MixMOOD: A systematic approach to class distribution mismatch in semi-supervised learning using deep dataset dissimilarity measures

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Abstract

In this work, we propose MixMOOD - a systematic approach to mitigate effect of class distribution mismatch in semi-supervised deep learning (SSDL) with MixMatch. This work is divided into two components: (i) an extensive out of distribution (OOD) ablation test bed for SSDL and (ii) a quantitative unlabelled dataset selection heuristic referred to as MixMOOD. In the first part, we analyze the sensitivity of MixMatch accuracy under 90 different distribution mismatch scenarios across three multi-class classification tasks. These are designed to systematically understand how OOD unlabelled data affects MixMatch performance. In the second part, we propose an efficient and effective method, called deep dataset dissimilarity measures (DeDiMs), to compare labelled and unlabelled datasets. The proposed DeDiMs are quick to evaluate and model agnostic. They use the feature space of a generic Wide-ResNet and can be applied prior to learning. Our test results reveal that supposed semantic similarity between labelled and unlabelled data is not a good heuristic for unlabelled data selection. In contrast, strong correlation between MixMatch accuracy and the proposed DeDiMs allow us to quantitatively rank different unlabelled datasets *ante hoc* according to expected MixMatch accuracy. This is what we call MixMOOD. Furthermore, we argue that the MixMOOD approach can aid to standardize the evaluation of different semi-supervised learning techniques under real world scenarios involving out of distribution data.

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Preprint. Under review.

1 Introduction

Training an effective deep learning solution typically requires a considerable amount of labelled data. In specific application domains such as medicine, high quality labelled data can be expensive to obtain leading to scarcely labelled data settings [1, 2]. Several approaches have been developed to address this data constraint including data augmentation, transfer, weakly and semi-supervised learning, among others [3, 4, 5]. Semi-supervised learning is an attractive approach for learning problems where little labelled data is available. It leverages the use of unlabelled data which is often cheap to obtain [6]. Formally, in a semi-supervised setting both labelled and unlabelled datasets are used. Labelled observations $X_l = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{n_l}\}$ and their corresponding labels $Y_l = \{y_1, \ldots, y_{n_l}\}$ make up the labelled dataset S_l. The set of unlabelled observations is represented as $X_u = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{n_u}\}$, therefore $S_u = X_u$. Semi-supervised deep learning (SSDL) approaches can be grouped into pre-training [7], self-training or pseudo-labelled [8] and regularization based. Regularization techniques include generative based approaches, along consistency loss term and graph based regularization [2]. A detailed survey on semi-supervised learning can be found in [6]. The practical implementation of SSDL techniques in different application domains has been however limited, given its moderate success in real-world settings [9]. In [9], authors call for more systematic and realistic evaluation of SSDL approaches. A class distribution mismatch between labelled and unlabelled data is among the most important aspects highlighted by the authors. The following example illustrates this problem. We can train a Convolutional Neural Network (CNN) to classify between pneumonia ill and healthy patients using chest X-ray images, as for example seen in [10]. The labelled dataset S_l can include a limited number of observations for each class. However, the unlabelled dataset S_u can include observations of patients with other lung pathologies. These observations correspond to what is known as out of distribution (OOD) data [11] which can potentially harm the performance of a SSDL solution [9].

1.1 Problem statement

The central premise of this work is the quantitative impact assessment of class distribution mismatch between labelled and unlabelled data on SSDL. This notion stipulates that a mismatch negatively affects the accuracy of models trained with SSDL algorithms [9]. A mismatch occurs when the unlabelled data contains observations that do not correspond to any of the classes present in the labelled data. It is not clear though what exactly the effect is when this mismatch occurs: does it always harm the model accuracy? Does it help to use unlabelled data that is, supposedly, semantically more similar to the labelled data? And if certain unlabelled datasets indeed harm accuracy of SSDL trained models, is there a reliable way to select the unlabelled data in an informed way *ante hoc*? In order to establish points of reference for what follows we adopt the definitions below. Given a dataset S_1 emanating from the data generating process $y = f(\boldsymbol{x})$, with $y \in \mathcal{Y} := \{1, ..., K\}$ being a set of labels, and a second dataset S_2 emanating from the data generating process $y' = g(\boldsymbol{x})$, with $y' \in \mathcal{Y}' := \{1, ..., K'\}$, we say that

Definition 1.1. *Inside of distribution (inside of distribution (IOD)) data:* Dataset S_2 is IOD relative to dataset S_1 if $f(\boldsymbol{x}) = g(\boldsymbol{x})$. In particular, we have that $\mathcal{Y} = \mathcal{Y}'$.

Definition 1.2. *Outside of distribution (OOD) data:* Dataset S_2 is OOD relative to dataset S_1 if $f(\boldsymbol{x}) \neq g(\boldsymbol{x})$. In particular, we have that $\mathcal{Y} \neq \mathcal{Y}'$.

Definition 1.3. *Class distribution mismatch in SSDL:* A class distribution mismatch occurs if the unlabelled data S_u used for SSDL is OOD relative to S_l.

In practice, $f(\boldsymbol{x})$ and $g(\boldsymbol{x})$ are typically not known explicitly. Thus, given two datasets S_1 and S_2 a definite formal verification of the class distribution mismatch property is not possible. Instead, it is usually *assumed* that two *different* datasets, e.g. CIFAR-10 and MNIST, emanate from different data generating processes. This working definition of OOD data follows the existing literature on class distribution mismatch in SSDL [9] as well as OOD detection in deep learning [12]. We adopt this working definition for the OOD scenarios of our test bed. Note that different degrees of OOD contamination for S_u are possible as we describe in Section 3.1.

1.2 Contribution

In order to address the questions outlined in Section 1.1 we present the MixMatch approach to out of distribution data (MixMOOD)[2]. It entails the following contributions:

- A systematic OOD ablation test bed. We demonstrate that including OOD data in the unlabelled training dataset for the MixMatch algorithm can yield different degrees of accuracy degradation compared to the exclusive use of IOD data. However, in most cases, using unlabelled data with OOD contamination still improves the results when compared to the default fully supervised configuration.
- Markedly, OOD data that is supposedly semantically similar to the IOD labelled data does not always lead to the highest accuracy gain.
- We propose and evaluate four Deep Dataset Dissimilarity Measure (DeDiM)s that can be used to rank unlabelled data according to the expected accuracy gain *prior* to SSDL training. They are cheap to compute and model-agnostic which make them amenable for practical application.
- Our test results reveal a strong correlation between the tested DeDiMs and MixMatch accuracy, making them informative for unlabelled dataset selection. This leads to MixMOOD which proposes the usage of tested DeDiMs to select the unlabelled dataset for improved MixMatch accuracy.

