Improved Regularization and Robustness for Fine-tuning in Neural Networks

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Abstract

A widely used algorithm for transfer learning is fine-tuning, where a pre-trained model is fine-tuned on a target task with a small amount of labeled data. When the capacity of the pre-trained model is much larger than the size of the target data set, fine-tuning is prone to overfitting and “memorizing” the training labels. Hence, an important question is to regularize fine-tuning and ensure its robustness to noise. To address this question, we begin by analyzing the generalization properties of fine-tuning. We present a PAC-Bayes generalization bound that depends on the distance traveled in each layer during fine-tuning and the noise stability of the fine-tuned model. We empirically measure these quantities. Based on the analysis, we propose regularized self-labeling—the interpolation between regularization and self-labeling methods, including (i) layer-wise regularization to constrain the distance traveled in each layer; (ii) self label-correction and label-reweighting to correct mislabeled data points (that the model is confident) and reweight less confident data points. We validate our approach on an extensive collection of image and text data sets using multiple pre-trained model architectures. Our approach improves baseline methods by 1.76% (on average) for seven image classification tasks and 0.75% for a few-shot classification task. When the target data set includes noisy labels, our approach outperforms baseline methods by 3.56% on average in two noisy settings.

1 Introduction

Learning from limited labeled data is a fundamental problem in many real-world applications (Ratner et al., 2016, 2017). A common approach to address this problem is fine-tuning a large model that has been pre-trained on publicly available labeled data (He et al., 2019). Since fine-tuning is typically applied to a target task with limited labels, this algorithm is prone to overfitting or “memorization” issues (Tan et al., 2018). These issues worsen when the target task contains noisy labels (Zhang et al., 2016). In this paper, we analyze regularization methods for fine-tuning from both theoretical and empirical perspectives. Based on the analysis, we propose a regularized self-labeling approach that improves the generalization and robustness properties of fine-tuning.

Previous works (Li et al., 2018a,b) have proposed regularization methods to constrain the distance between a fine-tuned model and the pre-trained model in the Euclidean norm. Li et al. (2020) provides extensive study to show that the performance of fine-tuning and the benefit of adding regularization depend on the hyperparameter choices. Salman et al. (2020) empirically find that performing adversarial training during the pre-training phase helps learn pre-trained models that transfer better to downstream tasks. The work of Gouk et al. (2021) generalizes the above ideas to various norm choices and finds that projected gradient descent methods perform well for implementing distance-based regularization. Additionally, they derive generalization bounds for fine-tuning using Rademacher complexity. These works focus on settings where there is no label noise in the target data set. When
Label noise is present, for example, due to applying weak supervision techniques (Ratner et al., 2016), an important question is to design methods that are robust to such noise. The problem of learning from noisy labels has a rich history of study in supervised learning (Natarajan et al., 2013). In contrast, little is known in the transfer learning setting. These considerations motivate us to analyze the generalization and robustness properties of fine-tuning.

In Section 4.1, we begin by conducting a PAC-Bayesian analysis of regularized fine-tuning. This is inspired by recent works that have found PAC-Bayesian analysis correlates with empirical performance better than Rademacher complexity (Jiang et al., 2020). We identify two critical measures for analyzing the generalization performance of fine-tuning. The first measure is the $\ell_2$ norm of the distance between the pre-trained model (initialization) and the fine-tuned model. The second measure is the perturbed loss of the fine-tuned model, i.e. its loss after the model weights get perturbed by random noise. First, we observe that the fine-tuned weights remain closed to the pre-trained model. Moreover, the top layers travel much further away from the pre-trained model than the bottom layers. Second, we find that fine-tuning from a pre-trained model implies better noise stability than training from a randomly initialized model. In Section 4.2, we evaluate regularized fine-tuning for target tasks with noisy labels. We find that fine-tuning is prone to “memorizing the noisy labels”, and regularization helps alleviate such memorization behavior. Moreover, we observe that the neural network has not yet overfitted to the noisy labels during the early phase of fine-tuning. Thus, its prediction could be used to relabel the noisy labels.

We propose an algorithm that incorporates layer-wise regularization and self-labeling for improved regularization and robustness based on our results. Figure 1 illustrates the two components. First, we encode layer-wise distance constraints to regularize the model weights at different levels. Compared to (vanilla) fine-tuning, our algorithm reduces the gap between the training and test accuracy, thus alleviating overfitting. Second, we add a self-labeling mechanism that corrects and reweights “noisy labels” based on the neural network’s predictions. Figure 1 shows that our algorithm effectively hinders the model from learning the incorrect labels by relabeling them to correct ones.

In Section 5, we evaluate our proposed algorithm for both transfer learning and few-shot classification tasks with image and text data sets. First, using ResNet-101 (He et al., 2016) as the pre-trained model, our algorithm outperforms previous fine-tuning methods on seven image classification tasks by 1.76% on average and 3.56% when their labels are noisy. Second, we find qualitatively similar results for applying our approach to medical image classification tasks (ChestX-ray14 (Wang et al., 2017; Rajpurkar et al., 2017)) and vision transformers (Dosovitskiy et al., 2020). Finally, we extend our approach to few-shot learning and sentence classification. For these related but different tasks and data modalities, we find an improvement of 0.75% and 0.46% over previous methods, respectively.

In summary, our contributions are threefold. First, we provide a PAC-Bayesian analysis of regularized fine-tuning. Our result implies empirical measures that explain the generalization performance of regularized fine-tuning. Second, we present a regularized self-labeling approach to enhance the generalization and robustness properties of fine-tuning. Third, we validate our approach on an extensive collection of classification tasks and pre-trained model architectures.

2 Related work

Fine-tuning is widely used in multi-task and transfer learning, meta-learning, and few-shot learning. Previous works (Li et al., 2018b,a) find that injecting $\ell_2$ regularization helps improve the performance of fine-tuning. Li et al. (2018b) propose a $\ell_2$ distance regularization method that penalizes the $\ell_2$ distance between the fine-tuned weights and the pre-trained weights. Li et al. (2018a) penalize the distance between the feature maps as opposed to the layer weights. Chen et al. (2019) design a regularization method that suppresses the spectral components (of the feature maps) with small
singular values to avoid negative transfer. Gouk et al. (2021) instead encode distance constraints in constrained minimization and use projected gradient descent to ensure the weights are close to the pre-trained model. Salman et al. (2020) show that fine-tuning from adversarially robust pre-trained models outperforms fine-tuning from (standard) pre-trained models.

The robustness of learning algorithms in the presence of label noise has been extensively studied in supervised learning (Natarajan et al., 2013). Three broad ideas for designing robust algorithms include defining novel losses, identifying noisy labels, and regularization methods. Zhang and Sabuncu (2018) design the robust Generalized Cross Entropy (GCE) loss which is a mixture of Cross Entropy (CE) and mean absolute error. The Symmetric Cross Entropy (SCE) (Wang et al., 2019) loss combines reverse cross-entropy with the CE loss. Ma et al. (2020) proposes APL, which normalizes the loss to be robust to noisy labels and combines active and passive loss functions. Thulasidasan et al. (2019) propose DAC, which identifies and suppresses the signals of noisy samples by abstention-based training. Liu et al. (2020) introduce ELR, an early learning regularization approach to mitigate label "memorization". Huang et al. (2020) propose a self-adaptive training method that corrects noisy labels and reweights training data to suppress erroneous signals. These works primarily concern the supervised learning setting. To the best of our knowledge, fine-tuning algorithms under label noise are relatively under-explored in transfer learning. Our approach draws inspiration from the semi-supervised learning literature, which has evaluated pseudo-labeling and self-training approaches given a limited amount of labeled data, and a large amount of unlabeled data (Zou et al., 2019; Xu et al., 2021; Tai et al., 2021). A very recent work considered a sharpness-aware approach and evaluated its performance for fine-tuning from noisy labels (Foret et al., 2021). It would be interesting to see if combining their approach with our ideas could lead to better results.

From a theoretical perspective, the seminal work of Ben-David et al. (2010) considers a setting where labeled data from many source tasks and a target task is available. They show that minimizing a weighted combination of the source and target empirical risks leads to the best result. In the supervised setting, Arora et al. (2019) provide data-dependent generalization bounds for neural networks. Nagarajan and Kolter (2018) and Wei and Ma (2019a,b) provide improved generalization bounds that depend only polynomially on the depth of the neural network characterized by a margin condition. Recent work has found that the PAC-Bayes theory provides generalization measures that correlate with empirical generalization performance better than other alternatives (Jiang et al., 2020). We defer a more extensive review of PAC-Bayesian generalization theory to Section A.

