Optimally Combining Classifiers Using Unlabeled Data

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Abstract

We develop a worst-case analysis of aggregation of classifier ensembles for binary classification. The task of predicting to minimize error is formulated as a game played over a given set of unlabeled data (a transductive setting), where prior label information is encoded as constraints on the game. The minimax solution of this game identifies cases where a weighted combination of the classifiers can perform significantly better than any single classifier.

1 Introduction

Suppose that we have a finite set, or ensemble, of binary classifiers $H = \{h_1, h_2, \ldots, h_p\}$, with each $h_i$ mapping data in some space $X$ to a binary prediction $\{-1, +1\}$. Examples $(x, y) \in X \times \{-1, +1\}$ are generated i.i.d. according to some fixed but unknown distribution $D$ – write the expectation with respect to $D$ or one of its marginal distributions as $E_D[\cdot]$.

Consider a statistical learning setting, in which we assume access to two types of i.i.d. data: a small set of training examples $S = \{(x'_1, y'_1), \ldots, (x'_m, y'_m)\}$ drawn from $D$ and a much larger set of unlabeled test examples $T = \{x_1, \ldots, x_n\}$ drawn i.i.d. according to the marginal distribution over $X$ induced by $D$. A typical use of the labeled set is to find an upper bound on the expected error rate for each of the classifiers. Specifically, we assume a set of lower bounds $\{b_i > 0\}_{i=1}^p$ such that the correlation $\text{corr}(h) := E_D[ yh(x) ]$ satisfies $\text{corr}(h) \geq b_i$.

If we ignore the test set, then the best we can do, in the worst case, is use the classifier with the largest correlation (smallest error). This corresponds to the common practice of Empirical Risk Minimization (ERM). However, in many cases we can glean useful information from the distribution of the test set that will allow us to greatly improve over ERM.

We motivate this statement by contrasting two simple cases, A and B. In both cases there are $p = 3$ classifiers and $n = 3$ unlabeled test examples. The correlation vector is $(\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$; equivalently, the classifier error rates are $33\%$. Based on that information the predictor knows that each classifier makes two correct predictions and one incorrect prediction.

So far, both cases are the same. The difference is in the relations between different predictions on the same example. In case A, each example has two predictions that are the same, and a third that is different. In this case it is apparent that the majority vote over the three classifiers has to be correct on all 3 examples, i.e. we can reduce the error from $\frac{1}{3}$ to $0$. In case B, all three predictions are equal for all examples. In other words, the three classification rules are equal on the three examples. In this case, there is no way to improve over the single rules.

These cases show that there is information in the unlabeled test examples that can be used to reduce error. In this paper, we give a complete characterization of the minimax predictions given the correlation vector $b$ and the unlabeled test examples.

Our development does not consider the instance space $X$ directly, but instead models the knowledge of the $p$ ensemble predictions on $T$ with a $p \times n$ matrix that we denote by $F$. Our focus is on how to use the matrix $F$ in conjunction with the correlation vector $b$, to make the minimax optimal predictions on the test examples.

The rest of the paper is organized as follows. In Section 2 we introduce some additional notation. In Section 3 we define the game between the predictor and nature and solve it, characterizing the minimax strategies for both sides by minimizing a convex objective we call the slack function. After linking the game to statistical learning in Section 4 in Section 5 we give some interpretation of the slack function and the minimax strategies. In Section 6 we focus
on computational issues in computing the minimax strategy. After discussing relations to other work in Section 7, we conclude in Section 8.

## 2 Preliminaries

The main tools we use in this paper are linear programming and uniform convergence. We therefore use a combination of matrix notation and probabilistic notation. The probabilistic notation was given in the introduction. The algorithm is described in a deterministic context where some inequalities are assumed to hold; probabilistic arguments are used to show that these assumptions are correct with high probability.

The ensemble’s predictions on the unlabeled data are denoted by $F$:

$$
F = \begin{pmatrix}
  h_1(x_1) & h_2(x_2) & \cdots & h_1(x_n) \\
  h_2(x_1) & h_2(x_2) & \cdots & h_2(x_n) \\
  \vdots & \vdots & \ddots & \vdots \\
  h_p(x_1) & h_p(x_2) & \cdots & h_p(x_n)
\end{pmatrix} \in [-1, +1]^{p \times n}
$$

(1)

Note that we allow $F$, as well as other variables defined below, to take any value in the range $[-1, +1]$ rather than just the two endpoints. This relaxation does not change the analysis, because intermediate values can be interpreted as the expected value of randomized predictions. For example, a value of $\frac{1}{2}$ indicates $\{+1$ w.p. $\frac{1}{2}, \ -1$ w.p. $\frac{1}{2}\}$. This interpretation extends to our definition of the empirical correlation on the test set, $\text{corr}(h) = \frac{1}{n} \sum_{i=1}^{n} h(x_i) y_i$.

We use vector notation for the rows and columns of $F$: $h_i = (h_i(x_1), h_i(x_2), \cdots, h_i(x_n))$ and $x_j = (h_1(x_j), h_2(x_j), \cdots, h_p(x_j))^\top$.

The true labels on the test data $T$ are represented by $z = (z_1; \ldots; z_n) \in [-1, 1]^n$. The labels $z$ are hidden from the predictor, but we assume the predictor has knowledge of a correlation vector $b \succeq 0^n$ such that $\frac{1}{n} \sum_{j} h_i(x_j) z_j \geq b_i$, i.e. $\frac{1}{n} F z \succeq b$.

