Abstract

When data analysts train a classifier and check if its accuracy is significantly different from random guessing, they are implicitly and indirectly performing a hypothesis test (two sample testing) and it is of importance to ask whether this indirect method for testing is statistically optimal or not. Given that hypothesis tests attempt to maximize statistical power subject to a bound on the allowable false positive rate, while prediction attempts to minimize statistical risk on future predictions on unseen data, we wish to study whether a predictive approach for an ultimate aim of testing is prudent. We formalize this problem by considering the two-sample mean-testing setting where one must determine if the means of two Gaussians (with known and equal covariance) are the same or not, but the analyst indirectly does so by checking whether the accuracy achieved by Fisher’s LDA classifier is significantly different from chance or not. Unexpectedly, we find that the asymptotic power of LDA’s sample-splitting classification accuracy is actually minimax rate-optimal in terms of problem-dependent parameters. Since prediction is commonly thought to be harder than testing, it might come as a surprise to some that solving a harder problem does not create a information-theoretic bottleneck for the easier one. On the flip side, even though the power is rate-optimal, our derivation suggests that it may be worse by a small constant factor; hence practitioners must be wary of using (admittedly flexible) prediction methods on disguised testing problems.

Keywords: classification accuracy, two sample testing, Fisher’s Linear Discriminant Analysis, permutation testing.
1 Introduction

The recent popularity of machine learning has resulted in the extensive teaching and use of prediction in theoretical and applied communities and the relative lack of awareness or popularity of the topic of Neyman-Pearson style hypothesis testing in the computer science and related “data science” communities. As a result, when practically faced with what is effectively a hypothesis testing problem, where statisticians would construct and study an appropriate test statistic for “direct” testing, data scientists often take a route involving the use of prediction (via estimating a classifier/regressor), and use that as a proxy for “indirect” hypothesis testing.

We study one example of this phenomenon in this paper, concerning arguably the most classical testing and prediction problems – we discuss two sample testing (are the two underlying distributions the same?) and classification (learning a classifier that separates the two distributions well, implicitly assuming they are not the same). These problems will be studied in the linear setting, when the underlying distributions are Gaussians – this statement will become clearer when we formally define the problem setups in Section 2. For now, it suffices to say that for Gaussians, the natural linear classifier is Fisher’s linear discriminant (also known as Fisher’s LDA).

Practitioners familiar with machine learning but not the hypothesis testing literature might not recognize the testing problem, and may instead find it intuitive to perform indirect testing in the following way – first estimate a classifier and then see if its accuracy is significantly different from chance and if it is, then conclude the distributions are different.

The central question that this paper seeks to answer is “what price does one pay for doing testing indirectly instead of directly?”. As we shall detail in Section 2, the notion of cost or price that is appropriate for the Neyman-Pearson hypothesis testing paradigm, is the power achievable at a fixed false positive level $\alpha$ (in other words, the lowest possible type-2 error achievable at some pre-specified target type-1 error). We would like to answer this question in a worst-case sense, relying on the minimax theory from frequentist statistics. So, more formally, we can restate our question as “how much power do we lose compared to the minimax power, for performing hypothesis testing indirectly after prediction?”. This question is interesting because prediction (learning a predictor) is in some sense a harder problem than testing – in one case we are chasing a real vector (the linear classifier) and in the other case we want a binary output (the result of the hypothesis test). We can use that estimated real vector to then do testing, but that may not be optimal (it may perform worse than a “direct” test). Indeed, Vapnik’s advice [1] for solving problems with limited information is:

When solving a given problem, try to avoid solving a more general problem as an intermediate step.

One could be tempted to conjecture that one is attempting to solve a harder problem than needed at first, and this could serve as a bottleneck for the easier problem. Surprisingly, our analysis shows that the aforementioned possible hurdle does not occur in the problems we study, and the prediction before testing does not seem to pose a significant bottleneck. Indeed, in from the perspective of minimax testing error rates, linear classification does allow
us to perform two sample mean testing optimally\(^1\) at least under Gaussianity assumptions under which such a detailed analysis is possible to carry out.

