Debiasing Linear Prediction

Nilesh Tripuraneni  
Department of EECS  
University of California, Berkeley

Lester Mackey  
Microsoft Research New England  
Cambridge, MA, USA

Abstract

Standard methods in supervised learning separate training and prediction: the model is fit independently of any test points it may encounter. However, can knowledge of the next test point \( x^\star \) be exploited to improve prediction accuracy? We address this question in the context of linear prediction, showing how debiasing techniques can be used transductively to combat regularization bias. We first lower bound the \( x^\star \) prediction error of ridge regression and the Lasso, showing that they must incur significant bias in certain test directions. Then, building on techniques from semi-parametric inference, we provide non-asymptotic upper bounds on the \( x^\star \) prediction error of two transductive, debiased prediction rules. We conclude by showing the efficacy of our methods on both synthetic and real data, highlighting the improvements test-point-tailored debiasing can provide in settings with distribution shift.

1 Introduction

We consider the task of prediction given independent datapoints \( ((y_i, x_i))_{i=1}^n \) from a linear model,

\[
y_i = x_i^\top \beta_0 + \epsilon_i, \quad E[\epsilon_i] = 0, \quad \epsilon_i \perp \perp x_i
\]

in which our observed targets \( y = (y_1, \ldots, y_n) \in \mathbb{R}^n \) and covariates \( X = [x_1, \ldots, x_n]^\top \in \mathbb{R}^{n \times p} \) are related by an unobserved parameter vector \( \beta_0 \in \mathbb{R}^p \) and noise vector \( \epsilon = (\epsilon_1, \ldots, \epsilon_n) \in \mathbb{R}^n \).

Most approaches to linear model prediction are inductive, divorcing the steps of training and prediction; for example, regularized least squares methods like ridge regression [15] and the Lasso [21] are fit independently of any knowledge of the next target test point \( x^\star \). This suggests a tantalizing transductive question: can knowledge of a single test point \( x^\star \), be leveraged to improve prediction for \( x^\star \)? In the random design linear model setting (1), we answer this question in the affirmative.

Specifically, in Section 2 we establish out-of-sample prediction lower bounds for the popular ridge and Lasso estimators, highlighting the significant dimension-dependent bias introduced by regularization. In Section 3 we demonstrate how this bias can be removed, by presenting two classes of debiased, transductive estimators which are trained using explicit knowledge of the test point \( x^\star \). We provide non-asymptotic risk bounds for these estimators in the random design setting, proving when \( n \) is sufficiently large, they achieve a dimension-free \( O(\frac{1}{n}) \) \( x^\star \)-prediction risk. In Section 4, we first validate our theory in simulation, demonstrating that debiasing the Lasso with fixed regularization improves prediction accuracy even when \( x^\star \) is drawn from the training distribution. We then demonstrate that under distribution shift, our debiased methods outperform even the popular cross-validated Lasso, cross-validated ridge, and cross-validated elastic net estimators (which find an optimal data-dependent tradeoff between bias and variance) on both synthetic data and a suite of five real datasets.

Preprint. Under review.
1.1 Related Work

Our work is inspired by two approaches to semiparametric inference in linear models: the debiased Lasso approach introduced by [27, 23, 17] and the orthogonal machine learning approach of [11]. The works [27, 23, 17] obtain small-width and asymptotically-valid confidence intervals for individual model parameters \((\beta_0)_j = (\beta_0, e_j)\) by debiasing an initial Lasso estimator [21]. The works [9, 8, 2] each consider a more closely related problem of obtaining prediction confidence intervals using a generalization of the estimator of [17].

The work of [11] describes a general-purpose procedure for extracting \(\sqrt{n}\)-consistent and asymptotically normal target parameter estimates in the presence of nuisance parameters. Specifically, Chernozhukov et al. [11] construct a two-stage estimator where one initially fits first-stage estimates of nuisance parameters using arbitrary ML estimators on a first-stage data sample. In the second-stage, these first-stage estimators are used to provide estimates of the relevant model parameters using an orthogonalized method-of-moments. Wager et al. [24] also consider the problem of treatment effect estimation using general ML procedures.

Our approach to prediction also bears some resemblance to semi-supervised learning – transferring predictive power between labelled and unlabelled examples [28]. In contrast with this, the goal of transductive learning is to predict solely the labels of the observed unlabeled features. Alquier and Hebiri [1] formulate a transductive version of the Lasso and Dantzig selector estimators in the fixed design setting focused only on predicting against a subset of points. Bellec et al. [5] also prove risk bounds for transductive and semi-supervised \(\ell_1\)-regularized estimators in the high-dimensional setting. A principal difference between our approaches is that we make no distributional assumptions upon the sequence of test points \(x_\star\) and do not assume simultaneous access to a large pool of test data. Rather our procedures receive access to only a single arbitrary test point \(x_\star\), and our aim is accurate prediction for that point. Previous works in this vein also do not address the issue of debiasing.

1.2 Problem Setup

Our principal aim in this work is to understand the \(x_\star\) prediction risk,

\[
R(x_\star, \hat{y}) = E[(y_\star - \hat{y})^2] - \sigma^2_\epsilon = E[(\hat{y} - \langle x_\star, \beta_0 \rangle)^2],
\]

of an estimator \(\hat{y}\) of the unobserved test response \(y_\star = x_\star^\top \beta_0 + \epsilon_\star\). Here, \(\epsilon_\star\) is independent of \(x_\star\) with variance \(\sigma^2_\epsilon\). We exclude the additive noise \(\sigma^2_\epsilon\) from our risk definition, as it is irreducible for any estimator. Importantly, to accommodate non-stationary learning settings, we make no distributional assumptions on \(x_\star\); in particular, \(x_\star\) need not be drawn from the training distribution. Hereafter, we will make use of several assumptions which are standard in the random design linear regression literature.

**Assumption 1** (Well-specified Model). The data \((X, y)\) is generated from the model (1).

**Assumption 2** (Bounded Covariance). The covariate vectors have common covariance \(\Sigma = E[XX^\top]\) with \(\Sigma_{ii} \leq 1/2; \sigma_{\text{max}}(\Sigma) \leq C_{\text{max}}\) and \(\sigma_{\text{min}}(\Sigma) \geq C_{\text{min}}\). We further define the precision matrix \(\Omega = \Sigma^{-1}\) and condition number \(C_{\text{cond}} = C_{\text{max}}/C_{\text{min}}\).

**Assumption 3** (Sub-Gaussian Design). Each covariate vector \(\Sigma^{-1/2}x_i\) is sub-Gaussian with parameter \(\kappa \geq 1\), in the sense that, \(E[\exp(v^\top x_i)] \leq \exp\left(\frac{x_i^2||\Sigma^{1/2}v||^2}{2}\right)\).

**Assumption 4** (Sub-Gaussian Noise). The noise \(\epsilon_i\) is sub-Gaussian with variance parameter \(\sigma^2_\epsilon\).

Throughout, we will use bold lower-case letters (e.g., \(x\)) to refer to vectors and bold upper-case letters to refer to matrices (e.g., \(X\)). We use \([p]\) for the set \(\{1, \ldots, p\}\). Vectors or matrices subscripted with an index set \(S\) indicate the subvector or submatrix supported on \(S\). The expression \(s_{\beta_0}\) indicates the number of non-zero elements in \(\beta_0\) and \(\text{supp}(\beta_0) = \{j : (\beta_0)_j \neq 0\}\). We will use \(\gtrsim, \ltrsim, \asymp\) to denote greater than, less than, and equal to up to a constant that is independent of \(p\) and \(n\).

2 Lower Bounds for Regularized Prediction

We begin by providing lower bounds on the \(x_\star\) prediction risk of Lasso and ridge regression; the corresponding predictions take the form \(\hat{y} = \langle x_\star, \hat{\beta} \rangle\) for a regularized estimate \(\hat{\beta}\) of the unknown
vector $\beta_0$. While our presentation focuses on the prediction risk (2), which features an expectation over $\hat{y}$, our proofs also provide identical constant probability lower bounds on \((\hat{y} - \langle x_*, \beta_0 \rangle)^2\).

### 2.1 Lower Bounds for Prediction with Ridge Regression

We first consider the prediction risk of the ridge estimator $\hat{\beta}_R(\lambda) = \arg\min_{\beta} \|y - X\beta\|^2 + \lambda \|\beta\|^2$ with regularization parameter $\lambda > 0$. In the asymptotic high-dimensional limit (with $n, p \to \infty$) and assuming the training distribution equals the test distribution, Dobriban et al. [13] compute the prediction risk of the ridge estimator in a dense random effects model. By contrast, we provide a non-asymptotic lower bound which does not impose any distributional assumptions on $x_*$ or on the underlying parameter vector $\beta_0$. Theorem 1, proved in Appendix B.1, isolates the error in the ridge estimator due to bias for any choice of regularizer $\lambda$.

**Theorem 1.** Under Assumption 1, suppose $x_i \overset{i.i.d.}{\sim} \mathcal{N}(0, I_p)$ with independent noise $\epsilon \sim \mathcal{N}(0, \sigma^2)$. Then, if $n \geq p \geq 20$, the ridge estimator with regularization parameter $\lambda$ satisfies

$$\mathbb{E}[|\langle x_*, \hat{\beta}_R(\lambda) - \beta_0 \rangle|^2] \geq \frac{\|\beta_0\|^2}{\sigma^2} + \frac{\lambda}{\lambda(n+\gamma)} \left(\frac{\lambda}{\lambda(n+\gamma)}\right)^2 \cdot \|x_*\|^2 \cdot \frac{\sigma^2}{n} \cdot \cos(x_*, \beta_0)^2.$$  

Notably, the dimension-free term $\|x_*\|^2 \cdot \frac{\sigma^2}{n}$ in this bound coincides with the $x_*$ risk of the ordinary least squares (OLS) estimator in this setting. The remaining multiplicative factor indicates that the ridge risk can be substantially larger if the regularization strength $\lambda$ is too large. In fact, our next result shows that, surprisingly, over-regularization can result even when $\lambda$ is tuned to minimize held-out prediction error over the training population. The same undesirable outcome results when $\lambda$ is selected to minimize $\ell_2$ estimation error; the proof can be found in Appendix B.2.

**Corollary 1.** Under the conditions of Theorem 1, if $x \overset{d}{=} x_1$ and $x$ is independent of $(X, y)$, then

$$\lambda_* \overset{\Delta}{=} \arg\min_{\lambda} \mathbb{E}[\|(\hat{\beta}_R(\lambda) - \beta_0)\|^2] = \arg\min_{\lambda} \mathbb{E}[\|\hat{\beta}_R(\lambda) - \beta_0\|^2] = \frac{p \sigma^2}{\|\beta_0\|^2} = \frac{p}{\text{SNR}} \text{ and } \mathbb{E}[\langle x_*, \hat{\beta}_R(\lambda_*), \beta_0 \rangle)^2] \geq \frac{p \sigma^2}{\text{SNR}} \cdot \|x_*\|^2 \cdot \frac{\sigma^2}{n} \cdot \cos(x_*, \beta_0)^2 \text{ whenever } n \geq \frac{1}{6} \frac{p}{\text{SNR}}.$$

Several insights can be gathered from the previous results:

- The expression $\mathbb{E}[\|\hat{y} - \hat{x}^\top \hat{\beta}_R(\lambda)\|^2] = \mathbb{E}[\|\hat{x} \cdot \hat{\beta}_R(\lambda) - \beta_0\|^2] + \sigma^2$ (where $\hat{y} = \hat{x}^\top \beta_0 + \epsilon$) minimized in Corollary 1 is the out-of-sample prediction error for a new datapoint $\hat{x}$ drawn from the training distribution. This is the population analog of held-out validation error or cross-validation error that is often minimized in practice.

- In the setting of Corollary 1, taking $\text{SNR} = \frac{1}{6} \frac{p}{n}$ yields

$$\mathbb{E}[\langle x_*, \hat{\beta}_R(\lambda_*), \beta_0 \rangle)^2] \geq p \cdot \|x_*\|^2 \cdot \frac{\sigma^2}{n} \cdot \frac{3 \cos(x_*, \beta_0)^2}{392}.$$  

More generally, if we take $\cos(x_*, \beta_0)^2 = \Theta(1)$, $\text{SNR} = o\left(\frac{p}{n}\right)$ and $\text{SNR} \geq \frac{1}{6} \frac{p}{n}$ then,

$$\mathbb{E}[\langle x_*, \hat{\beta}_R(\lambda_*), \beta_0 \rangle)^2] \geq \omega\left(\|x_*\|^2 \cdot \frac{\sigma^2}{n}\right).$$

If $\lambda$ is optimized for estimation error or for prediction error with respect to the training distribution, the ridge estimator must incur much larger test error then the OLS estimator in some test directions. Such behavior can be viewed as a symptom of over-regularization – the choice $\lambda_*$ is optimized for the training distribution and cannot be targeted to provide uniformly good performance over all $x_*$. In Section 3 we show how debiasing techniques can improve prediction in this regime.

The chief difficulty in lower-bounding the $x_*$ prediction risk in Theorem 1 lies in controlling the expectation over the design $X$, which enters nonlinearly into the prediction risk. Our proof circumvents this difficulty in two steps. First, the isotropy and independence properties of Wishart matrices are used to reduce the computation to that of a 1-dimensional expectation with respect to the unordered eigenvalues of $X$. Second, in the regime $n \geq p$, the sharp concentration of Gaussian random matrices in spectral norm is exploited to essentially approximate $\frac{p}{n}X^\top X \approx I_p$. In a similar fashion, the symmetry properties of Wishart matrices allow us to explicitly compute the optimal $\lambda_*$ in Corollary 1 (which is valid for all $n$).
2.2 Lower Bounds for Prediction with the Lasso

We next provide a strong lower bound on the out-of-sample prediction error of the Lasso estimator $\hat{\beta}_L(\lambda) = \arg\min_{\beta} \frac{1}{2n} \| y - X\beta \|_2^2 + \lambda \| \beta \|_1$, with regularization parameter $\lambda > 0$. There has been extensive work [see, e.g., 20] establishing minimax lower bounds for the in-sample prediction error and parameter estimation error of any procedure given data from a sparse linear model. However, our focus is on out-of-sample prediction risk for a specific procedure, the Lasso. The point $x_\star$ need not be one of the training points (in-sample) nor even be drawn from the same distribution as the covariates. Theorem 2, proved in Appendix C.1, establishes that a well-regularized Lasso program suffers significant biases even in a simple problem setting with i.i.d. Gaussian covariates and noise.

**Theorem 2.** Under Assumption 1, fix any $s \geq 0$, and let $x_\star \sim N(0, I_n \sigma^2)$ with independent noise $\epsilon \sim N(0, I_p)$ with independent components. Then, if $\hat{\beta}_L(\lambda)$ denotes the solution of the Lasso program, with regularization parameter chosen as $\lambda \geq (8 + 2\sqrt{2})\sigma_\epsilon \sqrt{\log(2cp)}/n$, and $p \geq 20$, there exist universal constants $c_1, c_2$ such that for all $n \geq c_1 s^2 \log(2cp)$ and for $x_\star \sim \mathcal{P}^\star$ independently of $X, \epsilon$,

$$
\sup_{\beta_0 \in \mathbb{B}_0(s)} \mathbb{E}[\| x_\star \|^2] \geq \sup_{\beta_0 \in \mathbb{B}_0(s)} \mathbb{E}[\| x_\star \|^2] \geq c_2 \lambda^2 \Lambda_s[\mathbb{E}[x_\star x_\star^\top]] \geq c_2 \lambda^2 \mathbb{E}[\| x_\star \|_2^2]
$$

where the trimmed norm $\| x_\star \|_2$ is the sum of the magnitudes of the $s$ largest magnitude entries of $x_\star$ and $\Lambda_s[\mathbb{E}[x_\star x_\star^\top]]$ is the maximum $s$-sparse eigenvalue of $\mathbb{E}[x_\star x_\star^\top]$.

We can instantiate this result in a useful setting when we consider a degenerate distribution $\mathcal{P}^\star$ concentrated along a fixed $x_\star$ (see Appendix C.2 for the proof):

**Corollary 2.** In the setting of Theorem 2, there exists a universal constant $c_3$ such that

$$
\sup_{\| x_\star \|_2 = 1} \sup_{\beta_0 \in \mathbb{B}_0(s)} \mathbb{E}[\| x_\star \|_2] \geq c_3 \lambda^2 s^2/2q \geq c_3 \lambda^2 s^2/2q \quad \text{for all } q \epsilon [1, \infty).
$$

We make several comments regarding these results:

- Together Theorem 2 and Corollary 2 yield an $\mathcal{P}^\star/x_\star$-specific lower bound — showing that given any potential direction $x_\star$, there will exist an underlying $s$-sparse parameter $\beta_0$ for which the Lasso performs poorly. Moreover, the magnitude of error suffered by the Lasso scales both with the regularization strength $\lambda$ and the norm of $x_\star$ along its top $s$ coordinates.

- The constraint on the regularization parameter in Theorem 2, $\lambda \gtrsim \sigma_\epsilon \sqrt{\log p/n}$, is a sufficient and standard choice to obtain consistent estimates with the Lasso (see Wainwright [25, Ch. 7] for example).

- Simplifying to the case of $q = 2$, we see that Corollary 2 implies the Lasso must incur $x_\star$ prediction error $\geq c_3 \lambda^2 s^2/2q$, matching upper bounds for Lasso prediction error. In particular such a bound is not dimension-free, possessing a dependence on $s \log p$, even though the Lasso is only required to predict well along a single direction.

The proof of Theorem 2 uses two key ideas. First, in this benign setting, we can show that $\hat{\beta}_L(\lambda)$ has support strictly contained in the support of $\beta_0$ with at least constant probability. We then adapt ideas from the study of debiased lasso estimation in [17], to sharply characterize the coordinate-wise bias of the Lasso estimator along the support of $\beta_0$. We show that when $(x_\star)_j > 0$ and $(\beta_0)_j = \lambda$, we have $\mathbb{E}[(\hat{\beta}_L(\lambda) - \beta_0)_j] = -\Omega(\lambda) < 0$ for each coordinate $j \in S$ (and similarly for $(x_\star)_j < 0$ and $(\beta_0)_j = -\lambda$). Thus the bias induced by regularization can coherently sum across the $s$ coordinates in the support of $\beta_0$. The argument for the case when $x_\star$ is drawn from a distribution $\mathcal{P}^\star$ is similar. This sign alignment between $x_\star$ and $\beta_0$ is also explored in the independent and concurrent work of [3, Thm. 2.2].

3 Upper Bounds for Transductive Prediction

Having established that regularization can lead to excessive prediction bias, we now introduce two classes of estimators which can mitigate this bias using knowledge of the single test direction $x_\star$. While our presentation focuses on the prediction risk (2), which features an expectation over $\hat{y}$, our proofs also provide identical high probability upper bounds on $(\hat{y} - (x_\star, \beta_0))^2$. 

4
3.1 Javanmard-Montanari (JM)-style Estimator

Our first approach to debiasing linear prediction is inspired by the debiased Lasso estimator of Javanmard and Montanari [17] which was to designed to construct confidence intervals for individual model parameters $(\beta_0)_j$. For prediction in the $x_*$ direction, we will consider the following generalization of the Javanmard-Montanari (JM) debiasing construction:

$$w = \arg\min_w \ w^T \Sigma_n w \ \text{s.t.} \ \|\Sigma_n w - x_*\|_\infty \leq \lambda_w. \quad (3)$$

$$\hat{y}_{JM} = \langle x_*, \hat{\beta} \rangle + \frac{1}{n} w^T X^\top (y - X\beta). \quad (4)$$

Here, $\hat{\beta}$ is any (ideally $\ell_1$-consistent) initial pilot estimate of $\beta_0$, like the estimate $\hat{\beta}_L(\lambda)$ returned by the Lasso. When $x_* = \epsilon_j$ the estimator (4) reduces exactly to the program in [17], and equivalent generalizations have been used in [9, 2, 8] to construct prediction intervals and to estimate treatment effects. Intuitively, $w$ approximately inverts the population covariance matrix along the direction defined by $x_*$ (i.e., $w \approx \Omega x_*$). The second term in (4) can be thought of as a high-dimensional one-step correction designed to remove bias from the initial prediction $\langle x_*, \hat{\beta} \rangle$; see [17] for more intuition on this construction. We can now state our primary guarantee for the JM-style estimator (4); the proof is given in Appendix D.1.

**Theorem 3.** Suppose Assumptions 1, 2, 3 and 4 hold and that the debiased estimator $\hat{y}_{JM}$ of (4) is fit with regularization parameter $\lambda_w = 8a\sqrt{C_{\text{cond}}\kappa^2}\|x_*\|_2 \sqrt{\frac{\log(p \lor n)}{n}}$ for some $a > 0$. Then there is a universal constant $c_1$ such that if $n \geq c_1 a^2 \log(2e(p \lor n)),$

$$E[(\hat{y}_{JM} - \langle \beta_0, x_* \rangle)^2] \leq O \left( \frac{\sigma^2 x_* \Omega x_*}{n} + \epsilon^2_{\beta, 1}(\lambda_w^2 + \|x_*\|_\infty^2 \frac{1}{\min\{n, p, \kappa^2\}}) \right) . \quad (5)$$

for $c_3 = \frac{a^2}{4} - \frac{1}{2}$ and $r_{\beta, 1} = (E[\|\|\beta_0\|_\infty^2\|])^{1/4}$, the $\ell_1$ error of the initial estimate. Here the $O(\cdot)$ masks constants depending only on $\kappa, C_{\text{min}}, C_{\text{max}}, C_{\text{cond}}$.

Intuitively, the first term in our bound (5) can be viewed as the variance of the estimator’s prediction along the direction of $x_*$, while the second term can be thought of as the (reduced) bias of the estimator. We consider the third term to be of higher-order since $a$ (and in turn $c_3$) can be chosen as a large constant. When the Lasso is used as the pilot regression procedure we can derive the following corollary to Theorem 3, also proved in Appendix D.2.

**Corollary 3.** Recall $s_{\beta_0} = \|\beta_0\|_0$. Under the conditions of Theorem 3, consider the JM-style estimator (4) with pilot estimate $\hat{\beta} = \hat{\beta}_L(\lambda)$ with $\lambda \geq 80\sigma \sqrt{\frac{\log(2e\pi\|\beta_0\|_0)}{n}}$. If $p \geq 20$, then there exist universal constants $c_1, c_2$ such that if $\|\beta_0\|_\infty / \sigma = o(e^{c_1 n})$ and $n \geq c_2 \max\{\frac{s_{\beta_0} \kappa^2}{\min\{C_{\text{min}}, a^2\}} \log(2e(p \lor n)),$

$$E[(\hat{y}_{JM} - \langle \beta_0, x_* \rangle)^2] \leq O \left( \frac{\sigma^2 x_* \Omega x_*}{n} + \lambda^2 s_{\beta_0}^2 (\lambda_w^2 + \|x_*\|_\infty^2 \frac{1}{\min\{n, p, \kappa^2\}}) \right) \right) \right)$$

Here the $O(\cdot)$ masks constants depending only on $\kappa, C_{\text{min}}, C_{\text{max}}, C_{\text{cond}}$.