We establish the following notation: $[a]_+ = \max(0, a)$ and $[a]_- = [-a]_+$, $[n] = \{1, 2, \ldots, n\}$, $1^n = (1; 1; \ldots; 1)$, and $0^n$ similarly. Also, write $I_n$ as the $n \times n$ identity matrix. All vector inequalities are componentwise.

The probability simplex in $d$ dimensions is denoted by $\Delta^d = \{ x \succeq 0^d : \sum_{i=1}^{d} x_i = 1 \}$.

## 3 The Transductive Binary Classification Game

We now describe our prediction problem, and formulate it as a two-player zero-sum game between a predictor and nature.

In this game, the predictor is the first player, who plays $g = (g_1; g_2; \ldots; g_n)$, a randomized label $g_i \in [-1, 1]$ for each example $\{x_i\}_{i=1}^{n}$. Nature then plays adversarially, setting the labels $z \in [-1, 1]^n$ under ensemble error constraints defined by $b$. The predictor’s goal is to minimize (and Nature’s to maximize) the worst-case expected classification error on the test data (w.r.t. the randomized labelings $z$ and $g$): $\frac{1}{2} (1 - \frac{1}{n} z^\top g)$. This is equivalently viewed as maximizing worst-case correlation $\frac{1}{n} z^\top g$.

To summarize concretely, we study the following game:

$$
V = \max_{g \in [-1, 1]^n} \min_{z \in [-1, 1]^n, \frac{1}{n} F z \succeq b} \frac{1}{n} z^\top g
$$

(2)

It is important to note that we are only modeling “test-time” prediction, and represent the information gleaned from the labeled data by the parameter $b$. Inferring the vector $b$ from training data is a standard application of Occam’s Razor, which we provide in Section 4.

\footnote{We are slightly abusing the term “correlation” here. Strictly speaking this is the expected value of the product without subtracting means and dividing by the product of the standard deviations. We prefer this to inventing a new term.}
Figure 1: The optimal strategies and slack function as a function of the ensemble prediction $x^\top \sigma^\ast$.

The minimax theorem (e.g. [CBL06], Theorem 7.1) applies to the game (2), since the constraint sets are convex and compact and the payoff linear. Therefore, it has a minimax equilibrium and associated optimal strategies $g^\ast, z^\ast$ for the two sides of the game, i.e. $\min_g \frac{1}{n} z^\top g^\ast = V = \max_g \frac{1}{n} z^\ast g$.

As we will show, both optimal strategies are simple functions of a particular weighting over the $p$ hypotheses – a nonnegative $p$-vector. Define this weighting as follows.

**Definition 1 (Slack Function).** Let $\sigma \geq 0^p$ be a weight vector over $H$ (not necessarily a distribution). The vector of ensemble predictions is $F^\top \sigma = (x_1^\top \sigma, \ldots, x_n^\top \sigma)$, whose elements' magnitudes are the margins. The prediction slack function is

$$\gamma(\sigma, b) = \gamma(\sigma) = \frac{1}{n} \sum_{j=1}^{n} [\left|x_j^\top \sigma\right| - 1]_+ - b^\top \sigma \quad (3)$$

**Definition 2 (Optimal Weight Vector).** The optimal weight vector $\sigma^\ast$ is any minimizer of the slack function: $\sigma^\ast \in \arg\min_{\sigma \geq 0^p} [\gamma(\sigma)]$.

Our main result uses these to describe the minimax equilibrium of the game (2).

**Theorem 3 (Solution of the Game).** The minimax value of the game (2) is $V = -\gamma(\sigma^\ast)$. The minimax optimal strategies are defined as follows: for all $i \in [n],$

$$g_i^\ast = g_i(\sigma^\ast) = \begin{cases} x_i^\top \sigma^\ast & \text{if } \left|x_i^\top \sigma\right| < 1 \\ \text{sgn}(x_i^\top \sigma^\ast) & \text{otherwise} \end{cases} \quad \text{and} \quad z_i^\ast = \begin{cases} 0 & \left|x_i^\top \sigma\right| < 1 \\ \text{sgn}(x_i^\top \sigma^\ast) & \left|x_i^\top \sigma\right| > 1 \end{cases} \quad (4)$$

The proof of this theorem involves linear program analysis. The minimax value of the game (proved in Lemma 8) and the optimal strategy for the predictor $g^\ast$ (Lemma 10) are our main objects of study and are completely characterized, and the theorem’s partial description of $z^\ast$ (proved in Lemma 9) will suffice for our purposes.

Theorem 3 illuminates the importance of the optimal weighting $\sigma^\ast$ over hypotheses. This weighting $\sigma^\ast \in \arg\min_{\sigma \geq 0^p} [\gamma(\sigma)]$ is the solution to a convex optimization problem (Lemma 13), and therefore we can efficiently compute it and $g^\ast$ to any desired accuracy. The ensemble prediction (w.r.t. this weighting) on the test set is $F^\top \sigma^\ast$, which is the only dependence of the optimal solution on $F$. More specifically, the minimax optimal prediction/label (4) on any test set example $x_j$ can be expressed as a function of the ensemble prediction $x_j^\top \sigma^\ast$. These functions are depicted in Figure 1.

