BETTER OPTIMIZATION CAN REDUCE SAMPLE COMPLEXITY: ACTIVE SEMI-SUPERVISED LEARNING VIA CONVERGENCE RATE CONTROL

Anonymous authors
Paper under double-blind review

ABSTRACT

Reducing the sample complexity associated with deep learning (DL) remains one of the most important problems in both theory and practice since its advent. Semi-supervised learning (SSL) tackles this task by leveraging unlabeled instances which are usually more accessible than their labeled counterparts. Active learning (AL) directly seeks to reduce the sample complexity by training a classification network and querying unlabeled instances to be annotated by a human-in-the-loop. Under relatively strict settings, it has been shown that both SSL and AL can theoretically achieve the same performance of fully-supervised learning (SL) using far less labeled samples. While empirical works have shown that SSL can attain this benefit in practice, DL-based AL algorithms have yet to show their success to the extent achieved by SSL. Given the accessible pool of unlabeled instances in pool-based AL, we argue that the labeling sample efficiency brought by AL algorithms that seek diversity is marginal when using SSL as the training scheme. Equipped with a few theoretical insights, we designed an AL algorithm that rather focuses on controlling the convergence rate of a classification network by actively querying instances to improve the rate of convergence upon inclusion to the labeled set. We name this AL scheme convergence rate control (CRC), and our experiments show that a deep neural network trained using a combination of CRC and a recently proposed SSL algorithm can quickly achieve high performance using far less labeled samples than SL. In contrast to a few works combining independently developed AL and SSL (ASSL) algorithms, our method is a natural fit to ASSL, and we hope our work can catalyze research combining AL and SSL as opposed to an exclusion of either.

1 INTRODUCTION

The data-hungry nature of supervised deep learning (DL) algorithms has spurred interest in active learning (AL), where a model can interact with a dedicated annotator and request unlabeled instances to be labeled. In the pool-based AL setting, a model initially has access to a set of unlabeled samples and can query instances which need be labeled for training. Under certain conditions on the task, AL can provably achieve up to exponential improvement in sample complexity and thus has great potential for reducing the number of labeled instances required to achieve high accuracy. This is especially important when the annotation task is extremely costly, for example, in medical imaging where only highly-specialized experts can diagnose a subject's condition.

Active learning algorithms have been extensively explored, but its ill-posed nature engendered various formulations including uncertainty-based sampling (Wang & Shang, 2014), aligning the labeled and unlabeled distributions (Gissin & Shalev-Shwartz, 2019) with connections to domain adaptation (Ben-David et al., 2010), and coreset (Sener & Savarese, 2018). Furthermore, there is no standard method in modeling a deep neural network's (DNN) uncertainty, and uncertainty-based AL has its own variants ranging from utilizing Bayesian networks (Kirsch et al., 2019) to using a model's predictive confidence (Wang & Shang, 2014). This ambiguous characterization of how much information a sample's label carries also motivated AL algorithms based on maximizing the expected change of a classification model (Huang et al., 2016; Ash et al., 2020).

Algorithm 1 Active Semi-Supervised Learning

for each query iteration $i = 1, ..., N$ **do**
  Train a classifier f_θ using some SSL algorithm on $(\mathcal{X}_L, \mathcal{X}_U)$ until convergence.
  Retrieve unlabeled samples $\mathcal{X}_u^* \subset \mathcal{X}_U$ using Alg. 2 and obtain their labels.
  Update labeled and unlabeled pools $\mathcal{X}_L \leftarrow \mathcal{X}_L \cup \mathcal{X}_u^*$, $\mathcal{X}_U = \mathcal{X}_U \backslash \mathcal{X}_u^*$.
end for

While AL comes with optimistic potentials, most algorithms outperform random sampling (passive learning) by only a small margin, with follow-up works (Gissin & Shalev-Shwartz, 2019; Sener & Savarese, 2018; Ducoffe & Precioso, 2018) reporting worse performance of certain AL algorithms than random sampling due to different architectures or datasets. Furthermore, the performance of AL algorithms are usually reported by training a model using supervised learning (SL) on the queried labeled data despite the availability of unlabeled data in pool-based AL. Semi-supervised learning (SSL) has recently shown impressive performance with a small number of labeled instances, and its most premature variant known as pseudo-labeling (Lee, 2013) has been combined with AL algorithms (Wang et al., 2017). One recent work (Song et al., 2019) uses a rather modern SSL algorithm (Berthelot et al., 2019) and shows the strength of combining AL with SSL which we name ASSL. However, their results are limited to independent combinations of AL and SSL.

In this work, we propose a novel query strategy which naturally blends in with SSL, and show that our AL algorithm can rapidly achieve the high performance of fully-supervised algorithms using very few labeled data. Our algorithm is inspired by recent developments in DNN theory, namely the neural tangent kernel (NTK) (Jacot et al., 2018). Experimental comparisons with diversity-seeking strategies and an algorithm with an objective similar to ours demonstrate how labeling instances based on our objective helps SSL attain high performance in a sample-efficient manner.