We make several remarks to further interpret this result:

- To simplify the presentation of the results (and match the setting of the lower bound in Theorem 2) consider the regime $n \geq s_{\beta_0}^2 \log p \log(p \lor n)$ in our algorithm and consider the regime $n \geq s_{\beta_0}^2 \log \log p \log(p \lor n).$ Then the upper bound in Theorem 3 can be succinctly stated as $O\left(\frac{\sigma^2 x_* \Omega x_*}{n}\right)$. In short, the debiased estimator attains a dimension-free rate for sufficiently large $n$. Under the same conditions the Lasso estimator suffers a prediction error of $\Omega(n^{-2} s_{\beta_0}^2 \frac{\log p}{n})$ as Theorem 2 and Corollary 2 establish.

- The estimator described in (3) and (4) is transductive in that it is tailored to an individual test-point $x_*$. The corresponding guarantees in Theorem 3 and Corollary 3 embody a computational-statistical tradeoff. In our setting, the detrimental effects of regularization can be mitigated at the cost of extra computation: the convex program in (3) must be solved for each new $x_*$.  

\[^{1}\text{In the event the constraints are not feasible we define } w = 0.\]
3.2 Orthogonal Moment (OM) Estimators

Our second approach to debiasing linear prediction is inspired by orthogonal moment (OM) estimation [11]. OM estimators are commonly used to estimate single parameters of interest (like a treatment effect) in the presence of high-dimensional or nonparametric nuisance. To connect our problem to this semiparametric world, we first frame the task of prediction in the \( x \) direction as one of estimating a single parameter, \( \theta_0 = x_0^\top \beta_0 \). Consider the linear model equation (1)

\[
y_i = x_i^\top \beta_0 + \epsilon_i = (x_i - U^\top \theta_0) + \epsilon_i
\]

with a data reparametrization defined by the matrix \( U = \|x_i\|_2 \cdot [u_1 \cdots u_p] \) for \( \frac{x_i}{\|x_i\|_2} = u_1 \) so that \( e_i^\top U \beta_0 = x_i^\top \beta_0 = \theta_0 \). Here, the matrix \( R \in \mathbb{R}^{(p-1) \times p} \) has orthonormal orthogonal to \( u_1 \) - these are obtained as the non-\( u_1 \) eigenvectors of the projector matrix \( I_p - u_1 u_1^\top \). This induces the data reparametrization \( x' = [t, z] = (U^{-1})^\top x \). In the reparametrized basis, the linear model becomes,

\[
y_i = \theta_0 t_i + z_i^\top f_0 + \epsilon_i, \quad t_i = g_0(z_i) + \eta_i, \quad q_0(z_i) \triangleq \theta_0 g_0(z_i) + z_i^\top f_0 \tag{6}
\]

where we have introduced convenient auxiliary equations in terms of \( g_0(z_i) \). To estimate \( \theta_0 = x_0^\top \beta_0 \) in the presence of the unknown nuisance parameters \( f_0, g_0, q_0 \), we introduce a thresholded-variant of the two-stage method of moments estimator proposed in [11]. The method of moments takes as input a moment function \( m \) of both data and parameters that uniquely identifies the target parameter of interest. Our reparameterized model form (6) gives us access to two different Neyman orthogonal moment functions described [11]:

\[
\begin{align*}
\text{f moments:} & \quad m(t_i, y_i, \theta, z_i^\top f, g(z_i)) = (y_i - t_i \theta - z_i^\top f)(t_i - g(z_i)) \\
\text{q moments:} & \quad m(t_i, y_i, \theta, q(z_i), g(z_i)) = (y_i - q(z_i) - \theta(t_i - g(z_i)))(t_i - g(z_i)).
\end{align*}
\tag{7}
\]

These orthogonal moment equations enable the accurate estimation of a target parameter \( \theta_0 \) in the presence of high-dimensional or nonparametric nuisance parameters (in this case \( f_0 \) and \( g_0 \)). We focus our theoretical analysis and present description on the set of \( f \) moments since the analysis is similar for the \( q \), although we investigate the practical utility of both in Section 4.

Our OM proposal to estimate \( \theta_0 \) now proceeds as follows. We first split our original dataset of \( n \) points into two\(^2\) disjoint, equal-sized folds \( (X^{(1)}, y^{(1)}) = \{ (x_i, y_i) : i \in \{1, \ldots, \frac{n}{2}\} \} \) and \( (X^{(2)}, y^{(2)}) = \{ (x_i, y_i) : i \in \{ \frac{n}{2} + 1, \ldots, n \} \} \). Then,

- The first fold \( (X^{(1)}, y^{(1)}) \) is used to run two first-stage regressions. We estimate \( \beta_0 \) by linearly regressing \( y^{(1)} \) onto \( X^{(1)} \) to produce \( \hat{\beta} \); this provides an estimator of \( f_0 \) as \( e_1^\top U \beta = \hat{\beta} \). Second we estimate \( g_0 \) by regressing \( t^{(1)} \) onto \( z^{(1)} \) to produce a regression model \( \hat{g}(\cdot) : \mathbb{R}^{p-1} \rightarrow \mathbb{R} \). Any arbitrary linear or non-linear regression procedure can be used to fit \( \hat{g}(\cdot) \).
- Then, we estimate \( \mathbb{E}[\eta_i^2] \) as \( \mu_2 = \frac{1}{n/2} \sum_{i=\frac{n}{2}+1}^n t_i(t_i - \hat{g}(z_i)) \) where the sum is taken over the second fold of data in \( (X^{(2)}, y^{(2)}) \); crucially \( (t_i, z_i) \) are independent of \( \hat{g}(\cdot) \) in this expression.
- If \( \mu_2 \leq \tau \) for a threshold \( \tau \) we simply output \( \hat{y}_{OM} = x_0^\top \hat{\beta} \). If \( \mu_2 \geq \tau \) we estimate \( \theta_0 \) by solving the empirical moment equation:

\[
\sum_{i=\frac{n}{2}+1}^n m(t_i, y_i, \hat{y}_{OM}, z_i^\top f, \hat{g}(z_i)) = 0 \implies \hat{y}_{OM} = \frac{1}{\mu_2} \sum_{i=\frac{n}{2}+1}^n (y_i - \hat{z}_i^\top f)(t_i - \hat{g}(z_i)) \tag{8}
\]

where the sum is taken over the second fold of data in \( (X^{(2)}, y^{(2)}) \) and \( m \) is defined in (7).

If we had oracle access to the underlying \( f_0 \) and \( g_0 \), solving the population moment condition \( \mathbb{E}_{t_i, y_i, z_i}[m(t_i, y_i, \theta, z_i^\top f_0, g_0(z_i))] = 0 \) for \( \theta \) would exactly yield \( \theta_0 = x_0^\top \beta_0 \). In practice, we first construct estimates \( \hat{f} \) and \( \hat{g} \) of the unknown nuisance parameters to serve as surrogates for \( f_0 \) and \( g_0 \) and then solve an empirical version of the aforementioned moment condition to extract \( \hat{y}_{OM} \). A key property of the moments in (7) is their Neyman orthogonality: they satisfy

\(^2\)In practice, we use \( K \)-fold cross-fitting to increase the sample-efficiency of the scheme as in [11]; for simplicity of presentation, we defer the description of this slight modification to Appendix G.4.
Then there exist universal constants

$$E[\nabla_x f^m(t_1, y_1, \theta_0, z^\top_1 f_0, g_0(z_1))] = 0$$

and

$$E[\nabla_g(z_1)[m(t_1, y_1, z^\top_1 f_0, g_0(z_1))]] = 0.$$ Thus the solution of the empirical moment equations is first-order insensitive to errors arising from using $f, g$ in place of $f_0$ and $g_0$. Data splitting is further used to create independence across the two stages of the procedure. In the context of testing linearly-constrained hypotheses of the parameter $\beta_0$, Zhu and Bradic [29] propose a two-stage OM test statistic based on the transformed $f$ moments introduced above; they do not use cross-fitting and specifically employ adaptive Dantzig-like selectors to estimate $f_0$ and $g_0$. Finally, note the thresholding step in the estimator is not present in prior work and is used to control the variance explosion that might arise from $\mu_2$ being too small. This is important since we are ultimately interested in providing non-asymptotic prediction risk bounds on the estimator. Before presenting the analysis of the OM estimator (8) we introduce another condition:

**Assumption 5.** The noise $\eta_i$ is independent of $z_i$.

Recall $\hat{g}$ is evaluated on the (independent) second fold data $z$. We now obtain our central guarantee for the OM estimator (proved in Appendix E.1).

**Theorem 4.** Let Assumptions 1, 2, 3, 4 and 5 hold, and assume that $g_0(z_i) = z_i^\top g_0$ in (6) for $g_0 = \arg\min_{g} E[(t_1 - z_1^\top g)^2]$. Then the thresholded orthogonal ML estimator $\hat{y}_{OM}$ of (8) with $\tau = \frac{1}{4}\sigma_n^2$ satisfies

$$E[(\hat{y}_{OM} - x_i^\top \beta)^2] \leq \|x_i\|_2^2 \left[ O\left(\frac{\sigma^2}{\sigma_n^2}\right) + O\left(\frac{\sigma^2}{\sigma_n^2}\right) + O\left(\frac{\sigma^2}{\sigma_n^2}\right) \right]$$

where $r_{\beta,2} = (E[\|\hat{\beta} - \beta_0\|_2^2])^{1/2}$ and $r_{\eta,2} = (E[\|\hat{\eta}(z_n) - g_0(z_n)^2\|])^{1/2}$. In the setting of Theorem 4, suppose $\hat{\beta}$ and $\hat{g}(z_i) = \hat{g}^\top z_i$ are fit with the ridge estimator with regularization parameters $\lambda_\beta$ and $\lambda_g$ respectively. Then there exist universal constants $c_1, c_2, c_3, c_4, c_5$ such that if $p \geq 20$, $c_1 \frac{n^2 C_{\max} e^{-nc_2/\kappa^4 C_{\max}}}{p C_{\max}} \leq \lambda_\beta \leq c_3 \left(C_{\max} e^{-nc_2/\kappa^4 C_{\max}}\right)^{1/3}$, and $c_4 \frac{n^2 C_{\max} e^{-nc_2/\kappa^4 C_{\max}}}{p C_{\max}} \leq \lambda_g \leq c_5 \frac{n^2 C_{\max} e^{-nc_2/\kappa^4 C_{\max}}}{p C_{\max}}$ for $n \geq c_6 \kappa^4 C_{\max} p$

$$E[(\hat{y}_{OM} - x_i^\top \beta_0)^2] \leq \|x_i\|_2^2 \left[ O\left(\frac{\sigma^2}{\sigma_n^2}\right) + O\left(\frac{\sigma^2}{\sigma_n^2}\right) + O\left(\frac{\sigma^2}{\sigma_n^2}\right) \right]$$

where the $O(\cdot)$ masks constants depending only on $C_{\min}, C_{\max}, C_{\cond}, \kappa$.

Similarly, when $\beta_0$ and $g_0$ are estimated using the Lasso we conclude the following (proved in Appendix E.2).

**Corollary 5 (OM Lasso).** In the setting of Theorem 4, suppose $\hat{\beta}$ and $\hat{g}(z_i) = \hat{g}^\top z_i$ are fit with the Lasso with regularization parameters $\lambda_\beta \geq 80\sigma_\epsilon \sqrt{\log(2ep/\sigma_\epsilon^2)}/n$ and $\lambda_g \geq 80\sigma_\eta \sqrt{\log(2ep/\sigma_\eta^2)}/n$ respectively. If $p \geq 20$, $s_{\beta_0} = \|\beta_0\|_0$, and $s_{g_0} = \|g_0\|_0$, then there exist universal constants $c_1, c_2$ such that if $\|\beta_0\|_\infty / \sigma_\epsilon = o(\epsilon^{-1})$, then for $n \geq \frac{c_3 \kappa^4}{C_{\min}} \max\{s_{\beta_0}, s_{g_0}\} \log(2ep)$,

$$E[(\hat{y}_{OM} - x_i^\top \beta_0)^2] \leq \|x_i\|_2^2 \left[ O\left(\frac{\sigma^2}{\sigma_n^2}\right) + O\left(\frac{\sigma^2}{\sigma_n^2}\right) + O\left(\frac{\sigma^2}{\sigma_n^2}\right) \right]$$

where the $O(\cdot)$ masks constants depending only on $C_{\min}, C_{\max}, C_{\cond}, \kappa$.

We make several comments regarding the aforementioned results.

---

3This assumption is not essential to our result and could be replaced by assuming $\eta_i$ satisfies $E[\eta_i | z_i] = 0$ and is almost surely (w.r.t. to $z_i$) sub-Gaussian with a uniformly (w.r.t. to $z_i$) bounded variance parameter.
Theorem 4 possesses a double-robustness property. In order for the dominant bias term $O(r^2g^2_{\hat{g},2})$ to be small, it is sufficient for either $\beta_0$ or $g_0$ to be estimated at a fast rate or both to be estimated at a slow rate. As before, the estimator is transductive and adapted to predicting along the direction $x_\star$.

In the case of ridge regression, to match the lower bound of Corollary 1, consider the setting where $n = \Omega(p^2)$, $\text{SNR} = o\left(\frac{\epsilon^2}{n}\right)$, $\cos(x_j, \beta_0)^2 = \Theta(1)$ and $\text{SNR} \geq \frac{\epsilon}{n}$. Then, the upper bound can be simplified to $O(\|x_\star\|_2^2 \frac{\epsilon^2}{p n})$. By contrast, Corollary 1 shows the error of the optimally-tuned ridge estimator is lower bounded by $\omega(\|x_\star\|_2^2 \frac{\epsilon^2}{p n})$; for example, the error is $\Omega(p\|x_\star\|_2^2 \frac{\epsilon^2}{p n})$ when $\text{SNR} = \frac{1}{6} \frac{\epsilon^2}{n}$. Hence, the performance of the ridge estimator can be significantly worse than its debiased counterpart.

If we consider the setting of Corollary 5 where $n \gtrsim s_{\beta_0}s_{g_0}(\log p)^2$ while we take $\lambda_\beta \asymp \sigma_\epsilon \sqrt{\log p/n}$ and $\lambda_g \asymp \sigma_n \sqrt{\log p/n}$, the error of the OML estimator attains the fast, dimension-free $O(\|x_\star\|_2^2 \frac{\epsilon^2}{n})$ rate. On the other hand, Corollary 2 shows the Lasso suffers prediction error $\Omega(\|x_\star\|_2^2 \frac{\epsilon^2}{n} \log p)$. Although Theorem 4 makes stronger assumptions on the design of $X$ than the JM-style estimator introduced in (3) and (4), one of the primary benefits of the OM framework is its flexibility. All that is required for the algorithm are "black-box" estimates of $g_0$ and $\beta_0$ which can be obtained from more general ML procedures than the Lasso.

4 Experiments

We complement our theoretical analysis with a series of numerical experiments highlighting the failure modes of standard inductive prediction. In Section 4.1, we demonstrate that the theoretically-calibrated Lasso can be excessively biased even when a test point $x_\star$ is drawn from the training distribution and compare the performance of our debiased estimators in this synthetic data setting. In Section 4.2, we highlight the significant benefits of debiasing under distribution shift, i.e., when the test point does not reflect the training distribution. In our synthetic data experiments, we find that debiasing improves both ridge and Lasso estimators, not just when parameters are set to their theoretically motivated values but also when they are tuned to minimize cross-validation error. Finally, in Section 4.3 we demonstrate that debiasing consistently improves over cross-validated lasso, ridge, and elastic net prediction on five real-world prediction tasks.

On synthetic data we report the root mean square reducible error (RMSRE) $\sqrt{\frac{1}{n_{\text{test}}} \|\hat{y}_{\text{test}} - \hat{X}_{\text{test}}\beta_0\|_2^2}$ on the test set. For real datasets we report the root mean squared error (RMSE) $\sqrt{\frac{1}{n_{\text{test}}} \|\hat{y}_{\text{test}} - \hat{y}_{\text{test}}\|_2^2}$ on the test set. Throughout, we set $\tau = 0$ in the OM methods, as all denominators were stable. We refer the reader to Appendix G for further details on our experimental set-up. Python code to reproduce our experiments can be found at https://github.com/nileshstrip/DebLinPredCode.

4.1 Excess Lasso Bias without Distribution Shift

We construct problem instances for Lasso estimation by independently generating $x_i \sim \mathcal{N}(0, \Sigma)$, $\epsilon_i \sim \mathcal{N}(0, 1)$, and $(\beta_0)_j \sim \mathcal{N}(0, 1)$ for $j$ less than the desired sparsity level $s_{\beta_0}$ while $(\beta_0)_j = 0$ otherwise. We fit the Lasso estimator, JM-style estimator with Lasso pilot, and the OM f-moment estimator with Lasso first-stage estimators. We set all hyperparameters to theoretically-motivated values: $\lambda_\beta = \lambda_g = 4 \sqrt{\log p/n}$ for the Lasso regressions, and, inspired by the feasibility heuristic of [17], we set $\lambda_\omega$ to the smallest value between $\sqrt{\log p/n}$ and $.01 \sqrt{\log p/n}$ for which the JM-style program (3) was feasible. The RMSRE in each experiment was computed over 500 test datapoints (i.e., 500 independent $x_\star$’s) generated from the training distribution; each experiment was repeated 20 times, and the average RMSRE is reported.

---

4Note that in this regime, $\sqrt{\text{SNR}} = \|\beta_0\|_2/\sigma_\epsilon = o(1)$ and hence the condition $\|\beta_0\|_\infty/\sigma_\epsilon = O(1)$ in Corollary 4 is satisfied.
Figure 1: Lasso vs. debiased Lasso prediction without distribution shift. Hyperparameters are set according to theory (see Section 4.1). Left: $p = 200, s_{\beta_0} = 20$. Right: $p = 200, s_{\beta_0} = 100$. Error bars represent ±1 standard error of the mean computed over 20 different problem instances.

As Figure 1 demonstrates, both debiasing methods significantly reduce the prediction risk of the Lasso estimator when the hyperparameters are calibrated to their theoretical values, even for a dense $\beta_0$ (where $s_{\beta_0} = 2$).

4.2 Benefits of Debiasing under Distribution Shift

The no distribution shift simulations of Section 4.1 corroborate the theoretical results of Corollaries 3 and 5. However, since our debiased estimators are tailored to each individual test point $x_*$, we expect these methods to provide an even greater gain when the test distribution deviates from the training distribution.

In Figure 2, we consider two cases where the test distribution is either mean-shifted or covariance-shifted from the training distribution and evaluate the ridge estimator with the optimal regularization parameter for the training distribution, $\lambda_* = \frac{p\sigma_x^2}{|\beta_0|^2}$. We independently generated $x_i \sim \mathcal{N}(0, I_p)$, $\epsilon_i \sim \mathcal{N}(0, 1)$, and $\beta_0 \sim \mathcal{N}(0, \frac{1}{\sqrt{p}} I_p)$. In the case with a mean-shifted test distribution, we generated $x_* \sim \mathcal{N}(10\beta_0, I_p)$ for each problem instance while the covariance-shifted test distribution was generated by taking $x_* \sim \mathcal{N}(0, 100\beta_0\beta_0^\top)$. The first and second plots in Figure 2 show the OM estimator with $\lambda_*$-ridge pilot provides significant gains over the baseline $\lambda_*$-ridge estimator.

In Figure 3 we also consider two cases where the test distribution is shifted for Lasso estimation but otherwise identical to the previous set-up in Section 4.1. For covariance shifting, we generated $(x_*^i)_{i \in \text{supp}(\beta_0)} \sim \mathcal{N}(0, 100)$ for $i \in \text{supp}(\beta_0)$ and $(x_*^i)_i = 0$ otherwise for each problem instance. For mean shifting, we generated $x_* \sim \mathcal{N}(10\beta_0, I_p)$ for each problem instance. The first and second plots in Figure 3 show the debiasing effect of the OM and JM estimators improves prediction risk with respect to the Lasso when the regularization hyperparameters are selected via theory.

In practice, the regularization strength $\lambda$ is often set in a data-dependent manner to minimize an estimate of the prediction error, like cross-validation (CV) error. To assess the value of our proposed procedures in this practical setting, we also compared CV-tuned ridge or Lasso to OM and JM with
As the third and fourth in Figure 2 show, selecting \( \lambda \) via CV leads to over-regularization of the ridge estimator, and the debiased methods provide substantial gains over the base ridge estimator. We also highlight that CV ridge performs similarly to \( \lambda_* \)-ridge, which is to be expected as CV approximates the training distribution out-of-sample prediction error (see Corollary 1).

In the case of the Lasso, the third and fourth plots in Figure 3 show the residual bias of the CV Lasso also causes it to incur significant error in its test predictions, while the debiased methods provide substantial gains by adapting to each \( \mathbf{x}_* \).

### 4.3 Debiasing Cross-validated Prediction

Motivated by our findings on synthetic data, we conclude by reporting the performance of our methods on real data with and without distribution shift. We use both the ridge and Lasso estimators as base regression procedures, in addition to the popular elastic net estimator (which uses a combination of \( \ell_1 \) and \( \ell_2 \)-squared penalties). Five-fold CV was used to select hyperparameters for the Lasso and elastic net estimators, while leave-one-out CV was used for ridge regression.

For the OM estimators we exploited the flexibility of the framework by including a suite of methods for the auxiliary \( \mathbf{g} \) regressions: Lasso estimation, random forest regression, and a \( \mathbf{g} = 0 \) baseline. Amongst these, we select the method with the least estimated asymptotic variance, which can be done in a data-dependent way without introducing any extra hyperparameters into the implementation; see Appendix G for further details on the methodology and datasets. In our experiments we used 4 regression datasets with distributional shift – the Fertility dataset (\( n_{\text{train}} = 69, n_{\text{test}} = 31, p = 8 \)), the Forest Fires dataset (\( n_{\text{train}} = 320, n_{\text{test}} = 197, p = 10 \)), the Parkinson dataset (\( n_{\text{train}} = 1877, n_{\text{test}} = 3998, p = 17 \)), and the Wine dataset (\( n_{\text{train}} = 4898, n_{\text{test}} = 1599, p = 11 \)). We also included a higher-dimensional dataset without explicit distribution shift – the Triazines dataset (\( n_{\text{train}} = 139, n_{\text{test}} = 47, p = 60 \)). All datasets were acquired from the UCI dataset repository [14].

The \( \mathbf{f} \) and \( \mathbf{q} \) regressions were always fit with linear Lasso/ridge/elastic net estimation. In Table 1 we can see the orthogonal moment estimators generically provide gains over the CV Lasso, CV ridge regression, and CV elastic net on datasets with intrinsic distribution shift and perform comparably on a dataset without explicit distribution shift. On the Wine dataset, we see a substantial performance gain from 0.96-0.99 RMSE without debiasing to 0.77 RMSE with OM \( q \) debiasing. The gains on other datasets are smaller but still notable as they represent consistent improvements over the de facto standard of cross-validated prediction. Typically the OM methods also outperform the JM-style estimator.

