Kore Initial Clustering for Unsupervised Domain Adaptation

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Abstract: In unsupervised domain adaptation (UDA) literature, there exists an array of techniques to derive domain adaptive features. Among them, a particularly successful family of approaches of pseudo-labeling the unlabeled target data has shown promising results. Yet, the majority of the existing methods primarily focus on leveraging only the target domain knowledge for pseudo-labeling while insufficiently considering the source domain knowledge. Here, we hypothesize that quality pseudo labels obtained via classical K-means clustering considering both the source and target domains bring simple yet significant benefits. In particular, we propose to assign pseudo labels to the target domain’s instances better aligned with the source domain labels by a simple method that modifies K-means clustering by emphasizing the strengthened notion of centroids, namely, Kore Initial Clustering (KIC). The proposed KIC is readily utilizable with a wide array of UDA models, consistently improving the UDA performance on multiple UDA datasets including Office-Home and Office-31, demonstrating the efficacy of pseudo labels in UDA.

1 INTRODUCTION

Unsupervised Domain Adaptation (UDA), a learning framework that focuses on leveraging labeled source domain data to enhance the performance of unlabeled target domain data, has gained significant attention in recent literature for its benefit of not having supervision in target domain (Liu et al., 2022; Ren et al., 2022; Lee et al., 2022; Xie et al., 2022). The UDA scenario is especially beneficial in situations where labeling costs are high or labeling itself is unfeasible (Tarvainen and Valpola, 2017). The fundamental premise of UDA lies in minimizing the distribution difference between the source and target domains. Nevertheless, prior arts in UDA task have a number of disadvantages as follows:

First, many conventional methods in UDA required complex optimization processes or tuning of multiple hyperparameters (Sun and Saenko, 2016). This complexity posed challenges for researchers and practitioners in real-world applications. Second, while most existing methods solely focused on minimizing the distribution difference between the source and target domains, this did not always guarantee optimal performance. Especially when there was a substantial distribution difference between domains, such approaches proved to be inefficient (Tzeng et al., 2017). Finally, recent UDA studies have indeed paid attention to domain adaptation through cluster-
2 RELATED WORKS

Unsupervised Domain Adaptation. UDA aims to minimize the distributional difference between labeled data from a source domain and unlabeled data from a target domain (Ganin and Lempitsky, 2015; Xu et al., 2021; Sun et al., 2022). The main intention of UDA is to overcome the distributional discrepancy between these domains. To address this challenge, we have a variety of strategies. One method involves matching the higher-order statistics of features from both domains, thereby reducing their distributional divergence (Long et al., 2015). Another method ensures consistency in the prediction results of both source and target domain data, thereby bridging the domain gap (French et al., 2017). Lastly, pseudo-labeling involves creating synthetic labels for unlabeled data in the target domain. Using these pseudo-labels, models are retrained, which have shown efficacy in several UDA models (Saito et al., 2018). Despite these advancements, real-world domain disparities continue to manifest in diverse manners, posing a persistent challenge in UDA research.

Vision Transformer. Recently, the trend in the computer vision field has been showing a shift from traditional convolutional neural networks (CNNs) to the transformer structure, originally designed for natural language processing tasks. Among these, the Vision Transformer (ViT) introduced by Dosovitskiy et al. (Dosovitskiy et al., 2020) is considered a representative study. While traditional CNNs process images in a local and hierarchical manner, ViT divides the image into patches of fixed size, linearly embeds them, and then processes the sequence of embedded patches through transformer blocks (Carion et al., 2020). In UDA, reducing the distribution difference between the source and target domains (Du et al., 2021) is crucial, and the attention mechanism of ViT is better capturing and adapting to these domain differences. Specifically, ViT can focus attention on distant parts of an image regardless of spatial proximity, making it advantageous in detecting subtle differences between domains. After the initial success of ViT, various modifications have been proposed to optimize and apply its structure to different tasks and constraints (Touvron et al., 2021). Proposed by Liu et al. (Liu et al., 2021), the Swin Transformer divides images into non-overlapping windows and performs self-attention operations only within these windows, reducing computational load while capturing domain differences more finely. Yet, even with the advancements brought by the Swin Transformer, there remains challenges, especially in the context of UDA.
Pseudo-Label. Pseudo-labeling is a method of assigning temporary labels to unlabeled data based on model predictions. Because in UDA, it is essential to reduce the distribution discrepancy between labeled data from the source domain and unlabeled data from the target domain, pseudo-labeling provides a means to fine-tune these domain differences by assigning labels to the data in the target domain. (Ben-David et al., 2006). Pseudo-labeling can refine this domain alignment by providing labels to the target domain’s data. The basic approach using pseudo-labels involves generating predictions for the unlabeled data in the target domain using an initially trained model. The model makes these predictions as new labels and then re-trains in an iterative process. This approach aids the model in extracting information from the target domain’s data in UDA scenarios (Saito et al., 2017). We generate pseudo-labels on the target samples with a bias towards the source domain using a customized initial centroid computation for solving the UDA problem. This method proves effective in achieving high performance with data that has intricate domain characteristics or complex distributions.