3 Preliminaries

Problem setup. We begin by formally introducing the setup. Suppose we would like to solve a target task. We have a training data set of size \( n(t) \). Let \((x_1^{(t)}, y_1^{(t)}), \ldots, (x_{n(t)}, y_{n(t)})\) be the feature vectors and the labels of the training data set. We assume that every \( x_i^{(t)} \) lies in a \( d \)-dimensional space denoted by \( \mathcal{X} \subset \mathbb{R}^d \). Following standard terminologies in statistical learning, we assume all data are drawn from some unknown distribution supported on \( \mathcal{X} \times \mathcal{Y} \), where \( \mathcal{Y} \subseteq \mathbb{R} \) is the label space. Denote the underlying data distribution as \( \mathcal{P}(x) \).

For our result in Section 4.1, we consider feedforward neural networks, and our results can also be extended to convolutional neural networks (e.g., using ideas from Long and Sedghi (2020)). Consider an \( L \) layer neural network. For each layer \( i \) from 1 to \( L \), let \( \psi_i \) be the activation function and let \( W_i \) be the weight matrix at layer \( i \). Given an input \( x \) to the \( i \)-th layer, the output is then denoted as \( \phi_i(W_i z) \). Thus, the final output of the network is given by

\[
f_W(x) = \phi_L \circ \phi_{L-1} \circ \cdots \circ \phi_1(x), \text{ for any input } x \in \mathcal{X},
\]

where we use \( W = [W_1, \ldots, W_L] \) to include all the parameters of the network for ease of notation. The prediction error of \( f_W \) is measured by a loss function \( \ell(\cdot) \) that is both convex and 1-Lipschitz.

\[
\mathcal{L}(f_W) = \mathbb{E}_{(x,y) \sim \mathcal{P}(x)} [\ell(f_W(x), y)].
\]

(1)

Suppose we have access to a pre-trained source model \( \hat{W}(s) \). Using \( \hat{W}(s) \) as an initialization, we then fine-tune the layers \( W_1^{(s)}, \ldots, W_L^{(s)} \) to predict the target labels.

Applications. We consider seven image classification data sets described in Table 1. We use ResNets pre-trained on ImageNet as the initialization \( \hat{W}(s) \) (Russakovsky et al., 2015; He et al., 2016). We
perform fine-tuning using the pre-trained network on the above data sets. See Section 5.1 for further description of the training procedure.

**Modeling label noise.** In many settings, fine-tuning is applied to a target task whose labels may contain noise; for example, if the target labels are created using weak supervision techniques (Ratner et al., 2019; Saab et al., 2021). To capture such settings, we denote a noisy data set as \( x_1^{(t)}, y_1^{(t)}, \ldots, x_n^{(t)}, y_n^{(t)} \), where \( y_i^{(t)} \) is a noisy version of \( y_i^{(t)} \). We consider two types of label noise: *independent* noise and *correlated* noise. We say that the label noise is *independent* if it is independent of the input feature vector

\[
Pr(\tilde{y}_i^{(t)} = k | y_i^{(t)} = j, x_i^{(t)}) = Pr(\tilde{y}_i^{(t)} = k | y_i^{(t)} = j) = \eta_{j,k}
\]

for some fixed \( \eta_{j,k} \) between 0 and 1. On the other hand, we say that the label noise is *correlated* if it depends on the input feature vector (i.e. the above equation does not hold).

## 4 Our proposed approaches

Given the problem setup described above, next, we study the generalization and robustness properties of regularized fine-tuning methods. First, we present a PAC-Bayes generalization bound for regularized fine-tuning. This result motivates us to evaluate two empirical measures: the fine-tuned distance in each layer and the perturbed loss of the fine-tuned model. Second, we consider fine-tuning from noisy labels. We show that layer-wise regularization prevents the model from memorizing the noisy labels. We then suggest injecting predictions of the model during training, similar to self-training and pseudo-labeling. Finally, we incorporate both components into our regularized self-labeling approach, blending the strengths of both to improve the generalization performance and the robustness of fine-tuning.

### 4.1 Fine-tuning and regularization

We consider the following regularized fine-tuning problem, which constrains the network from traveling too far from the pre-trained initialization \( W^{(s)} \) (Li et al., 2018a,b; Gouk et al., 2021).

\[
\hat{W} \leftarrow \arg \min_{W} \mathcal{L}^{(t)}(f_W) \quad \text{s.t. } \|W_i - \hat{W}^{(s)}_i\|_F \leq D_i, \quad \forall \ i = 1, \ldots, L. 
\]

Above, \( D_i \) is a hyperparameter that constrains how far the \( i \)-th layer \( W_i \) can travel from the pre-trained initialization \( \hat{W}^{(s)}_i \). Previous works have observed that stronger regularization reduces the generalization gap during fine-tuning (cf. Figure 2). Next, we analyze the generalization error of \( W \), that is, \( \mathcal{L}^{(t)}(f_W) - \mathcal{L}^{(t)}(f_{\hat{W}}) \), where \( \mathcal{L}^{(t)}(f_W) \) is the test loss of \( f_W \) according to equation (1) and \( \mathcal{L}^{(t)}(f_{\hat{W}}) \) is the empirical loss of \( f_{\hat{W}} \) on the training data set.

**PAC-Bayesian analysis.** We begin by analyzing the generalization error of \( f_{\hat{W}} \) using PAC-Bayesian

![Figure 2: The training and test accuracy of fine-tuning using early stopping vs. optimizing (2) and (3) on the Indoor data set.](image-url)
tools (McAllester, 1999a,b). This departs from the previous work of Gouk et al. (2021), which bases on their analysis using Rademacher complexity. This change of perspective is inspired by several recent works that have found PAC-Bayesian bounds to better correlate with empirical performance than Rademacher complexity bounds (Jiang et al., 2020). We refer the interested reader to Section A for further references from this line of work. After presenting our result, we provide empirical measures of our result and discuss the practical implication.

**Theorem 4.1** (PAC-Bayes generalization bound for fine-tuning). Suppose for every $i = 1, \ldots, L$, $\|W_i^{(x)}\|_2 \leq B_i$, for a fixed $B_i > 1$. Suppose the feature vectors in the domain $X$ are all bounded: $\|x\|_2 \leq C_1$ for every $x \in X$, for some $C_1 \geq 1$. Finally, suppose the loss function $\ell(\cdot)$ is 1-Lipschitz and bounded from above by a fixed constant $C_2$. Under these conditions, let $f_{\hat{W}}$ be the minimizer of regularized fine-tuning, solved from problem (3). Let $\varepsilon > 0$ be an arbitrary small value. Let $H$ be the maximum over the width over all the $L$ layers and the input dimension $d$. Then, with probability at least $1 - \delta$ for some small $\delta > 0$, the expected loss $\mathcal{L}^{(i)}(f_{\hat{W}})$ is upper bounded by

$$
\mathcal{L}^{(i)}(f_{\hat{W}}) \leq \hat{\mathcal{L}}^{(i)}(f_{\hat{W}}) + \varepsilon + C_2 \sqrt{\frac{\log \left(4LHc_2\right)}{\varepsilon}} \left(\sum_{i=1}^{L} \frac{\mathbb{E}_{x \sim \mathcal{D}_i} N_{36}^{(i)}(x_i) + B_i}{\varepsilon} \right)^2 \left(\sum_{i=1}^{L} D_i^2\right) + 3\ln \frac{n^{(i)}}{\varepsilon} + 8. \quad (4)
$$

**Relation to prior works.** Compared to the result of Gouk et al. (2021), we instead proceed by factoring the generalization error into a noise error (i.e. the $\varepsilon$ term in equation (4)) and a KL-divergence between $W^{(x)}$ and $\hat{W}$ (i.e. the final term in equation (4)). The proof of Theorem 4.1 is based on Neyshabur et al. (2018) and is presented in Appendix A. The difference between Theorem 4.1 and the result of Neyshabur et al. (2018) is that our result is stated for the (e.g. cross-entropy) loss function $\ell(\cdot)$ whereas Neyshabur et al. (2018) states the result using the soft margin loss.

Our result suggests that the fine-tuned distances $\{D_i\}_{i=1}^{L}$ and the perturbed loss (more precisely $\mathbb{E}_U \left[\ell(f_{\hat{W}_i+U}(x), y)\right]$ where every entry of $U$ is drawn from $\mathcal{N}(0, \sigma^2)$) are two important measures for fine-tuning. Next, we empirically evaluate these two measures on real-world data sets.

**Fine-tuned distances $\{D_i\}_{i=1}^{L}$.** First, we present our empirical finding for the fine-tuned distances in each layer. We fine-tune a ResNet-18 model (pre-trained on ImageNet) on seven data sets and calculate the Frobenius distance between $W_i^{(x)}$ and $\hat{W}_i$ for every layer $i$.