Since much of our focus has been on improving prediction with debiasing, we also report the performance of ordinary least squares (OLS) which produces an unbiased estimate of the entire parameter vector \( \mathbf{\beta}_0 \). OLS fares worse than most methods on each dataset due to a increase in variance. In contrast, our proposed procedures limit the variance introduced by focusing on debiasing a single parameter of interest, \( (\mathbf{x}_*, \mathbf{\beta}_0) \); this leads to a consistent reduction of RMSE for our OM procedures across the five datasets.

### Table 1: Model Performance

| Dataset       | OLS (RMSE) | OM (\( q = \text{Theory} \)) (RMSE) | OM (\( q = \text{CV} \)) (RMSE) |
|---------------|------------|--------------------------------------|----------------------------------|
| Fertility     | 1.06       | 0.66                                 | 0.52                             |
| Forest Fires  | 1.23       | 0.88                                 | 0.70                             |
| Parkinson     | 1.34       | 0.98                                 | 0.79                             |
| Triazines     | 0.96       | 0.62                                 | 0.49                             |
| Wine          | 1.12       | 0.74                                 | 0.57                             |

Figure 3: Lasso vs. debiased Lasso prediction (\( p = 200 \)) under mean (\( s_{\beta_0} = 100 \)) or covariance (\( s_{\beta_0} = 200 \)) train-test distribution shifts. Hyperparameters are set according to theory (1st and 2nd plots) or via CV (3rd and 4th plots). Error bars represent ±1 standard error of the mean computed over 20 different problem instances. See Section 4.2 for more details.
Table 1: Test set RMSE of OLS, CV-tuned ridge, Lasso, and elastic net, and debiased CV-tuned ridge, Lasso, and elastic net on five real-world datasets. All hyperparameters are set via CV. Error bars represent ±1 standard error of the mean computed over the test set.

| Method | Fertility | Fire | Parkinson | Wine | Triazines (no shift) |
|--------|-----------|------|-----------|------|----------------------|
| OLS    | 0.3988±0.0657 | 82.7147±35.5141 | 12.7916±0.1486 | 1.0118±0.0156 | 0.1716±0.0367 |
| Ridge  | 0.399±0.0665   | 82.3462±35.5955 | 12.5267±0.1448 | 0.9936±0.0155 | 0.1469±0.0285 |
| OM f (Ridge) | 0.3977±0.0653 | 81.9794±35.7872 | 12.0891±0.1366 | 0.7696±0.0145 | 0.1507±0.0242 |
| OM q (Ridge) | 0.3987±0.0665 | 82.3522±35.5519 | 12.4686±0.1439 | 0.9883±0.0154 | 0.1446±0.0296 |
| Lasso  | 0.4092±0.0716   | 82.0656±36.0321 | 12.2535±0.1356 | 0.9812±0.0155 | 0.1482±0.0237 |
| JM (Lasso) | 0.3988±0.0657 | 82.7147±35.5141 | 12.7916±0.1486 | 1.0118±0.0156 | 0.173±0.0367 |
| OM f (Lasso) | 0.3976±0.0657 | 81.794±35.6599 | 11.869±0.1339 | 0.9473±0.0152 | 0.1444±0.0239 |
| OM q (Lasso) | 0.3976±0.0657 | 81.794±35.6599 | 11.869±0.1339 | 0.7691±0.0144 | 0.147±0.0226 |
| Elastic | 0.4092±0.0716   | 81.8428±35.8333 | 12.2535±0.1356 | 0.9652±0.0154 | 0.1495±0.0238 |
| OM f (Elastic) | 0.398±0.0665 | 81.7719±35.6166 | 11.8369±0.1338 | 0.9507±0.0152 | 0.1445±0.0246 |
| OM q (Elastic) | 0.3976±0.0657 | 81.803±35.6048 | 11.8658±0.1341 | 0.769±0.0145 | 0.147±0.0228 |

5 Discussion and Future Work

We have highlighted the detrimental effects of bias in linear prediction and presented two transductive, debiased estimators that ameliorate this bias. We provided theoretical guarantees for these estimators and demonstrated their practical utility—especially under distribution shift—on both synthetic and real data. Promising directions for future work include improving the quality of our OM debiasing techniques using higher-order orthogonal moments [18] and exploring the utility of these debiasing techniques for other regularizers (e.g., group Lasso [26] penalties) and alternative models such as generalized linear models and kernel machines.

References

[1] Pierre Alquier and Mohamed Hebiri. Transductive versions of the lasso and the dantzig selector. *Journal of Statistical Planning and Inference*, 142(9):2485–2500, 2012.

[2] Susan Athey, Guido W Imbens, and Stefan Wager. Approximate residual balancing: debiased inference of average treatment effects in high dimensions. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 80(4):597–623, 2018.

[3] Pierre C Bellec and Cun-Hui Zhang. De-biasing the lasso with degrees-of-freedom adjustment. *arXiv preprint arXiv:1902.08885*, 2019.

[4] Pierre C Bellec, Guillaume Lecué, and Alexandre B Tsybakov. Slope meets lasso: improved oracle bounds and optimality. *arXiv preprint arXiv:1605.08651*, 2016.

[5] Pierre C Bellec, Arnak S Dalalyan, Edwin Grappin, Quentin Paris, et al. On the prediction loss of the lasso in the partially labeled setting. *Electronic Journal of Statistics*, 12(2):3443–3472, 2018.

[6] Peter J Bickel, Ya’acov Ritov, Alexandre B Tsybakov, et al. Simultaneous analysis of lasso and dantzig selector. *The Annals of Statistics*, 37(4):1705–1732, 2009.

[7] Adrian N. Bishop, Pierre Del Moral, and Angélique Niclas. An introduction to wishart matrix moments. *Foundations and Trends® in Machine Learning*, 11(2):97–218, 2018. ISSN 1935-8237. doi: 10.1561/2200000072. URL http://dx.doi.org/10.1561/2200000072.

[8] T Tony Cai, Zijian Guo, et al. Confidence intervals for high-dimensional linear regression: Minimax rates and adaptivity. *The Annals of statistics*, 45(2):615–646, 2017.

[9] Shih-Kang Chao, Yang Ning, and Han Liu. On high dimensional post-regularization prediction intervals, 2014.

[10] Xiangli Chen, Mathew Monfort, Anqi Liu, and Brian D Ziebart. Robust covariate shift regression. In *Artificial Intelligence and Statistics*, pages 1270–1279, 2016.
[11] Victor Chernozhukov, Denis Chetverikov, Mert Demirer, Esther Duflo, Christian Hansen, Whitney Newey, James Robins, et al. Double/debiased machine learning for treatment and causal parameters. Technical report, 2017.

[12] Steven Diamond and Stephen Boyd. CVXPY: A Python-embedded modeling language for convex optimization. *Journal of Machine Learning Research*, 17(83):1–5, 2016.

[13] Edgar Dobriban, Stefan Wager, et al. High-dimensional asymptotics of prediction: Ridge regression and classification. *The Annals of Statistics*, 46(1):247–279, 2018.

[14] Dheeru Dua and Casey Graff. UCI machine learning repository, 2017. URL http://archive.ics.uci.edu/ml.

[15] Arthur E. Hoerl and Robert W. Kennard. Ridge regression: Biased estimation for nonorthogonal problems. *Technometrics*, 12(1):55–67, 1970.

[16] Daniel Hsu, Sham M. Kakade, and Tong Zhang. Random design analysis of ridge regression. In *Conference on learning theory*, pages 9–1, 2012.

[17] Adel Javanmard and Andrea Montanari. Confidence intervals and hypothesis testing for high-dimensional regression. *The Journal of Machine Learning Research*, 15(1):2869–2909, 2014.

[18] Lester Mackey, Vasilis Syrgkanis, and Ilias Zadik. Orthogonal machine learning: Power and limitations. *arXiv preprint arXiv:1711.00342*, 2017.

[19] Philipp Moritz, Robert Nishihara, Stephanie Wang, Alexey Tumanov, Richard Liaw, Eric Liang, Melih Elibol, Zongheng Yang, William Paul, Michael I Jordan, et al. Ray: A distributed framework for emerging {AI} applications. In *13th {USENIX} Symposium on Operating Systems Design and Implementation ({OSDI} 18)*, pages 561–577, 2018.

[20] Garvesh Raskutti, Martin J Wainwright, and Bin Yu. Minimax rates of estimation for high-dimensional linear regression over $\ell_q$-balls. *IEEE transactions on information theory*, 57(10): 6976–6994, 2011.

[21] Robert Tibshirani. Regression shrinkage and selection via the lasso. *Journal of the Royal Statistical Society: Series B (Methodological)*, 58(1):267–288, 1996.

[22] Sara van de Geer. Statistical theory for high-dimensional models. *arXiv preprint arXiv:1409.8557*, 2014.

[23] Sara Van de Geer, Peter Bühlmann, Ya’acov Ritov, Ruben Dezeure, et al. On asymptotically optimal confidence regions and tests for high-dimensional models. *The Annals of Statistics*, 42(3):1166–1202, 2014.

[24] Stefan Wager, Wenfei Du, Jonathan Taylor, and Robert J Tibshirani. High-dimensional regression adjustments in randomized experiments. *Proceedings of the National Academy of Sciences*, 113(45):12673–12678, 2016.

[25] Martin J Wainwright. High-dimensional statistics: A non-asymptotic viewpoint.

[26] Ming Yuan and Yi Lin. Model selection and estimation in regression with grouped variables. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 68(1):49–67, 2006.

[27] Cun-Hui Zhang and Stephanie S Zhang. Confidence intervals for low dimensional parameters in high dimensional linear models. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 76(1):217–242, 2014.

[28] Xiaojin Jerry Zhu. Semi-supervised learning literature survey. Technical report, University of Wisconsin-Madison Department of Computer Sciences, 2005.

[29] Yinchu Zhu and Jelena Bradic. Linear hypothesis testing in dense high-dimensional linear models. *Journal of the American Statistical Association*, 113(524):1583–1600, 2018.

[30] Hui Zou and Trevor Hastie. Regularization and variable selection via the elastic net. *Journal of the royal statistical society: series B (statistical methodology)*, 67(2):301–320, 2005.
A Notation

We first establish several useful pieces of notation used throughout the Appendices. We will say that a mean-zero random variable \( x \) is sub-gaussian, \( x \sim sG(\kappa) \), if \( \mathbb{E}[\exp(\lambda x)] \leq \exp \left( \frac{\kappa^2 \lambda^2}{2} \right) \) for all \( \lambda \). We will say that a mean-zero random variable \( x \) is sub-exponential, \( x \sim sE(\nu, \alpha) \), if \( \mathbb{E}[\exp(\lambda x)] \leq \exp \left( \frac{\nu^2 \lambda^2}{2} \right) \) for all \( |\lambda| \leq \frac{1}{\alpha} \). We will say that a mean-zero random vector is sub-gaussian, \( \mathbf{x} \sim sG(\kappa) \), if \( \forall \mathbf{v} \in \mathbb{R}^p, \mathbb{E}[\exp(\mathbf{v}^\top \mathbf{x})] \leq \exp \left( \frac{\kappa^2 \|\mathbf{v}\|_2^2}{2} \right) \). Moreover a standard Chernoff argument shows if \( x \sim sE(\nu, \alpha) \) then \( \Pr[|x| \geq t] \leq 2 \exp \left( -\frac{1}{2} \min(\frac{t^2}{\nu^2}, \frac{t}{\alpha}) \right) \).

B Proofs for Section 2.1: Lower Bounds for Prediction with Ridge Regression

Here we provide lower bounds on the prediction risk of the ridge regression estimator. To do so, we show that under Gaussian design and independent Gaussian noise \( \epsilon \) the ridge regression estimator can perform poorly.

Recall we define the ridge estimator as \( \hat{\beta}_R(\lambda) = \arg \min_\beta \frac{1}{2} \left( \| \mathbf{y} - \mathbf{X} \beta \|_2^2 + \lambda \| \beta \|_2^2 \right) \) which implies \( \hat{\beta}_R(\lambda) = (\mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}_p)^{-1} \mathbf{X}^\top \mathbf{y} \). For convenience we further define \( \hat{\Sigma} = \mathbf{X}^\top \mathbf{X} / n, \hat{\Sigma}_\lambda = \mathbf{X}^\top \mathbf{X} / n + \frac{\lambda}{n} \mathbf{I}_p \) and \( \Pi_\lambda = \mathbf{I}_p - (\hat{\Sigma}_\lambda)^{-1} \hat{\Sigma} \). Note that under Assumption 1, \( \hat{\beta}_R(\lambda) - \beta_0 = -\Pi_\lambda \beta_0 + \frac{1}{\lambda/n} \mathbf{X}^\top \epsilon / n, \) which can be thought of as a standard bias-variance decomposition for the ridge estimator. We begin by stating a standard fact about Wishart matrices we will repeatedly use throughout this section.

**Proposition 5.** Let \( \mathbf{x}_i \overset{i.i.d.}{\sim} \mathcal{N}(0, \mathbf{I}_p) \) for \( i \in [n] \). Then the eigendecomposition of the sample covariance \( \hat{\Sigma}_n = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^\top = \mathbf{V}^\top \mathbf{D} \mathbf{V} \) satisfies the following properties:

- The orthonormal matrix \( \mathbf{V} \) is uniformly distributed (with respect to the Haar measure) over the orthogonal group \( O(p) \).
- The matrices \( \mathbf{V} \) and \( \mathbf{D} \) are independent. Moreover, by isotropy, \( \mathbf{D} \) is equivalent in distribution to the random matrix \( \frac{1}{\sqrt{\lambda/n}} \mathbf{z} \mathbf{I}_p \) where \( \mathbf{z} \) is an unordered eigenvalue of \( \hat{\Sigma}_n \).

**Proof.** Statements and proofs of these standard facts about Wishart matrices can be found in Bishop et al. [7].

### B.1 Theorem 1

We now provide the proof of our primary lower bound on the prediction risk of the ridge estimator.

**Proof of Theorem 1.** The first statement follows by using Lemma 1 and taking the expectation over \( \mathbf{X} \),

\[
\mathbb{E}[\langle \mathbf{x}_s, (\hat{\beta}_R(\lambda) - \beta_0) \rangle^2] = \mathbb{E}[\langle \mathbf{x}_s^\top \Pi_\lambda \beta_0 \rangle^2] + \frac{\sigma_x^2}{n} \mathbf{x}_s^\top \mathbb{E}[\langle (\hat{\Sigma}_\lambda)^{-1} \hat{\Sigma}(\hat{\Sigma}_\lambda)^{-1} \rangle] \mathbf{x}_s = \mathbb{E}[\langle \mathbf{x}_s^\top \Pi_\lambda \beta_0 \rangle^2] + \sigma_x^2 \frac{\|\mathbf{x}_s\|_2^2}{n} \mathbb{E}[\frac{\mathbf{z}}{\lambda/n}]^2
\]

The computation of the variance term uses the eigendecomposition of \( \Sigma \) and Proposition 5,

\[
\mathbb{E}[\langle (\hat{\Sigma}_\lambda)^{-1} \hat{\Sigma}(\hat{\Sigma}_\lambda)^{-1} \rangle] = \mathbb{E}[\mathbf{V}^\top \mathbb{E}[\langle \mathbf{D} + \lambda/n \mathbf{I}_p \rangle^{-2} \mathbf{D}] \mathbf{V}] = \mathbb{E}[\frac{\mathbf{z}}{(\lambda/n)^2}]^2 \mathbf{I}_p.
\]

We now lower bound the bias. Again by Proposition 5 and the eigendecomposition of \( \hat{\Sigma}_n \), \( \mathbb{E}[\hat{\Pi}_\lambda] = \mathbb{E}[\frac{\lambda/n}{\lambda/n}] \mathbf{I}_p \). Using Jensen’s inequality,

\[
\mathbb{E}[\langle (\beta_0^\top \Pi_\lambda \mathbf{x}_s)^2 \rangle] \geq \langle (\beta_0^\top \mathbb{E}[\Pi_\lambda] \mathbf{x}_s)^2 \rangle = \|\mathbf{x}_s\|_2^2 \|\beta_0\|_2^2 \cos(\langle \mathbf{x}_s, \beta_0 \rangle)^2 \mathbb{E}[\frac{\lambda/n}{\lambda/n}]^2.
\]

The final expectation over the unordered eigenvalue distribution can be controlled using the sharp concentration of Gaussian random matrices. Namely for \( n \geq p, \|\hat{\Sigma}_n - \Sigma\|_2 \leq 2\epsilon + \epsilon^2 \) for
\[ \epsilon = \sqrt{\frac{\epsilon}{n}} + \delta \] with probability at least \( 1 - 2e^{-n\delta^2/2} \) [25, Theorem 6.1, Example 6.2]. Taking \( \delta = 1/2\sqrt{p/n} \) and assuming that \( p \geq 20 \) we conclude that \( \| \tilde{\Sigma} - \Sigma \|_2 \leq 6\sqrt{\epsilon} \) with probability at least \( \frac{1}{2} \) - let \( \mathcal{E} \) denote this event. Note that by the Weyl inequalities, on the event \( \mathcal{E} \), all of the eigenvalues of \( \tilde{\Sigma} \) are uniformly close to the eigenvalues of \( \Sigma \). Hence if \( n \geq p \), on \( \mathcal{E} \) we must have that \( \tilde{\Sigma}_n \leq 7I_p \), and hence the unordered eigenvalue \( z \leq 7 \) as well. Thus it follows that \( \langle \mathbb{E}[1_{\lambda/n + z}] \rangle^2 \geq \langle \mathbb{E}[1_{\lambda/n + 7}]^2 \rangle \geq \langle \mathbb{E}[1_{\lambda/n}]^2 \rangle^2 \geq \frac{1}{4}(\lambda/n)^2 \). Combining the expressions yields the conclusion. \( \square \)

### B.2 Corollary 1

We now prove Corollary 1.

**Proof of Corollary 1.** The expression for \( \lambda_* = \arg\min_\lambda \mathbb{E}[\| \hat{\beta}_R(\lambda) - \beta_0 \|^2] \) can be computed using Lemma 2. Since, \( \arg\min_\lambda \mathbb{E}[\| \hat{\beta}_R(\lambda) - \beta_0 \|^2] = \mathbb{E}[\| \hat{\beta}_R(\lambda) - \beta_0 \|^2] + \sigma^2 \), equality of the minimizers follows for both expressions.

Define \( SNR = \frac{\| \beta_0 \|^2}{\sigma^2} \) and \( a = \sqrt{\frac{4C}{SNR}} \). If, in addition, \( n \geq a^2 \) and \( \lambda \geq \frac{7an}{\sqrt{n-a}} \), we claim,

\[
\mathbb{E}[\langle x_* , \hat{\beta}_R(\lambda) - \beta_0 \rangle^2] \geq C \cos(x_* , \beta_0)^2 \cdot \| x_* \|^2 \cdot \frac{\sigma^2}{a^2}.
\]

This lower bound follows by simply rearranging the lower bound from Theorem 1 – some algebraic manipulation gives the conditions that \( \lambda/n \geq a/\sqrt{n} \) \( \implies \lambda \geq a/\sqrt{n} \implies \lambda(1 - a/\sqrt{n}) \geq 7a\sqrt{n} \implies \lambda \geq \frac{7a\sqrt{n}}{1/\sqrt{n} - a} \).

After defining \( \lambda_* = \frac{p}{SNR} = b \) the previous inequality over \( \lambda_* \) to achieve the desired conclusion can be rearranged to \( b(\sqrt{n} - a) \geq 7an \implies n - b\sqrt{n} + b \leq n - \frac{b}{a}\sqrt{n} + b \leq 0 \). The corresponding quadratic equation in \( \sqrt{n} \) has roots \( r_+ = \frac{1}{14} \left( \frac{b}{a} + \frac{\sqrt{b^2 - 28a^2b}}{a} \right) \), \( r_- = \frac{1}{14} \left( \frac{b}{a} - \frac{\sqrt{b^2 - 28a^2b}}{a} \right) \). In order to ensure both roots are real we must have \( b \geq 28a^2 \implies p \geq 120C \). The condition that \( r_- \leq \sqrt{n} \leq r_+ \) can be equivalently expressed as,

\[
\left| \sqrt{n} - \frac{b}{14a} \right| \leq \frac{\sqrt{b^2 - 28a^2b}}{a} \iff \left| \sqrt{n} - \frac{1}{14} \frac{p}{\sqrt{4C}} \right| \leq \frac{p^2}{4C} - 28 \frac{p}{\sqrt{4CNR}}.
\]

Defining \( C \) such that \( \sqrt{n} - \frac{p}{14\sqrt{4C}} = 0 \implies C = \frac{p^2}{784a^{1.4}N} \). The remaining condition simplifies as, \( \sqrt{\frac{p^2}{4C} - 28 \frac{p}{\sqrt{4CNR}}} \geq 0 \implies 196n - 28 \frac{p}{\sqrt{4CNR}} \geq 0 \implies n \geq \frac{1}{7} \frac{p}{SNR} \). The condition \( p \geq 120C \implies n \geq \frac{1}{6} \frac{p}{SNR} \). Accordingly, under these conditions,

\[
\mathbb{E}[\langle x_* , \hat{\beta}_R(\lambda) - \beta_0 \rangle^2] \geq \frac{\cos(x_* , \beta_0)^2}{784} \| x_* \|^2 \cdot \frac{\sigma^2}{n}.
\]

\( \square \)

We first compute the (conditional on \( X \)) prediction risk of this estimator alongst \( x_* \) as,

**Lemma 1.** Let the independent noise distribution be Gaussian, \( \epsilon \sim \mathcal{N}(0, I, \sigma^2) \), and Assumption 1 hold. Then,

\[
\mathbb{E}[\langle x_* , \hat{\beta}_R(\lambda) - \beta_0 \rangle^2 | X] = (x_*^\top \Pi_\lambda \beta_0)^2 + \sigma^2 x_*^\top (\Sigma_\lambda)^{-1} \Sigma (\Sigma_\lambda)^{-1} x_* / n.
\]

**Proof.** Using the standard bias-variance decomposition \( \hat{\beta}_R(\lambda) - \beta_0 = -\Pi_\lambda \beta_0 + \Sigma_\lambda^{-1} X^\top \epsilon / n \), squaring and taking the expectation over \( \epsilon \) (which is mean-zero) gives the result. \( \square \)

We now calculate the optimal choice of the ridge parameter \( \lambda \) to minimize the parameter error in the \( \ell_2 \) distance.
Lemma 2. Under Assumption 1, let \( x_i \sim N(0, I_p) \) with independent noise \( \epsilon \sim N(0, I_n \sigma^2) \). Then,
\[
\mathbb{E} \left[ \left\| \hat{\beta}_R(\lambda) - \beta_0 \right\|^2 \right] = \| \beta_0 \|^2 \mathbb{E} \left[ \frac{\lambda}{\lambda + n \sigma^2} \right] + \frac{\sigma^2_p}{n} \mathbb{E} \left[ \frac{\lambda}{\lambda + n \sigma^2} \right]
\]
and the optimal \( \lambda_\star = \arg \min \lambda \mathbb{E} \left[ \left\| \hat{\beta}_R(\lambda) - \beta_0 \right\|^2 \right] \) is \( \lambda_\star = \frac{\sigma^2}{\| \beta_0 \|^2} \).