2 Background Theory

2.1 Sample Efficiencies of Active Learning and Semi-Supervised Learning

Here we informally describe some theoretical results describing the superiority of SSL to SL and AL to passive learning in terms of labeled sample complexity, that is, the number of labeled instances that can be used to attain ϵ-classification error. Because pool-based AL already subsumes unlabeled instances, it makes much more sense to perform SSL on the readily available unlabeled instances when training a classification network between each query iteration (Alg. 1). This section serves to motivate why AL and SSL algorithms should consider different objectives when used together.

It is well known that SL can find an ϵ-optimal classifier from a sufficiently rich class of hypotheses (e.g. classifiers which can be realized by deep neural networks) using $\tilde{\Theta}\left(\frac{1}{\epsilon}\right)$ i.i.d samples for the separable case and $\tilde{\Theta}\left(\frac{1}{\epsilon^2}\right)$ in the agnostic case (Massart & Nédélec, 2006; Vapnik & Izmailov, 2015)[1]. In contrast, actively adding instances to the (labeled) training set can sometimes improve the sample complexity sub-exponentially from $O(1/\epsilon)$ to $O(\text{poly} \log 1/\epsilon)$ (Balcan et al., 2010). When unlabeled instances are drawn i.i.d., Balcan & Urner (2016) show how labeling samples selected via binary search over $\tilde{O}(1/\epsilon)$ unlabeled instances can achieve exponential improvement over passive learning.

Göpfert et al. (2019) constructed a few examples which show how an SSL algorithm can use unlabeled instances to significantly improve the labeled sample complexity for a rather restricted class of data distributions. A corollary of one such example is that using $O(\log 1/\epsilon)$ labeled samples and $O(1/\epsilon^2)$ unlabeled samples can be used to obtain ϵ-error. Considering a target error $\epsilon \approx 6\%$ achieved by fully-supervised learning in CIFAR10 using $O(1/\epsilon) \approx 50,000$ labeled samples, a training set with only $O(\text{poly} \log(1/\epsilon)) \approx 250$ labeled samples and leaving the remaining $O(1/\epsilon) \approx 49,750$ samples unlabeled is analogous to the aforementioned sample complexities achievable in the respective AL and SSL settings, although their assumptions may not be satisfied.

Given two exponential efficiency improvements potentially attained by pool-based AL and SSL, it is less appealing to formulate the same objective for both AL and SSL algorithms, as their combined benefit is most likely marginal. Instead, we take the underlying intuitions to suggest using

[1] Here we slightly abuse the $\tilde{\Theta}$ notation to denote upper and lower bounds matching up to logarithmic factors.

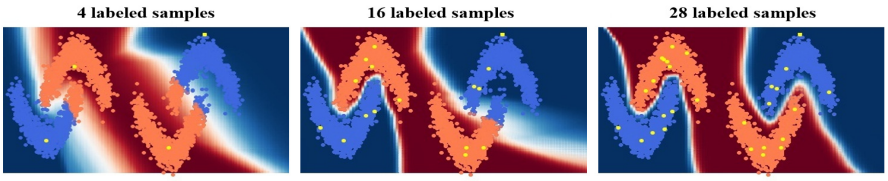

Figure 1: Illustration of how a Π-model's (Laine & Aila, 2017) decision boundary changes as the proposed algorithm enlarges the labeled set. The 4 initial pivot points were manually selected.

an AL algorithm that queries instances to help optimization. Specifically, we would like an AL algorithm to construct a labeled dataset such that a classifier $f^{(T)}$ trained for T iterations rapidly minimizes the optimization error $|f^{(T)} - f^{(\infty)}|$, and formulate an SSL objective $\mathcal{L}_n(f)$ to guide the target classifier $f^{(\infty)} \in \arg\min_f \mathcal{L}_n(f)$ towards a solution that minimizes $|f^{(\infty)} - f^*|$, where $f^* \in \arg\min_f \mathbb{E}\left[\mathcal{L}_n(f)\right]$ is the optimal classifier and $\mathcal{L}_n$ is the empirical loss computed over n samples. Together, the resulting model would ultimately minimize the generalization error's upper bound: $|f^{(T)} - f^*| \leq |f^{(T)} - f^{(\infty)}| + |f^{(\infty)} - f^*|$. The next section shows how we can carefully design labeled and unlabeled sets such that a classifier trained on this construction enjoys a fast rate of convergence by employing a recently developed tool known as the NTK.

