Classification as Direction Recovery: Improved Guarantees via Scale Invariance

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Abstract

Modern algorithms for binary classification rely on an intermediate regression problem for computational tractability. In this paper, we establish a geometric distinction between classification and regression that allows risk in these two settings to be more precisely related. In particular, we note that classification risk depends only on the direction of the regressor, and we take advantage of this scale invariance to improve existing guarantees for how classification risk is bounded by the risk in the intermediate regression problem. Building on these guarantees, our analysis makes it possible to compare algorithms more accurately against each other and suggests viewing classification as unique from regression rather than a byproduct of it. While regression aims to converge toward the conditional expectation function in location, we propose that classification should instead aim to recover its direction.

1 Introduction

The correct assignment of binary labels to data is a fundamental problem of machine learning. Practitioners naturally seek to minimize the portion of observations they misclassify, yet in practice, minimizing a loss function over binary labels and outcomes is computationally intractable. Therefore, modern approaches start with regression, which may be viewed as a convex relaxation of the original classification problem. They identify a real-valued function that minimizes a smooth surrogate risk criterion pre-selected by the algorithm designer, and they then threshold resulting predictions to arrive at binary classifications.

Several influential results in statistical machine learning relate the performance of a classifier to the performance of this intermediate regression procedure [Lugosi and Vayatis, 2004; Zhang, 2004; Bartlett et al., 2006]. Attempts to attack this problem theoretically have, with few exceptions, proceeded by relating the classification risk to the surrogate risk, reducing the analysis to the better understood problem of stochastic optimization [Hazan et al., 2014; Rosasco et al., 2004]. Results on surrogate risk convergence, when combined with this analysis, produce theoretical guarantees that provide guidance on the choice of surrogate loss for classification tasks.
In this paper, we aim to improve this guidance by taking advantage of a fundamental geometric
difference between classification and regression. In particular, we note that classification risk depends
only on the direction of a regressor, whereas surrogate risk depends also on its scale. By taking
advantage of the scale invariance of classification, we achieve tighter bounds relating classification
risk to surrogate risk. The precision gained in these bounds can help practitioners better compare
classification procedures and thus design better algorithms.

Throughout our analysis, we reframe the problem of classification as “direction recovery.” To
illustrate, suppose the conditional expectation function $E[Y|X]$ may be represented by some $\beta^*$ a
multidimensional vector space. Rather than aim to produce predictions close to $\beta^*$ in location, as
in traditional regression, we instead aim to produce predictions close to $\beta^*$ in direction. We show
that procedures designed to converge in direction to $\beta^*$ may achieve lower classification error than
those that only seek to minimize regression error, and that upper bounds for existing procedures may
be sharpened by studying convergence in direction. We hope this perspective shows the potential
of treating classification not only as a byproduct of regression, but as a unique problem deserving a
tailored approach.

1.1 Outline

The paper proceeds in four main sections. In Section 2, we identify slack in existing bounds of
classification risk and proceed to reduce the slack by introducing a notion of angle $\theta$ between a
regressor and its optimal value. We characterize how a small angle $\theta$ minimizes excess classification
risk. To achieve small angles in practice, we turn to surrogate loss minimization in Section 3. We
show that regularized least squares obtains the optimal classifier when features are uncorrelated, and
otherwise, study how regularization biases the predictor away from the optimal direction. Lastly, we
present simulations in Section 4 that exemplify how surrogate loss minimization can fail or succeed
to minimize the relevant angle.

1.2 Related Work

Recently, great attention has been paid to how bounds based on the excess risk alone can be systemat-
ically improved based on a margin condition, which says that the posterior probability of a positive
label does not concentrate near one-half [Mammen and Tsybakov 1999]. While these results are of
great conceptual and practical importance, and similarly illustrate how bounds based on the surrogate
risk can fail to adequately capture the classification problem, they rely on specific properties of the
distribution at hand. In contrast, our results will focus primarily on the structure of classification
problems in general, without attention to a specific class of distributions. Our results can, however,
be strengthened by combining them with a margin condition, and we illustrate this in the paper.
Perhaps most similar to our work in spirit is the example of Koltchinskii and Beznosova [2005], in which the excess classification risk decays exponentially fast, whereas the excess surrogate risk decays no faster than \( O(1/n) \). While they make use of a margin condition and a specific class of distributions, particular attention is paid to the discrepancy between classification and stochastic optimization, and scale invariance of the optimal set of classifiers is used analytically. Like the authors, in our paper we give attention to the subtle aspects of classification that meaningfully affect classifier performance. In the words of the authors,

“In classification problems, there are many relevant probabilistic, analytic and geometric parameters to play with when one studies the convergence rates... probably, we have not understood to the end [the] rather subtle interplay between various parameters that influence the behaviour of this type of classifier.”

We believe that a powerful such parameter is the notion of direction we introduce in this paper.

Finally, canonical results relating the classification error to the surrogate risk can be found in Bartlett et al. [2006], and the results there are foundational to the analysis in this paper.

