Implicit Class-Conditioned Domain Alignment for Unsupervised Domain Adaptation

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Abstract
We present an approach for unsupervised domain adaptation—with a strong focus on practical considerations of within-domain class imbalance and between-domain class distribution shift—from a class-conditioned domain alignment perspective. Current methods for class-conditioned domain alignment aim to explicitly minimize a loss function based on pseudo-label estimations of the target domain. However, these methods suffer from pseudo-label bias in the form of error accumulation. We propose a method that removes the need for explicit optimization of model parameters from pseudo-labels directly. Instead, we present a sampling-based implicit alignment approach, where the sample selection procedure is implicitly guided by the pseudo-labels. Theoretical analysis reveals the existence of a domain-discriminator shortcut in misaligned classes, which is addressed by the proposed implicit alignment approach to facilitate domain-adversarial learning. Empirical results and ablation studies confirm the effectiveness of the proposed approach, especially in the presence of within-domain class imbalance and between-domain class distribution shift.

1. Introduction
Supervised learning aims to extract statistical patterns from data by learning to approximate the conditional density $p(y|x)$. However, the generalization of the approximation is often sensitive to some dataset-specific factors. Dataset shift (Quionero-Candela et al., 2009) frequently arises from real-world applications and can manifest in many different ways, such as sample selection bias (Heckman, 1979; Torralba et al., 2011), class distribution shift (Webb & Ting, 2005), and covariate shift (Shimodaira, 2000). Unsupervised Domain Adaptation (UDA) aims to address domain shift with access to labeled data in the source domain and unlabeled data in the target domain (Pan & Yang, 2009). The fundamental algorithmic issue is to infer domain-invariant representations.

While considerable progress has been made in UDA (Ganin et al., 2016), they tend to focus on marginal distribution matching in the feature space, and less emphasis is made on discovering label distributions. In real-world applications, it is very common to have class imbalance within each domain and class distribution shift between different domains, necessitating the incorporation of label space distribution into adaptation. Explicit class-conditioned domain alignment (Xie et al., 2018; Pan et al., 2019; Liang et al., 2019a; Deng et al., 2019) has emerged as a key approach to promoting class-conditioned invariance by aligning prototypical representations of each class. While explicit alignment has the advantage of directly minimizing class-conditioned misalignment, it presents critical vulnerabilities to error accumulation (Chen et al., 2019a) and ill-calibrated probabilities (Guo et al., 2017) due to its dependence on explicit supervision from pseudo-labels provided by model predictions.

We propose Implicit Class-Conditioned Domain Alignment that removes the need for explicit pseudo-label based optimization. Instead, we use the pseudo-labels implicitly to sample class-conditioned data in a way that maximally aligns the joint distribution between features and labels. The primary advantage of the sampling-based implicit domain alignment is the ability to address within-domain class imbalance and between-domain class distribution shift, in addition to many other benefits such as applications in cost-sensitive learning.

The proposed method is simple, effective, and is supported by theoretical analysis on the empirical estimations of domain divergence measures. It also overcomes limitations of explicit alignment by allowing the domain adaptation algorithm to discover class-conditioned domain-invariance in an unsupervised way without explicit supervision from pseudo-labels.

The contributions of this paper are as follows: (i) We propose implicit class-conditioned domain alignment to address the challenge of within-domain class imbalance and between-domain class distribution shift, which overcomes the limitation of error accumulation in explicit domain align-
ment; (ii) We provide theoretical analysis on the empirical domain divergence and reveal the existence of a shortcut function that interferes with domain-invariant learning, which is addressed by the proposed approach; (iii) We show that the proposed approach is orthogonal to the choice of domain adaptation algorithms and offers consistent improvements to two adversarial domain adaptation algorithms; (iv) We report state-of-the-art UDA performance under extreme within-domain class imbalance and between-domain class distribution shift, and competitive results on standard UDA tasks.

2. Preliminaries

We follow the notations by (Ben-David et al., 2010) and define a domain as an ordered pair consisting of a distribution \( D \) on the input space \( \mathcal{X} \), and a labeling function \( f : \mathcal{X} \rightarrow \mathcal{Y} \) that maps \( \mathcal{X} \) to the label space \( \mathcal{Y} \). The source and target domains are denoted by \( (D_S, f_S) \) and \( (D_T, f_T) \), respectively.

In unsupervised domain adaptation, the model is trained on labeled data from the source domain, together with unlabeled data from the target domain. The goal is to obtain a model \( h \in \mathcal{H} \) which learns domain-invariant representations while simultaneously minimizing the classification error on \( D_S \).

Adversarial training is the prevailing approach for domain adaptation (Ganin et al., 2016). It formulates a minimax problem where the maximizer maximizes the estimation of the domain divergence between the empirical samples, and the minimizer minimizes the sum of the source error and the domain divergence estimation obtained from the maximizer.

While matching the marginal distribution is a good step towards domain-invariant learning, it is still susceptible to the problem of conditional distribution mismatching. Prototype-based class-conditioned domain alignment (Luo et al., 2017; Xie et al., 2018; Chen et al., 2019a; Pan et al., 2019; Liang et al., 2019a;b) is designed to address this problem. Let \( \mathcal{H} \) be a hypothesis space and \( \mathcal{Y} \) be the label space. The empirical estimation of the domain divergence measure \( \Delta_H \) is bounded by the error of the source domain error \( \epsilon_S(h) \) and the empirical domain divergence \( d_{\mathcal{H} \Delta H}(U_S, U_T) \) where \( U_S, U_T \) are unlabeled empirical samples drawn from \( D_S, D_T \).

In deep learning, minibatch-based optimization limits the amount of data available at each training step. This necessitates the analysis of the empirical estimations of \( d_{\mathcal{H} \Delta H} \) at the minibatch level, so as to shed light on the learning dynamics.

