcal{D}_s$. Under the SFDA setting, only the model $f_s$ trained on the source data is accessible, which consists of two parts: a feature extractor $g_s: \mathcal{X}_s \to \mathbb{R}^d$ and a classifier $h_s: \mathbb{R}^d \to \mathbb{R}^K$, i.e., $f_s(x) = h_s(g_s(x))$, where $d$ denotes the dimension of the feature space. In this work, with only the source model $f_s$ and unlabeled data $\{x^i_t\}_{i=1}^{n_t}$ available, our goal is to learn an objective function $f_t: \mathcal{X}_t \to \mathcal{Y}_t$ and to infer $\{y^i_t\}_{i=1}^{n_t}$.

3.2 Overall framework

An overview of our proposed framework is presented in Figure 1. The target model $f_t$ is initialized by the source model $f_s$, and the source model consists of two modules: the feature encoding module $g_s$ and the classifier module $h_s$. The target model uses the same classifier module, namely, $h_t = h_s$, and two new modules named PCC and mixup are introduced respectively. It is noted that our PCSR learn $f_t$ in an epoch-wise manner. As for each epoch stage, firstly, a balanced set of feature instances representing each class is obtained using inter-class balanced sampling. Then polycentric clustering is implemented to obtain accurate pseudo-labeling. After that, information maximization loss is used to reduce the gap between the feature distributions in the source and target domains. Meanwhile, the mixup operation is introduced to enhance the target domain with more interpolated samples.

3.3 Information maximization

We update the feature extractor $g_t$ using the information maximization (IM) loss \[12\], which reduces the feature distribution between the source and target domains so that the classification output of the target features has some certainty and global diversity. The IM loss consists of a conditional entropy term and a diversity term:

$$
L_{im} = -\mathbb{E}_{x \in \mathcal{X}_t} \sum_{k=1}^{K} \delta_k(f_t(x)) \log \delta_k(f_t(x)) + \sum_{k=1}^{K} \tilde{p}_k \log \tilde{p}_k
$$

(1)

Where $\delta_k(a)$ denotes the $k$-th element in the softmax output of the K-dimensional vector $a$. $\tilde{p} = \mathbb{E}_{x \in \mathcal{X}_t} [\delta_k(f_t(x))]$ is the average of the current batch’s softmax output.
3.4 Intra-class polycentric clustering

To reduce the gap between the source and target domains, a simple existing solution is to eliminate the noisy labels by selecting pseudo-labels with high confidence. However, this will bias the model toward majority classes and ignore minority classes, resulting in noisy labels for those hard data in the target domain. To reduce the noisy labels, an intra-class polycentric clustering strategy is proposed, which contains two steps.

**Inter-class balanced sampling.** Due to class imbalance in the target domain, instead of using the existing prediction results based on argmax operations, we adopt an inter-class balanced sampling strategy to construct each class of the target domain. Specifically, for the $k$-th class in the target domain, each sample in the target domain is represented by a feature vector $\hat{g}_t(x_t)$ and a classification result $p(x_t) = \delta(\hat{f}_t(x_t))$. Instead of choosing the top-1 feature, the top-$M$ $p(x_t)$ of the $k$-th class on the target domain $D_t$ are selected as potential representative features for aggregation. Then these top-$M$ are averaged to form an inter-class balanced feature clustering center $c_k$, and the initial pseudo-label $\hat{y}_t$ is obtained from the nearest centroid classifier as follows:

$$M_k = \arg \max_{x \in X_t} \delta_k(\hat{f}_t(x))$$

$$c_k^{(0)} = \frac{1}{M} \sum_{i \in M_k} \hat{g}_t(x_i)$$

$$\hat{y}_t = \arg \min_k D_f(\hat{g}_t(x), c_k^{(0)})$$

(2)

Where $\hat{f}_t = \hat{g}_t \circ h_t$ denotes the previously learned target hypothesis, $M = \max(1, \lfloor \frac{n_t}{r \times K} \rfloor)$. $r$ is the hyperparameter of the top-$M$ selection ratio and $K$ is the number of classes in the target domain. $D_f(a, b)$ measures the cosine distance between $a$ and $b$. Based on the above strategy, we can obtain balanced sampled feature instances for each class. Similar to SHOT [19], we perform iterative computations to obtain more robust clustering centers $c_k$ and pseudo-labels $\hat{y}_t$ as follows:

$$M_k = \arg \max_{x \in X_t} \delta_k(\hat{g}_t(x) \cdot c_k^{(0)})$$

$$c_k^{(1)} = \frac{1}{M} \sum_{i \in M_k} \hat{g}_t(x_i)$$

$$\hat{y}_t = \arg \min_k D_f(\hat{g}_t(x), c_k^{(1)})$$

(3)

Although the pseudo-labels and the centroids can be updated by Eq. (3) multiple times, we find that two rounds of updating are sufficient.

