SELECTIVE PREDICTION VIA TRAINING DYNAMICS

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ABSTRACT

Selective prediction is the task of rejecting inputs a model would predict incorrectly on through a trade-off between input space coverage and model utility. Current methods for selective prediction typically impose constraints on either the model architecture or the loss function; this inhibits their usage in practice. In contrast to prior work, we show that state-of-the-art selective prediction performance can be attained solely from studying the (discretized) training dynamics of a model. We propose a general framework that, given a test input, monitors metrics capturing the instability of predictions from intermediate models obtained during training w.r.t. the final model's prediction. In particular, we reject data points exhibiting too much disagreement with the final prediction at late stages in training. The proposed scoring mechanism is domain-agnostic (i.e., it works for both discrete and real-valued prediction) and can be flexibly combined with existing selective prediction approaches as it does not require any train-time modifications. Our experimental evaluation on image classification, regression, and time series forecasting problems shows that our method beats past state-of-the-art accuracy/utility trade-offs on typical selective prediction benchmarks.

1 INTRODUCTION

Machine learning (ML) is increasingly deployed in high-stakes decision-making environments, where it is critical to detect inputs for which the model produces an erroneous prediction. This is particularly true when deploying deep neural networks (DNNs) for applications with low tolerances for false-positives (i.e., classifying with a wrong label), such as healthcare (Challen et al., 2019; Mozannar and Sontag, 2020), self-driving (Ghodsi et al., 2021), and law (Vieira et al., 2021). This problem setup is captured by the selective prediction (SP) framework, which introduces a gating mechanism to abstain from predicting on individual test points in the presence of high prediction uncertainty (Geifman and El-Yaniv, 2017). Specifically, SP aims to (i) only accept inputs on which the ML model would achieve high utility, while (ii) maintaining high coverage / throughput, i.e., accepting as many inputs as possible.

Current selective prediction techniques take one of two directions: (i) augmentation of the architecture of the underlying ML model (Geifman and El-Yaniv, 2019); or (ii) training the model using a purposefully adapted loss function (Liu et al., 2019; Huang et al., 2020; Gangrade et al., 2021). The unifying principle behind these methods is to modify the training stage in order to accommodate selective prediction. While many ad-hoc experimentation setups are amenable to these changes, productionalized environments often impose data pipeline constraints which limit the applicability of existing methods. Such constraints include, but are not limited to, data access revocation, high (re)-training costs, or pre-existing architecture/loss modifications whose interplay with selective prediction adaptations are unexplored.

In this work, we instead show that *these modifications are unnecessary*. That is, our method not only outperforms existing work but **our method, the new state-of-the-art, can be easily applied on top of all existing models in contrast with past methods**. Moreover, our method is not restricted to classification problems but can be applied for real-valued prediction problems, too. This is an important contribution as recent SP approaches have solely focused on improving selective *classification*. We believe that our work will motivate additional future work on selective regression tasks in particular.

Our approach builds on the following observation: typical DNNs are trained iteratively e.g., using stochastic gradient descent. Hence, as training goes on, the optimization process yields a sequence of intermediate models. Current methods for selective prediction only rely on the final model. We however propose to take advantage of the information contained in these optimization trajectories for the purpose of selective prediction. For example, we observe that instability in SGD convergence

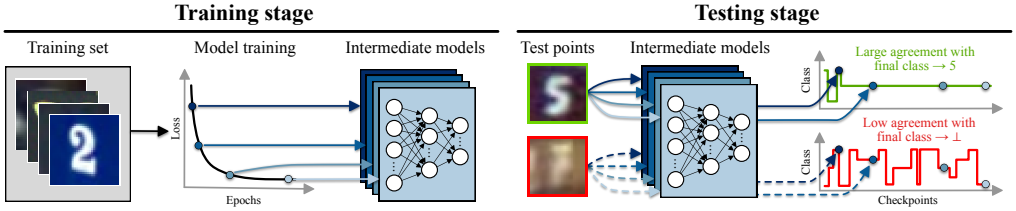

Figure 1: **Our proposed `SPTD` method for a classification example**. During the model training stage, we store checkpoints of intermediate models. At inference time, given a test input, we compute various metrics capturing the stability of intermediate predictions with respect to the final model prediction. Data points with high stability are accepted while data points with low stability are rejected.

is often indicative of potential in-separability or of noise in the data. Furthermore, work on example difficulty (Jiang et al., 2020; Toneva et al., 2018; Hooker et al., 2019; Agarwal et al., 2020) has highlighted faster convergence as indicative of easy-to-learn examples. We hypothesize such training time correlations with uncertainty also hold for test points and studying how test time predictions evolve over the intermediate checkpoints is useful for reliable uncertainty quantification.

With this hypothesis, we derive the first framework for **S**elective **P**rediction based on neural network **T**raining **D**ynamics (`SPTD`, see Figure 1 for a classification example). Through a formalization of this particular neural network training dynamics problem, we first note that a useful property of the intermediate models' predictions for a test point is whether they converge ahead of the final prediction. This convergence can be measured by deriving a prediction instability score measuring how strongly predictions of intermediate models agree with the final model. While the exact specifics of how we measure instability differs between domains (classification vs regression), our resulting score generalizes across domains and measures weighted prediction instability. This weighting allows us to emphasize instability late in training which we deem indicative of points that should be rejected. Note that this approach is transparent w.r.t. the training stage: our method only requires that intermediate checkpoints were recorded when a model was trained, which is an established practice (especially when operating in shared computing environments). Moreover, when compared to competing ensembling-based methods such as deep ensembles (Lakshminarayanan et al., 2017), our approach can match the same inference-time cost while being significantly cheaper to train.

To summarize, our main contributions are as follows:

1. We present a motivating synthetic logistic regression example showcasing the effectiveness of training dynamics information in the presence of a challenging classification task (Sec. 3.1).
2. We propose a novel method for selective prediction based on training dynamics (`SPTD`, Sec. 3.2). To that end, we devise an effective scoring mechanism capturing weighted prediction instability of intermediate models with the final prediction for individual test points. Our methods allow for selective classification, regression, and time series prediction. Moreover, `SPTD` can be applied to all existing models whose checkpoints were recorded during training.
3. We perform a comprehensive set of empirical experiments on established selective prediction benchmarks (Sec. 4). Our results obtained from all instances of `SPTD` demonstrate highly favorable utility/coverage trade-offs, establishing new state-of-the-art results in the field.

2 Background on Selective Prediction

Supervised Learning Setup. Our work considers the standard supervised learning setup. We assume access to a dataset $D = \{(\boldsymbol{x}_i, y_i)\}_{i=1}^{M}$ consisting of data points $(\boldsymbol{x}, y)$ with $\boldsymbol{x} \in \mathcal{X}$ and $y \in \mathcal{Y}$. We refer to $\mathcal{X} = \mathbb{R}^d$ as the covariate space of dimensionality d. For classification problems we define $\mathcal{Y} = \{1, 2, ..., C\}$ as the label space consisting of C classes. For regression and time series problems we instead define $\mathcal{Y} = \mathbb{R}$ and $\mathcal{Y} = \mathbb{R}^R$ respectively (with R being the prediction horizon). All data points $(\boldsymbol{x}, y)$ are sampled independently from the underlying distribution p defined over $\mathcal{X} \times \mathcal{Y}$. Our goal is to learn a prediction function $f : \mathcal{X} \to \mathcal{Y}$ which minimizes the empirical risk with respect to the underlying data distribution p and an appropriately chosen loss function $\ell : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$.

Selective Prediction Setup. Selective prediction alters the standard supervised learning setup by introducing a rejection state $\perp$ through a *gating mechanism* (El-Yaniv and Wiener, 2010). In particular, such a mechanism introduces a selection function $g : \mathcal{X} \to \mathbb{R}$ which determines if a model should predict on a data point $\boldsymbol{x}$. Given an acceptance threshold τ, the resulting predictive model can be summarized as:

$$(f,g)(\boldsymbol{x}) = \begin{cases} f(\boldsymbol{x}) & g(\boldsymbol{x}) \leq \tau \\ \perp & \text{otherwise.} \end{cases} \tag{1}$$

Selective Prediction Evaluation Metrics. Prior work evaluates the performance of a selective predictor (f,g) based on two metrics: the *coverage* of (f,g) (i.e., what fraction of points we predict on) and the *selective utility* of (f,g) on the accepted points. Note that the exact utility metric depends on the type of the underlying selective prediction task (e.g. accuracy, R^2, quantile loss). Successful SP methods aim to obtain both strong selective utility and high coverage. Note that these two metrics are at odds with each other: naïvely improving utility leads to lower coverage and vice-versa. The complete performance profile of a model can be specified using the risk–coverage curve, which defines the risk as a function of coverage (El-Yaniv and Wiener, 2010). These metrics can be formally defined as follows:

$$\text{coverage}(f,g) = \frac{|\{(\boldsymbol{x},y) : g(\boldsymbol{x}) \leq \tau\}|}{|D|} \qquad \text{utility}(f,g) = \sum_{\{(\boldsymbol{x},y) : g(\boldsymbol{x}) \leq \tau\}} u(f(\boldsymbol{x}),y) \tag{2}$$

where $u(\cdot,\cdot)$ corresponds to the specifically used utility function (e.g. accuracy, R^2, quantile loss).

2.1 Past & Related Work

Softmax Response Baseline (classification). The first work on selective classification is the softmax response (SR) mechanism (Hendrycks and Gimpel, 2016; Geifman and El-Yaniv, 2017). A threshold τ is applied to the maximum response of the softmax layer $\max_{y \in \mathcal{Y}} f(y|\boldsymbol{x})$. Given a confidence parameter δ and desired risk r^*, SR constructs (f,g) with test error no larger than r^* w.p. $\geq 1-\delta$. This approach however has been shown to produce over-confident results under mis-calibration (Guo et al., 2017).

Loss Modifications (classification). The first work to deliberately address selective classification via architecture modification is SelectiveNet (Geifman and El-Yaniv, 2019), which trains a model to jointly optimize for classification and rejection. A loss penalty is added to enforce a particular coverage constraint using a variant of the interior point method. To optimize selective accuracy over the full coverage spectrum in a single training run, Deep Gamblers (Liu et al., 2019) transform the original C-class problem into a $(C+1)$-class problem where the additional class represents model abstention. A similar approach is given by Self-Adaptive Training (SAT) (Huang et al., 2020) which also uses a $(C+1)$-class setup but instead incorporates an exponential average of intermediate predictions into the loss function. Other similar approaches include: performing statistical inference for the marginal prediction-set coverage rates using model ensembles (Feng et al., 2021), confidence prediction using an earlier snapshot of the model (Geifman et al., 2018), estimating the gap between classification regions corresponding to each class (Gangrade et al., 2021), and complete precision by classifying only when models consistent with the training data predict the same output (Khani et al., 2016).

Uncertainty Quantification (classification + regression). It was further shown by Lakshminarayanan et al. (2017); Zaoui et al. (2020) that model ensembles can provide state-of-the-art uncertainty quantification, a task closely related to selective prediction. This however raises the need to train multiple models from scratch. To reduce the cost of training multiple models, Gal and Ghahramani (2016) proposed abstention based on the variance statistics from several dropout enabled forward passes at test time. Another popular technique for uncertainty quantification, especially for regression and time series forecasting, is given by directly modeling the output distribution (Alexandrov et al., 2019) in a parametric fashion. Training with a parametric output distribution however can lead to additional training instability, often requiring extensive hyper-parameter tuning and distributional assumptions.

