
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 Γ on (X, Y) , what is the optimal decision rule minimizing the worst-case expected loss over Γ ? 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 marginal on X constrained to be the empirical marginal from the data, we develop a general minimax approach for supervised learning problems. While for some loss functions such as squared-error and log loss, the minimax approach rederives well-known regression models, for the 0-1 loss it results in a new linear classifier which we call the maximum entropy machine. The maximum entropy machine minimizes the worst-case 0-1 loss over the structured set of distribution, and by our numerical experiments can outperform other well-known linear classifiers such as SVM. We also prove a bound on the generalization worst-case error in this minimax framework.

1 Introduction

Supervised learning, the task of inferring a function that predicts a target Y from a feature vector $\mathbf{X} = (X_1, \dots, X_d)$ by using n labeled training samples $\{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$, has been a problem of central interest in machine learning. Given the underlying distribution $\hat{P}_{\mathbf{X}, Y}$, 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: What would be a good 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 genome-based classification task where we seek to predict a binary trait of interest Y from an observation of 3,000,000 SNPs, each of which can be considered as a discrete variable $X_i \in \{0, 1, 2\}$. Hence, to estimate the underlying distribution we need $O(3^{3,000,000})$ samples.

With no possibility of estimating the underlying P^* in such problems, several approaches have been proposed to deal with high-dimensional settings. The standard approach in statistical learning theory is empirical risk minimization (ERM) [1]. ERM learns the prediction rule by minimizing an approximated loss under the empirical distribution of samples. However, to avoid overfitting, ERM restricts the set of allowable decision rules to a class of functions with limited complexity measured through its VC-dimension. However, the ERM problem for several interesting loss functions such as 0-1 loss is computationally intractable [2].

This paper focuses on a complementary approach to ERM where 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:

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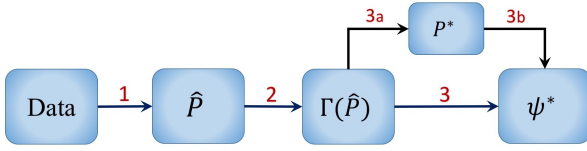


Figure 1: Minimax Approach

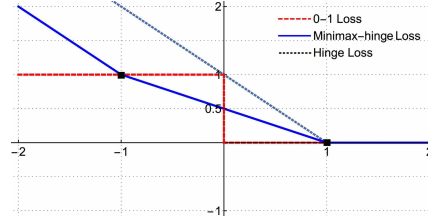


Figure 2: Minimax-hinge Loss

1. We compute the empirical distribution \hat{P} from the data,
2. We form a distribution set $\Gamma(\hat{P})$ based on \hat{P} ,
3. We learn a prediction rule ψ^* that minimizes the worst-case expected loss over $\Gamma(\hat{P})$.

An important example of the above minimax approach is the linear regression fitted via the least-squares method, which also minimizes the worst-case squared-error over all distributions with the same first and second order moments as empirically estimated from the samples. Some other special cases of this minimax approach, which are also based on learning a prediction rule from low-order marginal/moments, have been addressed in the literature: [3] solves a robust minimax classification problem for continuous settings with fixed first and second-order moments; [4] develops a classification approach by minimizing the worst-case hinge loss subject to fixed low-order marginals; [5] 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 functions.

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 [4] to

$$\operatorname{argmin}_{\psi \in \Psi} \max_{P \in \Gamma(\hat{P})} \mathbb{E} [L(Y, \psi(\mathbf{X}))]. \quad (1)$$

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

If we have to predict Y with no access to \mathbf{X} , (1) reduces to

$$\min_{a \in \mathcal{A}} \max_{P \in \Gamma(\hat{P})} \mathbb{E} [L(Y, a)], \quad (2)$$

where \mathcal{A} is the action space for loss function L . For L being the logarithmic loss function (log loss), Topsøe [6] reduces (2) to the entropy maximization problem over $\Gamma(\hat{P})$. This result is shown based on Sion's minimax theorem [7] which shows under some mild conditions one can exchange the order of min and max in the minimax problem. Note that when L is log loss, the maximin problem corresponding to (2) results in a maximum entropy problem. More generally, this result provides a game theoretic interpretation of the principle of maximum entropy introduced by Jaynes in [8]. By the principle of maximum entropy, one should select and act based on a distribution in $\Gamma(\hat{P})$ which maximizes the Shannon entropy.

Grünwald and Dawid [9] generalize the minimax theorem for log loss in [6] to other loss functions, showing (2) and its corresponding maximin problem have the same solution for a large class of loss functions. They further interpret the maximin problem as maximizing a generalized entropy function, which motivates generalizing the principle of maximum entropy for other loss functions: Given loss function L , select and act based on a distribution maximizing the generalized entropy function for L . Based on their minimax interpretation, the maximum entropy principle can be used for a general loss function to find and interpret the optimal action minimizing the worst-case expected loss in (2).

How can we use the principle of maximum entropy to solve (1) where we observe \mathbf{X} as well? A natural idea is to apply the maximum entropy principle to the conditional $P_{Y|\mathbf{X}=\mathbf{x}}$ 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*. The conditional entropy maximization for prediction problems was first introduced and interpreted by Berger et al. [10]. They indeed proved that the logistic regression model maximizes the conditional entropy over a particular set of distributions.

In this work, we extend the minimax interpretation from the maximum entropy principle [6, 9] to the maximum conditional entropy principle, which reveals how the maximum conditional entropy principle breaks Step 3 into two smaller steps:

- 3a. We search for P^* the distribution maximizing the conditional entropy over $\Gamma(\hat{P})$,
- 3b. We find ψ^* 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 [11], 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 \mathbf{X} and Y . However, they develop their theory targeting a broad class of distribution sets, which results in a convex problem, yet the number of variables is exponential in the dimension of the problem.

To overcome this issue, we propose a specific structure for the distribution set by matching the marginal $P_{\mathbf{X}}$ of all the joint distributions $P_{\mathbf{X}, Y}$ in $\Gamma(\hat{P})$ to the empirical marginal $\hat{P}_{\mathbf{X}}$ while matching only the cross-moments between \mathbf{X} and Y with those of the empirical distribution $\hat{P}_{\mathbf{X}, Y}$. We show that this choice of $\Gamma(\hat{P})$ has two key advantages: 1) the minimax decision rule ψ^* can be computed efficiently; 2) the minimax generalization error can be controlled by allowing a level of uncertainty in the matching of the cross-moments, which can be viewed as regularization in the minimax framework.

More importantly, by applying this idea for the generalized conditional entropy we generalize the duality shown in [10] among the maximum conditional Shannon entropy problem and the maximum likelihood problem for fitting the logistic regression model. 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 a classifier which we call the *maximum entropy machine (MEM)*. We also show how regularization in the empirical risk minimization problem can be interpreted as expansion of the uncertainty set in the dual maximum conditional entropy problem, which allows us to bound the generalization worst-case error in the minimax framework.

2 Two Examples

In this section, we highlight two important examples to compare the minimax approach with the ERM approach. These examples also motivate a particular structure for the distribution set in the minimax approach, which is discussed earlier in the introduction.

2.1 Regression: Squared-error

Consider a regression task to predict a continuous $Y \in \mathbb{R}$ from feature vector $\mathbf{X} \in \mathbb{R}^d$. A well-known approach for this task is the linear regression, where one considers the set of linear prediction rules $\{\psi : \exists \beta \in \mathbb{R}^d, \forall \mathbf{x} \in \mathbb{R}^d : \psi(\mathbf{x}) = \beta^T \mathbf{x}\}$. The ERM problem over this function class is the least-squares problem, where given samples $(\mathbf{x}_i, y_i)_{i=1}^n$ we solve

$$\min_{\beta} \frac{1}{n} \sum_{i=1}^n (y_i - \beta^T \mathbf{x}_i)^2. \quad (3)$$

Interestingly, the minimax approach for the squared-error loss also results in the linear regression and least-squares method. Consider the space of functions $\Psi = \{\psi : \mathbb{R}^d \rightarrow \mathbb{R}\}$ and define Γ as the following set of distributions fixing the cross-moments $\mathbb{E}[Y\mathbf{X}]$ and the $P_{\mathbf{X}}$ marginal using the data

$$\Gamma = \left\{ P_{\mathbf{X}, Y} : P_{\mathbf{X}} = \hat{P}_{\mathbf{X}}, \mathbb{E}[Y\mathbf{X}] = \frac{1}{n} \sum_{i=1}^n y_i \mathbf{x}_i, \mathbb{E}[Y^2] = \frac{1}{n} \sum_{i=1}^n y_i^2 \right\}, \quad (4)$$

where $\hat{P}_{\mathbf{X}}$ is the empirical marginal $P_{\mathbf{X}}$. Then, in Section 4 we show if we solve the minimax problem

$$\min_{\psi \in \Psi} \max_{P \in \Gamma} \mathbb{E} \left[(Y - \psi(\mathbf{X}))^2 \right] \quad (5)$$

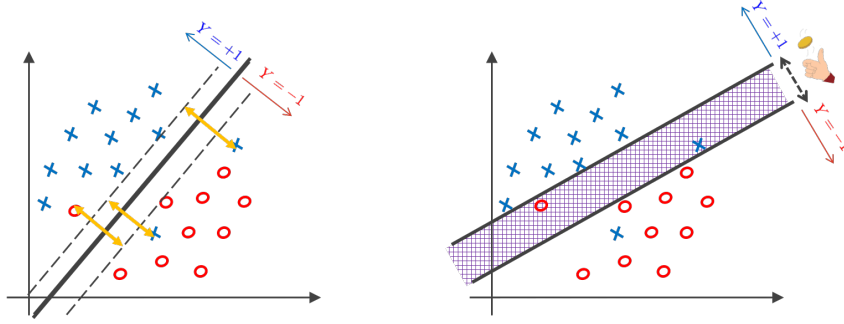


Figure 3: The deterministic linear prediction rule for SVM in the ERM approach (left picture) vs. the randomized linear prediction rule for MEM in the minimax approach (right picture)

the minimax optimal ψ^* is a linear function which is the same as the solution to the least-squares problem. This simple example motivates the minimax approach and Γ defined above by fixing the cross-moments and $P_{\mathbf{X}}$ marginal. Note that the maximin problem corresponding to (5) is

$$\max_{P \in \Gamma} \min_{\psi \in \Psi} \mathbb{E} \left[(Y - \psi(\mathbf{X}))^2 \right] = \max_{P \in \Gamma} \mathbb{E} [\text{Var}(Y|\mathbf{X})], \quad (6)$$

where $\mathbb{E}[\text{Var}(Y|\mathbf{X})]$ is in fact the generalized conditional entropy for the squared-error loss function.

