ABSTRACT

Active learning is an effective technique for reducing the labeling cost by improving data efficiency. In this work, we propose a novel batch acquisition strategy for active learning in the setting where the model training is performed in a semi-supervised manner. We formulate our approach as a data summarization problem via bilevel optimization, where the queried batch consists of the points that best summarize the unlabeled data pool. We show that our method is highly effective in keyword detection tasks in the regime when only few labeled samples are available.

Index Terms— Batch active learning, semi-supervised learning, bilevel optimization, coresets

1. INTRODUCTION

Many practical applications of supervised learning face the challenge of high labeling costs due to the involvement of human expertise. At the same time, gathering unlabeled data is often less expensive. Active learning is an extensively studied technique for improving data efficiency, which proceeds in rounds of label acquisition and model retraining. In each round of pool-based active learning, the goal is to select samples from the unlabeled data pool to be labeled by an expert, such that the generalization error of the model is maximally reduced when the newly acquired labels are also considered.

Prominent approaches to active learning include uncertainty sampling [15], margin-based selection [3] and expected informativeness [17]. Since acquiring labels one-by-one and retraining the model after each acquisition can be resource-intensive, batch active learning approaches [8, 2, 13] query the labels of multiple points in a single round. The challenge in this setup is to ensure the informativeness of individual points while also avoiding the redundancy in the selection.

While most active learning approaches work in the pool-based setup, they consider training the model on the labeled set and use the unlabeled data pool in the acquisition step only. Recent progress in semi-supervised learning (SSL) [21, 18, 4] has significantly reduced the number of labels required for training highly accurate models in the image domain. For example, MixMatch [4] allows reaching 89% test accuracy on CIFAR-10 with only 250 labeled points — meanwhile training in a supervised manner on 250 points would result in under 40% test accuracy. This suggests that ignoring the pool of unlabeled data and training in a supervised manner during active learning might lead to suboptimal acquisitions.

The idea of combining pool-based active learning with SSL, although quite natural, has received relatively little attention. Early attempts showed improved label efficiency for Gaussian fields [26] and SVMs [2, 14]. More closely related to our work, in the context of deep learning, Sener et al. [22] propose to acquire labels for the points solving the $k$-center problem in the last layer embedding of the network trained in a semi-supervised manner. Song et al. [23] show that combining MixMatch with well-known acquisition functions improves label efficiency in batch active learning. Gao et al. [6] propose a consistency-based batch selection and show the benefit of the strategy when applied with MixMatch. We provide an empirical comparison to these methods in Section 3.

In this work, we propose a novel batch data acquisition strategy via bilevel optimization for pool-based active learning when the model training is performed in a semi-supervised manner. Inspired by the recent work of Borsos et al. [5] on data summarization, we formulate the batch acquisition as a bilevel optimization problem with cardinality constraints. In this formulation, the points selected for labeling are the ones that best summarize the “pseudo-labeled” data pool, i.e., the labels are guessed by the model trained with SSL. Similarly to [5], we approach the resulting optimization problem via forward greedy selection through a proxy reformulation, which we extend to handle data augmentations efficiently. Our formulation naturally supports batch selection and ensures diversity within the selected batch. Our main contributions are the following:

- We demonstrate the effectiveness of SSL using MixMatch [4] in keyword detection tasks.
- We propose a novel data acquisition strategy for semi-supervised batch active learning.
- We show that our approach significantly outperforms other selection strategies in keyword detection tasks, requiring up to 30% fewer labels for achieving the same performance.
2. METHOD

Consider one round of batch active learning: given the labeled training set \( \mathcal{D}_{\text{train}} = \{(x_i, y_i)\}_{i=1}^{m} \) and the unlabeled data pool \( \mathcal{D}_{\text{pool}} = \{(x_j)\}_{j=m+1}^{n} \), the goal is to select and query the labels for a batch \( B \subset \mathcal{D}_{\text{pool}} \) such that the generalization error of the learner is maximally reduced with the newly acquired labels. Although several batch acquisition strategies have been proposed, as discussed in the previous section, the vast majority of these approaches operate in the supervised setting: the learner considers \( \mathcal{D}_{\text{train}} \) only while \( \mathcal{D}_{\text{pool}} \) is used for acquisition and is ignored during training.