2 Related work

In this work we address a combination of three overlapping problems that are often dealt with in parallel in the literature: class distribution mismatch in SSDL, OOD detection, and dataset dissimilarity measures.

2.1 Class distribution mismatch in SSDL

As previously highlighted, in [9] authors call for the need of a more extensive testing of SSDL techniques under real-world usage settings. One of them is the possible data distribution mismatch between the labelled and unlabelled training data. Real Mix was proposed [13] as a reply to this remark, implementing a masking coefficient to OOD data for the unlabelled dataset. The masking coefficient is used as a threshold of the softmax output of the model, discarding unlabelled data used only in the unsupervised term. The authors performed limited testing of the consequences of using OOD unlabelled data. The tested OOD dataset consists in the split CIFAR-10 dataset in two halves with different semantics. [14] explores a similar scenario. Four levels of OOD contamination were tested. We argue for the need of testing different OOD datasets to more extensively understand their impact on SSDL.

2.2 OOD data detection

In the context of machine learning, OOD data detection refers to the general problem of detecting observations that belong to a data distribution different from the distribution of the training data [15]. OOD detection can be considered as a generalization of outlier detection, since it considers individual and collective outliers [16]. Further variations of the OOD data detection problem are novel and anomaly data detection [17], with different applications such as rare event detection and artificial intelligence safety [18, 19]. Classical OOD and anomaly detection methods rely on density estimation, e.g. Gaussian Mixture Models [20], robust moment estimation, like the Minimum Covariance Determinant method [21], prototyping, e.g. k-nearest neighbor algorithm [20], as well as kernel based variants such as Support Vector Data Description [22]. Also, a variety of neural network based approaches for novelty detection can be found [20], with a data oriented philosophy. With the success of deep learning, recent works have addressed the generic problem of discriminative detection of OOD data for deep learning architectures. Discriminative OOD detectors can be categorized in output- and feature-based. A simple OOD detection approach is proposed in [23]. The authors

[2] All code and experimental scripts, with automatic download of test bed data for ease of reproduction, can be found at `https://github.com/peglegpete/mixmood`

frame OOD detection a prediction confidence. The proposed method relies on the softmax output, sampling the maximum value. [11] introduced OOD data detection in neural networks using input perturbations. A *temperature* coefficient T in the calculation of the softmax output and calibrated decision threshold δ for OOD data detection. More recently, [24] argue that deep networks with softmax output layers are over-confident for inputs very different from the training data and hence propose the usage of the Mahalanobis distance in latent space. Similarly [25] also exploit latent representations, defining what they refer to as learning certificates; neural networks that map feature vectors to zero for IOD data. A more challenging OOD detection setting was tested, where half of each tested dataset is used as IOD data, and the other half is used as OOD data, making OOD detection harder. Another approach to OOD detection is the use of generative adversarial learning. The generative model aims to approximate an implicit model of the IOD data, as seen in [26, 27]. The standard datasets used in these test beds include MNIST, SVHN, LSUN, CIFAR-10, CIFAR-100 and Tiny ImageNet. We provide a tabular overview of these works and the explored pairing of IOD and OOD datasets in the appendix for the interested reader. In the reviewed literature, we can see how dataset selection for benchmarking OOD detection commonly is not quantitatively assessed, making the comparison of the algorithms harder.

2.3 Dataset dissimilarity measures

Computing a notion of dissimilarity between two sets of points (known as shape matching [28]) is typically more computationally expensive than calculating the dissimilarity between a set of points and another single point. Strategies to reduce this burden are primarily centered around enriching the object space with a probability measure which helps guide attention to important areas of comparison [28]. When starting with raw datasets, as is typically the case when trying to decide which data to use for SSDL, additional pre-processing or modelling steps would be necessary to employ these object matching strategies. Methods to compute dissimilarities between raw datasets are, to the best of our knowledge, rare. [29] defines a dissimilarity measure based on the Euclidean distance between the frequency of a given feature function on two datasets, referred as the constrained measure distance. The calculation of the proposed measure can be efficiently performed through the usage of the covariance matrix of the feature function in the dataset. An optimized dataset measure is implemented for binary datasets. More recently, authors in [30] proposed a distance dissimilarity index based on the statistical significance difference of the distance distributions between the two datasets. To calculate it, each data point in the test set is matched with the training data. After exchanging the associated observations, changes in the topology are assessed, using the distance distribution. The confidence p-value of the difference between the two distributions is calculated and used as a dissimilarity measure.

Note that our requirements differ from the above OOD detection and dissimilarity measure methods: we are interested in computationally cheap, ante hoc and model agnostic quantification of the OOD degree between two *datasets*. Approaches that are computationally expensive or post hoc, that is being applied after the model has been trained, are not feasible to address class distribution mismatch before SSDL training. Closest to our work are the OOD detection ideas developed by [12]. The authors present introductory experiments on the correlation between OOD detection and the dataset dissimilarity using a genome distance [31]. We explore a similar comparison: the relationship between SSDL accuracy and OOD-IOD dissimilarity.

3 Proposed method and experiments

3.1 Systematic OOD ablation study

3.1.1 SSDL setup

The basis for all SSDL experiments in this paper is the MixMatch algorithm, a state of the art SSDL method [32]. MixMatch estimates pseudo-labels for unlabelled data X_u, and also implements an unsupervised regularization term. Pseudo-label $\widehat{\boldsymbol{y}}_j$ estimation is performed with the average model output of a transformed input x_j, with K number of different transformations. The pseudo-labels $\widehat{\boldsymbol{y}}$ are further sharpened with a temperature parameter ρ. To further augment the data using both labelled and unlabelled samples, MixMatch makes use of the MixUp algorithm by [33] which builds linear interpolations between labelled and unlabelled observations. For supervised and semi-

Table 1: Results for the class distribution mismatch experiment. Each result entry in the table represents the mean and variance of accuracy across ten random experimental runs per entry. For a detailed description of symbols and the experiment see Section 3.1.2.

