DIRECT ACQUISITION OPTIMIZATION FOR LOW-BUDGET ACTIVE LEARNING

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ABSTRACT

Active Learning (AL) has gained prominence in integrating data-intensive machine learning (ML) models into domains with limited labeled data. However, its effectiveness diminishes significantly when the labeling budget is especially low. In this paper, we empirically verify the performance degradation of existing AL algorithms in the extremely low-budget settings, and then introduce *Direct Acquisition Optimization* (DAO), a novel AL algorithm that optimizes sample selections based on expected true loss reduction. Specifically, DAO utilizes influence functions to update model parameters and incorporates an additional acquisition strategy to mitigate bias in loss estimation. This approach facilitates a more accurate estimation of the overall error reduction, without extensive computations or reliance on labeled data. Experiments demonstrate the effectiveness of DAO in both low and higher budget settings, outperforming state-of-the-arts approaches across seven benchmarks.

1 INTRODUCTION

Active learning (AL) explores how adaptive data collection can reduce the amount of data needed by machine learning (ML) models (Settles, 2009; Schröder & Niekler, 2020; Ren et al., 2021; Zhan et al., 2022). It is particularly useful when labeled data is scarce or expensive to obtain, which significantly limits the adaptability of modern deep learning (DL) models due to their data-hungry nature (van der Ploeg et al., 2014). In these cases, AL algorithms selectively choose the most beneficial data points for labeling, thereby maximizing the effectiveness of the training process even if the data is limited in number. In fact, AL has been broadly applied in many fields (Adadi, 2021), such as medical image analysis (Budd et al., 2021), astronomy (Škoda et al., 2020), and physics (Ding et al., 2023), where unlabeled samples are plentiful but the process of labeling through human expert annotations or experiments is highly cost-intensive. In these contexts, judiciously selecting samples for labeling can significantly lower the expenses involved in compiling the datasets (Ren et al., 2021).

Many active learning algorithms have emerged over the past decades, with early seminal contributions from Lewis (1995); Tong & Koller (2001); Roy & McCallum (2001), and a shift that focuses more on deep active learning – a branch of AL that targets more towards DL models in more recent years (Huang, 2021). Depending on the optimization objective, AL algorithms can be classified into two categories. The first category includes heuristic objectives that are not exactly the same as the evaluation metric, i.e. error reduction. Examples in this category are diversity (Sener & Savarese, 2017), uncertainty (Gal et al., 2017), and hybrids of both (Ash et al., 2019). Second category includes criteria that is exactly the same as the evaluation metric, where notable approaches include expected error reduction (EER) (Roy & McCallum, 2001) and its more recent follow-up works (Killamsetty et al., 2021; Mussmann et al., 2022).

Despite the popularity of the first type of AL algorithms, existing works (Mittal et al., 2019; Hacohen et al., 2022) as well as our empirical analysis in Appendix A show that these methods often suffer heavily in low-budget settings, where the total (accumulative) sampling quota is less than 1% of the number of unlabeled data points, making them less suitable for the extreme data scarcity scenarios. In terms of the methods from the second category, their higher running time and reliance on the availability of a *validation* or *hold-out* set remain significant limitations, constraining their applicability in many data-scarcity scenarios as well. For example, EER (Roy & McCallum, 2001) re-trains the classifier for each candidate with all its possible labels, where in each time also evaluates the updated model on all the unlabeled data, making its runtime intractable especially for deep neural networks. And GLISTER (Killamsetty et al., 2021), despite being much more computationally efficient, requires a *labeled, hold-out* set for its sample selection process, formulated as a mixed discrete-continuous bi-level optimization problem, to be optimized properly. While these constraints might not be a huge limitation a few years ago, it poses a more important challenge currently as we are adopting deep learning models to more areas, where labeled data may be extremely expensive to acquire. More importantly, it is also worth noticing that under these scenarios, the highly limited labeled data should have been better utilized for training than being reserved for AL algorithms.

Above limitations highlight a critical gap between the capabilities of current AL methodologies and the urgent demands from real-world applications, underscoring the need for developing novel AL strategies that can operate both relatively efficient while presenting little to none reliance on the labeled set. To this end, we introduce **Direct Acquisition Optimization (DAO)**, a novel AL algorithm that selects new samples for labeling by efficiently estimating the expected loss reduction. Compared to EER and GLISTER, DAO solves the pain points of prohibitive running time and the reliance on a separate labeled set through utilizing *influence function* (Ling, 1984) in model parameters updates, and a more accurate, efficient unbiased estimator of loss reduction through importance-weighted sampling. In summary, DAO optimizes sample selections based on expected error reduction while operating efficiently through influence function-based model parameters approximation and true overall reduced error estimation. Thorough experiments demonstrating DAO's superior performance in the low-budget settings, out-performing current popular AL methods across seven benchmarks.

2 Related Work

Active learning. AL has gained a lot of attraction in recent years, with its goal to achieve better model performance with fewer training data (Settles, 2009; Schröder & Niekler, 2020; Ren et al., 2021). There have been different selection criteria including uncertainty, diversity, query-by-committee, version space and information-theoretic heuristics (Liu et al., 2022; Zhan et al., 2022). The uncertainty-based approaches are arguably the most popular and easiest to implement, which includes selection criteria such as least confidence (Lewis, 1995), minimum margin (Scheffer et al., 2001; Roth & Small, 2006; Citovsky et al., 2021), maximum entropy (Joshi et al., 2009; Settles, 2009) and others (Gal et al., 2017). At their core, these methods select points where the classifier is least certain. However, uncertainty-based methods can be biased towards the current learner. Diversity-based methods (Settles, 2009; Bilgic & Getoor, 2009; Guo, 2010; Luo et al., 2013; Elhamifar et al., 2013; Mac Aodha et al., 2014; Yang et al., 2015; Sener & Savarese, 2017; Sinha et al., 2019; Agarwal et al., 2020; Wu et al., 2021), on the other hand, aim to select the most representative samples of the dataset. In addition, query-by-committee (Seung et al., 1992; Abe, 1998) and version space-based (Mitchell, 1982) methods, keep a pool of models, and then select samples that maximize the disagreements between them. Information-theoretic methods (Hoi et al., 2006; Barz et al., 2018) typically utilize mutual information as the criterion. Hybrid method that combines both uncertainty and diversity criteria, such as BADGE (Ash et al., 2019), has also been developed to take advantage of both worlds. As shown later in the paper, we visually observe that the selections of our proposed DAO, although not explicitly optimized towards any of these heuristics, display characteristics of an hybrid approach.

EER-based acquisition criterion. Alternatively, EER was proposed to select new training examples that result in the lowest expected error on future test examples, which directly optimizes the metric by which the model will be evaluated (Roy & McCallum, 2001). In essence, EER employs sample selection based on the estimated impact of adding a new data point to the training set, rather than evaluating performance against a separate validation set, meaning that it does not inherently require a validation hold-out set. However, its necessity to retrain the model for every possible candidate sample and every possible label renders its cost intractable in the context of deep neural networks (Budd et al., 2021; Škoda et al., 2020; Ding et al., 2023). More recent look-ahead EER-based AL algorithms (Mussmann et al., 2022) focus on addressing this efficiency concern. However, these methods either rely on a small set of validation data to be used for the evaluation of the expected loss reduction (Killamsetty et al., 2021), or can still be quite slow when the size of labeled and unlabeled sets are large (Mohamadi et al., 2022). In this paper, we present DAO, a novel AL algorithm that improves upon EER through optimizations on both model updates as well as loss estimation, efficiently and effectively broadening the applicability of EER-based algorithm.