Centroid of Clustering. The choice of initial centroids can significantly affect the convergence and quality of the clustering results. In UDA as well, it is essential to reduce the distributional discrepancy between the source and target domains (Zhang and Lee, 2022). To address this, a method combining Self-Supervised Learning (SSL) and clustering to generate anchor vectors or cluster centroids has been proposed (Mahapatra et al., 2022). These anchor vectors play a pivotal role in bridging the gap between the known classes (seen classes) from the source domain and the unknown classes (unseen classes) from the target domain. The research emphasizes the importance of having accurate anchor vectors to solve the UDA problem and introduces self-supervised loss terms to ensure the uniqueness and consistency of these vectors. Additionally, to provide focused attention to the data from the target domain during the clustering phase, the research integrates saliency maps, enhancing the quality of information derived from image features. Based on the potential of centroid clustering to facilitate domain alignment, we believed that applying it to UDA could yield promising outcomes.

3 METHODS

In this section, we first investigate pseudo-labeling for unsupervised domain adaptation. Then we discuss the issues associated with K-means clustering and the initialization of centroids. Finally, we describe the proposed method named Kore Initial Clustering (KIC) which aligns the source and target domains by estimating initial centroids in clustering for cross-domain adaptation.

3.1 Pseudo-Labeling

Unsupervised Domain Adaptation (UDA) typically involves transferring knowledge from a labeled source domain to an unlabeled target domain. Pseudo labeling helps create a form of pseudo-supervision in the target domain by assigning labels to unlabeled data based on the predictions of the model trained on the source domain. One common challenge in UDA is obtaining reliable pseudo-labels for unlabeled data in the target domain. A weighted clustering strategy is a technique that assigns different weights to data points during the pseudo-labeling process, aiming to improve the overall reliability of the assigned labels. In this paper, we use a weighted clustering strategy (Du et al., 2021) to obtain the centroid $c_k$ of the $k$-th class. Suppose that we have feature extractor $G_v$, classifier $F_n$ and $n_t$ unlabeled target samples $\{x_t^i\}_{i=1}^{n_t}$ drawn from the target distribution $\mu_t$:

$$c_k = \frac{\sum_{n=1}^{2} \sum_{x^i < \chi_n^k} \delta_k (F_n(G(x^i))) G(x^i)}{\sum_{n=1}^{2} \sum_{x^i < \chi_n^k} \delta_k (F_n(G(x^i)))},$$

where $\delta_k$ represents the corresponding $k$-th element of the softmax output $\delta$. Then, pseudo labels could be obtained by the nearest centroid strategy.

3.2 K-means Clustering

Clustering-based pseudo-labeling (Lee, 2013) is a technique used in machine learning to generate labels for unlabeled data points by first clustering the data and then assigning labels based on the clusters. A widely adopted methodology in UDA involves the integration of clustering algorithms, such as K-means clustering (MacQueen et al., 1967), in conjunction with pseudo-labeling. This combined approach is employed to effectively leverage the untapped potential residing within the unlabeled data of the target domain. K-means clustering is popular in UDA for several reasons: its simplicity makes it easy to understand and implement, and it can be easily integrated into the UDA pipeline. In K-means clustering, the algorithm aims to partition a given dataset into $K$ clusters, where each cluster is represented by its centroid. The centroid initialization step plays a crucial role in the performance and convergence of the algorithm. The choice of initial centroids can significantly impact the clustering results, as poorly selected initial
centroids can lead to suboptimal clustering. Random initialization in K-means randomly selects K data points as initial centroids, but it can be sensitive to the random seed and produce different outcomes for different runs. On the other hand, K-means++ initialization (Arthur and Vassilvitskii, 2007) improves random initialization by selecting centroids based on the distance to the nearest centroid. While K-means++ initialization generally produces improved clustering results compared to random initialization, it does not take advantage of any available source domain knowledge to estimate initial centroids for clustering in the target domain. To address this, in our study, we propose a method utilizing K-means clustering to refine the pseudo-labeling process further.

