Beyond the Final Linear Layer: Enhancing Decision Boundaries

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Abstract

SSL leverages an abundance of unlabeled data to improve deep learning based model performance under limited training data regimes. This paper presents a novel extension to any image classification architecture which improves accuracy in low-label regimes. We extend the FixMatch [1] training scheme with our novel last layers and demonstrate test accuracy improvement. The novelty consists of 2 elements: first we replace the last linear layer with a GMM trained via backprop, and second, we impose class-wise constraints on the embedding space the GMM operates on. These methods match published SOTA 250 label CIFAR-10 [2] results and come close to matching SOTA in the 40 label regime without the significant model complexity of methods like SimMatchV2 [3]. Our method achieves 94.8% and 94.2% accuracy with 250 and 40 CIFAR-10 labels respectively. Our code is available at: https://github.com/mmajurski/ssl-gmm

1. Introduction

SSL leverages an abundance of unlabeled data to improve deep learning based model performance under limited training data regimes [4, 5, 6]. Image classification has become a playground for exploring new SSL ideas. The early successes of deep learning based methods relied on large annotated datasets to enable models to learn the relevant features to perform the task, i.e. image classification build on top of ImageNet [7]. With data annotation becoming a significant bottleneck, especially in application domains outside of the standard benchmarks, another learning paradigm was needed.

There are several flavors of SSL. Contrastive learning methods leverage the intuition that similar instances should be close in the representation space, while different instances are farther apart [8, 9]. Consistency regularization borrows the intuition that modified views of the same instance should have similar representations and predictions [1, 10, 11, 12]. Pseudo-labeling methods like FixMatch [1] fall within the consistency regularization domain.

This work argues that pseudo-labeling methods can be improved with better calibration of the network logits used to filter the pseudo-labels into reliable and unreliable. Neural networks are known to be overconfident in their predictions [13], and this affects the pseudo-labeling process. Potentially allowing for the inclusion of more incorrect pseudo-labels any specific logit threshold would otherwise have. This work demonstrates the better calibrated replacements for a models final linear layer can improve the final accuracy of pseudo-labeling based SSL algorithms in very label scarce regimes.

With that goal in mind, this work proposes replacing the final linear (fully connected) layer of the neural network with one of a few options, all of which have explicit modeling of class cluster centroids. First, a nearest neighbor (k=1) kmeans layer. Second, an axis-aligned differentiable Gaussian Mixture Model (GMM) trained via back prop. Third, an identity covariance axis-aligned differentiable GMM trained via back prop. These three methods represent differing levels of prescription about how the final embedding space should be arranged.

Additionally, to assist these cluster based final embedding classification layers, we explore the effect of different constraints on the embedding space. All of the embedding space constraints are based on specifying how many of the first 4 gaussian moments are identity/zero. Moment1 (cluster mean position) should have zero distance to the learned cluster centroids. Moment2 (cluster variance) should be the identity matrix. Moment3 (cluster skew) should be zero. Moment4 (cluster kurtosis) should be the identity matrix. We explore how no constraints, moment1, moment1-2, and moment1-4 impact the final learned model accuracy.

This paper contributes a simple easy to implement improvement to pseudo-labeling methods where very few annotations are available, replace the last linear layer with

a kmeans layer which explicitly models class cluster centers. We demonstrate this methodology using CIFAR-10 and CIFAR-100 [2] with 40 and 400 labels respectively. Additionally, we explore and demonstrate that high level prescriptive constraints on the embedding space produce significantly worse outcomes than allowing the embedding space to take on whatever emergent structure the training process produces. Finally, because the embedding constraint penalties are applied to all unlabeled data and not just the valid pseudo-labels, our method extracts training signal from every unlabeled data point, unlike FixMatch [1] and other methods which only learn from the valid pseudo-labels.

2. Related Work

Semi-Supervised learning has recently show great progress in learning high quality models, in some cases match fully supervised performance, for a number of benchmarks [11]. The goal of SSL is to produce a trained model of equivalent accuracy to fully supervised training, with vastly reduced data annotation requirements.

2.1. Pseudo-Labeling

Self-supervised learning was among the initial approaches employed in the context of semi-supervised learning to annotate unlabeled images. This technique involves the initial training of a classifier with a limited set of labeled samples and incorporates pseudo-labels into the gradient descent process, exceeding a predefined threshold [14, 15, 16, 17, 18, 19]. A closely related method to self-training is co-training, where a given dataset is represented as two distinct feature sets [20]. These independent sample sets are subsequently trained separately using two distinct models, and the sample predictions surpassing predetermined thresholds are utilized in the final model training process [20, 21]. A notably advanced approach to pseudo-labeling is the Mean Teacher algorithm [22], which leverages exponential moving averages of model parameters to acquire a notably more stable target prediction. This refinement has a substantial impact on enhancing the convergence of the algorithm.

2.2. Consistency Regularization

Consistency regularization operates on the premise that when augmenting an unlabeled sample, its label should remain consistent. This approach implicitly enforces a smoothness assumption, promoting coherence between unlabeled samples and their basic augmentations [23]. In other words, the model should be able to predict the unlabeled sample x exactly the same way it predicts the class for Augmented(x) [1, 24, 25, 26]. In addition to evaluating image-wise augmentations, recent research has

demonstrated that incorporating class-wise and instance-based consistencies yields superior performance outcomes [9, 27]. Finally, pseudo-labeling filtering based on consistence between strongly augmented views shows convergence improvement [12].

2.3. Embedding Clustering/Constraints

Several papers have attempted to improve the quality of pseudo-labels to either improve the final model accuracy, or to improve the rate of convergence. Rizve et al. [28] explores how uncertainty aware pseudo-label selection/filtering can be used to reduce the label noise. Incorrect pseudo-labels can be viewed as a network calibration issue [28] where better network logit calibration might improve results [29]. Other work has attempted to improve the pseudo-labeling process by imposing curriculum [11] or by including a class-aware contrastive term [8]. Previous work has leveraged the concept of explicit class cluster centers for conditioning semantic similarity [27]. Recent work has extended purely clustering based methods like DINO [30] into semi-supervised methods [31].

3. Methodology

In this section, we explore the details of our proposed embedding constraints and final linear layer replacements.

3.1. Fully Connected Replacements

3.1.1 KMeans

3.1.2 Differentiable Axis Aligned Gaussian Mixture Model

3.2. Embedding Constraints

3.2.1 L2

3.2.2 mean/covar

4. Experiments

4.1. Ablation Study

5. Conclusions

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