PabLO: Improving Semi-Supervised Learning with Pseudolabeling Optimization

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ABSTRACT

Modern semi-supervised learning (SSL) methods frequently rely on pseudolabeling and consistency regularization. The main technical challenge in pseudolabeling is identifying the points that can reliably be labeled. Existing methods use ad-hoc or hand-crafted notions of confidence and threshold selection functions to choose points. Though such hand-designed strategies shine on benchmark datasets, they may not fare well in specialized settings. To address this challenge we propose a framework to learn confidence functions and thresholds explicitly aligned with the SSL task, obviating the need for manual designs. Our approach formulates an optimization problem over a flexible space of confidence functions and thresholds, allowing us to obtain optimal scoring functions—while remaining compatible with the most popular and performant SSL techniques today. Extensive empirical evaluation of our method shows up to 11% improvement in test accuracy over the standard baselines while requiring substantially fewer training iterations.

1 Introduction

Obtaining high-quality labeled data is a major bottleneck in machine learning. The semi-supervised learning (SSL) paradigm tackles this problem by training models on a small amount of labeled data and a large quantity of unlabeled data (Chapelle et al., 2006; Zhu, 2005; van Engelen and Hoos, 2019). While SSL as a field dates back decades and includes a wide variety of approaches, modern SSL methods frequently rely on a pair of ideas: pseudolabeling (McLachlan, 1975; Amini et al., 2023; Rosenberg et al., 2005; Lee, 2013; Rizve et al., 2021) and consistency regularization (Laine and Aila, 2017; Bachman et al., 2014; Sajjadi et al., 2016; Fan et al., 2021; Kukačka et al., 2017). SSL techniques marrying these ideas have delivered strong performance on a number of benchmark datasets.

The major challenge when using approaches that rely on pseudolabeling is determining which points should be labeled. Such methods use various notions of confidence and corresponding thresholds to select points. The goal is to avoid inducing errors (which can cascade and dramatically hurt the model being trained) while not being so conservative as to produce extremely slow convergence. A wide variety of ad-hoc strategies have been proposed for both the confidence function and the method used to set the thresholds. These include maximum softmax probability (MSP) scores for confidence as well as using fixed thresholds (Sohn et al., 2020), class-wise and adaptive thresholds (Zhang et al., 2021; Wang et al., 2023; Xu et al., 2021; Chen et al., 2023), and instance-dependent thresholds (Li et al., 2023) for thresholding. While such hand-designed strategies have been tuned to produce good performance on popular benchmarks, ***practitioners may struggle using them for SSL in specialized settings.***

A prospective solution addressing this challenge is a framework that can produce suitable confidence functions and thresholds that are *explicitly aligned* with the SSL task. This obviates the need for experimenting with manually-designed notions of confidence and threshold schemes. To develop such a framework, we are inspired by a strategy for learning confidence functions in a different context, threshold-based auto-labeling (TBAL) (Vishwakarma et al., 2024). TBAL is a fundamentally different problem, whose goal is data development rather than building a high-quality model, as in SSL. Nevertheless, building on principles used for TBAL (Vishwakarma et al., 2024), we introduce a framework that *learns confidence functions and thresholds* that can be coupled with pseudolabeling-based SSL techniques.

Our approach involves two aspects. First, we formulate an optimization problem over a flexible space of confidence functions and thresholds to optimize the quantity/quality tradeoff in pseudolabeling. The space we optimize over is

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broad enough to subsume many existing manually-designed approaches. That is, we *learn confidence functions and thresholds*. Second, we develop strategies to make the framework compatible with SSL approaches. For example, we address an important question: what is the role of *pseudolabel accumulation* in SSL performance?

Experimentally, we couple our framework to some of the most prominent SSL techniques in use today, including Fixmatch (Sohn et al., 2020) and Freematch (Wang et al., 2023). We observed accuracy lifts of up to 11%, 6%, and 3% on popular benchmarks like SVHN, CIFAR-10, and CIFAR-100 respectively, along with substantial improvements in convergence speed. Our main contributions are,

1. We formulate the goal of maximizing pseudolabel quality and quantity as an optimization problem over a flexible space of scoring functions and thresholds, allowing us to characterize the optimal scoring functions.
2. From this framework we derive a practical method to learn scoring functions and thresholds, optimizing for the quality and quantity of pseudolabels. This method can be flexibly integrated with existing SSL methods that rely on pseudolabeling.
3. We provide extensive empirical evaluation and obtain strong results: the combination of our method with baseline SSL approaches outperforms the baselines, achieving **substantial improvements in test accuracy, by up to 11%, and requires substantially fewer iterations**.

2 Background and Problem Setup

We begin with notation, then provide useful background and a statement of our goal.

Notation. Consider a feature space $\mathcal{X}$ and label space $\mathcal{Y} = \{1, \ldots, k\}$ in a k-class classification task. As usual in semi-supervised learning, we have access to a set $X_u = \{\mathbf{x}_u\}_{u=1}^{n_u}$ of unlabeled data drawn from the distribution P_x over $\mathcal{X}$. We also have access to $D_l = \{(\mathbf{x}_l, y_l)\}_{l=1}^{N_l}$, a set of labeled data points drawn from the joint distribution P_{xy}, with $n_l \ll N_u$. Let $h : \mathcal{X} \to \mathcal{Y}$ denote a model and $g : \mathcal{X} \to T^k \subseteq \mathbb{R}^k$ be an associated confidence function giving a score $g(\mathbf{x})$ indicating the confidence of h on its prediction for any data point $\mathbf{x}$. For any $\mathbf{x}$ the hard label prediction is $\hat{y} := h(\mathbf{x})$. When the prediction $\hat{y}$ is used as a pseudolabel we denote it as $\tilde{y}$. In general, for a vector $\mathbf{v} \in \mathbb{R}^d$, $\mathbf{v}[i]$ denotes its $i-$th component. The vector $\mathbf{t}$ denotes thresholds over the scores k-classes, and $\mathbf{t}[y]$ is its $y-$th entry, i.e., the score for class y.

2.1 Pseudolabeling-based Semi-Supervised Learning

Given, as above, a large collection of unlabeled data X_u and a small set of labeled points D_l, inductive semi-supervised learning (SSL) seeks to learn a classifier $\hat{h}_{\text{ssl}}$ from the model class $\mathcal{H}$. The promise of SSL is that by effectively using X_u in the learning process it can learn a better classifier than its supervised counterpart, which learns only from D_l.

In many recent pseudolabeling-based SSL techniques, in each iteration of training, a batch of labeled and unlabeled data is obtained, then the sum of the losses $\widehat{\mathcal{L}} = \widehat{\mathcal{L}}_s + \lambda_u \widehat{\mathcal{L}}_u + \lambda_r \widehat{\mathcal{L}}_r$ is minimized w.r.t to the model h. Here $\widehat{\mathcal{L}}_s$ is the supervised loss, $\widehat{\mathcal{L}}_u$ unsupervised loss, and $\widehat{\mathcal{L}}_r$ is (the sum of) regularization term(s). The constants λ_u, λ_r are hyperparameters controlling the relative importance of the corresponding terms.

Supervised loss. Given a batch of labeled data D_l^b the supervised loss is computed as follows, $\widehat{\mathcal{L}}_s(h|D_l^b) = \frac{1}{|D_l^b|} \sum_{(x,y) \in D_l^b} H(y, h, \mathbf{x})$. Here $H(y, h, \mathbf{x})$ is the standard cross-entropy loss between the 1-hot representation of y and the softmax output of h on input $\mathbf{x}$.