2.2 Neural Tangent Kernel

The neural tangent kernel (NTK) (Jacot et al., 2018) is a theoretical tool developed to understand how overparametrized networks can be well-optimized and generalize to unseen data. In particular, the training dynamics of DNNs parameterized by θ_t at any iteration t follows a closed form expression

$$\frac{df_{\theta_t}(\mathcal{X})}{dt} = -\hat{\mathcal{K}}^{(t)}(\mathcal{X}, \mathcal{X})\left(f_{\theta_t}(\mathcal{X}) - \mathcal{Y}\right). \tag{1}$$

when minimizing the mean-squared error (MSE) loss using gradient descent, where $\hat{\mathcal{K}}^{(t)}(\mathcal{X}, \mathcal{X}) = \left[\nabla_\theta f_{\theta_t}(x)^T \nabla_\theta f_{\theta_t}(x')\right]_{(x,x') \in \mathcal{X} \times \mathcal{X}}$ is the empirical NTK (Arora et al., 2019) with $\nabla_\theta f_{\theta_t}(x)^T \nabla_\theta f_{\theta_t}(x') \in \mathbb{R}^{C \times C}$ vectorized over a set of instances $\mathcal{X}$. If we let the width of all layers grow to infinity, a remarkable property holds in which the training dynamics can be characterized using a matrix independent of time, namely the NTK $\mathcal{K}$:

$$\frac{df_{\theta_t}(\mathcal{X})}{dt} = -\mathcal{K}(\mathcal{X}, \mathcal{X})\left(f_{\theta_t}(\mathcal{X}) - \mathcal{Y}\right) \tag{2}$$

with probability 1 over random initialization[2]. For any network of finite width d trained for t iterations, the relation (2) holds with probability $\geq 1 - \delta_d$, where $\delta_d \to 0$ as $d \to \infty$.

Assuming a network that satisfies the differential equation, the transient solution is given by

$$f_{\theta_t}(\mathcal{X}) = \sum_i c_i v_i \exp\left(-\lambda_i(\mathcal{X}) t\right) \tag{3}$$

for some constants c_i and eigenvalue/vector pairs (λ_i, v_i) of the NTK $\mathcal{K}(\mathcal{X}, \mathcal{X})$. Notice how the NTK, and in turn the convergence rate, depends on the set of instances $\mathcal{X}$ it is computed over. This sparks the intuition that the rate of convergence can be *controlled* by carefully designing a labeled set.

3 Active Learning via Convergence Rate Control

3.1 Convergence Rate Control

Inspired by the aforesaid NTK's characterization of the model's training dynamics when supervised on the dataset it is computed over, we propose to move unlabeled instances $\mathcal{X}_u^*$ selected from a

[2]Formally, the dynamics $\frac{df_{\theta_t}(\mathcal{X})}{dt}$ converges to the RHS in probability as the network's width sequentially grows to infinity when initialized using He initialization.

pool of unlabeled samples $\mathcal{X}_U$ that maximize the rate of convergence of the SGD dynamics to the labeled set $\mathcal{X}_L$, hence the name convergence rate control (CRC). While Eq. 3 is a solution to the time-inhomogeneous ODE in Eq. 2, the performance of infinitely-wide networks fall behind their finite-width counterparts. We thus replace the eigen-pair (λ, v) of the true NTK $\mathcal{K}$ with its empirical NTK $\hat{\mathcal{K}}^{(T)}$ in Eq. 1 using a model trained for T epochs until its validation accuracy saturates.

Maximizing the eigenvalues of the NTK is a multi-objective problem, and CRC takes a worst-case approach to select unlabeled instances that maximize the smallest eigenvalue of the NTK:

$$\max_{\mathcal{X}_u \subset \mathcal{X}_U} \min_{i \in |\mathcal{X}_L \cup \mathcal{X}_u|} \lambda_i \left(\hat{\mathcal{K}}^{(T)} \left(\mathcal{X}_u \cup \mathcal{X}_L, \mathcal{X}_u \cup \mathcal{X}_L \right) \right). \tag{4}$$

In general, the eigenvalue distribution is not necessarily supported over positive values, and we observed that considering only positive eigenvalues consistently results in higher performance than when considering both negative and positive eigenvalues. CRC thus scores unlabeled instances as the minimum over positive eigenvalues. Each block $\hat{\mathcal{K}}^{(T)}(x, x') \in \mathbb{R}^{C \times C}$ is replaced by its trace computed as $\sum_c \hat{\mathcal{K}}_{cc}^{(T)}(x, x')$, which we numerically found to be an accurate replacement to the block matrices in computing the minimum eigenvalue, to reduce both computational and memory complexities. The solution to Eq. 4 can then be found using dedicated GPU-implementations available in popular DL frameworks such as PyTorch. This algorithm is detailed in Alg. 2.

A labeled sample's influence on a DNN's predictive behavior is abstruse. Intuitively, a labeled sample may be most informative when it is near a region separating different classes; however, this does not guarantee that a DNN learns such a decision boundary effectively. Furthermore, it is unclear whether a sample in some other region could better enhance a classifier's performance when added to the labeled set, especially when considering SSL algorithms which complicate DL analysis. Contrary to the above intuition, Rebuffi et al. (2019) demonstrates how a DNN trained with a SSL objective (Laine & Aila, 2017) learns a decision boundary using only 4 manually selected pivot points not on the class-separating region. Figure 1 illustrates how the classifier's decision boundary progressively forms near low-density regions as CRC enlarges the labeled set.

