A Minimax Approach to Supervised Learning

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Abstract

Given a task of predicting \( Y \) from \( X \), a loss function \( L \), and a set of probability distributions \( \Gamma \), what is the optimal decision rule minimizing the worst-case expected loss over \( \Gamma \)? In this paper, we address this question by introducing a generalization of the principle of maximum entropy. Applying this principle to sets of distributions with a proposed structure, we develop a general minimax approach for supervised learning problems, that reduces to the maximum likelihood problem over generalized linear models. Through this framework, we develop two classification algorithms called the minimax SVM and the minimax Brier classifier. The minimax SVM, which is a relaxed version of the standard SVM, minimizes the worst-case 0-1 loss over the structured set of distribution, and by our numerical experiments can outperform the SVM. We also explore the application of the developed framework in robust feature selection.

1 Introduction

Supervised learning, the task of inferring a function that predicts a target \( Y \) from a feature vector \( X = (X_1, \ldots, X_d) \) by using \( n \) labeled training samples \( \{(x_1, y_1), \ldots, (x_n, y_n)\} \), has been a problem of central interest in machine learning. Given the underlying distribution \( \tilde{P}_{X,Y} \), the optimal prediction rules had long been studied and formulated in the statistics literature. However, the advent of high-dimensional problems raised this important question that what would be an optimal prediction rule when we do not have enough samples to estimate the underlying distribution?

To understand the difficulty of learning in high-dimensional settings, consider a classification task for a genome-wide association studies (GWAS) problem where we seek to predict a binary label \( Y \) from an observation of 3,000,000 SNPs, each of which is a categorical variable \( X_i \in \{0, 1, 2\} \). Hence, to estimate the underlying distribution we need \( O(3^{3,000,000}) \) samples, that is impossible.

With no possibility of estimating the underlying \( P^* \) in such problems, several methods have been proposed to deal with high-dimensional settings. A standard approach in statistical learning is the empirical risk minimization (ERM) [1]. ERM learns the prediction rule by minimizing an approximated loss under the empirical distribution of samples \( \hat{P} \). However, to avoid overfitting ERM restricts the set of allowable decision rules to a class of functions with limited complexity, such as hypothesis classes of small VC dimension or spaces of norm-bounded linear functions.

As a complementary approach to ERM, one can learn the prediction rule through minimizing a decision rule’s worst-case loss over a larger set of distributions \( \Gamma(\hat{P}) \) centered at the empirical distribution \( \hat{P} \). In other words, instead of restricting the class of decision rules, we consider and evaluate all possible decision rules, but based on a more stringent criterion that they will have to perform well over all distributions in \( \Gamma(\hat{P}) \). As seen in Figure[1] this minimax approach can be broken into three main steps: First, we compute the empirical distribution \( \hat{P} \) from the data; Second, we form a distribution set \( \Gamma(\hat{P}) \) based on \( \hat{P} \); Finally, we learn a prediction rule \( \psi^* \) that minimizes the worst-case expected loss over \( \Gamma(\hat{P}) \).

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Some special cases of this minimax approach, which are based on learning a prediction rule from low-order marginal/moments, have been addressed in the literature: [2] solves a robust minimax classification problem for continuous settings with fixed first and second-order moments; [3] develops a classification approach by minimizing the worst-case hinge loss subject to fixed low-order marginals; and [4] fits a model minimizing the maximal correlation under fixed pairwise marginals to design a robust classification scheme. In this paper, we develop a general minimax approach for supervised learning problems with arbitrary loss function.

To formulate Step 3 in Figure 1, given a general loss function $L$ and set of distribution $\Gamma(\hat{P})$ we generalize the problem formulation discussed at [3] to

$$\arg\min_{\psi \in \Psi} \max_{P \in \Gamma(\hat{P})} \mathbb{E} \left[ L(Y, \psi(X)) \right].$$

(1)

Here, $\Psi$ is the space of all decision rules. Notice the difference with the ERM setting where $\Psi$ was restricted to smaller function classes while $\Gamma(\hat{P}) = \{\hat{P}\}$.

If we have to predict $Y$ with no access to $X$, (1) will reduce to the formulation studied at [5]. There, the authors propose to use the principle of maximum entropy [6], for a generalized definition of entropy, to find the optimal prediction minimizing the worst-case loss. By the principle of maximum entropy, we should select and predict based on a distribution in $\Gamma(\hat{P})$ that maximizes the entropy function.

How can we use the principle of maximum entropy to solve (1) when we observe $X$ as well? A natural idea is to apply the maximum entropy principle to the conditional $P_{Y|X=x}$ instead of the marginal $P_Y$. This idea motivates a generalized version of the principle of maximum entropy, which we call the principle of maximum conditional entropy. In fact, this principle breaks Step 3 in Figure 1 into two smaller steps: First, we search for $P^*$ the distribution maximizing the conditional entropy over $\Gamma(\hat{P})$; Then, we find $\psi^*$ the optimal decision rule for $P^*$.

Although the principle of maximum conditional entropy characterizes the solution to (1), computing the maximizing distribution is hard, in general. In [7], the authors propose a conditional version of the principle of maximum entropy, for the specific case of Shannon entropy, and draw the principle’s connection to (1). They call it the principle of minimum mutual information, by which one should predict based on the distribution minimizing mutual information among $X$ and $Y$. However, they develop their theory targeting a broad class of distribution sets, which results in a convex problem yet with an exponential number of variables in the dimension of the problem.

In this paper, we propose to fix the marginal $P_X$ across the distributions in $\Gamma(\hat{P})$ to find the right structure for the distribution set. Note that for a prediction task the goal is to learn the conditional distribution $P_{Y|X}$. Thus, through convex duality we require to learn only the dual variables corresponding to the constraints $\Gamma(\hat{P})$ enforces on $P_{Y|X}$. Therefore, if the empirical marginal $\hat{P}_X$ provides sufficient knowledge of the underlying $\hat{P}_X$ to learn those dual variables, we can learn a predictive model. Moreover, by imposing this specific structure on $\Gamma(\hat{P})$, (1) reduces to an unconstrained convex problem with a number of variables linear in the number of constraints on $P_{Y|X}$ in $\Gamma(\hat{P})$.

More importantly, by applying the described idea for the generalized conditional entropy we provide a generalization of the duality derived in [8] between maximum conditional (Shannon) entropy and maximum likelihood for logistic regression. This generalization justifies all generalized linear models via a unified minimax framework. In particular, we show how under quadratic and logarithmic loss...
functions our framework leads to the linear regression and logistic regression models respectively. Through the same framework, we also derive two classification algorithms which we call the minimax SVM and the minimax Brier classifier. The minimax SVM, which is a relaxed version of the standard SVM, minimizes the worst-case 0-1 loss and by our numerical experiments outperforms the SVM. Note that ERM with the 0-1 loss is known to be NP-hard [9]. The minimax Brier classifier justifies making binary classification using the Huber penalty and extends this binary classification technique to a multi-class version. Finally, we discuss the framework application in robust feature selection.

2 Principle of Maximum Conditional Entropy

In this section, we provide a conditional version of the key definitions and results developed in [5]. We propose the principle of maximum conditional entropy to break Step 3 into 3a and 3b in Figure 1. We also define and characterize Bayes decision rules under different loss functions to address Step 3b.

2.1 Decision Problems, Bayes Decision Rules, Conditional Entropy

Consider a decision problem. Here the decision maker observes \( X \in \mathcal{X} \) from which she predicts a random target variable \( Y \in \mathcal{Y} \) using an action \( a \in \mathcal{A} \). Let \( P_{X,Y} = (P_X, P_{Y|X}) \) be the underlying distribution for the random pair \((X, Y)\). Given a loss function \( L : \mathcal{Y} \times \mathcal{A} \to [0, \infty], \) \( L(y,a) \) indicates the loss suffered by the decision maker by deciding action \( a \) when \( Y = y \). The decision maker uses a decision rule \( \psi : \mathcal{X} \to \mathcal{A} \) to select an action \( a = \psi(x) \) from \( \mathcal{A} \) based on an observation \( x \in \mathcal{X} \). We will in general allow the decision rules to be random, i.e. \( \psi \) is random. The main purpose of extending to the space of randomized decision rules is to form a convex set of decision rules. Later in Theorem[2], this convexity is used to prove a saddle-point theorem.