**Polycentric clustering.** According to the above strategy, class-balanced prototype and robust pseudo-labels can be obtained. However, for those ambiguous data located nearby the decision boundary, they may not be effectively represented by a coarse monocentric prototype. In this paper, polycentric clustering is proposed to get more accurate pseudo-labels with a predefined number of clustering centers. Specifically, the classical k-means algorithm [26] is introduced to achieve intra-class clustering of the target domain, assuming that the number of clustering centers is $P$ and $\{c_k^i\}_{i=1}^P$ is defined as the multiple clustering centers of the $k$-th class. The k-means algorithm is used to obtain multiple clustering centers
of each class \( \{c^i_k\}_{i=1}^P \) and obtain more robust pseudo-labels \( \hat{y}_t \):

\[
M_k = \arg \max_{x \in X_t} \frac{\max_{1 \leq i \leq P} (\exp(\hat{g}_t(x) \cdot c_k^i))}{\sum_{j=1}^K \max_{1 \leq i \leq P} (\exp(\hat{g}_t(x) \cdot c_j^i))}
\]

\[
\{c^i_k\}_{i=1}^P = \text{Kmeans}(\hat{g}_t(x_m))
\]

(4)

Empirically, we find that iterating this process for two rounds is sufficient. Given the generated pseudo-labeling, the loss function for computing the intra-class polycentric clustering pseudo-labeling is as follows.

\[
\mathcal{L}_{pcc} = -\mathbb{E}_{x \in X_t} \sum_{k=1}^K \mathbb{I}_{[\hat{y}_t = k]} \log \delta_k (f_t(x))
\]

(5)

### 3.5 Structural regularization by mixup training

As mentioned above, we consider intra-class polycentric clustering to mitigate negative transfer, but this ignores the target domain’s data structure and still suffers from the noisy labels. According to [48], even though the target data is shifted in the feature space, the target data of the same class is still expected to form a cluster in the embedding space. Therefore, we consider paired target structure information by MixUp [50] to reduce the intra-domain variation, and the new instance \( \{x, y\} \) generated by the MixUp operation \( \text{Mix}((X_1, Y_1), (X_2, Y_2)) \) can be defined as:

\[
x = \lambda x_1 + (1 - \lambda)x_2; \quad x_1 \in X_1, x_2 \in X_2
\]

\[
y = \lambda y_1 + (1 - \lambda)y_2; \quad y_1 \in Y_1, y_2 \in Y_2
\]

(6)

\( \lambda \) denotes the mixup coefficient. The structured loss is optimized by using interpolation consistency training [41]:

\[
\mathcal{L}_{\text{mix}} = \mathbb{E}_{x_i, x_j \in X_t} l_{ce}(\lambda f_t^i(x_i) + (1 - \lambda) f_t^j(x_j), f_t(\lambda x_i) + (1 - \lambda) x_j)
\]

(7)

Where \( \lambda \) obeys Beta distribution sampling, \( \lambda \in \text{Beta}(\alpha, \alpha) \), and the hyperparameter is empirically set to 0.3, following the setup of [50]. \( l_{ce} \) represents the cross-entropy loss. \( f_t^i \) indicates that no gradient calculation is required, but only the value of \( f_t \) is provided. This loss function can supply more augmented samples for the target domain, allowing for better generalization ability.

Integrating all the loss function equations introduced, we can derive the final loss function as follows.

\[
\mathcal{L}_t = \mathcal{L}_{im} + \mathcal{L}_{pcc} + \beta \mathcal{L}_{\text{mix}}
\]

(8)

Where \( \beta \) is a hyperparameter experimentally set to 1.0.

Algorithm 1 summarizes our method’s training process.
Algorithm 1 Polycentric Clustering and Structural Regularization for SFDA

**Input:** Pre-trained source model $f_s(h_s, g_s)$; target data $X_t$; max epoch number $T_{\text{max}}$; Number of clustering centers $P$.