Training Dynamics Approaches (classification) Huang et al. (2017); Chen et al. (2017) first proposed the usage of training dynamics to construct checkpoint ensembles to boost model utility. Our work is closest in spirit to Swayamdipta et al. (2020) which relies on using training dynamics from an example difficulty viewpoint by considering the variance of logits. However, their approach does not consider selective prediction and requires access to true label information. Adila and Kang (2022) harness similar training dynamics based signals for out-of-distribution detection.

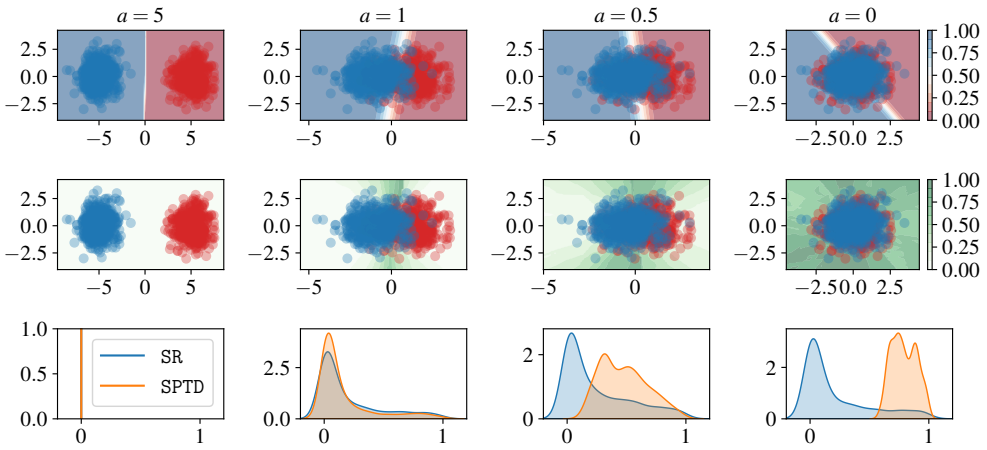

Figure 2: **Synthetic example of anomaly scoring based on `SR` vs `SPTD`**. The first row shows a test set from the generative Gaussian model as well as the learned decision boundary separating the two Gaussians. For small a, the decision boundary is unrightfully overconfident. The second row shows the same data set but instead depicts the scores yielded by applying `SPTD` to the full domain. `SPTD` highlights rightful rejection regions more clearly than the overconfident `SR` score: as $a \to 0$ we see that larger regions are flagged as exhibiting noisy training dynamics (with stronger shades of green indicating stronger disagreement). The bottom row shows the distribution of the `SR` and `SPTD` scores, clearly showing that `SPTD` leads to improved uncertainty under stronger label ambiguity.

3 Selective Prediction via Neural Net Training Dynamics

We now introduce our selective prediction algorithms based on neural network training dynamics. We start by presenting a motivating example showcasing the effectiveness of analyzing training trajectories for a logistic regression problem. Following this, we formalize our selective classification scoring rule based on training-time prediction disagreements. We refer to the class of methods we propose as `SPTD`.

3.1 Method Intuition: Prediction Disagreements Generalize Softmax Response

Stochastic iterative optimization procedures, such as Stochastic Gradient Descent (SGD), yield a sequence of models that is iteratively derived by minimizing a loss function. Current methods for selective prediction disregard the properties of this iterative process and only rely on the final model that it outputs. However, the optimization trajectories contain information that we can use to determine prediction reliability. In particular, on hard optimization tasks, the presence of stochasticity from SGD and the potential in-separability / ambiguity of the data often leads to noisy optimization behavior. As a result, intermediate predictions produced over the course of training might widely disagree in what the right prediction would be for a given data point. Our class of selective prediction approaches explicitly make use of these training dynamics by formalizing rejection scores based on the observed frequency of prediction disagreements with the final model throughout training.

To illustrate and reinforce this intuition that training dynamics contain meaningfully more useful information for selective prediction than the final model, we present a synthetic logistic regression example. First, we generate a mixture of two Gaussians each consisting of 1000 samples:

$$D = \{(\boldsymbol{x}_i, 0)\}_{i=1}^{1000} \cup \{(\boldsymbol{x}_j, 1)\}_{j=1}^{1000} \quad \text{where} \quad \boldsymbol{x}_i \sim \mathcal{N}([a \quad 0]^\top, \boldsymbol{I}) \quad \text{and} \quad \boldsymbol{x}_j \sim \mathcal{N}([-a \quad 0]^\top, \boldsymbol{I})$$

Note that a controls the distance between the two 2-dimensional Gaussian clusters, allowing us to specify the difficulty of the learning task. Then, we train a logistic regression model using SGD for 1000 epochs for each $a \in \{0, 0.5, 1, 5\}$. Finally, we compute both the softmax response score (`SR`) score, the typical baseline for selective classification, as well as our `SPTD` score (details in Section 3.2).

We showcase the results from this experiment in Figure 2. We see that if the data is linearly separable ($a = 5$) the learned decision boundary is optimal and the classifier's built-in confidence score `SR`

Algorithm 1: SPTD for classification

Require: Intermediate models $[f_1,...,f_T]$, query point $\boldsymbol{x}$, weighting parameter $k \in [0,\infty)$.

for $t \in [T]$ **do**
  if $f_t(\boldsymbol{x}) = f_T(\boldsymbol{x})$ **then** $a_t \leftarrow 0$ **else** $a_t \leftarrow 1$
  $v_t \leftarrow (\frac{t}{T})^k$
end for
$g \leftarrow \sum_t v_t a_t$
if $g \leq \tau$ **then** $f(\boldsymbol{x}) = f_T(\boldsymbol{x})$ **else** $f(\boldsymbol{x}) = \perp$

Algorithm 2: SPTD for regression

Require: Intermediate models $[f_1,...,f_T]$, query point $\boldsymbol{x}$, weighting parameter $k \in [0,\infty)$.

for $t \in [T]$ **do**
  $a_t \leftarrow ||f_t(\boldsymbol{x}) - f_T(\boldsymbol{x})||$
  $v_t \leftarrow (\frac{t}{T})^k$
end for
$g \leftarrow \sum_t v_t a_t$
if $g \leq \tau$ **then** $f(\boldsymbol{x}) = f_T(\boldsymbol{x})$ **else** $f(\boldsymbol{x}) = \perp$

reflects well-calibrated uncertainty. Moreover, the optimization process is stable as SPTD yields low scores over the full domain. However, as we move the two Gaussians closer to each other (i.e., by reducing a) we see that the SR baseline increasingly suffers from overconfidence: large parts of the domain are very confidently classified as either 0 (red) or 1 (blue) with only a small ambiguous decision region (white). However, the optimization trajectory is highly unstable with the decision boundary changing abruptly between successive optimization steps. SPTD identifies the region of datapoints exhibiting large prediction disagreement due to this training instability and correctly rejects them (as those are regions also subject to label ambiguity in this case). In summary, we observe that SPTD provides improved uncertainty quantification in ambiguous classification regions (which induce training instability) and reduces to the SR solution as the classification task becomes easier. Hence, we expect SPTD to generalize SR performance, which is supported by this logistic regression experiment.

3.2 Method Overview: Measuring Prediction Instability During Training

We proceed to describe the statistics we collect from intermediate checkpoints that we later devise our scores on. The objective of these statistics is to capture how unstable the prediction for a datapoint was over the training checkpoints. Let $[f_1,f_2,...,f_T]$ be a sequence of intermediate checkpoints, and $\mathcal{D} = D_{\text{train}} \cup D_{\text{test}}$ be the set of all data points. We define a prediction disagreement score as some function $a_t : \mathcal{X} \to \mathbb{R}^+$ with $a_t(\boldsymbol{x}) = 0$ if $f_t(\boldsymbol{x}) = f_T(\boldsymbol{x})$. Note that the exact $a_t(\cdot)$ we use depends on the problem domain (classification vs regression) and we define our choices below. In the following, when conditioning on $\boldsymbol{x}$ is understood from context, we drop the explicit dependence on $\boldsymbol{x}$ and write a_t.

For a fixed data point $\boldsymbol{x}$, our approach takes a given sequence of prediction disagreements $[a_1,...,a_T]$ and associates a weight v_t to each disagreement a_t to capture how severe a disagreement at step t is. To derive this weighting we ask: How indicative of $\boldsymbol{x}$ being incorrectly classified is a disagreement at step t? Related work in the example difficulty literature (see Appendix A for details) found that easy-to-optimize samples are learned early in training and converge faster. While prior work specifically derived these convergence insights for training points only, the novelty of our method is to show such conclusions for training points also generalize to test points. Hence, we propose to use $v_t = (\frac{t}{T})^k$ for $k \in [0,\infty)$ to penalize late prediction disagreements as more indicative of a test point we will not predict correctly on. With this weighting, our methods compute a weighted sum of the prediction disagreements, which effectively forms our selection function $g(\cdot)$:

$$g(\boldsymbol{x}) = \sum_t v_t a_t(\boldsymbol{x}) \tag{3}$$

Instability for Classification. For discrete prediction problems (i.e., classification) we define the label disagreement score as $a_t = 1 - \delta_{f_t(\boldsymbol{x}), f_T(\boldsymbol{x})}$ where δ is the Dirac-delta function: a_t is hence 1 if the intermediate prediction f_t at checkpoint t disagrees with the final prediction f_T for $\boldsymbol{x}$, else 0. The resulting algorithm using this definition of a_t for classification is given in Algorithm 1. We remark that continuous metrics such as the maximum softmax score, the predictive entropy, or the gap between the two most confident classes could be used as alternate measures for monitoring stability (see Appendix C for a discussion). However, these measures only provide a noisy proxy and observing a discrete deviation in the predicted class provides the most direct signal for potential mis-classification.

Instability for Regression. One key advantage of our method over many previous ones is that it is applicable to *any* predictive model, including regression. Here, we propose the following prediction disagreement score measuring the distance of intermediate predictions to the final model's prediction:

$a_t = ||f_t(\boldsymbol{x}) - f_T(\boldsymbol{x})||$.[1] The resulting algorithm using this definition of a_t for regression is given in Algorithm 2. We again highlight the fact that Algorithm 2 only differs from Algorithm 1 in the computation of the prediction disagreement a_t (line 2 in both algorithms).

Instability for Time Series Prediction. We can further generalize the instability sequence used for regression to time series prediction problems by computing the regression score for all time points on the prediction horizon. In particular, we compute $a_{t,r} = ||f_t(\boldsymbol{x})_r - f_T(\boldsymbol{x})_r||$ for all $r \in \{1,...,R\}$. Recall that for time series problems $f_t(\boldsymbol{x})$ returns a vector of predictions $y \in \mathbb{R}^R$ and we use the subscript r on $f_t(\boldsymbol{x})_r$ to denote the vector indexing operation. Our selection function is then given by computing Equation 3 for each r and summing up the instabilities over the prediction horizon: $g(\boldsymbol{x}) = \sum_r \sum_t v_t a_{t,r}(\boldsymbol{x})$. The full algorithm therefore shares many conceptual similarities with Algorithm 2 and we provide the detailed algorithm as part of Algorithm 3 in the Appendix. Note that the presented generalization for time series is applicable to any setting in which the variability of predictions can be computed. As such, this formalism can extend to application scenarios beyond time series prediction such as object detection / segmentation.