$\mathbf{S_{IOD}}$	$\mathbf{T_{OOD}}$	$\mathbf{S_{uOOD}}$	$\mathbf{\%_{uOOD}}$	$\mathbf{n_l}$ 60	100	150
MNIST	Fully supervised baseline			0.457 ± 0.108	0.559 ± 0.125	0.645 ± 0.101
	SSDL baseline (no OOD data)			$\mathbf{0.704 \pm 0.096}$	$\mathbf{0.781 \pm 0.065}$	$\mathbf{0.831 \pm 0.0626}$
	HH	OH	50	0.679 ± 0.108	0.769 ± 0.066	0.802 ± 0.054
			100	0.642 ± 0.111	0.746 ± 0.094	0.798 ± 0.07
	Sim	SVHN	50	0.637 ± 0.098	0.745 ± 0.081	0.801 ± 0.0699
			100	0.482 ± 0.113	0.719 ± 0.058	0.765 ± 0.072
	Dif	TI	50	0.642 ± 0.094	0.739 ± 0.074	0.809 ± 0.066
			100	0.637 ± 0.097	0.732 ± 0.074	0.804 ± 0.071
		G	50	0.606 ± 0.0989	0.713 ± 0.087	0.786 ± 0.065
			100	0.442 ± 0.099	0.461 ± 0.073	0.542 ± 0.062
		SAP	50	0.631 ± 0.102	0.735 ± 0.082	0.813 ± 0.057
			100	0.48 ± 0.0951	0.524 ± 0.09	0.563 ± 0.095
CIFAR-10	Fully supervised baseline			0.380 ± 0.024	0.445 ± 0.042	0.449 ± 0.022
	SSDL baseline (no OOD data)			$\mathbf{0.453 \pm 0.046}$	0.474 ± 0.019	0.501 ± 0.033
	HH	OH	50	0.444 ± 0.040	0.472 ± 0.039	0.525 ± 0.050
			100	0.443 ± 0.023	0.472 ± 0.047	0.499 ± 0.054
	Sim	TI	50	0.435 ± 0.054	0.473 ± 0.039	$\mathbf{0.543 \pm 0.040}$
			100	0.417 ± 0.020	$\mathbf{0.480 \pm 0.039}$	0.498 ± 0.042
	Dif	SVHN	50	0.419 ± 0.027	0.464 ± 0.044	0.469 ± 0.056
			100	0.385 ± 0.034	0.418 ± 0.035	0.440 ± 0.046
		G	50	0.409 ± 0.047	0.454 ± 0.048	0.491 ± 0.032
			100	0.297 ± 0.029	0.306 ± 0.034	0.302 ± 0.038
		SAP	50	0.438 ± 0.029	0.455 ± 0.037	0.485 ± 0.034
			100	0.236 ± 0.031	0.246 ± 0.032	0.232 ± 0.022
FashionMNIST	Fully supervised baseline			0.571 ± 0.073	0.704 ± 0.066	0.720 ± 0.093
	SSDL baseline (no OOD data)			$\mathbf{0.715 \pm 0.049}$	$\mathbf{0.760 \pm 0.044}$	0.756 ± 0.069
	HH	OH	50	0.714 ± 0.049	0.721 ± 0.104	0.765 ± 0.053
			100	0.660 ± 0.061	0.711 ± 0.090	0.747 ± 0.061
	Sim	FP	50	0.707 ± 0.039	0.724 ± 0.030	0.778 ± 0.078
			100	0.546 ± 0.101	0.542 ± 0.099	0.540 ± 0.105
	Dif	TI	50	0.690 ± 0.065	0.745 ± 0.093	0.792 ± 0.058
			100	0.690 ± 0.073	0.728 ± 0.066	$\mathbf{0.794 \pm 0.056}$
		G	50	0.644 ± 0.061	0.689 ± 0.075	0.755 ± 0.055
			100	0.352 ± 0.025	0.366 ± 0.065	0.361 ± 0.057
		SAP	50	0.671 ± 0.072	0.708 ± 0.095	0.729 ± 0.088
			100	0.276 ± 0.069	0.297 ± 0.046	0.283 ± 0.059

supervised loss functions, the cross-entropy and the Euclidean distance, are used, respectively. The regularization coefficient γ controls the direct influence on unlabelled data. Unlabelled data also influences the labelled data term since unlabelled data is used also to artificially augment the dataset with the Mix Up algorithm. This loss term is used at training time, for testing, a regular cross entropy loss is implemented. We documented a detailed description of the MixMatch algorithm in the appendix along with all hyperparameters used throughout the experiments. Both follow the reference and values recommended in [32].

3.1.2 SSDL with OOD data ablation test bed

To assess the effect of OOD unlabelled data S_u on the accuracy of SSDL models trained with MixMatch, we construct an ablation test bed with four variables: base data S_{IOD} which constitutes the original task to be learned, the type of OOD data T_{OOD}, the OOD data source $S_{\text{u,OOD}}$, the relative amount of OOD data among the unlabelled data $\%_{\text{u,OOD}}$, and the amount n_l of labelled observations. Each of the four axes is explored by varying only one of the variables at a time while keeping the others constant. This allows us to isolate the effect of the individual variables. We consider three configurations for S_{IOD} comprising MNIST, CIFAR-10 and FashionMNIST. A total of three configurations for T_{OOD} (*half-half (HH), similar (Sim)* and *different (Dif)*) are tested. We derived the possible types of OOD data from the existing literature cited in Section 2. In the *half-half* setting half of the classes and associated inputs are taken to be the S_{IOD} data whereas the other half of classes are taken to be the $S_{\text{u,OOD}}$ data. *Similar* is a $S_{\text{u,OOD}}$ dataset that is supposedly semantically related to S_{IOD}, e.g. MNIST and SVHN. *Different* is a $S_{\text{u,OOD}}$ dataset that is supposedly semantically unrelated to S_{IOD}, e.g. MNIST and Tiny ImageNet. There are five configurations for $S_{\text{u,OOD}}$ as explained above: the other half *(OH)*, a similar dataset, and three different datasets including two noise baselines. They include Street View House Numbers *(SVHN)*, Tiny ImageNet *(TI)*, Gaussian noise *(G)*, salt and pepper noise *(SAP)* and Fashion Product *(FP)*. Please see Table 1 for the per task pairings. Each configuration represents a multi-class classification task with $|\mathcal{Y}| = 5$, that is a random subset of half of the classes of base data S_{IOD}. An overview for all the datasets used in