**Initialization:** Initialize $f_t(h_t, g_t)$ using $f_s(h_s, g_s)$.

1: for $\text{epoch}_\text{idx} = 1$ to $T_{\text{max}}$ do
2: Obtain feature prototypes and initial pseudo-labels using inter-class balanced sampling using Eq. (2) Eq.(3).
3: Compute multiple clustering centers and pseudo-labels based on $P$ and k-means algorithm using Eq.(4).
4: for $\text{iter}_\text{idx} = 1$ to the number of target samples $N_b$ do
5: Calculate IM loss according to the Eq.(1).
6: Apply MixUp to performing structural regularization operations by Eq.(7).
7: end for
8: Update $f_t$ via minimizing Eq.(8).
9: end for

4 Experiment and Analysis

4.1 Experimental setup

**DataSets.** We conduct experiments on three datasets, including Office-31 [32], Office-Home [40], and VisDA-C [29]. Office-31 is divided into three domains: Amazon(A), Webcam(W), and DSLR(D), with 31 categories. Office-Home contains 65 categories and consists of four domains: Artistic images(A), Clip Art(C), Product images(P), and Real-World images(R). VisDA-C is a more challenging dataset, with 152K synthetic images generated by rendering 3D models in the source domain while the target domain has 55K real object images, which are divided into 12 shared classes.

**Implementation details.** To ensure a fair comparison with the related approaches, we employ ResNet-50 [11] pre-trained on Image-Net [6] as the backbone for Office-31 and Office-Home, and ResNet-101 [11] as the backbone for VisDA-C. Similar to the previous work, for all datasets, we apply the gradient descent (SGD) optimizer with momentum 0.9 and weight decay $1e^{-3}$, the batch size is set to 64, and the input image size is reshaped to $224 \times 224$. The learning rate is set to $1e^{-2}$ for Office-31 and Office-Home, and $1e^{-3}$ for VisDA-C, and 30 epochs are trained for all the settings. For the hyperparameter settings, we set the hyperparameter $r$ of the selection ratio to 3 on all datasets, and the predefined number of clustering centers $P$ is set to 3 for Office-31 and Office-Home, and 4 for VisDA-C. All experiments are built on a TITAN Xp with Pytorch-3.8. The source code of the proposed algorithm is available in https://github.com/Gxinuu/PCSR.

4.2 Quantitative comparison

Tables 1-3 show the experimental results on the three datasets mentioned above. The best results in SFDA shown in bolded font and the sub-optimal results underlined. In Table 1, our method achieves comparable results to 3C-GAN on Office-31 and even obtains more competitive performance. Note that 3C-GAN highly relies on the extra synthesized data. And Office-31 is a small-scale dataset whose image number of each class is around 40 on average. Therefore, it is hard for our method to aggregate valid polycentric clustering. Yet
we still achieve the best results on 3 of 6 tasks.

As shown in Table 2, our method achieves the latest performance (72.8%) and is higher than the second best NRC by a margin of 0.6% on Office-Home, achieving the best/second-best results on 10 out of 12 individual tasks. Our method is even superior to some of the traditional domain adaptation methods which require source data. This can be attributed to the fact that due to the increased amount of data, more finely polycentric clustering and more comprehensive structure information is available to support our approach.

To further demonstrate the effectiveness of our proposed PCSR, we conduct evaluation experiments on the large dataset VisDA-C and illustrate the results in Table 3. Our method significantly outperforms SHOT, surpassing it by 2.7%. We can find that class-balanced performance has been improved with our strategy. Especially for the challenging class ‘truck’, our method achieves 66.4%, which outperforms SHOT applied monocentric clustering by 23.7%. The reason is that the polycentric clustering strategy introduces more fine-grained feature clustering centers and the generalization ability of the target model is improved by structural regularization. The results demonstrate the effectiveness of our approach, and our method also outperforms domain adaptation methods with access to source data on both Office-Home and VisDA-C.

