Pearls from Pebbles: Improved Confidence Functions for Auto-labeling

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Abstract

Auto-labeling techniques produce labeled data with minimal manual annotations using the representations from self-supervised models and confidence scores. A popular technique, threshold-based auto-labeling (TBAL) trains model using these representations and manual annotations, and assigns model's prediction as label to the points where model's confidence score is greater than certain threshold. However, the model's scores can be overconfident and lead to poor performance. We show that, calibration, a common remedy for the overconfidence problem, falls short in tackling this problem for TBAL. Thus, instead of using existing calibration methods, we introduce a framework for optimal confidence functions for TBAL and develop `Colander`, a method designed to maximize auto-labeling performance. We perform an extensive empirical evaluation of `Colander` and other confidence functions, using representations from CLIP and text embedding models for image and text data respectively. We find `Colander` achieves up to 60% improvement on coverage (the proportion of points labeled by model) over the baselines while maintaining error level below 5% and using the same amount of labeled data.

1 Introduction

The demand for labeled data in machine learning (ML) is perpetual. Threshold-based auto-labeling (TBAL) is a promising solution to obtain high-quality labeled data at low cost [41, 37, 49] using model's confidence scores and self-supervision. It powers industry products like Amazon SageMaker Ground Truth [41]. The confidence function is critical to the TBAL workflow. Existing TBAL systems rely on common choices like softmax outputs from neural networks [37, 49]. These functions *are not well aligned with the objective of the auto-labeling system*. Using them results in substantially suboptimal coverage (Figure 1(a)). For this reason, we ask:

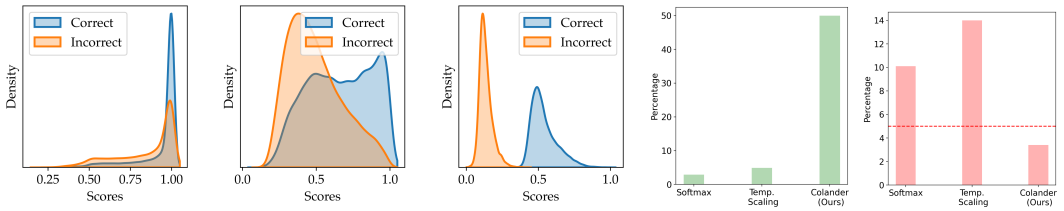
> What are the right choices of confidence functions for TBAL and how can we obtain them?

An ideal confidence function for auto-labeling will achieve the maximum coverage at a given auto-labeling error tolerance and thus will bring down the labeling cost significantly. Finding such an ideal function, however, is difficult because of the *inherent tension* between accuracy and coverage.

Overconfidence further stymies hopes of balancing accuracy and coverage. While overconfidence is a challenge in general, it is exacerbated in TBAL: since models are trained on a small amount of labeled data, making the problem of designing confidence functions even more challenging. Figure 1(a) shows that softmax scores are overconfident, resulting in poor auto-labeling performance.

Several methods have been introduced to address overconfidence [10]. Applying these miss out on significant performance (Figure 1(b)), since the calibration goal differs from auto-labeling. From the auto-labeling standpoint, we seek minimum overlap between the correct and incorrect model prediction scores.

Submitted to 38th Conference on Neural Information Processing Systems (NeurIPS 2024). Do not distribute.



(a) Softmax (b) Temp. Scaling (c) `Colander` (Ours) (d) Coverage (e) Auto-labeling Err.

Figure 1: Scores distributions (Kernel Density Estimates) of a CNN model trained on CIFAR-10 data. (a) softmax scores of the vanilla training procedure (SGD) (b) scores after post-hoc calibration using temperature scaling and (c) scores from our `Colander` procedure applied on the same model. For training the CNN model we use 4000 points drawn randomly and 1000 validation points (of which 500 are used for Temp. Scaling and `Colander`). The test accuracy of the model is 55%. Figures (d) and (e) show the coverage and auto-labeling error of these methods. The dotted-red line corresponds to a 5% error threshold.

We tackle these challenges by ***proposing a framework to learn suitable confidence functions*** for TBAL. We summarize our contributions as follows,

1. We propose a principled framework to study the choices of confidence functions suitable for auto-labeling and provide a practical method (`Colander`) to learn confidence functions for efficient and reliable auto-labeling.
2. We systematically study commonly used choices of scoring functions and calibration methods and demonstrate that they lead to poor auto-labeling performance.
3. Through extensive empirical evaluation on real-world datasets, we show that using the confidence scores obtained using our procedure boosts auto-labeling performance significantly in comparison to common choices of confidence functions and calibration methods.

2 Background and Motivation

Notation. Let $[m] := \{1, 2, \ldots, m\}$ for any natural number m. Let X_u be a set of unlabeled points drawn from some instance (feature) space $\mathcal{X}$. This could either be the space of raw features or the representation space from some self-supervised model. Let $\mathcal{Y} = \{1, \ldots, k\}$ be the label space. There is an unknown ground truth labeling function $f^* : \mathcal{X} \to \mathcal{Y}$. Let $\mathcal{O}$ be a *noiseless* oracle that provides the true label for any point $\mathbf{x} \in \mathcal{X}$. Denote the model (hypothesis) class by $\mathcal{H}$, where each $h \in \mathcal{H}$ is a function $h : \mathcal{X} \to \mathcal{Y}$. Each classifier h also has an associated *confidence function* $g : \mathcal{X} \to \Delta^k$ that quantifies the confidence of the prediction by model $h \in \mathcal{H}$ on any data point $\mathbf{x} \in \mathcal{X}$. Here, Δ^k is a $(k-1)$-dimensional probability simplex. Let $\mathbf{v}[i]$ denote the i^{th} component for any vector $\mathbf{v} \in \mathbb{R}^d$. For any point $\mathbf{x} \in \mathcal{X}$ the prediction is $\hat{y} := h(\mathbf{x})$ and the associated confidence is $g(\mathbf{x})[\hat{y}]$. The vector $\mathbf{t}$ denotes scores over k-classes, and $\mathbf{t}[y]$ denotes its y^{th} entry, i.e., score for class y. Table 2 contains a summary of the notation.

Threshold-based Auto-labeling. Threshold-based auto-labeling (TBAL) seeks to obtain labeled datasets while reducing the labeling burden on humans. The input is a pool of unlabeled data X_u. It outputs, for each $\mathbf{x} \in X_u$, a label $\tilde{y} \in \mathcal{Y}$. The output label could be either y, from the oracle (representing a human-obtained label), or $\hat{y}$, from the model. Let N_u be the number of unlabeled points, $A \subseteq [N_u]$ the set of indices of auto-labeled points, and $X_u(A)$ be these points. Let N_a denote the size of the auto-labeled set A. The *auto-labeling error*, denoted by $\widehat{\mathcal{E}}(X_u(A))$, and the *coverage*, denoted by $\widehat{\mathcal{P}}(X_u(A))$, are defined as follows:

$$\widehat{\mathcal{E}}(X_u(A)) := \frac{1}{N_a} \sum_{i \in A} \mathbb{1}(\tilde{y}_i \neq f^*(\mathbf{x}_i)), \quad \text{and} \quad \widehat{\mathcal{P}}(X_u(A)) := |A|/N_u = N_a/N_u. \tag{1}$$

The goal of an auto-labeling algorithm is to label the dataset so that $\widehat{\mathcal{E}}(X_u(A)) \leq \epsilon_a$ while maximizing coverage $\widehat{\mathcal{P}}(X_u(A))$ for any given $\epsilon_a \in [0, 1]$. The TBAL algorithm proceeds iteratively. In each iteration, it queries labels for a subset of unlabeled points from the oracle. It trains a classifier from the model class $\mathcal{H}$ on the oracle-labeled data acquired till that iteration. It then uses the model's confidence scores on the validation data to identify the region in the instance space, where the current classifier is confidently accurate and automatically labels the points in this region.

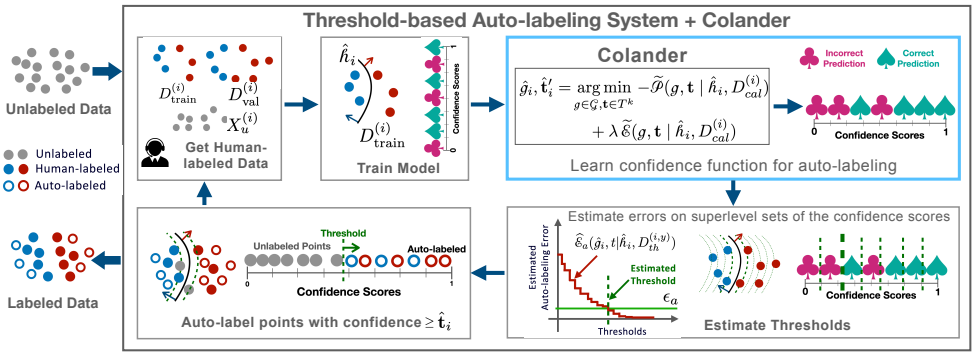


Figure 2: Threshold-based Auto-labeling with `Colander`: takes unlabeled data as input, selects a small subset of data points, and obtains human labels for them to create $D^{(i)}_{\text{train}}$ and $D^{(i)}_{\text{val}}$ for the ith iteration. Trains model $\hat{h}_i$ on $D^{(i)}_{\text{train}}$. In contrast to the standard TBAL procedure, here we randomly split $D^{(i)}_{\text{val}}$ into two parts, $D^{(i)}_{\text{cal}}$ and $D^{(i)}_{\text{th}}$. `Colander` kicks in, takes $\hat{h}_i$ and $D^{(i)}_{\text{cal}}$ as input and learns a coverage maximizing confidence function $\hat{g}_i$ for $\hat{h}_i$. Using $D^{(i)}_{\text{th}}$ and $\hat{g}_i$ auto-labeling thresholds $\hat{\mathbf{t}}_i$ are determined to ensure the auto-labeled data has error at most ϵ_a. After obtaining the thresholds the rest of the steps are the same as standard TBAL. The whole workflow runs until all the data is labeled or another stopping criterion is met.