Table 2: Distance measures between the labelled and unlabelled datasets S_l and S_u. Numbers in italics correspond to results with $p > 0.5$ for the Wilcoxon test. For a detailed description of symbols and the experiment see Section 3.2.1

$\mathbf{S_l}$	$\mathbf{S_u}$	$\%_{\mathbf{uOOD}}$	$\mathbf{d}_{\ell_2}$	$\mathbf{d}_{\ell_1}$	$\mathbf{d_{JS}}$	$\mathbf{d_C}$
MNIST	OH	50	*0.011 ± 0.006*	*0.459 ± 0.28*	*0.266 ± 0.221*	*0.811 ± 0.512*
		100	*0.014 ± 0.019*	*0.38 ± 0.507*	1.001 ± 0.725	1.263 ± 0.665
	SVHN	50	*0.09 ± 0.017*	1.569 ± 0.504	6.789 ± 0.924	12.021 ± 1.757
		100	0.25 ± 0.053	4.702 ± 1.04	52.349 ± 3.292	42.026 ± 4.31
	TI	50	0.008 ± 0.023	1.519 ± 0.223	3.663 ± 0.772	5.512 ± 0.767
		100	0.217 ± 0.04	4.3 ± 0.636	10.305 ± 1.667	15.18 ± 2.698
	G	50	0.11 ± 0.0219	1.958 ± 0.534	14.785 ± 1.052	23.593 ± 1.859
		100	0.357 ± 0.081	5.987 ± 1.091	52.349 ± 4.253	86.21 ± 3.471
	SAP	50	0.089 ± 0.0311	2.479 ± 0.7433	15.116 ± 1.475	20.151 ± 1.619
		100	0.323 ± 0.07	6.308 ± 1.366	53.397 ± 4.253	77.456 ± 4.474
CIFAR-10	OH	50	*0.056 ± 0.023*	*0.915 ± 0.934*	*0.338 ± 0.325*	0.892 ± 0.402
		100	*0.061 ± 0.04*	0.769 ± 0.461	*0.451 ± 0.41*	0.648 ± 0.407
	TI	50	0.082 ± 0.037	*0.928 ± 0.815*	*0.388 ± 0.243*	*0.423 ± 0.362*
		100	*0.056 ± 0.048*	*0.992 ± 0.517*	*0.469 ± 0.426*	0.415 ± 0.232
	SVHN	50	*0.055 ± 0.032*	*0.948 ± 0.699*	*0.665 ± 0.565*	*0.414 ± 0.357*
		100	*0.075 ± 0.036*	1.291 ± 0.925	0.736 ± 0.658	0.581 ± 0.343
	G	50	*0.107 ± 0.083*	1.344 ± 1.156	1.708 ± 0.421	3.001 ± 0.696
		100	0.127 ± 0.087	1.531 ± 0.767	5.855 ± 0.552	8.703 ± 0.926
	SAP	50	0.1146 ± 0.044	1.854 ± 0.894	2.299 ± 0.691	2.56 ± 0.762
		100	0.208 ± 0.05	5.502 ± 1.156	8.225 ± 0.866	9.554 ± 0.489
FashionMNIST	OH	50	*0.02 ± 0.012*	*0.34 ± 0.162*	*0.669 ± 0.566*	*0.575 ± 0.423*
		100	0.059 ± 0.032	0.801 ± 0.402	0.305 ± 0.237	0.774 ± 0.343
	FP	50	0.105 ± 0.0526	2.168 ± 0.774	7.263 ± 0.622	5.305 ± 0.405
		100	0.195 ± 0.0457	4.819 ± 1.077	9.056 ± 0.462	11.286 ± 0.751
	TI	50	*0.04 ± 0.03*	*0.798 ± 0.542*	*0.897 ± 0.516*	0.897 ± 0.516
		100	0.065 ± 0.03	1.66 ± 0.45	1.4 ± 0.488	1.912 ± 0.683
	G	50	*0.047 ± 0.03*	*0.533 ± 0.347*	2.819 ± 0.703	3.843 ± 0.704
		100	0.074 ± 0.041	1.325 ± 0.631	9.042 ± 0.699	15.511 ± 0.445
	SAP	50	0.036 ± 0.022	0.52 ± 0.303	2.799 ± 0.497	2.799 ± 0.497
		100	0.076 ± 0.044	1.411 ± 0.548	8.464 ± 0.553	8.464 ± 0.553

our experiments can be found in the appendix. Finally, we vary the relative amount of OOD data $\%_{\text{u,OOD}}$ between 0, 50 and 100 as well as the amount of labelled datapoints n_l between 60, 100 and 150. Note that for each result entry you can see in Table 1 we performed ten experimental runs and report the accuracy mean and variance of the models performing best on the test data from each run, as overfitting is very likely to happen with a low n_l. For each run we sampled a disjunct subset of data from S_{IOD} and $S_{\text{u,OOD}}$ to obtain the required number of labelled n_l and unlabelled n_u samples for the run. Descriptive statistics (mean and standard deviation) for standardization of the neural networks inputs were only computed from these subsets to keep the simulation realistic and not use any information from the global training data. All other parameters (number of unlabelled observations $n_u = 3000$, neural network architecture , the set of optimization hyperparameters, number of training epochs) are kept constant across all experiments to enable direct comparison with respect to the variable parameters of the system and not to achieve state of the art performance with MixMatch on the given data. Note that it is possible to extend the test bed to other effects of interest. Some of these ideas we address at the end in Section 5. A description of all hyperparameters and the computing infrastructure used for all experiments as well as their approximate runtimes are documented in the appendix.

3.2 Proposed method: MixMOOD ante hoc ranking of $S_{\text{u,OOD}}$ benefit

In this experiment we compute the proposed DeDiMs between the inputs of the IOD labeled data and the inputs of the OOD unlabelled data. In addition, we compute the correlations between the distance measures and SSDL performance under the different OOD configurations from the ablation experiments before. The motivation behind these distance experiments is to validate whether the measures can be used to rank different $S_{\text{u,OOD}}$ prior to SSDL learning according to their expected benefit for the resulting model accuracy. We refer to this as MixMOOD.