### 4.3 Ablation studies

**Number of clustering centers P.** In Figure 3, we show the results using different $P \in \{1,2,3,4,$}
Table 3: Classification accuracies (%) on VisDA-C for ResNet101-based methods.

| Method          | SF | plane | bicycle | bus | car | horse | knife | person | plant | sktbrd | train | truck | Per-class |
|-----------------|----|-------|---------|-----|-----|-------|-------|--------|-------|--------|-------|-------|-----------|
| ResNet-101(2016) | ✓  | 55.1  | 53.3    | 61.9| 59.1| 80.6  | 17.9  | 79.7   | 31.2  | 81.0   | 26.5  | 73.5  | 8.5       |
| CDAN(2018)      | ✓  | 85.2  | 66.9    | 83.0| 50.8| 84.2  | 74.9  | 88.1   | 74.5  | 83.4   | 76.0  | 81.9  | 38.0      |
| SAFN(2019)      | ✓  | 93.6  | 61.3    | 84.1| 70.6| 94.1  | 79.0  | 91.8   | 79.6  | 89.9   | 56.9  | 89.0  | 24.4      |
| SWD(2019)       | ✓  | 90.8  | 82.5    | 81.7| 70.5| 91.7  | 69.5  | 86.3   | 77.5  | 84.7   | 63.6  | 85.6  | 29.2      |
| MCC(2020)       | ✓  | 88.7  | 80.3    | 80.5| 71.5| 90.1  | 93.2  | 85.0   | 71.6  | 89.4   | 73.8  | 85.0  | 36.9      |
| RWO(T2020)      | ✓  | 95.1  | 80.3    | 83.7| 90.0| 92.4  | 68.0  | 92.5   | 82.2  | 87.9   | 78.4  | 90.4  | 68.2      |
| Source-only     | ✓  | 64.1  | 24.9    | 53.0| 66.5| 67.9  | 9.1   | 84.5   | 21.1  | 62.8   | 29.8  | 83.5  | 9.3       |
| SFDA(2021)      | ✓  | 86.9  | 81.7    | 84.6| 63.9| 93.1  | 91.4  | 86.6   | 71.9  | 84.5   | 58.2  | 74.5  | 42.7      |
| SHOT(2020a)     | ✓  | 94.3  | 88.5    | 80.7| 57.3| 93.1  | 94.9  | 80.7   | 80.3  | 91.5   | 89.1  | 86.3  | 58.2      |
| 3C-GAN(2020)    | ✓  | 94.8  | 73.4    | 68.8| 74.8| 93.1  | 95.4  | 88.6   | 84.7  | 89.1   | 84.7  | 83.5  | 48.1      |
| G-SFDA(2021b)   | ✓  | 96.1  | 88.3    | 85.5| 74.1| 97.1  | 95.4  | 89.5   | 79.4  | 95.4   | 92.9  | 89.1  | 42.6      |
| HCL(2021a)      | ✓  | 93.3  | 85.4    | 80.7| 68.5| 91.0  | 88.1  | 86.0   | 78.6  | 86.6   | 88.8  | 80.0  | 74.7      |
| ours            | ✓  | 96.2  | 89.8    | 82.5| 61.0| 95.3  | 96.4  | 87.5   | 81.8  | 91.7   | 92.3  | 86.2  | 66.4      |

Table 4: Ablation of the losses on Office-Home.

| Loss     | L_{im} | L_{pcc} | L_{mix} | Avg. |
|----------|--------|---------|---------|------|
| ✓        | ✓      | ✓       | ✓       | 59.6 |
| ✓        | ✓      |         | ✓       | 70.5 |
| ✓        | ✓      | ✓       |         | 72.1 |
| ✓        | ✓      | ✓       |         | 72.5 |
| ✓        | ✓      | ✓       |         | 72.8 |

Ablation study on losses. We validate the effectiveness of our methods on Office-Home. Results are shown in Table 4. The classification accuracy is 59.6% when the source-only model is used. We start with applying the information maximization loss, where makes the classification output of the target features becomes more certainty and more global diversity. This achieves 70.5% accuracy. In the third row, based on the information maximization loss, with the intra-class polycentric feature clustering, more accurate pseudo labels are obtained, and the performance increases by 12.5% to 72.1%. And using structural regularization, the model is enforced to maintain consistency, and the performance achieves 72.5%. The model’s performance is optimized when all three are used simultaneously. This demonstrates the validity of each loss function.

t-SNE visualization. To visually the effectiveness of our method, we compare the t-
5 Conclusion

In this paper, we have proposed a polycentric clustering and structure regularization (PCSR) strategy for source-free domain adaptation. Specifically different from the previous monocentric clustering, our PCSR strategy reduced the negative transfer of hard data in the target domain by considering intra-class polycentric clustering through inter-class-balanced sampling. In addition, structural regularization of the target domain interpolates the target data for consistent training, and improves the model’s robustness. The experimental results on three benchmark datasets have demonstrated the effectiveness of our approach. For future work, we intend to apply the method to other vision tasks, such as semantic segmentation and target detection.
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