Unsupervised loss and consistency regularization. For the unlabeled batch X_u^b, pseudolabels $\tilde{y} = h(\mathbf{x})$ are computed for each $\mathbf{x} \in X_u^b$. Then, a pseudlabeling mask $S(\mathbf{x}, g, \mathbf{t} \mid h) = \mathbb{1}(g(\mathbf{x})[\tilde{y}] \geq \mathbf{t}[\tilde{y}])$, is 1 for points having confidence score bigger than predetermined threshold corresponding to the predicted class. Recent methods, couple this loss and consistency regularization together by doing pseudolabeling on weakly augmented data using weak transform ω and then defining the cross-entropy loss on the strongly augmented data using strong transformation Ω. The loss is

$$\widehat{\mathcal{L}}_u(h \mid g, \mathbf{t}, \widetilde{D}_u^b) = \frac{1}{|\widetilde{D}_u^b|} \sum_{(x,\tilde{y}) \in \tilde{D}_u^b} S(\omega(\mathbf{x}), g, \mathbf{t}|h) \cdot H(\tilde{y}, h, \Omega(\mathbf{x})).$$

Regularization. A regularization term (or a sum of multiple regularizers) is often included along with the above two losses to encourage desired behavior. For instance, Freematch (Wang et al., 2023) adds a self-adaptive class fairness regularizer to encourage diverse predictions during the initial training phase. Similarly, a regularizer is introduced in (Mishra et al., 2024) to encourage calibration in model's confidence scores. Including such regularizers has been fruitful in pseudolabeling-based SSL.

2.2 Problem Statement

The success of pseudolabeling-based SSL hinges heavily on maximizing the quality and quantity of the pseudolabels. These are defined as follows:

Pseudolabeling coverage (quantity). Given a set of points X, the pseudolabeling coverage is the fraction of points that were pseudolabeled using h, g and $\mathbf{t}$. This measurement captures the quantity of pseudolabels and is defined as

$$\widehat{\mathcal{P}}(g, \mathbf{t} \mid h, X) := \frac{1}{|X|} \sum_{(\mathbf{x}) \in X} S(\mathbf{x}, g, \mathbf{t} \mid h)\,, \quad \mathcal{P}(g, \mathbf{t}|h) := \mathbb{E}_{\mathbf{x}}[S(\mathbf{x}, g, \mathbf{t} \mid h)]. \tag{1}$$

Pseudolabeling error (quality). This is the fraction of pseudolabeled points that received wrong labels. This metric captures the quality of pseudolabels:

$$\widehat{\mathcal{E}}(g, \mathbf{t} \mid h, D) := \frac{\sum_{(\mathbf{x}, y, \tilde{y}) \in D} S(\mathbf{x}, g, \mathbf{t} \mid h) \cdot \mathbb{1}(h(\mathbf{x}) \neq y)}{\sum_{(\mathbf{x}, y, \tilde{y}) \in D} S(\mathbf{x}, g, \mathbf{t} \mid h)}, \tag{2}$$

$$\mathcal{E}(g, \mathbf{t} \mid h) = \frac{\mathbb{E}_{\mathbf{x}}[S(\mathbf{x}, g, \mathbf{t} \mid h) \cdot \mathbb{1}(h(\mathbf{x}) \neq y)]}{\mathcal{P}(g, \mathbf{t}|h)}. \tag{3}$$

Goal. In pseudolabeling-based SSL aim is to learn a classifier $\hat{h}_{\text{ssl}}$ that generalizes well on the unseen data i.e. has high test accuracy. It is common wisdom in the literature that maximizing the quality and quantity of the pseudolabeled points during the training procedure will lead to a better model. Departing from the hand-crafting strategies to achieve this objective, we seek learnable solutions to confidence scores and thresholding to achieve high coverage at low error, that will eventually lead to a classification model $\hat{h}_{\text{ssl}}$ with much higher test accuracy.

3 Methodology

Our approach is to integrate learnable confidence functions and thresholds into existing pseudolabeling-based SSL pipelines. To do so, we build on a recently-developed technique (Vishwakarma et al., 2024) to improve the performance of threshold-based auto-labeling (TBAL) (SGT, 2022; Vishwakarma et al., 2023; Qiu et al., 2023) systems. In order to make such an approach compatible with SSL, we apply a simple notion—*accumulating pseudolabels*—that may also be useful for other methods.

3.1 Pseudolabeling Optimization Framework

The fundamental problem in pseudolabeling is, given a classifier $\hat{h}_i$, to correctly identify the points in the pool of unlabeled data X_u where the predictions of $\hat{h}_i$ are correct. Since the classifier is frequently undertrained during the SSL process, it may not have high accuracy. That is, it might only be accurate in some small part of the feature space, which we hope to identify via the confidence scores and appropriate thresholds. As discussed earlier, existing solutions (Lee, 2013; Sohn et al., 2020; Wang et al., 2023) use maximum softmax probability (MSP) from the model $\hat{h}_i$ in concert with heuristics for thresholds that are either fixed or vary dynamically based on the learning status of the model. Some recent works have observed that MSP scores tend to be miscalibrated and proposed solutions to obtain more calibrated scores (Mishra et al., 2024; Loh et al., 2023), which also led to performance gains.

Theoretical Framework. Instead of trying to improve calibration or heuristics for thresholding, we propose to express the objective of pseudolabeling as an optimization problem over the space of confidence functions and thresholds. The objective is to maximize the quantity i.e. the pseudolabeling coverage (eq. (1)) while keeping the pseudolabeling error low (eq. (3)) i.e. have high quality.

More specifically, one approach to formalizing this optimization problem is to seek to maximize the pseudolabeling coverage while ensuring pseudolabeling error is at most $\epsilon \in (0, 1)$, for some hyperparameter ϵ. In other words, given the classifier $\hat{h}_i$ in any iteration i of SSL, then,

$$g_i^\star, \mathbf{t}_i^* \in \underset{g \in \mathcal{G}, \mathbf{t} \in T^k}{\arg\max}\, \mathcal{P}(g, \mathbf{t}|\hat{h}_i) \quad \text{s.t. } \mathcal{E}(g, \mathbf{t}|\hat{h}_i) \leq \epsilon,$$

are the optimal confidence functions and thresholds for pseudolabeling using $\hat{h}_i$'s predictions. The *quality* of the pseudolabels can be controlled using ϵ. This follows the recipe for TBAL (Vishwakarma et al., 2024), with one additional complication: for SSL, it is not clear what value of ϵ is suitable, while in TBAL ϵ is a system-level constant provided as input.

The most attractive property of this framework is that, irrespective of the choice of ϵ, it will provide the scores and threshold that yield maximum pseudolabeling coverage at that error level. This frees us from making arbitrary choices of confidence scores, calibration techniques, and thresholding heuristics. Instead, solving the optimization problem over a flexible enough space will subsume specific strategies. Next, we discuss how to make the framework tractable.