Figure 3a shows the ratio of the fine-tuned distances to the pre-trained weights in each layer. First, we observe that the fine-tuned distances are relatively small compared to the pre-trained network. This means that fine-tuning stays within a small local region near the pre-trained model. Second, we find that $D_i$ varies across layers. $D_i$ is smaller at lower layers and is larger at higher layers. This observation aligns with the folklore intuition that different layers in Convolutional neural networks play a different role (Guo et al., 2019). Bottom layers extract higher-level representations of features.
and stay close to the pre-trained model. Top layers extract class-specific features and vary among different tasks. Thus, top layers travel further away from the pre-trained model.

Based on the above empirical finding, we propose layer-wise constraints as regularization. In particular, the constraints for the bottom layers should be small, and the constraints for the top layers should be large. In practice, we find that an exponentially increasing scheme involving a base distance parameter $D$ and a scale factor $\gamma$ works well. This is summarized in the following regularized fine-tuning problem:

$$\hat{W} \leftarrow \arg \min_{W} \mathcal{L}(f_W)$$

s.t. $$\|W_i - \hat{W}_i\|_F \leq D \cdot \gamma^{i-1}, \quad \forall i = 1, \ldots, L.$$  \hspace{1cm} (5)

where the scale factor $\gamma > 1$ according to Figure 3a. The previous work of Gouk et al. (2021) uses the same distance parameter in equation (6), i.e., $D_i = D$, $\forall i = 1, \ldots, L$. In our experiments, we have observed that such constant regularization constraints are only active at the top layers. With layer-wise regularization, we instead extend the constraints to the bottom layers as well. In Table 8 (cf. Section B.3), we compare the value of $\sum_{i=1}^{L} D_i^2$ between constant regularization and layer-wise regularization. We find that layer-wise regularization leads to a smaller value of $\sum_{i=1}^{L} D_i^2$, thus indicating a tighter generalization bound according to Theorem 4.1.

**Perturbed loss** $\mathbb{E}_U \left[ \ell(f_{\hat{W} + U_{\theta}}(x), y) \right]$. Second, we compare the perturbed loss of models fine-tuned from random, pre-trained, and adversarially robust pre-trained model initializations. The perturbed loss is measured by the average loss on the training set, after perturbing each entry of the layer weights by a Gaussian random variable $N(0, \sigma^2)$.

In Table 3b, we report the perturbed losses for both the CUB-200-2011 and the Indoor data set. The results show that models fine-tuned from pre-trained initializations are more stable than models fine-tuned from random initializations.

**Explaining why adversarial robustness helps fine-tuning.** Recent work (Salman et al., 2020) found that performing adversarial training in the pre-training phase leads to models that transfer better to downstream tasks. More precisely, the adversarial training objective is defined as

$$\mathcal{L}_{\text{adv}}^{(s)}(\theta) = \min_{W} \frac{1}{n^{(s)}} \sum_{i=1}^{n^{(s)}} \max_{\|\delta\|_2 \leq \varepsilon} \ell(f_W(x_i^{(s)} + \delta), y_i^{(s)}).$$

Let $\hat{W}_{\text{adv}}^{(s)}$ be a fine-tuned neural network using a pre-trained model from adversarial training. We measure the perturbed loss of $\hat{W}_{\text{adv}}^{(s)}$ using the pre-trained model provided by Salman et al. (2020) on the CUB-200-2011 and Indoor data set. Table 3b shows that $f_{\hat{W}_{\text{adv}}^{(s)}}$ often incurs lower perturbed losses than models fine-tuned from random and pre-trained initializations. In Section B.3, we additionally observe that the layers of $\hat{W}_{\text{adv}}^{(s)}$ generally have lower Frobenious norms compared to $W^{(s)}$. Thus, the improved noise stability and the smaller layer-wise norms together imply a tighter generalization bound for adversarial training. We leave a thorough theoretical analysis of adversarial training in the context of fine-tuning to future works.
Average weight injected by self label-reweighting.

We observe that the test accuracy increases at first, meaning the network learns from the correct labels during training. The model will prioritize data points with correct labels in its gradient by assigning smaller weights to large-loss data points. More precisely, given a data point \((x_i, y_i)\) with an incorrect label, we reweight it by \(\omega_i = \exp(-\ell(f_W(x_i(t)), \hat{y}_i(t))/\tau)\), where \(\tau\) is a temperature parameter. In the implementation, we normalize the weights of every data point in every mini-batch \(B\):

\[
\hat{L}_B(f_W) = \frac{1}{\sum_{i \in B} \omega_i} \sum_{i \in B} \omega_i \cdot \ell(f_W(x_i(t)), \hat{y}_i(t)).
\]
We selected the MIT-Indoor data set (Sharif Razavian et al., 2014) as the benchmark data set and evaluate our proposed algorithm in a wide range of tasks and pre-trained networks. First, we conduct experiments on the miniImageNet benchmark (Vinyals et al., 2016) following the setup which can be found in Section B.2. We consider both independent random noise and correlated noise of Tian et al. (2020). Section B.1 describes the label flipping process. For few-shot image classification, we simulate the correlated noise by using the predictions of an auxiliary network as noisy labels. Section B.1 describes the label flipping process. For few-shot image classification, we generate the independent random noise by flipping the labels uniformly with a given noise rate. We evaluate our proposed algorithm under two different kinds of label noise to test the robustness of fine-tuning. Additionally, our approach can achieve a similar performance boost for fine-tuning vision transformer models on noisy labeled data. Finally, we show our algorithms improve the robustness of fine-tuning in the presence of noisy labels compared to previous methods. Our extensive evaluation confirms that our approach applies to a broad range of settings, validating our algorithmic insights. Due to space constraints, we defer the ablation studies to Section B.3. Our code is available at https://github.com/NEU-StatsML-Research/Regularized-Self-Labeling.

Algorithm 1 Regularized self-labeling (REGSL)

Input: Input noisy data \((x_1^{(t)}, \hat{y}_1^{(t)}), \ldots, (x_n^{(t)}, \hat{y}_n^{(t)})\), network model \(f_W\), constraint distance \(D\), distance scale factor \(\gamma\), re-weight start step \(E_c\), re-weight temperature \(\tau\), label correction start step \(E_c\), label correction threshold \(p_t\), and fine-tuning steps \(T\)

1: Initialize model parameters with pre-trained weights \(W = \tilde{W}^0\) and the start step \(t = 0\)
2: while \(t < T\) do
3: Fetch a mini-batch of data \((x_i^{(t)}, \hat{y}_i^{(t)}))_{i=1}^m\) for each data point \(i\) in the batch do
4: Calculate the predicted probability \(p_i = \text{softmax}(f_W(x_i^{(t)}))\)
5: if \(t > E_c\) and \(\text{max}(p_i) > p_t\) and \(\text{arg max}(p_i) \neq \hat{y}_i^{(t)}\) then
6: Correct the label \(\hat{y}_i^{(t)} = \arg \max(p_i)\)
7: end if
8: Calculate loss \(\ell(t) = \ell(f_W(x_i^{(t)}), \hat{y}_i^{(t)})\)
9: if \(t > E_c\) then Calculate the weight \(\omega_t = \exp(-\ell(t)/\tau)\) else Set the weight \(\omega_t = 1\)
10: end if
11: Update \(f_W\) by SGD on \(L = -\frac{1}{\omega_t} \sum \omega_i \ell_i\) and \(t = t + 1\)
12: end for
13: Project the weights \(W_i\) of each layer inside the layer-wise constraint region as in Equation 6
14: end while

Figure 5b compares the average weight of data points with the correct label to data points with an incorrect label. We find that with our reweighting scheme, the average weight of incorrectly labeled data points is much lower than the average weight of correctly labeled data points. Thus, the reweighting scheme expands the gradient of correctly labeled data points, thus reducing the fraction of noisy data points in the training set.

The pseudo-code for our final approach, which combines both layer-wise regularization and self-labeling, is presented in Algorithm 1.

5 Experiments

We evaluate our proposed algorithm in a wide range of tasks and pre-trained networks. First, we show that our algorithm outperforms the baselines by 1.75% on average over seven transfer learning tasks and can generalize to a more distant task of medical images. Second, our algorithm improves the robustness of fine-tuning in the presence of noisy labels compared to previous methods. Our algorithm improves over numerous baselines by 3.56% on average under both independent and correlated label noise. Moreover, our approach can achieve a similar performance boost for fine-tuning vision transformer models on noisy labeled data. Finally, we show our algorithms improve over fine-tuning baselines by 0.75% on average for the related task of few-shot classification. Our extensive evaluation confirms that our approach applies to a broad range of settings, validating our algorithmic insights. Due to space constraints, we defer the ablation studies to Section B.3. Our code is available at https://github.com/NEU-StatsML-Research/Regularized-Self-Labeling.