**Definition 3.1.** Let \( B_S, B_T \) be minibatches from \( U_S \) and \( U_T \), respectively, where \( B_S \subseteq U_S, B_T \subseteq U_T \), and \( |B_S| = |B_T| \). The empirical estimation of \( d_{\mathcal{H} \Delta H}(B_S, B_T) \) over the minibatches \( B_S, B_T \) is defined as

\[
\hat{d}_{\mathcal{H} \Delta H}(B_S, B_T) = \sup_{h, h' \in \mathcal{H}} \left| \sum_{B_T} [h \neq h'] - \sum_{B_S} [h \neq h'] \right|. 
\]

**Theorem 3.2** (The decomposition of \( \hat{d}_{\mathcal{H} \Delta H}(B_S, B_T) \)). Let \( \mathcal{H} \) be a hypothesis space and \( \mathcal{Y} \) be the label space of the classification task where \( B_S, B_T \) are minibatches drawn from \( U_S, U_T \), respectively, and \( Y_S, Y_T \) are the label set of \( B_S, B_T \). We define three disjoint sets on the label space: the shared labels \( Y_C := Y_S \cap Y_T \), and the domain-specific labels \( Y_S' := Y_S - Y_C \), \( Y_T' := Y_T - Y_C \). We also define the following disjoint sets on the input space where \( B_S' := \{ x \in B_S \mid y \in Y_C \}, B_S'' := \{ x \in B_S \mid y \notin Y_C \}, B_T' := \{ x \in B_T \mid y \in Y_C \}, B_T'' := \{ x \in B_T \mid y \notin Y_C \} \). The empirical \( \hat{d}_{\mathcal{H} \Delta H}(B_S, B_T) \) divergence can be decomposed into class aligned divergence and class-misaligned divergence:

\[
\hat{d}_{\mathcal{H} \Delta H}(B_S, B_T) = \sup_{h, h' \in \mathcal{H}} \left| \xi^C(h, h') + \xi^C(h, h') \right|, 
\]

where

\[
\xi^C(h, h') = \sum_{B_S'} [h \neq h'] - \sum_{B_S''} [h \neq h'], 
\]

\[
\xi^C(h, h') = \sum_{B_T'} [h \neq h'] - \sum_{B_T''} [h \neq h']. 
\]
Misaligned: \[3, 6\] \hspace{1cm} \text{Aligned:} \[4, 4\]

Figure 1. Illustration of the domain discriminator shortcut. The domain discriminator aims to distinguish between different domains (red and blue), where the decision boundary is represented by dashed lines. But misaligned samples create a shortcut where the domain labels can be directly determined by the misaligned class labels (3 and 6). The decision boundary of the resulting shortcut is independent of the covariate that causes the domain difference, which does not contribute to adversarial domain-invariant learning.

The proof is provided in supplementary materials.

Remark 3.3 (The domain discriminator shortcut). Let the ordered triple \((x, y_c, y_d)\) denote data sample \(x\), and its associating class label \(y_c\) and domain label \(y_d\), respectively, where \(x \in \mathcal{X}, \ y_c \in \mathcal{Y}\) and \(y_d \in \{0, 1\}\). Let \(f_c\) be a classifier that maps \(x\) to a class label \(y_c\). Let \(f_d\) be a domain discriminator that maps \(x\) to a binary domain label \(y_d\). For the empirical class-misaligned divergence \(\xi(x, h, h')\) with sample \(x \in \mathcal{B}_S \cup \mathcal{B}_T\), there exists a domain discriminator shortcut function

\[
f_d(x) = \begin{cases} 1 & f_c(x) \in \mathcal{Y}_S \\ 0 & f_c(x) \in \mathcal{Y}_T, \end{cases}
\]

such that the domain label can be solely determined by the domain-specific class labels. This shortcut interferes with adversarial domain adaptation because the model could bypass the optimization for domain-invariant representations, but rather optimize for a shortcut function that is independent of the covariate contributing to the domain difference.

Figure 2 depicts the proposed implicit class-conditioned domain alignment framework. We aim to align \(p_S(x)\) and \(p_T(x)\) at the input and label space jointly with the factorization \(p(x, y) = p(x|y)p(y)\) while ensuring that the sampled classes are aligned between the two domains. The alignment distribution \(p(y)\) is pre-specified, e.g., uniform distribution, to ensure samples are aligned in the shared label space in spite of different empirical label distributions of the two domains. This implicit alignment procedure minimizes the class-misaligned divergence \(\xi(x, h, h')\), providing a more reliable empirical estimation of domain divergence. For the unlabeled target domain, we use the model predictions to sample class-conditioned data from \(p_T(x|y)\) to approximate \(p_T(x|y)\).

### 3.2. Class-Aligned Sampling Strategy

Algorithm 1 presents the proposed sampling procedure that selects class-aligned examples for minibatch training. It is a type of stratified sampling where the dataset is partitioned into mutually exclusive subgroups to reflect the label information in a class-aligned manner.

First, we predict pseudo-labels of the target domain using the classifier \(f_c(\cdot; \theta)\) parameterized by \(\theta\). The pseudo-labels will be later used in class-conditioned sampling. Second, we sample a set \(Y\) from the label space \(\mathcal{Y}\) where \(p(y)\) defines the probability with which we pick the classes to align so as to ensure the empirical samples of the source and target domains share the same \(Y\). This in turn minimizes the class-misaligned divergence \(\xi(x, h, h')\). Third, for each class \(y_i \in Y\), we sample class-conditioned examples for the source...
We use uniform sampling $p_f$.

This algorithm addresses class imbalance within each domain and the disparity measures of the two domains.

and target domains, respectively, and store them in $(X'_S, Y'_S)$ and $X'_T$. This is equivalent to performing a table lookup to select a subset $B_i$ where all examples belong to class $y_i$, followed by random sampling in $B_i$. We use pseudo-labels to sample the target domain due to the lack of ground-truth labels. Once we obtained the class-aligned minibatch, we use it to train unsupervised domain alignment algorithm and repeat this process until the model converges.