3.2 Practical Considerations

Summing the network's gradients over all layers for each instance pair is infeasible for modern network architectures, and we compare one realization of using all parameters with the final layer's to compute the NTK. A comparison of one realization using the NTK computed over all layers vs. using just the final layer averaged over 3 trials (Tab. 1) shows how the final layer performs just as well as when all layers were used but with much faster ($\times 100$) queries. If we assume that the shallow layers saturate more quickly than deeper layers, justified by the 'lower layers learn first' phenomenon (Raghu et al., 2017), the NTK estimate computed at the network's last layer is a prediction of the training dynamics corresponding to a single layer perceptron attached to a (slowly-changing) feature extractor. In this perspective, the final accuracy is mostly affected by the final layer which determines how high-level features are recognized, and designing a labeled set using the NTK estimated over the last layer would sufficiently capture the model's training dynamics.

Query step	0	1	2
Last	53.12±5.50	67.14±4.28	71.98±4.04
All	50.47	68.25	74.03

Table 1: CRC performances when NTK is computed over final vs. all layers with $G = 5$ at $Q = 50$. Initial performance difference is due to using a randomly initialized model and not random sampling.

One reason why estimating the training dynamics over all layers could be *worse* than using the last is that the former requires a network trained in the next SSL phase to learn a similar low-level representation to that obtained in the previous SSL phase. However, it was observed by Raghu et al. (2017) that two randomly initialized networks trained on the same dataset have similar final layers but extremely different intermediate representations. Because our networks are retrained from scratch between each query iteration, it is highly likely that the next network will have very different intermediate representations, and these middle layers would provide noisy estimates as to how much

Algorithm 2 Convergence Rate Control (solving equation 4)

Inputs: Unlabeled pool $\mathcal{X}_U$, query-size Q, group-size G.
Output: New pool $\mathcal{X}_u^*$ to be labeled.
for $t = 1, \cdots Q/G$ **do**
  $\mathcal{X}_u^{(t)} \leftarrow G$ unlabeled instances randomly sampled from $\mathcal{X}_U$.
  $s(\mathcal{X}_u^{(t)}) \leftarrow \lambda_{\min}^{+}\left(\mathcal{X}_L \cup \mathcal{X}_u^{(t)}\right)$ using the empirical NTK computed over final layers.
end for
Store Q/G highest groups: $t_1^*, \ldots t_{Q/G}^* \leftarrow \arg\max(s)$.
return $\mathcal{X}_u^* \leftarrow \mathcal{X}_u^{(t_1^*)} \cup \cdots \cup \mathcal{X}_u^{\left(t_{Q/G}^*\right)}$.

the model's functional representation would be affected by the enlarged dataset. Since we are seeking to modify a dataset in order to amplify a model's performance, it is reasonable that we enlarge the labeled set based on how much the additional samples would affect the model's final layers. Had we designed the experiments such that a model is continuously trained from its previous SSL phase, computing the NTK over all layers may have been beneficial at the expense of computation.

3.3 Myopic vs. Batch-Mode Active Learning

Myopic AL policies refer to algorithms that score unlabeled instances based on their individual importance. Considering how an expert annotator 'in-the-loop' must label queried samples, it is desirable that an AL algorithm queries large batches based on their collective importance. Myopic policies usually degrade in performance as the query size Q increases, as they may repetitively sample identical instances (Kirsch et al., 2019), and it has been of great interest in designing a computationally efficient batch-AL algorithm. CRC (Alg. 2) is a batch-mode AL algorithm as it computes $\lambda_{\min}$ over groups of unlabeled instances $\mathcal{X}_u$. To cope with the combinatorial complexity associated with the outer-maximization in Eq. 4, we randomly sample candidate groups $\mathcal{X}_u$ without replacement. This randomization significantly reduces the search space, potentially yielding highly sub-optimal solutions, and we introduce a hyperparameter G such that G divides Q, and search over candidate groups $|\mathcal{X}_u| = G$, selecting Q/G groups at each query step. The group size controls whether the outer maximization is solved more accurately ($G = 1$) without considering the collective significance of a group, or the inner-minimization incorporates the collective importance of all queried samples ($G = Q$) at the expense of a substantially smaller search space. This trade-off is established in Tab. 2 when $Q = 100$ over a single realization for $G = 2, 5$ and average over 3 trials for $G = 10$. Our relatively small group-sizes make the cubic complexity of the inner-minimization negligible, and a larger group size is consequently faster due to less ($Q \to Q/G$) eigen-decomposition operations and inefficient batch-gradient computations in autograd packages. All experiments hereon use $G = 5$ for $Q = 50$ and $G = 10$ considering the speed vs. performance trade-off.

Query step	1	2	3
$G = 2$	75.15	87.07	87.66
$G = 5$	83.93	86.61	89.59
$G = 10$	83.38 ± 1.14	85.71 ± 1.50	88.07 ± 0.06

Table 2: Effect of different group sizes with $Q = 100$.

