An Analysis of Random Design Linear Regression

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Abstract

The random design setting for linear regression concerns estimators based on a random sample of covariate/response pairs. This work gives explicit bounds on the prediction error for the ordinary least squares estimator and the ridge regression estimator under mild assumptions on the covariate/response distributions. In particular, this work provides sharp results on the "out-of-sample" prediction error, as opposed to the "in-sample" (fixed design) error. Our analysis also explicitly reveals the effect of noise vs. modeling errors. The approach reveals a close connection to the more traditional fixed design setting, and our methods make use of recent advances in concentration inequalities (for vectors and matrices). We also describe an application of our results to fast least squares computations.

1 Introduction

In the random design setting for linear regression, one is given pairs $(X_1, Y_1), \ldots, (X_n, Y_n)$ of covariates and responses, sampled from a population, where each X_i are random vectors and $Y_i \in \mathbb{R}$. These pairs are hypothesized to have the linear relationship

$$Y_i = X_i^\top \beta + \epsilon_i$$

for some linear map β , where the ϵ_i are noise terms. The goal of estimation in this setting is to find coefficients $\hat{\beta}$ based on these (X_i, Y_i) pairs such that the expected prediction error on a new draw (X, Y) from the population, measured as $\mathbb{E}[(X^{\top}\hat{\beta} - Y)^2]$, is as small as possible.

The random design setting stands in contrast to the fixed design setting, where the covariates X_1, \ldots, X_n are fixed (non-random), with only the responses Y_1, \ldots, Y_n being treated as random. Thus, the covariance structure of the design points is completely known and need not be estimated, making the conditions simpler for establishing finite sample guarantees and for studying techniques such as dimension reduction and feature selection. However, the fixed design setting does not directly address out-of-sample prediction, which is of primary concern in some applications.

In this work, we show that the *ordinary least squares estimator* can be readily understood in the random design setting almost as naturally as it is in the fixed design setting. Our analysis

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provides a simple decomposition that decouples the estimation of the covariance structure from another quantity resembling the fixed design risk; it is revealed that the accuracy of the covariance estimation has but a second-order effect once $n \ge d$, whereupon the prediction error converges at essentially the same d/n rate as in the fixed design setting. Moreover, the prediction errors of the optimal linear predictor—which need not be the same as the Bayes predictor $x \mapsto \mathbb{E}[Y|X = x]$ can be separated into (deterministic) approximation errors and zero-mean noise, which our analysis can treat separately in a simple way. The decomposition allows for the straightforward application of exponential tail inequalities to all its constituent parts, and we comment on the consequences of natural subgaussian moment assumptions that afford sharper tail inequalities, which we also provided in this work. Finally, because many of the tail inequalities applicable here also hold under relaxed independence assumptions, such as martingale dependence, the sampling assumptions in the random design regression can be relaxed to these more general conditions as well.

The basic form of our analysis for ordinary least squares also generalizes to give an analysis of the *ridge estimator*, which is applicable in infinite-dimensional covariate spaces. This analysis, which we specialize to the case where β perfectly models the Bayes predictor, is somewhat more involved because establishing the accuracy of the empirical second-moment matrix is more delicate. Nevertheless, its core still rests upon the same (or similar) exponential tail inequalities used in the analysis of ordinary least squares.

Related work. Many classical analyses of the ordinary least squares estimators in the random design setting (e.g., in the context of non-parametric estimators) do not actually show O(d/n) convergence of the mean squared error to that of the best linear predictor. Rather, the error relative to the Bayes error is bounded by some multiple (e.g., eight) of the error of the optimal linear predictor relative to Bayes error, plus a O(d/n) term (Györfi et al., 2004):

$$\mathbb{E}\left[(X^{\top}\hat{\beta}_{ols} - \mathbb{E}[Y|X])^2\right] \le 8 \cdot \mathbb{E}\left[(X^{\top}\beta - \mathbb{E}[Y|X])^2\right] + O(d/n).$$

Such bounds are appropriate in non-parametric settings where the error of the optimal linear predictor also approaches the Bayes error at an O(d/n) rate. Beyond these classical results, analyses of ordinary least squares often come with non-standard restrictions on applicability or additional dependencies on the spectrum of the second moment matrix (see the recent work of Audibert and Catoni (2010b) for a comprehensive survey of these results). A result of Catoni (2004, Proposition 5.9.1) gives a bound on the excess mean squared error of the form

$$\mathbb{E}\left[(X^{\top} \hat{\beta}_{\text{ols}} - X^{\top} \beta)^2 \right] \le O\left(\frac{d + \log(\det(\hat{\Sigma}) / \det(\Sigma))}{n} \right)$$

where $\Sigma = \mathbb{E}[XX^{\top}]$ is the second-moment matrix of X and $\hat{\Sigma}$ is its empirical counterpart. This bound is proved to hold as soon as every linear predictor with low empirical mean squared error satisfies certain boundedness conditions.

This work provides ridge regression bounds explicitly in terms of the vector β (as a sequence) and in terms of the eigenspectrum of the of the second moment matrix (e.g. the sequence of eigenvectors of $\mathbb{E}[XX^{\top}]$). Previous analyses of ridge regression made certain boundedness assumptions (*e.g.*, Zhang, 2005; Smale and Zhou, 2007). For instance, Zhang assumes $||X|| \leq B_X$ and $|Y - X^{\top}\beta| \leq$

 B_{bias} almost surely, and gives the bound

$$\mathbb{E}[(X^{\top}\hat{\beta}_{\lambda} - X^{\top}\beta)^{2}] \leq \lambda \|\hat{\beta}_{\lambda} - \beta\|^{2} + O\left(\frac{d_{1,\lambda} \cdot (B_{\text{bias}} + B_{X}\|\hat{\beta}_{\lambda} - \beta\|)^{2}}{n}\right)$$

where $d_{1,\lambda}$ is a notion of effective dimension at scale λ (same as that in (1)). The quantity $\|\hat{\beta}_{\lambda} - \beta\|$ is then bounded by assuming $\|\beta\| < \infty$. Smale and Zhou separately bound $\mathbb{E}[(X^{\top}\hat{\beta}_{\lambda} - X^{\top}\beta_{\lambda})^2]$ by $O(B_X^2 B_Y^2 / \lambda^2 n)$ under the more stringent conditions that $|Y| \leq B_Y$ and $\|X\| \leq B_X$ almost surely; this is then used to bound $\mathbb{E}[(X^{\top}\hat{\beta}_{\lambda} - X^{\top}\beta)^2]$ under explicit boundedness assumptions on β . Our result for ridge regression is given explicitly in terms of $\mathbb{E}[(X^{\top}\beta_{\lambda} - X^{\top}\beta)^2]$ (the first term in Theorem 3), which can be bounded even when $\|\beta\|$ is unbounded. We note that $\mathbb{E}[(X^{\top}\beta_{\lambda} - X^{\top}\beta)^2]$ is precisely the bias term from the standard fixed design analysis of ridge regression, and therefore is natural to expect in a random design analysis.

Recently, Audibert and Catoni (2010a,b) derived sharp risk bounds for the ordinary least squares estimator and the ridge estimator (in addition to specially developed PAC-Bayesian estimators) in a random design setting under very mild assumptions. Their bounds are proved using PAC-Bayesian techniques, which allows them to achieve exponential tail inequalities under simple moment conditions. Their non-asymptotic bound for ordinary least squares holds with probability at least $1 - \delta$ and requires $\delta > 1/n$. This work makes stronger assumptions in some respects, allowing for δ to be arbitrarily small (through the use of vector and matrix tail inequalities). The analysis of Audibert and Catoni (2010a) for the ridge estimator is established in an asymptotic sense and bounds the excess *regularized* mean squared error rather than the excess mean squared error itself. Therefore, the results are not directly comparable to those provided here.

Our results can be readily applied to the analysis of certain techniques for speeding up overcomplete least squares computations, originally studied by Drineas et al. (2010). Central to this earlier analysis is the notion of statistical leverage, which we also use in our work. In the appendix, we show that these computational techniques can be readily understood in the context of random design linear regression.

Outline. The rest of the paper is organized as follows. Section 2 sets up notations and the basic data model used in the analyses. The analysis of ordinary least squares is given in Section 3, and the analysis of ridge regression is given in Section 4. Appendix A presents the exponential tail inequalities used in the analyses, and Appendix B discusses the application to fast least squares computations.

2 Preliminaries

2.1 Notations

The Euclidean norm of a vector x is denoted by ||x||. The induced spectral norm of a matrix A is denoted by ||A||, *i.e.*, $||A|| := \sup\{||Ax||: ||x|| = 1\}$; its Frobenius norm is denoted by $||A||_{\rm F}$, *i.e.*, $||A||_{\rm F}^2 = \sum_{i,j} A_{i,j}^2$. For any symmetric and positive semidefinite matrix M (*i.e.*, $M = M^{\top}$ and $M \succeq 0$), let $||x||_M$ denote the norm of a vector x defined by

$$\|x\|_M := \sqrt{x^\top M x}$$

The *j*-th eigenvalue of a symmetric matrix A is denoted by $\lambda_j(A)$, where $\lambda_1(A) \ge \lambda_2(A) \ge \ldots$ and the smallest and largest eigenvalues of a symmetric matrix A are denoted by $\lambda_{\min}(A)$ and $\lambda_{\max}(A)$, respectively.

2.2 Linear regression

Let X be a random vector of covariates (features) and $Y \in \mathbb{R}$ be a response variable (label), both sampled from some (unknown) underlying joint distribution. We are interested in linear predictors of the response variable from the covariates, with performance measured under a standard probabilistic model of the covariate/response pairs.

In the context of linear regression, the quality of a linear prediction $X^{\top}w$ of Y from X is typically measured by the squared error $(X^{\top}w - Y)^2$. The mean squared error of a linear predictor w is given by

$$L(w) := \mathbb{E}\left[(X^{\top}w - Y)^2 \right]$$

where the expectation is taken over both X and Y. Let

$$\varSigma := \mathbb{E}[XX^\top]$$

be the second moment matrix of X.

We assume that Σ is invertible, so there is a unique minimizer of L given by

$$\beta := \Sigma^{-1} \mathbb{E}[XY].$$

The excess mean squared error of w over the minimum is

$$L(w) - L(\beta) = ||w - \beta||_{\Sigma}^{2}.$$

2.3 Data model

We are interested in estimating a vector $\hat{\beta}$ of coefficients from *n* observed random covariate/response pairs $(X_1, Y_1), \ldots, (X_n, Y_n)$. We assume these pairs are independent copies of (X, Y), *i.e.*, sampled i.i.d. from the (unknown) distribution over (X, Y). The quality of an estimator $\hat{\beta}$ will be judged by its excess loss $\|\hat{\beta} - \beta\|_{\Sigma}^2$, as discussed above.

We now state conditions on the distribution of the random pair (X, Y).

2.3.1 Response model

The response model we consider is a relaxation of the typical Gaussian model by allowing for model approximation error and general subgaussian noise. In particular, define the random variables

$$\eta(X) := Y - \mathbb{E}[Y|X]$$
 and $\operatorname{bias}(X) := \mathbb{E}[Y|X] - X^{\top}\beta$,

where $\eta(X)$ corresponds to the response noise, and bias(X) corresponds to the approximation error of β . This gives the modeling equation

$$Y = X^{\top}\beta + \operatorname{bias}(X) + \eta(X).$$

Conditioned on X, the noise $\eta(X)$ is a random, while the approximation error bias(X) is deterministic.

We assume the following condition on the noise $\eta(X)$.

Condition 1 (Subgaussian noise). There exist a finite $\sigma_{\text{noise}} \ge 0$ such that for all $\lambda \in \mathbb{R}$, almost surely:

$$\mathbb{E}\left[\exp(\lambda \eta(X)) \mid X\right] \le \exp\left(\lambda^2 \sigma_{\text{noise}}^2/2\right).$$

In some cases, we make the further assumption on the approximation error bias(X). The quantity B_{bias} in the following only appears in lower order terms (or as $log(B_{bias})$) in the main bounds.

Condition 2 (Bounded approximation error). There exist a finite $B_{\text{bias}} \ge 0$ such that for all $\lambda \in \mathbb{R}$, almost surely:

$$\|\Sigma^{-1/2}X \operatorname{bias}(X)\| \le B_{\operatorname{bias}}\sqrt{d}.$$

It is possible to relax this condition to moment bounds, simply by using a different exponential tail inequality in the analysis. We do not consider this relaxation for sake of simplicity.

2.3.2 Covariate model

We separately consider two conditions on X. The first requires that X has subgaussian moments in every direction after *whitening* (the linear transformation $x \mapsto \Sigma^{-1/2} x$).

Condition 3 (Subgaussian projections). There exists a finite $\rho_{1,cov} \ge 1$ such that:

$$\mathbb{E}\left[\exp\left(\alpha^{\top} \Sigma^{-1/2} X\right)\right] \le \exp\left(\rho_{1, \text{cov}} \cdot \|\alpha\|^{2}/2\right) \quad \forall \alpha \in \mathbb{R}^{d}.$$

The second condition requires that the squared length of X (again, after whitening) is never more than a constant factor greater than its expectation.

Condition 4 (Bounded statistical leverage). There exists a finite $\rho_{2,cov} \geq 1$ such that almost surely:

$$\frac{\|\Sigma^{-1/2}X\|}{\sqrt{d}} = \frac{\|\Sigma^{-1/2}X\|}{\sqrt{\mathbb{E}[\|\Sigma^{-1/2}X\|^2]}} \le \rho_{2,\text{cov}}.$$

This condition can be seen as being analogous to a Bernstein-like condition (*e.g.*, an assumed almost-sure upper bound on a random variable and a known variance; in the above, $\rho_{2,cov}$ is the ratio of these two quantities).