This algorithm addresses class imbalance within each domain as well as class distribution shift between different domains by specifying the sampling strategy $p(y)$ in the label space. We use uniform sampling $p(y)$ for all experiments in this paper, and leave more advanced specifications and their applications to cost-sensitive domain adaptation as future work.

3.2.2. INTEGRATING IMPLICIT ALIGNMENT INTO CLASSIFIER-BASED DOMAIN DISCREPANCY MEASURE

Section 3.2.1 describes the implicit alignment algorithm from a sampling perspective, where we sample minibatches in a way that maximizes class alignment implicitly. This sampling strategy is independent of the choice of domain divergence measures. In this section, we show how to integrate the sampling approach into Margin Disparity Discrepancy (MDD) (Zhang et al., 2019b)—a state-of-the-art classifier-based domain discrepancy measure—to further facilitate implicit alignment. MDD is defined as

$$d_{f,f'}(S,T) = \sup_{f' \in \mathcal{F}} \left( \text{disp}_{D_f}(f', f) - \text{disp}_{D_{f'}}(f', f) \right),$$

where $f$ and $f'$ are two independent scoring functions that predict class probabilities, and $\text{disp}(f', f)$ is a disparity measure between the scores provided by the classifiers $f'$ and $f$. The domain divergence is to estimate the discrepancy between the disparity measures of the two domains.

Following notations in Theorem A.2, we define the empirical MDD on class-misaligned samples as

$$\hat{d}_{f,f'}(B_S, B_T) = \sup_{f' \in \mathcal{F}} \left( \sum_{B_S} \text{disp}(f', f) - \sum_{B_S} \text{disp}(f', f) \right).$$

Because $B_S$ and $B_T$ are disjoint in the label space, there exists a shortcut solution

$$\text{disp}(f'(x), f(x)) = \begin{cases} 0 & f_c(x) \in Y_S, \\ 1 & f_c(x) \in \overline{Y_T}, \end{cases}$$

which maximizes the divergence estimation of Eq. (8). Although class-aligned sampling can mitigate this problem, it is difficult to fully eliminate the impact of misalignment due to imperfect pseudo-labels. To further eliminate the detrimental impact of class-misalignment, we introduce a masking scheme on the scoring functions $f$ and $f'$ defined as

$$\hat{d}_{f,f'}(B_S, B_T) = \sup_{f' \in \mathcal{F}} \left( \sum_{B_T} \text{disp}(f' \odot \omega, f \odot \omega) - \sum_{B_S} \text{disp}(f' \odot \omega, f \odot \omega) \right),$$

where $f \odot \omega$ denotes element-wise multiplication between the output of $f$ and $\omega$. The alignment mask $\omega$ is a binary vector that denotes whether the $i$-th class is present in the sampled classes $Y$ (i.e., the classes that we intend to align in the current minibatch). By doing so, we simultaneously align the source and target domains (i) in the input space and (ii) in the functional approximations of the domain divergence by masking the scoring functions $f$ and $f'$.

4. Experiments

4.1. Setup

Datasets. We evaluate on Office-31, Office-Home and VisDA2017. Office-31 (Saenko et al., 2010) has three domains (Amazon, DSLR and Webcam) with 31 classes. We use three versions of Office-Home (Venkateswara et al., 2017) that contains four domains (Art, Clip Art, Prduct, and Real-world) with 65 classes: (i) “standard”: the standard Office-Home dataset. (ii) “balanced” (Tan et al., 2019): a subset of the standard dataset where each class has the same number of examples. (iii) “RS-UT”: Reversely-unbalanced Source (RS) and Unbalanced-Target (UT) distribution (Tan et al., 2019) where both domains are imbalanced, but the majority class in the source domain is the minority class in the target domain. VisDA2017 (synthetic—real) (Peng et al., 2017) is a large-scale dataset with 12 classes and more than 200k images.

Model architecture. We use ResNet-50 (He et al., 2016) pre-trained from ImageNet (Russakovsky et al., 2015) as the backbone, and use hyper-parameters from (Zhang et al., 2019b)
Table 1. Per-class average accuracy on Office-Home dataset with RS-UT label shifts (ResNet-50).

| Methods                                      | Rw→Pr | Rw→Cl | Pr→Rw | Pr→Cl | Cl→Rw | Cl→Pr | Avg |
|----------------------------------------------|-------|-------|-------|-------|-------|-------|-----|
| Source Only†                                | 69.77 | 38.35 | 67.31 | 35.84 | 53.31 | 52.27 | 52.81 |
| BSP (Chen et al., 2019c)†                   | 72.80 | 23.82 | 66.19 | 20.05 | 32.59 | 30.36 | 40.97 |
| PADA (Cao et al., 2018)†                    | 60.77 | 32.28 | 57.09 | 26.76 | 40.71 | 38.34 | 42.66 |
| BBSE (Lipton et al., 2018)†                 | 61.10 | 33.27 | 62.66 | 31.15 | 39.70 | 38.08 | 44.33 |
| MCD (Saito et al., 2018)†                   | 66.03 | 33.17 | 62.95 | 29.99 | 44.47 | 39.01 | 45.94 |
| DAN (Long et al., 2015)†                    | 69.35 | 40.84 | 66.93 | 34.66 | 53.55 | 52.09 | 52.90 |
| F-DANN (Wu et al., 2019)†                   | 68.56 | 40.57 | 67.32 | 37.33 | 55.84 | 53.67 | 53.88 |
| JAN (Long et al., 2017)†                    | 67.20 | 43.60 | 68.87 | 39.21 | 57.98 | 48.57 | 54.24 |
| DAN (Gan et al., 2016)†                     | 71.60 | 46.51 | 68.40 | 38.07 | 58.83 | 58.05 | 56.91 |
| MDD (random sampler)                        | 71.21 | 44.78 | 69.31 | 42.56 | 52.10 | 52.70 | 55.44 |
| MDD (source-balanced sampler)               | 76.06 | 47.38 | 71.56 | 40.03 | 57.46 | 58.54 | 58.50 |
| COAL (Tan et al., 2019)†                    | 73.65 | 42.58 | 73.26 | 40.61 | 59.22 | 57.33 | 58.40 |
| MDD+Explicit Alignment (basic)†             | 69.52 | 44.70 | 69.59 | 40.27 | 53.02 | 53.39 | 55.08 |
| MDD+Explicit Alignment (moving avg.)†        | 71.37 | 45.26 | 69.69 | 40.28 | 52.92 | 52.69 | 55.37 |
| MDD+Explicit Alignment (curriculum)†        | 70.02 | 45.48 | 69.71 | 40.86 | 53.26 | 52.99 | 55.39 |
| MDD+Implicit Alignment                      | 76.08 | 50.04 | 74.21 | 45.38 | 61.15 | 63.15 | 61.67 |