3.4 Relation to Gradient-based Methods

The proposed algorithm can be interpreted as measuring the importance of unlabeled instances by how much they would change a model's parameters. Two AL algorithms are similar in this manner in that they seek to label instances which affect the model the most: expected gradient length (EGL) (Huang et al., 2016) and BADGE (Ash et al., 2020). EGL first computes the gradient of the cross-entropy loss over all unlabeled instances, replacing the ground truth target with an expectation over a posterior distribution determined by the trained model, then selects instances with the greatest norm. BADGE uses an embedding of the loss' gradients using predicted classes, computed over the parameters in just

the final layer, and uses kmeans++ to enforce diversity. Nonetheless, both algorithms only estimate the benefit due to candidate unlabeled samples and do not consider the labeled set's influence.

4 EXPERIMENTS

4.1 IMPLEMENTATION DETAILS

Our SSL implementation is primarily based on a publicly-available PyTorch implementation[3] of FixMatch (Sohn et al., 2020) and guided by suggestions made in Oliver *et al.* (Oliver et al., 2018). In particular, we used the WRN-28-2 architecture further motivated by the derivation of NTK as a network in its infinite width limit. FixMatch is a variant of MixMatch (Berthelot et al., 2019), replacing standard augmentations with more powerful augmentation techniques when computing the SSL loss. In short, FixMatch enforces consistency between a classification model's predictions on perturbed inputs which effectively yields a more robust model with small Jacobian norm (Athiwaratkun et al., 2019) in junction with other SSL algorithms including mean teacher (Tarvainen & Valpola, 2017). Furthermore, the hyperparameters in FixMatch were kept the same across different dataset sizes in their original report, making our experimental comparisons convenient.

The initial pool of labeled instances significantly affected the downstream SSL task and subsequent AL queries, especially for uncertainty-based algorithms (see section 4.2). It is practical to assume that a model would initially have access to a small pool of labeled images with an equal number of classes. Thus, we randomly sampled a balanced number of images per class in the first query iteration and use the AL algorithms in subsequent queries without enforcing balanced classes. Between each query step, the classification network is trained until either its validation accuracy does not improve for 50 epochs or 310 epochs is reached, except for confidence and EGL maxed at 350 for their low performances. All experiments are repeated 3 times with mean $\pm$ std performances reported unless stated otherwise. Our implementation will be open-sourced upon publication.

4.2 BASELINE ALGORITHMS

Both AL and SSL algorithms demand much more time than standard supervised learning, and an extensive comparison of all ASSL combinations is beyond our compute availability. We resort to comparing the proposed algorithm with 3 other AL algorithms, 2 of which scores unlabeled instances based on how much they reduce a model's uncertainty, and the other because of its similarity to CRC. Uncertainty-based AL (Wang & Shang, 2014) is one of the simplest DL-based AL algorithm that selects the unlabeled instance with lowest confidence in its prediction: $\mathcal{X}_u^* = \arg\min_{\{x \in \mathcal{X}_U\}} \max_y f_{\theta,y}(x)$ In the same work, Wang & Shang (2014) proposed to also use entropy as a measure of the model's uncertainty in unlabeled samples. EGL (Huang et al., 2016) retrieves instances that modify a model the most: $\mathcal{X}_u^* = \arg\max_{\{x \in \mathcal{X}_U\}} \mathbb{E}_{y \sim \hat{p}(\cdot;x,\theta)} \left[\|\nabla_\theta H\left(y, f_\theta(x)\right)\|^2 \right]$ where $\hat{p}(y; x_i, \theta) = f_{\theta,y}(x_i)$ is the model's confidence in class y and H is the cross entropy function.

4.3 ACTIVE SEMI-SUPERVISED LEARNING

Here we report the sample efficiencies obtained by using non-random query strategies on the CIFAR10 dataset in Tab. 3. For reference, a model trained using FixMatch attains accuracy ranging from 10% to 84% using 1 labeled image per class and an average of 94.93% accuracy using 25 labeled image per class. Note however, that this is expected to be an upper bound on our experiments, as the original implementation trains a model for 1024 epochs (roughly $\times 3 \sim 5$ more than ours) and training images are sampled guaranteeing an equal number of images per class.

One difficulty arising from the ASSL setting is class imbalance. In contrast to standard AL settings that consider much larger query sizes, the small query size in ASSL significantly impacts the class distribution, resulting in occasional performance drop for certain query strategies. Entropy has repeatedly achieved state-of-the-art performance (Gissin & Shalev-Shwartz, 2019; Wang et al., 2017; Ash et al., 2020) in AL settings despite its simplicity, and our experiments show the same holds for ASSL. Conforming with our motivation in section 2.1, CRC performed comparable or better than entropy although it does not explicitly enforce diversity on the labeled set. Furthermore, while