We call a (randomized) decision rule \( \psi_{bayes} \) a Bayes decision rule if for all decision rules \( \psi \) and for all \( x \in \mathcal{X} \):

\[
\mathbb{E}[L(Y, \psi_{bayes}(X)) | X = x] \leq \mathbb{E}[L(Y, \psi(X)) | X = x].
\]

It should be noted that \( \psi_{bayes} \) depends only on \( P_{Y|X} \), i.e. it remains a Bayes decision rule under a different \( P_X \). Although we are not generally guaranteed that a Bayes decision rule exists, we can define conditional entropy of \( Y \) given \( X = x \) as

\[
H(Y | X = x) := \inf_{\psi} \mathbb{E}[L(Y, \psi(X)) | X = x],
\]

and the conditional entropy of \( Y \) given \( X \) as

\[
H(Y | X) := \sum_x P_X(x) H(Y | X = x). \tag{3}
\]

We can also define an (unconditional) entropy [5]

\[
H(Y) := \inf_{a \in \mathcal{A}} \mathbb{E}[L(Y, a)]. \tag{4}
\]

Note that \( H(Y | X = x) \) and \( H(Y | X) \) are both concave in \( P_{Y|X} \). Applying Jensen’s inequality, this concavity implies that

\[
H(Y | X) \leq H(Y),
\]

which motivates the following definition for the information that \( X \) carries about \( Y \),

\[
I(X; Y) := H(Y) - H(Y | X), \tag{5}
\]

i.e. the reduction of expected loss in predicting \( Y \) by observing \( X \). In [10], the author has defined the same concept to which he calls a coherent dependence measure. It can be seen that \( I(X; Y) = \mathbb{E}_{P_X} [D(P_{Y|X}, P_Y)] \) where \( D \) is the divergence measure corresponding to the loss \( L \), defined for any two probability distributions \( P_Y, Q_Y \) with Bayes actions \( a_P, a_Q \) as [5]

\[
D(P_Y, Q_Y) := E_P[L(Y, a_Q)] - E_P[L(Y, a_P)] = E_P[L(Y, a_P)] - H_P(Y). \tag{6}
\]
2.2 Examples

2.2.1 Logarithmic Loss

For any $y \in \mathcal{Y}$ and distribution $Q_Y$, define

$$L_{\log}(y, Q_Y) = -\log Q_Y(y).$$

(7)

It can be seen that under the logarithmic loss $H_{\log}(Y)$, $H_{\log}(Y|X)$, $I_{\log}(X; Y)$ are the well-known unconditional, conditional Shannon entropy and mutual information \[^{[11]}\]. The divergence measure is the well-known KL-divergence. Also, the Bayes decision rule for every distribution $P_{X,Y}$ is given by

$$\psi_{\Bayes}(x) = P_{Y|X}(\cdot|x).$$

(8)

2.2.2 0-1 loss function

The 0-1 loss function is defined for any $y, \hat{y} \in \mathcal{Y}$ as

$$L_{0-1}(y, \hat{y}) = \mathbb{I}(\hat{y} \neq y).$$

Then, we can show

$$H_{0-1}(Y) = 1 - \max_{y \in \mathcal{Y}} P_Y(y), \quad H_{0-1}(Y|X) = 1 - \sum_{x \in \mathcal{X}} \max_{y \in \mathcal{Y}} P_{X,Y}(x, y).$$

Under the 0-1 loss function, the Bayes decision rule for a distribution $P_{X,Y}$ is the well-known maximum a posteriori (MAP) rule, i.e.

$$\psi_{\Bayes}(x) = \arg \max_{y \in \mathcal{Y}} P_{Y|X}(y|x).$$

(9)

2.2.3 Quadratic loss function

The quadratic loss function is defined as $L_2(y, \hat{y}) = (y - \hat{y})^2$. It can be seen

$$H_2(Y) = \text{Var}(Y), \quad H_2(Y|X) = \mathbb{E}[\text{Var}(Y|X)], \quad I_2(X; Y) = \text{Var}(\mathbb{E}[Y|X]).$$

Also, the Bayes decision rule for any $P_{X,Y}$ is the well-known minimum mean-square error (MMSE) estimator that is

$$\psi_{\Bayes}(x) = \mathbb{E}[Y|X = x].$$

(10)

2.2.4 Brier loss function

Unlike logarithmic loss and 0-1 loss functions, the quadratic loss function does not make perfect sense for a discrete variable $Y$. The Brier loss function \[^{[12]}\] is an adjusted version of the quadratic loss function targeting a discrete $Y$, where for any distribution $Q_Y$ on $Y$ and an outcome $y \in \mathcal{Y}$,

$$L_{\BR}(y, Q_Y) = \|\delta_y - q_Y\|^2_2.$$

(11)

Here $\delta_y$ denotes a vector of size $|\mathcal{Y}|$, 1 at index $y$ and 0 elsewhere, and $q_Y$ stands for the vector of probabilities for $Q_Y$. Then,

$$H_{\BR}(Y) = 1 - \|P_Y\|^2_2, \quad H_{\BR}(Y|X) = 1 - \mathbb{E}\left[|P_{Y|X}(Y|X)\right],$$

Given the distribution $P_{X,Y}$ the Bayes decision rule is uniquely

$$\psi_{\Bayes}(x) = P_{Y|X}(\cdot|x).$$

(12)

**Connection to the maximal correlation:** Consider the well-known Pearson correlation coefficient $\rho(X, Y) = \frac{\text{Cov}(X, Y)}{\sqrt{\text{Var}(X)\text{Var}(Y)}}$ that measures the linear dependence among random variables $X$ and $Y$. To extend this correlation measure to a measure for non-linear dependence, the HGR (Hirschfeld-Gebelein-Rényi) maximal correlation has been proposed in the probability literature \[^{[13][15]}\]. The HGR maximal correlation of two random variables $X, Y$ is defined as

$$\rho_m(X; Y) = \sup_{f,g} \rho(f(X), g(Y)),$$

(13)

where the supremum is taken over all functions $f$, $g$ with finite non-zero variance. In \[^{[15]}\], it has been shown the maximal correlation satisfies several interesting properties. Here, we connect this measure to the information under the Brier loss $I_{\BR}(X; Y)$. 

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4
We also assume the continuity of Bayes decision rules for distributions in $\Gamma^*$. We call any solution where $\Psi$ is the space of all randomized mappings from $X$ to $A$, and $E_P$ denotes the expected value over distribution $P$. Note that by a randomized mapping $\psi$ we mean a random selection of members of $F$, the space of deterministic functions from $X$ to $A$, according to a certain distribution.

We call any solution $\psi^*$ to the above problem a robust Bayes decision rule against $\Gamma$. When $\Gamma$ is convex, the following theorem guarantees the existence of a saddle point for (16), under some mild conditions. Therefore, Theorem 2 motivates a generalization of the maximum entropy principle to find robust Bayes decision rules.

**Theorem 2.** Suppose that $\Gamma$ is convex and that under any $P \in \Gamma$ there exists a Bayes decision rule. We also assume the continuity of Bayes decision rules for distributions in $\Gamma$ (See the Appendix for the exact condition). Then, if $P^*$ maximizes $H(Y|X)$ over $\Gamma$, a Bayes decision rule for $P^*$ will be a robust Bayes decision rule against $\Gamma$.

**Proof.** Refer to the Appendix for the proof.

**Corollary 1.** For a binary $Y \in \{0,1\}$,

$$I_{BR}(X;Y) = 2p_0(1-p_0)\rho_m^2(X;Y).$$

2.3 Principle of Maximum Conditional Entropy & Robust Bayes decision rules

Given a distribution set $\Gamma$, consider the following minimax problem to find a decision rule minimizing the worst-case expected loss over $\Gamma$:

$$\arg\min_{\psi \in \Psi} \max_{P \in \Gamma} E_P[L(Y, \psi(X))],$$

where $\Psi$ is the space of all randomized mappings from $X$ to $A$ and $E_P$ denotes the expected value over distribution $P$. Note that by a randomized mapping $\psi$ we mean a random selection of members of $F$, the space of deterministic functions from $X$ to $A$, according to a certain distribution.