3 METHODOLOGY

Different from the heuristics-based AL algorithms that optimize criteria such as diversity or uncertainty, DAO is built upon the EER formulation with the selection objective being the largest reduced error evaluated on the entire unlabeled set. More specifically, DAO majorly improves upon two aspects: (1) instead of re-training the classifier, we employ influence function (Cook & Weisberg, 1982), a concept with rich history in statistical learning, to formulate the new candidate sample as a small perturbation to the existing labeled set, so that the model parameters can be estimated without re-training; and (2) instead of reserving a separate, relatively large labeled set for validation (Killamsetty et al., 2021), we sample a very small subset directly from the *unlabeled* set and estimate the loss reduction through bias correction.

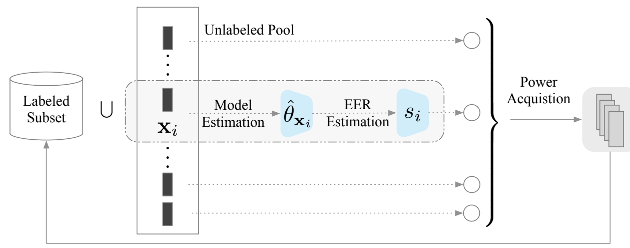


Figure 1: Schematic of the algorithmic framework of DAO.

Essentially, when considering each candidate from the unlabeled set, we optimize the EER framework on two of its core components, which are model parameter update and true loss estimation. Additionally, we upgrade EER, which only supports single sequential acquisition, to offer DAO in both single and batch acquisition variants by incorporating stochastic samplings to the sorted estimated loss reductions. We illustrate our algorithmic framework in Fig. 1. In the following parts of this section, we first introduce a formal problem statement in §3.1, and then dive into each specific component of DAO from §3.2 to §3.5.

3.1 PROBLEM STATEMENT

The optimal sequential active learning acquisition function can be formulated as selecting a budget number of samples $\mathbf{x}_t^{\text{train}}$ from the current unlabeled set $\mathcal{U}_t$ at each round t such that

$$\mathbf{x}_t^{\text{train}} = \underset{\mathbf{x}_{\mathcal{S}_i} \subset \mathcal{U}_{t-1}}{\arg\min}\, \mathbb{E}_{(y_{\mathcal{S}_i}|f^*, \mathbf{x}_{\mathcal{S}_i})} \left[L_{\text{true}}(f_{t|\mathbf{x}_{\mathcal{S}_i}, y_{\mathcal{S}_i}}) \right] \tag{1}$$

where f^* represents an optimal oracle that maps from any subset of the unlabeled data $\mathbf{x}_{\mathcal{S}_i} \subset \mathcal{U}_{t-1}$ to their ground-truth labels $y_{\mathcal{S}_i}$, and $f_{t|\mathbf{x}_{\mathcal{S}_i}, y_{\mathcal{S}_i}}$ is the model that has been trained on the union of the current labeled set $\mathcal{L}_{t-1}$ and the current unlabeled candidates $\mathbf{x}_{\mathcal{S}_i} \subset \mathcal{U}_{t-1}$. In addition, $L_{\text{true}}(f_{t|\mathbf{x}_{\mathcal{S}_i}, y_{\mathcal{S}_i}}) = \frac{1}{|\mathcal{U}_{t-1,i}|} \sum_{\mathbf{x} \in \mathcal{U}_{t-1,i}} \ell(\mathbf{x}; f_{t|\mathbf{x}_{\mathcal{S}_i}, y_{\mathcal{S}_i}})$ represents the loss estimator that can predict the *unbiased* error of $f_{t|\mathbf{x}_{\mathcal{S}_i}, y_{\mathcal{S}_i}}$, where ℓ denotes the loss function. It is numerically the same as if $f_{t|\mathbf{x}_{\mathcal{S}_i}, y_{\mathcal{S}_i}}$ has been tested on the entire unlabeled set $\mathcal{U}_{t-1,i}$, where $\mathcal{U}_{t-1,i} = \mathcal{U}_{t-1} \setminus \mathbf{x}_{\mathcal{S}_i}$. Such formulation represents the optimal AL criterion and aligns with any existing sequential active learning algorithm — of which the goal is to select the new data points that can most significantly improve the current model performance (Roy & McCallum, 2001).

Unfortunately, Eq. (1) cannot be directly implemented in practice. Because, first, we do not have access to the optimal oracle f^* to reveal the labels $y_{\mathcal{S}_i}$ of $\mathbf{x}_{\mathcal{S}_i} \subset \mathcal{U}_{t-1}$; second, even if we had f^* and therefore $y_{\mathcal{S}_i}$, we cannot afford the cost of retraining model f_{t-1} on each $\mathcal{L}_{t-1} \cup \mathbf{x}_{\mathcal{S}_i}$ to obtain the updated $f_{t|\mathbf{x}_{\mathcal{S}_i}, y_{\mathcal{S}_i}}$; and third, we do not have the unbiased true loss estimator L_{true}, which demands evaluating $f_{t|\mathbf{x}_{\mathcal{S}_i}, y_{\mathcal{S}_i}}$ on the entire $\mathcal{U}_{t-1,i}$.

Therefore, the goal of DAO is to solve the above challenges and efficiently and accurately approximate Eq. (1) for the sample selection strategy. It is also worth noting that, when $\mathbf{x}_t^{\text{train}}$ represents a *set* of newly acquired data points, the above formulation becomes eligible for batch active learning, which is more suitable for deep neural networks (Huang, 2021).

3.2 LABEL APPROXIMATION VIA SURROGATE

In this section, we address the first challenge when approximating Eq. (1). As we do not know the true label or true label distribution $p(y|\mathbf{x}, f^*)$ of each unlabeled sample $\mathbf{x}$, the best we can do is provide an approximation for $p(y|\mathbf{x})$. To this end, we introduce the concept of a *surrogate* (Kossen et al., 2021), which is a model parameterized by some potentially infinite set of parameters θ. Specifically, $p(y|\mathbf{x})$ can be approximated using the marginal distribution $\pi(y|\mathbf{x}) = \mathbb{E}_{\pi(\theta)}[\pi(y|\mathbf{x}, \theta)]$ with some proposal distribution $\pi(\theta)$ over model parameters θ. In other words, we have:

$$p(y|\mathbf{x}) \approx \int_{\theta} \pi(\theta)\pi(y|\mathbf{x}, \theta)\,\mathrm{d}\theta \tag{2}$$

As the sample selection process continues, new labeled points should also be used to train and update the surrogate model $\pi(\theta)$ for better approximation of the true outcomes.

Although ideally, a more capable surrogate is preferred for better ground truth approximations, we acknowledge that the choice of surrogate model can be very sensitive to the computational constraints. Therefore, if running time is at center of the concerns during sample acquisitions, using f_t at step t also as the surrogate could be an efficient alternative, as we don't need to update a second model, nor do we need to run forward pass on the both models. However, this will come with the cost that π_t never disagrees with f_t, which causes performance degradation for the unbiased true loss estimation, which will be illustrated with more details in §3.4. Therefore, in short, we do not recommend replicating f_t as surrogate in practice, unless the computational constraint is substantial.