We conclude our methods section by remarking that our scores can be motivated from multiple different perspectives. In particular, we provide a formal treatment on the connection between selective prediction and forging (Thudi et al., 2022) in Appendix B leading to the same selection function $g(\cdot)$ as above.

4 Empirical Evaluation

We present a comprehensive empirical study demonstrating the effectiveness of SPTD across domains.

4.1 Classification

Datasets & Training. We evaluate our proposed approach on image dataset benchmarks that are common in the selective classification literature: CIFAR-10/CIFAR-100 (Krizhevsky et al., 2009), StanfordCars (Krause et al., 2013), and Food101 (Bossard et al., 2014). For each dataset, we train a deep neural network following the ResNet-18 architecture (He et al., 2016) and checkpoint each model after processing 50 mini-batches of size 128. All models are trained over 200 epochs (400 epochs for StanfordCars) using the SGD optimizer with an initial learning rate of 10^{-2}, momentum 0.9, and weight decay 10^{-4}. Across all datasets, we decay the learning rate by a factor of 0.5 in 25-epoch intervals.

Baselines. We compare our method (SPTD) to common SC techniques previously introduced in Section 2: Softmax Response (SR) and Self-Adaptive Training (SAT). Based on recent insights from Feng et al. (2023), we (i) train SAT with additional entropy regularization; and (ii) derive SAT's score by applying Softmax Response (SR) to the underlying classifier (instead of logit-thresholding the abstention class). We refer to this method as SAT+ER+SR. We do not include results for SelectiveNet, Deep Gamblers, or Monte-Carlo Dropout as previous works (Huang et al., 2020; Feng et al., 2023) have shown that SAT+ER+SR strictly dominates these methods. In contrast to recent SC works, we do however include results with Deep Ensembles (DE) (Lakshminarayanan et al., 2017), a relevant baseline from the uncertainty quantification literature. Our hyper-parameter tuning procedure is documented in Appendix D.1.

Our empirical results show that computing and thresholding the proposed weighted instability score from SPTD provides a strong score for selective classification. In the following, we first study the accuracy/coverage trade-off with comparison to past work. Then, we present exemplary training-dynamics-derived label evolution curves for individual examples from all datasets. Next, we examine our method's sensitivity to the checkpoint selection strategy and the weighting parameter k. Finally, we analyze distributional training dynamics patterns of both correct and incorrect data points.

Accuracy/Coverage Trade-off. Consistent with standard evaluation schemes for selective classification, our main experimental results examine the accuracy/coverage trade-off of SPTD. We present our performance results with comparison to past work in Table 1 where we demonstrate SPTD's effectiveness on CIFAR-10, CIFAR-100, StanfordCars, and Food101. We document the results obtained by

[1] We also explore a more robust normalization by considering the average prediction computed over the last l checkpoints: $a_t = ||f_t(\boldsymbol{x}) - \frac{1}{n}\sum_{c\in\{T-l,T-l+1,...,T\}} f_c(\boldsymbol{x})||$. Across many l, we found the obtained results to be statistically indistinguishable from the results obtained by normalizing w.r.t. the last checkpoint f_T only.

Table 1: **Selective accuracy achieved across coverage levels**. We find that SPTD-based methods outperforms current SOTA error rates across multiple datasets with full-coverage accuracy alignment. Numbers are reported with mean values and standard deviation computed over 5 random runs. **Bold** numbers are best results at a given coverage level across all methods and underlined numbers are best results for methods relying on a single training run only. Datasets are consistent with Feng et al. (2023).

	Cov.	SR	SAT+ER+SR	DE	SPTD	DE+SPTD
CIFAR-10	100	**92.9 (±0.0)**	**92.9 (±0.0)**	**92.9 (±0.0)**	**92.9 (±0.0)**	**92.9 (±0.1)**
	90	96.4 (±0.1)	96.3 (±0.1)	**96.8 (±0.1)**	96.5 (±0.0)	**96.7 (±0.1)**
	80	98.1 (±0.1)	98.1 (±0.1)	**98.7 (±0.0)**	98.4 (±0.1)	**98.8 (±0.1)**
	70	98.6 (±0.2)	99.0 (±0.1)	**99.4 (±0.1)**	99.2 (±0.0)	**99.5 (±0.0)**
	60	98.7 (±0.1)	99.4 (±0.0)	99.6 (±0.1)	**99.6 (±0.2)**	**99.8 (±0.0)**
	50	98.6 (±0.2)	99.7 (±0.1)	99.7 (±0.1)	99.8 (±0.0)	**99.9 (±0.0)**
	40	98.7 (±0.0)	99.7 (±0.0)	99.8 (±0.0)	99.8 (±0.1)	**100.0 (±0.0)**
	30	98.5 (±0.0)	99.8 (±0.0)	99.8 (±0.0)	99.8 (±0.1)	**100.0 (±0.0)**
	20	98.5 (±0.1)	99.8 (±0.1)	99.8 (±0.0)	**100.0 (±0.0)**	**100.0 (±0.0)**
	10	98.7 (±0.0)	99.8 (±0.1)	99.8 (±0.1)	**100.0 (±0.0)**	**100.0 (±0.0)**
CIFAR-100	100	**75.1 (±0.0)**	**75.1 (±0.0)**	**75.1 (±0.0)**	**75.1 (±0.0)**	**75.1 (±0.0)**
	90	78.2 (± 0.1)	78.9 (± 0.1)	80.2 (± 0.0)	80.4 (± 0.1)	**81.1 (± 0.1)**
	80	82.1 (± 0.0)	82.9 (± 0.0)	84.7 (± 0.1)	84.6 (± 0.1)	**85.0 (± 0.2)**
	70	86.4 (± 0.1)	87.2 (± 0.1)	88.6 (± 0.1)	**88.7 (± 0.0)**	**88.8 (± 0.1)**
	60	90.0 (± 0.0)	90.3 (± 0.2)	90.2 (± 0.2)	90.1 (± 0.0)	**90.4 (± 0.1)**
	50	92.9 (± 0.1)	93.3 (± 0.0)	94.8 (± 0.0)	94.6 (± 0.0)	**94.9 (± 0.0)**
	40	95.1 (± 0.0)	95.2 (± 0.1)	**96.8 (± 0.1)**	**96.9 (± 0.1)**	**96.9 (± 0.0)**
	30	97.2 (± 0.2)	97.5 (± 0.0)	**98.4 (± 0.1)**	**98.4 (± 0.1)**	**98.5 (± 0.0)**
	20	97.8 (± 0.1)	98.3 (± 0.1)	**99.0 (± 0.0)**	98.8 (± 0.2)	**99.2 (± 0.1)**
	10	98.1 (± 0.0)	98.8 (± 0.1)	99.2 (± 0.1)	**99.4 (± 0.1)**	**99.6 (± 0.1)**

	Cov.	SR	SAT+ER+SR	DE	SPTD	DE+SPTD
Food101	100	**81.1 (±0.0)**	**81.1 (±0.0)**	**81.1 (±0.0)**	**81.1 (±0.0)**	**81.1 (±0.0)**
	90	85.3 (±0.1)	85.5 (±0.2)	86.2 (±0.1)	85.7 (±0.0)	**86.7 (±0.0)**
	80	87.1 (±0.0)	89.5 (±0.0)	90.3 (±0.0)	89.9 (±0.0)	**91.3 (±0.1)**
	70	92.1 (±0.1)	92.8 (±0.1)	**94.5 (±0.1)**	93.7 (±0.0)	**94.6 (±0.0)**
	60	95.2 (±0.1)	95.5 (±0.1)	**97.0 (±0.0)**	**97.0 (±0.0)**	**97.0 (±0.0)**
	50	97.3 (±0.1)	97.5 (±0.0)	98.2 (±0.0)	**98.3 (±0.2)**	**98.5 (±0.0)**
	40	98.7 (±0.0)	98.7 (±0.2)	**99.1 (±0.0)**	99.1 (±0.1)	**99.2 (±0.1)**
	30	99.5 (±0.0)	99.7 (±0.2)	99.2 (±0.0)	99.6 (±0.0)	**99.7 (±0.0)**
	20	99.7 (±0.1)	99.7 (±0.2)	**99.9 (±0.1)**	**99.8 (±0.0)**	**99.9 (±0.1)**
	10	99.8 (±0.0)	99.8 (±0.1)	**99.9 (±0.1)**	**99.9 (±0.1)**	**99.9 (±0.1)**
StanfordCars	100	**77.6 (±0.0)**	**77.6 (±0.0)**	**77.6 (±0.0)**	**77.6 (±0.0)**	**77.6 (±0.0)**
	90	83.0 (±0.1)	83.0 (±0.2)	**83.7 (±0.1)**	83.3 (±0.1)	**83.7 (±0.2)**
	80	87.6 (±0.0)	88.0 (±0.1)	88.7 (±0.1)	**89.3 (±0.0)**	**89.7 (±0.0)**
	70	90.8 (±0.0)	92.2 (±0.1)	92.4 (±0.1)	**93.6 (±0.0)**	93.4 (±0.1)
	60	93.5 (±0.1)	95.2 (±0.1)	95.3 (±0.0)	**96.2 (±0.0)**	**96.3 (±0.0)**
	50	95.3 (±0.0)	96.9 (±0.2)	96.4 (±0.1)	**97.0 (±0.1)**	**97.1 (±0.3)**
	40	96.8 (±0.0)	97.8 (±0.0)	**97.8 (±0.2)**	**97.8 (±0.1)**	**97.8 (±0.0)**
	30	97.5 (±0.1)	98.2 (±0.2)	**98.6 (±0.0)**	98.2 (±0.2)	**98.9 (±0.0)**
	20	98.1 (±0.0)	98.4 (±0.1)	**98.9 (±0.2)**	98.6 (±0.0)	**99.0 (±0.0)**
	10	98.2 (±0.1)	98.7 (±0.1)	**99.5 (±0.1)**	98.5 (±0.1)	**99.5 (±0.0)**

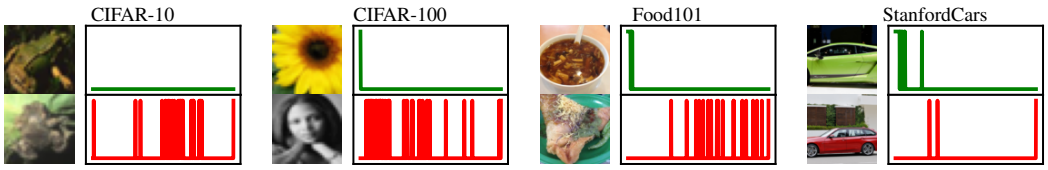

Figure 3: **Most characteristic examples across datasets**. For each dataset, we show the samples with the most stable and most unstable (dis-) agreement with the final label along with their corresponding a_t indicator function. Correct points are predominantly characterized by disagreements early in training while incorrect points change their class label throughout (but importantly close to the end of) training. We provide additional examples from all datasets in Figure 21 in the Appendix.

