REGULARIZATION IN HIGH-DIMENSIONAL REGRESSION AND CLASSIFICATION VIA RANDOM MATRIX THEORY

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ABSTRACT. We study general singular value shrinkage estimators in high-dimensional regression and classification, when the number of features and the sample size both grow proportionally to infinity. We allow models with general covariance matrices that include a large class of data generating distributions. As far as the implications of our results are concerned, we find exact asymptotic formulas for both the training and test errors in regression models fitted by gradient descent, which provides theoretical insights for early stopping as a regularization method. In addition, we propose a numerical method based on the empirical spectra of covariance matrices for the optimal eigenvalue shrinkage classifier in linear discriminant analysis. Finally, we derive optimal estimators for the dense mean vectors of high-dimensional distributions. Throughout our analysis we rely on recent advances in random matrix theory and develop further results of independent mathematical interest.

CONTENTS

1. INTRODUCTION

In recent years scientists in many different disciplines have access to very high-dimensional data sets. The abundance of data together with the significant increase in computing power has allowed them to perform analyses that would have been impossible some decades ago. On the other hand, it is known that classical statistical theory does not provide accurate explanations of the performance of the methods used when the data dimension increases to infinity (see, for example, Yao et al.

[2015]). As a result, serious effort has been put in the last years by statisticians to develop theory that better captures the relevant aspects in this setting and suggest better procedures for estimation, testing and prediction. Many of the methods that have successfully been used in practice rely on incorporating prior knowledge to the estimation procedure. A common hypothesis in many applications is that each predictor variable has a small effect on the outcome, a statement that will be made precise later. A widely used method in this scenario is ridge regression and ridge-regularized discriminant analysis. Those methods were studied in detail in Dobriban and Wager [2018], where the authors provide exact asymptotic formulas for the limiting out-of-sample predictive risk. In this paper, we vastly extend their results to more general shrinkage methods.

For the case of regression the main assumption, which was also used in Dobriban and Wager [2018], is that we observe i.i.d. data points $(x_i, y_i) \in \mathbb{R}^p \times \mathbb{R}$ from a linear model $y_i = w^\top x_i + \varepsilon_i$. We will use the notation $X = (x_1, \cdots, x_n) \in \mathbb{R}^{p \times n}$. To model the assumption that each predictor variable has a small effect on the outcome the authors suggested the so-called Random Regression Coefficient Hypothesis (RRC), namely that the coefficent vector w has i.i.d. coordinates with mean 0 and variance $\alpha^2 p^{-1}$. We study estimates based on general shrinkage of the spectrum of the predictor matrix of the form $\hat{w} = \sum h(\lambda_i) u_i v_i^\top n^{-1/2} y$, where $\sum \sqrt{\lambda_i} u_i v_i^\top$ is the singular-value-decomposition of $n^{-1/2} X$. These include as special cases the ridge regression estimate, but also the estimated coefficient vector after any step of descent-based optimization schemes. The extensions we provide here have important implications about early stopping in gradient descent-trained models and the interplay between the regularization parameter and the optimal stopping time in training. Early stopping has been used by practitioners in the deep learning community for a while (see Bengio [2012] for an explanation) as a regularization method. In many cases it has been observed that instead of fully minimizing the loss function in a regression or classification task, it is better for out-of-sample predictions to stop the decent optimization algorithm after fewer iterations. In our models this will become apparent for under-regularized ridge-regression with exact asymptotic formulas. For the case of simple linear regression with identity covariance matrix and no l_2 regularization parameter the learning curves have been studied in Advani and Saxe [2017]. For general covariance matrix asymptotic limits are derived in Ali et al. [2018], but their formulas are rather intractable. Here we are going to get as a byproduct of our main theorems a more general analysis of the problem under an arbitrary covariance matrix of the predictor variables and the inclusion of an l_2- penalty and provide explicit formulas for the limits for a more general class of estimators. We are also going to verify that no singular value shrinkage method can perform better than ridge regression with the Bayes optimal regularization parameter as a simple corollary of Theorem 1. A common assumption that allows us to use the asymptotic results of random matrix theory is that we are working in a regime with p-dimensional features and n data points such that $p, n \to \infty, pn^{-1} \to \gamma > 0$. This assumption will be of great importance throughout this paper. In addition, we assume that the spectral distribution of the population covariance matrix Σ of the predictor variables converges weakly to a deterministic limiting spectral measure H supported on $[0, \infty)$. The model will be explained in detail in Section 3.

For the case of classification using linear discriminant analysis in the dense setting that we consider in this paper, to the best of our knowledge, not much work has been

done that departs from the ridge-regularized method proposed in Dobriban and Wager [2018]. The main assumption is that we have observed data points from two Gaussian distributions in $\mathbb{R}^p$ with $\mathcal{N}(\delta, \Sigma), \mathcal{N}(-\delta, \Sigma)$, where the coordinates of δ are i.i.d. with mean zero and variance $\alpha^2 p^{-1}$. We then estimate $\delta, \hat{\Sigma}$ from the data and use them to classify new data points based on Bayes' rule. Since one main problem with the performance of discriminant analysis in high-dimensions is the noise in the estimation of the covariance matrix, one might attempt to perform eigenvalue shrinkage to the empirical covariance matrix before using it for a classification task in the same way as the authors do for covariance estimation in Ledoit and Wolf [2004], Ledoit and Wolf [2012] and Ledoit and Wolf [2017]. Usually this is done by doing the spectral decomposition $\hat{\Sigma} = \sum_{i=1}^{p} \hat{\lambda}_i u_i u_i^\top$ and then using a function h to shrink the eigenvalues and produce the estimate $h(\hat{\Sigma}) = \sum_{i=1}^{p} h(\hat{\lambda}_i) u_i u_i^\top$. Two questions arise naturally in discriminant analysis, if one uses such a method. The first one concerns the asymptotic prediction accuracy and the second one concerns whether it is possible to improve the performance by selecting a novel shrinkage method, since optimality of shrinkage functions has only been studied (as we will see below) for specific losses that do not include the classification error of discriminant analysis. Our theorems in Section 4 will answer both questions later on. For this it will be necessary to prove convergence of certain trace functionals involving both the true and empirical covariance matrices of the predictor variables, a result of independent mathematical interest.

1.1. **Our Contributions.** We derive results of independent mathematical interest for the convergence of some trace functionals that include both the population and the sample covariance matrices in Proposition 1. This will be particularly useful for the proof of our main theorem (Theorem 1), which gives the asymptotic prediction risk for a large class of estimators for the coefficient vector w, but also has other important applications that we discuss. For instance, we explain in Corollary 1 how it can be used to recover the optimal shrinkage function for covariance estimation in Frobenius norm derived heuristically in Ledoit and Péché [2011] and used in Ledoit and Wolf [2012]. Another interesting application is related to optimal shrinkage for estimation of means of high-dimensional distributions. This is done in Proposition 4, where we suggest an empirical Bayes estimator with strong theoretical motivation. Moreover, Theorem 1 implies the optimality of ridge regression with a suitable parameter among all singular value shrinkage-based methods. Finally, Theorem 1 can be used to prove Proposition 2, which describes the test error evolution in gradient descent training. This gives us important insights about the early stopping regularization method used in neural networks. In particular, even in this very simplistic setting the regime we are studying explains some attributes of the overtraining phenomenon seen in much more complex models.

For classification we prove Proposition 5 as the main tool for our analysis. We use it to derive asymptotic formulas for the classification error of high-dimensional linear discriminant analysis under general nonlinear shrinkage functions for covariance estimation in Theorem 2. After that, we study an optimization problem that gives the optimal shrinkage function for classification and explain how the optimum behaves for different values of signal-to-noise ratio. We also study a relaxation of the problem that can be solved analytically and show that a combination of the shrinkage for covariance estimation in Ledoit and Wolf [2012] and ridge-regularization is close to optimal in the sense that it provides the solution to this relaxation.

This important observation can be used to approximate the optimal shrinkage at the same computational cost as tuning a ridge parameter for LDA. Before the development of the tools that we present here this analysis was impossible for general nonlinear shrinkage functions. Proposition 5 that gives exact asymptotics for $\lim_{p\to\infty} p^{-1}tr\left(\Sigma h(\hat{\Sigma})\Sigma h(\hat{\Sigma})\right)$ for any continuous function h, where Σ is the population covariance matrix and $\hat{\Sigma}$ is the sample covariance matrix was particularly useful for this purpose.

1.2. **Related Work.** In the same direction as Dobriban and Wager [2018], the authors in Hastie et al. [2019] study least-norm high-dimensional regression in a setting similar to ours. They also consider random kernel features interpolators and study the asymptotic risk. For that purpose the predictor variables are generated as $x_i = \phi(Wz_i), z_i \sim \mathcal{N}(0, I_d)$, where $W \in \mathbb{R}^{p\times d}$ is a matrix with i.i.d. entries with distribution $\mathcal{N}(0, d^{-1})$ and d is an integer that grows proportionally to p, n. This corresponds to the linearization of a two-layer neural network with random weights in the first layer. Interesting behaviour arises with this model for minimum-norm regression due to the double descent shape of the risk curve. Random features regression is also studied in Mei and Montanari [2019] for learning an unknown function over the d-dimensional sphere via ridge regression.

As mentioned earlier, incorporating prior knowledge is usually extremely important for extending statistical methods to high dimensions. A different set of hypotheses are related to sparsity, according to which only a relatively small number of parameters in a regression or classification task are nonzero (Hastie et al. [2015]). One of the first papers that showed that even in the extremely high-dimensional regime with $p >> n$ it is possible, under certain assumptions, to recover (with high probability) the coefficient vector was Candes et al. [2006]. Other papers in the vast literature in this direction are, for example, Bayati and Montanari [2011], where the authors derive the asymptotic risk for LASSO, or Donoho and Montanari [2016], where the authors study the asymptotic variance of M-estimators.

As far as high-dimensional classification is concerned, in Bickel et al. [2004] it is explained that classification using the full sample covariance matrix gives poor performance and a Naive Bayes classifier is suggested instead. In Fan and Fan [2008] the authors argue that such independence rules may not be enough and suggest that feature selection rules are necessary. In Bickel et al. [2008] the closely related problem of covariance estimation is studied and thresholding-based methods are examined. For high-dimensional logistic regression, which is another commonly used classification method, high-dimensional phenomena are studied in Candès and Sur [2018],Sur and Candès [2019], Sur et al. [2019]. The authors consider extremely important questions such as the existence and asymptotic distribution of the Maximum-Likelihood Estimator for logistic regression when the number of features grows proportionally to the sample size. The asymptotic loss for a large class of binary classifiers (including logistic regression and maximum margin classifiers) in the high-dimensional regime considered here was studied in Taheri et al. [2020].

Eigenvalue shrinkage and thresholding methods have been used in solving many problems. First of all, shrinkage methods for covariance estimation have been studied previously by many researchers. The authors in Ledoit and Wolf [2004] proposed a well-conditioned shrinkage estimator for the empirical covariance matrix based on a linear shrinkage method. In Ledoit and Wolf [2012] the authors extended their method to the study the optimal (with respect to some loss) rotation invariant

nonlinear shrinkage estimator for a covariance matrix using results from random matrix theory and in Ledoit and Wolf [2017] kernel estimation was used to improve the numerical stability and speed of the optimal nonlinear shrinkage procedure. Finally, optimal shrinkage functions for a spiked covariance model for 26 different loss functions were obtained (for most of them analytically) in Donoho et al. [2018]. A closely related application in symmetric matrix denoising via singular value thresholding can be found in Donoho et al. [2014] and Gavish and Donoho [2014].

1.3. **Organization of the Paper.** In Section 2 we review some useful results from random matrix theory. Some of those results have been used in Dobriban and Wager [2018], but here we will be required to develop more mathematical tools to derive our results. This is done, for example, in Proposition 1, which generalizes the results of Ledoit and Péché [2011], or in Proposition 6. In Section 3 we derive a general formula for the asymptotics of out-of-sample predictive risk in regularized linear regression. As mentioned earlier we will apply those results to understand early stopping and study the training and test error evolution. In Section 4 we carry out a similar study for Discriminant Analysis. Furthermore, we explain how to numerically solve for the optimal shrinkage function. Finally, we summarize our most important results and propose some directions that might be useful to explore in the future in Section 5. Proofs of more technical results can be found in Section 6.

Acknowledgements

2. Results from Random Matrix Theory

We review some basic results about the asymptotics of the eigenvalue distributions of random matrices.

For a probability measure μ supported on the real line the Stieltjes transform is defined as $m_\mu(z) = \int (x - z)^{-1} \mu(dx)$ for $z \in \mathbb{C}$ away from the support of μ.

The spectral distribution of a Hermitian $p \times p$ matrix A with eigenvalues (in decreasing order) $\lambda_1(z), \cdots, \lambda_p(A)$ is defined as the measure $F_A(x) = p^{-1} \sum_{i=1}^{p} \delta_{\lambda_i(A)}$. This is, of course, a measure supported on the real line. For empirical covariance matrices the spectral disribution is characterized asymptotically by the Marcenko-Pastur theorem. In the general form presented below it can be found in Silverstein and Bai [1995].

