Improving Semi-supervised Deep Learning by using Automatic Thresholding to Deal with Out of Distribution Data for COVID-19 Detection using Chest X-ray Images

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Abstract—Semi-supervised learning (SSL) leverages both labeled and unlabeled data for training models when the labeled data is limited and the unlabeled data is vast. Frequently, the unlabeled data is more widely available than the labeled data, hence this data is used to improve the level of generalization of a model when the labeled data is scarce. However, in real-world settings unlabeled data might depict a different distribution than the labeled dataset distribution. This is known as distribution mismatch. Such problem generally occurs when the source of unlabeled data is different from the labeled data. For instance, in the medical imaging domain, when training a COVID-19 detector using chest X-ray images, different unlabeled datasets sampled from different hospitals might be used. In this work, we propose an automatic thresholding method to filter out-of-distribution data in the unlabeled dataset. We use the Mahalanobis distance between the labeled and unlabeled datasets using the feature space built by a pre-trained Image-net Feature Extractor (FE) to score each unlabeled observation. We test two simple automatic thresholding methods in the context of training a COVID-19 detector using chest X-ray images. The tested methods provide an automatic manner to define what unlabeled data to preserve when training a semi-supervised deep learning architecture.

I. INTRODUCTION

Deep Neural Networks (DNNs) have shown outstanding results on many supervised learning problems, but this practice requires large labeled datasets [21]. This decreases considerably the number of problems that supervised learning can solve in many areas where labeled data is scarce. For example, the usage of labeled medical images requires expensive human effort (professional human annotators), thus building a labeled dataset is costly [7].

To overcome this problem Semi-supervised Learning (SSL) algorithms have proven to be an alternative to building models less prone to over-fitting training data [6]. This approach leverages both labeled and unlabeled data, providing a way to train models without the need of large labeled datasets [32]. Unlabeled samples are in general easier to collect, as it usually does not require annotators. Hence, building an Semi-supervised Deep Learning (SSDL) model can be a cheaper alternative to Supervised Deep Learning (SDL).

Unlabeled data is available from many different sources. In semi-supervised learning, it is usually assumed that the labeled and unlabeled datasets follow a similar distribution. This is known as the Independent and Identically Distributed (IID) assumption. However, the risk that this assumption is violated under real-world usage settings can be high when using unlabeled data sampled from different sources. The phenomenon where the distribution of the labeled dataset is not similar to the distribution in the unlabeled dataset is called distribution mismatch [23]. An unlabeled observation that is very unlikely to belong to the labeled data distribution can be referred to as an Out of Distribution (OOD) observation.

The accurate detection of COVID-19 is a critical task to control the pandemic. Fortunately, COVID-19 detection using chest X-ray images can be considered an inexpensive method for its detection, as X-ray imaging systems are more widely available than other medical imaging technologies [5]. Nevertheless, scarcely labeled data is a limitation faced to train a deep learning based COVID-19 detector [1].

The problem of distribution mismatch between the labeled and unlabeled datasets for training a COVID-19 detector using chest X-ray was analyzed in [7]. In such work, a simple method to score each unlabeled chest X-ray image with respect to the labeled dataset was proposed. However, the method was tested using a previously known fixed threshold [7].

In this work, an automatic thresholding technique is proposed. This technique is used to filter the OOD data in the unlabeled dataset, using the scores proposed in [7]. The tested thresholding techniques use the scores to estimate the optimal threshold between the In-Distribution (IOD) and OOD data. Furthermore, we propose a simple method to improve the data quality in the unlabeled dataset in a semi-supervised setting by removing the OOD data. We evaluate the filter by using a small labeled dataset from the target clinic along with a large unlabeled dataset from the same or a different clinic.

II. STATE OF THE ART

In Section II-A we enlist recent major categories for SSL for deep learning architectures. As the aim of this work refers to training SSL methods under distribution mismatch settings,
we later examine the literature around OOD detection for deep learning models in Section II-B.

A. Semi-supervised Learning approaches for Deep Learning Architectures in Image Analysis

In SSL the training datasets uses both labeled observations \( S^{(l)} \) and unlabeled observations \( S^{(u)} \). Using SSL can be useful under real-world usage settings where collecting labeled data is expensive, or time-consuming. SSL leverages unlabeled data which is frequently more widely available and less expensive to obtain [25]. We refer to SSDL when SSL is implemented to train a set of layers in a deep learning model.