2 Bounding Excess Classification Risk

In this section, we present a new bound on excess classification risk. To begin, we describe our setting and motivation for why these bounds are useful in practice. Then we show evidence of slack in existing bounds that can be substantially reduced, and finally, we reduce that slack to achieve tighter bounds.

2.1 Setting

Consider a setting where features \( X \) fix a linear conditional expectation function \( f^*(X) = \mathbb{E}[Y|X] \) of a binary outcome \( Y \in \{-1, 1\} \). A machine learner minimizes a surrogate convex loss function \( \phi \) over data \((X, Y)\) to construct an estimate \( f(X) \) of \( f^*(X) \). The sign of \( f \) fixes their classification decisions \( \hat{Y} \equiv \text{sign } f \). Although they are minimizing \( \phi \)-loss, ultimately they care about classification loss: the probability that \( f \) takes a different sign than \( Y \).

Luckily, it has been shown that minimizing the convex surrogate loss successfully can constrain classification error. These guarantees are used in practice for machine learners to ultimately select their learning procedure. We discuss one contemporary approach to bound the classification error in the next section, as well as show slack in that approach which can be reduced to achieve tighter bounds. In practice, these tighter bounds can aid investigations of how learning procedures perform.
2.2 Finding slack in existing bounds for excess classification risk

Contemporary bounds generally relate the excess classification risk to some increasing function $\psi$ of the excess $\phi$-risk, taking the form

$$P(\text{sign } f \neq Y) - P(\text{sign } f^* \neq Y) \leq \psi(\mathbb{E}\phi(f,Y) - \mathbb{E}\phi(f^*,Y))$$

(1)

(cf. Thms. 1 and 3 of [Bartlett et al. 2006]). Since the slack is revealed from following the proof behind this bound, we sketch the main idea.

The argument on which this bound is based relies first on fixing a value of $f^*$ and then computing the associated excess classification risk of an arbitrary $f$,

$$P(\text{sign } f \neq Y) - P(\text{sign } f^* \neq Y) = E[|f^*|\{\text{sign } f \neq \text{sign } f^*\}]$$

(2)

[Bartlett et al. 2006] show how to bound the step function (2) by a smooth convex function based on $\phi$-risk. We illustrate their bound in Figure 1 for a given $f^*$ and shade the associated slack in green (when $\text{sign } f = \text{sign } f^*$) and in yellow (when $\text{sign } f \neq \text{sign } f^*$). The way that we will ultimately reduce this slack is by noting that the LHS of (2) depends only on whether $f^*$ and $f$ share the same sign. Therefore, we have the opportunity to rewrite the bound (1) in terms of a predictor $g$ that i) satisfies $\text{sign } g = \text{sign } f$ so that the LHS of (1) is unchanged but ii) that corresponds to a tighter convex bound on the RHS of (1). To do so, we will choose $g$ among the rescalings of $f$, i.e., among all vectors pointing in the direction of $f$.

Figure 1: Illustration of upper bound for a given $f^*$. The green and yellow regions correspond to slack that we aim to reduce.
Figure 2: Top-down view of projection $Z$ on plane spanned by $(\tilde{\beta}, \beta^*)$. Dashed lines correspond to the classification boundaries associated with each $\beta \in \{\tilde{\beta}, \beta^*\}$. Points to the right are positively classified by $\beta$ while those to the left are negatively classified. Thus, the two sectors between the dashed lines (with combined measure of $\frac{\theta}{\pi}$) designate observations that are classified differently by $\tilde{\beta}$ and $\beta^*$.

2.3 Tightening the bound: a first example

In order to illustrate the relevance of the direction of $f$ to its associated classification loss, we present a visual example. In particular, we consider the problem of learning a linear classification rule in the presence of features that satisfy a notion of symmetry called rotational invariance.

Definition 1. The law of $X$ is rotation invariant if it satisfies $P(X \in S) = P(RX \in S)$ for any measurable set $S$ and any rotation $R$ of its coordinates.

Note that rotational invariance is a stronger condition than uncorrelated features. This property allows us to exactly characterize the probability that a linear predictor $\tilde{\beta}$ yields a different classification from the optimal $\beta^*$, based on the angle $\theta(\tilde{\beta}, \beta^*)$ between them. The probability grows in $\theta$ as follows.

Lemma 1. If the law of $X$ is rotation invariant, we have

$$P(\text{sign}(\beta^*, X) \neq \text{sign}(\tilde{\beta}, X)) = \frac{\theta(\tilde{\beta}, \beta^*)}{\pi}$$

Proof. We have

$$P(\text{sign}(\beta^*, X) \neq \text{sign}(\tilde{\beta}, X)) = P\left(\text{sign} \left(\tilde{\beta}, \frac{X}{\|X\|_2}\right) \neq \text{sign} \left(\beta^*, \frac{X}{\|X\|_2}\right)\right)$$