Theorem. *Let $Z \in \mathbb{R}^{p \times n}$ be a matrix with i.i.d. mean 0 and variance 1 entries and $\Sigma \in \mathbb{R}^{p \times p}$ a covariance matrix that is either deterministic or random but independent of Z and $X = \Sigma^{1/2} Z$. We assume that the spectral distribution of Σ converges weakly to a deterministic probability measure H supported on $[0, \infty)$. If $p, n \to \infty$ such that $pn^{-1} \to \gamma > 0$, then the spectral distribution of the matrix $n^{-1} X X^\top$ converges weakly almost surely to a deterministic probability measure $F_{\gamma, H}$ with Stieltjes transform that satisfies*

$$m_{\gamma, H}(z) = \int \frac{dH(t)}{t(1 - \gamma - \gamma z m_{\gamma, H}(z)) - z}.$$

We will often omit the subscripts and just write m for the Stieltjes transform, since it will be clear from our setting what the subscripts correspond to. In many cases it is useful to work with the companion Stieltjes transform which is defined as $\underline{m}_{\gamma,H}(z) = -(1-\gamma)z^{-1} + \gamma m_{\gamma,H}(z)$ and corresponds to the Stieltjes transform of the limiting spectral distribution of $n^{-1}X^\top X$. For any $x \in \mathbb{R} - \{0\}$ Silverstein and Choi [1995] proved that the limit $\lim_{\epsilon\downarrow 0} \underline{m}_{\gamma,H}(x + i\epsilon) = \tilde{m}_{\gamma,H}(x) = f(x) + ig(x)$ exists. They also proved that F has a continuous density away from 0 given by $F' = Im(\tilde{m})(\gamma\pi)^{-1} = g(\gamma\pi)^{-1}$.

This theorem has far-reaching implications in statistics. The references Johnstone [2006] and Paul and Aue [2014] provide interesting reviews.

For the case $H = \delta_1$ the equation for the Stieltjes transform is quadratic and can be solved explicitly. For other measures H it is possible to solve numerically for the limiting spectral density, as explained in detail in Dobriban [2015]. The author also provides software implementations of the methods.

A generalization of the Marcenko-Pastur equation is given in Ledoit and Péché [2011] and we mention an implication of their main result below. For the rest of this Section we are going to use the notation $S_n = n^{-1}XX^\top$.

Theorem. *With the assumptions above, if the entries of Z have uniformly bounded 12-th moments, H has support contained in a compact interval $[h_1, h_2]$ and all the eigenvalues of Σ eventually lie in $[h_1, h_2]$, then for any bounded continuous function u and any $z \in \mathbb{C}^+$ we have*

$$\frac{1}{p}tr\left(u(\Sigma)\left(S_n - z\right)^{-1}\right) \xrightarrow{a.s.} \int \frac{u(t)dH(t)}{t(1 - \gamma - \gamma z m_{\gamma,H}(z)) - z}. \tag{1}$$

For $g(t) = 1$ we recover the Marcenko-Pastur equation.

The authors used this result to study the overlap of the eigenvectors of $n^{-1}XX^\top$ with their population counterparts. Another significant application of this result in statistics was the nonlinear shrinkage method for covariance estimation mentioned earlier. Furthermore, it was used by Dobriban and Wager [2018] in their analysis of the asymptotics of ridge regression and ridge-regularized linear discriminant analysis.

An extension that we are going to use is proved below. This is an important result of independent mathematical interest. For our purposes it is going to be the main tool in providing limits for regularized high-dimensional linear regression risk. *To avoid technical complications arising from the fact that the density of the Marcenko-Pastur can be unbounded when $\gamma = 1$, we are going to assume for the rest of the paper that $\gamma \neq 1$.*

Proposition 1. *With the same assumptions as above for any bounded continuous function h on $[0, \infty)$ we have*

$$\frac{1}{p}tr\left(\Sigma h\left(S_n\right)\right) \xrightarrow{a.s.} M_{\gamma,H}(h),$$

where

$$M_{\gamma,H}(h) = \int h(x)\frac{g(x)}{\pi\gamma x(f(x)^2 + g(x)^2)}dx + \frac{h(0)}{\gamma\underline{m}(0)}I_{\gamma>1}.$$

Proof. We start the proof assuming $\gamma < 1$, but in the end we are going to show how to take into consideration the different behaviour that occurs for $\gamma > 1$.

First of all, by a simple density argument, namely that polynomials on a compact set are dense in the uniform convergence topology in the space of continuous functions, it is enough to prove the result for polynomial functions h. We will prove it for holomorphic functions in general using Cauchy's integral formula. The fact that we can restrict our attention to a compact subset of $[0, \infty)$ follows from the inequality

$$\limsup \|S_n\| \le \limsup \|\Sigma\| \left\| \frac{ZZ^\top}{n} \right\| \le h_2(1 + \sqrt{\gamma})^2.$$

Here we used the fact that $\limsup \|n^{-1}ZZ^\top\| = (1 + \sqrt{\gamma})^2$ by Bai and Silverstein [1998].

We observe that $1 + z\underline{m}(z) = \gamma(1 + zm(z))$.

By (1) we have

$$\frac{1}{p}tr\left(\Sigma\left(S_n - z\right)^{-1}\right) \xrightarrow{a.s.} \int \frac{t}{t(1 - \gamma - \gamma zm(z)) - z} dH(t)$$

$$= \frac{1}{1 - \gamma - \gamma zm(z)} \int (1 + \frac{z}{t(1 - \gamma - \gamma zm(z)) - z}) dH(t) \qquad (2)$$

$$= \frac{1}{1 - \gamma - \gamma zm(z)}(1 + zm(z)) = \frac{1}{\gamma}\frac{1 + z\underline{m}(z)}{1 - 1 - z\underline{m}(z)} = -\frac{1 + z\underline{m}(z)}{\gamma z\underline{m}(z)}.$$

Let Γ be a simple closed curve that encloses counterclockwise the support of $F_{\gamma,H}$.

We write

$$\frac{1}{p}tr\left(\Sigma h\left(S_n\right)\right) = -\frac{1}{2\pi i}\oint_\Gamma h(w)\frac{1}{p}tr\left(\Sigma\left(S_n - w\right)^{-1}\right)dw \qquad (3)$$

We clearly have that $\left\|\left(S_n - w\right)^{-1}\right\|$ is uniformly bounded almost surely for $w \in \Gamma$. In addition,

$$\left|\frac{d}{dw}\frac{1}{p}tr\left(\Sigma\left(S_n - w\right)^{-1}\right)\right| \le \|\Sigma\|\|(S_n - w)^{-2}\|.$$

As a consequence, the sequence of functions $p^{-1}tr\left(\Sigma\left(S_n - w\right)^{-1}\right)$ almost surely contains functions that are uniformly Lipschitz on Γ. We conclude that almost surely the convergence in (2) is uniform for $w \in \Gamma$. By the bounded convergence theorem and combining (2) and (3) it follows that

$$\frac{1}{p}tr\left(\Sigma h\left(S_n\right)\right) \xrightarrow{a.s.} \frac{1}{2\pi i}\oint_\Gamma h(w)\frac{1 + w\underline{m}(w)}{\gamma w\underline{m}(w)}dw \qquad (4)$$

We need to convert the contour integral to a real integral. To do this, we follow the idea of Bai and Silverstein [2008] and consider the curve Γ to approximate an interval on the real line in both directions. Then,

$$\lim_{\epsilon \to 0^+} \frac{1 + (x - i\epsilon)\underline{m}(x - i\epsilon)}{\gamma(x - i\epsilon)\underline{m}(x - i\epsilon)} - \frac{1 + (x + i\epsilon)\underline{m}(x + i\epsilon)}{\gamma(x + i\epsilon)\underline{m}(x + i\epsilon)}$$

$$= -2i\lim_{\epsilon \downarrow 0} Im\left(\frac{1 + (x + i\epsilon)\underline{m}(x + i\epsilon)}{\gamma(x + i\epsilon)\underline{m}(x + i\epsilon)}\right) = 2i\frac{g(x)}{\gamma x(f(x)^2 + g(x)^2)},$$

as a simple calculation shows.

To adjust the proof for the case $\gamma > 1$, we see that the only difference is that $\lim_{z \to 0} z\underline{m}(z) = 0$, so that we need to substitute the curve Γ with two other curves, one (call it Γ_1) contained in $\{z \in \mathbb{C} : Re(z) > 0\}$ enclosing counterclockwise the

support of the limiting spectral distribution $F_{\gamma,H}$ in the positive real axis, and the other (call it Γ_2) being a small circle around 0 with radius r.

Then, for the first curve the argument is the same as above and shows convergence to the same term exactly. For Γ_2 we have

$$\lim_{r\downarrow 0}\frac{1}{2\pi i}\oint_{\Gamma_2}h(w)\frac{1+w\underline{m}(w)}{\gamma w\underline{m}(w)}dw = \lim_{r\downarrow 0}\frac{1}{2\pi i}\oint_{\Gamma_2}\frac{h(w)}{\gamma w\underline{m}(w)}dw$$
$$= \lim_{r\downarrow 0}\frac{1}{2\pi}\int_0^{2\pi}\frac{h(r\exp(i\theta))}{\gamma\underline{m}(r\exp(i\theta))}d\theta = \frac{h(0)}{\gamma\underline{m}(0)}. \tag{5}$$

This completes the proof.

$\square$

Remarks

If $\Sigma = I$ we have $f(x)^2 + g(x)^2 = x^{-1}$ and the result is equivalent to the original Marcenko-Pastur theorem. In addition, if we consider functionals of the form $p^{-1}tr(f_1(\Sigma)f_2(S_n))$, it is straightforward to derive an analogous formula.

As an application of Proposition 1 that illustrates how it can be useful, we observe that one can recover the optimal nonlinear shrinkage function of Ledoit and Péché [2011]. There it was motivated heuristically as an asymptotic equivalent to an oracle that is the optimal rotation invariant estimator of the covariance matrix. We present this here from a different perspective, since a similar method will be applied in the Discriminant Analysis case to find the optimal shrinkage function there (numerically, since the formulas will be much more complicated).

Corollary 1. *If $\gamma \neq 1$, among the bounded continuous functions on an open set U that contains the support of $F_{\gamma,H}$, the one that minimizes the asymptotic (mean squared) Frobenius loss $\lim_{p\to\infty}p^{-1}\|\Sigma - h(S_n)\|_F^2$ satisfies*

$$h(x) = \frac{1}{x(f(x)^2 + g(x)^2)}, x \in supp(F_{\gamma,H}), x > 0.$$

If $x = 0$ and $\gamma > 1$, the optimal function at 0 evaluates to

$$h(0) = \frac{1}{(\gamma-1)\underline{m}(0)}.$$

Proof. We will use the well-known fact that

$$dF_{\gamma,H}(x) = \frac{g(x)}{\pi\gamma}dx + \max(1-\gamma^{-1},0)\delta_0.$$

The limit of the Frobenius loss is

$$\int t^2 dH(t) + \int h(x)^2 dF_{\gamma,H}(x) - 2\int h(x)\frac{g(x)}{\pi\gamma x(f(x)^2+g(x)^2)}dx - 2\frac{h(0)}{\gamma\underline{m}(0)}I_{\gamma>1}$$

$$= \int t^2 dH(t) + \int\left(h(x)^2 - 2h(x)\frac{1}{x(f(x)^2+g(x)^2)}\right)\frac{g(x)}{\pi\gamma}dx$$

$$+ \left((1-\gamma^{-1})h(0)^2 - 2\frac{h(0)}{\gamma\underline{m}(0)}\right)I_{\gamma>1}.$$

For $\gamma < 1$, we see that the integrand is minimized for $h(x) = (x(f(x)^2+g(x)^2))^{-1}$, which is going to be continuous close to the support of $F_{\gamma,H}$. For $\gamma > 1$, this is still

true away from 0, but at 0 we need to minimize

$$\left((1 - \gamma^{-1})h(0)^2 - 2\frac{h(0)}{\gamma \underline{m}(0)}\right).$$

This happens for $h(0) = (\gamma - 1)^{-1}\underline{m}(0)^{-1}$. The fact that we there exists such a continuous function h is trivial (for example, usually constructed by partitions of unity as in Munkres [1991]). This completes our proof.

$\square$

3. High-Dimensional Linear Regression

Regression Model and Assumptions

Data-Generating Distribution

Suppose that we observe n predictor variables $x_1, \cdots, x_n \in \mathbb{R}^p$ which are i.i.d. and there exist i.i.d. $z_1, \cdots, z_n \in \mathbb{R}^p$ with entries of mean 0, variance 1 and uniformly bounded 12-th moments such that $x_i = \Sigma^{1/2}z_i$. In addition, we assume that $p, n \to \infty$ with $pn^{-1} \to \gamma > 0$. As in the previous section, Σ is the population covariance matrix, which has bounded norm and spectral distribution that converges weakly to a probability measure H compactly supported on $[0, \infty)$. The target variables $y_1, \cdots, y_n$ are generated by a linear model as $y_i = w^\top x_i + \varepsilon_i$. As in the previous Section we are going to use the notation $S_n = n^{-1}XX^\top$.