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**Proof.** Refer to the Appendix for the proof.

**Principle of Maximum Conditional Entropy:** Given a set of distributions $\Gamma$, select and predict $Y$ based on a distribution in $\Gamma$ that maximizes the conditional entropy of $Y$ given $X$, i.e.

$$\arg\max_{P \in \Gamma} H(Y|X)$$

3 Prediction via Maximum Conditional Entropy Principle

Consider a prediction task with target variable $Y$ and feature vector $X = (X_1, \ldots, X_d)$. Note that we do not require the variables to be discrete. As discussed earlier, the maximum conditional entropy principle reduces (16) to (17). Notice that (16) and (17) formulate Steps 3 and 3a in Figure 1 respectively. However, a general formulation of (17) in terms of the joint distribution $P_{X,Y}$ leads to an exponential computational complexity in the feature dimension $d$.

The key question is therefore under what structures of $\Gamma(\hat{P})$ in Step 2 we can solve (17) efficiently. In this section, we propose a specific structure for $\Gamma(\hat{P})$, under which we provide an efficient solution to Steps 3a and 3b in Figure 1. In fact, we show (17) reduces to the maximum likelihood problem over a generalized linear model, under this specific structure.

To describe this structure, consider a set of distributions $\Gamma(Q)$ centered around a given distribution $Q_{X,Y}$, where for a given norm $\| \cdot \|$, mapping vector $\theta(Y)_{d \times 1}$,

$$\Gamma(Q) = \{ P_{X,Y} : P_X = Q_X, \forall 1 \leq i \leq t : \| E_P [\theta_i(Y)|X] - E_Q [\theta_i(Y)|X] \| \leq \epsilon_i \}.$$

Here $\theta$ encodes $Y$ with $t$-dimensional $\theta(Y)$, and $\theta_i(Y)$ denotes the $i$th entry of $\theta(Y)$. The first constraint in the definition of $\Gamma(Q)$ says that all distributions in $\Gamma(Q)$ share the same marginal on $X$,
as \(Q\); the second imposes constraints on the cross-moments between \(X\) and \(Y\), allowing for some uncertainty in estimation. When applied to our supervised learning framework, we will choose \(Q\) to be the empirical distribution \(\hat{P}\) and select \(\theta\) appropriately based on the loss function \(L\). However, for now we will consider the problem of solving (17) over \(\Gamma = \Gamma(Q)\) for general \(Q\) and \(\theta\).

To that end, we apply the Fenchel’s duality technique, also used at [16–18] to address f-divergence minimization problems. However, we consider a different version of convex conjugate for \(-H\), which is defined with respect to \(\theta\). Considering \(P_Y\) as the set of all probability distributions for the variable \(Y\), we define \(F_\theta: \mathbb{R}^t \to \mathbb{R}\) as the convex conjugate of \(-H(Y)\) with respect to the mapping \(\theta\),

\[F_\theta(z) := \max_{P \in P_Y} H(Y) + \mathbb{E}[\theta(Y)]^T z.\]  

(19)

**Theorem 3.** Define \(\Gamma(Q)\), \(F_\theta\) as given by (18), (19). Then the following duality holds

\[
\max_{P \in \Gamma(Q)} H(Y|X) = \min_{A \in \mathbb{R}^t \times d} \mathbb{E}_Q \left[ F_\theta(A X) - \theta(Y)^T A X \right] + \sum_{i=1}^t \epsilon_i \|A_i\|_*,
\]

(20)

where \(\|A_i\|_*\) denotes \(\|\cdot\|\)'s dual norm of the \(A\)'s \(i\)th row. Furthermore, for the optimal \(P^*\) and \(A^*\)

\[\mathbb{E}_{P^*}[\theta(Y) | X = x] = \nabla F_\theta(A^* x).\]  

(21)

**Proof.** The proof has been relegated to the the Appendix.

When applying Theorem 3 on a supervised learning problem with a specific loss function, \(\theta\) will be chosen such that \(\mathbb{E}_{P^*}[\theta(Y) | X = x]\) provides sufficient information to compute the Bayes decision rule \(\Psi^*\) for \(P^*\). This enables the direct computation of \(\Psi^*\), i.e. step 3 of Figure 1, without the need to explicitly compute \(P^*\) itself. Later in this section, we will discuss three examples to see how this technique applies to different loss functions.

We make the key observation that the problem in the RHS of (20), when \(\epsilon_i = 0\) for all \(i\)'s, is equivalent to minimizing the negative log-likelihood for fitting a generalized linear model [19] given by

- An exponential family distribution \(p(y|\eta) = h(y) \exp(\eta^T \theta(y) - F_\theta(\eta))\) with the log-partition function \(F_\theta\) and the sufficient statistic \(\theta(Y)\),
- A linear predictor, \(\eta(X) = AX\).
- A link function such that \(\mathbb{E}[\theta(Y)|X = x] = \nabla F_\theta(\eta(x))\).

Therefore, Theorem 3 reveals a duality between the maximum conditional entropy problem and the regularized maximum likelihood problem for the specified generalized linear model. This duality further provides a justification for generalized linear models, since given a generalized linear model
we can consider the convex conjugate of its log-partition function as the negative entropy in the maximum conditional entropy framework.

To interpret this duality geometrically, note that by solving the regularized maximum likelihood problem in the RHS of (20), we in fact minimize a regularized KL-divergence

\[
\arg\min_{P_Y \cdot \cdot (Q_X, P_Y | X) \in S_F} E_{Q_X} \left[ D_{KL}(Q_{Y|X} \parallel P_{Y|X}) \right] + \sum_{i=1}^{t} \epsilon_i \| A_i (P_{Y|X}) \|_*,
\]

where \( S_F = \{(Q_X, P_Y | X) | y) = h(y) \exp(\theta(Y)^T A x - F \theta(A x)) \} \) is the set of all exponential family distributions for the described GLM. This can be viewed as projecting \( Q \) onto \( S_F \) (See Figure 2).

Furthermore, considering the definition of divergence \( D \) given in (6), it can be seen that maximizing \( H(Y|X) \) over \( \Gamma(Q) \) in the LHS of (20) is equivalent to the following divergence minimization problem

\[
\arg\min_{P_Y \cdot \cdot (Q_X, P_Y | X) \in \Gamma(Q)} E_{Q_X} \left[ D(P_{Y|X}, U_{Y|X}) \right]
\]

where \( U_{Y|X} \) denotes the uniform conditional distribution. This can be interpreted as projecting the joint distribution \( (Q_X, U_{Y|X}) \) onto \( \Gamma(Q) \) (See Figure 2).

Notice the difference of divergence measures and the ordering of distributions between (23) and (22). Then, the duality shown in Theorem 1 implies the following corollary.

**Corollary 2.** The solution to (22) would also minimize (23), i.e. \( (22) \subseteq (23) \).

To connect the proposed framework to the ERM setting, suppose \( Q = \hat{P}_n \) is the empirical distribution of \( n \) samples drawn i.i.d. from the underlying distribution \( \hat{P} \). Then the problem in the RHS of (20) is equivalent to the ERM problem

\[
\min_{\psi \in \Psi(S_F)} E_Q[L_{log}(Y, \psi(X))] + R(\psi),
\]

where \( \Psi(S_F) \) denotes the set of the logarithmic-loss \( L_{log} \) Bayes decision rules corresponding to the distributions in \( S_F \). Also, \( R(\psi) = \sum_{i=1}^{t} \epsilon_i \| A_i(\psi) \|_* \) is the added regularizer. Then, an important question is how to bound the excess risk, that is the difference between the expected loss of the two decision rules \( \hat{\psi}_n \) and \( \hat{\psi} \) minimizing (24) for the empirical distribution \( Q = \hat{P}_n \) and the underlying distribution \( Q = \hat{P} \), respectively. Replacing the original regularizer \( \sum_{i=1}^{t} \epsilon_i \| A_i \|_* \) with the strongly-convex \( \lambda \sum_{i=1}^{t} \| A_i \|_*^2 \), we show the following theorem to bound the excess risk.