Practical Version. The optimization problem discussed earlier involves population-level quantities which are usually not accessible in practice. Thus we have to fall back to using their finite sample estimates and smooth variations to make the optimization problem tractable. We adapt the steps from (Vishwakarma et al., 2024) to obtain such a practical version of the optimization problem. There, the authors first estimate the coverage and error using a small amount held-out labeled data (called calibration data D_{cal}) curated from the validation data. They then introduce differentiable surrogates for the 0-1 variables. Let $\sigma(\alpha, z) := 1/(1+\exp(-\alpha z))$ denote the sigmoid function on $\mathbb{R}$ with scale parameter $\alpha \in \mathbb{R}$. The surrogates are as follows,

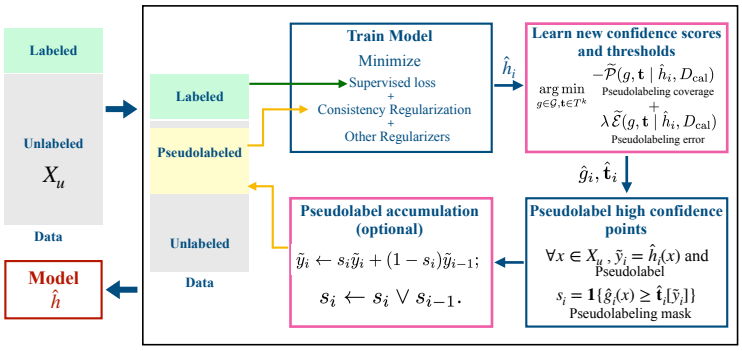

Figure 1: Updated workflow of pseudolabeling-based SSL with confidence function learning and pseudolabel accumulation.

$$\widetilde{\mathcal{P}}(g,\mathbf{t}|h,D_{\text{cal}}) := \frac{1}{|D_{\text{cal}}|}\sum_{(\mathbf{x},y,\tilde{y})\in D_{\text{cal}}} \sigma\big(\alpha, g(\mathbf{x})[\tilde{y}]-\mathbf{t}[\tilde{y}]\big), \tag{4}$$

$$\widetilde{\mathcal{E}}(g,\mathbf{t}\mid h,D_{\text{cal}}) := \frac{\sum_{(\mathbf{x},y,\tilde{y})\in D_{\text{cal}}} \mathbb{1}\big(y\neq\tilde{y}\big)\,\sigma\big(\alpha, g(\mathbf{x})[\tilde{y}]-\mathbf{t}[\tilde{y}]\big)}{\sum_{(\mathbf{x},y,\tilde{y})\in D_{\text{cal}}} \sigma\big(\alpha, g(\mathbf{x})[\tilde{y}]-\mathbf{t}[\tilde{y}]\big)}. \tag{5}$$

Using these surrogates the following practical optimization problem is obtained. It is also converted into unconstrained formulation by introducing the penalty term $\lambda\in\mathbb{R}^+$ controlling the relative importance of the pseudolabeling error and coverage.

$$\hat{g}_i,\hat{\mathbf{t}}_i \in \underset{g\in\mathcal{G},\mathbf{t}\in T^k}{\arg\min} \quad -\widetilde{\mathcal{P}}(g,\mathbf{t}\mid\hat{h}_i,D_{\text{cal}}) + \lambda\,\widetilde{\mathcal{E}}(g,\mathbf{t}\mid\hat{h}_i,D_{\text{cal}}) \tag{P1}$$

We use 2-layer neural nets as a choice of $\mathcal{G}$. The optimization problem (P1) is nonconvex, but differentiable and we solve it using Stochastic Gradient Descent (SGD). See Appendix B for more details on our choice of $\mathcal{G}$ and training details and hyperparameters.

3.2 Threshold Estimation

While we can obtain both the confidence scores and thresholds by solving (P1), we propose to adapt the threshold estimation procedure from (Vishwakarma et al., 2024) as it avoids potential generalization issues due to learning them simultaneously from the same data D_{cal} and ensures stricter control over the pseudolabeling errors. It is also decoupled from any particular choice of scoring function, hence it can replace the thresholding procedure in the existing SSL pipelines as well.

Our procedure is simple. It takes in a confidence function $\tilde{g}_i$ and another part of the held-out validation data referred to as D_{th}. It estimates thresholds for each class separately and estimates the pseudolabeling errors $\widehat{\mathcal{E}}(\tilde{g}_i,t\mid h,D_{\text{th}},\tilde{y})$ on the super level sets of $\tilde{g}_i$. Here we slightly abuse notation: instead of $\mathbf{t}\in T^k$, we use $t\in T$, to indicate the estimate of pseudolabeling error at threshold t for class y. To obtain a threshold $\tilde{\mathbf{t}}[y]$ for class y, the procedure finds the smallest $t\in T$ such that $\widehat{\mathcal{E}}(\tilde{g}_i,t\mid h,D_{\text{th}},\tilde{y}) + C_1\hat{\sigma}(\widehat{\mathcal{E}}) \leq \epsilon$. Here C_1 is a constant and $\hat{\sigma}(z)=\sqrt{z\cdot(1-z)}$ and $\widehat{\mathcal{E}}$ is used for brevity in place of $\widehat{\mathcal{E}}(\tilde{g}_i,t\mid h,D_{\text{th}},\tilde{y})$. Using the thresholds found using this procedure ensures pseudolabeling error remains below (or close to) the a tolerance level ϵ.

Remarks. Departing from fixed thresholds as in (Sohn et al., 2020), prior works have proposed adaptive and class-wise heuristic thresholding schemes based on the model's learning status, such as in (Djurisic et al., 2023; Zhang et al., 2021; Wang et al., 2023) and others. In contrast, our approach is a principled way to estimate adaptive and class-wise pseudolabeling thresholds while providing strict control over the quality of pseudolabels. This has been used in prior works in TBAL for the problem of creating reliable datasets and is backed by theoretical guarantees for the quality of pseudolabels produced (Vishwakarma et al., 2023, 2024).

Table 1: Details of the dataset we use in our experiments. k is the number of classes. N_l is the number of labeled data points used for training the backbone model h. N_u is the number of unlabelled data points used for consistency regularization and pseudolabeling for all the methods. N_{val} is the number of points used for model selection in all methods. N_{test} is the number of test data points. N_{cal} is the number of points used for learning the g function. N_{th} is the number of data points used for threshold estimation.

Dataset	**Backbone Model** h	k	N_u	N_{val}	N_{test}	N_l	N_{cal}	N_{th}	**Augmentation**
CIFAR-10	WRN-28-2	10	50K	6K	4K	250	1K	1K	Weak, Strong
CIFAR-100	WRN-28-2	100	50K	6K	4K	2500	3K	3K	Weak, Strong
SVHN	WRN-28-2	10	604,388	15,620	10,412	250	3K	3K	Weak, Strong

3.3 Pseudolabeling and Accumulation

In the usual pseudolabeling-based SSL setups, the pseudolabels inferred by the model for a mini-batch will be discarded after each iteration. Moreover, it is not guaranteed that a previously pseudolabeled point will get pseudolabled in the current iteration as well. Given the quality of pseudolabels is high, it is appealing to reuse the past pseudolabel for a point that did not get pseudolabeled in the current iteration. We propose to do so for techniques where the quality of pseudolabels is assured. We refer to this trick as "pseudolabel accumulation".

Mathematically, if $s_{i-1}, \tilde{y}_{i-1}$ are the previous mask and psuedolabels and $s_i, \tilde{y}_{i-1}$ are the current mask and pseudolabels for the same point, then with accumulation,

$$\tilde{y}_i \leftarrow s_i \tilde{y}_i + (1 - s_i)\tilde{y}_{i-1}; \quad \text{and} \quad s_i \leftarrow s_i \vee s_{i-1}.$$

Here $\vee$ is the boolean `or` operation and the steps are executed in the order. In words, if the point is pseudolabeled in current iteration, then it will use the current pseudolabel o.w. if the point was pseudolabeled in earlier iteration(s) it will use the pseudolabel from that iteration and mark the point as pseudolabeld. In case the point is not pseudolabeled in this iteration or any other iteration in the past it will remain unlabeled. While it is appealing to use this trick, its use is only warranted in settings ensuring high-quality pseudolabels. We try to understand the consequences of inclusion and exclusion of this trick in pseudolabeling-based SSL via experiments in discussed in the next section.