Now let $Z$ denote the projection of $X/\|X\|_2$ onto the plane spanned by $(\tilde{\beta}, \beta^*)$. We know $Z$ is uniformly distributed on the circle by rotation invariance, and the sign associated with $\tilde{\beta}$ and with $\beta^*$ will differ precisely when $Z$ belongs to a subset of the circle of measure $\theta/\pi$. This is illustrated in Figure 2 which visualizes the projection $Z$ from above. \qed
The key insight which leads to the angle \( \theta(\beta^*, \beta) \) on the RHS of (3) is that the classification rules \( x \mapsto \text{sign} \langle \beta, x \rangle \) and \( x \mapsto \text{sign} \langle \beta^*, x \rangle \) are invariant to rescaling the linear predictors \( \beta \) and \( \beta^* \). The angle, which corresponds to the distance between \( \beta / \| \beta \| \) and \( \beta^* / \| \beta^* \| \) along the surface of the unit sphere, emerges as a natural, scale invariant measure of the distance between the two predictors. In the following section, we will see that this intuition extends far beyond the simple case of rotationally invariant features.

2.4 The general angle criterion

In the general case, the situation is more nuanced. However, the key insight that the classifier \( 1 \{ f \geq 0 \} \) is invariant to rescaling \( f \) remains.

To begin, we need to know how to actually express the angle \( \theta \) between two vectors \( u \) and \( v \). In the following lemma, we use a geometric argument to write \( \sin \theta \) as the minimum distance between a rescaled \( u \) and a normalized \( v \).

**Lemma 2.** The angle \( \theta(u, v) \) between vectors \( u, v \in \mathbb{R}^d \) with \( \langle u, v \rangle > 0 \) satisfies

\[
\sin \theta(u, v) = \inf_{t \geq 0} \left\| tu - \frac{v}{\|v\|_2} \right\|
\]

and \( \theta(-u, v) = \pi - \theta(u, v) \) for all \( u, v \in \mathbb{R}^d \).

**Proof.** As seen in Figure 3, the distance \( \left\| tu - \frac{v}{\|v\|_2} \right\| \) is minimized when \( t = t^* \), where \( t^* u \) is equal to the orthogonal projection of \( v/\|v\| \) onto the line spanned by \( u \). As seen, \( (v/\|v\|, 0, t^* u) \) forms a right triangle with hypotenuse of length 1, and \( (t^* u, v/\|v\|) \) is opposite the angle \( \theta(u, v) \).

Now that we no longer require the law of \( X \) to be rotation invariant, we must deal directly with \( L^2(\mathbb{P}) \).

This requires us to define the relevant angle of a predictor with respect to the norm \( \| f \|_{2, \mathbb{P}} = \mathbb{E}[f^2]^{1/2} \) in the probability space. Motivated by Lemma 2, we generalize our notion of the relevant angle.
\[ \theta_{2,p}(\beta, \beta^*) \text{ to } L^2(\mathbb{P}) \text{ by the relation} \]

\[
\sin \theta_{2,p}(u, v) = \inf_{t > 0} \left\| tu - \frac{v}{\|v\|_2} \right\|_{2,p}, \tag{4}
\]

when \( \mathbb{E}[uv] > 0 \) and \( \theta_{2,p}(u, v) = \pi - \theta_{2,p}(-u, v) \) when \( \mathbb{E}[uv] < 0 \).

Equipped with the suitable notion of angle, we can establish a main result. Here we bound the excess classification risk of an arbitrary predictor \( f \) according to the direction of \( f \). Note that while the \( L^2(\mathbb{P}) \) distance and the square loss are essential ingredients in its proof, the result applies to any predictor, however it is obtained.

**Theorem 1.** Let \( f^* = \mathbb{E}[Y \mid X] \). Then, the excess classification risk is bounded as

\[
\mathbb{P}(Y \neq \text{sign } f) - \mathbb{P}(Y \neq \text{sign } f^*) \leq \|f^*\|_{2,p} \sin \theta_{2,p}(f, f^*). \]

We prove this result using the canonical bound given by Theorem 1 in [Bartlett et al. 2006], which relates the classification risk in excess of \( f^* \) to the excess surrogate loss. Stated for the square loss, the result reduces to the following.

**Theorem 2** (Bartlett et al. [2006, Thm. 1]).

\[
\mathbb{P}(Y \neq \text{sign } f) - \mathbb{P}(Y \neq \text{sign } f^*) \leq \|f - f^*\|_{2,p}.
\]

We use the canonical theorem to prove our new result.

**Proof of Theorem** Let \( C_f \) denote the convex cone of functions \( g \) satisfying \( \text{sign } g = \text{sign } f \) almost surely. For any \( g \in C_f \) we can apply Theorem 2 to obtain

\[
\mathbb{P}(Y \neq \text{sign } f) - \mathbb{P}(Y \neq \text{sign } f^*) = \mathbb{P}(Y \neq \text{sign } g) - \mathbb{P}(Y \neq \text{sign } f^*)
\leq \|g - f^*\|_{2,p}. \]

Optimizing over the bounds obtained in this manner yields

\[
\mathbb{P}(Y \neq \text{sign } f) - \mathbb{P}(Y \neq \text{sign } f^*) \leq \inf_{g \in C_f} \left\{ \|g - f^*\|_{2,p} \right\}. \tag{5}
\]