Weight and error distributions

The error terms are i.i.d. with mean 0, variance 1 and uniformly bounded $(4+\eta)$-th moments (for some $\eta > 0$), while the weight vector w has independent components with mean zero and variance $p^{-1}\alpha^2$. This is a way to describe the hypothesis discussed in the introduction that each predictor variable has a small effect on the outcome. We also assume that the normalized coordinates $\sqrt{p}w_i$ of the weight vector have uniformly bounded $(4 + \eta)$-th moments. The same assumptions are made in Dobriban and Wager [2018].

Out-of-sample risk

The out-of-sample prediction risk is defined as $\mathbb{E}[(y_0 - \hat{w}^\top x_0)^2 | X, y, w] = 1 + \|\Sigma^{1/2}(\hat{w}-w)\|^2$, where (x_0, y_0) is generated independently from the training sample by the same model.

Estimators that we consider

We write $X = (x_1, \cdots, x_n) \in \mathbb{R}^{p \times n}, y = (y_1, \cdots, y_n)^\top$. When we perform linear regression of X on y (assume for a moment that $XX^\top$ is invertible) we estimate the weights by $\hat{w} = (XX^\top)^{-1}Xy$.

If $n^{-1/2}X = \sum_{i=1}^p \sqrt{\lambda_i}u_i v_i^\top$ is the singular value decomposition of $n^{-1/2}X$, we can rewrite $\hat{w} = \sum_{i=1}^p (\sqrt{n\lambda_i})^{-1}u_i v_i^\top y$. Similarly, ridge regression with parameter $\lambda \geq 0$ gives $\hat{w}_\lambda = \sum_{i=1}^p \sqrt{n^{-1}\lambda_i}(\lambda_i + \lambda)^{-1}u_i v_i^\top y$. Thus, ridge regression can be treated as a shrinkage method for the singular values of X before performing a linear regression. More examples of this phenomenon will be studied later.

Motivated by this we look at estimators of the form

$$\hat{w} = \sum_{i=1}^p h(\lambda_i)u_i v_i^\top \frac{y}{\sqrt{n}},$$

where h is a bounded continuous function in an open interval containing the support of $F_{\gamma,H}$.

Our first important result is below. The functions f, g are defined as in Section 2.

Theorem 1. *The out-of-sample prediction risk under the assumptions described above converges almost surely to*

$$1 + \int \left[\alpha^2 (\sqrt{x} h(x) - 1)^2 + \gamma h(x)^2 \right] \frac{g(x)}{\gamma \pi x (f(x)^2 + g(x)^2)} dx + \frac{\alpha^2 + \gamma h(0)^2}{\gamma \underline{m}(0)} I_{\gamma > 1}.$$

The proof is given in Section 6. The two most important steps at the proof are to first control the deviations of the quadratic form in the out-of-sample risk around the expectation using a consequence of the Marcinkiewicz-Zygmund inequality and then derive asymptotic formulas for the expectations of the terms that appear using Proposition 1.

Remark Observe that the function g is nonnegative, as $(\pi\gamma)^{-1}g$ is the density of the generalized Marcenko-Pastur distribution $F_{\gamma,H}$. The function $\alpha^2(\sqrt{x}h(x) - 1)^2 + \gamma h(x)^2$ is quadratic in h and is minimized when $h(x) = \sqrt{x}(x + \gamma\alpha^{-2})^{-1}$. This shrinkage function corresponds to ridge regression with parameter $\lambda^* = \gamma\alpha^{-2}$. One intuitive explanation for why this should be true is the following: From the Bayesian perspective, if we impose a normal prior distribution on the coefficient vector w and the residual vector ε, after observing the data points (x_i, y_i) the posterior of w is going to be normal. The posterior mean is exactly the ridge regression estimate with the parameter above. In the case of a general prior distribution on w the optimal shrinkage function should not change asymptotically, since the limit arising in Theorem 1 is universal. In particular, we never made assumptions about the strict shape of the distribution of the coefficients except for the first two moments, when deriving the asymptotic formula of the error. Choosing the optimal parameter λ^* may not be a straightforward task when $p > n$ and there has been significant amount of work in the literature dedicated to this question and the closely related heritability problem. For instance, the reader can refer to Janson et al. [2017] and Dicker and Erdogdu [2016] and the references therein.

3.1. **Learning Curves in Ridge Regression.** In the introduction we argued that Theorem 1 will allow us to study the learning curves for high-dimensional regression for any covariance matrix Σ and any regularization parameter λ trained by gradient descent, which we do here.

Before we present our result, we need to describe the dynamics of descent in linear regression. The weights $\hat{w}(t)$, which we initialize at 0 are iteratively updated to minimize over $\beta \in \mathbb{R}^p$ the function

$$\frac{\|y - X^\top \beta\|}{2n} + \frac{\lambda \|\beta\|^2}{2}.$$

Taking small steps against the gradient of this function with step size dt gives

$$\hat{w}(t + dt) = \hat{w}(t) - dt \left(\frac{X(X^\top \hat{w} - y)}{n} + \lambda \hat{w} \right).$$

Assuming $dt \to 0$ we get an ordinary differential equation for $\hat{w}(t)$ described by

$$\frac{d\hat{w}}{dt} = -\left(\frac{XX^\top}{n} + \lambda\right)\hat{w} + \frac{Xy}{n} \Rightarrow \hat{w}(t) = \left(I - \exp\left(-t\left(S_n + \lambda\right)\right)\right)\left(S_n + \lambda\right)^{-1}\frac{Xy}{n}.$$

Notice that $\lim_{t\to\infty}\hat{w}(t)$ recovers the usual weight for ridge regression. We conclude that Theorem 1 provides asymptotic formulas for the out-of-sample prediction risk at all points in time during the training. In particular, early stopping provides regularization via singular value shrinkage of $n^{-1/2}X$. Using the notation we introduced above, we can apply our results for $h(x) = (1 - \exp(-t(x + \lambda)))\sqrt{x}(x + \lambda)^{-1}$.

Proposition 2. *The prediction risk using gradient descent for time t in ridge regression with regularization parameter λ converges almost surely to*

$$1 + \int [\alpha^2(\sqrt{x}h(x) - 1)^2 + \gamma h(x)^2]\frac{g(x)}{\gamma\pi x(f(x)^2 + g(x)^2)}dx + \frac{\alpha^2}{\gamma\underline{m}(0)}I_{\gamma>1},$$

where $h = h(x; t, \lambda) = (1 - \exp(-t(x + \lambda)))\sqrt{x}(x + \lambda)^{-1}$.

In Figure 1 verify experimentally that our theorem produces the right result for $p = 500, n = 1500, \alpha = 1$ and $H = 0.5(\delta_1 + \delta_4)$. The regularization parameter was set to the optimal $\lambda = 1/3$. In Figure 2 we do the same for $p = 1000, n = 1500, \alpha = 2$ an autoregressive covariance matrix with $\Sigma_{ij} = 2^{-|i-j|}$. For this example we chose $\lambda = 0$, which corresponds to unregularized linear regression.
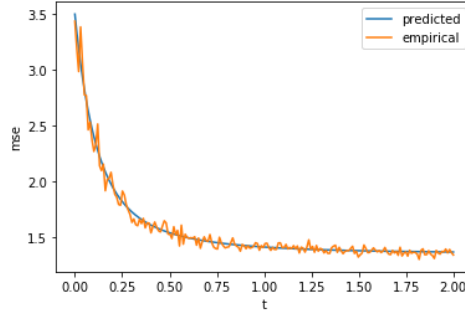

FIGURE 1. Predicted vs Empirical out-of-sample MSE evolution for $p = 500, n = 1500, \alpha = 1$ and $H = 0.5(\delta_1 + \delta_4)$. Here the ridge parameter is chosen as the optimal $\lambda = 1/3$.

Observe that the first term in the integral is decreasing in t and roughly corresponds to a bias term, as we see from the proof. The second term in the integral is increasing in t and behaves as a variance term.

As a special case we recover a result of Advani and Saxe [2017] which we state in Corollary 2.

Corollary 2. *If $\lambda = 0$ (unregularized linear regression), for $\Sigma = I_p$, the evolution of the prediction risk during training is given by*

$$1 + \int \alpha^2 \exp(-2tx) + \gamma\frac{(1 - \exp(-tx))^2}{x}dF_\gamma(x).$$
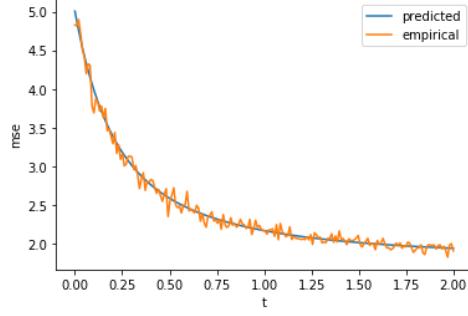
FIGURE 2. Predicted vs Empirical out-of-sample MSE evolution
for $p = 1000, n = 1500, \alpha = 2, \lambda = 0$ and $\Sigma_{ij} = 2^{-|i-j|}$.

*Here $F_\gamma = F_{\gamma,\delta_1}$ is the measure on the real line that is absolutely continuous with
respect to the Lebesgue measure for $\gamma \leq 1$ with density*

$$\frac{dF_\gamma(x)}{dx} = \frac{\sqrt{\left((1+\sqrt{\gamma})^2 - x\right)\left(x - (1-\sqrt{\gamma})^2\right)}}{2\pi\gamma x}, (1 - \sqrt{\gamma})^2 \leq x \leq (1 + \sqrt{\gamma})^2.$$

If $\gamma > 1$, F_γ has an additional mass $1 - \gamma^{-1}$ at 0.

When γ increases the effect of the second term will become more significant and
in general will require stopping earlier in the training to achieve better performance.
For $\alpha = 0.5$ and three different values of γ the asymptotic prediction risk is seen
in the plot below in the null case $H = \delta_1$ and with $\lambda = 0$. We observe that it is
optimal to stop early, since going beyond a certain point results to overtraining,
which increases the prediction risk. We also see that, as we explained, the higher
γ is, the earlier the overtraining phenomenon starts to impact the performance of
the model. Furthermore, if α increases the optimal training time always increases,
keeping the other parameters fixed. In other words, the smaller the fraction of
the variance explained by pure noise is, the longer the optimal training period.
Overtraining becomes more rare, since the gradient descent tries to update the
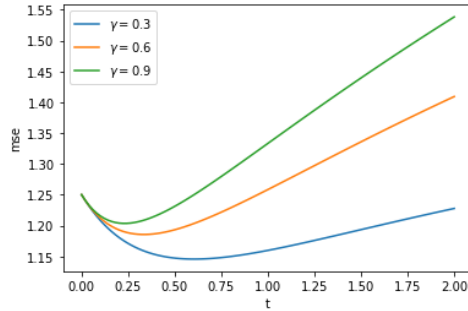weights in directions governed mostly by signal and less by noise.

FIGURE 3. Out-of-sample MSE evolution for $\alpha = 0.5, H = \delta_1, \lambda = 0$
as a function of training time.

To examine the tradeoff between λ and the optimal stopping time, we plot for $\gamma = \alpha = 0.5$ the prediction risk as a function of t, λ. In this case the optimal λ is $\gamma \alpha^{-2} = 2$. In the plot below we see that close to $\lambda = \lambda^* = 2$ training for longer times is required and leads to lower prediction risk values, but when the regularization parameter is much smaller and not close to the optimum it might be very easy to overtrain.
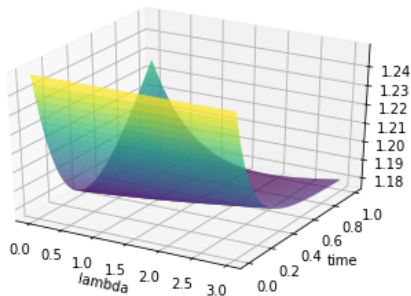

FIGURE 4. MSE surface

We also have the following easy consequence, which tells us that for the case of over-regularized ridge regression, under the assumptions we have made, fully training the model is optimal. In other words, the most significant gains from stopping early are for λ much smaller than the optimal parameter.

