

Understanding Uncertainty Sampling

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Abstract

Uncertainty sampling is a prevalent active learning algorithm that queries sequentially the annotations of data samples which the current prediction model is uncertain about. However, the usage of uncertainty sampling has been largely heuristic: (i) There is no consensus on the proper definition of “uncertainty” for a specific task (classification or regression) under a specific loss (binary loss, cross-entropy loss, squared loss, etc.); (ii) There is no theoretical guarantee that prescribes a standard protocol to implement the algorithm, for example, how to handle the sequentially arrived annotated data under the framework of empirical risk minimization or optimization algorithms such as stochastic gradient descent. In this work, we systematically examine uncertainty sampling algorithms under both stream-based and pool-based active learning. We propose a notion of equivalent loss which depends on the used uncertainty measure and the original loss function through a partial differential equation and establish that an uncertainty sampling algorithm essentially optimizes against such an equivalent loss. The perspective verifies the properness of existing uncertainty measures (including entropy uncertainty, least confidence uncertainty, margin-based uncertainty, etc.) from two aspects: surrogate property and loss convexity. It can also be used to develop new uncertainty measures. Furthermore, we propose a new notion for designing uncertainty measures called *loss as uncertainty*. The idea is to use the conditional expected loss given the features as the uncertainty measure. Such an uncertainty measure has nice analytical properties and, more importantly, a generality to cover both classification and regression problems (in contrast to the existing case-by-case design of uncertainty measures). These developments enable us to provide the first generalization bound for uncertainty sampling algorithms under both stream-based and pool-based settings, in the full generality of the underlying model and problem. Lastly, we establish some connection between certain variants of the uncertainty sampling algorithms with risk-sensitive objectives and distributional robustness, which can partly explain the advantage of uncertainty sampling algorithms when the sample size is small.

1 Introduction

Active learning is a machine learning paradigm where the learning algorithm interactively queries humans (or some other information source) to annotate new data points. Different from supervised learning, an active learning algorithm begins with all the data samples unlabeled and adaptively decides which samples to query for labels. The study of active learning is motivated by the great availability of unlabeled data and the prohibitive cost of getting all the data labeled. Its goal is to improve data efficiency and reduce the labeling cost by querying only a small proportion of the data but still getting a satisfying performance.

The study of active learning algorithms can be categorized according to two standards: scenarios and querying strategies (Settles, 2009). The scenarios of active learning are determined by how the data is generated and observed. The *query synthesis* scenario allows the learner to generate de novo examples rather than samples from a distribution (Angluin, 1988). While query synthesis is practical for many problems, labeling arbitrarily generated instances could be awkward for human experts (Baum and Lang, 1992). Comparatively, if the data is generated from a fixed unknown distribution, then we call it either

stream-based sampling or *pool-based sampling*, depending on the way that unlabeled samples arrive. If the samples arrive in a sequence, the learner queries the labels from a stream (Atlas et al., 1989; Cohn et al., 1994). Otherwise, the learner can observe the pool of unlabeled samples (Lewis, 1995). In this paper, we focus on stream-based and pool-based scenarios.

The second criterion to categorize the active learning algorithms is the querying strategy, among which *uncertainty sampling* is “perhaps the simplest and most commonly used query framework” (Settles, 2009). Roughly speaking, the uncertainty sampling strategy is to query the samples that the model is uncertain about (Lewis, 1995). Other strategies include query-by-committee (Seung et al., 1992), expected model change (Settles et al., 2007), expected error reduction (Roy and McCallum, 2001), and expected variance reduction (Wang et al., 2015). Although rigorous theoretical results have been obtained for some of the other querying strategies (Balcan et al., 2006; Hanneke et al., 2014), theoretical understanding of the uncertainty sampling strategy is still lacking. Some initial yet intriguing results have been established for various kinds of uncertainty measurements. Mussmann and Liang (2018b) show that the threshold-based uncertainty sampling (i.e., to query only the samples of which the uncertainty is above a threshold) can be interpreted as performing a preconditioned stochastic gradient step on a smoothed version of the population zero-one loss that converges to the population zero-one loss. The non-convexity of the zero-one loss implies that the threshold-based uncertainty sampling could be trapped in local minima, suggesting the necessity of a warm start. Tifrea et al. (2022) consider a similar threshold-based uncertainty, where the threshold is chosen implicitly via querying the least confident several samples under the Bayes optimal hypothesis. For a handcrafted linearly separable distribution, Tifrea et al. (2022) prove a finite-sample lower bound on the logistic regression in the high-dimensional case for the empirical risk minimization algorithm as Lewis (1995), and claim the less efficiency of uncertainty sampling against passive learning both theoretically and empirically. Apart from the pool-based setting and the threshold-based uncertainty, Raj and Bach (2022) design their algorithm in the stream-based setting with a margin-based uncertainty. They prove that the stream-based algorithm will converge with an $O(1/T)$ error rate under a strictly linearly separable data distribution.

Despite all those efforts, there has been no systematic theoretical understanding of data efficiency or even the convergence of uncertainty sampling. Besides, existing theoretical works are restricted to particular forms of uncertainty sampling algorithms. In addition, all existing theoretical results are made for linear classifiers. And there is little theoretical understanding of the probabilistic-based uncertainty measurements (Dagan and Engelson, 1995; Culotta and McCallum, 2005) or the regression problem. In this paper, we propose a general framework to analyze uncertainty sampling algorithms and introduce a notion of *equivalent loss*. We establish that the uncertainty sampling algorithms essentially optimize against such an equivalent loss objective. By inspecting the surrogate and the optimization properties of the equivalent loss, we not only recover existing theoretical results but also generalize to uncertainty sampling algorithms under other contexts such as multi-class classification and regression. Our contribution can be summarized as follows:

- We introduce the equivalent loss as a loss function specified through a partial differential equation in terms of the used uncertainty and the original loss function. Then we establish that uncertainty sampling algorithms essentially optimize against this equivalent loss.
- For binary classification, we examine the existing uncertainty measures and theoretical results through the lens of equivalent loss. Specifically, we show that the error rate of the margin-based uncertainty in Raj and Bach (2022) will converge to zero regardless of the underlying data distribution, compared to their assumption that the data needs to be strictly separable. We recover the non-convexity observations of the threshold-based models (Mussmann and Liang, 2018b; Tifrea et al., 2022). We also analyze the probabilistic uncertainty models, showing their Fisher

consistency.

- We generalize this notion to the multi-classification and the regression problems with our *loss-as-uncertainty* principle. Equipped with such an uncertainty measure, the convergence can be proved for any convex and non-negative loss functions for binary classification, multi-class classification, and regression.
- We also study several other variants of uncertainty sampling algorithms and draw connections with risk-sensitive loss and distributional robustness. Specifically, we show the exponential-loss-as-uncertainty will be minimizing the softmax of the loss, the top- k -max uncertainty sampling essentially minimizes the conditional value at risk (CVaR), and the mixture of uniform and uncertainty sampling recovers a distributionally robust optimization formulation.

2 Problem Setup

Consider the problem of predicting the label Y from the feature X , where (X, Y) is independently drawn from an unknown distribution \mathcal{P} . We denote the marginal distribution of X to be \mathcal{P}_X and the conditional distribution of Y on X is $\mathcal{P}_{Y|X}$. Let \mathcal{X} and \mathcal{Y} denote the support of X and Y respectively. Suppose $\mathcal{X} \in \mathbb{R}^d$ is a bounded set with an upper bound of M_X with respect to the Euclidean norm. For a binary classification problem, $\mathcal{Y} = \{-1, +1\}$. For a K -nary classification problem, $\mathcal{Y} = [K] = \{1, \dots, K\}$. For a regression problem, we assume $\mathcal{Y} = [-M_Y, M_Y]$ is a bounded set with an upper bound of M_Y .

For the canonical setting of supervised learning, a full dataset of both features and labels is completely revealed to the learner at the beginning. For active learning, the learner starts with only observations of the features X 's and needs to decide which of the labels Y 's to query or whether to query the labels Y 's. In this paper, we consider two mainstream settings for active learning.

- **Stream-based setting.** The dataset \mathcal{D}_T^X consists of T i.i.d. features $\{X_t\}_{t=1}^T$ from \mathcal{P}_X . The samples arrive sequentially. At each time t , upon the arrival of X_t , the learner decides whether to query the sample: if so, Y_t is revealed to the learner; otherwise, it moves on to the next time period. The feature and the label (if queried) of the t -th time period will be discarded (but not cached) after the time period. Without loss of generality, we still assume the presence of the label Y_t sampled from $\mathcal{P}_{Y|X=X_t}$; it may just not be revealed to the learner depending on the querying decision.
- **Pool-based setting.** The dataset \mathcal{D}_n^X consists of n i.i.d. features $\{X_i\}_{i=1}^n$ from \mathcal{P}_X . The whole dataset \mathcal{D}_n^X is revealed all at once to the learner at the beginning. The learner queries samples from the dataset sequentially. Unlike the stream-based setting, the information from past queries will be retained and can be repeatedly utilized by the learner.

Throughout the paper, we consider a parameterized family of hypotheses denoted by $\mathcal{F} = \{f_\theta(\cdot) : \theta \in \Theta, f_\theta(\cdot) : \mathcal{X} \rightarrow \mathcal{Y}\}$. We assume the parameter set Θ has an upper bound of M_Θ under the Euclidean norm. We denote the loss function $l : \mathcal{Y} \times \mathcal{Y} \rightarrow \mathbb{R}$, i.e., $l(\hat{Y}, Y)$ measures the loss of predicting Y with \hat{Y} . With a slight overload of the notation, we denote $l(\theta; (X, Y)) = l(f_\theta(X), Y)$ as the prediction loss of the model $f_\theta(\cdot)$ on the sample (X, Y) .

For uncertainty sampling algorithms, a key component is an uncertainty function/measure $U(\theta; X) : \mathcal{X} \rightarrow [0, \infty)$. The uncertainty function quantifies the uncertainty about a sample X given the model parameter θ . The specification of the uncertainty function usually depends on both the underlying hypothesis class \mathcal{F} and the loss function l ([Dagan and Engelson, 1995](#); [Culotta and McCallum, 2005](#); [Dasgupta et al., 2005](#); [Balcan et al., 2007](#); [Mussmann and Liang, 2018b](#); [Raj and Bach, 2022](#); [Tifrea et al., 2022](#)).

2022). The general idea is to spend more querying efforts on those samples that the current model is uncertain about, in the hope to maximize the improvement of the model learning.

3 Uncertainty Sampling for Binary Classification

3.1 Generic algorithm under stream-based setting

We begin our discussion with the binary classification problem. In the following, we present a generic algorithm of uncertainty sampling under the stream-based setting. Specifically, Algorithm 1 queries the data samples based on the model uncertainty and updates the model parameter according to a gradient descent procedure. It takes the uncertainty function $U(\theta; X)$ as an input. At each time t , the algorithm observes only the feature X_t and calculates the uncertainty $U(\theta_t; X_t)$. Here, without loss of generality, we assume the uncertainty is between $[0, 1]$. Then, with probability $U(\theta_t; X_t)$, the algorithm queries the label of the sample and performs a gradient descent update; with probability $1 - U(\theta_t; X_t)$, the algorithm does not make a query and hence not update the parameters. In this way, a larger value of uncertainty will encourage the querying of a sample.

Algorithm 1 Uncertainty sampling with gradient descent update (stream-based version)

Input: Dataset $\mathcal{D}_T = \{(X_t, Y_t)\}_{t=1}^T$, step sizes $\{\eta_t\}_{t=1}^T > 0$, uncertainty function $U(\theta; X) : \mathcal{X} \rightarrow [0, 1]$

- 1: Initialize θ_1 ; $\bar{\theta}_1 \leftarrow \theta_1$
- 2: **for** $t = 1, \dots, T$ **do**
- 3: Observe X_t and calculate $U(\theta_t; X_t)$
- 4: Generate $\xi_t \sim \text{Unif}[0, 1]$
- 5: **if** $\xi_t \leq U(\theta_t; X_t)$ **then**
- 6: Query the label Y_t and update

$$\theta_{t+1} \leftarrow \theta_t - \eta_t \cdot \frac{\partial l(\theta; (X_t, Y_t))}{\partial \theta} \Big|_{\theta=\theta_t}$$

- 7: **else**
- 8: Do not query the label Y_t and let $\theta_{t+1} \leftarrow \theta_t$
- 9: **end if**
- 10: $\bar{\theta}_{t+1} \leftarrow (1 - \frac{1}{t+1})\bar{\theta}_t + \frac{1}{t+1}\theta_{t+1}$
- 11: **end for**

Output: $\bar{\theta}_{T+1}$

The core idea of the algorithm is to query only the samples that the model is uncertain about, and the uncertainty function quantifies such uncertainty. In the following, we review three examples of the uncertainty function used in the literature as special cases of the generic algorithm.

Example 1 (Probabilistic model (Dagan and Engelson, 1995; Culotta and McCallum, 2005)). A probabilistic model outputs $q(\theta; X) : \mathcal{X} \rightarrow [0, 1]$ to estimate the true conditional probability $\mathbb{P}(Y = +1|X)$. The entropy uncertainty (Dagan and Engelson, 1995) considers the entropy of $q(\theta; X)$:

$$U(\theta; X) := -[q(\theta; X) \log(q(\theta; X)) + (1 - q(\theta; X)) \log(1 - q(\theta; X))],$$

where $q = q(X; \theta) \in (0, 1)$. The least confidence uncertainty (Culotta and McCallum, 2005) considers

$$U(\theta; X) := 1 - \max\{q(X; \theta), 1 - q(X; \theta)\} = \min\{q(X; \theta), 1 - q(X; \theta)\}.$$

These two uncertainties are often accompanied by the following cross-entropy loss that trains the probabilistic model

$$l(\theta; (X, Y)) = -[\mathbb{1}\{Y = +1\} \log q(\theta; X) + \mathbb{1}\{Y = -1\} \log(1 - q(\theta; X))]$$

where $\mathbb{1}\{\cdot\}$ is the indicator function. Equivalently, we can also represent the loss function by $l(\hat{Y}, Y) = -\log\left(\frac{1+\hat{Y}\cdot Y}{2}\right)$ where $\hat{Y} = 2q(\theta; X) - 1 \in [-1, 1]$ is the predicted expectation.

For a probabilistic model, $q(\theta; X)$ reflects the confidence of the prediction. When $q(\theta; X)$ is close to 1, the model is confident that $Y = +1$, while $q(\theta; X)$ is close to 0, it is confident that $Y = -1$. For both ends, the uncertainty is small for both the entropy uncertainty and the least confidence uncertainty. When the model is less confident about the prediction and outputs $q(\theta; X)$ close to $\frac{1}{2}$, the uncertainty becomes larger.

Example 2 (Margin-based model (Raj and Bach, 2022)). Another class of classification model is margin-based, such as support vector machines (SVMs). Consider a linear SVM model that predicts Y with the sign of $\theta^\top X$. The margin-based uncertainty function is defined by

$$U_\mu(\theta; X) := \frac{1}{1 + \mu|\theta^\top X|}$$

where $\mu > 0$ is a hyper-parameter. The associated loss function for learning such margin-based models is squared margin loss

$$l(\theta; (X, Y)) = (\max\{0, 1 - Y \cdot \theta^\top X\})^2.$$

Equivalently, the loss function can be written in the form of

$$l(\hat{Y}, Y) = (\max\{0, 1 - Y \cdot \hat{Y}\})^2,$$

where $\hat{Y} = \theta^\top X$.

For linear classifiers, $|\theta^\top x|$ is proportional to the distance from a sample to the classification hyperplane. The margin-based uncertainty captures the intuition that the closer a sample is to the classification hyperplane, the more uncertain the learner is about the sample.

Example 3 (Threshold-based uncertainty (Orabona et al., 2011; Mussmann and Liang, 2018b; Tifrea et al., 2022)). The pool-based version of Example 2 works with a fixed set of samples and results in a threshold-based uncertainty function. At each time step, the algorithm will query the most uncertain sample in the given dataset with index $i_t = \arg \min_{i \in \mathcal{U}_t} |\theta^\top X_i|$ where the set \mathcal{U}_t contains the indices of unqueried samples at time t . Such a procedure can be captured by the following uncertainty function

$$U(\theta; X) := \mathbb{1}\{|\theta^\top X| \leq \gamma\}.$$

where $\gamma > 0$ is a hyper-parameter that may change over time. Tifrea et al. (2022) analyze this uncertainty function and derive some negative theoretical results on its performance. Specifically, they consider the following loss for a logistic regression model

$$l(\theta; (X, Y)) = \log(1 + \exp(-Y \cdot \theta^\top X)).$$

Equivalently, the loss can be written as

$$l(\hat{Y}, Y) = \log(1 + \exp(-Y \cdot \hat{Y})),$$

where $\hat{Y} = \theta^\top X$.

As in the margin-based model, the quantity $|\theta^\top x|$ reflects the confidence of the prediction, and thus it is inversely proportional to the uncertainty. The threshold-based uncertainty queries only those samples where the confidence is smaller than the threshold γ .

3.2 Equivalent loss

Now we show a general property of Algorithm 1 that, with this selective querying procedure, the algorithm essentially optimizes against an alternative loss function which we name as the equivalent loss; and the alternative loss is jointly determined by the uncertainty function U and the original loss function l . Specifically, if we combine the two cases of *query* and *not query* for the update step in Algorithm 1, we obtain the following

$$\mathbb{E}_{\xi_t}[\theta_{t+1}|\theta_t, X_t, Y_t] = \theta_t - \eta_t \cdot U(\theta_t; X_t) \cdot \frac{\partial l(\theta; (X_t, Y_t))}{\partial \theta} \Big|_{\theta=\theta_t}$$

where the expectation is taken with respect to ξ_t which is the *sampling* random variable that determines whether to query the sample.

Suppose (for the moment) there exists a loss function \tilde{l} such that

$$\frac{\partial \tilde{l}(\theta; (x, y))}{\partial \theta} = U(\theta; X) \cdot \frac{\partial l(\theta; (x, y))}{\partial \theta} \quad (1)$$

holds for all $\theta \in \Theta$ and $(x, y) \in \mathcal{X} \times \mathcal{Y}$ (we will discuss the existence of \tilde{l} in the following subsection). Then the parameter update can be written as

$$\mathbb{E}_{\xi_t}[\theta_{t+1}|\theta_t, X_t, Y_t] = \theta_t - \eta_t \cdot \frac{\partial \tilde{l}(\theta; (X_t, Y_t))}{\partial \theta} \Big|_{\theta=\theta_t}.$$

Proposition 1. Suppose there exists \tilde{l} satisfying (1). Then Algorithm 1 essentially performs stochastic gradient descent (SGD) with respect to the loss function \tilde{l} .

Definition 1. We say \tilde{l} is the *equivalent loss* for the uncertainty function U and the original loss function l , if it satisfies (1).

The equivalent loss \tilde{l} can be viewed as a surrogate loss of the original loss l twisted by the uncertainty function U . If \tilde{l} exists, it provides a convenient handle to understand and analyze the algorithm. In the following, we derive the equivalent loss \tilde{l} for the previous examples.

Example 1 (Continued). Example 1 considers a probabilistic model $q(\theta; X)$ that estimates the true conditional probability $\mathbb{P}(Y = +1|X)$, and the loss function is the cross-entropy loss.

- For the entropy uncertainty, the equivalent loss

$$\tilde{l}(\theta; (X, Y)) = q \log(q) + (1 - q) \log(1 - q) - \mathbb{1}\{Y = +1\} \cdot \text{Li}_2(q) - \mathbb{1}\{Y = -1\} \cdot \text{Li}_2(1 - q) + \text{Li}_2(1),$$

where $q = q(\theta; X)$ stands for the prediction model and the function $\text{Li}_2(z) = -\int_0^z \frac{\log(1-u)}{u} du$ is the Spence's function.

- For the least confidence uncertainty, the equivalent loss

$$\tilde{l}(\theta; (X, Y)) = \begin{cases} -\mathbb{1}\{Y = -1\} \cdot \log(2(1 - q)) - q + \log(2), & \text{if } q < \frac{1}{2}; \\ -\mathbb{1}\{Y = +1\} \cdot \log(2q) - (1 - q) + \log(2), & \text{if } q \geq \frac{1}{2}. \end{cases}$$

where $q = q(\theta; X)$ stands for the prediction model.

Example 2 (Continued). For the margin-based model, the equivalent loss for the margin-based uncertainty function (defined in Example 2) and the squared margin loss is

$$\tilde{l}_\mu(\theta; (X, Y)) = \begin{cases} -\frac{2}{\mu}(\frac{1}{\mu} - 1) \log(1 - \mu Y \cdot \hat{Y}) - \frac{2}{\mu}Y \cdot \hat{Y} + C, & \text{if } Y \cdot \hat{Y} \leq 0; \\ -\frac{2}{\mu}(\frac{1}{\mu} + 1) \log(1 + \mu Y \cdot \hat{Y}) + \frac{2}{\mu}Y \cdot \hat{Y} + C, & \text{if } Y \cdot \hat{Y} \in (0, 1); \\ 0, & \text{if } Y \cdot \hat{Y} \geq 1, \end{cases}$$

where the prediction $\hat{Y} = \theta^\top X$, the constant $C = \frac{2}{\mu}(\frac{1}{\mu} + 1) \log(1 + \mu) - \frac{2}{\mu}$, and the hyper-parameter $\mu > 0$ is the same one that defines the margin-based uncertainty function.

Example 3 (Continued). The equivalent loss for the threshold-based uncertainty and the logistic loss function is given by the following:

$$\tilde{l}_\gamma(\theta; (X, Y)) = \begin{cases} \log(1 + \exp(\gamma)), & \text{if } Y \cdot \hat{Y} \leq -\gamma, \\ \log(1 + \exp(-Y \cdot \hat{Y})), & \text{if } Y \cdot \hat{Y} \in (-\gamma, \gamma), \\ \log(1 + \exp(-\gamma)), & \text{if } Y \cdot \hat{Y} \geq \gamma \end{cases}$$

where the prediction $\hat{Y} = \theta^\top X$ and the hyper-parameter γ is the same one that specifies the threshold-based uncertainty function.

For these three examples, the derivation of the equivalent loss is standard and it is by solving the partial differential equation (PDE) (1), and we defer the details to Appendix A.1. We remark that these equivalent loss functions specify the objective function that Algorithm 1 optimizes, and they are jointly determined by the pair of the uncertainty function and the original loss function.