While we cannot tractably minimize over all \( g \) in the cone \( C_f \), we can minimize over the \( g \) that rescale \( f \), noting that these rescalings satisfy \( \{tf \mid t > 0\} \subset C_f \). This gives us the bound

\[
\mathbb{P}(Y \neq \text{sign } f) - \mathbb{P}(Y \neq \text{sign } f^*) \leq \inf_{t > 0} \left\{ \|tf - f^*\|_{2,p} \right\}
= \|f^*\|_{2,p} \inf_{t > 0} \left\{ \left\| \frac{tf}{\|f\|_2} - \frac{f^*}{\|f^*\|_2} \right\|_{2,p} \right\}. \]
Making the change of variable $t' = \|f^*\|_{2,p} t$ gives
\[
\begin{align*}
&= \|f^*\|_{2,p} \inf_{t' > 0} \left\{ \left\| t' f - \frac{f^*}{\|f^*\|_{2,p}} \right\| \right\} \\
&= \|f^*\|_{2,p} \sin \theta_{2,p}(f, f^*),
\end{align*}
\]
by our definition of $\theta_{2,p}$. This is what we aimed to show.

In fact, Bartlett et al. [2006] proved stronger versions of Theorem 2 under the low-noise condition (also sometimes called a margin condition), and the same machinery can be applied to yield stronger versions of our Theorem 1. To state these, we first introduce the low-noise condition. It characterizes the extent to which the best prediction of the outcome is close to the classification boundary.

**Definition 2.** Given $\alpha \in [0, 1]$ the pair $(X,Y)$ is said to satisfy the $\alpha$-noise condition if for some $C > 0$, $f^* = \mathbb{E}[Y|X]$ satisfies
\[
\mathbb{P}(|f^*| < \varepsilon) \leq C\varepsilon^{\alpha/(1-\alpha)},
\]
for all sufficiently small $0 < \varepsilon < c$.

Under the above condition, Bartlett et al. [2006] proved the following improvement on their bound.

**Theorem 3** (Special case of Bartlett et al. [2006, Theorem 3]). Suppose $(X,Y)$ satisfies the $\alpha$-noise condition with constants $c, C > 0$. Then
\[
\mathbb{P}(\text{sign } f \neq Y) - \mathbb{P}(\text{sign } f^* \neq Y) \leq \frac{\|f - f^*\|_{2,p}^{1+\alpha}}{4c'}
\]
for some $c'$ which depends only on $c$ and $C$.

Repeating the proof of Theorem 1 and replacing our use of Theorem 2 with the improved Theorem 3 gives the following improved result.

**Theorem 4.** Suppose $(X,Y)$ satisfies the $\alpha$-noise condition with constant $c > 0$. Then, for the same $c'$ appearing in Theorem 3 it holds that
\[
\mathbb{P}(\text{sign } f \neq Y) - \mathbb{P}(\text{sign } f^* \neq Y) \leq \inf_{g \in C_f} \left\{ \frac{\|g - f^*\|_{2,p}^{1+\alpha}}{4c'} \right\}
\]
\[
\leq \frac{\|f^*\|_{2,p}^{1+\alpha}}{4c'} \left( \sin \theta_{2,p}(f, f^*) \right)^{1+\alpha}
\]

**Remark.** An interesting aspect of the bounds in Theorems 3 and Theorem 1 is that they are never weaker than the corresponding bounds of Bartlett et al. [2006], which relate classification risk to the excess square loss, on which they are based. As such, since $\|f^*\|_{2,p}$ is a problem-invariant constant,
procedures that are tailored to minimization of \( \theta_{2,P}(f,f^*) \) will yield stronger bounds than those based only on control of the excess mean squared error.

Remark. For the rotationally invariant case, we show in the appendix that excess classification error is given precisely by

\[
\frac{1}{\pi} \left( \int_0^\theta \sin t \, dt \right) \mathbb{E}|\langle X, \beta^* \rangle |.
\]

We explain how this implies a convergence rate of \( \frac{1}{\sqrt{n}} \), whereas the standard bound by Bartlett et al. [2006] only guarantees a rate of \( \frac{1}{\sqrt{n}} \). Therefore, we see that rotation invariant linear classification produces fast rates, even without imposition of a margin condition. This demonstrates how an angle-based analysis of learning procedures can improve convergence guarantees from traditional bounds.

3 Relationship between surrogate loss minimization and \( \theta \)

3.1 Defining classification calibration

Thus far, we have related excess classification risk to the angle \( \theta \) between a predictor \( \hat{\beta} \) and the optimal \( \beta^* \), showing that the excess risk is guaranteed to be small when \( \theta \) is small. Now we turn our attention to how \( \theta \) is actually determined. In particular, we consider procedures that minimize a surrogate loss function \( \phi \) over a set \( S \subset \mathbb{R}^d \) of linear predictors and present guarantees on their maximum associated values of \( \theta \).

Procedures that are guaranteed to achieve \( \sin(\theta) = 0 \) in the population are of particular interest, as they converge to the optimal classifier. We call these “classification calibrated.” In the case of minimizing surrogate risk over \( S \), we define this special trait as follows.