Corollary 3. *For $\lambda \geq \gamma \alpha^{-2}$ the out-of-sample risk of ridge regression is decreasing as a function of t.*

Proof. It is enough to show that for any $x \geq 0, \lambda \geq \gamma \alpha^{-2}$

$$H(t) = (\sqrt{x}h(x;t,\lambda) - 1)^2 + \frac{\gamma}{\alpha^2}h(x;t,\lambda)^2$$

is decreasing in t, with $h(x;t,\lambda)$ as in Proposition 2.
We have

$$H'(t) = 2\sqrt{x}\exp(-t(x+\lambda))[xh(x;t,\lambda) - \sqrt{x} + \frac{\gamma}{\alpha^2}h(x;t,\lambda)],$$

so it is enough to show that $h(x;t,\lambda) \leq \sqrt{x}(x + \frac{\gamma}{\alpha^2})^{-1}$. This obviously holds, since

$$h(x;t,\lambda) \leq \frac{\sqrt{x}}{x+\lambda} \leq \frac{\sqrt{x}}{x+\frac{\gamma}{\alpha^2}}.$$

$\square$

In Figure 5 and 6 we show how early stopping can tremendously increase performance if the regularization is too small. In fact, in Ali et al. [2018] the authors use a coupling argument to provide bounds on optimally tuned versus early-stopped regression and show that the ratio of the risks is at most 1.22 (out-of-sample). In Yao et al. [2007] the authors also derive probabilistic upper bounds for non-parametric regression. Data-dependent stopping rules are studied in Raskutti et al. [2014]. Probabilistic upper bounds have also been studied in . It is also obvious that for $\lambda \geq \lambda^* = \gamma \alpha^{-2}$ early stopping cannot influence the performance.
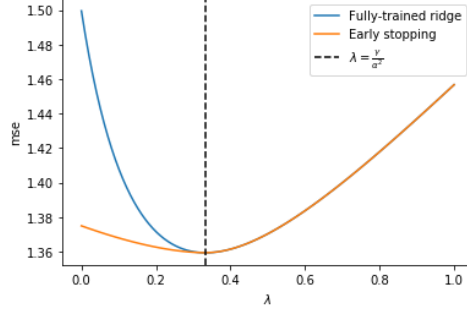
FIGURE 5. Fully-trained ridge regression vs Early Stopping MSE as a function of the regularization parameter λ. As in Figure 1 we chose $\gamma = 1/3, \alpha = 1$ and $H = 0.5(\delta_1 + \delta_4)$
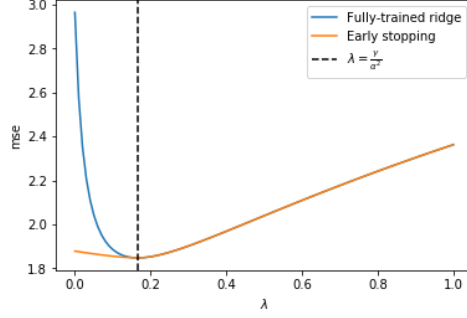

FIGURE 6. Fully-trained ridge regression vs Early Stopping MSE as a function of the regularization parameter λ. As in Figure 2 we chose $\gamma = 2/3, \alpha = 2$ and $\Sigma_{ij} = 2^{-|i-j|}$

In Section 6 we prove the analogous result for the training error evolution, which we state next. Here $\underline{F}_{\gamma,H}$ is the companion measure with Stieltjes transform $\underline{m}_{\gamma,H}$. The main ingredient is again, as in Theorem 1, to control the deviations of the quadratic forms that appear around the mean using the Marcinkiewicz-Zygmund inequality. The means turn out to be simply linear spectral statistics of S_n and the companion matrix $n^{-1} X^\top X$, hence we can use the Marcenko-Pastur Theorem to derive almost sure limits as $p, n \to \infty$.

Proposition 3. *At the point t in time, the training error $E_n(\hat{w}) = n^{-1} \|y - X^\top \hat{w}\|^2$ converges almost surely to*

$$\int \left[\frac{x}{x+\lambda}(1 - \exp(-t(x+\lambda))) - 1 \right]^2 d\underline{F}_{\gamma,H}(x)$$

$$+ \alpha^2 \int x \left[\frac{x}{x+\lambda}(1 - \exp(-t(x+\lambda))) - 1 \right]^2 dF_{\gamma,H}(x). \tag{6}$$

In particular, at the end of training $(t \to \infty)$ it is

$$\int \frac{\lambda^2}{(x+\lambda)^2} d\underline{F}_{\gamma,H} + \alpha^2 \lambda^2 \int \frac{x}{(x+\lambda)^2} dF_{\gamma,H}(x).$$

Remarks

The function is decreasing in t as we should expect and increasing in α. For $\lambda \downarrow 0$ we can recover the training error for the unregularized linear regression as $\underline{F}_{\gamma,H}(\{0\}) = \max(1 - \gamma, 0)$ at the end of training regardless of Σ. In this case $(S_n + \lambda)^{-1}$ converges to the Moore-Penrose pseudoinverse of the empirical covariance matrix. This explains the severe overfitting phenomenon observed when the number of features exceeds the sample size. Moreover, notice that in the beginning of training, that is when $t \to 0^+$, the prediction risk is $1 + \alpha^2 \int x dF_{\gamma,H}(x)$ for both the training and test sets, which is the variance of the target variable y. For the prediction risk, for instance, the surface in Figure 4 starts always close to 1.25 when $t = 0$.

If we use a different optimization scheme similar estimators arise. For instance, for Nesterov's accelerated gradient method we can use the second order differential equation derived in Su et al. [2014] to see that the evolution of weights during training is essentially the same as in gradient descent, but with an additional term that is a Bessel function of the empirical covariance matrix S_n. Obviously the same method can be applied to provide asymptotics.

4. High-Dimensional Discriminant Analysis

At this point we study regularization methods for linear discriminant analysis based on random matrix theory. Linear Discriminant Analysis, introduced by Fischer, has been one of the most commonly used classification methods. For example, it has been used in areas such as finance (Bramhandkar [1989]) and biology (Golub et al. [1999]). Our methods can potentially be extended to study regularization in quadratic discriminant analysis, which is again a very popular method used by scientists (for instance, Zhang [1997]).

First of all, it is essential to derive asymptotic formulas for the classification error for regularized Linear Discriminant Analysis. Once we have done that we will be able to write down an optimization program to find the optimal shrinkage function for the covariance matrix.

Classification Model and Assumptions We will build on the model from Dobriban and Wager [2018]. We assume that we have data generated by two different distributions with equal probabilities. The distributions are assumed to be Gaussian with means $\mu_1 = \delta, \mu_2 = -\delta \in \mathbb{R}^p$.

Assumptions on the means

We assume that the coordinates of δ are independent and identically distributed random variables with mean 0 and variance $\alpha^2 p^{-1}$. Notice that this is similar to the assumption made in linear regression that each predictor variable has a small effect on the outcome. In particular, each predictor variable contributes a small effect in the distance between class means. In the reference above the authors allow the means to be centered around a point different from zero, but this has no affect on the analysis. We assume that the coordinates of $\sqrt{p}\delta$ have uniformly bounded moments of order $4 + \eta$ for some fixed $\eta > 0$.

Assumptions on the covariance matrix

The two Gaussian distributions have covariance matrix Σ which we assume has a spectral distribution that converges weakly to a measure H supported on the

real line and there exist deterministic constants $b, B > 0$ with $0 < b < \lambda_{\min}(\Sigma) \le \lambda_{\max}(\Sigma) < B < \infty$.

Labeled data points

Suppose that there are n data points $(x_1, y_1), \cdots, (x_n, y_n)$ such that the first $n/2$ of them, which were generated by the first distribution, have labels $y_i = 1$, while the other half have labels $y_i = -1$ and were generated by the second distribution. As always, the setting we are interested in is when $p, n \to \infty$ and $p/n \to \gamma > 0$. We will use the notation $x_i = \Sigma^{1/2} z_i + \delta y_i$ and $S_n = n^{-1} \sum_{i=1}^n \Sigma^{1/2} z_i z_i^\top \Sigma^{1/2}$.

To classify new data points the Bayes oracle estimator is $\hat{y}(x) = sign(\delta^\top \Sigma^{-1} x)$. Of course, Σ, δ have to be estimated from the data. For δ we use the estimate

$$\hat{\delta} = \frac{1}{n} \sum_{i=1}^{\frac{n}{2}} x_i - \frac{1}{n} \sum_{i=\frac{n}{2}+1}^{n} x_i.$$

If we replace Σ by the empirical covariance matrix $\hat{\Sigma}$, then, as the Marcenko-Pastur theorem indicates, there will be significant noise in the estimation. In addition, if $\gamma > 1$, the empirical covariance matrix will not be invertible. For this reason the author in Friedman [1989] recommends to use $(\hat{\Sigma} + \lambda)^{-1}$ instead. This is a linear shrinkage method. However, it has been observed (for example, in Ledoit and Wolf [2012] and Lam et al. [2016]) that employing nonlinear shrinkage methods for covariance estimation can greatly enhance the accuracy. For our problem this would mean using the estimator $\hat{y} = sign(\hat{\delta}^\top h(\hat{\Sigma}) x)$. What is more, it was explained in great detail in Donoho et al. [2018] that optimal shrinkage depends heavily on the choice of loss function that is used in the estimation. As a consequence, choosing an optimal shrinkage for, say, the Frobenius or Stein loss, does not imply that the shrinkage is optimal for classification purposes. This leads naturally to the questions that we examine in this section, namely we try to answer the following: *How does the choice of shrinkage function affect the classification accuracy? How do well-known shrinkage methods perform asymptotically? What is the optimal shrinkage function for Discriminant Analysis?*

Improved Mean Estimation

First of all, as mentioned in the Introduction, we explain how estimation of δ can be improved by a shrinkage estimator that relies on the sample mean and the sample covariance. To motivate the estimator we impose a Gaussian prior on δ. Since $y_i x_i | \delta \sim \mathcal{N}(\delta, \Sigma)$, the posterior density of δ is proportional to

$$\exp\left(-\frac{\sum_{i=1}^n (y_i x_i - \delta) \Sigma^{-1} (y_i x_i - \delta)}{2} - \frac{p \|\delta\|^2}{2\alpha^2} \right),$$

hence $\delta | y_1 x_1, \cdots, y_n x_n$ is Gaussian and the posterior mean is given by

$$\mathbb{E}[\delta | y_1 x_1, \cdots, y_n x_n] = \frac{\alpha^2 n}{p} \left(\Sigma + \frac{n\alpha^2}{p} \right)^{-1} \hat{\delta}.$$

If Σ was known we could use this formula, but for unknown Σ we might again try to use an estimator of the form

$$\hat{\delta}^{(r)} = r(\hat{\Sigma})\hat{\delta}.$$

Surprisingly, if we try to minimize over r the distance $\left\| \hat{\delta}^{(r)} - \delta \right\|$ we get the following result proved in Section 6, which is true without the Gaussian assumption on δ.

Proposition 4. *The continuous function h that asymptotically minimizes $\left\|\hat{\delta}^{(r)} - \delta\right\|$ is given by*

$$r(x) = \frac{\frac{\alpha^2}{\gamma}}{\frac{\alpha^2}{\gamma} + \frac{1}{x(f(x)^2 + g(x)^2)}}, x \in supp(F_{\gamma, H}) - \{0\}.$$

If $\gamma > 1$ the value of the optimal r at 0 is given by:

$$r(0) = \frac{\frac{\alpha^2}{\gamma}}{\frac{\alpha^2}{\gamma} + \frac{1}{(\gamma-1)\underline{m}(0)}}$$

The surprising nature of this result is that r comes from plugging in the optimal shrinkage function for covariance estimation in Frobenius loss from Ledoit and Wolf [2012] for Σ in the posterior mean derived above, although one might expect that trying to approximate $(\Sigma + \gamma^{-1}\alpha^2)^{-1}$ directly might be better. Notice that for the classifier $\hat{y} = sign(\hat{\delta}^{\top} h(\hat{\Sigma})x)$ if h is chosen optimally using $\hat{\delta}$ instead of a better estimate $\hat{\delta}^{(r)}$ there should be no effect in the accuracy, hence the use of $\hat{\delta}$ is justified for the vector of means.

We now return to the problem of the asymptotic classification error. We prove the following result in Section 6 using random matrix theory. This result is of independent mathematical interest, but also the main ingredient in deriving the asymptotic formula of the classification error. Notice that using a polarization argument the result can easily be extended to provide asymptotics for functionals of the form $p^{-1}tr(\Sigma h_1(S_n)\Sigma h_2(S_n))$.

Proposition 5. *There exists a continuous function $K : supp(F_{\gamma, H}) \times supp(F_{\gamma, H}) \to \mathbb{R}$ such that for any bounded continuous function h defined in an open set containing $supp(F_{\gamma, H})$ we have*

$$\frac{1}{p}tr\left(\Sigma h\left(S_n\right)\Sigma h\left(S_n\right)\right) \xrightarrow{a.s.} T_{\gamma, H}(h),$$

where

$$T_{\gamma, H}(h) = \int \frac{h^2(x)g(x)}{\gamma \pi x^2(f(x)^2 + g(x)^2)^2}dx + \int \int K(x, y)h(x)h(y)dxdy, \quad (7)$$

if $\gamma < 1$. If $\gamma > 1$ there is an additional term equal to

$$\frac{1}{\gamma}\left[\frac{\underline{m}'(0)}{\underline{m}(0)^4} - \frac{1}{\underline{m}(0)^2}\right]h^2(0) + \frac{2h(0)}{\gamma \underline{m}(0)^2}\int u_h(x)dx$$

$$u_h(x) = \frac{f(x)^2 + g(x)^2 - 2f(x)\underline{m}(0) - x\underline{m}(0)(f(x)^2 + g(x)^2)}{\pi x^2(f(x)^2 + g(x)^2)^2}g(x)h(x). \quad (8)$$

The function K is explicitly defined as

$$K(x, y) = -\frac{g(x)g(y)}{\gamma \pi^2 xy(f(x)^2 + g(x)^2)(f(y)^2 + g(y)^2)}$$

$$+2\frac{f(x)\left[f(y)^2 + g(y)^2\right] - f(y)\left[f(x)^2 + g(x)^2\right]}{\gamma \pi^2 xy(y - x)\left[f(x)^2 + g(x)^2\right]^2\left[f(y)^2 + g(y)^2\right]^2}g(x)g(y).$$

When the covariance matrix Σ is identity, we can actually see that all terms in $T_{\gamma,I}$ cancel out, except for $\int h^2(x)g(x)/(\gamma\pi x^2(f(x)^2+g(x)^2)^2)dx$, which simplifies to $\int h(x)g(x)/\gamma\pi dx$, and (for $\gamma > 1$) $\gamma^{-1}\left[(\underline{m}'(0)-\underline{m}(0)^2)/\underline{m}(0)^4\right]h^2(0)$, which simplifies to $(1-\gamma^{-1})h(0)^2$. This agrees the limit of $p^{-1}tr(h(S_n)^2)$ under the standard Marcenko-Pastur distribution. This result is going to play the role of Proposition 1 in the case of regression, but the proofs for Discriminant Analysis are far more involved.