3 Proposed Method (`Colander`)

3.1 Auto-labeling optimization framework

In any iteration of TBAL, we have a model $\hbar$ trained on a subset of data labeled by the oracle. This model may not be highly accurate. However, it could be accurate in some regions of the instance space, and with the help of a confidence function g, we want to identify the points where the model is correct and auto-label them. As we saw earlier, arbitrary choices of g perform poorly on this task. Instead, we propose a framework to find the right function from a sufficiently rich family.

Optimization problem. Let $\sigma(\alpha, z) := 1/(1+\exp(-\alpha z))$ denote the sigmoid function on $\mathbb{R}$ with scale parameter $\alpha \in \mathbb{R}$. It is easy to see that, for any g, y and $\mathbf{t}$, $g(\mathbf{x})[y] \geq \mathbf{t}[y] \iff \sigma(\alpha, g(\mathbf{x})[y] - \mathbf{t}[y]) \geq 1/2$. Using this fact, we define the following surrogates of the auto-labeling error and coverage:

$$\widetilde{\mathscr{P}}(g, \mathbf{t} | \hbar, D_{\text{cal}}) := \frac{1}{|D_{\text{cal}}|} \sum_{(\mathbf{x},y)\in D_{\text{cal}}} \sigma\big(\alpha, g(\mathbf{x})[\hat{y}] - \mathbf{t}[\hat{y}]\big), \tag{2}$$

$$\widetilde{\mathscr{E}}(g, \mathbf{t} \mid \hbar, D_{\text{cal}}) := \frac{\sum_{(\mathbf{x},y)\in D_{\text{cal}}} \mathbb{1}\big(y \neq \hat{y}\big)\, \sigma\big(\alpha, g(\mathbf{x})[\hat{y}] - \mathbf{t}[\hat{y}]\big)}{\sum_{(\mathbf{x},y)\in D_{\text{cal}}} \sigma\big(\alpha, g(\mathbf{x})[\hat{y}] - \mathbf{t}[\hat{y}]\big)}, \tag{3}$$

and the surrogate optimization problem as follows,

$$\underset{g\in\mathcal{G}, \mathbf{t}\in T^k}{\arg\min} \quad -\widetilde{\mathscr{P}}(g, \mathbf{t} \mid \hbar, D_{\text{cal}}) + \lambda\, \widetilde{\mathscr{E}}(g, \mathbf{t} \mid \hbar, D_{\text{cal}}) \tag{P1}$$

Here, $\lambda \in \mathbb{R}^+$ is the penalty term controlling the relative importance of the auto-labeling error and coverage. We tune it with the procedure discussed in Appendix B.4. The gap between the surrogate and actual coverage diminishes as $\alpha \to \infty$. We discuss this in the Appendix. Our framework is flexible with respect to the choice of $\mathcal{G}$. We use 2-layer neural nets for $\mathcal{G}$ and use representations from the last two layers of $\hat{h}$ as input for g. See Appendix for further details.

Solving the surrogate optimization. The optimization problem (P1) is non-convex. Nevertheless, it is differentiable and we can apply gradient-based methods. We solve for g and $\mathbf{t}$ simultaneously using Adam [19]. Appendix B.4 lists the detailed procedure of our method in a TBAL system.

4 Empirical Evaluation

We conduct extensive empirical evaluation with variety of train-time and post-hoc calibration methods, and feature choices. We use *Vanilla* training with SGD [1, 3, 10]. *Squentropy* [16], *Correctness*

Train-time	Post-hoc	MNIST		CIFAR-10		20 Newsgroups		Tiny-ImageNet	
		Err (↓)	**Cov (↑)**	**Err (↓)**	**Cov (↑)**	**Err (↓)**	**Cov (↑)**	**Err (↓)**	**Cov (↑)**
Vanilla	Softmax	**4.1±0.7**	85.0±2.5	4.8±0.2	14.0±2.1	6.0±0.6	48.2±1.6	11.1±0.3	32.6±0.5
	TS	7.8±0.6	94.2±0.5	7.3±0.3	23.2±0.7	9.7±0.6	60.7±2.3	16.3±0.5	37.4±1.5
	Dirichlet	7.9±0.7	93.2±2.2	7.7±0.5	22.4±1.2	9.4±0.9	59.4±1.8	17.1±0.4	33.3±2.0
	SB	6.7±0.5	92.6±1.5	6.1±0.4	18.6±1.1	8.1±0.6	58.1±1.8	15.7±0.6	35.4±1.2
	Top-HB	7.4±1.4	93.1±3.6	6.0±0.7	15.6±1.9	9.2±1.0	59.0±2.0	16.6±0.5	37.6±2.2
	Ours	4.2±1.5	**95.6±1.4**	**3.0±0.2**	**78.5±0.2**	**2.5±1.1**	**80.6±0.7**	**1.4±2.1**	**59.2±0.8**
CRL	Softmax	4.7±0.4	86.0±4.5	5.2±0.3	15.9±0.8	5.8±0.5	48.3±0.3	10.4±0.4	32.5±0.6
	TS	8.0±0.8	94.8±0.8	6.8±0.8	20.3±1.1	9.5±1.0	61.7±1.6	15.8±0.6	37.4±1.7
	Dirichlet	8.6±0.6	93.1±1.6	7.7±0.2	20.9±1.1	8.7±0.9	58.0±1.4	16.3±0.4	33.1±1.9
	SB	7.4±0.8	93.1±2.7	5.9±0.9	17.9±1.5	8.9±1.1	57.9±3.9	15.0±0.4	35.5±1.2
	Top-HB	7.7±0.8	94.1±1.5	4.4±0.5	12.3±0.4	8.8±1.0	58.8±2.7	16.5±0.5	38.9±1.6
	Ours	**4.5±1.4**	**95.6±1.3**	**2.2±0.6**	**77.9±0.2**	**1.8±1.2**	**81.3±0.5**	**2.8±2.1**	**61.2±1.4**
FMFP	Softmax	4.8±0.8	84.2±4.1	4.9±0.4	15.6±1.7	5.4±0.7	45.4±1.9	10.5±0.3	32.4±1.4
	TS	8.0±0.6	95.3±1.6	6.5±0.3	21.0±1.5	9.5±0.5	57.7±2.2	16.2±1.1	37.7±1.8
	Dirichlet	8.2±1.3	94.0±2.2	6.9±0.4	21.7±1.2	8.9±1.0	56.6±2.4	17.4±0.8	33.0±1.8
	SB	7.2±1.1	93.1±2.3	6.1±0.5	19.5±1.0	8.6±0.4	55.8±1.3	15.5±0.6	36.1±0.5
	Top-HB	7.1±0.6	93.3±4.9	5.2±0.5	14.2±2.4	9.0±0.7	57.9±2.4	16.2±0.4	37.4±1.1
	Ours	**4.6±0.8**	**95.7±0.2**	**3.0±0.4**	**77.4±0.2**	**2.5±0.9**	**80.8±0.6**	**1.8±2.0**	**60.8±1.4**
Squentropy	Softmax	**3.7±1.0**	88.2±3.9	5.2±0.5	21.2±1.8	4.6±0.4	52.0±1.2	7.8±0.3	36.2±0.8
	TS	6.2±1.1	95.6±0.9	6.9±0.6	28.2±2.5	8.3±0.6	66.6±1.4	13.3±0.1	44.9±1.0
	Dirichlet	6.5±1.2	95.9±0.8	7.3±0.3	29.4±1.1	7.8±0.6	64.0±1.3	14.1±0.3	42.5±0.7
	SB	6.0±0.8	95.3±1.2	6.2±0.4	23.8±1.9	7.8±0.7	63.0±2.9	13.0±0.5	45.2±2.0
	Top-HB	5.3±0.4	96.4±0.9	4.3±0.5	15.8±1.4	8.2±0.8	66.5±2.2	13.7±0.1	45.9±1.4
	Ours	4.1±0.8	**97.2±0.5**	**2.3±0.5**	**79.0±0.3**	**3.3±0.8**	**82.9±0.4**	**0.6±0.2**	**66.5±0.7**

Table 1: In every round the error was enforced to be below 5%; 'TS' stands for Temperature Scaling, 'SB' stands for Scaling Binning, 'Top-HB' stands for Top-Label Histogram Binning. The column Err stands for auto-labeling error and Cov stands for the coverage. Each cell value is mean ± std. deviation observed on 5 repeated runs with different random seeds.