SPTD, SAT, SR, and DE across the full coverage spectrum. We see that SPTD outperforms both SAT and SR and performs similarly as DE. To further boost performance across the accuracy/coverage spectrum, we combine SPTD and DE by applying SPTD on each ensemble member from DE and then average their scores. More concretely, we estimate $\texttt{DE+SPTD} = \frac{1}{m}\sum_{m=1}^{M} \texttt{SPTD}_m$ where $\texttt{SPTD}_m$ computes g on each ensemble member $m \in [M]$. This combination leads to new state-of-the-art selective classification performance and showcases that SPTD can be flexibly applied on top of established training pipelines.

Individual Evolution Plots. To analyze the effectiveness of our disagreement metric proposed in Section 3, we examine the evolution curves of our indicator variable a_t for individual datapoints in Figure 3. In particular, for each dataset, we present the most stable and the most unstable data points from the test sets and plot the associated label disagreement metric a_t over all checkpoints. We observe that easy-to-classify examples only show a small degree of oscillation while harder examples show a higher frequency of oscillations, especially towards the end of training. This result matches our intuition: our model should produce correct decisions on data points whose prediction is mostly constant throughout training and should reject data points for which intermediate models predict inconsistently. Moreover, as depicted in Figure 4, we also show that our score g yields distinct distributional patterns for both correctly and incorrectly classified points. This separation enables strong coverage/accuracy trade-offs via our thresholding procedure.

Checkpoint Weighting Sensitivity. One important hyper-parameter of our method is the weighting of intermediate predictions. Recall from Section 3 that SPTD approximates the expected stability for correctly classified points via a weighting function $v_t = (\frac{t}{T})^k$. In Figure 12 in the Appendix, we observe

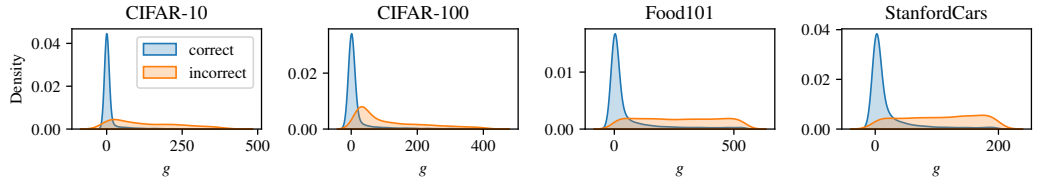

Figure 4: **Distribution of g for different datasets**. We see that correct predictions concentrate at 0 (indicating training dynamics stability) while incorrect predictions spread over a wide score range.

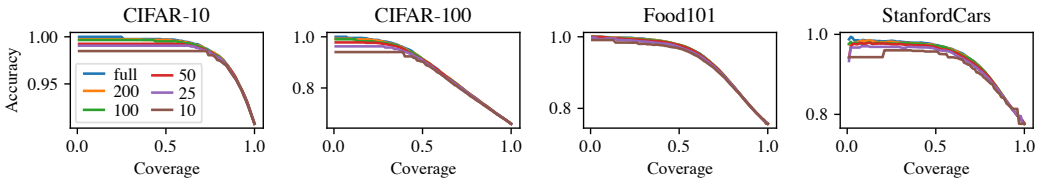

Figure 5: **Coverage/error trade-off of `SPTD` for varying total number of checkpoints**. `SPTD` delivers consistent performance independent of the checkpointing resolution at high coverage. At low coverage, a more detailed characterization of training dynamics boosts performance.

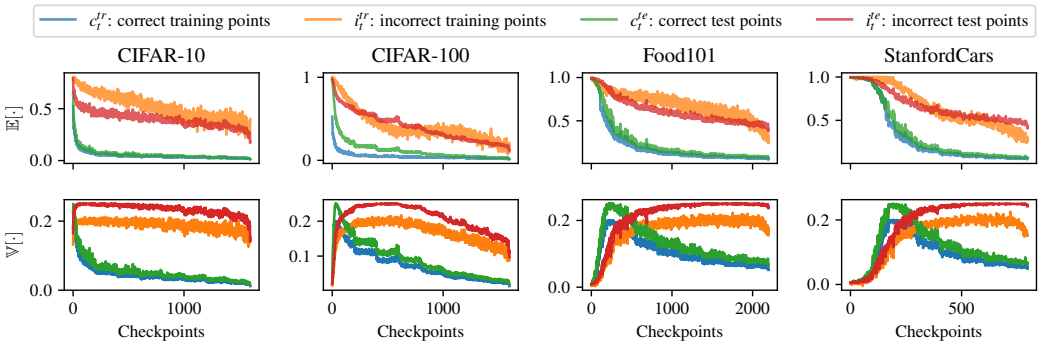

Figure 6: **Monitoring expectations $\mathbb{E}[\cdot]$ and variances $\mathbb{V}[\cdot]$ for correct/incorrect training and test points**. We observe that correctly classified points (cold colors) have both their expectations and variances quickly decreasing to 0 as training progresses. Incorrectly classified points (warm colors) both exhibit large expectations and variances and stay elevated over large periods while training.

that `SPTD` is robust to the choice of k and that $k \in [1,3]$ performs best. At the same time, we find that increasing k too much leads to a decrease in accuracy at medium coverage levels. This result emphasizes that (i) large parts of the training process contain valuable signals for selective classification; and that (ii) early label disagreements arising at the start of optimization should be de-emphasized by our method.

Checkpoint Selection Strategy. The second important hyper-parameter of our method is the checkpoint selection strategy. In particular, to reduce computational cost, we study the sensitivity of `SPTD` with respect to the checkpointing resolution in Figure 5. Our experiments demonstrate favorable coverage/error trade-offs between 25 and 50 checkpoints when considering the full coverage spectrum. However, when considering the high coverage regime in particular (which is what most selective prediction works focus on), even sub-sampling 10 intermediate models is sufficient for SOTA selective classification. Hence, with only observing the training stage, our method's computational overhead reduces to only 10 forward passes at test time when the goal is to reject at most $30\% - 50\%$ of incoming data points. In contrast, `DE` requires to first train M models (with $M = 10$ being a typical and also our particular choice for `DE`) and perform inference on these M models at test time. Further increasing the checkpointing resolution does offer increasingly diminishing returns but also leads to improved accuracy-coverage trade-offs, especially at low coverage.

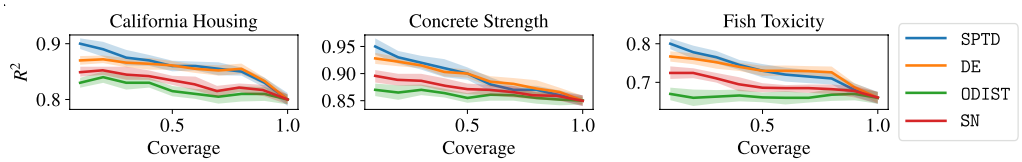

Figure 7: **R^2/coverage trade-off across various regression datasets**. SPTD offers comparable performance to DE but provides improved results at low coverage.

Examining the Convergence Behavior of Training and Test Points. The effectiveness of SPTD relies on our hypothesis that correctly classified points and incorrectly classified points exhibit distinct training dynamics. We verify this hypothesis in Figure 6 where we examine the convergence behavior of the disagreement distributions of correct (c_t^{tr}) / incorrect (i_t^{tr}) training and correct (c_t^{te}) / incorrect (i_t^{te}) test points. We observe that the expected disagreement for both correctly classified training c_t^{tr} and test points c_t^{te} points converge to 0 over the course of training. The speed of convergence is subject to the difficulty of the optimization problem with more challenging datasets exhibiting slower convergence in predicted label disagreement. We also see that the variances follow an analogous decreasing trend. This indicates that correctly classified points converge to the final label quickly and fast convergence is strongly indicative of correctness. In contrast, incorrectly classified points i_t^{tr} and i_t^{te} show significantly larger mean and variance levels. This clear separation in distributional evolution patterns across correct and incorrect points leads to strong selective prediction performance in our SPTD framework.

4.2 Regression Experiments

Datasets Our experimental suite for regression considers the following datasets: California housing dataset (Pace and Barry, 1997) ($N = 20640$, $D = 8$), the concrete compressive strength dataset (Yeh, 2007) ($N = 1030$, $D = 9$), and the fish toxicity dataset (Ballabio et al., 2019) ($N = 546$, $D = 9$).

Model Setup & Baselines We split all datasets into 80% training and 20% test sets after a random shuffle. Then, we train a fully connected neural network with layer dimensionalities $D \to 10 \to 7 \to 4 \to 1$. Optimization is performed using full-batch gradient descent using the Adam optimizer with learning rate 10^{-2} over 200 epochs and weight decay 10^{-2}. We consider the following baseline methods for rejecting input samples: (i) approximating the predictive variance using deep ensembles (DE) (Lakshminarayanan et al., 2017; Zaoui et al., 2020); (ii) SelectiveNet (SN) which explicitly optimizes utility given a desired coverage constraint; and (iii) training the model with a Gaussian parametric output distribution (ODIST) via maximum likelihood maximization (Alexandrov et al., 2019).

Main results We document our results in Figure 7. We see that the ODIST only delivers subpar results (likely due to mis-calibration) and does not provide a meaningful signal for selective prediction. On the other hand, DE and SPTD perform comparably with SPTD outperforming DE at low coverage. We stress again that SPTD's training cost is significantly cheaper than DE's while matching the inference-time cost when sub-sampling a reduced set of checkpoints. We observe the same key insights for our time series forecasting panel and discuss these results in Appendix D.2.9.

5 Conclusion

In this work we have proposed SPTD, a selective prediction technique that relies on measuring prediction instability of test points over intermediate model states obtained during training. Our method offers several advantages over previous works. In particular (i) it can be applied to all existing models whose checkpoints were recorded (hence the potential for immediate impact); (ii) it is composable with existing selective prediction techniques; (iii) it can be readily applied to both discrete and real-valued prediction problems; and (iv) it is computationally more efficient than competing ensembling-based approaches. We verified the performance of SPTD using an extensive empirical evaluation, leading to new state-of-the-art performance in the field. We believe future work can further improve our approach by providing a theoretically rigorous understanding of convergence patterns for correct and incorrect points. Moreover, we expect training dynamics information to be useful for identifying and mitigating other open problems in trustworthy machine learning (e.g., unfairness, privacy, mechanistic interpretability).

ETHICS STATEMENT

Modern neural networks often produce overconfident decisions (Guo et al., 2017). This limitation, amongst other shortcomings, prevents neural nets from being readily applied in high-stakes decision-making. Selective prediction is one paradigm enabling the rejection of data points. In particular, samples that with high error predictions should be rejected. Since our work improves over current state-of-the-art methods, our work can be used to enhance the trustworthiness of deep neural networks in practice. While modern selective precition techniques mitigates overconfidence, recent work has also shown that selective classification algorithms disproportionately reject samples from minority groups (Jones et al., 2020). This finding suggests that improvements to the overall coverage comes at a fairness cost. As a result, the connection between fairness and sample rejection still warrants further investigation.

