A Active learning, in more detail

First, we will give an additional task description of Active Learning (AL) in Appendix A.1 introducing necessary concepts and mathematical notation for our compared query methods which are discussed in Appendix A.2. Finally, we give intuitions where the connection of AL to Self-Supervised Learning (Self-SL) and Semi-Supervised Learning (Semi-SL) lies in Appendix A.3 and Appendix F.4.

A.1 From supervised to active learning

In supervised learning, we are given a labeled dataset of sample-target pairs $(x, y) \in \mathcal{L}$ sampled from an unknown joint distribution $p(x, y)$. Our goal is to produce a prediction function $p(Y|x, \theta)$ parametrized by θ, which outputs a target value distribution for previously unseen samples from $p(x)$. Choosing θ might amount, for example, to optimizing a loss function which reflects the extent to which $\text{argmax}_c p(Y = c|x, \theta) = y$ for $(x, y) \in \mathcal{L}$. However, in pool-based AL we are additionally given a collection of unlabeled samples $\mathcal{U}$, sampled from $p(x, y)$. By using a query method (QM), we hope to leverage this data efficiently through querying and successively labeling the most informative samples $(x_1, ..., x_B)$ from the pool. This should lead to a prediction function better reflecting $p(Y|x)$ than if random samples were queried.

From a more abstract perspective, the goal of AL is to use the information of the labeled dataset $\mathcal{L}$ and the prediction function $p(Y|x, \theta)$, to find the samples giving the most information where $p(Y|x)$ deviates from $p(Y|x, \theta)$. This is also reflected by the way performance in AL is measured – which is the relative performance gain of the prediction function with queries from a QM compared to random queries. Making the prediction function implicitly the gauge for measuring the "success" of an AL strategy.

At the heart of AL is an optimization problem: AL is a game of reducing cost – one trades in computation cost with the expectation of lowering labeling cost which is deemed to be the bottleneck.

A.2 Query methods

A comprehensive overview of AL and its methods is out of the scope of this paper, we refer interested readers to [50] as a basis and [40] for an overview of current research. Most QMs fall into two categories following either: explorative strategies, which enforce queried samples to explore the distribution of $p(x)$; and uncertainty-based strategies, which make direct use of the prediction function $p(Y|x, \theta)$. [2] The principled combination of both strategies, especially to allow larger query sizes for uncertainty-based QM, is an open research question.
In our work, we focus exclusively on QMs which induce no changes to the prediction function and add no additional HPs except for Bayesian QMs modeled with dropout. This immediately rules out QMs like Learning-Loss [55] or TA-VAAL [30], changing the prediction function, and QMs like VAAL [51], introducing new HPs. The QMs we use for our comparisons are currently state-of-the-art in AL on classification tasks. Further, they require no additional hyperparameters (HPs) to be set for the query function which is hard to evaluate in practice due to the validation paradox.

For this chapter we follow the notation introduced in [31], where e.g. X represents a random variable and x represents a concrete sample of variable X.

Random Draws samples from the pool $\mathcal{U}$ randomly which follows $p(x, y)$. Therefore it can be interpreted as an exploratory QM.

Core-Set This method is based on the finding that the decision boundaries of convolutional neural networks are based on a small set of samples. To find these samples, the Core-Set QM queries samples that minimize the maximal shortest path from unlabeled to labeled sample in the representation space of the classifier [49]. This is also known as the K-Center problem, for which we use the K-Center greedy approximation. It draws queries especially from tails of the data distribution,

[2] This is conceptually similar to the exploration and exploitation paradigm seen in Reinforcement Learning and there actually exist strong parallels between Reinforcement Learning and Active Learning – so much so that Reinforcement Learning has been proposed to use in AL and AL-based strategies have been proposed to be used in Reinforcement Learning.

to cover the whole dataset as well as possible. Therefore we classify it as an explorative strategy.

Entropy The Entropy QM greedily queries the samples x with the highest uncertainty of the model as shown in Equation (1) with C being the number of classes.

$$H(Y|x,\theta) = \sum_{c=1}^{C} p(Y=c|x,\theta) \cdot \log(p(Y=c|x,\theta)) \tag{1}$$

BALD Uses a bayesian model and selects greedily a query of samples with the highest mutual information between the predicted labels Y and weights Θ for a sample x following [19]. From the weight variable Θ the concrete values $\theta \sim p(\theta|\mathcal{L})$ are then obtained by MC sampling of a bayesian dropout model [19].

$$\begin{aligned} \mathrm{MI}(Y;\Theta|x,\mathcal{L}) = &\sum_{c=1}^{C}(p(Y=c|x,\mathcal{L}) \cdot \log(p(Y=c|x,\mathcal{L})) \\ &- \mathbb{E}_{p(\theta|\mathcal{L})}\left[H(Y|x,\theta)\right]) \end{aligned} \tag{2}$$

Where $p(Y|x,\mathcal{L}) = \mathbb{E}_{p(\theta|\mathcal{L})}\left[p(Y|x,\theta)\right]$.

BADGE Uses the K-MEANS++ initialization algorithm on the last layer gradient embeddings $\mathcal{G} = \{\nabla_{\theta_{L-1}}\mathcal{L}(\hat{y}(x), p(Y|x,\theta)|x \in \mathcal{U}\}$ to obtain B centers. These are likely to have diverse directions (which capture diversity due to diverse parameter updates) and large loss gradients (capturing uncertainty due to large loss changes) [2].

A.3 Connection to self-supervised learning

The high-level concept of Self-SL pre-training is to obtain a model by training it with a proxy task that is not dependent on annotations, leading to representations that generalize well to a specific task. This allows the induction of information from unlabeled data into the model in the form of an initialization, which can be interpreted as a form of bias. Usually, these representations are supposed to be clustered based on some form of similarity, which is often induced directly by the proxy task and also the reason why different proxy tasks are useful for different downstream tasks. Several different Self-SL pre-training strategies were developed based on different tasks s.a. generative models or clustering [12, 13, 21, 25], with contrastive training being currently the de facto standard in image classification. For a more thorough overview over Self-SL we refer the interested reader to [41]. Based on this, we use the popular contrastive SimCLR [13] training strategy as a basis for our Self-SL pre-training.

A.4 Connection to semi-supvervised learning

In Semi-SL the core idea is to regularize $p(Y|x,\theta)$ by inducing information about the structure of $p(x)$ using the unlabeled pool additionally to the labeled dataset. Usually, this leads to the representations of unlabeled samples with the clustering being more in line with the structure of the supervised task [39]. Several different Semi-SL methods were developed based on regularizations on unlabeled samples, which often fall into the category of enforcing consistency of predictions against perturbations and/or reducing the uncertainty of predictions (for more information, we refer to [45]). For a more thorough overview of Semi-SL we refer interested readers to [7, 45] In our experiments, we use FixMatch [52] as a Semi-SL method, which combines both aforementioned principles of consistency and uncertainty reduction in a simple manner.

B Active learning literature, in more detail

We will discuss the current literature landscape of deep active classification with a focus on our proposed key-pitfalls as shown in Figure 1b.

The rules for evaluation of each of the five pitfalls (P1-P5) are:

P1 Data distribution	Use of multiple datasets for evaluation featuring class-imbalanced datasets.
P2 Starting budget	Evaluation or ablating the influence of the starting budget on multiple datasets explicitly.
P3 Query size	Evaluation or ablating the influence of the query size on multiple datasets explicitly.
P4 Performant baselines	Performance is close to ours or Munjal et al. [44] for ST models on CIFAR-10/100(see Appendix H for details).[3]
P4 HP Optim. & Val. Split	The use of a dedicated validation set to configure the classifier.
P5 Self-SL	Benchmarking AL with a performant Self-SL training paradigms.
P5 Semi-SL	Benchmarking AL with a performant Semi-SL training paradigm

Munjal et al. [44] Evaluate the performance of AL methods and compare against and with well finetuned baseline models using AutoML.

P1 Data Distribution: Perform experiments on CIFAR-10, CIFAR-100 and limited experiments on ImageNet. They perform an ablation on CIFAR-100 with an artificial imbalanced dataset.
→ (✔) due to limited imbalanced datasets.

P2 Starting Budget: Perform no experiments at all regarding the starting budget.
→ **X**

P3 Query Size: Perform ablations on CIFAR-10/100 comparing query sizes of 5% (2500) to 10% (5000). → ✔

P4 Performant Baselines: They achieve performance on CIFAR-10/100 on par with ours (see Appendix H). → ✔

P4 HP Optim. & Val. Split They explicitly use a validation set and finetune their hyperparameters based on the validation set performance using AutoML.
→ ✔

P5 Self-SL: They do not consider using models pre-trained with Self-SL.
→ **X**

P5 Semi-SL: They do not consider using models trained with semi-supervised training paradigms.
→ **X**

Mittal et al. [43] Evaluate the performance of AL methods and set them into context with semi-supervised training paradigms.

P1 Data Distribution: Perform experiments on CIFAR-10, CIFAR-100.
→ **X**

P2 Starting Budget: Perform experiments both on the standard setting with starting budget of 5000 (10%) on CIFAR-10/100 as well as 250 (CIFAR-10) and 500 (CIFAR-100).
→ (✔) due to limited settings.

P3 Query Size: They do not consider speicifally ablating the query size.
→ **X**

[3] We only base this on ST models, as getting good performance with Self-SL and Semi-SL for low data settings can be achieved without taking HP configuration into account, as they can simply be taken from a paper focusing on them which often use very large validation sets.

P4 Performant Baselines: Their random baseline is more performant on CIFAR10/100 than most of the literature. However, not as good as Munjal et al. [44] or ours (see Appendix H).
→ (✔) due to performance being good but no on par with ours.

P4 HP Optim. & Val. Split They do not state optimizing their hyperparameters based on a validation set.
→ **X**

P5 Self-SL: They do not consider using models pre-trained with Self-SL.
→ **X**

P5 Semi-SL: They evaluate AL with and against the semi-supervised training paradigm 'Unsupervised Data Augmentation for Consistency Training'.
→ ✔

Bengar et al. [6] Evaluate the performance of AL methods and set them into context with self-supervised training paradigms.

P1 Data Distribution: They perform experiments on CIFAR-10/100 and TinyImageNet. All of which are class balanced datasets.
→ **X** due to only evaluating balanced datasets.

P2 Starting Budget: They use 3 different starting budgets on each of their three datasets. CIFAR-10: 0.1%, 1%, 10%; CIFAR-100: 1%, 2%, 10%; Tiny ImageNet: 1%, 2%, 10% (% of the whole dataset).
→ ✔

P3 Query Size: Each of the three different starting budgets has a different query size resulting in overlapping experiments. Therefore it would be possible to draw some conclusions about the influence of the query size.
→ (✔) due missing selective evaluation of query size.

P4 Performant Baselines: Their supervised random baseline is performing worse on CIFAR-10/100 than most models in the literature (see Appendix H).
→ **X**

P4 HP Optim. & Val. Split: They do not state optimizing their hyperparameters based on a validation set.

P5 Self-SL: They evaluate AL methods with and against one self-supervised training paradigm (SimSiam).
→ ✔

P5 Semi-Supervise Learning: They do not consider using models trained with semi-supervised training paradigms.
→ **X**

Gao et al. [20] Evaluate the performance of AL methods against and in the context of semi-supervised training paradigms. Further, they propose a new query method designed for AL with models that are trained with a Semi-SL training paradigm.

P1 Data Distribution: They perform experiments on CIFAR-10/100 and ImageNet.
→ **X** due to only evaluating balanced datasets.

P2 Starting Budget: They perform a specific ablation about the importance of the starting budget on CIFAR-10 with multiple settings and discuss it.
→ ✔

P3 Query Size: In addition to the standard experiments, they perform experiments with query sizes of 50 and 250. However, they do not specifically discuss its importance.
→ (✔) due missing selective evaluation of query size.

P4 Performant Baselines: The performance of their supervised random baseline models in the main comparison is not close to our performance on CIFAR-10/100.
→ **X**

P4 HP Optim. & Val. Split: They do not state optimizing their hyperparameters based on a validation set.
→ **X**

P5 Self-SL: They do not consider using models pre-trained with Self-SL.
→ **X**

P5 Semi-SL: They evaluate AL with and against the semi-supervised training paradigm (MixMatch).
→ ✔

Yi et al. [54] They propose to use self-supervised pre-text as a basis for query functions.

P1 Data Distribution: Perform experiments on CIFAR-10, an imbalanced version of CIFAR-10, Caltech-101 and ImageNet.
→ ✔

P2 Starting Budget: One experiment is performed where they select the starting budget with their proposed Active Learning method on CIFAR-10. Otherwise, they do not evaluate the performance under different starting budgets.
→ **X**

P3 Query Size: They do not evaluate the performance with regard to different query sizes.
→ **X**

P4 Performant Baselines: Their supervised random baseline models are not close to the performance of our random baseline models on CIFAR-10 (see Appendix H).
→ **X**

P4 HP Optim. & Val. Split: They do not state optimizing their hyperparameters based on a validation set.
→ **X**

P5 Self-SL: They consider several different Self-SL paradigms (‘Rotation Prediction’, ‘Colorization’, ‘Solving jigsaw puzzles’ and ‘SimSiam’) based on which they select rotation prediction for their experiments.
→ (✔) due to selection of non state-of-the-art Self-SL paradigm.

P5 Semi-Supervise Learning: They do not consider using models trained with semi-supervised training paradigms.
→ **X**

Krishnan et al. [35] They propose to use a supervised contrastive training paradigm as a basis for two AL methods.