We propose a batch acquisition strategy that takes full advantage of the unlabelled data by operating in a semi-supervised setup. Oblivious to the specific algorithm used for SSL, our method relies on a single assumption: training with the SSL algorithm has lower generalization error than training in supervised manner only (Assumption 1). While in our experiments we rely on MixMatch, we abstract the details of the SSL algorithm for the sake of the presentation.

**Bilevel formulation.** Let \( f \) denote the base model and \( \theta^*_\text{SSL} \) its optimal parameters learned in a semi-supervised manner, and assume that the supervised cost function for the \( c \)-classification problem is the cross-entropy loss, denoted by \( \ell \). Using the model \( f_{\theta^*_\text{SSL}} \), we can generate soft pseudo-labels for the unlabeled pool by \( \tilde{y}_x := f_{\theta^*_\text{SSL}}(x) \) for all \( x \in \mathcal{D}_{\text{pool}} \). Given the labeled \( \mathcal{D}_{\text{train}} \) and the pseudo-labeled \( \mathcal{D}_{\text{pool}} \), we formulate our batch selection strategy as follows: summarize \( \mathcal{D}_{\text{pool}} \) by selecting a batch \( B \subset \mathcal{D}_{\text{pool}} \) of size \( b \) such that when \( f \) is trained in a supervised manner on \( \mathcal{D}_{\text{train}} \cup B \), it generalizes well to \( \mathcal{D}_{\text{train}} \cup \mathcal{D}_{\text{pool}} \). Formally, we select \( B \) as the solution of the following optimization problem:

\[
\begin{aligned}
\min_{B \subset \mathcal{D}_{\text{pool}} | |B| = b} & \sum_{(x,y) \in \mathcal{D}_{\text{train}}} \ell(f_{\theta^*}(x), y) + \sum_{x \in \mathcal{D}_{\text{pool}}} \ell(f_{\theta^*}(x), \tilde{y}_x) \\
\text{s.t. } & \theta^* \in \arg \min_{\theta} \sum_{x,y \in \mathcal{D}_{\text{train}}} \ell(f_{\theta}(x), y) + \sum_{x \in B} \ell(f_{\theta}(x), \tilde{y}_x),
\end{aligned}
\]

which is an instance of a cardinality-constrained bilevel optimization problem: while the lower level objective captures training in supervised manner on \( \mathcal{D}_{\text{train}} \cup B \), the upper level problem serves as a proxy for the generalization error due to Assumption 1. Let us denote the lower level objective by \( F(B, \theta) \) and the upper level objective by \( G(\theta) \).

The summary \( B \), containing the most important points of \( \mathcal{D}_{\text{pool}} \) for supervised training, is also known as “coreset” in the literature [1,2]. In order to motivate acquiring labels for points in \( B \), consider the following cases for \( x \in B \): (i) if \( f_{\theta^*_\text{SSL}} \) misclassifies \( x \), then acquiring the correct label will induce a large model change, as \( x \) belongs to the pool’s most influential points; (ii) even if \( f_{\theta^*_\text{SSL}} \) classifies \( x \) correctly, it might do so with low confidence, thus acquiring hard labels for \( x \) can benefit SSL method to propagate labels in the neighborhood of \( x \). One of the core challenges in batch active learning is to ensure that a diverse batch containing no redundant points is selected for labeling. We note that, under Assumption 1, this is automatically guaranteed by our formulation in Eq. (1), since the batch is selected to minimize a proxy (upper level objective) to the generalization error.

The combinatorial optimization problem in Eq. (1) is an instance of the coreset generation framework recently proposed by Borsos et al. [3] restricted to unweighted points. The authors propose a forward greedy heuristic based on minimizing the first order Taylor expansion of the global objective in Eq. (1): suppose the set of points \( B' \subset \mathcal{D}_{\text{pool}} \) has already been selected; first, the inner optimization problem \( \theta^*_{B'} \in \arg \min_{\theta} F(B', \theta) \) is solved, and the next point to be added is greedily chosen by:

\[
x^* = \arg \max_{x \in \mathcal{D}_{\text{pool}} \setminus B'} (f_{\theta^*}(x), \tilde{y}_x)^\top \left( \frac{\partial^2 F(B', \theta)}{\partial \theta \partial \theta} \right)^{-1} \nabla G(\theta),
\]

where the gradients and partial derivatives are evaluated at \( \theta^*_{B'} \). Then \( x^* \) is added to \( B' \) and the iteration resumes with re-solving the inner optimization problem.