5.1 Experimental setup

Data sets. First, we evaluate fine-tuning on seven image classification data sets and one medical image data set. The statistics of the seven image data sets are described in Table 1. For the medical imaging task, we consider the ChestX-ray14 data set contains 112120 frontal-view chest X-ray images labeled with 14 different diseases (Wang et al., 2017; Rajpurkar et al., 2017). Second, we evaluate Algorithm 1 under two different kinds of label noise to test the robustness of fine-tuning. We selected the MIT-Indoor data set (Sharif Razavian et al., 2014) as the benchmark data set and randomly flipped the labels of the training samples. The results for the other data sets are similar, which can be found in Section B.2. We consider both independent random noise and correlated noise in our experiments. We generate the independent random noise by flipping the labels uniformly with a given noise rate. We simulate the correlated noise by using the predictions of an auxiliary network as noisy labels. Section B.1 describes the label flipping process. For few-shot image classification, we conduct experiments on the miniImageNet benchmark (Vinyals et al., 2016) following the setup of Tian et al. (2020).
Architectures. We use the ResNet-101 (He et al., 2016) network for transfer learning tasks and ResNet-18 (He et al., 2016) network for ChestX-ray data set. We use ResNet-18 network for the label-noise experiments and extend the our algorithm to the vision transformer (ViT) model (Dosovitskiy et al., 2020). The ResNet models are pre-trained on ImageNet (Russakovsky et al., 2015) and the ViT model is pre-trained on ImageNet-21k data set (Dosovitskiy et al., 2020). For the few-shot learning tasks, we use ResNet-12 pre-trained on the meta-training data set as in the previous work (Tian et al., 2020). We set four different values of $D_i$ for the four blocks of the ResNet models in our algorithm. We describe the fine-tuning procedure and the hyperparameters in Section B.1.

Baselines. For the transfer learning tasks, we use the Frobenius norm for distance regularization. We present ablation studies to compare the Frobenius norm and other norms in Section B.3, we compare our algorithm with fine-tuning with early stop (Fine-tuning), fine-tuning with weight decay ($\ell_2$-Norm), label smoothing (LS) method formulated in Müller et al. (2019), $\ell_2$-SP (Li et al., 2018b), and $\ell_2$-PGM (Gouk et al., 2021). For testing the robustness of our algorithm, in addition to the baselines described above, we adopt several baselines that have been proposed in the supervised learning setting, including GCE (Zhang and Sabuncu, 2018), SCE (Wang et al., 2019), DAC (Thulasidasan et al., 2019), APL (Ma et al., 2020), ELR (Liu et al., 2020) and self-adaptive training (SAT) (Huang et al., 2020). We compare with the same baselines to transfer learning in few-shot classification tasks. We describe the implementation and hyper-parameters of baselines in Section B.1.

### 5.2 Experimental results

**Improved regularization for transfer learning.** We report the test accuracy of fine-tuning ResNet-101 on seven data sets in Table 2. We observe that our method performs the best among six regularized fine-tuning methods on average. Our proposed layer-wise regularization method provides an improvement of 1.76% on average over distance-based regularization (Gouk et al., 2021). In particular, our approach outperforms $\ell_2$-PGM by 2 ~ 3% on both Stanford-Dogs and MIT-Indoor data sets. This suggests that adding appropriate distance constraints for all the layers is better than applying only one constraint to the top layers. In Table 10 (cf. Section B.3), we note that using the MARS norm of Gouk et al. (2021) yields comparable results to using the $\ell_2$ norm with our approach.

Next, we apply our approach to medical image classification, a more distant transfer task (relative to the source data set ImageNet). We report the mean AUROC (averaged over predicting all 14 labels) on the ChestX-ray14 data set in Table 6a (cf. Section B.2). With layer-wise regularization, we see an 0.39% improvement over the baseline methods. Finally, we extend our approach to text classification. The results are consistent with the above and can be found in Table 7 (cf. Section B.2).

**Improved robustness under label noise.** Next, we report the test accuracy of our approach on the Indoor data set with independent and correlated noise in Table 3. We find that our approach consistently outperforms baseline methods by 1 ~ 3% for various settings involving label noise. First, our method (REGSL) improves the performance by over 4% on average compared to distance-based regularization (Gouk et al., 2021). This result implies our method is more robust to label noise in the training labels. Second, our method outperforms previous supervised training methods by 3.56% on average. This result suggests that regularization is critical for fine-tuning. Taken together, our results suggest that regularization and self-labeling complement each other during fine-tuning. This is reinforced by our ablation study in Section B.3; We study the influence of each component of our algorithm and find that removing any component degrades performance.

We further apply our approach to fine-tuning pre-trained ViT (Dosovitskiy et al., 2020) from noisy labels, under the same setting as Table 3. Table 6b shows the result (cf. Section B.2). First, we find that

| Aircrafts | CUB-200-2011 | Caltech-256 | Stanford-Cars | Stanford-Dogs | Flowers | MIT-Indoor |
|-----------|--------------|-------------|---------------|---------------|---------|------------|
| Fine-tuning | \(73.96 \pm 0.34\) | \(80.31 \pm 0.26\) | \(79.41 \pm 0.23\) | \(82.89 \pm 0.35\) | \(92.92 \pm 0.15\) | \(74.78 \pm 0.97\) |
| $\ell_2$-Norm | \(74.84 \pm 0.15\) | \(80.90 \pm 0.16\) | \(79.67 \pm 0.31\) | \(83.00 \pm 0.10\) | \(92.76 \pm 0.26\) | \(76.57 \pm 0.70\) |
| LS | \(74.19 \pm 0.41\) | \(82.22 \pm 0.17\) | \(81.10 \pm 0.13\) | \(89.66 \pm 0.10\) | \(93.72 \pm 0.04\) | \(76.84 \pm 0.31\) |
| $\ell_2$-SP | \(74.09 \pm 0.98\) | \(81.49 \pm 0.36\) | \(84.13 \pm 0.09\) | \(88.96 \pm 0.09\) | \(93.06 \pm 0.28\) | \(78.11 \pm 0.37\) |
| $\ell_2$-PGM | \(74.90 \pm 0.26\) | \(81.23 \pm 0.32\) | \(83.25 \pm 0.33\) | \(88.92 \pm 0.39\) | \(93.23 \pm 0.34\) | \(77.31 \pm 0.30\) |

**REGSL (ours)** | \(75.32 \pm 0.23\) | \(82.24 \pm 0.21\) | \(84.90 \pm 0.16\) | \(89.14 \pm 0.22\) | \(89.58 \pm 0.13\) | \(93.82 \pm 0.35\) | \(79.30 \pm 0.31\) |
We found that regularization and self-labeling complement each other in our experiments, leading to significant improvement over previous methods, which either use regularization methods or use noisy labels. We proposed a self label-correction and label-reweighting approach in the noisy setting. This approach performs well on both pre-trained ResNets and ViTs; empirical measures, which we empirically computed. The analysis inspired us to consider layer-wise regularization. We then evaluated the performance of regularized fine-tuning from constant regularization. We leave the details to Section B.3.

Ablation studies. We study the influence of removing each component in Algorithm 1 contribute to the final performance. The importance of each component depends on the noise rate. In particular, if the noise rate is higher than 40%, label-correction is the most critical component. Other ablation studies we present include: comparing the $\ell_2$ norm and the MARS norm in our algorithm and comparing the distance parameters between layer-wise and miniImageNet benchmark (Vinyals et al., 2016). We find that our layer-wise regularization method achieves 0.75% improvement on average compared to previous regularization methods. Additionally, regularization methods generally improve the performance of fine-tuning by over 1%.

Extension to few-shot classification. We extend our approach to a few-shot image classification task. We compare our approach to the baseline regularization methods. In Table 4, we report the average accuracy of 600 sampled tasks from the meta-test split of the miniImageNet benchmark (Vinyals et al., 2016). We find that our layer-wise regularization method achieves 0.75% improvement on average compared to previous regularization methods. Additionally, regularization methods generally improve the performance of fine-tuning by over 1%.