Proof. We first compute the (expected) mean-squared error. Using Lemma 1, summing over \( x_\star = e_i \), and taking a further expectation over \( X \) we have that,
\[
\mathbb{E} \left[ \left\| \hat{\beta}_R(\lambda) - \beta_0 \right\|^2 \right] = \mathbb{E} \left[ \sum_{i=1}^p (e_i^\top \Pi_\lambda \beta_0)^2 \right] + \frac{\sigma^2_p}{n} \mathbb{E} \left[ \sum_{i=1}^p e_i^\top (\Sigma_\lambda)^{-1} \Sigma (\Sigma_\lambda)^{-1} e_i \right]
\]

The computation of both the bias and variance terms exploits Proposition 5 along with the eigendecomposition of \( \Sigma_n \). For the bias term,
\[
\mathbb{E} \left[ \sum_{i=1}^p (e_i^\top \Pi_\lambda \beta_0)^2 \right] = \mathbb{E} [\beta_0^\top \Pi_\lambda^2 \beta_0] = \mathbb{E} [\beta_0^\top V^\top (\mathbb{E}[I_p - 2(D + \lambda I_p)^{-1} D + (D + \lambda I_p)^{-2} D^2]) V \beta_0] = \| \beta_0 \|^2 v
\]
where \( v = \mathbb{E}[\frac{\lambda}{\lambda + n \sigma^2}] \). Similarly for the variance term,
\[
\frac{\sigma^2_p}{n} \mathbb{E} \left[ \sum_{i=1}^p e_i^\top (\Sigma_\lambda)^{-1} \Sigma (\Sigma_\lambda)^{-1} e_i \right] = \frac{\sigma^2_p}{n} \mathbb{E}[\text{Tr} \left( (\Sigma_\lambda)^{-1} \Sigma (\Sigma_\lambda)^{-1} \right)] = \frac{\sigma^2_p}{n} \mathbb{E}[\text{Tr} [\Sigma V \Sigma V^\top \mathbb{E}[I_p] V^\top]] = \frac{\sigma^2_p}{n} \mathbb{E}[w]
\]
where \( E[w] = \mathbb{E}[\frac{\lambda}{\lambda + n \sigma^2}] \). Combining we have that,
\[
\mathbb{E} \left[ \left\| \hat{\beta}_R(\lambda) - \beta_0 \right\|^2 \right] = \| \beta_0 \|^2 \mathbb{E} \left[ \frac{\lambda}{\lambda + n \sigma^2} \right] + \frac{\sigma^2_p}{n} \mathbb{E} \left[ \frac{\lambda}{\lambda + n \sigma^2} \right]
\]
In general this expression is a complicated function of \( \lambda \), however conveniently,
\[
\frac{d}{d\lambda} \mathbb{E} \left[ \left\| \hat{\beta}_R(\lambda) - \beta_0 \right\|^2 \right] = 2\lambda n \| \beta_0 \|^2 \mathbb{E} \left[ \frac{\lambda}{\lambda + n \sigma^2} \right] - 2n^2 \frac{\sigma^2_p}{n} \mathbb{E} \left[ \frac{\lambda}{(\lambda + n \sigma^2)^3} \right] \implies \lambda_\star / p = \frac{\sigma^2}{\| \beta_0 \|^2}.
\]

C Proofs for Section 2.2: Lower Bounds for Prediction with the Lasso

Here we provide the proof of Theorem 2.

Proof of Theorem 2. Let \( v_\star \) denote the maximum \( s \)-sparse eigenvector of \( \mathbb{E}[x_i x_i^\top] \) (which is normalized as have \( \| v \|_2 = \| v \|_1 = 1 \)) and \( \lambda_\star \mathbb{E}[x_i x_i^\top] \) its corresponding eigenvalue. We begin by restricting \( \beta_0 \) to have support on these \( s \) coordinates of \( v_\star \), denoted by \( S \); we subsequently choose the magnitude of the elements \( \beta_0 \). Now under the conditions of the Proposition, we can guarantee support recovery of the Lasso solution, \( S_{\beta_0} \subseteq S_{\beta_0} \equiv S \), with probability at least \( 1/2 \) by Proposition 7. Denote this event by \( S \).

Thus, for this choice of \( \beta_0 \),
\[
\mathbb{E}[\langle x_\star, \hat{\beta}_L(\lambda) - \beta_0 \rangle^2] \geq \mathbb{E}[\langle (x_\star)_S, (\hat{\beta}_L(\lambda) - \beta_0)_S \rangle^2 I[S]] = \mathbb{E}[\langle (x_\star)_S, I[S](\hat{\beta}_L(\lambda) - \beta_0)_S \rangle^2 I[S]]
\]
\[
\langle I[S](\hat{\beta}_L(\lambda) - \beta_0)_S \rangle, \mathbb{E}[x_i x_i^\top] \mathbb{E}[I[S]](\hat{\beta}_L(\lambda) - \beta_0)_S \rangle
\]
using Jensen’s inequality and independence of $x_i$ and $\hat{\beta}_L(\lambda)$ in the inequality.

We now focus on characterizing the bias of the Lasso solution $\hat{\beta}_L(\lambda)$ on the coordinates contained in $S$ (in fact using properties of the debiased Lasso estimator). Consider a single coordinate $i \in S$, and without loss of generality assume that $(x_i)_i > 0$, in which case we choose $(\beta_0)_i > 0$. We will argue that the magnitude of $(\hat{\beta}_L)_i$ can be chosen so that $E[|\hat{\beta}_L(\lambda) - \beta_0|] < c < 0$ for appropriate $c$ under the conditions of the theorem. Note that under our assumptions $\kappa = C_{\text{max}} = C_{\text{min}} = 1$ for the following.

Recall, since $y = X\beta_0 + \epsilon$, from the KKT conditions applied to the Lasso objective we have that,

$$
\frac{1}{n} X^T (X^T \hat{\beta}_L(\lambda) - y) + \lambda v = 0, \quad v \in \partial \left( \|\hat{\beta}_L(\lambda)\|_1 \right) \implies (I - \Sigma_n)(\hat{\beta}_L(\lambda) - \beta_0) + \frac{1}{n} X^T \epsilon - \lambda v = \hat{\beta}_L(\lambda) - \beta_0
$$

We can now use this relation to control the coordinate-wise Lasso bias,

$$
E[I|S](\hat{\beta}_L(\lambda) - \beta_0)_i] = E[(\hat{\beta}_L(\lambda) - \beta_0)_i|S \cap \{(\hat{\beta}_L(\lambda))_i > 0\}] + E[(\hat{\beta}_L(\lambda) - \beta_0)_i|S \cap \{(\hat{\beta}_L(\lambda))_i \leq 0\}] = E[[Z + \Delta - \lambda v)_i|S \cap \{(\hat{\beta}_L(\lambda))_i > 0\}] + E(((\hat{\beta}_L(\lambda) - \beta_0)_i|S \cap \{(\hat{\beta}_L(\lambda))_i \leq 0\}] \leq E[[Z_i] + |\Delta_i|] - \lambda E[I|S \cap \{(\hat{\beta}_L(\lambda))_i > 0\}] - (\beta_0)_i E[I|S \cap \{(\hat{\beta}_L(\lambda))_i \leq 0\}] \leq E[[Z_i] + |\Delta_i|] - \min(\lambda, (\beta_0)_i) \text{Pr}[S].
$$

At this point we fix the magnitude of $(\beta_0)_i = \lambda$ for $i \in S$. We can now bound the expectations of our first two terms. For the first term $Z_i = \frac{1}{n} e_i^T X^T \epsilon$ where $\epsilon \sim N(0, \sigma_2^2 I_n)$ and $v = Xe_i \sim N(0, \sigma_2^2 I_n)$ independently of $\epsilon$. Thus,

$$
E[|Z_i|] = \frac{1}{n} \sqrt{E[(v^T \epsilon)^2]} = \frac{\sigma}{\sqrt{n}}.
$$

For the second term,

$$
E[|\Delta_i|] \leq \sqrt{E[||(\Sigma_n - I)e_i||_2^2]} \sqrt{E[||\hat{\beta}_L - \beta_0||^2_2]}
$$

From the proof of Lemma 4, with $x_i = e_i$ and $\Omega = I$, we have that $Pr[||\Sigma_n - I|| \geq t] \leq 2p \cdot \exp(-\frac{n}{2} \cdot \text{min}(\frac{t}{\sqrt{2}}, \frac{t}{\sqrt{2}}))$ where $\kappa = 8$. Note for $n \geq (a/\kappa')^2 \log p$, $a \sqrt{\frac{\log p}{n}} \leq \kappa'$. Defining $A = ||(\Sigma_n - I)e_i||_\infty$,

$$
E[A^2] = \int_0^\infty 2t \text{Pr}[A > t] \leq \left( \int_0^{\sqrt{\log p}/n} t \cdot 1 + \int_{\sqrt{\log p}/n}^{\kappa'} t \cdot p \cdot t \exp \left( -\frac{n}{2} \left( \frac{t}{\kappa'} \right)^2 \right) + \int_{\kappa'}^{\infty} p \cdot t \exp \left( -\frac{n}{2} \left( \frac{t}{\kappa'} \right)^2 \right) \right)
$$

$$
\leq 4 \left[ \frac{a^2 \log p}{2} + \frac{\kappa'^2 p}{2} - \frac{a^2}{2\kappa'^2} \frac{\log p}{n} + 2\kappa'^2 e^{-n/2} (2 + n)p \cdot n^2 \right] \leq \left( 8\kappa'^2 + \frac{20\kappa'^2}{p \log p \cdot n} \right) \frac{\log p}{n} \leq \kappa'^2 \log p
$$

where the last sequence of inequalities follows by choosing $a = 2\kappa'$, assuming $n \geq \max\{4 \log p, 2\}$, and then assuming $p \geq 20$. Using Lemma 9 and 14 we have that,

$$
E[||\hat{\beta}_L(\lambda) - \beta_0||^2_2] \leq \left( \frac{49\lambda s_{\beta_0}}{4} \right)^2 + \left( \frac{49}{8} (8 + 2\sqrt{2}) \sigma_2 \right)^2 + \left( \frac{a^4}{\lambda^2} + 24^2 s_{\beta_0} \kappa \right) \left( 2e^{-c_2/2n} \right)
$$

using our choice of $(|\beta_0)_i = \lambda$ for each of the $s$ non-zero coordinates in $\beta_0$ (so $||\beta_0||_1 \leq s_{\beta_0}\lambda$). Here $\lambda_*$ is the lower bound on $\lambda$ from the Theorem statement. Under the assumption that $n \geq c_1 s_{\beta_0} \log(2e^p)$ and $p \geq 20$, there exists $c_1$ such that $(\frac{a^4}{\lambda^2} + 24^2 s_{\beta_0} \kappa) \left( 2e^{-c_2/2n} \right) \leq (8 + 2\sqrt{2})^2 \sigma_2^2 / n + 2\lambda^2 s_{\beta_0}^2$. Once again using $p \geq 20$ and that $\lambda \geq \lambda_*$ we have that,

$$
E[||\hat{\beta}_L(\lambda) - \beta_0||^2_1] \leq 300\lambda^2 s_{\beta_0}^2.
$$
Assembling, we conclude that,
\[
\mathbb{E}[\mathbf{I}[S](\hat{\beta}_L(\lambda) - \beta_0)_i] \leq \mathbb{E}[|\mathbf{Z}_i| + |\Delta_i|] - \min(\lambda, (\beta_0)_i) \Pr[|S| \geq \sqrt{\frac{\sigma_v}{n} + 300\lambda s\beta_0} \sqrt{\frac{\log(2ep)}{n}} - \frac{1}{2}\lambda] \leq -\frac{2}{5}\lambda.
\]

The last inequality holds using that \(\lambda_{\beta} \geq \lambda_v\) and \(n \geq c_1s_{\beta_0}^2 \log(2ep)\) for sufficiently large \(c_1\).

This allows us to conclude that \((\mathbf{v}_i^\top \mathbb{E}[\mathbf{I}[S](\hat{\beta}_L(\lambda) - \beta_0)_S])^2 \geq \frac{1}{100} \lambda_{\beta}^2 \mathbf{v}_i^\top \mathbf{v}_i \geq \frac{1}{100} \lambda_{\beta}^2\). Finally if we consider a spectral decomposition of \(\mathbb{E}[\mathbf{x}_i \mathbf{x}_i^\top]_S\) we can conclude that, \(\langle \mathbb{E}[\mathbf{I}[S](\hat{\beta}_L(\lambda) - \beta_0)_S] \rangle \mathbb{E}[\mathbf{x}_i \mathbf{x}_i^\top]_S \mathbb{E}[\mathbf{I}[S](\hat{\beta}_L(\lambda) - \beta_0)_S] \geq \mathbb{E}_{i}[\mathbb{E}[\mathbf{x}_i \mathbf{x}_i^\top]] (\mathbf{v}_i^\top (\hat{\beta}_L(\lambda) - \beta_0)_S)^2\), which yields the desired conclusion after combining with (10). The final inequality in the display, \(\mathbb{E}_{i}[\mathbb{E}[\mathbf{x}_i \mathbf{x}_i^\top]] \geq \mathbb{E}[\mathbf{x}_i \mathbf{x}_i^\top]_S^2\) follows by Jensen’s inequality and the variational characterization of the \(s\)-sparse eigenvalues.

C.2 Corollary 2 and Supporting Lemmas

We now provide a short proof of the supporting corollary.

**Proof of Corollary 2.** This follows from Theorem 2 since for a fixed \(\mathbf{x}_*\) we have that \(\mathbb{E}[\mathbf{x}_*] = \mathbf{x}_*\) and \(\sup_{\|\mathbf{x}\|_2 = 1} \|\mathbf{x}\|_2^2 \geq s^{2-2/\eta}\).

The construction of this lower bound utilizes a support recovery result which requires the following conditions on the sample design matrix \(\mathbf{X} \in \mathbb{R}^{n \times p}\).

**Condition 1.** (Lower Eigenvalue on Support). The smallest eigenvalue of the sample covariance sub-matrix indexed by \(S\) is bounded below:
\[
\sigma_{\min}\left(\frac{\mathbf{X}_S^\top \mathbf{X}_S}{n}\right) \geq c_{\min} > 0.
\]

**Condition 2.** (Mutual Incoherence). There exists some \(\alpha \in [0, 1)\) such that
\[
\max_{j \in S} \| (\mathbf{X}_S^\top \mathbf{X}_S)^{-1} \mathbf{X}_S^\top \mathbf{X}\mathbf{e}_j \|_1 \leq \alpha.
\]

**Condition 3.** (Column Normalization). There exists some \(C\) such that
\[
\max_{j=1,\ldots,p} \frac{\|\mathbf{X}\mathbf{e}_j\|_2}{\sqrt{n}} \leq C.
\]

Importantly all of these conditions can be verified w.h.p when \(n \gtrsim s_{\beta_0} \log p\) for covariates \(\mathbf{x}_i \sim \mathcal{N}(0, \mathbf{I}_p)\) using standard matrix concentration arguments. To state our first lower bound it is also convenient to define \(\Pi_{S^c}(\mathbf{X}) = \mathbf{I}_n - \mathbf{X}_S(\mathbf{X}_S^\top \mathbf{X}_S)^{-1} \mathbf{X}_S^\top\), which is a type of orthogonal projection matrix.

Given these conditions we can state a conditional (on \(\mathbf{X}\)) support recovery result.

**Proposition 6.** Let Conditions (1), (2) and (3) hold for the sample covariance matrix \(\mathbf{X}\), the independent noise distribution be Gaussian, \(\epsilon \sim \mathcal{N}(0, \mathbf{I}_n \sigma^2_e)\), and Assumption 1 hold (with \(s_{\beta_0} \)-sparse underlying parameter \(\beta_0\)). Then, for any choice of regularization parameter \(\lambda = \frac{2\sigma_\epsilon}{1 - \alpha} \sqrt{\frac{2\log(p - s_{\beta_0})}{n}} + \delta\) for \(\delta > 0\), the support of \(\hat{\beta}_L(\lambda)\) is strictly contained in the support of \(\beta_0\):
\[
S_{\hat{\beta}_L(\lambda)} \subseteq S_{\beta_0}
\]
with probability at least \(1 - 4e^{-n\delta^2/2}\).

**Proof.** Conditions (1) and (2), and the fact that \(\lambda \geq \frac{2\sigma_\epsilon}{1 - \alpha} \|\mathbf{X}_S^\top \Pi_{S^c}(\mathbf{X}) \mathbf{e}\|_\infty\) are sufficient show a support recovery result. Under these conditions, for all \(s\)-sparse \(\beta_0\), there is a unique optimal solution.
to the Lagrangian Lasso program $\hat{\beta}_L(\lambda)$ and the support of $\hat{\beta}_L(\lambda)$, $S_{\hat{\beta}_L(\lambda)}$, is contained within the support $S_{\beta_0}$ (no false inclusion property) [25, Theorem 7.21]. We can simplify the condition on the regularization parameter from Proposition [25, Theorem 7.21] using a standard union bound/Gaussian tail bound argument (using Assumption 4) along with the column normalization condition (Condition (3)) to show that $\lambda = \frac{2\log(p - s_{\beta_0})}{n} + \delta$ satisfies $\lambda \geq \frac{2}{1 - \alpha} \|X_{S_\perp} \Pi_{S_\perp}(X) \|_{\infty}$ with probability at least $1 - 4e^{-n\delta^2/2}$ (over the randomness in $e$) [25, Corollary 7.22]. Combining yields the desired conclusion. 

The aforementioned result holds conditional on $X$. However, we can verify that Conditions, (1), (2), (3) hold true w.h.p. even if we sample $x_i \sim N(0, I_p)$ (see Lemma 3). Thus, we can show a Lasso prediction error bound that holds in expectation over all the randomness in the training data $(X, e)$. To do so we introduce the following standard result showing Conditions (1), (2), (3) can be verified w.h.p. for i.i.d. covariates from $N(0, I_p)$.

**Lemma 3.** Let $x_i \overset{i.i.d.}{\sim} N(0, I_p)$ for $i \in [n]$. Then there exists a universal constant $c_{2}$, such that for $n \geq c_{2} s_{\beta_0} \log p$ and $p \geq 20$, Conditions 1, 2, 3 each hold with probability at least $\frac{99}{100}$.

**Proof.** The proofs of these follow by standard matrix concentration arguments. Condition (3) can be verified w.h.p. for $C = 1$ (as a function of $n$) identically to Lemma 8 for $n \gtrsim \log p$. Condition (2) can also be verified w.h.p. for $\alpha = \frac{1}{2}$ for $n \gtrsim s_{\beta_0} \log(p - s_{\beta_0})$, see for example [25, Ch.7, p.221, Exercise 19]. While finally, Condition (1) can also be verified w.h.p. for $c_{\min} = \frac{1}{2}$ when $n \gtrsim s_{\beta_0}$ using standard operator norm bounds for Gaussian ensembles (see for example, [25, Theorem 6.1, Example 6.3]).

Combining Lemma 3 and Proposition 6 yields the desired conclusion which we formalize below.

**Proposition 7.** Under Assumption 1, suppose $x_i \overset{i.i.d.}{\sim} N(0, I_p)$ with independent noise $e \sim N(0, \sigma^2 I)$. Then, if $\hat{\beta}_L(\lambda)$ denotes the solution of the Lasso program, with regularization parameter chosen as $\lambda \geq 8\sigma \sqrt{\log p/n}$, there exists a universal constant $c_1$ such that for all $n \gtrsim c_1 s_{\beta_0} \log p$,

$$S_{\hat{\beta}_L(\lambda)} \subseteq S_{\beta_0}$$

with probability at least $\frac{1}{2}$. 

**Proof.** The proof follows using the independence of $e$ and $X$, by combining the results of Proposition 6 and Lemma 3 with a union bound (and taking $n$ sufficiently large). 

# D Proofs for Section 3.1: Javanmard-Montanari (JM)-style Estimator

In this section we provide the proof of the prediction risk bounds for the JM-style estimator.

## D.1 Theorem 3

We provide the proof of Theorem 3.

**Proof of Theorem 3.** Recall that we will use $r_{\beta, 1} = (\mathbb{E}_{X, e}[\|\hat{\beta} - \beta_0\|_1^4])^{1/4}$. This estimator admits the error decomposition,

$$\hat{y}_{JM} - \langle x_*, \beta_0 \rangle = \frac{1}{n} w^T X^T e + \langle x_* - \Sigma_n w, \hat{\beta} - \beta_0 \rangle$$

and hence,

$$\mathbb{E}_{X, e}[\|\hat{y}_{JM} - \langle x_*, \beta_0 \rangle\|_2^2] \leq 2 \left( \mathbb{E}_{X, e}[\|\frac{1}{n} w^T X^T e\|_2^2] + \mathbb{E}_{X, e}[\|\langle x_* - \Sigma_n w, \hat{\beta} - \beta_0 \rangle\|_2^2] \right)$$
The first term can be thought of as the variance contribution while the second is the contribution due to bias. For the variance term, we begin by evaluating the expectation over $\epsilon$. Using independence (w.r.t. to $X$) and sub-gaussianity of $\epsilon$,

$$E_{X,\epsilon}[\frac{1}{n} w^T X^T \epsilon]^2] = \frac{1}{n} E_X E_{\epsilon}[(\sum_{i=1}^n w^T x_i \epsilon_i)^2 | X] = \frac{\sigma^2}{n} E_X [w^T \Sigma_n w]$$

Now using Applying Corollary 6 and defining $\kappa'_1 = 8\kappa^2/C_{\min}||x_*||_2^2$ we have that,

$$E_X [w^T \Sigma_n w] \leq x_*^T \Omega x_* + \frac{3\kappa'_1}{\sqrt{n}}$$

using the condition $n \geq 2$.

Turning to the bias term, by the Holder inequality and Cauchy-Schwarz inequality, $E_{X,\epsilon}[||x_* - \Sigma_n w, \hat{\beta} - \beta_0||^2] \leq E_{X,\epsilon}[||x_* - \Sigma_n w||_2^2 ||\hat{\beta} - \beta_0||_2^2] \leq \sqrt{E_X [||x_* - \Sigma_n w||_4^4] E_X [||\hat{\beta} - \beta_0||_4^4]}$.

We begin by evaluating the first expectation $E_X [||x_* - \Sigma_n w||_4^4]$ which follows from Corollary 6,

$$\sqrt{E_X [||x_* - \Sigma_n w||_4^4]} \leq \lambda_w^2 + \sqrt{2||x_*||_\infty^2 (p \vee n)^{-c_3}}$$

for $n \geq a^2 \log(p \vee n)$ and $c_3 = a^2/4 - \frac{1}{2}$ with $\kappa'_2 = 8\kappa^2/C_{\cond}||x_*||_2$. By definition of the base estimation procedure we can assemble to obtain the desired error is bounded by,

$$\leq O\left(\frac{\sigma^2 x_* \Omega x_*}{n} + \frac{\sigma^2 \kappa'_1}{n^{3/2}} + r^2 \beta_1 ((\lambda_w^2 + ||x_*||_\infty^2 (p \vee n)^{-c_3}))\right)$$

where $\lambda_w = a\kappa'_2 \sqrt{\frac{\log(p \vee n)}{n}}$.