**Proxy reformulation.** Since in the applications of interest \( f \) is a deep neural network, the inverse-Hessian vector product in Eq. (2) is computationally intensive. The authors in [3] empirically show that, for several settings, the coreset selection can be solved in reformulation via a proxy model that is related to \( f \). For neural networks, the chosen proxy model relies on the corresponding Neural Tangent Kernel (NTK) [11], which is a fixed kernel related to the training of the network in the infinite-width limit with gradient descent. Their reformulation, however, is only practical for small core-set sizes, as the time complexity depends cubically on the number of selected points. Moreover the reformulation does not support data augmentations, which are crucial in the inner objective of Eq. (1) for the good performance in our setting.

We thus propose a proxy formulation which eliminates the cubic dependence on the number of selected points and supports data augmentations. Analogously to [3], we rely on the NTK corresponding to the neural network at hand. However, instead of using the representor theorem as in [3], we propose to low-rank approximate the kernel matrix via the Nyström method. For mapping to Nyström features, we select the subset of samples \( U = \{u_1, \ldots, u_m\} \) from \( \mathcal{D}_{\text{train}} \cup \mathcal{D}_{\text{pool}} \) at random, and calculate \( K^U \), where \( K^U_{i,j} = k(u_i, u_j) \) for \( i,j \in [m] \) and \( k \) is the NTK. We obtain the Nyström features for \( x \) by \( z_x := (K^U)^{1/2} [k(x, u_1), \ldots, k(x, u_m)]^\top \). Let us further denote \( h_w(x) := \sigma(w^\top z_x) \), where \( w \in \mathbb{R}^{m \times c} \) and \( \sigma \) is the softmax function. We propose the following reformulation:

\[
\begin{aligned}
\min_{B \subset \mathcal{D}_{\text{pool}} | |B| = b} & \sum_{(x,y) \in \mathcal{D}_{\text{train}}} \ell(h_w(x), y) + \sum_{x \in \mathcal{D}_{\text{pool}}} \ell(h_w(x), \tilde{y}_x) \\
\text{s.t. } & \theta^*_{w} = \arg \min_w \sum_{(x,y) \in \mathcal{D}_{\text{train}}} \ell(h_w(x), y) + \sum_{x \in B} \ell(h_w(x), \tilde{y}_x) + \lambda \|w\|^2
\end{aligned}
\]

The inner optimization problem has thus a strongly convex objective — multi-class logistic regression with weight de-
(b) Speech Commands [24]

Fig. 1: Supervised (with and without data augmentations) and semi-supervised learning with MixMatch [4] with labeled samples chosen uniformly at random.

Fig. 2: First round of batch selection by our method (Bilevel) on Free Spoken Digit. Color codes (top left) denote predictions by the model trained on the initial pool, digits denote the true classes.

cay — related to the original neural network via working on the Nyström features of the corresponding NTK. In this formulation, using data augmentations in the inner objective is straightforward. We optimize the inner objective for \( nr_{it} = 10^3 \) steps using Adam [12] with batch size 64 and set \( \lambda = 10^{-4} \). Similarly to [5], we approximate the inverse Hessian-vector product in the selection rule (Eq. (2)) via 30 conjugate gradient steps [20]. We summarize our batch selection strategy in Algorithm 1. We note that we use the proxy conjugate gradient steps [20]. We summarize our batch selection strategy in Algorithm 1. We note that we use the proxy conjugate gradient steps [20].

Algorithm 1 Batch Active Learning via Bilevel Optimization

Input: Labeled data \( D_{train} \), unlabeled pool \( D_{pool} \), model \( f_{\theta_{SSL}} \) trained with SSL, batch size \( b \), \( \lambda, nr_{it} \).
Output: Batch \( B \) for label query.