Table 3: Top-1 test accuracy of fine-tuning ResNet-18 on the Indoor data set with various settings of noisy labels in the training set. Results are averaged over 3 random seeds.

| Data sets | Methods | 20% | independent noise | 40% | 60% | 80% | correlated noise | 25.18% |
|-----------|---------|-----|------------------|-----|-----|-----|----------------|--------|
| Indoor    | Fine-tuning | 65.02±0.39 | 57.49±0.39 | 44.60±0.95 | 27.09±0.19 | 67.49±0.74 |
|           | LS      | 67.04±0.58 | 58.98±0.57 | 48.56±0.53 | 25.82±0.90 | 68.06±0.76 |
|           | $\ell_2$-PGM | 69.45±0.19 | 62.74±0.60 | 51.24±0.15 | 30.15±0.94 | 68.86±0.27 |
|           | GCE     | 70.45±0.40 | 64.73±0.21 | 54.10±0.16 | 29.58±0.26 | 68.88±0.18 |
|           | SCE     | 69.43±0.20 | 64.68±0.45 | 55.07±0.52 | 29.85±0.44 | 69.00±1.22 |
|           | DAC     | 64.45±0.31 | 59.73±0.27 | 47.44±0.09 | 26.69±0.34 | 68.06±1.32 |
|           | APL     | 70.05±0.41 | 66.22±0.10 | 52.51±0.66 | 30.90±0.37 | 68.31±0.77 |
|           | SAT     | 68.98±0.63 | 63.43±0.72 | 52.84±0.38 | 29.60±0.53 | 67.06±0.55 |
|           | ELR     | 71.43±0.80 | 66.34±0.48 | 55.22±0.73 | 31.24±0.19 | 69.38±0.49 |
|           | REGSL (ours) | 72.51±0.46 | 68.13±0.16 | 57.59±0.55 | 34.08±0.79 | 70.12±0.83 |

Table 4: Test accuracy with 95% confidence interval for fine-tuning ResNet-12 over 600 meta-test splits of miniImageNet.

| Methods | miniImageNet |
|---------|---------------|
|         | 5-way-1-shot   | 5-way-5-shot   |
| Fine-tuning | 60.56±0.78 | 76.42±0.36 |
| $\ell_2$-Norm | 60.93±0.81 | 76.57±0.55 |
| LS | 61.31±0.77 | 76.73±0.62 |
| $\ell_2$-SP | 61.48±0.76 | 77.02±0.62 |
| $\ell_2$-PGM | 61.35±0.83 | 77.33±0.59 |
| REGSL (ours) | 61.71±0.77 | 78.03±0.54 |

Our work concerns the theory and the empirical performance of fine-tuning for transfer learning. Due to its technical nature, there is very little negative societal impact. Since transfer learning is commonly used in practice, one avenue that deserves attention for these applications is to carefully evaluate bias or fairness metrics before applying our proposed approaches.
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A Proof of Theorem 4.1

Background. PAC-Bayesian generalization theory offers a nice way to blend data-dependent properties such as noise stability and sharpness into generalization bounds. Recent works (e.g., Bartlett et al. (2017); Neyshabur et al. (2018)) introduced generalization bounds for multi-layer neural networks in an attempt to explain why neural network models generalize well despite having more trainable parameters than the number of training examples. On the one hand, the VC dimension of a neural network is known to be roughly equal to its number of parameters (Bartlett et al., 2019). On the other hand, the number of parameters is not a good capacity measure for neural nets, as evidenced by the popular work of Zhang et al. (2016). The bounds of Bartlett et al. (2017) (and follow-up works) provide a more meaningful notion of “capacity” compared to VC-dimension.

While these bounds constitute an improvement compared to classical learning theory, it is unclear if these bounds are tight or non-vacuous. One response to this criticism is a computational framework from Dziugaite and Roy (2017). That work shows that directly optimizing the PAC-Bayes bound leads to a much smaller bound and low test error simultaneously (see also Zhou et al. (2018) for a large-scale study). The recent work of Jiang et al. (2020) further compared different complexity notions and noted that the ones given by PAC-Bayes tools correlate better with empirical performance. In particular, we will use the following classical result (McAllester, 1999a,b).

Theorem A.1 (Theorem 1 in McAllester (1999a)). Let \( \mathcal{H} \) be some hypothesis class. Let \( P \) be a prior distribution on \( \mathcal{H} \) that is independent of the training set. Let \( Q_S \) be a posterior distribution on \( \mathcal{H} \) that may depend on the training set \( S \). Suppose the loss function is bounded from above by \( C \). With probability \( 1 - \delta \) over the randomness of the training set, the following holds

\[
\mathbb{E}_{h \sim Q_S} [\mathcal{L}(h)] \leq \mathbb{E}_{h \sim Q_S} [\hat{\mathcal{L}}(h)] + C \sqrt{\frac{\text{KL}(Q_S \mid \mid P)}{n} + 3 \ln \frac{n}{\delta} + 8 n}.
\] (8)

We remark that the original statement in McAllester (1999a) requires the loss function is bounded between 0 and 1. The above statement modifies the original statement and instead applies to a loss function bounded between 0 and \( C \), for some fixed constant \( C > 0 \). This is achieved by rescaling the loss by \( 1/C \), leading the \( C \) factor in the right hand side of equation (8). To invoke the above result in our setting, we set the prior distribution \( P = N(W^{(s)}, \sigma^2 \text{Id}) \), where \( W^{(s)} \) are the weights of the pre-trained network. The posterior distribution \( Q_S \) is centered at the fine-tuned model as \( N(\bar{W}, \sigma^2 \text{Id}) \). Based on the above result, we present the proof of Theorem 4.1.

Proof of Theorem 4.1. First, we show that the KL divergence between \( P \) and \( Q_S \) is equal to \( \frac{1}{2\sigma^2} ||\bar{W} - \bar{W}^{(s)}||^2 \). We expand the definition using the density of multivariate normal distributions.

\[
\text{KL}(P \mid \mid Q_S) = \mathbb{E}_{W \sim P} \left[ \log \frac{\text{Pr}(W \sim P)}{\text{Pr}(W \sim Q_S)} \right]
\]

\[
= \mathbb{E}_{W \sim P} \left[ \log \frac{\exp(-\frac{1}{2\sigma^2} ||W - W^{(s)}||^2)}{\exp(-\frac{1}{2\sigma^2} ||W - \bar{W}||^2)} \right]
\]

\[
= -\frac{1}{2\sigma^2} \mathbb{E}_{W \sim P} \left[ ||W - W^{(s)}||^2 - ||W - \bar{W}||^2 \right]
\]

\[
= \frac{1}{2\sigma^2} \mathbb{E}_{W \sim P} \left[ (W^{(s)} - \bar{W}, 2W - W^{(s)} - \bar{W}) \right]
\]

\[
= \frac{1}{2\sigma^2} ||\bar{W} - W^{(s)}||^2 \leq \frac{\sum_{i=1}^{L} D_i^2}{2\sigma^2},
\]

where the last line uses the fact that \( ||\bar{W}_i - W_i^{(s)}||_p \leq D_i \), for all \( 1 \leq i \leq L \).

Next, let the dimension of \( W_i \) be \( d_{i-1} \) times \( d_i \), for every \( i = 1, 2, \ldots, L \). In particular, \( d_0 \) is equal to the dimension of the input data points. Let \( H = \max_{0 \leq i \leq L} d_i \) be the maximum matrix dimension size across all the \( L \) layers. Let \( e = \sigma \sqrt{2H \log(2L \cdot H/\delta)} \). We show that for any \( \delta > 0 \) and any \( L \)-layer feedforward neural network parameterized by \( W = [W_1, W_2, \ldots, W_L] \), with probability at least \( 1 - \delta \), the perturbation \( Q_S \) increases the loss function \( \hat{\mathcal{L}}(h) \) by at most

\[
C_1 \cdot e \cdot \left( \sum_{i=1}^{L} \prod_{j=1}^{i} \left( ||W_j||_2 + e \right) \right),
\] (9)
Consider some data point \((x, y)\) evaluated at a neural network function \(f_W\). Let \(U_i\) be a Gaussian perturbation matrix on \(W_i\) with mean zero and entrywise variance \(\sigma^2\), for \(i = 1, \ldots, L\). Denote by \(U = [U_1, U_2, \ldots, U_L]\). Since \(\ell(x, y)\) is 1-Lipschitz over \(x\), we get
\[
|\ell(f_{W+U}(x), y) - \ell(f_W(x), y)| \leq \|f_{W+U}(x) - f_W(x)\|_2. \tag{10}
\]

Since \(U_i \in \mathbb{R}^{d_{i-1} \times d_i}\) is a random matrix with i.i.d. entries sampled from the standard Gaussian distribution, we can upper bound the operator norm of \(U_i\) by applying well-known concentration results. In particular, by equation (4.1.8) and section (4.2.2) of Tropp (2015), we get
\[
\Pr \left[ \frac{1}{\sigma} \|U_i\|_2 \geq t \right] \leq (d_{i-1} + d_i) \cdot \exp \left( - \frac{-t^2}{2 \max(d_{i-1}, d_i)} \right). \tag{11}
\]

Thus, for all \(i = 1, 2, \ldots, L\), with probability at most \(\delta / L\), we have that
\[
\frac{1}{\sigma} \|U_i\|_2 \leq \sqrt{2H \log(2L \cdot H/\delta)}. \tag{12}
\]

In particular, the right hand side above is obtained by setting \(2H \exp \left( - \frac{-t^2}{2H} \right) = \delta / L\) and solve for \(t = \sqrt{2H \log(2L \cdot H/\delta)}\). Since the right hand side of equation (11) is at most \(2H \exp \left( - \frac{-t^2}{2H} \right)\), by union bound, we conclude that with probability at most \(1 - \delta\), for all \(i = 1, 2, \ldots, L\), the operator norm of \(U_i\) is at most \(\sigma \cdot \sqrt{2H \log(2L \cdot H/\delta)}\).