We refer to our method as `PabLO` . A more formal listing of the steps is detailed in Algorithm 1, deferred to Appendix A due to space constraints.

4 Experiments

We evaluate our method empirically to verify the following claims:

C1. Our method `PabLO` produces models with improved test accuracy while taking fewer iterations.

C2. In certain cases, we may wish to produce a high-quality dataset using pseudolabeling (rather than a single high-quality model). For such scenarios, `PabLO` achieves much higher dataset coverage and accuracy.

Additionally, we study the following ablations:

A1. We seek to understand the role of pseudolabel accumulation in our method and in baselines.

A2. We study the effect of varying ϵ for our method.

A3. We study our technique's dependence on the amount of data used in learning g and thresholds.

4.1 Experimental Setup

First, we provide a brief description of the experimental setup, with details deferred to Appendix B.

Methods. We use two simple base methods capturing the core ideas of pseudolabeling (PL) and consistency regularization (CR). The first is *Fixmatch* (Sohn et al., 2020) which uses fixed thresholds on MSP scores for PL along with CR. *Freematch* (Wang et al., 2023) improves upon it by using adaptive, class-wise thresholds and class fairness regularization (CFR) along with CR, and is a promising method among others using dynamic thresholds for PL. We include their combinations with recently proposed *Bayesian Model Averaging (BAM)* (Loh et al., 2023) and *Margin Regularization (MR)*[2] (Mishra et al., 2024) to improve calibration in SSL. We replace the pseudolabeling component by our method `PabLO` to obtain *Fixmatch + Ours* (a combination of `PabLO` and CR) and *Freematch + Ours* (a combination of `PabLO` , CR, and CFR). We provide implementations of these in the code submitted along with the paper.

Datasets. We experiment with 3 datasets: *CIFAR-10* (Krizhevsky et al., 2009) is an image dataset with 10 classes. *CIFAR-100* (Krizhevsky et al., 2009) is an extended version of CIFAR-10 with 100 classes. *SVHN* (Netzer et al., 2011)

[2]We assign this name for convenience.

Table 2: Top-1 Accuracy for CIFAR-10, CIFAR-100 and SVHN averaged across 3 random seeds. The best accuracy is **bolded**

Dataset	CIFAR-10	CIFAR-100	SVHN
# Labels	250	2500	250
Fixmatch	88.15 ± 1.27	50.07 ± 1.12	96.54 ± 0.05
Fixmatch + MR	87.85 ± 1.10	44.75 ± 1.36	96.58 ± 0.04
Fixmatch + BaM	86.44 ± 1.47	44.58 ± 0.41	95.99 ± 0.06
Fixmatch + Ours	$\mathbf{93.03 \pm 0.44}$	$\mathbf{53.17 \pm 1.27}$	$\mathbf{96.61 \pm 0.16}$
Freematch	90.17 ± 0.13	57.21 ± 0.78	85.25 ± 1.70
Freematch + MR	90.17 ± 0.45	57.23 ± 1.18	84.65 ± 1.03
Freematch + BaM	88.34 ± 0.99	51.98 ± 1.74	86.28 ± 1.75
Freematch + Ours	$\mathbf{93.08 \pm 0.05}$	$\mathbf{60.96 \pm 0.53}$	$\mathbf{96.48 \pm 0.33}$

is a 10-class image dataset of digits from Google street view. More details are summarized in Table 1. We use a portion of the validation data (N_{val}) for our method, split into N_{cal}, used to calibrate the function g, and N_{th}, used to estimate the threshold.

Models and Training. The backbone encoder is a Wide ResNet-28-2 for all the datasets. We use the default hyperparameters and dataset-specific settings (learning rates, batch size, optimizers and schedulers) following previous baseline recommendations (Wang et al., 2022). We run till 25K iterations—in contrast to the extremely large number of iterations (2^{20}) in prior works—which may be unrealistic in practice due to resource constraints. For confidence functions class $\mathcal{G}$ we use a class of 2-layer neural nets and provide it last two layers representations from h as input, as in (Vishwakarma et al., 2023). We train it using SGD, the hyperparameters are deferred to Appendix B. For our method we use pseudolabeling error tolerance $\epsilon = 5\%$ across all settings.

4.2 Results and Discussion

To verify our main claims, we compare the baselines, their combinations with our method, and methods that induce calibrated scores in SSL. We run all methods with three random seeds and report the mean and std. deviation of accuracy across three runs. The results are reported in Table 2.

C1. Test accuracy improvements. Since our method maximizes the pseudolabeling coverage and accuracy, it will provide a larger quantity of accurate pseudolabels for model training. Therefore, we expect it to yield a model with better test accuracy than the baselines while taking fewer training iterations. We report the test accuracies at the end of 25K iterations in Table 2. First, as expected, we see that integrating our method into the base methods improves test accuracy across all settings. For CIFAR-10, using it with Fixmatch provides 6% improvement over Fixmatch alone, and using it with Freematch yields 3% improvement over Freematch alone. Similar improvements are observed in the much harder setting of CIFAR-100, while a numerically similar 3% improvement in top-1 accuracy on a 100-class problem is more significant. SVHN is an easier setting and here the improvements are marginal with Fixmatch but using it with Freematch improves the performance by 11%.

C2. Improved pseudolabeling coverage and accuracy. Since our method is designed to explicitly maximize coverage and accuracy of pseudolabels, we expect it to maintain high pseudolabeling accuracy from the beginning and pseudolabel as many points as possible with the current classification model. To test this, we log the pseudolabeling coverage and accuracy in each iteration on the batch of unlabeled data used in that iteration. We refer to these as batch pseudolabeling coverage (batch-pl-cov) and batch pseudolabeling accuracy(batch-pl-acc). We show these for CIFAR-10 and CIFAR-100 data settings in Figure 2 and 3. These results are aligned with our expectations i.e. the batch-pl-acc is high right from the beginning and is maintained close to the desired level of 95% (with $\epsilon = 5\%$) throughout for CIFAR-10. However, for CIFAR-100 possibly due to high class cardinality it drops to around 70%. This is similar to some of the baselines but yields much higher coverage. This means that our method indeed improves the utilization of unlabeled data. Similar results hold for SVHN from Figure 7.

We also perform ablations that give insights into the role of various parts of it. We run all the ablation experiments on the CIFAR-10 data setting.

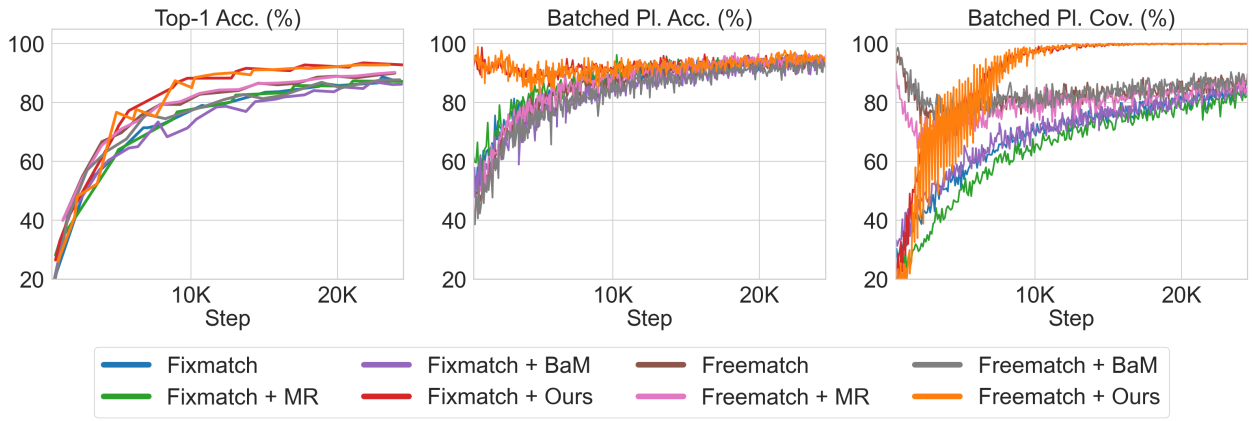

Figure 2: Left to Right: Top-1 accuracy, Batched pseudolabeling accuracy and Batched pseudolabeling coverage of our method and baselines on CIFAR-10. We plot the values for every 200 steps.