P1 Data Distribution: Perform experiments on Fashion-MNIST, SVHN and CIFAR-10 and an imbalanced version of CIFAR-10.
→ (✔) due to imbalanced CIFAR-10 being simulated.

P2 Starting Budget: They do not evaluate the performance under different starting budgets.
→ **X**

P3 Query Size: They do not evaluate the performance with regard to different query sizes.
→ **X**

P4 Performant Baselines: Their supervised random baseline models are not close to the performance of our random baseline models on CIFAR-10 (see Appendix H).
→ **X**

P4 HP Optim. & Val. Split: They do not state optimizing their hyperparameters based on a validation set.
→ **X**

P5 Self-SL: They do not consider using models pre-trained with Self-SL.
→ **X**

P5 Semi-Supervise Learning: They do not consider using models trained with semi-supervised training paradigms.
→ **X**

Kim et al. [30] They propose task-aware active learning which is a combination of learning loss active learning and variational adversarial active learning.

P1 Data Distribution: Perform experiments on CIFAR-10, CIFAR-100, CALTECH 101 and imbalanced CIFARS.
→ ✔

P2 Starting Budget: They do not evaluate the performance under different starting budgets.
→ (✔)

P3 Query Size: They do not evaluate the performance with regard to different query sizes.
→ (✔)

P4 Performant Baselines: Their supervised random baseline models perform good but not on par with ours on CIFAR-10 and 100.
→ (✔)

P4 HP Optim. & Val. Split: They do not state optimizing their hyperparameters based on a validation set.
→ **X**

P5 Self-SL: They do not consider using models pre-trained with Self-SL.
→ **X**

P5 Semi-SL: They do not consider using models trained with semi-supervised training paradigms.
→ **X**

Beck et al. [4] Evaluate several AL methods in different settings to gain an understanding which AL methods outperform random queries. Further, they provide the Al toolkit DISTIL.

P1 Data Distribution: Perform experiments on CIFAR-10, CIFAR-100, Fashion-MNIST, SVHN and MNIST. → **X** due to no class imbalance.

P2 Starting Budget: They perform one experiment, where they evaluate a lower starting budget for MNIST.
→ (✔) due limited dataset.

P3 Query Size: They evaluate three different query sizes on CIFAR-10, but do so only for Random, Entropy and BADGE.
→ (✔) due to limited scope.

P4 Performant Baselines: Their supervised random baseline models perform good but no par with our random baseline models on CIFAR-10/100 (see Appendix H).
→ (✔) due to limited scope.

P4 HP Optim. & Val. Split: They do not state optimizing their hyperparameters based on a validation set.
→ **X**

P5 Self-SL: They do not consider using models pre-trained with Self-SL.
→ **X**

P5 Semi-SL: They do not consider using models trained with semi-supervised training paradigms.
→ **X**

Zhan et al. [58] Evaluate a multitude of different AL methods and provide the AL toolkit *DeepAL*$^+$.

P1 Data Distribution: Perform experiments on Tiny ImageNet, CIFAR-10 (and CIFAR-10 imbalanced), CIFAR-100, Fashion-MNIST, EMNIST and SVHN. Further Experiments are performed on an Histopathological image Classification Task (BreakHis) and Chest X-Ray Pneumonia classification (Pneumonia-MNIST) as well as the Waterbird dataset adopted from object recognition with correlated backgrounds.
→ ✔

P2 Starting Budget: They do not evaluate the performance under different starting budgets.
→ **X**

P3 Query Size: They evaluate multiple different query sizes on CIFAR-10 and analyze the difference.
→ ✔

P4 Performant Baselines: Their supervised random baseline models are not close to the performance of our random baseline models on CIFAR-10/100.
→ **X**

P4 HP Optim. & Val. Split: They do not state optimizing their hyperparameters based on a validation set.
→ **X**

P5 Self-SL: They do not consider using models pre-trained with Self-SL.
→ **X**

P5 Semi-SL: They do not consider using models trained with semi-supervised training paradigms.
→ **X**

Chan et al. [11] Evaluate how AL methods interact with self- and semi-supervised training paradigms and how and whether they yield a benefit. The experiments in this paper differ from standard AL experiments by using only one query cycle, making it hard to compare systematically.

P1 Data Distribution: Perform experiments on CIFAR-10 and CIFAR-100.
→ **X**

P2 Starting Budget: Experiments are performed with a fixed starting budget of 3 samples per class or 2 samples per class in one case. This does not allow for evaluate of the influence of the starting budget on AL methods.
→ **X**

P3 Query Size: They query all samples for their final performance in one query step. This does not allow for evaluation of the influence of the query size on AL methods.
→ **X**

P4 Performant Baselines: Their supervised random baseline models perform on par with our random baseline models on CIFAR-10/100.
→ ✔

P4 HP Optim. & Val. Split: They do not state optimizing their hyperparameters based on a validation set.
→ **X**

P5 Self-SL: They use Debiased Contrastive Learning as self-supervised pretext task.
→ ✔

P5 Semi-SL: They use Pseudo-labeling and FixMatch as semi-supervised training paradigms.
→ ✔

Table 1: Number of Samples for each class in CIFAR-10 LT dataset. Validation and test sets are balanced.

Class	Train Split
airplane	4500
automobile (but not truck or pickup truck)	2913
bird	1886
cat	1221
deer	790
dog	512
frog	331
horse	214
ship	139
truck (but no pickup truck)	90

C Dataset details

Each dataset is split into a training, a validation and a test split.
For CIFAR-10/100 (LT) datasets the test split of size 10000 observations is already given and for MIO-TCD and ISIC-2019 we use a custom test split of 25% random observations of the entire dataset size. For MIO-TCD and ISIC-2019 the train, validation and test splits are imbalanced.
The validation split for all CIFAR-10 and CIFAR-100 datasets are 5000 randomly drawn observations corresponding to 10% of the entire dataset. For CIFAR-10 LT the validation split also consists of 5000 samples obtained from the dataset before the long-tail distribution is applied onto the training split. The CIFAR-10 LT validation split is therefore balanced. For MIO-TCD and ISIC-2019 the validation splits consist of 15% of the entire dataset.
The shared training & pool dataset for CIFAR-10/100 consists of 45000 observations. For CIFAR-10 LT the training & pool datasets consist of 12,600 observations. For MIO-TCD and ISIC-2019 the training & pool datasets consist of 60% the dataset.

C.1 Dataset descriptions

1. CIFAR-10: natural images containing 10 classes, label distribution is uniform
   Splits: (Train:45000; Val: 5000; Test; 10000)
   Whole Dataset: 60000
2. CIFAR-100: natural images containing 100 classes, label distribution is uniform
   Splits: (Train:45000; Val: 5000; Test; 10000)
   Whole Dataset: 60000
3. CIFAR-10 LT: natural images containing 10 classes, label distribution of test and validation split is uniform, label distribution of train split is artifically altered with imbalance factor $\rho = 50$ according to [10]. The resulting label distribution is shown in Tab. 1.
   Splits: (Train:$\sim$12,600; Val: 5000; Test; 10000)
   Whole Dataset: 27600
4. ISIC-2019: dermoscopic images containing 8 classes, label distribution of the dataset is imbalanced and shown in Tab. 2
   Splits: (Train:15200; Val: 3799; Test; 6332)
   Whole Dataset: 25331
5. MIO-TCD: natural images of traffic participants containing 11 classes, label distribution of the dataset is imbalanced and shown in Tab. 3
   Splits: (Train:311498; Val: 77875; Test; 129791)
   Whole Dataset: 519164

Table 2: Number of Samples for each class in ISIC-2019

Class	Whole Dataset
Melanoma	4522
Melanocytic nevus	12875
Basal cell carcinoma	3323
Benign keratosis	867
Dermatofibroma	197
Vascular lesion	63
Squamos cell carcinoma	64

Table 3: Number of samples for each class in MIO-TCD

Class	Whole Dataset
Articulated Truck	10346
Background	16000
Bicycle	2284
Bus	10316
Car	260518
Motorcycle	1982
Non-motorized vehicle	1751
Pedestrian	6262
Pickup truck	50906
Single unit truck	5120
Work van	9679

D Experimental setup, in more detail

Here we detail the most crucial information for reprocubility, re-implementation and checking our implementation. When in doubt, trust the information documented here with regard to what we wanted to do in our code.

D.1 Initial dataset setup

Before we do anything else the datasets are split according to Figure 4 resulting in a tain split, a validation split and a test split. Each dataset has 3 different validation splits while always using the same test split. This is to ensure comparability across these splits without relying on cross-validation. The exact splits for each dataset are detailed in Appendix C. After that the final datasets use for training and validation are then labeled according to the 'label strategy', which is described in Figure 5. For all balanced datasets, we use class balanced label strategies since the label strategy only leads to different outcomes for imbalanced datasets. For CIFAR-10 LT we use the label strategy on the train split only, whereas for MIO-TCD and ISIC-2019 we use the label strategy on both train and validation split. The amount of data which is labeled for the final datasets of each split is then dependent upon the label-regime (described in more detail in Appendix D.2).

D.2 Label regimes

The exact label regimes are obtained by first taking the corresponding splits and then using the proper label strategy (see Figure 5) in combination with the starting budget and validation set size according to Tab. 4.

D.3 Model architecture and training

On each training step the model is trained from its initialization to avoid a 'mode collapse' [32]. Further we select the checkpoint with the best validation set performance in the spirit of [19]. A ResNet-18 [24] is the backbone for all of our experiments with weight decay disabled on bias parameters. If not otherwise noted, a nesterov momentum optimizer with momentum of 0.9 is used.

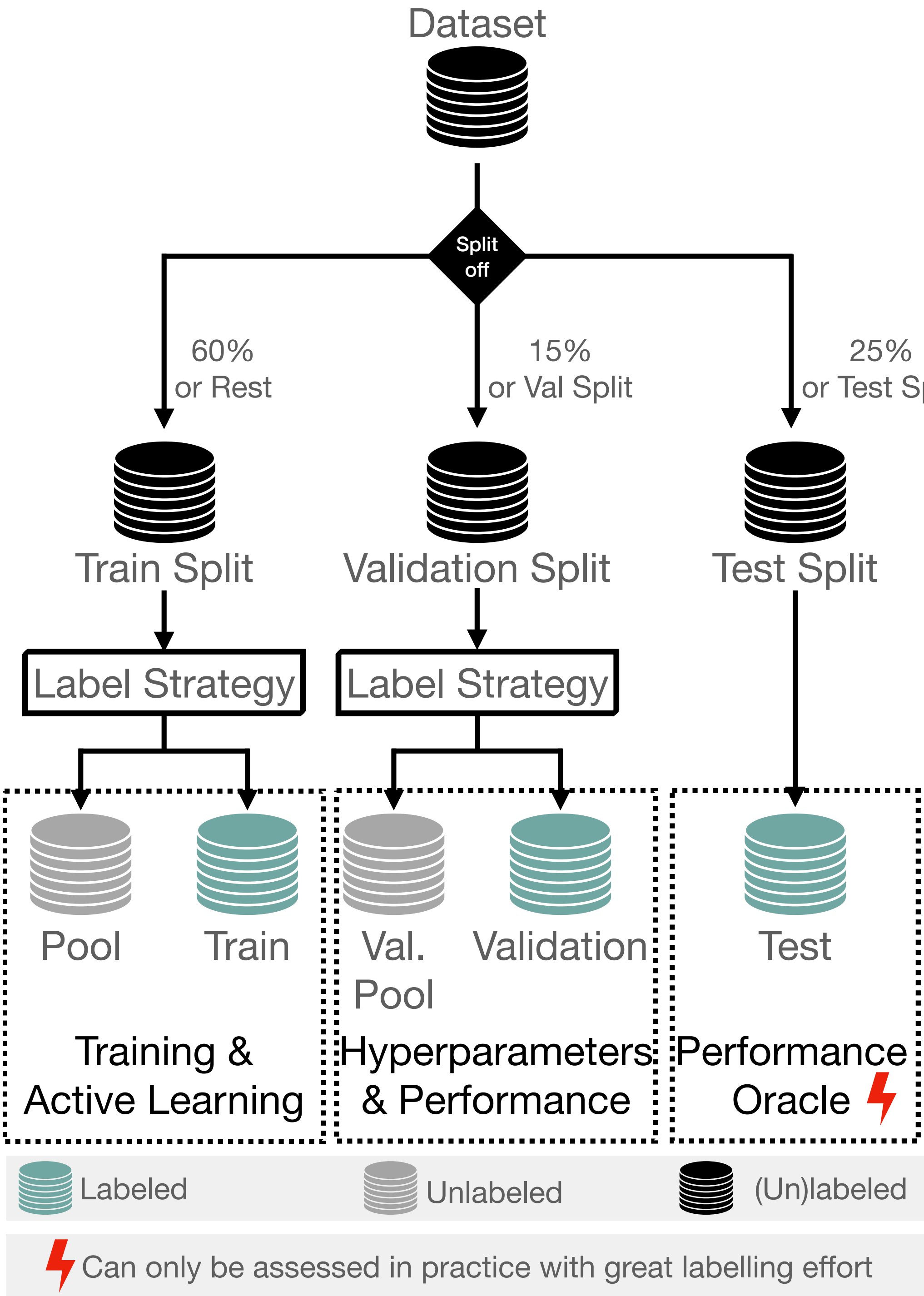


Figure 4: Description of the three different data splits and their use-cases. The complete separation of a validation split allows to compare across label regimes and incorporate techniques for performance evaluation s.a. Active Testing [34]. For evaluation and development the test split should be as big as possible since QM recommendations are based on the test set performance making it a form of "oracle". An estimate of the size a dataset is required to have to measure specific performance differences can be derived using Hoeffding's inequality [26, 45].