3.3 Surrogate property of the equivalent loss

The derivation of equivalent loss makes it clear the objective function of the uncertainty sampling procedure. Then a natural question is whether the equivalent loss is a “suitable” loss for the binary classification problem. Recall that the practical goal of training a binary classifier is commonly to achieve a high classification accuracy, i.e., to optimize the binary loss $l_{01}(\hat{Y}, Y) := \mathbb{1}(\hat{Y} \neq Y)$. While the binary loss is in general computationally intractable (Arora et al., 1997), the margin loss, the logistic loss, and the cross-entropy loss can all be viewed as a *surrogate* loss of the binary loss that enjoys better computational structure such as convexity. In this light, the equivalent loss derived from uncertainty sampling can also be viewed as a surrogate of the binary loss. Following the principles of Bartlett et al. (2006), we can examine the suitability of an equivalent loss and hence certify the properness of the uncertainty function.

Definition 2 (Surrogate loss (Bartlett et al., 2006)). A loss function $l(\cdot, \cdot)$ is said to be a surrogate of the binary loss if there exists a continuous, non-negative, and non-decreasing function ψ such that for any measurable function $f : \mathcal{X} \rightarrow \mathcal{Y}$ and any probability distribution \mathcal{P} on $\mathcal{X} \times \mathcal{Y} = \mathcal{X} \times \{-1, +1\}$,

$$\psi \left(L_{01}(f) - \inf_{g \in \mathcal{G}} L_{01}(g) \right) \leq \mathbb{E}[l(f(X), Y)] - \inf_{g \in \mathcal{G}} \mathbb{E}[l(g(X), Y)], \quad (2)$$

where \mathcal{G} is the set of all measurable functions, and $L_{01}(f) := \mathbb{E}[l_{01}(f(X), Y)]$ denotes the expected binary loss. All the expectations are taken with respect to the distribution \mathcal{P} .

The definition establishes a connection between the oracle generation bound under the loss l and that under the binary loss. It can thus verify the properness of a loss l by whether training a model with l can also lead to a performance guarantee for the binary loss. An important property of the link function ψ is that if $z \rightarrow 0$ as $\psi(z) \rightarrow 0$, then the loss function is classification-calibrated (Bartlett et al., 2006). This ensures that the minimizer of the loss l among all the measurable functions will be the Bayes optimal classifier; the property is also known as the Fisher consistency.

Theorem 1 (Theorem 3 in Bartlett et al. (2006)). *For any loss function l that can be expressed as $l(\hat{Y}, Y)$, one can construct a link function ψ . Furthermore, the constructed link function is mini-max optimal in the sense that for any non-negative loss l , any $|\mathcal{X}| \geq 2$, any risk level $\zeta \in [0, 1]$, and any precision $\epsilon > 0$, there exists a probability distribution on $\mathcal{X} \times \{-1, +1\}$ such that $L_{01}(f) - \inf_{g \in \mathcal{G}} L_{01}(g) = \zeta$ and*

$$\psi(\zeta) \leq \mathbb{E}[l(f(X), Y)] - \inf_{g \in \mathcal{G}} \mathbb{E}[l(g(X), Y)] \leq \psi(\zeta) + \epsilon.$$

The loss l is classification-calibrated (Fisher consistent) if and only if for any $z \in (0, 1]$, $\psi(z) > 0$.

Bartlett et al. (2006) provide a way to derive the link function ψ (See our Appendix A.2 for more details). They further prove that this surrogate property's link function is mini-max optimal by the existence of a probability distribution to make the surrogate upper bound arbitrarily tight. They also establish some equivalence between the link function and the Fisher consistency. While such a conclusion is only stated for margin-based models where $l(\hat{Y}, Y) = l(\hat{Y} \cdot Y)$ in (Bartlett et al., 2006), their analysis in Theorem 1 indeed applies to more general loss functions such as the cross entropy written as loss $l(\hat{Y}, Y) = \mathbb{1}\{Y = +1\} \cdot l(\hat{Y}, +1) + \mathbb{1}\{Y = -1\} \cdot l(\hat{Y}, -1)$.

In the following proposition, we re-examine the previous examples and calculate the corresponding link functions against binary loss.

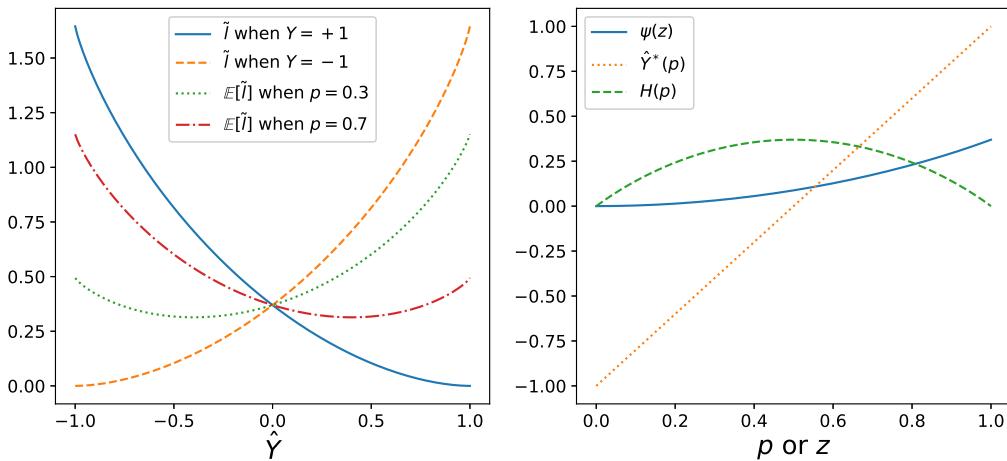


Figure 1: Probabilistic model with entropy uncertainty (Example 1). The left subfigure shows $\tilde{l}(\hat{Y}, +1)$, $\tilde{l}(\hat{Y}, -1)$, and two different expected losses for positive probability $p = 0.3$ and $p = 0.7$. The minima of these expectations are the values $H(p)$, and the minimizing arguments are the values $\hat{Y}^*(p)$. The right subfigure shows $H(p)$ and \hat{Y}^* as a function of p , and the surrogate link function $\psi(z)$.

Proposition 2. *All the equivalent losses in Example 1, Example 2, and Example 3 are surrogate losses for binary loss. Specifically,*

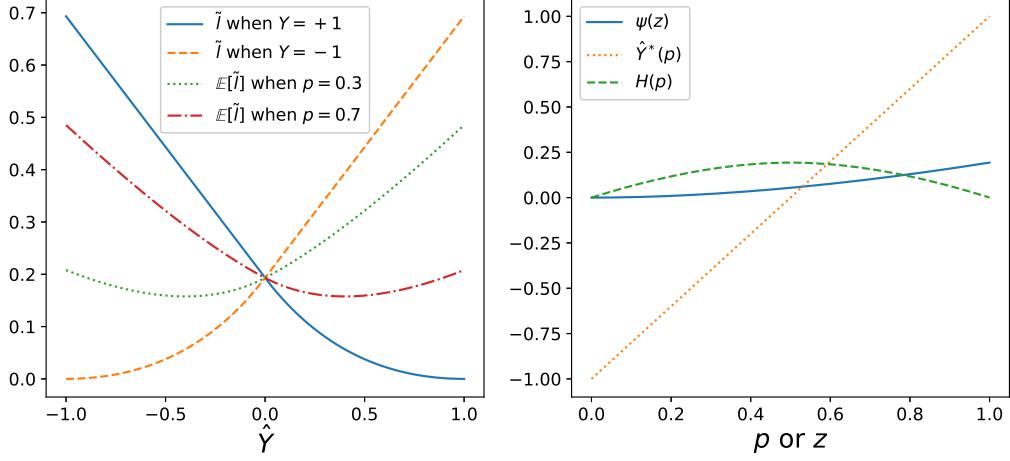


Figure 2: Probabilistic model with least confidence uncertainty ([Culotta and McCallum, 2005](#)).

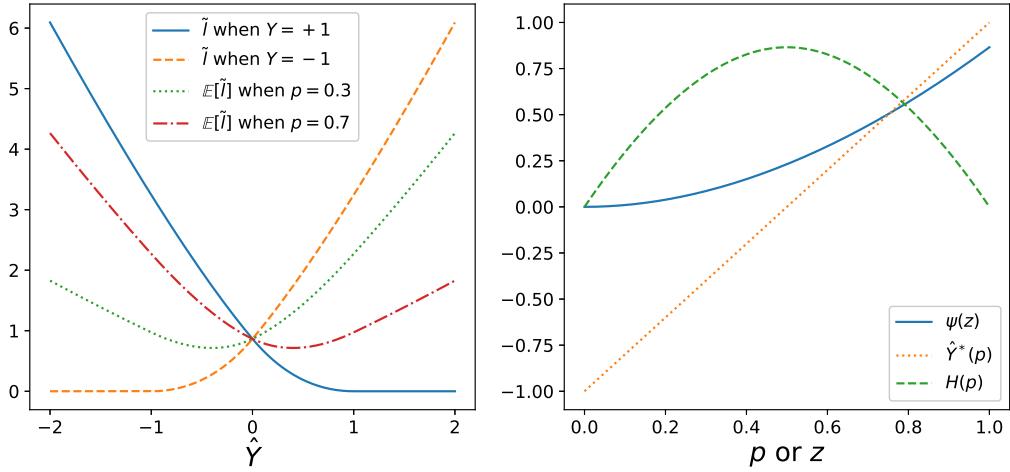


Figure 3: Margin-based model ([Raj and Bach, 2022](#)) with $\mu = 0.5$.

- Example 1 – entropy uncertainty (see Figure 1). The link function

$$\begin{aligned}\psi(z) &= \frac{1+z}{2} \cdot \text{Li}_2\left(\frac{1+z}{2}\right) + \frac{1-z}{2} \cdot \text{Li}_2\left(\frac{1-z}{2}\right) - \text{Li}_2\left(\frac{1}{2}\right) \\ &\quad - \frac{1+z}{2} \cdot \log(1+z) - \frac{1-z}{2} \cdot \log(1-z) \\ &= \log(2) \cdot z^2 + o(z^2) \quad \text{as } z \rightarrow 0.\end{aligned}$$

where $\text{Li}_2(z)$ is the Spence's function as defined earlier.

- Example 1 – least confidence uncertainty (see Figure 2)

$$\psi(z) = \frac{1+z}{2} \log(1+z) - \frac{z}{2} = \frac{z^2}{2} + o(z^2) \quad \text{as } z \rightarrow 0.$$

- Example 2 – margin-based uncertainty (see Figure 3)

$$\psi_\mu(z) = \frac{2}{\mu^2} (1 + \mu z) \log(1 + \mu z) - \frac{2}{\mu} z = 2z^2 + o(z^2) \quad \text{as } z \rightarrow 0.$$

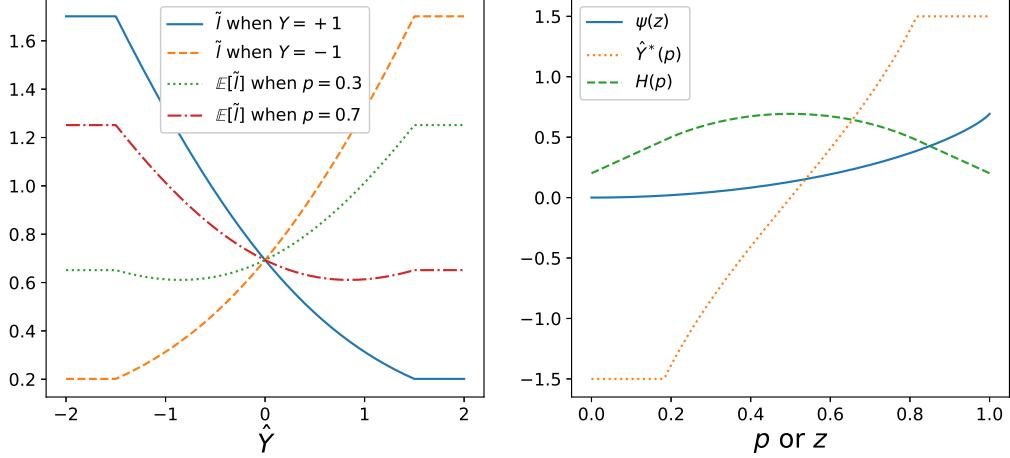


Figure 4: Threshold-based model (Tifrea et al., 2022) with $\gamma = 1.5$.

- Example 3 – threshold-based uncertainty (see Figure 4)

$$\psi_\gamma(z) = \begin{cases} \frac{1}{2} [(1+z) \log(1+z) + (1-z) \log(1-z)], & \text{if } z \leq z_0; \\ \frac{1}{2} [(1+z) \log(1+z_0) + (1-z) \log(1-z_0)], & \text{if } z \geq z_0, \end{cases}$$

where z_0 is a constant determined by the threshold γ

$$z_0 := 2 \left(\exp\left(\frac{\gamma}{1+\exp(\gamma)}\right) + \exp\left(\frac{-\gamma}{1+\exp(-\gamma)}\right) \right)^{-1} - 1.$$

As $z \rightarrow 0$, $\psi_\gamma(z) = z^2 + o(z^2)$.

As noted earlier, the link function helps to transfer the excessive risk bound under the equivalent loss to that under the binary loss. In the next subsection, we pursue such a roadmap by first establishing the convergence rate under the equivalent loss and then transferring it to a performance guarantee under the binary loss.

3.4 Convergence analysis for convex loss

From the perspective of equivalent loss, the stream-based uncertainty sampling of Algorithm 1 can be viewed as a stochastic gradient descent algorithm to minimize the objective function $\mathbb{E}[\tilde{l}(\theta; (X, Y))]$. Now we establish the convergence rate against such an objective.

Definition 3 (Loss convexity). A loss function $l(\theta; (X, Y))$ is said to be a *convex* loss if it is convex with respect to θ for any $X \in \mathcal{X}$ and $Y \in \mathcal{Y}$.

When the equivalent loss is convex, we let

$$\tilde{\theta}^* := \arg \min_{\theta \in \Theta} \mathbb{E} [\tilde{l}(\theta^*, (X, Y))]$$

and have the following convergence bound.

Proposition 3. Suppose that (i) for the original loss, $\left\| \frac{\partial l(\theta; (X, Y))}{\partial \theta} \right\|_2 \leq G$ for all $\theta \in \Theta$ almost surely for $(X, Y) \sim \mathcal{P}$; (ii) for the initial point, $\|\theta_1 - \tilde{\theta}^*\|_2 \leq D$; (iii) the equivalent loss is a convex loss. Then

with the step size $\eta_t = \frac{D}{G\sqrt{T+1}}$, Algorithm 1 yields the following bound

$$\mathbb{E} \left[\tilde{l}(\bar{\theta}_{T+1}, (X, Y)) \right] \leq \frac{1}{T} \sum_{t=1}^T \mathbb{E} \left[\tilde{l}(\theta_t, (X, Y)) \right] \leq \mathbb{E} \left[\tilde{l}(\tilde{\theta}^*, (X, Y)) \right] + \frac{GD}{\sqrt{T+1}}.$$

We would like to draw a comparison between the bound in Proposition 3 and the bound obtained by a standard SGD algorithm against the equivalent loss objective. Note that Algorithm 1 queries only part of the samples, but it achieves the same order of $\frac{1}{\sqrt{T}}$ as the standard SGD which naively queries all the samples. The sacrifice here is the larger variance which is reflected by the constant G in the bound; comparatively, the corresponding gradient variance will be smaller for the standard SGD against the equivalent loss objective.

The analysis of Proposition 3 follows the standard analysis of stochastic gradient descent, and it states in the expectation sense. For high probability bounds, a typical concentration argument will yield a similar bound with an additional $\log(T)$ factor. We note that the rate of $O(1/\sqrt{T})$ can be further improved to $O(1/T)$ for strongly convex functions. Furthermore, if we only consider the last iteration θ_{T+1} rather than the average $\bar{\theta}_{T+1}$, Shamir and Zhang (2013) give an expectation bound of $O(\log(T)/\sqrt{T})$ (or $O(\log(T)/T)$) for non-smooth convex (or strongly convex) functions.

Theorem 2. Suppose the equivalent loss \tilde{l} induced by Algorithm 1 is a surrogate loss for the binary loss with link function ψ . Also, the parameter space Θ satisfies the conditions in Proposition 3, and the step size $\eta_t = \frac{D}{G\sqrt{T+1}}$. Then we have

$$\mathbb{E} \left[L_{01}(f_{\bar{\theta}_{T+1}}) \right] - \inf_{g \in \mathcal{G}} L_{01}(g) \leq \psi^{-1} \left(\frac{GD}{\sqrt{T+1}} + \left(\mathbb{E}[\tilde{l}(f_{\tilde{\theta}^*}(X), Y)] - \inf_{g \in \mathcal{G}} \mathbb{E}[\tilde{l}(g(X), Y)] \right) \right),$$

where $L_{01}(f) = \mathbb{E}[l_{01}(f(X), Y)]$ denotes the expected binary loss as earlier, and the expectation is with respect to the training data and the algorithm's randomness. Here \mathcal{G} is the set of all measurable functions.

Theorem 2 exemplifies how the performance guarantee under the equivalent loss \tilde{l} (Proposition 3) can induce an excessive risk bound under the binary loss through the link function ψ . There are two terms on the right-hand side which correspond to estimation error and approximation error, respectively. The first term comes from the SGD learning procedure, and it captures the estimation suboptimality of $\bar{\theta}_{T+1}$ against the best parameter $\tilde{\theta}^*$. While such an error bound on the estimation suboptimality will generally involve the complexity of the hypothesis class, the online nature of the stream-based setting enables a neat analysis alike other online convex optimization algorithms. The second term captures the approximation suboptimality between the best parameter $\tilde{\theta}^*$ in the prescribed hypothesis class and the best one in the class of all measurable functions. The term will shrink as we enlarge the hypothesis class. We note that this approximation term is not pertaining to the uncertainty sampling algorithm or the equivalent loss, but it also appears in the standard supervised learning setting when transforming the excessive risk bound under margin/cross-entropy loss to that under binary loss.

We make the following two remarks based on Theorem 2:

- Convergence rate: We note that the link function plays a key role in transforming the excessive risk bound: it determines the convergence rate under the binary loss. For all the examples calculated so far (See Proposition 2), the link function $\psi(z) = \Theta(z^2)$ as $z \rightarrow 0$, which implies that $\psi^{-1}(z) \sim \Theta(z^{-\frac{1}{2}})$. Thus it will lead to a convergence rate of $O(T^{-\frac{1}{4}})$ under the binary loss. This does not mean a performance deterioration of uncertainty sampling. For comparison, under the supervised learning regime, the margin loss corresponds to a link function $\psi(z) = \Theta(z)$, while the cross-entropy loss and the logistic loss, among others, all correspond to a link function $\psi(z) = \Theta(z^2)$.

More importantly, we emphasize that T in the bound represents the number of arrived samples in Algorithm 1 but not the number of queried samples. That is, the uncertainty sampling algorithm achieves the same rate of theoretical convergence for the cross-entropy loss but uses potentially much fewer queried samples. For the margin loss, we provide a short discussion in the next section arguing why it is not compatible with the existing uncertainty sampling algorithms.

- Convexity: An important condition in obtaining the bound is the convexity of the loss function with respect to the underlying parameter. While the non-convexity induced by the neural networks is commonly acknowledged as a *benign* non-convexity, the non-convexity induced by the loss function such as the binary loss or the truncated loss which may cause bad local minima is the type of non-convexity we try to avoid. This gives a new perspective to understanding the existing uncertainty functions:
 - The equivalent loss for either the entropy uncertainty or the least confidence uncertainty is convex with respect to the predicted probability $q = q(\theta; X)$ for Example 1.
 - The equivalent loss is convex for the squared margin loss in Example 2. The convexity can thus explain why [Raj and Bach \(2022\)](#) develop the algorithm based on the squared margin loss rather than the vanilla margin loss: any margin-based uncertainty $U(\theta; X) = h(|\theta^\top X|)$ for some non-decreasing function $h(\cdot)$ will induce a non-convex equivalent loss when the original loss is the margin loss (see Proposition 4).
 - The equivalent loss is non-convex for the truncated loss in Example 3 (see Figure 4), which provides an explanation for the bad performance of uncertainty sampling ([Tifrea et al., 2022](#)).

This discussion underlines that in addition to the surrogate property, we desire the equivalent loss induced by the uncertainty function also has a convexity structure.

3.5 Two more examples

We conclude our discussion of the binary classification problem with two more examples.

Example 4 (Margin loss with margin-based uncertainty induces non-convexity). As noted earlier, all the link functions calculated so far for the equivalent losses have that $\psi(z)$ is of order z^2 as $z \rightarrow 0$. For the standard supervised learning problem, the margin loss (also known as the Hinge loss) has $\psi(z) = z$. In fact, we can calculate the link function for the equivalent loss associated with the margin loss and the margin-based uncertainty as follows. The margin loss is

$$l(\theta; (X, Y)) = \max\{0, 1 - Y \cdot \theta^\top X\}$$

and the margin-based uncertainty is

$$U_\mu(\theta; X) = \frac{1}{1 + \mu|\theta^\top X|}.$$

Then the equivalent loss is

$$\tilde{l}(\theta; (X, Y)) = \begin{cases} \frac{1}{\mu} \log(1 - \mu \cdot Y \cdot \theta^\top X) + \frac{1}{\mu} \log(1 + \mu), & \text{if } Y \cdot \theta^\top X \leq 0; \\ -\frac{1}{\mu} \log(1 + \mu \cdot Y \cdot \theta^\top X) + \frac{1}{\mu} \log(1 + \mu), & \text{if } Y \cdot \theta^\top X \in (0, 1); \\ 0, & \text{if } Y \cdot \theta^\top X \geq 1. \end{cases}$$

And its link function is

$$\psi_\mu(z) = \frac{\log(1 + \mu)}{\mu} \cdot z,$$

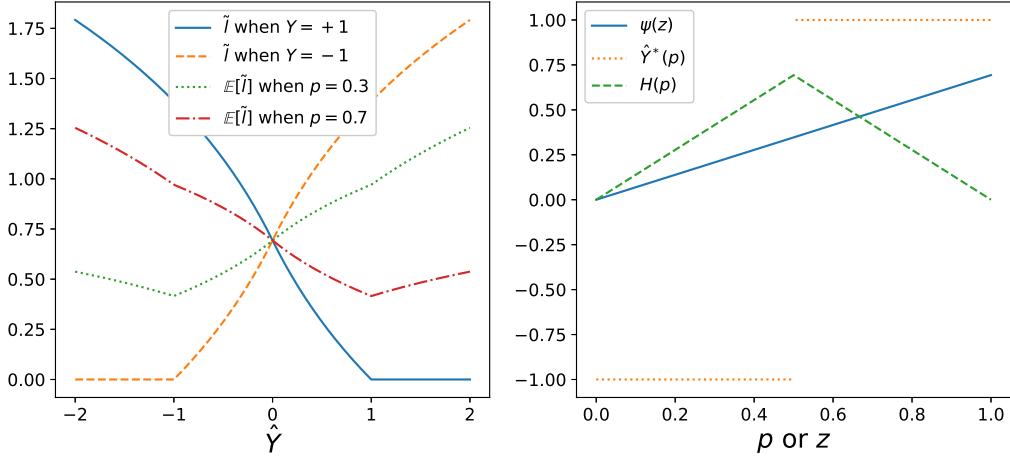


Figure 5: Margin loss with the margin-based uncertainty when $\mu = 0.5$.

which is of the desirable linear order. However, as plotted in Figure 5, the equivalent loss is non-convex with respect to the margin $\theta^\top X$. Thus Proposition 3 no longer applies, and practically, the loss may induce bad local minima. This also justifies the choice of the squared margin loss in (Raj and Bach, 2022). In the following proposition, it establishes that for the margin loss, if the induced equivalent loss is convex, then any differentiable margin-based uncertainty function must be constant.