**Theorem 4.** Let the regularizer \( R(\psi) = \lambda \sum_{i=1}^{t} \| A_i(\psi) \|_*^2 \). Take \( \| \cdot \| / \| \cdot \|_* \) to be the \( \ell_p/\ell_q \) pair for \( \frac{1}{p} + \frac{1}{q} = 1 \), \( 1 < q \). Assume that \( \| X \|_p \leq B \) and \( \| \theta(Y) \|_\infty \leq L \). Then, for any \( \delta \), with probability at least \( 1 - \delta \)

\[
E_{\hat{P}}[L(Y, \hat{\psi}_n(X))] - E_{\hat{P}}[L(Y, \hat{\psi}(X))] = O \left( \frac{t L^2 B^2 \log(\frac{1}{\delta})}{(q-1)\lambda n} \right).
\]

**Proof.** Due to the definition given in (19), \( \nabla F_\theta(z) = E_{\hat{P}}[\theta(Y)] \) for some distribution \( P \). Therefore, \( \| \nabla F_\theta(z) \|_\infty \leq L \) and \( F_\theta(z) - \theta(Y)^T z \) is \( 2L \)-Lipschitz in each entry \( z_i \). Then, the theorem is an immediate consequence of Theorem 1 in [20].

\( \square \)

In the remaining of this section, we apply the described framework to the loss functions discussed at Subsection 2.2.

### 3.1 Logarithmic Loss: Logistic Regression

For classifying \( Y \in \mathcal{Y} = \{1, \ldots, t+1\} \), let \( \theta(Y) \) be the one-hot encoding of variable \( Y \), i.e. \( \theta_i(Y) = \mathbb{I}(Y = i) \) for \( 1 \leq i \leq t \). Here, we exclude \( i = t + 1 \) as \( \mathbb{I}(Y = t + 1) = 1 - \sum_{i=1}^{t} \mathbb{I}(Y = i) \). Given this \( \theta \), for the logarithmic loss

\[
F_\theta(z) = \log(1 + \sum_{j=1}^{t} \exp(z_j)), \quad \forall 1 \leq i \leq t : \left( \nabla F_\theta(z) \right)_i = \exp(z_i) / (1 + \sum_{j=1}^{t} \exp(z_j)),
\]

\( (26) \)
that gives the multinomial logistic regression model [21]. Also, the RHS of (20) would be the regularized maximum likelihood problem for this specific GLM. This discussion is well-studied in the literature and straightforward using the duality result shown in [8].

3.2 0-1 Loss: Minimax SVM

Consider the same classification setting and $\theta$ described at the beginning of last subsection. We show in the Appendix that for the 0-1 loss we can calculate the gradient of $F_\theta$ using the following procedure. Given $z \in \mathbb{R}^t$, let $\tilde{z} = (z, 0)$. Let $\sigma$ be the permutation sorting $\tilde{z}$ in a descending order, i.e. $i \leq j : \tilde{z}_\sigma(i) \geq \tilde{z}_\sigma(j)$. We find the smallest $k$ where $\sum_{i=1}^{k} \tilde{z}_\sigma(i) - \tilde{z}_\sigma(k+1) > 1$. If this does not hold for any $k$, let $k = t + 1$. Then,

$$\nabla F_\theta(z)_i = \begin{cases} 1/k & \text{if } \sigma(i) \leq k, \\ 0 & \text{Otherwise}. \end{cases}$$

(27)

Knowing that $F_\theta(0) = t/(t+1)$ that is the 0-1 entropy of a uniformly distributed $Y$, the characterization of $F_\theta$ is complete.

With $\nabla F_\theta$ characterized, for Step 3b in Figure 1 we should apply the MAP rule to the output of $\nabla F_\theta$. We can also learn the linear predictor (Step 3a) through applying the gradient descent to solve the RHS of (20). The classifier minimizes the worst-case 0-1 loss over $\Gamma(Q)$. In particular, if $Y$ is binary, i.e. $t + 1 = 2$

$$F_\theta(z) = \max \{ 0, \frac{z + 1}{2}, z \}.$$  

(28)

Then, if $Y = \{-1, 1\}$, the RHS problem of (20) would be

$$\min_{\alpha} \mathbb{E}_Q \left[ \max \left\{ 0, \frac{1 - Y \alpha^T X}{2}, -Y \alpha^T X \right\} \right] + \epsilon \| \alpha \|_\alpha.$$ 

(29)

Since $\max \{ 0, \frac{1-z}{2}, -z \} \leq \max \{ 0, 1-z \}$, if we replace $\epsilon \| \alpha \|_\alpha$ with $\lambda \| \alpha \|_2^2$ in (29), we get a relaxation of the standard SVM formulated with the hinge loss [22]. We therefore call this classification algorithm the minimax SVM. Note that unlike the standard SVM, the minimax SVM can be naturally extended to a multi-class classification algorithm through (27).

3.3 Brier Loss: Minimax Brier Classifier

Consider the same classification setting and $\theta$ defined in the last two subsections. In the Appendix, we show we can characterize the gradient of $F_\theta$ for the Brier loss by repeating the same procedure as in the minimax SVM with two modifications. First, we change the level for finding the smallest $k$ as $\sum_{i=1}^{k} \tilde{z}_\sigma(i) - \tilde{z}_\sigma(k+1) > 2$, and second we modify (27) as

$$\nabla F_\theta(z)_i = \begin{cases} (2 - \sum_{j=1}^{k} \tilde{z}_\sigma(j))/(2k) + \tilde{z}_\sigma(i)/2 & \text{if } \sigma(i) \leq k, \\ 0 & \text{Otherwise}. \end{cases}$$

(30)

As discussed in Subsection 2.2.4 the robust Bayes decision rule is the conditional $P_{Y|X}^*$ of the distribution maximizing the conditional Brier entropy. Therefore, to make prediction, we can apply the MAP rule to the probability vector $\nabla F_\theta$ returns. We call this classification algorithm the minimax Brier Classifier (mmBC). For the binary case when $t = 1$, it can be seen

$$F_\theta(z) = \frac{z}{2} = \begin{cases} \frac{1}{8} z^2 & \text{if } |z| \leq 2, \\ \frac{1}{2} |z| - \frac{1}{2} & \text{Otherwise}, \end{cases}$$

(31)

which is the Huber penalty function [23]. This binary classification problem is the same classification problem formulated with the modified Huber loss function at [24]. Through the developed minimax framework, we can naturally extend this binary classification technique to a multi-class classification algorithm.
Based on Corollary 1 for a binary $Y$ the conditional Brier entropy-maximizing distribution is the distribution minimizing maximal correlation between $X$ and $Y$ in $\Gamma(\hat{P})$. Assuming some extra conditions, [4] solves the minimax problem of finding the maximal correlation-minimizing distribution, but for a larger class of distributions where only pairwise marginals are fixed. One can see that their proposed solution is based on replacing the Huber function in (31) with the following quadratic function

$$F_\theta(z) - \frac{z}{2} = \frac{1}{8} z^2,$$  

and the condition under which their solution solves the original problem is that for the $\mathbf{A}^*$ minimizing the RHS of (20), $|\mathbf{A}^* \mathbf{x}| \leq 1$ for every input $\mathbf{x}$.

In [4], the authors also show for a binary prediction problem over a convex set of distributions $\Gamma$, there exists a randomized prediction rule based on the maximal correlation-minimizing distribution, achieving a worst-case misclassification rate of at most twice the minimum worst-case misclassification rate. Here, we generalize their result to a multi-class version using the connection between the Brier information and the maximal correlation shown in Theorem 1.

**Theorem 5.** Consider a prediction problem for $Y \in \mathcal{Y} = \{1, \ldots, t\}$. Let $\mathbf{p}^*$ denote the conditional $P_{Y|\mathbf{X}}$ of the distribution maximizing $H_{BR}(Y|\mathbf{X})$ over a convex set of distributions $\Gamma$. Define the randomized decision rule $\psi_{BR}$:

$$\forall i, 1 \leq i \leq t : \quad \psi_{BR}(\mathbf{x}) = i, \quad \text{w.p.} \quad \frac{P_{i|\mathbf{x}}^2}{\sum_{j=1}^t P_{j|\mathbf{x}}^2}. \tag{33}$$

Then the worst-case misclassification rate of $\psi_{BR}$ is bounded by twice the minimum worst-case misclassification rate over $\Gamma$, i.e.

$$\max_{\mathbf{p} \in \Gamma} P(\psi_{BR}(\mathbf{X}) \neq Y) \leq 2 \min_{\psi \in \Psi} \max_{\mathbf{p} \in \Gamma} P(\psi(\mathbf{X}) \neq Y).$$

**Proof.** The proof has been relegated to the Appendix.

Hence, we can predict by applying this randomized decision rule to the probability vector that $\nabla F_\theta$ returns. We call this classification algorithm the minimax Randomized Brier Classifier (mRBC).