3.3 Model Parameters Update without Re-training

At acquisition round t, suppose we have labeled set $\mathcal{L}_{t-1}$ and unlabeled set $\mathcal{U}_{t-1}$ as the results from the previous round $t-1$, and new sample $\mathbf{x}_i \in \mathcal{U}_{t-1}$ that is currently under consideration for acquisition, the goal of this section is to estimate the parameters of model $f_{t|\mathbf{x}_i, y_i}$ that could has been obtained after training f_{t-1} on the combined dataset $\{\mathcal{L}_{t-1} \cup \mathbf{x}_i\}$. In other words, if we suppose the conventional full training converges to parameters $\hat{\theta}_{\mathbf{x}_i}$, we have:

$$\hat{\theta}_{\mathbf{x}_i} = \arg\min_{\theta\in\Theta} \frac{1}{|\mathcal{L}_{t-1}|+1} \sum_{\mathbf{x}\in\{\mathcal{L}_{t-1}\cup\mathbf{x}_i\}} \ell(\mathbf{x};\theta) \tag{3}$$

where recall that $\ell(\mathbf{x};\theta)$ denotes the loss of θ on $\mathbf{x}$. The core of our approach is that, instead of re-training as showed in Eq. (3), we can approximate the effect of adding a new sample as upweighting the influence function by $\frac{1}{|\mathcal{L}_{t-1}|+1}$ (Koh & Liang, 2017) and then directly estimate the updated model parameters.

Following Cook & Weisberg (1982), we have the influence function defined as:

$$\mathcal{I}_{\text{up,params}}(\mathbf{x}_i) := \left.\frac{d\hat{\theta}_{\epsilon,\mathbf{x}_i}}{d\epsilon}\right|_{\epsilon=0} = -H_{\hat{\theta}}^{-1}\nabla_\theta \ell(\mathbf{x}_i;\hat{\theta})$$

where $H_{\hat{\theta}}$ is the positive definite Hessian matrix (Koh & Liang, 2017). Next, we can estimate the model parameters after adding this new sample $\mathbf{x}_i$, as:

$$\hat{\theta}_{\mathbf{x}_i} - \hat{\theta} \approx \frac{1}{|\mathcal{L}_{t-1}|+1}\mathcal{I}_{\text{up,params}}(\mathbf{x}_i) = -\frac{1}{|\mathcal{L}_{t-1}|+1} H_{\hat{\theta}}^{-1}\nabla_\theta \ell(\mathbf{x}_i;\hat{\theta})$$

where $\nabla_\theta \ell(\mathbf{x}_i;\hat{\theta})$ could be approximated as the expected gradient of sample $\mathbf{x}_i$: By a slight abuse of notation of the training loss function ℓ, we denote

$$\nabla_\theta \ell(\mathbf{x}_i;\hat{\theta}) \approx \sum_{k=1}^{K} \nabla_\theta \ell(\mathbf{x}_i, \hat{y}_k;\hat{\theta}) \cdot \hat{p}_k \tag{4}$$

In Eq. (4), $\hat{y}_k$ and $\hat{p}_k$ represent model's label prediction and likelihood (e.g. confidence) respectively while K represents the total number of classes in the ground truths.

In practice, the inverse of $H_{\hat{\theta}}$ cannot be computed due to its prohibitive $O(np^2 + p^3)$ runtime (Liu et al., 2021), with p being the number of model parameters. The computation unavoidably becomes especially intensive when f is a deep neural network model (Fu et al., 2018). Luckily, we have two optimization methods, conjugate gradients (CG) (Martens et al., 2010) and stochastic estimation (Agarwal et al., 2017) at our disposal.

Conjugate gradients. As mentioned earlier, by assumption we have $H_{\hat{\theta}} \succ 0$ and $\nabla_\theta \ell(\mathbf{x}';\hat{\theta})$ as a vector. Therefore, we can calculate the inverse Hessian vector product (IHVP) through first transforming the matrix inverse into an optimization problem, i.e.

$$H_{\hat{\theta}}^{-1}\nabla_\theta \ell(\mathbf{x}_i;\hat{\theta}) \equiv \arg\min_{t}\; t^T H_{\hat{\theta}} t - v^T t$$

and then solving it with CG (Martens et al., 2010), which speeds up the runtime effectively to $O(np)$.

Stochastic estimation. Besides CG, we can also efficiently compute the IHVP using the stochastic estimation algorithm developed by Agarwal et al. (2017). From Neumann series, we have $A^{-1} \approx \sum_{i=0}^{\infty}(I - A)^i$ for any matrix A. Similarly, suppose we define the first j terms in the Taylor expansion of $H_{\hat{\theta}}^{-1}$ as

$$H_{\hat{\theta},j}^{-1} = \sum_{i=0}^{j}(I - H_{\hat{\theta}})^i = I + (I - H_{\hat{\theta}})H_{\hat{\theta},j-1}^{-1}$$

we have $H_{\hat{\theta},j}^{-1} \rightarrow H_{\hat{\theta}}^{-1}$ as $j \rightarrow \infty$. The core idea of the stochastic estimation is that the Hessian matrix $H_{\hat{\theta}}$ can be substituted with any unbiased estimation when computing $H_{\hat{\theta}}^{-1}$. In practice, we sample n_{ihvp} data points from the existing labeled set $\mathcal{L}_{t-1}$ and use $\nabla_{\theta}^2\ell(\mathbf{x}_i; \hat{\theta})$ as the estimator of $H_{\hat{\theta}}$ (Liu et al., 2021). Notice that since n_{ihvp} is usually very small (in our experiments we used $n_{\text{ihvp}} = 8$), it does not create a constraint on the size of the current labeled set, which does not interfere with the low-budget settings.

Finally, we can approximate the model parameters after the addition of $\mathbf{x}_i$ as

$$\hat{\theta}_{\mathbf{x}_i} = \hat{\theta} - \frac{1}{n+1}H_{\hat{\theta}}^{-1}\nabla_{\theta}\ell(\mathbf{x}_i; \hat{\theta}) \tag{5}$$

which does not require any re-training. And we will demonstrate in §5.2 that this parameter update strategy provides much better approximations than the naive single backpropagation as seen in the existing AL literature (Killamsetty et al., 2021).

3.4 Efficient Unbiased Loss Estimation

Referring back to Eq. (1), the last challenge that we need to address is to gain access to the unbiased true loss estimator L_{true}. In other words, we want to predict the *true* performance of $f_{t|\mathbf{x}_i,y_i}$ on the unlabeled set $\mathcal{U}_{t,i}$ without exhaustive testing. Strictly, such evaluation cannot be drawn until $f_{t|\mathbf{x}_i,y_i}$ is evaluated on the entire unlabeled set $\mathcal{U}_{t,i}$. However, this is infeasible in practice.

Such approximation is typically carried out in other approaches (Killamsetty et al., 2021; Mussmann et al., 2022) by randomly sampling a labeled validation set $\mathcal{V}$ at the beginning of the entire acquisition process, which will later be used for evaluations in all the subsequent acquisition episodes. Despite the simplicity as well as being i.i.d., which makes the estimated loss unbiased by nature, this approximation method suffers from large variance as the size of $\mathcal{V}$ is usually much smaller than $\mathcal{U}$, which unavoidably hurts the acquisition performance. It is also contradictory to the goal of AL in general, especially under the low-budget settings, as discussed in §1.

