On Challenges in Unsupervised Domain Generalization

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Abstract

Domain Generalization (DG) aims to learn a model from a labeled set of source domains which can generalize to an unseen target domain. Although an important stepping stone towards building general purpose models, the reliance of DG on labeled source data is a problem if we are to deploy scalable ML algorithms in the wild. We thus propose to study a novel and more challenging setting which shares the same goals as that of DG, but without source labels. We name this setting as Unsupervised Domain Generalization (UDG), where the objective is to learn a model from an unlabeled set of source domains that can *semantically cluster* images in an unseen target domain. We will investigate the challenges involved in solving UDG as well as potential methods to address the same. Our work could lay a solid foundation for solving two key problems – *unsupervised learning under domain shift* and *imbalanced clustering*. We outline the experimental protocol via which we seek to establish a competitive baseline for further research in this area.

1 Introduction

There is a growing need for generalizable models that learn with limited supervision. Safety-critical systems such as self-driving cars require robust models that are invariant to changes between train and test distributions such as weather (38), illumination (5) and location (36). To this end, considerable research has been conducted in domain generalization (DG) (1; 19; 2; 10; 22; 28; 11) in recent years. DG has been formulated as learning a model from a labeled set of source domains that can generalize to an unseen target domain. While an important step towards deploying machine learning algorithms in the wild, the necessity of labeled source data in the formulation of DG is a bottleneck. Data labeling can be a time-consuming process – and in certain niche applications like healthcare that require subject matter experts, it can quickly get infeasible, especially on multiple source domains. There is clearly tremendous incentive to build models which obviate the need of labeling images in the source domain (even if partially on some of the source domains) and can generalize to unseen target domains (1).

We thus propose in this work to study a new problem setting which we name Unsupervised Domain Generalization (UDG), where the objective is to learn a model from an unlabeled set of source domains such that it can *semantically cluster* images in an unseen target domain. A mathematical formulation of our problem setting is provided in Section 2.1. Despite the potential applicability of

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Table 1: Comparison with other related settings in literature

Setting	Source			Target		
	Unlabeled	Partially Labeled	Labeled	Unlabeled	Partially Labeled	Labeled
Domain Adaptation (DA) (40)	×	×	✓	×	×	✓
Semi-supervised DA (33)	×	×	✓	×	✓	×
Unsupervised DA (41)	×	×	✓	✓	×	×
Domain Generalization (44)	×	×	✓	×	×	×
CDS (17)	×	✓	×	✓	×	×
UCDS (27)	✓	×	×	✓	×	×
UDG (Ours)	✓	×	×	×	×	×

the problem setting in real-world scenarios, there surprisingly has not been a principled approach to study it. To the best of our knowledge, ours is the first such effort.

Considering the nature of the constraints in the UDG problem, we have preliminarily identified two key challenges to be addressed herein – *unsupervised learning under domain shift* and *cluster imbalance* (see Figure 1). Existing DG methods (which require labeled source domains) address the domain shift problem. We investigate in this work whether the ideas in existing DG solutions can be translated and adapted to tackling UDG. We expand on this in the next section. UDG is also related to Unsupervised Clustering under Domain Shift (UCDS) (27), a slightly relaxed setting where in addition to unlabeled source images, access to unlabeled images in the target domain is also allowed. Various related settings in domain shift literature are summarized in Table 1.

The second challenge that needs we recognize is that of cluster imbalance. An implicit assumption among contemporary deep clustering methods (29; 7; 23; 30; 35) that are designed for a single domain is that the clusters ought to be balanced. This is, in part, to avoid trivial (or empty) clusters, and also due to the nature of existing clustering benchmark datasets which are all balanced: CIFAR-10 & CIFAR-100 (18), STL-10 (4), ImageNet-10 (15) and ImageNet-Dogs (6). While important for making initial forays, this is too strong an assumption for real-world datasets. For example, Figure 1 illustrates the strong imbalance present inside each domain in the PACS (19) dataset (this is one of the simpler DG datasets, to put this in context).