Ranking Loss (CRL) [30] and *FMFP* [53] as train-time methods. We pipe these with `Colander` and other post-hoc methods *Temperature scaling* [10], *Top-Label Histogram-Binning* [12], *Scaling-Binning* [24] and *Dirichlet Calibration* [22]. We use raw features for *MNIST* [26] and *CIFAR-10* [20], CLIP [38] embeddings for *Tiny-ImageNet* and FlagEmbedding [50] for *20 Newsgroups* [29] The results are reported in Table 1.

TBAL with `Colander` consistently achieves significantly higher coverage compared to vanilla training and softmax scores, especially on more complex datasets like Tiny-ImageNet, outperforming baseline models across all data settings. Post-hoc calibration techniques slightly improve coverage but at the cost of higher error, as their goal of mitigating overconfidence is not aligned with TBAL's needs. Importantly, `Colander` is compatible with different train-time methods and amplifies performance gains, particularly when paired with Squentropy, where coverage increases by 6-7% and error decreases, outperforming other train-time approaches. In contrast, methods focused on ordinal ranking objectives, such as CRL and FMFP, perform poorly in the TBAL setting due to challenges like limited training data and reduced effectiveness in differentiating between correct and incorrect predictions when training error reaches zero after a few rounds.

5 Conclusion

We studied confidence scoring functions used in threshold-based auto-labeling (TBAL) and showed that the commonly used choices and calibration methods can often be a bottleneck, leading to poor performance. We proposed `Colander` to learn confidence functions that are aligned with the TBAL objective. We evaluated `Colander` extensively against common baselines on several real-world datasets and found that it improves the performance of TBAL significantly. A limitation of `Colander` is that, similar to other post-hoc methods it also requires validation data to learn the scores. Reducing (or eliminating) this dependence could be an interesting future work.

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Supplementary Material Organization

The supplementary material is organized as follows. We provide deferred details of background and motivation section in Appendix A of the method in Appendix B. Then, in Appendix C, we provide additional experimental results and details of the experiment protocol and hyperparameters used for the experiments. Our code with instructions to run, is uploaded along with the paper.

Contents

A Appendix to Section 2

A.1 Detailed Comparison with Active Learning and Self Training

To illustrate the differences between TBAL and the combination of Active Learning (AL) and Self-Training for the task of data labeling, we run an experiment on the 2 concentric circles data setting as used in [49]. The details are as follows:

Data setting. We generate two concentric circles with points in the outer circle belonging to one class and the inner circle belonging to the other class. The total number of points generated is 10,000 of which we use 2000 for validation.

Methods. We run TBAL, AL+Self-Training, and AL+Self-Training+SC, using logistic regression. The combination of AL+Self-Training means, in each iteration, the algorithm queries human-labeled data points and pseudo-labels the points in the unlabeled data using self-training and adds both the human-labeled and pseudo-labeled points in the training pool. With this procedure, AL+Self-Training first learns the best classifier ($\hat{h}_{\mathrm{al-st}}$) with the given budget of maximum training points (N_t) that can be queried from humans. Then it auto-labels all the remaining unlabeled points with this classifier's predictions. For AL+Self-Training+SC, we do selective auto-labeling using $\hat{h}_{\mathrm{al-st}}$, i.e., only auto-label the points where the classifier will have an error at most ϵ_a. We use ϵ_a =1% here.

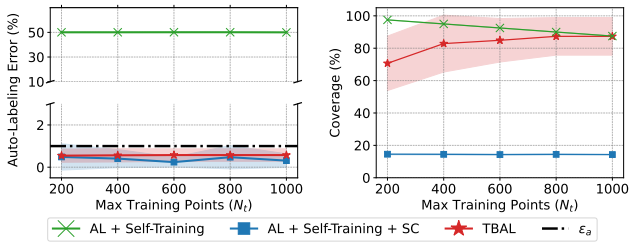


Figure 3: Results of experiment on 2-concentric circles to show the differences between TBAL, AL and ST.

Results and Discussion. The Figure 3 shows auto-labeling error and coverage achieved by these methods when run with different choices of human-labeled data budget for training. First, we can see that even with linear classifiers TBAL is able to auto-label a huge chunk of the data (high coverage) while maintaining auto-labeling error below the tolerance level of 1% On the other hand, methods like AL+Self-Training (+SC) that try to first learn the optimal classifier in the given function class either have high auto-labeling error or very low coverage. These results are also consistent with the observations in [49] on the comparison between TBAL and AL, AL+SC. While such findings confirm the notion that there are differences—and, at least in some settings, advantages—for the TBAL approach compared to other techniques, we reiterate that our goal is to understand and improve the role of the confidence function within TBAL, rather than comparing TBAL to other techniques.

A.2 Details of the motivating experiment in Section 2

We run TBAL for a single round on the CIFAR-10 dataset with a SimpleCNN classification model with around 5.8M parameters [17]. We randomly sampled 4,000 points for training the classifier and randomly sampled 1,000 points as validation data. We train the model to zero training error using minibatch SGD with learning rate 1e-3, weight decay 1e-3 [13, 21], momentum 0.9, and batch size 32. The trained model has validation accuracy around 55%, implying we could hope to get coverage around 55%. We run the auto-labeling procedure with an error tolerance of 5%.

B Appendix on Our Method

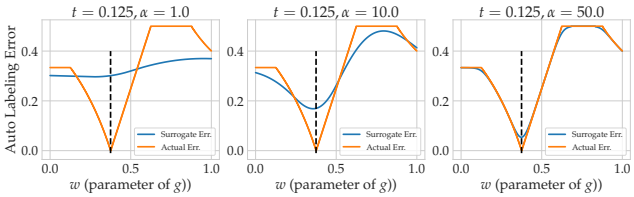
B.1 Detailed Algorithms

See Algorithms 1 and 2.

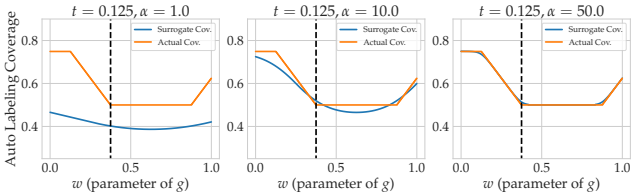
B.2 Tightness of surrogates.

The surrogate auto-labeling error and coverage introduced to relax the optimization problem (**??**) is indeed a good approximation of the actual auto-labeling error and coverage. To see this, we use a toy data setting of $x \sim \text{Uniform}(0, 1)$ with $1-$dimensional threshold classifier $h_\theta(x) = \mathbb{1}(x \geq \theta)$. For any x, let true labels $y = h_{0.5}(x)$ and consider the confidence function $g_w(x) = |w - x|$. Let $\hat{y} = h_{0.25}(x)$ and consider the points on the side where $\hat{y} = 1$. We plot actual and surrogate errors in Figure 4(a) and the surrogate and actual coverage in Figure 4(a).

for three choices of α. As expected, the gap between the surrogates and the actual functions diminishes as we increase the α.



(a) Auto-labeling error and surrogate error at various α.



(b) Auto-labeling coverage and surrogate coverage at various α.

Figure 4: Illustration of the tightness of surrogate error and coverage functions based on the choice of α.

B.3 Active Querying Strategy.

We employ the margin-random query approach to select the next batch of training data. This method involves sorting points based on their margin (uncertainty) scores and selecting the top Cn_b points, from which n_b points are randomly chosen. This strategy provides a straightforward and computationally efficient way to balance the exploration-exploitation trade-off. It's important to acknowledge the existence of alternative active-querying strategies; however, we adopt the margin-random approach as our standard to maintain a focus on evaluating various choices of confidence functions for auto-labeling. Note that while we use the new confidence scores computed using post-hoc methods for auto-labeling, we do not use these scores in active querying. Instead, we use the softmax scores from the model for this. We do this to avoid conflating the study with the study of active querying strategies. We use $C = 2$ for all experiments.

B.4 TBAL procedure with `Colander`

We take the workflow of TBAL and plugin our method `Colander` to learn the new confidence function and threshold. We discuss the updated workflow below and place the detailed Algorithms 1 and 2 in the Appendix B due to space constraints.

1. Initialization. First select n_s points randomly from X_u and obtain human labels for them to create initial training data $D^{(1)}_{\text{train}}$. This is written as $\text{RandomQuery}(X_u, n_s)$ in Algorithm 1. The procedure $\text{RandomQuery}(X_u, n_s)$ selects n_s points randomly from X_u and obtains human labels for them to create $D^{(1)}_{\text{train}}$.

2. Train classification model. After obtaining human-labeled training data $D^{(i)}_{\text{train}}$ for the current round i, the procedure $\text{TrainModel}(\mathcal{H}, D^{(i)}_{\text{train}})$ trains a model from model class $\mathcal{H}$ on the training data $D^{(i)}_{\text{train}}$. Any training procedure can be used here. We use methods listed in Section **??** for model training. This step outputs a model $\hat{h}_i$ trained on $D^{(i)}_{\text{train}}$.

3. Learn new confidence function using `Colander`. The model $\hat{h}_i$ obtained in the previous step also produces softmax scores that can be used to for auto-labeling. However, as we saw earlier in Section 2, using these scores may lead to poor auto-labeling performance. Thus, we plug in our procedure `Colander` to learn new scores that are designed to maximize the auto-labeling performance. We first randomly splits the validation data $D_{\text{val}}^{(i)}$ into $D_{\text{cal}}^{(i)}$ and $D_{\text{th}}^{(i)}$ using procedure RANDOMSPLIT$(D_{\text{val}}^{(i)}, \nu)$. The part $D_{\text{cal}}^{(i)}$ has a fraction ν of the points from $D_{\text{val}}^{(i)}$. Then we consider problem P1 with $\hat{h}_i$ and $D_{\text{cal}}^{(i)}$. We solve it to obtain the post-hoc confidence function $\hat{g}_i$.