Different from the existing works, we propose to sample a subset $\mathcal{C}$ from current $\mathcal{L}_{t-1}$ in each acquisition round based on an alternative acquisition function, and then correct the bias in the loss induced from this acquisition function. In the meantime, we also want to keep the variance low, so that the final corrected loss enjoys both low bias and low variance, which is more preferable than the zero bias but high variance that the random i.i.d. sampling has.

Specifically, continuing with the notations from §3.1, let $\mathcal{C} = \{\mathbf{x}_{t,1}, \ldots, \mathbf{x}_{t,m}, \ldots, \mathbf{x}_{t,n_{\mathcal{C}}}\}$, where $\mathcal{C} \subset \mathcal{U}_{t-1}$, be the subset containing $n_{\mathcal{C}}$ samples selected for this true loss estimation at each round t. Farquhar et al. (2021) shows that if $\mathbf{x}_{t,m}$ is sampled in proportion to the true loss of each data point, the bias originated from this selection can be corrected through the Monte Carlo estimator $\hat{R}_{\text{LURE}}$[1]. Following our notations, it takes the form:

$$\hat{R}_{\text{LURE}} = \frac{1}{n_{\mathcal{C}}}\sum_{m=1}^{n_{\mathcal{C}}} v_m \ell\left(\mathbf{x}_{t,m}; f\right) \tag{6}$$

where recall that ℓ denotes the loss of f, and the importance weight v_m is

$$v_m = 1 + \frac{|\mathcal{U}_{t-1}| - n_{\mathcal{C}}}{|\mathcal{U}_{t-1}| - m}\left(\frac{1}{(|\mathcal{U}_{t-1}| - m + 1)q_t^*(m)} - 1\right) \tag{7}$$

with $q_t^*(m)$ being the acquisition distribution of index m at round t. Importantly, the variance can be significantly reduced if the acquisition distribution $q_t^*(m)$ is proportion to the true loss of each

[1]LURE stands for Levelled Unbiased Risk Estimator

data point. Again, this is not feasible as we do not have access to the labels for $\mathcal{U}_{t-1}$. However, following Kossen et al. (2021), we can approximate $q_t^*(m)$ with

$$q_t(m) = -\sum_y \pi(y|\mathbf{x}_{t,m}) \log f(\mathbf{x}_{t,m})$$

for classification tasks when the loss function is the cross-entropy loss, and where π is conveniently just our surrogate discussed in §3.2. Referring back to the discussion we had on choosing a good surrogate π, with $f(\mathbf{x})$ being designed to approximate $p(y|\mathbf{x})$ as well, the surrogate π should ideally be different from f so that more diversity is introduced in the acquisitions.

To put all components together, our loss correction process involves selecting samples in $\mathcal{C}$ following

$$\mathbf{x}_{t,m} \propto -\sum_y \pi_{t-1}(y|\mathbf{x}) \log f_{t-1}(y|\mathbf{x}) \tag{8}$$

where π_{t-1} is the surrogate model π at round $t-1$. Finally, the corrected loss s_i can be approximated using $\hat{R}_{\text{LURE}}$ as

$$s_i = \frac{1}{n_\mathcal{C}} \sum_{m=1}^{n_\mathcal{C}} \hat{v}_m \ell\left(\mathbf{x}_{t,m}; f_t\right) \tag{9}$$

where $\hat{v}_m$, which depends on the choice of $\mathbf{x}_{t,m}$, is the approximated version of the original v_m defined in Eq. (7). Specifically, $\hat{v}_m$ takes the form

$$\hat{v}_m = 1 + \frac{|\mathcal{U}_{t-1}| - n_\mathcal{C}}{|\mathcal{U}_{t-1}| - m} \left(\frac{1}{(|\mathcal{U}_{t-1}| - m + 1) q_t(m)} - 1 \right) \tag{10}$$

where $q_t(m)$ is the acquisition function defined in Eq. (8).

3.5 Batch Acquisition via Stochastic Sampling

In §3.1, we briefly discussed that when $\mathbf{x}_t^{\text{train}}$ represents a set of data points (instead of a single one), the formulation in Eq. (1) essentially represents the *batch* active learning scenario. Suppose the acquisition budget per round is k, although selecting the top k samples with the lowest estimated losses (or highest expected error reduction) is straightforward, this approach is sub-optimal. This is because top-k acquisition, while effective to some degree due to its greedy nature, overlooks the crucial interactions among data points in batch acquisitions. Specifically, while aiming to select the most informative unlabeled points, top-k acquisition may lead to redundant choices, diminishing the overall benefit of the acquisition. Inspired by Kirsch et al. (2021), we propose to similarly perturb the original ranking of the estimated true losses so that the batch sampling provides better acquisitions when the most informative data points may be duplicated. Suppose at acquisition episode t, we rank the set of estimated true loss of each unlabeled data point in ascending orders as $\{\hat{l}_{\text{true},i}\}_{\mathbf{x}_i \in \mathcal{U}_{t-1}}$, such that $\hat{l}_{\text{true},i} \leq \hat{l}_{\text{true},j}, \forall i \leq j$ and $\mathbf{x}_i, \mathbf{x}_j \in \mathcal{U}_{t-1}$, we can perturb the ranking with three strategies: soft-rank, soft-max, and power acquisition, to improve batch performance from the naive top-k sampling.

Algorithm 1 Direct Acquisition Optimization (DAO)

input Episode t, unlabeled set $\mathcal{U}_{t-1}$, labeled set $\mathcal{L}_{t-1}$, model f_{t-1}, surrogate π_{t-1}, budget k, n_{ihvp} (§3.3), and $n_\mathcal{C}$ (§3.4)
output Acquisition set $\mathcal{A}_t = \{\mathbf{x}_{t,1}^{\text{train}}, \ldots, \mathbf{x}_{t,k}^{\text{train}}\}$ ▷ Eq. (1)
Approximate $p(y|\mathbf{x})$ for all $\mathbf{x} \in \mathcal{U}_{t-1}$ ▷ §3.2, Eq. (2)
Initialize array S where $|S| = |\mathcal{U}_{t-1}|$
for $i = 1$ **to** $|\mathcal{U}_{t-1}|$ **do**
  Let $\mathcal{U}_{t,i} = \mathcal{U}_{t-1} \setminus \{\mathbf{x}_i\}$
  Randomly sample n_{ihvp} data points from $\mathcal{U}_{t,i}$
  Approximate parameters of $f_{t|\mathbf{x}_i, y_i}$ ▷ §3.3, Eq. (5)
  Acquire n_c samples from $\mathcal{U}_{t,i}$ ▷ §3.4, Eq. (8)
  Compute s_i and add to S ▷ §3.4, Eq. (9)
end for
Sort S in ascending order
if $k > 1$ **then**
  Perturb S ▷ Methods showed in §3.5
end if
Return top-k samples in S as $\mathcal{A}_t$

Soft-rank acquisition. Soft-rank acquisition relies on the relative ordering of the scores while ignoring the absolute score values. It samples the data point ranked at index i with probability $p_{\text{softrank}}(i) = i^{-\beta}$, where β is the "coldness" parameter and is kept as 1 throughout this paper. It is not hard to notice that $p_{\text{softrank}}(i)$ is invariant to $\hat{l}_{\text{true},i}$, as long as the relative ranking remains the same. More conveniently, with sampled Gumbel noise $\epsilon_i \sim \text{Gumbel}(0; \beta^{-1})$, taking the top-$k$ data points from the perturbed ranked list

$$\hat{l}_{\text{true},i}^{\text{softrank}} = -\log i + \epsilon_i$$

is equivalent to sampling $p_{\text{softrank}}(i)$ without replacement (Huijben et al., 2022).