3 Ordinary least squares

We now work in a finite dimensional setting where $X \in \mathbb{R}^d$ The *empirical mean squared error* of a linear predictor w is

$$\hat{L}(w) := \frac{1}{n} \sum_{i=1}^{n} (X_i^{\top} w - Y_i)^2.$$

Let

$$\hat{\Sigma} := \sum_{i=1}^{n} X_i X_i^{\top} / n$$

be the empirical second moment matrix of X_1, \ldots, X_n . Throughout, we denote empirical expectations by $\hat{\mathbb{E}}[\cdot]$; so, for instance,

$$\hat{L}(w) = \hat{\mathbb{E}}(X^{\top}w - Y)^2$$
 and $\hat{\Sigma} = \hat{\mathbb{E}}[XX^{\top}].$

If $\hat{\Sigma}$ is invertible, then the unique minimizer, $\hat{\beta}_{ols}$, is is given by ordinary least squares:

$$\hat{\beta}_{\text{ols}} := \hat{\Sigma}^{-1} \hat{\mathbb{E}}[XY].$$

3.1 Review: the fixed design setting

In the fixed design setting, the X_i are regarded as deterministic vectors in \mathbb{R}^d , so the only randomness involved is the sampling of the Y_i . Here, $\Sigma_{\text{fixed}} := \sum_{i=1}^n X_i X_i^\top / n = \hat{\Sigma}$ (a deterministic quantity, assumed without loss of generality to be invertible), and

$$\beta_{\text{fixed}} := \Sigma_{\text{fixed}}^{-1} \left(\frac{1}{n} \sum_{i=1}^{n} X_i \mathbb{E}[Y_i] \right)$$

is the unique minimizer of

$$L_{\text{fixed}}(w) := \mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n} (X_i^{\top}w - Y_i)^2\right].$$

Here, we are interested in the excess squared error:

$$L_{\text{fixed}}(w) - L_{\text{fixed}}(\beta) = ||w - \beta_{\text{fixed}}||_{\Sigma_{\text{fixed}}}^2$$

In this case, the analysis under suitable modifications of Condition 1 is standard.

Proposition 1 (Fixed design). Suppose Σ_{fixed} is invertible and $X \in \mathbb{R}^d$. If $\operatorname{var}(Y_i) = \sigma^2$, then:

$$\mathbb{E}\left[\|\hat{\beta}_{\text{ols}} - \beta_{\text{fixed}}\|_{\Sigma_{\text{fixed}}}^2\right] = \frac{d\sigma^2}{n}$$

(where the expectation is over the randomness in the Y_i 's). Instead, suppose that there exists $\sigma_{noise} > 0$ such that

$$\mathbb{E}\left[\exp\left(\sum_{i=1}^{n}\alpha_{i}(Y_{i}-\mathbb{E}[Y_{i}])\right)\right] \leq \exp\left(\|\alpha\|^{2}\sigma_{\text{noise}}^{2}/2\right)$$

for all $(\alpha_1, \ldots, \alpha_n) \in \mathbb{R}^n$. For $\delta \in (0, 1)$, we have that with probability at least $1 - \delta$,

$$\|\hat{\beta}_{\text{ols}} - \beta_{\text{fixed}}\|_{\Sigma_{\text{fixed}}}^2 \le \frac{\sigma_{\text{noise}}^2 \cdot \left(d + 2\sqrt{d\log(1/\delta)} + 2\log(1/\delta)\right)}{n}.$$

Proof. The claim follows immediately from the definitions of $\hat{\beta}_{ols}$ and β_{fixed} , and by Lemma 14.

Our results for the random design setting will be directly comparable to the bound obtained here for fixed design.

Remark 1 (Approximation error in the fixed design setting). Note that modeling error has no effect on the bounds above. That is, there is no dependence on the modeling error with regards to the excess loss in the fixed design setting.

3.2 Out-of-sample prediction error: correct model

Our main results are largely consequences of the decompositions in Lemma 1 and Lemma 2, combined with probability tail inequalities given in Appendix A.

First, we present the results for the case where bias(X) = 0, *i.e.*, when the linear model is correct.

Lemma 1 (Random design decomposition; correct model). Suppose $\hat{\Sigma} \succ 0$ and $\mathbb{E}[Y|X] = X^{\top}\beta$, then

$$\|\hat{\beta}_{\text{ols}} - \beta\|_{\Sigma}^{2} = \left\|\hat{\mathbb{E}}\left[\hat{\Sigma}^{-1}X\eta(X)\right]\right\|_{\Sigma}^{2}$$
$$\leq \left\|\Sigma^{1/2}\hat{\Sigma}^{-1}\Sigma^{1/2}\right\|\left\|\hat{\mathbb{E}}\left[\hat{\Sigma}^{-1/2}X\eta(X)\right]\right\|^{2}.$$

Proof. Since $Y - X^{\top}\beta = \eta(X)$, we have

$$\mathbb{\hat{E}}[XY] - \mathbb{\hat{\Sigma}}\beta = \mathbb{\hat{E}}[X\eta(X)].$$

.

Hence, using the definitions of $\hat{\beta}_{ols}$,

$$\hat{\beta}_{ols} - \beta = \hat{\mathbb{E}} \left[\hat{\Sigma}^{-1} X \eta(X) \right]$$

Furthermore,

$$\Sigma^{1/2}\left(\hat{\beta}_{\rm ols}-\beta\right) = \Sigma^{1/2}\hat{\Sigma}^{-1/2} \,\hat{\mathbb{E}}\left[\hat{\Sigma}^{-1/2}X\,\eta(X)\right].$$

Observe $\|\Sigma^{1/2}\hat{\Sigma}^{-1/2}\| = \|\hat{\Sigma}^{-1/2}\Sigma^{1/2}\| = \|\Sigma^{1/2}\hat{\Sigma}^{-1}\Sigma^{1/2}\|^{1/2}$, and the conclusion follows.

This decomposition shows that as long as $\|\Sigma^{1/2}\hat{\Sigma}^{-1}\Sigma^{1/2}\| = O(1)$, then the rate at which $\|\hat{\beta}_{ols} - \beta\|_{\Sigma}^2$ tends to zero is controlled by $\|\hat{\mathbb{E}}[\hat{\Sigma}^{-1/2}X\eta(X)]\|^2$, which is essentially the fixed design excess loss.

To state our main bound, we first define the following quantities for all $\delta \in (0, 1)$:

$$n_{1,\delta} := 70\rho_{1,\text{cov}}^2 \left(d\log 41 + \log(2/\delta)\right)$$

$$n_{2,\delta} := 4\rho_{2,\text{cov}}^2 d\log(d/\delta)$$

$$K_{1,\delta,n} := \frac{1}{1 - \frac{10\rho_{1,\text{cov}}}{9} \left(\sqrt{\frac{32(d\log 41 + \log(2/\delta))}{n}} + \frac{2(d\log 41 + \log(2/\delta))}{n}\right)}$$

$$K_{2,\delta,n} := \frac{1}{1 - \sqrt{\frac{2\rho_{2,\text{cov}}^2 d\log(d/\delta)}{n}}}.$$

Note that $1 < K_{1,\delta,n} < \infty$ and $1 < K_{2,\delta,n} < \infty$, respectively, when $n > n_{1,\delta}$ and $n > n_{2,\delta}$. Furthermore,

$$\lim_{n \to \infty} K_{1,\delta,n} = 1, \qquad \lim_{n \to \infty} K_{2,\delta,n} = 1.$$

Our first result follows.

Theorem 1 (Correct model). Fix any $\delta \in (0, 1)$. Suppose that Conditions 1 and 3 hold and that $\mathbb{E}[Y|X] = \beta \cdot X$. If $n > n_{1,\delta}$, then with probability at least $1 - 2\delta$, we have

• (Matrix errors)

$$\left\| \Sigma^{1/2} \hat{\Sigma}^{-1} \Sigma^{1/2} \right\| \le K_{1,\delta,n} \le 5;$$

• (Excess loss)

$$\|\hat{\beta}_{\text{ols}} - \beta\|_{\Sigma}^2 \le K_{1,\delta,n} \cdot \frac{\sigma_{\text{noise}}^2 \cdot \left(d + 2\sqrt{d\log(1/\delta)} + 2\log(1/\delta)\right)}{n}.$$

Suppose that Conditions 1 and 4 hold and that bias(X) = 0. If $n > n_{2,\delta}$, then with probability at least $1 - 2\delta$, we have

• (Matrix errors)

$$\left\| \Sigma^{1/2} \hat{\Sigma}^{-1} \Sigma^{1/2} \right\| \le K_{2,\delta,n} \le 5;$$

• (Excess loss)

$$\|\hat{\beta}_{\text{ols}} - \beta\|_{\Sigma}^2 \le K_{2,\delta,n} \cdot \frac{\sigma_{\text{noise}}^2 \cdot \left(d + 2\sqrt{d\log(1/\delta)} + 2\log(1/\delta)\right)}{n}.$$

Remark 2 (Accuracy of $\hat{\Sigma}$). Observe that $\|\Sigma^{1/2}\hat{\Sigma}^{-1}\Sigma^{1/2}\| \leq 5$ is not a particularly stringent condition on accuracy. In particular, a scaling of $\rho_{1,\text{cov}} = \Theta(\sqrt{n})$ (or $\rho_{2,\text{cov}} = \Theta(\sqrt{n})$) would imply $\|\Sigma^{1/2}\hat{\Sigma}^{-1}\Sigma^{1/2}\|$ is constant.

3.3 Out-of-sample prediction error: misspecified model

Now we state our results in the general case where $bias(X) \neq 0$ is allowed, *i.e.*, a misspecified linear model. Again, we begin with a basic decomposition.

Lemma 2 (Random design decomposition; misspecified model). If $\hat{\Sigma} \succ 0$, then

$$\|\hat{\beta}_{\text{ols}} - \beta\|_{\Sigma} = \left\| \hat{\mathbb{E}} \left[\hat{\Sigma}^{-1} X(\text{bias}(X) + \eta(X)) \right] \right\|_{\Sigma}$$

$$\leq \left\| \hat{\mathbb{E}} \left[\hat{\Sigma}^{-1} X \text{bias}(X) \right] \right\|_{\Sigma} + \left\| \hat{\mathbb{E}} \left[\hat{\Sigma}^{-1} X \eta(X) \right] \right\|_{\Sigma}$$

$$\|\hat{\beta}_{\text{ols}} - \beta\|_{\Sigma}^{2} \leq 2 \left\| \hat{\mathbb{E}} \left[\hat{\Sigma}^{-1} X \text{bias}(X) \right] \right\|_{\Sigma}^{2} + 2 \left\| \hat{\mathbb{E}} \left[\hat{\Sigma}^{-1} X \eta(X) \right] \right\|_{\Sigma}^{2}.$$

Furthermore,

$$\left\| \hat{\mathbb{E}} \left[\hat{\varSigma}^{-1} X \operatorname{bias}(X) \right] \right\|_{\varSigma}^{2} \leq \left\| \varSigma^{1/2} \hat{\varSigma}^{-1} \varSigma^{1/2} \right\|^{2} \cdot \left\| \hat{\mathbb{E}} \left[\varSigma^{-1/2} X \operatorname{bias}(X) \right] \right\|^{2}$$

and

$$\left\| \hat{\mathbb{E}} \left[\hat{\mathcal{L}}^{-1} X \eta(X) \right] \right\|_{\Sigma}^{2} \leq \left\| \mathcal{L}^{1/2} \hat{\mathcal{L}}^{-1} \mathcal{L}^{1/2} \right\| \left\| \hat{\mathbb{E}} \left[\hat{\mathcal{L}}^{-1/2} X \eta(X) \right] \right\|^{2}.$$

Proof. Since $Y - X^{\top}\beta = bias(X) + \eta(X)$, we have

$$\hat{\mathbb{E}}[XY] - \hat{\Sigma}\beta = \hat{\mathbb{E}}[X(\operatorname{bias}(X) + \eta(X))].$$

Using the definitions of $\hat{\beta}_{ols}$, multiplying both sides on the left by $\Sigma^{1/2} \hat{\Sigma}^{-1}$ (which exists given the assumption $\hat{\Sigma} \succ 0$) gives

$$\Sigma^{1/2} \left(\hat{\beta}_{ols} - \beta \right) = \Sigma^{1/2} \hat{\Sigma}^{-1/2} \hat{\mathbb{E}} \left[\hat{\Sigma}^{-1/2} X_i (bias(X_i) + \eta_i) \right]$$

= $\Sigma^{1/2} \hat{\Sigma}^{-1} \Sigma^{1/2} \hat{\mathbb{E}} \left[\Sigma^{-1/2} X_i bias(X_i) \right] + \Sigma^{1/2} \hat{\Sigma}^{-1/2} \hat{\mathbb{E}} \left[\hat{\Sigma}^{-1/2} X_i \eta_i \right].$

The claims now follow.

Our main result for ordinary least squares, with approximation error, follows.

Theorem 2 (Misspecified model). Fix any $\delta \in (0, 1)$. Suppose that Conditions 1, 2, and 3 hold. If $n > n_{1,\delta}$, then with probability at least $1 - 3\delta$, the following holds:

• (Matrix errors)

$$\left| \Sigma^{1/2} \hat{\Sigma}^{-1} \Sigma^{1/2} \right\| \le K_{1,\delta,n} \le 5$$

• (Approximation error contribution)

$$\left\| \hat{\mathbb{E}} \left[\hat{\mathcal{L}}^{-1} X \operatorname{bias}(X) \right] \right\|_{\mathcal{L}}^{2} \leq K_{1,\delta,n}^{2} \left(\frac{4\mathbb{E} \left[\| \mathcal{L}^{-1/2} X \operatorname{bias}(X) \|^{2} \right] \left(1 + 8 \log(1/\delta) \right)}{n} + \frac{3B_{\operatorname{bias}}^{2} d \log^{2}(1/\delta)}{n^{2}} \right)$$

(See Remark 4 below for interpretation).