We can now instantiate the result of the previous theorem in the setting where the Lasso estimator is used as the base-regression procedure.

**D.2 Corollary 3 and Supporting Lemmas**

We provide the proof of Corollary 3.

**Proof of Corollary 3.** The second expectation $E_{X,\epsilon}[||\hat{\beta}_L(\lambda) - \beta_0||_4^4]$ can be evaluated using Lemmas 12 and 14 from which we find,

$$r_{\beta,1}^2 = \sqrt{E_{X,\epsilon}[||\hat{\beta}_L(\lambda) - \beta_0||_4^4]} \leq O\left(\frac{\lambda_{\beta_1} s_\beta_1}{\epsilon_{\min}} \right)^2 + O\left(\frac{\sigma_x}{\sqrt{n}}\right)^2 + O\left(\frac{\sigma_x^4}{\lambda_{\beta}} + ||\beta_0||_4^2\right)\left(e^{-c_3^{-n}}\right)$$

Assuming $p \geq 20$ and $n \geq c_2 \frac{\sigma_x^4}{\epsilon_{\min}} s \log(2ep)$, there exists sufficiently large $c_2$ such that

$$\left(\frac{\sigma_x^4}{\lambda_{\beta}} + ||\beta_0||_4^2\right)\left(e^{-c_3^{-n}}\right) \leq O\left(\frac{\sigma_x^2}{\sqrt{n}} + ||\beta_0||_4^2 e^{-nc/(4\epsilon_x^4)}\right) \leq O\left(\frac{\sigma_x^2}{\sqrt{n}} + ||\beta_0||_4^2\right)$$

for some sufficiently small $c_1$. Thus we have $r_{\beta,1}^2 \leq O\left(\frac{\lambda_{\beta_1} s_\beta_1}{c_{\min}} + \frac{\sigma_x^2}{n}\right) = O\left(\frac{\lambda_{\beta_1} s_\beta_1}{c_{\min}}\right)$ due to the lower bound on $\lambda_\beta$. Combining with Theorem 3 gives the result,

$$O\left(\frac{\sigma_x^2 x_* \Omega x_*}{n} + \frac{\lambda_{\beta_1} s_\beta_1}{c_{\min}}\right)\left(\lambda_w^2 + ||x_*||_\infty^2 (p \vee n)^{-c_3}\right)$$

We collect several useful lemmas which follow from standard concentration arguments useful both in the analysis of the upper bound on the JM estimator and in the Lasso lower bound.

To begin we show the convex program defining the JM estimator is feasible with high probability. For convenience we define the event $F(a)$ to be the event that the convex program defining the JM estimator in (3) with choice of regularization parameter $\lambda_w = a\sqrt{\log p/n}$ possesses $w_0 = \Omega x_*$ as a feasible point.
Lemma 4. Let Assumption 2 and 3 hold for the design $X$ and assume $n \geq a^2 \log(p \lor n)$ with $\kappa_2' = 8\kappa^2/\sqrt{\text{cond}}\|x_*\|_2$. If $x_* \in \mathbb{R}^p$ then for $w_0 = \Omega x_*$,

$$\Pr\left[ \|\hat{\Sigma}_n w_0 - x_*\|_\infty \geq a\kappa_2' \sqrt{\log(p \lor n)/n} \right] \leq 2(p \lor n)^{-c_2}$$

for $c_2 = \frac{a^2}{2} - 1$. Hence the convex program in (3) with regularization parameter $\lambda_w = a\kappa_2' \sqrt{\log(p \lor n)/n}$ admits $w_0$ as a feasible point with probability at least $1 - 2(p \lor n)^{-c_2}$.

Proof. This follows from a standard concentration argument for sub-exponential random variables. Throughout we will use $\hat{x}_\ell = \Omega^{1/2} x_\ell$. Consider some $j \in [p]$ and define $z_j = e_j^\top \Omega^{1/2} \hat{x}_\ell \cdot \Sigma^{1/2} x_* - e_j^\top \Sigma^{1/2} x_*$ which satisfies $\mathbb{E}[z_j^2] = 0$, is independent over $\ell \in [n]$, and for which $e_j^\top (\hat{\Sigma}_n w_0 - x_*) = \frac{1}{n} \sum_{t=1}^n z_j^t$. Since $e_j^\top \Omega^{1/2} \hat{x}_\ell \sim sG(\kappa\|e_j^\top \Omega^{1/2} \|_2) \sim sG(\kappa/\sqrt{\text{cond}})$, and $(x_*)^\top \Omega^{1/2} \hat{x}_\ell \sim sG(\kappa\|\Sigma^{1/2} x_*\|_2) \sim sG(\kappa\sqrt{\text{cond}}\|x_*\|_2)$, $z_j$ is a mean-zero sub-exponential random variable approximately by Lemma 7. Defining $\kappa_2' = 8\kappa^2/\sqrt{\text{cond}}\|x_*\|_2$, applying the tail bound for sub-exponential random variables, and taking a union bound over the $p$ coordinates implies that,

$$\Pr[\|\hat{\Sigma}_n w_0 - x_*\|_\infty \geq t] \leq 2p \exp\left[ -\frac{n}{2} \min((t/k_2'),(t/k_2')) \right].$$

Choosing $t = a\kappa_2' \sqrt{\log(p \lor n)/n}$, assuming $n \geq a^2 \log(p \lor n)$, gives the conclusion

$$\Pr[\|\hat{\Sigma}_n w_0 - x_*\|_\infty \geq a\kappa_2' \sqrt{\log(p \lor n)/n}] \leq 2(p \lor n)^{-a^2/2+1}$$

and the conclusion follows. \hfill \Box

We can now provide a similar concentration argument to bound the objective of the JLM program.

Lemma 5. Let Assumption 2 and 3 hold for the design $X$. Let $w$ be the solution of the convex program in (3) with regularization parameter set as $\lambda_w$. If $x_* \in \mathbb{R}^p$, then,

$$\Pr[\|w^\top \Sigma_n w - x_*\Omega x_* + t\|_\infty \geq \|x_*\Omega x_*\|_\infty] \leq 2 \exp\left[-n/2 \min((t/k_1'),(t/k_1'))\right]$$

for $k_1' = 8\kappa^2/\sqrt{\text{cond}}\|x_*\|_2^2$.

Proof. The argument once again follows from a standard concentration argument for sub-exponential random variables. Considering,

$$(x,\Omega)^\top \Sigma_n \Omega x_* = [(x,\Omega)^\top \Sigma_n \Omega x_* - x,\Omega x_*] + x,\Omega x_* = \frac{1}{n} \sum_{j=1}^n (z_j^2 - x,\Omega x_* ) + x,\Omega x_*$$

where $z_j = x,\Omega x_j$ is mean-zero with $s_j \sim sG(\kappa\|\Omega^{1/2} x_*\|_2) \sim sG(\kappa/\sqrt{\text{cond}}\|x_*\|_2)$. Since $\mathbb{E}[z_j^2] = x,\Omega x_*$, Lemma 7 implies $z_j^2 \sim x,\Omega x_* \sim sG(8\kappa^2/\sqrt{\text{cond}}\|x_*\|_2^2)$ and is mean-zero. The sub-exponential tail bound gives,

$$\Pr\left[ \frac{1}{n} \sum_{j=1}^n z_j^2 \geq x,\Omega x_* + t \right] \leq \exp\left[-n/2 \min((t/k_1'),(t/k_1'))\right]$$

where $k_1' = 8\kappa^2/\sqrt{\text{cond}}\|x_*\|_2^2$. Hence, since on the event $\mathcal{F}(a)$, we have that $w^\top \Sigma_n w \leq (x,\Omega)^\top \Sigma_n \Omega x_*$ (recall $w_0 = \Omega x_*$ is feasible on $\mathcal{F}(a)$),

$$\Pr[w^\top \Sigma_n w \geq x,\Omega x_* + t] \leq \Pr\left\{ w^\top \Sigma_n w \geq x,\Omega x_* + t \cap \mathcal{F}(a) \right\} + \Pr\left\{ w^\top \Sigma_n w \geq x,\Omega x_* + t \cap \mathcal{F}(a)^c \right\} \leq \Pr\left[ \frac{1}{n} \sum_{j=1}^n z_j^2 \geq x,\Omega x_* + t \right] + 0 \leq \exp\left[-n/2 \min((t/k_1'),(t/k_1'))\right],$$

since by definition on the event $\mathcal{F}(a)^c$ the convex program outputs $w = 0$ and $x,\Omega x_* \geq 1/C_{\text{max}} > 0$. \hfill \Box
Finally we can easily convert these tail bounds into moment bounds.

**Corollary 6.** Let Assumption 2 and 3 hold for the design \( \mathbf{X} \). Let \( \mathbf{w} \) be the solution of the convex program in (3) with regularization parameter set as \( \lambda = \alpha n^{\frac{1}{2}} \sqrt{\log(p/v)} \). If \( \mathbf{x}_* \in \mathbb{R}^p \), then,

\[
E[\mathbf{w}^T \Sigma_n \mathbf{w}] \leq \mathbf{x}_* \mathbf{\Omega x}_* + \frac{3\kappa'_1}{\sqrt{n}}
\]

for \( \kappa'_1 = 8\kappa^2/C_{\min} \| \mathbf{x}_* \|^2 \). Moreover, assuming \( n \geq a^2 \log(p \vee n) \),

\[
\sqrt{E[\|\hat{\Sigma}_n \mathbf{w} - \mathbf{x}_*\|_4^4]} \leq \lambda_\mathbf{w}^2 + \sqrt{2}\|\mathbf{x}_*\|^2_{\infty}(p \vee n)^{-c_2}
\]

for \( c_2 = a^2/2 - 1 \) with \( \kappa'_2 = 8\kappa^2\sqrt{C_{\text{cond}}} \| \mathbf{x}_* \|^2 \).

**Proof.** Using Lemma 5 we have that,

\[
E[\mathbf{w}^T \Sigma_n \mathbf{w}] = \mathbf{x}_* \mathbf{\Omega x}_* + \int_0^\infty \Pr[\mathbf{w}^T \Sigma_n \mathbf{w} \geq \mathbf{x}_* \mathbf{\Omega x}_* + t]
\]

\[
\leq \mathbf{x}_* \mathbf{\Omega x}_* + \int_0^{\kappa'_1} \left[ \exp \left(-n/2(t/\kappa'_1)^2 \right) dt + \int_{\kappa'_1}^\infty \left[ \exp \left(-n/2(t/\kappa'_1)^2 \right) \right] dt \right]
\]

\[
\leq \mathbf{x}_* \mathbf{\Omega x}_* + \frac{2\kappa'_1}{\sqrt{n}} + \frac{2\kappa'_1 e^{-n/2}}{n} \leq \mathbf{x}_* \mathbf{\Omega x}_* + \frac{3\kappa'_1}{\sqrt{n}}
\]

which holds for \( n \geq 2 \).

Similarly, directly applying Lemma 4 we obtain,

\[
E[\|\hat{\Sigma}_n \mathbf{w} - \mathbf{x}_*\|_4^4] \leq E[\|\hat{\Sigma}_n \mathbf{w} - \mathbf{x}_*\|_4^4 1[F(a)]] + E[\|\hat{\Sigma}_n \mathbf{w} - \mathbf{x}_*\|_4^4 1[F^c(a)]] \leq \lambda_\mathbf{w}^4 + \|\mathbf{x}_*\|_4^4 \Pr[F^c(a)] \leq \lambda_\mathbf{w}^4 + 2\|\mathbf{x}_*\|_4^4 (p \vee n)^{-c_2}
\]

\( c_2 = a^2/2 - 1 \), since the convex program outputs \( \mathbf{w} = 0 \) on the event \( F^c(a) \). The conclusion follows using subadditivity of \( \sqrt{\cdot} \).

---

**E Proofs for Section 3.2: Orthogonal Moment Estimators**

We begin by providing the consistency proofs for the orthogonal moment estimators introduced in Section 3.2. However, first we make a remark which relates the assumptions on the design we make to the properties of the noise variable \( \eta \).

**Remark 1.** Under the random design assumption on \( \mathbf{x} \), if we consider \( \mathbf{x}' = [t, \mathbf{z}] = (\mathbf{U}^{-1})^\top \mathbf{x} \), then by Assumption 3, \( \mathbf{g}_0 = \arg\min_{\mathbf{g}} E[(t - \mathbf{z}^\top \mathbf{g}_0)^2] \) can be thought of as the best linear approximator interpreted in the regression framework. Hence it can also be related to the precision matrix and residual variance as:

\[
\mathbf{\Omega}_{\mathbf{e}_t} = \frac{(1, -\mathbf{g}_0)}{\sigma_\mathbf{e}_t^2}.
\]

In this setting, we have that \( E[\eta^2] = \Sigma_{tt} - \mathbf{g}_0^\top \Sigma_{tz} \mathbf{g}_0 \geq 0 \). Moreover from the variational characterization of the minimum eigenvalue we also have that \( E[\eta^2] \geq C_{\min}/\|\mathbf{x}_*\|_2 \). Thus \( \|\mathbf{g}_0\|^2_2 \leq \frac{\Sigma_{tt}}{C_{\min}} \leq C_{\text{cond}}/\|\mathbf{x}_*\|_2 \) and \( E[\eta^2] \leq \Sigma_{tt} \leq C_{\max}/\|\mathbf{x}_*\|_2 \). Moreover, the treatment noise \( \eta \) is also a sub-Gaussian random variable, since \( \eta = t - \mathbf{z}^\top \mathbf{g}_0 = (1, -\mathbf{g}_0)^\top \mathbf{x}' \). Recall by Assumption 2 that \( E[(\mathbf{x}'^\top \mathbf{v})^p] \leq \kappa^2 p \|\mathbf{\Sigma}^{1/2} \mathbf{v}\|^2_2 \) while \( \eta = (1, -\mathbf{g}_0)^\top \mathbf{x}' \). Thus we have that \( E[\eta^p] = \kappa^2 p C_{\max} (1 + \|\mathbf{g}_0\|^2_2)^p/\|\mathbf{x}_*\|^2_2 \leq O((\kappa^2 C_{\text{cond}} C_{\max}/\|\mathbf{x}_*\|_2^2)^p) \). Similarly \( E[(\mathbf{z}^\top \mathbf{g}_0)^{2p}] \leq (\kappa^2 \|\mathbf{g}_0\|^2_2 C_{\max}/\|\mathbf{x}_*\|_2^2)^p \).
We now present the Proof of Theorem 4.

**Proof of Theorem 4.** To begin we rescale the $x_i$ such that is has unit-norm (and restore the scaling in the final statement of the proof). In order to calculate the mean-squared error of our prediction $\mathbb{E}[(\hat{y}_{OM} - x_i^\top \beta_0)^2]$, it is convenient to organize the calculation in an error expansion in terms of the moment function $m$. For convenience we define the following (held-out) prediction errors $\Delta_f(z_i) = z_i^\top (\hat{f} - f_0)$, and $\Delta_g(z_i) = g(z_i) - g_0(z_i)$ of $f$ and $g(\cdot)$ which are trained on first-stage data but evaluated against the second-stage data. Note that as assumed in the Theorem, $g_0(z) = z^\top g_0$. Also note the moment equations only depend on $f$ and $g(\cdot)$ implicitly through the evaluations $z^\top \hat{f}$ and $g(z)$, so derivatives of the moment expressions with respect to $z^\top \hat{f}$ and $g(z)$, refer to derivatives with respect to scalar. Recall the sums of the empirical moment equation here only range over the second fold of data, while $\hat{f}$ and $g$ are fit on the first fold. The empirical moment equations can be expanded (exactly) as,

$$
\frac{1}{n/2} \sum_{i=1}^{n/2} \nabla_g m(t_i, y_i, \theta_0, z_i^\top \hat{f}, g(z_i)) (\theta_0 - \hat{y}_{OM}) = \frac{1}{n/2} \sum_{i=1}^{n/2} m(t_i, y_i, \theta_0, z_i^\top \hat{f}, g(z_i))
$$

since by definition $\frac{1}{n/2} \sum_{i=1}^{n/2} m(t_i, y_i, \hat{y}_{OM}, z_i^\top \hat{f}, g(z_i)) = 0$. Then we further have that,

$$
\frac{1}{n/2} \sum_{i=1}^{n/2} m(t_i, y_i, \theta_0, z_i^\top \hat{f}, g(z_i)) = \frac{1}{n/2} \sum_{i=1}^{n/2} \nabla_m(t_i, y_i, \theta_0, z_i^\top \hat{f}, g(z_i)) + \frac{1}{n/2} \sum_{i=1}^{n/2} \nabla_z m(t_i, y_i, \theta_0, z_i^\top \hat{f}, g(z_i))(\nabla_f + \nabla_g)
$$

We first turn to controlling the moments of $A, B_1, B_2, C$. We use as convenient shorthand $\zeta = \kappa^2 C_{\text{max}}$. Similarly we also use $r_{f,2} = (\mathbb{E}[(\Delta_f(z))^2])^{1/4}$. 

1. For $A = \frac{1}{n/2} \sum_{i=1}^{n/2} \eta_i \epsilon_i$, note that $\mathbb{E}[m(t_i, y_i, \theta_0, z_i^\top \hat{f}, g_0(z_i))|z_i] = 0$ so it follows that,

$$
\mathbb{E}[A^2] = \mathbb{O} \left( \frac{1}{n} \mathbb{E}[\eta^2 \epsilon^2] \right) = \mathbb{O} \left( \frac{\sigma^2_{\eta} \sigma^2_{\epsilon}}{n} \right)
$$

2. For $B_1 = \frac{1}{n/2} \sum_{i=1}^{n/2} \Delta_f(z_i) \eta_i$. Note $\mathbb{E}[\nabla_{z^\top} m(t_i, y_i, \theta_0, z_i^\top f_0, g_0(z_i))|z_i] = 0$ since $\mathbb{E}[\eta_i|z_i] = 0$. So we have using sub-gaussianity of the random vector $z$, sub-gaussianity of $\eta$ and independence that,

$$
\mathbb{E}[B_1^2] = \mathbb{O} \left( \frac{1}{n} \mathbb{E}[(\Delta_f(z))^2 \eta^2] \right) \leq \mathbb{O} \left( \frac{1}{n} r_{f,2}^2 \sigma^2_{\eta} \right)
$$

3. For $B_2 = \sum_{i=1}^{n} \Delta_g(z_i) \epsilon_i$. Note $\mathbb{E}[\nabla_{g(z)} m(t_i, y_i, \theta_0, z_i^\top f_0, g_0(z_i))|z_i] = 0$ using independence of $\epsilon_i$ and the fact $\mathbb{E}[\epsilon_i] = 0$. Once again using independence,

$$
\mathbb{E}[B_2^2] = \mathbb{O} \left( \frac{1}{n} \mathbb{E}[(\Delta_g(z))^2 \epsilon^2] \right) \leq \mathbb{O} \left( \frac{1}{n} \sigma^2_{\epsilon} \sigma^2_{\eta} \right)
$$

22
4. For $C = \frac{1}{n} \sum_{i=1}^{n} \Delta_{\beta}(z_i) \Delta_f(z_i)$. Note that in general for the remainder term $E[\nabla_{x, g(z)} m(t_i, y_i, \theta_0, z_i^f, g_0(z_i)) | z_i] \neq 0$; however in some cases we can exploit unless we can exploit unconditional orthogonality: $E[\nabla_{x, g(z)} m(t_i, y_i, \theta_0, z_i^f, g_0(z_i)) | z_i] = 0$ to obtain an improved rate although this is not mentioned in the main text.

- In the absence of unconditional orthogonality, we have by the Cauchy-Schwarz inequality that,

$$E[C^2] \leq O\left(\sqrt{E[(\Delta_{\beta}(z_i))^4]} \sqrt{E[(\Delta_f(z_i))^4]}\right) \leq O(r_{f, 2}^2 r_{g, 2}^2)$$

- In the presence of unconditional orthogonality we have that,

$$E[C^2] = \frac{1}{n} r_{f, 2}^2 r_{g, 2}^2$$

as before using Cauchy-Schwarz but cancelling the cross-terms.

Now we can amalgamate our results. Before doing so note that $r_{f, 2} \leq \zeta r_{\beta, 2}$ since in the description of the algorithm the estimator is defined by rotating an estimate of $\beta_0$ in the base regression procedure (and consistency of the (held-out) prediction error is preserved under orthogonal rotations).

First define the event $J = \{ J \leq \frac{1}{4} \sigma_n^2 \}$. For the orthogonal estimator defined in the algorithm, on the event $J$ the estimator will output the estimate from the first-stage base regression using $\hat{y}_{om} = x_\star^T \beta_0$. So introducing the indicator of this event, and using Cauchy-Schwarz, we have that,

$$E[(\hat{y}_{om} - \theta_0)^2] = \left[E[(\hat{y}_{om} - \theta_0)^2 1(J)] + \sqrt{E[\|\Delta_{\beta}(x_\star)\|^4]} \right] \Pr[\bar{J}]$$

$$\leq \left[O\left(\frac{E[A^2 + B^2 + C^2]}{(\sigma_n^2)^2} \right) + O(r_{f, 2}^2) \sqrt{O(((\frac{\xi}{\sigma_n^2})^4 + \frac{\xi^2}{(\sigma_n^2)^2} r_{f, 2}^2) \cdot \frac{1}{n^2})}\right]$$

$$\leq \|x_\star\|^2 \left[O\left(\frac{\sigma_n^2 \sigma_n^2 + \zeta r_{\beta, 2}^2 \sigma_n^2 + r_{g, 2}^2 \sigma_n^2}{(\sigma_n^2)^2 n}\right) + O(((\frac{\xi}{\sigma_n^2})^2 + \frac{\xi^2}{(\sigma_n^2)^2} r_{g, 2}^2, \cdot \frac{1}{n}) \cdot r_{f, 2}^2) + \right.$$ $O\left(\frac{\zeta^2 r_{\beta, 2}^2 \sigma_n^4}{(\sigma_n^2)^2 n}\right)$ with unconditional orthogonality

$$O\left(\frac{\zeta^2 r_{\beta, 2}^2 \sigma_n^4}{(\sigma_n^2)^2 n}\right)$ without unconditional orthogonality

where $\Pr[\bar{J}]$ is computed using Lemma 6. If we consider the case without unconditional orthogonality, and assume since $C_{max} \geq \sigma_n^2 \geq C_{min}$, the above results simplifies (ignoring conditioning-dependent factors) to the theorem statement,

$$\|x_\star\|^2 \left[O\left(\frac{\sigma_n^2}{\sigma_n^2} \right) + O\left(\frac{r_{\beta, 2}^2 \sigma_n^2}{(\sigma_n^2)^2 n}\right) + O\left(\frac{r_{g, 2}^2 \sigma_n^4 + r_{g, 2}^2 \sigma_n^4}{(\sigma_n^2)^2 n}\right) \right]$$

\[\square\]

**Lemma 6.** Let Assumptions 2, 3, and 5 hold and suppose $g_0(z) = z^T g_0$ in (6). Defining $J = \frac{1}{n} \sum_{i=1}^{n} J_i = \frac{1}{n} \sum_{i=1}^{n} t_i (t_i - \tilde{g}(z_i))$ as in the description of first-order OM estimator with $\tau \leq \frac{1}{4} E[y_i^2]$, then,

$$\Pr \left[ \frac{1}{n} \sum_{i=1}^{n} J_i \leq \tau \right] \leq O \left( ((\frac{\xi}{\sigma_n^2})^4 + \frac{\xi^2}{(\sigma_n^2)^2} r_{g, 2}^2) \cdot \frac{1}{n^2} \right)$$

where $\xi = C_{cond} C_{max} \kappa^2$ and $\zeta = \kappa^2 C_{max}$ and $r_{g, 2} = (E[\|\Delta_{\beta}(z_i)\|^4])^{1/4}$.