**Definition 3.** A procedure that minimizes the \( \phi \)-risk \( \mathbb{E}[\phi(Y, \langle \beta, X \rangle)] \) over \( S \) is **classification calibrated** if its constrained minimizer \( \hat{\beta} \) is also a global minimizer of the classification risk \( \mathbb{P}[^{\text{sign}}(\beta, X) \neq Y] \).

Note that this definition does not require the procedure to identify the global minimizer of the \( \phi \) risk. In fact, in our simulations we will provide examples of when the global minimizer of \( \phi \)-risk is not contained in \( S \), but the constrained minimizer in \( S \) yields the global minimum of classification risk nonetheless.

In this section, we study classification calibration in settings with well-specified models that are regularized so that \( S \) is a ball of positive radius \( r \), i.e.,

\[
S = \{ v \in \mathbb{R}^d \mid \|v\| \leq r \}.
\]
In the following lemma, we start by noting that this choice of $S$ contains a global minimizer of the classification risk. The question therefore becomes, when does minimizing the surrogate loss $\phi$ within $S$ identify this global minimizer?

**Lemma 3.** $S$ contains a global minimizer of the classification risk.

**Proof.** Since $\text{sign}(\beta, X) = \text{sign}(c\beta, X)$ for any $c > 0$, recall that the classifications associated with any given $\beta$ are invariant to rescaling $\beta$. This is illustrated in Figure 4. Since $S$ contains a neighborhood of the origin, it follows that it is guaranteed to contain a rescaled $\tilde{\beta} = c\beta^* \in S$ of some global minimizer $\beta^*$ of the classification risk. \qed

### 3.2 Studying $\theta$ under Square Loss Minimization

In this section, we will investigate the case where $\phi$ is the square loss $\phi(Y, f(X)) = (Y - f(X))^2$. We consider de-meaned features $X$ that may or may not be correlated and then characterize the population square loss in terms of their covariance matrix $\Sigma = \mathbb{E}[XX^\top]$. Then, we will bound the angle between the constrained population minimizer $\tilde{\beta}$ and the unconstrained population minimizer $\beta^*$ in terms of $\Sigma$, showing that when features are uncorrelated, the angle is 0. Finally, we will investigate whether the excess misclassification risk can be controlled in terms of $\beta^*$, $\tilde{\beta}$, and $\Sigma$ alone.

#### 3.2.1 Characterizing the population loss

We will show that the population loss associated with a linear predictor $\beta$ can be expressed in terms of $\Sigma$. We begin with the following lemma as an intermediate step to computing the mean square loss.
Lemma 4. If $E[XX^\top] = \Sigma$ then $E \langle X, v \rangle^2 = v^\top \Sigma v$.

Proof in appendix.

This result makes it possible for us to express the mean square loss associated with a linear predictor $\beta$ in terms of $\Sigma$ and $\beta^*$, the orthogonal projection of $Y$ onto the span of the features. We will see then that choosing $\beta$ to minimize the mean square loss corresponds to minimizing the expression $(\beta^* - \beta)^\top \Sigma (\beta^* - \beta)$.

Lemma 5. Let $\beta^*$ be the orthogonal projection of $Y$ onto the span of the features, $\{ \langle \gamma, X \rangle \ | \ \gamma \in \mathbb{R}^d \}$ in $L^2(\mathbb{P})$. Then

$$
E(Y - \langle \beta, X \rangle)^2 = E(Y - \langle \beta^*, X \rangle)^2 + E((\langle \beta^*, X \rangle - \langle \beta, X \rangle)^2
= C + (\beta^* - \beta)^\top \Sigma (\beta^* - \beta),
$$

where $C$ is a constant independent of $\beta$.

Proof in appendix.

These lemmas have particularly useful implications in cases where the features are uncorrelated and standardized, that is, when $X$ is isotropic according to the following definition.

Definition 4. A random vector $X \in \mathbb{R}^d$ is called isotropic if $E[XX^\top] = I$.

When this holds, then the following corollary proves that minimizing the mean square loss in the population corresponds to choosing $\beta$ to minimize its distance from $\beta^*$.

Corollary 1. The $\beta$ that minimizes $E(Y - \langle \beta, X \rangle)^2$ also minimizes $\| \beta^* - \beta \|^2$.

Proof in appendix.

3.2.2 Bounding the angle

We now shift our attention to bounding the angle between a linear predictor $\beta$ and the best linear predictor $\beta^*$.

We see that in the isotropic case, minimizing square loss recovers a $\tilde{\beta}$ whose angle with $\beta^*$ is 0. That is, minimizing square loss gives the optimal classifier.

Proposition 1. If $X$ is isotropic, then the minimizer $\tilde{\beta} \in S$ of the square loss $E(Y - \langle \beta, X \rangle)^2$ satisfies

$$
\sin \theta(\tilde{\beta}, \beta^*) = 0
$$

This follows easily from the following, more general result given a feature covariance matrix $\Sigma$. 