2.2 Classification: 0-1 Loss

0-1 loss is a loss function of central interest for the classification task. In the binary classification problem, the empirical risk minimization problem over linear decision rules is commonly formulated as

$$\min_{\beta} \frac{1}{n} \sum_{i=1}^n \mathbf{1}(y_i \beta^T \mathbf{x}_i \leq 0) \quad (7)$$

where $\mathbf{1}$ denotes the indicator function. This ERM problem to minimize the number of misclassifications over the training samples is known to be non-convex and NP-hard [2]. To resolve this issue in practice, the 0-1 loss is replaced with a surrogate loss function. The hinge loss is an important example of a surrogate loss function which is empirically minimized by the Support Vector Machine (SVM) [12] and is defined for a binary $Y \in \{-1, +1\}$ as

$$\ell_{\text{hinge}}(y, \beta^T \mathbf{x}) = \max\{0, 1 - \beta^T \mathbf{x} y\}. \quad (8)$$

On the other hand, one can change the loss function from squared-error to 0-1 loss and solve the minimax problem (5) instead of empirical risk minimization. Then, by swapping the order of min and max as

$$\min_{\psi \in \Psi} \max_{P \in \Gamma} \mathbb{E} [L_{0-1}(Y, \psi(\mathbf{X}))] = \max_{P \in \Gamma} \min_{\psi \in \Psi} \mathbb{E} [L_{0-1}(Y, \psi(\mathbf{X}))] = \max_{P \in \Gamma} H_{0-1}(Y|\mathbf{X}), \quad (9)$$

we reduce the 0-1 loss minimax problem to the maximization of a concave objective $H_{0-1}(Y|\mathbf{X})$ over a convex set of probability distributions Γ . Therefore, unlike the ERM problem with 0-1 loss, this minimax problem can be solved efficiently by the MEM method. In fact, MEM solves the maximum conditional entropy problem by reducing it to a convex ERM problem. For a binary $Y \in \{-1, +1\}$, the new ERM problem has a loss function to which we call the *minimax hinge loss* defined as

$$\ell_{\text{mmhinge}}(y, \beta^T \mathbf{x}) = \max\left\{0, \frac{1 - \beta^T \mathbf{x} y}{2}, -\beta^T \mathbf{x} y\right\}. \quad (10)$$

As seen in Figure 2, the minimax hinge loss is different from the hinge loss, and while the hinge loss is an adhoc surrogate loss function, the minimax hinge loss emerges naturally from the minimax framework. Another notable difference between the ERM and minimax frameworks is that while

the linear prediction rule coming from the ERM framework is deterministic, the prediction rule resulted from the minimax approach is randomized linear (See Figure 3). Indeed, the relaxation from the deterministic rules to the randomized rules is an important step to overcome the computational intractability of 0-1 loss minimization problem in the minimax approach. We will discuss the details of the randomized prediction rule for MEM later in Section 4. Therefore, 0-1 loss provides an important example where, unlike the ERM problem, the generalized maximum entropy framework developed at [9] results in a computationally tractable problem which is well-connected to the loss function.

3 Principle of Maximum Conditional Entropy

In this section, we provide a conditional version of the key definitions and results developed in [9]. 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 for different loss functions to address Step 3b.

3.1 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 $L : \mathcal{Y} \times \mathcal{A} \rightarrow [0, \infty]$, $L(y, a)$ indicates the loss suffered by the decision maker by deciding action a when $Y = y$. The decision maker uses a decision rule $\psi : \mathcal{X} \rightarrow \mathcal{A}$ 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. ψ 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 1, this convexity is used to prove a saddle-point theorem.

We call a (randomized) decision rule ψ_{Bayes} a Bayes decision rule if for all decision rules ψ and for all $x \in \mathcal{X}$:

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

It should be noted that ψ_{Bayes} depends only on $P_{Y|X}$, i.e. it remains a Bayes decision rule under a different P_X . The (unconditional) entropy of Y is defined as [9]

$$H(Y) := \inf_{a \in \mathcal{A}} \mathbb{E}[L(Y, a)]. \quad (11)$$

Similarly, we can define conditional entropy of Y given $X = x$ as

$$H(Y|X = x) := \inf_{\psi} \mathbb{E}[L(Y, \psi(X))|X = x], \quad (12)$$

and the conditional entropy of Y given X as

$$H(Y|X) := \sum_x P_X(x) H(Y|X = x) = \inf_{\psi} \mathbb{E}[L(Y, \psi(X))]. \quad (13)$$

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 ,

$$I(X; Y) := H(Y) - H(Y|X), \quad (14)$$

i.e. the reduction of expected loss in predicting Y by observing X . In [13], 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 [9]

$$D(P_Y, Q_Y) := E_P[L(Y, a_Q)] - E_P[L(Y, a_P)] = E_P[L(Y, a_Q)] - H_P(Y). \quad (15)$$

3.2 Examples

3.2.1 Logarithmic loss

For an outcome $y \in \mathcal{Y}$ and distribution Q_Y , define logarithmic loss as $L_{\log}(y, Q_Y) = -\log Q_Y(y)$. It can be seen $H_{\log}(Y)$, $H_{\log}(Y|X)$, $I_{\log}(X; Y)$ are the well-known unconditional, conditional Shannon entropy and mutual information [14]. Also, the Bayes decision rule for a distribution $P_{X,Y}$ is given by $\psi_{\text{Bayes}}(x) = P_{Y|X}(\cdot|x)$.

3.2.2 0-1 loss

The 0-1 loss function is defined for any $y, \hat{y} \in \mathcal{Y}$ as $L_{0-1}(y, \hat{y}) = \mathbf{1}(\hat{y} \neq y)$. Then, we can show

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

The Bayes decision rule for a distribution $P_{X,Y}$ is the well-known maximum a posteriori (MAP) rule, i.e. $\psi_{\text{Bayes}}(x) = \operatorname{argmax}_{y \in \mathcal{Y}} P_{Y|X}(y|x)$.

3.2.3 Quadratic loss

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

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

The Bayes decision rule for any $P_{X,Y}$ is the well-known minimum mean-square error (MMSE) estimator that is $\psi_{\text{Bayes}}(x) = \mathbb{E}[Y|X = x]$.

3.3 Principle of Maximum Conditional Entropy & Robust Bayes decision rules

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

$$\operatorname{argmin}_{\psi \in \Psi} \max_{P \in \Gamma} \mathbb{E}_P[L(Y, \psi(X))], \quad (16)$$

where Ψ is the space of all randomized mappings from \mathcal{X} to \mathcal{A} and \mathbb{E}_P denotes the expected value over distribution P . We call any solution ψ^* to the above problem a robust Bayes decision rule against Γ . The following results motivate a generalization of the maximum entropy principle to find a robust Bayes decision rule. Refer to the Appendix for the proofs.

Theorem 1.A. (Weak Version) Suppose Γ is convex and closed, and let L be a bounded loss function. Assume \mathcal{X}, \mathcal{Y} are finite and that the risk set $S = \{[L(y, a)]_{y \in \mathcal{Y}} : a \in \mathcal{A}\}$ is closed. Then there exists a robust Bayes decision rule ψ^* against Γ , which is a Bayes decision rule for a distribution P^* that maximizes the conditional entropy $H(Y|X)$ over Γ .

Theorem 1.B. (Strong Version) Suppose Γ is convex and that under any $P \in \Gamma$ there exists a Bayes decision rule. We also assume the continuity in Bayes decision rules for distributions in Γ (See the Appendix for the exact condition). Then, if P^* maximizes $H(Y|X)$ over Γ , any Bayes decision rule for P^* is a robust Bayes decision rule against Γ .

Principle of Maximum Conditional Entropy: Given a set of distributions Γ , predict Y based on a distribution in Γ that maximizes the conditional entropy of Y given X , i.e.

$$\operatorname{argmax}_{P \in \Gamma} H(Y|X) \quad (17)$$

Note that while the weak version of Theorem 1 guarantees **only the existence** of a saddle point for (16), the strong version further guarantees that **any** Bayes decision rule of the maximizing distribution results in a robust Bayes decision rule. However, the continuity in Bayes decision rules does not hold for the discontinuous 0-1 loss, which requires considering the weak version of Theorem 1 to address this issue.

4 Prediction via Maximum Conditional Entropy Principle

Consider a prediction task with target variable Y and feature vector $\mathbf{X} = (X_1, \dots, X_d)$. We do not require the variables to be discrete. As discussed earlier, the maximum conditional entropy principle reduces (16) to (17), which formulate steps 3 and 3a in Figure 1, respectively. However, a general formulation of (17) in terms of the joint distribution $P_{\mathbf{X},Y}$ 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 addition, we prove a bound on the generalization worst-case risk for the proposed $\Gamma(\hat{P})$. In fact, we derive these results by reducing (17) 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 $Q_{\mathbf{X},Y}$, where for a given norm $\|\cdot\|$, mapping vector $\boldsymbol{\theta}(Y)_{t \times 1}$,

$$\Gamma(Q) = \{ P_{\mathbf{X},Y} : P_{\mathbf{X}} = Q_{\mathbf{X}}, \quad \forall 1 \leq i \leq t : \|\mathbb{E}_P[\theta_i(Y)\mathbf{X}] - \mathbb{E}_Q[\theta_i(Y)\mathbf{X}]\| \leq \epsilon_i \}. \quad (18)$$

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

To that end, we use a similar technique as in the Fenchel's duality theorem, also used at [15–17] to address divergence minimization problems. However, we consider a different version of convex conjugate for $-H$, which is defined with respect to $\boldsymbol{\theta}$. Considering \mathcal{P}_Y as the set of all probability distributions for the variable Y , we define $F_{\boldsymbol{\theta}} : \mathbb{R}^t \rightarrow \mathbb{R}$ as the convex conjugate of $-H(Y)$ with respect to the mapping $\boldsymbol{\theta}$,

$$F_{\boldsymbol{\theta}}(\mathbf{z}) := \max_{P \in \mathcal{P}_Y} H(Y) + \mathbb{E}[\boldsymbol{\theta}(Y)]^T \mathbf{z}. \quad (19)$$

Theorem 2. Define $\Gamma(Q)$, $F_{\boldsymbol{\theta}}$ as given by (18), (19). Then the following duality holds

$$\max_{P \in \Gamma(Q)} H(Y|\mathbf{X}) = \min_{\mathbf{A} \in \mathbb{R}^{t \times d}} \mathbb{E}_Q [F_{\boldsymbol{\theta}}(\mathbf{A}\mathbf{X}) - \boldsymbol{\theta}(Y)^T \mathbf{A}\mathbf{X}] + \sum_{i=1}^t \epsilon_i \|\mathbf{A}_i\|_*, \quad (20)$$

where $\|\mathbf{A}_i\|_*$ denotes $\|\cdot\|$'s dual norm of the \mathbf{A} 's i th row. Furthermore, for the optimal P^* and \mathbf{A}^*

$$\mathbb{E}_{P^*}[\boldsymbol{\theta}(Y) | \mathbf{X} = \mathbf{x}] = \nabla F_{\boldsymbol{\theta}}(\mathbf{A}^* \mathbf{x}). \quad (21)$$