Before we delve into the details, it is worth mentioning that even though this paper is a theoretical endeavor, the question was initially practically motivated. Many scientific questions are naturally posed as two sample tests – examples abound in epidemiology and neuroscience. As a hypothetical example from the latter, consider a particular region of interest in the brain, say the hippocampus. Say we are interested in determining whether the hippocampus responds differently under two situations (say listening to loud harsh sounds vs soft smooth sounds), or for a person with a medical condition (patient) and a person without the condition (control) – the condition could be as varied as depression, autism, Parkinson’s disease, etc. Then, one collects and analyzes brain data for the same patient under the two contrasting stimuli (to study the effect of change in that stimulus), or for different normal and ill patients under the same stimulus (to study effect of onset of disease). It is increasingly common in the field of neuroscience, see [2], to assess whether there is a significant difference between the two sets of data collected by learning a classifier to differentiate between them (because, for instance, they may be more familiar with the problem of classification than that of two sample testing). Neuroscientists call this style of brain decoding, as pattern discrimination and a positive answer can be seen as preliminary evidence that the mental process of interest might occur within the portion of the brain being studied – see [3] for a recent discussion of related issues. The results of our paper would then reassure the neuroscientist that their use of prediction instead of testing, even in the high dimensional setting (where dimensionality is large relative to sample size), should not reduce their power much. At the same time, it should also serve as a warning that a constant factor loss of power might be possible, and for scientific disciplines in which data is not plenty, the scientist should be wary of using prediction techniques for disguised hypothesis testing problems.

**Paper Outline.** In Section 2 we formally define both problems and provide some relevant background information. In Section 3 we discuss lower bounds for two sample testing. In Section 4 we study the power of linear classification for two sample mean testing. In Section 7 we discuss related problem settings, before concluding in Section 9.

**Notation** Let \( \mathcal{N}_d(\mu, \Sigma) \) refer to the \( d \)-variate Gaussian distribution with mean \( \mu \in \mathbb{R}^d \) and \( d \times d \) positive definite covariance matrix \( \Sigma \). With a slight abuse of notation, we shall also use \( \mathcal{N}_d(z; \mu, \Sigma) \) to denote the corresponding Gaussian pdf at a point \( z \) which is given by \((2\pi)^{-d/2}\det(\Sigma)^{-1/2}\exp(-\frac{1}{2}(z - \mu)^T \Sigma (z - \mu))\). \( \| \cdot \| \) refers to the standard Euclidean 2-norm. Let \( \mathbb{I}[-] \) denote the standard 0-1 indicator function, \( \mathbb{R} \) denote the reals, \( \mathbb{E} \) denote expectation.

### 2 Background

In this section, we introduce the two main topics that we touch upon in this paper – two sample mean testing and Fisher’s linear discriminant analysis (LDA). In both these problems, we will be working in the high-dimensional setting, which means the number of dimensions and

\(^1\)In this paper, by *optimally* we typically mean rate-optimally, i.e. we ignore constant factors.
points can both go to infinity simultaneously (we will think of them as being polynomially related since we avoid sparsity assumptions).

2.1 Two Sample Mean Testing

Consider the problem of testing whether two $d$-variate Gaussian distributions $P$ with density $p(x) \overset{\text{def}}{=} \mathcal{N}_d(x; \mu_0, \Sigma)$ and $Q$ with density $q(y) \overset{\text{def}}{=} \mathcal{N}_d(y; \mu_1, \Sigma)$ are identical or not. Given $n$ i.i.d. samples $X_1, ..., X_n \in \mathbb{R}^d$ and $Y_1, ..., Y_n \in \mathbb{R}^d$ from $P$ and $Q$ respectively, we want to differentiate between the null hypothesis that they are the same and the alternate hypothesis that they are different:

$$H_0 : P = Q \text{ vs. } H_1 : P \neq Q.$$  

Since we assume that $P, Q$ are Gaussians with equal covariance, this boils down to

$$H_0 : \mu_0 = \mu_1 \text{ vs. } H_1 : \mu_0 \neq \mu_1.$$  

Two-sample testing is a fundamental decision-theoretic problem, having a long history in statistics – for example, the past century has seen a wide adoption of the t-statistic by [4] to decide if two samples have different population means. It was introduced in the parametric setting for univariate Gaussians, but it has been generalized to multivariate non-Gaussian settings as well. If we assume that $\Sigma$ is known, then Hotelling’s t-statistic is

$$T_H = \left(\hat{\mu}_0 - \hat{\mu}_1\right)^T \Sigma^{-1} \left(\hat{\mu}_0 - \hat{\mu}_1\right)$$

Remark 1. We assume that we have the same number of points drawn from $P, Q$. However if instead we had $n_1, n_2$ points respectively, all of the claimed results will still hold (almost identically) in spirit, whenever $n_1/(n_1 + n_2)$ converges to a constant in $(0, 1)$. This fact can be simply verified by looking at the more general expressions for power derived in [5, 6, 7]. We choose to avoid this complication since it is unnecessary for this paper’s main message.