3.2.1 Deep dataset dissimilarity measures

In this work we implement a set of DeDiMs. They make use of dataset subsampling, as image datasets are usually large, following a sampling approach for comparing two populations, as seen in [34]. We compute the dissimilarity measures in the feature space of a generic Wide-ResNet pre-

trained on ImageNet, making our proposed approach agnostic to the SSDL model to be trained. This enables an evaluation of the unlabelled data before training the SSDL model. The proposed measures in this work are meant to be simple and quick to evaluate with practical use in mind. We propose and test the implementation of two Minkowski based dissimilarity measures, $d_{\ell_2}(S_a, S_b, \tau, \mathcal{C})$ and $d_{\ell_1}(S_a, S_b, \tau, \mathcal{C})$, corresponding to the Euclidean and Manhattan distances, respectively, between two datasets S_a and S_b. Additionally, we implement and test two non-parametric density based distances; Jensen-Shannon (d_{JS}) and cosine distance (d_C). For all the proposed dissimilarity measures, the parameter τ_c defines the sub-sample size used to compute the dissimilarity between the two datasets S_a and S_b and $\mathcal{C}$ the total number of samples to compute the mean sampled dissimilarity measure. The general procedure for all the implemented distances is as follows.

- We randomly sub-sample each one of the datasets S_a and S_b, with a sample size of τ, creating the sampled datasets $S_{a,\tau}$ and $S_{b,\tau}$.
- We transform an input observation $\boldsymbol{x}_j \in S_i$, with $\boldsymbol{x}_j \in \mathbb{R}^n$, with n the dimensionality of the input space, using the feature extractor f, yielding $\boldsymbol{h}_j = f(\boldsymbol{x}_j)$.

  Where $\boldsymbol{h}_i \in \mathbb{R}^{n'}$ is the feature vector of n' dimensions, with $n' < n$. For instance, the implemented feature extractor uses the Wide-ResNet architecture, extracting $n' = 512$ features. This yields the two feature sets $H_{a,\tau}$ and $H_{b,\tau}$

For the Minkowski based distances $d_{\ell_2}(S_a, S_b, \tau, \mathcal{C})$, $d_{\ell_1}(S_a, S_b, \tau, \mathcal{C})$, we perform the following steps for the sets of features obtained in the previous description $H_{a,\tau}$ and $H_{b,\tau}$:

- For each element in $h_j \in H_{a,\tau}$, find the closest element $h_k \in H_{b,\tau}$, using the ℓ_p distance, for $d_{\ell_p}(S_a, S_b, \tau, \mathcal{C})$, with $p = 1$ or $p = 2$ for the Manhattan and Euclidean distances, respectively: $\widehat{d}_j = \underset{k}{\operatorname{argmin}} \|\boldsymbol{h}_j - \boldsymbol{h}_k\|_p$. We do this for a number of $\mathcal{C}$ samples, yielding a list of distance calculations $\widehat{d}_1, \widehat{d}_2, ..., \widehat{d}_{\mathcal{C}}$.
- We compute a reference list of distances for the same list of samples of the dataset S_a to itself (intra-dataset distance), computing $d_{\ell_p}(S_a, S_a, \tau, \mathcal{C})$. This yields a list of reference distances $\check{d}_1, \check{d}_2, ..., \check{d}_{\mathcal{C}}$. In our case S_a corresponds to the labelled dataset S_l, as the distance to different unlabelled datasets S_u is to be computed.
- To ensure that the absolute differences between the reference and inter-dataset distances $d_c = \left|\widehat{d}_c - \check{d}_c\right|$ are statistically significant, we compute the p significance value with a Wilcoxon test.
- Computing the distance between two datasets $d_{\ell_p}(S_a, S_b, \tau, \mathcal{C})$ results in the average reference substracted distance $\overline{d}$ and its corresponding confidence p value.

As for the density based distances implemented we follow a similar sub-sampling approach, with these steps:

- For each dimension $r = 1, ..., n'$ in the feature space, we compute the normalized histogram $p_{r,a}$, in the sample $H_{a,\tau}$. Similarly, we compute the set of density functions $p_{r,b}$ for $r = 1, ..., n'$, using the observations in the sample $H_{b,\tau}$.
- We compute the sum of the distances between the density functions $p_{r,a}$ and $p_{r,b}$, to yield the distance approximation for the sample j: $\widehat{d}_j = \sum_{r=1}^{n'} \delta_g(p_{r,a}, p_{r,b})$. We do this for all the $\mathcal{C}$ samples, yielding the list of inter-dataset distances: $\widehat{d}_1, \widehat{d}_2, ..., \widehat{d}_{\mathcal{C}}$. To lower the computational burden, we assume that the dimensions are statistically independent.
- Similar to the Minkowski distances, we compute the intra-dataset distances for the dataset S_a, in this context the labelled dataset S_l, to obtain the list of reference distances $\check{d}_1, \check{d}_2, ..., \check{d}_{\mathcal{C}}$.
- Similarly, to verify that the inter- and intra-dataset distance difference $d_c = \left|\widehat{d}_c - \check{d}_c\right|$ are statistically significant, we compute the p significance value with a Wilcoxon test. The distance computation yields the sample mean distance $\overline{d}$ and its confidence value p.

The proposed dissimilarity measures do not hold for a mathematical metric or pseudo-metric, as the distance of an object to itself is not strictly zero (but tends to be close) and symmetry properties

are not fulfilled for the sake of evaluation speed [35]. Despite these relaxations we will see that these dissimilarity measures, especially the two that are density based, are an effective proxy for $S_{\text{u,OOD}}$ benefit. To quantitatively measure how related the distances between S_l and S_u and the yielded SSDL accuracy are, we calculate the Pearson coefficient between the distance measures and the SSDL accuracy. This verifies the linear correlation between them. Table 3 describes the Pearson coefficient for each implemented dissimilarity measure and each SSDL configuration. In summary, as part of MixMOOD we propose to quantitatively rank a set of possible unlabelled datasets $S_{u,1}, S_{u,2}, ..., S_{u,k}$ according to a dissimilarity measure $d(S_l, S_u)$, instead of using qualitative based heuristics. In all the tests of this work, we used $n' = 512$, $\tau = 80$ and $\mathcal{C} = 30$.