Proposition 4. *Consider the margin loss and an uncertainty function that can be expressed by $U(\theta; X) = h(|\theta^\top X|)$ where $h(\cdot)$ is a non-increasing, non-negative, and piece-wise differentiable function. Then $h(\cdot)$ must be a constant function,*

$$h(\cdot) \equiv C$$

for some $C > 0$ if the equivalent loss is continuous and convex.

The non-decreasing requirement is natural for that we want to assign a larger uncertainty value to a sample with a smaller margin. The proposition gives a negative result on designing uncertainty functions for the margin loss in that there does not exist a non-trivial uncertainty function that retains the convexity structure for the equivalent loss. While Proposition 3 and Theorem 2 provide positive results on establishing the convergence rate of the uncertainty sampling algorithm, Proposition 4 and Example 3 give negative results on the non-convexity issue associated with some uncertainty functions.

Going beyond analyzing the existing uncertainty functions, we can apply the machinery to derive new uncertainty functions such as the following example.

Example 5 (Exponential loss with exponential uncertainty). The loss function and the uncertainty function are defined by

$$l(\theta; (X, Y)) = \exp(-Y \cdot \theta^\top X).$$

$$U_\mu(\theta; X) = \exp(-\mu|\theta^\top X|).$$

The equivalent loss takes a similar shape as the exponential loss:

$$\tilde{l}_\mu(\theta; (X, Y)) = \begin{cases} \frac{1}{1+\mu} \cdot \exp(-(1+\mu)Y \cdot \theta^\top X) + \frac{\mu}{1+\mu}, & \text{if } Y \cdot \theta^\top X \geq 0; \\ \frac{1}{1-\mu} \cdot \exp(-(1-\mu)Y \cdot \theta^\top X) - \frac{\mu}{1-\mu}, & \text{if } Y \cdot \theta^\top X < 0. \end{cases}$$

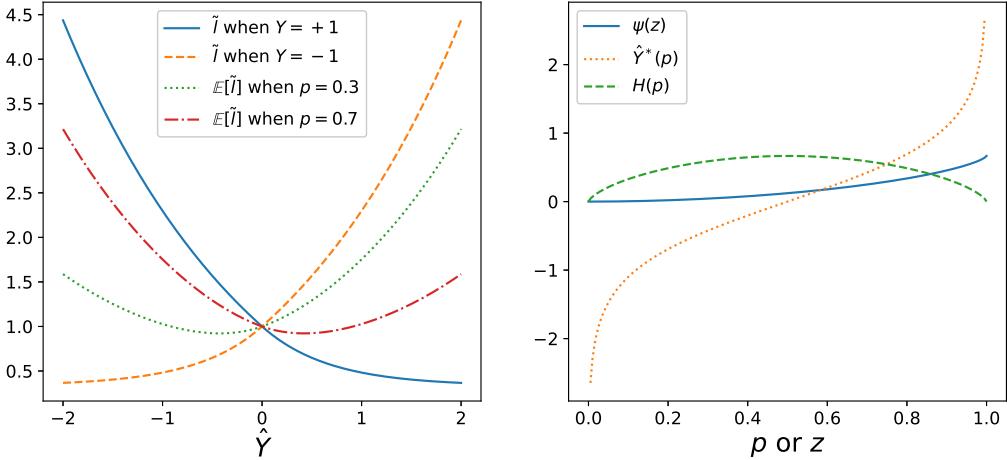


Figure 6: Exponential loss and exponential uncertainty with $\mu = 0.5$.

The link function for the surrogate property is

$$\psi_\mu(z) = \frac{1}{1-\mu^2} \left(1 - \mu z - (1-z)^{\frac{1+\mu}{2}} (1+z)^{\frac{1-\mu}{2}} \right) = z^2 + o(z^2) \quad \text{as } z \rightarrow 0.$$

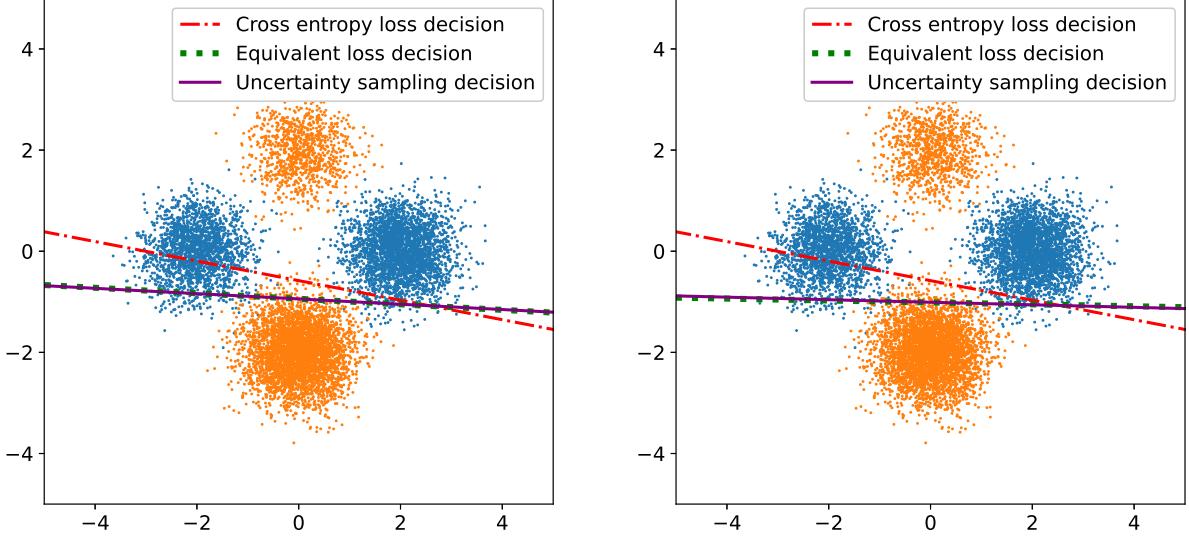
See Figure 6 for a visualization of these functions.

We note that this equivalent property not only maintains the convexity of the exponential loss but also exhibits a strong convexity when both Θ and \mathcal{X} are bounded. This is a property that does not hold for equivalent losses derived upon margin-based loss but can be helpful in accelerating the convergence rate of gradient-based algorithms.

3.6 Numerical illustration

After previous theoretical discussions, we utilize a numerical example to demonstrate the equivalence between the uncertainty sampling and the equivalent loss and the convexity conditions. We adopt the synthetic data generation from [Mussmann and Liang \(2018b\)](#), where the feature points follow a mixture of two-dimensional Gaussian distributions. All the Gaussians are of $(0.5, 0.5)$ standard deviance, where the centers are located at 4 distinct positions: $(-2, 0), (2, 0), (0, -2), (0, 2)$. The percentages of the four Gaussians are 20%, 30%, 40%, 10%, where the former two are aligned with positive labels while the latter two are negative. For each example, we start from random initialization, apply both the original loss minimization and the equivalent loss minimization algorithms on the synthetic data, and plot their final decision boundaries. As for the uncertainty sampling, we also choose the random initial points, set the step size to be small enough (10^{-4}), and run sufficiently many iterations (10^7). The final decision boundaries obtained by the uncertainty sampling are compared with the two empirical risk minimization boundaries.

Figure 7, 8, 9, 10, and 11 show the final decision boundaries obtained by different algorithms. We can observe that the uncertainty sampling algorithm achieves almost the same decision boundary as the equivalent loss minimization rather than the original loss. Besides, Figure 9 and 10 imply that their corresponding equivalent losses are non-convex and of local minimum, which coincides with our theoretical computation. A noteworthy fact is that although we show the non-convexity of the logistic regression model under the cross entropy loss and the probabilistic uncertainties, Figure 7a and 7b show that they might be of no local minimum or be able to avoid from being trapped into them.



(a) Example 1 cross-entropy loss and entropy uncertainty.

(b) Example 1 cross-entropy loss and least confidence uncertainty.

Figure 7: The decision boundaries of the original loss, the equivalent loss, and the uncertainty sampling. The synthetic data are generated from a mixture of two-dimensional Gaussian distributions as in [Mussmann and Liang \(2018b\)](#).

4 Loss as Uncertainty: Multi-Class Classification and Regression

In the previous section, we discuss the problem of binary classification and propose the notion of equivalent loss to verify the properness of an uncertainty function. However, the discussion, along with the uncertainty functions, has been quite specialized to the problem of binary classification and therefore can be hardly applied to the more general multi-class classification and regression problems. In particular, for binary classification, the uncertainty function and the loss function can be expressed by a single-variable function of either the predicted probability q or the margin $\theta^\top X$. While this usually ensures the existence of the equivalent loss \tilde{l} , the structure no longer holds for multi-class classification and regression problems. In this section, we develop a general principle for designing uncertainty functions – “loss as uncertainty”, which umbrellas binary classification, multi-class classification, and regression problems as special cases. The idea is, rather than handcrafting uncertainty functions case-by-case, we propose using *conditional expected loss* as the uncertainty function. Such an uncertainty function endows nice analytical properties for the learning problem, and it provides a guideline for the uncertainty quantification/calibration of a prediction model.

4.1 Loss as uncertainty

We first define the conditional loss which marginalizes Y given the feature X .

Definition 4 (Conditional loss). Define the conditional (expected) loss as

$$L(\theta; X) := \mathbb{E}[l(\theta; (X, Y))|X]$$

where the expectation is taken with respect to the conditional distribution of $Y|X$ with $(X, Y) \sim \mathcal{P}$.

Note that the conditional loss is a function of the parameter θ and the feature X . Suppose we let the uncertainty function simply be the conditional loss. Then we have the equivalent loss being exactly the square of the original loss.

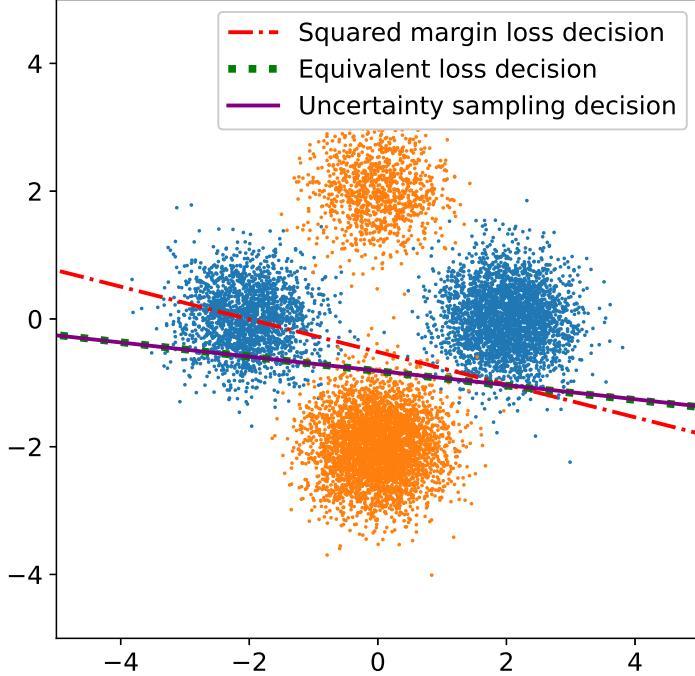


Figure 8: Decision boundaries of Example 2 squared margin loss and margin-based uncertainty when $\mu = 1$.

Proposition 5. Suppose the uncertainty function $U(\theta; X) = L(\theta; X)$. Then Algorithm 1 essentially performs stochastic gradient descent with respect to the loss function $\mathbb{E}[\tilde{L}(\theta; X)]$ where the expectation is with respect to $X \sim \mathcal{P}_X$ and the equivalent loss

$$\tilde{L}(\theta; X) := \frac{1}{2}(L(\theta; X))^2.$$

Compared to Proposition 1, the loss-as-uncertainty design performs SGD against a loss that marginalizes out the label Y . It results in a small twist in the proof, but it is not essential. Importantly, the result holds for all differentiable conditional loss $L(\theta; X)$, and saves us from finding the solution to PDE (1) case-by-case. In other words, the result applies generally to the problem of binary classification, multi-class classification, and regression. It reduces the design of the uncertainty function to a calibration problem of estimating the conditional loss $L(\theta; X)$. In terms of uncertainty sampling for regression problems, a similar uncertainty that measures conditional variance has already been proposed (Settles, 2009). Settles (2009) justifies such a variance uncertainty by showing the equivalence between variance and entropy under the Gaussian distribution assumption, while for more general distributions, the equivalence does not hold. We provide a different but more general explanation that the conditional variance is the conditional loss (when the estimation is the true conditional mean) regardless of the underlying distribution.

We provide the following two motivations for ‘‘loss as uncertainty’’:

Convexity: The design retains the convexity of the original loss. Suppose that the original loss l is non-negative and convex. Then it leads to the non-negativity and convexity of the conditional loss L . Consequently,

$$\frac{\partial^2 \tilde{L}}{\partial \theta^2} = \frac{\partial L}{\partial \theta} \cdot \left(\frac{\partial L}{\partial \theta} \right)^\top + \frac{\partial^2 L}{\partial \theta^2} \succeq 0.$$

More generally, it is easy to verify that the convexity is still retained for \tilde{L} if the uncertainty function

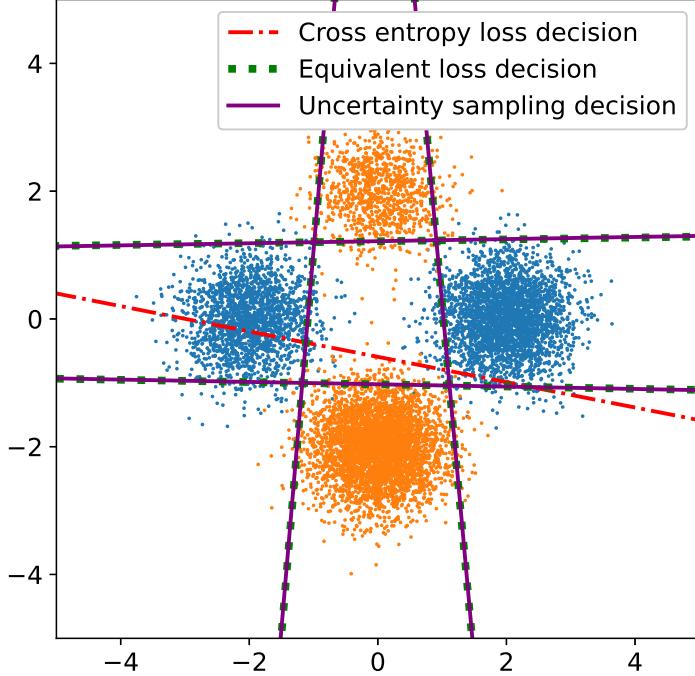


Figure 9: Decision boundaries of Example 2 logistic loss and threshold-based uncertainty when $\gamma = 2$.

$U(\theta; X) = h(L(\theta; X))$ for some non-decreasing and non-negative scalar function $h(\cdot)$.

Existence of solution to (1): The PDE (1) becomes a multi-variate one for multi-class classification for that there will be one predicted probability for each class. And multi-variable functions generally do not have an *indefinite integral*, whereas the single-variable case is guaranteed by the fundamental theorem of calculus. If we aim to find a well-defined equivalent loss that always produces the same gradient as the uncertainty sampling in expectation, a necessary condition is that the path integral of its derivatives $\sum_{j=1}^d U \cdot \frac{\partial l}{\partial \theta_j} d\theta_j$ should depend not on the chosen path but only on the starting and the ending points. Assume that both U and l are smooth functions of θ . From the basics of differential forms and algebraic topology (Bott et al., 1982), such a requirement is equivalent to finding some U such that the exchangeability holds,

$$\frac{\partial U}{\partial \theta_i} \cdot \frac{\partial l}{\partial \theta_j} = \frac{\partial U}{\partial \theta_j} \cdot \frac{\partial l}{\partial \theta_i}, \quad \forall i \neq j,$$

where a natural choice is $U = h(l)$ such that $h(\cdot)$ has an anti-derivative. Consequently, this leads to the choice of $h(\cdot)$ as a non-decreasing and non-negative function with the special case of the identity function. We defer more discussions to Appendix B.5.

4.2 Oracle case

Now we analyze Algorithm 1 with the choice of $U(\theta; X) = L(\theta; X)$. Here we assume the algorithm has an oracle access to $L(\theta; X)$. Note that this entails the knowledge of the conditional distribution $\mathcal{P}_{Y|X}$. In the next subsection, we analyze the case where such oracle is not available and one needs to calibrate the conditional loss to obtain an estimate of $L(\theta; X)$.

With slight overload of notation, we write

$$L(f) = \mathbb{E}[l(f(X), X)|X], \tilde{L}(f) = \frac{1}{2} (\mathbb{E}[l(f(X), X)|X])^2 = \frac{1}{2} L^2(f)$$

for some hypothesis f .

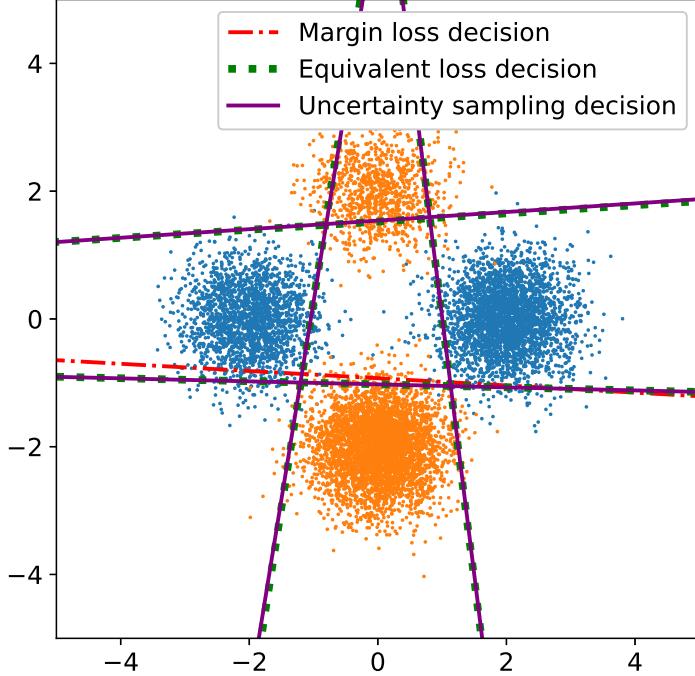


Figure 10: Decision boundaries of Example 4 margin loss and margin-based uncertainty when $\mu = 10$.

Also, without loss of generality, we assume the loss is non-negative. Then for any two hypotheses f and g , we have

$$\tilde{L}(f) - \tilde{L}(g) = \frac{1}{2}L^2(f) - \frac{1}{2}L^2(g) = \frac{1}{2}(L(f) + L(g))(L(f) - L(g)) \geq \frac{1}{2}(L(f) - L(g))^2 \quad (3)$$

where the last inequality comes from the non-negativeness of L .

Proposition 6 (Loss as uncertainty). *For any measurable hypothesis f , we have the following bound for $U(\theta; X) = L(\theta; X)$,*

$$\mathbb{E}[L(f)] - \inf_{g \in \mathcal{G}} \mathbb{E}[L(g)] \leq \sqrt{2 \left(\mathbb{E}[\tilde{L}(f)] - \inf_{g \in \mathcal{G}} \mathbb{E}[\tilde{L}(g)] \right)}$$

where \mathcal{G} denotes the class of all measurable functions as before, and the expectation is taken with respect to $X \sim \mathcal{P}_X$.

Proposition 6 presents the link function between \tilde{L} and L , and this gives a handle of transforming a performance guarantee with respect to the squared conditional loss \tilde{L} to that with respect to an original loss L . Then one can derive similar results as Proposition 3 and Theorem 2.

Furthermore, a careful examination of the derivation in (3) leads to an improved link function, and consequently a faster convergence rate. Let

$$g^* := \arg \min_{g \in \mathcal{G}} \mathbb{E}[L(g)]$$

denotes the best measurable hypothesis, and

$$\epsilon^* := \arg \min_{x \in \mathcal{X}} \mathbb{E}[l(g^*(X), X) | X = x]$$

be the pointwise minimum conditional risk. Then the following proposition expresses the link function with ϵ^* .

