Towards optimally abstaining from prediction

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Abstract

A common challenge across all areas of machine learning is that training data is not distributed like test data, due to natural shifts, “blind spots,” or adversarial examples. We consider a model where one may abstain from predicting, at a fixed cost. In particular, our transductive abstention algorithm takes labeled training examples and unlabeled test examples as input, and provides predictions with optimal prediction loss guarantees. The loss bounds match standard generalization bounds when test examples are i.i.d. from the training distribution, but add an additional term that is the cost of abstaining times the statistical distance between the train and test distribution (or the fraction of adversarial examples). For linear regression, we give a polynomial-time algorithm based on Celis-Dennis-Tapia optimization algorithms. For binary classification, we show how to efficiently implement it using a proper agnostic learner (i.e., an Empirical Risk Minimizer) for the class of interest. Our work builds on a recent abstention algorithm of Goldwasser, Kalais, and Montasser [8] for transductive binary classification.

1 Introduction

For learning of a class of functions $F$ of bounded complexity, statistical learning theory guarantees low error if test examples are distributed like training examples. Thus abstention is not necessary for standard realizable prediction. However, when the test distribution $Q$ is not the same as the distribution of training examples $P$, abstaining from prediction may be beneficial if the cost of abstaining $\alpha$ is substantially less than the cost of an error. This is particularly important when there are “blind spots” where $Q(x) > P(x) = 0$. Such an extreme covariate shift scenario was analyzed for binary classification in recent work by Goldwasser, Kalais, and Montasser [8] (henceforth GKKM).

Abstaining from predicting may be useful because it is well-known to be impossible to guarantee accuracy on test examples from arbitrary $Q \neq P$ (under the common assumption that $Q(x)/P(x)$ is upper-bounded, abstention is not necessary) [6]. Whether one is classifying images or predicting the probability of success of a medical procedure, training data may miss important regions of test examples. For instance, an image classifier may be trained on publicly available data but may be also used on people’s private images or even adversarial spam/phishing images [19]. For a regression example, a model may be used to predict the success probability of a medical treatment across a population, yet examples from people that are considered high-risk for the treatment may be absent from the training data.

We begin by discussing binary classification, and then move to regression. In particular, for any distribution $P$ over examples $x \in X$ and any true classifier $f : X \to \{0, 1\}$ in $F$ of VC-dimension $d$, the so-called Fundamental Theorem of Statistical Learning (FTSL) guarantees $\tilde{O}(d/n)$ error rate [4] on future examples from $P$ using any classifier $h \in F$ that agrees with $f$ on $n$ noiseless labeled examples [see, e.g., [18]].

$^{1}$The $\tilde{O}$ notation hides logarithmic factors.
In Chow’s original abstention model [5], a selective classifier is allowed to either make a prediction $\hat{y}$ at a loss of $\ell(y, \hat{y}) \geq 0$ or abstain from predicting at a fixed small loss $\alpha > 0$. Following GKKM, we consider a transductive abstention algorithm that takes as input $n$ unlabeled test examples and $n$ labeled training examples and predicts on a subset of the $n$ test labels, abstaining on the rest. The goal is to minimize the average loss on the test set. (Unfortunately, the natural idea to abstain on test points whose labels are not uniquely determined by the training data can lead to abstaining on all test points even when $P = Q$.) GKKM give an algorithm with guarantees that naturally extend the FTSL to $Q \neq P$ albeit at an additional cost. The word transductive refers to the common prediction model where one wishes to classify a given test set rather a standard classifier that generalizes to future examples, though the two models are in fact equivalent in terms of expected error as we discuss. The term covariate shift is appropriate here as it describes settings in which $Q \neq P$ but both train and test labels are consistent with the same $f \in F$. Without abstention, both transductive learning and covariate shift have been extensively studied [see, e.g., 1].

The principle behind our approach is illustrated through an example of Figure [1]. Suppose $P$ is the distribution $Q$ restricted to a set $S \subset X$ which contains, say, 90% of the test set, so that 10% of the unlabeled test examples are in blind spots. Say we have learned a standard classifier $h \in F$ from the $n$ labeled training examples. Hypothetically, if we knew $S$, then we could predict $h(x_i)$ for test $x_i \in S$ and abstain from predicting on $x_i \notin S$. If abstaining costs $\alpha$, then the FTSL would naturally guarantee test loss $\leq 0.1\alpha + O(d/n)$, because one abstains on 10% of the test examples and the remaining test examples are distributed just like $P$. The difficulty is that $S$ may be too complex to learn. To circumvent this, we suggest a conceptually simple but theoretically powerful approach: choose the set of points to abstain on so as to minimize the worst-case loss over any true function $f \in F$ that is also consistent with the training data. In particular, given a predictor $h$ and a set of test points not abstained on, (ignoring efficiency) one could compute the worst-case loss over all $f \in F$ that are consistent with the labeled training examples. This approach achieves optimal worst-case guarantees and, in particular, inherits the natural loss guarantee one attains from abstaining outside of $S$ discussed above. Converting this theoretical insight into an efficient algorithm is the focus of this paper, and different algorithms are needed for the case of classification and regression.

**Interpretation.** In the case of known $P, Q$, one may say there is a known unknown: the region of large $Q(x)/P(x)$. In our model, however, even though this region is an unknown unknown, we achieve essentially the same bounds as if we knew $P$ and $Q$. Thus, perhaps surprisingly, there is little additional loss for not knowing $P$ and $Q$. GKKM give related guarantees, but their model has an inherent cost for unknown unknowns. In particular, even when $P = Q$ their guarantees are $O(\sqrt{d/n})$ compared to the $O(d/n)$ of FTSL, and they give a lower-bound showing $\Omega(\sqrt{d/n})$ is inherent in their “PQ” learning model. In the PQ model, the error rate on $Q$ (mistakes that are not abstained on) and the abstention rate on future examples from $P$ are separately bounded. In Appendix C, we show that the Chow model is stronger than PQ-learning in the sense that our guarantees imply PQ-bounds similar to theirs, but the reverse does not hold. Hence, the algorithms and guarantees in this paper extend the FTSL in both the Chow and PQ models. We also note that abstaining on predictions can either help reduce inaccuracies on marginal groups or be a source of unfairness towards a person or group of people, and it should not serve as an excuse not to collect representative data.

### 1.1 Classification results

For classification, suppose $Y = \{0, 1\}$, $\ell(y, \hat{y}) := |y - \hat{y}|$ is the 0-1 loss (more general losses are considered in the body), and $F$ is a family of functions of VC-dimension $d$. There is also a deterministic Empirical Risk Minimization (ERM) oracle that computes $\operatorname{ERM}(x, y) \in \arg \min_{g \in F} \sum_i \ell(y_i, g(x_i))$ on any dataset $x \in X^n, y \in Y^n$ (even noisy). While it is NP-hard to efficiently compute ERM for many simple classes like disjunctions, previous reductions to ERM have proven useful with off-the-shelf classifiers (e.g., neural networks) albeit without theoretical guarantees.

The inputs to the learner are labeled training examples $\bar{x} \in X^n, \bar{y} = f(\bar{x}) \in Y^n$, and unlabeled test examples $x \in X^n$. For transductive learning, the goal is to predict labels for the $n$ test examples $x$. A transductive abstention algorithm is also given the predictor $h := \operatorname{ERM}(\bar{x}, \bar{y})$, which has 0 training error, and selects a vector $a \in [0, 1]^n$ for the probability of abstaining on test examples $x$. Its loss is
We generalize Theorem 1 in multiple ways. First, we point out a stronger bound in terms of a

\[ \text{Theorem 1 (Classification)} \]

The total variation distance

\[ D_{TV}(\Omega) := \sum_{i=1}^{n} a_i \alpha + (1 - a_i) \ell(f(x_i), h(x_i)). \]  

(1)

Our Min-Max Abstention (MMA) reduction, mentioned above, attempts to minimize the maximum test loss among classifiers consistent with the training data. In particular, it (approximately) solves the following convex optimization problem for \( \alpha \):

\[ \min_{a \in [0,1]^n} \max_{g \in V} \ell_x(g, h, a). \]  

(2)

Here, \( V := \{ g \in F : \forall i \ g(\bar{x}_i) = f(\bar{x}_i) \} \) is the version space of classifiers consistent with the training labels; thus \( h, f \in V \). In other words, MMA minimizes the worst-case test loss it could possibly incur based on the labeled training and unlabeled test data. A key insight is that MMA has no unknowns, so MMA will achieve a max in (2) as low as if it knew \( P, Q \) and even \( f \).

To solve (2), one must be able to maximize loss over \( V \). Fortunately, GKKM showed how to solve that using a simple subroutine, which we call FLIP, that calls ERM.

**Theorem 1 (Classification).** For \( Y = \{0, 1\} \), any \( n, d \in \mathbb{N} \), any \( F \) of VC dimension \( d \), any \( f \in F \), and any distributions \( P, Q \) over \( X \),

\[ \mathbb{E}_{\bar{x} \sim P^n, x \sim Q^n} [\ell_x(f, h, \hat{a})] \leq \alpha|P - Q|_{TV} + \frac{2d \log 3n}{n}, \]

where \( h = \text{ERM}(\bar{x}, f(\bar{x})) \) and \( \hat{a} = \text{MMA}(\bar{x}, f(\bar{x}), x, h, \text{FLIP}) \in [0,1]^n \) can be computed in time \( \text{poly}(n) \) using the ERM oracle for \( F \).

The total variation distance \( |P - Q|_{TV} \), also called the statistical distance, is a natural measure of non-overlap that ranges from 0 when \( P = Q \) to 1 when \( P \) and \( Q \) have disjoint supports. The \( \alpha|P - Q|_{TV} \) term arises because the learner may need to abstain where \( P \) and \( Q \) do not overlap, and the other term derives directly from the same bound one gets in the case where \( P = Q \) (so \( |P - Q|_{TV} = 0 \)). These bounds are stated in terms of expected loss, because unfortunately as we show in Lemma 8 high probability bounds require \( \Omega(\alpha/\sqrt{n}) \) loss because of the variance in how \( Q \) samples are distributed. All proofs, unless otherwise stated, are deferred to Appendix F.

We generalize Theorem 1 in multiple ways. First, we point out a stronger bound in terms of a divergence \( D_k(P\|Q) \), \( k \geq 1 \), that measures the excess of \( Q(x) \) over \( k \cdot P(x) \). It generalizes the total variation distance \( |P - Q|_{TV} \) between distributions \( P, Q \):

\[ D_k(P\|Q) := \sum_{x} \max(Q(x) - k \cdot P(x), 0) \in [0,1] \]  

(3)

\[ |P - Q|_{TV} := D_1(P\|Q) = \frac{1}{2} \sum_{x} |P(x) - Q(x)| \]  

(4)
Note that if $Q(x) \leq k \cdot P(x)$ for all $x$, then $D_k(P\|Q) = 0$.