REPRODUCIBILITY STATEMENT

In accordance with contemporary works on selective prediction, our experimental setup uses widely used and publicly accessible datasets from the vision and regression domain. Baseline results were obtained using open-source implementations of the respective papers as published by the authors. Hyper-parameter tuning is performed as described in original works and documented in Appendix D.1. Moreover, our method implementation will be open sourced as part of the reviewing process.

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A Extended Discussion on Example Difficulty

A related line of work is identifying *difficult* examples, or how well a model can generalize to a given unseen example. Jiang et al. (2020) introduce a per-instance empirical consistency score which estimates the probability of predicting the ground truth label with models trained on data subsamples of different sizes. Unlike our approach, however, this requires training a large number of models. Toneva et al. (2018) quantifies example difficulty through the lens of a forgetting event, in which the example is misclassified after being correctly classified. However, the metrics that we introduce in § 3, are based on the disagreement of the label at each checkpoint with the final predicted label. Other approaches estimate the example difficulty by: prediction depth of the first layer at which a k-NN classifier correctly classifies an example (Baldock et al., 2021), the impact of pruning on model predictions of the example (Hooker et al., 2019), and estimating the leave-one-out influence of each training example on the accuracy of an algorithm by using influence functions (Feldman and Zhang, 2020). Closest to our method, the work of Agarwal et al. (2020) utilizes gradients of intermediate models during training to rank examples by difficulty. In particular, they average pixel-wise variance of gradients for each given input image. Notably, this approach is more costly and less practical than our approach and also does not study the accuracy/coverage trade-off which is of paramount importance to selective prediction.

B Connection to Forging

Running SGD on different datasets could lead to the same final model (Hardt et al., 2016; Bassily et al., 2020; Thudi et al., 2022). For example, this is intuitive when two datasets were sampled from the same distribution. We would then expect that training on either dataset should not affect significantly the model returned by SGD. For our selective prediction problem, this suggests an approach to decide which points the model is likely to predict correctly on: identify the datasets that it could have been trained on (in lieu of the training set it was actually trained on). Thudi et al. (2022) solves this problem by brute-forcing through different mini-batches to determine if a mini-batch can be used to reproduce one of the original training steps. Even then, this is only a sufficient condition to show a datapoint could have plausibly been used to train: if the brute-force fails, it does not mean the datapoint could not have been used to obtain the final model. As an alternative, we propose to instead characterize the optimization behaviour of training on a dataset, i.e, conditions most datapoints that were (plausibly) trained on would satisfy based on training dynamics. Our modified hypothesis is then that the set of datapoints we optimized for coincides significantly with the set of points the model predicts correctly on.

B.1 A Framework for Being Optimized

In this section we derive an upper-bound on the probability that a datapoint could have been used to obtain the model's checkpointing sequence. This yields a probabilistically necessary (though not sufficient) characterization of the points we explicitly optimized for. This bound, and the variables it depends on, informs what we will later use to characterize "optimizing" a datapoint, and, hence, our selective classification methods.

Let us denote the set of all datapoints as $\mathcal{D}$, and let $D \subset \mathcal{D}$ be the training set. We are interested in the setting where a model f is plausibly sequentially trained on D (e.g., with stochastic gradient descent). We thus also have access to a sequence of T intermediate states for f, which we denote $[f_1,...,f_T]$. In this sequence, note that f_T is exactly the final model f.

Now, let p_t represent the random variable for outputs on D given by an intermediate model f_t where the outputs have been binarized: we have 0 if the output agrees with the final prediction and 1 if not. In other words, p_t is the distribution of labels given by first drawing $\boldsymbol{x} \sim D$ and then outputting $1-\delta_{f_t(\boldsymbol{x}),f_T(\boldsymbol{x})}$ where δ denotes the Dirac delta function. Note that we always have both a well-defined mean and variance for p_t as it is bounded. Furthermore, we always have the variances and expectations of $\{p_t\}$ converge to 0 with increasing t: as $p_T = 0$ always and the sequence is finite convergence trivially occurs. To state this formally, let $v_t = \mathbb{V}_{\boldsymbol{x}\sim D}[p_t]$ and let $e_t = \mathbb{E}_{\boldsymbol{x}\sim D}[p_t]$ denote the variances and expectations over points in D. In particular, we remark that $e_T = 0$, $v_T = 0$, so both e_t and v_t converge. More formally, for all $\epsilon > 0$ there exists an $N \in \{1,...,T\}$ such that $v_t < \epsilon$ for all $t > N$. Similarly, for all $\epsilon > 0$ there exists a (possibly different) $N \in \{1,...,T\}$ such that $e_t < \epsilon$ for all $t > N$.

However, the core problem is that we do not know how this convergence in the variance and expectation occurs. More specifically, if we knew the exact values of e_t and v_t, we could use the following bound on the probability of a particular data point being in D. We consequently introduce the notation $[a_1,...,a_T]$ where $a_t = 1 - \delta_{f_t(\boldsymbol{x}),f_T(\boldsymbol{x})}$ which we call the "label disagreement (at t)". Note that the a_t are defined with respect to a given input, while p_t represent the distribution of a_t over all inputs in D.

Lemma 1. *Given a datapoint $\boldsymbol{x}$, let $\{a_1,...,a_T\}$ where $a_t = 1 - \delta_{f_t(\boldsymbol{x}),f_T(\boldsymbol{x})}$. Assuming not all $a_t = e_t$ then the probability $\boldsymbol{x} \in D$ is $\leq \min_{v_t \ s.t \ a_t \neq e_t} \frac{v_t}{|a_t - e_t|^2}$.*

Proof. By Chebyshev's inequality we have the probability of a particular sequence $\{a_1, \dots, a_T\}$ occurring is $\leq \frac{v_t}{|a_t - e_t|^2}$ for every t (a bound on any of the individual a_t occurring as that event is in the event $|p_t - e_t| \geq |a_t - e_t|$ occurs). By taking the minimum over all these upper-bounds we obtain our upper-bound. □

We do not guarantee Lemma 1 is tight. Though we do take a minimum to make it tighter, this is a minimum over inequalities all derived from Chebyshev's inequality[2]. Despite this potential looseness, using the bound from Lemma 1, we can design a naïve selective classification protocol based on the "optimized = correct (often)" hypothesis and use the above bound on being a plausible training datapoint as our characterization of optimization; for a test input $\boldsymbol{x}$, if the upper-bound on the probability of being a datapoint in D is lower than some threshold τ reject, else accept. However, the following question prevents us from readily using this method: *How do $\mathbb{E}[p_t]$ and $\mathbb{V}[p_t]$ evolve during training?*

To answer this question, we propose to examine how the predictions on plausibly training points evolve during training. Informally, the evolution of $\mathbb{E}[p_t]$ represents knowing how often we predict the final label at step t, while the evolution of $\mathbb{V}[p_t]$ represents knowing how we become more consistent as we continue training. Do note that the performance of this optimization-based approach to selective classification will depend on how unoptimized incorrect test points are. In particular, our hypothesis is that incorrect points often appear sufficiently un-optimized, yielding distinguishable patterns for $\mathbb{E}[p_t]$ and $\mathbb{V}[p_t]$ when compared to optimized points. We verify this behavior in Section 4 where we discuss the distinctive label evolution patterns of explicitly optimized, correct, and incorrect datapoints.

B.1.1 Last Disagreement Model Score For Discrete Prediction (s_{MAX})

Here, we propose a selective classification approach based on characterizing optimizing for a datapoint based off of Lemma 1. Recall the bound given in Lemma 1 depends on expected values and variances for the p_t (denoted e_t and v_t respectively). In Section 4 we observe that e_t quickly converge to 0, and so by assuming $e_t = 0$ always[3] the frequentist bound on how likely a datapoint is a training point becomes $\min_{t \ s.t \ a_t=1} \frac{v_t}{|a_t - e_t|^2} = \min_{t \ s.t \ a_t=1} v_t$. Using this result for selective classification, we would impose acceptance if $\min_{t \ s.t \ a_t=1} v_t \geq \tau$. Moreover, in Section 4, we further observe that v_t monotonically decreases in a convex manner (after an initial burn-in phase). Hence, imposing $\min_{t \ s.t \ a_t=1} v_t \geq \tau$ simply imposes a last checkpoint that can have a disagreement with the final prediction.

Based on these insights, we propose the following selective classification score: $s_{\max} = \max_{t \ s.t \ a_t=1} \frac{1}{v_t}$. Note that this score directly follows from the previous discussion but flips the thresholding direction from $\min_{t \ s.t \ a_t=1} v_t \geq \tau$ to $\max_{t \ s.t \ a_t=1} \frac{1}{v_t} \leq \tau$ for consistency with the anomaly scoring literature (Ruff et al., 2018). Finally, we choose to approximate the empirical trend of v_t as observed in Section 4 with $v_t = 1 - t^k$ for $k \in [1, \infty)$. Based on the choice of k, this approximation allows us to (i) avoid explicit estimation of v_t from validation data; and (ii) enables us to flexibly specify how strongly we penalize model disagreements late in training.

To summarize, our first algorithm for selective classification is hence given by:

1. Denote $L = f_T(\boldsymbol{x})$, i.e. the label our final model predicts.
2. If $\exists t \ s.t \ a_t = 1$ then compute $s_{\max} = \max_{t \ s.t \ a_t=1} \frac{1}{v_t}$ as per the notation in § B.1 (i.e $a_t = 1$ iff $f_t(x) \neq L$), else accept $\boldsymbol{x}$ with prediction L.
3. If $s_{\max} \leq \tau$ accept $\boldsymbol{x}$ with prediction L, else reject ($\perp$).

[2] One could potentially use information about the distribution of points not in D to refine this bound.

[3] We considered removing this assumption and observe comparable performance.

Algorithm 3: SPTD for time series forecasting

Require: Intermediate models $[f_1,...,f_T]$, query point $\boldsymbol{x}$, weighting $k \in [0,\infty)$, prediction horizon R.

for $t \in [T]$ **do**
  for $r \in [R]$ **do**
    $a_{t,r} \leftarrow ||f_t(\boldsymbol{x})_r - f_T(\boldsymbol{x})_r||$
  end for
  $v_t \leftarrow (\frac{t}{T})^k$
end for
$g \leftarrow \sum_r \sum_t v_t a_{t,r}$
if $g \leq \tau$ **then** $f(\boldsymbol{x}) = L$ **else** $f(\boldsymbol{x}) = \perp$

Note once again, as all our candidate $\frac{1}{v_t}$ increase, the algorithm imposes a last intermediate model which can output a prediction that disagrees with the final prediction: hereafter, the algorithm must output models that consistently agree with the final prediction.

B.1.2 Overall Disagreement Model Score (s_{SUM})

Note that the previous characterization of optimization, defined by the score s_{MAX}, could be sensitive to stochasticity in training and hence perform sub-optimally. That is, the exact time of the last disagreement, which s_{MAX} relies on, is subject to high noise across randomized training runs. In light of this potential limitation we propose the following "summation" algorithm which computes a weighted sum over training-time disagreements to get a more consistent statistic. Do note that typically to get a lower-variance statistic one would take an average, but multiplying by scalars can be replaced by correspondingly scaling the threshold we use. Hence, our proposed algorithm is:

1. Denote $L = f_T(\boldsymbol{x})$, i.e. the label our final model predicts.
2. If $\exists t \; s.t \; a_t = 1$, compute $s_{\text{sum}} = \sum_{t=1}^{T} \frac{a_t}{v_t}$, else accept $\boldsymbol{x}$ with prediction L.
3. If $s_{\text{sum}} \leq \tau$ accept $\boldsymbol{x}$ with prediction L, else reject ($\perp$).