\footnote{For completeness, Corollary 12 in the appendices specifies $z_i^\ast$ when $\left|x_i^\top \sigma\right| = 1$.}
4 Bounding the Correlation Vector

In the analysis presented above we assumed that a correlation vector $\mathbf{b}$ is given and that it is guaranteed to be a lower bound on the true correlations on the test set. In this section we analyze how $\mathbf{b}$ can be calculated from a labeled training set.

The algorithm that we use is the natural one: we compute the empirical correlation for the $p$ classifiers and add a uniform penalty term to guarantee that the $\mathbf{b}$ is a lower bound on the correlation of the test data.

For each classifier, we have three quantities to consider:
- The true correlation: $\text{corr}(h) = \mathbb{E}_D [y h(x)]$
- The correlation on the training set: $\hat{\text{corr}}_{\text{trn}}(h) = \frac{1}{m} \sum_{i=1}^{m} h(x_i') y_i'$
- The correlation on the test set: $\hat{\text{corr}}_{\text{tst}}(h) = \frac{1}{n} \sum_{i=1}^{n} h(x_i) y_i$

Using Chernoff bounds, we can bound the probability that each of the empirical correlations is $\epsilon$ far from the true correlation. For each individual classifier we have the inequalities

\[
\begin{align*}
\Pr (\hat{\text{corr}}_{\text{trn}} > \text{corr}(h) + \epsilon_{\text{trn}}) & \leq e^{-2m\epsilon^2} \\
\Pr (\hat{\text{corr}}_{\text{tst}} < \text{corr}(h) - \epsilon_{\text{tst}}) & \leq e^{-2n\epsilon^2}
\end{align*}
\]

Let $\delta$ denote the probability we allow for failure. If we set $\epsilon_{\text{trn}} = \sqrt{(\ln(p/\delta))/2m}$ and $\epsilon_{\text{tst}} = \sqrt{(\ln(p/\delta))/2n}$, we are guaranteed that all of the inequalities hold concurrently with probability at least $1 - \delta$.

We thus set the correlation bound to:

\[
b_i = \hat{\text{corr}}(h_i) - \sqrt{(\ln(p/\delta))/2m} - \sqrt{(\ln(p/\delta))/2n}
\]

and have that $\mathbf{b}$ is a good correlation vector with probability $1 - \delta$.

5 Discussion

Given $\sigma$, we partition the examples $\mathbf{x}$ into three subsets, depending on the value of the ensemble prediction: the hedged set $H(\sigma) := \{\mathbf{x} : |\mathbf{x}^\top \sigma| < 1\}$, the clipped set $C(\sigma) := \{\mathbf{x} : |\mathbf{x}^\top \sigma| > 1\}$, and the borderline set $B(\sigma) \triangleq \{\mathbf{x} : |\mathbf{x}^\top \sigma| = 1\}$. Using these sets, we now give some intuition regarding the optimal choice of $g$ and $z$ given in $[4]$, for some fixed $\sigma$.

Consider first examples $\mathbf{x}$ in $H(\sigma)$. The optimal strategy for the predictor is to predict with the ensemble average $\mathbf{x}^\top \sigma$, which is a number between $-1$ and $+1$. Making such an intermediate prediction might seem to be a type of calibration, but this view is misleading. The optimal strategy for the adversary in this case is to set $z_i = 0$, equivalent to predicting $\pm 1$ with probability $1/2$ each. The reason that the learner hedges is because if $g < \mathbf{x}^\top \sigma$, the adversary would respond with $z = 1$ and with $z = -1$ if $g > \mathbf{x}^\top \sigma$. In either case, the loss of the predictor would increase. In other words, our ultimate rationale for hedging is not calibration, but rather “defensive forecasting” in the spirit of $[\text{VTS05}]$.

Next we consider the clipped set $\mathbf{x} \in C(\sigma)$. In this case, Nature’s optimal strategy is to predict deterministically, and so the learner matches Nature. It is interesting to note that with all else held equal, increasing the margin $|\mathbf{x}_j^\top \sigma|$ beyond 1 is sub-optimal for the learner. Qualitatively, the reason is that while $\mathbf{x}_j^\top \sigma$ continues to increase, the prediction for the learner is clipped, and so the value for the learner does not increase with the ensemble prediction.

5.1 Subgradient Conditions

For another perspective on the result of Theorem $[3]$ consider the subdifferential set of the slack function $\gamma$ at an arbitrary weighting $\sigma$:

\[
\partial \gamma(\sigma) = \left\{ \frac{1}{n} \left( \sum_{\mathbf{x}_j \in C(\sigma)} \mathbf{x}_j \text{sgn}(\mathbf{x}_j^\top \sigma) + \sum_{\mathbf{x}_j \in B(\sigma)} c_j \mathbf{x}_j \text{sgn}(\mathbf{x}_j^\top \sigma) \right) - \mathbf{b}, \quad \forall c_j \in [0,1] \right\}
\]
Note that the hedged set plays no role in the gradient. Since the slack function $\gamma(\cdot)$ is convex (Lemma 13), the sub-differential set (5) at any $\sigma^*$ contains $\vec{0}$, i.e.,

$$\exists c_j \in [0, 1] \text{ s.t. } n b - \sum_{j: x_j^T \sigma^* > 1} x_j + \sum_{j: x_j^T \sigma^* < -1} x_j = \sum_{j: |x_j^T \sigma^*| = 1} c_j x_j \text{ sgn}(x_j^T \sigma^*)$$

The geometric interpretation of this equation is given in Figure 5.1. The optimal weighting $\sigma^*$ partitions the examples into five sets: hedged, positive borderline and positive clipped, and negative borderline and negative clipped. Taking the difference between the sum of the positive clipped and the sum of the negative clipped examples gives a vector that is approximately $b$. By adding a weighted sum of the borderline examples, $b$ can be obtained exactly.