Generate pseudo-labels \( \hat{y}_x = f_{\theta_{SSL}}(x) \) for all \( x \in D_{pool} \).
Initialize \( w \in \mathbb{R}^{m \times c} \) randomly, set \( B = \emptyset \).
for \( b \in [1, ..., b] \) do
    for \( it \in [1, ..., nr_{it}] \) do
        Sample minibatch \( S \) from \( D_{train} \cup B \) w/ data augm.
        Generate Nyström features \( \tilde{z}_x \) for all \( x \in S \).
        Update \( w \) by SGD on the inner obj. of Eq. (3) with \( \tilde{z}_S \).
    end for
    Select \( x^* \) by Eq. (2) with \( \theta \) replaced by \( w \) and \( f_0 \) by \( h_w \).
    Set \( B = B \cup \{ x^* \} \).
end for

3. EXPERIMENTS

We evaluate our proposed method for keyword detection tasks on the Free Spoken Digit Dataset [10] (2700 utterances of length max 1 second, 10 classes) and on Speech Commands V2 [24] (~85000 utterances of 1 second, 35 classes). We pad the utterances to the length of 1 second, resample to 16 kHz and compute the mel spectrogram features with a window length of 2048 samples (128 ms), a hop length of 512 (32 ms) and with 32 bins. The resulting \( 32 \times 32 \) spectrograms allow us to use ResNets proposed in the image domain for CIFAR-10 without architectural modifications. We employ the following augmentations independently with probability 0.5: (i) random change of amplitude by a factor of \( u \sim U[0.8, 1.2] \), (ii) changing the speed of the audio by a factor of \( u \sim U[0.8, 1.2] \), (iii) random shifts in the time domain by \( t \sim U[-250, 250] \) ms, (iv) adding background noise sequences provided with Speech Commands with SNR \( r \sim U[0, 40] \) dB. We train a Wide ResNet-28 [25] without dropout on the resulting mel spectrograms.

First, we demonstrate the effectiveness of SSL in the domain of keyword detection. Our SSL algorithm of choice is MixMatch [4] with Wide ResNet-28, which has been shown to provide large performance gains in the image domain. We use two augmentations for label guessing for MixMatch and set the cost tradeoff parameter to 10, while we keep all other hyperparameters as proposed in [4]. We train MixMatch for 10⁵ iterations with Adam using batch size 64 and linearly decaying learning rate from \( 10^{-3} \) to \( 10^{-5} \).

We evaluate MixMatch by comparing to supervised training on a small number of labeled samples chosen uniformly at random, where each class is represented by at least one sample. Figures [1a,1b] show 20% and 35% gaps between MixMatch and supervised training in the test accuracy on the two datasets. Note that training the same model on the full labeled training set achieves 100% test accuracy on Free Spoken Digit Dataset and 96% on Speech Commands, respectively. These large performance gaps between supervised and semi-supervised training motivate that pool-based active learning should be leveraged together with SSL.

We compare our proposed batch acquisition strategy to other batch selection methods for active learning with SSL, including k-center selection based on last layer embeddings [22], consistency-based batch selection [6], max-entropy selection and random sampling. For max-entropy selection, we select the top \( b \) samples with highest predictive entropy, where predictions are averaged over 2 data augmen-
Fig. 3: Semi-supervised batch active learning with 10 labels acquired per active learning round. We report the average test accuracy over 6 random seeds, where bands represent one standard deviation. When combined with MixMatch, our proposed acquisition strategy consistently outperforms competing approaches.

Table 1: Semi-supervised batch active learning with batch size of 10. Results reported at 60 acquired labels for Free Spoken Digit and 200 for Speech Commands.

| Method           | Free Spoken Digit | Speech Commands |
|------------------|-------------------|-----------------|
| Uniform          | 91.33 ± 3.98      | 88.13 ± 0.79    |
| Max-Entropy      | 87.56 ± 7.44      | 78.52 ± 4.62    |
| k-center         | 92.67 ± 2.37      | 81.45 ± 3.20    |
| Consistency      | 96.61 ± 2.80      | 82.06 ± 3.98    |
| Bilevel (ours)   | 98.89 ± 1.13      | 90.58 ± 0.97    |

4. CONCLUSION

We presented a novel batch acquisition strategy for pool-based active learning when the model training is performed in a semi-supervised manner. We formalized our approach as a cardinality-constrained bilevel optimization problem and provided a reformulation suitable for deep neural networks trained with data augmentations. We demonstrated the empirical effectiveness of our method on keyword detection tasks, where we observed significant performance gains in the regime of working with a small labeled data pool.

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