ROBUST SEMI-SUPERVISED LEARNING WITH OUT OF DISTRIBUTION DATA

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ABSTRACT
Semi-supervised learning (SSL) based on deep neural networks (DNNs) has recently been proven effective. However, recent work [Oliver et al., 2018] shows that the performance of SSL could degrade substantially when the unlabeled set has out-of-distribution examples (OODs). In this work, we first study the key causes about the negative impact of OOD on SSL. We found that (1) OODs close to the decision boundary have a larger effect on the performance of existing SSL algorithms than the OODs far away from the decision boundary and (2) Batch Normalization (BN), a popular module in deep networks, could degrade the performance of a DNN for SSL substantially when the unlabeled set contains OODs. To address these causes, we proposed a novel unified robust SSL approach for many existing SSL algorithms in order to improve their robustness against OODs. In particular, we proposed a simple modification to batch normalization, called weighted batch normalization, capable of improving the robustness of BN against OODs. We developed two efficient hyperparameter optimization algorithms that have different tradeoffs in computational efficiency and accuracy. The first is meta-approximation and the second is implicit-differentiation based approximation. Both algorithms learn to reweight the unlabeled samples in order to improve the robustness of SSL against OODs. Extensive experiments on both synthetic and real-world datasets demonstrate that our proposed approach significantly improves the robustness of four representative SSL algorithms against OODs, in comparison with four state-of-the-art robust SSL approaches. We performed an ablation study to demonstrate which components of our approach are most important for its success.

1 Introduction
Deep learning models (e.g., AlexNet [Krizhevsky et al., 2012], ResNet [He et al., 2016]) have been shown to be successful on several supervised learning task, such as computer vision [Szegedy et al., 2015], natural language processing [Graves, 2013], and speech recognition [Graves et al., 2013]. However, these successes often require huge labeled datasets to train deep learning model well, and labeling a large amount of unlabeled data can be expensive. Therefore, it is natural to consider semi-supervised learning (SSL) [Zhu, 2005] to address this challenge. SSL algorithms provide a framework of learning representation from the large unlabeled set. SSL is an active research area and a variety of SSL algorithms have been proposed, such as Entropy Minimization (EntMin) [Grandvalet and Bengio, 2005], Pseudo-label based methods [Lee, 2013][Arazo et al., 2019][Berthelot et al., 2019], and consistency based methods [Sajjadi et al., 2016][Laine and Aila, 2016][Tarvainen and Valpola, 2017][Miyato et al., 2018].

Despite the positive results of the above SSL methods, they are designed based on the assumption that both labeled and unlabeled sets are drawn from the same distribution. Fig1(a) shows an example of this conventional SSL. However, this assumption may not hold in many real-world applications, such as web classification [Yang et al., 2011] and medical diagnosis [Yang et al., 2015], where some unlabeled examples have unknown or novel classes unseen in the labeled data. As illustrated in Fig1(b), in a image classification task, labeled images contains three classes (vehicle, airplane and boat), but unlabeled images include three novel classes (cat, deer, and dog) that are not present in the labeled images.
When the unlabeled set contains OODs, the performance of deep SSL can degrade substantially and is sometimes even worse than a simple supervised learning (SL) approaches [Oliver et al., 2018].

To handle noisy unlabeled data for SSL, a general idea is to assign a weight to each unlabeled example about its cost value and minimize a weighted training or validation loss. There are two main approaches to this. The first is model-based and second is learning to reweight. The former approach considers a parametric function to predict the weights and estimates the parameters based on the training and/or validation sets. In particular, [Chen et al., 2020] proposed to weight the unlabeled examples based on an estimation of predictive uncertainty for each unlabeled example in order to discard the potentially irrelevant samples of low confidence scores and estimate the parameters by optimizing a regularized training loss. [Guo et al., 2020] proposed to weight the unlabeled examples using a neural network and estimate the parameters based on the labeled data via bi-level optimization.

The latter (our proposed) approach applies meta-learning techniques and assigns the weights of unlabeled examples based on their meta-gradient directions derived from a loss function on a clean validation set, by treating the weights as hyperparameters. This is designed based on the basic assumption that: “The best example weighting should minimize the loss of a set of unbiased clean validation examples that are consistent with the evaluation procedure” [Ren et al., 2018]. It is common to obtain a dataset composed of two parts, including a relatively small but accurately labeled set and a large but coarsely labeled set that may come from inexpensive crowdsourcing services or other noisy sources. We note that this idea has been originally applied to address noisy labels for robust SL, demonstrating state-of-the-art performance in a number of real-world benchmark datasets [Ren et al., 2018]. Our proposed work is the first one that demonstrates the effectiveness of learning to reweight for robust SSL against OODs. We conducted extensive experiments on both synthetic and real-world benchmark datasets and the results demonstrate that our proposed robust SSL approach significantly improves the robustness of four representative SSL algorithms against OODs, in comparison with four state-of-the-art robust SSL approaches. We performed an ablation study to demonstrate which components of our approach are most important for its success.

2 Background & Related Work

In this section, we introduce the background of SSL and review recent advances in robust SSL.

Semi-Supervised Learning (SSL). Given a training set with a labeled set of examples \( D = \{ x_i, y_i \}_{i=1}^n \) and an unlabeled set of examples \( U = \{ x_j \}_{j=1}^m \). For any classifier model \( f(x, \theta) \) used in SSL, where \( x \in \mathbb{R}^C \) is the input data, and \( \theta \) refers to the parameters of the classifier model. The loss functions of many existing methods can be formulated as the following general form:

\[
\sum_{(x_i, y_i) \in D} l(f(x_i, \theta), y_i) + \sum_{x_j \in U} r(f(x_j, \theta)),
\]

where \( l(\cdot) \) is the loss function for labeled data (such as cross entropy), and \( r(\cdot) \) is the loss function (regularization function) on the unlabeled set, the goal of SSL methods is to design the regularization function, we introduce some popular SSL method as following. Pseudo-labeling [Lee, 2013] designed the regularization function as a standard supervised loss function with producing “pseudo-labels” as target label. II-Model [Laine and Aila, 2017, Sajjadi et al., 2016] designed a consistency regularization function that push the distance between the prediction for an unlabeled sample and its stochastic perturbation (e.g., data augmentation, dropout [Srivastava et al., 2014]) to be small. Mean Teacher [Tarvainen and Valpola, 2017] proposed to obtain a more stable target output \( f(x, \theta) \) for unlabeled set by setting
the target via an exponential moving average of parameters from previous training steps. Instead to design a stochastic function $f(x, \theta)$, Virtual Adversarial Training (VAT) [Miyato et al., 2018] proposed to approximate a tiny perturbation to unlabeled samples, which would most affect the output of the prediction function. MixMatch [Berthelot et al., 2019], UDA [Xie et al., 2019] choose the pseudo-labels to design the regularization function based on predictions of augmented samples, such as shifts, cropping, image flipping, and mix-up [Zhang et al., 2017]. However, the performance of most existing SSL can degrade substantially when the unlabeled dataset contains OODs examples [Oliver et al., 2018].