• (Noise contribution) and

$$\left\| \hat{\mathbb{E}} \left[\hat{\mathcal{L}}^{-1} X \eta(X) \right] \right\|_{\Sigma}^{2} \leq K_{1,\delta,n} \cdot \frac{\sigma_{\text{noise}}^{2} \cdot \left(d + 2\sqrt{d \log(1/\delta)} + 2\log(1/\delta) \right)}{n}$$

• (Excess loss)

$$\|\hat{\beta}_{ols} - \beta\|_{\Sigma} \leq \underbrace{\left\|\hat{\mathbb{E}}\left[\hat{\Sigma}^{-1}X\operatorname{bias}(X)\right]\right\|_{\Sigma}}_{\sqrt{approximation\ error\ contribution}} + \underbrace{\left\|\hat{\mathbb{E}}\left[\hat{\Sigma}^{-1}X\eta(X)\right]\right\|_{\Sigma}}_{\sqrt{noise\ contribution}};$$
$$\|\hat{\beta}_{ols} - \beta\|_{\Sigma}^{2} \leq 2\left\|\hat{\mathbb{E}}\left[\hat{\Sigma}^{-1}X\operatorname{bias}(X)\right]\right\|_{\Sigma}^{2} + 2\left\|\hat{\mathbb{E}}\left[\hat{\Sigma}^{-1}X\eta(X)\right]\right\|_{\Sigma}^{2}.$$

Instead, if Conditions 1, 2, and 4 hold, then the above claims hold with $n_{2,\delta}$ and $K_{2,\delta,n}$ in place of $n_{1,\delta}$ and $K_{1,\delta,n}$.

Remark 3. Since $\beta = \arg \min_{w} \mathbb{E}[(X^{\top}w - Y)^2]$, the excess loss bound $\|\hat{\beta}_{ols} - \beta\|_{\Sigma}$ can be translated into an oracle inequality with the following identity:

$$\mathbb{E}[(X^{\top}\hat{\beta}_{\text{ols}} - Y)^2] = \inf_{w} \mathbb{E}[(X^{\top}w - Y)^2] + \|\hat{\beta}_{\text{ols}} - \beta\|_{\Sigma}^2.$$

Remark 4 (Approximation error interpretation). Under Condition 4, the term which governs the approximation error, the quantity $\mathbb{E}[||\Sigma^{-1/2}X||^2 \operatorname{bias}(X)^2]$, is bounded as

$$\mathbb{E}\left[\|\mathcal{L}^{-1/2}X\operatorname{bias}(X)\|^2\right] \le \rho_{2,\operatorname{cov}}^2 \cdot d \cdot \mathbb{E}\left[\operatorname{bias}(X)^2\right].$$

A similar bound can be obtained under Conditions 2 and 3; see Lemma 7.

Remark 5 (Comparison to fixed design). The bounds in Theorems 1 and 2 reveal the relative effect of approximation error $\mathbb{E}[\operatorname{bias}(X)^2]$ and stochastic noise (through $\sigma_{\operatorname{noise}}^2$). The main leading factors, $K_{1,\delta,n}$ and $K_{2,\delta,n}$, quickly approach 1 after $n > n_{1,\delta}$ and $n > n_{2,\delta}$, respectively. If we disregard $K_{1,\delta,n}$ and $K_{2,\delta,n}$, then the bounds from Theorem 1 essentially match the those in the usual fixed design and Gaussian noise setting (where the conditional response Y|X is assumed to have a normal $\mathcal{N}(X^{\top}\beta, \sigma_{\operatorname{noise}}^2)$ distribution); see Proposition 1 for comparison.

Remark 6 (The $\sigma_{\text{noise}} = 0$ case and a tight upper bound). If $\sigma_{\text{noise}} = 0$ (no stochastic noise), then the excess loss is entirely due to approximation error. In this case,

$$\|\hat{\beta}_{\text{ols}} - \beta\|_{\Sigma}^{2} = \left\|\hat{\mathbb{E}}\left[\hat{\Sigma}^{-1}X\operatorname{bias}(X)\right]\right\|_{\Sigma}^{2} = \|\hat{\mathbb{E}}[\Sigma^{1/2}\hat{\Sigma}^{-1}X\operatorname{bias}(X)]\|^{2}.$$

Furthermore, Theorem 2 bounds this as:

$$\left\| \hat{\mathbb{E}} \left[\hat{\Sigma}^{-1} X \operatorname{bias}(X) \right] \right\|_{\Sigma}^{2} \leq K_{1,\delta,n}^{2} \left(\frac{4\mathbb{E} \left[\| \Sigma^{-1/2} X \operatorname{bias}(X) \|^{2} \right] \left(1 + 8 \log(1/\delta) \right)}{n} + \frac{3B_{\operatorname{bias}}^{2} d \log^{2}(1/\delta)}{n^{2}} \right).$$

Note that $\Sigma^{1/2} \hat{\Sigma}^{-1} \Sigma^{1/2} \approx I$ for large enough *n*. In particular, with probability greater than $1 - \delta$, if $n > cn_{1,\delta}$ where *c* is a constant (or $n > cn_{2,\delta}$), we have that:

$$\frac{1}{2} \|\hat{\mathbb{E}}[\Sigma^{-1/2}X\operatorname{bias}(X)]\|^2 \le \|\hat{\mathbb{E}}[\Sigma^{1/2}\hat{\Sigma}^{-1}X\operatorname{bias}(X)]\|^2 \le 2\|\hat{\mathbb{E}}[\Sigma^{-1/2}X\operatorname{bias}(X)]\|^2$$

(which follows from the arguments provided in Lemmas 3 and 4). Furthermore, observe that $\mathbb{E}[\|\hat{\mathbb{E}}[\Sigma^{-1/2}X\operatorname{bias}(X)]\|^2] = (1/n)\mathbb{E}[\|\Sigma^{-1/2}X\operatorname{bias}(X)\|^2]$ (where the outside expectation is with respect to the sample X_1, \ldots, X_n). Hence, the bound given for the approximation error contribution is essentially tight, up to constant factors and lower order terms, for constant δ .

3.4 Analysis of ordinary least squares

We separately control $\|\Sigma^{1/2}\hat{\Sigma}^{-1}\Sigma^{1/2}\|$ under Condition 3 and Condition 4.

Lemma 3. For all $\delta \in (0,1)$, if Condition 3 holds and $n > n_{1,\delta}$, then

$$\Pr\left[\hat{\Sigma} \succ 0 \land \|\Sigma^{1/2}\hat{\Sigma}^{-1}\Sigma^{1/2}\| \le K_{1,\delta,n}\right] \ge 1 - \delta$$

and that $K_{1,\delta,n} \leq 5$.

Proof. Let $\widetilde{X}_i := \Sigma^{-1/2} X_i$ for i = 1, ..., n, and $\widetilde{\Sigma} := (1/n) \sum_{i=1}^n \widetilde{X}_i \widetilde{X}_i^{\top}$. Let E be the event that

$$\lambda_{\min}(\widetilde{\Sigma}) \ge 1 - \frac{\rho_{1,\text{cov}}}{1 - 2/0.05} \left(\sqrt{\frac{32 \left(d \log(1 + 2/0.05) + \log(2/\delta) \right)}{n}} + \frac{2 \left(d \log(1 + 2/0.05) + \log(2/\delta) \right)}{n} \right).$$

By Lemma 16 (with $\eta = 0.05$), $\Pr[E] \geq 1 - \delta$. Now assume the event E holds. The lower bound on n ensures that $\lambda_{\min}(\tilde{\Sigma}) > 0$, which implies that $\hat{\Sigma} = \Sigma^{1/2} \tilde{\Sigma} \Sigma^{1/2} \succ 0$. Moreover, since $\Sigma^{1/2} \hat{\Sigma}^{-1} \Sigma^{1/2} = \tilde{\Sigma}^{-1}$,

$$\left\| \Sigma^{1/2} \hat{\Sigma}^{-1} \Sigma^{1/2} \right\| = \left\| \widetilde{\Sigma}^{-1} \right\| = \frac{1}{\lambda_{\min}(\widetilde{\Sigma})} \le K_{1,\delta,n}.$$

Lemma 4. For all $\delta \in (0,1)$, if Condition 4 holds and $n > n_{2,\delta}$, then

$$\Pr\left[\hat{\Sigma} \succ 0 \land \|\Sigma^{1/2}\hat{\Sigma}^{-1}\Sigma^{1/2}\| \le K_{2,\delta,n}\right] \ge 1 - \delta$$

and that $K_{2,\delta,n} \leq 5$.

Proof. Analogous to the proof of Lemma 3 (using Lemma 17 in place Lemma 16). \Box

Under Condition 1, we control $\|\hat{\mathbb{E}}[\hat{\Sigma}^{-1/2}X\eta(X)]\|^2$ using a tail inequality for certain quadratic forms of subgaussian random vectors (Lemma 14).

Lemma 5. Suppose Condition 1 holds. Fix $\delta \in (0,1)$. Conditioned on $\hat{\Sigma} \succ 0$, we have that with probability at least $1 - \delta$,

$$\left\|\hat{\mathbb{E}}[\hat{\mathcal{L}}^{-1/2}X\eta(X)]\right\|^2 \le \frac{\sigma_{\text{noise}}^2\left(d + 2\sqrt{d\log(1/\delta)} + 2\log(1/\delta)\right)}{n}$$

Proof. We condition on X_1, \ldots, X_n , and consider the matrix $A \in \mathbb{R}^{d \times n}$ whose *i*-th column is $(1/\sqrt{n})\hat{\Sigma}^{-1/2}X_i$, so $A^{\top}A = I$. From Conditions 1 and Lemma 14, the result follows.

We control $\|\mathbb{E}[\Sigma^{-1/2}X \operatorname{bias}(X)]\|^2$ using a tail inequality for sums of random vectors (Lemma 15), **Lemma 6.** Suppose Condition 1 holds. Fix $\delta \in (0,1)$. With probability at least $1 - \delta$,

$$\left\|\hat{\mathbb{E}}[\Sigma^{-1/2}X\operatorname{bias}(X)]\right\|^{2} \leq \frac{4\mathbb{E}\left[\|\Sigma^{-1/2}X\operatorname{bias}(X)\|^{2}\right]\left(1+8\log(1/\delta)\right)}{n} + \frac{3B_{\operatorname{bias}}^{2}d\log^{2}(1/\delta)}{n^{2}}.$$

Proof. The optimality β implies $\mathbb{E}[X_i \operatorname{bias}(X_i)] = \mathbb{E}[X \operatorname{bias}(X)] = 0$ for all $i = 1, \ldots, n$. Using this fact and the bound $\|\Sigma^{-1/2}X \operatorname{bias}(X)\| \leq B_{\operatorname{bias}}\sqrt{d}$ from Condition 2, Lemma 15 implies:

$$\Pr\left[\left\|\hat{\mathbb{E}}[\Sigma^{-1/2}X\operatorname{bias}(X)]\right\| \leq \sqrt{\frac{\mathbb{E}\left[\|\Sigma^{-1/2}X\operatorname{bias}(X)\|^2\right]\left(1+\sqrt{8\log(1/\delta)}\right)^2}{n}} + \frac{4B_{\operatorname{bias}}\sqrt{d}\log(1/\delta)}{3n}\right] \geq 1-\delta,$$
d the claim follows

and the claim follows

The expectation $\mathbb{E}[\|\Sigma^{-1/2}X\operatorname{bias}(X)\|^2]$ that appears in the previous lemma can be bounded in terms of $\mathbb{E}[bias(X)^2]$ under our conditions.

Lemma 7. If Conditions 2 and 3 hold, then for any $\lambda > 0$,

$$\mathbb{E}\left[\|\Sigma^{-1/2}X\operatorname{bias}(X)\|^2\right] \le \rho_{1,\operatorname{cov}} \cdot d \cdot \mathbb{E}[\operatorname{bias}(X)^2]$$
$$\cdot \left(1 + \sqrt{\frac{\log\max\left\{\frac{B_{\operatorname{bias}}^2d}{\lambda\rho_{1,\operatorname{cov}}\mathbb{E}[\operatorname{bias}(X)^2]}, 1\right\}}{d}} + \frac{\log\max\left\{\frac{B_{\operatorname{bias}}^2d}{\lambda\rho_{1,\operatorname{cov}}\mathbb{E}[\operatorname{bias}(X)^2]}, 1\right\} + \lambda}{d}\right).$$

If Condition 4 holds, then

$$\mathbb{E}\left[\|\Sigma^{-1/2}X\operatorname{bias}(X)\|^2\right] \le \rho_{2,\operatorname{cov}}^2 \cdot d \cdot \mathbb{E}\left[\operatorname{bias}(X)^2\right]$$

Proof. For the first part of the claim, we assume Conditions 3 and 1 hold. Let E be the event that

$$\left\|\Sigma^{-1/2}X\right\|^2 \le \rho_{1,\text{cov}} \cdot \left(d + \sqrt{d\log(1/\delta)} + \log(1/\delta)\right).$$

By Lemma 14, $\Pr[E_{\delta}] \ge 1 - \delta$. Therefore

$$\mathbb{E}\left[\|\Sigma^{-1/2}X\operatorname{bias}(X)\|^{2}\right] = \mathbb{E}\left[\|\Sigma^{-1/2}X\operatorname{bias}(X)\|^{2} \cdot \mathbb{1}[E_{\delta}]\right] + \mathbb{E}\left[\|\Sigma^{-1/2}X\operatorname{bias}(X)\|^{2} \cdot \left(1 - \mathbb{1}[E_{\delta}]\right)\right]$$

$$\leq \rho_{1,\operatorname{cov}} \cdot \left(d + \sqrt{d\log(1/\delta)} + \log(1/\delta)\right) \cdot \mathbb{E}\left[\operatorname{bias}(X)^{2} \cdot \mathbb{1}[E_{\delta}]\right]$$

$$+ B_{\operatorname{bias}}^{2} \cdot d \cdot \mathbb{E}\left[\left(1 - \mathbb{1}[E_{\delta}]\right)\right]$$

$$\leq \rho_{1,\operatorname{cov}} \cdot \left(d + \sqrt{d\log(1/\delta)} + \log(1/\delta)\right) \cdot \mathbb{E}[\operatorname{bias}(X)^{2}] + B_{\operatorname{bias}}^{2} \cdot d \cdot \delta.$$

Choosing $\delta := \min\{\lambda \rho_{1,\text{cov}} \mathbb{E}[\text{bias}(X)^2] / (B_{\text{bias}}^2 d), 1\}$ completes the proof of the first part.