Proof. Refer to the the supplementary material for the proof. \square

When applying Theorem 2 on a supervised learning problem with a specific loss function, $\boldsymbol{\theta}$ will be chosen such that $\mathbb{E}_{P^*}[\boldsymbol{\theta}(Y) | \mathbf{X} = \mathbf{x}]$ provides sufficient information to compute the Bayes decision rule Ψ^* for P^* . This enables the direct computation of ψ^* , i.e. step 3 of Figure 1, without the need to explicitly compute P^* itself. For the loss functions discussed at Subsection 3.2, we choose the identity $\boldsymbol{\theta}(Y) = Y$ for the quadratic loss and the one-hot encoding $\boldsymbol{\theta}(Y) = [\mathbf{1}(Y = i)]_{i=1}^t$ for the logarithmic and 0-1 loss functions. Later in this section, we will discuss how this theorem applies to these 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 [18] given by

- An exponential-family distribution $p(y|\boldsymbol{\eta}) = h(y) \exp(\boldsymbol{\eta}^T \boldsymbol{\theta}(y) - F_{\boldsymbol{\theta}}(\boldsymbol{\eta}))$ with the log-partition function $F_{\boldsymbol{\theta}}$ and the sufficient statistic $\boldsymbol{\theta}(Y)$,
- A linear predictor, $\boldsymbol{\eta}(\mathbf{X}) = \mathbf{A}\mathbf{X}$,

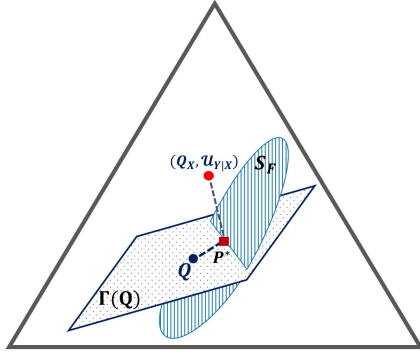


Figure 4: Duality of Maximum Conditional Entropy/Maximum Likelihood in GLMs

- A mean function, $\mathbb{E}[\boldsymbol{\theta}(Y)|\mathbf{X} = \mathbf{x}] = \nabla F_{\boldsymbol{\theta}}(\boldsymbol{\eta}(\mathbf{x}))$.

Therefore, Theorem 2 reveals a duality between the maximum conditional entropy problem over $\Gamma(Q)$ and the regularized maximum likelihood problem for the specified generalized linear model. This duality further provides a minimax justification for generalized linear models and fitting them using maximum likelihood, since we can consider the convex conjugate of its log-partition function as the negative entropy in the maximum conditional entropy problem.

4.1 Generalization Bound on the Worst-case Risk

By establishing the objective's Lipschitzness and boundedness through appropriate assumptions, we can apply standard results to bound the rate of uniform convergence for the problem in the RHS of (20). Here we consider the uniform convergence of the empirical averages, when $Q = \hat{P}_n$ is the empirical distribution of n samples drawn i.i.d. from the underlying distribution \tilde{P} , to their expectations when $Q = \tilde{P}$.

In the supplementary material, we prove the following theorem which bounds the generalization worst-case risk, by interpreting the mentioned uniform convergence on the other side of the duality. Here $\hat{\psi}_n$ and $\tilde{\psi}$ denote the robust Bayes decision rules against $\Gamma(\hat{P}_n)$ and $\Gamma(\tilde{P})$, respectively. As explained earlier, by the maximum conditional entropy principle we can learn $\hat{\psi}_n$ by solving the RHS of (20) for the empirical distribution and then applying (21).

Theorem 3. *Consider a loss function L with the entropy function H and suppose $\boldsymbol{\theta}(Y)$ includes only one element, i.e. $t = 1$. Let $M = \max_{P \in \mathcal{P}_Y} H(Y)$ be the maximum entropy value over \mathcal{P}_Y . Also, take $\|\cdot\|/\|\cdot\|_*$ to be the ℓ_p/ℓ_q pair where $\frac{1}{p} + \frac{1}{q} = 1$, $1 \leq q \leq 2$. Given that $\|\mathbf{X}\|_2 \leq B$ and $|\boldsymbol{\theta}(Y)| \leq L$, for any $\delta > 0$ with probability at least $1 - \delta$*

$$\max_{P \in \Gamma(\hat{P})} \mathbb{E}[L(Y, \hat{\psi}_n(\mathbf{X}))] - \max_{P \in \Gamma(\tilde{P})} \mathbb{E}[L(Y, \tilde{\psi}(\mathbf{X}))] \leq \frac{8BLM}{\epsilon\sqrt{n}} \left(1 + \sqrt{\frac{\log(2/\delta)}{2}}\right). \quad (22)$$

Theorem 3 states that though we learn the prediction rule $\hat{\psi}_n$ by solving the maximum conditional problem for the empirical case, we can bound the excess Γ -based worst-case risk. This generalization result justifies the constraint of fixing the marginal $P_{\mathbf{X}}$ across the proposed $\Gamma(Q)$ and explains the role of the uncertainty parameter ϵ in bounding the generalization worst-case risk.

4.2 Geometric Interpretation of Theorem 2

By solving the regularized maximum likelihood problem in the RHS of (20), we in fact minimize a regularized KL-divergence

$$\operatorname{argmin}_{P_{Y|\mathbf{X}} \in S_F} \mathbb{E}_{Q_{\mathbf{X}}}[D_{\text{KL}}(Q_{Y|\mathbf{X}} \| P_{Y|\mathbf{X}})] + \sum_{i=1}^t \epsilon_i \|\mathbf{A}_i(P_{Y|\mathbf{X}})\|_*, \quad (23)$$

where $S_F = \{P_{Y|\mathbf{X}}(y|\mathbf{x}) = h(y) \exp(\boldsymbol{\theta}(y)^T \mathbf{A}\mathbf{x} - F_{\boldsymbol{\theta}}(\mathbf{A}\mathbf{x})) \mid \mathbf{A} \in \mathbb{R}^{t \times s}\}$ is the set of all exponential-family conditional distributions for the specified generalized linear model. This can be viewed as projecting $Q_{Y|X}$ onto S_F (See Figure 4).

Furthermore, it can be seen that for a label-invariant entropy function $H(Y)$, the Bayes act for the uniform distribution \mathcal{U}_Y leads to the same expected loss under any distribution P_Y on Y . Based on the divergence D 's definition in (15), maximizing $H(Y|\mathbf{X})$ over $\Gamma(Q)$ in the LHS of (20) is therefore equivalent to the following divergence minimization problem

$$\operatorname{argmin}_{P_{Y|\mathbf{X}}: (Q_{\mathbf{X}}, P_{Y|\mathbf{X}}) \in \Gamma(Q)} \mathbb{E}_{Q_{\mathbf{X}}} [D(P_{Y|\mathbf{X}}, \mathcal{U}_{Y|\mathbf{X}})]. \quad (24)$$

Here $\mathcal{U}_{Y|\mathbf{X}}$ denotes the uniform conditional distribution over Y given any $x \in \mathcal{X}$. This can be interpreted as projecting the joint distribution $(Q_{\mathbf{X}}, \mathcal{U}_{Y|\mathbf{X}})$ onto $\Gamma(Q)$ (See Figure 4). Then, the duality shown in Theorem 2 implies the following corollary.

Corollary 1. *The solution to (23) would also minimize (24), i.e. (23) \subseteq (24).*

4.3 Examples

4.3.1 Logarithmic Loss: Logistic Regression

To gain sufficient information for the Bayes decision rule under the logarithmic loss, for $Y \in \mathcal{Y} = \{1, \dots, t+1\}$, let $\boldsymbol{\theta}(Y)$ be the one-hot encoding of Y , i.e. $\boldsymbol{\theta}_i(Y) = \mathbf{1}(Y = i)$ for $1 \leq i \leq t$. Here, we exclude $i = t+1$ as $\mathbf{1}(Y = t+1) = 1 - \sum_{i=1}^t \mathbf{1}(Y = i)$. Then

$$F_{\boldsymbol{\theta}}(\mathbf{z}) = \log\left(1 + \sum_{j=1}^t \exp(\mathbf{z}_j)\right), \quad \forall 1 \leq i \leq t: (\nabla F_{\boldsymbol{\theta}}(\mathbf{z}))_i = \exp(\mathbf{z}_i) / \left(1 + \sum_{j=1}^t \exp(\mathbf{z}_j)\right), \quad (25)$$

which is the logistic regression model [19]. Also, the RHS of (20) will be the regularized maximum likelihood problem for logistic regression. This particular result is well-studied in the literature and straightforward using the duality shown in [10].

4.3.2 0-1 Loss: maximum entropy machine

To get sufficient information for the Bayes decision rule under the 0-1 loss, we again consider the one-hot encoding $\boldsymbol{\theta}$ described for the logarithmic loss. We show in the Appendix that if $\tilde{\mathbf{z}} = (\mathbf{z}, 0)$ and $\tilde{z}_{(i)}$ denotes the i th largest element of $\tilde{\mathbf{z}}$,

$$F_{\boldsymbol{\theta}}(\mathbf{z}) = \max_{1 \leq k \leq t+1} \frac{k-1 + \sum_{j=1}^k \tilde{z}_{(j)}}{k}. \quad (26)$$

In particular, if Y is binary where $t = 1$

$$F_{\boldsymbol{\theta}}(z) = \max\left\{0, \frac{z+1}{2}, z\right\}. \quad (27)$$

Then, if $Y \in \mathcal{Y} = \{-1, 1\}$ the maximum likelihood problem (20) for learning the optimal linear predictor $\boldsymbol{\alpha}^*$ given n samples $(\mathbf{x}_i, y_i)_{i=1}^n$ will be

$$\min_{\boldsymbol{\alpha}} \frac{1}{n} \sum_{i=1}^n \max\left\{0, \frac{1-y_i \boldsymbol{\alpha}^T \mathbf{x}_i}{2}, -y_i \boldsymbol{\alpha}^T \mathbf{x}_i\right\} + \epsilon \|\boldsymbol{\alpha}\|_*. \quad (28)$$

The first term is the empirical risk of a linear classifier over the minimax-hinge loss $\max\{0, \frac{1-z}{2}, -z\}$ as shown in Figure 2. In contrast, the standard SVM is formulated using the hinge loss $\max\{0, 1-z\}$:

$$\min_{\boldsymbol{\alpha}} \frac{1}{n} \sum_{i=1}^n \max\{0, 1 - y_i \boldsymbol{\alpha}^T \mathbf{x}_i\} + \epsilon \|\boldsymbol{\alpha}\|_*, \quad (29)$$

We therefore call this classification approach the maximum entropy machine. However, unlike the standard SVM, the maximum entropy machine is naturally extended to multi-class classification.