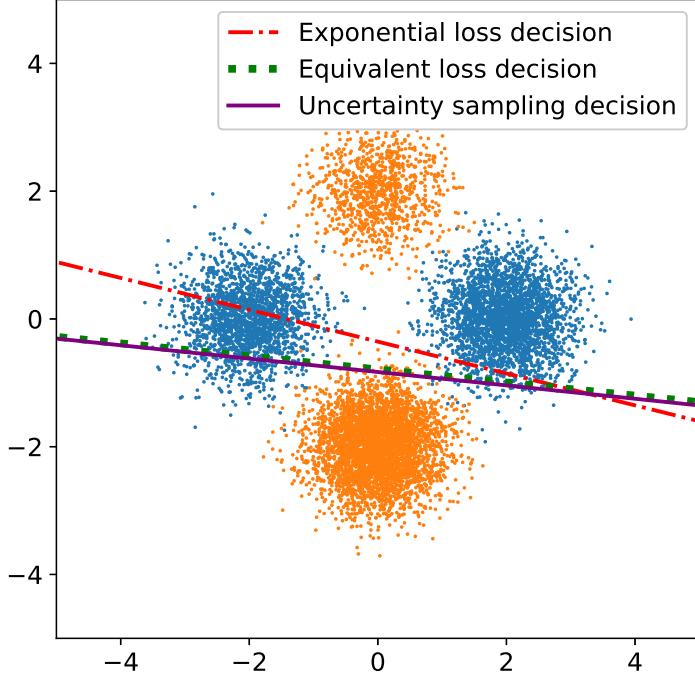


Figure 11: Decision boundaries of Example 5 exponential loss and exponential uncertainty when $\mu = 0.9$.

Proposition 7 (Improved link function and convergence rate). *Under the same setup as Proposition 6, we have*

$$\mathbb{E}[L(f)] - \inf_{g \in \mathcal{G}} \mathbb{E}[L(g)] \leq \frac{2}{\epsilon^*} \cdot \left(\mathbb{E}[\tilde{L}(f)] - \inf_{g \in \mathcal{G}} \mathbb{E}[\tilde{L}(g)] \right).$$

The error bound in Proposition 7 becomes smaller when ϵ^* grows larger, i.e., the data become more noisy and inseparable. This seems to contradict the results of (Mussmann and Liang, 2018a; Tifrea et al., 2022) that the data efficiency of uncertainty sampling algorithms is in strong negative correlation with the error rate of the final classifier. However, we should note that Proposition 7 is stated with respect to the excessive risks' relationships of any hypothesis f rather than the excessive risk itself, while the latter term is dealt by the SGD's convergence analysis as in Proposition 3. The convergence analysis is made with respect to the number of periods/observed features T rather than the number of queried samples. If the data become more separable from the decision boundary, the expected loss as the querying probability will decrease, leading to a smaller number of queries and higher data efficiency; thus it reconciles Mussmann and Liang (2018a)'s observation.

Results such as Proposition 6 and Proposition 7 are not restricted to the binary classification problem but are generally applicable to the multi-class classification problem and the regression problem. While the existing development of uncertainty sampling algorithms has mainly focused on the classification problem, few uncertainty measurements have been proposed for the regression problem. Our result here gives a pointer for such development; for example, one can use the estimated mean-squared error itself as the uncertainty measure for the regression problem.

4.3 Estimated loss and loss calibration

The analysis of the oracle case in previous can also be adapted to a setting where one uses the estimated conditional loss as uncertainty. Specifically, consider

$$U(\theta; X) = \hat{L}(\theta; X)$$

where $\hat{L}(\theta; X)$ is an estimate of $L(\theta; X)$. Then although the equivalent loss relation does not hold exactly, one can still analyze the estimation error of Algorithm 1.

Suppose the estimates satisfy

$$\mathbb{E} \left[|\hat{L}(\theta_t; X) - L(\theta_t; X)| \right] \leq \delta_t \quad (4)$$

where the expectation is taken with respect to both θ_t and $X \sim \mathcal{P}_X$ that is independent of θ_t .

Theorem 3 (Convergence rate under estimated conditional loss). *Let $U(\theta; X) = \hat{L}(\theta; X) \in [0, 1]$ such that (4) holds. Under the same condition as Proposition 3, Algorithm 1 yields the following bound*

$$\mathbb{E} \left[\tilde{L}(\bar{\theta}_{T+1}; X) \right] \leq \min_{\theta \in \Theta} \mathbb{E} \left[\tilde{L}(\theta; X) \right] + \frac{GD}{\sqrt{T}} + \frac{D}{T} \sum_{t=1}^T \delta_t,$$

where the expectation is taken with respect to both X and $\bar{\theta}_{T+1}$.

The estimate $\hat{L}(\theta_t; X)$ can be obtained from a separate validation dataset by adapting uncertainty quantification methods (Kuleshov et al., 2018; Kumar et al., 2019; Hüllermeier and Waegeman, 2021; Foygel Barber et al., 2021). We note that compared to the model calibration literature, the condition (4) aims for an *individual calibration* objective in that it measures the calibration/estimation error for each X , and then takes expectation, rather than a *population/average calibration* or *group calibration* objective.

5 Pool-Based Setting

In this section, we analyze the uncertainty sampling algorithm under the pool-based setting and continue to adopt the conditional loss as the uncertainty function. Different from the stream-based setting, the features for all the samples are given at the beginning. To distinguish between the number of samples and the number of steps for the gradient descent algorithm, we use $i = 1, \dots, n$ to index the samples and $t = 1, \dots, T$ to index the gradient descent time steps.

Algorithm 2 presents the pool-based uncertainty sampling algorithm. At each time step, the algorithm calculates the uncertainty for each sample in the data pool \mathcal{D}_n given the current model parameter θ_t . Then the algorithm samples an index according to the probability distribution proportional to the uncertainty and queries the label of the sampled index. Based on this new label, the algorithm updates the model parameter via gradient descent.

5.1 Repeated-query v.s. single-query

For the pool-based setting in our paper, we consider a repeated-query setting where the learner may query the same sample X_i multiple times. Practically, this captures the situation where different human experts may provide different labels for the same sample feature X .

Proposition 8. *With the uncertainty function $U(\theta; X) = L(\theta; X)$ and a proper choice of the step size η_t , Algorithm 2 essentially performs stochastic gradient descent to minimize*

$$\mathbb{E}_{\hat{\mathcal{P}}_X^n} \left[\tilde{L}(\theta; X) \right] \coloneqq \frac{1}{n} \sum_{i=1}^n (\mathbb{E} [l(\theta; (X, Y)) | X = X_i])^2 \quad (5)$$

where the subscript $\hat{\mathcal{P}}_X^n$ denotes the empirical distribution of \mathcal{D}_n^X .

Algorithm 2 Uncertainty sampling with gradient descent update (pool-based version)

Input: Unlabeled dataset $\mathcal{D}_n^X = \{X_i\}_{i=1}^n$, step size $\{\eta_t\}_{t=1}^T > 0$, uncertainty function $U(\theta; X)$

- 1: Initialize θ_1 ; $\bar{\theta}_1 \leftarrow \theta_1$
- 2: **for** $t = 1, \dots, T$ **do**
- 3: Calculate the uncertainty $U(\theta_t; X_i)$ for each $X_i \in \mathcal{D}_n$
- 4: Sample $i_t \in [n]$ according to the probability distribution $\propto U(\theta_t; X_i)$
- 5: Query a label Y_t of X_{i_t}
- 6: Update the parameter via gradient descent

$$\theta_{t+1} \leftarrow \theta_t - \eta_t \cdot \frac{\partial l(\theta; (X_{i_t}, Y_t))}{\partial \theta} \Big|_{\theta=\theta_t}$$

$$7: \quad \bar{\theta}_{t+1} \leftarrow (1 - \frac{1}{t+1})\bar{\theta}_t + \frac{1}{t+1}\theta_{t+1}$$

8: **end for**

Output: $\bar{\theta}_{T+1}$

We remark that the choice of the step size involves an adjustment based on the normalizer of the probability distribution,

$$S_t = \sum_{i=1}^n U(\theta_t; X_i).$$

This ensures the length of the step size does not scale with the uncertainty level. We defer more details to the proof in Appendix B.9.

The repeated-query setting is entailed by the objective (5), which optimizes the empirical conditional loss that marginalizes out Y . In theory, the analysis still goes through for the single-query setting, and accordingly, Algorithm 2 performs SGD to minimize

$$\frac{1}{n} \sum_{i=1}^n (l(\theta; (X, Y)))^2.$$

But this will require $U(\theta; X_i) = l(\theta; (X_i, Y_i))$ for $i \in [n]$. This uncertainty function is not as practical for that it depends on the realized label Y_i , and thus it will be generally hard to estimate this quantity without observing Y_i .

5.2 Theoretical analysis

We describe a general challenge in analyzing pool-based uncertainty sampling. The algorithm dynamic works as follows:

$$\theta_t \rightarrow (X_t, Y_t) \rightarrow \theta_{t+1}.$$

At each time t , we observe a new sample and use the sample to update the model parameter. If (X_t, Y_t) is sampled uniformly from the data pool or from the distribution \mathcal{P} , it can be viewed as an exogenous randomness. Such an exogeneity provides great convenience in analyzing the convergence behavior of θ_t under online algorithms. However, for the uncertainty sampling algorithm, the parameter θ_t determines the uncertainty value and consequently the sampling distribution of (X_t, Y_t) ; and this makes the update dynamics more complicated. In this light, our perspective of equivalent loss and the notion of loss as uncertainty becomes helpful. Specifically, while the sampling distribution of (X_t, Y_t) bears dependence on the parameter θ_t , one can absorb the sampling distribution into the gradient and make the sample (X_t, Y_t) exogenous again, but against an alternative objective of \tilde{l} or \tilde{L} .

Therefore, the error bound of $\bar{\theta}_{T+1}$ in Algorithm 2 can be derived in a few standard steps:

- Establish a convergence result like Proposition 3 for Algorithm 2. Note that the objective here is the empirical conditional loss but no longer the expected loss, but this will not change the nature of the analysis.
- Develop a generalization argument to connect the empirical condition loss with the expected loss.
- Use the link function argument to transform the excessive risk bound under \tilde{L} to the original loss L or binary loss L_{01} .

5.3 Numerical experiments

To show that our *loss as uncertainty* principle can be a practical option for the multi-class classification and the regression problems, we test our pool-based algorithm Algorithm 2 (denoted by *active*) on 5 UCI datasets (Kelly et al., 2021) in comparison with the uniform sampling algorithm (marked as *passive*). Our implementation of Algorithm 2 drops out the adjusting term S_t to simplify the step sizes to be constant. The source code and data can be found on <https://github.com/liushangnoname/Uncertainty-Sampling>.

Estimation of loss: In order to get an estimation of the conditional expected loss, we carry out the non-parametric estimator in Liu et al. (2023) with a little adaptation to the active learning setting. Liu et al. (2023) is focused on supervised learning, where they split out an independent validation set to calibrate the error. Their argument is that the independence of the validation set is crucial to avoid an underestimated error, while in our active learning setting, we can still apply the “loss as uncertainty” principle even if the error estimation is not calibrated as long as the estimation reflects the relative quantitative relationships. On the contrary, the preciousness of the labels encourages us to utilize every label for gradient descent training. We henceforth do not split the labels into validation and training in our active learning implementation.

Multi-class classification: We test two types of classifiers: logistic regression with cross-entropy loss and support vector machine with margin loss. We choose 3 datasets where the linear classifiers get acceptable performance on prediction accuracy, named Dry Bean, Waveform Version 1, and Covertype. For the Covertype dataset, we randomly pick 10000 samples from the whole set. We run 30 trials, where the dataset is randomly split according to an 80-20 proportion for training and testing each time. For each trial, the uncertainty sampling and the uniform sampling share the same Gaussian initialization and the same constant step sizes. The averaged accuracy v.s. step numbers result is shown in Figure 12, 13, and 14. For the Dry Bean and the Covertype datasets, uncertainty sampling with the “loss as uncertainty” principle outperforms uniform sampling, while for the Waveform dataset, the performances are similar.

Regression: As for the regression problem, we test the kernelized linear regression model, where the kernel is chosen among linear, polynomial, and radial basis functions. Two datasets named Forest Fires and QSAR Aquatic Toxicity are examined, where the datasets are chosen so that the kernelized linear regression is of acceptable performance and computational cost. The results are shown in Figure 15. Although for the QSAR dataset, our uncertainty sampling does not achieve dominant performance, it still reaches the same level as the uniform sampling. For the Forest Fires, our algorithm shows its superiority to passive learning.

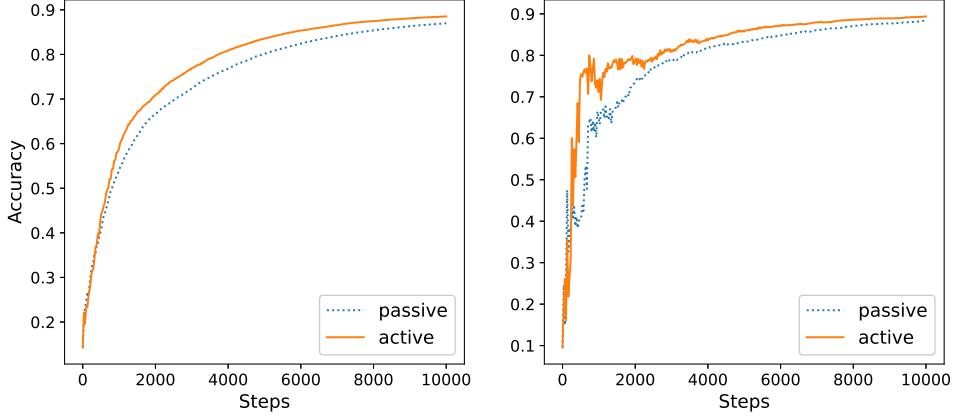


Figure 12: Accuracy v.s. step number curves for the Dry Bean dataset. The accuracy is averaged across 30 independent trials with an 80-20 train-test split. Left: logistic regression. Right: support vector machine.

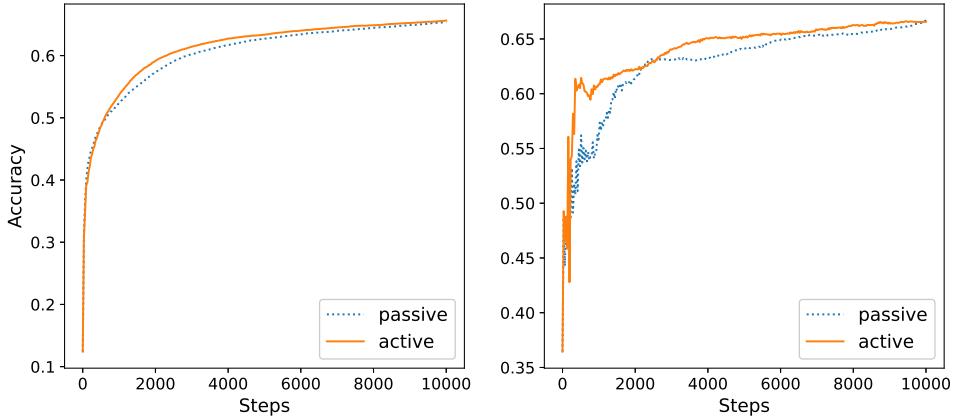


Figure 13: Accuracy v.s. step number curves for the Covertype dataset. Left: logistic regression. Right: support vector machine.

6 Other Variants of Uncertainty Sampling

6.1 Exponential loss as uncertainty

Now we explore an alternative choice for the uncertainty function for Algorithm 2 where

$$U(\theta; X) = \exp(L(\theta; X)).$$

To generate some intuitions, we first make some derivations under the oracle case where we have direct access to $\mathbb{E}_{\hat{P}_n}[l(\theta; (X, Y))|X = X_i] = l(\theta; (X_i, Y_i))$. To simplify the notation, we abbreviate the gradient we take at time step t to g_t :

$$g_t := \left. \frac{\partial l(\theta; (X_{it}, Y_{at}))}{\partial \theta} \right|_{\theta=\theta_t}.$$

If we define the uncertainty as the exponential of the conditional expected loss and utilize the structure

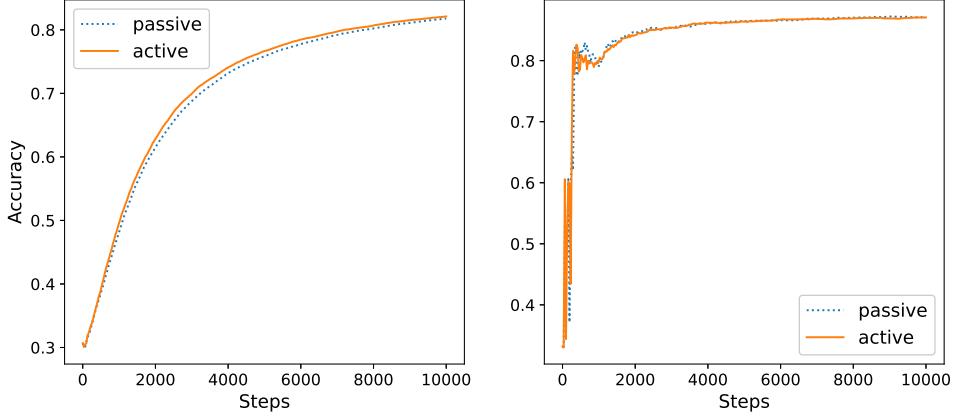


Figure 14: Accuracy v.s. step number curves for the Waveform dataset. Left: logistic regression. Right: support vector machine.

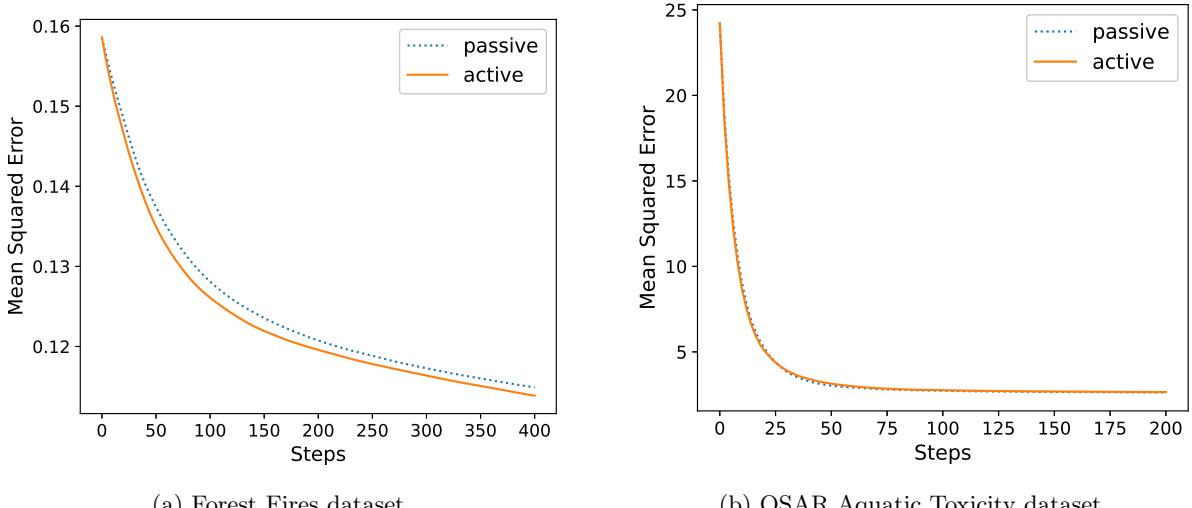


Figure 15: Mean squared error v.s. step number curves for the regression task. The mean squared error is averaged across 30 independent trials with an 80-20 train-test split. Left: Forest Fires dataset. Right: QSAR Aquatic Toxicity dataset.

of the softmax distribution, then the conditional expectation of the gradient g_t is

$$\mathbb{E}[g_t | \mathcal{F}_t] = \sum_{i=1}^n \frac{\exp(l(\theta_t; (X_i, Y_i))) \cdot \nabla_\theta l(\theta_t; (X_i, Y_i))}{\sum_{j=1}^n \exp(l(\theta_t; (X_j, Y_j)))} = \nabla_\theta \left(\log \left(\sum_{i=1}^n \exp(l(\theta_t; (X_i, Y_i))) \right) \right).$$

By viewing the overall equivalent loss as the log-sum-exp (softmax) function

$$\tilde{L} := \log \left(\sum_{i=1}^n \exp(l(\theta; (X_i, Y_i))) \right),$$

we have

$$\mathbb{E}[g_t | \mathcal{F}_t] = \nabla_\theta \tilde{L}(\theta_t).$$

Proposition 9. *With the uncertainty function $U(\theta; X) = \exp(L(\theta; X))$, Algorithm 2 essentially performs*

stochastic gradient descent to minimize

$$\log \left(\sum_{i=1}^n \exp(L(\theta; X_i)) \right).$$

We note that the objective in Proposition 9 is risk-sensitive rather than risk-neutral such as expectation. In the following section, we continue to study two more variants of uncertainty sampling that relate to the risk profile and robustness of the underlying loss.

6.2 Top- k -max uncertainty sampling

Some variant of the uncertainty sampling algorithm queries the most uncertain samples, in replacement of the *sampling* step in Algorithm 2. Algorithm 3 describes such a variant: at each time step, the algorithm randomly picks one of the m most uncertain samples and queries the sample. Then the algorithm performs a gradient descent step based on the queried sample.

Algorithm 3 Top- k -max uncertainty sampling (pool-based setting)

Input: Unlabeled dataset $\mathcal{D}_n = \{X_i\}_{i=1}^n$, step size $\{\eta_t\}_{t=1}^T > 0$, uncertainty function $U(\theta; X)$, $m \in \mathbb{N}$

- 1: Initialize θ_1
- 2: **for** $t = 1, \dots, T$ **do**
- 3: Calculate the uncertainty $U(\theta_t; X_i)$ for each $X_i \in \mathcal{D}_n$
- 4: Let $\{i_{t1}, \dots, i_{tn}\}$ be a permutation of $\{1, 2, \dots, n\}$ such that

$$U(\theta_t; X_{i_{t1}}) \geq U(\theta_t; X_{i_{t2}}) \geq \dots \geq U(\theta_t; X_{i_{tn}})$$

- 5: Randomly sample i_t from $\{i_{t1}, \dots, i_{tm}\}$ – the m largest uncertainty indices
- 6: Query a label Y_t of X_{i_t}
- 7: Update the parameter via gradient descent

$$\theta_{t+1} \leftarrow \theta_t - \eta_t \cdot \frac{\partial l(\theta; (X_{i_t}, Y_t))}{\partial \theta} \Big|_{\theta=\theta_t}$$

- 8: **end for**

Output: θ_{T+1}

Proposition 10. *With the uncertainty function $U(\theta; X) = L(\theta; X)$, Algorithm 3 essentially performs stochastic gradient descent to minimize*

$$\text{CVaR}_{\hat{\mathcal{P}}_X^n}^\alpha (\mathbb{E}[l(\theta; (X, Y)) | X]) \quad (6)$$

where the subscript $\hat{\mathcal{P}}_X^n$ denotes the empirical distribution of \mathcal{D}_n^X and the risk level $\alpha = \frac{m}{n}$.