Robust SSL. The robustness in SSL against different noise types has been studied in the literature, including label noise [Yan et al., 2016], distribution shift [Chen et al., 2019] and distribution mismatch (OOD involved) [Oliver et al., 2018]. To improve the robustness of SSL against OODs, [Yan et al., 2016] applied a set of weak annotators to approximate the ground-truth labels as pseudo-labels to learn a robust SSL model. [Chen et al., 2019] proposed a distributionally robust model that estimates a parametric weight function based on both the discrepancy and the consistency between the labeled data and the unlabeled data. [Chen et al., 2020] proposed a uncertainty-based robust SSL that learns a parametric weight function to predict OODs based on epistemic uncertainty [Gal and Ghahramani, 2016]. [Guo et al., 2020] proposed a safe SSL that adapts a model based approach [Shu et al., 2019] into robust SSL perspective.

There are three main limitations of existing methods for robust SSL. First, it lacks a study of potential causes about the impact of OODs on SSL, and as a result the interpretation of robust SSL methods becomes difficult. Second, despite the success of the learning-to-reweight approach for robust SL against noisy labels, it is unknown whether this approach is also effective for robust SSL against OODs. Third, existing algorithms for learning-to-reweight are generally designed based on lower-order approximations of the objective in the inner loop of meta learning, due to vanishing gradients or memory constraints. As a result, the loss of high-order information could degrade the learning performance significantly in some applications, as demonstrated in our experiments. Our main technical contributions over existing methods are summarized as follows:

- **Our work is the first one that investigates the key and potential causes about the negative impact of OODs on SSL performance. In particular, we found that 1) OODs lying close to class boundary have more influence on SSL performance than those far from the boundary in most cases; 2) OODs far from the decision boundary can degrade SSL performance substantially if the deep learning model includes a batch normalization (BN) layer.**

- **To address the above causes, we first proposed a simple modification to BN, called weighted batch normalization, to improve the robustness of BN against OODs, and then developed a unified robust SSL approach to improve the robustness of many existing SSL algorithms by learning to reweight the unlabeled samples based on meta optimization.**

- **We proposed two efficient hyperparameter optimization algorithms for our proposed robust SSL approach, including meta-approximation and implicit-differentiation based, that have different tradeoffs on computational efficiency and accuracy. The first algorithm was designed based on lower-order approximations of the objective in the inner loop of meta optimization. The second algorithm was designed based on higher-order approximations of the objective and is scalable to a large number of inner optimization steps for learning of massive weight parameters, but is less efficient than the first algorithm.**

![Fig 2](image_url) (a) Faraway OODs (b) Boundary OODs

Fig 2: (a) OODs far away from decision boundary and (b) OODs close to decision boundary.
3 Impact of OOD on SSL Performance

We have conducted an extensive empirical analysis on both synthetic and real-world datasets and have discovered several key and potential causes about the impact of OODs for many popular SSL algorithms, such as Pseudo-Label (PL) [Lee, 2013], Π-Model [Laine and Aila, 2016], Mean Teacher (MT) [Tarvainen and Valpola, 2017], Virtual Adversarial Training (VAT) [Miyato et al., 2018]. This section illustrates our discoveries using the following synthetic datasets for the example SSL algorithm VAT. We considered two moons datasets that have OODs (yellow triangle points) far away and close to the decision boundary, respectively, as shown in Fig 2. A multi-layer perceptron neural network (MLP) that has three layers was used as a backbone and the impact of OOD based on three following different model was analyzed.

- **SSL-NBN (MLP without Batch Normalization).** Fig 2(a) and (b) demonstrate a limited influence of OODs on the decision boundary when they far away from the true boundary, but a substantial influence of OODs on the decision boundary when they are close to the true boundary.

- **SSL-BN (MLP with Batch Normalization).** Fig 2(a) and (b) demonstrate a significant influence of OODs on the decision boundary for SSL-BN, for both OODs that are close or far away to the true boundary. To explain this pattern, OODs would influence the estimation of mean and variance on BN process, which result in (1) accumulated errors on \( \text{running\_mean} \) and \( \text{running\_variance} \) estimation; (2) bad representation of BN, i.e., can not learn a good BN parameters (\( \gamma \) and \( \beta \)). Besides, SSL-BN performs worse than SSL-NBN when OODs are close to the true decision boundary.

- **SSL-FBN (MLP with freezed Batch Normalization for unlabeled examples).** Freezed BN (FBN) is a common trick used on SSL implementation to be robust on conventional SSL problems [Oliver et al., 2018]. FBN means that we will not update \( \text{running\_mean} \) and \( \text{running\_variance} \) in the training phase. Although it can reduce some effect OODs for BN, we still can not learn good BN parameters (\( \gamma \) and \( \beta \)) such that the OOD would hurt the SSL performance as well: SSL-FBN worse than SSL-NBN in both scenarios.

Here, we summarize the impact of OOD on SSL in general,

1. OODs close to decision boundary (Boundary OODs) would hurt SSL performance in most cases.
2. OODs faraway from the decision boundary (Faraway OODs) would hurt SSL performance if the model involved BN. Freeze BN can reduce some impact of OOD, but OOD would still influence SSL performance.
3. OOD faraway from the decision boundary will not hurt SSL performance if there is no BN in the model.

To address OOD’s above issues, we proposed a novel robust SSL framework, the results are shown in the red curve in Fig 2, more synthetic experiment refer to Appendix.