Using Theorem 1.A¹, we prove that for 0-1 loss the robust Bayes decision rule exists and is randomized in general, where given the optimal linear predictor $\tilde{\mathbf{z}} = (\mathbf{A}^* \mathbf{x}, 0)$ randomly predicts a label according to the following $\tilde{\mathbf{z}}$ -based distribution on labels

$$\forall 1 \leq i \leq t+1: \quad p_{\sigma(i)} = \begin{cases} \tilde{z}_{(i)} + \frac{1 - \sum_{j=1}^{k_{\max}} \tilde{z}_{(j)}}{k_{\max}} & \text{if } \sigma(i) \leq k_{\max}, \\ 0 & \text{Otherwise.} \end{cases} \quad (30)$$

Here σ is the permutation sorting $\tilde{\mathbf{z}}$ in the ascending order, i.e. $\tilde{z}_{\sigma(i)} = \tilde{z}_{(i)}$, and k_{\max} is the largest index k satisfying $\sum_{i=1}^k [\tilde{z}_{(i)} - \tilde{z}_{(k)}] < 1$. For example, in the binary case discussed, the maximum entropy machine first solves (28) to find the optimal α^* and then predicts label $y = 1$ vs. label $y = -1$ with probability $\min\{1, \max\{0, (1 + \mathbf{x}^T \alpha^*)/2\}\}$.

We can also find the conditional-entropy maximizing distribution via (21), where the gradient of F_{θ} is given by

$$\forall 1 \leq i \leq t: \quad (\nabla F_{\theta}(\mathbf{z}))_i = \begin{cases} 1/k_{\max} & \text{if } \sigma(i) \leq k_{\max}, \\ 0 & \text{Otherwise.} \end{cases} \quad (31)$$

Note that F_{θ} is not differentiable if $\sum_{i=1}^{k_{\max}} [\tilde{z}_{(i)} - \tilde{z}_{(k_{\max}+1)}] = 1$, but the above vector is still in the subgradient $\partial F_{\theta}(\mathbf{z})$. Although we can find the $H(Y|X)$ -maximizing distribution, there could be multiple Bayes decision rules for that distribution. Since the strong result in Theorem 1 does not hold for the 0-1 loss, we are not guaranteed that all these decision rules are robust against $\Gamma(\hat{P})$. However, as we show in the appendix the randomized decision rule given by (30) will be robust.

4.3.3 Quadratic Loss: Linear Regression

Based on the Bayes decision rule for the quadratic loss, we choose $\theta(Y) = Y$. To derive F_{θ} , note that if we let \mathcal{P}_Y in (19) include all possible distributions, the maximized entropy (variance for quadratic loss) and thus the value of F_{θ} would be infinity. Therefore, given a parameter ρ , we restrict the second moment of distributions in $\mathcal{P}_Y = \{P_Y : \mathbb{E}[Y^2] \leq \rho^2\}$ and then apply (19). We show in the Appendix that an adjusted version of Theorem 2 holds after this change, and

$$F_{\theta}(z) - \rho^2 = \begin{cases} z^2/4 & \text{if } |z/2| \leq \rho \\ \rho(|z| - \rho) & \text{if } |z/2| > \rho, \end{cases} \quad (32)$$

which is the Huber function [20]. To find $\mathbb{E}[Y|\mathbf{X}]$ via (21), we have

$$\frac{dF_{\theta}(z)}{dz} = \begin{cases} -\rho & \text{if } z/2 \leq -\rho \\ z/2 & \text{if } -\rho < z/2 \leq \rho \\ \rho & \text{if } \rho < z/2. \end{cases} \quad (33)$$

Given the samples of a supervised learning task if we choose the parameter ρ large enough, by solving the RHS of (20) when $F_{\theta}(z)$ is replaced with $z^2/4$ and set ρ greater than $\max_i |\mathbf{A}^* \mathbf{x}_i|$, we can equivalently take $F_{\theta}(z) = z^2/4 + \rho^2$. Then, (33) reduces to the linear regression model and the maximum likelihood problem in the RHS of (20) is equivalent to

- Least squares when $\epsilon = 0$.
- Lasso [21, 22] when $\|\cdot\|/\|\cdot\|_*$ is the ℓ_{∞}/ℓ_1 pair.
- Ridge regression [23] when $\|\cdot\|$ is the ℓ_2 -norm.
- (overlapping) Group lasso [24, 25] with the $\ell_{1,p}$ penalty when $\Gamma_{\text{GL}}(Q)$ is defined, given subsets I_1, \dots, I_k of $\{1, \dots, d\}$ and $1/p + 1/q = 1$, as

$$\Gamma_{\text{GL}}(Q) = \{P_{\mathbf{X}, Y} : P_{\mathbf{X}} = Q_{\mathbf{X}}, \quad (34)$$

$$\forall 1 \leq j \leq k: \quad \|\mathbb{E}_P[Y \mathbf{X}_{I_j}] - \mathbb{E}_Q[Y \mathbf{X}_{I_j}]\|_q \leq \epsilon_j \}.$$

See the Appendix for the proofs. Another type of minimax, but non-probabilistic, argument for the robustness of lasso-like regression algorithms can be found in [26, 27].

¹We show that given the specific structure of $\Gamma(Q)$ Theorem 1.A holds whether \mathcal{X} is finite or infinite.

Dataset	MEM	SVM	DCC	MPM	TAN	DRC
adult	17	22	18	22	17	17
credit	12	16	14	13	17	13
kr-vs-kp	7	3	10	5	7	5
promoters	5	9	5	6	44	6
votes	4	5	3	4	8	3
hepatitis	17	20	19	18	17	17

Table 1: Methods Performance (error in %)

5 Robust Feature Selection

Using a minimax criterion over a set of distributions Γ , we solve the following problem to select the most informative subset of k features,

$$\operatorname{argmin}_{|S| \leq k} \min_{\psi \in \Psi_S} \max_{P \in \Gamma} \mathbb{E}_P[L(Y, \psi(\mathbf{X}_S))] \quad (35)$$

where \mathbf{X}_S denotes the feature vector \mathbf{X} restricted to the indices in S . Here, we evaluate each feature subset based on the minimum worst-case loss over Γ . Applying Theorem 1, (35) reduces to

$$\operatorname{argmin}_{|S| \leq k} \max_{P \in \Gamma} H(Y | \mathbf{X}_S), \quad (36)$$

which under the assumption that the marginal $H(Y)$ is fixed across all distributions in Γ is equivalent to selecting a subset S maximizing the worst-case generalized information $I(\mathbf{X}_S; Y)$ over Γ , i.e.

$$\operatorname{argmax}_{|S| \leq k} \min_{P \in \Gamma} I(\mathbf{X}_S; Y). \quad (37)$$

To solve (36) when $\Gamma = \Gamma(\hat{P}_n)$ defined at (18), where \hat{P}_n is the empirical distribution of samples $(\mathbf{x}_i, y_i)_{i=1}^n$, we apply the duality shown in Theorem 2 to obtain

$$\operatorname{argmin}_{\mathbf{A} \in \mathbb{R}^{t \times s}: \|\mathbf{A}\|_{0, \infty} \leq k} \frac{1}{n} \sum_{i=1}^n [F_{\theta}(\mathbf{A}\mathbf{x}_i) - \theta(y_i)^T \mathbf{A}\mathbf{x}_i] + \sum_{i=1}^t \epsilon_i \|\mathbf{A}_i\|_*. \quad (38)$$

Here by constraining $\|\mathbf{A}\|_{0, \infty} = \|(\|\mathbf{A}^{(1)}\|_{\infty}, \dots, \|\mathbf{A}^{(s)}\|_{\infty})\|_0$ where $\mathbf{A}^{(i)}$ denotes the i th column of \mathbf{A} , we impose the same sparsity pattern across the rows of \mathbf{A} . Let $\|\cdot\|_*$ be the ℓ_1 -norm and relax the above problem to

$$\operatorname{argmin}_{\mathbf{A} \in \mathbb{R}^{t \times s}} \frac{1}{n} \sum_{i=1}^n [F_{\theta}(\mathbf{A}\mathbf{x}_i) - \theta(y_i)^T \mathbf{A}\mathbf{x}_i] + \sum_{i=1}^t \epsilon_i \|\mathbf{A}_i\|_1. \quad (39)$$

Note that if for the uncertainty parameters ϵ_i 's, the solution \mathbf{A}^* to (39) satisfies $\|\mathbf{A}^*\|_{0, \infty} \leq k$ due to the tendency of ℓ_1 -regularization to produce sparse solutions, \mathbf{A}^* is the solution to (38) as well. In addition, based on the generalization bound established in Theorem 3, by allowing some gap we can generalize this sparse solution to (35) with $\Gamma = \Gamma(\tilde{P})$ for the underlying distribution \tilde{P} .

It is noteworthy that for the quadratic loss and identity θ , (39) is the same as the lasso. Also, for the logarithmic loss and one-hot encoding θ , (39) is equivalent to the ℓ_1 -regularized logistic regression. Hence, the ℓ_1 -regularized logistic regression maximizes the worst-case mutual information over $\Gamma(Q)$, which seems superior to the methods maximizing a heuristic instead of the mutual information $I(\mathbf{X}_S; Y)$ [28, 29].

6 Numerical Experiments

We evaluated the performance of the maximum entropy machine on six binary classification datasets from the UCI repository, compared to these five benchmarks: Support Vector Machines (SVM), Discrete Chebyshev Classifiers (DCC) [4], Minimax Probabilistic Machine (MPM) [3], Tree Augmented

Naive Bayes (TAN) [30], and Discrete Rényi Classifiers (DRC) [5]. The results are summarized in Table 1 where the numbers indicate the percentage of error in the classification task.

We implemented the maximum entropy machine by applying the gradient descent to (28) with the regularizer $\lambda \|\alpha\|_2^2$. We determined the value of λ by cross validation. To determine the lambda 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 $\{2^{-10}, \dots, 2^{10}\}$. Using the tuned lambda, we trained the algorithm 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 maximum entropy machine results in the best performance for four of the six datasets. Also, note that except a single dataset the maximum entropy machine outperforms 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 $y = \text{sign}(\gamma^T \mathbf{x} + z)$ 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 MEM which shows the MEM can outperform SVM and DRC in high-dimensional settings as well.