Proposition 10 gives the objective of Algorithm 3 when using the conditional loss as the uncertainty function. Here the conditional value-at-risk is defined by

$$\text{CVaR}_{\mathcal{Q}}^\alpha(\xi) := \mathbb{E}[\xi | \xi \geq \mathcal{Q}_\alpha^{-1}(\xi)]$$

where the underlying random variable ξ follows the distribution \mathcal{Q} , and $\mathcal{Q}_\alpha^{-1}(\xi)$ denotes the α -quantile of ξ . Note that Algorithm 3 uses loss as uncertainty, and by querying the most uncertain samples, it focuses on the samples with the largest conditional loss, which naturally leads to the CVaR objective. We remark that the CVaR is a risk-sensitive objective rather than a risk-neutral one such as expectation/average.

While the result is presented for the oracle case of $U(\theta; X) = L(\theta; X)$, we may expect similar risk-sensitive behavior for the uncertainty sampling algorithm when the used $U(\theta; X)$ is strongly correlated with $L(\theta; X)$. Also, the risk level $\alpha = \frac{m}{n}$ partly explains why the arg-max strategy (where $m = 1$) may have volatile behavior: it may focus on the very tail part of the loss.

6.3 Distributionally robust optimization as a variant of uncertainty sampling

In this section, we establish some equivalence between distributionally robust optimization under χ^2 -divergence and a variant of uncertainty sampling. Algorithm 4 implements a mixture of uniform sampling and uncertainty sampling (Algorithm 3). At each time step, the algorithm queries a sample uniformly randomly with probability $1 - \gamma$, and follows the top- k -max uncertainty sampling with probability γ . It is a natural algorithm in that it softly combines uncertainty sampling with the standard learning procedure of uniform sampling.

Algorithm 4 Mixture of uniform and uncertainty sampling (pool-based setting)

Input: Unlabeled dataset $\mathcal{D}_n = \{X_i\}_{i=1}^n$, step size $\{\eta_t\}_{t=1}^T > 0$, uncertainty function $U(\theta; X)$, threshold $\gamma \in (0, 1)$, $m \in \mathbb{N}$

```

1: Initialize  $\theta_1$ 
2: for  $t = 1, \dots, T$  do
3:   Generate  $\xi_t \sim \text{Unif}[0, 1]$ 
4:   if  $\xi_t \leq 1 - \gamma$  then
5:     %% with probability  $1 - \gamma$ , do uniform sampling
6:     Randomly pick an index  $i_t$  from  $\{1, 2, \dots, n\}$ 
7:   else
8:     %% with probability  $\gamma$ , do uncertainty sampling
9:     Calculate the uncertainty  $U(\theta_t; X_i)$  for each  $X_i \in \mathcal{D}_n$ 
10:    Let  $\{i_{t1}, \dots, i_{tn}\}$  be a permutation of  $\{1, 2, \dots, n\}$  such that

```

$$U(\theta_t; X_{i_{t1}}) \geq U(\theta_t; X_{i_{t2}}) \geq \dots \geq U(\theta_t; X_{i_{tn}})$$

```

11:    Randomly sample  $i_t$  from  $\{i_{t1}, \dots, i_{tm}\}$  – the  $m$  largest uncertainty indices
12:  end if
13:  Query a label  $Y_t$  of  $X_{i_t}$ 
14:  Update the parameter via gradient descent

```

$$\theta_{t+1} \leftarrow \theta_t - \eta_t \cdot \frac{\partial l(\theta; (X_{i_t}, Y_t))}{\partial \theta} \Big|_{\theta=\theta_t}$$

15: **end for**

Output: θ_{T+1}

Proposition 11. *With the uncertainty function $U(\theta; X) = L(\theta; X)$, Algorithm 4 essentially optimize the following distributionally robust objective*

$$\max_{\mathbf{p} \in \mathcal{U}(\mathcal{P})} \sum_{i=1}^n p_i \cdot \mathbb{E}[l(\theta; (X, Y)) | X = X_i], \quad (7)$$

where $\mathcal{U}(\mathcal{P})$ is the ambiguity set for the probability vector $\mathbf{p} = (p_1, \dots, p_n)$. It is defined by

$$\mathcal{U}(\mathcal{P}) := \left\{ \mathbf{p} \left| \sum_{i=1}^n p_i = 1, 0 \leq p_i \leq \frac{m + (n-m)\gamma}{mn}, D_\phi\left(\mathbf{p} \middle\| \left(\frac{1}{n}, \dots, \frac{1}{n}\right)^\top\right) \leq \frac{\gamma^2 n(n-m)}{2nm} \right. \right\},$$

where $D_\phi(\mathbf{p} \parallel \mathbf{q}) = \sum_{i=1}^n q_i \phi\left(\frac{p_i}{q_i}\right)$ is the ϕ -divergence with $\phi(z) = \frac{1}{2}(z-1)^2$.

Proposition 11 gives the objective of the mixture of uncertainty sampling and uniform sampling. Note that when we employ loss as uncertainty, the samples with larger losses will be more frequently sampled and optimized over. This intuition is aligned with the design of the above distributionally robust optimization formulation which assigns larger weights to samples with larger losses. There is a small difference between these two in that uncertainty sampling uses the conditional expected loss whereas the robust objective uses the empirical loss, yet the difference is not essential. The distributionally robust objective (7) bears certain equivalence to the variance regularized objective (Namkoong and Duchi, 2017; Duchi et al., 2021)

$$\frac{1}{n} \sum_{i=1}^n L(\theta; X_i) + \sqrt{\frac{\gamma^2(n-m)}{m} \cdot \text{Var}_{\hat{\mathcal{P}}_X^n}(L(\theta; X))},$$

where the latter objective (called variance regularized empirical risk) can act as a high probability upper bound for the population risk (Bartlett et al., 2002; Maurer and Pontil, 2009). To avoid a vain upper bound, the theory of distributionally robust optimization suggests a choice of $\gamma = \sqrt{\frac{Cm}{n(n-m)}}$ so that $\frac{\gamma^2(n-m)}{m} = \frac{C}{n}$, and this will render Algorithm 4 a strong tendency to the uniform sampling.

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A Derivation of equivalent losses and surrogate link function

This section will present the detailed calculations of the equivalent losses and the surrogate link functions of all the listed examples in previous sections. The subscript of μ or γ will sometimes be omitted for simplicity when the text is clear.

A.1 Equivalent loss in Section 3.2

Example 1 (Equivalent loss of (Dagan and Engelson, 1995; Culotta and McCallum, 2005)). Both the loss and the uncertainty function can be expressed as a function of predicted probability $q(X; \theta)$. By the chain rule,

$$\begin{aligned}\frac{\partial \tilde{l}}{\partial \theta} &= \frac{\partial \tilde{l}}{\partial q} \cdot \frac{\partial q}{\partial \theta}, \\ U \cdot \frac{\partial l}{\partial \theta} &= U \cdot \frac{\partial l}{\partial q} \cdot \frac{\partial q}{\partial \theta}.\end{aligned}$$

Hence if we can find some \tilde{l} such that

$$\frac{\partial \tilde{l}}{\partial q} = U \cdot \frac{\partial l}{\partial q},$$

then we have accomplished the task.

The indicator function $\mathbb{1}\{Y = +1\}$ where $Y \in \{-1, +1\}$ can be transformed into $\frac{Y+1}{2}$ which we denote as p by a slightly abuse of notations. Then the derivative of the original cross-entropy loss can be presented as

$$\frac{\partial l}{\partial q} = -\frac{p}{q} + \frac{1-p}{1-q} = \frac{q-p}{q(1-q)}.$$

We start with the entropy uncertainty $U = -q \log(q) - (1-q) \log(1-q)$ in Dagan and Engelson (1995).

$$\begin{aligned}U(q) \cdot \frac{\partial l}{\partial q} &= p \log(q) - (1-p) \log(1-q) - (1-p) \cdot \frac{q \log(q)}{1-q} + p \cdot \frac{(1-q) \log(1-q)}{q} \\ &= p \log(q) - (1-p) \log(1-q) - (1-p) \cdot \frac{(q-1) \log(q) + \log(q)}{1-q} + p \cdot \frac{-q \log(1-q) + \log(1-q)}{q} \\ &= p \log(q) - (1-p) \log(1-q) + (1-p) \log(q) - (1-p) \cdot \frac{\log(q)}{1-q} - p \log(1-q) + p \cdot \frac{\log(1-q)}{q} \\ &= \log(q) - \log(1-q) - (1-p) \cdot \frac{\log(q)}{1-q} + p \cdot \frac{\log(1-q)}{q}.\end{aligned}$$

Then by calculating its indefinite integral, we have

$$\int U(q) \cdot \frac{\partial l}{\partial q} dq = q \log(q) + (1-q) \log(1-q) - p \cdot \text{Li}_2(q) - (1-p) \cdot \text{Li}_2(1-q) + C,$$

where $\text{Li}_2(z)$ is the Spence's function,

$$\text{Li}_2(z) = - \int_0^z \frac{\log(1-z)}{z} dz.$$

Since we are interested in the excessive risk (which is the expected difference between those hypotheses and the optimal measurable function), the selection of C does not matter. We simply select $C = \text{Li}_2(1) = \frac{\pi^2}{6}$ to make the equivalent loss vanish at $p = q = 0$ and $p = q = 1$, which yields the equivalent loss \tilde{l} presented in Section 3.2.

We continue with the least confident uncertainty $U = \min\{q, 1-q\}$ in Culotta and McCallum (2005).

For $q \in [0, \frac{1}{2}]$, we have

$$\begin{aligned} U(q) \cdot \frac{\partial l}{\partial q} &= \frac{q-p}{1-q} \\ &= \frac{q-1+1-p}{1-q} \\ &= -1 + \frac{1-p}{1-q}. \end{aligned}$$

Its indefinite integral is simple:

$$\int U(q) \cdot \frac{\partial l}{\partial q} dq = -q - (1-p) \log(1-q) + C, \quad \forall q \in [0, 0.5].$$

Similarly, we can compute the indefinite integral for $q \in [0.5, 1]$:

$$\int U(q) \cdot \frac{\partial l}{\partial q} dq = q - p \log(q) + C, \quad \forall q \in [0.5, 1].$$

The equivalent loss function is piece-wise continuous. We select the constants properly to avoid the jump discontinuity at $q = \frac{1}{2}$. To let the values at $q = \frac{1}{2}$ match each other, we select the constants so that

$$\tilde{l} = \begin{cases} -(1-p) \cdot \log(2(1-q)) - q + \log(2), & \text{if } q < 0.5; \\ -p \cdot \log(2q) - (1-q) + \log(2), & \text{if } q \geq 0.5. \end{cases}$$

Again, we don't choose the overall constant deliberately. The $\log(2)$ term is simply to make the equivalent loss vanish at $p = q = 0$ and $p = q = 1$.

Example 2 (Equivalent loss of (Raj and Bach, 2022)). For the SVM-based methods, both the loss and the uncertainty function can be expressed as a function of $Y \cdot \hat{Y}$, where $\hat{Y} = \theta^\top X$. By the similar chain rule arguments in Example 1, we can find the equivalent loss with respect to θ as long as we can find that with respect to $Y \cdot \hat{Y}$. To simplify the notations, we denote $Y \cdot \hat{Y} = Y\theta^\top X$ by s . As a reminder, we again state the squared Hinge loss

$$l(s) = \begin{cases} (1-s)^2, & \text{if } s \leq 1; \\ 0, & \text{if } s \geq 1, \end{cases}$$

and the uncertainty function

$$U_\mu(s) = \begin{cases} (1-\mu s)^{-1}, & \text{if } s \leq 0; \\ (1+\mu s)^{-1}, & \text{if } s \geq 0. \end{cases}$$

We compute the amount $U \cdot \frac{\partial l}{\partial s}$ and its indefinite integral in three parts.

For $s \geq 1$, the result is straightforward: the equivalent loss must be a constant. We select the constant to be zero for some notation convenience.

For $s \in [0, 1]$,

$$\begin{aligned} U_\mu(s) \cdot \frac{\partial l}{\partial s} &= -2(1-s) \cdot \frac{1}{1+\mu s} \\ &= -2 \frac{-\frac{1}{\mu}(\mu s + 1) + \frac{1}{\mu} + 1}{1+\mu s} \\ &= \frac{2}{\mu} - 2\left(\frac{1}{\mu} + 1\right) \cdot \frac{1}{1+\mu s}. \end{aligned}$$

Its indefinite integral is

$$\int U_\mu(s) \cdot \frac{\partial l}{\partial s} ds = \frac{2}{\mu} \cdot s - \frac{2}{\mu} \left(\frac{1}{\mu} + 1 \right) \cdot \log(1 + \mu s) + C,$$

where we select $C = \frac{2}{\mu} - \frac{2}{\mu} \left(\frac{1}{\mu} + 1 \right) \cdot \log(1 + \mu)$ so that the values at $s = 1$ coincide.

For $s \leq 0$, we can complete the calculation similarly:

$$\begin{aligned} U_\mu(s) \cdot \frac{\partial l}{\partial s} &= -2(1-s) \cdot \frac{1}{1-\mu s} \\ &= -2 \frac{-\frac{1}{\mu}(1-\mu s) - \frac{1}{\mu} + 1}{1-\mu s} \\ &= -\frac{2}{\mu} + 2\left(\frac{1}{\mu} - 1\right) \cdot \frac{1}{1-\mu s}. \end{aligned}$$

The indefinite integral is

$$\int U_\mu(s) \cdot \frac{\partial l}{\partial s} ds = -\frac{2}{\mu} \cdot s - \frac{2}{\mu} \left(\frac{1}{\mu} - 1 \right) \cdot \log(1 - \mu s) + C,$$

where the constant is selected to be the same as $s \in [0, 1]$ to match at $s = 0$.

Example 3 (Equivalent loss of Tifrea et al. (2022)). The uncertainty function is probably the simplest case: an indicator function of whether $|s| = |Y \cdot \hat{Y}| = |Y\theta^\top X|$ is no greater than a certain threshold γ . Then for those s 's that satisfy the threshold requirement, the equivalent loss is identical to the original loss (which is the logistic loss, as a reminder), while for those s 's outside the threshold area, the equivalent loss must be constant. We select those constants to avoid abrupt changes at the threshold, resulting in the expressions in Section 3.2.

Example 4 (Equivalent loss of margin loss and margin-based uncertainty). We recall that the original loss and the uncertainty function w.r.t. $s = \hat{Y} \cdot Y$ are

$$l(s) = \max\{0, 1 - s\},$$

$$U_\mu(s) = \begin{cases} \frac{1}{1+\mu s}, & \text{if } s \geq 0; \\ \frac{1}{1-\mu s}, & \text{if } s \leq 0. \end{cases}$$

For the $s \geq 1$ part, the indefinite integral must be constant. We select the constant to be zero.

For the $s \in (0, 1)$ part,

$$U_\mu(s) \cdot \frac{\partial l}{\partial s} = -\frac{1}{1+\mu s},$$

which indicates that

$$\int U_\mu(s) \cdot \frac{\partial l}{\partial s} ds = -\frac{1}{\mu} \log(1 + \mu s) + C, \quad \forall s \geq 0.$$

We select the constant to be $\frac{1}{\mu} \log(1 + \mu)$ so that there is no discontinuity at $s = 1$.

For the $s \leq 0$ part,

$$U_\mu(s) \cdot \frac{\partial l}{\partial s} = -\frac{1}{1-\mu s},$$

resulting in

$$\int U_\mu(s) \cdot \frac{\partial l}{\partial s} ds = \frac{1}{\mu} \log(1 - \mu s) + C, \quad \forall s \geq 0.$$

We set the constant to be $\frac{1}{\mu} \log(1 + \mu)$ to keep the continuity at $s = 0$.

Example 5 (Equivalent loss of exponential loss and exponential uncertainty). Similarly, we state the

original loss and the uncertainty function concerning s :

$$l(s) = \exp(-s),$$

$$U_\mu(s) = \begin{cases} \exp(-\mu s), & \text{if } s \geq 0; \\ \exp(\mu s), & \text{if } s \leq 0. \end{cases}$$

Then, for $s \geq 0$,

$$U_\mu(s) \cdot \frac{\partial l}{\partial s} = -\exp(-(1+\mu)s),$$

of which the indefinite integral is

$$\int U_\mu(s) \cdot \frac{\partial l}{\partial s} ds = \frac{\exp(-(1+\mu)s)}{1+\mu} + C, \quad \forall s \geq 0.$$

We select $C = \frac{\mu}{1+\mu}$ so that the value at $s = 0$ is 1.

On the contrary, for $s \leq 0$,

$$U_\mu(s) \cdot \frac{\partial l}{\partial s} = -\exp(-(1-\mu)s),$$

leading to

$$\int U_\mu(s) \cdot \frac{\partial l}{\partial s} ds = \frac{\exp(-(1-\mu)s)}{1-\mu} + C, \quad \forall s \leq 0.$$

The constant is chosen to be $C = -\frac{\mu}{1-\mu}$ to meet the value at $s = 0$.

A.2 Surrogate property and proof of Proposition 2

In this subsection, we summarize the arguments in [Bartlett et al. \(2006\)](#) and provide their surrogate link function computation method for the margin-based models such as the SVM. Such a surrogate property induces a mini-max optimal bound on the excessive 0-1 risk (see Theorem 3 in [Bartlett et al. \(2006\)](#)). For simplicity, in this subsection, we omit the dependence on X and θ , since all the excessive risk analyses hold for any certain but fixed hypothesis f_θ and sample point $X = x$.

We start with the standard definitions of [Bartlett et al. \(2006\)](#). Assume that the loss $l(\hat{Y}, Y)$ is of the form $l(\hat{Y} \cdot Y)$ (which is the case in all of our examples). By denoting the probability of a positive Y by p , the expected loss induced by predicting \hat{Y} is

$$C_p(\hat{Y}) := pl(\hat{Y}) + (1-p)l(-\hat{Y}).$$

For any fixed probability value p , the inferior of the expected loss is denoted by

$$H(p) := \inf_{\hat{Y}} C_p(\hat{Y}).$$

If we restrict the prediction \hat{Y} to be not Bayes-optimal (that is, to be of the different sign as $2p - 1$) and take the inferior, we get

$$H^-(p) := \inf_{\hat{Y} \cdot (2p-1) \leq 0} C_p(\hat{Y}).$$

Note that a binary classification loss l is said to be classification-calibrated ([Bartlett et al., 2006](#)) (or Fisher consistent ([Lin, 2004](#))) if $H^-(p) > H(p)$ for any $p \neq \frac{1}{2}$.

[Bartlett et al. \(2006\)](#) provide a way of computing the surrogate link function $\psi : [0, 1] \rightarrow \mathbb{R}$ via

$$\tilde{\psi}(z) = H^- \left(\frac{1+z}{2} \right) - H \left(\frac{1+z}{2} \right),$$

$$\psi(z) = \tilde{\psi}^{**}(z),$$

where g^{**} is the Fenchel-Legendre biconjugate of the function g , characterized by

$$\text{epi } g^{**} = \overline{\text{co}} \text{ epi } g.$$

Note that those functions are convex if and only if their Fenchel-Legendre biconjugate are themselves (Bartlett et al., 2006).

Equipped with such a surrogate link function ψ , Bartlett et al. (2006)'s Theorem 3 shows that it can be an upper bound for the excessive 0-1 risk: for any measurable function f and any probability distribution on $\mathcal{X} \times \mathcal{Y} = \mathcal{X} \times \{-1, +1\}$,

$$\psi \left(L_{01(f)} - \inf_{g \in \mathcal{G}} L_{01}(g) \right) \leq \mathbb{E}[l(f(X), Y)] - \inf_{g \in \mathcal{G}} \mathbb{E}[l(g(X), Y)],$$

where \mathcal{G} is the set of all measurable functions.

Such an upper bound is mini-max optimal in the sense that for any non-negative loss l , any $|\mathcal{X}| \geq 2$, any 0-1 risk level $\zeta \in [0, 1]$, and any precision $\epsilon > 0$, there exists a probability distribution on $\mathcal{X} \times \{-1, +1\}$ such that $L_{01(f)} - \inf_{g \in \mathcal{G}} L_{01}(g) = \zeta$, and

$$\psi(\zeta) \leq \mathbb{E}[l(f(X), Y)] - \inf_{g \in \mathcal{G}} \mathbb{E}[l(g(X), Y)] \leq \psi(\zeta) + \epsilon.$$

Equipped with such powerful tools, all we need to do is to find the surrogate link functions of those active learning models. But before we proceed to the particular calculation, we notice that the analysis in Bartlett et al. (2006) is designed for the margin-based models, while our Example 1 is not based on the margin but on the probability. To generalize the arguments to the probabilistic models, we transform the probability into the expectation to enable the margin-based analysis. We denote the predicted expectation of Y in a probabilistic model by

$$\hat{Y} := \hat{\mathbb{E}}[Y] = 2q - 1.$$

Example 1 (Surrogate link function of Dagan and Engelson (1995); Culotta and McCallum (2005)). Remind that the original loss can be expressed as

$$l(\hat{Y} \cdot Y) = -\log \left(\frac{1 + \hat{Y} \cdot Y}{2} \right).$$

The entropy uncertainty is

$$\begin{aligned} U &= -[q \log(q) + (1 - q) \log(1 - q)] \\ &= - \left[\frac{1 + \hat{Y}}{2} \log \left(\frac{1 + \hat{Y}}{2} \right) + \frac{1 - \hat{Y}}{2} \log \left(\frac{1 - \hat{Y}}{2} \right) \right] \\ &= - \left[\frac{1 + \hat{Y} \cdot Y}{2} \log \left(\frac{1 + \hat{Y} \cdot Y}{2} \right) + \frac{1 - \hat{Y} \cdot Y}{2} \log \left(\frac{1 - \hat{Y} \cdot Y}{2} \right) \right]. \end{aligned}$$

Then the equivalent loss is

$$\tilde{l} = \text{Li}_2(1) - \text{Li}_2 \left(\frac{1 + \hat{Y} \cdot Y}{2} \right) + \frac{1}{2} \left[(1 + \hat{Y} \cdot Y) \log \left(\frac{1 + \hat{Y} \cdot Y}{2} \right) + (1 - \hat{Y} \cdot Y) \log \left(\frac{1 - \hat{Y} \cdot Y}{2} \right) \right],$$

where $\text{Li}_2(\cdot)$ is the Spence's function. One can take an easy check that this loss is actually identical to the equivalent loss we provide in Section 3.2 if $\hat{Y} = 2q - 1$.