### 5.2 Better than ERM Without Clipping

We now make some simple observations about the minimax solution.

First, note that no $\sigma$ such that $\|\sigma\|_1 < 1$ can be optimal, because in such a case $-\gamma(\sigma) > -\gamma\left(\frac{\sigma}{\|\sigma\|_1}\right)$; therefore, $\|\sigma^*\|_1 \geq 1$.

Consider next a situation where we do not know the matrix $F$. Then $\|\sigma^*\|_1 = 1$. This can be shown by proving the contra-positive; assume the negation $\|\sigma^*\|_1 > 1$. Then there exists a vector $x \in [-1, +1]^p$ such that $x^T \sigma^* = \|\sigma^*\|_1 > 1$. If each of the columns of $F$ is equal to $x$, then $\sigma^*$ cannot be optimal since $-\gamma\left(\frac{\sigma^*}{a}\right) > -\gamma(\sigma^*)$.

In other words, if we want to protect ourselves against the worst case $F$, then we have to set $\|\sigma\|_1 = 1$ so as to ensure that $C(\sigma)$ is empty. In this case, the slack function simplifies to $\gamma(\sigma) = -b^T \sigma$, over the probability simplex. Minimizing this is achieved by setting $\sigma_i$ to be $1$ at $\arg \max \sigma_i$ and zero elsewhere. As might be expected, in the case that $F$ is unknown, the optimal strategy is to use the classifier with the minimal error guarantee.

This is because $C(\sigma^*)$ is empty, and the set of all $\sigma$ such that this is true is of wider interest. We name it the Zero Box Region: $\text{ZBR} = \{\sigma : C(\sigma) = 0\}$. Another clean characterization of the ZBR can be made by using a duality argument similar to that used to prove Theorem 3.

**Theorem 4.** The best weighting in ZBR satisfies

$$\max_{\substack{|F^T \sigma| \leq 1^n, \\ \sigma \geq 0^p}} b^T \sigma = \max_{g \in [-1, 1]^n} \min_{\frac{1}{n} P z \geq b} \frac{1}{n} z^T g.$$
lar, the optimal $\sigma^* \in \text{ZBR}$ if and only if the hypercube constraint $z \in [-1,1]^n$ is superfluous, i.e. when $V = \min_{\frac{1}{n} F z \geq b} \max_{g \in [-1,1]^n} \frac{1}{n} z^\top g$.

The ZBR is where the optimal strategy is always to hedge and never to incorporate any clipping. Consider a situation in which the solution is in ZBR, $\sigma^* = 1^p$, and all of the predictions are binary: $F \in \{-1, +1\}^{p \times n}$. This is an ideal case for our method; instead of the baseline value $\max_i b_i$ obtained when $F$ is unknown, we get a superior value of $\sum_i b_i$.

In fact, we referred to such a case in the introduction, and we will present a formal version here. Take $F$ in $\sigma$-classifiers for a fixed $F$ in $\sigma$-classifiers has led to a $p$-fold improvement over random guessing.

Of course, this particular case is extremal in some ways; in order to be in ZBR, there must be many cancellations of independent label noise on example $i$. Indeed, by definition of $g(\sigma)$, the slack function value $-\gamma(\sigma) = b^\top \sigma - \frac{1}{n} \|F^\top \sigma - g(\sigma)\|_1 \leq \max_{\sigma^* \geq 0} \left[ b^\top \sigma^* - \frac{1}{n} \|F^\top \sigma^* - g(\sigma)\|_1 \right]$, which is simply the dual problem (Lemma 11) of the worst-case correlation suffered by $g(\sigma)$: $
abla_{z \in [-1,1]^n, \frac{1}{n} F z \geq b} \frac{1}{n} z^\top [g(\sigma)]$. We now state this formally.

**Observation 5.** For any weight vector $\sigma \geq 0^p$, the worst-case correlation after playing $g(\sigma)$ is bounded by

$$\min_{z \in [-1,1]^n, \frac{1}{n} F z \geq b} \frac{1}{n} z^\top [g(\sigma)] \geq -\gamma(\sigma)$$

**5.3 Independent Label Noise**

An interesting variation on the game is to limit the adversary to $z_i \in [-\alpha_i, \alpha_i]^n$ for some $\bar{\sigma} = (\alpha_1, \ldots, \alpha_n) \in [0, 1]^n$. This corresponds to assuming a level $1 - \alpha_i$ of independent label noise on example $i$: the adversary is not allowed to set the label deterministically, but is forced to flip example $i$’s label independently with probability $\frac{1}{2} (1 - \alpha_i)$.

Solving the game in this case gives the result (proof in appendices) that if we know some of the ensemble’s errors to be through random noise, then we can find a weight vector $\sigma$ that would give us better performance than without such information.