Let \(z_i\) be the input to the \(i\)-th layer of \(f_W\). Let \(\tilde{z}_i\) be the input to the \(i\)-th layer of \(f_{W+U}\). We can expand the right hand side of equation (10) as
\[
\begin{align*}
\|\psi_L(W_L + U_L)\tilde{z}_L - \psi_L(W_Lz_L)\|_2 & \leq \|W_L + U_L\|_2 \|\tilde{z}_L - z_L\|_2 - \|W_L\|_2 \|z_L\|_2\| \quad \text{(since } \psi_L(\cdot) \text{ is 1-Lipschitz)} \\
& \leq \|W_L\|_2 \|\tilde{z}_L - z_L\|_2 - \|W_L\|_2 \|z_L\|_2 + \|U_L\|_2 \|z_L\|_2\| \quad \text{(by triangle inequality)} \\
& \leq \|W_L\|_2 \|\tilde{z}_L - z_L\|_2 - \|W_L\|_2 \|z_L\|_2 + \sigma \cdot \sqrt{2H \log(2L \cdot H/\delta)} \|\tilde{z}_L\|_2, \tag{14}
\end{align*}
\]
where the last step is by equation (12). Recall from Section 3 that the \(i\)-th layer takes an input \(z\) and outputs \(\psi_i(W_i z)\), for every \(i = 1, \ldots, L\). Because we have assumed that \(\psi_i(\cdot)\) is 1-Lipschitz, for all \(i = 1, \ldots, L - 1\), we can bound
\[
\|\tilde{z}_L\|_2 = \phi_{L-1} \circ \phi_{L-2} \cdots \phi_1(x) \leq \prod_{i=1}^{L-1} \|W_i + U_i\|_2 \cdot \|x\|_2 \\
\leq \left( \prod_{i=1}^{L-1} \|W_i + U_i\|_2 \right) \cdot C_1 \quad \text{(since } \|x\|_2 \leq C_1 \text{ for } x \in X) \\
\leq \left( \prod_{i=1}^{L-1} (\|W_i\|_2 + e) \right) \cdot C_1. \quad \text{(by equation (12))}
\]

Applying the above to equation (14), we have shown
\[
\|f_{W+U}(x) - f_W(x)\|_2 \leq \|W_L\|_2 \|\tilde{z}_L - z_L\|_2 + \sigma \cdot \sqrt{2H \log(2L \cdot H/\delta)} \cdot \left( \prod_{i=1}^{L-2} (\|W_i\|_2 + e) \right) \cdot C_1. \tag{15}
\]

Next, we can expand the difference between \(\tilde{z}_L = \psi_{L-1}((W_{L-1} + U_{L-1})\tilde{z}_{L-1})\) and \(z_L = \psi_{L-1}(W_{L-1}z_{L-1})\) similar to equation (13). In general, for any \(i = 1, 2, \ldots, L\), we get
\[
\|\tilde{z}_i - z_i\|_2 \leq \|W_{i-1}\|_2 \|\tilde{z}_{i-1} - z_{i-1}\|_2 + \sigma \cdot \sqrt{2H \log(2L \cdot H/\delta)} \cdot \left( \prod_{j=i}^{L-2} (\|W_j\|_2 + e) \right) \cdot C_1. \tag{16}
\]

By repeatedly applying equation (16) together with equation (15) (relaxing \(\|W_i\|_2\) to \(\|W_i\|_2 + e\)), we can show that with probability at least \(1 - \delta\),
\[
\|f_{W+U}(x) - f_W(x)\|_2 \leq \sigma \cdot C_1 \sqrt{2H \log(2L \cdot H/\delta)} \cdot \left( \sum_{i=1}^{L} \prod_{j=i}^{L-1} (\|W_j\|_2 + e) \right). 
\]
Combined with equation (10), we have shown that equation (9) holds. Finally, with equation (9) and the fact that the loss function $\ell(\cdot)$ is bounded from above by some fixed value $C_2$, we can bound the expectation of $\bar{L}(h)$ for some $h \sim Q_S$ as

$$E_{h \sim Q_S} \left[ \bar{L}(h) \right] \leq \bar{L}(f_W) + (1 - \delta) \cdot \sigma \cdot C_1 \sqrt{2H \log \left( \frac{2L \cdot H}{\delta} \right)} \cdot \left( \sum_{i=1}^L \prod_{j=1}^i \frac{\|\hat{W}_j\|_2 + e}{\|W_i\|_2 + e} \right) + \delta \cdot C_2. \tag{17}$$

Note that the above inequality applies for any (small) value of $\delta$. Thus, we can minimize the right hand side by appropriately setting $\delta$. For our purpose, we will show that there exists some $\delta$ such that the right hand side of equation (17) (leaving out $\bar{L}(f_W)$) is at most

$$2\sigma C_1 \left( \sum_{i=1}^L \prod_{j=1}^i \frac{\|\hat{W}_j\|_2 + e}{\|W_i\|_2 + e} \right) \cdot \sqrt{2H \log (4L \cdot H \cdot C_2)}. \tag{18}$$

To see that the above is true, we will abstract away the precise scalars and instead write the right hand side of equation (17) as $g(\delta) = (1 - \delta)A_1 \sqrt{\log(A_2/\delta)} + C_2\delta$, for some fixed $A_1$ and $A_2$ that does not depend on $\delta$. We note that subject to

$$C_2\delta \leq (1 - \delta)A_1 \sqrt{\log(A_2/\delta)}, \tag{19}$$

g(\delta) is at most

$$g(\delta) \leq 2(1 - \delta)A_1 \sqrt{\log(A_2/\delta)} \leq 2A_1 \sqrt{\log \left( \frac{A_2}{\delta} \right)}. \tag{20}$$

Therefore, we only need to lower bound $\delta$ based on the constraint (19). In particular, the largest possible $\delta^*$ under constraint (19) is achieved when both sides equal:

$$C_2\delta^* = (1 - \delta^*)A_1 \sqrt{\log(A_2/\delta^*)} \geq \frac{A_1}{2} \sqrt{\log(A_2)},$$

which implies that $\delta^* \geq \frac{A_1}{2\sqrt{\log(A_2)}}$. Thus, we have shown that $g(\delta^*)$ is less than equation (18), using equation (20) and the lower bound on $\delta^*$. Additionally, $A_1$ is on the order of a fixed constant based on $\sigma$ defined below.

Using a similar argument since our bound on the perturbed loss holds point-wise for every $x \in \mathcal{X}$, we can likewise prove that with probability $1 - \delta$, 

$$E_{h \sim Q_S} \left[ \bar{L}(h) \right] \geq \bar{L}(f_W) - 2\sigma C_1 \left( \sum_{i=1}^L \prod_{j=1}^i \frac{\|\hat{W}_j\|_2 + e}{\|W_i\|_2 + e} \right) \cdot \sqrt{2H \log (4L \cdot H \cdot C_2)}.$$ 

By applying equation (18) and the above to equation (8) in Theorem A.1, we thus conclude that for any $\sigma$, with probability at least $1 - 2\delta$ over the training data set, the following holds

$$\mathcal{L}(f_W) \leq \mathcal{L}(f_W) + 4\sigma \cdot C_1 \cdot \sqrt{2H \log (4L \cdot H \cdot C_2)} \left( \sum_{i=1}^L \prod_{j=1}^i \frac{\|\hat{W}_j\|_2 + e}{\|W_i\|_2 + e} \right) + C_2 \cdot \left( \frac{\sum_{i=1}^L \frac{\|\hat{W}_i\|_2}{\|W_i\|_2 + e}}{\sum_{i=1}^L \|W_i\|_2 + e} \right). \tag{21}$$

Since $\|\hat{W}_i\|_2 \leq B_i$ and $\|\hat{W}_i - W_i\|_F \leq D_i$, for any $i = 1, \ldots, L$, we have that $\|\hat{W}_i\|_2 \leq B_i + D_i$. Thus, we can upper bound the above by replacing every $\|\hat{W}_i\|_2$ with $B_i + D_i$.