[3]https://github.com/kekmodel/FixMatch-pytorch

Accuracy (%)	Q=50			Q=100		
# Labeled images	100	150	200	200	300	400
Random	69.81±4.77	82.14 ±2.30	82.41±0.68	85.04±1.53	**87.09**±1.25	87.14±1.06
Entropy	72.43±8.21	82.41±2.89	83.38±1.93	**85.51**±1.47	86.89±0.47	86.87±1.22
Confidence	52.54±7.71	49.55±7.77	46.52±4.04	77.05±4.66	75.14±4.40	-
EGL	57.18±7.41	56.67±10.53	69.09±13.12	79.95±3.11	80.41±2.77	81.20±5.10
CRC†	**78.41**±3.16	**83.67**±3.24	**86.51**±1.52	83.38±1.11	85.71±1.40	**88.08**±0.05

Table 3: ASSL performances using $Q \in \{50, 100\}$ when the initial labeled set is randomly sampled.

both CRC and EGL scores instances by estimating how much they would affect the model's training dynamics, only CRC outperformed random sampling. Our results suggest that actively enlarging the labeled set can definitively reduce the labeled sample complexity in the SSL setting, without having to construct a labeled set consisting of images representative of their class.

Existing DL-based AL algorithms have performed comparably to random sampling when using large query sizes, and our experiments show the same for entropy and CRC with $Q = 100$ in the ASSL setting. A proper AL algorithm should achieve higher performance at the same number of labeled samples if the query size is small since it would be taking more query steps in order to claim its superiority to random sampling; however, we observed that only CRC satisfies this property. EGL's low performance had been reported on image classification tasks (Gissin & Shalev-Shwartz, 2019; Sener & Savarese, 2018; Ducoffe & Precioso, 2018) under the AL setting. Our experimental design of retraining networks from scratch may have had negative influence on EGL, similar to how it affected the NTK estimate over all layers. We attribute confidence's low performance to the poor calibration of DNNs (Guo et al., 2017), inadequately capturing the model's uncertainty on unlabeled instances. A successful application of confidence-based query may require incorporating calibration while training classification networks or before performing such queries.

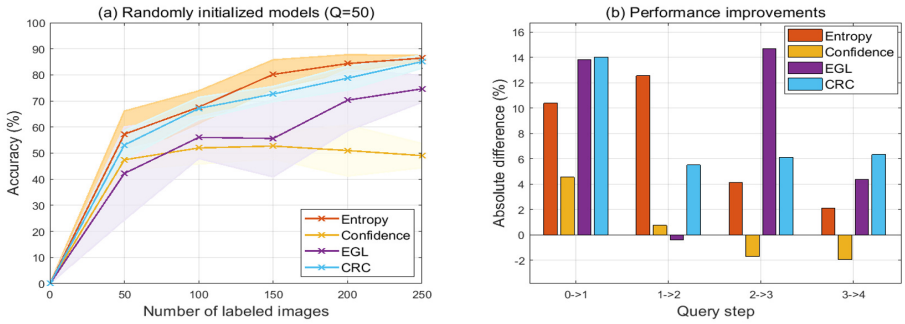

Figure 2: Performances when the initial AL queries were performed using a randomly initialized model. The figure on the right underscores performance gains in consecutive query steps.

In principle, all query strategies using a randomly initialized network should behave similarly to random sampling. As shown in Fig. 2, however, sampling the initial labeled set using a randomly initialized model adversely affected all subsequent queries. While entropy and CRC overcome this initial disadvantage after a few query iterations, other baselines tend to under-perform random sampling due to this initial disadvantage that affects subsequent queries. This phenomenon has not been reported in previous works, and whether this is an artifact of our ASSL setting or the architecture/hyperparameters used deserves future notice.

4.4 Convergence Rate and Time Horizon Prediction

The proposed CRC algorithm is designed to query unlabeled instances that improve the rate of convergence a DNN in the following SSL phase. To see if our algorithm achieves this purpose, we plot the empirical NTK's minimum eigenvalues used to score unlabeled instance groups against the number of training epochs until the test *loss* reaches its global minimum in Fig. 3 (a) to show how the minimum eigenvalues are predictive of the time horizon. Global minimum here refers to the value for

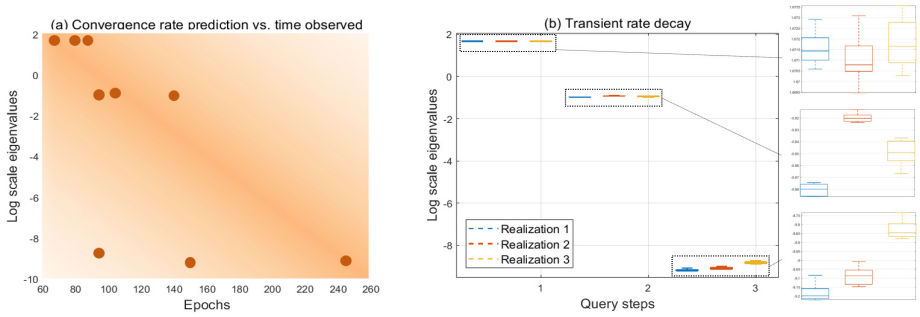

Figure 3: Minimum eigenvalues' distribution in log-scale ($Q = 50$). Left figure shows how informative the minimum eigenvalues are in terms of predicting the number of epochs required for convergence, and right figure illustrates how the minimum eigenvalues' distribution concentrates towards zero. Negative linear slope implies (a) exponential convergence as predicted by Eq. 3 and (b) slower convergence rate with increasing labeled set size.