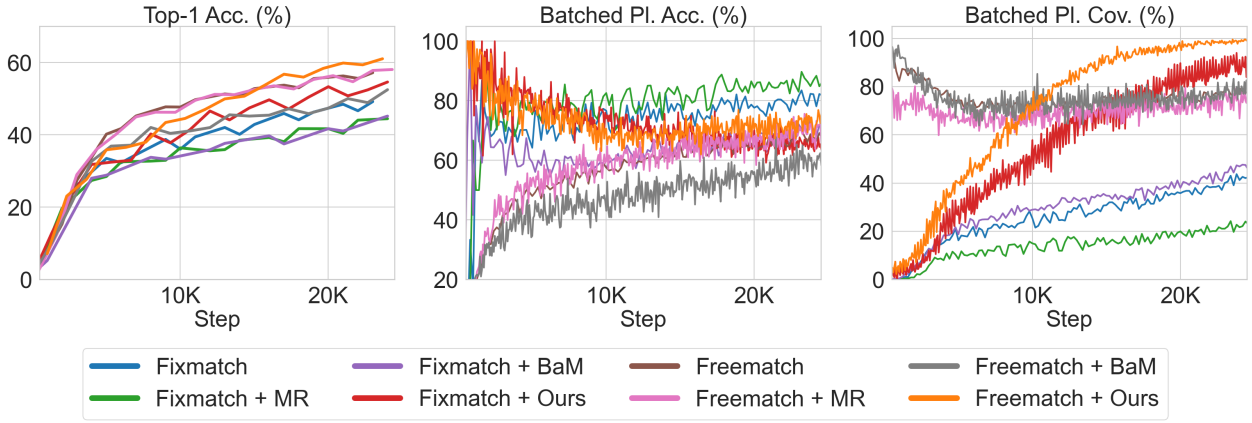

Figure 3: Left to Right: Top-1 accuracy, Batched pseudolabeling accuracy and Batched pseudolabeling coverage of our method and baselines on CIFAR-100. We plot the values for every 200 steps.

A1. Is pseudolabel accumulation helpful? Accumulation allows the methods to use old pseudolabel for points that couldn't get pseudolabeled in the current iteration. Thus we expect accumulation could help in improving the utilization of unlabeled data and could lead to better test accuracy in cases where the pseudolabel quality is assured to be high in all iterations. We run two variations of our method and baselines — with accumulation and without it and report the results in Table 3. We observe that our method has similar test accuracy irrespective of accumulation. However, with accumulation it achieves better coverage in early iterations as observed in Figure 6. These results are not surprising, since our method ensures high quality of pseudolabels while maximizing coverage, it is able to eventually catch up with the version using accumulation, leading to similar final test accuracies. On the other hand, having accumulation hurts the performance of baseline models. This might be because the pseudo labels generated by the baseline models are not accurate especially in the earlier iterations, thus degrading the overall performance. Overall, we believe accumulation is going to be helpful when we have pseudolabels with high accuracy. The plots for coverage and accuracy over the entire run are in Figures 8, 9 in the Appendix B.

Table 3: Results on CIFAR-10 with and without pseudolabel accumulation (Acc) for all the methods.

Method	Acc—True	Acc—False
Fixmatch	66.30 ± 1.68	88.15 ± 1.27
Fixmatch + MR	64.24 ± 1.93	87.85 ± 1.10
Fixmatch + BaM	84.50 ± 2.60	86.44 ± 1.47
Freematch	85.17 ± 4.74	90.17 ± 0.13
Freematch + MR	80.67 ± 2.39	90.17 ± 0.45
Freematch + BaM	88.92 ± 0.49	88.34 ± 0.99
Fixmatch + Ours	**93.03 ± 0.44**	**93.34 ± 0.50**
Freematch + Ours	**93.08 ± 0.05**	**93.01 ± 0.24**

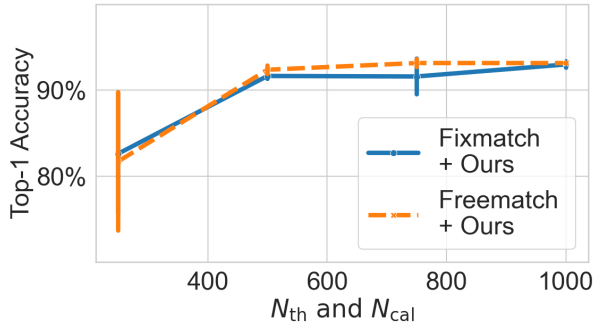

Figure 4: Top-1 accuracy of our method with different N_{th} and N_{cal}.

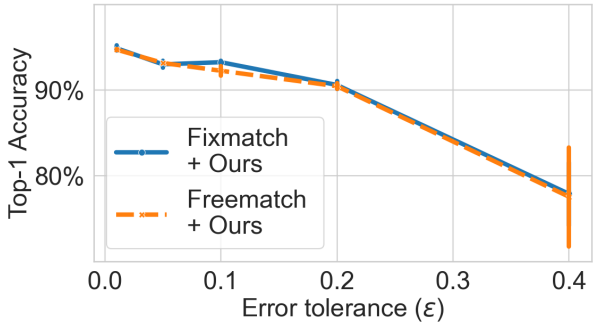

Figure 5: Top-1 accuracy of our method with different error tolerance ϵ.

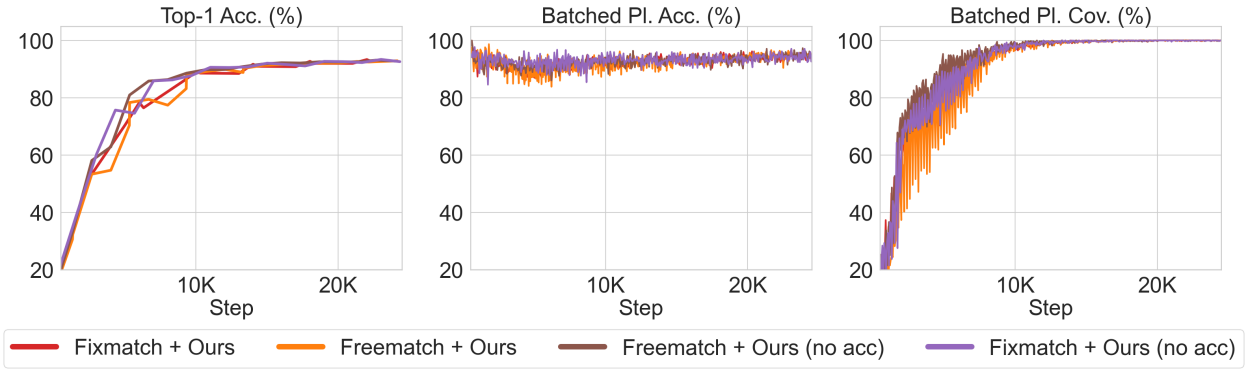

Figure 6: Left to Right: Top-1 Accuracy, Batched pseudolabeling Accuracy and Batched pseudolabeling coverage of our method with and without pseudolabeling accumulation enabled.