Soft-max acquisition. In contrast to soft-rank, soft-max acquisition uses the actual scores, i.e., the estimated true losses, instead of their relative orderings. However, this acquisition does not rely on the semantics of the actual values, resulting in the transformed true loss simply being:

$$\hat{l}_{\text{true},i}^{\text{softmax}} = \hat{l}_{\text{true},i} + \epsilon_i$$

where ϵ_i remains the same Gumbel noise as in the soft-rank acquisition. Statistically, choosing the top-k data points from this perturbed ranked list is equivalent to sample from $p_{\text{softmax}}(i) = e^{\beta i}$ without replacement.

Power acquisition. While neither soft-rank or soft-max acquisitions take the semantic meaning of the actual score values into account when designing the acquisition distribution, power acquisition uses the value directly when determining the perturbed values. Specifically, the power acquisition perturbs the scores as

$$\hat{l}_{\text{true},i}^{\text{power}} = \log \hat{l}_{\text{true},i} + \epsilon_i$$

where again ϵ_i is the Gumbel noise, and choosing the top-k indices from this new list is equivalent to sampling from $p_{\text{power}}(i) = i^{\beta}$ without replacement. Results comparing DAO with different batch acquisition strategies discussed above are showed in Appendix B. Combining all the components, the pseudocode of DAO is summarized in Algorithm 1.

4 Experiments

We evaluate DAO on seven classification benchmarks including digit recognition datasets MNIST (LeCun et al., 1998), Street-View House Numbers recognition (SVHN) (Sermanet et al., 2012), object classification datasets STL-10 (Coates et al., 2011), CIFAR-10, CIFAR-100 (Krizhevsky et al., 2009), as well as domain-specific datasets Fashion-MNIST (Xiao et al., 2017) and Stanford Cars (Cars196) (Krause et al., 2013).

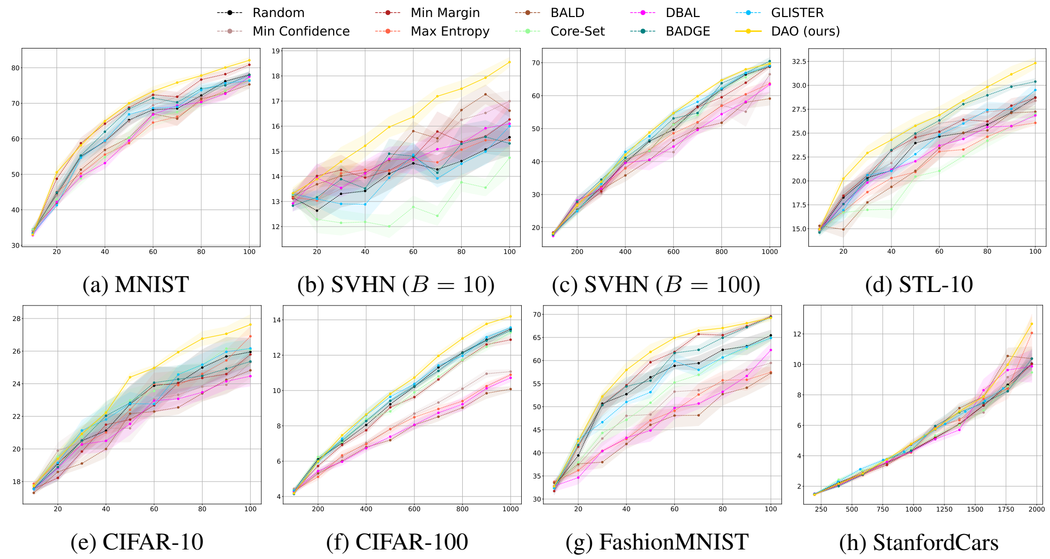
4.1 Experimental Setup

Baselines. To ensure fair comparisons, besides baseline methods that we empirically surveyed in Appendix A, we also include other state-of-the-arts AL methods, including Deep Bayesian Active Learning (DBAL) (Gal et al., 2017) and GLISTER (Killamsetty et al., 2021), where GLISTER is a direct competitor that also optimizes the EER framework. For all the baselines, we used the default/recommended parameters and their official implementations if publically available. In terms of earlier works such as least confidence (Lewis, 1995), minimum margin (Scheffer et al., 2001), and maximum entropy (Settles, 2009), we used the peer-reviewed deep active learning framework DeepAL+ (Zhan et al., 2022). All experiments are repeated ten times with different random seeds.

Implementation details. Throughout the section, we set ResNet-18 (He et al., 2016) as the model f to be trained from scratch. We employed VGG16 (Simonyan & Zisserman, 2014), initialized with random weights, as our surrogate π. We used stochastic estimation (Agarwal et al., 2017) when estimating the updated model parameters, as discussed in §3.3. We choose $n_{\text{ihvp}} = 8$ when approximating the unbiased estimator of $H_{\hat{\theta}}$, and set $n_{\mathcal{C}} = 16$ for biased loss correction as in §3.4.

4.2 Performance under Low Budgets

Digit recognition. First, we demonstrate DAO's effectiveness through two digit recognition benchmarks: MNIST (LeCun et al., 1998) and SVHM (Sermanet et al., 2012). MNIST is a collection of handwritten digits consisting of 60k training and 10k test images, while SVHN is a more challenging dataset containing over 600k real-world house numbers images taken from street views. Both datasets contain 10 classes corresponding to digits from 0 to 9. Based on insights from Appendix A, we define a general rule of low-budget setting as *one image per class*, which translates to initial label size $|\mathcal{L}_{\text{init}}^{\text{MNIST}}| = 10$ and per-episode budget $B_{\text{MNIST}} = 10$ for MNIST. Given that SVHN is more challenging, and there are ten times more unlabeled images than in MNIST (600k vs. 60k), we experiment both 10 and 100 for our initial labeled size and per-round budget for SVHN. The results are shown in Fig. 2b and 2c.



(a) MNIST (b) SVHN ($B = 10$) (c) SVHN ($B = 100$) (d) STL-10

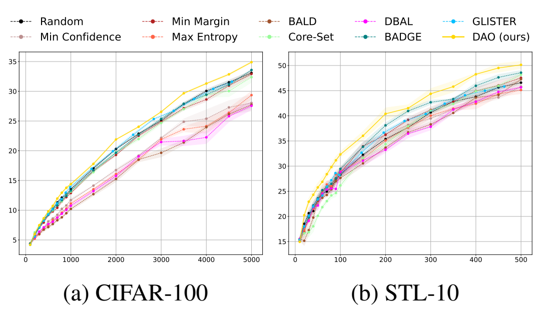
(e) CIFAR-10 (f) CIFAR-100 (g) FashionMNIST (h) StanfordCars

Figure 2: Experiment results comparing DAO with existing AL algorithms across seven benchmarks. In all subplots, horizontal axis represents the accumulative size of the labeled set, while vertical axis indicates classification accuracy.