4 The Proposed Robust SSL

4.1 Robust SSL Framework

**Robust Loss.** Consider the semi-supervised classification problem with training data (labeled \( D \) and unlabeled \( U \)) and classifier \( f(x; \theta) \). Generally, the optimal classifier parameter \( \theta \) can be extracted by minimizing the ssl loss (Eq. (1)) calculated on the training set. In the presence of unlabeled OOD data, sample re-weighting methods enhance the robustness of training by imposing weigh \( w_j \) on the \( j \)-th unlabeled sample loss,

\[
\sum_{(x_i, y_i) \in D} l(f(x_i; \theta), y_i) + \sum_{x_j \in U} w_j r(f(x_j; \theta)),
\]

where we denote \( \mathcal{L}_U \) is the robust unlabeled loss, and we treat weight \( w \) as hyperparameter. Our goal is to learn a perfect sample weight \( w \) (i.e., \( w = 0 \) for OODs, \( w = 1 \) for In-distribution (ID) sample).

**Weighted Batch Normalization.** In practice, most Deep SSL model would use deep CNN (e.g., ResNet, WideResNet), which usually contains BN to learn useful representations. At the same time, some faraway OODs would indeed affect the SSL performance. To address this issue, we proposed a weight Batch Normalization (W-BN) that estimate batch

\[^2\text{In test phrase, BN would use running\_mean and running\_variance instead the mean and variance of input batch.}\]
mean and batch variance with sample weight $w_i$,

$$
\mu_{WB} \leftarrow \frac{1}{\sum_{i=1}^{m}w_i} \sum_{i=1}^{m} w_i x_i \\
\sigma^2_{WB} \leftarrow \frac{1}{\sum_{i=1}^{m}w_i} \sum_{i=1}^{m} w_i (x_i - \mu_{WB})^2
$$

$$
\hat{x}_i \leftarrow \frac{x_i - \mu_{WB}}{\sqrt{\sigma^2_{WB}} + \epsilon} \\
y_i \leftarrow \gamma x_i + \beta \equiv \text{WBN}_{\gamma,\beta}(x_i)
$$

**Proposition 1.** Give ID samples $I = \{x_i\}_{i=1}^m$, OODs $O = \{x_i\}_{i=1}^m$, and the mixed data of ID samples and OOD samples $IO = I \cup O$. Under the faraway OOD condition: $|\mu_{IO} - \mu_I|_2 > L$, where $L$ is a large number ($L \gg 0$), we have:

1. $\|\mu_{B}(IO) - \mu_{B}(I)\|_2 > \frac{L}{2}$ and $BN_{I}\circ(x_i) \approx \gamma \frac{x_i - \mu_{IO}}{|\mu_{IO} - \mu_I|_2} + \beta$, which is totally different from $BN_{I}\circ(x_i)$;

2. Given perfect weight $w$, then $\mu_{B}(I) = \mu_{WB}(IO)$ and $BN_{I}(x_i) = WBN_{IO}(x_i)$

where $\mu_{B}(I)$ is the mean of data $I$ by BN, $\mu_{WB}(IO)$ is the mean of data $IO$ by W-BN; $BN_{I}(x_i)$ is the output by BN with data $I$ for sample $x_i$, $WBN_{IO}(x_i)$ is the output by W-BN with data $IO$ for sample $x_i$.

**Proof.** See Appendix.

The above proposition shows that when unlabeled set contains OODs, the original BN would not learn a good representation due to inaccurate mean and variance estimation, while our W-BN can learn a good representation respect to in distribution. Therefor, our robust SSL framework uses W-BN instead of original BN to optimize the net parameter $\theta$ by calculated by minimizing the following robust loss:

$$
\mathcal{L}_T(\theta, w) = \sum_{(x_i,y_i) \in D} l(f(x_i; \theta), y_i) + \sum_{x_j \in \mathcal{U}} w_j r(f_W(x_j; \theta))
$$

where $f_W(x_j; \theta)$ denote the forward operation with W-BN.

**Robust learning objective.** However, these weights (hyperparameters) introduce a new challenge: manually tuning or grid-search for each $w_i$ is intractable, mainly if the unlabeled dataset’s size is enormous. We develop an algorithm that learns the weights $w_i$ for each unlabeled data point to address this. Formally, we address the following hyperparameter optimization problem:

$$
\min_w \mathcal{L}_V(\theta^*(w), w), \\
\text{s.t.}\quad \theta^*(w) = \arg\min_{\theta} \mathcal{L}_T(\theta, w)
$$

Denote $\mathcal{L}_V = \mathcal{L}_V(\theta^*(w), w)$ is the supervised loss over a labeled dataset, e.g., $\mathcal{L}_V \triangleq \sum_{(x_i,y_i) \in V} l(f(x_i, \theta^*), y_i)$. Intuitively, the problem given in Eq. (3) aims to minimize the supervised loss evaluated on the validation set w.r.t. the weights of unlabeled samples $w$, while being given model parameters $\theta^*(w)$ which minimize the overall training loss $\mathcal{L}_T(\theta, w)$.
Adaptive approximation. However, Calculating the optimal \( \theta^* \) and \( w \) requires two nested loops of optimization, which is expensive and intractable to obtain the exact solution [Franceschi et al., 2018], especially when optimization involves deep learning models and large datasets, adaptive gradient-based methods like Stochastic Gradient Descent (SGD) have shown to be very effective [Bengio, 2000]. Here we adopt an online approximation strategy to adaptively learn the optimal \( \theta^* \) and \( w \). Specifically, we nest the Hyperparameter optimization problem (Eq. (3)) on each iteration, and first learn an approximation optimal \( \theta^*_t(w) \) based on current \( \theta_t \) and \( w_t \), then we update hyperparameter \( w_{t+1} \) on the basis of the net parameter \( \theta^*_t(w) \) and weight \( w_t \) obtained in the last iteration. After we get \( w_{t+1} \), we can update net parameter via gradient descent. The main steps of our robust SSL framework are shown in Fig [3].

Cluster Re-weight. Directly optimize multiple weight \( w \) is not efficiently on the large dataset. We proposed a Cluster Re-weight (CRW) method to learn weight \( w \) efficiently. Specifically, we use an unsupervised cluster algorithm (e.g., K-means algorithm) to embed unlabeled samples into \( K \) clusters, and assign weight to each cluster such that we can reduce weight dimension form \( |M| \) to \( |K| \), where \( |K| \ll |M| \). In practice for high dimensional data, we may use a pre-train model to do embedding first then apply cluster method.