For the second part, note that under Condition 4, we have $\|\Sigma^{-1/2}X\|^2 \leq \rho_{2,cov}^2 d$ almost surely, so the claim follows immediately.

4 Ridge regression

In infinite dimensional spaces, the ordinary least squares estimator is not applicable (note that our analysis hinges on the invertibility of $\hat{\Sigma}$). A natural alternative is the *ridge estimator*: instead of minimizing the empirical mean squared error, the ridge estimator minimizes the *empirical regularized mean squared error*.

For a fixed $\lambda > 0$, the regularized mean squared error and the empirical regularized error of a linear predictor w are defined as

$$L_{\lambda}(w) := \mathbb{E}(X^{\top}w - Y)^2 + \lambda \|w\|^2 \quad \text{and} \quad \hat{L}_{\lambda}(w) := \hat{\mathbb{E}}(X_i^{\top}w - Y_i)^2 + \lambda \|w\|^2$$

The minimizer β_λ of the regularized mean squared error is given by

$$\beta_{\lambda} := (\Sigma + \lambda I)^{-1} \mathbb{E}[XY].$$

The ridge estimator $\hat{\beta}_{\lambda}$ is the minimizer of the empirical regularized mean squared error, and is given by

$$\hat{\beta}_{\lambda} := (\hat{\Sigma} + \lambda I)^{-1} \hat{\mathbb{E}}[XY].$$

It is convenient to define the λ -regularized matrices Σ_{λ} and $\hat{\Sigma}_{\lambda}$ as

 $\Sigma_{\lambda} := \Sigma + \lambda I$ and $\hat{\Sigma}_{\lambda} := \hat{\Sigma} + \lambda I$

so that

$$\beta_{\lambda} = \Sigma_{\lambda}^{-1} \mathbb{E}[XY]$$
 and $\hat{\beta}_{\lambda} = \hat{\Sigma}_{\lambda}^{-1} \hat{\mathbb{E}}[XY].$

Due to the random design, $\hat{\beta}_{\lambda}$ is not generally an unbiased estimator of β_{λ} ; this is a critical issue in our analysis.

Throughout this section, we assume that our representation is rich enough so that

$$\mathbb{E}[Y|X] = X^\top \beta.$$

However, we will not require that $\|\beta\|^2$ be finite. The specific conditions (in addition to Condition 1) are given as follows.

Condition 5 (Ridge conditions).

- 1. $\mathbb{E}[Y|X] = X^{\top}\beta$ almost surely. That is, the regression function is perfectly modeled by β .
- 2. There exists $\rho_{\lambda} \geq 1$ such that almost surely,

$$\frac{\|\Sigma_{\lambda}^{-1/2}X\|}{\sqrt{\mathbb{E}\|\Sigma_{\lambda}^{-1/2}X\|^2}} = \frac{\|\Sigma_{\lambda}^{-1/2}X\|}{\sqrt{\sum_{j}\frac{\lambda_j(\Sigma)}{\lambda_j(\Sigma)+\lambda}}} \le \rho_{\lambda}$$

where $\lambda_1(\Sigma), \lambda_2(\Sigma), \ldots$ are the eigenvalues of Σ .

3. There exists $B_{\text{bias}_{\lambda}} \geq 0$ such that the approximation error $\text{bias}_{\lambda}(X)$ due to β_{λ} , defined as

$$\operatorname{bias}_{\lambda}(X) := X^{\top}(\beta - \beta_{\lambda}),$$

is bounded almost surely as

$$|\operatorname{bias}_{\lambda}(X)| \leq B_{\operatorname{bias}_{\lambda}}.$$

Remark 7. The second part is analogous to the bounded statistical leverage condition (Condition 4) except with λ -whitening (the linear transformation $x \mapsto \Sigma_{\lambda}^{-1/2} x$) instead of whitening. Note that $\sum_{j} \lambda_{j}(\Sigma)/(\lambda_{j}(\Sigma) + \lambda) \to d$ (the dimension of the covariate space) and $\Sigma_{\lambda} \to \Sigma$ as $\lambda \to 0$.

Remark 8. As with the quantity B_{bias} from Condition 2 in the ordinary least squares analysis, the quantity B_{bias} here only appears in lower order terms in the results.

4.1 Review: ridge regression in the fixed design setting

Again, in the fixed design setting, $X_1, \ldots X_n$ are fixed (non-random) points, and, again, define $\Sigma_{\text{fixed}} := \sum_{i=1}^n X_i X_i^{\top} / n$ (a deterministic quantity). Here, $\hat{\beta}_{\lambda}$ is an unbiased estimate of the minimizer of the true regularized loss, *i.e.*,

$$\beta_{\lambda,\text{fixed}} := \mathbb{E}[\hat{\beta}_{\lambda}] = (\Sigma_{\text{fixed}} + \lambda I)^{-1} \mathbb{E}\left[\frac{1}{n} \sum_{i=1}^{n} X_i Y_i\right].$$

where the expectation is with respect to the Y_i 's.

The following bias-variance decomposition is useful:

$$\mathbb{E}_{\hat{\beta}_{\lambda}} \| \hat{\beta}_{\lambda} - \beta \|_{\Sigma_{\text{fixed}}}^2 = \| \beta_{\lambda,\text{fixed}} - \beta \|_{\Sigma_{\text{fixed}}}^2 + \mathbb{E}_{\hat{\beta}_{\lambda}} \| \beta_{\lambda,\text{fixed}} - \hat{\beta}_{\lambda} \|_{\Sigma_{\text{fixed}}}^2$$

where the expectation is with respect to the randomness in the Y_i 's. Here, the first term represents the bias due to regularization and the second is the variance.

The following straightforward lemma provides a bound on the risk of ridge regression.

Proposition 2. Denote the singular values of Σ_{fixed} by $\lambda_{j,\text{fixed}}$ (in decreasing order) and define the effective dimension as

$$d_{\lambda,\text{fixed}} = \sum_{j} \left(\frac{\lambda_{j,\text{fixed}}}{\lambda_{j,\text{fixed}} + \lambda} \right)^2.$$

If $\operatorname{var}(Y_i) = \sigma^2$, then

$$\mathbb{E}_{\hat{\beta}_{\lambda}} \| \hat{\beta}_{\lambda} - \beta \|_{\Sigma_{\text{fixed}}}^2 = \sum_{j} \beta_j^2 \frac{\lambda_{j,\text{fixed}}}{(1 + \lambda_{j,\text{fixed}}/\lambda)^2} + \frac{\sigma^2 d_{\lambda,\text{fixed}}}{n}$$

where the expectation is with respect to the Y_i 's.

Remark 9 (Approximation error). Again, note that modeling error has no effect on the fixed design excess loss for ridge regression.

The results in the random design case are comparable to this bound, in certain ways.

4.2 Out-of-sample prediction error: ridge regression

Due to the random design, $\hat{\beta}_{\lambda}$ may be a biased estimate of β_{λ} . For the sake of analysis, this motivates us to consider another estimate, $\bar{\beta}_{\lambda}$, which is the conditional expectation of $\hat{\beta}_{\lambda}$ (conditioned on X_1, \ldots, X_n). Precisely,

$$\bar{\beta}_{\lambda} := \mathbb{E}[\hat{\beta}_{\lambda} | X_1, \dots, X_n] = \hat{\Sigma}_{\lambda}^{-1} \hat{\mathbb{E}}[X(\beta \cdot X)] = \hat{\Sigma}_{\lambda}^{-1} \hat{\Sigma}\beta$$

where the expectation is with respect to the Y_i 's. These definitions lead to the following natural decomposition.

Lemma 8 (Random design ridge decomposition). Assume Condition 5 holds. We have that

$$\begin{aligned} \|\hat{\beta}_{\lambda} - \beta\|_{\Sigma} &\leq \|\beta_{\lambda} - \beta\|_{\Sigma} + \|\bar{\beta}_{\lambda} - \beta_{\lambda}\|_{\Sigma} + \|\bar{\beta}_{\lambda} - \hat{\beta}_{\lambda}\|_{\Sigma} \\ \|\hat{\beta}_{\lambda} - \beta\|_{\Sigma}^{2} &\leq 3\left(\|\beta_{\lambda} - \beta\|_{\Sigma}^{2} + \|\bar{\beta}_{\lambda} - \beta_{\lambda}\|_{\Sigma}^{2} + \|\bar{\beta}_{\lambda} - \hat{\beta}_{\lambda}\|_{\Sigma}^{2}\right). \end{aligned}$$

Remark 10 (Special case: ordinary least squares $(\lambda = 0)$). Here, $\bar{\beta}_{\lambda} = \beta_{\lambda} = \beta$ if $\hat{\Sigma}$ is invertible and $\lambda = 0$, in which case the constant 3 can be replaced by 2 in the second inequality.

Proof. A norm obeys the triangle inequality, and $(a + b + c)^2 \leq 3(a^2 + b^2 + c^2)$.

Our main result for ridge regression provides a bound on each of these terms.

Theorem 3 (Ridge regression). Suppose that Conditions 1 and 5 hold. Let $\lambda_1(\Sigma), \lambda_2(\Sigma), \ldots$ denote the eigenvalues of Σ , and define the following notions of effective dimensions:

$$d_{1,\lambda} := \sum_{j} \frac{\lambda_j(\Sigma)}{\lambda_j(\Sigma) + \lambda} \quad and \quad d_{2,\lambda} := \sum_{j} \left(\frac{\lambda_j(\Sigma)}{\lambda_j(\Sigma) + \lambda}\right)^2.$$
(1)

Define the λ -whitened error matrix as

$$\Delta_{\lambda} := \Sigma_{\lambda}^{-1/2} (\hat{\Sigma} - \Sigma) \Sigma_{\lambda}^{-1/2}$$
⁽²⁾

and

$$K_{\lambda,\delta,n} := \frac{1}{1 - \left(\sqrt{\frac{4\rho_{\lambda}^2 d_{1,\lambda} \log(d_{1,\lambda}/\delta)}{n}} + \frac{\rho_{\lambda}^2 d_{1,\lambda} \log(d_{1,\lambda}/\delta)}{n}\right)}.$$

Suppose that $\delta \in (0, 1/8)$, $\lambda \leq \lambda_{\max}(\Sigma)$, and

 $n \ge 16\rho_{\lambda}^2 d_{1,\lambda} \log(d_{1,\lambda}/\delta).$

(see Remark 15 below). There exists a universal constant 0 < c < 40 (explicit constants are provided in the lemmas) such that following claims hold with probability at least $1 - 4\delta$:

• (Matrix errors)

$$\left\| \Sigma_{\lambda}^{1/2} \hat{\Sigma}_{\lambda}^{-1} \Sigma_{\lambda}^{1/2} \right\| \le \frac{1}{1 - \left\| \Delta_{\lambda} \right\|} \le K_{\lambda, \delta, n} \le 4$$

and

$$\|\Delta_{\lambda}\|_{\mathrm{F}} \leq c \left(1 + \sqrt{\log(1/\delta)}\right) \sqrt{\frac{\mathbb{E}[\|\Sigma_{\lambda}^{-1/2}X\|^4] - d_{2,\lambda}}{n}} + \frac{c(\rho_{\lambda}^2 d_{1,\lambda} + \sqrt{d_{2,\lambda}})\log(1/\delta)}{n}.$$

• (First term)

$$\|\beta_{\lambda} - \beta\|_{\Sigma}^{2} = \sum_{j} \beta_{j}^{2} \frac{\lambda_{j}(\Sigma)}{(1 + \lambda_{j}(\Sigma)/\lambda)^{2}}.$$

• (Second term)

$$\begin{split} \|\bar{\beta}_{\lambda} - \beta_{\lambda}\|_{\Sigma}^{2} &\leq cK_{\lambda,\delta,n}^{2} \left(1 + \log(1/\delta)\right) \frac{\mathbb{E}[\|\Sigma_{\lambda}^{-1/2} (X \operatorname{bias}_{\lambda}(X) - \lambda\beta_{\lambda})\|^{2}]}{n} \\ &+ \frac{cK_{\lambda,\delta,n}^{2} (\rho_{\lambda}^{2} d_{1,\lambda} B_{\operatorname{bias}_{\lambda}}^{2} + \|\beta_{\lambda} - \beta\|_{\Sigma}^{2}) \log^{2}(1/\delta)}{n^{2}} \end{split}$$

Furthermore (for interpretation),

$$\mathbb{E}[X \operatorname{bias}_{\lambda}(X) - \lambda \beta_{\lambda}] = 0$$

and

$$\mathbb{E}[\|\Sigma_{\lambda}^{-1/2}(X\operatorname{bias}_{\lambda}(X) - \lambda\beta_{\lambda})\|^{2}] \le \|\beta_{\lambda} - \beta\|_{\Sigma}^{2}(2\rho_{\lambda}^{2}d_{1,\lambda} + 2)$$

(see Remark 13 below).