4. Threshold estimation. The scores from the new confidence function $\hat{g}_i$ on $D_{\text{th}}^{(i)}$ are used to estimate auto-labeling thresholds in Algorithm 2. This procedure finds thresholds for each class separately. It first splits the points in $D_{\text{th}}^{(i)}$ according to the ground truth class into subsets $D_{\text{th}}^{(i,y)}$. Then, for each class y, it finds the auto-labeling threshold $\hat{\mathbf{t}}[y]$ by selecting the minimum threshold t such that the estimate of auto-labeling error plus a confidence interval, estimated on points in $D_{\text{th}}^{(i,y)}$ having scores above t, is at most the given error tolerance ϵ_a. While we get thresholds as output from `Colander`, it is important to estimate them again from the held-out data $D_{\text{th}}^{(i)}$ to ensure the auto-labeling error constraint is not violated.

5. Auto-labeling. This is a simple step. We computes the scores on the remaining unlabeled data $X_u^{(i)}$ using the function $\hat{g}_i$ and any point $\mathbf{x} \in X_u^{(i)}$ having score above $\hat{\mathbf{t}}[\hat{y}]$ is assigned auto-label $\hat{y} = \hat{h}_i(\mathbf{x})$, and the points that did not meet this criterion remain unlabeled.

6. Remove auto-labeled points. The points that got auto-labeled in the previous steps are removed from the unlabeled pool. To make the validation data consistent with this unlabeled pool for the next round, the points in the validation data that fall into the auto-labeling region are also removed.

7. Get more human-labeled data. Lastly, it calls the procedure ACTIVEQUERY$(\hat{h}_i, X_u^{(i)}, n_b)$ to select n_b points from the remaining unlabeled pool using an active learning strategy. This newly acquired human-labeled data is added into the training data $D_{\text{train}}^{(i)}$. The details of the querying strategy are in Appendix B. The procedure then moves to step 2 and runs the loop until there are no more unlabeled points left or it has queried the stipulated number of human-labels N_t.

B.5 Glossary

The notation is summarized in Table 2 below.

Symbol	Definition
$\mathbb{1}(E)$	indicator function of event E. It is 1 if E happens and 0 otherwise.
$\mathcal{X}$	feature space.
$\mathcal{Y}$	label space i.e. $1, 2, \ldots k$.
$\mathcal{H}$	hypothesis space (model class for the classifiers).
$\mathcal{G}$	class of confidence functions.
k	number of classes.
$\mathbf{x}, y$	$\mathbf{x}$ is an element in $\mathcal{X}$ and y is its true label.
h	a hypothesis (model) in $\mathcal{H}$.
g	confidence function $g : \mathcal{X} \to \Delta^k$.
X_u	given pool of unlabeled data points.
$X_u^{(i)}$	unlabeled data left at the beginning of ith round.
$\hat{h}^{(i)}$	ERM solution and auto-labeling thresholds respectively in ith round.
$D_{\text{query}}^{(i)}$	labeled data queried from oracle (human) in the ith round.
$D_{\text{train}}^{(i)}$	training data to learn $\hat{h}^{(i)}$ in the ith round.
$D_{\text{val}}^{(i)}$	validation data in the ith round.
$D_{\text{cal}}^{(i)}$	calibration data in the ith round to learn a post-hoc g.
$D_{\text{th}}^{(i)}$	part of validation data in the ith round to estimate threshold $\mathbf{t}$.
$D_{\text{auto}}^{(i)}$	part of $X_u^{(i)}$ that got auto-labeled in the ith round.
D_{out}	Output labeled data, including auto-labeled and human labeled data.
$\mathbf{t}$	k dimensional vector of thresholds.
$\mathbf{t}[y]$	yth entry of $\mathbf{t}$ i.e. the threshold for class y.
$g(\mathbf{x})[y]$	the confidence score for class y output by confidence function g on data point $\mathbf{x}$.
$\hat{y}$	predicted class for data point $\mathbf{x}$.
f^*	unknown groundtruth labeling function.
N_u	number of unlabeled points, i.e. size of X_u.
N_t	number of manually labeled points that can be used for training h.
N_a	Total auto-labeled points in D_{out}.
ν	fraction of D_{val} that can be used for training post-hoc calibrator.
A	indices of points that are auto-labeled.
$X_u(A)$	subset of points in X_u with indices in A, i.e. the set of auto-labeled points.
$\tilde{y}_i$	label assigned to the ith point by the algorithm. It could be either y_i or $\hat{y}_i$.
y_i	groundtruth label for the ith point.
$\hat{y}_i$	predicted label for the ith point by classifier.
ϵ_a	auto-labeling error tolerance.
$\mathcal{E}(g, \mathbf{t} \mid h)$	population level auto-labeling error, see eq. (**??**).
$\mathcal{P}(g, \mathbf{t} \mid h)$	population level auto-labeling coverage, see eq. (**??**).
$\widehat{\mathcal{E}}(g, \mathbf{t} \mid h, D)$	estimated auto-labeling error, see eq. (**??**).
$\widehat{\mathcal{P}}(g, \mathbf{t} \mid h, D)$	estimated auto-labeling coverage, see eq. (**??**).
$\widetilde{\mathcal{E}}(g, \mathbf{t} \mid h, D)$	surrogate estimated auto-labeling error, see eq. (3).
$\widetilde{\mathcal{P}}(g, \mathbf{t} \mid h, D)$	surrogate estimated auto-labeling coverage, see eq. (2).

Table 2: Glossary of variables and symbols used in this paper.

Algorithm 1 Threshold-based Auto-Labeling (TBAL)

Input: Unlabeled data X_u, labeled validation data D_{val}, auto labeling error tolerance ϵ_a, N_t training data query budget, seed data size n_s, batch size for active query n_b, calibration data fraction ν, set of confidence thresholds T, coverage lower bound ρ_0, label space $\mathcal{Y}$.

Output: Auto-labeled dataset D_{out}

procedure TBAL($X_u, D_{\text{val}}, \epsilon_a, N_t, n_s, n_b, \nu, \rho_0, T, \mathcal{Y}$)
  ▷ /*** Initialization. ***/
  $D^{(1)}_{\text{query}} \leftarrow$ RANDOMQUERY(X_u, n_s) ▷ Randomly select n_s points and get manual labels for them.
  $X^{(1)}_u \leftarrow X_u \setminus \{\mathbf{x} : (\mathbf{x}, y) \in D^{(1)}_{\text{query}}\}$ ▷Remove the manually labeled points from the unlabeled pool.
  $D^{(1)}_{\text{val}} \leftarrow D_{\text{val}}; D^{(0)}_{\text{train}} \leftarrow \emptyset$ ▷Validation data for the first round is full D_{val}.
  $D_{\text{out}} \leftarrow D^{(1)}_{\text{query}}; n^{(1)}_t \leftarrow n_s; i \leftarrow 1$ ▷Include the manually labeled data in Step 2. in the output data D_{out}.
  ▷ /*** Run the auto-labeling loop ***/
  ▷ /* Until no more unlabeled points are left or the budget for manually labeled training data is exhausted. */
  while $X^{(i)}_u \neq \emptyset$ and $n^{(i)}_t \leq N_t$ **do**
    $D^{(i)}_{\text{train}} \leftarrow D^{(i-1)}_{\text{train}} \cup D^{(i)}_{\text{query}}$ ▷Include the manually labeled points in the training data.
    $\hat{h}_i \leftarrow$ TRAINMODEL$(\mathcal{H}, D^{(i)}_{\text{train}})$ ▷Train a classification model.
    $D^{(i)}_{\text{cal}}, D^{(i)}_{\text{th}} \leftarrow$ RANDOMSPLIT$(D^{(i)}_{\text{val}}, \nu)$ ▷Randomly split the current validation data into two parts.
    ▷ /*** `Colander` block, to learn the new confidence function $\hat{g}_i$***/
    $\hat{g}_i, \hat{\mathbf{t}}'_i \leftarrow \arg\min_{g \in \mathcal{G}, \mathbf{t} \in T^k} -\widetilde{\mathcal{P}}(g, \mathbf{t} \mid \hat{h}_i, D^{(i)}_{\text{cal}}) + \lambda \widetilde{\mathcal{E}}(g, \mathbf{t} \mid \hat{h}_i, D^{(i)}_{\text{cal}})$ ▷ `Colander` procedure.
    ▷ /*** Estimate auto-labeling thresholds using $\hat{g}_i$ and $D^{(i)}_{\text{th}}$. See Algorithm 2. ***/
    $\hat{\mathbf{t}}_i \leftarrow$ ESTTHRESHOLD$(\hat{g}_i, \hat{h}_i, D^{(i)}_{\text{th}}, \epsilon_a, \rho_0, T, \mathcal{Y})$
    ▷ /*** Auto-label the points having scores above the thresholds. ***/
    $\widetilde{D}^{(i)}_u \leftarrow \{(\mathbf{x}, \hat{h}_i(\mathbf{x})) : \mathbf{x} \in X^{(i)}_u\}$
    $D^{(i)}_{\text{auto}} \leftarrow \{(\mathbf{x}, \hat{y}) \in \tilde{D}^{(i)}_u : \hat{g}_i(\mathbf{x})[\hat{y}] \geq \hat{\mathbf{t}}_i[\hat{y}]\}$
    $X^{(i)}_u \leftarrow X^{(i)}_u \setminus \{\mathbf{x} : (\mathbf{x}, \hat{y}) \in D^{(i)}_{\text{auto}}\}$ ▷Remove auto-labeled points from the unlabeled pool.
    $\widetilde{D}^{(i)}_{\text{val}} \leftarrow \{(\mathbf{x}, \hat{h}_i(\mathbf{x})) : (\mathbf{x}, y) \in D^{(i)}_{\text{val}}\}$
    $D^{(i+1)}_{\text{val}} \leftarrow \{(\mathbf{x}, \hat{y}) \in \tilde{D}^{(i)}_{\text{val}} : \hat{g}_i(\mathbf{x})[\hat{y}] < \hat{\mathbf{t}}_i[\hat{y}]\}$ ▷Remove validation points in the auto-labeling region.
    ▷ /*** Get the next batch of manually labeled data using an active querying strategy. ***/
    $D^{(i+1)}_{\text{query}} \leftarrow$ ACTIVEQUERY$(\hat{h}_i, X^{(i)}_u, n_b)$
    $X^{(i+1)}_u \leftarrow X^{(i)}_u \setminus \{\mathbf{x} : (\mathbf{x}, y) \in D^{(i+1)}_{\text{query}}\}$ ▷Remove manually labeled data from the unlabeled pool.
    $D_{\text{out}} \leftarrow D_{\text{out}} \cup D^{(i)}_{\text{auto}} \cup D^{(i+1)}_{\text{query}}$ ▷Add the auto-labeled and manually labeled points in the output data.
    $n^{(i+1)}_t \leftarrow n^{(i)}_t + n_b$
    $i \leftarrow i + 1$
  end while
  return D_{out}
end procedure