**Proposition 6** (Independent Label Noise).

$$\max_{g \in [-1,1]^n} \min_{-\bar{\sigma} \leq z \leq \bar{\sigma}} \frac{1}{n} z^\top g = \max_{\sigma \geq 0^p} \frac{1}{n} \sum_{j=1}^n \alpha_j \left[ |x_j^\top \sigma| - 1 \right]_+ > \max_{\sigma \geq 0^p} [-\gamma(\sigma)] = V$$

Our prediction tends to clip – predict with the majority vote – more on examples with more known random noise, because it gains in minimax correlation by doing so. This mimics the Bayes-optimal classifier, which is always a majority vote.

Indeed, this statement’s generalization to the asymmetric-noise case can be understood with precisely the same intuition. The sign of the majority vote affects the clipping penalty in the same way:

\[\text{For instance, by setting } F_{ij} = 2 \times 1((i + j) \text{ is even}) - 1.\]
Proposition 7 (Asymmetric Label Noise). For some \( l, u \geq 0^n \),

\[
\max_{g \in \{-1,1\}^n} \min_{-\frac{1}{\gamma(x)} \leq u, \frac{1}{\gamma(x)} \geq b} \frac{1}{n} z^\top g = \max_{\sigma \geq 0^n} b^\top \sigma - \frac{1}{n} \sum_{j=1}^n \left( u_j [x_j^\top \sigma - 1]^+ + b_j [-x_j^\top \sigma - 1]^+ \right) > V
\]

6 Computational Issues

Theorem 3 makes clear that our ability to produce \( g^* \) is dependent on our ability to find the optimal weighting \( \sigma^* \), i.e. to minimize the slack function \( \gamma(\sigma) \) over \( \sigma \geq 0^n \). We discuss two extreme approaches to performing this minimization.

The most straightforward approach is to treat the problem as a linear programming problem and use an LP solver. The main problem with this approach is that it requires storing all of the examples in memory. As unlabeled examples are typically much more plentiful than labeled examples, this approach could be infeasible without further modification.

A different approach that exploits the structure of the equilibrium uses stochastic gradient descent. The fact that the slack function is convex guarantees that this approach will converge to the global minimum. The convergence rate might be suboptimal, particularly near the intersections of hyperplanes in the piecewise-linear slack function surface. But the fact that SGD is a constant-memory algorithm is very attractive. In fact, the entire arsenal of stochastic convex optimization comes into play theoretically and practically — the slack function is a sum of i.i.d. random variables. As such, it has a natural limiting object \( \mathbb{E}_{x \sim D} \left[ |x^\top \sigma| - 1 \right]^+ - b^\top \sigma \) amenable to standard optimization techniques.

7 Related Work

Our duality-based formulation would incorporate constraints far beyond the linear ones we have imposed so far, since all our results hold essentially without change in a general convex analysis context. Possible extensions in this vein include other loss functions as in multiclass and abstaining settings, specialist experts, and more discussed in the next section.

Weighted majority votes are a nontrivial ensemble aggregation method that has received focused theoretical attention for classification. Of particular note is the literature on boosting for forming ensembles, in which the classic work of [CBFH93] demonstrated this to result in optimal prediction error in the experts setting as well, and similar results have been shown in related settings ([Vov90, AP13]).

One class of philosophically related methods to ours uses moments of labeled data in the statistical learning setting to find a minimax optimal classifier; notably among linear separators ([LGBJ01]) and conditional label distributions under log loss ([IzLi04]). Our formulation instead uses only one such moment and focuses on unlabeled data, and is able to handle a rich class of dependence structure among classifier predictions, not just low-order moments.

There is also a long tradition of analyzing worst-case binary prediction of online sequences, from which we highlight [FMG92], which shows universal optimality for bit prediction of a piecewise linear function similar to Fig. 1. The work of [CBFH93] demonstrated this to result in optimal prediction error in the experts setting as well, and similar results have been shown in related settings ([Vov90, AP13]).

Our emphasis on the benefit of considering global effects (our transductive setting) even when data are i.i.d. is in the spirit of the idea of shrinkage estimators, well known in statistical literature since the James-Stein estimator ([EM77]).
8 Conclusions and Open Problems

In this paper we have shown a new way for utilizing unlabeled examples when combining an ensemble of classifiers. We show that in some cases the performance of the combined classifiers is guaranteed to be much better than that of any of the individual rules.

We have shown that the optimal solution is characterized by a convex function we call the slack function. Minimizing this slack function is computationally tractable, and can potentially be solved in a streaming model using stochastic gradient descent. The analysis introduces a margin similar to the one used in support vector machines. Curiously, the goal of the optimization problem is to minimize, rather than maximize, the number of examples with large margin.

Directions we are considering for future research include:

• Is there an algorithm that combines the convergence rate of the linear programming approach with the small memory requirements of SGD?

• In problems with high Bayes error, what is the best way to leverage the generalized algorithm which limits the adversary to a sub-interval of $[-1, +1]$?

• Can the algorithm and its analysis be extended to infinite concept classes?

• Allowing the classifiers to abstain can greatly increase the representational ability of the combination. Is there a systematic way to build and combine such “specialist” classifiers?
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A Proof of Theorem 3

We prove Theorem 3 in two steps. In Section A.1 we prove the equation for the minimax value of the game and in Section A.2 we prove the optimal strategies of the two sides.

A.1 Value of the Game

It is expedient to first calculate the value of the game, which we do through duality manipulations.