2.2 Fisher’s Linear Discriminant Classifier

Consider the problem of learning a classifier to differentiate between two $d$-variate Gaussian distributions $P$ with density $p(x) \overset{\text{def}}{=} \mathcal{N}_d(x; \mu_0, \Sigma)$ and $Q$ with density $q(y) \overset{\text{def}}{=} \mathcal{N}_d(y; \mu_1, \Sigma)$. In this paper, we assume that $\Sigma$ is known – we briefly discuss the difficulties of unknown $\Sigma$ in Section 7. Given $n$ i.i.d. samples $X_1, ..., X_n \in \mathbb{R}^d$ and $Y_1, ..., Y_n \in \mathbb{R}^d$ from $P$ and $Q$ respectively, we want to classify a new point $Z$ i.e. we need to predict whether it came from $P$ or $Q$.

Let $P, Q$ correspond to labels 0, 1 respectively. If $\mu_0$ and $\mu_1$ are also known, then the optimal classifier is given by Bayes rule:

$$I \left[ \log \frac{q(Z)}{p(Z)} > 0 \right] = I \left[ \left(\mu_0 - \mu_1\right)^T \Sigma^{-1} \left(Z - \frac{(\mu_0 + \mu_1)}{2}\right) > 0 \right]$$
We denote \( \delta \overset{\text{def}}{=} \Sigma^{-1/2}(\mu_0 - \mu_1) \) and \( \mu \overset{\text{def}}{=} \frac{\mu_0 + \mu_1}{2} \) so that we can write the Bayes rule as

\[
I[\delta^T \Sigma^{-1/2}(Z - \mu) > 0]
\]

Then, Fisher’s Linear Discriminant Analysis (LDA) classification rule is given by

\[
\text{LDA}_{n,n}(Z) \overset{\text{def}}{=} I[\hat{\delta}^T \Sigma^{-1/2}(Z - \hat{\mu}) > 0]
\]

where \( \hat{\delta} \) and \( \hat{\mu} \) are the corresponding plugin empirical estimators of \( \delta \) and \( \mu \) using \( \hat{\mu}_0 \overset{\text{def}}{=} \frac{1}{n} \sum_i X_i/n \) and \( \hat{\mu}_1 \overset{\text{def}}{=} \frac{1}{n} \sum_i Y_i/n \) and the subscript \( n,n \) is to remind the reader of the implicit dependence of \( \text{LDA}_{n,n}(Z) \) on the \( n \) input data points from each class. It has its roots in Fisher’s work \([8, 9]\) and was later developed further by Wald \([10]\) and Anderson \([11]\) (due to which it is also sometimes called the Anderson statistic).

Define the error of LDA conditioned on the input data as:

\[
\mathcal{E}_n \overset{\text{def}}{=} \frac{(\mathcal{E}_1 + \mathcal{E}_2)}{2} \tag{1}
\]

where

\[
\mathcal{E}_1 \overset{\text{def}}{=} \Pr_{Z \sim \mathcal{P}}(\text{LDA}_{n,n}(Z) = 1 \mid X_1^n, Y_1^n),
\]

\[
\mathcal{E}_2 \overset{\text{def}}{=} \Pr_{Z \sim \mathcal{Q}}(\text{LDA}_{n,n}(Z) = 0 \mid X_1^n, Y_1^n).
\]

Clearly, \( \mathcal{E}_n \) is a non-constant random variable that depends on the input data. Next, define the (unconditional) error of LDA as

\[
E_n \overset{\text{def}}{=} (E_1 + E_2)/2 \tag{2}
\]

where

\[
E_1 \overset{\text{def}}{=} \mathbb{E}_{n,n} \left[ \Pr_{Z \sim \mathcal{P}}(\text{LDA}_{n,n}(Z) = 1 \mid X_1^n, Y_1^n) \right],
\]

\[
E_2 \overset{\text{def}}{=} \mathbb{E}_{n,n} \left[ \Pr_{Z \sim \mathcal{Q}}(\text{LDA}_{n,n}(Z) = 0 \mid X_1^n, Y_1^n) \right].
\]

where \( \mathbb{E}_{n,n} \) denotes the expectation with respect to the \( n \) input points from each class, and \( X_1^n, Y_1^n \) denote the input datasets. Note that since the input data has already been integrated out, \( E, E_1, E_2 \) do not depend on the input data and are only functions of \( n, d, \|\delta\| \).