• (Third term)

$$\begin{split} \|\bar{\beta}_{\lambda} - \hat{\beta}_{\lambda}\|_{\Sigma}^{2} &\leq \frac{K_{\lambda,\delta,n}^{2} \sigma_{\text{noise}}^{2}}{n} \left(d_{2,\lambda} + \sqrt{d_{2,\lambda}} \|\Delta_{\lambda}\|_{\text{F}} \right) \\ &+ \frac{2K_{\lambda,\delta,n}^{3/2} \sigma_{\text{noise}}^{2}}{n} \sqrt{\left(d_{2,\lambda} + \sqrt{d_{2,\lambda}} \|\Delta_{\lambda}\|_{\text{F}} \right) \log(1/\delta)} + \frac{2K_{\lambda,\delta,n} \sigma_{\text{noise}}^{2}}{n} \log(1/\delta); \end{split}$$

• (Excess loss)

$$\begin{aligned} \|\hat{\beta}_{\lambda} - \beta\|_{\Sigma} &\leq \underbrace{\|\beta_{\lambda} - \beta\|_{\Sigma}}_{\sqrt{first \ term}} + \underbrace{\|\bar{\beta}_{\lambda} - \beta_{\lambda}\|_{\Sigma}}_{\sqrt{second \ term}} + \underbrace{\|\bar{\beta}_{\lambda} - \hat{\beta}_{\lambda}\|_{\Sigma}}_{\sqrt{third \ term}}; \\ \|\hat{\beta}_{\lambda} - \beta\|_{\Sigma}^{2} &\leq 3\left(\|\beta_{\lambda} - \beta\|_{\Sigma}^{2} + \|\bar{\beta}_{\lambda} - \beta_{\lambda}\|_{\Sigma}^{2} + \|\bar{\beta}_{\lambda} - \hat{\beta}_{\lambda}\|_{\Sigma}^{2}\right). \end{aligned}$$

Remark 11 (Overall form). For a fixed λ , the overall bound roughly has the form

$$\begin{split} \|\hat{\beta}_{\lambda} - \beta\|_{\varSigma} &\leq \|\beta_{\lambda} - \beta\|_{\varSigma} \cdot \left(1 + O\left(\sqrt{K_{\lambda,\delta,n}^2 \cdot \frac{\rho_{\lambda}^2 d_{1,\lambda} \log(1/\delta)}{n}}\right)\right) \\ &+ \sqrt{K_{\lambda,\delta,n}^2 \cdot \frac{\sigma_{\text{noise}}^2 \left(d_{2,\lambda} + 2\sqrt{d_{2,\lambda} \log(1/\delta)} + 2\log(1/\delta)\right)}{n}} + \text{lower order } o(1/\sqrt{n}) \text{ terms} \end{split}$$

where $\|\beta_{\lambda} - \beta\|_{\Sigma} = \sqrt{\sum_{j} \beta_{j}^{2} \lambda_{j}(\Sigma) / (1 + \lambda_{j}(\Sigma) / \lambda)^{2}}.$

Remark 12 (Special case: ordinary least squares $(\lambda = 0)$). Theorem 1 is essentially a special case for $\lambda = 0$ (with minor differences in constants and lower order terms). To see this, note that $d_{2,\lambda} = d_{1,\lambda} = d$ and take $\rho_{\lambda} = \rho_{2,\text{cov}}$ so that Condition 4 holds. It is clear that the first and second terms from Theorem 3 are zero in the case of ordinary least squares, and the third term gives rise to a nearly identical excess loss bound (in comparison to Theorem 1). In particular, the dependencies on all terms which are $\Theta(1/n)$ are identical (up to constants), and the terms which depend on $\|\Delta_{\lambda}\|_{\text{F}}$ are lower order (relative to 1/n).

Remark 13 (Comparison to fixed design). The random design setting behaves much like the fixed design, with the notable exception of the second term in the decomposition. This term behaves much like modeling error (in the finite dimensional case), since X bias_{λ}(X) - $\lambda\beta_{\lambda}$ is mean 0. Furthermore, since

$$\mathbb{E}[\|\mathcal{L}_{\lambda}^{-1/2}(X\operatorname{bias}_{\lambda}(X) - \lambda\beta_{\lambda})\|^{2}] \le \|\beta_{\lambda} - \beta\|_{\mathcal{L}}^{2}(2\rho_{\lambda}^{2}d_{1,\lambda} + 2)$$

this second term is a lower order term compared to the first term $\|\beta_{\lambda} - \beta\|_{\Sigma}^2$. Note that $\|\beta_{\lambda} - \beta\|_{\Sigma}^2$ is precisely the bias term from the fixed design analysis, except with the eigenvalues $\lambda_j(\Sigma)$ in place of the eigenvalues of the fixed design matrix.

Remark 14 (Random design effects and scaling λ). Note that above condition allows one to see the effects of scaling λ , such as the common setting of $\lambda = \Theta(1/\sqrt{n})$. As long as $\rho_{\lambda}^2 d_{1,\lambda}$ scales in a mild way with λ , then the random design has little effect.

Remark 15 (Conditions: $\lambda \leq \lambda_{\max}(\Sigma)$ and $\delta \in (0, 1/8)$). These conditions allow for a simplified expression for the matrix error term $\|\Sigma_{\lambda}^{1/2} \hat{\Sigma}_{\lambda}^{-1} \Sigma_{\lambda}^{1/2}\|$ (through $\|\Delta_{\lambda}\|$) and are rather mild. The proof of Lemma 10 provides the general expression, even if these conditions do not hold.

4.3 Analysis of ridge regression

Recall the definitions of $d_{2,\lambda}$, $d_{1,\lambda}$, and Δ_{λ} from (1) and (2) in Theorem 3. First, we bound the Frobenius and spectral norms of Δ_{λ} in terms of $d_{2,\lambda}$, $d_{1,\lambda}$, and the quantities from Condition 5. Then, assuming $\|\Delta_{\lambda}\| < 1$, we proceed to bound the various terms in the decomposition from Lemma 8 using these same quantities.

Lemma 9 (Frobenius error concentration). Assume Condition 5 holds. With probability at least $1 - \delta$,

$$\|\Delta_{\lambda}\|_{\rm F} \le \left(1 + \sqrt{8\log(1/\delta)}\right) \sqrt{\frac{\mathbb{E}[\|\Sigma_{\lambda}^{-1/2}X\|^4] - d_{2,\lambda}}{n}} + \frac{(4/3)(\rho_{\lambda}^2 d_{1,\lambda} + \sqrt{d_{2,\lambda}})\log(1/\delta)}{n}.$$

Proof. Define the λ -whitehed random vectors

$$X_{i,w} := \Sigma_{\lambda}^{-1/2} X_i$$

so that the random matrices

$$M_i := X_{i,w} X_{i,w}^{\top} - \Sigma_{\lambda}^{-1/2} \Sigma \Sigma_{\lambda}^{-1/2}$$

have expectation zero. In these terms, $\Delta_{\lambda} = (1/n) \sum_{i=1}^{n} M_i$. Observe that $\|\Delta_{\lambda}\|_{\rm F}^2$ is the inner product

$$\|\Delta_{\lambda}\|_{\mathrm{F}}^{2} = \langle \Delta_{\lambda}, \Delta_{\lambda} \rangle$$

where $\langle A, B \rangle := \operatorname{tr}(AB^{\top}).$

We apply Lemma 15, treating M_i as random vectors with inner product $\langle \cdot, \cdot \rangle$, to bound $\|\Delta_{\lambda}\|_{\mathrm{F}}^2$ with probability at least $1 - \delta$. Note that $\mathbb{E}[M_i] = 0$ and, by Condition 5, that

$$\mathbb{E}[\|M_i\|_{\mathrm{F}}^2] = \mathbb{E}[\langle X_{i,w}X_{i,w}^\top, X_{i,w}X_{i,w}^\top\rangle] - \langle \Sigma_w, \Sigma_w\rangle$$
$$= \mathbb{E}[\|X_{i,w}\|^4] - \operatorname{tr}(\Sigma_w^2)$$
$$= \mathbb{E}[\|\Sigma_\lambda^{-1/2}X\|^4] - d_{2,\lambda}.$$

Also,

$$\|X_{i,w}X_{i,w}^{\top}\|_{\mathbf{F}}^{2} = \|X_{i,w}\|^{4} \le \rho_{\lambda}^{4}d_{1,\lambda}^{2}$$

and

$$\|\Sigma_w\|_{\mathbf{F}}^2 = \langle \Sigma_w, \Sigma_w \rangle = d_{2,\lambda}$$

so that

$$||M_i||_{\mathbf{F}} \le ||X_{i,w}X_{i,w}^{\top}||_{\mathbf{F}} + ||\Sigma_w||_{\mathbf{F}} \le \rho_{\lambda}^2 d_{1,\lambda} + \sqrt{d_{2,\lambda}}$$

Therefore, Lemma 15 implies the claim, so the proof is complete.

Lemma 10 (Spectral error concentration). Assume Condition 5 holds. Suppose that $\lambda \leq \lambda_1(\Sigma)$ and that $\delta \in (0, 1/8)$. With probability at least $1 - \delta$,

$$\|\Delta_{\lambda}\| \le \sqrt{\frac{4\rho_{\lambda}^2 d_{1,\lambda} \log(d_{1,\lambda}/\delta)}{n}} + \frac{2\rho_{\lambda}^2 d_{1,\lambda} \log(d_{1,\lambda}/\delta)}{3n}$$

Remark 16. The condition that $\lambda \leq \lambda_1(\Sigma)$ is only needed to simplify the bound on $\|\Delta_{\lambda}\|$; it ensures a lower bound on $d_{1,\lambda}$ (since $d_{1,\lambda} \to 0$ as $\lambda \to \infty$), but this can be easily removed with a somewhat more cumbersome bound.

Proof. Define $M_i = \Sigma_{\lambda}^{-1/2} (X_i X_i^{\top} - \Sigma) \Sigma_{\lambda}^{-1/2}$. Note that by Condition 5, $\lambda_{\max}(M_i) \leq \|\Sigma_{\lambda}^{-1/2} X_i\|^2 \leq \rho_{\lambda}^2 d_{1,\lambda},$ $\lambda_{\max}(-M_i) \leq \lambda_{\max}(\Sigma_{\lambda}^{-1/2} \Sigma \Sigma_{\lambda}^{-1/2}) \leq \frac{\lambda_1(\Sigma)}{\lambda_1(\Sigma) + \lambda} \leq \rho_{\lambda}^2 d_{1,\lambda},$ $\lambda_{\max}(\mathbb{E}[M_i^2]) \leq \lambda_{\max}(\mathbb{E}[(\Sigma_{\lambda}^{-1/2} X_i X_i^{\top} \Sigma_{\lambda}^{-1/2})^2]) \leq \rho_{\lambda}^2 d_{1,\lambda} \lambda_{\max}(\Sigma_{\lambda}^{-1/2} \Sigma \Sigma_{\lambda}^{-1/2}) \leq \rho_{\lambda}^2 d_{1,\lambda},$ $\operatorname{tr}(\mathbb{E}[M_i^2]) \leq \operatorname{tr}(\mathbb{E}[(\Sigma_{\lambda}^{-1/2} X_i X_i^{\top} \Sigma_{\lambda}^{-1/2})^2]) \leq \rho_{\lambda}^2 d_{1,\lambda} \operatorname{tr}(\Sigma_{\lambda}^{-1/2} \Sigma \Sigma_{\lambda}^{-1/2}) = \rho_{\lambda}^2 d_{1,\lambda} \sum_j \frac{\lambda_j(\Sigma)}{\lambda_j(\Sigma) + \lambda} = \rho_{\lambda}^2 d_{1,\lambda}.$

From Lemma 18, for $t \ge 2.6$

$$\Pr\left[\lambda_{\max}\left(\frac{1}{n}\sum_{i=1}^{n}M_{i}\right) > \sqrt{\frac{2\rho_{\lambda}^{2}d_{1,\lambda}t}{n}} + \frac{\rho_{\lambda}^{2}d_{1,\lambda}t}{3n}\right] \le d_{1,\lambda} \cdot e^{-t/2}.$$

The claim follows for $t = 2 \log(d_{1,\lambda}/\delta)$ for $\delta \leq 1/8$.

Now we bound the (second and third) terms in the decomposition from Lemma 8.