Second, we show this implies generalization by using a transductive abstaining algorithm to bound the expected loss with respect to future examples from $Q$. That is, to go alongside classifier $h : X \to \{0, 1\}$, we can output abstainer $\alpha : X \to [0, 1]$ that gives a probability of abstaining on each test example. Here, the generalization loss is,

$$\ell_Q(f, h, \alpha) := \mathbb{E}_{x \sim Q} \left[ \alpha \alpha(x) + (1 - \alpha(x)) \ell(f(x), h(x)) \right].$$

These two generalizations are summarized by the following theorem, which we state for classification but also has a regression analog.

**Theorem 2** (Generalization for classification). Fix $Y = \{0, 1\}$ and $F$ of VC dimension $d$. For any $f \in F$, and any distributions $P, Q$ over $X$,

$$\mathbb{E}_{\bar{x} \sim P^n, \bar{y} \sim Q^n} \left[ \ell_Q(f, h, \alpha) \right] \leq \min_{k \geq 1} D_k(P\|Q) + \frac{2dk \log 3n}{n} \leq \alpha |P - Q|_{TV} + \frac{2d \log 3n}{n},$$

where $h = \text{ERM}(\bar{x}, f(\bar{x}))$ and abstainer $\alpha : X \to [0, 1]$ can be computed in time $\text{poly}(n)$ using ERM and is defined by $\alpha(x') := \text{MMA}(\bar{x}, f(\bar{x}), (x', x_2, \ldots, x_n), h, \text{FLIP})$.

These guarantees use the same algorithm—to predict on a new test example $x'$, it simply runs MMA with a modified test set where we have replaced the first test example by $x'$ and returns the probability of abstaining on it.

Third, as in GKKM, guarantees hold with respect to a “white-box” adversarial model in which there is only a training distribution $P$ and an adversary who may corrupt any number of test examples (but they are still labeled by $f$). More specifically, natural train and test sets $\bar{x}, z \sim P^n$ are drawn, and an adversary may form an arbitrary test set $x \in X^n$. We achieve guarantees as low as if one knew exactly which examples were corrupted and abstained on those:

**Theorem 3** (Adversarial classification). For any $f \in F$ with $d = \text{VC}(F)$, any $n \in \mathbb{N}, \delta \geq 0$ and any distribution $P$ over $X$, with probability $\geq 1 - \delta$ over $\bar{x}, z \sim P^n$, the following holds simultaneously for all $x \in X^n$:

$$\ell_x(f, h, \hat{\alpha}) \leq \frac{\alpha}{n} |\{i : x_i \neq z_i\}| + \frac{2d \log 2n + \log 1/\delta}{n},$$

where $h = \text{ERM}(\bar{x}, f(\bar{x}))$ and $\hat{\alpha} = \text{MMA}(\bar{x}, f(\bar{x}), x, h, \text{FLIP}) \in [0, 1]^n$ can be computed in time $\text{poly}(n)$ using ERM.

In their adversarial setting, GKKM again has $\tilde{O}(\sqrt{d/n})$ bounds. Our presentation actually begins in this adversarial setting as it in some sense most general–adversarial robustness implies robustness to covariate shift.

### 1.2 Linear regression results

For selective linear regression, the classic problem with transductive abstention, we give a more involved but fully polynomial-time algorithm. (GKKM did not discuss regression.) Here, $Y = [-1, 1], X = B_d(1)$ is taken to be the unit ball in $d$ dimensions. There is now a joint distribution $\nu$ over $X \times Y$ such that: $f(x) := E_{\nu}[y|x] = w \cdot x$ for some vector $w$ with $\|w\| \leq 1$. We write $(\bar{x}, \bar{y}) \sim \nu^n$ to indicate that the $n$ labeled training examples are drawn from $\nu$. The loss for selective regression $\ell_x(h, f, a)$ is still defined as in (1) except that $\ell(f(x), h(x)) := |f(x) - h(x)|^2$. Note that we are considering loss with respect to $f$ rather than $y$ which means that it may approach 0 for identical train and test distributions. Indeed, the additional loss term we will face due to the covariate shift is again $\alpha|P - Q|_{TV}$, where $P$ and $Q$ are the marginal distributions over $X$ for $\nu$ and the test distribution, respectively.

**Theorem 4** (Linear regression). Let $Y = [-1, 1], n, d \in \mathbb{N}, \delta > 0$, and $X = B_d(1)$. Let $P, Q$ be distributions over $X$ and $\nu$ be a distribution over $X \times Y$ with marginal $P$ over $X$. Let $f(x) := \mathbb{E}_{(x, y) \sim \nu}[y|x] = w \cdot x$ for some $w \in B_d(1)$. Then,

$$\mathbb{E}_{(\bar{x}, \bar{y}) \sim \nu^n, x \sim Q^n} \left[ \ell_x(f, h, \hat{\alpha}) \right] \leq \alpha |P - Q|_{TV} + \frac{\kappa \log n}{\sqrt{n}}.$$
where $\kappa$ is a constant, $h = \text{ERM}(\bar{x}, \bar{y})$ and \( \hat{a} = \text{MMA}(\bar{x}, \bar{y}, x, h, \text{CDT}) \in [0, 1]^n \) can be computed in time $\text{poly}(n, d)$.

A technical challenge is that, as a subroutine, we need to find a linear model maximizing squared error, which is a non-convex problem. Fortunately, this step can be formulated as a Celsis-Dennis-Tapia (CDT) problem, for which efficient algorithms are known \cite{4,5}. Our information theoretic results generalize to more general regression in a straightforward fashion, however the algorithm for maximizing loss is non-convex and we only know how to implement it efficiently for linear regression.

**Contributions and organization.** The main contributions of this work are: (1) introducing and analyzing an approach for optimally abstaining in classification and regression, and (2) giving an efficient abstention algorithm for linear regression and an efficient reduction for binary classification (optimal in our model). After reviewing related work, we formulate the problem in a manner that applies to both types of prediction: binary classification and regression. Section 2 gives information-theoretic bounds for selective prediction. Section 3 covers the general MMA reduction. We then focus on classification, where Section 4 gives bounds and an efficient reduction to ERM. Finally, Section 5 gives bounds and a polynomial-time abstention algorithm for linear regression.

### 1.3 Related work

There is relatively little theoretical work on selective classification tolerant to distributional shift. Early work had algorithms that could learn certain binary classes $F$ with very strong absolute abstention and error guarantees \cite{12,13,16}. However, it was impossible to learn other simple concept classes, even rectangles, in their models. GKKM was the first work to provide abstention guarantees for arbitrary classes of bounded VC dimension, achieving this with bounds that depended on $|P - Q|_{TV}$. They showed that unlabeled examples (i.e., transductive learning) were provably necessary. In their PQ-learning model, specific to binary classification, they simultaneously guarantee $O(\sqrt{d/n})$ errors ($h(x) \neq f(x)$ which are not abstentions) from distribution $Q$ and $\leq \epsilon$ rejections on future examples from distribution $P$. While this latter condition may seem counter-intuitive at first, it implies guarantees in terms of total variation distance similar to the ones we give. However, they show that this approach to deriving bounds necessarily suffers from a $\Omega(\sqrt{d/n})$ inherent loss. We circumvent this lower-bound in the Chow cost model by directly optimizing over $Q$ without regard to rejections on $P$. Appendix C details this comparison.

Other related work is either about selective classification or distributional shift, but not both. Work on selective classification, also called “reliable learning” and “classification with a reject option,” \cite{5,2,7} study the benefits of abstaining in a model with fixed small cost $\alpha > 0$. The goal is to abstain in regions where the model is inaccurate. Finally, among the large body of prior work on transductive learning, the closest is work on transfer learning (without abstentions) \cite{11}. Prior work on distributional shift without abstention [see, e.g., the book\cite{14}] has developed refined notions of distributional discrepancy with respect to classes of binary or real-valued functions \cite{12}. Since the focus of our work is on abstention, we use total-variation distance. In future work, it would be interesting to see if these notions could be adapted to our setting.

Note that while our work addresses adversarial examples, it is very different from the recent line of work focused on robustness to small perturbations of the input \cite{17,9}. While our algorithms are not robust to such perturbations, they may at least abstain from predicting on such examples rather than misclassifying them.

### 1.4 Definitions

A table of our notation is given in Appendix A for convenience. Many of the definitions are common to classification and regression. Let $X$ denote the instance space and $Y$ denote the label space, and let $F$ be a known family of functions from $X$ to $Y$. There is an unknown target function $f \in F$ to be learned.

We use boldface to indicate vectors (indexing examples), e.g., $a = (a_1, \ldots, a_k)$. We denote by $f(a) = (f(a_1), \ldots, f(a_k))$ for function $f$. Throughout the paper, we assume that $\alpha$ and $F$ are fixed.

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2To avoid measure-theoretic issues, for simplicity we assume that $X$ is finite or countably infinite.
and known. Let \( [n] = \{1, 2, \ldots, n\} \) and \( 1[\phi] \) denotes the indicator that is 1 if predicate \( \phi \) holds and 0 otherwise.

There is a general base loss \( \ell : Y \times Y \to \mathbb{R}_+ \). We extend the definition of loss to loss on a sequence \( x \) and with abstention indices \( A \subseteq [n] \):

\[
\ell_x(f, h) := \frac{1}{n} \sum_{i=1}^{n} \ell(f(x_i), h(x_i)), \quad \ell_x(f, h, A) := \frac{1}{n} \sum_{i \in A} \ell(f(x_i), h(x_i)).
\]

We assume access to a deterministic algorithm returning \( \text{ERM}(x, y) \in \arg\min_{g \in F} \sum_i \ell(y_i, g(x_i)) \) that runs in unit time on any dataset \( x \in X^n, y \in Y^n \) (even noisy).

The algorithms all take labeled training examples \( x \in X^n, y \in Y^n \) and unlabeled test examples \( x \in X^n \) as input. For binary classification, as discussed, \( Y = \{0, 1\} \), there are train and test distributions \( P, Q \) over \( X \), and all examples are assumed to be labeled by \( f \), so \( \bar{y} = f(\bar{x}) \). Here, the version space of classifiers with 0 training error is defined to be \( \text{VS}(\bar{x}, \bar{y}) := \{g \in F : g(\bar{x}) = \bar{y}\} \).