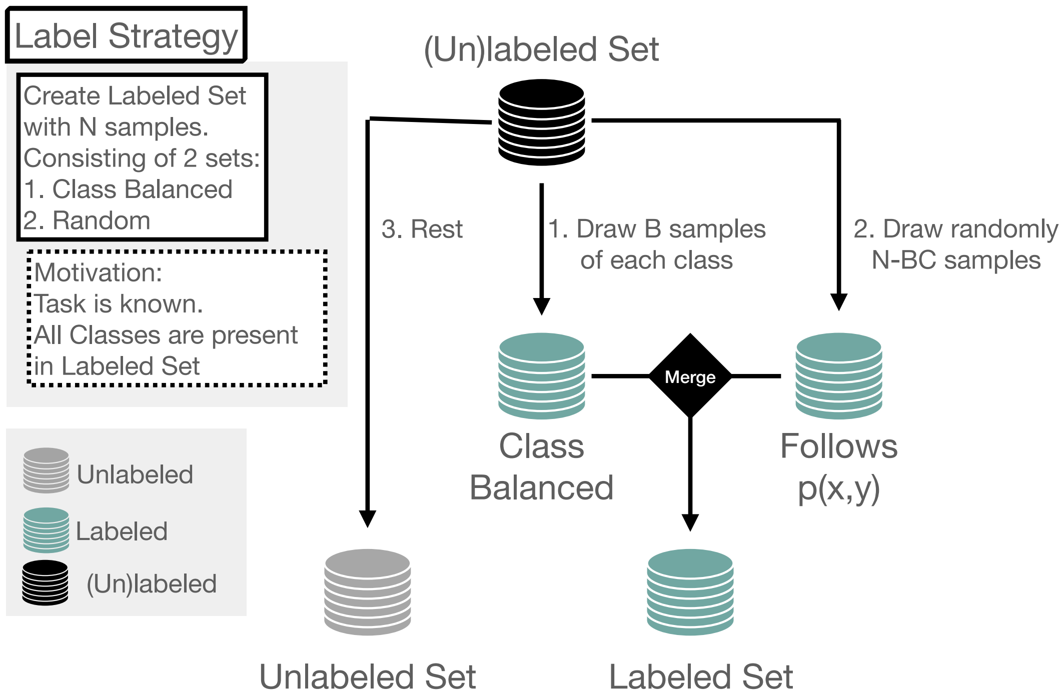


Figure 5: The Label Strategy used on the two roll-out datasets MIO-TCD and ISIC-2019 and for train and pool set on CIFAR-10 LT. For class balanced datasets this strategy does not induce meaningful changes to balanced starting budgets.

Table 4: The exact values for all label regimes. Final Budget denotes the amount of labeled training samples at the end of the AL pipeline.

Dataset	CIFAR-10			CIFAR-100			CIFAR-10 LT			MIO-TCD			ISIC-2019		
Label Regime	Low	Mid	High	Low	Mid	High	Low	Mid	High	Low	Mid	High	Low	Mid	High
Starting Budget	50	250	1000	500	1000	5000	50	250	1000	55	275	1100	40	200	800
Query Size	50	250	1000	500	1000	5000	50	250	1000	55	275	1100	40	200	800
Final Budget	500	2500	10000	5000	10000	25000	500	2500	10000	550	2750	11000	400	2000	8000
Validation Set Size	250	1250	5000	2500	5000	5000	250	1250	5000	275	1375	5500	200	800	3799

For Self-SL models we use a two layer MLP as a classification head to make better use of the Self-SL representations with further details in Appendix D.5. To obtain bayesian models we add dropout on the final representations before the classification head with probability ($p = 0.5$) following [19]. For all experiments on imbalanced datasets, we use the weighted CE-Loss following [44] based on the implementation in SK-Learn [9] if not otherwise noted. Models trained purely on the labeled dataset upsample it to a size of 5500 following [32] if the labeled train set is smaller.

Bayesian Models All steps that require bayesian properties of the models including the prediction are obtained by drawing 50 MC samples following [19, 32].

ST ST models are trained for 200 epochs with Cosine Annealing and 10 epochs warmup.

Self-SL Self-SL pre-trained models are trained for 80 epochs with a reduction of the learning rate with a factor of 10 every 20 epochs (MultiStepLR) and using a Mulit-Layer-Percpeptron (MLP) classification head (detailed description in Appendix D.5). The complete setup of the training for SimCLR is described in Appendix D.4.

Semi-SL Semi-SL training is identical to the one proposed with the FixMatch method [52], except that we do not use exponentially moving average models and restrict the training step from 1e6 to 2e5. The FixMatch implementation in our experiments is based on the open-source implementation

Table 5: HPs of the SimCLR pre-text training on each dataset. HP for CIFAR datasets are directly taken [13] whereas MIO-TCD and ISIC-2019 HP are adapted from ImageNet experiments.

Dataset	CIFAR-10/CIFAR100/CIFAR-10 LT	MIO-TCD	ISIC-2019
Epochs	1000	200	1000
Optimizer	LARS	LARS	
Scheduler	Cosine Annealing	Cosine Annealing	
Warmup Epochs	10	10	
Temperature	0.5	0.1	
Batch Size	512	256	
Learning Rate	1	0.3	
Weight Decay	1E-4	1E-6	
Transform. Gauss Blur	False	True	
Transform. Color Jitter	Strength=0.5	Strength=1.0	

Table 6: MLP Head Ablation for Self-SL models on CIFAR-10, over all labeled training set a small improvement for Multi-Layer-Perceptron is measurable compared to Linear classification head models. Reported as mean (std).

Labeled Train Set	Classification Head	Accuracy (Val) %	Accuracy (Test) %
50	Linear	69.87(1.62)	69.90(2.18)
50	2 Layer MLP	71.47(3.06)	71.54(0.56)
500	Linear	84.67(0.36)	83.51(0.45)
500	2 Layer MLP	85.37(0.16)	84.60(0.37)
1000	Linear	87.13(0.69)	85.97(0.64)
1000	2 Layer MLP	87.69(0.55)	86.57(0.42)
5000	Linear	90.77(0.44)	90.20(0.21)
5000	2 Layer MLP	91.12(0.32)	90.25(0.24)

of [4] and MixMatch for distribution alignment [5]. We always select the final Semi-SL model of the training for testing and querying. On imbalanced datasets we change the supervised term to the weighted CE-Loss and use distribution alignment on every dataset except for CIFAR-10 (where it does not improve performance [52]). The HP sweep for our Semi-SL models includes weight decay and learning rate.

Hyperparameters All information with regard to the final HPs and our proposed methodology of finding them is detailed in Appendix E

D.4 Self-supervised SimCLR pre-text training

Our implementation wraps the Pytorch-Lightning-Bolts implementation of SimCLR: https://lightning-bolts.readthedocs.io/en/latest/models/self_supervised.html#simclr . The training of our SimCLR models is performed by excluding the validation splits. Therefore three models are trained on each dataset, one for each different validation split. In Tab. 5 we give a list of the HPs used on each of our five different datasets. All other HPs are taken from [13]. Further, we did not optimize the HPs for SimCLR at all, meaning that on MIO-TCD and ISIC-2019 Self-SL models could perform even better than reported here.

D.5 MLP head for self-supervised pretrained models

The MLP Head used for the Self-SL models has 1 hidden layer of size 512 uses ReLU nonlinearities and BatchNorm. The results on CIFAR-10 based on which this design decision is based on is shown in Tab. 6.

[4] https://github.com/kekmodel/FixMatch-pytorch
[5] https://github.com/google-research/mixmatch

D.6 List of data transformations

Standard The standard augmentations we use are based on the different datasets.
For CIFAR datasets these are in order of execution: RandomHorizontalFlip, RandomCrop to 32x32 with padding of size 4.

For MIO-TCD we use the standard ImageNet transformations: RandomResizedCrop to 224x224, Random Horizontal Flip.

For ISIC-2019 we use ISIC transformations which are: Resize to 300x300, RandomHorizontalFlip, RandomVerticalFlip, ColorJitter(0.02, 0.02, 0.02, 0.01) ,RandomRotation(rotation=(-180, 180), translate=(0.1, 0.1), scale=(0.7, 1.3)), RandomAffine(-180, 180), RandomCrop to 224x224.
These are based on the ISIC-2018 challenge best single model submission:
https://github.com/JiaxinZhuang/Skin-Lesion-Recognition.Pytorch

RandAugmentMC We use the same set of image transformations used in RandAugment [17] with the parameters N=2 and M=10. A detailed list of image transformations alongside the corresponding values can be seen in [52] (Table 12).

The RandAugmentMC transformations were used additionally after the corresponding standard transformations for each dataset. RandAugmentMC(CIFAR) also adds cutout as a final transformation.

RandAugmentMC weak Works identical as RandAugmentMC and uses the same set of image transformations as for RandAugmentMC but changed its parameters to N=1 and M=2. Therefore the maximal range of values is divided by a factor of 5.

RandAugmentMC weak does not use cutout in difference to RandAugmentMC on CIFAR datasets.

D.7 Performance measure

As a measure of performance on CIFAR-10, CIFAR-100 and CIFAR-10 LT we use the accuracy while on MIO-TCD and ISIC-2019 we use balanced accuracy which is identical to mean recall shown in Equation (3).

$$\text{Mean Recall} = \sum_{c=1}^{C} \frac{1}{C} \frac{\text{TP}_c}{\text{TP}_c + \text{FN}_c} \tag{3}$$

Where C denotes the number of classes TP_c is the number of true positives for class c and FN_c being the number of samples belonging to class c being wrongly misclassified as another class.

D.8 Computational effort

Experiments were executed on a Cluster with access to multiple NVIDIA graphics cards. All ST and Self-SL pre-trained experiments used a single Nvidia RTX 2080 (10.7GB video-ram) graphic cards except for the BADGE experiments on CIFAR-100 and MIO-TCD which required more video-ram using Nvidia Titan RTX (23.6GB video-ram). The Semi-SL models on the CIFAR-10/100 (LT) datasets used also a single Nvidia RTX 2080 while on MIO-TCD and ISIC-2019 the Nvidia Titan RTX was utilized. For the results in our main table (excluding the HP optimization), the overall runtime was:

- All ST experiments: 1800 GPU hours
- All Self-SL pre-trained experiments: 1350 GPU hours[6]
- All Semi-SL experiments[7]: 11200 GPU hours

E Proposed hyperparameter optimization

Our proposed HP optimization for AL is based on the notion of minimizing HP selection effort by simplifying and reducing the search space. We use SGD Optimizer with Nesterov momentum of 0.9

[6]Excluding the pre-training
[7]For only 2 label regimes and exluding MIO-TCD and ISIC-2019

Table 7: Final HPs for each dataset and label regime for our ST models based on our HP tuning. HPs denoted with a * are fixed across datasets and HP denoted with a + are pre-selected for each dataset while all other HP are obtained via sweeping.

Dataset	CIFAR-10			CIFAR-100			CIFAR-10 LT			MIO-TCD			ISIC-2019		
Label Regime	Low	Mid	High	Low	Mid	High	Low	Mid	High	Low	Mid	High	Low	Mid	High
Epochs*		200			200			200			200			200	
Optimizer*		SGD Nesterov 0.9			SGD Nesterov 0.9			SGD Nesterov 0.9			SGD Nesterov 0.9			SGD Nesterov 0.9	
Scheduler*		Cosine Annealing			Cosine Annealing			Cosine Annealing			Cosine Annealing			Cosine Annealing	
Warmup Epochs*		10			10			10			10			10	
Loss*		CE-Loss			CE-Loss			CE-Loss			CE-Loss			CE-Loss	
Sampling+		standard			standard			oversampling		oversampling			oversampling		
Batch Size+		1024			1024			1024			512			512	
Learning Rate		0.1			0.1			0.1		0.01	0.01	0.1		0.1	
Weight Decay		5E-3			5E-3			5E-3		5E-3	5E-4	5E-3		5E-3	
Data Augmentation		RandAugmentMC (CIFAR)			RandAugmentMC (CIFAR)			RandAugmentMC (CIFAR)			RandAugmentMC (ImageNet)			RandAugmentMC (ISIC)	

Table 8: Final HPs for each dataset and label regime for our Self-SL models based on our HP tuning. Overall Performance was remarkably stable with regard to HPs and stronger augmentations did not necessarily improve performance in the same way as for ST models. This is presumably due to the pre-trained representations. HP denoted with a * are fixed across datasets and HP denoted with a + are pre-selected for each dataset while all other HP are obtained via sweeping.