A2. Does error tolerance affect performance? In our method, the error tolerance parameter ϵ is a knob to control the amount of noise in pseudolabels. A common wisdom in pseudolabeling is higher noise will lead to worse performance, which is our expectation too. To see this, we run our method with $\epsilon \in \{0.01, 0.05, 0.1, 0.2, 0.4\}$ in the CIFAR-10 setting. We run each setting with 3 random seeds and report the results in Figure 5. The results are as expected — higher values of ϵ lead to degraded test accuracy due to high noise in the pseudolabels and with decreasing ϵ leads to improved accuracy. These results also suggest that prioritizing the quality (accuracy) of pseudolabels over quantity is a better choice in pseudolabeling. The results are also summarized in Table 6 and Figure 11.

A3. How much data is needed to learn the g and $\mathbf{t}$? We take N_{cal} and N_{th} from the validation data to learn the confidence function g and estimate the thresholds $\mathbf{t}$ respectively. Intuitively larger values of these should lead to good g and $\mathbf{t}$ that can extract the expected level of pseudolabeling coverage and accuracy from the classifier at hand. However, the task of learning good g and estimating thresholds is not super hard and we expect it will take fewer samples to be successful. To understand this better we run our method with N_{cal} and N_{th} in $\{250,\ 500,\ 750,\ 1000\}$ on CIFAR-10 setting for 3 random seeds and report the result in Fig 4. We observe that our method can achieve desired performance with just 500 labeled points (i.e 50 labels per class). This is interesting because we can achieve 90% accuracy by just using 250 points (N_l) for training h and a total of 1K for learning g. Refer Table 5 and Figure 10 for more details.

5 Related Work

Semi-supervised learning (SSL). There is a rich literature on SSL spanning multiple decades (Zhu, 2005; Chapelle et al., 2006; Singh et al., 2008; Oliver et al., 2018). This literature comprises of a wide variety of approaches. Among these significant focus has been placed on self-training (also called pseudolabeling) (Scudder, 1965; Blum and Mitchell, 1998; Rosenberg et al., 2005; Lee, 2013; Oymak and Gulcu, 2020; Amini et al., 2023), generative models (Nigam et al., 2000; Adams and Ghahramani, 2009; Kingma et al., 2014), graph-based strategies (Blum and Chawla, 2001; Niyogi, 2013; Subramanya and Talukdar, 2022), and transductive approaches (Vapnik et al., 1998; Joachims, 1999). Due to their simplicity, pseudolabeling-based approaches have gained prominence and are widely used in application areas such as NLP (Karamanolakis et al., 2021), speech recognition (Kahn et al., 2020), and protein prediction (El-Manzalawy et al., 2016). Our paper focuses on recent variants of this, discussed next.

Pseudolabeling based SSL. These methods generate artificial labels for unlabeled data and use them for training the model. A crucial challenge here is the issue of confirmation bias (Arazo et al., 2020) i.e., when a model starts to reinforce its own mistakes. To overcome this and to maintain high quality of pseudolabels, confidence-based thresholding is applied. Here only the unlabeled data where confidence is higher than a particular threshold is used (Sohn et al., 2020). Due to the limitations of fixed thresholds, adaptive thresholds based on the classifier's learning status have been introduced to improve performance (Xu et al., 2021; Zhang et al., 2021; Wang et al., 2023). Nearly all of these methods also use some form of consistency regularization (Laine and Aila, 2017; Bachman et al., 2014; Sajjadi et al., 2016; Fan et al., 2021; Kukačka et al., 2017) where the core idea is that the model should produce similar prediction when presented with different versions (perturbations) of inputs and all the present SSL methods (Xie et al., 2020; Wang et al., 2023; Sohn et al., 2020; Zhang et al., 2021; Chen et al., 2023; Xu et al., 2021).

Confidence functions and calibration. Miscalibration (overconfidence) in neural networks plagues various applications (Nguyen et al., 2015; Hendrycks and Gimpel, 2017; Guo et al., 2017), including SSL. To mitigate this in general, a range of solutions have been proposed, including training-time methods (Moon et al., 2020; Kumar et al., 2018; Hui et al., 2023; Corbière et al., 2019; Foret et al., 2021) and post-hoc methods (Guo et al., 2017; Kumar et al., 2019; Gupta and Ramdas, 2022; Kull et al., 2019; Zadrozny and Elkan, 2002). In pseudolabeling based SSL, recent works (Rizve et al., 2021; Loh et al., 2023; Mishra et al., 2024) noted the issue of miscalibration. To promote calibration, Loh et al. (2023) use Bayesian neural nets by replacing the model's final layer with a Bayesian layer. Rizve et al. (2021) improve pseudolabeling with negative labels and an uncertainty-aware pseudolabel selection technique. Mishra et al. (2024) incorporate a regularizer in pseudolabeling to encourage calibration.

While calibration is a reasonable goal in general, it may not be sufficient to address the overconfidence problem in SSL and other applications. In pseudolabeling, we seek the use of scores that can easily segregate the model's correct and incorrect predictions, which is closely related to the ordinal ranking criterion (Hendrycks and Gimpel, 2017; Moon et al., 2020; Foret et al., 2021; Corbière et al., 2019). Rather than experimenting with several such choices, ideally we would have a flexible framework that can learn confidence functions explicitly optimizing pseudolabeling objectives. To do this we build upon the principles used to learn confidence functions in threshold-based auto-labeling (TBAL) (Vishwakarma et al., 2024) to create labeled datasets.

6 Conclusion

We built a framework, inspired by ideas from autolabeling, that learns confidence functions and thresholds explicitly aligned with the SSL task. This approach eliminates the need for manual designs and hand-crafted notions of confidence, which can be limited in specialized data settings. By formulating an optimization problem over a flexible space of confidence functions and thresholds, we characterized optimal scoring functions and achieved up to 11% improvement in test accuracy over standard baselines, while also reducing training iterations. A thorough empirical evaluation demonstrates the effectiveness of our method, providing a more adaptable and robust solution for SSL in various settings.

7 Limitations

Our method requires marginally more time compared to base SSL techniques for learning the confidence function and thresholds. We believe the extra time taken by our method can be reduced with more efficient implementations.

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Supplementary Material

We provide formal algorithm in Appendix A. Additional experimental results and details are in Appendix B.

A Appendix to the Method Section

The full algorithm we use is:

Algorithm 1 Pseudolabeling Based SSL with `PabLO`

Input: Labeled data for training D_l, Validation data D_{val}, unlabeled pool X_u, error tolerance ϵ, use-accumulation flag, num_iters, batch size B, replication factor μ, weak ω and strong Ω augmentations.

Output: $\hat{h}_{\text{ssl}}$, model with the best validation accuracy.