Lemma 11 (Second term in ridge decomposition). Assume Condition 5 holds. If $\|\Delta_{\lambda}\| < 1$, then

1.
$$\|\bar{\beta}_{\lambda} - \beta_{\lambda}\|_{\Sigma}^{2} \leq \frac{1}{(1 - \|\Delta_{\lambda}\|)^{2}} \|\hat{\mathbb{E}}[\Sigma_{\lambda}^{-1/2}(X \operatorname{bias}_{\lambda}(X) - \lambda\beta_{\lambda})]\|^{2};$$

2. with probability at least $1 - \delta$,

$$\begin{split} \|\bar{\beta}_{\lambda} - \beta_{\lambda}\|_{\Sigma}^{2} &\leq \frac{1}{(1 - \|\Delta_{\lambda}\|)^{2}} \left((4 + 32\log(1/\delta)) \frac{\mathbb{E}[\|\varSigma_{\lambda}^{-1/2}(X\operatorname{bias}_{\lambda}(X) - \lambda\beta_{\lambda})\|^{2}]}{n} \\ &+ \frac{6(\rho_{\lambda}^{2}d_{1,\lambda}B_{\operatorname{bias}_{\lambda}}^{2} + \|\beta_{\lambda} - \beta\|_{\Sigma}^{2})\log^{2}(1/\delta)}{n^{2}} \right). \end{split}$$

Furthermore,

$$\mathbb{E}[\|\Sigma_{\lambda}^{-1/2}(X\operatorname{bias}_{\lambda}(X) - \lambda\beta_{\lambda})\|^{2}] \leq \|\beta_{\lambda} - \beta\|_{\Sigma}^{2}(2\rho_{\lambda}^{2}d_{1,\lambda} + 2).$$

Proof. Since $\bar{\beta}_{\lambda} = \hat{\Sigma}_{\lambda}^{-1} \hat{\Sigma} \beta$ and $\beta_{\lambda} = \hat{\Sigma}_{\lambda}^{-1} \hat{\Sigma}_{\lambda} \beta_{\lambda} = \hat{\Sigma}_{\lambda}^{-1} (\hat{\Sigma} \beta_{\lambda} + \lambda \beta_{\lambda})$, we have that

$$\begin{split} \|\bar{\beta}_{\lambda} - \beta_{\lambda}\|_{\Sigma}^{2} &= \|\hat{\Sigma}_{\lambda}^{-1} \left(\hat{\Sigma}\beta - (\hat{\Sigma}\beta_{\lambda} + \lambda\beta_{\lambda})\right)\|_{\Sigma}^{2} \\ &\leq \|\Sigma^{1/2}\Sigma_{\lambda}^{-1/2}\|^{2} \|\Sigma_{\lambda}^{1/2}\hat{\Sigma}_{\lambda}^{-1} \left(\hat{\Sigma}\beta - (\hat{\Sigma}\beta_{\lambda} + \lambda\beta_{\lambda})\right)\|^{2} \\ &\leq \|\Sigma_{\lambda}^{1/2}\hat{\Sigma}_{\lambda}^{-1} \left(\hat{\Sigma}\beta - (\hat{\Sigma}\beta_{\lambda} + \lambda\beta_{\lambda})\right)\|^{2} \\ &= \|\Sigma_{\lambda}^{1/2}\hat{\Sigma}_{\lambda}^{-1}\Sigma_{\lambda}^{1/2}\|^{2} \|\Sigma_{\lambda}^{-1/2} \left(\hat{\Sigma}\beta - (\hat{\Sigma}\beta_{\lambda} + \lambda\beta_{\lambda})\right)\|^{2} \\ &= \|\Sigma_{\lambda}^{1/2}\hat{\Sigma}_{\lambda}^{-1}\Sigma_{\lambda}^{1/2}\|^{2} \|\hat{\mathbb{E}}[\Sigma_{\lambda}^{-1/2}(X\operatorname{bias}_{\lambda}(X) - \lambda\beta_{\lambda})]\|^{2}. \end{split}$$

The first claim now follows from Lemma 13.

Now we prove the second claim using Lemma 15. First, note that for each i,

$$\|\Sigma_{\lambda}^{-1/2}(X_i \operatorname{bias}_{\lambda}(X_i) - \lambda \beta_{\lambda})\| \le \|\Sigma_{\lambda}^{-1/2}X_i \operatorname{bias}_{\lambda}(X_i)\| + \|\lambda \Sigma_{\lambda}^{-1/2} \beta_{\lambda}\|$$

Each term can be further bounded using Condition 5 as

$$\|\mathcal{L}_{\lambda}^{-1/2}(X_i \operatorname{bias}_{\lambda}(X_i))\| \le \rho_{\lambda} \sqrt{d_{1,\lambda}} |\operatorname{bias}_{\lambda}(X_i)| \le \rho_{\lambda} \sqrt{d_{1,\lambda}} B_{\operatorname{bias}_{\lambda}}$$

and

$$\|\lambda \Sigma_{\lambda}^{-1/2} \beta_{\lambda}\|^{2} = \sum_{j} \beta_{j}^{2} \frac{\lambda^{2} \lambda_{j}^{2}}{(\lambda + \lambda_{j})^{3}} \leq \sum_{j} \beta_{j}^{2} \frac{\lambda^{2} \lambda_{j}}{(\lambda + \lambda_{j})^{2}} = \|\beta_{\lambda} - \beta\|_{\Sigma}^{2}.$$

By Lemma 15, we have that with probability at least $1 - \delta$,

$$\begin{aligned} \|\hat{\mathbb{E}}[\Sigma_{\lambda}^{-1/2}(X\operatorname{bias}_{\lambda}(X) - \lambda\beta_{\lambda})]\| &\leq \sqrt{\frac{\mathbb{E}[\|\Sigma_{\lambda}^{-1/2}(X\operatorname{bias}_{\lambda}(X) - \lambda\beta_{\lambda})\|^{2}]}{n}} \left(1 + \sqrt{8\log(1/\delta)}\right) \\ &+ \frac{(4/3)(\rho_{\lambda}\sqrt{d_{1,\lambda}}B_{\operatorname{bias}_{\lambda}} + \|\beta_{\lambda} - \beta\|_{\Sigma})}{n}\log(1/\delta) \end{aligned}$$

 \mathbf{SO}

$$\begin{split} \|\hat{\mathbb{E}}[\boldsymbol{\Sigma}_{\lambda}^{-1/2}(\boldsymbol{X}\operatorname{bias}_{\lambda}(\boldsymbol{X}) - \lambda\boldsymbol{\beta}_{\lambda})]\|^{2} &\leq \frac{2\mathbb{E}[\|\boldsymbol{\Sigma}_{\lambda}^{-1/2}(\boldsymbol{X}\operatorname{bias}_{\lambda}(\boldsymbol{X}) - \lambda\boldsymbol{\beta}_{\lambda})\|^{2}]}{n} \left(1 + \sqrt{8\log(1/\delta)}\right)^{2} \\ &+ \frac{(8/3)(\rho_{\lambda}\sqrt{d_{1,\lambda}}B_{\operatorname{bias}_{\lambda}} + \|\boldsymbol{\beta}_{\lambda} - \boldsymbol{\beta}\|_{\boldsymbol{\Sigma}})^{2}}{n^{2}}\log^{2}(1/\delta) \\ &\leq \frac{4\mathbb{E}[\|\boldsymbol{\Sigma}_{\lambda}^{-1/2}(\boldsymbol{X}\operatorname{bias}_{\lambda}(\boldsymbol{X}) - \lambda\boldsymbol{\beta}_{\lambda})\|^{2}]}{n} \left(1 + 8\log(1/\delta)\right) \\ &+ \frac{6(\rho_{\lambda}^{2}d_{1,\lambda}B_{\operatorname{bias}_{\lambda}}^{2} + \|\boldsymbol{\beta}_{\lambda} - \boldsymbol{\beta}\|_{\boldsymbol{\Sigma}}^{2})}{n^{2}}\log^{2}(1/\delta). \end{split}$$

Finally,

$$\mathbb{E}[\|\Sigma_{\lambda}^{-1/2}(X\operatorname{bias}_{\lambda}(X) - \lambda\beta_{\lambda})\|^{2}] \leq 2\mathbb{E}[\|\Sigma_{\lambda}^{-1/2}X\operatorname{bias}_{\lambda}(X)\|^{2}] + 2\|\beta_{\lambda} - \beta\|_{\Sigma}^{2}$$
$$\leq 2\rho_{\lambda}^{2}d_{1,\lambda}\mathbb{E}[\operatorname{bias}_{\lambda}(X)^{2}] + 2\|\beta_{\lambda} - \beta\|_{\Sigma}^{2}$$
$$= \|\beta_{\lambda} - \beta\|_{\Sigma}^{2}(2\rho_{\lambda}^{2}d_{1,\lambda} + 2)$$

which proves the last claim.

Lemma 12 (Third term in ridge decomposition). Assume Condition 1 holds. Let $A := [X_1|\cdots|X_n]$ be the random matrix whose *i*-th column is X_i . Let

$$M := \frac{1}{n^2} A^{\top} \hat{\varSigma}_{\lambda}^{-1} \Sigma \hat{\varSigma}_{\lambda}^{-1} A$$

We have

$$\Pr\left[\|\bar{\beta}_{\lambda} - \hat{\beta}_{\lambda}\|_{\Sigma}^{2} \le \sigma_{\text{noise}}^{2} \operatorname{tr}(M) + 2\sigma_{\text{noise}}^{2} \sqrt{\operatorname{tr}(M)} \|M\| \log(1/\delta) + 2\sigma_{\text{noise}}^{2} \|M\| \log(1/\delta) \mid X_{1}, \dots, X_{n}\right] \ge 1 - \delta$$

Furthermore, if $\|\Delta_{\lambda}\| < 1$, then

$$\operatorname{tr}(M) \leq \frac{1}{n} \cdot \frac{1}{(1 - \|\Delta_{\lambda}\|)^2} \cdot \left(d_{2,\lambda} + \sqrt{d_{2,\lambda}} \|\Delta_{\lambda}\|_{\mathrm{F}} \right) \quad and \quad \|M\| \leq \frac{1}{n} \cdot \frac{1}{1 - \|\Delta_{\lambda}\|}$$

Proof. Let $Z := (\eta(X_1), \ldots, \eta(X_n))$ be the random vector whose *i*-th component is $\eta(X_i)$. By definition of $\hat{\beta}_{\lambda}$ and $\bar{\beta}_{\lambda}$,

$$\|\hat{\beta}_{\lambda} - \bar{\beta}_{\lambda}\|_{\Sigma}^{2} = \|\hat{\Sigma}_{\lambda}^{-1}(\hat{\mathbb{E}}[XY] - \hat{\mathbb{E}}[X\mathbb{E}[Y|X]])\|_{\Sigma}^{2}$$
$$= \|\hat{\Sigma}_{\lambda}^{-1}(\hat{\mathbb{E}}[X\eta(X)])\|_{\Sigma}^{2}$$
$$= \|(1/n)\hat{\Sigma}_{\lambda}^{-1}AZ\|_{\Sigma}^{2}$$
$$= \|M^{1/2}Z\|^{2}.$$

By Lemma 14, we have that with probability at least $1 - \delta$ (conditioned on X_1, \ldots, X_n),

$$\begin{split} \|\bar{\beta}_{\lambda} - \hat{\beta}_{\lambda}\|_{\Sigma}^{2} &\leq \sigma_{\text{noise}}^{2} \operatorname{tr}(M) + 2\sigma_{\text{noise}}^{2} \sqrt{\operatorname{tr}(M^{2}) \log(1/\delta)} + 2\sigma_{\text{noise}}^{2} \|M\| \log(1/\delta) \\ &\leq \sigma_{\text{noise}}^{2} \operatorname{tr}(M) + 2\sigma_{\text{noise}}^{2} \sqrt{\operatorname{tr}(M)} \|M\| \log(1/\delta) + 2\sigma_{\text{noise}}^{2} \|M\| \log(1/\delta). \end{split}$$

The second step uses the fact that M is positive semi-definite and therefore

$$\operatorname{tr}(M^2) = \sum_j \lambda_j(M)^2 \le \sum_j \lambda_j(M) \cdot \lambda_{\max}(M) = \operatorname{tr}(M) ||M||$$

where we use the notation $\lambda_j(H)$ to denote the *j*-th largest eigenvalue of a symmetric matrix H. This gives the first claim. Now observe that since $(1/n)AA^{\top} = \hat{\Sigma}$,

$$\begin{split} \|M\| &= \frac{1}{n^2} \cdot \|\Sigma^{1/2} \hat{\Sigma}_{\lambda}^{-1} A\|^2 \\ &\leq \frac{1}{n^2} \cdot \|\Sigma^{1/2} \Sigma_{\lambda}^{-1/2} \|^2 \|\Sigma_{\lambda}^{1/2} \hat{\Sigma}_{\lambda}^{-1/2} \|^2 \|\hat{\Sigma}_{\lambda}^{-1/2} A\|^2 \\ &= \frac{1}{n} \cdot \|\Sigma^{1/2} \Sigma_{\lambda}^{-1/2} \|^2 \|\Sigma_{\lambda}^{1/2} \hat{\Sigma}_{\lambda}^{-1/2} \|^2 \|\hat{\Sigma}_{\lambda}^{-1/2} \hat{\Sigma}^{1/2} \|^2 \\ &\leq \frac{1}{n} \cdot \|\Sigma_{\lambda}^{1/2} \hat{\Sigma}_{\lambda}^{-1/2} \|^2 \\ &= \frac{1}{n} \lambda_{\max} (\Sigma_{\lambda}^{1/2} \hat{\Sigma}_{\lambda}^{-1} \Sigma_{\lambda}^{1/2}) \\ &\leq \frac{1}{n} \cdot \frac{1}{1 - \|\Delta_{\lambda}\|} \end{split}$$

where the last inequality follows from the assumption $\|\Delta_{\lambda}\| < 1$ and Lemma 13. Moreover,

$$\operatorname{tr}(M) = \frac{1}{n^2} \cdot \operatorname{tr}(A^{\top} \hat{\Sigma}_{\lambda}^{-1} \Sigma \hat{\Sigma}_{\lambda}^{-1} A) = \frac{1}{n} \cdot \operatorname{tr}(\hat{\Sigma}_{\lambda}^{-1} \hat{\Sigma} \hat{\Sigma}_{\lambda}^{-1} \Sigma).$$