which the loss never falls below until training completes. We additionally plot how the minimum eigenvalues' distribution progresses as the labeled set is enlarged, with Fig. 3 (b) showing that the eigenvalue distribution concentrates towards 0 as the labeled set grows, implying slower convergence rates. A similar observation was made by Nitanda & Suzuki (2020) where the authors showed how the true NTK's eigenvalues concentrate towards zero as the training set size increases, whereas our plot is over a union of labeled and queried groups. This figure illustrates how all candidate datasets will inevitably have eigenvalue distributions concentrated near zero, but the enlarged dataset chosen by CRC will have the fastest convergence rate among all considered candidates.

5 Conclusion

This work motivated the combination of AL with SSL, using the former for optimization and latter objective to restrict the hypothesis space to those that generalize well. We then proposed an AL algorithm inspired by the NTK, and demonstrated how controlling the convergence rate of the training dynamics can significantly improve sample efficiency. To the best of our knowledge, this work is the first practical application of NTK outside of supervised learning, where it has been shown that the true NTK is inferior to its DNN counterpart. In contrast to most DL-based AL experiments which have been conducted using relatively small networks, this work demonstrates that DL can benefit from AL even when modern architectures are used. Our algorithm outperformed uncertainty-based AL algorithms which enforce diversity and an AL algorithm with a similar goal of maximizing the model's change. The proposed algorithm's superiority was also demonstrated in the batch-AL setting, where an optional hyperparameter can be used to control the trade-off between computational complexity and performance.

Our CRC algorithm is developed under the assumption that a well-optimized network $f^{(\infty)}$ induced by the SSL objective is a good approximation of a model f^* that generalizes well. Incorporating the interplay between AL and SSL seems promising in further reducing the sample complexity, designing either an SSL algorithm best fit for some fixed AL algorithm or a joint ASSL scheme. For example, CRC provides an estimate on the number of epochs required for convergence, and a learning rate schedule best fit for the estimated time horizon could be used (Ge et al., 2019).

The proposed CRC algorithm can be extended in several directions, applying generalization guarantees characterized by the NTK to an online (streaming) setting where unlabeled instances cannot be stored. Another exciting direction to pursue would be to use the True NTK (Arora et al., 2019; Novak et al., 2020) to estimate the training dynamics. While CRC is motivated by controlling the transient solution using an estimated proxy of the training dynamics, the true NTK would enable an exact computation of the ODE solution. Of utmost importance would be that this could allow AL queries to be performed offline, that is, without having to train a model between each query iteration, alleviating the long training times associated with ASSL.

REFERENCES

Sanjeev Arora, Simon S Du, Wei Hu, Zhiyuan Li, Russ R Salakhutdinov, and Ruosong Wang. On exact computation with an infinitely wide neural net. In H. Wallach, H. Larochelle, A. Beygelzimer, F. dAlché-Buc, E. Fox, and R. Garnett (eds.), *Advances in Neural Information Processing Systems 32*, pp. 8141–8150. Curran Associates, Inc., 2019.

Jordan T. Ash, Chicheng Zhang, Akshay Krishnamurthy, John Langford, and Alekh Agarwal. Deep batch active learning by diverse, uncertain gradient lower bounds. In *International Conference on Learning Representations*, 2020.

Ben Athiwaratkun, Marc Finzi, Pavel Izmailov, and Andrew Gordon Wilson. There are many consistent explanations of unlabeled data: Why you should average. In *International Conference on Learning Representations*, 2019.

Maria-Florina Balcan and Ruth Urner. *Active Learning – Modern Learning Theory*, pp. 8–13. Springer New York, New York, NY, 2016. ISBN 978-1-4939-2864-4. doi: 10.1007/978-1-4939-2864-4_769.

Maria-Florina Balcan, Steve Hanneke, and Jennifer Vaughan. The true sample complexity of active learning. *Machine Learning*, 80:111–139, 09 2010. doi: 10.1007/s10994-010-5174-y.

Shai Ben-David, John Blitzer, Koby Crammer, Alex Kulesza, Fernando Pereira, and Jennifer Vaughan. A theory of learning from different domains. *Machine Learning*, 79:151–175, 2010.

David Berthelot, Nicholas Carlini, Ian Goodfellow, Nicolas Papernot, Avital Oliver, and Colin Raffel. Mixmatch: A holistic approach to semi-supervised learning. *arXiv preprint arXiv:1905.02249*, 2019.

Melanie Ducoffe and Frederic Precioso. Adversarial active learning for deep networks: a margin based approach. 02 2018.

Rong Ge, Sham M Kakade, Rahul Kidambi, and Praneeth Netrapalli. The step decay schedule: A near optimal, geometrically decaying learning rate procedure for least squares. In H. Wallach, H. Larochelle, A. Beygelzimer, F. dAlché-Buc, E. Fox, and R. Garnett (eds.), *Advances in Neural Information Processing Systems 32*, pp. 14977–14988. Curran Associates, Inc., 2019.