Recalling our previous candidates for v_t, we have the s_{SUM} places higher weight on late disagreements. This gives us a biased average of the disagreements which intuitively approximates the expected last disagreement but now is less susceptible to noise. More generally, this statistic allows us to perform selective classification by utilizing information from all the disagreements during training. In Section D.2.10, we experimentally show that s_{SUM} leads to more robust selective classification results compared to s_{MAX}. We remark that the sum score s_{SUM} corresponds exactly to our score g proposed as part of SPTD, showcasing the strong connection of our method to forging.

C Alternate Metric Choices

We briefly discuss additional potential metric choices that we investigated but which lead to selective classification performance worse than our main method.

C.1 Jump Score s_{JMP}

We also consider a score which captures the level of disagreement between the predicted label of two successive intermediate models (i.e., how much jumping occurred over the course of training). For $j_t = 0$ iff $f_t(\boldsymbol{x}) = f_{t-1}(\boldsymbol{x})$ and $j_t = 1$ otherwise we can compute the jump score as $s_{\text{jmp}} = 1 - \sum v_t j_t$ and threshold it as in § B.1.1 and § B.1.2.

C.2 Variance Score s_{VAR} for Continuous Metrics

Finally, we consider monitoring the evolution of continuous metrics that have been shown to be correlated with example difficulty. These metrics include (but are not limited to):

- Confidence (conf): $\max_{c \in \mathcal{Y}} f_t(\boldsymbol{x})$

- Confidence gap between top 2 most confident classes (gap): $\max_{c\in\mathcal{Y}} f_t(\boldsymbol{x}) - \max_{c\neq\hat{y}} f_t(\boldsymbol{x})$
- Entropy (ent): $-\sum_{c=1}^{C} f_t(\boldsymbol{x})_c \log(f_t(\boldsymbol{x})_c)$

Jiang et al. (2020) show that example difficulty is correlated with confidence and entropy. Moreover, they find that difficult examples are learned later in the training process. This observation motivates designing a score based on these continuous metrics that penalises changes later in the training process more heavily. We consider the maximum softmax class probability known as confidence, the negative entropy and the gap between the most confident classes for each example instead of the model predictions. Assume that any of these metrics is given by a sequence $z=\{z_1,...,z_T\}$ obtained from T intermediate models. Then we can capture the uniformity of z via a (weighted) variance score $s_{\text{var}}=\sum_t w_t(z_t-\mu)^2$ for mean $\mu=\frac{1}{T}\sum_t z_t$ and an increasing weighting sequence $w=\{w_1,...,w_T\}$.

In order to show the effectiveness of the variance score s_{var} for continuous metrics, we provide a simple bound on the variance of confidence $\max_{y\in\mathcal{Y}} f_t(\boldsymbol{x})$ in the final checkpoints of the training. Assuming that the model has converged to a local minima with a low learning rate, we can assume that the distribution of model weights can be approximated by a Gaussian distribution.

We consider a linear regression problem where the inputs are linearly separable.

Lemma 2. *Assume that we have some Gaussian prior on the model parameters in the logistic regression setting across m final checkpoints. More specifically, given T total checkpoints of model parameters $\{\boldsymbol{w}_1,\boldsymbol{w_2},...,\boldsymbol{w}_T\}$ we have $p(W=\boldsymbol{w}_t)=\mathcal{N}(\boldsymbol{w}_0 \mid \boldsymbol{\mu}, s\boldsymbol{I})$ for $t\in\{T-m+1,...,T\}$ and we assume that final checkpoints of the model are sampled from this distribution. We show that the variance of model confidence $\max_{y\in\{-1,1\}} p(y \mid \boldsymbol{x}_i,\boldsymbol{w}_t)$ for a datapoint $(\boldsymbol{x}_i,y_i)$ can be upper bounded by a factor of probability of correctly classifying this example by the optimal weights.*

Proof. We first compute the variance of model predictions $p(y_i \mid \boldsymbol{x}_i,W)$ for a given datapoint $(\boldsymbol{x}_i,y_i)$. Following previous work (Schein and Ungar, 2007; Chang et al., 2017), the variance of predictions over these checkpoints can be estimated as follows:

Taking two terms in Taylor expansion for model predictions we have $p(y_i \mid \boldsymbol{x}_i, W) \simeq p(y_i \mid \boldsymbol{x}_i,\boldsymbol{w}) + g_i(\boldsymbol{w})^\top (W-\boldsymbol{w})$ where W and $\boldsymbol{w}$ are current and the expected estimate of the parameters and $g_i(\boldsymbol{w})=p(y_i \mid \boldsymbol{x}_i,\boldsymbol{w})(1-p(y_i \mid \boldsymbol{x}_i,\boldsymbol{w}))\boldsymbol{x}_i$ is the gradient vector. Now we can write the variance with respect to the model prior as:

$$\mathbb{V}(p(y_i \mid \boldsymbol{x}_i,W)) \simeq \mathbb{V}\big(g_i(\boldsymbol{w})^\top (W-\boldsymbol{w})\big) = g_i(\boldsymbol{w})^\top F^{-1} g_i(\boldsymbol{w})$$

where F is the variance of posterior distribution $p(W \mid X,Y)\sim\mathcal{N}(W \mid \boldsymbol{w},F^{-1})$. This suggests that the variance of probability of correctly classifying $\boldsymbol{x}_i$ is proportional to $p(y_i \mid \boldsymbol{x}_i,\boldsymbol{w})^2(1-p(y_i \mid \boldsymbol{x}_i,\boldsymbol{w}))^2$. Now we can bound the variance of maximum class probability or confidence as below:

$$\begin{aligned}\mathbb{V}\left(\max_{y\in\{-1,1\}} p(y \mid \boldsymbol{x}_i,W)\right) &\leq \mathbb{V}(p(y_i \mid \boldsymbol{x}_i,W)) + \mathbb{V}(p(-y_i \mid \boldsymbol{x}_i,W)) \\ &\approx 2p(y_i \mid \boldsymbol{x}_i,\boldsymbol{w})^2(1-p(y_i \mid \boldsymbol{x}_i,\boldsymbol{w}))^2 \boldsymbol{x}_i^\top F^{-1}\boldsymbol{x}_i\end{aligned}$$

□

We showed that if the probability of correctly classifying an example given the final estimate of model parameters is close to one, the variance of model predictions following a Gaussian prior gets close to zero, we expect a similar behaviour for the variance of confidence under samples of this distribution.

D Extension of Empirical Evaluation

D.1 Full Hyper-Parameters

We document full hyper-parameter settings for our method (`SPTD`) as well as all baseline approaches in Table 2.

Table 2: **Hyper-parameters used for all algorithms for classification.**

Dataset	SC Algorithm	Hyper-Parameters
CIFAR-10	Softmax Response (SR)	N/A
	Self-Adaptive Training (SAT)	$E = 100$
	Deep Ensembles (DE)	$M = 10$
	Selective Prediction Training Dynamics (SPTD)	$T = 1600$, $k = 2$
CIFAR-100	Softmax Response (SR)	N/A
	Self-Adaptive Training (SAT)	$E = 100$
	Deep Ensembles (DE)	$M = 10$
	Selective Prediction Training Dynamics (SPTD)	$T = 1600$, $k = 2$
Food101	Softmax Response (SR)	N/A
	Self-Adaptive Training (SAT)	$E = 100$
	Deep Ensembles (DE)	$M = 10$
	Selective Prediction Training Dynamics (SPTD)	$T = 2200$, $k = 3$
StanfordCars	Softmax Response (SR)	N/A
	Self-Adaptive Training (SAT)	$E = 100$
	Deep Ensembles (DE)	$M = 10$
	Selective Prediction Training Dynamics (SPTD)	$T = 800$, $k = 5$

Table 3: **Cost vs Performance Tradeoff.** We report both the time and space complexities for all SC methods at training and test time along with their selective classification performance as per our results in Table 1 and Figure 5. We denote with M the number of distinct DE models and with T the number of SPTD checkpoints. Although SR and SAT are the cheapest methods to run, they also perform the poorest at selective classification. SPTD is significantly cheaper to train than DE and achieves competitive performance at $T \approx M$. Although DE+SPTD is the most expensive model, it also provides the strongest performance.

Method	Train Time	Train Space	Inference Time	Inference Space	Performance Rank
SR	$O(1)$	$O(1)$	$O(1)$	$O(1)$	5
SAT	$O(1)$	$O(1)$	$O(1)$	$O(1)$	4
DE	$O(M)$	$O(M)$	$O(M)$	$O(M)$	=2
SPTD	$O(1)$	$O(T)$	$O(T)$	$O(T)$	=2
DE+SPTD	$O(M)$	$O(MT)$	$O(MT)$	$O(MT)$	1

D.2 Additional Selective Prediction Results

D.2.1 Extended Synthetic Experiments

We extend the experiment from Figure 2 to all tested SC methods in Figure 8. We also provide an extended result using Bayesian Linear Regression in Figure 9.

D.2.2 Full Score Distribution

We extend the experiment from Figure 4 to all tested SC methods in Figure 10.

D.2.3 CIFAR-100 Results With ResNet-50

We further provide a full set of results using the larger ResNet-50 architecture on CIFAR-100 in Figure 4.

D.2.4 Applying SPTD on Top of SAT

Our main set of results suggest that applying SPTD on top of DE further improves performance. The same effect holds when applying SPTD on top of non-ensemble-based methods such as SAT. We document this result in Figure 11.

Table 4: **Selective accuracy achieved across coverage levels for CIFAR-100 with ResNet-50**.

Cov.	SR	SAT+ER+SR	DE	SPTD	DE+SPTD
100	**77.0 (±0.0)**	**77.0 (±0.0)**	**77.0 (±0.0)**	**77.0 (±0.0)**	**77.0 (±0.0)**
90	79.2 (± 0.1)	79.9 (± 0.1)	81.2 (± 0.0)	81.4 (± 0.1)	**82.1 (± 0.1)**
80	83.1 (± 0.0)	83.9 (± 0.0)	85.7 (± 0.1)	85.6 (± 0.1)	**86.0 (± 0.2)**
70	87.4 (± 0.1)	88.2 (± 0.1)	89.6 (± 0.1)	**89.7 (± 0.0)**	**89.8 (± 0.1)**
60	90.5 (± 0.0)	90.8 (± 0.2)	**90.7 (± 0.2)**	90.6 (± 0.0)	**90.9 (± 0.1)**
50	93.4 (± 0.1)	93.8 (± 0.0)	95.3 (± 0.0)	95.1 (± 0.0)	**95.4 (± 0.0)**
40	95.4 (± 0.0)	95.5 (± 0.1)	**97.1 (± 0.1)**	**97.2 (± 0.1)**	**97.2 (± 0.0)**
30	97.4 (± 0.2)	97.7 (± 0.0)	**98.6 (± 0.1)**	**98.6 (± 0.1)**	**98.7 (± 0.0)**
20	97.9 (± 0.1)	98.4 (± 0.1)	99.0 (± 0.0)	99.2 (± 0.1)	**99.2 (± 0.1)**
10	98.1 (± 0.0)	98.8 (± 0.1)	99.2 (± 0.1)	**99.4 (± 0.1)**	**99.6 (± 0.1)**

D.2.5 Ablation on k

We provide a comprehensive ablation on the weighting parameter k in Figures 12 and 13.