**Proof.** To begin we rescale the $x_\star$ such that is has unit-norm (and restore the scaling in the final statement of the proof). We begin by establishing concentration of the $J$ term which justifies the thresholding step in the estimator using a 4th-moment Markov inequality. We have that $J =$
\[ \frac{1}{n} \sum_{i=1}^{n} \nabla \phi(t_i, y_i, \theta_0, z_i^\top \hat{f}_i, \hat{g}(z_i)) = \frac{1}{n} \sum_{i=1}^{n} t_i (t_i - \hat{g}(z_i)) = \frac{1}{n} \sum_{i=1}^{n} J_i. \]

Note that we assume 
\[ t_i = z_i^\top g_0 + \eta_i. \]

The, for an individual term we have that, 
\[ J_i = (z_i^\top g_0 + \eta_i) (\Delta_y(z_i) + \eta_i) = \frac{\eta_i^2 + z_i^\top g_0 \eta_i + z_i^\top g_0 (\Delta_y(z_i))}{a_i} b_i. \]

Recall by Remark 1, that \( \eta = (1, -g_0)^\top x' \), and that \( \|g_0\|^2_2 = O(C_{\text{cond}}) \). Using sub-gaussianity of \( x' \) we have that \( \eta_i \sim \mathbb{N}(8C_{\text{cond}} \kappa_2 C_{\max}, 8C_{\text{cond}} \kappa_2 C_{\max}^2) \) by Lemma 7. Similarly, \( z_i^\top g_0 \eta_i \sim \mathbb{N}(8C_{\text{cond}} \kappa_2 C_{\max}, 8C_{\text{cond}} \kappa_2 C_{\max}^2) \) since \( z_i^\top g_0 \sim \mathbb{G}(C_{\max} \kappa_2 C_{\text{cond}}) \). We introduce \( \xi = C_{\text{cond}} C_{\max} \kappa_2 \) and \( \zeta = \kappa_2 C_{\max} \).

Analyzing each term, we have that,

- For the first terms, \( \mathbb{E}[\eta_i^2] = \mathbb{E}[\eta^2] \). Similarly for the second term, note \( \mathbb{E}[b_i] = 0 \) since \( \eta_i \) is conditionally (on \( z \)) mean-zero. Hence we have that each \( a_i \) is mean-zero and \( a_i \sim \mathbb{N}(16 \xi, 16 \zeta) \).

- For the final term, note \( \mathbb{E}[(z_i^\top g_0 (\Delta_y(z_i)))^4] \leq O(\xi^2 r^4 g) \) by Cauchy-Schwarz.

Since, \( J = \frac{1}{n} \sum_{i=1}^{n} a_i + b_i + c_i \), if \( \left| \frac{1}{n} \sum_{i=1}^{n} b_i + c_i \right| \leq \epsilon' \) and \( \frac{1}{n} \sum_{i=1}^{n} a_i \geq \epsilon' + \tau \) then \( \frac{1}{n} \sum_{i=1}^{n} J_i \geq \tau \).

So a union bound gives,
\[
\Pr \left[ \frac{1}{n} \sum_{i=1}^{n} J_i \leq \tau \right] \leq \Pr \left[ \frac{1}{n} \sum_{i=1}^{n} a_i < + \epsilon' + \tau \right] + \Pr \left[ \frac{1}{n} \sum_{i=1}^{n} b_i + c_i \geq \epsilon' \right]
\]

Using a sub-exponential tail bound for the first term and the 4th-moment Markov–Kolmogorov inequality for the second we obtain,

- For the first term
\[
\Pr \left[ \frac{1}{n} \sum_{i=1}^{n} a_i - \mathbb{E}[\eta^2] \leq - (\epsilon' - \tau + \mathbb{E}[\eta^2]) \right] \leq O(\exp \left( -c n \min \left( \frac{t^2}{\epsilon'}, \frac{t}{\xi} \right) \right))
\]

for some universal constant \( c \) (that may change line to line).

- For the second term
\[
\Pr \left[ \left| \frac{1}{n} \sum_{i=1}^{n} b_i \right| \geq + \epsilon' \right] \leq O(\frac{\xi^2 r^4}{(\epsilon')^2 n^2})
\]

Taking \( \epsilon' = \frac{1}{4} \sigma^2_n \) and \( \tau \leq \frac{1}{4} \sigma^2_n \) it follows that \( t \geq \frac{1}{2} \sigma^2_n \). Hence the second term can be simplified to \( O(\exp \left( -c n \min \left( \frac{t^2}{\epsilon'}, \frac{t}{\xi} \right) \right) = O(\max \left( \frac{\xi^2}{(\xi')^2}, \frac{\xi^2}{(\xi')^2} \right)^2 \frac{1}{n^2} \) \). Hence the desired bound becomes,
\[
\Pr \left[ \frac{1}{n} \sum_{i=1}^{n} J_i \leq \epsilon \right] \leq O\left( \frac{\xi^4 r^4}{(\xi')^4 n^4} \right) + O(\exp \left( -c n \min \left( \frac{t^2}{\epsilon'}, \frac{t}{\xi} \right) \right) = O\left( \left( \frac{\xi}{(\xi')}^4 + \frac{\xi^2}{(\xi')^2} \right)^2 \cdot \frac{1}{n^2} \right). \]

**E.2 Corollaries 4 and 5**

We conclude the section by presenting the proofs of Corollary 4 and Corollary 5 which instantiate the OM estimators when both first-stage regressions are estimated with the Lasso.

First we prove Corollary 4.

**Proof of Corollary 4.** It suffices to compute \( r_{\beta, 2} \) and \( r_{\tilde{g}, 2} \). By using Lemma 18,
\[
r_{\beta, 2} \leq O \left( \frac{\sigma^2_n}{n} \right)
\]

24
by utilizing condition on $\lambda_\beta$ in the theorem statement and that $\|\beta_0\|_\infty/\sigma_\epsilon \leq O(1)$ and $n \geq \Omega(n^4 C_{cond}^2)$. Similarly, for the case of $r_{g,2}$ in the case the estimator is parametric Lasso estimator it follows that $r_{g,2} = (\mathbb{E}[|z^T (g_0 - g)|^4])^{1/4} \leq O(\sqrt{C}E(\|g_0 - g\|_2^4))^{1/4}$ where $\zeta = \kappa^2 C_{max}$. Similar to above we obtain that,

$$r_{g,2} \leq O(\frac{s_{g}^2}{n})$$

since we can verify that the conditions of Lemma 18 also hold when $t$ is regressed against $z$ under the hypotheses of the result. In particular, note since the regression for $g$ is performed between $t$ and $z$ (which up to an orthogonal rotation is a subvector of the original covariate $x$ itself), the minimum eigenvalue for this regression is lower-bounded by the minimum eigenvalue of $X$. Moreover by Remark 1, $\|g_0\|_2 \leq \sqrt{C_{cond}}$.

\textbf{Proof of Corollary 5.} It suffices to compute $r_{\beta,2}$ and $r_{g,2}$. The computation for $r_{\beta,2}$ is similar to the one for $r_{\beta,1}$. By combining Lemma 12 and Lemma 14, and assuming $p \geq 20$ and $n \geq \frac{C_{max}}{C_{min}} \cdot s \log(2ep)$, there exists sufficiently large $c$ such that,

$$r_{\beta,2} \leq O\left(\frac{\lambda_\beta \sqrt{s}}{C_{min}} + O\left(\frac{\sigma_\epsilon}{\sqrt{n}}\right) + \frac{1}{n \lambda_\beta \sqrt{s}}\right) + O\left(\frac{\sigma_\epsilon}{\sqrt{n}} + \|\beta_0\|_1 e^{-nc/(8\kappa^4)}\right) = O\left(\frac{\lambda_\beta \sqrt{s}}{C_{min}}\right) + O(\|\beta_0\|_1 e^{-nc/(8\kappa^4)}) \leq O\left(\frac{\lambda_\beta \sqrt{s}}{C_{min}}\right)$$

using the lower bound on $\lambda_\beta$ in the theorem statement and that $\|\beta_0\|_\infty/\sigma_\epsilon = o(e^{c/n})$ for some sufficiently small $c_1$. Similarly, for the case of $r_{g,2}$ in the case the estimator is parametric Lasso estimator it follows that $r_{g,2} = (\mathbb{E}[|z^T (g_0 - g)|^4])^{1/4} \leq O(\sqrt{C}E(\|g_0 - g\|_2^4))^{1/4}$ where $\zeta = \kappa^2 C_{max}$. Similar to above we obtain that,

$$r_{g,2} \leq O\left(\frac{\lambda_\beta \sqrt{s}}{C_{min}}\right) + O(\|g_0\|_1 e^{-nc/(8\kappa^4)}) \leq O\left(\frac{\lambda_\beta \sqrt{s}}{C_{min}}\right)$$

since we can verify that the conditions of Lemma 12 and Lemma 14 also hold when $t$ is regressed against $z$ under the hypotheses of the result. In particular, note since the regression for $g$ is performed between $t$ and $z$ (which up to an orthogonal rotation is a subvector of the original covariate $x$ itself), the strong-restricted eigenvalue for this regression is lower-bounded by the strong-restricted eigenvalue of $X$. Moreover by Remark 1, $\|g_0\|_1 \leq s_{g_0} \|g_0\|_2 \leq s_{g_0} \sqrt{C_{cond}}$.

\section{Auxiliary Lemmas}

We now introduce a standard concentration result we will repeatedly use throughout,

\textbf{Lemma 7.} Let $x, y$ be mean-zero random variables that are both sub-Gaussian with parameters $\kappa_1$ and $\kappa_2$ respectively. Then $z = xy - \mathbb{E}[xy] \sim s\mathbb{E}(8\kappa_1 \kappa_2, 8\kappa_1 \kappa_2)$.

\textbf{Proof.} Using the dominated convergence theorem,

$$\mathbb{E}[e^{\lambda z}] = 1 + \sum_{k=2}^{\infty} \frac{\lambda^k \mathbb{E}[(xy - \mathbb{E}[xy])^k]}{k!}$$

$$\leq 1 + \sum_{k=2}^{\infty} \frac{\lambda^k 2^{k-1} (\mathbb{E}[|xy|^k] + \mathbb{E}[|xy|^k])}{k!}$$

$$\leq 1 + \sum_{k=2}^{\infty} \frac{\lambda^k 2^k \sqrt{\mathbb{E}[x^{2k}] \mathbb{E}[y^{2k}]}}{k!}$$

$$\leq 1 + \sum_{k=2}^{\infty} \frac{\lambda^k 2^k (2\kappa_1 \kappa_2)^k (2k) \Gamma(k)}{k!} = 1 + \frac{44\kappa_1 \kappa_2}{2} \sum_{k=0}^{\infty} (4\lambda \kappa_1 \kappa_2)^k$$

$$\leq 1 + 4(4\lambda \kappa_1 \kappa_2)^2 = 1 + 64\lambda^2 \kappa_1^2 \kappa_2^2 \quad \text{for } |\lambda| \leq \frac{1}{8\kappa_1 \kappa_2}$$

$$\leq e^{(\lambda - 8\kappa_1 \kappa_2)^2} \leq e^{(\lambda - 8\kappa_1 \kappa_2)^2}/2$$

\qed
where we have used the fact a sub-Gaussian random variable $x$ with parameter $\kappa$ satisfies $\mathbb{E}[|x|^2] \leq (2\kappa^2)^{k/2}k\Gamma(k/2)$ (which itself follows from integrating the sub-gaussian tail bound), along with the Cauchy-Schwarz and Jensen inequalities.

### F.1 Random Design Matrices and Lasso Consistency

Here we collect several useful results we use to show consistency of the Lasso estimator in the random design setting.

Note Assumption 2 ensures the population covariance for the design $X$ satisfies $\Sigma_{ii} \leq 1/2$, and a standard sub-exponential concentration argument establishes the result for a random design matrix under Assumption 3. Accordingly, we introduce,

**Definition 1.** The design matrix $X \in \mathbb{R}^{n \times p}$ satisfies the 1-column normalization condition if

$$\max_{i \in [p]} \|Xe_i\|^2/n = \Sigma_{ii} \leq 1$$

and we have that,

**Lemma 8.** Let $\kappa' = 8\sqrt{2}\kappa$. If Assumptions 2 and 3 hold, then

$$\Pr \left[ \max_{i \in [p]} (\hat{\Sigma}_n)_{ii} - \Sigma_{ii} \geq t \right] \leq p \exp \left( -\frac{n}{2} \min(\frac{t^2}{\kappa'^2}, \frac{t}{\kappa'}) \right)$$

and if $n \geq 2a \max(\kappa^2, \kappa') \log p$, then with probability at least $1 - p^{-a}$

$$\max_{i \in [p]} (\hat{\Sigma}_n)_{ii} \leq 1.$$  

**Proof.** Note that $x_i = x^\top e_i$ satisfies $\mathbb{E}[(\exp(\lambda x_i))] \leq \exp(\lambda^2 \kappa^2 \Sigma_{ii}/2)$. For fixed $i$ we have that $(\hat{\Sigma}_n)_{ii} = \frac{1}{n} \sum_{i=1}^n (x_i^2 - \Sigma_{ii})$. Since $x_i \sim sG(\kappa \sqrt{\Sigma_{ii}})$, using Lemma 7 along with a sub-exponential tail bound we have that,

$$\Pr \left[ (\hat{\Sigma}_n)_{ii} \geq \Sigma_{ii} + t \right] \leq \exp \left( -\frac{n}{2} \min(\frac{t^2}{\kappa'^2}, \frac{t}{\kappa}) \right)$$

defining $\kappa' = 8\kappa \sqrt{\Sigma_{ii}} \leq 4\sqrt{2}\kappa$. Since $\Sigma_{ii} \leq \frac{1}{2}$ using a union bound over the $p$ coordinates we have that $\max_{i \in [p]} (\hat{\Sigma}_n)_{ii} \geq 1$, with probability less than $p \exp \left( -\frac{n}{2} \min(\frac{t^2}{\kappa'^2}, \frac{t}{\kappa}) \right)$. If $t = \frac{1}{2}$ and $n \geq 2a \max(\kappa^2, \kappa') \log p$ the stated conclusion holds. \qed

Similarly, although the sample covariance will not be invertible for $p > n$ we require it to be nonsingular along a restricted set of directions. To this end we introduce the strong restricted eigenvalue condition (or SRE condition) defined in [4, Equation 4.2] which is most convenient for our purposes.

**Definition 2.** Given a symmetric covariance matrix $Q \in \mathbb{R}^{p \times p}$ satisfying $\max_{i \in [p]} Q_{ii} \leq 1$, an integer $s$, and parameter $L$, the strong restricted eigenvalue of $Q$ is,

$$\phi_{SRE}^2(Q, s, L) \equiv \min_{\theta} \left\{ \frac{\langle \theta, Q\theta \rangle}{\|\theta\|^2_{2}} : \theta \in \mathbb{R}^p, \|\theta\|_1 \leq (1 + L)\sqrt{s}\|\theta\|_2 \right\}.$$  

In general the cone to which $\theta$ belongs in Definition 2 is more constraining than the cone associated with the standard restricted eigenvalue condition of Bickel et al. [6]. Interestingly, due to the inclusion of the 1-column normalization constraint in Definition 2, up to absolute constants, the SRE condition is equivalent to the standard RE condition (with the 1-column normalization constraint also included in its definition) [4, Proposition 8.1].

Importantly, using further equivalence with $s$-sparse eigenvalue condition, [4, Theorem 8.3] establishes the SRE condition holds with high probability under the sub-gaussian design assumption.
We define the sequence of sets, with the fact that

\[ \text{Theorem 8. Bellec et al. [4, Theorem 8.3]. Let Assumptions 2 and 3 hold. Then there exist absolute constants } c_1, c_2 > 0 \text{ such that for } L \geq 0, \text{ if } n \geq \frac{c_1 \kappa^2 (2 + L)^2 s \log(2e\sigma/s)}{c_{\min}} \text{, then with probability at least } 1 - 3 \exp(-c_2 n/\kappa^4), \text{ we have that} \]

\[ \max_{i \in [p]} (\Sigma_n)_{ii} \leq 1 \]

and

\[ \phi_{SRE}^2(\Sigma_n, s, L) \geq \frac{c_{\min}}{2} \]

This result follows from [4, Theorem 8.3], the stated implication therein that the weighted restricted eigenvalue condition implies the strong restricted eigenvalue condition with adjusted constants, along with the fact that \( \phi_{SRE}^2(\Sigma, s, L) \geq C_{\min} \).

We define the sequence of sets,

\[ \mathcal{E}_n(s, L) = \{ X \in \mathbb{R}^{n \times p} : \phi_{SRE}^2(\Sigma_n, s, L) \geq \frac{c_{\min}}{2}, \max_{i \in [p]} \Sigma_{ii} \leq 1, \Sigma = X^T X/n \} \]

characterizing the class of design matrices satisfying both Definitions 1 and 2.

There are many classical results on \( \ell_1/\ell_2 \) consistency of the Lasso program,

\[ \hat{\beta}_L = \arg\min_{\beta \in \mathbb{R}^p} \frac{1}{2} \| y - X\beta \|^2 + \lambda \| \beta \|_1 \]

for sparse regression (see for example [22, Ch. 6]) when the model is specified as \( y = X\beta_0 + \epsilon \) for \( \epsilon \) i.i.d. that are sub-Gaussian with variance parameter \( \sigma^2 \). Such classical results have the confidence level of the non-asymptotic error tied directly to the tuning parameter. However, recently [4], through a more refined analysis, has obtained optimal rates for the Lasso estimator over varying confidence levels for a fixed regularization parameter. These results allow us to provide clean upper bounds on the Lasso parameter error in expectation.

**Lemma 9.** Let \( s \in [p] \), assume that the deterministic design matrix \( X \in \mathcal{E}_n(s, 7) \), and let Assumption 4 hold with \( \epsilon_i \sim \mathcal{N}(0, \sigma^2) \). If \( \hat{\beta}_L(\lambda) \) denotes the Lasso estimator with \( \lambda \geq (8 + 2\sqrt{2}) \sigma \sqrt{\frac{\log(2e\sigma/s)}{n}} \), \( 1 \leq q \leq 2 \), and \( \| \beta_0 \|_q \leq s \) then letting \( \phi_0^q = \phi_{SRE}^q(s, 7) \),

\[ \mathbb{E}[\| \hat{\beta}_L(\lambda) - \beta_0 \|_q^k] \leq \left( \frac{49\lambda s^{1/q}}{8\phi_0^q} \right)^k + \left( \frac{49}{8} \frac{(8 + 2\sqrt{2})\sigma}{s^{1-1/q}\sqrt{n}} \right)^k \frac{k(k - 1)}{2} \]

**Proof.** The proof follows easily by integrating the tail bound in Bellec et al. [4, Theorem 4.2], which provides that,

\[ \| \hat{\beta}_L(\lambda) - \beta_0 \|_q \leq \frac{49}{8} \left( \frac{1}{\log(1/\delta_0)} \left. \| \epsilon \|_q \right|_{\delta_0} \right) \mathbb{E}[\| \epsilon \|_q^k] \]

with probability at least \( 1 - \delta_0/2 \), where \( \delta(\lambda) = \exp\left(-\frac{\lambda \sqrt{n}}{8(8 + 2\sqrt{2})\sigma} \right) \), which satisfies \( \delta(\lambda) \leq \frac{s^p}{n^{p/4}} \).

Now, define \( \delta_0^* \) as the smallest \( \delta_0 \in (0, 1) \) for which \( \frac{1}{\phi_0^q} = \frac{\log(1/\delta_0^*)}{s^{1-1/q}\sqrt{n}} \), in which case \( \delta_0^* = (\delta(\lambda))^{s^{p/4}} \).

Then, \( Z_q = \frac{s\lambda \log(1/\delta_0)}{49s^{1/4}} \leq \log(1/\delta_0) \) with probability at least \( 1 - \delta_0/2 \), for all \( \delta_0 \in (0, \delta_0^*]. \)

Equivalently, \( \Pr[Z_q > t] \leq \frac{e^t}{T} \) for all \( t \geq T = \log(1/\delta_0^*) = \frac{1}{\phi_0^q} \log(1/\delta_0) \). Thus,

\[ \mathbb{E}[Z_q^k] = \int_0^\infty \int_0^T k t^{k-1} \Pr[Z_q > t] dt = \int_0^T k t^{k-1} + \int_T^\infty k t^{k-1} e^{-t} \leq \frac{T^k + \int_0^\infty k t^{k-1} e^{-t}}{2} \leq \frac{T^k + \int_0^T k t^{k-1} e^{-t}}{2} \leq \frac{k(k - 1)}{2} \]
which implies the conclusion,
\[
\|\hat{\beta}_L(\lambda) - \beta_0\|^2 \leq \left( \frac{49}{8} T\lambda s^{1/q} \right)^k + \left( \frac{49}{8} \lambda s^{1/q} \right)^k \frac{k(k-1)}{2} \leq \left( \frac{49\lambda s^{1/q}}{8\phi_0^2} \right)^k + \left( \frac{49 (8 + 2\sqrt{2})\sigma^2}{8 \cdot s^{1/q} \sqrt{n}} \right)^k \frac{k(k-1)}{2}
\]
where \( \lambda \geq (8 + 2\sqrt{2})\sigma^2 \sqrt{\log(2p\sigma^2)/n} \). \( \Box \)

Although the main results of Bellec et al. [4] are stated for Gaussian noise distributions, Bellec et al. [4, Theorem 9.1] also provides a complementary high-probability upper bound for the empirical process \( \frac{1}{n} \epsilon^T X u \) when \( \epsilon \) is sub-gaussian:

**Lemma 10.** Bellec et al. [4, Theorem 9.1] Let \( \delta_0 \in (0, 1) \), and let Assumption 4 hold (with variance parameter renamed to \( \sigma^2 \)) and assume the deterministic design matrix \( X \in \mathbb{R}^{n \times p} \) satisfies \( \max_{i \in [p]} \|X_i\|_2 / \sqrt{n} \leq 1 \). Then with probability at least \( 1 - \delta_0 \), for all \( u \in \mathbb{R}^p \),
\[
\frac{1}{n} \epsilon^T X u \leq 40\sigma\max \left( \sum_{j=1}^p u_j^2 \frac{\log(2p/j)}{n}, \frac{\|X u\|_2 \sqrt{\pi/2} + \sqrt{2\log(1/\delta_0)}}{\sqrt{n}} \right)
\]

The upper bound contains an additional, additive \( \sqrt{\pi/2} \) correction along with a change in absolute constants with respect to Bellec et al. [4, Theorem 4.1]. Hence we trace through the proof of Bellec et al. [4, Theorem 4.2] to derive a corresponding statement of Bellec et al. [4, Theorem 4.2] for sub-gaussian distributions.