† Source: Data of these baseline methods are cited from (Tan et al., 2019).
‡ Methods using explicit class-conditioned domain alignment.

2019b) for MDD-based domain discrepancy measure. The batch size is 31 for Office-31 and 50 for Office-Home.

**Baselines.** Our main explicit alignment baselines are COAL (Tan et al., 2019), PACET (Liang et al., 2019b) and MCS (Liang et al., 2019a), state-of-the-art explicit alignment methods based on domain discriminator discrepancy. As our domain discrepancy measure is MDD, we re-implement various MDD-based explicit alignment for fair comparison.

**Computational efficiency.** We only update pseudo-labels periodically, i.e., every 20 steps, instead of at every training step. We show in the supplementary materials that our method does not require more frequent pseudo-label updates.

### 4.2. Evaluating Extreme Class Distribution Shift

We use Office-Home (RS-UT), described in Figure 3 (a), to evaluate the performance of different methods under extreme within-domain class imbalance and between-domain class distribution shift where the majority classes in the source domain are minority classes in the target domain. Table 1 presents the per-class average accuracy on Office-Home (RS-UT). Our main baseline is the explicit alignment method “covariate and label shift co-alignment” (COAL) designed to address data imbalance and class distribution shift. Our proposed implicit domain alignment works the best.

#### 4.2.1. The Impact of Class Distribution Shift

Many baseline methods suffer from class distribution shift, and their performances degrade to “Source Only” training as they do not take into account within-domain class imbalance and between-domain class distribution shift. For MDD-based methods, after we apply balanced sampling for the source domain, the per-class average accuracy improved from 55.44% to 58.50%, which indicates balanced sampling is helpful for class distribution shift, despite only in the source domain.

#### 4.2.2. The Effectiveness of Implicit Alignment

The effectiveness of implicit alignment is demonstrated through the comparison between “MDD+Implicit Alignment” and “MDD (source-balanced sampler)”. Both methods use the same sampling procedure for the source. The only difference is that implicit alignment aligns the two domains by sampling aligned classes in the target domain, whereas “source-balanced sampler” only takes random samples from the target domain. Table 1 shows that implicit alignment performs better than “source-balanced sampler” because it is better-aligned, which confirms the effectiveness of implicit alignment. Besides, the proposed method also outperforms MDD-based explicit alignment, which validates the effectiveness of implicit alignment over the explicit alignment.

Figure 3 (b) compares the baseline, implicit and explicit alignments on Office-Home (balanced) and Office-Home (RS-UT). We observe that implicit alignment performs the best on both datasets. More importantly, implicit alignment is more robust to class distribution shift which greatly out-performs other methods under RS-UT distribution shift and has a smaller performance drop from the balanced version of Office-Home.
Table 2. Accuracy (%) on Office-31 (standard) for unsupervised domain adaptation (ResNet-50). We repeated each experiment 5 times with different random seeds and report the average and the standard error of the accuracy.

| Method                     | A → W | D → W | W → D | A → D | D → A | W → A | Avg  |
|----------------------------|-------|-------|-------|-------|-------|-------|------|
| Source only                | 68.4±0.2 | 96.7±0.1 | 99.3±0.1 | 68.9±0.2 | 62.5±0.3 | 60.7±0.3 | 76.1 |
| DAN (Long et al., 2015)    | 80.5±0.4 | 97.1±0.2 | 99.6±0.1 | 78.6±0.2 | 63.6±0.3 | 62.8±0.2 | 80.4 |
| DANN (Ganin et al., 2016)  | 82.0±0.4 | 96.9±0.2 | 99.1±0.1 | 79.7±0.4 | 68.2±0.4 | 67.4±0.5 | 82.2 |
| ADDA (Tzeng et al., 2017)  | 86.2±0.5 | 96.2±0.3 | 98.4±0.3 | 77.8±0.3 | 69.5±0.4 | 68.9±0.5 | 82.9 |
| JAN (Long et al., 2017)    | 85.4±0.3 | 97.4±0.2 | 99.8±0.2 | 84.7±0.3 | 68.6±0.3 | 70.0±0.4 | 84.3 |
| MADA (Pei et al., 2018)    | 90.0±0.1 | 97.4±0.1 | 99.6±0.1 | 87.8±0.2 | 70.3±0.3 | 66.4±0.3 | 85.2 |
| GTA (Sankaranarayanan et al., 2018) | 89.5±0.5 | 97.9±0.3 | 99.8±0.4 | 87.7±0.5 | 72.8±0.3 | 71.4±0.4 | 86.5 |
| MCD (Saito et al., 2018)   | 88.6±0.2 | 98.5±0.1 | 100.0±0.0 | 92.2±0.2 | 69.5±0.1 | 69.7±0.3 | 86.5 |
| CDAN (Long et al., 2018)   | 94.1±0.1 | 98.6±0.1 | 100.0±0.0 | 92.9±0.2 | 71.0±0.3 | 69.3±0.3 | 87.7 |
| MDD (Zhang et al., 2019b)  | 94.5±0.3 | 98.4±0.1 | 100.0±0.0 | 93.5±0.2 | 74.6±0.3 | 72.2±0.1 | 88.9 |
| PACET (Li et al., 2019b)‡  | 90.8    | 97.6    | 99.8    | 90.8    | 73.5    | 73.6    | 87.4 |
| CAT (Deng et al., 2019)‡    | 94.4±0.1 | 98.0±0.2 | 100.0±0.0 | 90.8±1.8 | 72.2±0.2 | 70.2±0.1 | 87.6 |
| MDD (source-balanced sampler) | 90.4±0.4 | 98.7±0.1 | 99.9±0.1 | 90.4±0.2 | 75.0±0.5 | 73.7±0.9 | 88.0 |
| MDD+Explicit Alignment‡    | 92.3±0.1 | 98.1±0.1 | 99.8±0.0 | 92.3±0.3 | 74.6±0.2 | 72.9±0.7 | 88.4 |
| MDD+Implicit Alignment‡     | 90.3±0.2 | 98.7±0.1 | 99.8±0.0 | 92.1±0.5 | 75.3±0.2 | 74.9±0.3 | 88.8 |