One can estimate \( E \) in a few different ways. One simple way is via sample splitting – we form the LDA classifier using the first \( n/2 \) samples of each class, and estimate its test error using the remaining \( n/2 \) samples of each class. We denote the sample-splitting error as \( \hat{E}^S \) defined as

\[
\hat{E}^S \overset{\text{def}}{=} \frac{(\hat{E}_1^S + \hat{E}_2^S)}{2} \tag{3}
\]

where

\[
\hat{E}_1^S \overset{\text{def}}{=} \frac{1}{n/2} \sum_{i=1}^{n/2} \mathbb{1}[\text{LDA}_{n/2,n/2}(X_{n/2+i}) = 1],
\]

\[
\hat{E}_2^S \overset{\text{def}}{=} \frac{1}{n/2} \sum_{i=1}^{n/2} \mathbb{1}[\text{LDA}_{n/2,n/2}(Y_{n/2+i}) = 0].
\]
where LDA\(_{n/2,n/2}\) represents the LDA classifier formed from the first \(n/2\) points of each class. It is clear from the definitions that the LDA classifier will have a true accuracy significantly above half if and only if \(\mu_0 \neq \mu_1\). This implies that one can actually use \(\hat{E}^S\) as a test statistic for two sample testing. We shall derive the power of such a test in Section 4 and compare it to the best possible power (in a minimax sense).

**Remark 2.** For clarity, we only deal with the case of equal sample sizes and when the prior probability of drawing a sample from \(P\) and \(Q\) is equal. When we have an unbalanced prior probabilities of sampling from each class \((\alpha_0, \alpha_1) \neq (1/2, 1/2)\) where \(\alpha_0 + \alpha_1 = 1\), one can verify that these results carry forward in the same spirit. To explain, we would observe \(n_0\) and \(n_1\) points in each class, where \(n_0/(n_0+n_1)\) converges to \(\alpha_0 \in (0,1)\) and the overall error in Eq.(2) would be \(\alpha_0E_0 + \alpha_1E_1\) and one can generalize our results using the expressions of [12] to achieve similar conclusions, or more specifically, Eq.(3.8) in [13].

### 3 Lower bounds for two sample testing

Before we present our analysis of the power of indirect two sample testing (via classification), we first begin by understanding the fundamental minimax lower bounds for two sample testing. [14] prove that when the two random variables \(X', Y' \in \mathbb{R}^d\) are both Gaussian with identity covariance, with a mean difference of \(\delta' \in \mathbb{R}^d\), the minimax power (over all tests having access to \(n\) points from each, that have type-1 error at most \(\alpha\)) for testing \(\delta' = 0\) vs \(\delta' \neq 0\) is given by

\[
\Phi \left( -\frac{\sqrt{d}}{\sqrt{d + n\|\delta'\|^2}} z_{\alpha} + \frac{\|\delta'\|^2}{\sqrt{8 \frac{d}{n} + 8 \|\delta'\|^2 / n}} \right) + o(1)
\]

where \(\Phi\) is the standard Gaussian CDF, \(z_{\alpha}\) is the point representing the right \(\alpha\)-quantile of the standard Gaussian distribution, i.e. \(\Phi(-z_{\alpha}) = \alpha\) and \(\Phi(z_{\alpha}) = 1 - \alpha\). This paper treats \(z_{\alpha}\) as a constant (for example, \(z_{\alpha} \approx 2\) for \(\alpha = 0.05\)).

The way we translate this lower bound into our setting is as follows. Given a dataset \(\{X_i, Y_i\}\) from Gaussians that have mean difference \(\delta\) and common covariance \(\Sigma\), we form standardized variables \(X_i' \overset{\text{def}}{=} \Sigma^{-1/2}X_i\) and \(Y_i' \overset{\text{def}}{=} \Sigma^{-1/2}Y_i\). Then the mean difference between \(X', Y'\) is \(\delta' = \Sigma^{-1/2}\delta\) and \(X', Y'\) also have identity covariance. Now we can apply the aforementioned lower bound of [14]. Resubstituting \(\|\delta'\|^2 = \delta^T\Sigma^{-1}\delta\) we then get a lower bound for power given by

\[
\Phi \left( -\frac{\sqrt{d}}{\sqrt{d + n\delta^T\Sigma^{-1}\delta}} z_{\alpha} + \frac{\delta^T\Sigma^{-1}\delta}{\sqrt{8 \frac{d}{n} + 8 \delta^T\Sigma^{-1}\delta / n}} \right) + o(1)
\]