By setting $\sigma = \frac{\sqrt{\log(4L \cdot H \cdot C_2)}}{6\sigma C_1 \cdot \sqrt{2H \log (4L \cdot H \cdot C_2)}}$ where $\alpha = \left( \sum_{i=1}^L \prod_{j=1}^i \frac{(B_j + D_j)}{B_i + D_i} \right)$, we get $e \leq \frac{1}{6\alpha}$ since $C_1 \geq 1$. To finish the proof, we will show

$$\sum_{i=1}^L \prod_{j=1}^i \frac{(B_j + D_j + e)}{B_i + D_i + e} \leq 3\alpha/2.$$
We divide each dataset into the training set, the validation set, and the test set for data split. We extend the details of our experiment setup. First, we introduce the data sets in our experiments. For CUB-200-2011 and Flowers, we adopt the standard splitting of data given in the Aircrafts dataset (Maji et al., 2013). For Caltech-256 dataset (Griffin et al., 2007), we use the setting in Li et al. (2018b) that randomly samples 30, 20, 20 images of each class for training, validation, and test set, respectively. For other data sets, we split 10% of the training set as the validation set and use the standard test set. We describe the statistics of the seven data sets in Table 1. When fine-tuning on the seven data sets, we preserve the original pixel and resize the shorter side to 256 pixels. The image samples are normalized with the mean and std values over ImageNet data (Russakovsky et al., 2015). Moreover, we apply commonly used

Thus, plugging in the value of $\sigma$ above, we conclude that the second term in equation (21) is at most $\varepsilon$. By applying the value of $\sigma$ to the third term in equation (21), we conclude

$$\mathcal{L}(f_W) \leq \hat{\mathcal{L}}(f_W) + \varepsilon + C_2 \sqrt{\frac{4 \varepsilon^2 C^2 H \log(4LHC_2)}{n} \left( \sum_{i=1}^{L} \frac{\Pi_{j=1}^{L} (D_i + D_j)}{n_{ij}} \right)^2 + \frac{3 \ln n^{(i)}}{n^{(i)}} + 8}.$$ 

Thus, we have proved equation (4) is true. The proof is complete.

**Implication.** Our result implies a tradeoff in setting the distance parameter $D_i$. While a larger $D_i$ increases the network’s “capacity”, the generalization bound gets worse as a result.

### B Extended experimental setup and results

#### B.1 Additional details of the experimental setup

We extend the details of our experiment setup. First, we introduce the data sets in our experiments and describe the pre-processing steps. Second, we present the model architectures and the fine-tuning procedures. Third, we describe the baselines in detail. Finally, we describe the implementation and the hyperparameters for our algorithm and the baselines.

**Data sets.** We evaluate fine-tuning on seven image classification data sets covering multiple applications, including fine-grained object recognition, scene recognition, and general object recognition. We divide each dataset into the training set, the validation set, and the test set for data split. We adopt the standard splitting of data given in the Aircrafts dataset (Maji et al., 2013). For Caltech-256 dataset (Griffin et al., 2007), we use the setting in Li et al. (2018b) that randomly samples 30, 20, 20 images of each class for training, validation, and test set, respectively. For other data sets, we split 10% of the training set as the validation set and use the standard test set. We describe the statistics of the seven data sets in Table 1. When fine-tuning on the seven data sets, we preserve the original pixel and resize the shorter side to 256 pixels. The image samples are normalized with the mean and std values over ImageNet data (Russakovsky et al., 2015). Moreover, we apply commonly used
data augmentation methods on the training samples, including random scale cropping and random flipping. The images are resized to $224 \times 224$ as the input for the model. The training and batch size are both 16.

To test the robustness of fine-tuning, we evaluate Algorithm 1 under two different settings with label noise. We select MIT-Indoor dataset (Sharif Razavian et al., 2014) as the benchmark dataset and randomly flipped the labels of the training samples. The results for the other datasets are similar, which can be found in Appendix B.2. We consider two scenarios of label noise in our experiments, independent random noise and correlated noise. Random label noise is generated by flipping the labels of a given proportion of training samples to other classes uniformly. For the correlated noise setting, the label noise is dependent on the sample. We simulate the correlated noisy label by training an auxiliary network on a held-out dataset to a certain accuracy. We then use the prediction of the auxiliary network as noisy labels. For few-shot learning, we conduct experiments on a few-shot image recognition benchmark, miniImageNet (Vinyals et al., 2016) and follow the meta training and meta test setup in Tian et al. (2020).

**Architectures.** For image data sets, we use ResNet-101 (He et al., 2016) network which is pre-trained on ImageNet dataset (Russakovsky et al., 2015). For the label-noise experiments, we mainly use ResNet-18 (He et al., 2016) network. In the transfer learning and label-noise experiments, we fine-tune the model with Adam optimizer (Kingma and Ba, 2014) with an initial learning rate 0.0001 for 30 epochs and decay the learning rate by 0.1 every 10 epochs. We report the average Top-1 accuracy on the test set of 3 random seeds. For the few-shot learning tasks, we use ResNet-12 pre-trained on the meta-training dataset as in the previous work (Tian et al., 2020). To fine-tune on the meta-test sets, we use Adam optimizer (Kingma and Ba, 2014) with an initial learning rate $5\times 10^{-5}$ and fine-tune the model on the training set for 25 epochs. We report the average classification accuracies on 600 sampled tasks from the meta-test split.

**Baselines.** For the transfer learning tasks, we focus on using the Frobenius norm for distance regularization. We present ablation studies to compare the Frobenius norm and other norms in Appendix B.2. We compare our algorithm with fine-tuning with early stop (Fine-tuning), fine-tuning with weight decay ($\ell^2$-Norm), label smoothing (LS) method formulated in (Müller et al., 2019), $\ell^2$-SP (Li et al., 2018b), and $\ell^2$-PGM (Gouk et al., 2021). For testing the robustness of our algorithm, in addition to the baselines described above, we adopt several baselines that have been proposed in the supervised learning setting, including GCE (Zhang and Sabuncu, 2018), SCE (Wang et al., 2019), DAC (Thulasidasan et al., 2019), APL (Ma et al., 2020), ELR (Liu et al., 2020) and self-adaptive training (SAT) (Huang et al., 2020). We compare with the same fine-tuning baselines in transfer learning for the few-shot classification tasks.

**Implementation and hyperparameters.** For all baselines and data sets, all regularization hyperparameters are searched on the validation dataset by the Optuna optimization framework (Akiba et al., 2019). In our proposed algorithm, we search the constraint distance $D$ in $[0.05, 10]$ and the distance scale factor $\gamma$ in $[1, 5]$ by sampling. For setting layer-wise constraints, we set four different constraints for the four blocks of the ResNet. Concretely, ResNet-101 has four blocks, with 10, 13, 67, and 10 convolutional layers for each block, respectively. For every block, we set the same constraint value for all the layers within the block. Therefore, there are four distance values $(D \cdot \gamma, D \cdot \gamma^2, D \cdot \gamma^3)$ each block. Similar constraints are set for ResNet-18 and ResNet-12 models in the experiments. The search space for other hyperparameters is shown as follows. Re-weight start step $E_r$ is searched in $\{3, 5, 8, 10, 13\}$. Re-weight temperature factor $\gamma$ is searched in $\{3.0, 2.0, 1.5, 1.0\}$. Label correction

| Methods          | Mean AUROC     |
|------------------|----------------|
| Fine-tuning      | 0.8159 ± 0.0667|
| $\ell^2$-Norm    | 0.8198 ± 0.0644|
| LS               | 0.7885 ± 0.0578|
| $\ell^2$-SP      | 0.8231 ± 0.0658|
| $\ell^2$-PGM     | 0.8235 ± 0.0636|
| REGSL (ours)     | 0.8274 ± 0.0654|

Table 6: Left: Mean AUROC of fine-tuning ResNet-18 on the ChestX-ray14 data set. Right: Top-1 accuracy of fine-tuning ViT on the indoor data set. Results are averaged over 3 random seeds.
We present additional results. First, we apply our algorithm to another data set with label noise (same as Table 3). Second, we find that our approach also improves upon self-labeling by 1.17% averaged over two settings. We report the results for baselines by running the official open-sourced implementations. We describe the start step $E_c$ is searched in $\{5, 8, 10, 13, 15\}$. Label correction threshold $p$ is set as 0.90 in all experiments. The validation set sizes used for evaluating these hyperparameters choices range from 536 to 5120 (cf. Table 1). For the results in Table 2, we search for 20 different trials of the hyperparameters for the proposed algorithm and the baselines. For the results in Table 3, we search 20 times on the self-labeling parameters and 20 times on the regularization parameters. For the few-show learning experiments in Table 4, we use the validation set of Mini-ImageNet, following the training procedure of Dhillon et al. (2019) and search for 20 different trials.

We report the results for baselines by running the official open-sourced implementations. We describe the hyperparameters space for baselines as follows. For GCE (Zhang and Sabuncu, 2018), we search the factor $q$ in their proposed symmetric cross entropy loss. The factor $\alpha$ is searched in $\{0.1, 0.10, 0.50, 1.0\}$, and the factor $A$ is searched in $\{2, 4, 6, 8\}$. For DAC (Thulasidasan et al., 2019), we search the start abstention epoch in $\{3, 5, 8, 10, 15\}$ and set the other hyperparameters as the same in their paper. For APL (Ma et al., 2020), we choose the active loss as normalized cross entropy loss and the passive loss as reversed cross entropy loss. We search the loss factor $\alpha$ in $\{1, 10, 100\}$ and $\beta$ in $\{0.1, 1.0, 10\}$. For ELR (Liu et al., 2020), we search the momentum factor $\beta$ in $\{0.5, 0.7, 0.9, 0.99\}$ and the weight factor $\lambda$ in $\{0.05, 0.3, 0.5, 0.7\}$. For SAT (Huang et al., 2020), the start epoch is searched in $\{3, 5, 8, 10, 13\}$, and the momentum is searched in $\{0.6, 0.8, 0.9, 0.99\}$. We use the same number of trials in tuning hyperparameters for baselines.