3.3 Weighted Cross Entropy

A recurring challenge arises when distinguishing between source and target domains. Specifically, while the source and target might be rendered indistinguishable through alignment techniques, there’s no guarantee that the data points from these domains will cluster densely. This sparse clustering can hinder the model’s ability to discriminate between different classes effectively. Recognizing this limitation, we propose a subtle approach: the incorporation of a weighted cross-entropy loss. The weighted cross entropy loss increases the shared information between the observed distribution of target inputs and the pseudo-label distribution (Prabhu et al., 2021).

The essence of this loss function lies in its ability to capture the uncertainty associated with each prediction. Entropy, a well-established measure of uncertainty in probability distributions, is leveraged for this purpose. For a given sample \( k \), its entropy is

\[
H(p^{(k)}) = - \sum_i p_i^{(k)} \log(p_i^{(k)}),
\]

where \( p_i^{(k)} \) represents the predicted probabilities for each class \( i \) by sample \( k \).

Drawing from this entropy calculation, we assign a weight to each sample. The underlying idea is to give more importance to samples that the model deems challenging or is less certain about. Thus, the normalized weight \( w_k \) for sample \( k \) is defined as

\[
w_k = \frac{1 + e^{-H(p^{(k)})}}{\sum_j 1 + e^{-H(p^{(j)})}}.
\]

This ensures that samples characterized by higher entropy (and thus, greater uncertainty) are assigned more substantial weights. By balancing the conventional cross-entropy loss with these weights, we create a loss function that dynamically adjusts based on the model’s confidence in its predictions.

By adopting this weighted cross-entropy loss, we provide the model with a refined training signal. This encourages the model to pay heightened attention to challenging samples, thereby increasing its robustness. This enhancement is important when dealing with diverse data sources, as it supports better generalization and adaptability across different domains.

Figure 3: An overview of our proposed framework. Both source samples and target samples are passed through an embedding layer respectively consisting of both patch embeddings and positional embeddings. Then the resulting source and target data are passed into the backbone model for training and evaluation. The KIC module, consisting of linear interpolation of the source and target points - weighted towards the source points - is performed on the features/logits extracted from the evaluated results to create initial centroids for K-means clustering. The pseudo-labels created from the K-means clustering are then compared to the target prediction labels to calculate a weighted cross entropy loss.
3.4 Kore Initial Clustering

In this work, our goal is to address the potential drawbacks associated with the clustering-based pseudo-labeling described in Section 3.2 by estimating initial centroids for target domain using linear interpolation toward source domain. To achieve this objective, we introduce the Kore Initial Clustering (KIC) method, considering its applicability to a broad Unsupervised Domain Adaptation (UDA) framework. An overview of our proposed approach is illustrated in Fig. 3. The training procedure consists of four steps:

1. **Initial Points.** Utilizing features and logits from the UDA framework, initial points for each domain are computed using weighted clustering (Equation 1).

2. **Initial Centroids.** Initial centroids are created by combining information from both the source and target domains. This is achieved through linear interpolation, where the initial points from each domain are linearly combined using the equation:

   \[ c_k = \alpha c_k^t + (1 - \alpha)c_k^s, \]  

   Here, \( c_k^t \) and \( c_k^s \) represent the initial points of the \( k \)-th class for the target and source domains respectively, and \( \alpha \) is the interpolation factor. In our model, we set \( \alpha \) to be more biased towards source domain with a weight of 0.9.

3. **Pseudo-Labeling with K-means.** K-means clustering, using estimated initial centroids for the target domain, is employed for pseudo-labeling. This ensures that labels are derived from the inherent structure of the data in the feature space. This approach provides a more informed way of labeling target domain data compared to using the existing K-means clustering method with random initialization for centroids.

4. **Loss Calculation.** Finally, the pseudo-labels generated from the K-means clustering are compared to the target prediction labels to calculate a weighted cross-entropy loss.

### Table 1: Comparison with SoTA methods on Office-Home. * indicates the results of experiments where the batch size was adjusted to 16, deviating from the original experimental setup. The best performance is marked as bold.