Dataset	CIFAR-10			CIFAR-100			CIFAR-10 LT			MIO-TCD			ISIC-2019		
Label Regime	Low	Mid	High	Low	Mid	High	Low	Mid	High	Low	Mid	High	Low	Mid	High
Epochs*		80			80			80			80			80	
Optimizer*		SGD Nesterov 0.9			SGD Nesterov 0.9			SGD Nesterov 0.9			SGD Nesterov 0.9			SGD Nesterov 0.9	
Scheduler*		MulitStepLR			MulitStepLR			MulitStepLR			MulitStepLR			MulitStepLR	
Warmup Epochs*		0			0			0			0			0	
Loss*		CE-Loss			CE-Loss			CE-Loss			CE-Loss			CE-Loss	
Sampling+		standard			standard			oversampling		oversampling			oversampling		
Batch Size+		64			64			64			256			128	
Learning Rate		0.001			0.001		0.01	0.01	0.001	0.001	0.01	0.001	0.01	0.001	0.01
Weight Decay		5E-3			5E-3		5E-4	5E-4	5E-3		5E-3		5e-3	5E-4	5e-3
Data Augmentation		RandAugmentMC weak (CIFAR)			RandAugmentMC weak (CIFAR)			Standard (CIFAR)		RandAugmentMC weak (ImageNet)	Standard (ImageNet)	Standard (ImageNet)		Standard (ISIC)	

and select a number of epochs that always allow a complete fit of the model. The scheduler is also fixed across experiments as are the warmup epochs if used. Secondly, we pre-select the batchsize for each dataset since it is usually not a critical HP as long as it is big enough for BatchNorm to work properly.

ST For our ST models the final HP for each dataset and label regime are shown in Tab. 7.
HP sweep: weight decay: (5E-3, 5E-4); learning rate: (0.1, 0.01); data transformation: (RandAugmentMC, Standard)

Self-SL For our Self-SL pre-trained models the final HP for each dataset and label regime are shown in Tab. 8.
HP sweep: weight decay: (5E-3, 5E-4); learning rate: (0.01, 0.001); data transformation: (RandAugmentMC weak, Standard)

Semi-SL For our Semi-SL models we follow [52] with regard to HP selection as closely as possible. The final HP for each dataset and label regime are shown in Tab. 9.
HP sweep: weight decay and learning rate.

Table 9: Final HPs for each dataset and label regime for our Semi-SL models based on our HP tuning. HP denoted with a * are fixed across datasets and HP denoted with a + are pre-selected for each dataset while all other HP are obtained via sweeping. – denotes not performed experiments.

Dataset	CIFAR-10			CIFAR-100			CIFAR-10 LT			MIO-TCD			ISIC-2019		
Label Regime	Low	Mid	High	Low	Mid	High	Low	Mid	High	Low	Mid	High	Low	Mid	High
Optimization Steps*		2E5	–		2E5	–		2E5	–		2E5	–		2E5	–
Optimizer*		SGD Nesterov 0.9	–		SGD Nesterov 0.9	–		SGD Nesterov 0.9	–		SGD Nesterov 0.9	–		SGD Nesterov 0.9	–
Scheduler*		Cosine Annealing	–		Cosine Annealing	–		Cosine Annealing	–		Cosine Annealing	–		Cosine Annealing	–
Warmup Steps+		0	–		0	–		0	–		3000	–		3000	–
Loss+		CE-Loss	–		CE-Loss	–		weigthed CE-Loss	–		weigthed CE-Loss	–		weigthed CE-Loss	–
Sampling*		standard	–		standard	–		standard	–		standard	–		standard	–
λ_u^*		1	–		1	–		1	–		1	–		1	–
μ^*		7	–		7	–		7	–		7	–		7	–
τ^*		0.95	–		0.95	–		0.95	–		0.95	–		0.95	–
Distribution Alignment+		False	–		True	–		True	–		True	–		True	–
Batch Size*		64	–		64	–		64	–		64	–		64	–
Learning Rate		0.03	–		0.03	–		0.03	–			–			–
Weight Decay		5E-4	–		5E-4	–	1E-3	5E-4	–			–			–
Data Augmentation+		Standard (CIFAR)	–		Standard (CIFAR)	–		Standard (CIFAR)	–		Standard (ImageNet)	–		Standard (ISIC)	–
Unlabeled Augmentation+		RandAugmentMC (CIFAR)	–		RandAugmentMC (CIFAR)	–		RandAugmentMC (CIFAR)	–		RandAugmentMC (ImageNet)	–		RandAugmentMC (ISIC)	–

F Detailed results

F.1 Main results

General observations: For all datasets, the overall performance of models was primarily determined by the training strategy and the HP selection, with the benefits of AL being generally smaller compared to the proper selection of both. For the three toy datasets, Semi-SL generally performed best, followed by Self-SL and ST last, whereas, for the two real-world datasets, Semi-SL showed no substantial improvement over ST in the first training stage and, therefore, further runs were omitted. Also, the absolute performance gains for Self-SL models with AL are generally smaller compared to ST models. For Semi-SL, there were generally only very small performance gains or substantially worse performance with AL observed. Concerning the effect of AL, the high-label regime proved to work for ST models on all datasets and Self-SL models. On the two real-world datasets, MIO-TCD and ISIC-2019, a dip in performance at 7k samples for all ST models could be observed. This behavior is ablated in Appendix I.1.

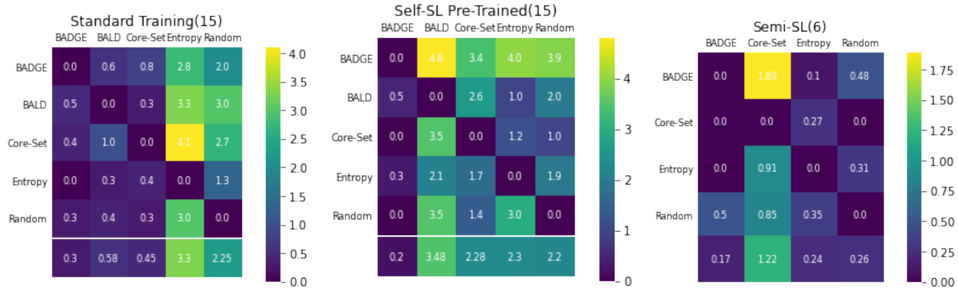
Evaluation using the pair-wise penalty matrix: We use the pair-wise penalty matrix (PPM) to compare whether the performance of one query method significantly outperforms the others. It is essentially a measure of how often one method significantly outperforms another method based on a t-test with $\alpha = 0.05$ (more info in [2, 4]). This allows to aggregate results over different datasets and label regimes, with the disadvantage being that the absolute performance is not taken into consideration. When reading a PPM, each row i indicates the number of settings in which method i beats other methods, while column j indicates the number of settings in which method j is beaten by another method.

We show the PPMs aggregated over all datasets and label regimes for each training paradigm in Figure 6.

For all methods, BADGE is the QM that is least often outperformed by other QMs. Further, for Self-SL models, it is never significantly outperformed by Random, whereas it is seldomly significantly outperformed for ST models. Based on this, we deem BADGE to be the best of our compared QMs for both ST and Self-SL models. Since BADGE is more often outperformed by Random (0.5) on the Semi-SL datasets and the additional high training cost for each iteration, we believe that Random is the better choice in many cases.

Evaluation using the area under the budget curve: For each of the following subsections, we added the area under the budget curve (AUBC) for each dataset and label regime to allow assessing the absolute performance each QM brings. Generally, higher values are better. For more information, we refer to [57, 58].

The results on the dataset for AUBC also show that BADGE is always one of the best performing AL methods. This is in line with the findings based on the PPM.



(a) (b) (c)

Figure 6: PPMs aggregated over all experiments for Standard Models (a), Self-Sl Pre-Trained Models (b) and Semi-SL models(c).
The value in the title (X) gives the highest possible value in a cell and the lowest row is the mean value across a column j without row $i = j$ signaling how often on average on QM is outperformed by another.

F.1.1 CIFAR-10

The AUBC values are shown in Tab. 10.

Table 10: Area Under Budget Curve values for CIFAR-10.

	Label Regime	Low-Label		Medium-Label		High-Label	
		Mean	STD	Mean	STD	Mean	STD
Training	Query Method						
ST	BADGE	0.4730	0.0105	0.7289	0.0025	0.8599	0.0016
	BALD	0.4744	0.0106	0.7253	0.0051	0.8578	0.0017
	Entropy	0.4307	0.0018	0.6859	0.0042	0.8498	0.0025
	Core-Set	0.4681	0.0038	0.7282	0.0043	0.8629	0.0017
	Random	0.4720	0.0144	0.7309	0.0068	0.8526	0.0030
Self-SL	BADGE	0.8282	0.0016	0.8728	0.0018	0.9086	0.0012
	BALD	0.8005	0.0056	0.8692	0.0011	0.9093	0.0010
	Entropy	0.8002	0.0090	0.8663	0.0017	0.9071	0.0010
	Core-Set	0.8224	0.0026	0.8670	0.0009	0.9015	0.0009
	Random	0.8117	0.0040	0.8669	0.0009	0.8989	0.0007
Semi-SL	BADGE	0.9349	0.0010	0.9488	0.0022	–	–
	Entropy	0.9193	0.0082	0.9497	0.0007	–	–
	Core-Set	0.9343	0.0018	0.9442	0.0007	–	–
	Random	0.9326	0.0050	0.9478	0.0002	–	–

ST Results are shown in Figure 7.

Self-SL Results are shown in Figure 8.

Semi-SL Results are shown in Figure 9.