4 Results

Table 1 shows the results of the distribution mismatch experiment described in Section 3.1. We make a number of observations. First, in the majority of cases using IOD unlabelled data or a 50-50 mix of IOD and OOD unlabelled data beats the fully supervised baseline. The gains range from 15% to 25% for MNIST, 10% to 15% for CIFAR-10 and 7% to 13% for FashionMNIST across all $S_{\text{u,OOD}}$ and n_l. As expected, in most of the cases the accuracy is degraded when including OOD data in S_u, with a more dramatic hit when noisy datasets (SAP, G) are used as OOD data contamination. Second, it is not always the case that $T_{\text{OOD}} = \text{HH}$, when $S_{\text{u,OOD}}$ is supposedly most similar to S_{IOD}, yields the best MixMatch performance. This is observed for CIFAR-10, when $n_l = 100$ and $n_l = 150$, where OOD unlabelled data from Tiny ImageNet results in more accurate models than using the other half of CIFAR-10 as $S_{\text{u,OOD}}$. It is interesting that an $S_{\text{u,OOD}}$ dataset of type *different* can be more beneficial than a $S_{\text{u,OOD}}$ dataset of type *similar* which is also the case for FashionMNIST and Tiny ImageNet

Table 3: Correlation results for the dissimilarity measures between S_l and S_u with OOD contamination and SSDL accuracy.

$\mathbf{S_l}$	$\mathbf{n_l}$	$\mathbf{d_{\ell_1}}$	$\mathbf{d_{\ell_2}}$	$\mathbf{d_{JS}}$	$\mathbf{d_C}$
MNIST	60	-0.876	-0.898	-0.969	-0.944
	100	-0.805	-0.83	-0.786	-0.948
	150	-0.794	-0.822	-0.81	-0.944
CIFAR-10	60	-0.823	-0.853	-0.944	-0.921
	100	-0.826	-0.878	-0.966	-0.947
	150	-0.808	-0.838	-0.952	-0.927
FashionMNIST	60	-0.2	-0.268	-0.735	-0.789
	100	-0.264	-0.326	-0.781	-0.824
	150	-0.286	-0.347	-0.785	-0.827

versus Fashion Product at $n_l = 150$. This contradicts the common heuristic that unlabelled data that appears semantically more related to the labelled data is always the better choice for SSDL. Rather, as we demonstrate in the second set of results below, a notion of distance between labelled and unlabelled data offers a more consistent and quantifiable proxy for the expected benefit of different unlabelled datasets.

The second set of results demonstrate the potential of using distance measures as a systematic and quantitative ranking heuristic when selecting unlabelled datasets for the MixMatch algorithm. The exact distances, as described in Section 3.2, for all OOD configurations from the ablation study can be found in Table 2. We can observe that these distances trace the accuracy results found in Table 1. This correlation is quantified in Table 3 with the cosine based density measure d_c correlating particularly well with the accuracy results of Table 1. Also, the p-values are consistently lower for the density based distances, meaning that density based distances can be enjoyed with more confidence as seen in Table 2. We suspect that this is related to the quantitative approximation of the distribution mismatch implemented both in the d_{JS} and d_{C} distances which we plan to explore in future work.

5 Conclusions and recommendations

In this work we extensively tested the behavior of the MixMatch algorithm under various OOD unlabelled data settings. We introduced MixMOOD, which uses quantitative data selection heuristics, DeDiMs, to rank unlabelled datasets *ante hoc* according to their expected benefit to SSDL. Our results lead us to the following conclusions and recommendations:

- Real-world usage scenarios of SSDL can include different degrees of OOD data contamination: for instance, with a deep learning model trained for medical imaging analysis, unlabelled data can include images within the same domain, but capturing different pathologies not present in

the labelled data. This scenario has been simulated with the *half-half* setting which resulted in a subtle accuracy degradation in most cases. However, the accuracy gain obtained vis-a-vis the fully supervised baseline is still substantial, making the application of SSDL attractive in such a setting.

- Another plausible real-world scenario for SSDL is the inclusion of widely available unlabelled datasets, e.g. built with web crawlers, where the domain shift can be more substantial. This scenario has been simulated with the OOD types similar and different. We can observe that notions of semantic similarity between labelled and unlabelled dataset pairings, e.g. (MNIST-SVHN) or (FashionMNIST-Fashion Product), do not necessarily imply an SSDL accuracy gain. Distance measures, in particular d_C, are an accurate and systematic proxy for SSDL accuracy. This is visible when comparing the accuracy and distance results of the previous pairings to (MNIST-Tiny ImageNet) and (FashionMNIST-Tiny ImageNet) which have higher accuracies and, also, surprisingly, lower measurements.
- Overall, the implemented DeDiMs correlate strongly with the yielded SSDL accuracy, in particular density based measures, recommended for its usage in MixMOOD. This approach can be applied in SSDL prior to learning to aid the unlabelled data selection process and mitigate the class distribution mismatch problem. The facts that they are model agnostic, simple and fast to compute make them particularly suitable for practical application in SSDL.
- Finally, the proposed test bed and distance measures can be used for a more systematic quantitative evaluation of SSDL algorithms.

In future work, this test bed can also be applied to other SSDL variants, depth-first analyses (e.g. fewer tasks with more training epochs), additional axes of test bed variables (e.g. n_u) and more testing around the appropriate dissimilarity measures parameters.

Broader Impact

We note that this study constitutes a breadth-first ablation exploration. Our goal was to present a comprehensive test bed to better understand the class distribution mismatch problem and provide a more systematic and quantitative approach for mitigating it. So far these results are limited to the MixMatch algorithm. The extension and usage of the proposed method needs further assessment, specially for its use in particular domains, where social and human costs are considerable.

Acknowledgments and Disclosure of Funding

The authors would like to thank Sören Becker for detailed feedback on a first draft of this paper.

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A MixMatch: Detailed description of the SSL algorithm used in this paper

In MixMatch, the consistency loss term minimizes the distance of the pseudo-labels and the model predictions over the unlabelled dataset X_u. Pseudo-label $\widehat{\boldsymbol{y}}_j$ estimation is performed with the average model output of a transformed input x_j, with K number of different transformations. $K = 2$ is advised in [32]. The estimated pseudo-labels $\widehat{\boldsymbol{y}}$ might be too *unconfident*. To tackle this, pseudo-label sharpening is performed with a temperature ρ. The dataset with the estimated and sharpened pseudo-labels was defined as $\widetilde{S}_u = \left(X_u, \widetilde{Y}\right)$, with $\widetilde{Y} = \left\{\widetilde{\boldsymbol{y}}_1, \widetilde{\boldsymbol{y}}_2, \ldots, \widetilde{\boldsymbol{y}}_{n_u}\right\}$.