4.2 Hyperparameter Optimization Approximation

In this section, We developed two efficient hyperparameter optimization algorithms that have different tradeoffs in computational efficiency and accuracy.

Implicit Differentiation. Directly calculate the weight gradient \( \frac{\partial L_v(\theta^*(w), w)}{\partial w} \) by chain rule:

\[
\frac{\partial L_v(\theta^*(w), w)}{\partial w} = \frac{\partial L_v}{\partial w} + \frac{\partial L_v}{\partial \theta^*(w)} \times \frac{\partial \theta^*(w)}{\partial w} \tag{4}
\]

where (a) is the weight direct gradient, (b) is the parameter direct gradient, which are easy to compute. The difficult part is the term (c) (best-response Jacobian). We approximate (c) by using the Implicit function theorem,

\[
\frac{\partial \theta^*}{w} = \left[ \frac{\partial L_T}{\partial \theta \partial \theta^T} \right]^{-1} \times \frac{\partial L_T}{\partial w \partial \theta^T} \tag{5}
\]

However, computing Eq. (5) is challenging when using deep nets because it requires to invert a high dimensional Hessian (term (d)), which often require \( \mathcal{O}(m^3) \) operations. Therefore, we give the Neumann series approximations [Lorraine et al., 2020] of term (d) which we empirically found to be effective for SSL,

\[
\left[ \frac{\partial L_T}{\partial w \partial \theta^T} \right]^{-1} \approx \lim_{p \to \infty} \sum_{p=0}^{p} \left[I - \frac{\partial L_T}{\partial \theta \partial \theta^T} \right]^p \tag{6}
\]

where \( I \) is identity matrix.

Meta approximation. Here we proposed the meta-approximation method to jointly update both network parameters \( \theta \) and hyperparameter \( w \) in an iterative manner. At iteration step \( t \), we approximate \( \theta^*_t \approx \theta^*_t \) on training set via low order approximation, where \( J \) is inner loop gradient steps, Eq. (7) shows each gradient step update,

\[
\theta^*_t(w_t) = \theta^*_t \times \alpha \nabla \theta L_T(\theta^*_t, w_t) \tag{7}
\]

then we update hyperparameter \( w_{t+1} \) on the basis of the net parameter \( \theta^*_t \) and weight \( w_t \) obtained in the last iteration. To guarantee efficiency and general feasibility, the outer loop optimization to update weight is employed by one gradient step on validation set \( V \).

\[
w_{t+1} = w_t - \beta \nabla_w L_V(\theta^*_t, w_t) \tag{8}
\]

Complexity. Compared with regular optimization on a single-level problem, our robust SSL requires \( J \) extra forward and backward passes of the classifier network. To compute weight gradient via bi-level optimization, Meta approximation requires an extra forward and backward passes. Therefore, compared with the regular training procedures of SSL, our robust SSL with Meta approximation needs approximately \((2 + J) \times \) training time. For Implicit Differentiation, the training time is complex to estimate, we show the running time in Fig [5](c) on experiment part. Our Robust SSL framework is detailed in Algorithm [1].

Connections between implicit-differentiation and meta-approximation. For Implicit Differentiation method, consider first order (i.e., \( P = 1 \)) approximate for inverse Hessian, we can formulate weight gradient as,

\[
\frac{\partial L_v(w)}{\partial w} \approx \frac{\partial L_v}{\partial w_t} - \frac{\partial L_v}{\partial w_t} \times \frac{\partial L_v^2}{\partial \theta^*_t \partial w_t} \times \frac{\partial L_v}{\partial \theta^*_t} \tag{9}
\]
And for Meta approximation method, consider one gradient step ($J = 1$) on inner loop to approximate $\theta^*_t(w)$, we have weight gradient,

$$\frac{\partial \mathcal{L}_V(w)}{\partial w} \approx \frac{\partial \mathcal{L}_V}{\partial \theta_t} - \frac{\partial \mathcal{L}_V}{\partial \theta_t \partial w_t} \times \frac{\partial \mathcal{L}_V}{\partial \theta_t^*}$$  \hspace{1cm} (10)

we found the similarity between weight gradient from Implicit Differentiation (Eq. (9)) and Meta approximation method (Eq. (10)), but Implicit Differentiation still needs more computation to estimate the implicit gradient. We designed these two efficient hyperparameter optimization algorithms have different tradeoffs on computational efficiency and accuracy. Meta approximation was designed based on lower-order approximations of the objective in the inner loop of meta optimization due to vanishing gradients or memory constraints. Implicit Differentiation was designed based on higher-order approximations of the objective and is scalable to a large number of inner optimization steps for learning of massive weight parameters, but is less efficient than Meta approximation.

**Algorithm 1: Robust SSL**

```
Input: $\mathcal{D}, \mathcal{U}$
Output: $\theta, w$
1 $t = 0$;
2 Set learning rate $\alpha$, $\beta$, and Hessian approximation $P$;
3 Initialize model parameters $\theta$ and weight $w$;
4 Apply K-means do K-clusters for $\mathcal{U}$;
5 if Model includes BN layer then
   Apply Weight Batch Normalization instead of BN;
7 repeat
   **** Inner loop optimization, initial $\theta^*_0 = \theta_t$ ****
   for $j = 1, \ldots, J$ do
   10 $\theta^*_j(w) = \theta_{t-1} - \alpha \nabla_w \mathcal{L}_T(\theta^*_{t-1}, w_t)$
   **** Outer loop optimization, set $\theta^*_0 = \theta^*_t$ ****
   if Meta Approximation then
   13 update weight via $w_{t+1} = w_t - \beta \nabla_w \mathcal{L}_V(\theta^*_t(w), w_t)$;
   else if Implicit Differentiation then
   15 Approximate inverse Hessian via Eq. (6);
   16 Calculate best-response Jacobian by Eq. (5);
   17 Calculate weight gradient $\nabla_w \mathcal{L}_V$ via Eq. (4);
   19 update weight via $w_{t+1} = w_t - \beta \cdot \nabla_w \mathcal{L}_V$;
   **** Update net parameters ****
20 $\theta_{t+1} = \theta_t - \alpha \nabla_\theta \mathcal{L}_T(\theta_t, w_{t+1})$
21 $t = t + 1$
until convergence
return $\theta_{t+1}, w_{t+1}$
```

5 Experiment

To test the effectiveness of our proposed robust SSL approach, we designed SSL settings with both OODs close to decision boundary and OODs far way from decision boundary based on MNIST, FashionMNIST, and CIFAR10 benchmarks for image classification using deep CNNs.