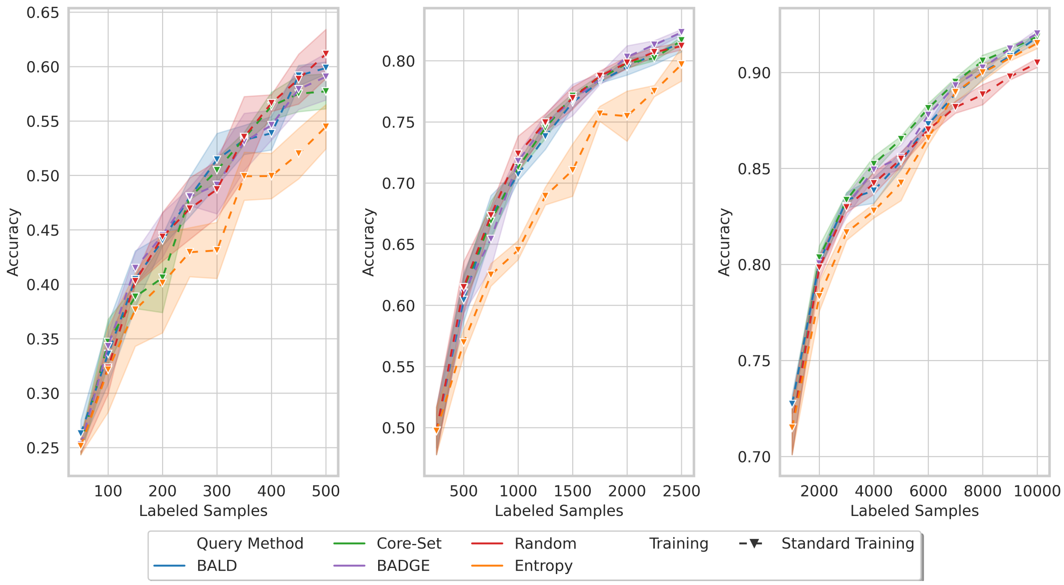


Figure 7: CIFAR-10 ST

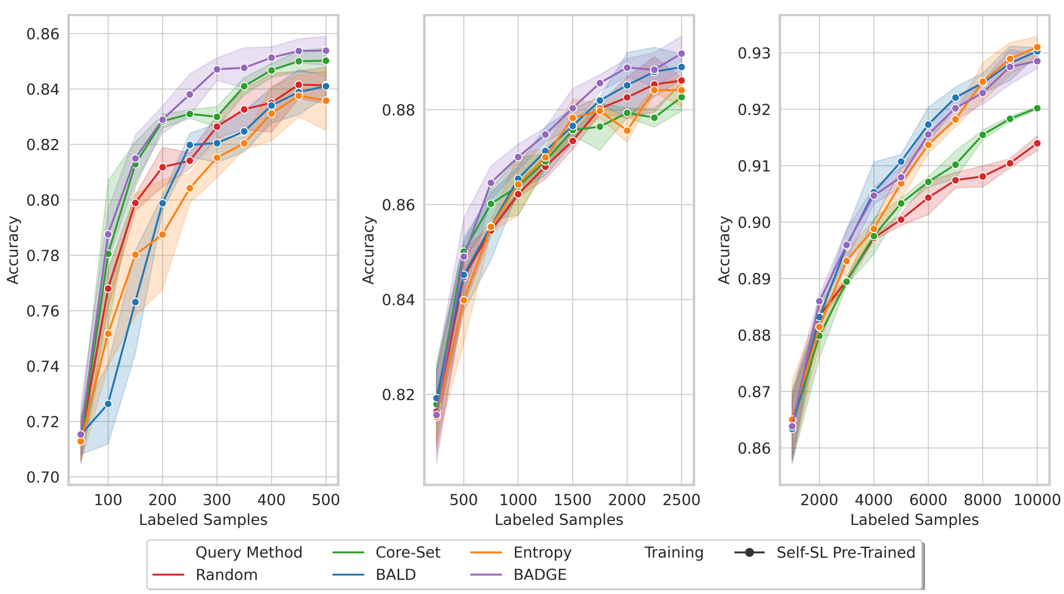


Figure 8: CIFAR-10 Self-SL

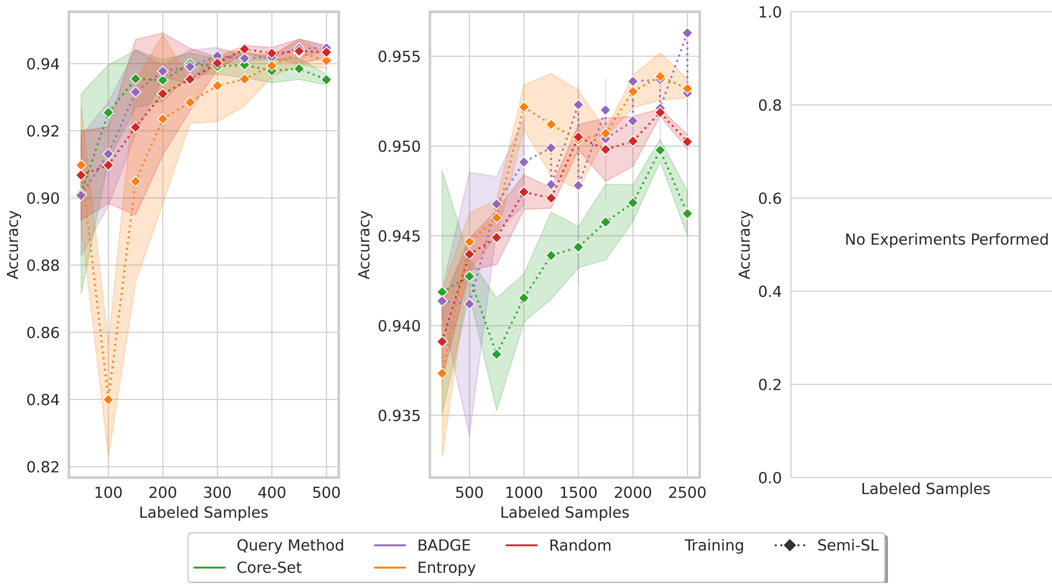


Figure 9: CIFAR-10 Semi-SL

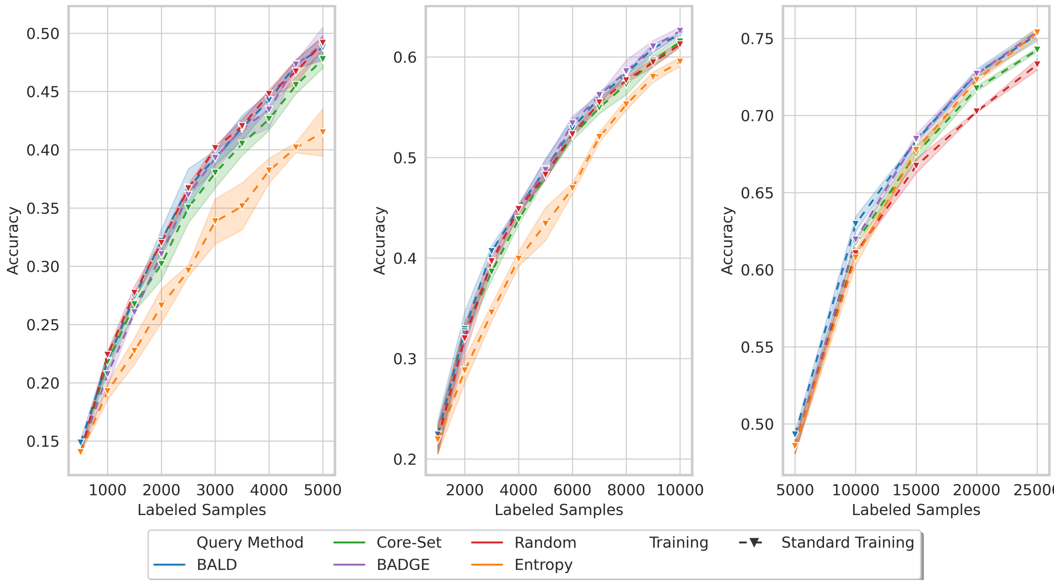


Figure 10: CIFAR-100 ST

F.1.2 CIFAR-100

The AUBC values are shown in Tab. 11.

Table 11: Area Under Budget Curve values for CIFAR-100.

	Label Regime	Low-Label		Medium-Label		High-Label	
		Mean	STD	Mean	STD	Mean	STD
Training	Query Method						
ST	BADGE	0.3525	0.0042	0.4855	0.0044	0.6627	0.0017
	BALD	0.3586	0.0007	0.4865	0.0019	0.6658	0.0002
	Entropy	0.3036	0.0095	0.4440	0.0007	0.6569	0.0021
	Core-Set	0.3458	0.0010	0.4767	0.0031	0.6560	0.0004
	Random	0.3599	0.0027	0.4791	0.0044	0.6474	0.0015
Self-SL	BADGE	0.5397	0.0030	0.6020	0.0019	0.6858	0.0021
	BALD	0.5028	0.0043	0.5754	0.0027	0.6784	0.0009
	Entropy	0.5111	0.0066	0.5857	0.0028	0.6857	0.0032
	Core-Set	0.5337	0.0044	0.5917	0.0032	0.6804	0.0013
	Random	0.5365	0.0017	0.5970	0.0017	0.6757	0.0013
Semi-SL	BADGE	0.5562	0.0033	0.6222	0.0041	–	–
	Entropy	0.5328	0.0158	0.6152	0.0038	–	–
	Core-Set	0.5220	0.0101	0.6083	0.0061	–	–
	Random	0.5713	0.0066	0.6307	0.0016	–	–

ST Results are shown in Figure 10.

Self-SL Results are shown in Figure 11.

Semi-SL Results are shown in Figure 12.

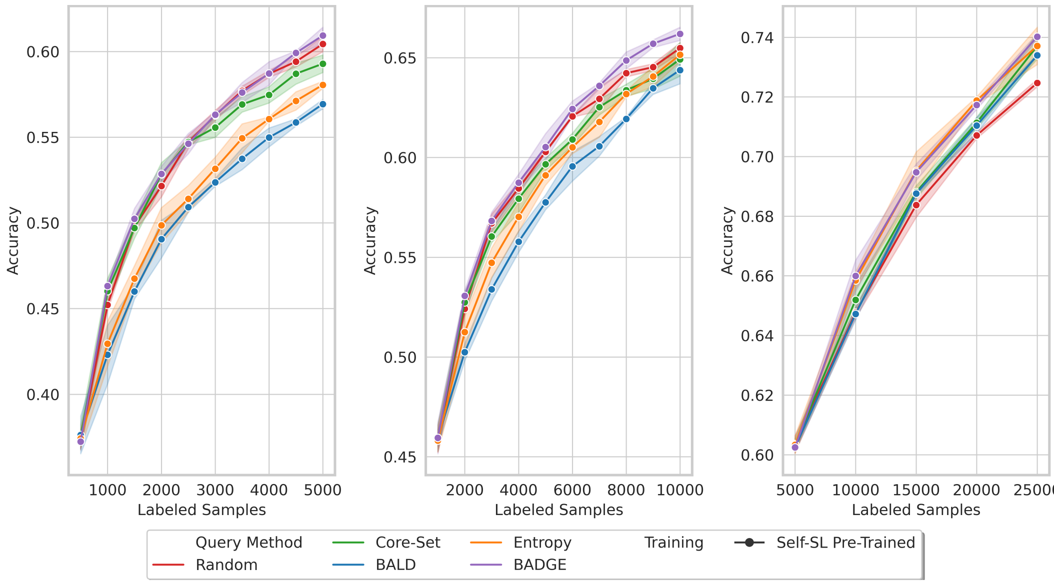


Figure 11: CIFAR-100 Self-SL

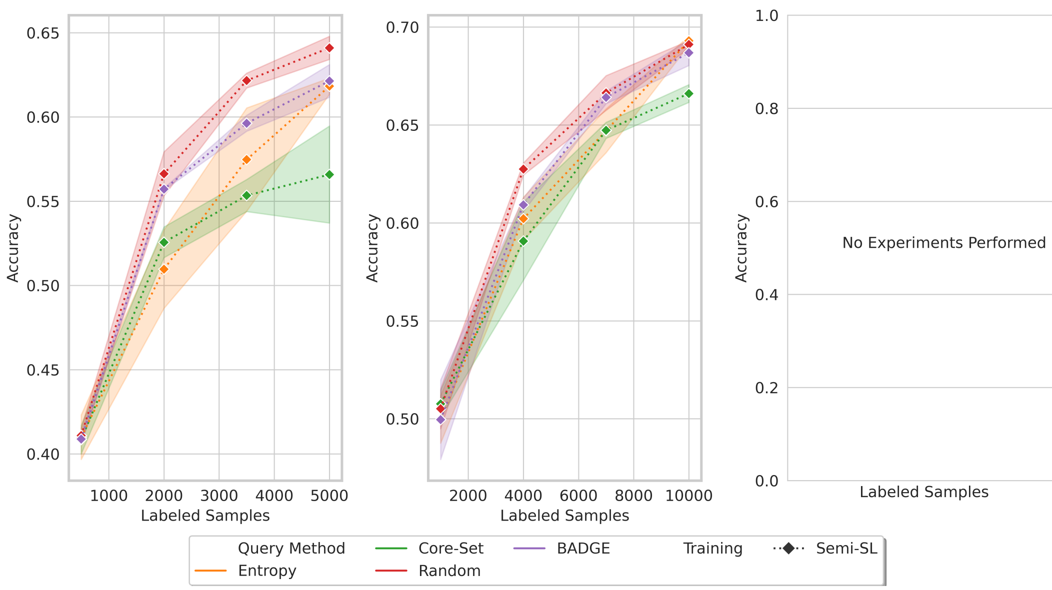


Figure 12: CIFAR-100 Semi-SL

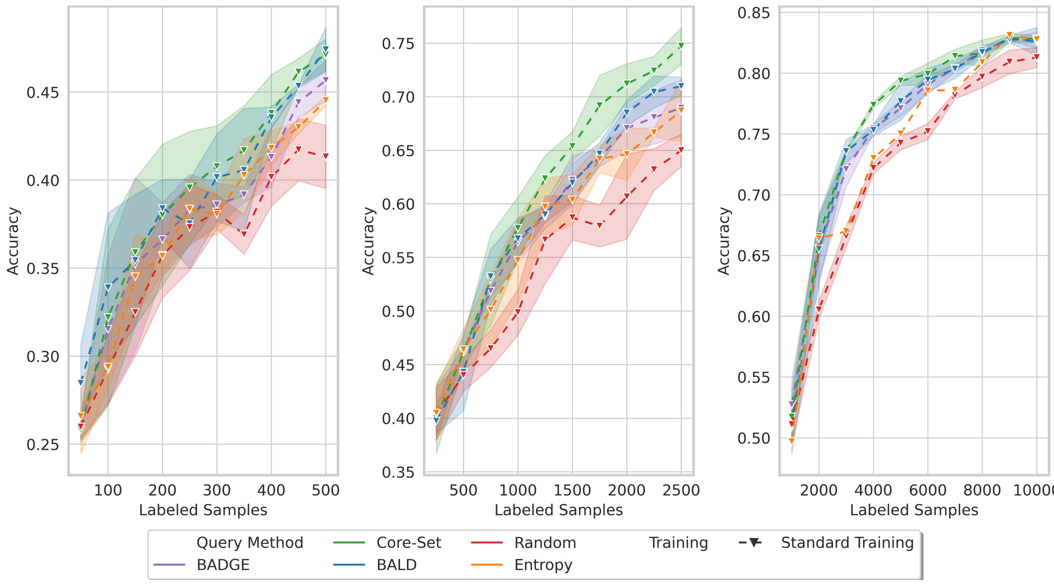


Figure 13: CIFAR-10 LT ST

F.1.3 CIFAR-10 LT

The AUBC values are shown in Tab. 12.

Table 12: Area Under Budget Curve values for CIFAR-10 LT.

	Label Regime	Low-Label		Medium-Label		High-Label	
		Mean	STD	Mean	STD	Mean	STD
Training	Query Method						
ST	BADGE	0.3788	0.0152	0.5887	0.0098	0.7577	0.0004
	BALD	0.3919	0.0111	0.5935	0.0141	0.7590	0.0034
	Entropy	0.3740	0.0064	0.5793	0.0114	0.7454	0.0023
	Core-Set	0.3939	0.0249	0.6162	0.0200	0.7667	0.0058
	Random	0.3615	0.0118	0.5446	0.0214	0.7263	0.0044
Self-SL	BADGE	0.5373	0.0233	0.6501	0.0026	0.7704	0.0093
	BALD	0.5431	0.0202	0.6549	0.0097	0.7742	0.0036
	Entropy	0.5282	0.0225	0.6450	0.0090	0.7707	0.0061
	Core-Set	0.5298	0.0182	0.6171	0.0154	0.7555	0.0032
	Random	0.5397	0.0208	0.6173	0.0097	0.7554	0.0069
Semi-SL	BADGE	0.7233	0.0166	0.7616	0.0087	–	–
	Entropy	0.6934	0.0289	0.7590	0.0101	–	–
	Core-Set	0.6825	0.0103	0.7608	0.0108	–	–
	Random	0.6965	0.0264	0.7363	0.0077	–	–

ST Results are shown in Figure 13.

Self-SL Results are shown in Figure 14.

Semi-SL Results are shown in Figure 15.