Algorithm 2 Estimate Auto-Labeling Threshold

Input: Confidence function $\hat{g}_i$, classifier $\hat{h}_i$, Part of validation data $D_{\text{th}}^{(i)}$ for threshold estimation, auto labeling error tolerance ϵ_a, set of confidence thresholds T, coverage lower bound ρ_0, label space $\mathcal{Y}$.

Output: Auto-labeling thresholds $\hat{\mathbf{t}}_i$, where $\hat{\mathbf{t}}_i[y]$ is the threshold for class y.

procedure ESTTHRESHOLD($\hat{g}_i, \hat{h}_i, D_{\text{th}}^{(i)}, \epsilon_a, \rho_0, T, \mathcal{Y}$)
  ▷ /*** Estimate thresholds for each class. ***/
  for $y \in \mathcal{Y}$ **do**
    $D_{\text{th}}^{(i,y)} \leftarrow \{(\mathbf{x}', y') \in D_{\text{th}}^{(i)} : y' = y\}$ ▷Group points class-wise.
    ▷ /*** Only evaluate thresholds with est. coverage at least ρ_0. ***/
    $T'_y \leftarrow \{t \in T : \widehat{\mathcal{P}}\big(\hat{g}_i, t \mid \hat{h}_i, D_{\text{th}}^{(i,y)}\big) \geq \rho_0\} \cup \{\infty\}$
    ▷ /*** Estimate auto-labeling error at each threshold. Pick the smallest threshold with the sum of estimated error and C_1 times the standard deviation is below ϵ_a. C_1 is set to 0.25 here. ***/
    $\hat{\mathbf{t}}_i[y] \leftarrow \min\{t \in T'_y : \widehat{\mathcal{E}}_a(\hat{g}_i, t | \hat{h}_i, D_{\text{th}}^{(i,y)}) + C_1 \hat{\sigma}(\hat{h}_i, t, D_{\text{th}}^{(i,y)}) \leq \epsilon_a\}$
  end for
  return $\hat{\mathbf{t}}_i$
end procedure

C Additional Experiments and Details

Choice of $\mathcal{G}$. Our framework is flexible with respect to the choice of function class $\mathcal{G}$. In this work, we use neural networks with at least two layers on model class $\mathcal{H}$. We use representations from the last two layers of as input for the functions in $\mathcal{G}$. Let $\mathbf{z}^{(1)}(\mathbf{x}; h) \in \mathbb{R}^k$ and $\mathbf{z}^{(2)}(\mathbf{x}; h) \in \mathbb{R}^{d_2}$ be the outputs of the last and the second-last layer of the net h for input $\mathbf{x}$ and let $\mathbf{z}(\mathbf{x}; h) := [\mathbf{z}^{(1)}(\mathbf{x}; h), \mathbf{z}^{(2)}(\mathbf{x}; h)]$ denote the concatenation. This input is passed to network $\mathcal{G}_{nn_2} : \mathbb{R}^{k+d_2} \mapsto \Delta^k$; it outputs confidence scores for the k classes. Specifically g is defined as $g(\mathbf{x}) := \texttt{softmax}\big(\mathbf{W}_2 \texttt{tanh}(\mathbf{W}_1 \mathbf{z}(\mathbf{x}; h))\big)$. Here $\mathbf{W}_1 \in \mathbb{R}^{(k+d_2)\times 2(k+d_2)}$ and $\mathbb{R}^{2(k+d_2)\times k}$ are the learnable weight matrices. As usual, for $\mathbf{v} \in \mathbb{R}^d$, $\texttt{softmax}(\mathbf{v})[i] := \exp(\mathbf{v}[i])/(\sum_j \exp(\mathbf{v}[j]))$ and $\texttt{tanh}(\mathbf{v})[i] := (\exp(2\mathbf{v}[i]) - 1)/(\exp(2\mathbf{v}[i]) + 1)$.

C.1 Experiments on N_t, N_v and ν

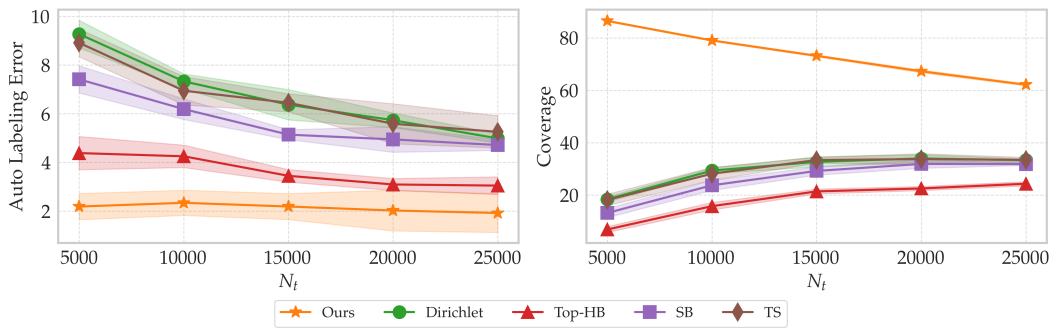


Figure 5: Autolabeling error and coverage of different post-hoc methods on CIFAR-10 for various N_t

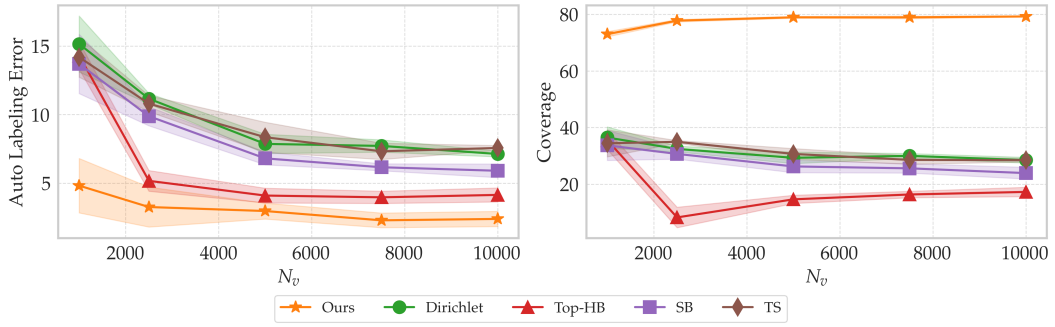


Figure 6: Autolabeling error and coverage of different post-hoc methods on CIFAR-10 for various N_v

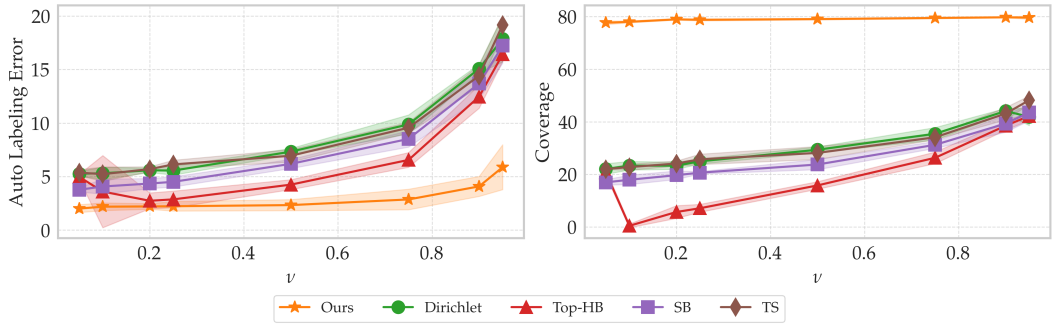


Figure 7: Autolabeling error and coverage of different post-hoc methods on CIFAR-10 for various ν

We need to understand the effect of training data query budget i.e. N_t, the total validation data N_v, and the data that can be used for calibrating the model i.e. the calibration data fraction ν on the

auto-labeling objective. As varying these hyperparameters on each train-time method is expensive, we experimented with only Squentropy as it was the best-performing method across settings for various datasets.