The above theorem suggests the minimax Brier classification as a natural extension of the results proven in [4] for the binary case.

### 3.4 Quadratic Loss: Linear Regression

For a regression problem on $Y \in \mathcal{Y} = \mathbb{R}$, let $\theta(Y) = Y$ be the identity function, so $t = 1$. To derive $F_\theta$ for the quadratic loss, note that if we let $\mathcal{P}_Y$ in (19) include all possible distributions, the maximized entropy (variance for quadratic loss) and thus the $F_\theta$ value would be infinity. Therefore, in (19) we restrict $\mathcal{P}_Y$ to $\{ P_Y : \mathbb{E}[Y^2] \leq \rho^2 \}$ given a parameter $\rho$. We show in the Appendix that a slightly adjusted version of Theorem 3 remains valid after this change, and

$$F_\theta(z) - \rho^2 = \begin{cases} 
\frac{z^2}{4} & \text{if } |z|/2 \leq \rho \\
\rho(|z| - \rho) & \text{if } |z|/2 > \rho,
\end{cases} \tag{34}$$

which is the Huber function [23]. To find the Bayes decision rule via (21), note that

$$\frac{dF_\theta(z)}{dz} = \begin{cases} 
-\rho & \text{if } z/2 \leq -\rho \\
z/2 & \text{if } -\rho < z/2 \leq \rho \\
\rho & \text{if } \rho < z/2.
\end{cases} \tag{35}$$

Given the samples in a supervised learning problem if we choose the parameter $\rho$ large enough, by solving the RHS of (20) when $F_\theta(z)$ is replaced with $z^2/4$ and set $\rho$ greater than $\max_i |\mathbf{A}^* \mathbf{x}_i|$, we can equivalently take $F_\theta(z) = z^2/4 + \rho^2$ which by (21) gives the linear regression model. Then, the RHS of (20) would be equivalent to

- Simple linear regression when $\epsilon = 0$.
- Lasso [25] when $\| \cdot \| / \| \cdot \|_*$ is the $\ell_\infty/\ell_1$ pair.
We implemented the three mmSVM, mmBC, and mmRBC by applying gradient descent to solve

We evaluated the performance of the minimax SVM (mmSVM), the minimax Brier Classifier (mmBC), and the minimax Randomized Brier Classifier (mmRBC), on six binary classification datasets from the UCI repository, compared to these five benchmarks: Support Vector Machines (SVM), Discrete Chebyshev Classifiers (DCC) [3], Minimax Probabilistic Machine (MPM) [2], Tree Augmented Naive Bayes (TAN) [31], and Discrete Rényi Classifiers (DRC) [4]. The results are summarized in Table 1, where the numbers indicate the percentage of error in the classification task.

To determine this coefficient, we used a randomly-selected 70% of the training set for training and the RHS of (20) with an added regularizer $\lambda\|\alpha\|^2$. We determined the value of $\lambda$ by cross validation. To determine this coefficient, we used a randomly-selected 70% of the training set for training and

- Ridge regression [21] when $\|\cdot\|$ is the $\ell_2$-norm.
- Group lasso [26] with the $\ell_{1,p}$ regularizer when we adjust $\Gamma(Q)$’s definition for disjoint subsets $I_1, \ldots, I_k$ of $\{1, \ldots, d\}$ as

$$\Gamma_GL(Q) = \{ P_{X,Y} : P_X = Q_X, \forall 1 \leq j \leq k : \| \mathbb{E}_P [Y|X_{I_j}] - \mathbb{E}_Q [Y|X_{I_j}] \|_q \leq \epsilon_j \}. \tag{36}$$

Here, $q$ is chosen such that $1/p + 1/q = 1$. Also, $X_{I_j}$ denotes the subvector including the $I_j$ entries of $X$. See the Appendix for the proof of the group lasso case. Another type of minimax, but non-probabilistic, justification of the robustness of lasso and group lasso as regression algorithms can be found in [27, 28].

4 Robust Feature Selection

Using a minimax criterion over a set of distributions $\Gamma$, we solve the following problem to select the most informative subset of $k$ features. Here, we evaluate a feature subset based on its minimum worst-case loss over $\Gamma$.

$$\arg\min_{|S| \leq k} \min_{\psi \in \Psi_S} \max_{P \in \Gamma} \mathbb{E}_P [L(Y, \psi(X_S))], \tag{37}$$

where $X_S$ denotes the feature vector $X$ restricted to the indices in $S$. Theorem 2 reduces (37) to

$$\arg\min_{|S| \leq k} \max_{P \in \Gamma} H(Y|X_S), \tag{38}$$

which under the assumption that $H(Y)$ is fixed across all distributions in $\Gamma$ becomes equivalent to selecting a subset $S$ maximizing the worst-case generalized information $I(X_S;Y)$ over $\Gamma$, i.e.

$$\arg\max_{|S| \leq k} \min_{P \in \Gamma} I(X_S;Y). \tag{39}$$

To solve (38) when $\Gamma = \Gamma(Q)$ [18], we apply the duality shown in Theorem 3 to obtain

$$\arg\min_{A \in \mathbb{R}^{r \times s} : \|A\|_{0,\infty} \leq k} \mathbb{E}_Q \left[ F_\theta(A \Phi(X)) - \theta(Y)^T A \Phi(X) \right] + \sum_{i=1}^t \epsilon_i \|A_i\|_{\ast}. \tag{40}$$

Here by constraining $\|A\|_{0,\infty} = \|\|A^{(1)}\|_{\infty}, \ldots, \|A^{(s)}\|_{\infty}\|_0$ where $A^{(i)}$ denotes the $i$th column of $A$, we impose the same sparsity pattern across the rows of $A$. Approximating the $\ell_0$ with the convex $\ell_1$ and taking $\|\cdot\|_\ast$ to be the $\ell_1$-norm, we can approximate the solution by

$$\arg\min_{A \in \mathbb{R}^{r \times s}} \mathbb{E}_Q \left[ F_\theta(A \Phi(X)) - \theta(Y)^T A \Phi(X) \right] + \lambda \|A\|_{1,\infty}. \tag{41}$$

It is noteworthy that for the quadratic loss and identity $\theta$, (41) is the same as the lasso [25]. Also, for the logarithmic loss and one-hot encoding $\theta$, (41) is equivalent to the $\ell_1$-regularized logistic regression. Hence, the $\ell_1$-regularized logistic regression maximizes the worst-case mutual information over $\Gamma(Q)$, which seems superior to the heuristic techniques for maximizing an approximation of the mutual information $I(X_S;Y)$ in the literature [29, 30].

5 Numerical Experiments

We evaluated the performance of the minimax SVM (mmSVM), the minimax Brier Classifier (mmBC), and the minimax Randomized Brier Classifier (mmRBC), on six binary classification datasets from the UCI repository, compared to these five benchmarks: Support Vector Machines (SVM), Discrete Chebyshev Classifiers (DCC) [3], Minimax Probabilistic Machine (MPM) [2], Tree Augmented Naive Bayes (TAN) [31], and Discrete Rényi Classifiers (DRC) [4]. The results are summarized in Table 1, where the numbers indicate the percentage of error in the classification task.

We implemented the three mmSVM, mmBC, and mmRBC by applying gradient descent to solve the RHS of (20) with an added regularizer $\lambda\|\alpha\|^2$. We determined the value of $\lambda$ by cross validation. To determine this coefficient, we used a randomly-selected 70% of the training set for training and
the rest 30% of the training set for testing. We tested the values in \(\{2^{-10}, \ldots, 2^{10}\}\). Using the tuned lambda, we trained the algorithms over all the training set and then evaluated the error rate over the test set. We performed this procedure in 1000 Monte Carlo runs each training on 70% of the data points and testing on the rest 30% and averaged the results.