We now present our main theorem for this chapter, the proof of which is again in Section 6. The general strategy in the proof is as follows: Firstly we write down a formula for the classification error that depends only on quadratic forms of δ and $\hat{\delta}$. Then we control the deviations of the quadratic forms using again the Marcinkiewicz-Zygmund inequality. Finally, we derive limits for the expectations of the quadratic forms using the generalized Marcenko-Pastur distribution, Proposition 1 and Proposition 5.

Theorem 2. *Assume that in order to perform discriminant analysis we use a shrinkage function $h \geq 0$ for the eigenvalues of the sample covariance matrix $\hat{\Sigma}$, which is bounded and continuous in an open interval containing $supp(F_{\gamma,H})$. In particular, we use the classification rule $\hat{y}(x) = sign(\hat{\delta}^\top h(\hat{\Sigma})x)$. Then, the out-of-sample classification error converges almost surely to $\Phi(-\sqrt{\Theta(h;\gamma,H)})$, where Φ is the standard normal c.d.f. and*

$$\Theta(h) = \frac{\alpha^4\left(\int h(x)dF_{\gamma,H}\right)^2}{\alpha^2 M_{\gamma,H}(h^2)+\gamma T_{\gamma,H}(h)}.$$

In real applications we do not know what the actual functions f,g are. However, they can be estimated from the data using kernel estimation. This is explained in Jing et al. [2010], where the the authors recommend using a bounded and non-negative density function with absolutely integrable derivative and window size $h \to 0$ that satisfies $\lim nh^{\frac{5}{2}} = \infty$. As mentioned in the Introduction, in Ledoit and Wolf [2017] use a similar method to approximate the optimal shrinkage function for covariance and precision matrix estimation.

We verify the correctness of our theorem in a simulation in Figure 7. There we plot the classification error as a function of the signal strength α for unregularized and optimally regularized LDA. We see that the empirical estimate of the classification error and the asymptotical value predicted by our theorem are remarkably close. As one might expect, for $\alpha \to 0$ all methods give approximately 50% accuracy, while for α large the accuracy of the methods tends to 100%.

(A) $H = \frac{\delta_1 + \delta_4}{2}$ (B) $H = \frac{\delta_1 + \delta_2 + \delta_3 + \delta_4 + \delta_5}{5}$
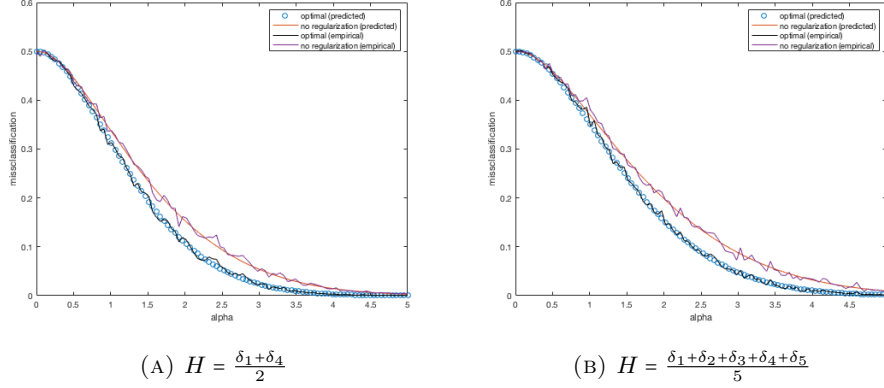
FIGURE 7. Empirical vs theoretical classification error for $p = 1000, n = 2000$ as a function of the signal strength α for two different choices of limiting spectral distribution H for the population covariance matrix.

4.1. **Optimization with respect to the shrinkage function.** Setting $s = \alpha^2/\gamma$ (which plays the role of a signal-to-noise ratio here), we would like to maximize

$$\frac{\left(\int h(x)dF_{\gamma,H}(x)\right)^2}{sM_{\gamma,H}(h^2) + T_{\gamma,H}(h)}.$$

Due to the invariance of this ratio under rescalings of h, we can assume that we have fixed $\int h dF_{\gamma,H} = 1$ and the problem now becomes

$$\underset{h \geq 0}{\text{minimize}} \quad G(h) = sM_{\gamma,H}(h^2) + T_{\gamma,H}(h)$$

$$\text{subject to} \quad \int h dF_{\gamma,H} = 1.$$

The optimization program above describes the tradeoff between the minimizer of M and the minimizer of T. In particular, if $\alpha \to \infty$ or $\gamma \to 0$, the solution approximates the solution to

$$\underset{h \geq 0}{\text{minimize}} \quad G(h) = M_{\gamma,H}(h^2)$$

$$\text{subject to} \quad \int h dF_{\gamma,H} = 1.$$

Up to rescalings, $h(x)$ for $x > 0$ is the same as the optimal shrinkage for covariance estimation, as wee see by examining when equality holds in the Cauchy-Schwartz:

$$\int \frac{h^2 g}{\gamma \pi x(f^2 + g^2)}dx \int x(f^2 + g^2)\frac{g}{\gamma \pi}dx \geq \left(\int \frac{hg}{\gamma \pi}dx\right)^2.$$

This proves the claim for $\gamma < 1$. For $\gamma > 1$ we also need to take into account the value of $h(0)$, but it is straightforward to extend the argument.

We conclude that, when the signal is strong, the optimal shrinkage function for covariance estimation in Frobenius norm is approximately the same as the optimal shrinkage function for linear discriminant analysis. When the signal is low, other shrinkage functions might perform better. All things considered, the last theorem vastly generalizes the results of the references mentioned and allows us to compute sharp asymptotics for the accuracy of complicated shrinkage estimators like the

ones from Ledoit and Péché [2011], when applied to classification via discriminant analysis.

We now for simplicity restrict our attention to $\gamma < 1$ and study more thoroughly the behaviour of the optimal shrinkage function. Since

$$\frac{1}{p} tr\left(\Sigma h(S_n)\Sigma h(S_n)\right) \geq \left(\frac{tr\left(\Sigma h(S_n)\right)}{p}\right)^2 \xrightarrow{a.s.} (M_{\gamma,H}(h))^2,$$

we can write down the following relaxation:

$$\begin{aligned} \underset{h \geq 0}{\text{minimize}} \quad & M_{\gamma,H}(h^2) + \frac{\gamma}{\alpha^2}(M_{\gamma,H}(h))^2 \\ \text{subject to} \quad & \int h \, dF_{\gamma,H} = 1. \end{aligned}$$

This optimization problem can easily be solved analytically. Below we make an interesting remark about the solution: If h_0 is the solution to this optimization problem, we have for any u such that $\int u \, dF_{\gamma,H} = 0$

$$\frac{d}{dt} M_{\gamma,H}((h_0 + tu)^2) + \frac{\gamma}{\alpha^2}(M_{\gamma,H}(h_0 + tu))^2|_{t=0} = 0 \tag{9}$$
$$\Rightarrow \int \frac{h_0 u g}{\gamma \pi x(f^2 + g^2)} dx + \frac{\gamma}{\alpha^2} \int \frac{h_0 g}{\gamma \pi x(f^2 + g^2)} dx \int \frac{u g}{\gamma \pi x(f^2 + g^2)} dx = 0$$

We conclude that, since this holds for all u with $\int u g \, dx = 0$, it must be that for some constant A

$$\frac{g}{\gamma \pi}\left[\frac{h_0}{x(f^2 + g^2)} + \frac{\gamma}{\alpha^2}\frac{1}{x(f^2 + g^2)}\int \frac{h_0 g}{\gamma \pi x(f^2 + g^2)} dx\right] = A\frac{g}{\gamma \pi}.$$

In other words, for suitably chosen constants A, B we have for all $x \in supp(F_{\gamma,H})$

$$h_0(x) = Ax(f(x)^2 + g(x)^2) - B.$$

This is the optimal shrinkage for covariance estimation with shift and rescaling. Since rescalings of h do not affect the classification error we can take $A = 1$. After this the solution can be viewed as a combination of ridge regularization (with negative parameter) and the optimal shrinkage for covariance estimation in Frobenius norm.

Solving the optimization problem To solve for h numerically, we may approximate h by piecewise constant functions defined on small intervals that cover $supp(F_{\gamma,H})$. The problem then becomes a convex quadratic program in the values assigned to each interval. In fact, the condition $h \geq 0$ should be redundant, as the optimal shrinkage function should be positive. This procedure, of course, does not impose continuity, but, if a continuous minimizer exists, one might expect that this procedure should approximate that. In addition, it is possible to modify Theorem 2 to account for problems with finitely many discontinuities, but at this point we ignore this detail.

Estimation of α^2

In order to solve numerically for the optimal shrinkage function in practice one needs to estimate f, g and α^2. As mentioned f, g can be estimated using kernel

estimation. We now explain the missing part, namely estimation of α^2. With the assumptions made it is immediate to see that

$$\left\|\hat{\delta}\right\|^2 - \alpha^2 - \frac{tr(\Sigma)}{n} \xrightarrow{a.s.} 0.$$

Since $n^{-1}(tr(\Sigma) - tr(\hat{\Sigma})) \xrightarrow{a.s.} 0$, we conclude that

$$\left\|\hat{\delta}\right\|^2 - \frac{tr(\hat{\Sigma})}{n} \xrightarrow{a.s.} \alpha^2.$$

We compare the asymptotic missclassification risk for limiting spectral distribution $H = 0.5(\delta_{0.75} + \delta_{15})$ and $\gamma = 0.75$. The estimators that we consider are the optimal shrinkage estimator that minimizes the asymptotic risk, the optimal shrinkage for covariance and precision estimation of Ledoit and Péché [2011] with respect to the Frobenius loss (the latter being $h(\lambda) = (\gamma - 1 - 2\lambda f(\lambda))/\lambda$) -which we call ledoit-peche 1 and ledoit-peche 2 respectively- the optimal ridge-regularized estimator of the form $(\hat{\Sigma} + \lambda)^{-1}$ and the unregularized sample covariance estimator.
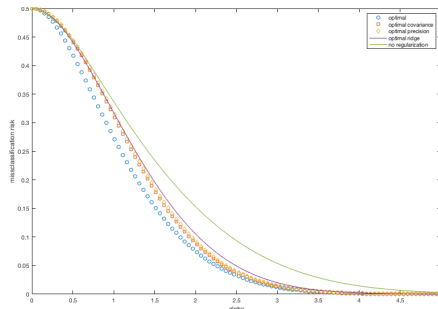

FIGURE 8. Comparison of different shrinkage estimators for LDA for $\gamma = 0.75, H = 0.5(\delta_{0.5} + \delta_{15})$.

We observe that the optimal covariance and optimal precision shrinkage functions perform very similarly and slightly better than optimally ridge-regularized shrinkage. The worst is unregularized, as one might expect.

5. CONCLUSIONS AND FUTURE WORK

In the first part of the paper we studied general singular value shrinkage methods for regularization of regression in high-dimensional statistics. For this purpose we derived results of independent mathematical interest for the convergence of some trace functionals that include both the population and the sample covariance matrices, as in Theorem 1. Before the development of these tools this was only possible for the case of ridge regression. We also presented important applications of Theorem 1. Firstly, we explained how it can be used to recover the optimal shrinkage function for covariance estimation derived heuristically in Ledoit and Péché [2011] and used in Ledoit and Wolf [2012]. Secondly, we proved the optimality of ridge regression with parameter γ/α^2 in this setting among all shrinkage-based methods for general coefficient distributions. Furthermore, our results allowed us to analyze methods such as early stopping in models with arbitrary predictor covariance matrices. In particular, we studied the test error evolution in gradient descent

training, which gave us important insights about the early stopping regularization methods used in the deep learning community and by practitioners. Even in this very simplistic setting the regime we are studying explains some attributes of the overtraining phenomenon seen in much more complex models. Within our model early stopping may provide important benefits and achieve performance comparable to optimally tuned ridge regression for parameters much smaller than the optimal. As a direction of future work, it might be interesting to examine if similar results could be established for larger classes of models, for example for shallow neural networks. This will be a step closer to the extremely complex models that have been used in the last decade in the most successful applications of deep learning.