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Theorem 5. In general, the minimizer \( \tilde{\beta} \in S \) of the square loss satisfies
\[
\sin \theta(\tilde{\beta}, \beta^*) \leq \inf_{a \geq 0} \|a\Sigma - I\|_{op}
\]

Proof in appendix.

3.3 Studying \( \theta \) under General Loss Minimization

When we consider minimizing a general surrogate loss function \( \phi \) in a setting where the law of \( X \) is rotation invariant, then we can guarantee convergence to the optimal classifier.

Proposition 2. Suppose that the following conditions hold.

(i) The law of \( X \) is rotation invariant.

(ii) \( P(Y = 1|X) = \eta(\langle X, \beta^* \rangle) \) for some \( \beta^* \in \mathbb{R}^d \).

(iii) The loss function \( \phi(Y, f) \) is convex in \( f \).

Then the constrained minimizer \( \tilde{\beta} \) of \( \beta \mapsto \mathbb{E}[\phi(Y, \langle \beta, X \rangle)] \) subject to \( \|\beta\| \leq r \) is unique and satisfies \( \tilde{\beta} = c\beta^* \) from some \( c \in \mathbb{R} \).

Proof in appendix. In the simulations in the following section, we present evidence that this result cannot be completely relaxed without further assumptions.

4 Application

In this section, we construct simulations that illustrate classification-calibration in practice. We also present evidence on future investigations to characterize when surrogate loss minimization can recover optimal classifiers.

In these simulations we construct features \( X \) that are either normally or uniformly distributed, and that may or may not be correlated. According to a fixed true \( \beta^* \), these ultimately determine true underlying probabilities \( p^* \) of a binary outcome \( Y \). We then construct \( Y \) according to binomial draws of \( p^* \). This data-generating process defines primitives \((\beta^*, p^*)\) that are unobserved by a machine learner, as well as data \((X, Y)\) that are observed.

The machine learner constructs models of the data-generating process to predict \( Y \) from \( X \). We suppose the learner passes training instances of \((X, Y)\) through a procedure that minimizes a convex loss function \( \phi \), either square or logistic loss, and thus produces estimated regressors \( f_{\phi}(\langle \beta, X \rangle) \) in a test set. To measure the success of their procedure, we compute excess \( \phi \)-risk, \( \mathbb{E}[\phi(Y f_{\phi}(X))] - \mathbb{E}[\phi(Y f^*(X))] \) as well as excess 0-1 risk, \( \mathbb{P}[\text{sign}(\langle \tilde{\beta}, X \rangle) \neq Y] - \mathbb{P}[\text{sign}(\langle \beta^*, X \rangle) \neq Y] \).
Figure 5: Minimizing square loss when \( p^* \) is linear in \( X \). Gray lines correspond to correctly specified models without binding norm constraints, and they are therefore associated with excess risks that converge to zero in panels (a) and (b). In panel (a) we see that the misspecified models trained on uncorrelated features (solid red and solid orange lines) have excess 0-1 risk converging to zero despite the fact that panel (b) shows they do not recover a globally minimized \( \phi \)-risk. Meanwhile, when features are correlated (dashed lines), the misspecified models do not yield zero excess risk neither according to 0-1 loss nor square loss.

We consider cases where \( p^* \) is linear or nonlinear in \( X \). This allows us to explore two kinds of misspecification: one where the models are only misspecified through a norm restriction, and the other where the estimating model itself is structurally different from the data-generating process.

### 4.1 \( p^* \) is linear in features

We first consider the linear case \( p^* = \frac{1}{2} + \beta^* X \) for which minimizing square loss produces a well-specified model. Recall that in Proposition 1 we showed that when \( X \) is isotropic, then models minimizing square loss are classification calibrated. That is, they recover the optimal classifier even when their norm constraint \( r \) prevents them from recovering the optimal regressor. Meanwhile, when features are not isotropic (Theorem 5), then more restrictive choices of \( r \) prevent the convergence of the classifications to the optimal.

We demonstrate these results in Figure 5 where we plot excess 0-1 classification risk and excess \( \phi \) risk. Features are distributed as \( U(-\frac{1}{8}, \frac{1}{8}) \) and they fix \( p^* = \frac{1}{2} + (\beta^*, X) \) with \( \beta^* = (1, -3) \). Consider first when there is no binding norm restriction, \( r = \infty \). The model is correctly specified regardless of whether features are correlated, and as the gray lines show, both 0-1 and \( \phi \) excess risks converge to 0 as the training size grows. Meanwhile, when we impose a misspecified norm constraint on the models (red and orange lines), then \( \phi \) excess risks no longer converge to 0. Yet 0-1 excess risk still does converge to 0 so long as the features are uncorrelated (solid red and orange lines), marking the cases where models are classification calibrated.
We separately minimized logistic loss to model the same data generating process. While the functional form is misspecified in this case, we were surprised to see that a notion of Proposition 1 still held. As seen in Figure 6 these models were again classification calibrated in the isotropic case. This suggests future exploration of a wider class of surrogate loss functions that yield optimal classifiers associated with linear predictors.