For regression, \( Y = [-1, 1] \) and there is a train distribution \( \nu \) over \( X \times Y \) with marginal \( P \) over \( X \), and it is assumed that \( f(\bar{x}) := \mathbb{E}_{(\bar{x}, \bar{y}) \sim \nu} [\bar{y} | \bar{x}] \in F \). The test distribution similarly has marginal \( Q \) over \( X \). The version space is \( \text{VS}_\alpha \) is somewhat more complicated and is defined in Section 5.

With respect to \( V \subseteq F \) (which we will generally take to be the version space), we denote the worst-case test loss of a given classifier \( h \) (with a given abstention set \( A \) ) on the test set, denoted by \( L_\infty \):

\[
L_x(V, h) := \max_{g \in V} \ell_x(g, h), \quad L_x(V, h, A) := \max_{g \in V} \ell_x(g, h, A).
\]

2 Information-theoretic bounds for classification and regression

This section bounds the statistical loss (ignoring computation time) of choosing where to abstain \( A \) so as to minimize the upper-bound \( L_x(V, h, A) \) on test loss, where the predictor \( h \) (used when not abstaining) is first fit on training data and \( V \subseteq F \) is a general version space containing the target \( f \). For noiseless binary classification, \( V \) would simply be those classifiers consistent with \( f \), and \( V \) is a bit different for regression. Now, for “normal” test data \( z \sim P^n \) iid from the train distribution, a standard generalization bound would apply to the worst-case test loss \( \mathbb{E}_{z \sim P^n}[L_x(V, h)] \) (e.g., \( \tilde{O}(d/n) \) for binary classification with 0-1 loss). Our bounds are stated in terms of this quantity \( \mathbb{E}_{z \sim P^n}[L_x(V, h)] \) and can be viewed as the overhead due to \( P \neq Q \).

2.1 Learning with adversarial test examples

We begin with the adversarial setting of GKKM since it is particularly simple and will imply bounds in a distributional case. Here, there is only one distribution \( P \). First, nature picks \( n \) “natural” iid train and test examples \( \bar{x}, \bar{z} \sim P^n \). As mentioned, if there were no adversary, a learning algorithm might output some \( h \) in a version space \( V \) and would have a test error guarantee of \( L_x(V, h) \).

Instead, a computationally-unlimited adversary armed with knowledge of \( x, \bar{y}, z, f \), and the learning algorithm (and its random bits), chooses an arbitrary test set \( x \in X^n \) by corrupting as many or few test examples as desired. If \( we know \ z \), the adversary could corrupt any \( \gamma \) fraction of examples, we could of course guarantee loss \( \leq \gamma \alpha + L_x(V, h) \) by abstaining on the modified examples where \( x_i \neq z_i \). While the learning algorithm does not see \( z \), it can still achieve the same guarantee:

**Lemma 1.** (Adversarial loss) For any \( n \in \mathbb{N}, V \subseteq F, f \in V, z, x \in X^n, h : X \to Y \) and all \( A^* \in \arg\min_{A \subseteq [n]} L_x(V, h, A) \):

\[
\ell_x(f, h, A^*) \leq \frac{\alpha}{n} |\{i : x_i \neq z_i\}| + L_x(V, h).
\]

What this means is that if the natural training and test distributions are iid from the same distribution, then no matter which examples an adversary chooses to corrupt—\( x \) may be arbitrary—if one chooses \( A \) to minimize \( L_x(V, h, A) \), one guarantees the same exact bound \( \gamma \alpha + L_x(V, h) \). Moreover, the adversary has no control over \( L_x(V, h) \).
We state bounds in terms of The question then becomes, how difficult is it to find a function in
3 The reduction (for classification and regression) where the above holds simultaneously for all
Lemma 2. [Covariate shift] For any distributions \( P, Q \) over train and test examples, respectively. For the reasons mentioned above, we focus on the (transductive) abstention problem where \( h \) and version space \( V \) are determined from training data, and we focus on the expected test error. Below we give a bound of the form \( \alpha |P - Q|_{TV} + \mathbb{E}_{x \sim P^n}[L_x(V, h)] \). Note that the second term is a standard generalization bound for transductive learning with test data from \( P \) – the worst case test loss (e.g., \( \tilde{O}(d/n) \) for binary classification). Hence, the first term represents the overhead for \( P \neq Q \). In fact, we get can state a tighter bound.

We state bounds in terms of \( D_k \) divergence for \( k \geq 1 \), defined in Eq. (3), which generalizes statistical distance recalling that \( D_1(P||Q) = |P - Q|_{TV} \). To see why total variation bounds are loose, consider a distribution \( P \) which is uniform on \( X = [0, 1] \) and \( Q \) which is uniform on \([0, 1/2] \), so \( |P - Q|_{TV} = 1/2 \). Clearly the error rate of any \( h \) under \( Q \) is at most twice the error rate under \( P \), and depending on \( \alpha \) it may be significantly cheaper not to abstain. In particular, let \( \epsilon = \mathbb{E}_{x \sim P^n}[\ell_x(f, h)] \) be the error of \( h \) over \( P \). As long as \( \epsilon < \alpha/2 \), the error upper bound \( 2\epsilon \) from not abstaining at all is lower than \( \alpha |P - Q|_{TV} = \alpha/2 \). The guarantee we give is:

Lemma 2. [Covariate shift] For any distributions \( P, Q \) over \( X \), any \( h : X \to N, n \in N, V \subseteq F, f \in V \),

\[
\mathbb{E}_{x \sim Q^n}[\ell_x(f, h, A^*)] \leq \min_{k \geq 1} \alpha D_k(P||Q) + k \cdot \mathbb{E}_{z \sim P^n}[L_z(V, h)] \leq \alpha |P - Q|_{TV} + \mathbb{E}_{z \sim P^n}[L_z(V, h)],
\]

where the above holds simultaneously for all \( A^* \in \arg \min_{A \subseteq [n]} L_x(V, h, A) \).

In the above example, \( D_2(P||Q) = 0 \) for \( P, Q \) uniform over \([0, 1] \) and \([0, 1/2] \), respectively.

3 The reduction (for classification and regression)

The approach is conceptually simple: it chooses where to abstain so as to minimize the upper-bound on test loss \( L_x(V, h, A) \). The algorithm MMA, in particular, shows that if one can maximize loss, then one has a separation oracle that can be used to minimize this upper bound using standard techniques. In particular, the ellipsoid algorithm is used, though simpler algorithms would suffice\(^3\).

The question then becomes, how difficult is it to find a function in \( F \) that maximizes loss. For classification, this can be done using an ERM oracle and a label-flipping “trick” used by \( [8] \). For linear regression, this can be done in polynomial time (no ERM oracle is required, and ERM is trivial for linear regression) using existing CDT solvers. We first relax from binary to fractional abstention.

Fractional abstention. Loss may be slightly lower if one is allowed fractional abstentions, or equivalently to abstain at random. This can be described by a probability \( a_i \in [0, 1] \) for each test example \( x_i \), which indicates that we abstain with probability \( a_i \) and classify according to \( h \) with probability \( 1 - a_i \). As described in the introduction, the definitions of \( \ell \) and \( L \) are extended to fractional abstention vectors \( a \in [0, 1]^n \) in the natural way:

\[
\ell_x(f, h, a) := \frac{1}{n} \sum_{i=1}^n a_i c_i + (1 - a_i) \ell(f(x_i), h(x_i)) \quad \text{and} \quad L_x(V, h, a) := \max_{g \in F} \ell_x(g, h, a).
\]

Our task is to optimize abstention given a fixed \( h \) and \( x \) and a fixed set of candidate function \( g \in V \) (e.g., a version space), assuming one can maximize loss, i.e., find \( g \in V \) realizing \( \max_{g \in V} \ell(g, h, \hat{a}) = L_x(V, h, \hat{a}) \).

\(^3\)Perceptron-like algorithms would suffice as we require only optimization to polynomial (not exp.) accuracy.
Algorithm MMA

Input: $\tilde{x}, x \in X^n, \tilde{y}, y \in Y^n, h : X \to Y$, and approximate loss-maximizer $O$
Output: $a \in [0,1]^n$

Find and output point in convex set $K$:

$$K := \left\{ a \in [0,1]^n : L_\infty(\text{VS}(\tilde{x}, \tilde{y}), h, a) \leq \min_{a \in [0,1]^n} L_\infty(\text{VS}(\tilde{x}, \tilde{y}), h, a) + 1/n \right\}$$

by running the Ellipsoid algorithm using the following separation oracle $\text{SEP}(a)$ to $K$:

1. If $a \notin [0,1]^n$, i.e., $a_i \notin [0,1]$, then output unit vector $v$ with $v_i = 1$ if $a_i > 1$ or $v_i = -1$ if $a_i < 0$.
2. Otherwise, output separator

$$v := (c - \ell(g(x_1), h(x_1)), \ldots, c - \ell(g(x_n), h(x_n)),$$

where $g := O(\tilde{x}, \tilde{y}, h, a)$. // $g \in \text{VS}(\tilde{x}, \tilde{y})$ maximizes $\ell_x(g, h, a)$ to within $1/(3n)$.

Figure 2: The reduction MMA for computing abstention probabilities using an approximate loss maximization oracle $O$ whose output $g \in \text{VS}(\tilde{x}, \tilde{y})$ maximizes $\ell_x(g, h, a)$ to within $1/3n$. Ellipsoid runtime analysis is in Lemma[3]

Lemma 3 (Reduction). For any bounded loss $\ell : Y^2 \to [0,1]$, any $V := \text{VS}(\tilde{x}, \tilde{y}) \subseteq Y^X$, any $h : X \to Y$, and any $x \in X^n$, the Ellipsoid algorithm can be used in MMA to find $\hat{a}$ such that,

$$L_\infty(V, h, \hat{a}) \leq \min_{a} L_\infty(V, h, a) + \frac{1}{n},$$

in $\text{poly}(n)$ time and calls to approximate loss maximization oracle $O$ provided that its outputs $g = O(\tilde{x}, \tilde{y}, h, a) \in V$ all satisfy $\ell_x(g, h, a) \geq \max_{g' \in V} \ell_x(g', h, a) - \frac{1}{3n}$.

This can be done using any standard optimization algorithm, e.g., the ellipsoid algorithm, with $O$ serving as a separation oracle. Optimizing to within less than $1/n$ is not generally significant for learning purposes. Note that the Ellipsoid method is more commonly defined with a separation-membership oracle that either claims membership in the convex set $K$ or finds a separator. As we describe in Appendix F.3 containing the proof of Lemma[3] for such optimization problems the Ellipsoid can be used with such an oracle by outputting the query with best objective value.