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References

- [1] Vladimir Vapnik. *The nature of statistical learning theory*. Springer Science & Business Media, 2013.
- [2] Vitaly Feldman, Venkatesan Guruswami, Prasad Raghavendra, and Yi Wu. Agnostic learning of monomials by halfspaces is hard. *SIAM Journal on Computing*, 41(6):1558–1590, 2012.
- [3] Gert RG Lanckriet, Laurent El Ghaoui, Chiranjib Bhattacharyya, and Michael I Jordan. A robust minimax approach to classification. *The Journal of Machine Learning Research*, 3:555–582, 2003.
- [4] Elad Eban, Elad Mezuman, and Amir Globerson. Discrete chebyshev classifiers. In *Proceedings of the 31st International Conference on Machine Learning (ICML-14)*, pages 1233–1241, 2014.
- [5] Meisam Razaviyayn, Farzan Farnia, and David Tse. Discrete rényi classifiers. In *Advances in Neural Information Processing Systems 28*, pages 3258–3266, 2015.
- [6] Flemming Topsøe. Information-theoretical optimization techniques. *Kybernetika*, 15(1):8–27, 1979.
- [7] Maurice Sion. On general minimax theorems. *Pacific J. Math*, 8(1):171–176, 1958.
- [8] Edwin T Jaynes. Information theory and statistical mechanics. *Physical review*, 106(4):620, 1957.
- [9] Peter D. Grünwald and Philip Dawid. Game theory, maximum entropy, minimum discrepancy and robust bayesian decision theory. *The Annals of Statistics*, 32(4):1367–1433, 2004.
- [10] Adam L Berger, Vincent J Della Pietra, and Stephen A Della Pietra. A maximum entropy approach to natural language processing. *Computational linguistics*, 22(1):39–71, 1996.
- [11] Amir Globerson and Naftali Tishby. The minimum information principle for discriminative learning. In *Proceedings of the 20th conference on Uncertainty in artificial intelligence*, pages 193–200, 2004.
- [12] Corinna Cortes and Vladimir Vapnik. Support-vector networks. *Machine learning*, 20(3):273–297, 1995.
- [13] Philip Dawid. Coherent measures of discrepancy, uncertainty and dependence, with applications to bayesian predictive experimental design. *Technical Report 139, University College London*, 1998. <http://www.ucl.ac.uk/Stats/research/abs94.html>.
- [14] Thomas M Cover and Joy A Thomas. *Elements of information theory*. John Wiley & Sons, 2012.
- [15] Yasemin Altun and Alexander Smola. Unifying divergence minimisation and statistical inference via convex duality. In *Learning Theory: Conference on Learning Theory COLT 2006, Proceedings*, 2006.
- [16] Miroslav Dudík, Steven J Phillips, and Robert E Schapire. Maximum entropy density estimation with generalized regularization and an application to species distribution modeling. *Journal of Machine Learning Research*, 8(6):1217–1260, 2007.
- [17] Ayse Erkan and Yasemin Altun. Semi-supervised learning via generalized maximum entropy. In *AISTATS*, pages 209–216, 2010.

- [18] Peter McCullagh and John A Nelder. *Generalized linear models*, volume 37. CRC press, 1989.
- [19] Jerome Friedman, Trevor Hastie, and Robert Tibshirani. *The elements of statistical learning*, volume 1. Springer, 2001.
- [20] Peter J Huber. *Robust Statistics*. Wiley, 1981.
- [21] Robert Tibshirani. Regression shrinkage and selection via the lasso. *Journal of the Royal Statistical Society. Series B (Methodological)*, pages 267–288, 1996.
- [22] Scott Shaobing Chen, David L. Donoho, and Michael A. Saunders. Atomic decomposition by basis pursuit. *SIAM Journal on Scientific Computing*, 20(1):33–61, 1998.
- [23] Arthur E Hoerl and Robert W Kennard. Ridge regression: Biased estimation for nonorthogonal problems. *Technometrics*, 12(1):55–67, 1970.
- [24] Ming Yuan and Yi Lin. Model selection and estimation in regression with grouped variables. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 68(1):49–67, 2006.
- [25] Laurent Jacob, Guillaume Obozinski, and Jean-Philippe Vert. Group lasso with overlap and graph lasso. In *Proceedings of the 26th annual international conference on machine learning*, pages 433–440, 2009.
- [26] Huan Xu, Constantine Caramanis, and Shie Mannor. Robust regression and lasso. In *Advances in Neural Information Processing Systems*, pages 1801–1808, 2009.
- [27] Wenzhuo Yang and Huan Xu. A unified robust regression model for lasso-like algorithms. In *Proceedings of The International Conference on Machine Learning*, pages 585–593, 2013.
- [28] Hanchuan Peng, Fuhui Long, and Chris Ding. Feature selection based on mutual information criteria of max-dependency, max-relevance, and min-redundancy. *Pattern Analysis and Machine Intelligence, IEEE Transactions on*, 27(8):1226–1238, 2005.
- [29] Pablo Estévez, Michel Tesmer, Claudio Perez, Jacek M Zurada, et al. Normalized mutual information feature selection. *Neural Networks, IEEE Transactions on*, 20(2):189–201, 2009.
- [30] CK Chow and CN Liu. Approximating discrete probability distributions with dependence trees. *Information Theory, IEEE Transactions on*, 14(3):462–467, 1968.
- [31] Ralph Rockafellar. Characterization of the subdifferentials of convex functions. *Pacific Journal of Mathematics*, 17(3):497–510, 1966.
- [32] Peter L Bartlett and Shahar Mendelson. Rademacher and gaussian complexities: Risk bounds and structural results. *Journal of Machine Learning Research*, 3(Nov):463–482, 2002.
- [33] Sham M Kakade, Karthik Sridharan, and Ambuj Tewari. On the complexity of linear prediction: Risk bounds, margin bounds, and regularization. In *Advances in neural information processing systems*, pages 793–800, 2009.
- [34] Andreas Maurer. A vector-contraction inequality for rademacher complexities. In *Algorithmic Learning Theory (ALT)*, pages 3–17, 2016.

7 Appendix

7.1 Proof of Theorem 1

7.1.1 Weak Version

First, we list the assumptions of the weak version of Theorem 1:

- Γ is convex and closed,
- Loss function L is bounded by a constant C ,
- \mathcal{X}, \mathcal{Y} are finite,
- Risk set $S = \{ [L(y, a)]_{y \in \mathcal{Y}} : a \in \mathcal{A} \}$ is closed.

Given these assumptions, Sion’s minimax theorem [7] implies that the minimax problem has a finite answer H^* ,

$$H^* := \sup_{P \in \Gamma} \inf_{\psi \in \Psi} \mathbb{E}[L(Y, \psi(X))] = \inf_{\psi \in \Psi} \sup_{P \in \Gamma} \mathbb{E}[L(Y, \psi(X))]. \quad (40)$$

Thus, there exists a sequence of decision rules $(\psi_n)_{n=1}^{\infty}$ for which

$$\lim_{n \rightarrow \infty} \sup_{P \in \Gamma} \mathbb{E}[L(Y, \psi_n(X))] = H^*. \quad (41)$$

As we supposed, the risk set S is closed. Therefore, the randomized risk set² $S_r = \{ [L(y, \zeta)]_{y \in \mathcal{Y}} : \zeta \in \mathcal{Z} \}$ defined over the space of randomized acts \mathcal{Z} is also closed and, since L is bounded, is a compact subset of $\mathbb{R}^{|\mathcal{Y}|}$. Therefore, since \mathcal{X} and \mathcal{Y} are both finite, we can find a randomized decision rule ψ^* which on taking a subsequence $(n_k)_{k=1}^\infty$ satisfies

$$\forall x \in \mathcal{X}, y \in \mathcal{Y} : L(y, \psi^*(x)) = \lim_{k \rightarrow \infty} L(y, \psi_{n_k}(x)). \quad (42)$$

Then ψ^* is a robust Bayes decision rule against Γ , because

$$\sup_{P \in \Gamma} \mathbb{E}[L(Y, \psi^*(X))] = \sup_{P \in \Gamma} \lim_{k \rightarrow \infty} \mathbb{E}[L(Y, \psi_{n_k}(X))] \leq \lim_{k \rightarrow \infty} \sup_{P \in \Gamma} \mathbb{E}[L(Y, \psi_{n_k}(X))] = H^*. \quad (43)$$

Moreover, since Γ is assumed to be convex and closed (hence compact), $H(Y|X)$ achieves its supremum over Γ at some distribution P^* . By the definition of conditional entropy, (43) implies that

$$E_{P^*}[L(Y, \psi^*(X))] \leq \sup_{P \in \Gamma} \mathbb{E}[L(Y, \psi^*(X))] \leq H^* = H_{P^*}(Y|X), \quad (44)$$

which shows that ψ^* is a Bayes decision rule for P^* as well. This completes the proof.

7.1.2 Strong Version

Let's recall the assumptions of the strong version of Theorem 1:

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

Note: A particular structure used in our paper is given by fixing the marginal P_X across Γ . Under this structure, the condition of the continuity in Bayes decision rules reduces to the continuity in Bayes acts over P_Y 's in $\Gamma_{Y|X}$. It can be seen that while this condition holds for the logarithmic and quadratic loss functions, it does not hold for the 0-1 loss.

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

$$\mathbb{E}_{P^*}[L(Y, \psi^*(X))] \leq \mathbb{E}_{P^*}[L(Y, \psi(X))], \quad (45)$$

and

$$\mathbb{E}_{P^*}[L(Y, \psi^*(X))] \geq \mathbb{E}_P[L(Y, \psi^*(X))]. \quad (46)$$

Clearly, inequality (45) holds due to the definition of the Bayes decision rule. To show (46), 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 Γ is convex. Let ψ_λ be a Bayes decision rule for P_λ . Due to the linearity of the expected loss in the probability distribution, we have

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

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 Γ . Applying the assumption of the continuity in Bayes decision rules, we have

$$\mathbb{E}_P[L(Y, \psi^*(X))] - \mathbb{E}_{P^*}[L(Y, \psi^*(X))] = \lim_{\lambda \rightarrow 0} \mathbb{E}_P[L(Y, \psi_\lambda(X))] - \mathbb{E}_{P^*}[L(Y, \psi_\lambda(X))] \leq 0, \quad (47)$$

which makes the proof complete.

² $L(y, \zeta)$ is a short-form for $E[L(y, A)]$ where $A \in \mathcal{A}$ is a random action distributed according to ζ .