**Lemma 11.** Let \( s \in [p], \gamma \in (0, 1) \) and \( \tau \in (0, 1 - \gamma] \) and assume the SRE(s, \( c_0 \)) condition holds \( c_0(\gamma, \tau) = \frac{1 + \gamma + \tau}{1 - \gamma - \tau} \). Let \( \lambda \geq \frac{40\sigma}{\gamma} \sqrt{\log(2p\sigma^2)/n} \). Then on the event in Lemma 10, for \( 1 \leq q \leq 2 \),
\[
\|\hat{\beta}_L(\lambda) - \beta_0\|_2 \leq \left( \frac{C_{\gamma,\tau}(s, \lambda, \delta_0)}{\tau} \lambda^s + \pi(1 + \tau + \gamma)^2 \gamma^2 \pi n \lambda \right)^{2/q - 1} \left( \frac{C_{\gamma,0}(s, \lambda, \delta_0)}{1 + \gamma} \lambda^s \sqrt{s} + \pi(1 + \gamma)^2 \gamma^2 \lambda^{2} \sqrt{2sn} \right)^{2 - 2/q}
\]
where \( C_{\gamma,\tau} = (1 + \gamma + \tau)^2 \left( \frac{\log(1/\delta_0)}{\gamma \log(1/\delta(\lambda))} \right) \frac{1}{\phi_0(s, c_0(\gamma, \tau))} \).

**Proof.** The argument simply requires tracing through the proof of Bellec et al. [4, Theorem 4.2] to accommodate the additional \( O\left( \frac{1}{\sqrt{n}} \right) \) term (and is nearly identical to Bellec et al. [4, Theorem 4.2]), so we only highlight the important modifications.

Following the proof of Bellec et al. [4, Theorem 4.2] we have,
\[
2\tau\lambda \|\hat{\beta}_L(\lambda) - \beta_0\|_1 + 2\|X(\hat{\beta}_L(\lambda) - \beta_0)\|_2^2/n \leq \Delta^* \tag{11}
\]
where \( \Delta^* = 2\tau\lambda \|\hat{\beta}_L(\lambda) - \beta_0\|_1 + \frac{2}{n} \epsilon^T X(\hat{\beta}_L(\lambda) - \beta_0) + 2\lambda \|\beta_0\|_1 - 2\lambda \|\hat{\beta}_L(\lambda)\|_1 \). Letting \( u = \hat{\beta}_L(\lambda) - \beta_0 \), we obtain
\[
\Delta^* \leq 2\lambda \left( (1 + \gamma) \|\hat{\beta}_L(\lambda) - \beta_0\|_1 - (1 - \tau) \sum_{j=s+1}^p u_j^2 \right) + 2\max(F(u), G(u))
\]
where \( F(u) = \gamma \left( \sqrt{s} \|u\|_2 + \sum_{j=s+1}^p u_j^2 \right) \) and \( G(u) = \frac{40\sigma}{\gamma} \left( \frac{\|X u\|_2}{\sqrt{n}} + \sqrt{2 \log(1/\delta_0)} \right) \). By definition of \( \delta(\lambda) = \exp\left( \frac{-40\lambda^2}{\gamma \log(1/\delta(\lambda))} \right) \) we have equivalently that, \( G(u) = \left( \lambda^s \gamma \sqrt{s} \sqrt{\log(1/\delta(\lambda))} / (\gamma \log(1/\delta(\lambda))) \right) + \frac{40\sqrt{\pi} \sqrt{2\gamma}}{\sqrt{n}} \|X u\|_2 / \sqrt{n} \).

We now consider two cases
1. $G(u) > F(u)$. Then,

$$||u||_2 \leq \left( \sqrt{\frac{\log(1/\delta_0)}{s \log(1/\delta(\lambda))}} + \frac{40 \sqrt{\pi/2\sigma}}{\lambda \sqrt{s} \sqrt{\gamma} \sqrt{n}} \right) ||Xu||_2 / \sqrt{n} \tag{12}$$

Thus,

$$\Delta^* \leq 2\lambda (1 + \tau) \sqrt{s} ||u||_2 + 2G(u)$$

$$2\lambda \sqrt{s}(1 + \tau + \gamma) \left( \sqrt{\frac{\log(1/\delta_0)}{s \log(1/\delta(\lambda))}} + \frac{40 \sqrt{\pi/2\sigma}}{\lambda \sqrt{s} \gamma \sqrt{n}} \right) ||Xu||_2 / \sqrt{n} \leq$$

$$2\lambda^2 s(1 + \tau + \gamma)^2 \left( \frac{\log(1/\delta_0)}{s \log(1/\delta(\lambda))} + \frac{800 \pi \sigma^2}{\lambda^2 s \gamma^2 \sqrt{n}} \right) + ||Xu||_2^2 / n =$$

$$2\lambda^2 s(1 + \tau + \gamma)^2 \left( \frac{\log(1/\delta_0)}{s \log(1/\delta(\lambda))} \right) + ||Xu||_2^2 / n + \frac{1600 \pi \sigma^2 (1 + \tau + \gamma)^2}{\gamma^2 n} \tag{13}$$

2. $G(u) \leq F(u)$. In this case,

$$\Delta^* \leq 2\lambda \left( (1 + \gamma + \tau) \sqrt{s} ||u||_2 - (1 - \gamma - \tau) \sum_{j=s+1}^p u_{2j}^* \right) = \Delta \tag{14}$$

Since $\Delta > 0$, $u$ belongs to the $SRE(s, c_0)$ cone and hence $\phi_0(s, c_0)||u||_2 \leq ||Xu||_2$. So,

$$\Delta^* \leq \Delta \leq \frac{2 (1 + \gamma + \tau) \lambda \sqrt{s}}{\phi_0(s, c_0)} ||Xu||_2 / \sqrt{n} \leq \left( \frac{(1 + \gamma + \tau) \lambda \sqrt{s}}{\phi_0(s, c_0)} \right)^2 + ||Xu||_2^2 / n \tag{15}$$

Assembling the two cases we conclude that,

$$2\tau ||\hat{\beta}_L(\lambda) - \beta_0||_1 \leq 2C_{\gamma, \tau}(s, \lambda, \delta_0) \lambda s + \frac{1600 \pi \sigma^2 (1 + \tau + \gamma)^2}{\gamma^2 n \lambda}$$

where $C_{\gamma, \tau}(s, \lambda, \delta_0) = (1 + \gamma + \tau)^2 \left( \frac{\log(1/\delta_0)}{s \log(1/\delta(\lambda))} \right) \vee \frac{1}{\phi_0^2(s, c_0(\gamma, \tau))}.$

Turning to upper bounding $u$ in the $\ell_2$ norm, we specialize to $\tau = 0$ and consider cases 1 and 2 from before.

1. $G(u) > F(u)$, then using Equations 11 and 13 we have,

$$||Xu||_2^2 / n \leq 2\lambda^2 s(1 + \gamma)^2 \left( \frac{\log(1/\delta_0)}{s \log(1/\delta(\lambda))} \right) + \frac{1600 \pi \sigma^2 (1 + \gamma)^2}{\gamma^2 n}$$

Combining the previous display with (12) we have,

$$||u||_2 \leq \left( \sqrt{2\lambda^2 s(1 + \gamma)^2 \left( \frac{\log(1/\delta_0)}{s \log(1/\delta(\lambda))} \right)} + \sqrt{n \log(1/\delta_0) / s \log(1/\delta(\lambda))} \right) \left( \frac{\log(1/\delta_0)}{s \log(1/\delta(\lambda))} + \frac{40 \sqrt{\pi/2\sigma}}{\lambda \sqrt{s} \gamma \sqrt{n}} \right)$$

$$= \sqrt{2s(1 + \gamma) \lambda} \left( \frac{\log(1/\delta_0)}{s \log(1/\delta(\lambda))} \right) + \frac{1600 \pi (1 + \gamma) \sigma^2}{\gamma^2 \lambda \sqrt{2sn}} + \sqrt{2s(1 + \gamma) \lambda} \frac{\log(1/\delta_0)}{s \log(1/\delta(\lambda))} \cdot \frac{1600 \pi \sigma^2 (1 + \gamma)}{\gamma^2 \lambda \sqrt{2sn}}$$

$$\leq 3 \left( \sqrt{2s(1 + \gamma) \lambda} \left( \frac{\log(1/\delta_0)}{s \log(1/\delta(\lambda))} \right) + \frac{1600 \pi \sigma^2 (1 + \gamma)}{\gamma^2 \lambda \sqrt{2sn}} \right)$$

using subadditivity of $\sqrt{\cdot}$.

2. $G(u) \leq F(u)$. Equations 11 and 14 implies that $\Delta \geq \Delta^* \geq 0$ a.s. Hence $u$ is contained in $SRE(s, 1 + \gamma/\gamma)$. and

$$||u||_2 \leq \frac{||Xu||_2}{n \phi_0(s, 1 + \gamma/\gamma)} \leq \frac{(1 + \gamma) \lambda \sqrt{s}}{\phi_0^2(s, 1 + \gamma/\gamma)}$$

using (11) and (15), and recalling we set $\tau = 0$. Assembling these two cases we conclude,

$$(1 + \gamma)||\hat{\beta}_L(\lambda) - \beta_0||_2 \leq 3 \left( C_{\gamma,0}(s, \lambda, \delta_0) \lambda \sqrt{s} + \frac{1600 \pi \sigma^2 (1 + \gamma)^2}{\gamma^2 \lambda \sqrt{2sn}} \right)$$

29
So using the norm interpolation inequality $||\hat{\beta}_L(\lambda) - \beta_0||_q \leq ||\hat{\beta}_L(\lambda) - \beta_0||_1^{2/q} ||\hat{\beta}_L(\lambda) - \beta_0||_2^{2-2/q}$,
\[
||\hat{\beta}_L(\lambda) - \beta_0||_q \leq \left( \frac{C_{\gamma,\tau}(s, \lambda, \delta_0)}{\gamma} \lambda s + \frac{1600 \pi \sigma^2 (1 + \tau + \gamma)^2}{\gamma^2 n \lambda} \right)^{2/q - 1} \left( 3 + \frac{C_{\gamma,0}(s, \lambda, \delta_0)}{1 + \gamma} \lambda \sqrt{s} + \frac{1600 \pi \sigma^2 (1 + \gamma)}{\gamma^2 n \lambda^2} \right)^{2-2/q}.
\]

We can now derive a corresponding moment bound for error as before\(^5\).

**Lemma 12.** Let $s \in [p]$, assume that the deterministic design matrix $X \in \mathcal{E}_n(s, 7)$, and let Assumption 4 hold (with variance parameter renamed to $\sigma^2$). If $\hat{\beta}_L(\lambda)$ denotes the Lasso estimator with $\lambda \geq 80 \sigma \sqrt{\frac{\log(2ep/s)}{n}}$, $1 \leq q \leq 2$, and $||\beta_0||_0 \leq s$, then letting $\phi_0^2 = \phi^2_{SRE}(s, 7)$,
\[
\mathbb{E}[||\hat{\beta}_L(\lambda) - \beta_0||_1^k] \leq 2^{k-1} \left( \frac{13 \lambda s}{\phi_0^2} \right)^k + \left( \frac{13 \pi \sigma}{\sqrt{n}} \right)^k \left( \frac{k(k-1)}{2} + \frac{250000}{n \lambda} \right)^k
\]
\[
\mathbb{E}[||\hat{\beta}_L(\lambda) - \beta_0||_2^k] \leq 2^{k-1} \left( \frac{5 \lambda \sqrt{s}}{\phi_0^2} \right)^k + \left( \frac{13 \pi \sigma}{\sqrt{n s}} \right)^k \left( \frac{k(k-1)}{2} + \frac{250000}{n \lambda \sqrt{s}} \right)^k
\]

**Proof.** We instantiate the result of Lemma 12 with $\gamma = 1/2$ and $\tau = 1/4$ in which case $c_0 = 7$, $(1 + \tau + \gamma) = 49/16$, $\frac{1 + \gamma}{1 - \gamma} = 3$, $1 + \gamma = 3/2$. Defining $D(\delta_0, \lambda, s) = \left( \frac{\log(1/\delta_0)}{s \log(1/\delta(\lambda))} \right)$ and $\phi_0^2 = \phi_{SRE}(s, 7)$, we have,
\[
||\hat{\beta}_L(\lambda) - \beta_0||_1 \leq 13D(\delta_0, \lambda, s) \lambda s + \frac{250000 \sigma^2}{n \lambda}
\]
\[
||\hat{\beta}_L(\lambda) - \beta_0||_2 \leq 5D(\delta_0, \lambda, s) \lambda \sqrt{s} + \frac{250000 \sigma^2}{n \lambda \sqrt{s}}
\]

with probability $1 - \delta_0$ where $\delta(\lambda) = \exp\left( -\left( \frac{\lambda \sqrt{s}}{80 \sigma} \right)^2 \right)$. Now, define $\delta_0^*$ as the smallest $\delta_0 \in (0, 1)$ for which $\frac{1}{\phi_0^2} = \frac{\log(1/\delta_0)}{s \log(1/\delta(\lambda))}$, in which case $\delta_0^* = (\delta(\lambda))^\frac{1}{\phi_0^2}$.

Then, $Z_1 = \frac{(||\hat{\beta}_L(\lambda) - \beta_0||_1 - 250000 \sigma^2 \chi s \log(1/\delta(\lambda)))}{\lambda \sqrt{s}} \leq \log(1/\delta_0)$ and $Z_2 = \frac{(||\hat{\beta}_L(\lambda) - \beta_0||_2 - 250000 \sigma^2 \chi s \log(1/\delta(\lambda)))}{\lambda \sqrt{s}}$ with probability at least $1 - \delta_0$, for all $\delta_0 \in (0, \delta_0^*]$. Equivalently, $\Pr[Z_q > t] \leq e^{-t}$ for all $t \geq T = \log(1/\delta_0^*) = \frac{1}{\phi_0^2} \log(1/\delta(\lambda))$ for $q \in \{1, 2\}$. As before,
\[
\mathbb{E}[Z_q^k] \leq T^k + k(k-1).
\]

Since $\mathbb{E}[||\hat{\beta}_L(\lambda) - \beta_0||_q^k] = \mathbb{E}[||\hat{\beta}_L(\lambda) - \beta_0||_q + c + c]^k] \leq 2^{k-1} \left( \mathbb{E}[||\hat{\beta}_L(\lambda) - \beta_0||_q + c] \right)^k + k(c)^k,
\]
we conclude,
\[
\mathbb{E}[||\hat{\beta}_L(\lambda) - \beta_0||_1^k] \leq 2^{k-1} \left( \frac{13 \lambda s}{\phi_0^2} \right)^k + \left( \frac{13 \pi \sigma}{\sqrt{n}} \right)^k \left( \frac{k(k-1)}{2} + \frac{250000 \sigma^2}{n \lambda} \right)^k \leq 2^{k-1} \left( \frac{13 \lambda s}{\phi_0^2} \right)^k + \left( \frac{13 \pi \sigma}{\sqrt{n}} \right)^k \left( \frac{k(k-1)}{2} + \frac{250000 \sigma^2}{n \lambda} \right)^k
\]
\[
\mathbb{E}[||\hat{\beta}_L(\lambda) - \beta_0||_2^k] \leq 2^{k-1} \left( \frac{5 \lambda \sqrt{s}}{\phi_0^2} \right)^k + \left( \frac{5 \pi \sigma}{\sqrt{n s}} \right)^k \left( \frac{k(k-1)}{2} + \frac{250000 \sigma^2}{n \lambda \sqrt{s}} \right)^k \leq 2^{k-1} \left( \frac{5 \lambda \sqrt{s}}{\phi_0^2} \right)^k + \left( \frac{5 \pi \sigma}{\sqrt{n s}} \right)^k \left( \frac{k(k-1)}{2} + \frac{250000 \sigma^2}{n \lambda \sqrt{s}} \right)^k
\]

\(^5\)for convenience we only state for the $\ell_1$ and $\ell_2$ norms an analogous result to Lemma 9 can be derived with more computation.
where \( \lambda \geq 80\sigma \sqrt{\frac{\log(2ep/s)}{n}}. \)

The aforementioned results establish Lasso consistency (in expectation) conditioned on the event \( X \in E_n(s, 7) \). Generalizing these results to an unconditional statement (on \( X \)) requires the following deterministic lemma to control the norm of the error vector \( \| \hat{\beta}_L(\lambda) - \beta_0 \|_1 \) on the “bad” events \( X \notin E_n(s, 7) \) where we cannot guarantee a “fast” rate for the Lasso.

**Lemma 13.** Let \( \hat{\beta}_L(\lambda) \) be the solution of the Lagrangian lasso, then

\[
\| \hat{\beta}_L(\lambda) - \beta_0 \|_1 \leq \frac{1}{2n} \| \epsilon \|_2^2/\lambda + 2\| \beta_0 \|_1.
\]

**Proof.** By definition we have that,

\[
\frac{1}{2n} \| y - X \hat{\beta}_L(\lambda) \|_2^2 + \lambda \| \hat{\beta}_L \|_1 \leq \frac{1}{2n} \| \epsilon \|_2^2 + \lambda \| \beta_0 \|_1 \implies \| \hat{\beta}_L(\lambda) \|_1 \leq \frac{1}{2n} \| \epsilon \|_2^2/\lambda + \| \beta_0 \|_1
\]

So by the triangle inequality we obtain that,

\[
\| \hat{\beta}_L(\lambda) - \beta_0 \|_1 \leq \frac{1}{2n} \| \epsilon \|_2^2/\lambda + 2\| \beta_0 \|_1.
\]

With this result in hand we can combine our previous results to provide our final desired consistency result for the Lasso.

**Lemma 14.** Let Assumptions 1, 2, 3, 4 hold (with variance parameter renamed to \( \sigma^2 \)). Then there exist absolute constants \( c_1, c_2 > 0 \) such that if \( n \geq c_1(k)^2 s \log(2ep/s), \) and \( \hat{\beta}_L(\lambda) \) is a solution of the Lagrangian Lasso then for \( q \in 1, 2 \)

\[
\mathbb{E}_{X, \epsilon} \left[ \| \hat{\beta}_L(\lambda) - \beta_0 \|_q^k \right] \leq \mathbb{E}_{X, \epsilon} \left[ \| \hat{\beta}_L(\lambda) - \beta_0 \|_q^k 1[X \in E_n(s, 7)] \right] + \left( \frac{\sigma^2k}{\lambda^k} + 2^{2k} \| \beta_0 \|_1^k \right) \left( 2e^{-\frac{c}{2n}} \right)
\]

where the first term can be bounded exactly as the conclusion of either Lemmas 9 or 12 with appropriate choice of regularization parameter \( \lambda_\beta \).

**Proof.** Consider the event \( \{ X \notin E_n(s, 7) \} \). For \( q \in 1, 2 \), we can split the desired expectation over the corresponding indicator r.v. giving,

\[
\mathbb{E}_{X, \epsilon} \left[ \| \hat{\beta}_L(\lambda) - \beta_0 \|_q^k \right] = \mathbb{E}_{X, \epsilon} \left[ \| \hat{\beta}_L(\lambda) - \beta_0 \|_q^k 1[X \in E_n(s, 7)] \right] + \mathbb{E}_{X, \epsilon} \left[ \| \hat{\beta}_L(\lambda) - \beta_0 \|_q^k 1[X \notin E_n(s, 7)] \right]
\]

(16)

The first term can be bounded using independence of \( X \) and \( \epsilon \) to integrate over \( \epsilon \) restricted to the set \( \{ X \notin E_n(s, 7) \} \) (by applying Lemmas 9 and 12). The second term can be bounded using Cauchy-Schwarz and Lemma 13 which provides a coarse bound on the Lasso performance which always holds,

\[
\mathbb{E}_{X, \epsilon} \left[ \| \hat{\beta}_L(\lambda) - \beta_0 \|_q^k 1[X \notin E_n(s, 7)] \right] \leq \sqrt{\mathbb{E}_{X, \epsilon} \left[ \| \hat{\beta}_L(\lambda) - \beta_0 \|_q^{2k} \right]} \sqrt{\mathbb{P}_X[X \notin E_n(s, 7)]}
\]

(17)

The hypotheses of Theorem 8 are satisfied, so \( \sqrt{\mathbb{P}_X[X \notin E_n(s, 7)]} \leq 2e^{-\frac{c}{2n}}. \) Using Lemma 13 along with the identity \( (a + b)^k \leq 2^{k-1}(a^k + b^k) \) we have that,

\[
\mathbb{E}_{X, \epsilon} \left[ \| \hat{\beta}_L(\lambda) - \beta_0 \|_q^{2k} \right] \leq \mathbb{E}_{X, \epsilon} \left[ \| \hat{\beta}_L(\lambda) - \beta_0 \|_1^{2k} \right] \leq 2^{2k-1} \cdot \mathbb{E}_{\epsilon} \left[ \sum_{j=1}^n c_j^2/n \right]^{2k} + 2^{2k} \| \beta_0 \|_1^{2k}
\]

(18)
With this result we first provide a conditional (on \( \mathbb{E}[Z] \)) concentration result providing control on the fluctuations which can be thought of as a standard bias-variance decomposition for the ridge estimator.

As previously noted the first term in Equation (19) is computed exactly as the final result of either Lemmas 9 or 12.

In (18), inserting the coarse bound in (18) into (17) and combining with (16) gives the result using subadditivity of \( \sqrt{\cdot} \),

\[
\mathbb{E}_{X, \epsilon} \left[ \| \beta_R(\lambda) - \beta_0 \|_q^k \right] \leq \mathbb{E}_{X, \epsilon} \left[ \| \beta_L(\lambda) - \beta_0 \|_q^k \mathbb{1}[X \in \mathcal{E}_n(s,7)] \right] + \left( \frac{\sigma^{2k} + 2^{2k} \| \beta_0 \|_1^k}{\lambda^k} \right) \left( 2e^{-\frac{n}{2}} \right)
\]

As previously noted the first term in Equation (19) is computed exactly as the final result of either Lemmas 9 or 12.

F.2 Random Design Matrices and Ridge Regression Consistency

Here we collect several useful results we use to show consistency of the ridge regression estimator in the random design setting. There are several results showing risk bounds for ridge regression in the random design setting, see for example Hsu et al. [16]. Such results make assumptions which do not match our setting and also do not immediately imply control over the higher moments of the \( \ell_2 \)-error which are also needed in our setting. Accordingly, we use a similar approach to that used for the Lasso estimator to show appropriate non-asymptotic risk bounds (in expectation) for ridge regression.