As developed in [6], [30] the most popular SSDL architectures can be classified as pre-training based [12], pseudo-labeled [13] and regularization-based [4]. In [6] a detailed description of SSDL methods can be found. Pre-training based methods frequently implement a set of proxy tasks (e.g., the estimation of the image rotation angle) to pre-train one or more layers of the deep learning model [26]. Later the model is fine-tuned using the labeled data [26].

Pseudo-labeled methods estimate a set of pseudo-labels, either by implementing an iterative process where the more confident estimations are re-used as labeled observations (e.g., boosting) or using a model ensemble [30].

Regularization-based SSDL, also known as intrinsically unsupervised methods [30], include an unlabeled data-based term in the loss function \( \mathcal{L}(S) \) to regularize the model during training. This is shown in Equation 1.

\[
\mathcal{L}(S) = \sum_{(x_i, y_i) \in S^{(l)}} \mathcal{L}_i(w, x_i, y_i) + \gamma \sum_{x_j \in S^{(u)}} \mathcal{L}_u(w, x_j)
\]

where \( w \) is the model’s weights array, and the labeled and unlabeled loss term are denoted by \( \mathcal{L}_l \) and \( \mathcal{L}_u \). The term \( \gamma \) weights the influence of unsupervised regularization.

Regularization-based methodologies have been the most popular ones to implement SSL for deep learning architectures [6]. Earlier regularization-based approaches include the pseudo-ensemble [2], temporal ensembling [20] and mean teacher [28]. More recently, regularized methods like MixMatch combine regularized SSDL with heavy data augmentation, yielding interesting results over previous architectures [4]. MixMatch combines pseudo-labeling with regularization based SSL by implementing the unlabeled loss term \( \mathcal{L}_u \) with a comparison of the estimated label of the model with the average output of the model using a number of simple transformations (e.g., image flipping). This averaged model output is referred to as a soft pseudo-label.

MixMatch has been extended to include more sophisticated approaches of data augmentation in FixMatch [27] and ReMixMatch [3]. Further within the MixMatch family, more recently in [17], the MixMatch approach is modified to include a pair loss which minimizes the distance between observations with high confidence pseudo-labels with high similarity. The authors reported accuracy gains ranging from 1 to 3 percent with respect to FixMatch.

In this work, we test our automatic OOD scoring algorithm with the MixMatch method. However, the proposed approach can be also combined with more recent developments within the MixMatch family.

B. Out of Distribution Data Detection

The task of detecting OOD data is frequently approached as a score estimation problem. The score can be used as a measure to discern how likely an observation belongs to the distribution of the labeled dataset [16].

In [7], OOD scoring methods are categorized as Deep Neural Network (DNN) output-based and feature or latent representation-based methods.

Output-based OOD scoring methods use the DNN output to estimate the OOD likelihood. For instance, [16] uses the softmax of the model’s output as a OOD score. Later, different calibration methods to improve the OOD score mapping were developed. Also, ensemble-based methods that use a number of model’s perturbations as the Monte Carlo Dropout (MCD) method developed in [14] can be categorized as output-based.

As for the feature space-based methods, Kimin et al. [22] proposed a simple method that compares the input observation to be scored with the training data, using the Mahalanobis distance. Later, Joost et al. [29] proposed a method referred as Deterministic Uncertainty Quantification (DUQ). The proposed method computes the centroids for each class in the training dataset (IOD dataset). For a new observation to be OOD scored, the method calculates the distance to each centroid. The shortest distance is used as the uncertainty or OOD score. For instance, Qing et al. [31] proposed a Multi-Task Curriculum Framework (MTCF) that enables SSL to achieve stable performance when the unlabeled dataset contains outliers by detecting them. The proposed method defines OOD scores to the observations in the unlabeled dataset. The scores are optimized with the DNN parameters, hence the scores are updated by using the DNN output. To threshold the OOD scores, the method uses Otsu’s thresholding method developed [24]. As a limitation, the thresholding method fails to improve the baseline accuracy when the number of IOD and OOD samples is imbalanced.