In the second part of the paper we provided sharp asymptotic formulas for regularization methods based on singular value shrinkage in high-dimensional classification. We were able to analyze asymptotically the performance of shrinkage methods proposed in the literature for covariance estimation (such as those in Ledoit and Wolf [2012]) in the case of discriminant analysis problems. With the tools previously available from random matrix theory this had been possible only for ridge-regularized linear discriminant analysis, so, to extend them, we had to derive results of independent mathematical interest. Our theorems also led to a procedure for finding numerically the optimal shrinkage function for classification in linear discriminant analysis. Finally, we examined and verified our results in extensive simulations. Extending our results to the case of quadratic discriminant analysis would be a natural next step. As a closely related direction for future work it might be interesting to explore how these results can be extended to other methods that are used frequently, such as logistic regression or support vector machines. As mentioned in the Introduction this question was considered in Taheri et al. [2020], but only for standard Gaussian features. Similar questions could be asked for more general covariance matrices and distributions such as those in our paper. Answering these questions will allow us to understand better how these commonly used methods generalize in very high dimensional settings.

6. Proofs of Main Results

6.1. **Proofs for Regression.** We will need the following lemma which is adapted from Lemma 7.8, Lemma 7.9 and Lemma 7.10 from Erdős and Yau [2017].

Lemma 1. *Let $q \geq 2$ and $X_1, \cdots, X_N, Y_1, \cdots, Y_N$ be independent random variables with mean 0, variance 1 and $2q$-th moment bounded by c_0. Then, for any deterministic $(b_i)_{1 \leq i \leq N}, (a_{ij})_{1 \leq i,j \leq N}$ we have for some positive constant $C_q = C_q(c_0)$:*

$$\left\| \sum_i b_i (X_i^2 - 1) \right\|_q \leq C_q \Big(\sum_i |b_i|^2 \Big)^{\frac{1}{2}} \tag{10}$$

$$\left\| \sum_{i,j} a_{ij} X_i Y_j \right\|_q \leq C_q \Big(\sum_{i,j} a_{ij}^2 \Big)^{\frac{1}{2}} \tag{11}$$

$$\left\| \sum_{i \neq j} a_{ij} X_i X_j \right\|_q \leq C_q \Big(\sum_{i \neq j} a_{ij}^2 \Big)^{\frac{1}{2}} \tag{12}$$

Proof of Theorem 1. Let us define

$$M_1 = \sum_{i=1}^{p} \sqrt{\lambda_i} h(\lambda_i) u_i u_i^\top, \quad M_2 = \sum_{i=1}^{p} h(\lambda_i) u_i v_i^\top.$$

We have

$$\hat{w} = \sum_{i=1}^{p} h(\lambda_i) u_i v_i^\top \frac{y}{\sqrt{n}} = \left[\sum_{i=1}^{p} h(\lambda_i) u_i v_i^\top \right] \frac{X^\top w + \varepsilon}{\sqrt{n}}$$

$$= \sum_{i=1}^{p} \sqrt{\lambda_i} h(\lambda_i) u_i u_i^\top w + \sum_{i=1}^{p} h(\lambda_i) u_i v_i^\top \frac{\varepsilon}{\sqrt{n}} = M_1 w + M_2 \frac{\varepsilon}{\sqrt{n}}.$$

The prediction risk is equal to

$$1 + (\hat{w} - w)^\top \Sigma (\hat{w} - w) = 1 + \left[(M_1 - I_p) w + M_2 \frac{\varepsilon}{\sqrt{n}} \right]^\top \Sigma \left[(M_1 - I_p) w + M_2 \frac{\varepsilon}{\sqrt{n}} \right]$$

$$= 1 + w^\top (M_1 - I_p) \Sigma (M_1 - I_p) w + \frac{1}{n} \varepsilon^\top M_2^\top \Sigma M_2 \varepsilon + 2 \frac{\varepsilon^\top}{\sqrt{n}} M_2^\top \Sigma (M_1 - I_p) w.$$

According to Lemma 1 for $q = (4 + \eta)/2$ we have

$$\mathbb{E} \left[\left(w^\top (M_1 - I_p) \Sigma (M_1 - I_p) w - \frac{\alpha^2}{p} tr \left((M_1 - I_p)^2 \Sigma \right) \right)^q \Big| M_1 \right] =$$

$$\mathcal{O} \left(\| (M_1 - I_p) \Sigma (M_1 - I_p) \|_F^q \frac{\alpha^{2q}}{p^q} \right) = \mathcal{O} \left(p^{-\frac{q}{2}} \| (M_1 - I_p) \Sigma (M_1 - I_p) \|^q \right). \tag{13}$$

Since $\limsup \max_{1 \le i \le p} \lambda_i = \limsup \| S_n \| \le \limsup \| \Sigma \| \| n^{-1} Z Z^\top \| \le \limsup \| \Sigma \| (1 + \sqrt{\gamma})^2$ almost surely, we conclude that almost surely $\sup_p \| \Sigma \| \| M_1 - I_p \| < \infty$. By Borel-Cantelli, since $q > 2$, this implies that

$$w^\top (M_1 - I_p) \Sigma (M_1 - I_p) w - \frac{\alpha^2}{p} tr \left((M_1 - I_p)^2 \Sigma \right) \xrightarrow{a.s.} 0.$$

A similar argument shows that

$$\frac{1}{n} \varepsilon^\top M_2^\top \Sigma M_2 \varepsilon - \frac{1}{n} tr \left(M_2^\top \Sigma M_2 \right) \xrightarrow{a.s.} 0.$$

By Lemma 1 for $q = (4 + \eta)/2$ and $n^{-1/2} \varepsilon^\top M_2^\top \Sigma (M_1 - I_p) w$ we get as before:

$$\mathbb{E} \left[\left(\frac{\varepsilon^\top}{\sqrt{n}} M_2^\top \Sigma (M_1 - I_p) w \right)^q \Big| M_1, M_2 \right] = \mathcal{O} \left(\frac{\alpha^q}{(pn)^{\frac{q}{2}}} \left[\| M_2^\top \Sigma (M_1 - I_p) \|_F^q | M_1, M_2 \right] \right)$$

$$= \mathcal{O} \left(\frac{\alpha^q}{n^{\frac{q}{2}}} \| M_2^\top \Sigma (M_1 - I_p) \|^q \right).$$

So, again by Borell-Cantelli, we derive that

$$\frac{\varepsilon^\top}{\sqrt{n}} M_2^\top \Sigma (M_1 - I_p) w \xrightarrow{a.s.} 0.$$

Finally, we see by Proposition 1

$$\frac{1}{p} tr \left((M_1 - I_p)^2 \Sigma \right) = \frac{1}{p} tr \left(\left(h (S_n) (S_n)^{\frac{1}{2}} - I_p \right)^2 \Sigma \right) \xrightarrow{a.s.} M_{\gamma, H} ((\sqrt{x} h(x) - 1)^2)$$

$$\frac{1}{n} tr \left(M_2^\top \Sigma M_2 \right) = \frac{1}{n} tr \left(\Sigma M_2 M_2^\top \right) = \frac{p}{n} \frac{1}{p} tr \left(\Sigma h (S_n)^2 \right) \xrightarrow{a.s.} \gamma M_{\gamma, H} (h(x)^2).$$

Combining everything we get that the risk converges almost surely to

$$M_{\gamma,H}((\sqrt{x}h(x)-1)^2) + \gamma M_{\gamma,H}(h(x)^2).$$

The proof is completed.

$\square$

The next result that we prove is the asymptotic formulas for the training error, namely Proposition 3.

Proof of Proposition 3. We have

$$\frac{\|y - X^\top \hat{w}\|^2}{n} = \frac{\|\varepsilon + X^\top w - X^\top \hat{w}\|^2}{n}.$$

We have $-\varepsilon + X^\top(\hat{w}(t) - w) = M_x w + M_\varepsilon \varepsilon$,
where

$$\begin{aligned}
M_x &= X^\top \left(I - \exp\left(-t\left(\frac{XX^\top}{n} + \lambda\right)\right)\right)\left(\frac{XX^\top}{n} + \lambda\right)^{-1}\frac{XX^\top}{n} - X^\top \\
&= \sqrt{n}\sum_{i=1}^{p}\left(\sqrt{\lambda_i}\frac{1 - \exp\left(-t(\lambda_i + \lambda)\right)}{\lambda_i + \lambda}\lambda_i - \sqrt{\lambda_i}\right)v_i u_i^\top.
\end{aligned} \tag{14}$$

$$\begin{aligned}
M_\varepsilon &= -I_n + X^\top \left(I - \exp\left(-t\left(\frac{XX^\top}{n} + \lambda\right)\right)\right)\left(\frac{XX^\top}{n} + \lambda\right)^{-1}\frac{X}{n} \\
&= -1 + \sum_{i=1}^{p}\left(\lambda_i\frac{1 - \exp\left(-t(\lambda + \lambda_i)\right)}{\lambda_i + \lambda}\right)v_i v_i^\top.
\end{aligned} \tag{15}$$

Thus, the training error is

$$E_n(\hat{w}) = \frac{w^\top M_x^\top M_x w + 2w^\top M_x^\top M_\varepsilon \varepsilon + \varepsilon^\top M_\varepsilon^\top M_\varepsilon \varepsilon}{n}.$$

The exact same argument based on Lemma 1 that we used in the previous proof implies that

$$\frac{w^\top M_x^\top M_x w}{n} - \frac{\alpha^2}{p}tr\left(\frac{M_x^\top M_x}{n}\right) \xrightarrow{a.s.} 0$$

$$\frac{w^\top M_x^\top M_\varepsilon \varepsilon}{n} \xrightarrow{a.s.} 0$$

$$\frac{\varepsilon^\top M_\varepsilon^\top M_\varepsilon \varepsilon}{n} - \frac{1}{n}tr\left(\frac{M_\varepsilon^\top M_\varepsilon}{n}\right) \xrightarrow{a.s.} 0$$

To finish the proof we use the fact that

$$\frac{1}{p}tr\left(\frac{M_x^\top M_x}{n}\right) \xrightarrow{a.s.} \int x\left[(1 - \exp\left(-t(x + \lambda)\right))\frac{x}{x + \lambda} - 1\right]^2 dF_{\gamma,H}(x),$$

which is clear from (14) and the Marcenko-Pastur theorem, since u_i's are the eigenvectors of $XX^\top/n$ and λ_i's the corresponding eigenvalues. Furthermore,

$$\frac{1}{n}tr\left(\frac{M_\varepsilon^\top M_\varepsilon}{n}\right) \xrightarrow{a.s.} \int\left[(1 - \exp\left(-t(x + \lambda)\right))\frac{x}{x + \lambda} - 1\right]^2 d\underline{F}_{\gamma,H}(x),$$

which follows from (15) by the same reasoning.

$\square$

6.2. **Proofs for Linear Discriminant Analysis.** Now we focus on the results that concern Discriminant Analysis. The assumptions are the same as in Section 4. First of all, we prove Proposition 4 for estimation of the mean vector.

Proof of Proposition 4. We will first prove the result for $\gamma < 1$, since minor changes are required to account for the mass at 0 when $\gamma > 1$. We have $\hat{\delta} = \Sigma^{1/2} n^{-1/2} u + \delta$, where $u \sim \mathcal{N}(0, I_n)$ is independent of the sample covariance matrix $\hat{\Sigma}$. Using Lemma 1 we have:

$$\left\| \hat{\delta}^{(r)} - \delta \right\|^2 = \left\| r(\hat{\Sigma}) \left(\frac{\Sigma^{\frac{1}{2}} u}{\sqrt{n}} + \delta \right) - \delta \right\|^2 = \frac{tr\left(\Sigma r^2(\hat{\Sigma})\right)}{n} + \frac{\alpha^2}{p} \left\| r(\hat{\Sigma}) - I_p \right\|_F^2 + o(1),$$

which (by Proposition 1 and the Marcenko-Pastur theorem converges almost surely to

$$\gamma M(r^2) + \alpha^2 \int (r(x) - 1)^2 dF_{\gamma,H} = \int \gamma \frac{r(x)^2}{x(f(x)^2 + g(x)^2)} + \alpha^2 (r(x) - 1)^2 dF_{\gamma,H}.$$

The integrand is quadratic in r and setting the derivative equal to 0 we see that it is minimized exactly for the function r that we claimed. If $\gamma > 1$ the only change in the proof is that we also need to minimize the contribution at 0, which equals

$$\frac{r^2(0)}{\underline{m}(0)} + \alpha^2 \frac{\gamma - 1}{\gamma} (r(0) - 1)^2.$$

□

We now prove Proposition 6, a very important result that we will need.

Proposition 6. *Let* $z_1, z_2 \in \mathbb{C}^+$. *Then,*

$$\frac{1}{p} tr \left(\Sigma \left(S_n - z_1 \right)^{-1} \Sigma \left(S_n - z_2 \right)^{-1} \right) \xrightarrow{a.s.}$$

$$-\frac{1}{\gamma z_1 z_2 \underline{m}(z_1) \underline{m}(z_2)} + \frac{\underline{m}(z_2) - \underline{m}(z_1)}{\gamma z_1 z_2 \underline{m}(z_1)^2 \underline{m}(z_2)^2 (z_2 - z_1)}.$$

Proof. Our proof is similar to the proof of the main theorem in Ledoit and Péché [2011], but it is way more complicated due to the nature of the functionals involved in the statement.