The main contributions of this proposal can be summarized as follows: (i) We introduce a new problem setting of Unsupervised Domain Generalization, where we are provided with an unlabeled set of source domains and we aim to learn a model that semantically clusters images on an unseen target domain; (ii) We outline the challenges in solving UDG – in particular, *unsupervised learning under domain shift* and *imbalanced clustering* and propose solutions to address these challenges as a first effort; and (iii) We plan to conduct empirical evaluation on standard benchmark datasets in the domain shift literature and seek to establish a solid baseline for the UDG problem.

2 Addressing Challenges in UDG

In this section, we give a mathematical formulation for UDG, describe how solutions from existing literature on domain generalization and clustering can transfer to our problem setting, and propose a potential methodology to tackle UDG.

2.1 Problem Formulation

Let $\mathcal{X} \in \mathcal{R}^{H \times W \times Ch}$ be the input space of images (where H and W are the height and width of the images, and Ch denotes the number of channels), and $\mathcal{F} \in \mathcal{R}^d$ be the hidden representation space. We assume access to M source domains $\{D_i^s\}_{i=1}^M$ where the i^{th} source domain D_i^s contains N_i unlabeled instances $\{x_j^i\}_{j=1}^{N_i}$. Using $\{D_i^s\}_{i=1}^M$, we learn a feature extractor $f_\theta : \mathcal{X} \rightarrow \mathcal{F}$ and a cluster classifier $f_\phi : \mathcal{F} \rightarrow \mathcal{C}$, where $\mathcal{C} \in \{1, \ldots C\}$ and C is the number of desired clusters. $f_\phi(f_\theta)$ can then be used to cluster images for an unseen target domain D^t. (We call this setting followed by recent work (29; 7; 23; 30; 35) as *semantic clustering* due to the evaluation procedure at test time, which involves checking for correct assignment to class labels.) We do not make any assumptions about the underlying distribution for either the source or the target domain. The number of classes are assumed to be the same across all domains for evaluation purposes.

2.2 Can Existing Solutions Transfer to UDG?

Based on preliminary studies, we identified two major challenges that we need to address to solve UDG - domain shift and cluster imbalance. In this section, we look at how existing methods in DG and clustering could help us in addressing these challenges.

Domain Generalization Multiple approaches have been considered to handle domain shift (44) - domain alignment, meta-learning, data augmentation, self-supervision and learning disentangled representations. Based on the success of meta-learning methods in DG (20; 8; 24; 21; 43; 3; 9; 25), we propose to examine it for our use case. The key idea behind using meta-learning for DG is that domain shift is simulated by dividing the source domains into meta-train and meta-test domains. The model is trained on the meta-source domains and optimized for performance on the meta-test domain. By training in this fashion across epochs, the model is expected to generalize to an unseen domain.

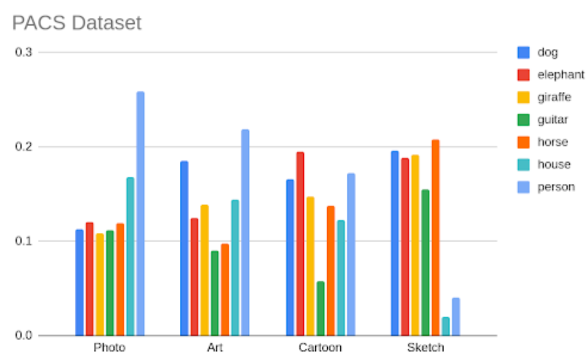

Figure 1: Imbalance across domains; Relative frequency for a particular class inside each domain

Clustering A plethora of deep learning-based methods have been proposed in clustering for datasets with no domain shift. The general norm in prevalent clustering methods is to train and test on the same dataset. UDG presents an additional challenge where a model is trained on one domain and tested on a completely different domain. Clustering methods broadly fall into two categories: (i) directly output a distribution over clusters, or (ii) learn a representation space that is amenable to being clustered using a simple technique like K-means. We plan to study methods from both categories (34; 35; 7; 29; 12; 23).

2.3 Curriculum Learning-based Meta-Learning Methodology for UDG

Hypothesis 1: Can existing methods to handle domain shift in DG be translated and adapted to tackle UDG?