4.2 $p^*$ is nonlinear in features

We next explored weakening the assumption that $p^*$ is linear in $X$ to see whether we could extend the result in Proposition 1 to cases where the law of $X$ is not rotation invariant. We learned that this result cannot be generalized without further assumptions.

In this new set of simulations, we adjusted the data-generating process by passing $\langle \beta^*, X \rangle$ through the logistic CDF function to construct the true underlying probabilities $p^*$. The results are depicted in Figure 7. We first considered specifications of $X$ satisfying rotation invariance: we constructed two features each independent and distributed as $N(0, 1)$. For both symmetric and non-symmetric choices of $\beta^*$, minimizing square or logistic loss produced classification-calibrated models regardless of whether square or logistic loss was minimized (black lines in each panel), supporting the result in Proposition 1. However, when we instead constructed features that are independent but distributed as $U(-1, 1)$, so that the law of $X$ is not rotation invariant, we saw that excess 0-1 risk does not necessarily converge to 0. This is depicted by the dashed red lines corresponding to $\beta^* = (1, -3)$.

![Figure 6: Minimizing logistic loss when $p^*$ is linear in $X$. Misspecified models in this case with a tight norm restriction (solid red and solid orange lines) are seen to be classification calibrated in the isotropic case, with excess 0-1 risk converging to zero. Meanwhile, tightening the norm restrictions leads to convergence toward non-zero values. This suggests that our results on square loss may be extended to other convex surrogate loss functions.](image-url)
Figure 7: Minimizing square and logistic loss when $p^*$ is a nonlinear transformation of $\langle \beta, X \rangle$. Adjusting the data-generating process is seen to affect convergence of excess 0-1 risk to zero, showing there is a limit to how much we can extend the result in Proposition 2. When features are uniformly distributed but $\beta$ is non-symmetric (dashed red line), models are not classification-calibrated regardless of whether $\phi$ is square or logistic loss.

Therefore, to guarantee convergence to the optimal classifier when $p^*$ is not linear in $X$ and the law of $X$ is not rotation invariant, we understood that additional assumptions are required.

5 Conclusion

In this paper, we used a geometric distinction between classification and regression problems to more precisely characterize how loss in one setting relates to loss in the other. Using the scale invariance of classification, we were able to improve the bounds used by theorists and practitioners to compare classification procedures against one another. We hope that this work will help inform decisions about which classification algorithms to deploy in practice, and that it may open the door for effective new algorithms that aim to directly predict the direction of the conditional expectation function rather than its location.
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6 Appendix

6.1 Proof of Lemma 4

Proof. We can expand

$$\langle X, v \rangle^2 = \left( \sum_{i=1}^{d} X_i v_i \right)^2$$

$$= \sum_{i=1}^{d} \sum_{j=1}^{d} X_i X_j v_i v_j$$

$$= v^T X X^T v.$$ 

Now take expectations and use $E[X X^T] = \Sigma$. □

6.2 Proof of Lemma 5

Proof. By definition of $\beta^*$ as the orthogonal projection of $Y$ onto the span of the features, the first equality follows from the Pythagorean theorem in $L^2(\mathbb{P})$. Then, the second follows from applying Lemma 4 to $E((\beta^*, X) - (\beta, X))^2 = E((\beta^* - \beta, X))^2$. □

6.3 Proof of Corollary 1

Proof. Following Lemma 5, the mean square loss is minimized when $(\beta^* - \beta)^T I (\beta^* - \beta) = \|\beta^* - \beta\|^2_2$ is minimized. □

6.4 Proof of Theorem 1

Proof. By Lemma 5, we know that $\tilde{\beta}$ minimizes

$$\beta \mapsto (\beta - \beta^*)^T \Sigma (\beta - \beta^*)$$

subject to $\|\beta\| \leq r$. This is a convex program; from the KKT conditions, we obtain that

$$\tilde{\beta} = (\Sigma + \lambda)^{-1} \Sigma \beta^*$$

where $\lambda = \lambda(r, \Sigma, \beta^*) \geq 0$ is a Lagrange multiplier.

Derivation. This is a feasible convex program as seen by taking $\beta = 0$, so the KKT conditions are necessary. The Lagrangian is

$$\mathcal{L}(\beta, \lambda) = (\beta - \beta^*)^T \Sigma (\beta - \beta^*) + \lambda (\beta^T \beta - \nu^2)$$
The dual feasibility condition is $\lambda \geq 0$ and the stationarity condition is

$$\frac{\partial L}{\partial \beta} = 0 \iff 2\Sigma^T(\beta - \beta^*) + 2\lambda\beta = 0 \iff \beta = (\Sigma + \lambda)^{-1}\Sigma\beta^*$$

where we used that $\Sigma^T = \Sigma$. This proves that the stated conditions must hold at the constrained minimizer $\tilde{\beta}$.