III. PROPOSED METHOD

In this work, we propose an automatic thresholding technique to filter the OOD data in the unlabeled dataset \( S^{(u)} \). To do so, we estimate the harm coefficient of each unlabeled observation \( s^{(u)} \), using the method developed in [7]. The method uses the Mahalanobis distance, which assumes a Gaussian distribution in the feature space. The Mahalanobis distance is used as previous work suggests that the Mahalanobis distance is faster and slightly yields more accuracy gain than the feature histograms method. The feature space used is a generic feature space built from a pre-trained Image-net model using the AlexNet architecture, given its low computational cost. We summarize the proposed method in [7] as follows:

1) Take the labeled observations in the matrix \( S^{(l)} \), and the unlabeled observation \( s^{(u)} \) to score. With a Fea-
true Extractor (FE) $h_{FE}$ of an Image-net pre-trained Alexnet architecture, we calculate the set of feature arrays for the labeled observations $H^{(l)} = h_{FE}(X^{(l)})$, and the feature array for the unlabeled input observation $h^{(u)} = h_{FE}(s^{(u)})$. The feature extractor we tested in this work yields 256 features, thus $h^{(u)} \in \mathbb{R}^{256}$ and $H^{(u)} \in \mathbb{R}^{N \times 256}$.

2) As a next step, the Mahalanobis distance is calculated as follows:

$$d_M \left( \bar{h}^{(l)}, h^{(u)} \right) = \left( \bar{h}^{(l)} - h^{(u)} \right)^T \Sigma_i^{-1} \left( \bar{h}^{(l)} - h^{(u)} \right)$$

(2)

Where $\Sigma_i^{-1}$ corresponds to the covariance matrix of the labeled feature set $H^{(l)}$ and $\bar{h}^{(l)}$ corresponds to the sample mean of such labeled feature set.

We define the histogram of the Mahalanobis distances of the observations within the unlabeled dataset as $p_d^{(u)}$. The set of distances between each unlabeled observation $s_j^{(u)}$ and the labeled dataset $S^{(l)}$ is defined by $D^{(u)}$.

The previous procedure shows the steps to calculate the set of distances $D^{(u)}$ to each observation in $S^{(u)}$. The larger distances are less favorable to use for training. Thus, when the unlabeled dataset has OOD data, the histogram of distances $p_d^{(u)}$ tends to form a bimodal Gaussian distribution, where one mode contains the IOD data and the other mode the OOD data. From there, we propose the usage of Otsu’s thresholding method and the K-means clustering, assuming one to two clusters, to find the optimal threshold in the distribution.

Otsu’s thresholding method is used to estimate an automatic thresholding in a histogram. In our case we use the previously estimated score density function $p_d^{(u)}$. The method assumes a Gaussian distribution in the input histogram, hence the performance to estimate the optimal threshold depends that the input data follows the mentioned distribution function. The approach consist in estimating the threshold by maximizing the between-class variance $\sigma_b^2(\tau)$. A more detailed explanation can be found in [24].

The K-means clustering estimates the nearest mean for the observations in the dataset. Therefore, the K-means algorithm is an iterative procedure that optimizes the means until stabilization is achieved [15]. In our case we use as input for the K-means the scores dataset for the unlabeled observations $D^{(u)}$. This algorithm can be represented by the equation $\arg \min_{C} \sum_{i=0}^{k} \sum_{x \in C_i} ||x - \mu_i||^2$, where $x \in D^{(u)}$ is the set of scores, $k$ the number of clusters, and $C$ the clusters.

The aforementioned methods, estimate the threshold assuming the unlabeled dataset $S^{(u)}$ contains OOD data. However, $S^{(l)}$ and $X^{(u)}$ may not depict distribution mismatch. As a result, the histogram $p_d^{(u)}$ will present a mono-modal Gaussian distribution. Therefore, we propose to use the Coefficient of Variation (CV) to estimate when $p_d^{(u)}$ depicts a mono-modal or a bi-modal distribution in order to select a dynamic threshold. The procedure is explained as follows:

1) Compute the set of Mahalanobis distances $D^{(u)}$.

2) Calculate the sample mean $\mu_{tot}$ and standard deviation $\sigma_{tot}$ from the set $D^{(u)}$.

3) Obtain the threshold $\tau$ using the one of the thresholding methods.

4) Using the threshold $\tau$ the set of distances $D^{(u)}$ is separated into two different sets:

$$D^{(u)}_h = \{D^{(u)}_i \leq \tau, 1 \leq i \leq N \} \quad \text{and} \quad (3)$$

$$D^{(u)}_g = \{D^{(u)}_i > \tau, 1 \leq i \leq N \} \quad \text{and} \quad (4)$$

where N is the number of elements in $D^{(u)}$.