5.1 Experiment Details

**Datasets.** We used two image classification benchmark datasets. (1) **MNIST**: a handwritten digit classification dataset, with with 50,000/10,000 training/validation/test samples. We split 100 images (each class has 10 images) from training set as labeled set $\mathcal{D}$ and set the rest 49,900 training images as unlabeled set $\mathcal{U}$. (2) **CIFAR10**: A natural image dataset with 45,000/5000/10,000 training/validation/test samples from 10 object classes. We split 4000 images (each class has 400 images) from training set as labeled set $\mathcal{D}$, and set the rest 41,000 training images as unlabeled set $\mathcal{U}$.

**Competitive methods.** We implemented two versions of our proposed robust SSL approach based on our two proposed hyperparameter optimization algorithms, including meta-approximation and implicit-differentiation based. We name these two versions as R-SSL-Meta and R-SSL-IFT, respectively. We compared these two versions (R-SSL-Meta and R-SSL-IFT) with four state-of-the-art robust SSL approaches, including USAD [Chen et al., 2020], DS3L [Guo et al., 2020], L2RW [Ren et al., 2018], and MWN [Shu et al., 2019]. The last two approaches L2RW and MWN were originally designed for robust SL. We adapted these two approaches to robust SSL by replacing the SL loss function.
with a SSL loss function. We note that the adapted method MWN is exactly the same as the robust SSL method DS3L, except that it uses a validation set optimize the parameters of a weight function about the cost values of unlabeled examples, but DS3L uses the labeled training set for the same optimization procedure instead.

We compared these robust approaches based on their performance on four representative SSL methods, including Pseudo-Label (PL) [Lee, 2013], Π-Model [Laine and Aila, 2016] [Sajjadi et al., 2016], Mean Teacher (MT) [Tarvainen and Valpola, 2017], and Virtual Adversarial Training (VAT) [Miyato et al., 2018]. One additional competitive method is the supervised learning method, named as ‘Sup’, that ignored all the unlabeled examples, named. As USAD and DS3L have not released their implementations, we implemented DS3L by ourselves and directly used the results of USAD for the CIFAR10 dataset from its original paper [Chen et al., 2020], as we used the same experiment settings for this dataset.

Setup. We set $J = 1$ for all R-SSL-Meta experiments, and $J = 3$, $P = 10$ for all R-SSL-IFT experiments. We used the standard LeNet model as the backbone on MNIST experiment. For a comprehensive and fair comparison on CIFAR10 experiment, we followed the same experiment setting of [Oliver et al., 2018] and used WRN-28-2 [Zagoruyko and Komodakis, 2016] as the backbone. All the compared methods were built upon the open-source Pytorch implementation by [Oliver et al., 2018]. More implementation details can be found in Appendix.

5.2 Results and Discussion

In all experiments, we report the performance over five runs. Denote OOD ratio=$U_{ood}/(U_{ood} + U_{in})$ where $U_{in}$ is ID unlabeled set, $U_{ood}$ is OOD unlabeled set, and $U = U_{in} + U_{ood}$.

Impact of faraway OODs on SSL performance (with batch normalization). We used FashionMNIST [Xiao et al., 2017] dataset to construct a set of OODs $U_{ood}$ far way from the decision boundary of the MNIST dataset, as FashionMNIST and MNIST have been shown very different and considered as cross-domain benchmark datasets [Meinke and Hein, 2019]. As shown in Fig 4(a)-(b), with the OOD ratio increase, the performance of the existing SSL method decreases rapidly, whereas our approach can still maintain clear performance improvement, i.e., the outperformance of our methods are fairly impressive(e.g., 10% increase with R-IFT-PI over PI model when OOD ratio = 75%). Compare with other robust SSL methods, our methods surprisingly improves the accuracy and suffers much less degradation under high OOD ratio.

Impact of boundary OODs on SSL performance (without batch normalization). We generate boundary OOD by mix up (fusion) existing ID unlabeled samples, i.e., $\hat{x}_{ood} = 0.5(x_i + x_j)$, where $x_i$, $x_j$ is ID images from different class, and $\hat{x}_{ood}$ can be regarded as boundary OOD [Guo et al., 2019]. As show in Fig 4(c)-(d), we get the similar result pattern that the accuracy of existing SSL methods decrease when OOD ratio increasing. Across different OOD ratio, particularly our method significantly outperformed among all (e.g.,

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The source code will be released soon.

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5 The source code will be released soon.
10% increase with Meta-VAT over VAT when OOD ratio = 75%). We also conduct the experiments based on other SSL algorithms, results are shown in Appendix.

**Impact of mixed OODs on SSL performance (with batch normalization).** We followed [Oliver et al., 2018] to adapt CIFAR10 for a 6-class classification task, using 400 labels per class. The ID classes are: "bird", "cat", "deer", "dog", "frog", "horse", and OOD classes are: "airline", "automobile", "ship", "truck". As our implementation follows [Oliver et al., 2018] that freeze BN layers for the WRN model, we freeze BN layers for all the methods for CIFAR10 for fair comparisons. In this dataset, the examples of the OOD classes were considered as OODs. As these OODs are from the same dataset, it may have OODs close to or far away from the decision boundary of the ID classes. We hence called this OODs as mixed-type OODs. The averaged accuracy of all compared methods v.s. OOD ratio is plotted in Fig 5. Across different OOD ratio, particularly our method significantly outperformed among all, strikingly exceeding the performance when OOD ratio is large (i.e., 4.5% increase with Ours-Meta over L2RW when OOD ratio = 75%). Unlike most SSL methods that degrade drastically when increasing the OOD ratio, ours achieves the stable performance even in 75% OOD ratio.

**Analysis of weight variation.** Fig 6(a) shows the weight learning curve of our R-VAT-Meta method on faraway OODs, which demonstrate that our method is robust to learn a good weight for unlabeled sample, i.e., small weight for OOD sample and large weight for ID sample.