### B.2 Extended experimental results

We present additional results. First, we apply our algorithm to another data set with label noise (same label noise as Table 3). Second, we apply our algorithm to sentence classification tasks.

**Additional results under label noise.** We report the test accuracy results of our algorithm on CUB-200-2011 and Flowers data sets with independent label noise in Table 5. From the table, we show that our algorithm still outperforms previous methods by a significant margin, which aligns with our results of the MIT-Indoor data set in Table 3.

**Results on ChestX-ray14.** We apply our approach to medical image classification, which is a more distant transfer task (relative to the source data set ImageNet). We report the mean AUROC (averaged over predicting all 14 labels) on the ChestX-ray14 data set in Table 6a. With layer-wise regularization, we see 0.39% improvement compared to the baseline methods.

**Results on ViT.** We apply our approach to fine-tuning pre-trained ViT (Dosovitskiy et al., 2020) from noisy labels, under the same setting as Table 3. Table 6b shows the result. First, we find that our approach improves upon the best regularization methods by 1.17% averaged over two settings. Second, we find that our approach also improves upon self-labeling by 13.57% averaged over two
settings. These two results again highlight that both regularization and self-labeling contribute to the final result. While regularization prevents the model from over-fitting to the random labels, self-labeling injects the belief of the fine-tuned model into the noisy data set.

**Extension to text classification.** We apply our algorithm in text data domains. We conduct an experiment on sentiment classification tasks using a three-layer feedforward neural network (or multi-layer perceptron). We considered six text classification data sets: SST (Socher et al., 2013), MR (Pang and Lee, 2005), CR (Hu and Liu, 2004), MPQA (Wiebe et al., 2005), SUBJ (Pang and Lee, 2004), and TREC (Li and Roth, 2002). We use SST as the source task and one of the other tasks as the target task. We compared our proposed algorithm with fine-tuning and L2-PGM (Gouk et al., 2021). In Table 7, we report the results evaluated under a setting with no label noise and a setting with independent label noise (same setting in Table 3). The results show our proposed algorithm can outperform these baseline methods under both settings.

**B.3 Ablation studies**

We describe several ablation studies. First, we compare the performance between using the Frobenius norm and the MARS norm proposed in Gouk et al. (2021). Second, we show the norm values of the adversarial robust pre-trained models in each layer and explain their improvement for fine-tuning on downstream tasks. Third, we compare our proposed layer-wise constraints and a constant and discuss their correlation to the generalization performance in Theorem 4.1. Fourth, we analyze the role of regularization in our proposed self label-correction method. Finally, we conduct an ablation study to study the influence of three components in our algorithm.

**Comparing layer-wise and constant regularization:** $\sum_{i=1}^{L} D_i^2$. To show the bound in Proposition 4.1 is nonvacuous, We compare the value of $\sum_{i=1}^{L} D_i^2$ from Equation 4 under both layer-wise constraints and constant regularization in Table 8. The values for every $D_i$ are from the parameters set in Table 2 for these data sets. We can see that layer-wise constraints incur a smaller value of $\sum_{i=1}^{L} D_i^2$ compared to constant regularization, which correlates with their better generalization performance.

**Comparing norms of adversarial robust pre-trained models.** We empirically observe that adversarially robust pre-trained models have lower Frobenius norms over each layer shown in Figure 6. The lower norms of robust models would induce smaller generation error, which explains their improvement in fine-tuning downstream tasks.

**Comparing label-correction precision with and without regularization.** We observe from Figure 5a that combining self-labeling and regularization is more effective than using just self-labeling. This is evidenced by the gap between correction with regularization and without regularization in the figure. In Table 9, we show the denominator of relabeling precision (i.e., the overall number of data points that are relabeled in line 7 of Algorithm 1) in the correction process. We find that the denominator is different between with and without regularization. The denominator is significantly smaller with regularization than without regularization, indicating that regularization prevents the model from over-fitting the noisy labels. The denominator decreases only with regularization. Without
Table 9: Denominator (total number of relabeled data points) and numerator (the number of correctly relabeled data) for calculating precision of label-correction in Figure 5a.

| Number of epoch | 1     | 4     | 7     | 10    | 13    | 16    | 19    | 21    |
|-----------------|-------|-------|-------|-------|-------|-------|-------|-------|
| denominator w/ regularization | 28    | 32    | 32    | 29    | 26    | 24    | 21    | 19    |
| numerator w/ regularization | 15    | 17    | 16    | 13    | 12    | 10    | 9     | 8     |
| denominator w/o regularization | 56    | 66    | 64    | 64    | 62    | 58    | 59    | 56    |
| numerator w/o regularization | 34    | 33    | 28    | 26    | 21    | 18    | 17    | 14    |

Table 10: Top-1 test accuracy of using different norms for fine-tuning ResNet-101 pre-trained on the ILSVRC-2012 subset of ImageNet. Results are averaged over 3 random seeds.

| Aircrafts       | CUB-200-2011 | Caltech-256 | Stanford-Cars | Stanford-Dogs | Flowers | MIT-Indoor |
|-----------------|--------------|-------------|---------------|---------------|---------|------------|
| PGM (MARS)      | 7.34±0.15    | 8.14±0.16   | 8.32±0.31     | 8.90±0.18     | 8.79±0.10 | 9.45±0.23  | 7.48±0.29 |
| PGM (ℓ²)        | 7.90±0.26    | 8.23±0.32   | 8.35±0.33     | 8.82±0.39     | 8.64±0.28 | 9.23±0.34  | 7.31±0.30 |
| Ours (MARS)     | 7.51±0.32    | 8.08±0.32   | 8.53±0.33     | 9.09±0.28     | 9.94±0.28 | 9.47±0.34  | 7.49±0.30 |
| Ours (ℓ²)       | 7.52±0.23    | 8.24±0.21   | 8.90±0.16     | 8.91±0.22     | 8.94±0.21 | 9.47±0.34  | 7.30±0.31 |

Table 11: Removing any component in our algorithm leads to worst performance. Results are on the Indoor data set with independent label noise. Results are averaged over 3 random seeds.

| Component           | Indoor 20% | independent noise 40% | indoor noise 60% | correlated noise 80% | correlated noise 25.18% |
|---------------------|------------|------------------------|------------------|----------------------|------------------------|
| REGSL (ours)        | 72.51±0.46 | 68.13±0.16             | 57.59±0.55       | 34.08±0.79           | 70.12±0.83             |
| w/o regularization  | 71.94±0.43 | 67.84±0.38             | 57.24±0.43       | 33.78±0.30           | 69.43±0.36             |
| w/o label correction| 70.92±0.41 | 59.10±0.24             | 47.81±0.35       | 28.42±0.46           | 69.78±0.34             |
| w/o label removal   | 70.32±0.65 | 66.57±0.76             | 55.37±0.28       | 29.43±0.88           | 67.96±0.49             |
| w/o self-labeling   | 70.23±0.25 | 64.40±0.58             | 54.20±0.68       | 32.54±0.43           | 69.05±0.09             |

Comparing ℓ² norm and the MARS norm. We report the results of using different norms for constraints in our algorithm in Table 10. We compare the performance of the Frobenius norm (ℓ²), and the MARS norm proposed in (Gouk et al., 2021). From the table, we show that the results of the two norms are similar. In the paper, we focus on the Frobenius norm for our discussion.

Influence of different components in REGSL. We study the influence of each component of our algorithm: layer-wise constraint, label correction, and label removal. We remove these components, respectively, and run the same experiments on the MIT-Indoor dataset with different kinds of label noise. Furthermore, we also include a row of results using only layer-wise constraints without self-labeling (containing label correction and removal). As shown in Table 11, removing any component from our algorithm could hurt the performance. This suggests that only incorporating these components can prevent both over-fitting and label memorization of models. In addition, We can see from Table 11 that when the noise rate is 20%, the self-labeling part (including label correction and removal) is more critical than regularization. When the noise rate is 40% or higher, the label correction part is the most important.

C Limitation

Our work focuses on the regularization and robustness properties of fine-tuning. We mainly focus on feedforward neural networks, including convolutional neural networks. Thus, we have not considered Other settings such as recurrent neural networks in this work. We mainly focus on independent label noise for evaluating the robustness. Other types of label noise, for example, using weak supervision, are not well-understood. This is left for future work. Finally, our treatment of label noise using self-labeling is based on empirical heuristics. It would be fascinating to come up with a more principled approach to tackle label noise.