As seen in the table, the minimax Brier Classifier and the minimax SVM result in the best performance for five and three out of the six datasets, respectively. Observe that although our main theoretical guarantee is for the randomized Brier classifier, the non-randomized Brier classifier has outperformed the randomized Brier classifier in all the datasets. Also, except a single dataset the minimax SVM outperforms the SVM.

To compare these methods in high-dimensional problems, we ran an experiment over synthetic data with \(n = 200\) samples and \(d = 10000\) features. We generated features by i.i.d. Bernoulli with \(P(X_i = 1) = 0.75\), and considered \(y = \text{sign}(\gamma^T x + z)\) where \(z \sim N(0, 1)\). Using the same approach, we evaluated 20.6% error rate for SVM, 20.4% error rate for DRC, 20.0% for the mmSVM and 19.4% for the mmBC, which shows the mmSVM and mmBC can outperform SVM and DRC in high-dimensional settings as well.

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6 Appendix

6.1 Proof of Theorem 1

In this proof, we use a known result for \( \rho_m(X; Z) \) for a Bernoulli \( Z \in \{0, 1\} \) with probabilities \( p_0, p_1 \) \cite{32}. For simplicity, we use \( p_x, z \) and \( p_{x|z} \) to denote \( P_X, Z(x, z) \) and \( P_{Z|X}(z|x) \), respectively. Then,

\[
\rho_m^2(X; Z) = \frac{1}{p_0 p_1} \sum_x p_x \left[ \frac{p_0^2 p_{z,1}^2 + p_1^2}{p_x} - 1 \right]
= \frac{1}{p_0 p_1} \sum_x p_x \left( \frac{p_0 p_{z,1}^2}{p_x} + p_1^2 \right) - 1
= \frac{1}{p_0 p_1} \sum_x p_x \left( \frac{p_0}{2} \left( p_{z,1}^2 + p_{z,0}^2 \right) + \frac{p_0 - p_1}{2} \left( p_{z,1} - p_{z,0} \right) \right) - 1
= \frac{1}{2p_0 p_1} \left( 1 - p_1 - p_0 - 2 \sum_x p_x p_{z|x} p_{z|x} \right)
= \frac{1}{2p_0 p_1} \left( p_1 p_0 - \sum_x p_x p_{z|x} p_{z|x} \right).
\]

Then, we have

\[
\sum_{i=0}^{t} p_i (1 - p_i) \rho_m^2(X; Y_i) = \sum_{i=0}^{t} p_i (1 - p_i) - \sum_x p_x p_{z|x} (1 - p_{z|x})
= \sum_{i=0}^{t} \left[ p_i - \sum_x p_x p_{z|x} + \sum_x p_x p_{z|x} \right]
= \mathbb{E} \left[ P_{Y|X}(Y|X) - P_{Y}(Y) \right]
= I_{BR}(X; Y).
\]

6.2 Proof of Theorem 2

First, let us recall the assumptions of Theorem 2.

- \( \Gamma \) is convex.
- For any distribution \( P \in \Gamma \), there exists a Bayes decision rule.
- We assume continuity in Bayes decision rules, i.e., if a sequence of distributions \( (Q_n)_{n=1}^{\infty} \) with the corresponding Bayes decision rules \( (\psi_n)_{n=1}^{\infty} \) converges weakly to \( Q \) with a Bayes decision rule \( \psi \), then under any \( P \in \Gamma \), the expected loss of \( \psi_n \) converges to the expected loss of \( \psi \).
- \( P^* \) maximizes the conditional entropy \( H(Y|X) \).

Let \( \psi^* \) be a Bayes decision rule for \( P^* \). We need to show that \( \psi^* \) is a robust Bayes decision rule against \( \Gamma \). To show this, it suffices to show that \( (P^*, \psi^*) \) is a saddle point of the mentioned minimax problem, i.e.,

\[
\mathbb{E}_{P^*}[L(Y, \psi^*(X))] \leq \mathbb{E}_{P^*}[L(Y, \psi(X))], \quad (42)
\]

and

\[
\mathbb{E}_{P^*}[L(Y, \psi^*(X))] \geq \mathbb{E}_P[L(Y, \psi^*(X))], \quad (43)
\]

Clearly, inequality \( 42 \) holds due to the definition of the Bayes decision rule. To show \( 43 \), let us fix an arbitrary distribution \( P \in \Gamma \). For any \( \lambda \in (0, 1] \), define \( P_\lambda = \lambda P + (1 - \lambda) P^* \). Notice that \( P_\lambda \in \Gamma \) since \( \Gamma \) is convex. Let \( \psi_\lambda \) be a Bayes decision rule for \( P_\lambda \). Due to the linearity of the expected loss in the probability distribution, we have

\[
\mathbb{E}_P[L(Y, \psi_{\lambda}(X))] - \mathbb{E}_{P^*}[L(Y, \psi_{\lambda}(X))] = \frac{\mathbb{E}_{P_\lambda}[L(Y, \psi_{\lambda}(X))] - \mathbb{E}_{P^*}[L(Y, \psi_{\lambda}(X))]}{\lambda}
\leq \frac{H_{P_\lambda}(Y|X) - H_{P^*}(Y|X)}{\lambda}
\leq 0,
\]

for any \( 0 < \lambda \leq 1 \). Here the first inequality is due to the definition of the conditional entropy and the last inequality holds since \( P^* \) maximizes the conditional entropy over \( \Gamma \). Applying the continuity assumption of the Bayes decision rules, we have

\[
\mathbb{E}_P[L(Y, \psi^*(X))] - \mathbb{E}_{P^*}[L(Y, \psi^*(X))] = \lim_{\lambda \to 0} \mathbb{E}_P[L(Y, \psi_{\lambda}(X))] - \mathbb{E}_{P^*}[L(Y, \psi_{\lambda}(X))] \leq 0, \quad (44)
\]

which makes the proof complete.
6.3 Proof of Theorem \[3\]

Let us recall the definition of the set \(\Gamma(Q)\):
\[
\Gamma(Q) = \{ P_{X,Y} : P_X = Q_X, \quad \forall 1 \leq i \leq t : \| \mathbb{E}_P[\theta_i(Y)X] - \mathbb{E}_Q[\theta_i(Y)X] \| \leq \epsilon_i \}. \tag{45}
\]

Defining \(\tilde{E}_i \equiv \mathbb{E}_Q[\theta_i(Y)X]\) and \(C_i \equiv \{ u : \| u - \tilde{E}_i \| \leq \epsilon_i \}\), we have
\[
\max_{P \in \Gamma(Q)} H(Y|X) = \max_{P, \forall i : w_i = \mathbb{E}_P[\theta_i(Y)X]} \mathbb{E}_{Q_X} [H_P(Y|X = x)] + \sum_{i=1}^t I_C(w_i) \tag{46}
\]
where \(I_C\) is the indicator function for the set \(C\) defined as
\[
I_C(x) = \begin{cases} 0 & \text{if } x \in C, \\ -\infty & \text{Otherwise.} \end{cases} \tag{47}
\]