Lemma 8. The value of the game \((2)\) is \(V\), as defined in Theorem 3.

To prove this, apply the minimax theorem ([CBL06], Theorem 7.1) to \((2)\) to yield the minimax dual game:

\[
\min_{\frac{1}{n}Fz \geq b} \max_{\frac{1}{n}g \in [-1,1]^n} \frac{1}{n} z^T g = \min_{\frac{1}{n}Fz \geq b} \frac{1}{n} \|z\|_1
\]

We now rewrite the problem \((7)\) slightly to make duality manipulations more transparent.

Define \(c = \frac{1}{2}2^{n}, A = [F, -F; -I_{2n}] \in [-1, 1]^{(p+2n) \times 2n}, \) and \(B = [nb; -1^{2n}] \in \mathbb{R}^{p+2n}.\) This will allow us to reparametrize the problem in terms of \(\zeta = ([z_1]^+, \ldots, [z_n]^+, [z_1]^-, \ldots, [z_n]^-)\).

With these definitions, the problem \((7)\) becomes

\[
\min_{A\zeta \geq B, \zeta \geq 0} \frac{1}{n} c^T \zeta
\]

This is clearly a linear program (LP); its dual program, equal to it by strong duality (since we assume a feasible solution exists; [Van96]) is

\[
\max_{\lambda \geq 0, c \geq A^T \lambda} \frac{1}{n} B^T \lambda
\]

Denote the solutions to \((8)\) and \((9)\) as \(\zeta^*\) and \(\lambda^*\).

Suppose the first \(p\) and last \(2n\) coordinates of \(\lambda\) are \(\sigma\) and \(\lambda_-\) respectively, so that \(\lambda = [\sigma; \lambda_-].\) Now rewriting the constraint \(A^T \lambda \leq c\) in terms of these coordinates, \((9)\) becomes

\[
\max_{\sigma \geq 0^p, \lambda_- \geq 0^{2n}} \left[ b^T \sigma - \frac{1}{n} \|\lambda_-\|_1 \right] \quad \text{s.t.} \quad [F^T \sigma; -F^T \sigma] - \lambda_- \leq 1^{2n}
\]

\[
= \max_{\sigma \geq 0^p, \lambda_- \geq 0^{2n}} \left[ b^T \sigma - \frac{1}{n} \|\lambda_-\|_1 \right] \quad \text{s.t.} \quad |F^T \sigma| - \lambda_- \leq 1^n
\]

From inspection of \((11)\), it is clear that given a setting of \(\sigma\), each coordinate of \(\lambda_-\) should be set to be as small as possible: \([\lambda_-]_i = \left[\|F^T \sigma\|_j - 1\right]_+.\) Therefore, \((11)\) is equivalent to

\[
\max_{\sigma \geq 0^p} \left[ b^T \sigma - \frac{1}{n} \sum_{j=1}^{n} \left[\|F^T \sigma\|_j - 1\right]_+ \right] = \max_{\sigma \geq 0^p} \left[ b^T \sigma - \frac{1}{n} \sum_{j=1}^{n} \left[\|x_j^T \sigma\| - 1\right]_+ \right] = \min_{\sigma \geq 0^p} \left[ \gamma(\sigma) \right]
\]

Therefore,

\[
\sigma^* = \arg \min_{\sigma \geq 0^p} \left[ \gamma(\sigma) \right]
\]

so we have proved Lemma 8.

---

4 We could use Fenchel duality, or a direct proof with the Lagrangian and minimax theorems. Instead we opt for LP duality, because it suffices.
A.2 Minimax Optimal Strategies

We can now derive \( z^* \) from LP complementary slackness conditions (proof in Section A.3).

**Lemma 9.** If \( \sigma^* \) is defined as in Theorem 3 then for every \( i \in [n] \),
\[
 z_i^* = \begin{cases} 
 0, & \text{if } \gamma = 0 \\
 \operatorname{sgn}(\gamma), & \text{if } \gamma > 0 
\end{cases}
\]

Finally, we study (2) directly to derive \( g^* \). The inner optimization problem in (2) (Nature’s decision, given some \( g \in [-1, 1]^m \)) is
\[
 \min_{z \in [-1, 1]^m} \frac{1}{n} z^\top g
\]

Taking the LP dual of this leads to reasoning similar to the proof of Lemma 8, whereby \( g^* \) can be derived.

**Lemma 10.** If \( \sigma^* \) is defined as in Theorem 3 then for every \( i \in [n] \),
\[
 g_i^* = \begin{cases} 
 [F^\top \sigma^*]_i, & \text{if } \gamma > 0 \\
 \operatorname{sgn}(\gamma), & \text{otherwise}
\end{cases}
\]

Proving Theorem 4 follows very similar lines.

**Proof of Theorem 4.** Let \( A = [F, -F] \in \mathbb{R}^{p \times 2n} \) and \( c = 1^{2n} \). Then the first assertion follows by LP duality, similar to the proof of Lemma 8.

\[
 \max_{\sigma \geq 0^p} b^\top \sigma = \max_{A^\top \sigma \leq c, \sigma \geq 0^p} b^\top \sigma = \min_{A \mathbb{R} \geq c, \mathbb{R} \geq 0^2} c^\top \zeta = \min_{F \mathbb{R} \geq c, \mathbb{R} \geq 0} \left[ \|\zeta^a\|_1 + \|\zeta^b\|_1 \right] = \min_{F \mathbb{R} \geq c, \mathbb{R} \geq 0} \|z\|_1
\]

\[
 = \min_{\frac{1}{n} F \mathbb{R} \geq c, \mathbb{R} \geq 0} \frac{1}{n} \|z\|_1 = \min_{\frac{1}{n} F \mathbb{R} \geq c, \mathbb{R} \geq 0} \|g\|_1
\]

where (a) is by strong LP duality and (b) uses the minimax theorem.