4 Binary classification

For the case of binary classification, the version space is defined as follows:

$$\text{VS}(\tilde{x}, \tilde{y}) := \{ g \in F : g(x_i) = y_i \text{ for all } i \leq n \}.$$  

We can use generalization bounds on $L_\infty(\text{VS}(\tilde{x}, \tilde{y}), h)$ to get directly:

Theorem 5 (Adversarial classification loss). For $Y = \{0,1\}$, $d = \text{VC}(F)$, $\ell(y, \hat{y}) = |y - \hat{y}|$, any $n \in \mathbb{N}$, $\delta > 0$, the following holds with probability $\geq 1 - \delta$ over $\tilde{x}, \tilde{z} \sim P^n$: For all $h \in \text{VS}(\tilde{x}, f(\tilde{x})), x \in X^n$, and all $A^* \in \text{argmin}_{A \subseteq [n]} L_\infty(\text{VS}(\tilde{x}, f(\tilde{x})), h, A)$,

$$\ell_x(f, h, A^*) \leq \frac{\alpha}{n} |\{i : x_i \neq z_i\}| + \frac{2d \log 2n + \log 1/2\delta}{n}.$$  

Proof. This follows directly from Lemma[1] and generalization bound Lemma[7] of Appendix[3].

Covariate shift bounds for classification were stated in Theorems[1] and[2]. Next, as observed in prior work [8], for binary classification with the 0-1 loss, one can use an ERM oracle which minimizes loss to maximize loss as needed above. This algorithm is called FLIP.
Lemma 4 (FLIP). For \( Y = \{0, 1\} \) with \( \ell(y, \hat{y}) = |y - \hat{y}| \) and any \( h \in F, \mathbf{x} \in X^n, \mathbf{y} = h(\mathbf{x}) \in Y^n, \) and any \( a \in [0, 1]^n \),

\[
\hat{g} = \text{ERM} \left( 4n^2 \text{ copies of } (\bar{x}_i, \bar{y}_i) \text{ and } 3n(1 - a_i) \text{ copies of } (x_i, 1 - h(x_i)), \text{ for each } i \right)
\]
satisfies \( \hat{g} \in \text{VS}(\mathbf{x}, \mathbf{y}) \) and \( \ell_x(\hat{g}, h, a) \geq \text{L}_x(\text{VS}(\mathbf{x}, \mathbf{y}), h, a) - 1/3n. \)

In other words, one creates an artificial weighted dataset consisting of numerous copies of the training data \((\bar{x}_i, \bar{y}_i)\) and a number of copies proportional to \(1 - a_i\) of each flipped test example \((x_i, 1 - y_i)\). Then the classifier output by ERM is in the version space with 0 training error, due to the high weight of each \((\bar{x}_i, \bar{y}_i)\), and approximately maximizes \( \ell_x(g, h, a) \). If \( \mathcal{O} \) can take weighted examples, then a dataset with only 2n samples would suffice. The proof appears in Appendix F.5.

5 Regression

In this section, we let \( Y = [-1, 1] \) and use the squared loss function \( \ell: Y^2 \rightarrow \mathbb{R}_+, \ell(y, \hat{y}) = (y - \hat{y})^2. \) For regression, since labels are noisy, we will not be able to use an exact version space and instead will need to define an \( \alpha \)-approximate version space for \( \alpha \geq 0; \text{VS}_\alpha(x, h) = \{ g \in F \mid \ell_x(g, h) \leq \alpha \}. \) For classes \( F \) that are convex and have bounded “Rademacher complexity”, the version space can be bounded (cf. Section 4 for the details). Unfortunately, the label flipping “trick” used for classification cannot be applied to maximize loss for regression. The loss here is continuous and convex in \( \bar{y} \), and any \( \ell \) to achieve a solution that is within an additive factor \( \varepsilon \) to \( \alpha \)-tightening the constraint set slightly and using an approximate optimal solution. As the running time is polynomial in \( \log(1/\varepsilon) \), choosing an \( \varepsilon \) smaller than the bounds obtained by the learning algorithm suffices. The details are provided in Appendix H.

Lemma 5 (Regression loss maximization). For \( X, Y, \ell \) as defined above, consider \( F \), the class of linear functions from \( X \rightarrow Y \). Assuming we have an exact oracle for the CDT problem, for any \( h \in F, \mathbf{x} \in X^n, \mathbf{y} \in Y^n, \mathbf{x} \in X^n, \alpha > 0, \) and \( a \in [0, 1]^n \), there exists a polynomial time algorithm that outputs \( \hat{g} \in \text{VS}_\alpha(\mathbf{x}, h) \) such that \( \ell_x(\hat{g}, h, a) = \text{L}_x(\text{VS}_\alpha(\mathbf{x}, h), h, a). \)

6 Conclusions

We have shown how transductive abstention can lead to algorithms with robustness to arbitrary covariate shift and adversarial test examples. A simple min-max approach is given to minimize the worst-case loss and is show how to efficiently implement this approach in certain cases such as linear regression. The min-max approach enjoys both optimal guarantees in terms of test loss and essentially no cost for not knowing the train and test distributions \( P \) and \( Q \) over \( X \).

In terms of future work, it would be interesting to generalize the abstention model to online and possibly agnostic settings, or at least understand the limits. GKKM showed a lower bound of \( \Omega(\sqrt{\text{OPT}}) \) for one agnostic model, though it is not clear what the right agnostic model is. Finally, it would be interesting to see if their are other applications of our min-max approach of formulating a learning problem as an optimization with no unknowns. It enables one to directly achieve upper bounds as good as if one knows the unknowns.
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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper’s contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes]
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] See introduction.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]

2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes]
   (b) Did you include complete proofs of all theoretical results? [Yes] In supplementary materials.

3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [N/A]
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [N/A]
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   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]
A Summary of notation

- \(X, Y\) sets of possible examples and labels, resp.
- \(F\) family of functions \(f: X \to Y\)
- \(f \in F\) unknown target function to be learned
- \(\bar{x} \in X^n, \bar{y} \in Y^n\) \(n\) training examples and labels (\(\bar{y} = f(\bar{x})\) for classification)
- \(x \in X^n\) \(n\) (unlabeled) test examples
- \(A \subseteq [n]\) subset of test examples to abstain on
- \(P, Q\) train and test distributions over \(X\)
  - \(\nu\) training distribution for regression over \(X \times Y\) with marginal \(P\) over \(X\) and \(f(x) := \mathbb{E}_{(\bar{x}, \bar{y}) \sim \nu}[\bar{y}|x] \in F\)
  - \(\alpha\) cost of abstaining instead of predicting
- \(\ell(y, \hat{y})\) non-negative base loss function \(\ell: Y^2 \to \mathbb{R}_+\)
- \(\ell_\bar{x}(f, h)\) test loss \(\frac{1}{n} \sum_i \ell(f(x_i), h(x_i))\)
- \(L_\bar{x}(V, h)\) worst possible loss \(\max_{g \in V} \ell_\bar{x}(g, h)\) over \(g \in V\)
- \(\ell_\bar{x}(f, h, A)\) test loss \(\frac{1}{n} |A| + \frac{1}{n} \sum_{i \notin A} \ell(f(x_i), h(x_i))\)
- \(L_\bar{x}(V, h, A)\) worst possible loss \(\max_{g \in V} \ell_\bar{x}(g, h, A)\) over \(g \in V\)
- \(\ell_\bar{x}(f, h, a)\) test loss \(\frac{1}{n} \sum_{i \in A} \ell(f(x_i), h(x_i))\)
- \(L_\bar{x}(V, h, a)\) worst possible loss \(\max_{g \in V} \ell_\bar{x}(g, h, a)\) over \(g \in V\)
- \(\text{VS}(\bar{x}, \bar{y}) \subseteq F\) classification version space \(\{g \in F : g(\bar{x}) = \bar{y}\}\)
- \(\text{VS}_\alpha(x, h)\) regression version space \(\{g \in F : \ell_\bar{x}(g, h) \leq \alpha\}\) (for \(\alpha > 0\))
- \(\text{ERM}(x, y)\) deterministic oracle to \(\arg\min_{h \in F} \sum_i \ell(y_i, h(x_i))\) for arbitrary \(x, y\)
- \(h = \text{ERM}(\bar{x}, \bar{y})\) predictor learned based on the labeled training data

B From transduction to generalization

One can trivially convert from transductive learning to generalization. In particular, given a transductive learner that classifies sets of \(n\) test examples, and given \(n - 1\) test examples, one can output an ordinary classifier \(h: X \to Y\) such that \(h(x)\) is simply the transductive learner’s label on \(x\) when \(x\) is added to the \(n - 1\) examples. The expected errors are the same, as long as the examples are permuted randomly before running the transductive learner. In this section, we point out that this works for abstention as well.

For this section, suppose we have a fixed test distribution \(Q\) over \(X\), fixed functions \(f, h: X \to Y\) with loss \(\ell: Y \times Y \to \mathbb{R}\), and an abstention algorithm that outputs a subset of test examples indices, i.e., \(A(x) \subseteq [n]\) for each test set \(x \in X^n\). For this section we will ignore any auxiliary inputs it takes which are chosen independently from \(x\), such as \(h\), the labeled training examples, and a version space.

For any distribution \(Q\) over \(X\), \(S \subseteq X\), and \(f, h: X \to Y\) we define the expected loss of \(h, S\) with respect to target \(f\) as,

\[
\ell_Q(f, h, S) := \alpha Q(S) + \mathbb{E}_{x \sim Q} [1|x \notin S] \ell(f(x), h(x))
\]
Lemma 6. For any $f, h : X \to Y$, distribution $Q$ over $X$ any transductive abstainer $a : X^n \to \{0, 1\}^n$, 
\[
E_{x \sim Q^n, i \in [n]} [\ell_Q(f, h, \alpha_i)] = E_{x \sim Q^n} [\ell_x(f, h, a(x))],
\]
where the expectation is over uniformly random $i$ and $\alpha_i(x) := a_i(x_1, \ldots, x_{i-1}, x, x_{i+1}, \ldots, x_n)$.

Proof. The proof follows from linearity of expectation, the fact that $(x_1, \ldots, x_{i-1}, x, x_{i+1}, \ldots, x_n) \sim Q^n$.

Since $\ell_Q$ is the generalization loss on future examples $x \sim Q$, this means that one can match the expected loss of any transductive abstainer on future examples drawn from $Q$.