Notice that U is a non-negative even function that only takes zero value at two endpoints, which implies that minimizing expected \tilde{l} is equivalent to minimizing expected l . The minimizer \hat{Y}^* can be easily obtained at the first-order stationary point

$$p \cdot \left(-\frac{1}{1 + \hat{Y}^*} \right) + (1 - p) \cdot \left(\frac{1}{1 - \hat{Y}^*} \right) = 0,$$

which is $\hat{Y}^* = 2p - 1$. Then

$$H(p) = \text{Li}_2(1) - [p\text{Li}_2(p) + (1 - p)\text{Li}_2(1 - p)] + [p\log(p) + (1 - p)\log(1 - p)],$$

where $\text{Li}_2(\cdot)$ is the Spence's function.

The computation of $H^-(p)$ is simple: the equivalent loss is convex, indicating that the inferior risk of the non-Bayes classifiers must be taken at $\hat{Y} = 0$. Therefore,

$$H^-(p) = \text{Li}_2(1) - \text{Li}_2\left(\frac{1}{2}\right) - \log(2).$$

By definition,

$$\tilde{\psi}(z) = -\text{Li}_2\left(\frac{1}{2}\right) + \frac{1+z}{2} \cdot \text{Li}_2\left(\frac{1+z}{2}\right) + \frac{1-z}{2} \cdot \text{Li}_2\left(\frac{1-z}{2}\right) - \left[\frac{1+z}{2} \cdot \log(1+z) + \frac{1-z}{2} \cdot \log(1-z) \right],$$

whose second-order derivative is

$$\frac{d^2\tilde{\psi}}{dz^2} = -\frac{1}{2} \left[\frac{(1-z)\log\left(\frac{1-z}{2}\right) + (1+z)\log\left(\frac{1+z}{2}\right)}{1-z^2} \right] \geq 0.$$

The convexity implies that

$$\psi(z) = \tilde{\psi}(z).$$

We need to note that the first-order derivative of ψ is

$$\frac{d\psi}{dz} = \frac{1}{2} \left[\text{Li}_2\left(\frac{1+z}{2}\right) - \text{Li}_2\left(\frac{1-z}{2}\right) \right] \geq 0,$$

which is zero if and only if $z = 0$. So the equivalent loss is classification-calibrated, and the surrogate link function around $z = 0$ is approximately

$$\psi(z) \sim \left. \frac{d^2\psi}{dz^2} \right|_{z=0} \cdot z^2 = \log(2) \cdot z^2.$$

Since $\psi(z)$ is bounded at $z \in [0, 1]$, we can conclude that $\psi(z) = \Theta(z^2)$, where Θ is the big theta notation referring to "of the same order as" rather than our denoted set of parameters.

The other example of the least confidence uncertainty $U = \min\{q, 1 - q\}$ can also be analyzed via $\hat{Y} = 2q - 1$. By definition,

$$U = \min \left\{ \frac{1+\hat{Y}}{2}, \frac{1-\hat{Y}}{2} \right\} = \frac{1-|\hat{Y}|}{2}.$$

The equivalent loss with respect to $\hat{Y} \cdot Y$ is

$$\tilde{l}(\hat{Y} \cdot Y) = \begin{cases} \frac{1}{2}(\hat{Y} \cdot Y - 2\log(1 + \hat{Y} \cdot Y)) + \log(2) - \frac{1}{2}, & \text{if } \hat{Y} \cdot Y \geq 0; \\ -\frac{1}{2} \cdot \hat{Y} \cdot Y + \log(2) - \frac{1}{2}, & \text{if } \hat{Y} \cdot Y \leq 0. \end{cases}$$

Again, one can quickly check that this equivalent loss is identical to the form we present in Section 3.2 with $\hat{Y} = 2q - 1$. We don't bother to adjust those constants explicitly to meet the non-negativity or any other requirements, since those equivalent losses are all bounded and we are interested in the excessive risk (which is one expected loss minus another).

W.l.o.g. assume that $p \geq \frac{1}{2}$. Then the first-order stationary point of $C_p(\hat{Y})$ should be

$$-\frac{1}{2} \cdot p \cdot \frac{1 - \hat{Y}^*}{1 + \hat{Y}^*} + \frac{1}{2}(1 - p) = 0,$$

which is $\hat{Y}^* = 2p - 1$. Then

$$H(p) = p \cdot \frac{1}{2} [(2p - 1) - 2\log(2p)] - (1 - p) \cdot \frac{1}{2} (1 - 2p) + \log(2) - \frac{1}{2} = p - \frac{1}{2} - p\log(2p) + \log(2) - \frac{1}{2}, \quad \forall p \geq \frac{1}{2}.$$

For $p \leq \frac{1}{2}$, the optimal \hat{Y}^* remains the same $2p - 1$, while $\forall p \leq \frac{1}{2}$,

$$\begin{aligned} H(p) &= -p \cdot \frac{1}{2}(2p - 1) + (1 - p) \cdot \frac{1}{2} [(1 - 2p) - 2\log(2(1 - p))] + \log(2) - \frac{1}{2} \\ &= \frac{1}{2} - p - (1 - p)\log(2(1 - p)) + \log(2) - \frac{1}{2}. \end{aligned}$$

By the convexity of \tilde{l} ,

$$H^-(p) = C_p(0) = \log(2) - \frac{1}{2}.$$

The derivation of $\tilde{\psi}$ only requires the $p \geq \frac{1}{2}$ part, hence

$$\tilde{\psi}(z) = H^-\left(\frac{1+z}{2}\right) - H\left(\frac{1+z}{2}\right) = -\frac{1}{2}z + \frac{1+z}{2}\log(1+z),$$

of which the second-order derivative is

$$\frac{d^2\tilde{\psi}}{dz^2} = \frac{1}{2(1+z)} \geq 0.$$

By the convexity of $\tilde{\psi}$, we have

$$\psi = \tilde{\psi}.$$

From the first-order derivative of ψ

$$\frac{d\psi}{dz} = \frac{1}{2}\log(1+z),$$

we know that the surrogate link function ψ is only tending to zero if and only if z itself tends zero. Thus, the equivalent loss is classification-calibrated. From the facts that

$$\left. \frac{d\psi}{dz} \right|_{z=0} = 0$$

and

$$\left. \frac{d^2\psi}{dz^2} \right|_{z=0} = \frac{1}{2},$$

we know that

$$\psi(z) \sim \frac{1}{2}z^2$$

around the zero point. From the boundedness of ψ , we can also conclude similarly to the entropy uncertainty case that

$$\psi(z) = \Theta(z^2),$$

where the big theta notation means “of the same order as”.

Example 2 (Surrogate link function of [Raj and Bach \(2022\)](#)). We start with finding the \hat{Y} that minimizes the expected equivalent loss. Remind that the equivalent loss can be written in the form of $\hat{Y} \cdot Y$:

$$\tilde{l}_\mu = \begin{cases} -\frac{2}{\mu}(\frac{1}{\mu} - 1) \log(1 - \mu\hat{Y} \cdot Y) - \frac{2}{\mu}\hat{Y} \cdot Y + C, & \text{if } \hat{Y} \cdot Y \leq 0; \\ -\frac{2}{\mu}(\frac{1}{\mu} + 1) \log(1 + \mu\hat{Y} \cdot Y) + \frac{2}{\mu}\hat{Y} \cdot Y + C, & \text{if } \hat{Y} \cdot Y \in (0, 1); \\ 0, & \text{if } \hat{Y} \cdot Y \geq 1, \end{cases}$$

where $C = \frac{2}{\mu}(\frac{1}{\mu} + 1) \log(1 + \mu) - \frac{2}{\mu}$. By the definition,

$$U_\mu \cdot \frac{\partial l}{\partial \hat{Y}} = \frac{\partial \tilde{l}_\mu}{\partial \hat{Y}}.$$

Since $U_\mu = (1 + \mu|\hat{Y}|)^{-1}$ is a positive and even function, minimizing the expected equivalent loss is identical to minimizing the expected original loss (which is, the squared Hinge loss). By direct calculation (or referring the Example 2 in [Bartlett et al. \(2006\)](#)), the minimizer should be

$$\hat{Y}^* = 2p - 1.$$

Without loss of generality, we assume $p \geq \frac{1}{2}$, which implies that $2p - 1 \geq 0$. Subject to that minimizer,

$$\begin{aligned} H(p) &= C \\ &+ p \cdot \left(-\frac{2}{\mu} \left(\frac{1}{\mu} + 1 \right) \log(1 + \mu(2p - 1)) + \frac{2}{\mu}(2p - 1) \right) \\ &+ (1 - p) \cdot \left(-\frac{2}{\mu} \left(\frac{1}{\mu} - 1 \right) \log(1 + \mu(2p - 1)) + \frac{2}{\mu}(2p - 1) \right). \end{aligned}$$

Since the equivalent loss is convex, the minimized risk of the non-Bayes classifier must be

$$H^-(p) = C_p(0) = C.$$

Hence we have

$$\begin{aligned} \tilde{\psi}(z) &= \frac{1+z}{2} \cdot \left(\frac{2}{\mu} \left(\frac{1}{\mu} + 1 \right) \log(1 + \mu z) + \frac{2}{\mu}z \right) + \frac{1-z}{2} \cdot \left(\frac{2}{\mu} \left(\frac{1}{\mu} - 1 \right) \log(1 + \mu z) + \frac{2}{\mu}z \right) \\ &= \frac{2}{\mu^2} \cdot (1 + \mu z) \log(1 + \mu z) - \frac{2}{\mu}z. \end{aligned}$$

The second-order derivative of $\tilde{\psi}$ is

$$\frac{d^2\tilde{\psi}}{dz^2} = \frac{2}{1 + \mu z} > 0,$$

which guarantees the convexity of $\tilde{\psi}$. Hence

$$\psi = \tilde{\psi}.$$

The first-order derivative of ψ is

$$\frac{d\psi}{dz} = \frac{2}{\mu} \log(1 + \mu z) \geq 0,$$

where the equality holds if and only if $z = 0$ for any $\mu > 0$, indicating the classification-calibration of the equivalent loss \tilde{l} . By a similar Taylor expansion argument, we can conclude that

$$\psi(z) \sim \left. \frac{d^2\psi}{dz^2} \right|_{z=0} \cdot z^2 = 2z^2.$$

Due to the boundedness of the surrogate link function, we have

$$\psi(z) = \Theta(z^2),$$

where the big theta notation stands for “of the same order as”.

Example 3 (Surrogate link function of Tifrea et al. (2022)). We briefly recall the equivalent loss with respect to \hat{Y}

$$\tilde{l}_\gamma = \begin{cases} \log(1 + \exp(\gamma)), & \text{if } Y \cdot \hat{Y} \leq -\gamma; \\ \log(1 + \exp(-Y \cdot \hat{Y})), & \text{if } Y \cdot \hat{Y} \in (-\gamma, \gamma); \\ \log(1 + \exp(-\gamma)), & \text{if } Y \cdot \hat{Y} \geq \gamma, \end{cases}$$

where the non-constant part is identical to that of a logistic loss. For sufficiently large threshold γ so that the minimizer locates in the non-constant part, we compute the first-order condition of the minimizer (which is just that of the logistic loss) as

$$-p \cdot \frac{\exp(-\hat{Y}^*)}{1 + \exp(-\hat{Y}^*)} + (1 - p) \cdot \frac{\exp(\hat{Y}^*)}{1 + \exp(\hat{Y}^*)} = 0,$$

which implies that

$$\hat{Y}^* = \log \left(\frac{p}{1 - p} \right).$$

For a small γ , the derivative of the expected equivalent loss suggests that the minimizer should be

$$\hat{Y}^* = \gamma \cdot \text{sign}(2p - 1).$$

Without loss of generality, we assume that $p \geq \frac{1}{2}$. Then

$$\hat{Y}^* = \begin{cases} \gamma, & \text{if } p \geq \frac{\exp(\gamma)}{1 + \exp(\gamma)}; \\ \log \left(\frac{p}{1 - p} \right), & \text{if } \frac{1}{2} \leq p \leq \frac{\exp(\gamma)}{1 + \exp(\gamma)}. \end{cases}$$

Substituting above results into $C_p(\hat{Y})$, we have

$$H(p) = \begin{cases} -[p \log(p) + (1 - p) \log(1 - p)], & \text{if } \frac{1}{2} \leq p \leq \frac{\exp(\gamma)}{1 + \exp(\gamma)}; \\ \log(1 + \exp(\gamma)) - \frac{\gamma \exp(\gamma)}{1 + \exp(\gamma)}, & \text{if } p \geq \frac{\exp(\gamma)}{1 + \exp(\gamma)}. \end{cases}$$

One can check that $C_p(0) \leq C_p(\hat{Y})$ for any $p \geq \frac{1}{2}$ and $\hat{Y} \leq 0$, implying that

$$H^-(p) = C_p(0) = \log(2).$$

Then

$$\tilde{\psi}(z) = \begin{cases} \frac{1}{2} [(1+z)\log(1+z) + (1-z)\log(1-z)], & \text{if } z \leq \frac{\exp(\gamma)-1}{\exp(\gamma)+1}; \\ \log\left(\frac{2}{1+\exp(\gamma)}\right) + \frac{\gamma \exp(\gamma)}{1+\exp(\gamma)}, & \text{if } z \geq \frac{\exp(\gamma)-1}{\exp(\gamma)+1}. \end{cases}$$

Apparently, $\tilde{\psi}(z)$ is non-convex as a whole: in the first part where z is small, the function is convex and strictly increasing, while in the second part, the function is a constant. We extend the values of $\tilde{\psi}(z)$ from small z 's to large z 's by defining another function

$$h(z) := \frac{1}{2} [(1+z)\log(1+z) + (1-z)\log(1-z)].$$

To compute $\psi(z)$, observe that the convex hull of the epigraph of $\tilde{\psi}$ can be determined by some specific point $z_0 \leq \frac{\exp(\gamma)-1}{\exp(\gamma)+1}$: at the left side of z_0 , the epigraph is identical to that of $h(z)$, while at the right side of z_0 , the epigraph is identical to that of the tangent at $(z_0, h(z_0))$. Such a tangent should contain the right-most point $(1, \tilde{\psi}(1))$, which means

$$h(z_0) + h'(z_0) \cdot (1 - z_0) = \tilde{\psi}(1).$$

Replacing the equation with concrete expressions, we have

$$\log(1+z_0) = h(z_0) + h'(z_0) \cdot (1 - z_0) = \tilde{\psi}(1) = \log(2) - \log\left(\exp\left(\frac{\gamma}{1+\exp(\gamma)}\right) + \exp\left(\frac{-\gamma}{1+\exp(-\gamma)}\right)\right).$$

Simplifying notations, we have

$$z_0 = 2 \cdot \left(\exp\left(\frac{\gamma}{1+\exp(\gamma)}\right) + \exp\left(\frac{-\gamma}{1+\exp(-\gamma)}\right) \right)^{-1} - 1.$$

Therefore,

$$\psi(z) = \begin{cases} \frac{1}{2} [(1+z)\log(1+z) + (1-z)\log(1-z)], & \text{if } z \leq z_0; \\ \frac{1}{2} [(1+z)\log(1+z_0) + (1-z)\log(1-z_0)], & \text{if } z \geq z_0, \end{cases}$$

where z_0 is some positive constant stated above. By examining the first-order derivative of $\psi(z)$, we can easily find out that the equivalent loss is classification-calibrated:

$$\frac{d\psi}{dz} = \begin{cases} \frac{1}{2} [\log(1+z) - \log(1-z)], & \text{if } z \leq z_0; \\ \frac{1}{2} [\log(1+z_0) - \log(1-z_0)], & \text{if } z \geq z_0. \end{cases}$$

By computing its Taylor expansions at $z = 0$, we have

$$\psi(z) \sim \left. \frac{d^2\psi}{dz^2} \right|_{z=0} \cdot z^2 = z^2.$$

Finally, we note that

$$\psi(z) = \Theta(z^2),$$

where the big theta notation suggests “at the same order as”.

Example 4 (Surrogate link function of margin loss and margin-based uncertainty). Similarly, the even

and positive uncertainty function U leads to the same minimizer of the expected equivalent loss as the expected original margin loss, while the latter by the arguments in Bartlett et al. (2006) is

$$\hat{Y}^* = \text{sign}\left(p - \frac{1}{2}\right),$$

for $p \neq \frac{1}{2}$. For $p = \frac{1}{2}$, any $\hat{Y} \in [-1, 1]$ will lead to the same expected equivalent loss.

We compute the $p \geq \frac{1}{2}$ part, gaining

$$H(p) = p \cdot 0 + (1-p) \cdot \frac{2}{\mu} \log(1+\mu) = (1-p) \cdot \frac{2}{\mu} \log(1+\mu), \quad \forall p \geq \frac{1}{2}.$$

The other part $p < \frac{1}{2}$ is

$$H(p) = p \cdot \frac{2}{\mu} \log(1+\mu) + (1-p) \cdot 0 = p \cdot \frac{2}{\mu} \log(1+\mu), \quad \forall p < \frac{1}{2}.$$

For computing the $H^-(p)$, assume that $p \geq \frac{1}{2}$. Then any $\hat{Y} \in [-1, 0]$ will be optimal among the non-Bayes classifiers, leading to

$$H^-(p) = \frac{2}{\mu} \log(1+\mu).$$

Hence,

$$\tilde{\psi}(z) = H^-\left(\frac{1+z}{2}\right) - H\left(\frac{1+z}{2}\right) = \frac{\log(1+\mu)}{\mu} z.$$

The linear function is of course convex, so

$$\psi = \tilde{\psi}.$$

Example 5 (Surrogate link function of exponential loss and exponential uncertainty). The equivalent loss concerning $\hat{Y} \cdot Y$ is

$$\tilde{l} = \begin{cases} -\frac{1}{1+\mu} \cdot \exp(-(1+\mu)\hat{Y} \cdot Y) + \frac{\mu}{1+\mu}, & \text{if } \hat{Y} \cdot Y \geq 0; \\ -\frac{1}{1-\mu} \cdot \exp(-(1-\mu)\hat{Y} \cdot Y) - \frac{\mu}{1-\mu}, & \text{if } \hat{Y} \cdot Y \leq 0. \end{cases}$$

Since the uncertainty function $U = \exp(-|\hat{Y}|)$ is even and positive, the minimizer of the expected equivalent loss $C_p(\hat{Y})$ is identical to that of the expected original loss. That is,

$$-p \exp(-\hat{Y}^*) + (1-p) \exp(\hat{Y}^*) = 0,$$

which implies that

$$\hat{Y}^* = \frac{1}{2} \log\left(\frac{p}{1-p}\right).$$

Without loss of generality, assume that $p \geq \frac{1}{2}$. Then

$$\begin{aligned} H(p) &= p \left[-\frac{1}{1+\mu} \cdot \exp\left(-\frac{1+\mu}{2} \log\left(\frac{p}{1-p}\right)\right) + \frac{\mu}{1+\mu} \right] \\ &\quad + (1-p) \left[-\frac{1}{1-\mu} \cdot \exp\left(\frac{1-\mu}{2} \log\left(\frac{p}{1-p}\right)\right) - \frac{\mu}{1-\mu} \right] \\ &= \frac{2}{1-\mu^2} \cdot p^{\frac{1-\mu}{2}} (1-p)^{\frac{1+\mu}{2}} + \frac{\mu}{1-\mu^2} \cdot (2p-1-\mu). \end{aligned}$$

Since the equivalent loss is convex with respect to $\hat{Y} \cdot Y$, the minimum of expected equivalent loss when

the prediction is non-Bayes is

$$H^-(p) = C_p(0) = 1.$$

Then by definition,

$$\begin{aligned}\tilde{\psi}(z) &= H^-\left(\frac{1+z}{2}\right) - H\left(\frac{1+z}{2}\right) \\ &= \frac{1}{1-\mu^2} \left(1 - \mu z - (1-z)^{\frac{1+\mu}{2}} (1+z)^{\frac{1-\mu}{2}}\right).\end{aligned}$$

The first-order derivative is

$$\frac{d\tilde{\psi}}{dz} = -\frac{\mu}{1-\mu^2} - \frac{1}{2(1+\mu)} \left(\frac{1-z}{1+z}\right)^{\frac{1+\mu}{2}} + \frac{1}{2(1-\mu)} \left(\frac{1+z}{1-z}\right)^{\frac{1-\mu}{2}},$$

which is zero at $z = 0$. The second-order derivative is

$$\frac{d^2\tilde{\psi}}{dz^2} = \frac{1}{1-z^2} \cdot (1-z)^{-\frac{1-\mu}{2}} (1+z)^{-\frac{1+\mu}{2}} \geq 0,$$

which implies two facts: $\tilde{\psi}(z)$ tends to zero if and only if z tends to zero, and $\tilde{\psi}(z)$ is convex (henceforth $\psi = \tilde{\psi}$). Thus, the equivalent loss is classification-calibrated.

From the facts that

$$\left.\frac{d\psi}{dz}\right|_{z=0} = 0$$

and

$$\left.\frac{d^2\psi}{dz^2}\right|_{z=0} = 1,$$

we can say that

$$\psi(z) \sim z^2$$

around $z = 0$. Due to the boundedness of ψ , we have

$$\psi(z) = \Theta(z^2),$$

where the big theta notation is “of the same order”.

A.3 Convexity and Proof of Proposition 4

In this subsection, we examine how the convexity requirements are fulfilled in the listed examples.