<table>
<thead>
<tr>
<th>Method</th>
<th>A→C</th>
<th>A→P</th>
<th>A→R</th>
<th>C→A</th>
<th>C→P</th>
<th>C→R</th>
<th>P→A</th>
<th>P→C</th>
<th>P→R</th>
<th>R→A</th>
<th>R→C</th>
<th>R→P</th>
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</thead>
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<td>63.8</td>
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<td>57.0</td>
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<tr>
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<td>92.6</td>
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### Table 2: Comparison with SOTA methods on Office-31. * indicates the results of experiments where the batch size was adjusted to 16, deviating from the original experimental setup. The best performance is marked as bold.

<table>
<thead>
<tr>
<th>Method</th>
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<th>D→W</th>
<th>W→D</th>
<th>A→D</th>
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<th>A→W</th>
<th>Avg</th>
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<tr>
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<td>96.3</td>
<td>70.9</td>
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<td>MCD (Saito et al., 2018)</td>
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</table>

After repeating the above steps, the model can effectively align the distributions of two domains. As we describe in the next section, achieving alignment of features from different domains is crucial for effective knowledge transfer. The Kore Initial Clustering (KIC) module aims to tackle this challenge by reliably estimating initial centroids for clustering through linear interpolation.

4 EXPERIMENTS AND RESULTS

To confirm the robustness and efficacy of our proposed model, we conduct experiments on prevalent benchmark datasets, including Office-Home (Venkateswarla et al., 2017), Office-31 (Saenko et al., 2010) and VisDA-2017 (Peng et al., 2017).

4.1 Implementation Details

We utilized the same backbone that was originally employed in previous experiments for our study. For PMTrans (Zhu et al., 2023), we use the Swin-based transformer (Liu et al., 2021) pre-trained on ImageNet (Deng et al., 2009) as the backbone which was used in their experiments. We experimented with two batch sizes, 16 and 32, for ViT-based PMTrans. However, we used a size of batch 16 for Swin-based method due to resource limitations. With the exception of a batch size, we used the original paper’s settings such
Table 3: Comparison with SOTA methods on VisDA-2017. * indicates the results of experiments where the batch size was adjusted to 16, deviating from the original experimental setup. The best performance is marked as bold.

<table>
<thead>
<tr>
<th>Method</th>
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<th>knife</th>
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<td>PMTrans-ViT + KIC*</td>
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<td>PMTrans-Swin (Zhu et al., 2023)</td>
<td>99.3</td>
<td>97.3</td>
<td>88.4</td>
<td>62.6</td>
<td>99.1</td>
<td>98.6</td>
<td>93.1</td>
<td>60.3</td>
<td>98.0</td>
<td>99.3</td>
<td>97.2</td>
<td>59.2</td>
<td>87.7</td>
</tr>
<tr>
<td>PMTrans-Swin + KIC*</td>
<td>99.4</td>
<td>88.3</td>
<td>88.1</td>
<td>78.9</td>
<td>98.8</td>
<td>98.3</td>
<td>95.8</td>
<td>70.3</td>
<td>94.6</td>
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<td>96.3</td>
<td>48.5</td>
<td>88.0</td>
</tr>
<tr>
<td>PMTrans-Swin + KIC</td>
<td>99.3</td>
<td>93.3</td>
<td>88.2</td>
<td>67.8</td>
<td>99.1</td>
<td>98.9</td>
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<td>97.4</td>
<td>99.1</td>
<td>97.0</td>
<td>57.5</td>
<td>88.3</td>
</tr>
</tbody>
</table>

as learning rate, the number of epochs, weight decay, and the optimizer. For each experiment, we utilized a single NVIDIA GeForce RTX 3090 GPU.

### 4.2 Results

We combine KIC module with the latest SOTA UDA method PMTrans (Zhu et al., 2023). Here we show the comparison between the original SOTA methods and the combination of KIC module with PMTrans. Note that, for a fair comparison, we utilized the results from the original papers.