C Comparison to GKKM’s PQ-learning

The “PQ learning” binary classification model of GKKM is different than Chow’s model of learning with a fixed cost $\alpha$ of abstention. In this section, we point out how our algorithm can be used to achieve PQ learning bounds (in expectation) that are similar to those of GKKM, and show how to use their PQ learning algorithm to achieve meaningful but suboptimal loss bounds in our setting of a rejection cost. This section follows GKKM and only considers binary classification with $Y = \{0, 1\}$ and $\ell(y, \hat{y}) = |y - \hat{y}|$.

PQ learning, rather than having a single loss with a fixed cost $\alpha$ for abstentions, considers two separate rates which we denote here by $\epsilon_1$ and $\epsilon_2$:

\[
\epsilon_1 = \epsilon_1(Q, h, f, A) := \Pr_{x \sim Q} [h(x) \neq f(x) \wedge x \notin A],
\]
\[
\epsilon_2 = \epsilon_2(P, A) := \Pr_{x \sim P} [x \in A]
\]

The first is the misclassification rate on future test examples from $Q$ (that are not abstained on), and the second (which they call false rejection rate) is the fraction of future examples from $P$ that are abstained on. Their Theorem 5.2 bounds $\epsilon_1 + \epsilon_2 \leq \tilde{O}(\sqrt{d/n})$ and their Theorem 5.4 shows $\epsilon_1 + \epsilon_2 \geq \Omega(\sqrt{d/n})$ in the worst case. Hence, in their model, there is a necessary additional cost to abstaining over the $\tilde{O}(d/n)$ rates common in noiseless learning of a $F$ of VC dimension $d$.

First note that their bound directly implies a bound on our loss, defined again as:

\[
\ell_Q(f, h, A) := c \Pr_{x \sim Q} [x \in A] + \Pr_{x \sim Q} [h(x) \neq f(x) \wedge x \notin A].
\]

Their $\epsilon_1 + \epsilon_2 \leq \tilde{O}(\sqrt{d/n})$ bound gives:

\[
\ell_Q(f, h, A) \leq c(\epsilon_2 + |P - Q|_{TV}) + \epsilon_1 \leq c|P - Q|_{TV} + \tilde{O}\left(\sqrt{d/n}\right).
\]

This is because the probability of abstaining under $Q$ is at most the probability of abstaining under $P$ plus $|P - Q|_{TV}$. While their Theorem A.5 gives a trade-off between $\epsilon_1$ and $\epsilon_2$, it only holds for $\epsilon_1 \geq \sqrt{d/n}$ which does not improve the above bound. Varying our parameter $\alpha$ is analogous to their trade-off.

Now, we bound $\mathbb{E}[\epsilon_1 + \epsilon_2] \leq \tilde{O}(\sqrt{d/n})$ using our model. To do so, consider the distribution $Q' = (1 - \lambda)P + \lambda Q$ for $\lambda = \sqrt{d/n} < 1/2$ supposing $n > 4d$. Use the $n$ labeled $P$-samples and $n$ unlabeled $Q$-samples to create a labeled training set of $n/2$ $P$-examples and a synthetic test set of $n/2$ unlabeled $Q'$-samples by, for each test example flipping a $\lambda$-biased coin to determine whether it should be from $P$ or $Q$. From the definitions $Q'$ and $\ell_{Q'}$, we also have,

\[
\ell_{Q'}(f, h, A) \geq (1 - \lambda)\epsilon c_2(P, A) + \lambda \epsilon_1(Q, h, f, A).
\]

Now, let us choose $\alpha$ so $\lambda = (1 - \lambda)c = \sqrt{d/n}$. Rearranging the above gives,

\[
\epsilon_1 + \epsilon_2 \leq \frac{1}{\lambda} \ell_{Q'}(f, h, A).
\]
Suppose one finds \( h, A \) such that,
\[
\ell_{Q'}(f, h, A) \leq c|P - Q'|_{TV} + \gamma,
\]
for some \( \gamma \). Combining with the fact that \( |P - Q'|_{TV} \leq \lambda \), gives:
\[
\ell_{Q'}(f, h, A) \leq c\lambda + \gamma.
\]
Putting this together with the chosen values of \( \alpha \) from \( \lambda = (1 - \lambda)c = \sqrt{d/n} \), gives,
\[
\epsilon_1 + \epsilon_2 \leq c + \frac{\gamma \lambda}{\alpha} \leq \frac{\sqrt{d/n}}{1 - \sqrt{d/n}} + \frac{\gamma}{\alpha} \leq O(\sqrt{d/n}) + \frac{\gamma}{\alpha}.
\]
Our Theorem 2 shows that our algorithm will output \( h, A \) satisfying (4 in expectation) for \( \gamma = O(d/n) \). This implies \( \mathbb{E}[\epsilon_1 + \epsilon_2] \leq O(\sqrt{d/n}) \), similar to GKKM. High probability bounds can be achieved by Markov’s inequality.

**Intuition.** The heart of the difference between the two models becomes clear in regions where \( P \) and \( Q \) overlap, e.g., where \( P(x) = \sqrt{d/n}Q(x) \). On such examples, \( PQ \)-learning either abstains and suffers a \( \sqrt{d/n} \) false rejection rate or classifies and may suffer \( \sqrt{d/n} \) error rate. In Chow’s model with a cost for abstention, the learner can selectively abstain without having to distinguish which examples are from \( P \) versus \( Q \) which is impossible. See the lower-bound of GKKM for further details.

**D Transductive bounds for binary classification with \( Q = P \)**

In this section, we bound the expected worst-case test error for binary classification, given training and test sets of size \( n \). This is a standard step used in proving generalization bounds, but we give the analysis for completeness. Recall that \( L \) is defined in Eq. (5).

**Lemma 7.** For any \( F \) of VC dimension \( d \), any \( f \in F \), and any distribution \( P \) over \( X \), and any \( \delta \in (0, 1] \),
\[
\mathbb{P}_{x, z \sim P^n} \left[ \max_{h \in VS(x, f(x))} L_z(\text{VS}(x, f(x)), h) < \frac{2d\log 2n + \log n}{n} \right] \leq 1 - \delta.
\]

**Proof.** We first establish Eq. (7). By Sauer’s Lemma, there are at most \( N = (2n)^d \) labelings of the \( 2n \) examples \( (x, z) \in X^{2n} \). For any \( k \geq 1 \), we claim:
\[
\mathbb{P}_{x, z \sim P^n} \left[ \max_{g \in VS(x, f(x))} \sum_i |g(z_i) - f(z_i)| \geq k \right] \leq N2^{-k}.
\]
To see the above, as is standard, one can imagine permuting these \( 2n \) examples without changing their joint distribution. For each of the \( < N \) labelings with more than \( k \) disagreements \( g \neq f \), the probability that all of these disagreements are in \( z \) is at most \( 2^{-k} \). By the union bound, the probability that any \( g \) have all disagreements in \( z \) is \( \leq N2^{-k} \), which is at most \( \delta \) for \( k \geq d\log 2n + \log \frac{1}{\delta} \) as in Eq. (9) of the Lemma.

Similarly, for Eq. (8), by the union bound over the \( \binom{N}{2} \) pairs of classifiers,
\[
\mathbb{P}_{x, z \sim P^n} \left[ \max_{g, h \in VS(x, f(x))} \sum_i |g(z_i) - h(z_i)| \geq k \right] \leq \left( \frac{N}{2} \right) 2^{-k}.
\]
By the union bound, the probability that any pair have all disagreements in \( z \) is \( \leq N^22^{-k-1} \), which is at most \( \delta \) for \( k \geq 2d\log 2n + \log \frac{1}{2\delta} \) as in Eq. (8) of the Lemma.
For Eq. (9), note that for non-negative integer random variable $W$, $E[W] = \sum_{k=1}^{\infty} P[W \geq k]$, so,

$$E_{x,x \sim P^n} \left[ \max_{g,h \in VS} \sum_i |g(z_i) - h(z_i)| \right] \leq \sum_{k=1}^{\infty} P_{x,z \sim P^n} \left[ \max_{g,h \in VS} \sum_i |g(z_i) - h(z_i)| \geq k \right] \leq \sum_{k=1}^{\infty} \min \left( 1, \left( \frac{N}{2} \right)^{2-k} \right).$$

Letting $K = \left\lfloor \lg \left( \frac{N}{2} \right) \right\rfloor = \lg \left( \frac{N}{2} \right) - \gamma$ for $\gamma = \lg \left( \frac{N}{2} \right) \in [0, 1)$, the last quantity above is,

$$K + \sum_{k=K+1}^{\infty} \left( \frac{N}{2} \right)^{2-k} = K + \left( \frac{N}{2} \right)^{2-K} = \lg \left( \frac{N}{2} \right) - \gamma + \lg \left( \frac{N}{2} \right)^{2-\lg \left( \frac{N}{2} \right) + \gamma} = \lg \left( \frac{N}{2} \right) - \gamma + 2^{\gamma}.$$

Using the fact that $2^\gamma - \gamma \leq 1$ for $\gamma \in [0, 1]$, this gives a bound of at most $1 + \lg \left( \frac{N}{2} \right) = \lg 2 \left( \frac{N}{2} \right) \leq \lg N^2$ which implies Eq. (9) of the Lemma since $N = (2n)^d$.

### E High-probability lower bound

In some scenarios, one’s goal is to minimize expected cost, such as when one regularly trains classifiers and costs are additive. In other prediction scenarios, it is desirable to have high probability guarantees on the accuracy of one’s classifier. As noted, Theorem 1 states bounds on expected loss rather than more standard high probability bounds. Unfortunately, the following lemma shows that this is for good reason.

**Lemma 8.** Let $X = \{1, 2\}$, and $F$ be consist of all 4 binary functions on $X$. Fix $P(1) = 1$ and $Q(1) = 1/2$, so $P$ is concentrated on 1 and $Q$ is uniform. Finally let $\mu$ be the uniform distribution over $F$. There is a constant $\kappa > 0$ such that, for any $c \in (0, 1/2)$, $n \geq 4$, for any transductive selective classification algorithm $L$ selecting $(h, a) := L(\tilde{x}, f(\tilde{x}), x)$:

$$\mathbb{P}_{f \sim \mu, \tilde{x} \sim P^n, x \sim Q^n} \left[ \ell_x(f, h, a) \geq c|P - Q|_{TV} + \frac{c}{\sqrt{n}} \right] \geq \kappa.$$

**Proof.** Let $m$ be the number of test 2’s. Suppose the selective classifier $h$ predict positively on $r$ of these $m$, negatively on $s$ of them, and abstains on the rest $(r, s \geq 0$ can be arbitrary reals such that $r + s \leq m$ if the classifiers make weighted predictions or if fractional abstentions are allowed). Imagine choosing $f(2)$ after choosing $f(1)$ and $\tilde{x}$. $x$. Since the training data reveals nothing about $f(2)$, it is conditionally uniform. Thus with probability $1/2$ over $\mu$, the algorithm’s total loss will be $c(m - r - s) + \max(r, s)$. However,

$$c(m - r - s) + \max(r, s) \geq c(m - r - s) + \frac{r + s}{2} = cm + (r + s) \left( \frac{1}{2} - c \right) \geq cm,$$

since $c \in (0, 1/2)$. Thus, with probability at least $1/2$, the algorithm’s loss will be $\geq cm$ regardless of its predictions and abstentions. It is well-known that with positive constant probability, say $\geq 2\kappa$, since $m$ is distributed like a standard binomial distribution (hence with standard deviation $\sqrt{m}/2$), $m \geq n/2 + \sqrt{n}$ for $n \geq 4$. Combined with the above, gives that with probability $\geq \kappa$, the average loss will be $\geq c/2 + c/\sqrt{n} = c|P - Q|_{TV} + c/\sqrt{n}$. \qed

### F Deferred proofs

We now prove the remaining deferred proofs.