Object classification. Next, we assess DAO on more general and complex object classification tasks. STL-10 (Coates et al., 2011) is a benchmark dataset derived from labeled examples in the ImageNet (Deng et al., 2009). Specifically, STL-10 contains 5k labeled 96×96 color images spread across 10 classes, as well as 8k images in the test split. CIFAR-10 (Krizhevsky et al., 2009) contains a collection of 60k 32x32 color images in 10 different classes, with 6k images per class. CIFAR-100 is similar to CIFAR-10, but covers a much wider range, containing 100 classes where each class holds 600 images. Continuing with the low-budget setting (*1 image per class*), we have $|\mathcal{L}_{\text{init}}^{\text{STL-10}}| = 10$, $B_{\text{STL-10}} = 10$ for STL-10, $|\mathcal{L}_{\text{init}}^{\text{CIFAR-10}}| = 10$, $B_{\text{CIFAR-10}} = 10$ for CIFAR-10 and $|\mathcal{L}_{\text{init}}^{\text{CIFAR-100}}| = 100$, $B_{\text{CIFAR-100}} = 100$ for CIFAR-100. The results are shown in Fig. 2d, 2e and 2f respectively.

Domain Specific Tasks The last part of our experiments involves case studies on applying DAO to domain-specific tasks, which simulates many real-world applications. Specifically, we use Fashion-MNIST (Xiao et al., 2017) and StanfordCars (Krause et al., 2013), also known as Cars196, in this experiment. FashionMNIST is structure-wise similar to MNIST, comprising 28×28 images of 70k fashion products from 10 categories, with 7k images per category. The training set contains 60k images, while the test set includes the rest. StanfordCars is a large collection of car images, containing 16,185 images with a near-balanced ratio on the train/test split, resulting in 8,144 and 8,041 images for training and testing. There are 196 classes in total, where each class consists of the year, make, model of a car (e.g., 2012 Tesla Model S). The results of both datasets are shown in Fig. 2g and 2h.

Results discussion. From Fig. 2, we notice that the proposed DAO outperforms popular AL state-of-the-arts by a clear margin across all seven benchmarks. Especially, with SVHN, when the budget is extremely low ($B = 10$, which is 0.0017% of the unlabeled size), DAO leads the performance by a very large gap, indicating its superior capability in the low-budget setting. Such performance does not degrade much as the budget constraint is relaxed. As shown in Fig. 2c, DAO still performs relatively well. The only experiment that DAO does not improve as much is the StanfordCars. However, the accuracy improvement from DAO is more smooth and has less variance, indicating better robustness when applied to the more challenging (StanfordCars has 196 classes) applications.



(a) CIFAR-100 (b) STL-10

Figure 3: Higher-budget experiment results comparing DAO with existing AL algorithms. In both subplots, horizontal axis represents the accumulative size of the labeled set, while vertical axis indicates classification accuracy.

4.3 PERFORMANCE UNDER HIGHER BUDGETS

To further evaluate the capabilities of the proposed DAO beyond its targeting focus on low-budget AL, we conducted additional experiments with higher budgets on the CIFAR-100 and STL10 datasets. Specifically, we keep the same experimental settings as previously, with the same initial labeled set and per-round acquisition budget, and repeated the process five times with different random seeds. However, we extended the number of rounds in each acquisition from 10 to 50, increasing the budget by five times. And to make the plot more clear, we plot every five rounds. As shown in Fig. 3, DAO consistently outperforms all other baselines throughout the entire acquisition process, demonstrating superior performance across both low and high budgets.

5 COMPONENT ANALYSIS AND ABLATION STUDIES

5.1 ABLATIONS ON DIFFERENT SURROGATES

To further understand how the surrogate model impacts the performance of DAO, we conducted additional experiments on CIFAR-10 using different surrogates. Specifically, we compared: (1) *VGG16*: The surrogate model currently used in the paper draft. (2) *ResNet18*: An efficient variant of DAO where the main model under training serves as the surrogate, i.e., $\pi_t = f_t$. In this case, the equation for approximating $q_t^*(m)$, the acquisition distribution of candidate index m at round t (the equation between lines 225 and 226), reduces from cross-entropy to entropy. (3) *SimpleCNN*: A simpler version of ResNet18 with six convolution blocks, each containing one Conv layer followed by BatchNorm and ReLU. and (4) *Oracle*: An unrealistic setting assuming access to an oracle surrogate model. We used the same experimental setup with CIFAR-10 as in our draft: starting with 10 labeled samples, acquiring 10 samples per round, and continuing for 10 rounds. The was repeated five times with different random seeds.

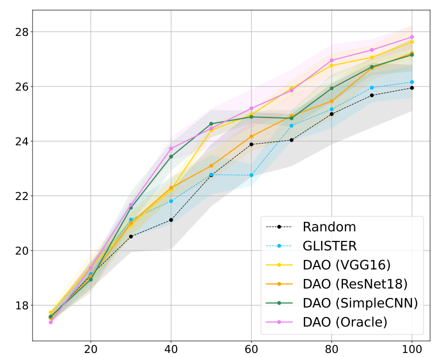


Figure 4: DAO performance when using different surrogate models.

As shown in Fig. 4, DAO with oracle surrogate performs the best, followed by VGG16 and SimpleCNN. ResNet18 performs the worst among all DAO variants, which aligns with our expectation that performance degrades when π_t never disagrees with f_t. However, all DAO variants outperform the random and GLISTER baselines by a clear margin. It is worth noting that while the oracle surrogate achieves the best results, the improvement over VGG16 and SimpleCNN is not substantial. We think this is likely because, when selecting samples for the unbiased loss estimation, the acquisition distribution $q_t^*(m)$ approximated with $q_t(m) = -\sum_y \pi(y|\mathbf{x}_{t,m}) \log f(\mathbf{x}_{t,m})$, does not solely depend on the surrogate quality. Although in the unrealistic case of an oracle surrogate, this creates an disadvantage, but in practical scenarios, this approximation provides better robustness in preventing the negative impact of poor quality of surrogate on unbiased loss estimation, especially in early stages where models might overfit.

Table 1: Surrogate model performance on unlabeled set during acquisition.

Budget	20	40	60	80	100
SimpleCNN	13.79	13.91	15.11	15.01	14.80
VGG16	18.50	20.07	21.02	22.44	22.75
ResNet18	**18.60**	**21.79**	**23.86**	**25.36**	**27.05**

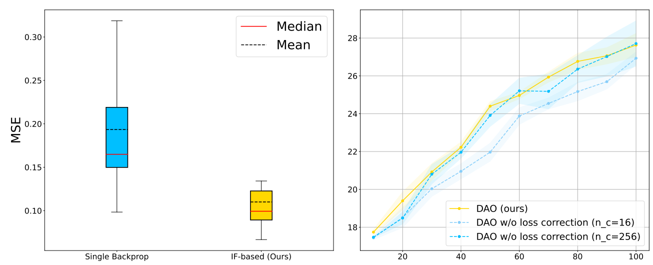
Additionally, we provide evaluations of the predictive accuracy of different surrogates on *unlabeled set* in Table 1. The results show that when the surrogate differs from the model being trained (i.e., $f \neq \pi$), its performance does not improve as significantly as that of f, indicating from a different angle that DAO specifically optimizes the sample selection that enhances the performance of the target model f.