For convenience of notation, we shall use \(\Psi^2 := \delta^T\Sigma^{-1}\delta\) to denote our signal to noise ratio. The way to interpret the above bound is as follows. The first term inside the parentheses is not of interest for our purposes, its magnitude being bounded by the constant \(z_{\alpha}\). The second term is what determines the rate at which the power approaches 1. When \(\delta = 0\), the power reduces to \(\Phi(-z_{\alpha}) = \alpha\) and if \(d, n\) are thought of as fixed, larger \(\delta\) leads to larger...
power. The key in high dimensions, however, is how the power depends jointly on the signal to noise ratio \( \Psi, d, n \). To see this clearer, in the low SNR regime when \( \Psi^2 << d/n \), the power lower bound morally simplifies to

\[
\Phi \left( -z_{\alpha} + \frac{n \Psi^2}{\sqrt{8d}} \right) + o(1) \quad (4)
\]

We can already see that at constant SNR, \( n \) only needs to scale faster than \( \sqrt{d/n} \) for test power to asymptotically approach unity – this \( \sqrt{d/n} \) scaling is unlike the \( d/n \) scaling one typically sees in prediction problems (for prediction error or classifier recovery). Let us now see how the power of the classification accuracy of Fisher’s LDA fares against the aforementioned minimax lower bounds for power.

4 Upper bounds for power of Fisher’s LDA

We begin by noting that \[13\] give an expression for the true (unknown) classification error \( E \) from Eq.(2):

\[
E_n = \Phi \left( -\frac{\Psi}{2} + \frac{1}{\sqrt{1 + \frac{2d}{n \Psi^2}}} \right) \quad (5)
\]

where we introduce the subscript \( n \) to remind us that this expression captures the error of the classifier if \( n \) points were used in training. This expression was proved by the authors to be asymptotically exact in the high-dimensional setting, under the so-called Raudys-Kolmogorov double asymptotics of \( n, d \to \infty \) with \( n/d \to c \in (0, \infty) \).

When conditioned on the data, the sample splitting error estimator \( \hat{E}^S \) in Eq.(3) is an unbiased estimator of \( E_{n/2} \), i.e.

\[
\mathbb{E}[\hat{E}^S | X_1^n, Y_1^n] = E_{n/2}.
\]

Marginalizing out the data, we see that

\[
\mathbb{E}[\hat{E}^S] = \mathbb{E}_{n/2, n/2}[E_{n/2}] = E_{n/2}.
\]

Further, note that \( \hat{E}^S \) is a sum of indicator functions (coin flips), each of which are (conditionally) i.i.d. given the training sample. Hence, conditional on the data we may conclude that \( \hat{E}^S \) is approximately normally distributed with mean \( E_{n/2} \) and conditional variance \( \frac{E_{n/2}(1-E_{n/2})}{n^2} \).

Since we are (morally) interested in the setting where the signal to noise ratio \( \Psi \) is small enough that the problem is hard, we may restrict our thinking to the regime where \( \Psi \) is near 0, \( E_{n/2} \) and \( E_{n/2} \) are close to 1/2, and we do not lose much accuracy when we conservatively approximate \( E_{n/2}(1-E_{n/2}) \) by its upper bound 1/4. Hence, unconditional on the training data, a reasonable asymptotic approximation is given by

\[
\hat{E}^S \sim \mathcal{N}\left( E_{n/2}, \frac{1}{2n} \right).
\]
Note that under $H_0$, we have

$$\hat{E}^S \sim \mathcal{N}\left(\frac{1}{2}, \frac{1}{2n}\right).$$

Hence, we define our test statistic to be the (scaled) difference between the estimated error and half:

$$T^S := \sqrt{n/2} - \sqrt{2n}\hat{E}^S = \sqrt{2n}(1/2 - \hat{E}^S)$$

which is distributed as a standard Gaussian $\mathcal{N}(0, 1)$ under the null, and a $\mathcal{N}(\sqrt{2n}(1/2 - E_{n/2}), 1)$ under the alternative. Hence, if $z_\alpha$ is the $1 - \alpha$ quantile of the standard Gaussian distribution, i.e. $\Pr(Z > z_\alpha) = \alpha$ for a standard Gaussian $Z$, then the corresponding test

$$\mathbb{I}\left[T^S > z_\alpha\right]$$

has an asymptotic type-1 error (probability of wrongly rejecting the null hypothesis when the null is true) controlled by $\alpha$, and it has power (probability of rightfully rejecting the null when the null is indeed false) given by

$$\Pr(T^S > z_\alpha) = \Pr\left(T^S - \sqrt{2n}(1/2 - E_{n/2}) > z_\alpha - \sqrt{2n}(1/2 - E_{n/2})\right)$$

$$\approx \Phi\left(\sqrt{2n}(1/2 - E_{n/2}) - z_\alpha\right)$$

where the $\approx$ is due to the variance approximation of $1/4$. Hence, the power comes down to how $E_{n/2}$ behaves around $1/2$ (the value achieved when $\Psi = 0$). Once more, since we are interested in the regime when $E_{n/2}$ is close to half (the testing problem is hard), we do not lose much accuracy with the following Taylor expansion:

$$\Phi(t) \approx \Phi(0) + \phi(0)t$$

where $\phi$ is the Gaussian pdf, hence $\phi(0) = 1/\sqrt{2\pi}$ and $\Phi(0) = 1/2$. From Eq.(5) when using $n/2$ points, we get

$$E_{n/2} = \Phi\left(-\frac{\Psi}{2} \frac{1}{\sqrt{1 + \frac{4d}{n\Psi^2}}}\right)$$

$$\approx 1/2 - \frac{\Psi}{2\sqrt{2\pi}} \frac{1}{\sqrt{1 + \frac{4d}{n\Psi^2}}}$$

and hence

$$1/2 - E_{n/2} \approx \frac{\Psi^2}{\sqrt{8\pi}} \frac{1}{\Psi^2 + \frac{4d}{n}}.$$
Substituting this back into Eq.(7), we get the power of $T^S$ can be approximately given by

$$
\Phi \left( \frac{\sqrt{2n}\Psi^2}{\sqrt{8\pi}} - \frac{1}{\sqrt{\Psi^2 + \frac{4d}{n}}} - z_\alpha \right) = \Phi \left( \frac{\Psi^2}{\sqrt{4\pi \frac{\Psi^2}{n} + 16\pi \frac{d}{n^2}}} - z_\alpha \right)
$$

Comparing this with the lower bound expression

$$
\Phi \left( \frac{\Psi^2}{\sqrt{8\frac{\Psi^2}{n} + \frac{8d}{n^2}}} - \sqrt{d} \frac{z_\alpha}{\sqrt{d + n\Psi^2}} \right) + o(1),
$$

we can conclude that using linear classification accuracy is essentially minimax optimal, up to small constant factors. Specifically, when $\Psi^2 << d/n$, i.e. we are in the low SNR regime when the errors are close to half, the asymptotic power of Fisher’s LDA is given by

$$
\Phi \left( \frac{n\Psi^2}{\sqrt{16\pi d}} - z_\alpha \right)
$$

which is just a small constant factor worse than the minimax lower bound in Eq.(4).

5 When $\Sigma$ is unknown

For two sample testing in the fixed $d$ setting, there are strong reasons to prefer Hotelling’s t-test. For example, it is known to be the “uniformly most powerful” test when $P, Q$ are univariate Gaussians under fairly general assumptions [15, 16, 17, 18]. In a seminal paper by [5], the authors proved that $T_H$ has asymptotic power tending to the (trivial) value of $\alpha$ in the high dimensional setting, when $d, n \to \infty$ with $d/n \to 1 - \epsilon$ for small $\epsilon$. This is the regime where $d < n$ so $\hat{\Sigma}$ is invertible, but they intuitively pointed out that with around $d$ samples, one would get a very ill-conditioned estimate of (the inverse of) the $d \times d$ matrix $\Sigma$ which has $d^2$ unknowns.

This motivated the study of alternate test statistics; for instance, the authors show that dropping $\hat{\Sigma}$ from the Hotelling test statistic entirely leads to a test that does have asymptotic power tending to 1 in the high-dimensional setting. Following that, [6] propose (in a similar spirit) the test statistic

$$
T_{SD} := (\hat{\mu}_0 - \hat{\mu}_1)^T \text{diag}(\hat{\Sigma})(\hat{\mu}_0 - \hat{\mu}_1)
$$

that replaces $\hat{\Sigma}$ by $\text{diag}(\hat{\Sigma})$ in Hotelling’s statistic also leads to high-dimensional consistency.

For the classification problem, there is a similar vein of results paralleling the results of two sample testing, even though this connection has seemingly not been explicitly mentioned in either set of papers to the best of our knowledge. For example, [19] prove that when $\Sigma$ is unknown, the error of Fisher’s LDA can be terrible in the high dimensional setting. They instead consider the “Naive Bayes” (NB) classification rule given by

$$
\text{NB}_{n,n}(Z) \overset{\text{def}}{=} \mathbb{I} \left[ \delta^T \text{diag}(\hat{\Sigma})^{-1/2}(Z - \hat{\mu}) > 0 \right]
$$

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which just assumes that the features are independent (similarly using \( \text{diag}(\hat{\Sigma}) \) as the estimator of \( \Sigma \) in the LDA rule). The show that NB can have a much better accuracy than LDA in the high dimensional setting (in the worst case).