When we vary the budget for training data N_t, we observe from Figure 5 that our method does not require a lot of data to train the base model, i.e. achieving low auto-labeling error and high coverage with a low budget. While other methods benefit from having more training data for auto-labeling objectives, it comes at the expense of reducing the available data for validation.

From figure 6, we observe that, while the coverage of our method remains the same across different N_v, it reduces for other methods. The cause of this phenomenon can be attributed to the fact that we are borrowing the data from the training budget as it limits the performance of the base model, which in turn limits the auto-labeling objective.

As we increase the percentage of data that can be used to calibrate the model, i.e., ν, we note from figure 7 that other methods improve the coverage, which can be understood from the fact that when more data is available for calibrating the model, the model becomes better in terms of the auto-labeling objective. But it's interesting to note that even with a low calibration fraction, our method achieves superior coverage compared to other methods. It is also important to note that the auto-labeling error increases as we increase ν. This is because when ν increases, the number of data points used to estimate the threshold decreases, leading to a less granular and precise threshold.

Feature	**Model**	**Error**	**Coverage**
Pre-logits	Two Layer	4.6 ± 0.3	82.8 ± 0.5
Logits	Two Layer	3.2 ± 1.3	82.8 ± 0.3
Concat	Two Layer	3.3 ± 0.8	82.9 ± 0.4

Table 3: Auto-labeling error and coverage for the 3 feature representations we could use for 20 Newsgroup. As we can see, the feature representation does not lead to a significant difference in auto-labeling error and coverage.

Feature	**Model**	**Error**	**Coverage**
Pre-logits	Two Layer	2.1 ± 0.5	79.0 ± 0.2
Logits	Two Layer	3.1 ± 0.4	76.5 ± 0.9
Concat	Two Layer	2.3 ± 0.5	79.0 ± 0.3

Table 4: Auto-labeling error and coverage for the 3 feature representations we could use for CIFAR10 SimpleCNN. As we can see, the feature representation does not lead to a significant difference in auto-labeling error and coverage.

C.2 Experiments on `Colander` input

Figure 14 illustrates that we could use logits (last layer's representations), pre-logits (second last layer's representations), or the concatenation of these two as the input to g. To help us decide which one we should use, we conduct a hyperparameter search for input features on the CIFAR-10 and 20 Newsgroup dataset using the Squentropy train-time method. Table 3 and 4 present the auto-labeling error and coverage of using the 3 types of feature representations. As we can see, all feature representation leads to a similar auto-labeling error and coverage, and in some cases, it is better to include pre-logits as well. Therefore, we use concatenated representation (Concat), allowing more flexibility.

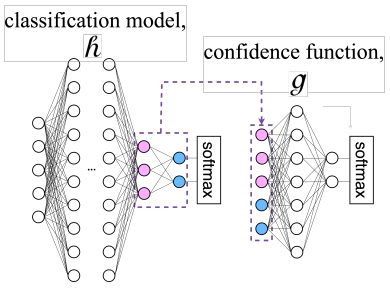


Figure 14: Our choice of g function.

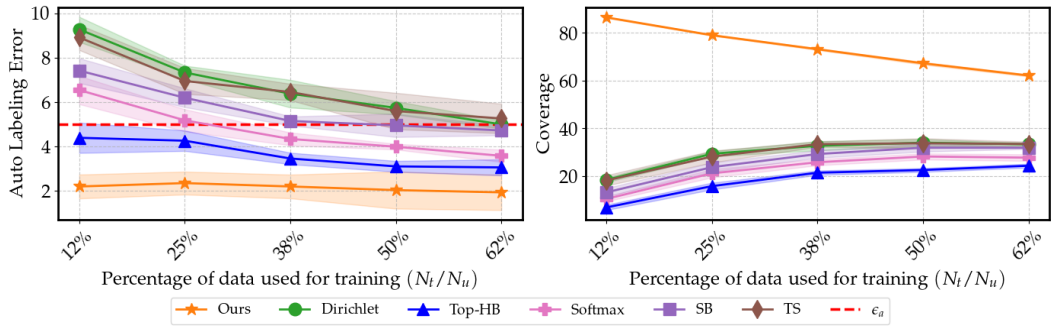


Figure 8: Auto-labeling error and coverage for different post-hoc methods on CIFAR-10 while we vary N_t. $N_u = 40,000$ is the size of the given unlabeled pool.

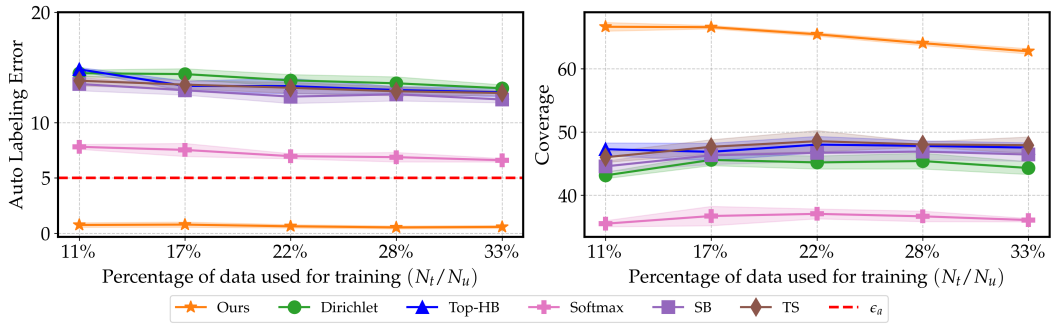


Figure 9: Auto-labeling error and coverage for different post-hoc methods on Tiny-ImageNet while we vary N_t. $N_u = 90,000$ is the size of the given unlabeled pool.

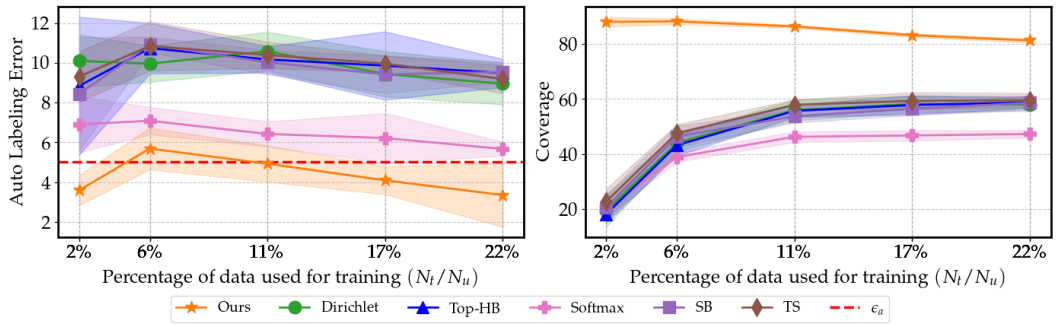


Figure 10: Auto-labeling error and coverage for different post-hoc methods on 20 Newsgroups while we vary N_t. $N_u = 9,052$ is the size of the given unlabeled pool.

C.3 Experiments on ϵ_a

We run TBAL with five values of $\epsilon_a \in \{0.01, 0.025, 0.05, 0.075, 0.1\}$ and report the results in Table 5. As expected the auto-labeling error is high with larger values of and smaller with small ϵ_a.

C.4 Experiments on multiple rounds

We further demonstrate that the performance gains are due to the use of Colander, even if methods use multiple rounds. To do so, we show the evolution of coverage and error over multiple rounds in Figure 15. The effects of using Colander are visible from the first round itself, and the following rounds improve performance further. We also run a single round (passive) variant of TBAL where we sample all the human-labeled points for training (N_t) randomly at once, train a classifier, do auto-labeling, and then stop. This setting avoids confounding due to multiple rounds. We observe that using Colander yields significantly higher coverage in comparison to the baselines (see Table 6).

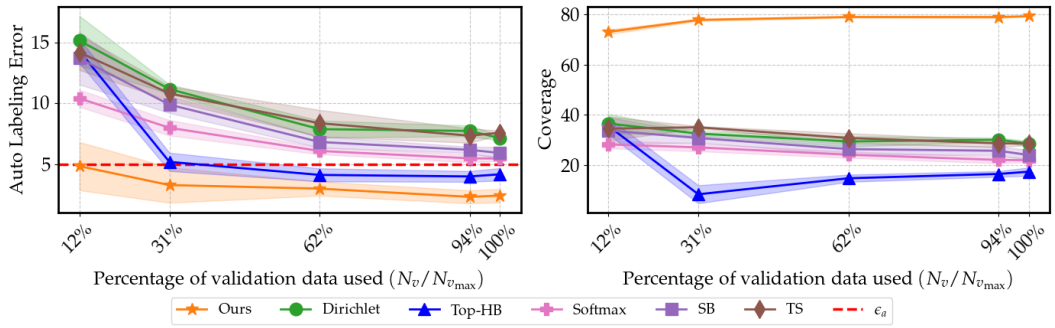


Figure 11: Auto-labeling error and coverage for different post-hoc methods on CIFAR-10 while we vary N_v. $N_{v_{\max}} = 8,000$ is the maximum number of points available for validation.