**Size of the clean validation set.** We make an attempt to explore the sensitive of clean validation set used in robust SSL approaches. Fig 6(b) plots the classification performance with varying the size of the clean validation set. Surprisingly, our methods are stable even when using 25 validation images, and the overall classification performance does not grow after having more than 1000 validation images.

**Comparison of our proposed hyperparameter optimization algorithms.** Note that meta-approximation (R-SSL-Meta) and implicit-differentiation (R-SSL-IFT) have different tradeoffs on computational efficiency and accuracy between. We find that implicit-differentiation is not always better than meta-approximation (e.g., Fig 4(a) (c) shows that R-VAT-Meta is better than R-VAT-IFT), and implicit-differentiation is more robust when reducing clean validation images (Fig 6(b)) or remove key technical components (Fig 6(d)-(e)). In addition, we design meta-approximation is a lower order approximation and implicit-differentiation is a higher order approximation such that implicit-differentiation method would has a large computation cost in practice, i.e., choose large $P$ and $J$ in practice. Fig 6(d) shows the the running time between meta-approximation and implicit-differentiation.

**Ablation Study.** We conducted additional experiments (see Fig 6(d)-(e)) in order to demonstrate the contributions of the key technical components, including Cluster Re-weight (CRW) and weight Batch Normalization (W-BN). The key findings obtained from this experiment are:

- W-BN plays an important role in our robust SSL framework to improve the robustness of BN against OODs.
- Remove CRW result in performance decrease, especially for VAT based approach, which demonstrate that CRW can further improve the accuracy and make the performance more robust.
- Implicit Differentiation method is more robust than Meta approximation when removing CRW or W-BN.

6 Conclusion

In this work, we proposed a novel unified robust SSL approach for many existing SSL algorithms in order to improve their robustness against OODs. In particular, we proposed weight batch normalization to improve the robustness of BN against OODs, and developed two efficient hyperparameter to learn to reweight the unlabeled samples in order to improve the robustness of SSL against OODs. The key findings from this study include:
• We investigate the key and potential causes about the negative impact of OODs on SSL performance: 1) boundary OODs have more influence on SSL performance than those faraway ODDs in most cases; 2) faraway ODDs can degrade SSL performance substantially if the deep learning model includes a BN layer.

• Our approach yielded the best performance on the extensive experiments among all other competitive counterparts. More impressively, R-SSL-Meta is more efficient and R-SSL-IFT performs more robust.

• Both W-BN and CRW can indeed help to improve the robustness of SSL against OOD.

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Appendix

Missing Proof

Proposition 1. Give ID samples \( \mathcal{I} = \{x_i\}_{i=1}^m \), OODs \( \mathcal{O} = \{\hat{x}_i\}_{i=1}^m \), and the mixed data of ID samples and OOD samples \( \mathcal{IO} = \mathcal{I} \cup \mathcal{O} \). Under the faraway OOD condition: \( \|\mu_\mathcal{O} - \mu_\mathcal{I}\|_2 > L \), where \( L \) is a large number \( (L \gg 0) \), we have:

1. \( \|\mu_\mathcal{IO} - \mu_\mathcal{I}\|_2 > \frac{L}{2} \) and BN\( \mathcal{IO}(x_i) \approx \gamma \frac{x_i - \mu_\mathcal{O}}{\|\mu_\mathcal{O} - \mu_\mathcal{I}\|_2} + \beta \), which is totally different from BN\( \mathcal{I}(x_i) \);

2. Given perfect weight \( w \), then \( \mu_\mathcal{B}(\mathcal{I}) = \mu_{WB}(\mathcal{IO}) \) and BN\( \mathcal{I}(x_i) = WBN_{\mathcal{IO}}(x_i) \)

where \( \mu_\mathcal{B}(\mathcal{I}) \) is the mean of data \( \mathcal{I} \) by BN, \( \mu_{WB}(\mathcal{IO}) \) is the mean of data \( \mathcal{IO} \) by W-BN; BN\( \mathcal{I}(x_i) \) is the output by BN with data \( \mathcal{I} \) for sample \( x_i \), WBN\( \mathcal{IO}(x_i) \) is the output by W-BN with data \( \mathcal{IO} \) for sample \( x_i \).

Proof. (1). The mean of \( \mathcal{I} \) by BN operation,

\[
\mu_\mathcal{B}(\mathcal{I}) = \frac{1}{m} \sum_{i=1}^{m} x_i = \mu_\mathcal{I}
\]

the mean of \( \mathcal{IO} \) by BN operation,

\[
\mu_\mathcal{B}(\mathcal{IO}) = \frac{1}{2m} \left( \sum_{i=1}^{m} x_i + \sum_{i=1}^{m} \hat{x}_i \right) \\
= \frac{1}{2} \mu_\mathcal{I} + \frac{1}{2} \mu_\mathcal{O}
\]

then we have,

\[
\|\mu_\mathcal{IO} - \mu_\mathcal{B}(\mathcal{I})\|_2 = \frac{1}{2} \mu_\mathcal{O} + \frac{1}{2} \mu_\mathcal{O} - \mu_\mathcal{I} \|_2 \\
= \frac{1}{2} \|\mu_\mathcal{O} - \mu_\mathcal{I}\|_2 > \frac{L}{2} \gg 0
\]

So we get \( \|\mu_\mathcal{IO} - \mu_\mathcal{I}\|_2 > \frac{L}{2} \).