This understated connection has important implications for extending the results of our paper. Indeed, from the aforementioned examples of high dimensional consistency resulting from using \( \text{diag}(\hat{\Sigma}) \) to replace \( \hat{\Sigma} \) in both two sample testing and classification, one should expect that the conclusions of this paper should also morally extend to the setting where \( \Sigma \) is unknown, when both the classifier and the two-sample test use the same substitute for \( \hat{\Sigma} \).

6 Permutation Testing

In practice, instead of using the kind of asymptotic approximations that we have analyzed, one often employs randomization tests also known as permutation tests. For a direct two sample test, we would do the following.

**Permutation Test:** Calculate \( T^* \) on the full data \( X,Y \). Repeat \( P \) times: Pool the samples \( X,Y \) into one bag, permute the samples, split it into two parts \( X^p,Y^p \). Evaluate the test statistic on each of these permuted samples, call this \( T^p \). Sort all the statistics \( T^*,T^1,...,T^P \); if the rank of \( T^* \) in the right \( \alpha \)-quantile (larger accuracy than \( 1 - \alpha \) fraction), then reject the null hypothesis.

We would like to note the two possible ways of applying permutation testing within the classification via sample splitting framework, because of the subtleties involved. The methods below differ in the italicized text.

**Method 1:** Split data into two halves, call these \( X^1,Y^1 \) and \( X^2,Y^2 \). Train the classifier on \( X^1,Y^1 \), call this \( f^* \). Evaluate accuracy of \( f^* \) on \( X^2,Y^2 \), call this \( a^* \). Repeat \( P \) times : Pool the samples \( X^2,Y^2 \) into one bag, permute the samples, and then split it into two parts, \( X^p,Y^p \). Evaluate the accuracy of \( f^* \), on this permuted data, call this \( a^p \). Sort all the accuracies \( a^*,a^1,...,a^P \); if the rank of \( a^* \) in the right \( \alpha \)-quantile (larger accuracy than \( 1 - \alpha \) fraction), then reject the null hypothesis.

**Method 2:** Split data into two halves, call these \( X^1,Y^1 \) and \( X^2,Y^2 \). Train the classifier on \( X^1,Y^1 \), call this \( f^* \). Evaluate accuracy of \( f^* \) on \( X^2,Y^2 \), call this \( a^* \). Repeat \( P \) times : Pool all samples \( X^1,Y^1,X^2,Y^2 \) into one bag, permute the samples, and then split it into 4 parts \( X^p,Y^p,X'^p,Y'^p \). Train a new classifier \( f^p \) on the first half, evaluate it on the second half, to get accuracy \( a^p \). Sort all the accuracies \( a^*,a^1,...,a^P \); if the rank of \( a^* \) in the right \( \alpha \)-quantile (larger accuracy than \( 1 - \alpha \) fraction), then reject the null hypothesis.

In our opinion, method 2 should be preferred to method 1, but their difference is rather subtle. The first method tests whether \( f^* \) is significantly different from chance. The second method tests whether any classifier can be learned that performs significantly different from chance. In other words, for testing the null hypothesis as we have stated it, permutation testing should be wrapped around the whole procedure of calculating a test statistic, not just around the second half of such a procedure. We currently don’t have a formal analysis to support this but we only expect minor (asymptotically negligible) differences between the finite-sample performance of the studied test and the permutation-variant, making the qualitative statements from our analysis carry forward to the permutation setting.

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\(^2\)In practice people choose \( P \) in the range of 100s to 1000s.
7 Related Settings

Here we discuss how our results may be extended to a larger context.

7.1 Leave one out classification accuracy

Another natural estimator for accuracy, as an alternative to sample-splitting, is a leave-one-out estimator $\hat{E}^L$, defined as

$$\hat{E}^L \overset{\text{def}}{=} (\hat{E}^L_1 + \hat{E}^L_2)/2$$

where

$$\hat{E}^L_1 \overset{\text{def}}{=} \frac{1}{n} \sum_{i=1}^{n} I[\text{LDA}_{n \setminus i}(X_i) = 1],$$

$$\hat{E}^L_2 \overset{\text{def}}{=} \frac{1}{n} \sum_{i=1}^{n} I[\text{LDA}_{n \setminus i}(Y_i) = 0].$$

where $\text{LDA}_{n \setminus i}$ (or $\text{LDA}_{n,n \setminus i}$) denotes the LDA classifier created from all points except $X_i$ (or all points except $Y_i$). We conjecture that a test statistic based on this might save the constant factor loss in power due to sample splitting.