Example 1 (Convexity of [Dagan and Engelson \(1995\)](#); [Culotta and McCallum \(2005\)](#)). W.l.o.g. we still assume $Y = 1$ to ease the burden of notations. For the entropy uncertainty, remind that we have already shown its partial derivative with respect to \hat{Y} by

$$\frac{\partial \tilde{l}}{\partial \hat{Y}} = \frac{1}{2} \log\left(\frac{1+\hat{Y}}{2}\right) + \frac{1}{2} \cdot \frac{1-\hat{Y}}{1+\hat{Y}} \log\left(\frac{1-\hat{Y}}{2}\right).$$

Continue to compute its partial derivative, we have

$$\frac{\partial^2 \tilde{l}}{\partial \hat{Y}^2} = -\frac{1}{(1+\hat{Y})^2} \cdot \log\left(\frac{1-\hat{Y}}{2}\right) \geq 0,$$

which ensures its convexity with respect to \hat{Y} .

For the least confidence uncertainty, the partial derivative is

$$\frac{\partial \tilde{l}}{\partial \hat{Y}} = \begin{cases} -\frac{1}{2} \cdot \frac{1-\hat{Y}}{1+\hat{Y}}, & \text{if } \hat{Y} \geq 0; \\ -\frac{1}{2}, & \text{if } \hat{Y} \leq 0, \end{cases}$$

which implies that \tilde{l} is at least C^1 continuous with respect to \hat{Y} . Furthermore,

$$\frac{\partial^2 \tilde{l}}{\partial \hat{Y}^2} = \begin{cases} \frac{1}{(1+\hat{Y})^2}, & \text{if } \hat{Y} > 0; \\ 0, & \text{if } \hat{Y} < 0. \end{cases}$$

Therefore, the equivalent loss is convex with respect to \hat{Y} .

We have shown the convexity with respect to \hat{Y} for both cases. If \hat{Y} is linear with respect to θ , then we can further conclude that the convexity regarding θ holds. But unlike the margin-based classifiers, the probabilistic models restrict that $\hat{Y} \in (-1, 1)$, where a popular model is the logistic regression model that predicts $\hat{Y} = \frac{\exp(\theta^\top X) - 1}{\exp(\theta^\top X) + 1}$. Unlike the original cross-entropy loss, the equivalent loss under the logistic regression model is no longer convex with respect to the parameter θ .

Example 2 (Convexity of [Raj and Bach \(2022\)](#)). Since the model is linear in the sense that $\hat{Y} = \theta^\top X$, we only need to check the convexity with respect to \hat{Y} . First, assuming $Y = 1$, the derivative of \tilde{l} with respect to \hat{Y} is

$$\frac{\partial \tilde{l}_\mu}{\partial \hat{Y}} = \begin{cases} \frac{2(\hat{Y}-1)}{1+\mu\hat{Y}}, & \text{if } \hat{Y} \leq 0; \\ \frac{2(\hat{Y}-1)}{1-\mu\hat{Y}}, & \text{if } \hat{Y} \in (0, 1); \\ 0, & \text{if } \hat{Y} \geq 1. \end{cases}$$

We can see that \tilde{l} is C^1 continuous with respect to \hat{Y} . We further compute that

$$\frac{\partial^2 \tilde{l}_\mu}{\partial \hat{Y}^2} = \begin{cases} \frac{2(1+\mu)}{(1+\mu\hat{Y})^2}, & \text{if } \hat{Y} < 0; \\ \frac{2(1-\mu)}{(1-\mu\hat{Y})^2}, & \text{if } \hat{Y} \in (0, 1); \\ 0, & \text{if } \hat{Y} > 1. \end{cases}$$

Hence the model is convex but not strongly convex.

Example 3 (Convexity of [Tifrea et al. \(2022\)](#)). The equivalent loss is non-convex for \hat{Y} since it is a truncated logistic loss outside a region, where the truncation is to set the loss to be a constant. By the linearity of \hat{Y} on θ , the model is also non-convex for θ .

Example 4 (Nonconvexity of margin loss and margin-based uncertainty). *Proof of Proposition 4.* Since the model is linear, we only need to examine the case where \tilde{l} is convex w.r.t. \hat{Y} . At the differentiable parts, the second-order derivative of the equivalent loss w.r.t. \hat{Y} is

$$\frac{\partial^2 \tilde{l}}{\partial \hat{Y}^2} = \frac{\partial}{\partial \hat{Y}} \left(\frac{\partial \tilde{l}}{\partial \hat{Y}} \right) = \frac{\partial U}{\partial \hat{Y}} \cdot \frac{\partial l}{\partial \hat{Y}} + U \cdot \frac{\partial^2 l}{\partial \hat{Y}^2} = \frac{\partial U}{\partial \hat{Y}} \cdot \frac{\partial l}{\partial \hat{Y}},$$

since the Hinge loss l is piece-wise linear w.r.t. \hat{Y} . For any fixed \hat{Y} , the actual outcome Y could possibly

be either +1 or -1, indicating that

$$\frac{\partial l}{\partial \hat{Y}} = \begin{cases} +1, & \text{if } \hat{Y} > -1, Y = -1; \\ -1, & \text{if } \hat{Y} < +1, Y = +1; \\ 0, & \text{otherwise.} \end{cases}$$

At the positive part $\hat{Y} > 0$, the uncertainty function is non-increasing, which restricts the term $\frac{\partial U}{\partial \hat{Y}}$ to be non-positive. But for the case $Y = -1$, the convexity requires the term $\frac{\partial U}{\partial \hat{Y}}$ to be non-negative. Henceforth

$$\frac{\partial U}{\partial \hat{Y}} = 0,$$

which implies that the uncertainty function must be piece-wise constants. To further ensure that U must be only one constant, we observe that the equivalent loss is now piece-wise linear with non-increasing slopes for $\hat{Y} > 0$ if $Y = -1$. In order to keep the loss continuous and convex, the slope must be constant everywhere. \square

Example 5 (Convexity of exponential loss and exponential uncertainty). Similar to the arguments in Example 2, we only need to compute the second-order derivatives (w.l.o.g. assume $Y = 1$):

$$\frac{\partial^2 \tilde{l}_\mu}{\partial \hat{Y}^2} = \begin{cases} (1 + \mu) \cdot \exp(-(1 + \mu)\hat{Y}), & \text{if } \hat{Y} < 0; \\ (1 - \mu) \cdot \exp(-(1 - \mu)\hat{Y}), & \text{if } \hat{Y} > 0. \end{cases}$$

The convexity thus holds.

A.4 Lipschitzness in Section 5

What is different from the stream-based case is the excessive equivalent risk decomposition, due to the distributions from which the SGD's samples are drawn. For the stream-based setting, the algorithm receives a newly drawn sample X from the underlying distribution \mathcal{P}_X , while for the pool-based setting, the sample set \mathcal{D}_n^X is determined and the sampling distribution is the empirical distribution $\hat{\mathcal{P}}_X^n$. As a consequence, the excessive risk for any loss function $l(f; (X, Y))$ (which can be transformed into the excessive risk for the conditional expectation $L(f; X) = \mathbb{E}_Y[l(f; (X, Y))]$) should be decomposed into five terms rather than two:

$$\begin{aligned} \mathbb{E}[l(\hat{f}; (X, Y))] - \mathbb{E}[l(g^*; (X, Y))] &= \mathbb{E}[L(\hat{f}; X)] - \mathbb{E}[L(g^*; X)] \\ &= \mathbb{E}[L(\hat{f}; X)] - \frac{1}{n} \sum_{i=1}^n L(\hat{f}; X_i) && \text{(generalization)} \\ &\quad + \frac{1}{n} \sum_{i=1}^n L(\hat{f}; X_i) - \inf_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n L(f; X_i) && \text{(optimization)} \\ &\quad + \inf_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n L(f; X_i) - \frac{1}{n} \sum_{i=1}^n L(f^*; X_i) && \text{(non-positive)} \\ &\quad + \frac{1}{n} \sum_{i=1}^n L(f^*; X_i) - \mathbb{E}[L(f^*; X)] && \text{(concentration)} \\ &\quad + \mathbb{E}[L(f^*; X)] - \mathbb{E}[L(g^*; X)] && \text{(approximation)}. \end{aligned}$$

Among the above five terms, the non-positive term and the concentration term can be dealt with easily: the non-positive term can be discarded immediately, and the concentration term can be handled by either

the standard concentration arguments to yield a high probability bound or the same as the generalization term. In this paper, we cope with the concentration term in the same way as the generalization term.

What matters most now remains three terms: generalization, optimization, and approximation. As in the stream-based setting, we do not discuss the approximation term in this paper, since it is beyond the scope of choosing the uncertainty function. We simply assume that there is no model misspecification so that the approximation term is zero. The optimization can be dealt with easily with the convexity condition as we do in Proposition 3. For the remaining generalization term, we summarize an easy-to-check criterion.

To begin with, we briefly review the classical statistical learning theory. The estimator \hat{f} we get in any algorithm is dependent on the data points \mathcal{D}_n^X , so we cannot directly get the generalization bound via the concentration inequalities that rely on the i.i.d. condition. To deal with such a dependence, classical statistical learning theory usually proves the uniform convergence to establish an upper bound on the generalization term. A popular way to uniform convergence is to compute the Rademacher complexity. The Rademacher complexity of a hypothesis class \mathcal{F} on \mathcal{X} can be defined as

$$\mathcal{R}_n(\mathcal{F}) := \mathbb{E} \left[\sup_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^n \sigma_i f(X_i) \right],$$

where σ_i 's are n i.i.d. samples from the uniform distribution on $\{-1, +1\}$ and X_i 's are n i.i.d. samples from the distribution \mathcal{P} on \mathcal{X} . If we further define the loss class as

$$\mathcal{L}_{L \circ \mathcal{F}} := \{x \mapsto L(f; x) | f \in \mathcal{F}\},$$

then a well-known high-probability upper bound for the generalization term (for example, see Theorem 5 in [Bousquet et al. \(2003\)](#)) is that for any $\delta > 0$, the following holds with probability at least $1 - \delta$:

$$\forall f \in \mathcal{F}, \quad \left| \mathbb{E}[L(f; X)] - \frac{1}{n} \sum_{i=1}^n L(f; X_i) \right| \leq 2\mathcal{R}_n(\mathcal{L}_{L \circ \mathcal{F}}) + \sqrt{\frac{\log(\frac{2}{\delta})}{2n}}. \quad (8)$$

The $1 - \delta$ high-probability bound 8 can handle the generalization term and the concentration term easily with an upper bound of $4\mathcal{R}_n(\mathcal{L}_{L \circ \mathcal{F}}) + O(\frac{\log(1/\delta)}{n})$.

The next question is: how to quickly get an upper bound on the Rademacher complexity of a loss class? We hope that $\mathcal{R}_n(\mathcal{L}_{L \circ \mathcal{F}})$ can be converted to $\mathcal{R}_n(\mathcal{F})$, since the Rademacher complexity of a function class \mathcal{F} is generally easier to compute. For example, for a linear function class with parameter L_2 norm upper bound M_Θ and feature space L_2 upper bound M_X , the Rademacher complexity is upper bounded by $\frac{M_\Theta M_X}{\sqrt{n}}$.

Luckily, if we can ensure the β_L -Lipschitzness of the conditionally expected loss L w.r.t. f , then by Ledoux-Talagrand's contraction inequality (see Corollary 3.17 in [Ledoux and Talagrand \(1991\)](#)), we have

$$\mathcal{R}_n(\mathcal{L}_{L \circ \mathcal{F}}) \leq \beta_L \mathcal{R}_n(\mathcal{F}). \quad (9)$$

Lipschitz condition of those examples in Section 3 are verified in Appendix A.4. As for the “loss as uncertainty” principle in Section 4, we note that the equivalent loss $\tilde{L} = \frac{1}{2}L^2 + C$ is $M_L \cdot \beta_L$ -Lipschitz if the original loss L is β_L -Lipschitz and bounded by M_L .

We start to check the Lipschitz condition for the equivalent loss in the examples. We recall that

$$\frac{\partial \tilde{l}}{\partial \hat{Y}} = U \cdot \frac{\partial l}{\partial \hat{Y}}.$$

Therefore, due to the fact that the uncertainty $U \in [0, 1]$, we have

$$\left| \frac{\partial \tilde{l}}{\partial \hat{Y}} \right| \leq \left| \frac{\partial l}{\partial \hat{Y}} \right|,$$

which implies the following:

Lemma 1. *If the uncertainty function $U \in [0, M_U]$ and the original loss $l(\hat{Y}, Y)$ is differentiable and β -Lipschitz with respect to \hat{Y} , then the equivalent loss $\tilde{l}(\hat{Y}, Y)$ is $M_U \cdot \beta$ -Lipschitz with respect to \hat{Y} .*

Moreover, the uncertainty function U is usually decreasing to be near zero when $|\hat{Y}|$ is large enough, which counteracts the effects of the rapid growth of many popular loss functions when $\hat{Y} \cdot Y$ is negative and far enough from zero. To see this, we have a closer look at the probabilistic model in Example 1.

Example 1 (Lipschitzness of [Dagan and Engelson \(1995\)](#); [Culotta and McCallum \(2005\)](#)). The original cross-entropy loss is not Lipschitz on the range $\hat{Y} \in (-1, 1)$ (or equivalently, $q \in (0, 1)$), since the derivative of the negative logarithm will explode near the zero point. But from direct computation, for the entropy uncertainty ([Dagan and Engelson, 1995](#)), we have (w.l.o.g. assume $Y = 1$)

$$\begin{aligned} \frac{\partial \tilde{l}}{\partial \hat{Y}} &= U \cdot \frac{\partial l}{\partial \hat{Y}} \\ &= - \left[\frac{1 + \hat{Y}}{2} \log \left(\frac{1 + \hat{Y}}{2} \right) + \frac{1 - \hat{Y}}{2} \log \left(\frac{1 - \hat{Y}}{2} \right) \right] \cdot \left(-\frac{1}{1 + \hat{Y}} \right) \\ &= \frac{1}{2} \log \left(\frac{1 + \hat{Y}}{2} \right) + \frac{1}{2} \cdot \frac{1 - \hat{Y}}{1 + \hat{Y}} \log \left(\frac{1 - \hat{Y}}{2} \right). \end{aligned}$$

Since the first-order partial derivative $\frac{\partial \tilde{l}}{\partial \hat{Y}}$ is non-positive and monotonically increasing, we only need to check the limit case $\hat{Y} \rightarrow -1^+$ to examine the Lipschitzness. We have

$$\left| \frac{\partial \tilde{l}}{\partial \hat{Y}} \right| \sim \left| \frac{1}{2} \log(1 + \hat{Y}) \right|,$$

which is much smaller than the original loss

$$\left| \frac{\partial l}{\partial \hat{Y}} \right| \sim \left| -\frac{1}{1 + \hat{Y}} \right|,$$

since by l'Hôpital's rule,

$$\lim_{\hat{Y} \rightarrow -1^+} \frac{\partial \tilde{l}}{\partial \hat{Y}} / \frac{\partial l}{\partial \hat{Y}} = \lim_{\hat{Y} \rightarrow -1^+} \left(-\frac{1}{1 + \hat{Y}} \right) / \left(-\frac{1}{(1 + \hat{Y})^2} \right) = \lim_{\hat{Y} \rightarrow -1^+} (1 + \hat{Y}) = 0.$$

Although we cannot say that the equivalent loss is Lipschitz with respect to the whole $(-1, 1)$, for any compact subset of $(-1, 1)$, the equivalent loss is Lipschitz. We shall see that the Lipschitz constant is reduced compared to the original loss.

As for the least confidence uncertainty, the situation is even better: the equivalent loss is Lipschitz over the entire set $\hat{Y} \in (-1, 1)$. To see this, we w.l.o.g. assume $Y = 1$, and the equivalent loss is

$$\tilde{l}(\hat{Y} \cdot Y) = \begin{cases} \frac{1}{2}(\hat{Y} - 2 \log(1 + \hat{Y})), & \text{if } \hat{Y} \geq 0; \\ -\frac{1}{2} \cdot \hat{Y}, & \text{if } \hat{Y} \leq 0. \end{cases}$$

Its partial derivative is

$$\frac{\partial \tilde{l}}{\partial \hat{Y}} = \begin{cases} -\frac{1}{2} \cdot \frac{1-\hat{Y}}{1+\hat{Y}}, & \text{if } \hat{Y} \geq 0; \\ -\frac{1}{2}, & \text{if } \hat{Y} \leq 0, \end{cases}$$

which implies that the equivalent loss is $\frac{1}{2}$ -Lipschitz.

Example 2 (Lipschitzness of [Raj and Bach \(2022\)](#)). From direct computation, the partial derivative w.r.t. \hat{Y} can be upper-bounded by

$$\left\| \frac{\partial \tilde{l}}{\partial \hat{Y}} \right\| \leq \frac{2}{\mu}.$$

By assuming an almost upper bound M_X on the feature space \mathcal{X} , the equivalent loss is of course $\frac{2M_X}{\mu}$ -Lipschitz w.r.t. θ .

Example 3 (Lipschitzness of [Tifrea et al. \(2022\)](#)). By the property of the logistic loss, the equivalent loss must be 1-Lipschitz w.r.t. \hat{Y} . Hence the equivalent loss is M_X -Lipschitz w.r.t. θ .

Example 4 (Lipschitzness of margin loss and margin-based uncertainty). The equivalent loss is 1-Lipschitz w.r.t. \hat{Y} , which indicates its M_X -Lipschitzness w.r.t. θ .

Example 5 (Lipschitzness of exponential loss and exponential uncertainty). The prediction $\hat{Y} = \theta^\top X$ has an upper bound of

$$|\hat{Y}| \leq M_X \cdot M_\Theta,$$

where M_X is the almost sure upper bound for X and M_Θ is the upper bound for Θ . Then the equivalent loss has an upper bound for its partial derivative w.r.t. \hat{Y} of $\exp((1-\mu)M_X \cdot M_\Theta)$. The final Lipschitzness constant w.r.t. θ is $M_X \cdot \exp((1-\mu)M_X \cdot M_\Theta)$.

B Proofs and Discussions

B.1 Proof of Proposition 1

Proof. Denote the σ -field generated by θ_t by \mathcal{F}_t . The general requirement for the SGD update to hold is that

$$\mathbb{E} [\theta_{t+1} - \theta_t | \mathcal{F}_t] = -\eta_t \cdot \frac{\partial \tilde{l}}{\partial \theta} \Big|_{\theta=\theta_t},$$

where η_t is the step size. To prove such a requirement, we first see that the only randomness that will affect θ_{t+1} conditioned on \mathcal{F}_t is

$$\mathbb{1}\{\xi_t \leq U(\theta_t; X_t)\}$$

that has a conditional expectation of

$$\mathbb{E} [\mathbb{1}\{\xi_t \leq U(\theta_t; X_t)\} | \mathcal{F}_t] = U(\theta_t; X_t).$$

From the definition that

$$\theta_{t+1} = \theta_t - \eta_t \cdot \mathbb{1}\{\xi_t \leq U(\theta_t; X_t)\} \cdot \frac{\partial \tilde{l}}{\partial \theta} \Big|_{\theta=\theta_t},$$

we can conclude the proof. \square

B.2 Proof of Proposition 3

Proof. To ease the notation, we denote $\mathbb{1}\{\xi_t \leq U(\theta_t; X_t)\} \cdot \frac{\partial l(\theta; (X_t, Y_t))}{\partial \theta} \Big|_{\theta=\theta_t}$ by g_t . By Proposition 1, we have

$$\mathbb{E}_{\xi_t} [g_t | \theta_t] = \nabla_\theta \tilde{l}(\theta_t; (X_t, Y_t)).$$

Take the expectation with respect to (X_t, Y_t) , we see that g_t is further applying SGD directly on the expected equivalent loss

$$\mathbb{E}_{\xi_t, (X_t, Y_t)} [g_t | \theta_t] = \mathbb{E}_{(X_t, Y_t)} \left[\nabla_\theta \tilde{l}(\theta_t; (X_t, Y_t)) \Big| \theta_t \right] = \nabla_\theta \mathbb{E}_{(X, Y)} [\tilde{l}(\theta_t; (X, Y)) | \theta_t].$$

Denote $\mathbb{E}_{(X, Y)} [\tilde{l}](\theta; (X, Y))$ by $R(\theta)$. Then from the definition, we have

$$\begin{aligned} \|\theta_{t+1} - \theta^*\|^2 &= \|\theta_t - \eta_t \cdot g_t - \theta^*\|^2 \\ &= \|\theta_t - \theta^*\|^2 - 2\eta_t \cdot g_t^\top (\theta_t - \theta^*) + \eta_t^2 \|g_t\|^2 \\ &= \|\theta_t - \theta^*\|^2 - 2\eta_t \cdot (g_t - \nabla R(\theta_t) + \nabla R(\theta_t))^\top (\theta_t - \theta^*) + \eta_t^2 \|g_t\|^2 \\ &\leq \|\theta_t - \theta^*\|^2 - 2\eta_t \cdot (g_t - \nabla R(\theta_t))^\top (\theta_t - \theta^*) + 2\eta_t \cdot (R(\theta^*) - R(\theta_t)) + \eta_t^2 \|g_t\|^2, \end{aligned}$$

where the last inequality follows from the convexity of $R(\cdot)$ such that $R(\theta^*) \geq R(\theta_t) + \nabla R(\theta_t)^\top (\theta^* - \theta_t)$. Assume that the parameters sequence $\{\theta_t\}_{t \geq 1}$ is adapted to an increasing sequence of σ -fields $\{\mathcal{F}_t\}_{t \geq 1}$. Since θ_{t+1} is completely determined by θ_t , ξ_t , and (X_t, Y_t) , taking the expectation conditioned on \mathcal{F}_t is equivalent to taking the expectation w.r.t. ξ_t and (X_t, Y_t) conditioned on knowing θ_t . By taking the expectation w.r.t. \mathcal{F}_t , we have

$$\begin{aligned} &\mathbb{E} [\|\theta_{t+1} - \theta^*\|^2 | \mathcal{F}_t] \\ &\leq \|\theta_t - \theta^*\|^2 - 2\eta_t \cdot \mathbb{E} [(g_t - \nabla R(\theta_t)) | \mathcal{F}_t]^\top (\theta_t - \theta^*) + 2\eta_t \cdot (R(\theta^*) - R(\theta_t)) + \eta_t^2 \mathbb{E} [\|g_t\|^2 | \mathcal{F}_t] \\ &= \|\theta_t - \theta^*\|^2 + 2\eta_t \cdot (R(\theta^*) - R(\theta_t)) + \eta_t^2 \mathbb{E} [\|g_t\|^2 | \mathcal{F}_t]. \end{aligned}$$