We therefore wish to bound

$$\inf_{t \in \mathbb{R}} \left\| t(\Sigma + \lambda)^{-1}\Sigma\beta^* - \frac{\beta^*}{\|\beta^*\|_2} \right\|_2.$$

Making the change of variable $t = t'/\|\beta^*\|$ this is

$$= \inf_{t' \in \mathbb{R}} \left\| t'(\Sigma + \lambda)^{-1}\Sigma\frac{\beta^*}{\|\beta^*\|_2} - \frac{\beta^*}{\|\beta^*\|_2} \right\|_2$$

$$\leq \inf_{t \in \mathbb{R}} \|t(\Sigma + \lambda)^{-1}\Sigma - I\|_{op}$$

$$\leq \inf_{t \in \mathbb{R}, \lambda \geq 0} \|t(\Sigma + \lambda)^{-1}\Sigma - I\|_{op}$$

Since the operator norm is equal to the maximum absolute eigenvalue, this is precisely

$$= \inf_{t \in \mathbb{R}, \lambda \geq 0} \max_{1 \leq k \leq d, \lambda \geq 0} \left| \frac{t\sigma_k}{\sigma_k + \lambda} - 1 \right|.$$

Choosing $t = (1 + \lambda)$ and interchanging max and sup, this is

$$\leq \max_{1 \leq k \leq d, \lambda \geq 0} \left| \frac{(1 + \lambda)\sigma_k}{\sigma_k + \lambda} - 1 \right|.$$

It can be seen by differentiating that for each $\sigma_k$ the inner expression is monotone increasing in $\lambda$ from 0 to $|\sigma_k - 1|$. Therefore, the above expression evaluates to

$$= \max_{1 \leq k \leq d} |\sigma_k - 1|$$

$$= \|\Sigma - I\|_{op}.$$

Finally, this entire argument holds when $\Sigma$ is replaced by $a\Sigma$ for any $a > 0$. Optimizing over all $a$, taking the limit as $a \downarrow 0$ if need be, gives the announced result.
6.5 Proof of Proposition 2

Proof. Firstly, note that since $Y \in \{\pm 1\}$ we may write

$$E \phi(Y, \langle \beta, X \rangle) = E [I\{Y = 1\} \phi(1, \langle \beta, X \rangle) + (1 - I\{Y = 1\}) \phi(-1, \langle \beta, X \rangle)].$$

Iterating expectations then yields

$$= E [P(Y = 1|X) \phi(1, \langle \beta, X \rangle) + (1 - P(Y = 1|X)) \phi(-1, \langle \beta, X \rangle)]
= E [\eta(\langle \beta^*, X \rangle) \phi(1, \langle \beta, X \rangle) + (1 - \eta(\langle \beta^*, X \rangle)) \phi(-1, \langle \beta, X \rangle)]
≡ EF_{\eta, \phi}(\langle \beta^*, X \rangle, \langle \beta, X \rangle),$$

by (ii). Now, let $g \in O_d(\mathbb{R})$ be any rotation such that $g\beta^* = \beta^*$. Note that these rotations form a group, $G$, for which $\{c\beta^* | c \in \mathbb{R}\}$ is the unique invariant subspace. Moreover, for any such rotation, $g^T = g^{-1}$ is also in $G$. By (i) we may then write

$$= EF_{\eta, \phi}(\langle \beta^*, g^T X \rangle, \langle \beta, g^T X \rangle)
= EF_{\eta, \phi}(\langle g\beta^*, X \rangle, \langle g\beta, X \rangle)
= EF_{\eta, \phi}(\langle \beta^*, X \rangle, \langle g\beta, X \rangle).$$

Note also that $\|g\tilde{\beta}\| = \|\tilde{\beta}\|$, so the set of constrained minimizers must contain $\{g\tilde{\beta} | g \in G\}$. However, the minimizer of a convex function over a strictly convex set is unique, so by (iii) we must have $g\tilde{\beta} = \tilde{\beta}$ for all $g \in G$. Thus $\tilde{\beta}$ must belong to the unique invariant subspace of $G$, from which we conclude that $\tilde{\beta} = c\beta^*$.

6.6 Elaborating on remark about excess classification risk in rotationally invariant case

Proof. Under rotational invariance, we have that $\|X\|$ is independent of $Z = X/\|X\|$. We can compute using (2) that

$$E[\|\beta^*, X\| I\{\text{sign } \langle \beta^*, X \rangle \neq \text{sign } \langle \beta, X \rangle\}]
= E[\|\beta^*\|_2 \|X\|_2 | \cos \theta(Z, \beta^*) I\{Z \in S\}]
= ||\beta^*\|_2 E \|X\|_2 E[\|X\|_2 \| \cos \theta(Z, \beta^*) I\{Z \in S\}]$$

$$= ||\beta^*\|_2 E \|X\|_2 \left(\frac{1}{\pi} \int_0^{\theta(\beta, \beta^*)} \sin t dt\right),$$
where the last step uses the fact that $Z$ is uniformly distributed on the sphere. Finally, a similar computation shows that $\|\beta^*\|_2 \mathbb{E} \|X\|_2 = \frac{\pi}{2} \mathbb{E}\left|\langle \beta^*, X \rangle\right|$, completing the proof of our claim. \qed