7.2 Proof of Theorem 2

Let us recall the definition of the set $\Gamma(Q)$:

$$\Gamma(Q) = \{ P_{\mathbf{X},Y} : P_{\mathbf{X}} = Q_{\mathbf{X}}, \quad \forall 1 \leq i \leq t : \|\mathbb{E}_P[\theta_i(Y)\mathbf{X}] - \mathbb{E}_Q[\theta_i(Y)\mathbf{X}]\| \leq \epsilon_i \}. \quad (48)$$

Defining $\tilde{\mathbf{E}}_i \triangleq \mathbb{E}_Q[\theta_i(Y)\mathbf{X}]$ and $C_i \triangleq \{\mathbf{u} : \|\mathbf{u} - \tilde{\mathbf{E}}_i\| \leq \epsilon_i\}$, we have

$$\max_{P \in \Gamma(Q)} H(Y|\mathbf{X}) = \max_{P, \mathbf{w}: \forall i: \mathbf{w}_i = \mathbb{E}_P[\theta_i(Y)\mathbf{X}]} \mathbb{E}_{Q_{\mathbf{X}}} [H_P(Y|\mathbf{X} = \mathbf{x})] + \sum_{i=1}^t I_{C_i}(\mathbf{w}_i) \quad (49)$$

where I_C is the indicator function for the set C defined as

$$I_C(x) = \begin{cases} 0 & \text{if } x \in C, \\ -\infty & \text{Otherwise.} \end{cases} \quad (50)$$

First of all, the law of iterated expectations implies that $\mathbb{E}_P[\theta_i(Y)\mathbf{X}] = \mathbb{E}_{Q_{\mathbf{X}}}[\mathbf{X}\mathbb{E}[\theta_i(Y)|\mathbf{X} = \mathbf{x}]]$. Furthermore, (49) is equivalent to a convex optimization problem where it is not hard to check that the Slater condition is satisfied. Hence strong duality holds and we can write the dual problem as

$$\min_{\mathbf{A}} \sup_{P_{Y|\mathbf{X}}, \mathbf{w}} \mathbb{E}_{Q_{\mathbf{X}}} \left[H_P(Y|\mathbf{X} = \mathbf{x}) + \sum_{i=1}^t \mathbb{E}[\theta_i(Y)|\mathbf{X} = \mathbf{x}] \mathbf{A}_i \mathbf{X} \right] + \sum_{i=1}^t [I_{C_i}(\mathbf{w}_i) - \mathbf{A}_i \mathbf{w}_i], \quad (51)$$

where the rows of matrix \mathbf{A} , denoted by \mathbf{A}_i , are the Lagrange multipliers for the constraints of $\mathbf{w}_i = \mathbb{E}_P[\theta_i(Y)\mathbf{X}]$. Notice that the above problem decomposes across $P_{Y|\mathbf{X}=\mathbf{x}}$'s and \mathbf{w}_i 's. Hence, the dual problem can be rewritten as

$$\min_{\mathbf{A}} \left[\mathbb{E}_{Q_{\mathbf{X}}} \left[\sup_{P_{Y|\mathbf{X}=\mathbf{x}}} H_P(Y|\mathbf{X} = \mathbf{x}) + \sum_{i=1}^t \mathbb{E}[\theta_i(Y)|\mathbf{X} = \mathbf{x}] \mathbf{A}_i \mathbf{X} \right] + \sum_{i=1}^t \sup_{\mathbf{w}_i} [I_{C_i}(\mathbf{w}_i) - \mathbf{A}_i \mathbf{w}_i] \right] \quad (52)$$

Furthermore, according to the definition of F_{θ} , we have

$$F_{\theta}(\mathbf{A}\mathbf{x}) = \sup_{P_{Y|\mathbf{X}=\mathbf{x}}} H(Y|\mathbf{X} = \mathbf{x}) + \mathbb{E}[\theta(Y)|\mathbf{X} = \mathbf{x}]^T \mathbf{A}\mathbf{x}. \quad (53)$$

Moreover, the definition of the dual norm $\|\cdot\|_*$ implies

$$\sup_{\mathbf{w}_i} I_{C_i}(\mathbf{w}_i) - \mathbf{A}_i \mathbf{w}_i = \max_{\mathbf{u} \in C_i} -\mathbf{A}_i \mathbf{u} = -\mathbf{A}_i \tilde{\mathbf{E}}_i + \epsilon_i \|\mathbf{A}_i\|_*. \quad (54)$$

Plugging (53) and (54) in (52), the dual problem can be simplified to

$$\begin{aligned} & \min_{\mathbf{A}} \mathbb{E}_{Q_{\mathbf{X}}} \left[F_{\theta}(\mathbf{A}\mathbf{X}) - \sum_{i=1}^t \mathbf{A}_i \tilde{\mathbf{E}}_i \right] + \sum_{i=1}^t \epsilon_i \|\mathbf{A}_i\|_* \\ & = \min_{\mathbf{A}} \mathbb{E}_Q [F_{\theta}(\mathbf{A}\mathbf{X}) - \theta(Y)^T \mathbf{A}\mathbf{X}] + \sum_{i=1}^t \epsilon_i \|\mathbf{A}_i\|_*, \end{aligned} \quad (55)$$

which is equal to the primal problem (49) since the strong duality holds. Furthermore, note that we can rewrite the definition given for F_{θ} as

$$F_{\theta}(\mathbf{z}) = \max_{\mathbf{E} \in \mathbb{R}^t} G(\mathbf{E}) + \mathbf{E}^T \mathbf{z}, \quad (56)$$

where we define

$$G(\mathbf{E}) = \begin{cases} \max_{P \in \mathcal{P}_Y: \mathbb{E}[\theta(Y)] = \mathbf{E}} H(Y) & \text{if } \{P \in \mathcal{P}_Y : \mathbb{E}[\theta(Y)] = \mathbf{E}\} \neq \emptyset \\ -\infty & \text{Otherwise.} \end{cases} \quad (57)$$

Observe that F_{θ} is the convex conjugate of the convex $-G$. Therefore, applying the derivative property of convex conjugates [31] to (53),

$$\mathbb{E}_{P^*}[\theta(Y)|\mathbf{X} = \mathbf{x}] \in \partial F_{\theta}(\mathbf{A}^* \mathbf{x}). \quad (58)$$

Here, ∂F_{θ} denotes the subgradient of F_{θ} . Assuming F_{θ} is differentiable at $\mathbf{A}^* \mathbf{x}$, (58) implies that

$$\mathbb{E}_{P^*}[\theta(Y)|\mathbf{X} = \mathbf{x}] = \nabla F_{\theta}(\mathbf{A}^* \mathbf{x}). \quad (59)$$

7.3 Proof of Theorem 3

First, we aim to show that

$$\max_{P \in \Gamma(\hat{P})} \mathbb{E}[L(Y, \hat{\psi}_n(\mathbf{X}))] \leq \mathbb{E}_{\hat{P}} \left[F_{\theta}(\hat{\mathbf{A}}\mathbf{X}) - \theta(Y)^T \hat{\mathbf{A}}\mathbf{X} \right] + \sum_{i=1}^t \epsilon_i \|\hat{\mathbf{A}}_{n_i}\|_* \quad (60)$$

where $\hat{\mathbf{A}}$ denotes the solution to the RHS of the duality equation in Theorem 2 for the empirical distribution \hat{P}_n . Similar to the duality proven in Theorem 2, we can show that

$$\begin{aligned} \max_{P \in \Gamma(\hat{P})} \mathbb{E}[L(Y, \hat{\psi}_n(\mathbf{X}))] &= \min_{\mathbf{A}} \mathbb{E}_{\hat{P}_X} \left[\sup_{P_{Y|\mathbf{X}} \in \mathcal{P}_Y} \mathbb{E}[L(Y, \hat{\psi}_n(\mathbf{X})) | \mathbf{X} = \mathbf{x}] + \mathbb{E}[\theta(Y) | \mathbf{X} = \mathbf{x}]^T \mathbf{A}\mathbf{X} \right] \\ &\quad - \mathbb{E}_{\hat{P}}[\theta(Y)^T \mathbf{A}\mathbf{X}] + \sum_{i=1}^t \epsilon_i \|\mathbf{A}_i\|_* \\ &\leq \mathbb{E}_{\hat{P}_X} \left[\sup_{P_{Y|\mathbf{X}=\mathbf{x}} \in \mathcal{P}_Y} \mathbb{E}[L(Y, \hat{\psi}_n(\mathbf{X})) | \mathbf{X} = \mathbf{x}] + \mathbb{E}[\theta(Y) | \mathbf{X} = \mathbf{x}]^T \hat{\mathbf{A}}\mathbf{X} \right] \\ &\quad - \mathbb{E}_{\hat{P}}[\theta(Y)^T \hat{\mathbf{A}}\mathbf{X}] + \sum_{i=1}^t \epsilon_i \|\hat{\mathbf{A}}_i\|_* \\ &= \mathbb{E}_{\hat{P}} \left[F_{\theta}(\hat{\mathbf{A}}\mathbf{X}) - \theta(Y)^T \hat{\mathbf{A}}\mathbf{X} \right] + \sum_{i=1}^t \epsilon_i \|\hat{\mathbf{A}}_i\|_*. \end{aligned}$$

Here we first upper bound the minimum by taking the specific $\mathbf{A} = \hat{\mathbf{A}}$. Then the equality holds because $\hat{\psi}_n$ is a robust Bayes decision rule against $\Gamma(\hat{P}_n)$ and therefore adding the second term based on $\hat{\mathbf{A}}\mathbf{x}$, $\hat{\psi}_n(\mathbf{x})$ results in a saddle point for the following problem

$$\begin{aligned} F_{\theta}(\hat{\mathbf{A}}\mathbf{x}) &= \sup_{P \in \mathcal{P}_Y} H(Y) + \mathbb{E}[\theta(Y)]^T \hat{\mathbf{A}}\mathbf{x} \\ &= \sup_{P \in \mathcal{P}_Y} \inf_{\zeta \in \mathcal{Z}} \mathbb{E}[L(Y, \zeta)] + \mathbb{E}[\theta(Y)]^T \hat{\mathbf{A}}\mathbf{x} \\ &= \sup_{P \in \mathcal{P}_Y} \mathbb{E}[L(Y, \hat{\psi}_n(\mathbf{x}))] + \mathbb{E}[\theta(Y)]^T \hat{\mathbf{A}}\mathbf{x}. \end{aligned}$$

Therefore, by Theorem 2 we have

$$\begin{aligned} \max_{P \in \Gamma(\hat{P})} \mathbb{E}[L(Y, \hat{\psi}_n(\mathbf{X}))] - \max_{P \in \Gamma(\tilde{P})} \mathbb{E}[L(Y, \tilde{\psi}(\mathbf{X}))] &\leq \quad (61) \\ \mathbb{E}_{\hat{P}} [F_{\theta}(\hat{\mathbf{A}}\mathbf{X}) - \theta(Y)^T \hat{\mathbf{A}}\mathbf{X}] + \sum_{i=1}^t \epsilon_i \|\hat{\mathbf{A}}_i\|_* - \mathbb{E}_{\tilde{P}} [F_{\theta}(\tilde{\mathbf{A}}\mathbf{X}) - \theta(Y)^T \tilde{\mathbf{A}}\mathbf{X}] - \sum_{i=1}^t \epsilon_i \|\tilde{\mathbf{A}}_i\|_*. \end{aligned}$$