**F.1 Proofs of main theorems from the introduction**

The main theorems are straightforward applications of the other theorems and lemmas in the paper.
Proof of Theorem 7 By Lemma 10,

\[ \mathbb{E}_{x \sim Q^n} \left[ \min_A L_{x}(V, h, A) \right] \leq \alpha |P - Q|_{TV} + \mathbb{E}_{x \sim P^n} [L_{x}(V, h)], \]

and by Eq. (9) of Lemma 7

\[ \mathbb{E}_{\hat{x}, z \sim P^n} [L_{x}(\text{VS}(\hat{x}, f(\hat{x})), h)] \leq \frac{2d \log 2n}{n}. \]

By Lemma 3 and Lemma 4 MMA together with FLIP find a solution within \(1/n\) of optimal, and the proof is completed using the fact that,

\[ \frac{2d \log 2n}{n} + \frac{1}{n} \leq \frac{2d \log 3n}{n}. \]

Proof of Theorem 3 This follows just as in the above proof, except using the expectation bound from Lemma 7 and using Lemma 2 instead of Lemma 10. By Lemma 6 the expected error of \(\alpha_1\) defined in that lemma is the same as the expected transductive loss \(\ell_x(f, h, a(x))\). (If the algorithm MMA is not symmetric, then one can shuffle the inputs first to make it symmetric.)

Proof of Theorem 1 By Lemma 10,

\[ \ell_x(h^*, A^*) \leq \alpha |P - Q|_{TV} + \mathbb{E}_{x \sim P^n} [L_{x}(V, h)], \]

and hence, if MMA minimizes the loss upper-bound of \(\hat{A}\) to \(1/n\), we will have a loss upper-bound of \(c|P - Q|_{TV} + 14c + 1/n\). By Lemma 5 one can efficiently maximize loss over the version space if one can solve the CDT problem exactly. As discussed, CDT can be solved to within \(\epsilon\) accuracy in time \(\text{poly}(\log 1/\epsilon)\). This is more than adequate for the approximate reduction required by Section 3 (see also Appendix H for details regarding the approximation of the CDT problem). To finish the proof, one simply observes that as the loss function is bounded, it suffices to set delta to 1/n.

F.2 Proofs from Section 2: information-theoretic loss bounds

In addition to proving Lemma 1 we expand on it to consider the possibility of jointly optimizing \((h, A)\) to minimize the worst-case loss. In particular, the Lemma below includes Lemma 1 as its second part.

Lemma 9. [Adversarial loss (expanded)] For any \(n \in \mathbb{N}, V \subseteq F, f \in V, z, x \in X^n,\)

\[ \ell_x(h^*, A^*) \leq \frac{\alpha}{n} \left| \{i : x_i \neq z_i\} \right| + L_x(V, f) \quad \text{for all } (h^*, A^*) \in \arg\min_{h \in F, A \subseteq [n]} L_x(V, h, A) \tag{10} \]

\[ \ell_x(h, A^*) \leq \frac{\alpha}{n} \left| \{i : x_i \neq z_i\} \right| + L_x(V, h) \quad \text{for all } h : X \to Y, A^* \in \arg\min_{A \subseteq [n]} L_x(V, h, A) \tag{11} \]
Proof. The idea is that, by minimizing $L_{\infty}(V, h, A)$, the resulting loss upper-bound is as low as if one knew $f$ and which points were modified $M := \{i : x_i \neq z_i\}$ and abstained on them. Formally, by definition of $L$, for all $(h^*, A^*) \in \arg\min_{h \in F, A \subseteq \{0, 1\}} L_{\infty}(V, h, A)$,

$$\ell_{\infty}(f, h^*, A^*) \leq L_{\infty}(V, h^*, A^*) = \min_{h, A} L_{\infty}(V, h, A) \leq L_{\infty}(V, f, M).$$

Since $x$ and $z$ agree outside of $M$,

$$L_{\infty}(V, f, M) = \frac{\alpha}{n} |M| + \max_{g \in V} \frac{1}{n} \sum_{i \notin M} \ell(g(z_i), f(z_i)) \leq \frac{\alpha}{n} |M| + \max_{g \in V} \ell_{\infty}(g, f) = \frac{\alpha}{n} |M| + L_{\infty}(V, f).$$

In the above we have used the fact that $\ell_{\infty}$ is first fit from the training data and $A$ is selected afterwards, which we refer to as (transductive) abstention. Abstention is practically appealing in that it is a post-processing step that can be added to any classifier. As we shall see for classification, the bound \[\text{(10)}\] is not significantly better than the transductive abstention bounds \[\text{(11)}.\]

Selective prediction versus abstention. The difference between the two bounds is that in the first case, the learner jointly optimizes for $h$ and $A$, which may be called (transductive) selective prediction, while in the second case, $h$ is first fit from the training data and $A$ is selected afterwards, which we refer to as (transductive) abstention. Abstention is practically appealing in that it is a post-processing step that can be added to any classifier. As we shall see for classification, the bound \[\text{(10)}\] is not significantly better than the transductive abstention bounds \[\text{(11)}.\]

F.3 Covariate shift analysis: Proof of Lemma 2

Before proving Lemma 2 we state a simpler lemma.

Lemma 10. [PQ loss] For any distributions $P, Q$ over $X$, any $h : X \rightarrow Y$, $n \in \mathbb{N}, V \subseteq F$, $f \in V$,

$$\mathbb{E}_{x \sim P^n} [\ell_{\infty}(f, h, A^*)] \leq \mathbb{E}_{x \sim Q^n} \left[ \min_A L_{\infty}(V, h, A) \right] \leq \alpha |P - Q|_{TV} + \mathbb{E}_{z \sim P^n} [L_{\infty}(V, h)],$$

where the above holds simultaneously for all $A^* \in \arg\min_{A \subseteq \{0, 1\}} L_{\infty}(V, h, A)$.

Note that this lemma follows directly from a tighter bound we prove in Lemma 2 the proof of this lemma serves as a "warm up" for that Lemma 2’s proof.

Proof. Let $A(x) = \arg\min_{A \subseteq \{0, 1\}} L_{\infty}(V, h, A) \subseteq 2^n$. The term \[\mathbb{E}_{x \sim Q^n} [\ell_{\infty}(f, h, A^*)]\] in the lemma is formally,

$$\mathbb{E}_{x \sim Q^n} \max_{A^* \in A(x)} \ell_{\infty}(f, h, A^*) \leq \mathbb{E}_{x \sim Q^n} \max_{A^* \in A(x)} L_{\infty}(V, h, A^*) = \mathbb{E}_{x \sim Q^n} \left[ \min_A L_{\infty}(V, h, A) \right]. \quad (12)$$

Thus, since we are minimizing over $A$, it suffices to give a (randomized) procedure for selecting $A$ knowing $x$ and even $P, Q$ that achieves in expectation,

$$\mathbb{E}_{x \sim Q^n, A} [L_{\infty}(V, h, A)] \leq \alpha |P - Q|_{TV} + \mathbb{E}_{z \sim P^n} [L_{\infty}(V, h)].$$

To see how, note that it is possible to pick $z \sim P^n$ by taking modifying an expected $|P - Q|_{TV}$ fraction of the points in $x$\footnote{Specifically, for each $i$, choose $z_i = x_i$ with probability $\min(1, P(z_i)/Q(z_i))$ and otherwise choose $z_i$ from the "adjustment" distribution $\rho(x) \propto \max(P(x) - Q(x), 0)$.} As in the proof of Lemma 1 letting $M := \{i : x_i \neq z_i\}$ be the set of modified indices,

$$\min_A L_{\infty}(V, h, A) \leq L_{\infty}(V, h, M) = L_{\infty}(V, h, M) \leq \frac{\alpha}{n} |M| + L_{\infty}(V, h).$$

The proof is completed by using the fact that $\mathbb{E} [\|M\|] = n \cdot |P - Q|_{TV}. \quad \Box$
Proof of Lemma 2. We show the inequality for any \( k \geq 1 \). We claim it suffices to exhibit joint distribution \((x, z, A) \sim \rho\) such that the marginal distribution over \( z \) is \( P^n \) and over \( x \) is \( Q^n \) and such that:

\[
\mathbb{E}_{(x, z, A) \sim \rho} \left[ \ell_{x}(V, h, A) \right] \leq \alpha D_k(P\|Q) + k \mathbb{E}_{(x, z) \sim \rho} \left[ L_{x}(V, h) \right].
\]

This is because, by Eq. (12), \( \mathbb{E}_{x \sim Q^n} \left[ f_{x}(f, h, A^*) \right] \) is at most,

\[
\mathbb{E}_{x \sim Q^n} \left[ \min_{A} L_{x}(V, h, A) \right] \leq \mathbb{E}_{(x, z) \sim \rho} \left[ L_{x}(V, h, A) \right] \leq \alpha D_k(P\|Q) + k \mathbb{E}_{(x, z) \sim \rho} \left[ L_{z}(V, h) \right] = \alpha D_k(P\|Q) + k \mathbb{E}_{z \sim Q^n} \left[ L_{z}(V, h) \right].
\]

We define \( \rho \) by defining a procedure for generating \((x, z, A) \sim \rho\). Begin with \( x \sim Q^n \). The procedure abstains independently on each test example with probability \( \alpha(x) := \max(1 - k\frac{P(x)}{Q(x)}, 0) \). The probability of abstaining on test examples \( x \sim Q \) is thus \( D_k(P\|Q) \):

\[
\mathbb{E}_{x \sim Q^n} \left[ \frac{|A|}{n} \right] = \sum_{x \in X} Q(x) \max(1 - k\frac{P(x)}{Q(x)}, 0) = \sum_{x \in X} \max(Q(x) - kP(x), 0) = D_k(P\|Q).
\]

Thus the expected cost due to abstaining is \( cD_k(P\|Q) \) and it suffices to show that,

\[
\mathbb{E}_{(x, z, A) \sim \rho} \left[ \max_{g \in V} \sum_{i \notin A} \ell(f(x_i), h(x_i)) \right] \leq k \mathbb{E}_{(x, z) \sim \rho} \left[ L_{x}(V, h) \right]. \quad (13)
\]

To complete the description of \( \rho \), we now explain how to generate \( z \). For each \( i \in A \), we will choose \( z_i = x_i \) with probability \( 1/k \) and otherwise, with probability \( 1 - 1/k \), choose \( z_i \sim \mu \).