Data augmentation is a key aspect in semi-supervised deep learning as found in [32]. To further augment data using both labelled and unlabelled samples, they implemented the Mix Up algorithm developed in [33]. Linear interpolation of a mix labelled observations and unlabelled (with its corresponding pseudo-labels) observations.

$$\left(S_l', \widetilde{S}_u'\right) = \Psi_{\text{MixUp}}\left(S_l, \widehat{S}_u, \alpha\right) \tag{1}$$

The Mix Up algorithm creates new observations from a linear interpolation of a mix of unlabelled (with its corresponding pseudo-labels) and labelled data. More specifically, it takes two labelled (or pseudo labelled) data pairs $(\boldsymbol{x}_a, y_a)$ and $(\boldsymbol{x}_b, y_b)$. The Mix Up method generates a new observation and its label $(\boldsymbol{x}', y')$ by following these steps:

1. Sample the Mix Up parameter λ from a Beta distribution $\lambda \sim \text{Beta}\,(\alpha, \alpha)$.
2. Ensure that $\lambda > 0.5$ by making $\lambda' = \max(\lambda, 1 - \lambda)$.
3. Create a new observation with a lineal interpolation of both observations: $\boldsymbol{x}' = \lambda' \boldsymbol{x}_a + (1 - \lambda')\, \boldsymbol{x}_b$.

With the augmented datasets $\left(S_l', \widetilde{S}_u'\right)$, the MixMatch training can be summarized as:

$$f_{\boldsymbol{w}} = T_{\text{MixMatch}}\left(S_l, S_u, \alpha, \gamma, \lambda\right) = \underset{\boldsymbol{w}}{\text{argmin}} \mathcal{L}\left(S, \boldsymbol{w}\right) \tag{2}$$

$$\mathcal{L}\left(S, \boldsymbol{w}\right) = \sum_{(\boldsymbol{x}_i, \boldsymbol{y}_i) \in S_l'} \mathcal{L}_l\left(\boldsymbol{w}, \boldsymbol{x}_i, \boldsymbol{y}_i\right) + r(t)\gamma \sum_{\left(\boldsymbol{x}_j, \widetilde{\boldsymbol{y}}_j\right) \in \widetilde{S}_u'} \mathcal{L}_u\left(\boldsymbol{w}, \boldsymbol{x}_j, \widetilde{\boldsymbol{y}}_j\right) \tag{3}$$

For supervised and semi-supervised loss functions, the cross-entropy $\mathcal{L}_l\left(\boldsymbol{w}, \boldsymbol{x}_i, \boldsymbol{y}_i\right) = \delta_{\text{cross-entropy}}\left(\boldsymbol{y}_i, f_{\boldsymbol{w}}\left(\boldsymbol{x}_i\right)\right)$ and the Euclidean distance $\mathcal{L}_u\left(\boldsymbol{w}, \boldsymbol{x}_j, \widetilde{\boldsymbol{y}}_j\right) = \left\|\widetilde{\boldsymbol{y}}_j - f_{\boldsymbol{w}}\left(\boldsymbol{x}_j\right)\right\|$, are usually implemented, respectively. The regularization γ controls the direct influence on unlabelled data. Since in the first epochs, unlabelled data based predictions are unreliable, the function $r(t) = t/\rho$ increases the unsupervised term contribution as the number of epochs progress. The coefficient ρ is referred as the rampup coefficient. Unlabelled data also influences the labelled data term $\mathcal{L}_l$, since unlabelled data is used also to artificially augment the dataset with the Mix Up algorithm. This loss term is used at training time, for testing, a regular cross entropy loss is implemented.

B MixMOOD pseudocode description

Note that based on our empirical results we recommend the use of density based deep dissimilarity measures, in particular cosine distance, as these displayed the best correlation with MixMatch accuracy.

Algorithm 1: MixMOOD for unlabelled dataset selection

Input: A list of unlabelled datasets $S_{u_1}, S_{u_2}, ..., S_{u_k}$
For each unlabelled dataset S_{u_i} do:

1. Randomly sub-sample each one of the datasets S_l and S_{u_i}, with a sample size of τ, creating the sampled datasets $S_{l,\tau}$ and $S_{u_i,\tau}$.
2. Transform all input observations in the two samples $\boldsymbol{x}_j \in S_i$, with $\boldsymbol{x}_j \in \mathbb{R}^n$, with n the dimensionality of the input space, using the feature extractor f, yielding $\boldsymbol{h}_j = f(\boldsymbol{x}_j)$. Where $\boldsymbol{h}_i \in \mathbb{R}^{n'}$ is the feature vector of n' dimensions, with $n' < n$. For instance, the implemented feature extractor uses the Wide-ResNet architecture, extracting $n' = 512$ features. This yields the two feature sets $H_{l,\tau}$ and $H_{u_i,\tau}$
3. For each dimension $r = 1, ..., n'$ in the feature space, compute the normalized histogram $p_{r,l}$, in the sample $H_{l,\tau}$. Similarly, we compute the set of density functions $p_{u_i,b}$ for $r = 1, ..., n'$, using the observations in the sample $H_{u_i,\tau}$.
4. Compute the sum of the distances between the density functions $p_{r,l}$ and p_{r,u_i}, to yield the distance approximation for the sample j: $\widehat{d}_j = \sum_{r=1}^{n'} \delta_g(p_{r,a}, p_{r,b})$. We do this for all the $\mathcal{C}$ samples, yielding the list of inter-dataset distances: $\widehat{d}_1, \widehat{d}_2, ..., \widehat{d}_{\mathcal{C}}$. To lower the computational burden, we assume that the dimensions are statistically independent.
5. Compute the intra-dataset distances for the dataset S_l, in this context the labelled dataset S_l, to obtain the list of reference distances $\check{d}_1, \check{d}_2, ..., \check{d}_{\mathcal{C}}$.
6. Compute the p significance value with a Wilcoxon test to verify that the inter- and intra-dataset distance difference $d_c = \left|\widehat{d}_c - \check{d}_c\right|$ are statistically significant. The distance computation yields the sample mean distance $\overline{d}_{u_i}$ and its confidence value p_{u_i}.