By rearranging the terms, we have

$$R(\theta_t) \leq R(\theta^*) + \frac{\|\theta_t - \theta^*\|^2 - \mathbb{E} [\|\theta_{t+1} - \theta^*\|^2 | \mathcal{F}_t]}{2\eta_t} + \frac{\eta_t}{2} \cdot \mathbb{E} [\|g_t\|^2 | \mathcal{F}_t], \quad (10)$$

where

$$\begin{aligned} \mathbb{E} [\|g_t\|^2 | \mathcal{F}_t] &= \left(\mathbb{1}\{\xi_t \leq U(\theta_t; X_t)\} \cdot \left\| \frac{\partial l(\theta; (X_t, Y_t))}{\partial \theta} \Big|_{\theta=\theta_t} \right\|^2 + \mathbb{1}\{\xi_t > U(\theta_t; X_t)\} \cdot 0 \right) \\ &\leq G^2. \end{aligned}$$

Summing up inequality 10 from $t = 1$ to $T + 1$ and taking the unconditional expectation on both sides, by the tower property of the conditional expectation we have

$$\frac{1}{T+1} \sum_{t=1}^{T+1} \mathbb{E} [R(\theta_t)] \leq R(\theta^*) + \frac{\|\theta_1 - \theta^*\|^2}{2\eta_t} + \frac{\eta_t}{2} \cdot G^2.$$

Assume $\|\theta_1 - \theta^*\| \leq D$. Substituting $\eta_t = \frac{D}{G\sqrt{T+1}}$ into the above inequality, we have

$$\frac{1}{T+1} \sum_{t=1}^{T+1} \mathbb{E} [R(\theta_t)] \leq R(\theta^*) + \frac{GD}{\sqrt{T+1}}.$$

By the convexity of $R(\cdot)$, we have

$$R(\bar{\theta}_{T+1}) = R\left(\frac{1}{T+1} \sum_{t=1}^{T+1} \theta_t\right) \leq \frac{1}{T+1} \sum_{t=1}^{T+1} R(\theta_t),$$

which finally verifies the proof. \square

B.3 Proof of Theorem 2

Proof. Since ψ is convex by the definition in [Bartlett et al. \(2006\)](#), we have

$$\psi\left(\mathbb{E}\left[L_{01}(f_{\bar{\theta}_{T+1}}) - \inf_{g \in \mathcal{G}} L_{01}(g)\right]\right) \leq \mathbb{E}\left[\psi\left(L_{01}(f_{\bar{\theta}_{T+1}}) - \inf_{g \in \mathcal{G}} L_{01}(g)\right)\right],$$

where the expectation is taken with respect to all the randomness in the algorithm. By the surrogate property (2), we have

$$\begin{aligned} \mathbb{E}\left[L_{01}(f_{\bar{\theta}_{T+1}}) - \inf_{g \in \mathcal{G}} L_{01}(g)\right] &\leq \psi^{-1}\left(\mathbb{E}\left[\psi\left(L_{01}(f_{\bar{\theta}_{T+1}}) - \inf_{g \in \mathcal{G}} L_{01}(g)\right)\right]\right) \\ &\leq \psi^{-1}\left(\mathbb{E}\left[\mathbb{E}_{X,Y}[\tilde{l}(f_{\bar{\theta}_{T+1}}(X), Y)] - \inf_{g \in \mathcal{G}} \mathbb{E}_{X,Y}[\tilde{l}(g(X), Y)]\right]\right) \\ &= \psi^{-1}\left(\mathbb{E}[\tilde{l}(f_{\bar{\theta}_{T+1}}(X), Y)] - \inf_{g \in \mathcal{G}} \mathbb{E}[\tilde{l}(g(X), Y)]\right) \\ &= \psi^{-1}\left(\mathbb{E}[\tilde{l}(f_{\bar{\theta}_{T+1}}(X), Y)] - \mathbb{E}[\tilde{l}(f_{\tilde{\theta}^*}(X), Y)] + \mathbb{E}[\tilde{l}(f_{\tilde{\theta}^*}(X), Y)] - \inf_{g \in \mathcal{G}} \mathbb{E}[\tilde{l}(g(X), Y)]\right). \end{aligned}$$

From the result in [Proposition 3](#), we can see that

$$\mathbb{E}[\tilde{l}(f_{\bar{\theta}_{T+1}}(X), Y)] - \mathbb{E}[\tilde{l}(f_{\tilde{\theta}^*}(X), Y)] \leq \frac{GD}{\sqrt{T+1}}.$$

\square

B.4 Proof of Proposition 5

Proof. The algorithm we are considering is under the stream-based setting ([Algorithm 1](#)), where the newly observed sample is directly taken from the unknown distribution \mathcal{P} . As discussed in [Section 3.4](#), we are directly applying SGD on the expected loss $L(\theta; X)$. Following the equivalent loss analyses, one can find the equivalent expected loss by

$$\frac{\partial \tilde{L}}{\partial \theta} = U \cdot \frac{\partial L}{\partial \theta} = L \cdot \frac{\partial L}{\partial \theta}.$$

Then

$$\tilde{L} = \frac{1}{2} L^2 + C,$$

where C is some constant. Since the constant does not affect the gradient, we choose $C = 0$ for simplicity. In other words, we are actually implementing SGD on the squared expected loss when we are applying the gradient-descent-update version of the uncertainty sampling algorithm. For those $U \geq 1$, we permanently query the label and compensate the ratio by increasing the original descent step size η to $\eta \cdot U$, keeping the SGD rule the same. \square

B.5 Discussions on existence of solution to Equation (1)

In Section 4.1, we have mentioned that the necessary and sufficient condition for the path integral of $\sum_{j=1}^d U \cdot \frac{\partial l}{\partial \theta_j} d\theta_j$ to not depend on the chosen path is the uncertainty U and loss l fulfill the exchangeability condition:

$$\frac{\partial U}{\partial \theta_i} \cdot \frac{\partial l}{\partial \theta_j} = \frac{\partial U}{\partial \theta_j} \cdot \frac{\partial l}{\partial \theta_i}, \quad \forall i \neq j.$$

To see why this happens, we give a very brief argument here without bothering to concretely introduce another system of concepts in differential forms and algebraic topology. For those interested readers, please refer to the textbook of differential forms in algebraic topology (Bott et al., 1982). By de Rham's theorem, we shall see the condition that the path integral of $\sum_{j=1}^d U \cdot \frac{\partial l}{\partial \theta_j} d\theta_j$ does not depend on the path choices is equivalent to saying that it is an *exact* form, where the term exact means that the form itself is the (exterior) derivative of another function. In other words, saying that the path integral of some differential form depends only on the starting and ending points equals saying that it is some gradient itself.

The next question is: how to find all the exact forms on some Euclidean parameter space Θ ? By Poincaré's lemma, on any open ball of \mathbb{R}^d , to say a 1-form is exact (where 1 means that it is a first-order gradient of a function) equals to say the form is a *closed* 1-form, where the term closed means that the form's exterior derivative is zero.

Before diving into finding closed forms, we try to intuitively tell what an exterior derivative is. We take \mathbb{R}^3 as an example. We shall see that the exterior derivative is a mimic of gradients, curls, and divergences. In the 3-dimensional Euclidean space, we can find the gradient of a smooth function F by

$$\nabla F = \left(\frac{\partial F}{\partial x}, \frac{\partial F}{\partial y}, \frac{\partial F}{\partial z} \right)^\top.$$

If we represent the gradient by independent vectors (dx, dy, dz) , then we have

$$\nabla F \simeq \frac{\partial F}{\partial x} dx + \frac{\partial F}{\partial y} dy + \frac{\partial F}{\partial z} dz,$$

which is exactly the definition of the exterior derivative dF .

If \mathbf{F} is now a vector field $(F_x, F_y, F_z)^\top$, then its curl is

$$\nabla \times \mathbf{F} = \left(\frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z}, \frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x}, \frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y} \right)^\top.$$

By representing it with independent vectors $(dy \wedge dz, dz \wedge dx, dx \wedge dy)$, we have

$$\nabla \times \mathbf{F} \simeq \left(\frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z} \right) dy \wedge dz + \left(\frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x} \right) dz \wedge dx + \left(\frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y} \right) dx \wedge dy.$$

By writing $\mathbf{F} \simeq F_x dx + F_y dy + F_z dz$, we have the same as the definition of exterior derivatives:

$$d(F_x dx + F_y dy + F_z dz) = \left(\frac{\partial F_z}{\partial y} - \frac{\partial F_y}{\partial z} \right) dy \wedge dz + \left(\frac{\partial F_x}{\partial z} - \frac{\partial F_z}{\partial x} \right) dz \wedge dx + \left(\frac{\partial F_y}{\partial x} - \frac{\partial F_x}{\partial y} \right) dx \wedge dy.$$

Finally, the divergence of a vector field $\mathbf{F} = (F_x, F_y, F_z)^\top$ is

$$\nabla \cdot \mathbf{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}.$$

Up to a vector $dx \wedge dy \wedge dz$, we have

$$\nabla \cdot \mathbf{F} \simeq d(F_x dy \wedge dz + F_y dz \wedge dx + F_z dx \wedge dy).$$

In a word, the exterior derivative is to extend the concept of “differential” from functions to vector fields.

All we have to do now is to find all the closed 1-forms. The closed forms are those of zero exterior derivatives. By the definition of exterior derivatives, we can compute the exterior derivative of $\sum_{j=1}^d U \cdot \frac{\partial L}{\partial \theta_j} d\theta_j$ as

$$\begin{aligned} d\left(\sum_{j=1}^d U \cdot \frac{\partial L}{\partial \theta_j} d\theta_j\right) &= \sum_{1 \leq i < j \leq d} \left(\frac{\partial}{\partial \theta_i} \left(U \cdot \frac{\partial L}{\partial \theta_j} \right) - \frac{\partial}{\partial \theta_j} \left(U \cdot \frac{\partial L}{\partial \theta_i} \right) \right) d\theta_i \wedge d\theta_j \\ &= \sum_{1 \leq i < j \leq d} \left(\frac{\partial U}{\partial \theta_i} \cdot \frac{\partial L}{\partial \theta_j} - \frac{\partial U}{\partial \theta_j} \cdot \frac{\partial L}{\partial \theta_i} \right) d\theta_i \wedge d\theta_j. \end{aligned}$$

which must be zero due to the definition of closed forms. This is the so-called requirement for exchangeability.

B.6 Proof of Proposition 6

Proof. $\forall \epsilon > 0$, we can find some $g_\epsilon \in \mathcal{G}$ such that

$$\mathbb{E}[L(g_\epsilon)] \leq \inf_{g \in \mathcal{G}} \mathbb{E}[L(g)] + \epsilon.$$

For every trajectory of X , the inequality (3) holds for any hypotheses f and g . Set $g = g_\epsilon$. Taking expectation w.r.t. $X \sim \mathcal{P}_X$ on both sides, we have

$$\mathbb{E}[\tilde{L}(f)] - \mathbb{E}[\tilde{L}(g_\epsilon)] \geq \frac{1}{2} \mathbb{E}[(L(f) - L(g_\epsilon))^2].$$

By Jensen’s inequality,

$$\begin{aligned} \frac{1}{2} (\mathbb{E}[L(f)] - \mathbb{E}[L(g_\epsilon)])^2 &\leq \frac{1}{2} \mathbb{E}[(L(f) - L(g_\epsilon))^2] \\ &\leq \mathbb{E}[\tilde{L}(f)] - \mathbb{E}[\tilde{L}(g_\epsilon)] \\ &\leq \mathbb{E}[\tilde{L}(f)] - \inf_{g \in \mathcal{G}} \mathbb{E}[\tilde{L}(g)]. \end{aligned}$$

Hence, we have $\forall \epsilon > 0$,

$$\mathbb{E}[L(f)] - \inf_{g \in \mathcal{G}} \mathbb{E}[L(g)] - \epsilon \leq \mathbb{E}[L(f)] - \mathbb{E}[L(g_\epsilon)] \leq 2 \sqrt{\mathbb{E}[\tilde{L}(f)] - \inf_{g \in \mathcal{G}} \mathbb{E}[\tilde{L}(g)]}.$$

Taking ϵ to be arbitrarily small, we complete the proof. \square

B.7 Proof of Proposition 7

Proof. The proof is straightforward from the first two equal signs of (3). We have assumed the pointwise minimum conditional risk of g^* is at least ϵ^* . Then for any $X \in \mathcal{X}$,

$$\tilde{L}(f) - \tilde{L}(g^*) = \frac{1}{2}(L(f) + L(g^*))(L(f) - L(g^*)) \geq \frac{\epsilon^*}{2}(L(f) - L(g^*)).$$

Taking expectation on $X \sim \mathcal{P}_X$ concludes the proof. \square

B.8 Proof of Theorem 3

Proof. We develop our proof based on that of Proposition 3. In the proof of Proposition 3, we utilize the term g_t to ease the burden of redundant notations. We keep the notation here but replace U with L :

$$g_t := \mathbb{1}\{\xi_t \leq L(\theta_t; X_t)\} \cdot \frac{\partial l(\theta; (X_t, Y_t))}{\partial \theta} \Big|_{\theta=\theta_t}.$$

Note that if we were able to carry on the parameter update based on g_t , then we would be doing SGD on the oracle equivalent expected loss \tilde{L} , and the analysis of Proposition 3 can be directly applied. But we are actually implementing the uncertainty based on an estimation of L , say \hat{L} . Note that the θ term in $\hat{L}(\theta; X)$ does not mean that the estimation model \hat{L} is also parametrized by θ but that the model estimates the conditional expected loss when the current hypothesis is θ . Therefore, the update is made w.r.t.

$$\hat{g}_t := \mathbb{1}\{\xi_t \leq \hat{L}(\theta_t; X_t)\} \cdot \frac{\partial l(\theta; (X_t, Y_t))}{\partial \theta} \Big|_{\theta=\theta_t}.$$

Denote $\mathbb{E}_Y[\tilde{L}]$ by R . By the definition of θ_{t+1} , we have

$$\begin{aligned} \|\theta_{t+1} - \theta_t\|^2 &= \|\theta_t - \eta_t \cdot \hat{g}_t - \theta^*\|^2 \\ &= \|\theta_t - \theta^*\|^2 - 2\eta_t \cdot (\hat{g}_t - g_t + g_t - \nabla R(\theta_t) + \nabla R(\theta_t))^\top (\theta_t - \theta^*) + \eta_t^2 \|\hat{g}_t\|^2 \\ &\leq \|\theta_t - \theta^*\|^2 - 2\eta_t \cdot (g_t - \nabla R(\theta_t))^\top (\theta_t - \theta^*) - 2\eta_t \cdot (\hat{g}_t - g_t)^\top (\theta_t - \theta^*) \\ &\quad + 2\eta_t \cdot (R(\theta^*) - R(\theta_t)) + \eta_t^2 \|\hat{g}_t\|^2, \end{aligned}$$

where the last inequality is derived from the convexity of R . Similar to the proof of Proposition 3, we take the expectation conditioned on \mathcal{F}_t on both sides, where \mathcal{F}_t is the σ -field generated by θ_t :

$$\begin{aligned} \mathbb{E} [\|\theta_{t+1} - \theta^*\|^2 | \mathcal{F}_t] &\leq \|\theta_t - \theta^*\|^2 + 2\eta_t \cdot \mathbb{E} [\|\hat{g}_t - g_t\| | \mathcal{F}_t] \cdot \|\theta_t - \theta^*\| \\ &\quad + 2\eta_t \cdot (R(\theta^*) - R(\theta_t)) + \eta_t^2 \mathbb{E} [\|\hat{g}_t\|^2 | \mathcal{F}_t]. \end{aligned}$$

Rearranging the terms, we have

$$R(\theta_t) \leq R(\theta^*) + \frac{\|\theta_t - \theta^*\|^2 - \mathbb{E} [\|\theta_{t+1} - \theta^*\|^2 | \mathcal{F}_t]}{2\eta_t} + \frac{\eta_t}{2} \cdot \mathbb{E} [\|\hat{g}_t\|^2 | \mathcal{F}_t] + \mathbb{E} [\|\hat{g}_t - g_t\| | \mathcal{F}_t] \cdot \|\theta_t - \theta^*\|. \quad (11)$$

Similar to the proof of Proposition 3, we can easily see from the definition that

$$\|\hat{g}_t\|^2 \leq \left\| \frac{\partial l(\theta; (X_t, Y_t))}{\partial \theta} \Big|_{\theta=\theta_t} \right\|^2 \leq G^2.$$

By assuming that $\|\theta_t - \theta^*\| \leq D$ for all $t \in [T+1]$, we take the unconditional expectation on both sides of inequality 11 and sum up from $t = 1$ to $t = T+1$, then

$$\frac{1}{T+1} \sum_{t=1}^{T+1} \mathbb{E}[R(\theta_t)] \leq R(\theta^*) + \frac{D^2}{2\eta_t} + \frac{\eta_t}{2} \cdot G^2 + D \cdot \frac{1}{T+1} \sum_{t=1}^{T+1} \delta_t.$$

By taking $\eta_t = \frac{D}{G\sqrt{T+1}}$ and the convexity of R , we have

$$\mathbb{E}[R(\bar{\theta}_{T+1})] \leq R(\theta^*) + \frac{GD}{\sqrt{T+1}} + \frac{D}{T+1} \sum_{t=1}^{T+1} \delta_t.$$

□

B.9 Proof of Proposition 8

Proof. We give the analysis here to show that Algorithm 2 is indeed an SGD update. To simplify the notation, we abbreviate the gradient we take at time step t as g_t :

$$g_t := \frac{\partial l(\theta; (X_{at}, Y_t))}{\partial \theta} \Big|_{\theta=\theta_t}.$$

We define the σ -field generated by θ_t to be \mathcal{F}_t . If we define the equivalent expected loss \tilde{L} to be $\frac{1}{2}L^2$ as we do in Section 4, we have

$$\begin{aligned} \mathbb{E} \left[\frac{S_t}{n} \cdot g_t \middle| \mathcal{F}_t \right] &= \frac{S_t}{n} \sum_{i=1}^n \frac{U(\theta_t; X_i)}{S_t} \nabla_\theta \mathbb{E} [l(\theta_t; (X_i, Y_i)) | X = X_i] \\ &= \mathbb{E}_{\hat{\mathcal{P}}_X^n} [U(\theta_t; X) \cdot \nabla_\theta L(\theta_t; X)] \\ &= \mathbb{E}_{\hat{\mathcal{P}}_X^n} [L(\theta_t; X) \cdot \nabla_\theta L(\theta_t; X)] \\ &= \mathbb{E}_{\hat{\mathcal{P}}_X^n} [\nabla_\theta \tilde{L}(\theta_t; X)] \\ &= \nabla_\theta \mathbb{E}_{\hat{\mathcal{P}}_X^n} [\tilde{L}(\theta_t; X)], \end{aligned} \tag{12}$$

which indicates that Algorithm 2 is indeed an SGD update w.r.t. the expected \tilde{L} under the empirical distribution $\hat{\mathcal{P}}_X^n$ with step sizes $\{\eta_t\}_{t=1}^T$. □

B.10 Proof of Proposition 10

Proof. Denote the indexes of the m -largest loss functions $l(\theta_t; (X_i, Y_i))$ by $\{i_{t1}, \dots, i_{tm}\}$. Denote the conditional expected loss as $\mathbb{E}[l(\theta; (X, Y)) | X]$ by $L(\theta; X)$. Then, the gradient of the objective (6) at $\theta = \theta_t$ is

$$\frac{1}{m} \sum_{k=1}^m \nabla_\theta L(\theta_t; X_{i_{tk}}).$$

On the other hand, the conditional expectation of the update is

$$\begin{aligned} \mathbb{E} [\theta_{t+1} - \theta_t | \theta_t] &= \mathbb{E} \left[-\eta_t \cdot \frac{\partial l(\theta; (X_{i_t}, Y_t))}{\partial \theta} \Big|_{\theta=\theta_t} \right] \\ &= -\eta_t \cdot \frac{1}{m} \sum_{k=1}^m \mathbb{E}_{Y_t} \left[\frac{\partial l(\theta; (X_{i_t}, Y_t))}{\partial \theta} \Big|_{\theta=\theta_t} \middle| \theta_t, i_t = i_{tk} \right] \\ &= -\eta_t \cdot \frac{1}{m} \sum_{k=1}^m \nabla_\theta \mathbb{E}_{Y_t} [l(\theta_t; (X_{i_t}, Y_t)) | \theta_t, i_t = i_{tk}] \\ &= -\eta_t \cdot \frac{1}{m} \sum_{k=1}^m \nabla_\theta L(\theta_t; X_{i_{tk}}), \end{aligned}$$

which completes the proof. □

B.11 Proof of Proposition 11

Proof. The sampling probability at step t is

$$p_{ti} = (1 - \gamma) \cdot \frac{1}{n} + \gamma \cdot \mathbb{1}\{i \in \{i_{t1}, \dots, i_{tm}\}\}.$$

Due to the envelope theorem, we only need to prove that \mathbf{p}_t is indeed the solution to the maximization problem at time step t :

$$\max_{\mathbf{p} \in \mathcal{P}_{\frac{\gamma^2 n(n-m)}{2m}, n, \frac{m+(n-m)\gamma}{m}}} \sum_{i=1}^n p_i \cdot L(\theta_t; X_i).$$

Such an optimality check can be easily done by checking the KKT condition, if one notices that the uncertainty set $\mathcal{P}_{\frac{\gamma^2 n(n-m)}{2m}, n, m}$ is a convex set and the objective is a linear function of p . In fact, if we remove the divergence constraint and only focus on the linear constraints, one can easily see that the maximization solution is \mathbf{p}_t , since it puts as much as possible weights on the largest m objectives. Since

$$D_{\frac{1}{2}(-1)^2} \left(\mathbf{p}_t \middle\| \left(\frac{1}{n}, \dots, \frac{1}{n} \right)^\top \right) = m \cdot \frac{1}{2n} \cdot \left(\gamma \left(\frac{n}{m} - 1 \right) \right)^2 + (n - m) \cdot \frac{1}{2n} \cdot \gamma^2 = \gamma^2 \cdot \frac{n - m}{2m},$$

which means that the divergence constraint is also fulfilled by the relaxed maximization point \mathbf{p}_t . Hence the relaxed solution is also the solution to the original maximization problem. \square