5.2 ACCURACY ON MODEL APPROXIMATION

First, we assess if estimating the model parameters updates through modelling the effect of adding a new sample as upweighting the influence function provides a more accurate model performance approximation than using single backpropagation as seen in GLISTER (Killamsetty et al., 2021). Specifically, we conduct the experiments on CIFAR-10 (Krizhevsky et al., 2009), with initial labeled size $|\mathcal{L}_{\text{init}}^{\text{CIFAR-10}}| = 100$ (randomly sampled from the train split), per-episode budget $B_{\text{CIFAR-10}} = 1$, and number of acquisition episode $E = 25$. We compare the updated models performance (accuracy) on the test split of CIFAR-10. Different from the experiments in §4, we do not apply any AL algorithm when acquiring the sample in each round. Instead, we randomly choose B sample in each acquisition round from the unlabeled set and then update the models through both methods with the same selected sample. To access the difference between models updated with our influence function-based method and single backpropagation, we compute the mean squared error (MSE) between the performance of each model and the model updated by conventional full training, which is defined in Eq. (3). As shown in Fig. 5a, the proposed method provides more accurate (smaller mean and median) and more robust (smaller std.) model approximations than single backpropagation, contributing to the performance gain we observe in §4.

5.3 Bias Correction vs. Random Sampling

Next, we conduct ablation studies on replacing the proposed loss estimation (§3.4) with the average loss of randomly sampled data points. More specifically, we replace the estimated loss s_i from averaging the corrected loss (Eq. (6)) of the acquired samples via an alternative acquisition criteria (Eq. (8)) with averaging losses of the samples acquired uniformly, i.e., at round t, we have $s_i^{\text{random}} = \frac{1}{M_{\text{random}}} \sum_{m=1}^{M_{\text{random}}} \ell(\mathbf{x}_{t,m}; f_t)$ where $\mathbf{x}_{t,m} \sim U(1, |\mathcal{U}_{t,i}|)$. We choose two $M_{\text{random}} = 16$ and 256, where former provides a direct comparison with our proposed loss estimation approach, and latter represents a brute-force solution that works relatively well but is often infeasible in practice due to intensive running time. The results are shown in Fig. 5b. We see that the proposed method performs even better than the conventional random-sampling loss estimation with large sampling size, while computationally being only 1/8 of the run time. Additionally, the variance of our method is much smaller, indicating more robust loss estimation and thus more robust acquisition performance.



(a) (b)

Figure 5: *Left*: MSE of the predictions accuracy on the test split of CIFAR-10 between models updated by single backpropagation, influence function, and the fully trained model. *Right*: Ablation results where the proposed loss estimation is replaced by the random sampling estimation defined in §5.3.

5.4 Different Batch Acquisition Strategies

We conducted additional ablation studies comparing various stochastic sampling methods as detailed in §3.5. Results are documented in Appendix B. Our findings reveal that the proposed algorithm, even when simply selecting the top k samples without applying any of the stochastic strategies, outperforms existing methods. Performance further improves with the implementation of these sampling strategies. It is important to note that we have not designed specific sampling strategies for our algorithm; instead, we utilized existing methods to showcase the efficacy of DAO framework.

5.5 Interpreting DAO with Other AL Criteria

In this section, we analyze the criterion optimized by DAO and compare it to common criteria such as diversity and uncertainty, using visual representations of the data samples collected by DAO. The detailed plots are available in Appendix C. Throughout multiple acquisition rounds, the data selected by DAO demonstrate notable diversity with uniform distribution across the sample space. However, in contrast to traditional uncertainty-based methods, selections within a single round by DAO also incorporate elements of uncertainty. This hybrid approach explains the performance improvements observed in §4 over algorithms that solely focus on diversity or uncertainty.

6 Conclusions

In this paper, we introduced Direct Acquisition Optimization, a novel algorithm designed to optimize sample selections in low-budget settings. DAO hinges on the utilization of influence functions for model parameter updates and a separate acquisition strategy to mitigate bias in loss estimation, represents a significant optimization of the EER method and its modern follow-ups. Through empirical studies, DAO has demonstrated superior performance in both low and higher budget settings, outperforming existing methods by a significant margin across seven datasets.

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APPENDIX

A LOW-BUDGET ACTIVE LEARNING: A MOTIVATING CASE STUDY

In this section, we provide an empirical analysis to demonstrate that commonly used heuristic-based AL algorithms do not work well under very low-budget settings. Specifically, we analyze (1) uncertainty sampling methods including least confidence (Lewis, 1995), minimum margin (Scheffer et al., 2001), maximum entropy (Settles, 2009), and Bayesian Active Learning by Disagreement (BALD) (Gal et al., 2017); (2) diversity sampling methods such as Core-Set (Sener & Savarese, 2017) and Variational Adversarial Active Learning (VAAL) (Sinha et al., 2019); and (3) hybrid method such as Batch Active learning by Diverse Gradient Embeddings (BADGE) (Ash et al., 2019).

We test the above methods on the CIFAR10 (Krizhevsky et al., 2009) dataset starting with an initial labeled set with size $|\mathcal{L}_{\text{init}}| = 10$, and conducted 50 acquisition rounds where after each round $B = 10$ new samples are selected and labeled. We use ResNet-18 (He et al., 2016) as our training model across all methods. And we repeated the acquisitions five times with different random seeds. The results are visualized in Fig. 6, where we plot the *relative* performance between each method and random sampling acquisition through a diverging color map.

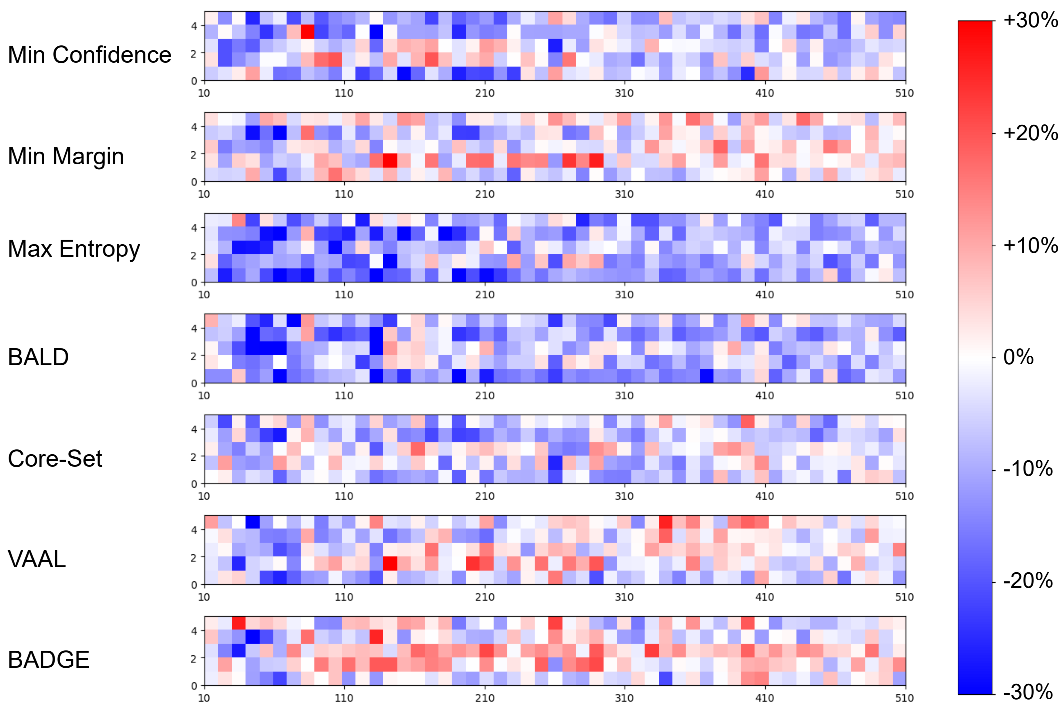


Figure 6: Existing methods fail to outperform random sampling with small budgets. This figure shows the relative performance between multiple methods and random acquisition. Within each subplot, x axis represents the accumulative acquisition size, while y axis indicates runs initiated with different random seeds. White color indicates on-par performance with random, blue indicates worse, and red indicates better.