$\widetilde{Y} \leftarrow [0] \times n_u$, $S \leftarrow [0] \times n_u$, $i \leftarrow 1$.
$D_{\text{cal}},\ D_{\text{th}} \leftarrow$ `draw_randomly`$(D_{\text{val}}, N_{\text{cal}},\ N_{\text{th}})$
while $i \leq$ num_iters **do**
  $D_l^b,\ X_u^b,\ I_u^b \leftarrow$ `draw_random_batch`$(\mu D_l, \mu X_u, B)$
  $X_{u,w}^b,\ X_{u,s}^b \leftarrow \omega(X_u^b),\ \Omega(X_u^b)$
  if use-`PabLO` **then**
    if $i\%F = 0$ **then**
      $\hat{g}_i \leftarrow$ `solve_opt_problem_P1`$(\hat{h}_i, D_{\text{cal}})$
      $\hat{\mathbf{t}}_i \leftarrow$ `estimate_thresholds`$(\hat{h}_i, \hat{g}_i, D_{\text{th}})$
      $\widetilde{Y}^f \leftarrow \hat{h}_i(\omega(X_u)), \quad S^f \leftarrow \mathbb{1}(\hat{g}_i(\omega(X_u)) \geq \hat{\mathbf{t}})$
      if use-accumulation **then**
        $\widetilde{Y},\ S \leftarrow S^f\widetilde{Y}^f + (1 - S^f)\widetilde{Y}; \quad S \leftarrow S \vee S^f$
      else
        $\widetilde{Y},\ S \leftarrow \widetilde{Y}^f,\ S^f$
      end if
    end if
    $\widetilde{Y}^b,\ S^b \leftarrow \widetilde{Y}[I_u^b],\ \ S[I_u^b]$
  else
    $\widetilde{Y}^b,\ S^b \leftarrow$ `baseline_pseudo_labeling`$(\hat{h}_i,\ X_{u,w}^b)$
    if use-accumulation **then**
      for $j \in I_u^b$ **do**
        $\widetilde{Y}[j] \leftarrow S^b[j]\widetilde{Y}^b[j] + (1 - S^b[j])\widetilde{Y}[j]$
        $S[j] \leftarrow S[j] \vee S^b[j]$
      end for
    end if
  end if
  $\widehat{\mathcal{L}}_s(\hat{h}_i) \leftarrow$ `supervised_loss`(h, D_l^b)
  $\widehat{\mathcal{L}}_u(\hat{h}_i) \leftarrow$ `unsupervised_loss`$(h, X_{u,w}^b X_{u,s}^b, \widetilde{Y}^b, S^b)$
  $\widehat{\mathcal{L}}_r(\hat{h}_i) \leftarrow$ `baseline_regularizers`$()$
  $\widehat{\mathcal{L}}(\hat{h}_i) \leftarrow \widehat{\mathcal{L}}_s(\hat{h}_i) + \lambda_u\widehat{\mathcal{L}}_u(\hat{h}_i) + \lambda_r\widehat{\mathcal{L}}_r(\hat{h}_i)$
  $\hat{h}_{i+1} \leftarrow$ `SGD_update`$(\widehat{\mathcal{L}}(\hat{h}_i)); \quad i \leftarrow i + 1$
  if $i\%$eval_freq $= 0$ **then**
    eval_acc $\leftarrow$ `evaluate_model`$(\hat{h}_i, D_{\text{val}})$
    If eval_acc is best so far then $\hat{h}_{\text{ssl}} = \hat{h}_i$.
  end if
end while

Table 4: Hyperparameters used for our method.

Method	Hyperparameter	Values
Learning g function	optimizer	SGD
	learning rate	0.01
	batch size	64
	max epoch	500
	weight decay	0.01
	momentum	0.9
Estimating $\mathbf{t}$	optimizer	SGD
	learning rate	0.01
	batch size	64
	max epoch	500
	weight decay	0.01
	momentum	0.9

Table 5: Results on CIFAR-10 with varying N_{cal} and N_{th}.

Method	$N_{\text{cal}} = N_{\text{th}} = 250$	$N_{\text{cal}} = N_{\text{th}} = 500$	$N_{\text{cal}} = N_{\text{th}} = 750$
Fixmatch + Ours	82.67 ± 7.08	91.74 ± 0.41	91.66 ± 2.11
Freematch + Ours	82.13 ± 7.93	92.33 ± 0.49	93.20 ± 0.53

B Additional Experiments and Details

Compute. For all our experiments, we used an NVIDIA RTX A6000 which has 48GB of VRAM and an NVIDIA RTX 4090 with 24GB of VRAM. The runtime depends on several factors including CPU I/O and GPU load, but on average, the baselines took around 8 hours, while our method took around 15 hours for 25K iterations.

Hyperparameters. For the baselines, we have used their default settings. To maintain consistency and experiment the efficiency of method, we used WRN-28-2 which is 1.4M parameter model for all the datasets. We summarize the main hyperparameters we have used in our method in Table 4.

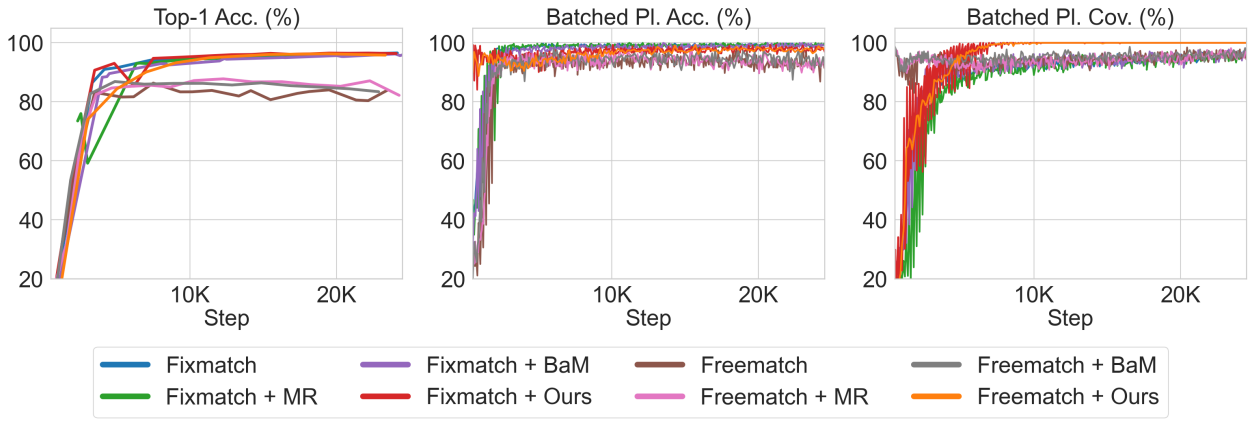

Figure 7: Left to Right: Top-1 Accuracy, Batched pseudolabeling Accuracy and batched pseudolabeling coverage of our method and various baselines on SVHN. We plots the values for every 200 steps.

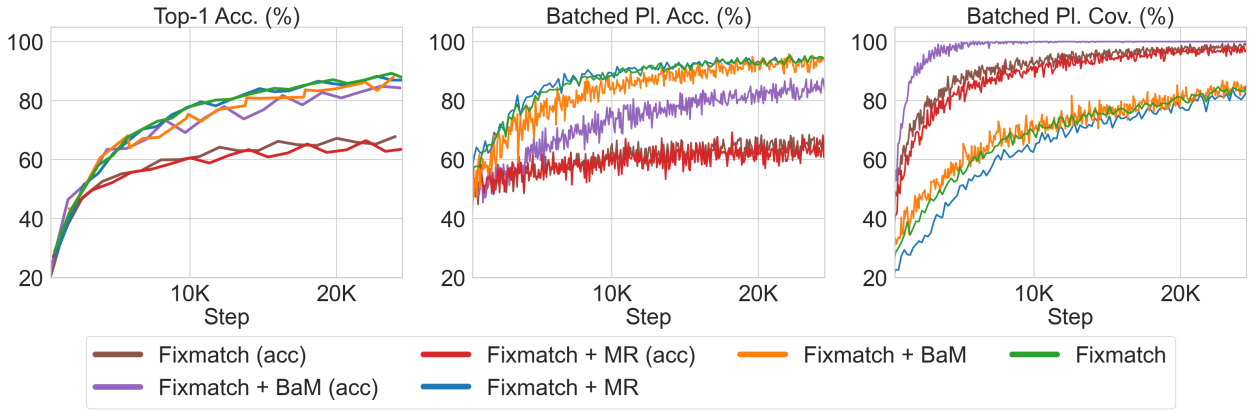

Figure 8: **(A1.)** Left to Right: Top-1 Accuracy, Batched pseudolabeling Accuracy and batched pseudolabeling coverage of Fixmatch with and without pseudolabeling accumulation enabled on CIFAR-10. It can be seen that enabling pseudolabeling accumulation worsen the performance of baseline methods in terms of accuracy and coverage.