To calculate the output of BN operation with batch \( \mathcal{I} \) for sample \( x_i \), we first calculate the variance

\[
\sigma^2_\mathcal{B}(\mathcal{I}) = \frac{1}{m} \sum_{i=1}^{m} (x_i - \mu_\mathcal{B}(\mathcal{I}))^2
\]

here we consider a common situation that \( \sigma^2_\mathcal{B}(\mathcal{I}), \sigma^2_\mathcal{B}(\mathcal{O}) \) have same magnitude level as \( \mu_\mathcal{I} \), i.e., \( \|\mu_\mathcal{O} - \sigma^2_\mathcal{B}(\mathcal{I})\|_2 > L \) and \( \|\mu_\mathcal{O} - \sigma^2_\mathcal{B}(\mathcal{O})\|_2 > L \). Then we have

\[
\sigma^2_\mathcal{B}(\mathcal{IO}) = \mathbb{E}[x^2] - (\mathbb{E}[x])^2 \\
= \frac{1}{2m} \left( \sum_{i=1}^{m} x_i^2 + \sum_{i=1}^{m} \hat{x}_i^2 \right) - \mu^2_\mathcal{B}(\mathcal{IO}) \\
= \frac{1}{2} \sigma^2_\mathcal{B}(\mathcal{I}) + \frac{1}{2} \sigma^2_\mathcal{B}(\mathcal{O}) + \frac{1}{4} (\mu_\mathcal{O} - \mu_\mathcal{I})^2 \\
\approx \frac{1}{4} (\mu_\mathcal{O} - \mu_\mathcal{I})^2
\]

and the BN output with ID samples

\[
BN_\mathcal{I}(x_i) = \gamma \frac{x_i - \mu_\mathcal{I}}{\sqrt{\sigma^2_\mathcal{B}(\mathcal{I})}} + \beta
\]

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the BN output when mix OODs and ID samples,

\[ \text{BN}_{\mathcal{IO}}(x_i) = \gamma \frac{x_i - \mu_{\mathcal{IO}}}{\sqrt{\sigma_{\mathcal{IO}}^2}} + \beta \]

\[ \approx \gamma \left( \frac{x_i - \mu_{\mathcal{IO}}}{\||\mu_{\mathcal{IO}} - \mu_I||_2} + \frac{x_i - \mu_I}{\||\mu_{\mathcal{IO}} - \mu_I||_2} \right) + \beta \]

(16)

\[ \approx \gamma \frac{x_i - \mu_{\mathcal{IO}}}{\||\mu_{\mathcal{IO}} - \mu_I||_2} + \beta \]  

(17)

Where the second term in Eq (16) is a small term when compare with the first term such that we can get the approximation in Eq. (17). And compare Eq. (15) and Eq. (17), we found that BN output would be significantly changed when OOD mix into the batch.

(2) Denote the perfect weight \( w = \{w_{\mathcal{I}}, w_{\mathcal{O}}\} \), where \( w_{\mathcal{I}} = 1, w_{\mathcal{O}} = 0 \), the mean of \( \mathcal{IO} \) by W-BN operation,

\[ \mu_{WB}(\mathcal{IO}) = \frac{\sum_{i=1}^{m} w_{\mathcal{I}} x_i + \sum_{i=1}^{m} w_{\mathcal{O}} \hat{x}_i}{\sum_{i=1}^{m} w_{\mathcal{I}} + \sum_{i=1}^{m} w_{\mathcal{O}}} \]

\[ = \frac{\sum_{i=1}^{m} 1 \cdot x_i + \sum_{i=1}^{m} 0 \cdot \hat{x}_i}{\sum_{i=1}^{m} 1 + \sum_{i=1}^{m} 0} \]

\[ = \mu_I \]

So we have \( \mu_{\mathcal{I}} = \mu_{WB}(\mathcal{IO}) \). The variance of \( \mathcal{IO} \) by W-BN operation,

\[ \sigma_{WB}^2(\mathcal{IO}) = \frac{\sum_{i=1}^{m} w_{\mathcal{I}} (x_i - \mu_{WB}(\mathcal{IO}))^2}{\sum_{i=1}^{m} w_{\mathcal{I}} + \sum_{i=1}^{m} w_{\mathcal{O}}} \]

\[ + \frac{\sum_{i=1}^{m} w_{\mathcal{O}} (x_i - \mu_{WB}(\mathcal{IO}))^2}{\sum_{i=1}^{m} w_{\mathcal{I}} + \sum_{i=1}^{m} w_{\mathcal{O}}} \]

\[ = \frac{\sum_{i=1}^{m} 1 \cdot (x_i - \mu_{WB}(\mathcal{I}))^2}{m} \]

\[ = \sigma_{\mathcal{I}}^2 \]

Consider the same parameters (\( \gamma \) and \( \beta \)) of BN and W-BN, and based on \( \mu_{\mathcal{I}} = \mu_{WB}(\mathcal{IO}) \) and \( \sigma_{\mathcal{I}}^2 = \sigma_{WB}^2(\mathcal{IO}) \), we have \( BN_{\mathcal{I}}(x_i) = WB_{\mathcal{I}}(\mathcal{IO}, x_i) \).

**Theorem 2.** (Cauchy, Implicit Function Theorem). If for some \( (w', \theta') \), \( \frac{\partial L_T}{\partial w'} |_{w', \theta'} = 0 \) and regularity conditions are satisfied, then surrounding \( (w', \theta') \) there is a function \( \theta^*(w) \) s.t. \( \frac{\partial L_T}{\partial \theta^*} |_{w, \theta^*(w)} = 0 \) and we have:

\[ \frac{\partial \theta^*(w)}{\partial w} = - \left[ \frac{\partial L_T}{\partial \theta \partial \theta^T} \right]^{-1} \times \frac{\partial L_T}{\partial w \partial \theta^T} \]

**Proof.** As \( \frac{\partial L_T}{\partial \theta^*} |_{w, \theta^*(w)} = 0 \), deriving the implicit equation with respect to \( w \) leads to the following equation,

\[ \frac{\partial^2 L_T}{\partial \theta \partial w} + \frac{\partial^2 L_T}{\partial \theta \partial \theta^T} \frac{\partial \theta^*}{\partial w} = 0 \]

where assuming \( \frac{\partial^2 L_T}{\partial \theta \partial \theta^T} \) invertible, characterizes the derivative of \( \theta \). Then we have,

\[ \frac{\partial \theta^*(w)}{\partial w} = - \left[ \frac{\partial L_T}{\partial \theta \partial \theta^T} \right]^{-1} \times \frac{\partial L_T}{\partial w \partial \theta^T} \]
Additional Experiment Details

In this section, we provide more experiment and implementation details.

Implementation Details. All the compared methods (except USAD [Chen et al., 2020]) were built upon the open-source Pytorch implementation by [Oliver et al., 2018]. As USAD and DS3L have not released their implementations, we implemented DS3L by ourselves and directly used the results of USAD for the CIFAR10 dataset from its original paper [Chen et al., 2020], as we used the same experiment settings for this dataset. For L2RW [Ren et al., 2018], we used the open-source Pytorch implementation and adapted it to the SSL settings. For MWN [Shu et al., 2019], we used the authors’ implementation and adapt to SSL.