The second assertion follows because \( V = -\gamma(\sigma^*) \) \( \equiv (c) \) \( b^\top \sigma^* \) \( \equiv (d) \) \( \max_{g \in [1, 1]^n} \min_{\frac{1}{n} F \mathbb{R} \geq c, \mathbb{R} \geq 0} \frac{1}{n} z^\top g \), where (c) uses the definition of ZBR and (d) is due to the first assertion.

A.3 Supporting Proofs

**Proof of Lemma 3.** By (12) and the discussion leading up to it, we already know \( \sigma^* \), and therefore only need establish the dependence of \( z^* \) on \( \sigma^* \). Applying LP complementary slackness ([Van96], Thm. 5.3) to (3) and (9), we get that for all \( j \in [2n] \),
\[
[c - A^\top \lambda^*]_j > 0 \implies \zeta^*_j = 0
\]
and
\[
\lambda^*_j > 0 \implies [A\zeta^* - B]_j = 0
\]

First we examine (14). The condition \( [c - A^\top \lambda^*]_j > 0 \) can be rewritten as
\[
c_j + [\lambda^*_j]_j - [F^\top \sigma^*; -F^\top \sigma^*]_j > 0
\]
For any example \( i \leq n \), if \( ||[F^T \sigma^*]_i|| < 1 \), then \( c_i - A^T \lambda^* \geq c_i - [F^T \sigma^*; -F^T \sigma^*]_i > 0 \) (since \( \lambda^*_+ \geq 0 \)). Similarly, \( c_{i+n} - [F^T \sigma^*; -F^T \sigma^*]_{i+n} > 0 \). By (14), this means \( \zeta^*_i = \zeta^*_i + n = 0 \), which implies \( z^*_i = 0 \) by definition of \( \zeta^* \). So we have shown that \( ||[F^T \sigma^*]_i|| < 1 \implies z^*_i = 0 \).

It remains only to prove that \( ||[F^T \sigma^*]_i|| > 1 \implies z^*_i = \text{sgn}([F^T \sigma^*]_i) \) for any \( i \in [n] \). We first show this is true for \( [F^T \sigma^*]_i > 1 \). In this case, from the constraints we need \( c \geq A^T \lambda^* \), in particular that

\[
0 \leq [c - A^T \lambda^*]_i = [\lambda^*_+]_i + (c_i - [F^T \sigma^*]_i)
\]  

By assumption, \( c_i - [F^T \sigma^*]_i = 1 - [F^T \sigma^*]_i < 0 \). Combined with (16), this means we must have \( [\lambda^*_+]_i > 0 \), i.e. \( \lambda^*_+ > 0 \). From (15), this means that

\[
[A^T z^* - B]_{i+n} = 0 \iff \zeta^*_i = 1
\]

Meanwhile,

\[
[c - A^T \lambda^*]_{i+n} = [\lambda^*_+]_i + (c_{i+n} - [-F^T \sigma^*]_i) = c_{i+n} + [F^T \sigma^*]_i > 0
\]

so from (14), \( \zeta^*_{i+n} = 0 \). Since \( \zeta^*_i = 1 \), this implies \( z^*_i = 1 = \text{sgn}([F^T \sigma^*]_i) \), as desired.

This concludes the proof for examples \( i \) such that \( [F^T \sigma^*]_i > 1 \). The situation when \( [F^T \sigma^*]_i < -1 \) is similar, but the roles of the \( i^{th} \) and \( (i+n)^{th} \) coordinates are reversed from (16) onwards in the above proof.

The proof of Lemma 10 relies on an independently useful supporting lemma describing Nature’s response to a given \( g \).

**Lemma 11.** For any \( g \in [-1, 1]^n \),

\[
\min_{\substack{z \in [-1, 1]^n, \lambda \geq 0^p, \lambda_- \geq 0^2n \atop \mathcal{F}z \geq b}} \frac{1}{n} z^T g = \max_{\sigma \geq 0^p} \left[ b^T \sigma - \frac{1}{n} \|F^T \sigma - g\|_1 \right]
\]

**Proof.** Manipulating the left-hand side of the lemma statement becomes easier if we rewrite the constraints. Define \( A, B, \zeta \) exactly as in Section A.1 and define \( g' = [g; -g] \in [-1, 1]^{2n} \) so that (13) becomes

\[
\min_{\substack{z \in [-1, 1]^n, \lambda \geq 0^p, \lambda_- \geq 0^2n \atop \mathcal{F}z \geq b}} \frac{1}{n} z^T g = \min_{A \zeta \geq B, \lambda \geq 0^p} \frac{1}{n} \zeta^T g' = \max_{\lambda \geq 0^p, g' \geq A^T \lambda} \frac{1}{n} B^T \lambda
\]  

(17)

where \( (a) \) is by strong LP duality ([Van96]).