7.2 Resubstitution classification accuracy

Since leave-one-out estimators are computationally intensive, one might be tempted to use the training data itself to test the classifier. This resubstitution error would be defined as

$$\hat{E}^R \overset{\text{def}}{=} (\hat{E}^R_1 + \hat{E}^R_2)/2$$

where

$$\hat{E}^R_1 \overset{\text{def}}{=} \frac{1}{n} \sum_{i=1}^{n} I[\text{LDA}_{n,n}(X_i) = 1],$$

$$\hat{E}^R_2 \overset{\text{def}}{=} \frac{1}{n} \sum_{i=1}^{n} I[\text{LDA}_{n,n}(Y_i) = 0].$$

where we first train on all the data and then test on all the data. Of course such an estimate would be overoptimistic, and would be scorned upon as an estimate of the true accuracy $E$ of the classifier. However, one might wonder if the null distribution would be similarly optimistically biased, nullifying the optimistic bias of $\hat{E}^R$. Our conjecture is that a test statistic based on resubstitution would actually be worse than both sample splitting and leave-one-out.

7.3 Non-linear Classification

Another natural setting is that of nonlinear classification. An examination of the test statistics used (Hotelling and its variants) shows that they are closely related to the statistics based on the kernel Maximum Mean Discrepancy of [20] and the kernel FDA of [21], when
specifically instantiated with the linear kernel. Similarly, for classification, a kernelized LDA was proposed by [22] which specializes to Fisher’s LDA when the linear kernel is employed.

Given the parallels observed in the other settings, one might naturally conjecture that the spirit of the results of this paper can be extended to such kernelized nonlinear settings as well.

7.4 Neyman-Pearson Classification

We would like to mention that while a Neyman-Pearson classification framework was proposed and analyzed in [23], the setting is quite different since that work considers the problem of minimizing probability of error for one class, subject to a bound on the probability of error of the other class. We are instead interested in minimizing probability of not detecting the two classes are different, subject to a bound on the probability of detecting them as different when they are actually the same. Thus, we consider a different connection to testing than [23] and a classification approach for our testing problem appears to be harder than testing (what label is it for each data point vs are all labels the same for all points).

8 Experiments

Here, we ran a couple of simple simulations to compare the performance of the algorithm (upper bound) with the theoretical lower bound. The setup is as follows: for each of $E$ difference choices of $d, n$, with $d/n = \kappa$, we draw $n$ samples from two $d$ dimensional identity-covariance Gaussians that have mean difference given by $\Psi \cdot (1, 1, 1, 1, ..., 1)$. We split the sample into two parts, train the classifier on the first and test it on the second. We use a cutoff $z_\alpha$ to determine if the test in Eq.(6) rejects or not. We then repeat this procedure $R$ times to determine the power, i.e. probability of rejecting while controlling level at $\alpha$. On all plots, higher is better.

8.1 Constant power

In the following experiment, we choose $E = 30, R = 200, z_\alpha = 2, \Psi = 3/d^{1/4}, \kappa = 1$ with $d, n$ varying from 20 to 600 in increments of 20. This setting was selected because it leads to (asymptotically) constant power according our theoretical analysis, for both upper and lower bounds, where the theoretical minimax power should approach

$$\Phi(-2 + 9/\sqrt{8}) \approx 0.88$$

and hence would be suitable for visualization on a graph ([14] already proved that the lower bound is asymptotically tight including all constants, so it serves as an excellent benchmark).

The slightly bumps in the blue curve are because we use $R$ repetitions to calculate the power (the number of times it rejected divided by $R$). The larger the $R$ used, the smoother the estimated curve would be. However, we can already make out from the above curve that it is tracking the minimax power accurately, but is consistently slightly lower.
8.2 Increasing power

In the following experiment, the setup is almost the same as the previous experiment, except that for each $1 \leq e \leq E$, we used $\Psi = \frac{e}{10d^{1/4}}$. In this setting, the theoretical prediction is that the power will increase from (near) zero in the first setting to (near) one in the last setting. (once more, we chose $\Psi$ so that we can visualize the effect easily without saturation near zero or one)

Once more, the power of the classifier accuracy is tracking the minimax power quite accurately, while always staying below it.
9 Conclusion

This paper gave a basic statistical analysis for the use of classification accuracy as a test statistic for two sample testing. Theoretically, we find that the classification accuracy of Fisher’s LDA is rate-optimal in the minimax sense for two sample mean testing of Gaussians with known covariance. We conjecture that such results should also hold when the covariance is unknown, and for nonlinear settings. Practically, the possible constant factor loss in power may be a worry in settings where sample sizes are low, dimensionality is high, signal to noise ratio is small, and practitioners may want to get the most from their data.

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