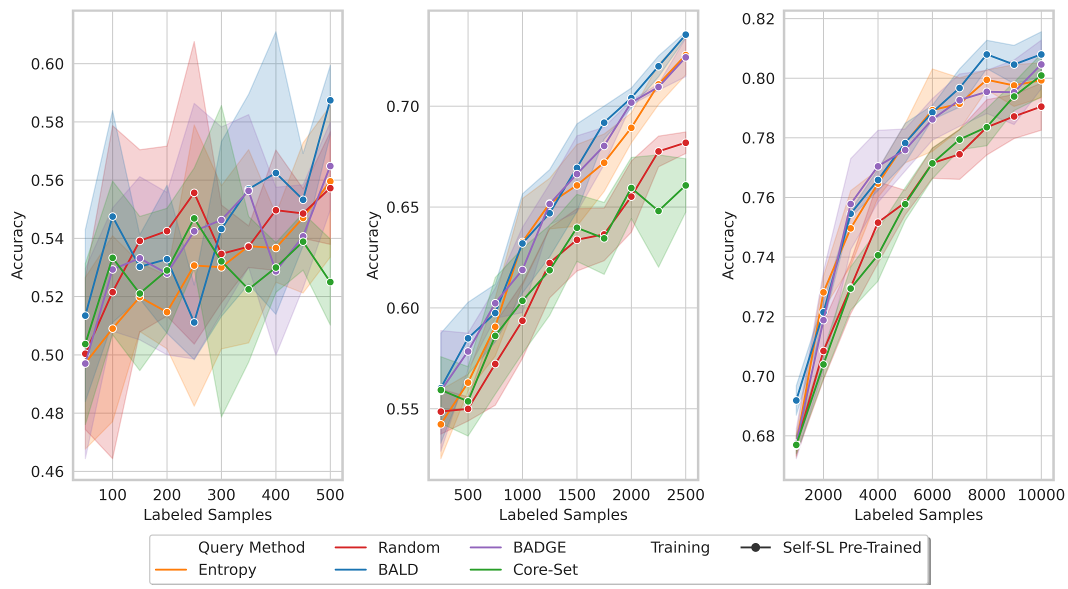


Figure 14: CIFAR-10 LT Self-SL

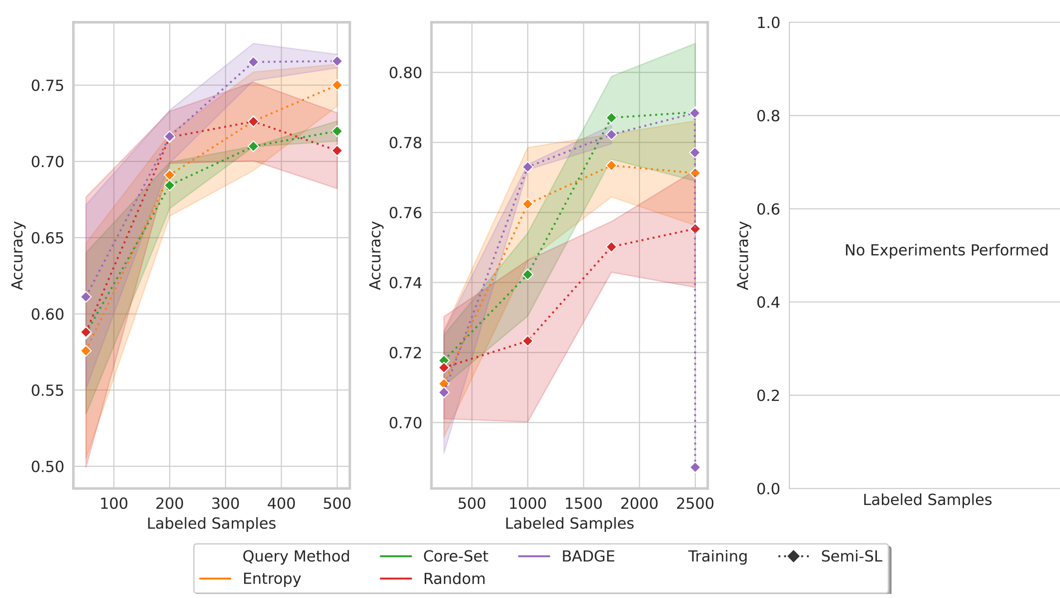


Figure 15: CIFAR-10 LT Semi-SL

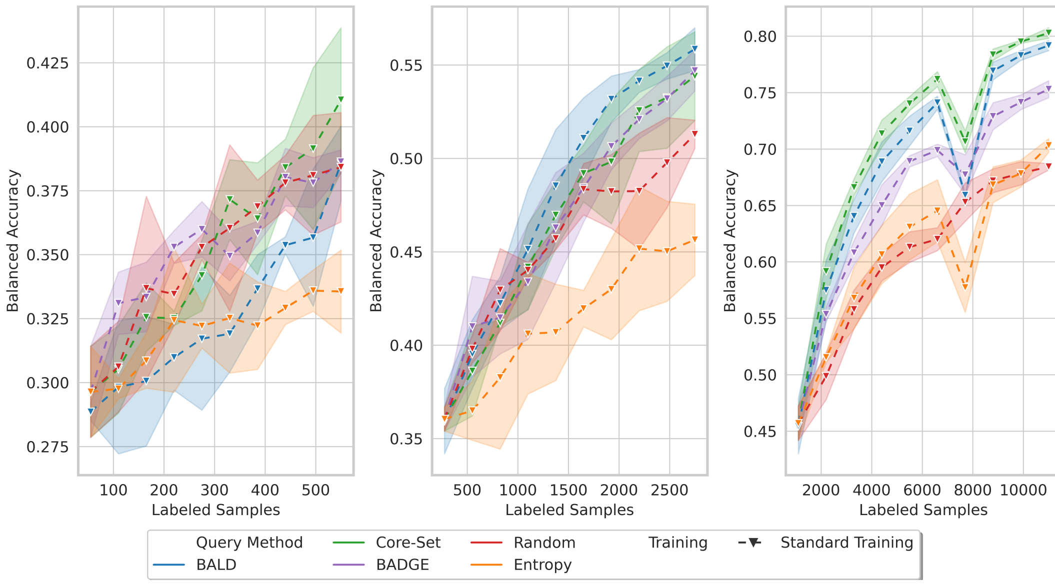


Figure 16: MIO-TCD ST

F.1.4 MIO-TCD

The AUBC values are shown in Tab. 13.

Table 13: Area Under Budget Curve values for MIO-TCD.

	Label Regime	Low-Label		Medium-Label		High-Label	
		Mean	STD	Mean	STD	Mean	STD
Training	Query Method						
ST	BADGE	0.3539	0.0041	0.4688	0.0153	0.6614	0.0080
	BALD	0.3254	0.0155	0.4830	0.0092	0.6884	0.0104
	Entropy	0.3201	0.0097	0.4134	0.0230	0.6078	0.0176
	Core-Set	0.3514	0.0134	0.4678	0.0181	0.7098	0.0056
	Random	0.3510	0.0151	0.4564	0.0140	0.6065	0.0120
Self-SL	BADGE	0.5446	0.0122	0.6365	0.0054	0.7174	0.0040
	BALD	0.4494	0.0102	0.5741	0.0138	0.6041	0.0092
	Entropy	0.5105	0.0092	0.6416	0.0075	0.6972	0.0029
	Core-Set	0.5060	0.0082	0.5900	0.0190	0.6699	0.0166
	Random	0.5298	0.0109	0.6124	0.0032	0.6975	0.0054

ST Results are shown in Figure 16.

Self-SL Results are shown in Figure 17.

Semi-SL We performed no AL experiments due to the bad performance of Semi-SL on the starting budgets. More information can be found in Appendix F.4.

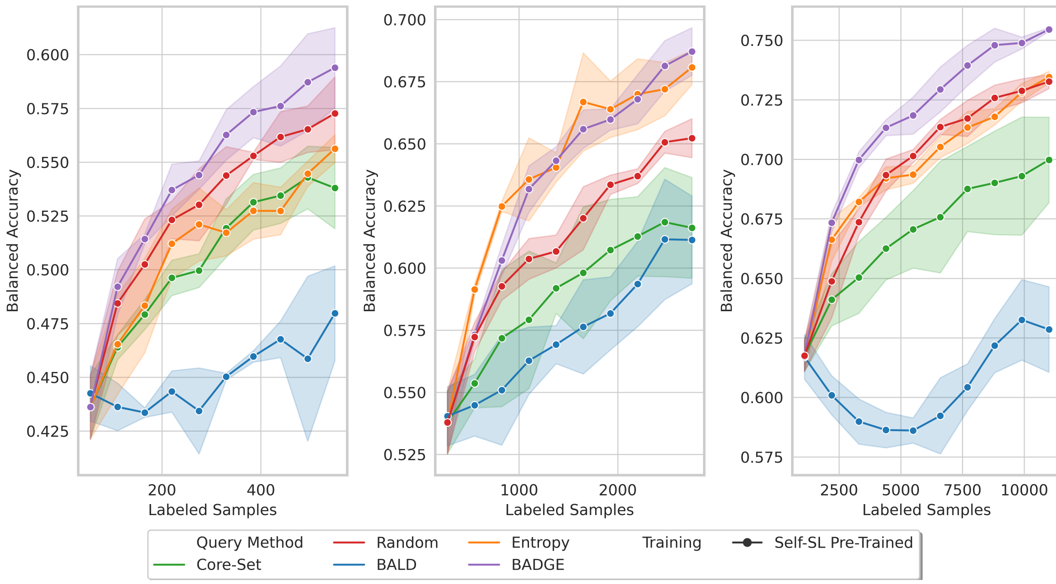


Figure 17: MIO-TCD Self-SL

F.1.5 ISIC-2019

The AUBC values are shown in Tab. 14.

Table 14: Area Under Budget Curve values for ISIC-2019.

	Label Regime	Low-Label		Medium-Label		High-Label	
		Mean	STD	Mean	STD	Mean	STD
Training	Query Method						
ST	BADGE	0.3204	0.0099	0.4331	0.0146	0.5628	0.0101
	BALD	0.3190	0.0133	0.4521	0.0211	0.5534	0.0052
	Entropy	0.3241	0.0067	0.4207	0.0335	0.5631	0.0061
	Core-Set	0.3426	0.0099	0.4501	0.0139	0.5708	0.0096
	Random	0.3376	0.0243	0.4116	0.0201	0.5273	0.0048
Self-SL	BADGE	0.3809	0.0168	0.4679	0.0174	0.5761	0.0063
	BALD	0.3949	0.0209	0.4847	0.0018	0.5914	0.0080
	Entropy	0.3666	0.0165	0.4659	0.0104	0.5872	0.0096
	Core-Set	0.3752	0.0205	0.4472	0.0071	0.5556	0.0069
	Random	0.3736	0.0092	0.4555	0.0053	0.5547	0.0066

ST Results are shown in Figure 18.

Self-SL Results are shown in Figure 19.

Semi-SL We performed no AL experiments due to the bad performance of Semi-SL on the starting budgets. More information can be found in Appendix F.4.

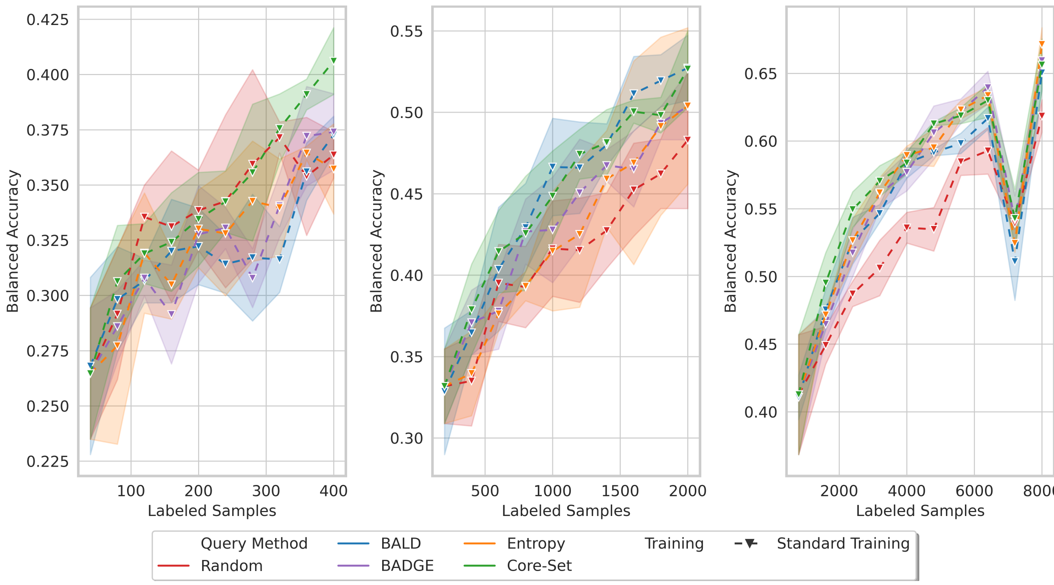


Figure 18: ISIC-2019 ST

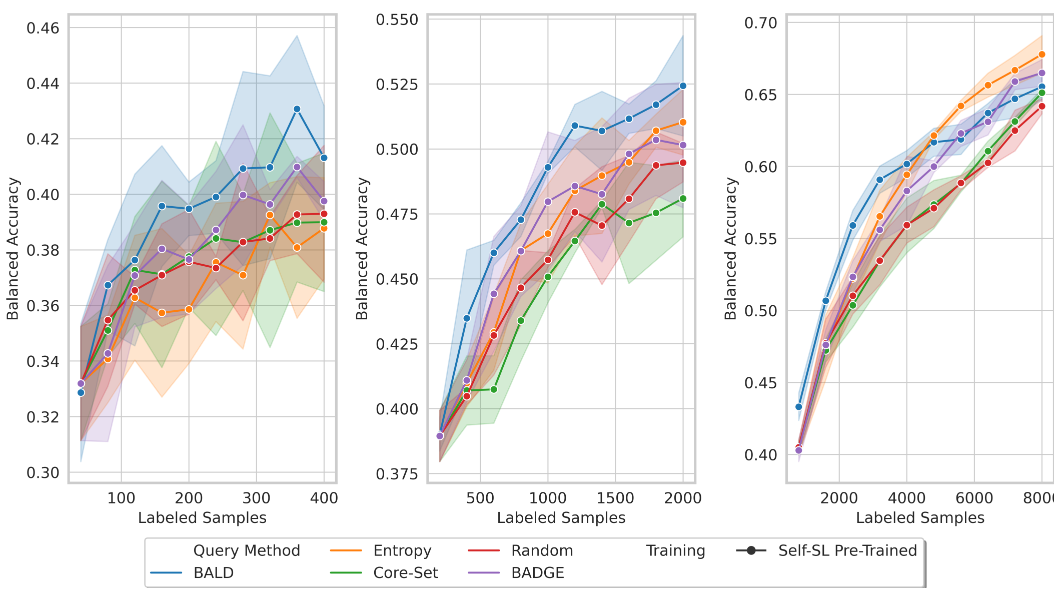


Figure 19: ISIC-2019 Self-SL Pre-Trained Models

F.2 Low-Label Query Size

To investigate the effect of query size in the low-label regime, we conduct an ablation with Self-SL pre-trained models on CIFAR-100 and ISIC-2019. For CIFAR-100 the query sizes are 50, 500 and 2000, while for ISIC-2019 they are 10, 40 and 160.