5) Compute the sample mean and standard deviation from the sets, which are defined as $\mu_h$ and $\sigma_h$ for the set $D_h^{(u)}$, and $\mu_g$ and $\sigma_g$ for the set $D_g^{(u)}$.

6) Calculate the CV, as follows:

$$CV_{tot} = \frac{\sigma_{tot}}{\mu_{tot}}, \quad CV_{uh} = \frac{\sigma_h}{\mu_h}, \quad CV_{ug} = \frac{\sigma_g}{\mu_g} \quad (5)$$

7) Compare the CV of $CV_{tot}$, and $CV_{uh}$ and $CV_{ug}$:

$$\alpha \cdot CV_{tot} \leq CV_{uh} + CV_{ug} \quad (6)$$

8) In case the previous step is false then the filter assumes that all the data in the unlabeled dataset is IOD and the filter’s output will correspond to the observations with distance $D^{(u)}$. Otherwise, the filter’s output is the observations whose distance is contained in $D_h^{(u)}$.

In step 6, the CV is a statistical measure that estimates the dispersion of data in a cluster. This coefficient is used to compare the variability of data between $D^{(u)}$, and the sets $D_h^{(u)}$ and $D_g^{(u)}$. For this reason, in step 7 both coefficients of variation are compared to choose the best-suited assumption. Moreover, in step 7 a constant $\alpha$ is defined, this value is used to increase a little the value of $CV_{tot}$. The suggested values of $\alpha$ should be around 1.12. This value was chosen due to experimentation.

In this work, we test two different thresholding methods using the Mahalanobis distances as scoring technique. MixMatch is used as the SSDL algorithm to train the model. In order to assess the filter the accuracy of the model using the filtered unlabeled dataset, the filter is tested under some controlled settings to evaluate the accuracy obtained after training the model using the data selected by the filter. The proposed method is tested using real-world data with distribution mismatch conditions in a medical imaging analysis such as the COVID-19 detection using chest X-ray images.

IV. DATASET DESCRIPTION

In this work, we assess the negative effect of distribution mismatch between the labeled and unlabeled dataset using the MixMatch algorithm. We use the medical imaging domain to test the proposed methods under real-world usage conditions, such as COVID-19 detection using chest X-ray images (binary classification between no pathology and pathology). We use different sources of COVID-19− (no pathology) and COVID-19+ (positive pathology) to recreate different distribution mismatch conditions. The observations of COVID-19+
TABLE I
COVID-19 Observation Sources Description Used in This Work.

| Source               | No. of Patients | Patient's Age Range (years) | No. of Observations | Hospital/clinic | Im. Resolution | Reference |
|----------------------|----------------|-----------------------------|---------------------|----------------|----------------|-----------|
| CR-Chavarria-ChestXray-2020 | 105            | 7 – 86                      | 105                 | Clinica Chavarria | 1907 × 1791 | [8]       |
| Chinese dataset      | 5856           | children                    | 5236                | No info.        | 1300 × 600   | [19]      |
| ChestX-ray8 dataset  | 62400          | 0 – 94                      | 224316              | Stanford Hospital | 1024 × 1024 | [8]       |
| Indiana dataset      | 4000           | adults                      | 8121                | Indiana Network for Patient Care | 1024 × 1024 | [11]      |

were collected from the open dataset available in [10]. This dataset currently has 105 COVID-19\(^+\) images. Images in the dataset do not have the same resolutions, which range from 400 × 400 to 2500 × 2500. Observations of COVID-19\(^-\) were collected from four different data sources. Such data sources are summarized in Table I. Figure 1 shows a sample of each dataset.

For the COVID-19\(^+\) images [10], the observations related to Middle East Syndrome (MERS), Acute Respiratory Distress Syndrome (ARDS), and Severe Acute Respiratory Syndrome (SARS) were removed and the letters in the radiographs were cropped. In the case of the Indiana dataset the lateral projections were discarded. The Indiana and Chinese datasets contained observations of different pathologies, therefore, we preserved only observations categorized as normal.

The configurations for the experiments were done using different combinations of labeled and unlabeled datasets, this is shown in Table II. The experiments were carried out using \(n_l = 20\) labeled samples and \(n_u = 90\) for the unfiltered unlabeled datasets. We used different sources for the labeled dataset and different contamination level to assess the impact of distribution mismatch in an unlabeled dataset. As the different sources of data were datasets of COVID-19\(^-\), the unlabeled datasets contained only COVID-19\(^-\) observations.