For any \( x \in X \), the probability of choosing any \( z_i = z \) is the sum of: (a) the probability of copying \( z_i \) from \( x_i = z \) which is the probability of choosing \( x_i = z \) \((Q(z))\) times the probability of not abstaining \((1 - \alpha(z))\) times the probability of copying \((1/k)\); plus (b) the probability of choosing \( z_i \sim \mu \) to be \( z \) which is the probability of choosing \( z \) from \( \mu(\mu(z)) \) times the probability of not copying (this value \( \beta \) is not crucial but it is \( \beta := 1 - \frac{1}{k}D_k(P\|Q) \) since probability of copying is the product of the probability of not abstaining \( 1 - D_k(P\|Q) \) and copying \( 1/k \)). This yields:

\[
\forall i \in [n] : \mathbb{P}_{(x, z, A) \sim \rho} [z_i = z] = Q(z)(1 - \alpha(z))\frac{1}{k} + \mu(z)\beta.
\]

Since the probability of not abstaining is \( 1 - \alpha(x) = \min(kP(x)/Q(x), 1) \), the above is

\[
\forall i \in [n] : \mathbb{P}_{(x, z, A) \sim \rho} [z_i = z] = \min(P(z), Q(z)/k) + \mu(z)\beta,
\]

which can be made to be \( P(z) \) by an appropriate choice of \( \mu \), in particular \( \mu(z) = \frac{1}{\beta} \max(0, P(z) - Q(z)/k) \).

Since the distribution of \( z_i \) is independent across \( i \), the above reasoning implies that \( \rho \)'s marginal distribution over \( z \) is \( P^n \). Again, define \( M := \{i \in [n] : z_i \neq x_i\} \). For any \( x, A \), pick any
though it is often called simply a separation oracle) is an oracle that given a

This is because, for any \(a \in K(\epsilon)\),

\[
L_\infty(V, h, a) = \max_{g \in V} \frac{1}{n} \sum_i \alpha \cdot a_i + (1 - a_i)\ell(g(x_i), h(x_i)) \leq \max_{g \in V} \frac{1}{n} \sum_i \alpha \cdot a_i^* + (1 - a_i^*)\ell(g(x_i), h(x_i)) + |a_i - a_i^*| \cdot |c - \ell(g(x_i), h(x_i))| \leq L_\infty(V, h, a) + \epsilon.
\]

The last step follows from the fact that \(|a_i - a_i^*| \leq \epsilon\) and that \(c, \ell(g(x_i) - h(x_i)) \in [0, 1]\). Thus \(Z \subseteq K(\epsilon)\). Also, it is not difficult to see that \(Z\) contains a cube of side \(\epsilon\) and thus also ball of radius \(r = \epsilon/2\). So \(R/r = 2\sqrt{n}/\epsilon\) and the ellipsoid algorithm runs in \(\text{poly}(n \log 1/\epsilon)\) time and queries to a separation oracle outputs \(\tilde{a} \in K(\epsilon)\).

Using this, we are now ready to prove Lemma 3

Proof of Lemma 3 Let \(\text{OPT} := \min_{a \in [0, 1]^n} L_\infty(V, h, a)\) and, for any \(\delta \geq 0\),

\[
K(\delta) := \{a \in [0, 1]^n : L_\infty(V, h, a) \leq \text{OPT} + \delta\}.
\]
It suffices to output \( \hat{a} \in K(1/n) \). To do so, we fix \( \epsilon := 1/(3n) \) simulate running the ellipsoid algorithm on \( K(\epsilon) \), which Lemma 11 shows would find \( \hat{a} \in K(\epsilon) \) in \( \leq T = \text{poly}(n) \) oracle calls and runtime, using an actual separation-membership oracle to \( K(\epsilon) \).

A separation-membership oracle both \textit{separates}: for \( a \notin K(\epsilon) \) it finds a vector \( v \) such that \( v \cdot b < v \cdot a \) for all \( b \in K(\epsilon) \), and computes \textit{membership}: identifying whether or not \( a \in K \). We first argue that \( \text{SEP} \) separates any \( a \notin K(2\epsilon) \). First, if \( a \not\in [0,1]^n \), \( v \) trivially separates \( a \) from \( [0,1]^n \supseteq K(\epsilon) \).

Next, we argue that \( \text{SEP}(a) \) separates any \( a \in [0,1]^n \setminus K(2\epsilon) \) from \( K(\epsilon) \). To see this, by definition of \( \ell_x(g,h,a) \),

\[
\forall b \in [0,1]^n, \quad v \cdot \frac{a - b}{n} = \ell_x(g,h,a) - \ell_x(g,h,b).
\]

And thus,

\[
\forall b \in K(\epsilon), \quad v \cdot \frac{a - b}{n} \geq \ell_x(g,h,a) - (\text{OPT} + 1/3n).
\]

On the other hand, by assumption on \( O \), for any \( a \notin K(2\epsilon) \),

\[
\ell_x(g,h,a) \geq L_x(V,h,a) - 1/3n > (\text{OPT} + 2/3n) - 1/3n = \text{OPT} + 1/3n.
\]

Combining these gives \( v \cdot (a - b) > 0 \) as needed for all \( b \in K(\epsilon) \) and \( a \in [0,1]^n \setminus K(2\epsilon) \).

The above has shown that \( \text{SEP} \) separates all \( a \notin K(2\epsilon) \) from \( K(\epsilon) \), thus it only fails to be a separation-membership oracle to \( K(\epsilon) \) for \( a \in K(2\epsilon) \). Such a failure must occur on one of the first \( T \) steps if we run the Ellipsoid algorithm using \( \text{SEP} \), because we know the Ellipsoid algorithm would otherwise find a point in \( K(\epsilon) \). But such a “failure” \( a \in K(2\epsilon) \) is useful to us as it is in \( K(1/n) \).

In particular, we adapt the Ellipsoid algorithm as follows. We run it for periods \( t = 1, 2, \ldots, T \) using \( \text{SEP} \), a good assumption on \( O \). Let \( a^{(t)} \) be the \( t \)-th input to \( \text{SEP} \). For \( a^{(t)} \in [0,1]^n \), denote \( g^{(t)} := O(\bar{x}, \bar{y}, h, a^{(t)}) \). At the end, the algorithm returns \( a^{(t)} \) with smallest \( \ell_x(g^{(t)}, h, a^{(t)}) \). Again using the assumption on \( O \), we have that

\[
L_x(V,h,a^{(t)}) - \epsilon \leq \ell_x(g^{(t)}, h, a^{(t)}) \leq L_x(V,h,a^{(t)}).
\]

This means that, among the \( a^{(t)} \), the algorithm outputs one within \( \epsilon \) of the smallest \( L_x(V,h,a^{(t)}) \). In particular, since one of them has \( L_x(V,h,a^{(t)}) \leq \text{OPT} + 2\epsilon \), it outputs one with \( L_x(V,h,a^{(t)}) \leq \text{OPT} + 3\epsilon = \text{OPT} + 1/n \) as required.

F.5 The flipping trick: Proof of Lemma 4

Next, we prove Lemma 4 that shows how to use ERM to approximately maximize test loss, an idea due to GKKM.

**Proof of Lemma 4.** Any \( g \) minimizing loss on the artificial dataset must be in \( \text{VS}(\bar{x}, \bar{y}) \) because if \( g \) erred on any training example, then its weighted loss would be at least \( 4n^2 \), while loss \( \leq 3n^2 \) is achievable (any \( g \in \text{VS} \)). Further, for any \( g \in \text{VS}(\bar{x}, \bar{y}) \),

\[
\ell_x(g,h,a) - \ell_x(\hat{g}, h, a) = \frac{1}{3n^2} \sum_i 3n(1 - a_i) (\ell(g(x_i), h(x_i)) - \ell(\hat{g}(x_i), h(x_i)))
\]

\[
\leq \frac{1}{3n^2} \sum_i 1 + [3n(1 - a_i)] (\ell(g(x_i), h(x_i)) - \ell(\hat{g}(x_i), h(x_i)))
\]

\[
= \frac{1}{3n} + \frac{1}{3n^2} \sum_i [3n(1 - a_i)] (\ell(\hat{g}(x_i), 1 - h(x_i)) - \ell(g(x_i), 1 - h(x_i))).
\]

But the term is at most \( 1/3n \), as required, since the last summation above is the error difference on the artificial dataset, which is non-positive by definition of ERM.

F.6 Proofs from Section 5: Regression

**Proof of Lemma 5.** Note that any \( h \in \mathcal{F} \) can be parametrized by a vector \( w \in \mathbb{R}^d \), such that \( \|w\| \leq 1 \). Let \( w_h \) denote such a parameterization of \( h \). Thus, the set \( \text{VS}_h(\bar{x}, h) \) can be characterized as functions
represented by $w \in \mathbb{R}^d$ subject to the following two quadratic constraints:

$$\frac{1}{n} \sum_{i=1}^{n} (w \cdot \bar{x}_i - w_h \cdot \bar{x}_i)^2 \leq \alpha, \quad (14)$$

$$\sum_{i=1}^{d} w_i^2 \leq 1. \quad (15)$$

These are both ellipsoid constraints; the latter is simply constraining $w$ to lie in the unit ball. In particular, we note that the function $w \mapsto ||w||^2$ is strictly convex. Recall the definition:

$$L_\alpha(VS_\alpha(\bar{x}, h), h, a) = \frac{c}{n} \sum_{i} a_i + \max_{g \in VS_\alpha(\bar{x}, h)} \frac{1}{n} \sum_{i=1}^{n} (1 - a_i) \cdot \ell(g(x_i), h(x_i)).$$

As $a$ is fixed and known, the maximizers $g$ of $L_\alpha(VS_\alpha(\bar{x}, h), h, a)$ are obtained by minimizing the following quadratic function with respect to $w$:

$$-\frac{1}{n} \sum_{i=1}^{n} (1 - a_i)(w \cdot x_i - w_h \cdot x_i)^2,$$

subject to the quadratic inequality constraints (14) and (15). Noting that the inequality constraint (15) is represented by a strictly convex quadratic function, this is an instance of the CDT problem, and can be solved by using the oracle.

\[ \square \]

### G Regression : Version Space

Let $Y = [-1, 1]$ and consider the squared loss function $\ell : Y^2 \rightarrow \mathbb{R}_+$, $\ell(y, \hat{y}) = (y - \hat{y})^2$.