Methods using explicit class-conditioned domain alignment.

4.3. Evaluating Standard Domain Adaptation Datasets

Table 2 and Table 3 summarize the results for the standard Office-31 and Office-Home datasets which have a small degree of class imbalance. Our method outperforms the baselines in 3 out of 6 domain pairs for Office-31, and 10 out of 12 domain pairs for Office-Home (standard). The proposed implicit alignment exhibits larger performance gains on the Office-Home dataset because the dataset is more difficult for domain adaptation, and it has 65 classes compared with the 31 classes in Office-31. We also report state-of-the-art results for VisDA in Table 4.

Similar to findings in Section 4.2, we observe source-balanced sampling is helpful when comparing “MDD (source-balanced sampler)” with the MDD standard baseline, even without extreme class distribution shift.

The proposed method outperforms the state-of-the-art explicit alignment methods—PACET and MCS—across all domain pairs. We find it ineffective to incorporate prototype-based explicit alignment into MDD. This is in contrast with domain-discriminator-based adversarial learning, where explicit alignment is shown to improve domain adaptation. This is because the classifier-based discrepancy MDD contains more abundant information than domain-discriminator-based discrepancy, owing to the availability of predictive probabilities provided by the classifiers. The rich information in domain discrepancy removes the need for prototype-based distances.

Table 4. VisDA2017 target accuracy (ResNet-50)

| Method                          | Acc. (%) |
|--------------------------------|----------|
| JAN (Long et al., 2017)         | 61.6     |
| GTA (Sankaranarayanan et al., 2018) | 69.5     |
| MCD (Saito et al., 2018)       | 69.8     |
| CDAN (Long et al., 2018)       | 70.0     |
| MDD (Zhang et al., 2019b)‡     | 74.6     |
| MDD+Explicit Alignment‡        | 67.1     |
| MDD+Implicit Alignment‡        | 75.8     |
Figure 4. The impact of class diversity and alignment on domain adaptation for Ar→Cl, Office-Home (standard).

Figure 5. The impact of pseudo-label errors on implicit and explicit alignment, Ar→Cl, Office-Home (standard).

**4.4. Ablation studies**

**4.4.1. Impact of class diversity and alignment**

We analyze the impact of class diversity and alignment by designing experiments along three dimensions: the number of unique labels in each minibatch, whether the classes are aligned, and whether we use pseudo-labels or ground-truth labels when sampling the target domain.

**Setup.** “Baseline (random)” randomly samples examples of both domains. “Baseline (S-sampled, T-random)” uses $N$-way sampler for the source domain, and randomly samples the target domain. “Aligned (pseudo-labels)” is the proposed implicit alignment approach. “Aligned (Oracle)” is the oracle form of implicit alignment where the target domain uses ground-truth labels for sampling.

**The impact of class diversity.** Minibatch-based class diversity determines the sampling distribution of the label space, and a greater diversity corresponds to a more stable measure of this sampling distribution. Figure 4 suggests a positive correlation between the model performance and class diversity: domain adaptation methods do not work well when the class diversity is very low—i.e., only sample 5 classes per batch among the 65 classes—and the alignment-based methods outperform the baseline as we increase class diversity.

**The impact of alignment.** We confirm the importance of the proposed implicit alignment algorithm from two perspectives. First, “Aligned (oracle)” consistently performs the best, which suggests perfect alignment can provide substantial benefits to unsupervised domain adaptation. Second, the comparison between “Aligned (pseudo-labels)” and “Baseline (S-sampled, T-random)” validates the effectiveness of pseudo-label based implicit alignment, although the pseudo-labels are approximations of the oracle.

**4.4.2. Robustness to pseudo-label errors**

We investigate whether implicit alignment is indeed more robust to pseudo-label errors when compared with explicit alignment. Figure 5 illustrates the relationship between pseudo-label accuracy at training step $t$ and the corresponding subsequent target accuracy at step $t + 1000$, i.e., after 1000 domain adaptation training steps. This process resembles a Markov chain that allows us to analyze the impact of pseudo-label accuracy on the learning dynamics.

It is evident that the drawbacks of explicit alignment are more severe when the pseudo-labels are less accurate, e.g., 10–40%, where implicit alignment has more considerable performance improvements than explicit alignment. This suggests that implicit alignment is more robust to erroneous pseudo-label predictions because it does not require explicit supervision from the pseudo-labels. Implicit and explicit methods eventually converge at 76% and 74%, respectively.

Although many recent techniques attempt to address pseudo-label bias in explicit alignment, they depend on the assumption that probabilities of model predictions are well-calibrated during training. They fail to address ill-calibrated probabilities (Guo et al., 2017), where the model tends to make confident mistakes on the target domain. Moreover, given that models do not initially perform well when training begins, for a random classifier, implicit alignment selects random samples that is equivalent to training without sampling. In contrast, explicit alignment optimizes model parameters from these random labels explicitly.