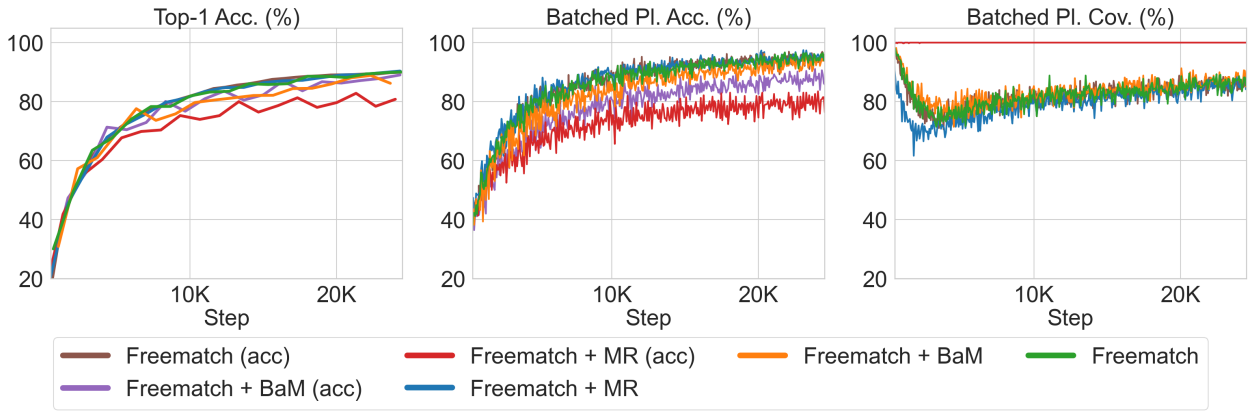

Figure 9: **(A1.)** Left to Right: Top-1 Accuracy, Batched pseudolabeling Accuracy and batched pseudolabeling coverage of Freematch with and without pseudolabeling accumulation enabled on CIFAR-10. It can be seen that enabling pseudolabeling accumulation worsen the performance of baseline methods in terms of accuracy and coverage.

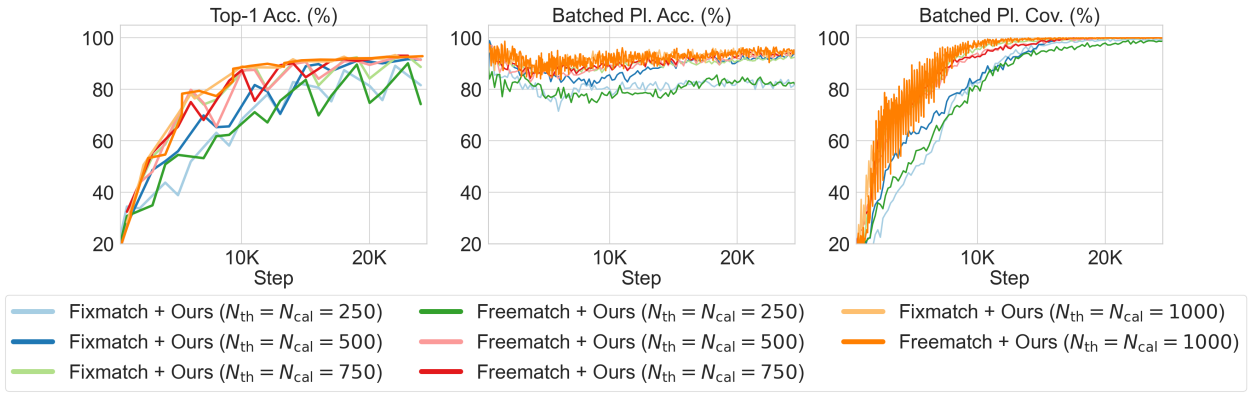

Figure 10: **(A3.)** Left to Right: Top-1 Accuracy, Batched pseudolabeling Accuracy and batched pseudolabeling coverage of our method with $N_{\text{th}} = N_{\text{cal}} \in \{250, 500, 750, 1000\}$ on CIFAR-10. We observe that having more calibration and threshold estimation points benefits the performance of our method.

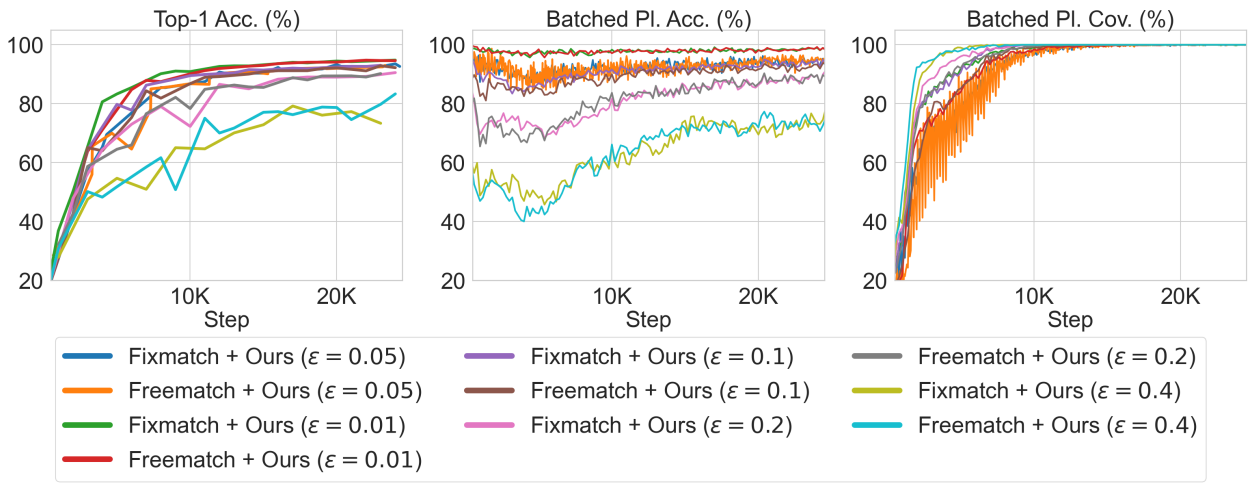

Figure 11: **(A2.)** Left to Right: Top-1 Accuracy, Batched pseudolabeling Accuracy and batched pseudolabeling coverage of our method with $\epsilon \in \{0.01, 0.05, 0.1, 0.2, 0.4\}$ on CIFAR-10. Although having a looser constraint on the error encourages more coverage, the pseudolabeling drops as a trade-off.

Table 6: Results on CIFAR-10 with varying ϵ.

Method	$\epsilon = 0.01$	$\epsilon = 0.1$	$\epsilon = 0.2$	$\epsilon = 0.4$
Fixmatch + Ours	**94.85 ± 0.28**	93.24 ± 0.18	90.52 ± 0.43	80.62 ± 1.22
Freematch + Ours	**94.67 ± 0.09**	92.11 ± 0.84	90.20 ± 0.65	82.23 ± 1.31