For regression, since labels are noisy, we will not be able to use an exact version space and instead will need to define an $\alpha$-approximate version space for $\alpha \geq 0$: $VS_\alpha(x, h) = \{ g \in F \mid \ell_\alpha(g, h) \leq \alpha \}$. We first discuss how to bound the version space for regression assuming that the family $F$ is convex, which means that for any $f, g \in F$, $\alpha f + (1 - \alpha)g \in F$ for every $\alpha \in [0, 1]$.

For a class of functions $G$, where each $g \in G$ is $g : X \rightarrow [0, 1]$, for a set $S = \{ x_1, \ldots, x_m \} \subseteq X$, the empirical Rademacher complexity of $G$ with respect to $S$ is defined as,

$$\hat{\text{RAD}}_S(G) = \mathbb{E}_{\sigma_1 \sim \cdots \sim (-1, 1)} \left[ \sup_{g \in G} \frac{1}{n} \sum_{i=1}^{n} \sigma_i g(x_i) \right],$$

where the $\sigma_i \in \{-1, 1\}$ are chosen uniformly and are known as Rademacher random variables. For any $n \in \mathbb{N}$ and for any distribution $P$ over $X$, define

$$\text{RAD}_n(G) = \mathbb{E}_{S \sim P^n}[\hat{\text{RAD}}_S(G)].$$

Lemma 12. Let $F$ be a class of functions from $X \rightarrow Y$ that is convex. Let $\text{RAD}_n(F)$ denote the Rademacher complexity of $F$. Let $\nu$ be any distribution over $X \times Y$ and let $f \in F$ be such that $\mathbb{E}[y|x] = f(x)$. Let $P$ be the marginal distribution of $\nu$ over $X$. Define

$$\varepsilon := 8\text{RAD}_n(F) + \sqrt{\frac{2\log(3/\delta)}{n}}.$$

For $(\bar{x}, \bar{y}) \sim \nu^n$ and $x \sim P^n$, if $h \in \arg \min_{g \in F} \ell_\alpha(\bar{y}, g(\bar{x}))$ then with probability at least $1 - \delta$,

1. $f \in \text{VS}_\varepsilon(\bar{x}, h)$
2. $\max_{g \in \text{VS}_\varepsilon(\bar{x}, h)} \ell_\varepsilon(g, h) \leq 14\varepsilon$
Before we prove Lemma 12, we state the following lemma.

**Lemma 13.** Let $F \subseteq Y^X$ be convex. Let $(\bar{x}, \bar{y})$ be the training data and $h \in \arg\min_{g \in F} \ell(\bar{y}, g(\bar{x}))$. Let $\ell : Y \times Y \to \mathbb{R}^+$ be the squared loss function, $\ell(y, \hat{y}) = (y - \hat{y})^2$. Then for any $f \in F$,

$$\ell_{\bar{x}}(f, h) \leq \ell(\bar{y}, f(\bar{x})) - \ell(\bar{y}, h(\bar{x}))$$

**Proof.** It is straightforward to check that,

$$\ell(\bar{y}, f(\bar{x})) - \ell(\bar{y}, h(\bar{x})) = \ell_{\bar{x}}(f, h) + \frac{\delta}{n} \sum_{i=1}^{n} (f(\bar{x}_i) - h(\bar{x}_i))(h(\bar{x}_i) - y_i)$$

We observe that the second term on the RHS above is non-negative, otherwise, $g := (1 - \alpha)h + \alpha f$ for a sufficiently small $\alpha > 0$ would have $\ell_{\bar{x}}(g, h) < \ell(\bar{y}, h(\bar{x}))$ contradicting the optimality of $h$. \hfill $\Box$

**Proof of Lemma 12** Note that $f \in F$ is such that $\mathbb{E}_D[y|x] = f(x)$. First consider the class of functions $F^1 := \{(x, y) \mapsto \frac{1}{2}\ell(g(x), y) \mid g \in F\}$ and $F^2 := \{x \mapsto \frac{1}{2}\ell(g(x), f(x)) \mid g \in F\}$. By using Talagrand’s lemma and the fact that $x \mapsto \frac{\ell}{2}$ is 1/2-Lipschitz for $x \in [0, 1]$, we get that $\text{RAD}_m(F^1) \leq \frac{1}{2}\text{RAD}_m(F)$ and $\text{RAD}_m(F^2) \leq \frac{1}{2}\text{RAD}_m(F)$ (see e.g. Lemma 5.7 from [13]). For a distribution $\nu$ over $X \times Y$, we denote by $\ell_\nu(g) = \mathbb{E}_{(x, y) \sim \nu}[\ell(y, g(x))]$. For the value of $\varepsilon$ set in the statement of the lemma, we have with probability at least $1 - \delta/3$, each of the following hold for every $g \in F$ (cf. Theorem 3.3 from [13]):

$$|\ell_\nu(g) - \ell_{\bar{y}, g(\bar{x})}| \leq \varepsilon/2,$$  \hfill (16)

$$|\ell_{\nu}(f) - \ell_{\bar{x}}(f, g)| \leq \varepsilon/2,$$  \hfill (17)

$$|\ell_{\nu}(f) - \ell_{\bar{x}}(f, g)| \leq \varepsilon/2.$$  \hfill (18)

By a simple union bound, all of the above hold for except with probability at most $\delta$. For the rest of the proof, we assume that the failure event does not occur.

Then, using Lemma 13 we have the following,

$$\ell_{\bar{x}}(f, h) \leq \ell_{\bar{x}}(\bar{y}, f(\bar{x})) - \ell_{\bar{x}}(\bar{y}, h(\bar{x}))$$

$$\leq \ell_{\nu}(f) - \ell_{\nu}(h) + \varepsilon$$

$$\leq \varepsilon.$$  \hfill Using (16)

As $\ell_{\nu}(f) = \min_{g \in F} \ell_\nu(g)$

This proves the first part of the result. For the second part, we will make repeated use of the following crude inequality when $\ell$ is the squared loss: for any $h \in F$, $\ell_{\bar{x}}(f, g) \leq 2\ell_{\bar{x}}(f, h) + 2\ell_{\bar{x}}(h, g)$. An analogous inequality holds when considering $\ell_{\nu}$. For the rest of the proof, denote by $V = \text{VS}_\nu(\bar{x}, h)$.

Then, we have

$$\max_{g \in V} \ell_{\bar{x}}(g, h) \leq 2\ell_{\bar{x}}(f, h) + 2\max_{g \in V} \ell_{\bar{x}}(f, g)$$

$$\leq 2\ell_{\bar{x}}(f, h) + 2\max_{g \in V} \ell_{\bar{x}}(f, g) + 2\varepsilon$$  \hfill Using (18)

$$\leq 2\ell_{\bar{x}}(f, h) + 2\max_{g \in V} \ell_{\bar{x}}(f, g) + 4\varepsilon$$  \hfill Using (17)

$$\leq 6\ell_{\bar{x}}(f, h) + 4\max_{g \in V} \ell_{\bar{x}}(g, h) + 4\varepsilon$$  \hfill Using (17)

$$\leq 10\max_{g \in V} \ell_{\bar{x}}(g, h) + 4\varepsilon \leq 14\varepsilon.$$  \hfill

In the last line above we used the fact that $f \in V$ to upper bound $\ell_{\bar{x}}(f, h)$ by $\max_{g \in V} \ell_{\bar{x}}(g, h)$. \hfill $\Box$

**H.** *Approximately solving the CDT Problem*

By slight abuse of notation, we will use the letter $g$ (suitably annotated) to denote a linear function and $w$ to denote the weight vector associated with the same linear function without explicit reference,
e.g. $\hat{g}$ is associated with $\hat{w}$, $\tilde{g}$ is associated with $\tilde{w}$, etc. Let $\hat{g}$ be the solution obtained by exactly solving the CDT problem as stated in Lemma 5.

We can instead tighten the constraints (14) and (15) by requiring that $w$ satisfy,

$$\frac{1}{n} \sum_{i=1}^{n} (w \cdot \bar{x}_i - w_h \cdot \bar{x}_i)^2 \leq \alpha - \epsilon,$$

(19)

$$\sum_{i=1}^{d} w_i^2 \leq 1 - \epsilon.$$  

(20)

Recall that the function we are minimizing in the CDT problem is given by:

$$F(w) = -\frac{1}{n} \sum_{i=1}^{n} (1 - a_i)(w \cdot x_i - w_h \cdot x_i)^2.$$  

(21)

Let $\tilde{g}$ denote a solution to the CDT problem with constraints (19) and (20) obtained using an approximate solver, which may violate the contraints by an additive factor of $\epsilon$. In particular, this means that $\tilde{g}$ satisfies the constraints (14) and (15). Furthermore, if $\hat{g}_\epsilon$ is the solution obtained by exactly solving the CDT problem with constraints (19) and (20), then we know that $F(\tilde{w}) \leq F(\hat{w}_\epsilon) + \epsilon$, again by the approximation guarantees given by the result of [3].

Let $\tilde{g}_{\lambda,\delta} = (1 - \delta)((1 - \lambda)\hat{g} + \lambda h)$. It can easily be checked that if we set $\lambda = 9\epsilon/\alpha$ and $\delta = \epsilon$, then using the fact that $F(w)$ is 8-Lipschitz for $w$ in the unit ball, $\tilde{g}_{\lambda,\delta}$ satisfies the constraints (19) and (20).

However, we note that $\|\hat{w}_{\lambda,\delta} - \hat{w}\|_2 = O(\lambda + \delta)$. Thus, we have, again using the Lipschitzness of $F$,

$$F(\tilde{g}) \leq F(\tilde{g}_\epsilon) + \epsilon$$

$$\leq F(\tilde{g}_{\lambda,\delta}) + \epsilon$$

$$\leq F(\tilde{g}) + O(\lambda + \delta).$$

The only observation that remains to be made is that $\epsilon$ may be set to be as small as we please since the running time of the approximate solver to the CDT problem provided by [3] runs in time polynomial in $\log(1/\epsilon)$. Certainly, this is more than sufficient for the results that we need to apply from Section 3.