Different combinations of data sources were used to build the unlabeled dataset to create different distribution mismatch conditions. As we noticed in our empirical tests that the Costa Rican dataset yielded the lowest performance when used for SSDL training, we used it as a OOD contamination source. The percentage of contamination in the test-bed range from 20 to 100 percent, as seen in Table II.

Regarding the test dataset, it consists of observations from the same source as the labeled dataset. Hence, it contains observations of COVID-19\(^+\) and its respective COVID-19\(^-\) source. The test dataset used a total of 40 observations, with 20 observations per class.

V. Experimental Design

A. Evaluation of using distribution mismatch datasets on MixMatch’s accuracy

The first experimentation test-bed is designed to assess the effect of using different unlabeled dataset and a target labeled datasets in the MixMatch’s performance. Hence, the prepared settings follow a controlled environment where the unlabeled datasets depicts different degrees of distribution mismatch. Table II shows the results of training MixMatch using an AlexNet model.

B. Evaluation of MixMatch’s accuracy using the Otsu’s and K-means methods for automatic thresholding

The experiment is designed to assess the MixMatch’s accuracy results when using the proposed methods to filter the OOD data in the unlabeled dataset. Hence, the MixMatch’s accuracy is measured using the filtered datasets with an AlexNet model. Table III shows the results of training the AlexNet model using MixMatch with the filtered datasets by the proposed methods. The filtering methods use the Mahalanobis distance to assign a score to each unlabeled sample. As previously mentioned, we assume that the OOD and IOD data tend to form a Gaussian mixture distribution or two clusters. Therefore the OOD data is filtered using the threshold estimated by Otsu’s thresholding method and the K-means clustering. Moreover, the proposed method evaluates whether the unlabeled dataset depicts contamination using the coefficient of variation of each cluster. To evaluate the ideal setting where all the OOD data is removed from the unlabeled dataset, we evaluate the accuracy yielded by using the real threshold (percentage of contamination using the Costa
unlabeled dataset from the Costa Rican data source. This accuracy degradation can be attributed to a different distribution between the labeled and unlabeled datasets.

Regarding the two proposed methods for automatic thresholding of the OOD data, described in Table III, we can see how, in general, both automatic thresholding methods tend to yield similar results when using the real unlabeled data contamination percentage. This suggests that both thresholding methods reach a similar OOD score to discard the unlabeled data, than using the real contamination value. The Otsu method, which assumes a Gaussian mixture distribution of the data, yields slightly better accuracy gains when used to filter the unlabeled data, however, with no statistical significance. Both methods can be considered a good alternative to automatically calculate the threshold to discard OOD data.

### VI. RESULTS

The results from the experiment in section V-A are presented in Table II. We can see how the different settings of unlabeled data affect the accuracy yielded by the MixMatch algorithm with an Alexnet back-bone.

For instance, the supervised model using a labeled dataset from Indiana and China yielded an accuracy of 67.2 and 65.5 respectively. The accuracy of these models was improved by using unlabeled data to 68.7 and 98.0 respectively. The unlabeled Costa Rica dataset yields the lowest accuracy when used along the labeled Indiana dataset. From there, in general, the accuracy is affected as we injected observations in the unlabeled dataset from the Costa Rican data source. This accuracy degradation can be attributed to a different distribution between the labeled and unlabeled datasets.

### VII. CONCLUSIONS

In this work, we analyzed the impact of training a SSDL model using a labeled and unlabeled dataset with distribution mismatch. The experiments were assessed under the medical imaging domain for COVID-19 detection. As an extension to the work in [7], we propose two simple methods to estimate...
the best threshold to discard unlabeled data, using OOD score proposed in [7].

The two thresholding methods evaluated in this work performed similarly, close to the accuracy yielded by filtering the unlabeled data with the real contamination percentage. Therefore, any of the tested methods can be used to find the best OOD score threshold.

The presented approach is meant to improve data quality before training the model. The approach is built upon a pre-trained model with Imagenet using the Mahalanobis distance in the feature space, as this configuration showed better results in [7]. The implemented proposed methods can be used to automatically filter harmful observations from the dataset when the unlabeled dataset is not highly contaminated. Furthermore, we proved that SSDL may improve the results of SDL model when the labeled dataset is small.

The approach does not require to train a deep learning model, which makes it less expensive alternative to increase the data quality in the unlabeled dataset.

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