As a result, we only need to bound the uniform convergence rate in the other side of the duality. Note that by the definition of F_{θ} ,

$$\forall P \in \mathcal{P}_Y, \mathbf{z} \in \mathbb{R}^t: \quad F_{\theta}(\mathbf{z}) - \mathbb{E}_P[\theta(Y)]^T \mathbf{z} \geq H_P(Y) \geq 0. \quad (62)$$

Hence, $\forall \mathbf{A}: F_{\theta}(\mathbf{A}\mathbf{X}) - \mathbb{E}[\theta(Y)]^T \mathbf{A}\mathbf{X} \geq 0$ and comparing the optimal solution to the RHS of the duality equation in Theorem 2 to the case $\mathbf{A} = \mathbf{0}$ implies that for any possible solution \mathbf{A}^*

$$\forall 1 \leq i \leq t: \quad \epsilon_i \|\mathbf{A}_i^*\|_q \leq \sum_{j=1}^t \epsilon_j \|\mathbf{A}_j^*\|_q \leq F_{\theta}(\mathbf{0}) = \max_{P \in \mathcal{P}_Y} H(Y) = M. \quad (63)$$

Hence, we only need to bound the uniform convergence rate in a bounded space where $\forall 1 \leq i \leq t: \|\mathbf{A}_i\|_q \leq \frac{M}{\epsilon_i}$. Also, applying the derivative property of the conjugate relationship indicates that $\partial F_{\theta}(\mathbf{z})$ is a subset of the convex hull of $\{\mathbb{E}[\theta(Y)]: P \in \mathcal{P}_Y\}$. Therefore, for any $u \in \partial F_{\theta}(\mathbf{z})$ we have $\|u\|_2 \leq L$, and $F_{\theta}(\mathbf{z}) - \theta(Y)\mathbf{z}$ is $2L$ -Lipschitz in \mathbf{z} . As a result, since $\|\mathbf{X}\|_p \leq B$ and $\|\theta(Y)\|_2 \leq L$ for any \mathbf{A}, \mathbf{A}' such that $\|\mathbf{A}_i\|_2 \leq \frac{M}{\epsilon_i}$,

$$\forall \mathbf{x}, \mathbf{x}', y, y': \quad [F_{\theta}(\mathbf{A}\mathbf{x}) - \theta(y)^T \mathbf{A}\mathbf{x}] - [F_{\theta}(\mathbf{A}'\mathbf{x}') - \theta(y')^T \mathbf{A}'\mathbf{x}'] \leq \sum_{i=1}^t \frac{4BML}{\epsilon_i}. \quad (64)$$

Consequently, we can apply standard uniform convergence results given convexity-Lipschitzness-boundedness [32, 33] as well as the vector contraction inequality from [34] to show that for any $\delta > 0$ with a probability at least $1 - \delta$

$$\begin{aligned} \forall \mathbf{A} \in \mathbb{R}^{d \times t}, \|\mathbf{A}_i\|_2 \leq \frac{M}{\epsilon_i} : \mathbb{E}_{\hat{P}} [F_{\theta}(\mathbf{A}\mathbf{X}) - \theta(Y)^T \mathbf{A}\mathbf{X}] & \quad (65) \\ -\mathbb{E}_{\hat{P}_n} [F_{\theta}(\mathbf{A}\mathbf{X}) - \theta(Y)^T \mathbf{A}\mathbf{X}] & \leq \frac{4BLM}{\sqrt{n}} \sum_{i=1}^t \frac{1}{\epsilon_i} \left(\sqrt{2}\sqrt{p-1} + \sqrt{\frac{\log(2/\delta)}{2}} \right). \end{aligned}$$

Therefore, considering $\hat{\mathbf{A}}$ and $\tilde{\mathbf{A}}$ as the solution to the dual problems corresponding to the empirical and underlying cases, for any $\delta > 0$ with a probability at least $1 - \delta/2$

$$\begin{aligned} \mathbb{E}_{\hat{P}} [F_{\theta}(\hat{\mathbf{A}}\mathbf{X}) - \theta(Y)^T \hat{\mathbf{A}}\mathbf{X}] + \sum_{i=1}^t \epsilon_i \|\hat{\mathbf{A}}_i\|_q & \quad (66) \\ -\mathbb{E}_{\hat{P}_n} [F_{\theta}(\hat{\mathbf{A}}\mathbf{X}) - \theta(Y)^T \hat{\mathbf{A}}\mathbf{X}] - \sum_{i=1}^t \epsilon_i \|\hat{\mathbf{A}}_i\|_q & \leq \frac{4BLM}{\sqrt{n}} \sum_{i=1}^t \frac{1}{\epsilon_i} \left(\sqrt{2(p-1)} + \sqrt{\frac{\log(4/\delta)}{2}} \right). \end{aligned}$$

Since $\hat{\mathbf{A}}$ is minimizing the objective for $Q = \hat{P}_n$,

$$\begin{aligned} \mathbb{E}_{\hat{P}_n} [F_{\theta}(\hat{\mathbf{A}}\mathbf{X}) - \theta(Y)^T \hat{\mathbf{A}}\mathbf{X}] + \sum_{i=1}^t \epsilon_i \|\hat{\mathbf{A}}_i\|_q & \quad (67) \\ -\mathbb{E}_{\hat{P}_n} [F_{\theta}(\tilde{\mathbf{A}}\mathbf{X}) - \theta(Y)^T \tilde{\mathbf{A}}\mathbf{X}] - \sum_{i=1}^t \epsilon_i \|\tilde{\mathbf{A}}_i\|_q & \leq 0. \end{aligned}$$

Also, since $\tilde{\mathbf{A}}$ does not depend on the samples, the Hoeffding's inequality implies that with a probability at least $1 - \delta/2$

$$\begin{aligned} \mathbb{E}_{\hat{P}_n} [F_{\theta}(\tilde{\mathbf{A}}\mathbf{X}) - \theta(Y)^T \tilde{\mathbf{A}}\mathbf{X}] + \sum_{i=1}^t \epsilon_i \|\tilde{\mathbf{A}}_i\|_q & \quad (68) \\ -\mathbb{E}_{\hat{P}} [F_{\theta}(\tilde{\mathbf{A}}\mathbf{X}) - \theta(Y)^T \tilde{\mathbf{A}}\mathbf{X}] - \sum_{i=1}^t \epsilon_i \|\tilde{\mathbf{A}}_i\|_q & \leq \sum_{i=1}^t \frac{2BML}{\epsilon_i} \sqrt{\frac{\log(4/\delta)}{2n}}. \end{aligned}$$

Applying the union bound, combining (66), (67), (68) shows that with a probability at least $1 - \delta$, we have

$$\begin{aligned} \mathbb{E}_{\hat{P}} [F_{\theta}(\hat{\mathbf{A}}\mathbf{X}) - \theta(Y)^T \hat{\mathbf{A}}\mathbf{X}] + \sum_{i=1}^t \epsilon_i \|\hat{\mathbf{A}}_i\|_q & \quad (69) \\ -\mathbb{E}_{\hat{P}} [F_{\theta}(\tilde{\mathbf{A}}\mathbf{X}) - \theta(Y)^T \tilde{\mathbf{A}}\mathbf{X}] - \sum_{i=1}^t \epsilon_i \|\tilde{\mathbf{A}}_i\|_q & \leq \sum_{i=1}^t \frac{4BLM}{\epsilon_i \sqrt{n}} \left(\sqrt{2(p-1)} + \frac{3}{2} \sqrt{\frac{\log(4/\delta)}{2}} \right). \end{aligned}$$

Given (61) and (69), the proof is complete. Note that we can improve the result in the case $q = 1$ by using the same proof and plugging in the Rademacher complexity of the ℓ_1 -bounded linear functions. Here we only replace $\sqrt{2(p-1)}$ in the above bound with $\sqrt{4 \log(2d)}$.

7.4 0-1 Loss: maximum entropy machine

7.4.1 F_{θ} derivation

Given the defined one-hot encoding θ we define $\tilde{\mathbf{z}} = (\mathbf{z}, 0)$ and represent each randomized decision rule ζ with its corresponding loss vector $\mathbf{L} \in \mathbb{R}^{t+1}$ such that $L_i = L_{0-1}(i, \zeta)$ denotes the 0-1 loss suffered by ζ when $Y = i$. It can be seen that \mathbf{L} is a feasible loss vector if and only if $\forall i : 0 \leq L_i \leq 1$ and $\sum_{i=1}^{t+1} L_i = t$. Then,

$$F_{\theta}(\mathbf{z}) = \max_{\substack{\mathbf{p} \in \mathbb{R}^{t+1}; \mathbf{1}^T \mathbf{p} = 1, \\ \forall i: 0 \leq p_i}} \min_{\substack{\mathbf{L} \in \mathbb{R}^{t+1}; \mathbf{1}^T \mathbf{L} = t, \\ \forall i: 0 \leq L_i \leq 1}} \sum_{i=1}^{t+1} p_i (\tilde{z}_i + L_i). \quad (70)$$

Hence, Sion's minimax theorem implies that the above minimax problem has a saddle point. Thus,

$$F_{\theta}(\mathbf{z}) = \min_{\substack{\mathbf{L} \in \mathbb{R}^{t+1}, \mathbf{1}^T \mathbf{L} = t, \\ \forall i: 0 \leq L_i \leq 1}} \max_{1 \leq i \leq t+1} \{\tilde{z}_i + L_i\}. \quad (71)$$

Consider σ as the permutation sorting $\tilde{\mathbf{z}}$ in a descending order and for simplicity let $\tilde{z}_{(i)} = \tilde{z}_{\sigma(i)}$. Then,

$$\forall 1 \leq k \leq t+1: \quad \max_{1 \leq i \leq t+1} \{\tilde{z}_i + L_i\} \geq \frac{1}{k} \sum_{i=1}^k [\tilde{z}_{\sigma(i)} + L_{\sigma(i)}] \geq \frac{k-1 + \sum_{i=1}^k \tilde{z}_{(i)}}{k}, \quad (72)$$

which is independent of the value of L_i 's. Therefore,

$$\max_{1 \leq k \leq t+1} \frac{k-1 + \sum_{i=1}^k \tilde{z}_{(i)}}{k} \leq F_{\theta}(\mathbf{z}). \quad (73)$$