Hyperparameter settings used in our experiments. For our approaches, we set $J = 1$ for all R-SSL-Meta, and $J = 3$; $P = 10$ for all R-SSL-IFT. For all robust SSL methods, we set weight learning rate $\beta = 0.1$, $K = 20$ for MNIST experiments, and set $\beta = 0.01$, $K = 10$ for CIFAR10 experiments. We trained all networks for 10,000 updates with a batch size of 100 for MNIST experiments, and 500,000 updates with a batch size of 100 for CIFAR10 experiments. We did not use any form of early stopping, but instead continuously monitored validation set performance and report test error at the point of lowest validation error. We show the specific hyperparameters used with four representative SSL methods on MNIST experiments in Table 1. For CIFAR10, we used the same hyperparameters as [Oliver et al., 2018].

Table 1: Hyperparameter settings used in MNIST experiments.

|                         | Shared                              | Supervised                      | Mean Teacher                  | VAT                               | Pseudo-Label                     |
|-------------------------|-------------------------------------|---------------------------------|--------------------------------|-----------------------------------|---------------------------------|
|                         | Learning decayed by a factor of      | Initial learning rate           | Initial learning rate          | Initial learning rate             | Initial learning rate           |
|                         | at training iteration 0.2            | 0.003                           | 0.003                          | 0.003                             | 0.003                           |
|                         | coefficient = 1 (Do not use rampup) | 1,000                           | Max consistency coefficient    | Max consistency coefficient        | Max consistency coefficient      |
|                         |                                     |                                 | 20                             | 8                                 | 0.3                             |
|                         |                                     |                                 | Exponential moving average     | VAT $\epsilon$                    | VAT $\xi$                       |
|                         |                                     |                                 | decay 0.95                      | 3.0                               | $10^{-6}$                       |
|                         |                                     |                                 |                                |                                    |                                 |
|                         |                                     |                                 |                                |                                    |                                 |
|                         |                                     |                                 |                                |                                    |                                 |

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4https://github.com/perrying/realistic-ssl-evaluation-pytorch
5https://github.com/danieltan07/learning-to-reweight-examples
6https://github.com/xjtushujun/meta-weight-net
Additional Experiments

Evaluation on Synthetic Dataset. We designed a synthetic experiment to illustrate that how OOD affects SSL performance. The experiment setting is same as the section of "Impact of OOD on SSL Performance" in main paper. We used Two Moons data with six labeled points and 2000 unlabeled (in-distribution) points, and considered two types of OOD: faraway OODs and boundary OODs. We conducted the experiment with OOD ratio = \{25\%, 50\%, 75\%\}, and reported the averaged accuracy rate with mean and standard deviation over ten runs. Table 2 shows our robust SSL (named R-SSL-IFT (Implicit Differentiation) and R-SSL-Meta (Meta approximation)) are more effective than the four baselines on test accuracy.

Comparisons on different orders of inverse Hessian approximation \(P\). We studied the performance for R-SSL-IFT with different \(P\) (inverse Hessian approximation order), shown in Table 3. The results demonstrate that a high order of inverse Hessian approximation (i.e., large \(P\)) is necessary to learn a good weighted gradient for R-SSL-IFT.

Our approaches based on Pseudo-Label. We conducted the experiments based on other representative SSL methods (Pseudo-Label and Mean Teacher) and the result are shown in Fig 7. We observed the same pattern as discussed in the main paper that our proposed methods outperformed the baselines significantly and the margin of improvements is the largest when the OOD ratio is high (e.g., 75\%). Note that as our proposed method R-SSL-IFT is not computationally efficient in the CIFAR10 experiments, we only show the result of our proposed method R-SSL-Meta, which is more efficient than R-SSL-IFT.

Number of clusters \((K)\). We analyzed the sensitivity of the number of clusters of used in our proposed robust SSL methods. Table 4 demonstrates that the test accuracies our our two proposed methods with varying number of clusters \(K\). The results indicate a low sensitivity of our proposed methods on the number of clusters. In the experiments, we chose \(K = 20\) for MNIST experiments and \(K = 10\) for CIFAR10 experiments.

Table 2: Test accuracies for two moons dataset, set \(P = 10\), \(J = 3\) for R-SSL-IFT and \(J = 1\) for R-SSL-Meta.

| Model       | Faraway OODs   | Boundary OODs |
|-------------|---------------|---------------|
|             | 25\% | 50\% | 75\% | 25\% | 50\% | 75\% |
| Supervised  | 84.4 ± 0.3  | 84.4 ± 0.3 | 84.4 ± 0.3 |
| SSL-NBN     | 100.0 ± 0.0 | 100.0 ± 0.0 | 100.0 ± 0.0 |
| SSL-BN      | 50.7 ± 1.5  | 50.7 ± 1.5  | 50.7 ± 1.5  |
| SSL-FBN     | 89.7 ± 0.7  | 89.7 ± 0.7  | 89.7 ± 0.7  |
| R-SSL-IFT   | 100.0 ± 0.0 | 100.0 ± 0.0 | 100.0 ± 0.0 |
| R-SSL-Meta  | 100.0 ± 0.0 | 100.0 ± 0.0 | 100.0 ± 0.0 |

Table 3: Test accuracies for different \(P\) at OOD ratio = 50\% on the synthetic dataset.

| Model       | Faraway OODs | Boundary OODs |
|-------------|--------------|---------------|
| R-SSL-IFT P=1 | 55.0 ± 2.1 | 83.9 ± 0.7 |
| R-SSL-IFT P=5 | 91.0 ± 3.1 | 93.9 ± 0.9 |
| R-SSL-IFT P=10 | 100.0 ± 0.0 | 100.0 ± 0.0 |

Table 4: Test accuracies for different numbers of clusters \(K\) on MNIST dataset with 50\% Boundary OODs.

| Model | R-VAT-Meta | R-VAT-IFT |
|-------|------------|-----------|
| \(K = 2\) | 93.7 ± 1.9 | 92.3 ± 0.6 |
| \(K = 5\) | 94.7 ± 0.7 | 93.2 ± 0.5 |
| \(K = 10\) | 95.3 ± 0.4 | 94.4 ± 0.7 |
| \(K = 20\) | 96.3 ± 0.5 | 95.3 ± 0.6 |