**4.4.3. Ablation study on MDD**

Table 5 presents the ablation study on Office-Home (RS-UT) that aims to assess the impact of different implicit alignment options: alignment in the domain divergence estimations in Section 3.2.1 (i.e., masking in MDD) and alignment in the input space in Section 3.2.1 (i.e., sampling class-conditioned examples). We observe that both alignment techniques are essential for domain adaptation because alignment should be enforced consistently across all aspects of adaptation. We report similar findings, in the supplementary material, on Office-Home (standard).

| Alignment options | Domains masking sampling | avg. acc. |
|-------------------|--------------------------|----------|
| Rw→Cl             | ×                        | 44.8     |
| ✓                 | ✓                        | 47.4     |
| ✓                 | ✓                        | 50.0     |
| Pr→Rw             | ✓                        | 69.3     |
| ✓                 | ✓                        | 72.7     |
| ✓                 | ✓                        | 72.0     |
| ✓                 | ✓                        | 74.2     |
Implicit Class-Conditioned Domain Alignment for Unsupervised Domain Adaptation

4.4.4. Generalization: Implicit Alignment Also Improves DANN

We design additional experiments to further demonstrate the effectiveness of the proposed approach on a different domain adaptation algorithm—DANN—on two synthetic domains with different degrees of class imbalance: “mild” (light-tailed class imbalance from a triangular-like distribution) and “extreme” (heavy-tailed class imbalance from a Pareto distribution). We synthetically manipulate the class distributions of SVHN and MNIST to simulate various interactions between within-domain class imbalance and between-domain class distribution shift. As illustrated in Fig 6, we simulate three types of distribution shift when $p_S(y) \neq p_T(y)$ (i) source-balanced, target-imbalanced; (ii) source-imbalanced, target-balanced; (iii) both-imbalanced.

Table 6, 7 and 8 present the results for the abovementioned scenarios and all experiments are repeated five times. The proposed implicit alignment approach significantly improves the performance of DANN regardless of the degree of imbalance or the type of distribution shift. Besides, implicit alignment offers greater improvements over DANN when the degree of imbalance is more severe, i.e., comparing “mild” with “extreme”. Implicit alignment overcomes this limitation of DANN and greatly improves the performance of the challenging task between SVHN and MNIST. We conclude that the proposed approach is independent of the choice of domain adaptation algorithms and helps both MDD and DANN.

Table 6. Per-class average accuracy (%) with mismatched prior where the source domain is balanced while the target domain is imbalanced.

| Method       | Source Only | DANN | DANN+implicit |
|--------------|-------------|------|---------------|
| SVHN→MNIST   | 67.4±7.3    | 78.2±2.8 | 88.6±0.7      |
| MNIST→SVHN   | 66.3±3.3    | 59.1±0.8 | 82.2±2.1      |

Table 7. Per-class average accuracy (%) with mismatched prior where the source domain is imbalanced while the target domain is balanced.

| Method       | Source Only | DANN | DANN+implicit |
|--------------|-------------|------|---------------|
| SVHN→MNIST   | 32.5±2.9    | 20.9±6.0 | 32.4±2.1      |
| MNIST→SVHN   | 28.2±2.3    | 20.5±3.1 | 28.9±3.3      |

Table 8. Per-class average accuracy (%) with mismatched prior where both domains are imbalanced.

| Method       | Source Only | DANN | DANN+implicit |
|--------------|-------------|------|---------------|
| SVHN→MNIST   | 60.9±5.2    | 67.6±0.8 | 88.6±0.6      |
| MNIST→SVHN   | 51.2±5.9    | 40.5±5.5 | 70.5±3.6      |

5. Related Work

We review related work on unsupervised domain adaptation and discuss their relations with our proposed method.

Instance-based importance-weighting (Chawla et al., 2002; Kouw & Loog, 2019) aims to minimize the target error directly from the source domain data, weighted at the example level or class level. Unlike our approach, importance-weighting only uses the source data to train the classifier without learning domain invariant representations.

Feature-based distribution adaptation is the prevailing approach to domain adaptation that aims to minimize the distribution discrepancy between the source and target domains. The domain difference can be measured in various ways, such as Maximum Mean Discrepancy (MMD) (Borgwardt et al., 2006), which is further minimized to achieve domain invariance. The minimization of such discrepancy can be carried out by directly minimizing the distance (Tzeng et al., 2014) or with the help of adversarial learning (Ganin et al., 2016).

Classifier-based distribution adaptation is a strong competitor to feature-based adaptation. It aims to minimize the discrepancy between two classifiers so that the learned representations respect the decision boundary of the classification task (Saito et al., 2018; Zhang et al., 2019b). We show that the proposed approach is beneficial to both classifier-based discrepancy MDD (Zhang et al., 2019b) and feature-based discrepancy DANN (Ganin et al., 2016).

Feature-classifier joint distribution adaptation aims to align the joint distribution between features and their corresponding predictions (Long et al., 2013; Tsai et al., 2018). The joint distribution can be represented in a multilinear map between features and classifier predictions (Long et al.,
Reinforced sample selection (Dong & Xing, 2018) is proposed for one-shot domain adaptation where a model actively selects labeled examples to train the domain adaptation model. In comparison, the advantage of our approach is in its simplicity that no reinforcement learning is required to obtain the sampling strategy.

6. Conclusion and Future Work

We introduce an approach for unsupervised domain adaptation—with a strong focus on practical considerations of within-domain class imbalance and between-domain class distribution shift—from a class-conditioned domain alignment perspective. We show theoretically that the proposed implicit alignment provides a more reliable measure of empirical domain divergence which facilitates adversarial domain-invariant representation learning, that would otherwise be hampered by the class-misaligned domain divergence. We show that our proposed approach leads to superior UDA performance under extreme within-domain class imbalance and between-domain class distribution shift, as well as competitive results on standard UDA tasks. We emphasize that the proposed method is robust to pseudo-label bias, simple to implement, has a unified training objective, and does not require additional parameter tuning. We also show that the proposed approach is orthogonal to the choice of domain adaptation algorithms and offers consistent improvements to feature-based and classifier-based domain adaptation algorithms.