On the other hand, if we let k_{\max} be the largest index satisfying $\sum_{i=1}^{k_{\max}} [\tilde{z}_{(i)} - \tilde{z}_{(k_{\max})}] < 1$ and define

$$\forall 1 \leq j \leq t+1: \quad L_{\sigma(j)}^* = \begin{cases} \frac{k_{\max} - 1 + \sum_{i=1}^{k_{\max}} \tilde{z}_{(i)}}{k_{\max}} - \tilde{z}_{(j)} & \text{if } \sigma(j) \leq k_{\max} \\ 1 & \text{if } \sigma(j) > k_{\max}, \end{cases} \quad (74)$$

we can simply check that \mathbf{L}^* is a feasible point since $\sum_{i=1}^{t+1} L_i^* = t$ and $L_{\sigma(k_{\max})}^* \leq 1$ so for all i 's $L_{\sigma(i)}^* \leq 1$. Also, $L_{\sigma(1)}^* \geq 0$ because $\tilde{z}_{(1)} - \tilde{z}_{(j)} < 1$ for any $j \leq k_{\max}$, so for all i 's $L_{\sigma(i)}^* \geq 0$. Then for this \mathbf{L}^* we have

$$F_{\theta}(\mathbf{z}) \leq \max_{1 \leq i \leq t+1} \{\tilde{z}_i + L_i^*\} = \frac{k_{\max} - 1 + \sum_{i=1}^{k_{\max}} \tilde{z}_{(i)}}{k_{\max}}. \quad (75)$$

Therefore, (73) holds with equality and achieves its maximum at $k = k_{\max}$,

$$F_{\theta}(\mathbf{z}) = \max_{1 \leq k \leq t+1} \frac{k-1 + \sum_{i=1}^k \tilde{z}_{(i)}}{k} = \frac{k_{\max} - 1 + \sum_{i=1}^{k_{\max}} \tilde{z}_{(i)}}{k_{\max}}. \quad (76)$$

Moreover, \mathbf{L}^* corresponds to a randomized robust Bayes act, where we select label i according to the probability vector $\mathbf{p}^* = \mathbf{1} - \mathbf{L}^*$ that is

$$\forall 1 \leq j \leq t+1: \quad p_{\sigma(j)}^* = \begin{cases} \frac{1 - \sum_{i=1}^{k_{\max}} \tilde{z}_{(i)}}{k_{\max}} + \tilde{z}_{(j)} & \text{if } \sigma(j) \leq k_{\max} \\ 0 & \text{if } \sigma(j) > k_{\max}. \end{cases} \quad (77)$$

Given F_{θ} we can simply derive the gradient ∇F_{θ} to find the entropy maximizing distribution. Here if the inequality $\sum_{i=1}^{k_{\max}} [\tilde{z}_{\sigma(i)} - \tilde{z}_{(k_{\max}+1)}] \geq 1$ holds strictly, which is true almost everywhere on \mathbb{R}^t ,

$$\forall 1 \leq i \leq t: \quad (\nabla F_{\theta}(\mathbf{z}))_i = \begin{cases} 1/k_{\max} & \text{if } \sigma(i) \leq k_{\max}, \\ 0 & \text{Otherwise.} \end{cases} \quad (78)$$

If the inequality does not strictly hold, F_{θ} is not differentiable at \mathbf{z} ; however, the above vector still lies in the subgradient $\partial F_{\theta}(\mathbf{z})$.

7.4.2 Sufficient Conditions for Applying Theorem 1.a

As supposed in Theorem 1.a, the space \mathcal{X} should be finite in order to apply that result. Here, we show for the proposed structure on $\Gamma(Q)$ one can relax this condition while Theorem 1.a still holds. It is

because, as shown in the proofs of Theorems 2 and 3, we have

$$\begin{aligned}
\inf_{\psi \in \Psi} \max_{P \in \Gamma(\tilde{P})} \mathbb{E}[L(Y, \psi(\mathbf{X}))] &= \inf_{\psi \in \Psi} \min_{\mathbf{A}} \mathbb{E}_{\tilde{P}_{\mathbf{X}}} \left[\sup_{P_{Y|\mathbf{X}} \in \mathcal{P}_{\mathcal{Y}}} \mathbb{E}[L(Y, \psi(\mathbf{X})) | \mathbf{X} = \mathbf{x}] \right. \\
&\quad \left. + \mathbb{E}[\boldsymbol{\theta}(Y) | \mathbf{X} = \mathbf{x}]^T \mathbf{A} \mathbf{X} \right] - \mathbb{E}_{\tilde{P}}[\boldsymbol{\theta}(Y)^T \mathbf{A} \mathbf{X}] + \sum_{i=1}^t \epsilon_i \|\mathbf{A}_i\|_* \\
&= \min_{\mathbf{A}} \mathbb{E}_{\tilde{P}_{\mathbf{X}}} \left[\inf_{\psi(\mathbf{x}) \in \mathcal{Z}} \sup_{P_{Y|\mathbf{X}} \in \mathcal{P}_{\mathcal{Y}}} \mathbb{E}[L(Y, \psi(\mathbf{x})) | \mathbf{X} = \mathbf{x}] \right. \\
&\quad \left. + \mathbb{E}[\boldsymbol{\theta}(Y) | \mathbf{X} = \mathbf{x}]^T \mathbf{A} \mathbf{X} \right] - \mathbb{E}_{\tilde{P}}[\boldsymbol{\theta}(Y)^T \mathbf{A} \mathbf{X}] + \sum_{i=1}^t \epsilon_i \|\mathbf{A}_i\|_*.
\end{aligned}$$

Therefore, given this structure the minimax problem decouples across different \mathbf{x} 's. Hence, the assumption of finite \mathcal{X} is no longer needed, because as long as $\boldsymbol{\theta}$ is a bounded function (which is true for the one-hot encoding $\boldsymbol{\theta}$), the rest of assumptions suffice to guarantee the existence of a saddle point given $\mathbf{X} = \mathbf{x}$ for any \mathbf{x} .

7.5 Quadratic Loss: Linear Regression

7.5.1 $F_{\boldsymbol{\theta}}$ derivation

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

$$F_{\boldsymbol{\theta}}(z) = \max_{\mathbb{E}[Y^2] \leq \rho^2} \mathbb{E}[Y^2] - \mathbb{E}[Y]^2 + z\mathbb{E}[Y] \quad (79)$$

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

$$F_{\boldsymbol{\theta}}(z) = \max_{|\mathbb{E}[Y]| \leq \rho} \rho^2 - \mathbb{E}[Y]^2 + z\mathbb{E}[Y] = \begin{cases} \rho^2 + z^2/4 & \text{if } |z/2| \leq \rho \\ \rho|z| & \text{if } |z/2| > \rho. \end{cases} \quad (80)$$

7.5.2 Applying Theorem 2 while restricting $\mathcal{P}_{\mathcal{Y}}$

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

$$\max_{\substack{P: P_{\mathbf{X}, Y} \in \Gamma(Q) \\ \forall \mathbf{x}: P_{Y|\mathbf{X}=\mathbf{x}} \in \mathcal{P}_{\mathcal{Y}}}} H(Y|\mathbf{X}) \quad (81)$$

In the case $\mathcal{P}_{\mathcal{Y}} = \{P_Y : \mathbb{E}[Y^2] \leq \rho^2\}$ Theorem 2 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 is still convex and strong duality holds as well. Also, when we move the constraints of $\mathbf{w}_i = \mathbb{E}_P[\boldsymbol{\theta}_i(Y)\mathbf{X}]$ to the objective function, we get a similar dual problem

$$\min_{\mathbf{A}} \sup_{\substack{P_{Y|\mathbf{X}, \mathbf{w}} \\ \forall \mathbf{x}: P_{Y|\mathbf{X}=\mathbf{x}} \in \mathcal{P}_{\mathcal{Y}}}} \mathbb{E}_{Q_{\mathbf{X}}} \left[H_P(Y|\mathbf{X} = \mathbf{x}) + \sum_{i=1}^t \mathbb{E}[\boldsymbol{\theta}_i(Y) | \mathbf{X} = \mathbf{x}] \mathbf{A}_i \mathbf{X} \right] + \sum_{i=1}^t [I_{C_i}(\mathbf{w}_i) - \mathbf{A}_i \mathbf{w}_i] \quad (82)$$

Following the next steps of the proof of Theorem 2, we complete the proof assuming the modification on $F_{\boldsymbol{\theta}}$ and the maximum conditional entropy problem.

7.5.3 Derivation of group lasso

To derive the group lasso problem, we slightly change the structure of $\Gamma(Q)$. First assume the subsets I_1, \dots, I_k are disjoint. Consider a set of distributions $\Gamma_{\text{GL}}(Q)$ with the following structure

$$\Gamma_{\text{GL}}(Q) = \{ P_{\mathbf{X}, Y} : P_{\mathbf{X}} = Q_{\mathbf{X}}, \quad (83) \\ \forall 1 \leq j \leq k : \|\mathbb{E}_P[Y\mathbf{X}_{I_j}] - \mathbb{E}_Q[Y\mathbf{X}_{I_j}]\| \leq \epsilon_j \}.$$

Now we prove a modified version of Theorem 2,

$$\max_{P \in \Gamma_{\text{GL}}(Q)} H(Y|\mathbf{X}) = \min_{\boldsymbol{\alpha}} \mathbb{E}_Q [F_{\theta}(\boldsymbol{\alpha}^T \mathbf{X}) - Y \boldsymbol{\alpha}^T \mathbf{X}] + \sum_{j=1}^k \epsilon_j \|\boldsymbol{\alpha}_{I_j}\|_*. \quad (84)$$

To prove this identity, we can use the same proof provided for Theorem 2. We only need to redefine $\tilde{\mathbf{E}}_j = \mathbb{E}_Q [Y \mathbf{X}_{I_j}]$ and $C_j = \{\mathbf{u} : \|\mathbf{u} - \tilde{\mathbf{E}}_j\| \leq \epsilon_j\}$ for $1 \leq j \leq k$. Notice that here $t = 1$. Using the same technique in that proof, the dual problem can be formulated as

$$\min_{\boldsymbol{\alpha}} \sup_{P_{Y|\mathbf{X}, \mathbf{w}}} \mathbb{E}_{Q_{\mathbf{X}}} [H_P(Y|\mathbf{X} = \mathbf{x}) + \mathbb{E}[Y|\mathbf{X} = \mathbf{x}] \boldsymbol{\alpha}^T \mathbf{X}] + \sum_{j=1}^k [I_{C_j}(\mathbf{w}_{I_j}) - \boldsymbol{\alpha}_{I_j} \mathbf{w}_{I_j}]. \quad (85)$$

Similarly, we can decouple and simplify the above problem to derive the RHS of (84). Then, if we let $\|\cdot\|$ be the ℓ_q -norm, we will get the group lasso problem with the $\ell_{1,p}$ regularizer.

If the subsets are not disjoint, we can create new copies of each feature corresponding to a repeated index, such that there will be no repeated indices after adding the new features. Note that since $P_{\mathbf{X}}$ has been fixed over $\Gamma_{\text{GL}}(Q)$ adding the extra copies of original features does not change the maximum-conditional entropy problem. Hence, we can use the result proven for the disjoint case and derive the overlapping group lasso problem.