**Result on Office-Home.** We summarize the results in Table 1. The proposed method excels particularly in improving performance in challenging domains where the accuracy predominantly lies in the mid-to-high 80s. Surprisingly, for P→C, we observed a dramatic improvement of 1.3% and it achieves SOTA performance. Domains that are difficult to adopt such as R→C and A→C achieve 0.9% and 0.4% improvements respectively compared to the existing SOTA method. Despite halving the batch size compared to the original paper, A→P demonstrated a performance boost of 1.1%. Likewise, R→A also showed an improvement of 0.9%. For the Swin-based PMTrans, training was conducted with a batch size of 32 in original paper, whereas our method utilized a batch size of 16. Despite this discrepancy, we achieved a 0.6% accuracy enhancement in C→A. In general, integrating UDA with our proposed approach significantly elevates classification accuracy across nearly all classes.

**Result on Office-31.** We summarize the results in Table 2. The proposed method achieves an average accuracy of 95.4% by increasing 0.4% compared to the existing SOTA method with the ViT-based approach. Similar to the results on Office-Home, the most significant improvements were noted in the most challenging classes such as D→A which improves 0.9% accuracy. For W→A, both ViT-based and Swin-based approaches, even when using a smaller batch size of 16 compared to the original paper, the proposed method achieves 0.5% and 0.4% improvement respectively.

**Result on VisDA-2017.** We summarize the results in Table 3. The proposed method improves an average accuracy of 88.3% by 0.4%. As observed, truck showed an 59.2% accuracy by improving 10.2% with ViT-based approach. We observed a 5% improvement in the performance on bicycles, reaching an accuracy of 93.3% and 2.8% improvement in plants with the Swin-based approach. Similarly, with the Vit-based approach, the enhancements were 3.6% and 4.6% respectively.

**Resource Efficiency.** The proposed method improves classification accuracy and also increases runtime efficiency and training speed. According to the PMTrans (Zhu et al., 2023), larger batch sizes lead to better representation of data distributions, typically resulting in superior performance in UDA tasks when using the PMTrans with various backbones. However, in our case, despite utilizing smaller batch sizes, we achieved superior performance. It demonstrates the effectiveness of the proposed method.

### 4.3 Ablation Study

**Comparison with K-means and KIC.** In this ablation study, we empirically validate that a standalone K-means clustering with random initial centroids cannot guarantee robust improvements; instead, a carefully designed initial centroid based on our KIC is a must. Specifically, we compare (1) PMTrans-ViT, (2) PMTrans-ViT + K-means which uses random initial centroids, and (3) PMTrans-ViT + KIC which uses our KIC centroids in Table 4 and Table 5. In Table 4 showing the results on Office-Home, we observe that PMTrans-ViT + K-means (89.2%) with random initial centroids do outperform the baseline PMTrans-ViT (88.9%) with no clustering, our PMTrans-ViT + KIC (89.3%) brings the best result on average. In addition, we see even more drastic boost from KIC on Office-31 in Table 5, where PMTrans-ViT + K-means
Table 4: The ablation study comparing the K-means with random initial centroids (PMTrans-ViT + K-means) and ours with KIC (PMTrans-ViT + KIC) on Office-Home. The best performance is marked as bold. We observe that the K-means with our domain adaptive KIC centroids lead to the best performance, and the K-means alone, while improving over the baseline (PMTrans-ViT), cannot.

| Method                     | A→C | A→P | A→R | C→A | C→P | C→R | P→A | P→C | P→R | R→A | R→C | R→P | Avg |
|----------------------------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| PMTrans-ViT (Zhu et al., 2023) | 90.5 | 89.0 | 89.4 | 94.5 | 85.7 | 88.2 | 94.9 |
| PMTrans-ViT + K-means      | 99.0 | 99.0 | 100.0 | 99.4 | 95.7 | 98.9 | 95.9 |
| PMTrans-ViT + KIC          | 99.2 | 99.3 | 100.0 | 99.8 | 96.6 | 98.9 | 95.6 |

(94.9%) brings no improvements over PMTrans-ViT (95.0%) but PMTrans-ViT + KIC (95.4%) made a significant improvement in every transfer setting.

5 CONCLUSION

In this work, we proposed a simple yet effective solution named KIC to derive domain adaptive initial centroids for K-means clustering which demonstrated robust performance on multiple UDA datasets. The underlying premise of KIC is to utilize the pseudo labels of the target data to pull the target initial centroids towards the source initial centroids. Our work naturally comes with a great versatility which can be easily added to existing UDA methods as we have shown and lead to SOTA results on multiple datasets. Thus, further research is needed to determine the relevance of our study to other clustering methods. We believe there exist an array of future work including more advanced clustering techniques which may further benefit from our KIC module.

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