D.2.6 Comparison With Logit-Variance Approaches

We showcase the effectiveness of SPTD against LOGITVAR (Swayamdipta et al., 2020), an approach that also computes predictions of intermediate models but instead computes the variance of the correct prediction. We adapt this method to our selective prediction approach (for which true labels are not available) by computing the variance over the maximum predicted logit instead of the true logit. In Figure 14, we see that the weighting of intermediate checkpoints introduced by SPTD leads to stronger performance over the LOGITVAR baseline approach.

D.2.7 Detection of Out-of-Distribution and Adversarial Examples

Out-of-distribution (OOD) and adversarial example detection are important disciplines in trustworthy ML related to selective prediction. We therefore provide preliminary evidence in Figure 15 that our method can be used for detecting OOD and adversarial examples. While these results are encouraging, we remark that adversarial and OOD samples are less well defined as incorrect data points and can come in a variety of different flavors (i.e., various kinds of attacks or various degrees of OOD-ness). As such, we strongly believe that future work is needed to determine whether a training-dynamics-based approach to selective prediction can be reliably used for OOD and adversarial sample identification. In particular, a study of the exact observed training dynamics for both types of samples seems vital to ensure improved detectability.

D.2.8 Estimating τ on Validation VS Test Data

Consistent with prior works (Geifman and El-Yaniv, 2017; Liu et al., 2019; Huang et al., 2020; Feng et al., 2023), we estimate τ directly on the test set. However, a realistically deployable approach has to compute thresholds based on a validation set for which labels are available. In the case of selective classification, the training, validation, and test sets follow the i.i.d. assumption, which means that an approach that sets the threshold based on a validation set should work performantly on a test set, too. Under consistent distributional assumptions, estimating thresholds on a validation set functions as an unbiased estimator of accuracy/coverage tradeoffs on the test set. By the same virtue, setting thresholds directly on the test set and observing the SC performance on that test set should be indicative for additional test samples beyond the actual provided test set. It is important to remark that the validation set should only be used for setting the thresholds and not for model selection / early stopping which would indeed cause a potential divergence between SC performance on the validation and test sets. Further note that violations of the i.i.d assumption can lead to degraded performance due to mismatches in attainable coverage as explored in Bar-Shalom et al. (2023).

To confirm this intuition, we present an experiment in Figure 16 and Figure 17 where we select 50% of the samples from the test set as our validation set (and maintain the other 50% of samples as our

new test set). We first generate 5 distinct such validation-test splits, set the thresholds for τ based on the validation set, and then evaluate selective classification performance on the test set by using the thresholds derived from the validation set. We compare these results with our main approach which sets the thresholds based on the test set directly (ignoring the validation set). We provide an additional experiment where we partition the validation set from the training set in Figure 18. We see that the results are statistically indistinguishable from each other, confirming that this evaluation practice is valid for the selective classification setup we consider.

D.2.9 TIME SERIES EXPERIMENTS

Datasets As part of our time series experiments, we mainly consider the M4 forecasting competition dataset (Makridakis et al., 2020) which contains time series aggregated at various time intervals (e.g., hourly, daily). In addition, we also provide experimentation on the Hospital dataset (Hyndman, 2015).

Models & Setup Our experimentation is carried out using the GluonTS time series framework (Alexandrov et al., 2019). We carry out our experimentation using the DeepAR model (Salinas et al., 2020), a recurrent neural network designed for time series forecasting. We train all models over 200 epochs and evaluate performance using the mean scaled interval score (MSIS) performance metric (Makridakis et al., 2020). Our baselines correspond to the same as presented for regression in Section 4.2: deep ensembles (`DE`), and output parameterization using a Student-t distribution (`ODIST`).

Main results Our time series results are shown in Figure 19 and are consistent with our results for regression: `ODIST` does not provide a meaningful signal for selective prediction while `SPTD` and `DE` perform similarly well. `SPTD` further improves results over `DE` at low converge.

D.2.10 COMPARING s_{MAX} AND s_{SUM}

As per our theoretical framework and intuition provided in Section 3, the sum score s_{SUM} should offer the most competitive selective classification performance. We confirm this finding in Figure 20 where we plot the accuracy/coverage curves across all datasets for both s_{MAX} and s_{SUM}. Overall, we find that the sum score s_{SUM} consistently outperforms the more noisy maximum score s_{MAX}.

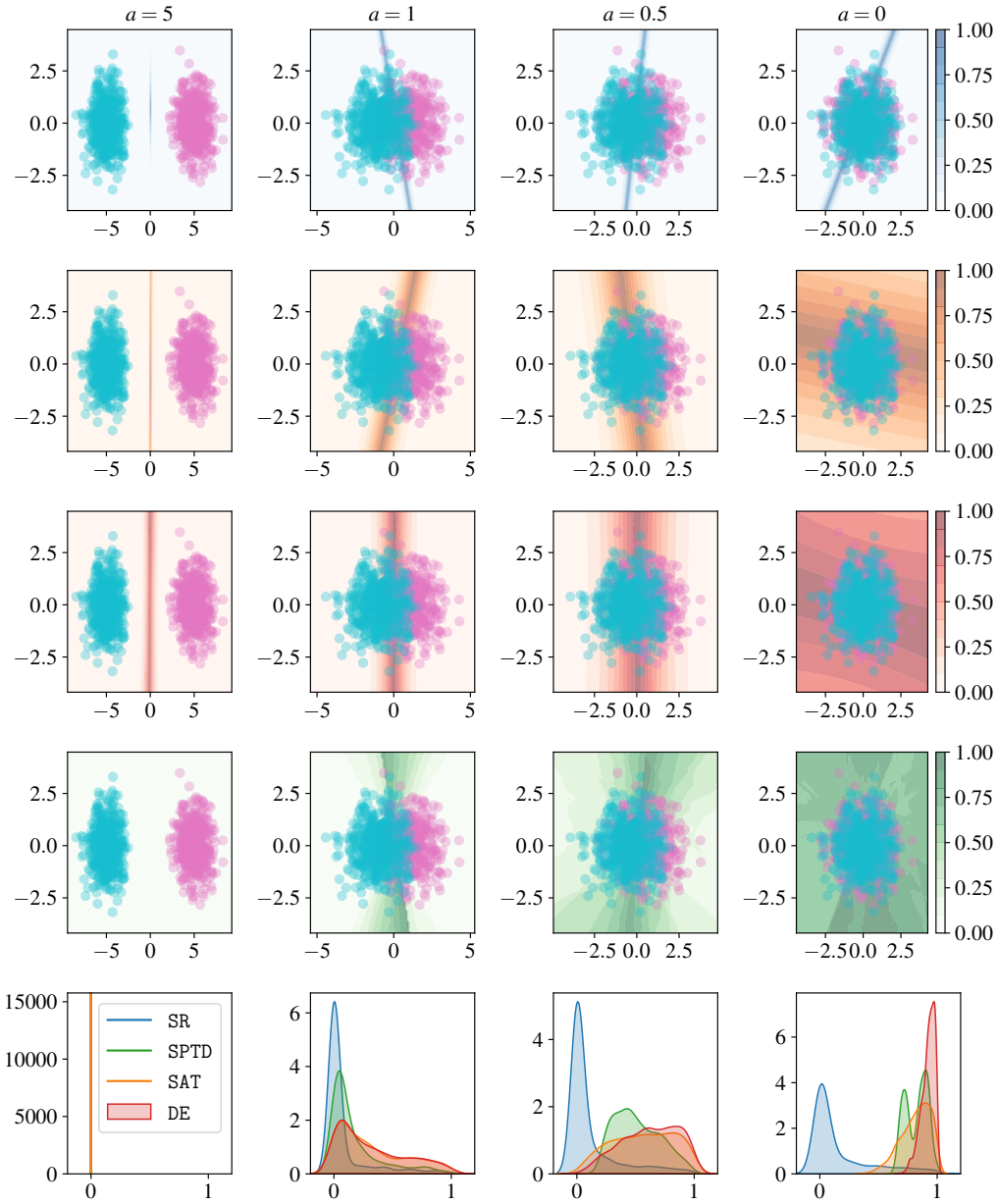

Figure 8: **Extended Gaussian experiment.** The first row corresponds to the anomaly scoring result of SR, the second to the result of SAT, the third to the result of DE, and the fourth to the result of SPTD. The bottom row shows the score distribution for each method over the data points. We see that all methods reliably improve over the SR baseline. At the same time, we notice that SAT and DE still assign higher confidence away from the data due to limited use of decision boundary oscillations. SPTD addresses this limitation and assigns more uniform uncertainty over the full data space.

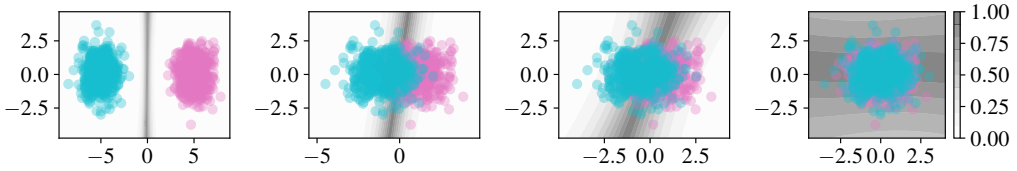

Figure 9: **Bayesian linear regression experiment on Gaussian data.** Results comparable to DE.

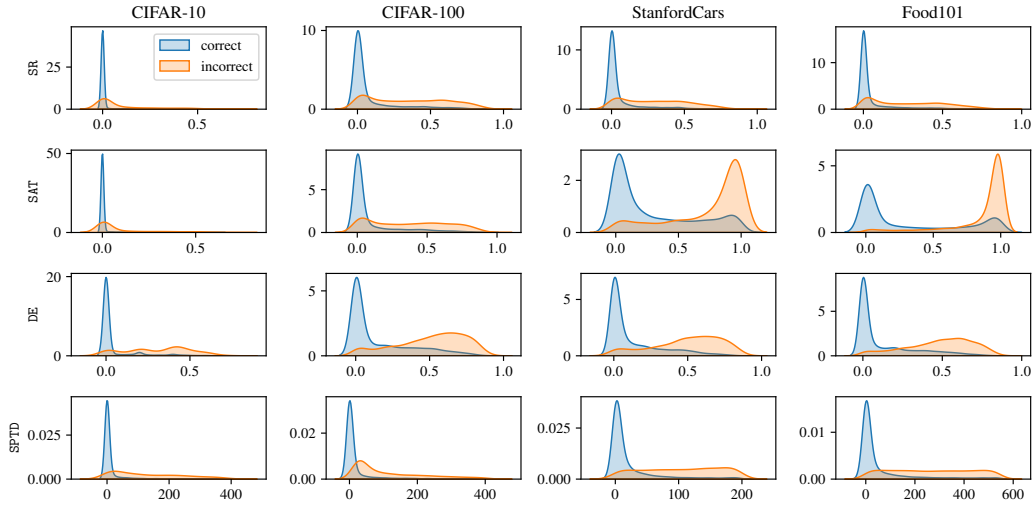

Figure 10: **Extended scores for correct and incorrect data points.** Since all methods are designed to address the selective prediction problem, they all manage to separate correct from incorrect points (albeit at varying success rates). We see that SPTD spreads the scores for incorrect points over a wide range with little overlap. We observe that for SR, incorrect and correct points both have their mode at approximately the same location which hinders performative selective classification. Although SAT and DE show larger bumps at larger score ranges, the separation with correct points is weaker as correct points also result in higher scores more often than for SPTD.