Meta-learning, by design of ‘learning to learn’, provides a natural way to generalize across domains. Hence, on the back of the success of meta-learning methods in DG (22; 8), we ask whether a meta-learning approach can be used for handling domain shift in UDG. As given in Algorithm 1, during training, we split the source domains into meta-source domains and meta-target domains, which are disjoint. We train a separate model for each meta-source domain and jointly optimize for domain shift by maximizing performance on a meta-target domain. We propose to experiment with and modify multiple state-of-the-art clustering objectives (35; 29; 34; 12; 23; 7). Unlike prevalent deep clustering algorithms, we do not plan to add an entropy term to our objective as it encourages uniformly distributed clusters. Specific experiments are discussed below.

Hypothesis 2: Can a curriculum learning strategy address cluster imbalance in UDG?

In order to address cluster imbalance, we propose to examine a curriculum based strategy, summarized in Algorithm 2. We first run the the algorithm described in 1 with two clusters and train

Algorithm 1: Meta-Clustering for UDG

Input: f_θ: Backbone network, k: Number of clusters
Output: f_θ^k: Backbone network trained on k clusters
$P(\mathcal{D})$: Distribution over domains
$f_\theta : \mathcal{R}^{H \times W \times Ch.} \rightarrow \mathcal{R}^d$
Clustering Head: $f_\phi : \mathcal{R}^d \rightarrow \mathcal{R}^k$
$f_\eta : f_\phi(f_\theta)$
while *convergence criteria not satisfied* **do**
  Sample meta-train domains $S_i \sim P(\mathcal{D})$
  Sample meta-test domain $T \sim P(\mathcal{D}) \mid T \neq S_i$
  forall S_i **do**
    Sample a batch $B_i = \{x_p^{(i)}\}_{p=1}^{n_i} \sim S_i$
    Evaluate $\nabla_\eta L_{cluster}(f_\eta)$ on B_i
    Compute adapted parameters: $\eta_i^{'} := \eta - \alpha \nabla_\eta L_{cluster}(f_\eta)$
  end
  Sample a batch $B_T = \{x_j^T\}_{j=1}^{n_T} \sim T$
  Update $\eta := \eta - \beta \nabla_\eta \sum_{S_i} L_{cluster}(f_{\eta_i^{'}})$ using B_T
end

Algorithm 2: Curriculum Learning for Handling Cluster Imbalance

$\mathcal{C}$: No. of classes in the dataset
$c_i = [2, 4, 8, \ldots, \mathcal{C}]$
Randomly initialized neural network $f_\theta : \mathcal{R}^{H \times W \times Ch.} \rightarrow \mathcal{R}^d$
Initialize $f_\theta^{(c_0)} \leftarrow f_\theta$
forall c_i **do**
  $f_\theta^{(c_i)} \leftarrow MetaClusteringUDG(f_\theta^{(c_{i-1})}, c_i)$ `/* See Algorithm 1 */`
end

until convergence. Then, we train with four clusters with the model trained on two clusters as an initialization, converge it. We do this till the number of clusters is equal to the number of classes. Our hypothesis is that at the highest level of two clusters, the imbalance would be minimal. This is equivalent to clustering the data into two *superclasses*. Once the representations are refined at this level, we train our model with more clusters and eventually train it with *C* clusters. Thus at each level, by refining the representation for that level, we expect the model to counteract cluster imbalance.

3 Experimental Protocol & Planned Implementation

In this section, we discuss about (i) baseline methods for UDG, (ii) datasets & metrics we plan to use (iii) evaluation protocol and (iv) implementation details

3.1 Baselines

We aim to explore and establish multiple baselines for our problem setting.

- **Random + K-Means**: The simplest baseline is to get the representations from a randomly initialized convolutional neural network (CNN) (13) and perform K-Means clustering on those representations. The random baseline is a sensible lower bound.
- **SSL + K-Means**: A second baseline is to use a self-supervised (SSL) (16) method to train on a dataset formed by aggregating all the source domains and test it on the target domain.
- **Deep Clustering**: Following the previous two relatively simple baselines, we then propose to use a state-of-the-art deep clustering method which has been designed for a single domain (35; 29; 34). We will follow the same evaluation strategy as that of the SSL baseline.
- **ACIDS w/o TA**: We will consider a modification to the UCDS setting from (27). (27) proposes a two-stage approach where a CNN is first trained on source domains and in the second stage is fine-tuned on the target domain. By discarding the target fine-tuning step, we obtain a strong baseline for UDG.