Aligning with the general perceptions that low-budget (Mittal et al., 2019; Hacohen et al., 2022) and cold-start (Zhu et al., 2019; Chandra et al., 2021) AL tasks are especially challenging, we empirically observe that almost all popular AL algorithms fail to outperform the naive random sampling when acquisition quota is less than 1% (500 out of 50,000 in the case of CIFAR10) of the unlabeled size. More specifically, when the quota is less than 0.2% (less than 100 data points for CIFAR-10), all methods fail to reliably outperform random sampling (as the beginning of each heatmap in Fig. 6 are almost all blue), which greatly motivates the development of DAO. We also include the more conventional line plot of the empirical analysis which may provide more detailed information of each run in Fig. 7.

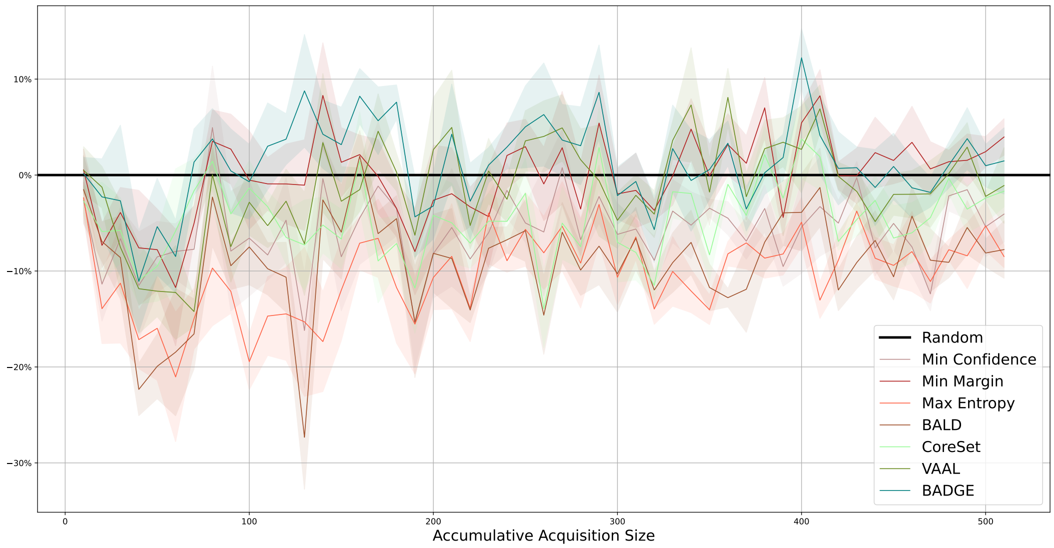
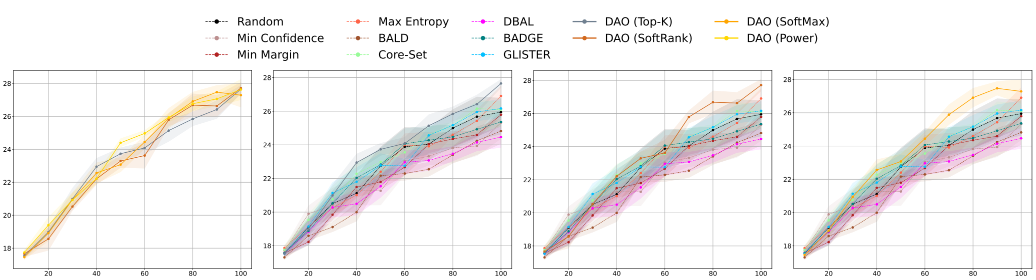


Figure 7: Relative performance between existing popular AL methods and random acquisition. horizontal axis represents the accumulative size of the labeled set, while vertical axis indicates relative performance in percentage.

B Experiments on Different Stochastic Batch Acquisitions

In this section, we provide more detailed results of §5.4. Specifically, we further study the performance of DAO when no batch sampling strategy or other sampling strategy is used and compare the results with existing popular AL algorithms. The results are shown in Fig. 8. For all experiments, we used the same low-budget setting as discussed in §4.



(a) (b) (c) (d)

Figure 8: CIFAR-10 experiment results on (a): DAO without batch acquisition strategy (using naive top-k selection) and with other sampling strategies (softmax and softrank, as discussed in §3.5); (b): DAO without sampling (top-k) vs. existing AL algorithms; (c): DAO with softrank sampling vs. existing AL algorithms; (d): DAO with softmax sampling vs. existing AL algorithms; In all subplots, horizontal axis represents the accumulative size of the labeled set, while vertical axis indicates classification accuracy.

C VISUALIZATIONS OF SAMPLES SELECTED BY DAO

In this section, we show the visual representations of the data samples collected by DAO as a complement to §5.5. Unlabeled and newly acquired data, in this case, images, or their latent space embeddings, are first dimensionally-reduced and then visualized in Fig. 9. We see that, DAO-selected data exhibit characteristics of diversity across the sample space over multiple acquisition rounds, while display uncertainty characteristics within single round.

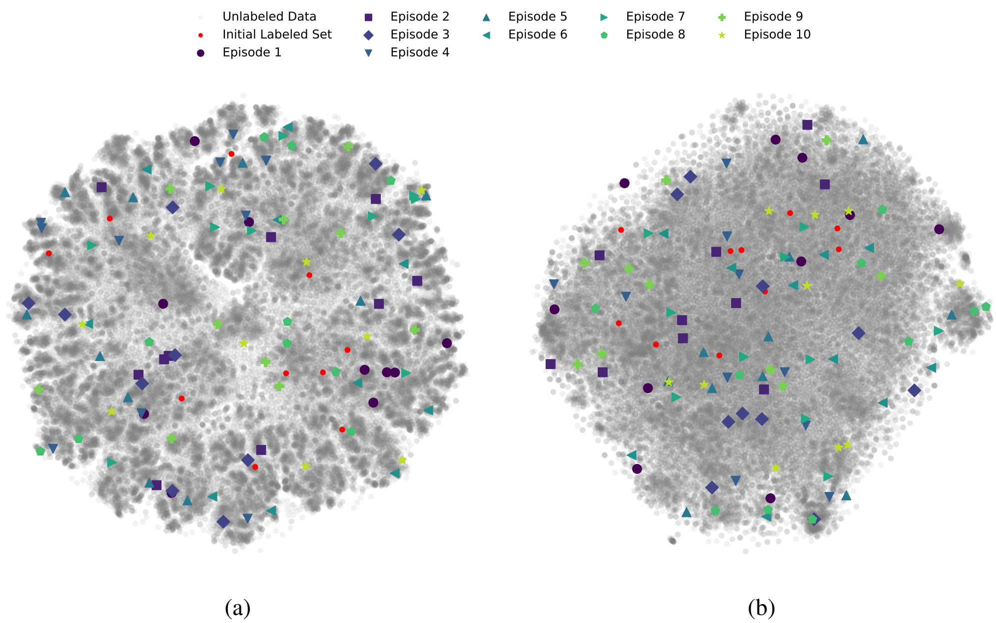


Figure 9: Visualizations of DAO acquisitions with dimensionality reduced from (a): raw images; and (b): latent space image embeddings.