Pick the unlabelled dataset $S_{u_{\text{best}}}$ with the lowest distance $\overline{d}_{u_{\text{lowest}}}$.
Result: $S_{u_{\text{best}}}$ the unlabelled dataset to yield the best accuracy for MixMatch

C Hyperparameters

C.1 Global

Table 4: Global hyperparameters which are kept constant throughout all experiments. This was done in order to isolate the effects of the changing OOD data configurations.

Description	Name in code	Value
Model architecture used in all tasks	`MODEL`	wide_resnet
Number of training epochs	`EPOCHS`	50
Batch size	`BATCH_SIZE`	16
Learning rate	`LR`	0.0002
Weight decay	`WEIGHT_DECAY`	0.0001
Rampup coefficient	`RAMPUP_COEFFICIENT`	3000
Optimizer	-	Adam with 1-cycle policy [36]

C.2 MixMatch

Table 5: MixMatch hyperparameters. All parameters were chosen following the recommendations by [32].

Symbol	Description	Name in code	Value
K	Number of augmentations	`K_TRANSFORMS`	2
T	Sharpening temperature	`T_SHARPENING`	0.5
α	Parameter for the Beta distribution	`ALPHA_MIX`	0.75
γ	Gamma for the loss weight	`GAMMA_US`	25
-	Whether to use balanced (5) or unbalanced (-1) loss for MixMatch	`BALANCED`	5

D Dataset descriptions

If you wish to reproduce any of the experiments datasets are automatically downloaded by the experiment script `ood_experiment_at_scale_script.sh` for your convenience based on which experiment you choose to run.

An overview of the different datasets can be found below. Note that we used the training split of each dataset as the basis to construct our own training and test splits for each experimental run.

Table 6: Information on the datasets used in the experiments. **Format** specifies the format the image files were provided in, $\mathbf{d}$ specifies the size of the images, $\mathbf{N}$ specifies the number of samples in the dataset, $|\mathcal{Y}|$ specifies the number of classes in the dataset, **Relative class distribution** specifies the relative class distribution in the dataset.

Dataset	Format	d	N	$\lvert\mathcal{Y}\rvert$	Relative class distribution
MNIST[37]	`.jpg`	28×28	42,000	10	Uniform
SVHN[38]	`.png`	32×32	73,557	10	0.07/0.19/0.14/0.12/0.1/ 0.09/0.08/0.07/0.07/0.07
Tiny ImageNet[39]	`.jpg`	64×64	100,000	200	Uniform
CIFAR-10[40]	`.jpg`	32×32	50,000	10	Uniform
FashionMNIST[41]	`.png`	28×28	60,000	10	Uniform
Fashion Product[42]	`.jpg`	60×80	44,441	5	0.48/0.25/0.21/0.05/0.01
Gaussian	`.png`	224×224	20,000	NA	NA
Salt and Pepper	`.png`	224×224	20,000	NA	NA

The Gaussian and Salt and Pepper datasets were created with the following parameters: a variance of 10 and mean 0 for the Gaussian noise, and an equal Bernoulli probability for 0 and 255 pixels, in the case of the Salt and Pepper noise.

D.1 Preprocessing

Each data point was preprocessed in the following way. After a subset of labelled and unlabelled data for an experimental run had been constructed the means and standard deviations (one pair for labelled data, one pair for unlabelled data) were calculated for this specific subset. Then, the labelled and unlabelled inputs were standardized by subtracting the respective mean and dividing by the respective standard deviation.

In addition, in situations when the size of the unlabelled images differed from the size of the labelled images up- or downsampling was used to align the unlabelled image size.

E Existing OOD detection methods and IOD-OOD data pairings

Table 7: OOD test benchmarks for different techniques. Datasets with * were randomly cut by half for in-distribution training labelled data and the other half was used as OOD unlabelled data. The table reveals how arbitrary different testbeds have been used for benchmarking OOD detection algorithms. IOD-OOD dataset pairs are indicated by number pairs in the table.

Method name	IOD data	OOD data
Max. value of Softmax layer [23]	CIFAR-10 [1] CIFAR-100 [2] MNIST [3]	SUN[1,2] Gaussian [1,2] Omniglot [3] notMNIST[3] Uniform noise[3]
Inhibited Softmax[43]	CIFAR-10[1] MNIST[2]	SVHN[1] LFW-A[1] notMNIST[2] Omniglot[2]
ODIN [11]	CIFAR-10[1] CIFAR-100[2]	TinyImageNet[1,2] LSUN[1,2] iSUN[1,2] Uniform[1,2] Gaussian[1,2]
Epistemic Uncertainty Estimation [25]	CIFAR *[1] FashionMNIST*[2] SVHN*[3] MNIST*[4]	CIFAR*[1] FashionMNIST*[2] SVHN*[3] MNIST*[4]
Mahalanobis latent distance [24]	CIFAR-10[1] CIFAR-100[2] SVHN[3]	SVHN[1,2] CIFAR-10[3] TinyImageNet[1,2,3] LSUN[1,2,3]

F Code archive and computing infrastructure

All training and evaluation code can be found at `https://github.com/peglegpete/mixmood`. Software dependencies are specified in the `requirements.txt` file in the same archive. We use the `mlflow` framework for experiment management and reproduction. After experiments have been completed you can extract results from all runs using the analysis scripts provided in the archive.

Experiments were run on three machines. Machine 1 has one 12GB NVIDIA TITAN X GPU, 24 Intel(R) Xeon(R) CPU E5-2687W v4 @ 3.00GHz and 32GB RAM. Machine 2 has four 16GB

NVIDIA T4 GPUs, 44 CPUs from the Intel Xeon Skylake family and 150GB RAM. Machine 3 has one 12GB NVIDIA TITAN V GPU, 24 Intel(R) Xeon(R) E5-2620 0 @ 2.00GHz CPU and 32GB RAM.

Experimental runs were parallelized using the ampersand option in `bash` executing 10 runs in parallel on a single GPU. With the current code base this requires up to 10 CPUs per GPU as well as approximately 25GB RAM per GPU. With this setup a single training epoch of 10 parallel experimental runs should last between 2 and 4 minutes per GPU, depending on which type of GPU is used.