Table 2: Clustering Accuracy for baseline approaches on PACS (19) using ResNet18

PACS	Photo	Art	Cartoon	Sketch	Average
Uniform	14.3	14.3	14.3	14.3	14.3
Random + K-Means	26.6	21.2	25.9	30.5	26.1
ACIDS w/o TA (27)	44.2	34.8	36.5	40.8	39.1
ImageNet + K-Means	97.7	55.4	54.7	44.6	63.1

- **ImageNet + K-Means**: We extract representations from an ImageNet pre-trained ResNet18 model for the target domain and cluster them using K-Means (see Table 2).

3.2 Datasets & Metrics

Datasets We propose to perform our experiments on three datasets which are commonly used in the domain shift literature for evaluation - PACS (19), OfficeHome (37) and Office31 (32). PACS comprises 9,991 images divided in 7 classes across 4 different domains: Photo, Art, Cartoon and Sketch. The Office-Home dataset contains about 15,500 images across 4 domains: Product, Art, Clipart and Real World. Each domain is divided into 65 different classes. The Office31 dataset contains 4,110 images divided into 31 classes across 3 different domains: Amazon, DSLR, and Webcam. Each of these datasets contain visually disparate domains across a wide spectrum and scale, thus providing an ideal benchmark for testing any method developed for UDG.

Metrics We plan on evaluating our proposed method on four metrics commonly used in clustering literature: clustering accuracy (ACC), normalized mutual information (NMI), Adjusted Rand Index (ARI) (30) and Silhouette score (SIL) (31). ACC, NMI and ARI metrics require ground truth labels, while SIL doesn't. SIL measures how similar an image is to its own cluster compared to other clusters based on distances in the representation space. Thus, a conjunction of all 4 metrics would give us a fair estimate of the quality of the clustering achieved.

Evaluation Protocol For our experiments, we will perform leave-one-domain-out evaluation where one domain is held-out as target, commonly done in DG literature. Multiple source domains may or may not be used during training. Due to the unavailability of labeled data anywhere in the UDG setting, we cannot perform validation. We thus train all models until convergence on the source data and use the trained model as a fixed feature extractor for the target domain.

Implementation Details We will use a randomly initialized ResNet-18 (14) model as our backbone network for all experiments. Although we will finetune hyperparameters, we expect to use the following based on related work (20) – SGD optimizer with learning rate $5e^{-4}$ and mini-batch size of 128, parameters α and β to $5e^{-4}$ and 1.0 respectively. We also plan to randomly crop the images, flip them horizontally and apply colour jitter. We will run all our experiments across multiple seeds and report the mean and std deviation.

4 Additional Experiments

We plan to conduct additional experiments to ascertain the robustness of the proposed algorithm as well as gain useful insight into the method. (i) To test whether the proposed curriculum strategy is useful, we will train and test on a single domain so that domain shift is controlled for. (ii) We also plan to test whether the proposed method is able to discover clusters for novel classes in the target domain that are not present in the source domain (iii) We could extend our work to settings where labeled data is available for a few domains by adding a cross-entropy loss term for those domains.

Best Practices Along with the basic meta-learning based solution that we propose, we expect to use the following best practices common in the domain shift literature. (i) **Domain-specific Batch Normalization** (26): We will compute batch statistics separately for each domain. The motivation is that the domain-shift can be reduced by aligning the different source feature distributions to a Gaussian reference distribution. (ii) **Domain Randomization** (39): Meta-learning approaches usually work better when there is a diverse range of tasks to learn from. In the same vein, we propose to use domain randomization (DR) to artificially increase the number of meta-source domains.

Visualizations We plan to visualize the representation space using t-SNE embeddings across training to monitor whether the model is getting progressively better as well as compare the final clustering after convergence with baseline methods. Another plot that might provide some insight into the method is to plot the meta-loss versus the clustering accuracy of the target domain per epoch similar to the one provided in (42).

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