To bound this trace expression, we first define the λ -whitened versions of Σ , $\hat{\Sigma}$, and $\hat{\Sigma}_{\lambda}$:

$$\Sigma_w := \Sigma_{\lambda}^{-1/2} \Sigma \Sigma_{\lambda}^{-1/2}$$
$$\hat{\Sigma}_w := \Sigma_{\lambda}^{-1/2} \hat{\Sigma} \Sigma_{\lambda}^{-1/2}$$
$$\hat{\Sigma}_{\lambda,w} := \Sigma_{\lambda}^{-1/2} \hat{\Sigma}_{\lambda} \Sigma_{\lambda}^{-1/2}.$$

We have the following identity:

$$\operatorname{tr}(\hat{\Sigma}_{\lambda}^{-1}\hat{\Sigma}\hat{\Sigma}_{\lambda}^{-1}\Sigma) = \operatorname{tr}(\hat{\Sigma}_{\lambda,w}^{-1}\hat{\Sigma}_{w}\hat{\Sigma}_{\lambda,w}^{-1}\Sigma_{w}).$$

By von Neumann's theorem (Horn and Johnson, 1985, page 423),

$$\operatorname{tr}(\hat{\Sigma}_{\lambda,w}^{-1}\hat{\Sigma}_w\hat{\Sigma}_{\lambda,w}^{-1}\Sigma_w) \leq \sum_j \lambda_j(\hat{\Sigma}_{\lambda,w}^{-1}\hat{\Sigma}_w\hat{\Sigma}_{\lambda,w}^{-1}) \cdot \lambda_j(\Sigma_w),$$

and by Ostrowski's theorem (Horn and Johnson, 1985, Theorem 4.5.9),

$$\lambda_j(\hat{\Sigma}_{\lambda,w}^{-1}\hat{\Sigma}_w\hat{\Sigma}_{\lambda,w}^{-1}) \leq \lambda_{\max}(\hat{\Sigma}_{\lambda,w}^{-2}) \cdot \lambda_j(\hat{\Sigma}_w).$$

Therefore,

$$\begin{aligned} \operatorname{tr}(\hat{\Sigma}_{\lambda,w}^{-1}\hat{\Sigma}_{w}\hat{\Sigma}_{\lambda,w}^{-1}\Sigma_{w}) &\leq \lambda_{\max}(\hat{\Sigma}_{\lambda,w}^{-2}) \cdot \sum_{j} \lambda_{j}(\hat{\Sigma}_{w}) \cdot \lambda_{j}(\Sigma_{w}) \\ &\leq \frac{1}{(1 - \|\Delta_{\lambda}\|)^{2}} \cdot \sum_{j} \lambda_{j}(\hat{\Sigma}_{w}) \cdot \lambda_{j}(\Sigma_{w}) \\ &= \frac{1}{(1 - \|\Delta_{\lambda}\|)^{2}} \cdot \sum_{j} \left(\lambda_{j}(\Sigma_{w})^{2} + \lambda_{j}(\Sigma_{w})(\lambda_{j}(\hat{\Sigma}_{w}) - \lambda_{j}(\Sigma_{w}))\right) \\ &\leq \frac{1}{(1 - \|\Delta_{\lambda}\|)^{2}} \cdot \left(\sum_{j} \lambda_{j}(\Sigma_{w})^{2} + \sqrt{\sum_{j} \lambda_{j}(\Sigma_{w})^{2}} \sqrt{\sum_{j} (\lambda_{j}(\hat{\Sigma}_{w}) - \lambda_{j}(\Sigma_{w}))^{2}}\right) \end{aligned}$$

where the second inequality follows from Lemma 13, and the third inequality follows from Cauchy-Schwarz. Since

$$\sum_{j} \lambda_j (\Sigma_w)^2 = \sum_{j} \left(\frac{\lambda_j(\Sigma)}{\lambda_j(\Sigma) + \lambda} \right)^2 = d_{2,\lambda}$$

and, by Mirsky's theorem (Stewart and Sun, 1990, Corollary 4.13),

$$\sum_{j} (\lambda_j(\hat{\Sigma}_w) - \lambda_j(\Sigma_w))^2 \le \|\hat{\Sigma}_w - \Sigma_w\|_{\mathrm{F}}^2 = \|\Delta_\lambda\|_{\mathrm{F}}^2$$

Hence,

$$\operatorname{tr}(M) = \frac{1}{n} \cdot \operatorname{tr}(\hat{\Sigma}_{\lambda,w}^{-1} \hat{\Sigma}_w \hat{\Sigma}_{\lambda,w}^{-1} \Sigma_w) \le \frac{1}{n} \cdot \frac{1}{(1 - \|\Delta_\lambda\|)^2} \cdot \left(d_{2,\lambda} + \sqrt{d_{2,\lambda} \cdot \|\Delta_\lambda\|_{\mathrm{F}}^2}\right)$$

which completes the proof.

Lemma 13. If $\|\Delta_{\lambda}\| < 1$, then

$$\lambda_{\max}(\varSigma_{\lambda}^{1/2} \hat{\varSigma}_{\lambda}^{-1} \hat{\varSigma}_{\lambda}^{1/2}) \le \frac{1}{1 - \|\Delta_{\lambda}\|}$$

Proof. Observe that $\Sigma_{\lambda}^{-1/2} \hat{\Sigma}_{\lambda} \Sigma_{\lambda}^{-1/2} = I + \Sigma_{\lambda}^{-1/2} (\hat{\Sigma}_{\lambda} - \Sigma_{\lambda}) \Sigma_{\lambda}^{-1/2} = I + \Sigma_{\lambda}^{-1/2} (\hat{\Sigma} - \Sigma) \Sigma_{\lambda}^{-1/2} = I + \Delta_{\lambda}$, and that

$$\lambda_{\min}(I + \Delta_{\lambda}) \ge 1 - \|\Delta_{\lambda}\| > 0$$

by Weyl's theorem (Horn and Johnson, 1985, Theorem 4.3.1) and the assumption $\|\Delta_{\lambda}\| < 1$. Therefore

$$\lambda_{\max}(\Sigma_{\lambda}^{1/2}\hat{\Sigma}_{\lambda}^{-1}\hat{\Sigma}_{\lambda}^{1/2}) = \lambda_{\max}\left((\Sigma_{\lambda}^{-1/2}\hat{\Sigma}_{\lambda}\hat{\Sigma}_{\lambda}^{-1/2})^{-1}\right) \le \frac{1}{1 - \|\Delta_{\lambda}\|}.$$

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References

- N. Ailon and B. Chazelle. Approximate nearest neighbors and the fast Johnson-Lindenstrauss transform. SIAM J. Comput., 39(1):302–322, 2009.
- J.-Y. Audibert and O. Catoni. Robust linear least squares regression, 2010a. arXiv:1010.0074.
- J.-Y. Audibert and O. Catoni. Robust linear regression through PAC-Bayesian truncation, 2010b. arXiv:1010.0072.
- O. Catoni. Statistical Learning Theory and Stochastic Optimization, Lectures on Probability and Statistics, Ecole d'Eté de Probabilitiés de Saint-Flour XXXI – 2001, volume 1851 of Lecture Notes in Mathematics. Springer, 2004.
- P. Drineas, M. W. Mahoney, S. Muthukrishnan, and T. Sarlós. Faster least squares approximation. Numerische Mathematik, 117(2):219–249, 2010.
- L. Györfi, M. Kohler, A. Kryżak, and H. Walk. A Distribution-Free Theory of Nonparametric Regression. Springer, 2004.
- Roger Horn and Charles R. Johnson. Matrix Analysis. Cambridge University Press, 1985.
- Daniel Hsu, Sham M. Kakade, and Tong Zhang. Dimension-free tail inequalities for sums of random matrices., 2011a. arXiv:0811.4413.
- Daniel Hsu, Sham M. Kakade, and Tong Zhang. A tail inequality for quadratic forms of subgaussian random vectors., 2011b. Forthcoming.
- B. Laurent and P. Massart. Adaptive estimation of a quadratic functional by model selection. *The* Annals of Statistics, 28(5):1302–1338, 2000.
- A. Litvak, A. Pajor, M. Rudelson, and N. Tomczak-Jaegermann. Smallest singular values of random matrices and geometry of random polytopes. *Advances in Mathematics*, 195:491–523, 2005.
- V. Rokhlin and M. Tygert. A fast randomized algorithm for overdetermined linear least-squares regression. Proc. Natl. Acad. Sci. USA, 105(36):13212–13217, 2008.
- S. Smale and D.-X. Zhou. Learning theory estimates via integral operators and their approximations. Constructive Approximations, 26:153–172, 2007.
- G. W. Stewart and Ji G. Sun. Matrix Perturbation Theory. Academic Press, 1990.
- J. Tropp. Freedman's inequality for matrix martingales, 2011. arXiv:1101.3039.
- T. Zhang. Learning bounds for kernel regression using effective data dimensionality. Neural Computation, 17:2077–2098, 2005.

A Exponential tail inequalities

The following exponential tail inequalities are used in our analysis. These specific inequalities were chosen in order to satisfy the general conditions setup in Section 2; however, our analysis can specialize or generalize with the availability of other tail inequalities of these sorts.

The first tail inequality is for positive semidefinite quadratic forms of a subgaussian random vector. We provide the proof for completeness.

Lemma 14 (Quadratic forms of a subgaussian random vector; Hsu et al., 2011b). Let $A \in \mathbb{R}^{m \times n}$ be a matrix and $\Sigma := AA^{\top}$. Let $X = (X_1, \ldots, X_n)$ be a random vector such that for some $\sigma \ge 0$,

$$\mathbb{E}\left[\exp\left(\alpha^{\top}X\right)\right] \le \exp\left(\|\alpha\|^{2}\sigma^{2}/2\right)$$

for all $\alpha \in \mathbb{R}^n$, almost surely. For all $\delta \in (0, 1)$,

$$\Pr\left[\|AX\|^2 > \sigma^2 \operatorname{tr}(\Sigma) + 2\sigma^2 \sqrt{\operatorname{tr}(\Sigma^2) \log(1/\delta)} + 2\sigma^2 \|\Sigma\| \log(1/\delta) \right] \le \delta.$$

Proof. Let Z be a vector of m independent standard Gaussian random variables (sampled independently of X). For any $\alpha \in \mathbb{R}^m$,

$$\mathbb{E}\left[\exp\left(Z^{\top}\alpha\right)\right] = \exp\left(\|\alpha\|^2/2\right).$$

Thus, for any $\lambda \in \mathbb{R}$ and $\varepsilon \geq 0$,

$$\mathbb{E}\left[\exp\left(\lambda Z^{\top}AX\right)\right] \geq \mathbb{E}\left[\exp\left(\lambda Z^{\top}AX\right) \mid \|AX\|^{2} > \varepsilon\right] \cdot \Pr\left[\|AX\|^{2} > \varepsilon\right]$$
$$\geq \exp\left(\frac{\lambda^{2}\varepsilon}{2}\right) \cdot \Pr\left[\|AX\|^{2} > \varepsilon\right]. \tag{3}$$

Moreover,

$$\mathbb{E}\left[\exp\left(\lambda Z^{\top}AX\right)\right] = \mathbb{E}\left[\mathbb{E}\left[\exp\left(\lambda Z^{\top}AX\right) \mid Z\right]\right]$$
$$\leq \mathbb{E}\left[\exp\left(\frac{\lambda^{2}\sigma^{2}}{2} \|A^{\top}Z\|^{2}\right)\right]$$
(4)

Let USV^{\top} be a singular value decomposition of A; where U and V are, respectively, matrices of orthonormal left and right singular vectors; and $S = \text{diag}(\sqrt{\rho_1}, \ldots, \sqrt{\rho_m})$ is the diagonal matrix of corresponding singular values. Note that

$$\|\rho\|_1 = \sum_{i=1}^m \rho_i = \operatorname{tr}(\Sigma), \quad \|\rho\|_2^2 = \sum_{i=1}^m \rho_i^2 = \operatorname{tr}(\Sigma^2), \quad \text{and} \quad \|\rho\|_\infty = \max_i \rho_i = \|\Sigma\|.$$

By rotational invariance, $Y := U^{\top}Z$ is an isotropic multivariate Gaussian random vector with mean zero. Therefore $||A^{\top}Z||^2 = Z^{\top}US^2U^{\top}Z = \rho_1Y_1^2 + \cdots + \rho_mY_m^2$. Let $\gamma := \lambda^2\sigma^2/2$. By a standard

bound for the moment generating function of linear combinations of χ^2 -random variables (*e.g.*, Laurent and Massart, 2000),

$$\mathbb{E}\left[\exp\left(\gamma\sum_{i=1}^{m}\rho_{i}Y_{i}^{2}\right)\right] \leq \exp\left(\|\rho\|_{1}\gamma + \frac{\|\rho\|_{2}^{2}\gamma^{2}}{1-2\|\rho\|_{\infty}\gamma}\right)$$
(5)

for $0 \leq \gamma < 1/(2\|\rho\|_{\infty})$. Combining (3), (4), and (5) gives

$$\Pr\left[\|AX\|^2 > \varepsilon\right] \le \exp\left(-\varepsilon\gamma/\sigma^2 + \|\rho\|_1\gamma + \frac{\|\rho\|_2^2\gamma^2}{1-2\|\rho\|_{\infty}\gamma}\right)$$

for $0 \le \gamma < 1/(2\|\rho\|_{\infty})$ and $\varepsilon \ge 0$. Choosing

$$\varepsilon := \sigma^2(\|\rho\|_1 + \tau) \text{ and } \gamma := \frac{1}{2\|\rho\|_{\infty}} \left(1 - \sqrt{\frac{\|\rho\|_2^2}{\|\rho\|_2^2 + 2\|\rho\|_{\infty}\tau}}\right),$$

we have

$$\Pr\left[\|AX\|^2 > \sigma^2(\|\rho\|_1 + \tau) \right] \le \exp\left(-\frac{\|\rho\|_2^2}{2\|\rho\|_\infty^2} \left(1 + \frac{\|\rho\|_\infty \tau}{\|\rho\|_2^2} - \sqrt{1 + \frac{2\|\rho\|_\infty \tau}{\|\rho\|_2^2}}\right)\right)$$
$$= \exp\left(-\frac{\|\rho\|_2^2}{2\|\rho\|_\infty^2} h_1\left(\frac{\|\rho\|_\infty \tau}{\|\rho\|_2^2}\right)\right)$$

where $h_1(a) := 1 + a - \sqrt{1 + 2a}$, which has the inverse function $h_1^{-1}(b) = \sqrt{2b} + b$. The result follows by setting $\tau := 2\sqrt{\|\rho\|_2^2 t} + 2\|\rho\|_{\infty} t = 2\sqrt{\operatorname{tr}(\Sigma^2)t} + 2\|\Sigma\|t$.