Daniel Gissin and Shai Shalev-Shwartz. Discriminative active learning, 07 2019.

Christina Göpfert, Shai Ben-David, O. Bousquet, S. Gelly, I. Tolstikhin, and Ruth Urner. When can unlabeled data improve the learning rate? In *COLT*, 2019.

Chuan Guo, Geoff Pleiss, Yu Sun, and Kilian Q. Weinberger. On calibration of modern neural networks. In *Proceedings of the 34th International Conference on Machine Learning - Volume 70*, ICML'17, pp. 1321–1330. JMLR.org, 2017.

Jiaji Huang, Rewon Child, Vinay Rao, Hairong Liu, Sanjeev Satheesh, and Adam Coates. Active learning for speech recognition: the power of gradients. 12 2016.

Arthur Jacot, Franck Gabriel, and Clement Hongler. Neural tangent kernel: Convergence and generalization in neural networks. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett (eds.), *Advances in Neural Information Processing Systems 31*, pp. 8571–8580. Curran Associates, Inc., 2018.

Andreas Kirsch, Joost van Amersfoort, and Yarin Gal. Batchbald: Efficient and diverse batch acquisition for deep bayesian active learning. In H. Wallach, H. Larochelle, A. Beygelzimer, F. dAlché-Buc, E. Fox, and R. Garnett (eds.), *Advances in Neural Information Processing Systems 32*, pp. 7026–7037. Curran Associates, Inc., 2019.

Samuli Laine and Timo Aila. Temporal ensembling for semi-supervised learning. In *ICLR (Poster)*. OpenReview.net, 2017.

Dong-Hyun Lee. Pseudo-label : The simple and efficient semi-supervised learning method for deep neural networks. *ICML 2013 Workshop : Challenges in Representation Learning (WREPL)*, 07 2013.

Pascal Massart and Élodie Nédélec. Risk bounds for statistical learning. *The Annals of Statistics*, 34, 10 2006. doi: 10.1214/009053606000000786.

Atsushi Nitanda and Taiji Suzuki. Optimal rates for averaged stochastic gradient descent under neural tangent kernel regime, 06 2020.

Roman Novak, Lechao Xiao, Jiri Hron, Jaehoon Lee, Alexander A. Alemi, Jascha Sohl-Dickstein, and Samuel S. Schoenholz. Neural tangents: Fast and easy infinite neural networks in python. In *International Conference on Learning Representations*, 2020.

Avital Oliver, Augustus Odena, Colin A Raffel, Ekin Dogus Cubuk, and Ian Goodfellow. Realistic evaluation of deep semi-supervised learning algorithms. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett (eds.), *Advances in Neural Information Processing Systems 31*, pp. 3235–3246. Curran Associates, Inc., 2018.

Maithra Raghu, Justin Gilmer, Jason Yosinski, and Jascha Sohl-Dickstein. Svcca: Singular vector canonical correlation analysis for deep learning dynamics and interpretability. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett (eds.), *Advances in Neural Information Processing Systems 30*, pp. 6076–6085. Curran Associates, Inc., 2017.

Sylvestre-Alvise Rebuffi, Sebastien Ehrhardt, Kai Han, Andrea Vedaldi, and Andrew Zisserman. Semi-supervised learning with scarce annotations. *Technical report*, 2019.

Ozan Sener and Silvio Savarese. Active learning for convolutional neural networks: A core-set approach. In *International Conference on Learning Representations*, 2018.

Kihyuk Sohn, David Berthelot, Chun-Liang Li, Zizhao Zhang, Nicholas Carlini, Ekin D. Cubuk, Alex Kurakin, Han Zhang, and Colin Raffel. Fixmatch: Simplifying semi-supervised learning with consistency and confidence. *arXiv preprint arXiv:2001.07685*, 2020.

Shuang Song, David Berthelot, and Afshin Rostamizadeh. Combining mixmatch and active learning for better accuracy with fewer labels, 12 2019.

Antti Tarvainen and Harri Valpola. Mean teachers are better role models: Weight-averaged consistency targets improve semi-supervised deep learning results. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett (eds.), *Advances in Neural Information Processing Systems 30*, pp. 1195–1204. Curran Associates, Inc., 2017.

Vladimir Vapnik and Rauf Izmailov. Learning using privileged information: Similarity control and knowledge transfer. *Journal of Machine Learning Research*, 16(61):2023–2049, 2015.

D. Wang and Y. Shang. A new active labeling method for deep learning. In *2014 International Joint Conference on Neural Networks (IJCNN)*, pp. 112–119, 2014.

Keze Wang, Dongyu Zhang, Ya Li, Ruimao Zhang, and L. Lin. Cost-effective active learning for deep image classification. *IEEE Transactions on Circuits and Systems for Video Technology*, 27: 2591–2600, 2017.