Let

$$R(z) = (S_n - z)^{-1}, R_{jk}(z) = \left(\frac{1}{n} \sum_{i \neq j,k} x_i x_i^\top - z \right)^{-1}.$$

We also define

$$a_{kj} = tr \left(\frac{x_k x_k^\top}{n} R(z_1) \frac{x_j x_j^\top}{n} R(z_2) \right).$$

The case $j = k$.

For $j = k$, we have

$$a_{jj} = \frac{x_j^\top R(z_1) x_j}{n} \frac{x_j^\top R(z_2) x_j}{n}.$$

Using $R_{jj}(z_1) - R(z_1) = R_{jj}(z_1) \frac{x_j x_j^\top}{n} R(z_1)$ we derive

$$\frac{x_j^\top R(z_1) x_j}{n} = 1 - \frac{1}{1 + \frac{x_j^\top R_{jj} x_j}{n}}.$$

In the proof of Lemma 2.2 in the reference above the authors prove that

$$\max_{j\in\{1,\cdots,n\}}\left|\frac{x_j^\top R_{jj}(z_1)x_j}{n}-\frac{1}{n}tr\left(R_{jj}(z_1)\Sigma\right)\right|\xrightarrow{a.s.}0.$$

As a result, since by the reference above

$$\max_{1\le j\le n}\left|\frac{1}{n}tr\left(R_{jj}(z_1)\Sigma\right)+1+\frac{1}{z_1\underline{m}(z_1)}\right|\xrightarrow{a.s.}0,$$

we have

$$\max_{j\in\{1,\cdots,n\}}\left|a_{jj}-(1+z_1\underline{m}(z_1))(1+z_2\underline{m}(z_2))\right|\xrightarrow{a.s.}0.$$

We conclude that

$$\frac{1}{p}\sum_{j=1}^n a_{jj}\xrightarrow{a.s.}\frac{1}{\gamma}(1+z_1\underline{m}(z_1))(1+z_2\underline{m}(z_2)). \tag{16}$$

The case $j\ne k$.

For $j\ne k$ we have

$$R(z_1)-R_{kj}(z_1)=-n^{-1}R(z_1)x_k x_k^\top R_{kj}(z_1)-n^{-1}R(z_1)x_j x_j^\top R_{kj}(z_1)$$

and, consequently,

$$\frac{x_k^\top R(z_1)x_j}{n}-\frac{x_k^\top R_{kj}(z_1)x_j}{n}$$

$$=-\frac{x_k^\top R(z_1)x_k}{n}\frac{x_k^\top R_{kj}(z_1)x_j}{n}-\frac{x_k^\top R(z_1)x_j}{n}\frac{x_j^\top R_{kj}(z_1)x_j}{n}$$

$$\Rightarrow\frac{x_k^\top R(z_1)x_j}{n}=\frac{\frac{x_k^\top R_{kj}(z_1)x_j}{n}\left(1-\frac{x_k^\top R(z_1)x_k}{n}\right)}{1+\frac{x_j^\top R_{kj}(z_1)x_j}{n}} \tag{17}$$

$$=\frac{x_k^\top R_{kj}(z_1)x_j}{n}\frac{1}{\left(1+\frac{x_j^\top R_{kj}(z_1)x_j}{n}\right)\left(1+\frac{x_k^\top R_{kk}(z_1)x_k}{n}\right)}.$$

We conclude that, for $j\ne k$,

$$a_{kj}=\frac{x_k^\top R_{kj}(z_1)x_j}{n}\frac{x_j^\top R_{kj}(z_2)x_k}{n}A_{kj}=tr\left(\frac{x_k x_k^\top}{n}R_{kj}(z_1)\frac{x_j x_j^\top}{n}R_{kj}(z_2)\right)A_{kj},$$

$$A_{kj}=\frac{1}{\left(1+\frac{x_j^\top R_{kj}(z_1)x_j}{n}\right)\left(1+\frac{x_k^\top R_{kk}(z_1)x_k}{n}\right)}\frac{1}{\left(1+\frac{x_j^\top R_{kj}(z_2)x_j}{n}\right)\left(1+\frac{x_k^\top R_{kk}(z_2)x_k}{n}\right)}. \tag{18}$$

Using the Hanson-Wright inequality from Rudelson et al. [2013] for the real and imaginary parts of $R_{kj}(z_1)$ we get that there exist absolute constants $C,c>0$ such that

$$\mathbb{P}\left(\left|\frac{x_j^\top R_{kj}(z_1)x_j}{n}-\frac{1}{n}tr\left(\Sigma R_{kj}(z_1)\right)\right|>t\mid R_{kj}\right)\le C\exp\left(-c\min\left(\frac{n^2t^2}{\|R_{jk}\|_F^2},\frac{nt}{\|R_{jk}\|}\right)\right).$$

Since $\|R_{kj}\|\le Im(z_1)^{-1}$, we conclude by the union bound that

$$\mathbb{P}\left(\max_{1\le k,j\le n}\left|\frac{x_j^\top R_{kj}(z_1)x_j}{n}-\frac{1}{n}tr\left(\Sigma R_{kj}(z_1)\right)\right|\ge t\right)$$

$$\le Cn^2\exp\left(-c\min\left(Im(z_1)^2 nt^2, Im(z_1)nt\right)\right).$$

We conclude that

$$\max_{1\le k,j\le n}\left|\frac{x_j^\top R_{kj}(z_1)x_j}{n} - \frac{1}{n}tr\left(\Sigma R_{kj}(z_1)\right)\right| \xrightarrow{a.s.} 0. \tag{19}$$

By Lemma 2.6 in Silverstein and Bai [1995] we have

$$\frac{1}{n}\left|tr\left(\Sigma R(z_1) - \Sigma R_{kk}(z_1)\right)\right| \le \frac{\|\Sigma\|}{nIm(z_1)}.$$

Applying this if we omit x_k we get

$$\frac{1}{n}\left|tr\left(\Sigma R_{kk}(z_1) - \Sigma R_{kj}(z_1)\right)\right| \le \frac{\|\Sigma\|}{nIm(z_1)}.$$

Combining the last two inequalities gives

$$\frac{1}{n}\left|tr(\Sigma R(z_1) - \Sigma R_{kj}(z_1))\right| \le \frac{2\|\Sigma\|}{nIm(z_1)}. \tag{20}$$

Using again

$$\frac{1}{n}tr(\Sigma R(z_1)) \xrightarrow{a.s.} -\frac{1 + z_1\underline{m}(z_1)}{z_1\underline{m}(z_1)},$$

(19) and (20) imply

$$\max_{1\le k,j\le n}\left|\frac{x_j^\top R_{kj}(z_1)x_j}{n} + 1 + \frac{1}{z_1\underline{m}(z_1)}\right| \xrightarrow{a.s.} 0.$$

Of course, the same convergence is true if we replace z_1 by z_2. We conclude that for $j \ne k$

$$\max_{1\le k,j\le n}\left|A_{kj} - z_1^2 z_2^2 \underline{m}(z_1)^2 \underline{m}(z_2)^2\right| \xrightarrow{a.s.} 0. \tag{21}$$

We now use the Hanson-Wright inequality twice and the exact same argument as above to get

$$\max_{1\le k\le n}\left|\frac{1}{p}tr\left(\sum_{j=1,j\ne k}^{n} R_{kj}(z_1)\frac{x_jx_j^\top}{n}R_{kj}(z_2)x_kx_k^\top\right) - \frac{1}{pn}tr\left(\Sigma R(z_1)\Sigma R(z_2)\right)\right| \xrightarrow{a.s.} 0. \tag{22}$$

Combining (21) and (22) we get

$$\frac{1}{p}\sum_{k\ne j} a_{kj} = z_1^2 z_2^2 \underline{m}(z_1)^2 \underline{m}(z_2)^2 \frac{1}{p}tr\left(\Sigma R(z_1)\Sigma R(z_2)\right) + o(1). \tag{23}$$

Let

$$E = \frac{1}{p}\sum_{1\le k,j\le n} a_{kj} = \frac{1}{p}tr\left((I_p + z_1 R(z_1)(I_p + z_2 R(z_2))))\right).$$

Then, by the Marcenko-Pastur theorem we know that

$$E \xrightarrow{a.s.} 1 + z_1 m(z_1) + z_2 m(z_2) + \frac{z_1 z_2(m(z_2) - m(z_1))}{z_2 - z_1}.$$

Notice that here we used the partial fraction decomposition $(x - z_1)^{-1}(x - z_2)^{-1} = (z_2 - z_1)^{-1}\left((x - z_2)^{-1} - (x - z_1)^{-1}\right)$, which immmplies that

$$R(z_1)R(z_2) = \frac{1}{z_2 - z_1}\left(R(z_2) - R(z_1)\right).$$

We conclude by (16) and (23) that

$$E = \frac{1}{\gamma}(1 + z_1\underline{m}(z_1))(1 + z_2\underline{m}(z_2)) + z_1^2z_2^2\underline{m}(z_1)^2\underline{m}(z_2)^2\frac{1}{p}tr\left(\Sigma R(z_1)\Sigma R(z_2)\right) + o(1).$$

The last two equations imply that

$$\lim_{p\to\infty} z_1^2z_2^2\underline{m}(z_1)^2\underline{m}(z_2)^2\frac{1}{p}tr\left(\Sigma R(z_1)\Sigma R(z_2)\right)$$

$$= -\frac{1}{\gamma}(1 + z_1\underline{m}(z_1))(1 + z_2\underline{m}(z_2)) + 1 + z_1 m(z_1) + z_2 m(z_2) + \frac{z_1 z_2(m(z_2) - m(z_1))}{z_2 - z_1}. \tag{24}$$

Using the equation for the companion Stieltjes transform

$$\gamma(1 + zm(z)) = 1 + z\underline{m}(z),$$

we can rewrite (24) after a straightforward manipulation:

$$\lim_{p\to\infty} z_1^2z_2^2\underline{m}(z_1)^2\underline{m}(z_2)^2\frac{1}{p}tr\left(\Sigma R(z_1)\Sigma R(z_2)\right)$$

$$= -\frac{1}{\gamma}z_1 z_2\underline{m}(z_1)\underline{m}(z_2) + \frac{z_1 z_2(\underline{m}(z_2) - \underline{m}(z_1))}{\gamma(z_2 - z_1)}. \tag{25}$$

This completes the proof. $\square$

This gives us the main tool in proving Proposition 5.

Proof of Proposition 5. As in Proposition 1 we only need to prove the result for analytic functions h in some open set that contains $supp(F_{\gamma,H})$. We write using the Cauchy integral formula:

$$\frac{1}{p}tr\left(\Sigma h\left(S_n\right)\Sigma h\left(S_n\right)\right) = \left(\frac{1}{2\pi i}\right)^2 \oint_\Gamma \oint_{\Gamma'} h(z_1)h(z_2)F_p(z_1, z_2)dz_1 dz_2,$$

where

$$F_p(z_1, z_2) = \frac{1}{p}tr\left(\Sigma\left(S_n - z_1\right)^{-1}\Sigma\left(S_n - z_2\right)^{-1}\right)$$

and Γ, Γ' are simple closed curves as the proof of Proposition 1 which we take to be non-intersecting (assume without loss of generality that Γ' contains Γ in the interior region). Since

$$\lim_{p\to\infty} F_p(z_1, z_2) = F(z_1, z_2) = -\frac{1}{\gamma z_1 z_2\underline{m}(z_1)\underline{m}(z_2)} + \frac{m(z_2) - \underline{m}(z_1)}{\gamma z_1 z_2\underline{m}(z_1)^2\underline{m}(z_2)^2(z_2 - z_1)},$$

the same reasoning as in Proposition 1 gives

$$\frac{1}{p}tr\left(\Sigma h\left(S_n\right)\Sigma h\left(S_n\right)\right) \xrightarrow{a.s.} \left(\frac{1}{2\pi i}\right)^2 \oint_\Gamma \oint_{\Gamma'} h(z_1)h(z_2)F(z_1, z_2)dz_1 dz_2.$$

We can rewrite

$$\left(\frac{1}{2\pi i}\right)^2 \oint_\Gamma \oint_{\Gamma'} h(z_1)h(z_2)F(z_1, z_2)dz_1 dz_2$$

$$= \left(\frac{1}{2\pi i}\right)^2 \oint_\Gamma \oint_{\Gamma'} h(z_1)h(z_2)\overline{F}(z_1, z_2)dz_1 dz_2 - \frac{1}{\gamma}\left(\frac{1}{2\pi i}\oint_\Gamma \frac{h(z)}{z\underline{m}(z)}dz\right)^2, \tag{26}$$

where

$$\overline{F}(z_1, z_2) = \frac{\underline{m}(z_2) - \underline{m}(z_1)}{\gamma z_1 z_2 \underline{m}(z_1)^2 \underline{m}(z_2)^2 (z_2 - z_1)}.$$

By the calculation in the first part we know that

$$\frac{1}{2\pi i} \oint_\Gamma -\frac{h(z)}{z\underline{m}(z)} dz = \frac{1}{2\pi i} \oint_\Gamma h(z) \frac{1 + z\underline{m}(z)}{(-z\underline{m}(z))} dz$$

$$= \int \frac{h(x)}{\pi x (f(x)^2 + g(x)^2)} g(x) dx + I_{\gamma > 1} \frac{h(0)}{\underline{m}(0)}. \tag{27}$$