The next lemma is a general tail inequality for sums of bounded random vectors. We use the shorthand $a_{1:k}$ to denote the sequence a_1, \ldots, a_k , and $a_{1:0}$ is the empty sequence.

Lemma 15 (Sums of random vectors). Let X_1, \ldots, X_n be a martingale difference vector sequence (i.e., $\mathbb{E}[X_i|X_{1:i-1}] = 0$ for all $i = 1, \ldots, n$) such that

$$\sum_{i=1}^{n} \mathbb{E}\left[\|X_i\|^2 \mid X_{1:i-1} \right] \le v \quad and \quad \|X_i\| \le b$$

for all i = 1, ..., n, almost surely. For all $\delta \in (0, 1)$,

$$\Pr\left[\left\|\sum_{i=1}^{n} X_{i}\right\| > \sqrt{v} \left(1 + \sqrt{8\log(1/\delta)}\right) + (4/3)b\log(1/\delta)\right] \le \delta$$

The proof of Lemma 15 is a standard application of Bernstein's inequality.

The last three tail inequalities concern the spectral accuracy of an empirical second moment matrix.

Lemma 16 (Spectrum of subgaussian empirical covariance matrix; Litvak et al., 2005; also see Hsu et al., 2011a). Let X_1, \ldots, X_n be random vectors in \mathbb{R}^d such that, for some $\gamma > 0$,

$$\mathbb{E}\left[X_{i}X_{i}^{\top} \mid X_{1:i-1}\right] = I \quad and$$
$$\mathbb{E}\left[\exp\left(\alpha^{\top}X_{i}\right) \mid X_{1:i-1}\right] \leq \exp\left(\|\alpha\|_{2}^{2}\gamma/2\right) \quad for \ all \ \alpha \in \mathbb{R}^{d}$$

for all $i = 1, \ldots, n$, almost surely.

For all $\eta \in (0, 1/2)$ and $\delta \in (0, 1)$,

$$\Pr\left[\lambda_{\max}\left(\frac{1}{n}\sum_{i=1}^{n}X_{i}X_{i}^{\top}\right) > 1 + \frac{1}{1-2\eta} \cdot \varepsilon_{\eta,\delta,n} \quad or \quad \lambda_{\min}\left(\frac{1}{n}\sum_{i=1}^{n}X_{i}X_{i}^{\top}\right) < 1 - \frac{1}{1-2\eta} \cdot \varepsilon_{\eta,\delta,n}\right] \le \delta$$

where

$$\varepsilon_{\eta,\delta,n} := \gamma \cdot \left(\sqrt{\frac{32 \left(d \log(1 + 2/\eta) + \log(2/\delta) \right)}{n}} + \frac{2 \left(d \log(1 + 2/\eta) + \log(2/\delta) \right)}{n} \right).$$

Lemma 17 (Matrix Chernoff bound; Tropp, 2011). Let X_1, \ldots, X_n be random vectors in \mathbb{R}^d such that, for some $b \ge 0$,

$$\mathbb{E}\left[\|X_i\|^2 \mid X_{1:i-1}\right] \ge 1 \quad and \quad \|X_i\| \le b$$

for all i = 1, ..., n, almost surely. For all $\delta \in (0, 1)$,

$$\Pr\left[\lambda_{\min}\left(\frac{1}{n}\sum_{i=1}^{n}X_{i}X_{i}^{\top}\right) < 1 - \sqrt{\frac{2b^{2}}{n}\log\frac{d}{\delta}}\right] \le \delta.$$

Lemma 18 (Infinite dimensional matrix Bernstein bound; Hsu et al., 2011a). Let M be a random matrix, and $\bar{b} > 0$, $\bar{\sigma} > 0$, and $\bar{k} > 0$ be such that, almost surely:

$$\mathbb{E}[M] = 0,$$

$$\lambda_{\max}(M) \le \bar{b},$$

$$\lambda_{\max}\left(\mathbb{E}[M^2]\right) \le \bar{\sigma}^2,$$

$$\operatorname{tr}\left(\mathbb{E}[M^2]\right) \le \bar{\sigma}^2 \bar{k}.$$

If M_1, \ldots, M_n are independent copies of M, then for any t > 0,

$$\Pr\left[\lambda_{\max}\left(\frac{1}{n}\sum_{i=1}^{n}M_{i}\right) > \sqrt{\frac{2\bar{\sigma}^{2}t}{n}} + \frac{\bar{b}t}{3n}\right] \leq \bar{k}\cdot t(e^{t}-t-1)^{-1}.$$

B Application to fast least squares computations

B.1 Fast least squares computations

Our main results can be used to analyze certain data pre-processing techniques designed for speeding up over-complete least squares computations (*e.g.*, Drineas et al., 2010; Rokhlin and Tygert, 2008). The goal of these randomized methods is to approximately solve the least squares problem

$$\min_{w \in \mathbb{R}^d} \frac{1}{N} \|Aw - b\|^2$$

for some large design matrix $A \in \mathbb{R}^{N \times d}$ and vector $b \in \mathbb{R}^N$. In these methods, the columns of A and the vector b are first subjected to a random rotation (orthogonal linear transformation) $\Theta \in \mathbb{R}^{N \times N}$. Then, the rows of $[\Theta A, \Theta b] \in \mathbb{R}^{N \times (d+1)}$ are jointly sub-sampled. Finally, the least squares problem is solved using just the sub-sampled rows.

Let $(X, Y) \in \mathbb{R}^d \times \mathbb{R}$ be a random pair distributed uniformly over the rows of $[\Theta A, \Theta b]$. It can be shown that the bounded statistical leverage condition (Condition 4) is satisfied with

$$\rho_{2,\text{cov}} = O\left(\sqrt{1 + \frac{\log(N/\delta')}{d}}\right)$$

with probability at least $1 - \delta'$ over the choice of the random rotation matrix Θ under a variety of standard ensembles (see below). We thus condition on the event that this holds. Now, let β be the solution to the original least squares problem, and let $\hat{\beta}_{ols}$ be the solution to the least squares problem given by a random sub-sample of the rows of $[\Theta A, \Theta b]$. We have, for any $w \in \mathbb{R}^d$,

$$L(w) = \mathbb{E}[(X^{\top}w - Y)^2] = \frac{1}{N} \|\Theta Aw - \Theta b\|^2 = \frac{1}{N} \|Aw - b\|^2.$$

Moreover, we have that $Y - X^{\top}\beta = bias(X)$, so $\mathbb{E}[bias(X)^2] = L(\beta)$. Therefore, Theorem 2 implies that if at least

$$n > n_{2,\delta} = O\left(\left(d + \log(N/\delta')\right) \cdot \log(d/\delta)\right)$$

rows of $[\Theta A, \Theta b]$ are sub-sampled, then $\hat{\beta}_{ols}$ satisfies the approximation error guarantee (with probability at least $1 - \delta$ over the random sub-sample):

$$L(\hat{\beta}_{ols}) - L(\beta) = O\left(\frac{d \cdot L(\beta) \cdot \log(1/\delta)}{n}\right) + \text{lower order } O(1/n^2) \text{ terms}.$$

It is possible to slightly improve these bounds with more direct arguments. Nevertheless, our analysis shows how these specialized results for fast least squares computations can be understood in the more general context of random design linear regression.

B.2 Random rotations and bounding statistical leverage

The following lemma gives a simple condition on the distribution of the random orthogonal matrix $\Theta \in \mathbb{R}^{N \times N}$ used to pre-process a data matrix A so that Condition 4 (bounded statistical leverage) is applicable to the uniform distribution over the rows of ΘA . Its proof is a straightforward application of Lemma 14. We also give two simple examples under which the required condition holds.

Lemma 19. Suppose $\Theta \in \mathbb{R}^{N \times N}$ is a random orthogonal matrix and $\sigma > 0$ is a constant such that for each i = 1, ..., N, for all $\alpha \in \mathbb{R}^N$, and almost surely:

$$\mathbb{E}\left[\exp\left(\alpha^{\top}\left(\sqrt{N}\Theta^{\top}e_{i}\right)\right)\right] \leq \exp\left(\|\alpha\|^{2}\sigma^{2}/2\right)$$

Let $A \in \mathbb{R}^{N \times d}$ be any matrix of rank d, and let $\Sigma := (1/N)(\Theta A)^{\top}(\Theta A) = (1/N)A^{\top}A$. There exists

$$\rho_{2,\text{cov}} \leq \sigma \sqrt{1 + 2\sqrt{\frac{\log(N/\delta)}{d}} + \frac{2\log(N/\delta)}{d}}$$

such that

$$\Pr\left[\max_{i=1,\dots,N} \|\mathcal{L}^{-1/2}(\Theta A)^{\top} e_i\| > \rho_{2,\mathrm{cov}} \sqrt{d}\right] \le \delta.$$

Proof. Let $Z_i := \sqrt{N} \Theta^{\top} e_i$ for each i = 1, ..., N. Let $U \in \mathbb{R}^{N \times d}$ be a matrix of left orthonormal singular vectors of A. We have

$$\|\Sigma^{-1/2}(\Theta A)^{\top} e_i\| = \|\sqrt{N}U^{\top}\Theta^{\top} e_i\| = \|U^{\top}Z_i\|.$$

By Lemma 14,

$$\Pr\left[\|U^{\top} Z_i\|^2 > \sigma^2 \left(d + 2\sqrt{d\log(N/\delta)} + 2\log(N/\delta)\right)\right] \le \delta/N.$$

Therefore, by a union bound,

$$\Pr\left[\max_{i=1,\dots,N} \|\mathcal{L}^{-1/2}(\Theta A)^{\top} e_i\|^2 > \sigma^2 \left(d + 2\sqrt{d\log(N/\delta)} + 2\log(N/\delta)\right)\right] \le \delta.$$

Example 1. Let Θ be distributed uniformly over all $N \times N$ orthogonal matrices. Fix any $i = 1, \ldots, N$. The random vector $V := \Theta^{\top} e_i$ is distributed uniformly on the unit sphere \mathbb{S}^{N-1} . Let L be a χ random variable with N degrees of freedom, so LV has an isotropic multivariate Gaussian distribution. By Jensen's inequality

$$\mathbb{E}\left[\exp\left(\alpha^{\top}(\sqrt{N}\Theta^{\top}e_{i})\right)\right] = \mathbb{E}\left[\exp\left(\alpha^{\top}(\sqrt{N}V)\right)\right]$$
$$= \mathbb{E}\left[\mathbb{E}\left[\exp\left(\frac{\sqrt{N}}{\mathbb{E}[L]}\alpha^{\top}(\mathbb{E}[L]V)\right) \mid V\right]\right]$$
$$\leq \mathbb{E}\left[\exp\left(\frac{\sqrt{N}}{\mathbb{E}[L]}\alpha^{\top}(LV)\right)\right]$$
$$\leq \exp\left(\frac{\|\alpha\|^{2}N}{2\mathbb{E}[L]^{2}}\right)$$
$$\leq \exp\left(\|\alpha\|^{2}\left(1 - \frac{1}{4N} - \frac{1}{360N^{3}}\right)^{-2}/2\right)$$

since

$$\mathbb{E}[L] \ge \sqrt{N} \left(1 - \frac{1}{4N} - \frac{1}{360N^3} \right).$$

Therefore, the condition is satisfied with $\sigma = 1 + O(1/N)$.

Example 2. Let N be a power of two, and let $\Theta := H \operatorname{diag}(S)/\sqrt{N}$, where $H \in \{\pm 1\}^{N \times N}$ is the $N \times N$ Hadamard matrix, and $S := (S_1, \ldots, S_n) \in \{\pm 1\}^N$ is a vector of N Rademacher variables $(i.e., S_1, \ldots, S_N \text{ i.i.d.})$ with $\Pr[S_1 = 1] = \Pr[S_1 = -1] = 1/2$. This random rotation is a key component of the fast Johnson-Lindenstrauss transform of Ailon and Chazelle (2009), also used by Drineas et al. (2010). For each $i = 1, \ldots, N$, the distribution of $\sqrt{N}\Theta^{\top}e_i$ is the same as that of S, and therefore

$$\mathbb{E}\left[\exp\left(\alpha^{\top}\left(\sqrt{N}\Theta^{\top}e_{i}\right)\right)\right] = \mathbb{E}\left[\exp\left(\alpha^{\top}S\right)\right] \leq \exp(\|\alpha\|^{2}/2)$$

where the last step follows by Hoeffding's inequality. Therefore, the condition is satisfied with $\sigma = 1$.