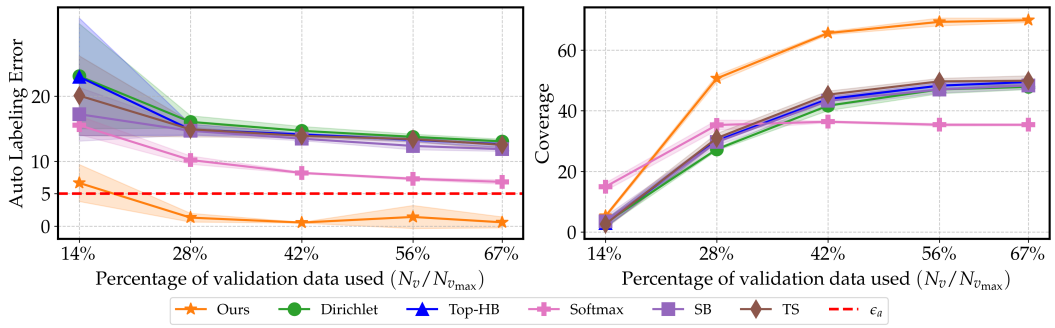


Figure 12: Auto-labeling error and coverage for different post-hoc methods on Tiny-ImageNet while we vary N_v. $N_{v_{\max}} = 18,000$ is the maximum number of points available for validation.

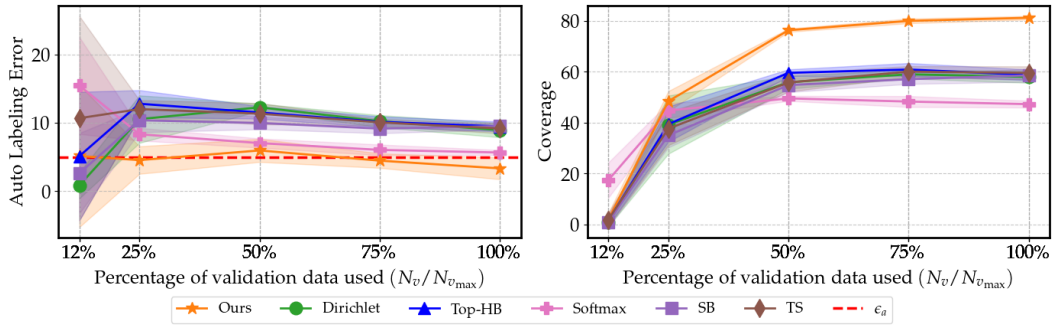


Figure 13: Auto-labeling error and coverage for different post-hoc methods on 20 Newsgroups while we vary N_v. $N_{v_{\max}} = 1,600$ is the maximum number of points available for validation.

This reinforces the fact that the gains in the multi-round TBAL are directly due to Colander, while multiple rounds of data selection, training, and auto-labeling are superior to doing everything in a single round.

Post-hoc Method	ϵ_a = 0.01		ϵ_a = 0.025		ϵ_a = 0.05		ϵ_a = 0.075		ϵ_a = 0.1	
	Err (↓)	Cov (↑)	Err (↓)	Cov (↑)	Err (↓)	Cov (↑)	Err (↓)	Cov (↑)	Err (↓)	Cov (↑)
Softmax	5.86 ± 0.38	12.73 ± 1.61	5.86 ± 0.38	12.73 ± 1.61	4.78 ± 0.21	14.01 ± 2.08	6.80 ± 0.47	16.73 ± 1.19	9.03 ± 0.17	21.28 ± 0.82
TS	8.19 ± 0.88	19.44 ± 1.16	8.19 ± 0.88	19.44 ± 1.16	7.26 ± 0.29	23.15 ± 0.7	9.24 ± 0.78	22.49 ± 0.74	11.63 ± 0.51	25.79 ± 1.97
Dirichlet	8.22 ± 0.4	16.94 ± 1.2	8.22 ± 0.4	16.94 ± 1.2	7.6 ± 0.48	22.36 ± 1.18	9.68 ± 0.82	18.65 ± 0.97	11.26 ± 1.16	24.91 ± 2.09
SB	6.15 ± 0.52	11.74 ± 0.57	6.15 ± 0.52	11.74 ± 0.57	6.09 ± 0.35	18.58 ± 1.13	7.81 ± 0.65	17.37 ± 1.3	9.13 ± 1.08	20.52 ± 1.11
Top-HB	5.76 ± 0.42	9.89 ± 0.55	5.76 ± 0.42	9.89 ± 0.55	5.95 ± 0.7	15.58 ± 1.92	7.45 ± 0.8	13.84 ± 0.78	8.71 ± 1.37	17.9 ± 0.56
Ours	**1.2 ± 0.18**	**78.33 ± 0.76**	**1.32 ± 0.21**	**78.75 ± 0.4**	**2.96 ± 0.2**	**78.48 ± 0.17**	**4.3 ± 0.23**	**78.94 ± 0.42**	**6.29 ± 0.5**	**78.97 ± 0.46**

Table 5: ϵ_a **variation.** Dataset: CIFAR-10, Train-time method: Vanilla.

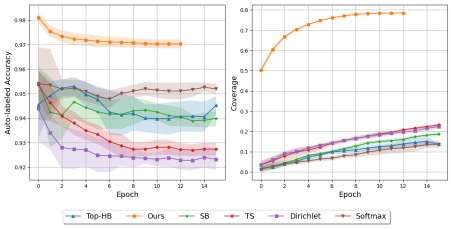


Figure 15: Clarification on multiple rounds. Per-epoch metrics for all post-hoc methods for CIFAR10. (left) Auto-labeling accuracy (right) Coverage. Train time method is vanilla and model is medium net.

Post-hoc method	Err (↓)	Coverage (↑)
Softmax	2.7 ± 0.54	11.06 ± 1.46
TS	3.04 ± 0.49	12.03 ± 1.98
Dirichlet	2.98 ± 0.32	11.22 ± 2.1
SB	2.72 ± 0.34	9.75 ± 1.33
Top-HB	1.83 ± 0.61	5.50 ± 1.08
Ours	**2.02 ± 0.28**	**49.62 ± 0.69**

Table 6: Results with single round of auto-labeling. Dataset and model: CIFAR-10 setting in the paper.

C.5 Experiments on different architectures

In TBAL it is not a priori clear what model the practitioner should use. The overall system is flexible enough to work with any chosen model class. Our focus is on evaluating the effect of various training time and post-hoc methods designed to improve the confidence functions for any given model. To answer the query, we ran experiments with Resnet18 and ViT models in the CIFAR-10 setting (see Table 7). As we expected there are variations in the results in the baselines due to model choices but our method maintains high performance irrespective of the classification model used. This is due to its ability to learn confidence scores tailored for TBAL.

Post-hoc Method	Err (↓)	Coverage (↑)
Softmax	14.02 ± 1.83	2.03 ± 0.31
TS	19.32 ± 2.51	2.54 ± 0.33
Dirichlet	17.27 ± 3.26	2.87 ± 0.55
SB	9.22 ± 10.91	0.46 ± 0.51
Top-HB	0.00 ± 0.00	0.00 ± 0.00
Ours	**2.62 ± 0.32**	**75.56 ± 0.15**

Post-hoc Method	Err (↓)	Coverage (↑)
Softmax	4.48 ± 0.23	33.24 ± 1.14
TS	6.38 ± 0.47	39.14 ± 1.96
Dirichlet	6.30 ± 0.41	37.99 ± 1.47
SB	5.16 ± 0.23	35.32 ± 1.36
Top-HB	4.46 ± 0.40	29.66 ± 0.74
Ours	**2.85 ± 0.25**	**78.56 ± 0.54**

Table 7: Model variation. CIFAR-10 dataset with ViT (Left) and ResNet18 (Right), Train-time method Vanilla.

C.6 Hyperparameters

The hyperparameters and their values we swept over are listed in Table 8 and 9 for train-time and post-hoc methods, respectively.

C.7 Train-time and post-hoc methods

C.7.1 Train-time methods

1. *Vanilla*: Neural networks are commonly trained by minimizing the cross entropy loss using stochastic gradient descent (SGD) with momentum [1, 3]. We refer to this as the Vanilla training method. We also include weight decay to mitigate the overconfidence issue associated with this method [10].

Method	Hyperparameter	Values
Common	optimizer	SGD
	learning rate	0.001, 0.01, 0.1
	batch size	32, 256
	max epoch	50, 100
	weight decay	0.001, 0.01, 0.1
	momentum	0.9
CRL	rank target	softmax
	rank weight	0.7, 0.8, 0.9
FMFP	optimizer	SAM

Table 8: Hyperparameters swept over for train-time methods. Those listed next to Common are the hyperparameters for the four train-time methods: Vanilla, CRL, FMFP, and Squentropy. Therefore, we do not list those again for each method. Note that for FMFP, we used SAM optimizer instead of SGD. For each method, we swept through all possible combinations of the possible values for each hyperparameter. Underlined values are only used on TinyImageNet since it is a complicated dataset containing 200 classes.