Future work includes extensions to cost-sensitive learning for domain adaptation, and other setups where the label space between the source and target domains are not identical, as well as other domain adaptation setups (Cao et al., 2018). It is also important to analyze the probability calibration of different domain adaptation models and develop well-calibrated methods for more effective use of pseudo-labels.

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A. Theory

Definition A.1. Let \( \mathcal{B}_S, \mathcal{B}_T \) be minibatches from \( \mathcal{U}_S \) and \( \mathcal{U}_T \), respectively, where \( \mathcal{B}_S \subseteq \mathcal{U}_S, \mathcal{B}_T \subseteq \mathcal{U}_T, \) and \( m_b = |\mathcal{B}_S| = |\mathcal{B}_T| \). The empirical estimation of \( d_{\Delta_H}(\mathcal{B}_S, \mathcal{B}_T) \) over the minibatches \( \mathcal{B}_S, \mathcal{B}_T \) is defined as

\[
\hat{d}_{\Delta_H}(\mathcal{B}_S, \mathcal{B}_T) = \frac{1}{m_b} \sum_{b \in \mathcal{B}_T} \left| \sum_{h \in \mathcal{B}_S} [h \neq h'] - \sum_{b \in \mathcal{B}_S} [h \neq h'] \right|.
\]

For simplicity, we drop the multiple \( \frac{1}{m_b} \) in the following analysis as it does not affect the result of optimization.

Theorem A.2 (The decomposition of \( \hat{d}_{\Delta_H}(\mathcal{B}_S, \mathcal{B}_T) \)). Let \( \mathcal{H} \) be a hypothesis space and \( Y \) be the label space of the classification task where \( \mathcal{B}_S, \mathcal{B}_T \) are minibatches drawn from \( \mathcal{U}_S, \mathcal{U}_T, \) respectively, and \( Y_S, Y_T \) are the label set of \( \mathcal{B}_S, \mathcal{B}_T \). We define three disjoint sets on the label space: the shared labels \( Y_C := Y_S \cap Y_T \), and the domain-specific labels \( Y_S' := Y_S - Y_C \), and \( Y_T' := Y_T - Y_C \). We also define the following disjoint sets on the input space where \( \mathcal{B}^C_S := \{ x \in \mathcal{B}_S \mid y \in Y_C \}, \mathcal{B}^C_T := \{ x \in \mathcal{B}_T \mid y \in Y_C \}, \mathcal{B}^C := \{ x \in \mathcal{B}_T \mid y \notin Y_C \}, \mathcal{B}^C := \{ x \in \mathcal{B}_T \mid y \notin Y_C \} \). The empirical \( \hat{d}_{\Delta_H}(\mathcal{B}_S, \mathcal{B}_T) \) divergence can be decomposed into class aligned divergence and class-misaligned divergence:

\[
\hat{d}_{\Delta_H}(\mathcal{B}_S, \mathcal{B}_T) = \sup_{h, h' \in \mathcal{H}} \left| \xi^C(h, h') + \xi^{\overline{C}}(h, h') \right|.
\]

where

\[
\xi^C(h, h') = \sum_{b \in \mathcal{B}_S^C} [h \neq h'] - \sum_{b \in \mathcal{B}_S} [h \neq h'],
\]

\[
\xi^{\overline{C}}(h, h') = \sum_{b \in \mathcal{B}_T^C} [h \neq h'] - \sum_{b \in \mathcal{B}_S} [h \neq h'].
\]

Proof. By definition, we have

\[
\hat{d}_{\Delta_H}(\mathcal{B}_S, \mathcal{B}_T) = \sup_{h, h' \in \mathcal{H}} \left| \sum_{b \in \mathcal{B}_T} [h \neq h'] - \sum_{b \in \mathcal{B}_S} [h \neq h'] \right|
\]

We rewrite the summation over all the samples \( \mathcal{B} \) into the sum of disjoint subsets \( \mathcal{B}^C \) and \( \mathcal{B}^{\overline{C}} \).

\[
\sum_{b \in \mathcal{B}_T} [h \neq h'] - \sum_{b \in \mathcal{B}_S} [h \neq h']
\]

\[
\left( \sum_{b \in \mathcal{B}^C_S} [h \neq h'] - \sum_{b \in \mathcal{B}^C} [h \neq h'] \right)
\]

\[
+ \left( \sum_{b \in \mathcal{B}^C_T} [h \neq h'] - \sum_{b \in \mathcal{B}^{\overline{C}}_S} [h \neq h'] \right)
\]

\[
= \xi^C(h, h') + \xi^{\overline{C}}(h, h').
\]

This completes the proof.
B. Experiments

B.1. Additional Evaluation Measures on Office-Home

Table 9. Evaluation on Office-Home (%) with ResNet-50.

|          | Ar→Cl MDD ours | Pr→Rw MDD ours |
|----------|----------------|----------------|
| accuracy | 54.91          | 77.46          |
| macro    |                |                |
| F1 score | 53.66          | 75.86          |
| weighted |                |                |
| F1 score | 53.97          | 77.24          |
| macro    |                |                |
| precision| 57.02          | 78.21          |
| weighted |                |                |
| precision| 58.85          | 79.60          |
| macro    |                |                |
| recall   | 56.41          | 76.30          |
| weighted |                |                |
| recall   | 54.91          | 77.65          |

Table 9 presents additional evaluation on Office-Home (standard). We re-implement MDD using identical batch sizes (50) and random seeds for fair comparison. The results show that our proposed method has consistent improvements across all evaluation measures, and the improvements are not a result of batch sizes or random seeds.