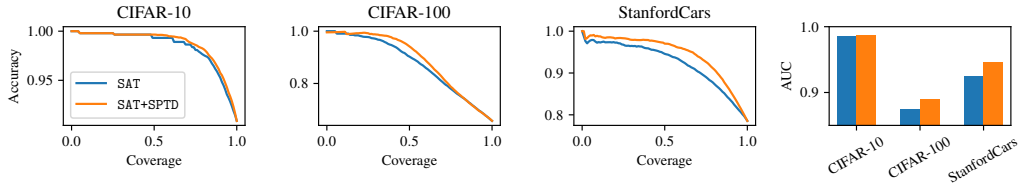

Figure 11: **Applying SPTD on top of SAT.** Similar as with DE, we observe that the application of SPTD improves performance.

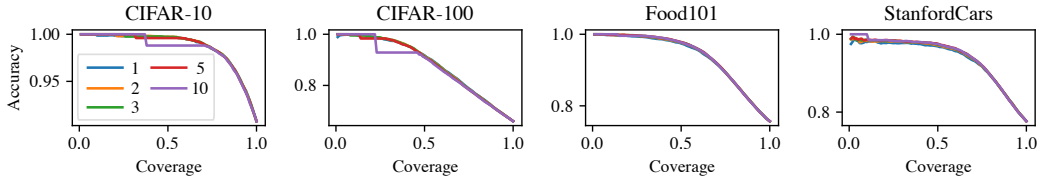

Figure 12: **Coverage/error trade-off of SPTD for varying checkpoint weighting k as used in v_t.** We observe strong performance for $k \in [1,3]$ across datasets.

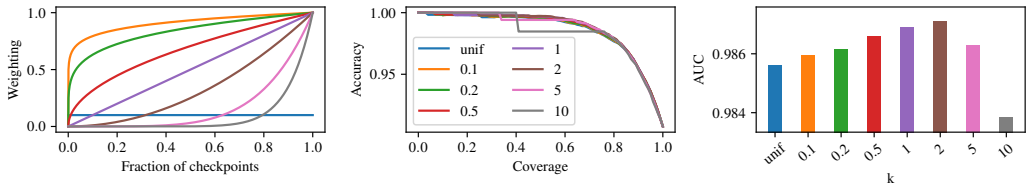

Figure 13: **Extended ablation results on k on CIFAR-10.** We now also consider $k \in (0,1]$ as well as a uniform weighting assigning the same weight to all checkpoints. We confirm that a convex weighting yields best performance.

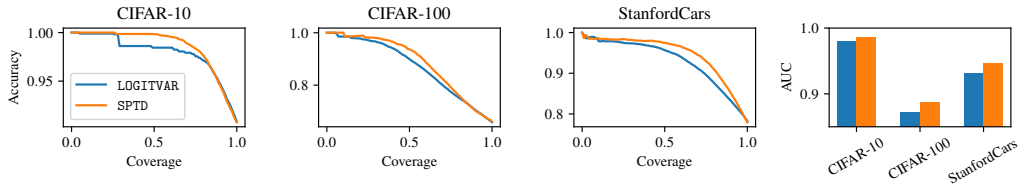

Figure 14: **Comparison of `LOGITVAR` vs `SPTD`.** We observe that `SPTD`, which incorporates weighting of intermediate checkpoints using v_t, outperforms `LOGITVAR`.

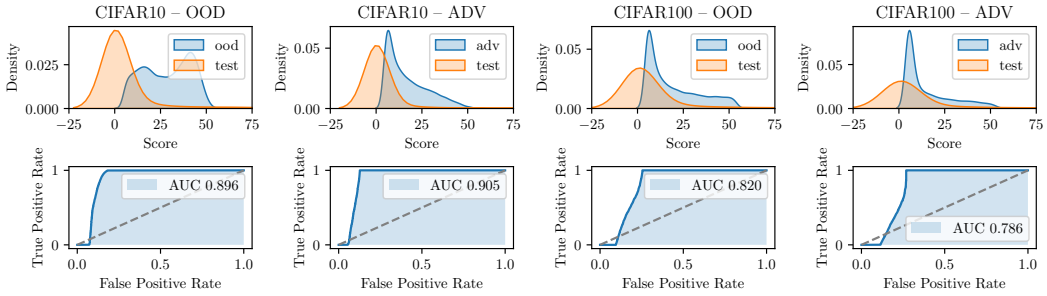

Figure 15: **Performance of `SPTD` on out-of-distribution (OOD) and adversarial sample detection on CIFAR-10 and CIFAR-100**. The first row shows the score distribution of the in-distribution test set vs the SVHN OOD test set or a set consisting of adversarial samples generated via a PGD attack in the final model. The second row shows the effectiveness of a thresholding mechanism by computing the area under the ROC curve. Our score enables separation of anomalous data points from in-distribution test points from the respective datasets.

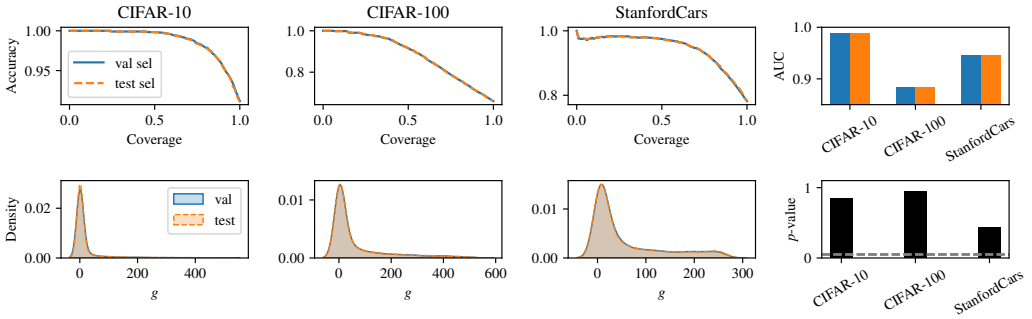

Figure 16: **SPTD accuracy/coverage trade-offs and score distributions on test data obtained by computing τ on a validation set or directly on the test set.** The first row shows the obtained accuracy/coverage trade-offs with the respective AUC scores. In the second row, we show the score distribution for both the picked validation and test sets, along with p-values from a KS-test to determine the statistical closeness of the distributions. Overall, we observe that both methods are statistically indistinguishable from each other.

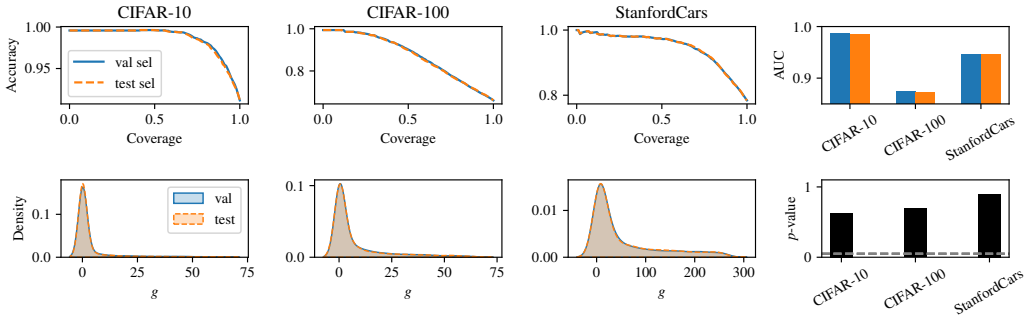

Figure 17: **SAT accuracy/coverage trade-offs and score distributions on test data obtained by computing τ on a validation set or directly on the test set.** Same as Figure 16 but with SAT.

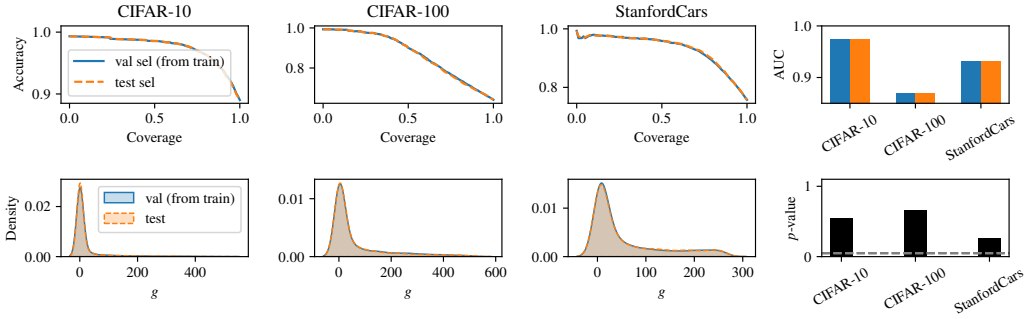

Figure 18: **SPTD accuracy/coverage trade-offs and score distributions on test data obtained by computing τ on a validation set or directly on the test set.** Same as Figure 16 but with the validation set is taken from the original training set.

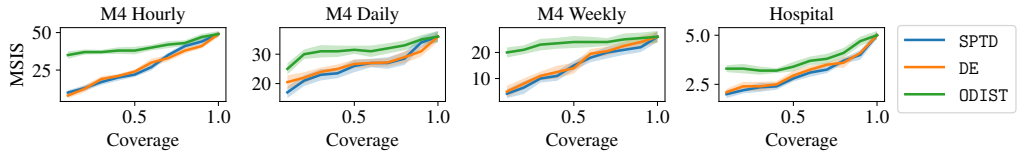

Figure 19: **MSIS/coverage trade-off across various time series prediction datasets**. `SPTD` offers comparable performance to `DE` but provides improved results at low coverage.

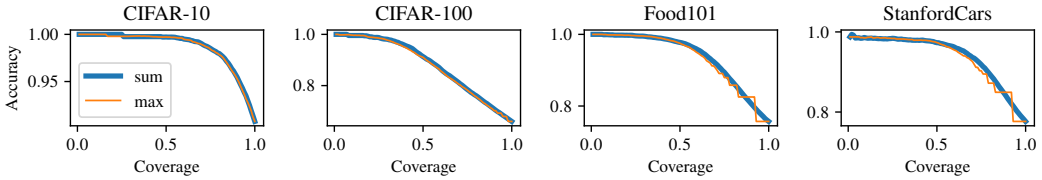

Figure 20: **Comparing s_{MAX} and s_{SUM} performance**. It is clear that s_{SUM} effectively denoises s_{MAX}.

(a) CIFAR-10 (b) CIFAR-100 (c) Food101 (d) StanfordCars

Figure 21: **Additional individual examples across datasets.**