2. *Squentropy* [16]: This method adds the average square loss over the incorrect classes to the cross-entropy loss. This simple modification to the Vanilla method leads to the end model with better test accuracy and calibration.

3. *Correctness Ranking Loss (CRL)* [30]: This method includes a term in the loss function of the vanilla training method so that the confidence scores of the model are aligned with the ordinal rankings criterion [15, 5]. The confidence functions satisfying this criterion produce high scores on points where the probability of correctness is high and low scores on points with low probabilities of being correct.

4. *FMFP* [53] aims to align confidence scores with the ordinal rankings criterion. It uses Sharpness Aware Minimizer (SAM) [6] to train the model, with the expectation that the flat minima would benefit the ordinal rankings objective of the confidence function.

C.7.2 Post-hoc methods

1. *Temperature scaling* [10]: This is a variant of Platt scaling [10], a classic and one of the easiest parametric methods for post-hoc calibration. It rescales the logits by a learnable scalar parameter and has been shown to work well for neural networks.

2. *Top-Label Histogram-Binning* [12]: Since TBAL assigns the top labels (predicted labels) to the selected unlabeled points, it is appealing to only calibrate the scores of the predicted label. Building upon a rich line of histogram-binning methods (non-parametric) for post-hoc calibration [52], this method focuses on calibrating the scores of predicted labels.

3. *Scaling-Binning* [24]: This method combines parametric and non-parametric methods. It first applies temperature scaling and then bins the confidence function values to ensure calibration.

4. *Dirichlet Calibration* [22]: This method models the distribution of predicted probability vectors separately on instances of each class and assumes the class conditional distributions are Dirichlet distributions with different parameters. It uses linear parameterization for the distributions, which allows easy implementation in neural networks as additional layers and softmax output.

Note: For binning methods, uniform mass binning [52] has been a better choice over uniform width binning. Hence, we use uniform mass binning as well.

C.8 Compute resources

Our experiments were conducted on machines equipped with the NVIDIA RTX A6000 and NVIDIA GeForce RTX 4090 GPUs.

C.9 Detailed dataset and model

1. The MNIST dataset [26] consists of 28×28 grayscale images of hand-written digits across 10 classes. It was used alongside the LeNet5 [27], a convolutional neural network, for auto-labeling.
2. The CIFAR-10 dataset [20] contains $3 \times 32 \times 32$ color images across 10 classes. We utilized its raw pixel matrix in conjunction with SimpleCNN [17], a convolutional neural network with approximately 5.8M parameters, for auto-labeling.
3. Tiny-ImageNet [25] is a color image dataset that consists of 100K images across 200 classes. Instead of using the $3 \times 64 \times 64$ raw pixel matrices as input, we utilized CLIP [38] to derive embeddings within the $\mathbb{R}^{512}$ vector space. We used a 3-layer perceptron (1,000-500-300) as the auto-labeling model.
4. 20 Newsgroups [29, 35] is a natural language dataset comprising around 18,000 news posts across 20 topics. We used the FlagEmbedding [50] to map the textual data into $\mathbb{R}^{1024}$ embeddings. We used a 3-layer perceptron (1,000-500-30) as the auto-labeling model.

C.10 Detailed experiments protocol

We predefined TBAL hyperparameters for each dataset-model pair and the hyperparameters we will sweep for each train-time and post-hoc method in Table 8 and Table 9 respectively. For a dataset-model pair, initially, we perform a hyperparameter search for the train-time method. Subsequently, we optimize the hyperparameters for post-hoc methods while keeping the train-time method fixed with the previously found optimum hyperparameter for that dataset-model pair.

We fix the hyperparameters for the train-time method while searching hyperparameters for the post-hoc method to alleviate computational budget throttle. We effectively reduce the search space to the sum of the cardinalities of unique hyper-parameter combinations across the two methods instead of a larger multiplicative product. Furthermore, due to the independent nature of these hyper-parameter combinations, TBAL runs can be highly parallelized to expedite the search process.

Since TBAL operates iteratively to acquire human labels for model training, selecting hyper-parameters at each round of TBAL could quickly become intractable and lose its practical significance. To better align with its practical usage, we only conducted a hyperparameter search for the initial TBAL round. The specific set of hyperparameters used for the search are reported in Table 9.

After completing the hyperparameter search for train-time and post-hoc methods, the determined hyperparameter combinations are subjected to a full evaluation across all iterations of TBAL. At the end of each iteration, the auto-labeled points are evaluated against their ground truth labels to determine their auto-labeling error. These points are then added to the auto-labeled set, where their ratio to the total amount of unlabeled data determines the coverage. This iterative process continues until all unlabeled data are exhaustively labeled by either the oracle or through auto-labeling in the final iteration. The auto-labeling error and coverage at the final iteration of TBAL are then recorded.

Since TBAL incorporates randomized components as detailed in Algorithm 1, we ran the algorithm 5 times, each with a unique random seed while maintaining the same hyperparameter combination. We then recorded the results from the final iteration of these runs and calculated the mean and standard deviation of both auto-labeling error and coverage. These figures are reported in Table 1.

A limitation of the grid search approach in hyper-parameter optimization becomes apparent when our predefined hyper-parameter choices result in sub-optimal coverage and auto-labeling errors. Using these sub-optimal hyper-parameters can adversely affect the multi-round iterative process in TBAL, prompting the need for repetitive searches to find more effective hyper-parameters. When encountering such scenarios, TBAL users should explore additional hyper-parameter options until satisfactory performance is achieved in the initial round. However, we opted for a more straightforward approach to hyper-parameter selection, mindful of the computational demands of repeatedly optimizing multiple hyper-parameters across different methods. In scenarios expressed conditionally, we retained the top-1 hyper-parameter combination for any given method if it achieved the highest coverage while adhering to the specified error margin (ϵ_a). If no hyper-parameter combinations yielded an auto-labeling error at most equal to the error margin (ϵ_a), we then chose the hyper-parameter combination with the lowest auto-labeling error, regardless of its coverage. In the case of ties, we resolved them through random selection. This process results in obtaining singular values for each choice of hyper-parameter after completing each method's hyper-parameter search.

D Broader Impact

This paper contributes to the advancement of the practice of creating labeled datasets in machine learning. While our work has various possible societal implications, we do not identify any specific concerns that require special attention in this context.

E Related Work

Data Labeling. We briefly discuss prominent methods for labeling. Crowdsourcing [40, 43] uses a crowd of non-experts to complete a set of labeling tasks. Works in this domain focus on mitigating noise in the obtained information, modeling label errors, and designing effective labeling tasks [9, 18, 28, 46, 45, 47, 4]. Weak supervision (WS), in contrast, emphasizes labeling through multiple inexpensive but noisy sources, not necessarily human [39, 7, 42, 48]. Works such as [39, 7] concentrate on binary or multi-class labeling, while [42, 48] extend WS to structured prediction tasks.

Auto-labeling occupies an intermediate position between weak supervision and crowdsourcing in terms of human dependency. It aims to minimize costs to obtain human labels while generating high-quality labeled data using a specific model. [37] use a TBAL-like algorithm and explore the cost of training for auto-labeling with large-scale model classes. Recent work [49] theoretically analyzes the sample complexity of validation data required to guarantee the quality of auto-labeled data.

Overconfidence and calibration. The issue of overconfidence [44, 33, 14, 2] is detrimental in several applications, including ours. Many solutions have emerged to mitigate the overconfidence and miscalibration problem. Gawlikowski et al. [8] provide a comprehensive survey on uncertainty quantification and calibration techniques for neural networks. Guo et al. [10] evaluated a variety of solutions ranging from the choice of network architecture, model capacity, weight decay regularization [21], histogram-binning and isotonic regression [51, 52] and temperature scaling [36, 34] which they found to be the most promising solution. The solutions fall into two broad categories: train-time and post-hoc. Train-time solutions modify the loss function, include additional regularization terms, or use different training procedures [23, 32, 31, 16]. On the other hand, post-hoc methods such as top-label histogram-binning [11], scaling binning [24], Dirichlet calibration [22] calibrate the scores directly or learn a model that corrects miscalibrated confidence scores.

Beyond calibration. While calibration aims to match the confidence scores with a probability of correctness, it is not the precise solution to the overconfidence problem in many applications, including our setting. The desirable criteria for scores for TBAL are closely related to the ordinal ranking criterion [15]. To get such scores, Corbière et al. [5] add a module in the net for failure prediction, Zhu et al. [53] switch to sharpness aware minimization [6] to learn the model; CRL [30] regularizes the loss.

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Method	Hyperparameter	Values
Temperature scaling	optimizer	Adam
	learning rate	0.001, 0.01, 0.1
	batch size	64
	max epoch	500
	weight decay	0.01, 0.1, 1
Top-label histogram binning	points per bin	25, 50
Scaling-binning	number of bins	15, 25
	learning rate	0.001, 0.01, 0.1
	batch size	64
	max epoch	500
	weight decay	0.01, 0.1, 1
Dirichlet calibration	regularization parameter	0.001, 0.01, 0.1
Ours	λ	10, 100
	features key	concat
	class-wise	independent
	optimizer	Adam
	learning rate	0.01, 0.1
	max epoch	500
	weight decay	0.01, 0.1, 1
	batch size	64
	regularize	false
	α	0.01, 0.1, 1

Table 9: Hyperparamters swept over for post-hoc methods. For each method, we swept through all possible combinations of the possible values for each hyperparameter.