As in Section A.1, partition the coordinates of \( \lambda \) as \( \lambda = [\lambda_+; \lambda_-] \) for \( \sigma \in \mathbb{R}^p \) and \( \lambda_- \in \mathbb{R}^{2n} \). Using similar manipulations to Section A.1 (17) is equal to

\[
\max_{\sigma \geq 0^p, \lambda_- \geq 0^2n} \left[ b^T \sigma - \frac{1}{n} \|\lambda_-\|_1 \right] \quad \text{s.t.} \quad [F^T \sigma; -F^T \sigma] - \lambda_- \leq g' = [g; -g]
\]  

(18)

It is clear that given a setting of \( \sigma \) and an example index \( i \leq n \), each coordinate of \( \lambda_- \) is set to be as small as possible: \( [\lambda_-]_i = [[F^T \sigma]_i - g_i]_+ \) and \( [\lambda_-]_{i+n} = [[-F^T \sigma]_i + g_i]_+ \), so that \( [\lambda_-]_i + [\lambda_-]_{i+n} = [F^T \sigma]_i - g_i \), and \( \|\lambda_-\|_1 = \sum_{i=1}^n \| [F^T \sigma]_i - g_i \|_1 = \|F^T \sigma - g\|_1 \). Therefore, (18) is equivalent to the right-hand side of the desired result.

Now Lemma 10 can be proved.

**Proof of Lemma 10.** From Lemma 11 the primal game (12) is equivalent to

\[
\max_{\sigma \geq 0^p} \left[ b^T \sigma - \frac{1}{n} \|g - F^T \sigma\|_1 \right]
\]  

(19)
From (19), it is clear that given a setting of $\sigma$, the $g^*(\sigma)$ that maximizes (19) is also the one that minimizes $\|g - F^T \sigma\|_1$ under the hypercube constraint:

$$g^*_i(\sigma) = \begin{cases} [F^T \sigma]_i, & \text{if } |[F^T \sigma]_i| < 1 \\ \text{sgn}([F^T \sigma]_i), & \text{otherwise} \end{cases}$$

The optimum $\sigma$ here is therefore

$$\sigma^* = \arg\max_{\sigma \geq 0} \left[ b^T \sigma - \frac{1}{n} \|g^*(\sigma) - F^T \sigma\|_1 \right]$$

$$= \arg\max_{\sigma \geq 0} \left[ b^T \sigma - \frac{1}{n} \sum_{j=1}^{n} \left[ |x_j^T \sigma| - 1 \right]_+ \right] = \arg\min_{\sigma \geq 0} |\gamma(\sigma)|$$

which finishes the proof.

By further inspection of the subgradient conditions described in the body of the paper, we can show the following result, which complements Theorem 3.

**Corollary 12.** For examples $j$ such that $|x_j^T \sigma^*| = 1$,

$$z_j^* = c_j \text{sgn}(x_j^T \sigma^*)$$

where $c_j \in [0, 1]$ are as defined in (6).

## B Miscellaneous Proofs

**Lemma 13.** The function $\gamma(\sigma)$ is convex in $\sigma$.

**Proof.** Note that for each $j$, the term $\left[ |x_j^T \sigma| - 1 \right]_+$ is convex in $\sigma$. Therefore, the average of $n$ terms is convex. As the term $-b^T \sigma$ is linear, the whole expression $\gamma(\sigma)$ is convex. (This is a special case of the Lagrangian dual function always being concave in the dual variables.)

**Proof of Prop. 6** The derivation here closely follows Section A.1. The game under consideration again has a minimax equilibrium:

$$\max_{g \in [-1,1]^n} \min_{{\bar{\sigma}} \leq \sigma \leq {\bar{\sigma}}, \frac{1}{2} Fz \geq b} \frac{1}{n} z^T g = \min_{{\bar{\sigma}} \leq \sigma \leq {\bar{\sigma}}, g \in [-1,1]^n} \max_{{\bar{\sigma}} \leq \sigma \leq {\bar{\sigma}}, \frac{1}{2} Fz \geq b} \frac{1}{n} z^T g = \min_{{\bar{\sigma}} \leq \sigma \leq {\bar{\sigma}}, \frac{1}{2} Fz \geq b} \frac{1}{n} \|z\|_1$$

(20)

Define $c, A, \zeta$ as in Section A.1 and $B = [nb; -{\bar{\sigma}}; -{\bar{\sigma}}] \in \mathbb{R}^{p+2n}$. With these definitions, the problem (20) becomes

$$\min_{A\zeta \geq B, \zeta \geq 0} \frac{1}{n} c^T \zeta = \max_{\lambda \geq 0, c \geq A^T \lambda} \frac{1}{n} B^T \lambda$$

(21)

Denote the solutions to this equation as $\zeta^*$ and $\lambda^*$.

Suppose the first $p$, next $n$ and last $n$ coordinates of $\lambda$ are $\sigma, \lambda_+, \lambda_-$ respectively, so that $\lambda = [\sigma; \lambda_+; \lambda_-]$. In terms of these coordinates, (21) becomes

$$\max_{\sigma \geq 0^p, \lambda_+ \geq 0^n, \lambda_- \geq 0^n} \left[ b^T \sigma - \frac{1}{n} \alpha^T (\lambda_+ + \lambda_-) \right] \text{ s.t. } [F^T \sigma; -F^T \sigma] - [\lambda_+; \lambda_-] \leq 1^{2n}$$

(22)

which is equivalent to the result.