Here the accuracies for the overlapping labeled samples are shown which are analyzed using a t-test.

CIFAR100 The results are shown in Tab. 15 and Tab. 16. When comparing the performance of the same QM using different query sizes only BALD and Core-Set lead to statistically significant difference in performance. While it is consistent across both comparisons for BALD with the the performance difference widening for larger labeled sets and more iterations the trend for Core-Set is not as clear.

ISIC-2019 The results are shown in Tab. 17 and Tab. 18. Entropy is the only QM showing a significant difference, indicating that a query size of 40 outperforms a query size of 10 for a training set size of 160. However, this behavior does not extend to the other training set sizes. Whereas, for BALD, there is a consistent trend that smaller query sizes lead to increased performance.

Table 15: Accuracies % for the low-label comparison for CIFAR100 with query sizes 50 and 500 at overlapping training set sizes. Reported as mean (std). Values with a significant difference (t-test) across query sizes are denoted with $*$.

Labeled Samples	1000		1500	
Query Size	50	500	50	500
BADGE	45.75 (0.75)	46.32 (0.20)	50.02 (0.92)	50.24 (0.61)
BALD	45.54 (0.20)	42.31 (1.71)	49.41 (0.39)*	46.00 (0.44)*
Core-Set	46.53 (0.76)	46.02 (0.74)	49.34 (0.72)	49.70 (0.60)
Entropy	43.82 (0.40)	42.95 (1.32)	47.05 (0.91)	46.75 (0.76)
Random	46.10 (0.41)	45.22 (0.34)	49.88 (0.26)	49.79 (0.27)

Table 16: Accuracies % for the low-label comparison for CIFAR100 with query sizes 500 and 2000 at overlapping training set sizes. Reported as mean (std). Values with a significant difference (t-test) across query sizes are denoted with $*$.

Labeled Samples	2500		4500	
Query Size	500	2000	500	2000
BADGE	54.62 (0.60)	55.03 (0.38)	50.92 (0.12)	59.98 (0.60)
BALD	50.92 (0.30)	49.96 (1.43)	55.86 (0.21)*	52.14 (1.36)*
Core-Set	54.72 (0.16)*	53.52 (0.33)*	58.71 (0.61)	58.28 (0.43)
Entropy	51.41 (0.53)	51.79 (0.76)	57.12 (0.53)	57.53 (0.43)
Random	54.71 (0.38)	54.38 (0.21)	59.98 (0.60)	59.48 (0.48)

Table 17: Accuracies % for the low-label comparison for ISIC-2019 with query sizes 10 and 40 at overlapping training set sizes. Reported as mean (std). Values with a significant difference (t-test) across query sizes are denoted with $*$.

Labeled Sample	80		120		160		200		240	
Query Size	10	40	10	40	10	40	10	40	10	40
BADGE	34.39 (0.86)	36.03 (0.39)	37.58 (1.93)	36.40 (1.10)	37.58 (2.51)	37.24 (2.15)	38.32 (1.59)	37.52 (1.16)	38.78 (1.64)	38.94 (2.97)
BALD	38.11 (1.42)	36.51 (1.26)	38.80 (1.19)	37.26 (4.90)	40.40 (1.76)	39.23(1.89)	42.15 (1.49)	40.09 (2.59)	42.26 (0.97)	40.18 (2.70)
Core-Set	35.57 (1.49)	35.38 (0.50)	36.87 (1.73)	36.52 (2.24)	38.55 (2.37)	38.19 (1.69)	38.41 (1.80)	37.19 (2.93)	39.04 (2.94)	38.30 (1.66)
Entropy	35.19 (0.63)	34.87 (0.91)	37.06 (1.63)	38.59 (2.06)	36.95 (1.13)*	39.67 (0.55)*	38.25 (3.11)	39.93 (2.38)	39.38 (2.62)	40.26 (2.49)
Random	36.10 (0.70)	35.69 (0.68)	37.57 (1.79)	37.65 (2.15)	37.43 (1.77)	40.62 (0.62)	38.41 (1.46)	40.29 (1.78)	3835 (2.43)	41.14 (0.37)

Table 18: Accuracies % for the low-label comparison for ISIC-2019 with query sizes 40 and 160 at overlapping training set sizes. Reported as mean (std). Values with a significant difference (t-test) across query sizes are denoted with $*$.

Labeled Samples	200		360	
Query Size	40	160	40	160
BADGE	37.52 (1.16)	38.11 (1.07)	42.90 (3.29)	42.86 (1.44)
BALD	40.09 (2.59)	39.67 (2.54)	44.49 (1.78)	42.83 (1.05)
Core-Set	37.79 (2.93)	37.71 (3.18)	39.56 (1.48)	39.47 (1.04)
Entropy	39.93 (2.38)	37.80 (1.46)	42.03 (1.16)	40.82 (1.46)
Random	40.29 (1.78)	40.80 (2.34)	42.10 (2.29)	42.10 (2.29)

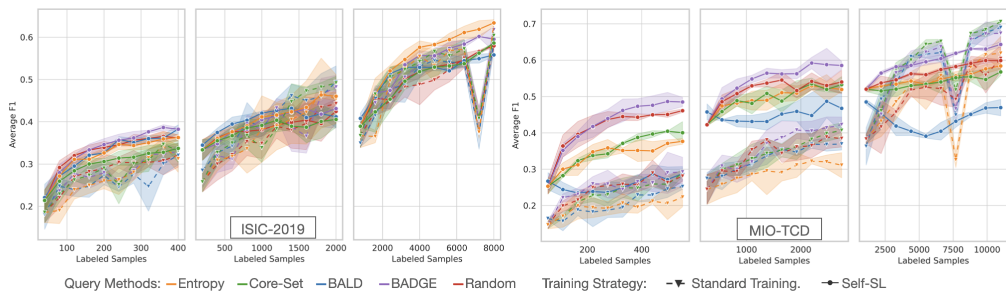


Figure 20: Macro-averaged F1-scores for ISIC-2019 and MIO-TCD datasets. Across the board, BADGE is still the best-performing QM which can also be seen in Table 19. Please interpret the results with care, as the model configurations are optimized for balanced accuracy.

Table 19: Area Under Budget Curve values based on macro-averaged F1-scores for ISIC-2019 and MIO-TCD (corresponding plots in Figure 20).

(a) ISIC-2019

	Label Regime	Low-Label		Mid-Label		High-Label	
		Mean	STD	Mean	STD	Mean	STD
Training	Query Method						
Standard Training	BADGE	0.2791	0.0081	0.3810	0.0167	0.5059	0.0054
	BALD	0.2587	0.0196	0.4050	0.0216	0.4866	0.0100
	Entropy	0.2652	0.0147	0.3763	0.0453	0.4988	0.0056
	Core-Set	0.2800	0.0105	0.3937	0.0082	0.5139	0.0141
	Random	0.2817	0.0153	0.3638	0.0292	0.4774	0.0035
Self-SL Pre-Trained	BADGE	0.3390	0.0107	0.3978	0.0053	0.5380	0.0067
	BALD	0.3273	0.0054	0.4065	0.0047	0.5173	0.0008
	Entropy	0.3232	0.0039	0.4081	0.0061	0.5586	0.0143
	Core-Set	0.3010	0.0129	0.3833	0.0094	0.5045	0.0123
	Random	0.3333	0.0033	0.3852	0.0153	0.5100	0.0059

(b) MIO-TCD

	Label Regime	Low-Label		Mid-Label		High-Label	
		Mean	STD	Mean	STD	Mean	STD
Training	Query Method						
Standard Training	BADGE	0.2503	0.0111	0.3604	0.0249	0.5759	0.0075
	BALD	0.2023	0.0127	0.3325	0.0082	0.5758	0.0116
	Entropy	0.1957	0.0208	0.2929	0.0218	0.5066	0.0290
	Core-Set	0.2301	0.0155	0.3450	0.0203	0.5945	0.0099
	Random	0.2446	0.0091	0.3438	0.0132	0.5085	0.0093
Self-SL Pre-Trained	BADGE	0.4295	0.0205	0.5487	0.0129	0.5994	0.0035
	BALD	0.2560	0.0132	0.4488	0.0236	0.4335	0.0088
	Entropy	0.3398	0.0104	0.4977	0.0095	0.5481	0.0078
	Core-Set	0.3525	0.0066	0.4970	0.0160	0.5375	0.0138
	Random	0.4175	0.0158	0.5194	0.0101	0.5681	0.0036

F.3 Macro averaged F1-scores

Additionally, we provide the macro-averaged F1-scores for ISIC-2019 and MIO-TCD dataset. A plot showing the performance of both ST and Self-SL models is shown in Figure 20 and the resulting AUBC values are shown in Tab. 19.

F.4 Semi-Supervised Learning

Results of FixMatch for all HPs on the whole validation splits are shown separately for MIO-TCD in Tab. 20 and ISIC-2019 in Tab. 21. Based on the performance which did not improve substantially over even ST models we decided to omit all further AL experiments.

Table 20: MIO-TCD FixMatch results reported on the test sets (balanced accuracy in %). Reported as mean (std).

FixMatch Sweep MIO-TCD			
Labeled Train Samples	Learning Rate	Weight Decay	Balanced Accuracy (Test)
55	0.3	5E-3	18.1(1.1)
		5E-4	28.0(0.4)
	0.03	5E-3	26.8(0.5)
		5E-4	29.7(2.4)
275	0.3	5E-3	20.2(6.2)
		5E-4	28.2(1.5)
	0.03	5E-3	31.4(0.7)
		5E-4	36.0(1.8)

Table 21: ISIC-2019 FixMatch results reported on the test sets (balanced accuracy in %). Reported as mean (std).

FixMatch Sweep ISIC-2019 Labeled Train Samples	Learning Rate	Weight Decay	Balanced Accuracy (Test)
40	0.3	5E-3	14.0(2.5)
		5E-4	26.9(1.5)
	0.03	5E-3	24.5(4.4)
		5E-4	31.3(1.7)
200	0.3	5E-3	15.2(3.6)
		5E-4	19.1(1.5)
	0.03	5E-3	26.3(0.8)
		5E-4	24.3(3.6)

G Discussion and further observations

The results are interpreted based on the assumption that a QM performing on a similar level as Random is not a drawback as long as it brings in other settings performance improvements over random queries. This mostly follows in line with the PPM as a performance metric but mostly focuses on the row that compares each QM with random queries. However, if a QM shows behavior leading to much worse behavior than random as Entropy does or shows signs of the cold start problem, we deem this as highly problematic. In these settings, one loses significant performance whilst paying a cost in computing and setup corresponding to AL. Therefore, we use random queries as a baseline for all QMs.
Based on this our recommendation for BADGE is given for Self-SL and ST trainings.
The main disadvantage of this approach is that absolute performance difference are not captured in this aggregated format.

H Comparing random-sampling baselines across studies

Here we compare the performance of random-sampling baselines on the most commonly utilized dataset CIFAR-10 and CIFAR-100 across different studies for ST, Self-SL and Semi-SL models along strategic point where overlap in between papers occurs. For CIFAR-10 the results of this comparison are shown for the high-label regime in Tab. 22 and the low- and mid-label regime in Tab. 23. Similarly for CIFAR-100 the results are shown in Tab. 24 for the high-label regime and Tab. 25 for the low- and mid-label regimes. Overall our ST random baselines outperform all other random baselines. Our Self-SL models also outperform the only other relevant literature [6] on CIFAR-10. Further, our Semi-SL models also outperform the relevant literature [20, 43] on CIFAR-10 and CIFAR-100.

Table 22: Comparison of random baseline model accuracy in % on the test set for the high label-regime for CIFAR-10 across different papers. Best performing models for each training strategy are **highlighted**. Values denoted with – represent not performed experiments. Values with a denoted with a * are reprinted from [44]. Values which are sourced from a graph are subject to human read-out error.