First of all, the law of iterated expectations implies that \(\mathbb{E}_P[\theta_i(Y)X] = \mathbb{E}_{Q_X} X \mathbb{E}[\theta_i(Y)|X = x] \). Furthermore, problem \[46\] is convex and it is not hard to check that the Slater condition is satisfied. Hence strong duality holds and we can write the dual problem as
\[
\min_A \sup_{P_{Y|X},w} \mathbb{E}_{Q_X} \left[ H_P(Y|X = x) + \sum_{i=1}^t \mathbb{E}[\theta_i(Y)|X = x]A_iX \right] + \sum_{i=1}^t [I_C(w_i) - A_iw_i], \tag{48}
\]
where the rows of matrix \(A\), denoted by \(A_i\), are the Lagrange multipliers for the constraints of \(w_i = \mathbb{E}_P[\theta_i(Y)\Phi(X)]\). Notice that the above problem decomposes across \(P_{Y|X=x}\)'s and \(w_i\)’s. Hence, the dual problem can be rewritten as
\[
\min_A \left[ \mathbb{E}_{Q_X} \left[ \sup_{P_{Y|X=x}} H_P(Y|X = x) + \sum_{i=1}^t \mathbb{E}[\theta_i(Y)|X = x]A_iX \right] + \sup_{w_i} [I_C(w_i) - A_iw_i] \right] \tag{49}
\]
Furthermore, according to the definition of \(F_\theta\), we have
\[
F_\theta(Ax) = \sup_{P_{Y|X=x}} H(Y|X = x) + \mathbb{E}[\theta(Y)|X = x]^TAX. \tag{50}
\]
Moreover, the definition of the dual norm \(\| \cdot \|_*\) implies
\[
\sup_{w_i} [I_C(w_i) - A_iw_i] = \max_{u \in C_i} A_iu = A_i\tilde{E}_i + \epsilon_i\|A_i\|_* \tag{51}
\]
Plugging \[50\] and \[51\] in \[49\], the dual problem can be simplified to
\[
\min_A \mathbb{E}_{Q_X} \left[ \sum_{i=1}^t A_i\tilde{E}_i \right] + \sum_{i=1}^t \epsilon_i\|A_i\|_* \tag{52}
\]
which is equal to the primal problem \[46\] since the strong duality holds. Furthermore, applying Danskin’s theorem to \[50\] implies that
\[
\mathbb{E}_{P_*}[\theta(Y)|X = x] = \nabla F_\theta(A^*X). \tag{53}
\]

6.4 \(F_\theta\) derivation for the 0-1 Loss, minimax SVM

Here, we derive \(\nabla F_\theta\) for the 0-1 loss function, where \(\theta\) is the described one-hot encoding that is \(\theta_i(Y) = 1(Y = i)\) for \(1 \leq i \leq t\). If \(P(Y = i) = p_i\) for \(1 \leq i \leq t+1\), then
\[
H(Y) + \mathbb{E}[\theta(Y)]^Tz = 1 - \max_{1 \leq l \leq t+1} p_l + \sum_{i=1}^t p_lz_i. \tag{54}
\]
Hence, due to the Danskin’s theorem,

\[ \nabla F_\theta(z) = \arg\max_{p \in \mathbb{R}^{t+1}: p \geq 0} \sum_{i=1}^{t} p_i z_i - \max_{1 \leq i \leq t+1} p_i \]  

(55)

To solve the above problem we define \( \tilde{z} = (z, 0) \) and rewrite the objective as

\[ \sum_{i=1}^{t+1} p_i \tilde{z}_i - \max_{1 \leq i \leq t+1} p_i. \]  

(56)

Then, the optimal solution \( p^* \) of (55) obeys the same order as the order of \( \tilde{z} \). Without loss of generality suppose that \( \tilde{z} \) is sorted in a descending order. Then, (55) is equivalent to

\[ \arg\max_{p \in \mathbb{R}^{t+1}: 1^T p = 1, \forall i \leq j: p_i \geq p_j} \sum_{i=1}^{t+1} p_i \tilde{z}_i - p_1 \]  

(57)

Note that under the constraint \( 1^T p = 1 \), for any \( m \leq t \)

\[ \sum_{i=1}^{t+1} p_i \tilde{z}_i - p_1 = (\tilde{z}_1 - \tilde{z}_{m+1} - 1)p_1 + \sum_{i=2}^{m} (\tilde{z}_i - \tilde{z}_{m+1})p_i + \tilde{z}_{m+1} - \sum_{j=m+2}^{t+1} (\tilde{z}_{m+1} - \tilde{z}_j)p_j. \]  

(58)

For the coefficients, we know \( \tilde{z}_{m+1} - \tilde{z}_j \) is non-negative if \( j > m \) and non-positive if \( j < m \). Let \( k \) be the smallest index for which \( \sum_{i=1}^{k} |\tilde{z}_i - \tilde{z}_{m+1}| > 1 \). If that does not hold for any \( k \), let \( k = t + 1 \).

Then, according to (58), for any solution \( p^* \) to (57)

\[ \forall i > k: p_i^* = 0. \]  

(59)

This is because if for some \( i \geq k + 1 \), \( p_i^* > 0 \) (let \( i \) be the largest index this happens), we construct a new feasible point \( p \) from \( p^* \) by setting \( p_i \) to be zero and for any \( j \leq k \) let \( p_j = p_j^* + p_i^*/k \). Then, for the new feasible point \( p \), we will get a larger objective, that is a contradiction to that \( p^* \) maximizes the above objective. Now, we claim that \( p_1^* = p_2^* = \ldots = p_k^* = 1/k \). If this is not true, then there is an index \( i < k \) where \( p_i^* - p_{i+1}^* > (i + 1)/k \) for some \( \epsilon > 0 \). Now if we modify the solution as \( p_j = p_j^* - \epsilon \) for any \( j \leq i \) and \( p_{i+1} = p_{i+1}^* + \epsilon \), we get a feasible point with the same order as \( p^* \), but since \( \sum_{j=1}^{i} |\tilde{z}_j - \tilde{z}_{i+1}| \leq 1 \) the objective of (57) grows because of (58), that is a contradiction.

Finally, this procedure characterizes the gradient as

\[ (\nabla F_\theta(z))_i = \begin{cases} 1/k & \text{if } i \leq k, \\ 0 & \text{Otherwise.} \end{cases} \]  

(60)

6.5 \( F_\theta \) derivation for the Brier Loss, minimax Brier classifier

Similar to the proof given for the 0-1 loss, we derive \( \nabla F_\theta \) for the Brier loss function with \( \theta \) the described one-hot encoding. If \( P(Y = i) = p_i \) for \( 1 \leq i \leq t + 1 \), then

\[ H(Y) + \mathbb{E}[(\theta(Y))^T z] = 1 - \sum_{i=1}^{t+1} [p_i^2] + \sum_{i=1}^{t} [p_i z_i]. \]  

(61)

Hence, due to the Danskin’s theorem,

\[ \nabla F_\theta(z) = \arg\max_{p \in \mathbb{R}^{t+1}: p \geq 0, 1^T p = 1} \sum_{i=1}^{t+1} [p_i z_i - p_i^2] - p_{i+1}^2 \]  

(62)

We define \( \tilde{z} = (z, 0) \) and rewrite the objective as

\[ \sum_{i=1}^{t+1} [p_i \tilde{z}_i - p_i^2]. \]  

(63)
Then, the optimal solution $\mathbf{p}^*$ of (62) obeys the same order as the order of $\tilde{z}$. To characterize the solution to (62), we use the KKT conditions. It is not hard to check the Slater condition holds here; thus, the KKT conditions are necessary and sufficient [33]. According to KKT conditions, for any optimal solution $\mathbf{p}^*$ there exists a dual solution $\lambda^* \geq 0$, $\beta^*$ where

$$\forall 1 \leq i \leq t + 1:\quad p_i^* = \frac{1}{2}(\tilde{z}_i + \lambda_i^* + \beta^*), \quad \lambda_i^* p_i^* = 0. \quad (64)$$

Since $\mathbf{p}^*$ has the same ordering as $\tilde{z}$, considering $\sigma$ as the permutation sorting $\tilde{z}$ in a descending order, we find the smallest $k$ such that $\sum_{i=1}^k [\tilde{z}_{\sigma(i)} - \tilde{z}_{\sigma(k+1)}] > 2$ or let $k = t + 1$ if the condition holds for no $k \leq t$. We claim that the following feasible $\mathbf{p}$ satisfies (64) and hence provides a solution to (62).

$$\forall 1 \leq i \leq t:\quad p_i = \begin{cases} \left(2 - \sum_{j=1}^k \tilde{z}_{\sigma(j)}\right)/2k + \tilde{z}_{\sigma(i)}/2 & \text{if } \sigma(i) \leq k, \\ 0 & \text{Otherwise.} \end{cases} \quad (65)$$

Note that due to the choice of $k$, $\mathbf{p}$ is a feasible point, i.e. $\mathbf{p} \geq 0$ and $1^T \mathbf{p} = 1$. Let $\beta = (2 - \sum_{j=1}^k \tilde{z}_{\sigma(j)})/k$ and $\lambda_{\sigma(i)} = 0$ for $i \leq k$. Then, for $i > k$ let $\lambda_{\sigma(i)} = -\tilde{z}_{\sigma(i)} - \beta = (2 - \sum_{j=1}^k \tilde{z}_{\sigma(j)} - \tilde{z}_{\sigma(i)})/k \geq 0$, due to the choice of $k$. Therefore, $\mathbf{p}$ satisfies the KKT conditions and the procedure returns a solution to (62).