As a consequence, to prove Proposition 5 it is enough to prove that

$$\left(\frac{1}{2\pi i}\right)^2 \oint_\Gamma \oint_{\Gamma'} h(z_1) h(z_2) \overline{F}(z_1, z_2) dz_1 dz_2$$

$$= \int \int \overline{K}(x, y) h(x) h(y) dx dy + \int \frac{h(x)^2 g(x)}{\gamma \pi x^2 (f(x)^2 + g(x)^2)^2} dx \tag{28}$$

$$+ \left[\frac{\underline{m}'(0)}{\gamma \underline{m}(0)^4} h(0)^2 + \frac{2h(0)}{\gamma \underline{m}(0)^2} \int h(x) \frac{f(x)^2 + g(x)^2 - 2f(x)\underline{m}(0)}{\pi x^2 (f(x)^2 + g(x)^2)^2} g(x) dx \right] I_{\gamma > 1}.$$

Here

$$\overline{K}(x, y) = K(x, y) + \frac{g(x)g(y)}{\gamma \pi^2 xy (f(x)^2 + g(x)^2)(f(y)^2 + g(y)^2)}.$$

Following the same idea as in the proof of Proposition 1, we can shrink the curve Γ' down to the real axis to get

$$A(z_2) = \frac{1}{2\pi i} \oint_{\Gamma'} h(z_1) \overline{F}(z_1, z_2) dz_1$$

$$= \lim_{\epsilon \downarrow 0} \int \frac{h(x)}{2\pi i} \left[\overline{F}(x - i\epsilon, z_2) - \overline{F}(x + i\epsilon, z_2) \right] dx + \frac{h(0)(\underline{m}(z_2) - \underline{m}(0))}{\gamma z_2^2 \underline{m}(0)^2 \underline{m}(z_2)^2} I_{\gamma > 1}$$

$$= \int \frac{2\underline{m}(z_2)f(x)g(x) - g(x)(f(x)^2 + g(x)^2)}{\gamma \pi x z_2 (z_2 - x)(f(x)^2 + g(x)^2)^2 \underline{m}(z_2)^2} h(x) dx + \frac{h(0)(\underline{m}(z_2) - \underline{m}(0))}{\gamma z_2^2 \underline{m}(0)^2 \underline{m}(z_2)^2} I_{\gamma > 1}. \tag{29}$$

The first term above comes from the support of $F_{\gamma, H}$ on $(0, \infty)$, while the second is from the mass at 0 when $\gamma > 1$. Let us focus on the contribution of the second term in the case $\gamma > 1$. We in turn shrink Γ to calculate the contribution of the second term

$$\frac{1}{2\pi i} \oint_\Gamma h(z_2) \frac{h(0)(\underline{m}(z_2) - \underline{m}(0))}{\gamma z_2^2 \underline{m}(0)^2 \underline{m}(z_2)^2} dz_2 = h(0)^2 \frac{\underline{m}'(0)}{\gamma \underline{m}(0)^4}$$

$$+ \frac{1}{\pi} \lim_{\epsilon \downarrow 0} \int Im \left[h(x - i\epsilon) \frac{h(0)(\underline{m}(x - i\epsilon) - \underline{m}(0))}{\gamma (x - i\epsilon)^2 \underline{m}(0)^2 \underline{m}(x - i\epsilon)^2} \right] dx \tag{30}$$

$$= h(0)^2 \frac{\underline{m}'(0)}{\gamma \underline{m}(0)^4} + \frac{h(0)}{\gamma \underline{m}(0)^2} \int h(x) \frac{f(x)^2 + g(x)^2 - 2f(x)\underline{m}(0)}{\pi x^2 (f(x)^2 + g(x)^2)^2} g(x) dx.$$

Comparing (28) and (30) we conclude that it remains to prove that

$$\frac{1}{2\pi i}\oint_\Gamma \int \frac{2\underline{m}(z_2)f(x)g(x)-g(x)(f(x)^2+g(x)^2)}{\gamma\pi x z_2(z_2-x)(f(x)^2+g(x)^2)^2\underline{m}(z_2)^2}h(z_2)h(x)dxdz_2$$

$$= \int\int \overline{K}(x,y)h(x)h(y)dxdy + \int h(x)^2 \frac{g(x)}{\gamma\pi x^2(f(x)^2+g(x)^2)^2}dx \qquad (31)$$

$$+ \left[\frac{h(0)}{\gamma\underline{m}(0)^2}\int h(x)\frac{f(x)^2+g(x)^2-2f(x)\underline{m}(0)}{\pi x^2(f(x)^2+g(x)^2)^2}g(x)dx\right]I_{\gamma>1}$$

.

Changing the order of integration we see that the second term comes by the contribution at 0 of the integrand in the case $\gamma > 1$ by the Cauchy integral formula. For the rest of the proof we focus on the contribution of the rest of the support of $F_{\gamma,H}$.

There are two types of terms we need to consider here. First of all, ignoring the singularity at $z_2 = x$ of the integrand and shrinking Γ as before gives a term equal to

$$\int\int \frac{1}{\pi}Im\left[\frac{2\underline{m}(y-i\epsilon)f(x)g(x)-g(x)(f(x)^2+g(x)^2)}{\gamma\pi xy(y-x)(f(x)^2+g(x)^2)^2\underline{m}(y-i\epsilon)^2}\right]h(x)h(y)dxdy$$

$$= \int\int \overline{K}(x,y)h(x)h(y)dxdy,$$

as we see by a straightforward calculation.

The last thing we need to take into account is the contribution of the singularity of $\frac{1}{z_2-x}$ at x. Let

$$k(z_2;x) = \frac{2\underline{m}(z_2)f(x)g(x)-g(x)(f(x)^2+g(x)^2)}{\gamma\pi x z_2(f(x)^2+g(x)^2)^2\underline{m}(z_2)^2}.$$

An important observation is that $k(\overline{z_2};x) = \overline{k(z_2;x)} \forall z_2 \in \mathbb{C}-\mathbb{R}$. The contribution of the singularity at x is equal to

$$\lim_{r\downarrow 0}\frac{1}{2\pi i}\int_0^\pi \frac{k(x+re^{i\theta};x)}{re^{i\theta}}h(x)h(x+re^{i\theta})rie^{i\theta}dr$$

$$+\frac{1}{2\pi i}\int_\pi^{2\pi}\frac{k(x+re^{i\theta};x)}{re^{i\theta}}h(x)h(x+re^{i\theta})rie^{i\theta}dr \qquad (32)$$

$$= \lim_{r\downarrow 0}\frac{1}{2\pi}\int_0^\pi \left[k(x+re^{i\theta};x)+k(x-re^{i\theta};x)\right]h(x)^2dx.$$

To finish the proof we use dominated convergence and the fact that

$$\lim_{r\downarrow 0}Re\left[k(x+re^{i\theta};x)\right] = \frac{g(x)\lim_{r\downarrow 0}Re\left[\frac{2\underline{m}(x+re^{i\theta})f(x)-f(x)^2-g(x)^2}{\underline{m}(x+re^{i\theta})^2}\right]}{\gamma\pi x^2(f(x)^2+g(x)^2)^2}$$

and (for $\theta \in [0,\pi]$)

$$\lim_{r\downarrow 0}Re\left[\frac{2\underline{m}(x+re^{i\theta})f(x)-f(x)^2-g(x)^2}{\underline{m}(x+re^{i\theta})^2}\right]$$

$$= Re\left[\frac{2(f(x)+ig(x))f(x)-f(x)^2-g(x)^2}{(f(x)+ig(x))^2}\right] = 1. \qquad (33)$$

As a consequence,

$$\lim_{r\downarrow 0} Re\left[k(x + re^{i\theta}; x)\right] = \frac{g(x)}{\gamma\pi x^2 (f(x)^2 + g(x)^2)^2}.$$

$\square$

We are now ready to prove the main theorem of Section 4, namely Theorem 2. With the machinery we have developed above, the proof is going to be rather straightforward. Since all of the concentration of measure results for quadratic forms that we will need in the next proof have been used a great number of times throughout the paper, for instance in the proof of Theorem 1 and Proposition 6, we will omit some details when we use them.

Proof of Theorem 2. Following the notation of Section 4 we have $\hat{\delta} = \delta + \Sigma^{1/2}u/\sqrt{n}$, where $u \sim \mathcal{N}(0, I_p)$ is independent of the sample covariance matrix $\hat{\Sigma}$. If we have a new data point $x = \Sigma^{1/2}z + \delta$, then the point is missclassified, using a shrinkage function h, if

$$\hat{\delta}^\top h\left(\hat{\Sigma}\right) \Sigma^{\frac{1}{2}} z \le -\hat{\delta}^\top h\left(\hat{\Sigma}\right)\delta.$$

This happens with probability

$$\Phi\left(-\frac{\hat{\delta}^\top h\left(\hat{\Sigma}\right)\delta}{\|\Sigma^{\frac{1}{2}}h\left(\hat{\Sigma}\right)\hat{\delta}\|}\right), \tag{34}$$

which is also, by symmetry, the missclassification rate of Discriminant Analysis in general.

Notice that

$$\frac{u^\top \Sigma^{\frac{1}{2}}}{\sqrt{n}} h\left(\hat{\Sigma}\right)\delta \xrightarrow{a.s.} 0,$$

since u, δ are independent (for example, by a $\frac{(4+\eta)}{2}$-th moment argument and Lemma 1 as in the proof of Theorem 1). This implies that

$$\hat{\delta}^\top h\left(\hat{\Sigma}\right)\delta - \delta^\top h\left(\hat{\Sigma}\right)\delta \xrightarrow{a.s.} 0.$$

Before we continue we observe that because $\hat{\Sigma}$ is a rank 1 perturbation of S_n and they are both independent of δ, we can replace $\hat{\Sigma}$ by S_n in all the asymptotics that follow and u by a standard normal random variable in $\mathbb{R}^n$).

By Lemma 1 and Borel-Cantelli as before, the above convergence result implies that

$$\hat{\delta}^\top h\left(S_n\right)\delta - \frac{\alpha^2}{p}tr\left(h\left(S_n\right)\right) \xrightarrow{a.s.} 0 \Rightarrow \hat{\delta}^\top h\left(S_n\right)\delta \xrightarrow{a.s.} \alpha^2 \int h(x)dF_{\gamma, H}(x). \tag{35}$$

Now we turn our focus to the asymptotics of

$$\|\Sigma^{\frac{1}{2}}h\left(S_n\right)\hat{\delta}\|^2.$$

Expanding the square of the norm we have

$$\|\Sigma^{\frac{1}{2}}h\left(S_n\right)\hat{\delta}\|^2 = \delta^\top h\left(S_n\right)\Sigma h\left(S_n\right)\delta + \frac{1}{n}u^\top \Sigma^{\frac{1}{2}}h\left(S_n\right)\Sigma h\left(S_n\right)\Sigma^{\frac{1}{2}}u \\ +2\delta^\top h\left(S_n\right)\Sigma h\left(S_n\right)\frac{\Sigma^{\frac{1}{2}}u}{\sqrt{n}}. \tag{36}$$

We have the following convergence results, all of which follow from Lemma 1 and Borel-Cantelli exactly in the same fashion as earlier:

$$\delta^{\top} h\left(S_{n}\right) \Sigma h\left(S_{n}\right) \frac{\Sigma^{\frac{1}{2}} u}{\sqrt{n}} \xrightarrow{a.s.} 0 \tag{37}$$

$$\delta^{\top} h\left(S_{n}\right) \Sigma h\left(S_{n}\right) \delta-\frac{\alpha^{2}}{p} tr\left(\Sigma h\left(S_{n}\right)^{2}\right) \xrightarrow{a.s.} 0$$
$$\Rightarrow \delta^{\top} h\left(S_{n}\right) \Sigma h\left(S_{n}\right) \delta \xrightarrow{a.s.} \alpha^{2} M_{\gamma, H}(h^{2}) \tag{38}$$

$$\frac{1}{n} u^{\top} \Sigma^{\frac{1}{2}} h\left(S_{n}\right) \Sigma h\left(S_{n}\right) \Sigma^{\frac{1}{2}} u-\frac{1}{n} tr\left(\Sigma h\left(S_{n}\right) \Sigma h\left(S_{n}\right)\right) \xrightarrow{a.s.} 0$$
$$\Rightarrow \frac{1}{n} u^{\top} \Sigma^{\frac{1}{2}} h\left(S_{n}\right) \Sigma h\left(S_{n}\right) \Sigma^{\frac{1}{2}} u \xrightarrow{a.s.} \gamma T_{\gamma, H}(h) \tag{39}$$

Using (37),(38),(39), we conclude from (36) that

$$\|\Sigma^{\frac{1}{2}} h\left(S_{n}\right) \hat{\delta}\|^{2} \xrightarrow{a.s.} \gamma T_{\gamma, H}(h)+\alpha^{2} M_{\gamma, H}(h^{2}).$$

The last result together with (35) and (34) imply Theorem 2.

$\square$

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