Information				Number Labeled Training Samples					
Paper	Training	Model	Source	1k	2k	5k	10k	15k	20k
QBC	ST	DenseNet121	Graph			74*	82.5*	-	-
VAAL	ST	VGG16	Graph	-	-	61.35*	68.17*	72.96*	75.99*
CoreSet	ST	VGG16	Graph	-	-	60*	68*	71*	74*
Agarwal et al.	ST	VGG16	Graph	-	-	61.5	68	72	76
Munjal-SR	ST	VGG16	Table	-	-	82.16	85.07	89.43	91.16
Mittal et al.	ST	WRN28-2	Graph	57	73	82.5	86	90.7	92
LLAL	ST	ResNet18	Graph	51	63	81*	87*	-	-
CoreCGN	ST	ResNet18	Graph	50	64	80*	85.5*	-	-
TA-VAAL	ST	ResNet18	Graph	50	65	81*	87.5*	-	-
Krishnan et al.	ST	ResNet18	Graph	47	60	78	86	-	-
Yi et al.	ST	ResNet18	Graph	47.5	56	78	86	-	-
Bengar et al.	ST	ResNet18	Graph	45	55	73	81	85	88
Beck et al.	ST	ResNet18	Graph	55	-	-	84	85	90.5
Zhan et al.	ST	ResNet18	Graph	45	-	-	76	-	-
Munjal-SR	ST	ResNet18	Table	-	-	84.69	88.45	89.98	92.29
Ours	ST	ResNet18	Table	**72.4**	**79.8**	**85.5**	**90.5**	-	-
Bengar et al.	Self-SL	ResNet18	Graph	**87**	88	89.5	90.5.	91	91.5
Ours	Self-SL	ResNet18	Table	86.2	**88.3**	**90.1**	**91.4**	-	-
Mittal et al.	Semi-SL	WRN28-2	Graph	88	91	92.5	93.8	94	94.5
Gao et al.	Semi-SL	WRN28-2	Graph	91.5	91	-	-	-	-
Ours	Semi-SL	ResNet18	Table	**94.7**	**95.0**	-	-	-	-

Table 23: Comparison of random baseline model accuracy in % on the test set for the low- and mid-label regime for CIFAR-10 across different papers. Best performing models for each training strategy are **highlighted**. Values denoted with – represent not performed experiments. Values which are sourced from a graph are subject to human read-out error.

Information				Number Labeled Training Samples				
Paper	Training	Model	Source	50	100	200	250	500
Chan et al.	ST	WRN28-2	Table	-	-	-	40.9	-
Mittal et al.	ST	WRN28-2	Graph	-	-	-	36	48
Bengar et al.	ST	ResNet18	Graph	-	-	-	-	38
Ours	ST	ResNet18	Table	**25.1**	**32.3**	**44.4**	**47.0**	**61.2**
Chan et al.	Self-SL	WRN28-2	Table	-	-	-	76.7	-
Bengar et al.	Self-SL	ResNet18	Graph	62	**77**	81	83	85
Ours	Self-SL	ResNet18	Table	**71.3**	76.8	**81.2**	81.4	84.1
Chan et al.	Semi-SL	WRN28-2	Table	-	-	-	**93.1**	-
Mittal et al.	Semi-SL	WRN28-2	Graph	-	-	-	82	85
Gao et al.	Semi-SL	WRN28-2	Table	-	47.9	89.2	90.2	-
Ours	Semi-SL	ResNet18	Graph	**90**	**91**	**93**	**93**	**94**

Table 24: Comparison of random baseline model accuracy in % on the test set for the high-label regime for CIFAR-100 across different papers. Best performing models for each training strategy are **highlighted**. Values denoted with – represent not performed experiments. Values which are sourced from a graph are subject to human read-out error.

Information				Number Labeled Training Samples			
Paper	Training	Model	Source	5k	10k	15k	20k
Agarwal et al.	ST	VGG16	Graph	28	35	41.5	46
Agarwal et al.	ST	ResNet18	Graph	29.5	38	45	49
Core-Set	ST	VGG16	Graph	27	37	42	49
VAAL	ST	VGG16	Graph	28	35	42	46
Munjal et al.	ST	VGG16	Graph	39.44	49	55	59
VAAL	ST	ResNet18	Graph	28	38	45	49
TA-VAAL	ST	ResNet18	Graph	43	52	60	63.5
Bengar et al.	ST	ResNet18	Graph	27	45	52	58
Beck et al.	ST	ResNet18	Graph	40	53	60	64
Zhan et al.	ST	ResNet18	Graph	-	39	-	-
Munjal et al.	ST	ResNet18	Table	?	61.1	**66.9**	69.8
Mittal et al.	ST	WRN28-2	Graph	44.9	58	64	68
Ours	ST	ResNet18	Table	**49.2**	**61.3**	66.7	**70.2**
Bengar et al.	Self-SL	ResNet18	Table	60	63	63.5	64
Ours	Self-SL	ResNet18	Table	**60.4**	**64.8**	**68.4**	**70.7**
Mittal et al.	Semi-SL	WRN28-2	Graph	59	65	70	71
Gao et al.	Semi-SL	WRN28-2	Table	**63.4**	67	68	70
Ours	Semi-SL	ResNet18	Graph	**63.5**	**68.5**	-	-

Table 25: Comparison of random baseline model accuracy in % on the test set for the low- and mid- label regime for CIFAR-100 across different papers. Best performing models for each training strategy are **highlighted**. Values denoted with – represent not performed experiments. Values which are sourced from a graph are subject to human read-out error.

Information				Number Labeled Training Samples			
Paper	Training	Model	Source	500	1000	2000	2500
Chan et al.	ST	WRN28-2	Table	-	-	-	33.2
Mittal et al.	ST	WRN28-2	Graph	9	12	24	27
TA-VAAL	ST	ResNet18	Graph	-	-	20	-
Bengar et al.	ST	ResNet18	Graph	9	12	17	-
Ours	ST	ResNet18	Table	**14.0**	**22.4**	**32.0**	**36.3**
Chan et al.	Self-SL	WRN28-2	Table	-	-	-	49.1
Bengar et al.	Self-SL	ResNet18	Table	**47**	**50**	**56**	-
Ours	Self-SL	ResNet18	Table	37.3	45.2	52.2	54.7
Chan et al.	Semi-SL	WRN28-2	Table	-	-	-	**67.6**
Mittal et al.	Semi-SL	WRN28-2	Graph	26	35.5	44.5	49
Ours	Semi-SL	ResNet18	Graph	**41**	-	**56.5**	-

I Detailed limitations

Additionally to the limitations already discussed in Sec. 4 we would like to critically reflect on the following points:

Query methods We only evaluate four different QMs which is only a small sub-selection of all the QMs proposed in the literature. We argue that this may not be optimal, however, deem it justified due to the variety of other factors which we evaluated. Further, we excluded all QMs which induce changes in the classifier (s.a. LLAL [55]) or add a substantial additional computational cost by training new components (s.a. VAAL [51]). These QMs might induce changes in the HPs for every dataset and were therefore deemed too costly to properly optimize.
We leave a combination of P4 with these QMs for future research.

Validation set size The potential shortcomings of our validation set were already discussed. However, we would like to point out that a principled inclusion of K-Fold Cross-Validation into AL might alleviate this problem. This would also give direct access to ensembles which have been shown numerous times to be beneficial with regard to final performance (also in AL) [5]. How this would allow us to assess performance gains in practice and also make use of improved techniques for performance evaluation s.a. Active Testing [34] in the same way as our proposed solution shown in Figure 4 is not clear to us. Therefore we leave this point up for future research.

Performance of ST models On the imbalanced datasets, the performance of our models is not steadily increasing for more samples which can be traced back to sub-optimal HP selection according to [44]. We believe that our approach of simplified HP tuning improves over the state-of-the-art in AL showcased by the superior performance of our models on CIFAR-10 and CIFAR-100. However, regularly re-optimizing HPs might be an alternative solution.

Performance of Self-SL models Our Self-SL models are outperformed on the low-label regime on CIFAR-100 by the Self-SL models by [6], whereas on the medium- and high-label regime our Self-SL models outperform them. We believe that this might be due to our fine-tuning schedule and the possibility that Sim-Siam improves over SimCLR on CIFAR-100. Since our Self-Sl models still outperform most Semi-SL models in the literature we believe that drawing conclusions from our results is still feasible. An interesting research direction would be to make better use of the Self-SL representations s.a. improved fine-tuning regimes [37].

No Bayesian Query Methods for Semi-SL The Semi-SL models were neither combined with BALD nor BatchBALD as query functions, even though we showed that small query sizes and BatchBALD can counteract the cold-start problem. Further our Semi-SL models had bigger query sizes by a factor of three, possibly additionally hindering performance gains obtainable with AL. However, in previous experiments with FixMatch, we were not able to combine it with Dropout whilst keeping the performance of models without dropout. This clearly might have been an oversight by us, but we would like to point out that in the works focusing on AL, using Semi-SL without bayesian QMs is common practice [20, 43]

Changing both starting budget and query size We correlated the two parameters (smaller query size for smaller starting budget etc.) since 1) in practice, we deem the size of the starting budget to be dependent on labeling cost (therefore, large query sizes for small starting budgets are unrealistic and vice versa) and 2) In this work, we are especially interested in smaller starting budgets ("cold-start" territory) compared to the ones in the literature, since AL typically shows robust performance for larger starting budgets. Theory shows that our adapted smaller query size for this case can only positively affect the result [19, 32]. The only possible confounder could be that we interpret the performance of a small starting budget too positively due to a hidden effect of the smaller query size. However, we performed the low-label query size ablation, showcasing that varying the query size for small starting budgets did not have considerable effects on performance for all QMs, except BALD, where, a clear performance increase for smaller query sizes was observed.

I.1 Instability of hyperparameters for class imbalanced datasets

The substantial dip in performance on MIO-TCD and ISIC-2019 for approx 7k samples shown in Figure 16 and Figure 18 is ablated in Tab. 26 where we show that simply changing the learning rate leads to stabilizing the performance on both datasets for these cases.

Table 26: Ablation study on the performance-dip on MIO-TCD and ISIC-2019 for ST models with regard to HP. Reported as mean (std).

Dataset	Labeled Train Set	Data Augmentation	Learning Rate	Weight Decay	Balanced Accuracy (Val)	Balanced Accuracy (Test)
ISIC-2019	7200	RandAugmentMC (ISIC)	0.1	5E-3	54.4(1.2)	52.6(1.9)
				5E-4	57.2(1.7)	55.4(0.9)
			0.01	5E-3	58.0(1.7)	55.6(1.0)
				5E-4	55.6(1.9)	54.5(2.1)
MIO-TCD	7700	RandAugmentMC (ImageNet)	0.1	5E-3	65.7(1.8)	64.3(1.1)
				5E-4	65.9(2.4)	63.6(2.7)
			0.01	5E-3	64.1(1.2)	62.9(1.0)
				5E-4	63.8(0.7)	62.2(1.1)

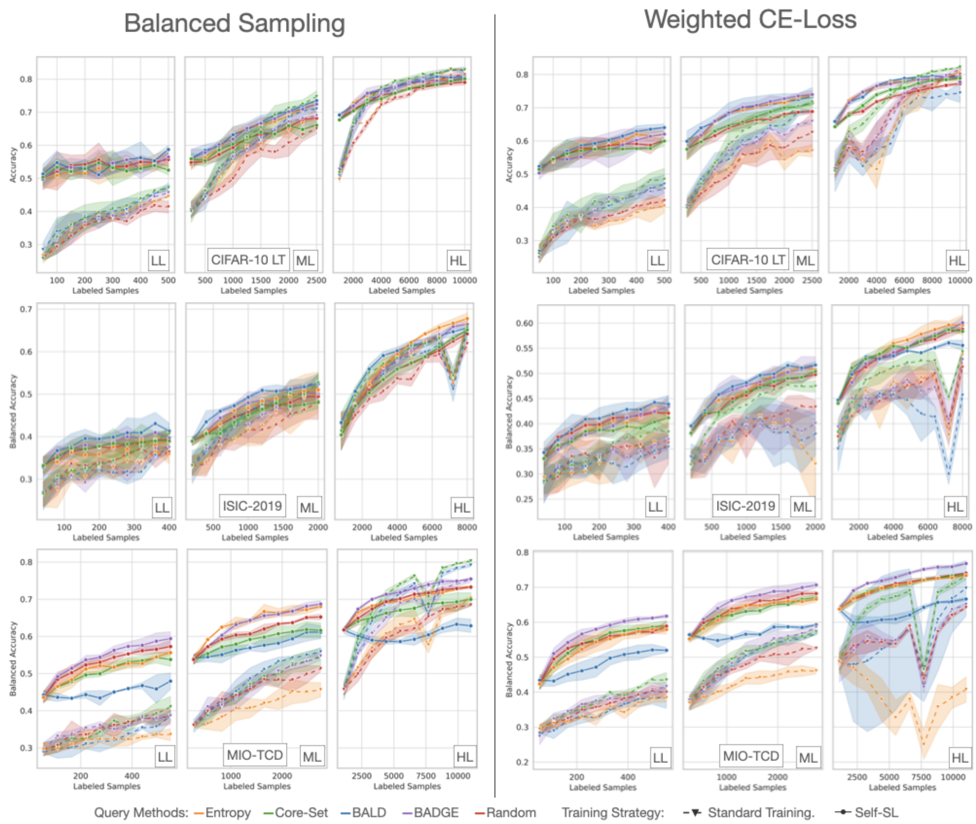


Figure 21: Comparison between balanced sampling and weighted cross-entropy-loss (weighted CE-Loss). Whereas the ST models overall seem to benefit more from balanced sampling, the Self-SL models perform slightly better for weighted CE-Loss. Generally the observed performance gains in the imbalanced settings are still present.

However, this dip in performance also arises using weighted Cross-Entropy (weighted CE-Loss) as a loss function as shown in the following ablation Figure 21.