B.2. Additional Ablation on Alignment Options

Table 10. The impact of different implicit alignment options, i.e., masking the classifier-based domain discrepancy measure and sampling examples from the source and target domains, on Ar→Cl and Cl→Pr, Office-Home (standard).

| Alignment options | Ar→Cl | Cl→Pr |
|--------------------|-------|-------|
| Domains            |       |       |
| masking            | ×     | ×     |
| sampling           | ×     | ×     |
| Accuracy           | 55.3  | 71.4  |
|                     |       |       |
|                     | ✓     | ✓     |
|                     | ✓     | ✓     |
|                     | ✓     | ✓     |
|                     | ✓     | ✓     |
|                     | ✓     | ✓     |

Table 10 presents the ablation study on Office-Home (standard) that aims to assess the impact of different implicit alignment options: alignment in the domain divergence estimations (i.e., masking in MDD) and alignment in the input space (i.e., sampling class-conditioned examples). We observe that both alignment techniques are essential for domain adaptation because alignment should be enforced consistently across all aspects of the domain adaptation training. This is consistent to findings in the main paper.

B.3. Learning Curve

Figure 7 shows the learning curve of the target domain accuracy for different methods. The proposed implicit alignment converges better than other methods.

B.4. Computational Efficiency

Table 11. The impact of pseudo-label update frequency on Ar→Cl, Office-Home (standard).

| pseudo-labels updated every $N$ steps | accuracy |
|--------------------------------------|----------|
| 5                                    | 56.0     |
| 10                                   | 56.7     |
| 20                                   | 56.2     |
| 50                                   | 55.2     |
| 100                                  | 56.3     |
| 500                                  | 55.7     |

Self-training requires estimating the target domain labels, which could be time-consuming depending on the size of the dataset. To improve the computational efficiency of our algorithm, we only update pseudo-labels periodically, i.e., every 20 steps, instead of at every training step. We show in Table 11 that different pseudo-label update frequencies exhibit similar performance on the target domain. Notably, implicit alignment outperforms the baseline method in spite of only updating the pseudo-labels every 500 training steps. This validates the robustness of implicit alignment.

For the experiments described in Section B.3, training the baseline methods take 31 hours (wall clock time), whereas implicit alignment takes 34 hours under the same training condition when the pseudo-labels are updated every 20 steps. The 10% computational overhead is rather restricted. Moreover, from an engineering perspective, partially updating and caching the pseudo-labels could further improve the computational efficiency, and we leave them as future work.
B.5. Impact of Batch Size

Table 12. Impact of batch size on target domain accuracy (%), Ar→Cl, Office-Home (standard). The MDD results are based on our re-implementation.

| batch size | baseline | implicit |
|------------|----------|----------|
| 8          | 48.9     | 49.7     |
| 16         | 52.7     | 52.8     |
| 32         | 54.9     | 56.2     |
| 50         | 55.3     | 56.2     |

Table 12 presents the impact of batch size on the target domain accuracy. We find that implicit alignment consistently improves the model performance over the MDD baseline across different batch sizes, and both methods work better with larger batch sizes.

B.6. Empirical Class Diversity

Figure 8. Empirical class diversity while training A→W (Office-31) with batch size 31.

Figure 8 shows the empirical class diversity comparing implicit alignment with the baseline. In both experiments, the batch size is identical with the total number of classes (i.e., 31). For the baseline method, random sampling only obtains about 19 unique classes per-batch, which is much smaller than the batch size, in spite of the batch sizes being the same with the total number of classes. This is because random sampling can be viewed as sampling with replacement in the label space, whereas the implicit alignment can be viewed as sampling without replacement in the label space, which naturally increases the empirical class diversity. The expected class diversity of the baseline is

\[ \mathbb{E}[|Y|] = n \left[ 1 - \left( \frac{n-1}{n} \right)^k \right], \tag{20} \]

where \( n \) is the number of unique classes and \( k \) is the size of the minibatch. The expected class diversity is 19.78 if \( n = 31 \) and \( k = 31 \), which is consistent with the empirical class diversity shown in Figure 8.

For the implicit alignment method shown in Figure 8, although it has low class diversity at training step 0 due to the random pseudo-labels, it has a sharp increase in class diversity for the first few hundred training steps, and eventually being able to sample 28 classes from the total of 31 classes. This confirms that implicit alignment is effective in improving empirical class diversity beyond random sampling.

C. Datasets

Figure 9 shows the frequencies of different classes for Cl→Rw on the Office-Home (standard) dataset. This dataset is under natural class imbalance where examples of different classes are not evenly distributed.

Figure 10 shows the frequencies of different classes for Cl→Rw on the Office-Home (RS-UT) dataset (Tan et al., 2019). In this dataset, the minority classes in the source domain are majority classes in the target domain, which creates extreme within-domain class imbalance and between-domain distribution shift.

Figure 10. Class distribution of Cl→Rw, Office-Home (RS-UT)
D. Model Architecture and Training Details

**Code.** We use PyTorch 1.2 as the training environment, and we observe that the adaptation performance on PyTorch 1.4 is slightly better PyTorch 1.2. The differences between PyTorch versions do not change the findings and the conclusions of this paper. Our code and training instructions are provided in https://github.com/xiangdal/implicit_alignment.

**Model architecture.** We use ResNet-50 (He et al., 2016) pre-trained from ImageNet (Russakovsky et al., 2015) as the backbone, and use hyper-parameters from (Zhang et al., 2019b) for MDD-based domain discrepancy measure. The backbone is followed by a 1-layer bottleneck. The classifier $f$ and auxiliary classifier $f'$ are both 2-layer networks.

**Optimization.** We use the SGD optimizer with learning rate 0.001, nesterov momentum 0.9, and weight decay 0.0005. We empirically find that SGD converges better than Adam for adversarial optimization. We use a gradient reversal layer for minimax optimization, and we use a training scheduler (Ganin et al., 2016) for gradient reversal layer defined as

$$
\lambda_p = \frac{0.2}{1 + \exp\left(-\frac{i}{1000}\right)} - 0.1, \tag{21}
$$

where $i$ denotes the step number. We used the same scheduler from (Zhang et al., 2019b) for all experiments and have not tried hyperparameter search for $\lambda_p$. The batch size is 31 for Office-31 and 50 for Office-Home.