### 6.6 Quadratic Loss: Linear Regression

#### 6.6.1 $F_\theta$ derivation

Here, we find $F_\theta(\mathbf{z}) = \max_{\mathbf{p} \in \mathcal{P}_Y} H(Y) + \mathbb{E}[\theta(Y)^T \mathbf{z}]$ for $\theta(Y) = Y$ and $\mathcal{P}_Y = \{P_Y : \mathbb{E}[Y^2] \leq \rho^2\}$. Since for quadratic loss $H(Y) = \text{Var}(Y) = \mathbb{E}[Y^2] - \mathbb{E}[Y]^2$, the problem is equivalent to

$$F_\theta(\mathbf{z}) = \max_{\mathbb{E}[Y^2] \leq \rho^2} \mathbb{E}[Y^2] - \mathbb{E}[Y]^2 + z \mathbb{E}[Y] \quad (66)$$

As $\mathbb{E}[Y]^2 \leq \mathbb{E}[Y^2]$, it can be seen for the solution $\mathbb{E}_{P_Y}[Y^2] = \rho^2$ and therefore we equivalently solve

$$F_\theta(\mathbf{z}) = \max_{\mathbb{E}[Y^2] \leq \rho^2} \rho^2 - \mathbb{E}[Y^2] + z \mathbb{E}[Y] = \begin{cases} \rho^2 + z^2/4 & \text{if } |z/2| \leq \rho \\ \rho |z| & \text{if } |z/2| > \rho. \end{cases} \quad (67)$$

#### 6.6.2 Applying Theorem 3 while restricting $\mathcal{P}_Y$

For the quadratic loss, we first change $\mathcal{P}_Y = \{P_Y : \mathbb{E}[Y^2] \leq \rho^2\}$ and then apply Theorem 3. Note that by modifying $F_\theta$ based on the new $\mathcal{P}_Y$ we also solve a modified version of the maximum conditional entropy problem

$$\max_{\mathbf{p}: \mathbf{p} \in \mathcal{P}_Y} H(Y|\mathbf{X}) \quad (68)$$

In the case $\mathcal{P}_Y = \{P_Y : \mathbb{E}[Y^2] \leq \rho^2\}$ Theorem 3 remains valid given the above modification in the maximum conditional entropy problem. This is because the inequality constraint $\mathbb{E}[Y^2|\mathbf{X} = \mathbf{x}] \leq \rho^2$ is linear in $P_Y|\mathbf{X} = \mathbf{x}$, and thus the problem remains convex and strong duality still holds. Also, when we move the constraints of $w_i = \mathbb{E}_P[\theta_i(Y)|\mathbf{X}]$ to the objective function, we get a similar dual problem

$$\min_{\mathbf{A}} \sup_{\mathbf{P}_{Y}: \mathbf{P}_{Y} \in \mathcal{P}_Y} \mathbb{E}_{\mathbf{Q}_X} \left[ H_P(Y|X = \mathbf{x}) + \sum_{i=1}^t \mathbb{E}[\theta_i(Y)|\mathbf{X} = \mathbf{x}] \mathbf{A}_i \mathbf{X} \right] + \sum_{j=1}^t \mathbb{E} [I_C_i(w_i)] - \mathbf{A}_i w_i \quad (69)$$

Following the next steps of the proof of Theorem 3 the proof remains valid given the modification on $F_\theta$ and the maximum conditional entropy problem.
6.6.3 Derivation of group lasso

To derive the group lasso, we slightly change the structure of $\Gamma(Q)$. Given disjoint subsets $I_1, \ldots, I_k$, consider a set of distributions $\Gamma_{GL}(Q)$ with the following structure
\[
\Gamma_{GL}(Q) = \{ P_{X,Y} : P_X = Q_X, \ \forall 1 \leq j \leq k : \| \mathbb{E}_P [Y|X_i] - \mathbb{E}_Q [Y|X_{I_j}] \| \leq \epsilon_j \}.
\]
Now we prove a modified version of Theorem 3, \[\text{max}_{P \in \Gamma_{GL}(Q)} H(Y|X) = \min_{\alpha} \mathbb{E}_Q \left[ F_0(\alpha^T X) - Y \alpha^T X \right] + \sum_{j=1}^k \epsilon_j \| \alpha_{I_j} \|.\] \[\text{(71)}\]
To prove this identity, we can use the same proof provided for Theorem 3. We only need to redefine $\tilde{E}_j = \mathbb{E}_Q [Y|X_{I_j}]$ and $C_j = \{ u : \| u - \tilde{E}_j \| \leq \epsilon_j \}$ for $1 \leq j \leq k$. Notice that here $t = 1$. Using the same technique in that proof, the dual problem is formulated as
\[
\min_{\alpha} \sup_{P_{Y|X}, w} \mathbb{E}_{Q_X} \left[ H_P(Y|X = x) + \mathbb{E}[Y|X = x] \alpha^T X \right] + \sum_{j=1}^k \left[ I_{C_j}(w_{I_j}) - \alpha_{I_j} w_{I_j} \right].
\]
\[\text{(72)}\]

Similar to the proof of Theorem 3, we can decouple and simplify the above problem to show (71). Then, considering the problem for the quadratic loss and taking $\| \cdot \|$ as the $l_q$-norm, we get the group lasso problem with the $\ell_{1,p}$ regularizer.

6.7 Proof of Theorem 5

Since entropy measures the infimum expected loss given a distribution, it is sufficient to show that under any distribution $P \in \Gamma$ the misclassification rate of $\psi_{BR}$ is bounded by the maximum Brier entropy over $\Gamma$ and the Brier entropy is generally bounded by twice the 0-1 entropy.

To show the first part, note that for any sequence $(a_i)_{i=1}^n$,
\[
\forall j : \quad 2a_j \leq \frac{a_j^2}{\sum a_i^2} + \sum a_i^2,
\]
\[
\Rightarrow \forall j : \quad 1 - \frac{a_j^2}{\sum a_i^2} \leq 1 - 2a_j + \sum a_i^2,
\]
\[
\Rightarrow \forall j : \quad 1 - \frac{a_j^2}{\sum a_i^2} \leq (1 - a_j)^2 + \sum_{i \neq j} a_i^2.
\]
Therefore, since the conditions of Theorem 3 hold, for any distribution $P \in \Gamma$
\[
P(\psi_{BR}(X) \neq Y) = \sum_{i,x} \mathbb{P}_{x,i} \left( 1 - \frac{P_{i|x}^2}{\sum_{j=1}^{\ell} P_{j|x}^2} \right) \leq \sum_{i,x} \mathbb{P}_{x,i} \left( (1 - P_{i|x})^2 + \sum_{j \neq i} P_{j|x}^2 \right) = \mathbb{E}_P \left[ L_{BR}(Y, P_{Y|X}) \right] \leq H_{BR}(P_{Y|X}).
\]
\[\text{(73)}\]
Also, note that for any sequence $(a_i)_{i=1}^n$,
\[
\forall i : \quad 2a_i \leq 1 + a_i^2 \Rightarrow \max_i a_i \leq 1 + \sum_i a_i^2 \Rightarrow 1 - \sum_i a_i^2 \leq 2(1 - \max_i a_i).
\]
Therefore, in general
\[
H_{BR}(Y) \leq 2 H_{0.1}(Y).
\]
\[\text{(74)}\]
Combining (\ref{eq:73}) and (\ref{eq:74}), we have
\[
\max_{P \in \Gamma} P(\psi_{BR}(X) \neq Y) \leq 2 \max_{P \in \Gamma} H_{0.1}(Y|X) = 2 \min_{\psi \in \Psi} \max_{P \in \Gamma} P(\psi(X) \neq Y).
\]