To begin recall we define the ridge estimator \( \beta_R(\lambda) = \arg\min_{\beta} \frac{1}{2} \left( \| y - X \beta \|_2^2 + \lambda \| \beta \|_2^2 \right) \) which implies \( \beta_R(\lambda) = (X^\top X + \lambda I_p)^{-1} X^\top y \). Throughout we also use \( \Sigma_n = X_n^\top X, \Sigma_\lambda = X_n^\top X / n + \frac{2}{n} I_p \) and \( \Pi_\lambda = I_p - (\Sigma_\lambda)^{-1} \Sigma_n \). Note that under Assumption 1, \( \beta_R - \beta_0 = -\Pi_\lambda \beta_0 + \Sigma_\lambda^{-1} X^\top \epsilon / n \), which can be thought of as a standard bias-variance decomposition for the ridge estimator.

We first introduce a standard sub-Gaussian concentration result providing control on the fluctuations of the spectral norm of the design matrix which follows immediately from Wainwright [25, Theorem 6.5].

**Lemma 15.** Let \( x_1, \ldots, x_n \) be i.i.d. random vectors satisfying Assumptions 2 and 3 with sample covariance \( \Sigma_n = \frac{1}{n} X^\top X \), then there exist universal constants \( c_1, c_2, c_3 \) such that for \( n \geq c_1 n^{4} C_{\text{cond}}^{2} \),

\[
\| \Sigma_n - \Sigma \|_2 \leq C_{\text{min}} \frac{1}{2}
\]

with probability at least \( 1 - c_2 e^{-c_3 n/(n^{4} C_{\text{cond}}^2)} \).

With this result we first provide a conditional (on \( X \)) risk bound for ridge regression. For convenience throughout this section we define the set of design matrices \( \mathcal{E}_n = \{ X : \forall v \text{ such that } \| v \|_2 = 1, v^\top \Sigma v \geq C_{\text{min}} \} \).

**Lemma 16.** Let Assumptions 2 and 4 hold (with variance parameter renamed to \( \sigma^2 \)) and assume a deterministic design matrix \( X \in \mathcal{E}_n \) and that \( n \geq p \). Then if \( \beta_R(\lambda) \) denotes the solution to the ridge regression program, with \( \lambda \leq \lambda_\star = \arg\min_{\lambda} \left( \frac{\lambda}{C_{\text{min}} + \lambda / n} \right)^4 \| \beta_0 \|_2^4 + \sigma^4 p^2 / n^2 \left( \frac{C_{\text{max}}}{C_{\text{min}} + \lambda / n} \right)^2 \),

\[
\left( \mathbb{E} \left[ \| \beta_R(\lambda) - \beta_0 \|_2^4 \right] \right)^{1/2} \leq O \left( \frac{\sigma^2 C_{\text{cond}} p}{C_{\text{min}} n} \right).
\]
Proof. Recall the standard bias variance decomposition $\hat{\beta}_R(\lambda) - \beta_0 = -\Pi_{\lambda}^2 + \frac{1}{\lambda} \Sigma_{\lambda}^{-1} X^T \epsilon/n$. So $\|\hat{\beta}_R(\lambda) - \beta_0\|_2 \leq 64 \left( (\beta_0 \Pi^2_\lambda \beta_0)^2 + (\epsilon^T X \Sigma_{\lambda}^{-1} \cdot \Sigma_{\lambda}^{-1} X^T \epsilon/n)^2 \right)$. Using the SVD of $X / \sqrt{n} = U^T \Lambda V$ we see that $\Sigma_{\beta_0} = V^T \Lambda V = V^T \Lambda D V$.

Further, on the event $\mathcal{E}_n$ we have that $\frac{1}{p} C_{\min} \leq d_i \leq \frac{3}{2} C_{\max}$ for $i \in [p]$ where $d_i = D_{ii}$ by the Weyl inequalities. So on $\mathcal{E}_n$, $\beta_0^T V^T (\text{diag}(\frac{\lambda/n}{\lambda + \lambda/n}))^2 V \beta_0 \leq O((\frac{\lambda/n}{\lambda + \lambda/n})^2 \|\beta_0\|^2_2)$. Define $S = \epsilon^T X \Sigma_{\lambda}^{-1} \cdot \Sigma_{\lambda}^{-1} X^T \epsilon/n$, we have that $S = U^T \text{diag}(\frac{\lambda/n}{\lambda + \lambda/n})^2 U \leq O(U^T \text{diag}(\frac{C_{\max}^2 (\frac{\lambda/n}{\lambda + \lambda/n})^2}) U)$ on $\mathcal{E}_n$, which also has at most rank $p$ since $\Lambda$ has at most $p$ non-zero singular values. Hence applying Lemma 19 we find that $\mathbb{E}(\epsilon^T S \epsilon)^2 \leq O(\sigma^4 p^2 (\frac{C_{\max}^2}{C_{\min}^2})^2)$. Combining, gives that

$$
\mathbb{E} \left( \left\| \hat{\beta}_R(\lambda) - \beta_0 \right\|_2^4 \right) \leq c_1 \left( \left( \frac{\lambda/n}{C_{\min}^2 + \lambda/n} \right)^4 \|\beta_0\|^4_2 + \sigma^4 p^2/n^2 \left( \frac{C_{\max}^2}{C_{\min}^2 + \lambda/n} \right)^2 \right).
$$

for some universal constant $c_1$. Since by definition $\lambda_*$ minimizes the upper bound in the above expression it is upper bounded by setting $\lambda = 0$ in the same expression so,

$$
\mathbb{E} \left( \left\| \hat{\beta}_R(\lambda) - \beta_0 \right\|_2^4 \right) \leq O \left( \sigma^4 p^2/n^2 \left( \frac{C_{\max}^2}{C_{\min}^2} \right)^2 \right).
$$

We can further check that the upper bound is decreasing over the interval $[0, \lambda_*$] and hence the conclusion follows. As an aside a short computation shows the optimal choice of $\lambda_* = (p_{\mathrm{cond}} C_{\max}^2 n \sigma^4/p \|\beta_0\|^2_2)^{1/3}$.

We now prove a simple result which provides a crude bound on the error of the ridge regression estimate we deploy when $X \notin \mathcal{E}_n$.

**Lemma 17.** Let $\hat{\beta}_R(\lambda)$ be the solution of the ridge regression program $\hat{\beta}_R(\lambda) = \arg \min_{\beta} \|y - X \beta\|^2_2 + \lambda \|\beta\|^2_2$, then

$$
\left\| \hat{\beta}_R(\lambda) - \beta_0 \right\|^2_2 \leq 4 \left( \|\epsilon\|^2_2/\lambda + \|\beta_0\|^2_2 \right).
$$

**Proof.** By definition we have that,

$$
\left\| y - X \hat{\beta}_R(\lambda) \right\|^2_2 + \lambda \left\| \hat{\beta}_R(\lambda) \right\|^2_2 \leq \|\epsilon\|^2_2 + \lambda \left\| \beta_0 \right\|^2_2 \implies \left\| \hat{\beta}_R(\lambda) \right\|^2_2 \leq \|\epsilon\|^2_2/\lambda + \left\| \beta_0 \right\|^2_2
$$

So we obtain that,

$$
\left\| \hat{\beta}_R(\lambda) - \beta_0 \right\|^2_2 \leq 2 \left( \left\| \hat{\beta}_R(\lambda) \right\|^2_2 + \left\| \beta_0 \right\|^2_2 \right) \leq 4 \left( \|\epsilon\|^2_2/\lambda + \|\beta_0\|^2_2 \right).
$$

Finally, we will prove the final result which will provide an unconditional risk bound in expectation for the ridge regression estimator.

**Lemma 18.** Let Assumptions 1, 2, 3, 4 hold (with variance parameter renamed to $\sigma^2$). Then there exist universal constants $c_1, c_2, c_3 > 0$ such that if $n \geq c_1 \kappa^4 C_{\text{cond}}^2 p$, and $\hat{\beta}_R(\lambda)$ a solution of the ridge regression program $\hat{\beta}_R(\lambda) = \arg \min_{\beta} \frac{\lambda/n}{C_{\min}^2 + \lambda/n}^4 \|\beta_0\|^4_2 + \sigma^4 p^2 \left( \frac{C_{\max}^2}{C_{\min}} + \lambda/n \right)^2$,

$$
\mathbb{E}_{X,\epsilon} \left[ \left\| \hat{\beta}_R(\lambda) - \beta_0 \right\|^2_2 \right] \leq \mathbb{E}_{X,\epsilon} \left[ \left\| \hat{\beta}_R(\lambda) - \beta_0 \right\|^2_2 \mathbb{1}[X \in \mathcal{E}_n] \right] + O \left( \frac{\lambda^2 \sigma^4 p}{\kappa^4} e^{-n^{c_3} \kappa^4 C_{\text{cond}}^2} \right).
$$

Moreover if $\|\beta_0\|_\infty = O(1)$ then,

$$
\sqrt{\mathbb{E}_{X,\epsilon} \left[ \left\| \hat{\beta}_R(\lambda) - \beta_0 \right\|^2_2 \right]} \leq O \left( \frac{\sigma^2 C_{\text{cond}} p}{C_{\min}} \right).
$$

where the $O$ hides universal constants in $C_{\max}, C_{\min}, C_{\text{cond}}, \kappa$ in the final statement.
Proof. Decomposing as
\[
\mathbb{E} \left[ \|\hat{\beta}_R(\lambda) - \beta_0\|^4_2 \right] = \mathbb{E}_{\mathbf{X}, \epsilon} \left[ \|\hat{\beta}_R(\lambda) - \beta_0\|^4_2 1_{\mathbf{X} \in \mathcal{E}_n} \right] + \mathbb{E}_{\mathbf{X}, \epsilon} \left[ \|\hat{\beta}_R(\lambda) - \beta_0\|^4_2 1_{\mathbf{X} \notin \mathcal{E}_n} \right]
\]
We can bound the second term explicitly using the Cauchy-Schwarz inequality as,
\[
\mathbb{E} \left[ \|\hat{\beta}_R(\lambda) - \beta_0\|^4_2 1_{\mathbf{X} \notin \mathcal{E}_n} \right] \leq \sqrt{\mathbb{E}_{\mathbf{X}, \epsilon} \left[ \|\hat{\beta}_R(\lambda) - \beta_0\|^2 \right]} \sqrt{\Pr[\mathbf{X} \notin \mathcal{E}_n]} \leq O\left( \frac{n^2 \sigma^4}{\lambda^2} + \|\beta_0\|^4_2 \right) e^{-\frac{C_{\text{cond}}^2 n}{\kappa^4}}
\]
using the crude upper bound from Lemma 17 to upper bound the first term and Lemma 15 to bound the probability in the second term.

For the second statement note that we can bound the first term using the using the independence of \(\mathbf{X}, \epsilon\) and Lemma 16, to conclude,
\[
\sqrt{\mathbb{E}_{\mathbf{X}, \epsilon} \left[ \|\hat{\beta}_R(\lambda) - \beta_0\|^2_2 1_{\mathbf{X} \in \mathcal{E}_n} \right]} \leq O\left( \frac{\sigma^2 C_{\text{cond}} p}{C_{\text{min}} n} \right).
\]
With the specific lower bound on \(\lambda\) in the theorem statement, when \(\|\beta_0\|_\infty / \sigma_\epsilon = O(1)\) and \(n \gtrsim \kappa^4 C_{\text{cond}}^2 p\) we have,
\[
\sqrt{\mathbb{E}_{\mathbf{X}, \epsilon} \left[ \|\hat{\beta}_R(\lambda) - \beta_0\|^4_2 1_{\mathbf{X} \in \mathcal{E}_n} \right]} \leq O\left( \frac{\sigma^2 C_{\text{cond}} p}{C_{\text{min}} n} \right).
\]

Finally, we prove a simple matrix expectation upper bound,

\textbf{Lemma 19.} Let \(\mathbf{S} \in \mathbb{R}^{n \times n}\) be a (deterministic) p.s.d. matrix with rank at most \(p\) satisfying \(\|\mathbf{S}\|_2 \leq z\), and let \(\epsilon \in \mathbb{R}^n\) satisfy Assumption 4. Then
\[
\mathbb{E} \left[ (\epsilon^\top \mathbf{S} \epsilon)^2 \right] \leq O(\sigma^4 z^2 p^2).
\]

\textbf{Proof.} This follows by a straightforward computation using the sub-Gaussianity of each \(\epsilon_i:\)
\[
\mathbb{E} \left[ (\epsilon^\top \mathbf{S} \epsilon)^2 \right] \leq O(\sum_i S_{ii}^2 \mathbb{E}[\epsilon_i^4] + \sum_{i \neq j} S_{ij}^2 \mathbb{E}[\epsilon_i^2 \epsilon_j^2] + \sum_{i \neq j} S_{ii} S_{jj} \mathbb{E}[\epsilon_i^2 \epsilon_j^2]) \leq O(\sigma^4 \|\mathbf{S}\|_F^4 + \sigma^4 \text{Tr}(\mathbf{S})^2) \leq O(\sigma^4 p^2 z^2).
\]

\section{G Experimental Details}

\subsection{G.1 Implementation Details}
All algorithms were implemented in Python (with source code to be released to be upon publication). The open-source library scikit-learn was used to fit the Lasso estimator, the cross-validated Lasso estimators, and the random forest regression models used in the synthetic/real data experiments. The convex program for the JM-style estimator was solved using the open-source library CVXPY equipped with the MOSEK solver [12].

Note the debiased estimators presented require either refitting the auxiliary regression for \(g(\cdot)\) (i.e. the Lasso estimator or a random forest) in the case of the OM estimators, or resolving the convex program in Eq. (3) for each new test point \(\mathbf{x}_*\). Although this presents a computational overhead in both our synthetic and real-data experiments, such computations are trivially parallelizable across the test points \(\mathbf{x}_*\). As such, we used the open-source library Ray to parallelize training of the aforementioned models [19]. All experiments were run on 48-core instances with 256 GB of RAM.

\subsection{G.2 Data Preprocessing and Cross-Validation Details}
In all of the experiments (both synthetic and real data) the training covariates (in the design \(\mathbf{X}\)) was first centered and scaled to have features with mean zero and unit variance. Subsequently the vector of \(y\) values was also centered by subtracting its mean; that is \(y \rightarrow y - \bar{y}\). After any given model was fit
the mean \( \bar{y} \) was added back to the (y-centered) prediction \( \theta \) of the model. On account of this centering, the Lasso estimators were not explicitly fit with an intercept term (we found the performance was unchanged by not performing the demeaning and instead explicitly fitting the intercept for the Lasso baseline). In each case the cross-validated Lasso estimator was fit, the regularization parameter was selected by cross validation over a logarithmically spaced grid containing a 100 values spaced between \( 10^{-6} \) and \( 10^3 \). The cross-validated ridge estimator was fit by using leave-one-out cross-validation to select the regularization parameter over a logarithmically spaced grid containing a 100 values spaced between \( 10^{-2} \) and \( 10^6 \) for the synthetic experiments, while a range of \( 10^{-6} \) and \( 10^1 \) was used for the real data. The \( \ell_1 \) and \( \ell_1/\ell_2 \) ratio parameter for the elastic net were also set using cross-validation by letting the \( \ell_1 \) regularization parameter over a logarithmically spaced grid containing a 100 values spaced between \( 10^{-6} \) and \( 10^3 \), while the \( \ell_1/\ell_2 \) ratio parameter was allowed to range over \([1.1, 5, 7, 9, 95, 99.1]\). In the case of the real data experiments the random forest regressors (RF) used in the \( g(\cdot) \) models were fit using a default value of 50 estimators in each RF.

G.3 JM-style Estimator Details

Note that \( \lambda_w \) was chosen for the JM-style estimator using the heuristic to search for the smallest \( \lambda_w \) in a set for which the convex program in Eq. (3) is feasible. If no such value existed (i.e. all the programs were infeasible) we defaulted to simply predicting using the base Lasso regression in all cases (which is equivalent to using \( w = 0 \)).

G.4 OM Estimators Details

As described in the main text, the OM estimators use 2-fold data-splitting. Such a procedure can be sample-inefficient since only a fraction of the data is used in each stage of the procedure. For the OM methods used in the experiments we instead used a more general \( K \)-fold cross-fitting as described in [11], with \( K = 5 \) and \( K = 10 \).

The OM methods can be fit exactly as described in the paper with the following modifications. First the original dataset is split into \( K \) equally-sized folds we denote as \((X_{I_1}, y_{I_1}), \ldots, (X_{I_K}, y_{I_K})\); here the index sets range over the datapoints as \( I_1 = \{1, \ldots, \frac{n}{K} \}, I_2 = \{ \frac{n}{K} + 1, \ldots, \frac{2n}{K} \} \) etc... We also use \((X_{I_{-i}}, y_{I_{-i}})\) to describe \( K \)-leave-one-out subsets of the original folds which contain the union of datapoints in all but the \( i \)th fold of data.

Then, \( K \) sets of first-stage regressions are trained on the \( K \)-leave-one-out subsets to produce \((f^{-1}, g^{-1}), \ldots, (f^{-K}, g^{-K})\); explicitly the pair \( (f^{-i}, g^{-i}) \) is fit on \((X_{I_{-i}}, y_{I_{-i}})\). Finally the empirical moment equations can be solved for \( \hat{g}_{OM} \) by summing over the entire dataset, but evaluating the \((f^{-i}, g^{-i})\) model on only the \( i \)th fold:

\[
\sum_{i \in K} \sum_{j \in I_i} m(t_j, y_j, \hat{g}_{OM}, z_j f^{-i}, g^{-i}(z_j)) = 0.
\]

The estimator for the variance \( \mu_2 \) can also be computed in an analogous fashion, \( \sum_{i \in K} \sum_{j \in I_i} t_j (t_j - g^{-i}(z_j)) \). More details on this procedure can be found in Chernozhukov et al. [11] and Mackey et al. [18]. Note that since \( K \) is chosen to be constant, our theoretical guarantees also apply to this estimator up to constant factors.

Also though the thresholding step (with the parameter \( \tau \)) is used in our theoretical analysis to control against the denominator \( \mu_2 \) being too small, we found in practice the estimate of \( \mu_2 \) concentrated quickly and was quite stable. Hence we found explicitly implementing the thresholding step was unnecessary and we did not include this in our implementation.

G.4.1 OM \( q \) moments

In Section 3.2 we focus our analysis on the OM \( f \) moments but also introduce the first-order orthogonal \( q \) moments, whose practical efficacy we explore in our real data experiments. For completeness we include the details of the algorithm to predict with \( q \)-moments here. The primary difference with respect to the \( f \)-moments is with respect to how the \( q \) or \( f \) regression is fit, the \( g \) regression is handled identically. For simplicity, we present the algorithm in parallel to how the \( f \) moments are introduced in the main text (without the \( K \)-fold cross-fitting), although \( K \)-fold cross-fitting is used in practice exactly as described above.
After the data reparametrization we have \( x_i = [t_i, z_i] = (U^{-1})^T x_i \). In the reparametrized basis, the linear model becomes,

\[
y_i = \theta t_i + z_i^T f_0 + \epsilon_i \quad t_i = g_0(z_i) + \eta_i
\]

where \( q_0(z_i) = \theta g_0(z_i) + z_i^T f_0 \).

- The first fold \((X^{(1)}, y^{(1)})\) is used to run two first-stage regressions. We estimate \( q_0 \) using a linear estimator (such as the Lasso) by directly regressing \( y^{(1)} \) onto \( z^{(1)} \) to produce the vector \( \hat{q} \). Second we estimate \( g_0(\cdot) \) by regressing \( t^{(1)} \) onto \( z^{(1)} \) to produce a regression model \( \hat{g}(\cdot) : \mathbb{R}^{p-1} \rightarrow \mathbb{R} \).
- Then, we estimate \( E[\eta_i^2] \) as \( \mu_2 = \frac{1}{n} \sum_{i=1}^{n} (t_i - \hat{g}(z_i))^2 \) where the sum is taken over the second fold of data; crucially \((t_i, z)\) are (statistically) independent of \( \hat{g}(\cdot) \) in this expression.
- If \( \mu_2 \leq \tau \) for a threshold \( T \) we simply output \( \hat{y}_{OM} = x_i^T \hat{\beta} \). If \( \mu_2 \geq \tau \) we estimate \( \theta \) by solving the empirical moment equation:

\[
\sum_{i=n/2+1}^{n} m(t_i, y_i, \hat{y}_{OM}, z_i^T \hat{q}, \hat{g}(z_i)) = 0 \implies \hat{y}_{OM} = \frac{1}{\mu_2} \sum_{i=n/2+1}^{n} (y_i - z_i^T \hat{q}) (t_i - \hat{g}(z_i))
\]

where the sum is taken over the second fold of data and \( m \) is defined in (7).

### G.4.2 Synthetic Data Experiment Details

The experiments on synthetic data were conducted as described in the main text in Section 4. In each case for the JM-style estimator the base regression was fit using the cross-validated Lasso, while the auxiliary parameter for the regression was chosen to be the smaller of \( \sqrt{\log p/n} \) and \( 0.01 \sqrt{\log p/n} \) for which the convex program in Eq. (3) was feasible. The OM \( f \) moments were fit as described above using 5-fold cross-fitting with the Lasso estimator (with either theoretically-calibrated values for the hyperparameters or hyperparameters chosen by cross-validation) used for both the first-stage regressions.

### G.4.3 Real Data Experiment Details

**OM methods** The OM \( f \) and \( q \) moments were implemented as above with 10-fold cross-fitting. However to exploit the generality of the OM framework in addition to allowing \( \hat{g}(\cdot) \) to be estimated via the cross-validated Lasso estimator, we also allowed \( \hat{g}(\cdot) \) to be estimated via random forest regression, and a \( g = 0 \) baseline. However, note that \( \hat{f} \) and \( \hat{q} \) were always fit with the cross-validated Lasso (a linear estimator) since our primary purpose is to investigate the impacts of debiasing linear prediction with the \( \hat{f} \) and \( \hat{q} \) moments.

For each \( x_i \) we fit a cross-validated Lasso estimator, a random forest regressor, and a \( \hat{g} = 0 \) baseline on each of the \( K \)-leave-one-subsets of data. We adaptively chose between these models in a data-dependent fashion by selecting the method that produced the minimal (estimated) variance for \( \hat{y}_{OM} \). We used a plug-in estimate of the asymptotic variance which can be computed as,

\[
q\text{-var}(\text{method}) = \frac{\sum_{i \in K} \sum_{j \in I_i} (t_j - \bar{g}_{\text{method}}(z_j))^2}{V}
\]

and

\[
f\text{-var}(\text{method}) = \frac{\sum_{i \in K} \sum_{j \in I_i} t_i (t_j - \bar{g}_{\text{method}}(z_j))}{V}
\]

where \( V_{\text{method}} = \sum_{i \in K} \sum_{j \in I_i} (t_j - \bar{g}_{\text{method}}(z_j))^2 - \left( \sum_{i \in K} \sum_{j \in I_i} (t_j - \bar{g}_{\text{method}}(z_j))^2 \right)^2 \) for each method. These asymptotic variance expressions can be computed from a general formula for the asymptotic variance from Mackey et al. [18, Theorem 1]. Upon selecting the appropriate \( \hat{g}(\cdot) \) method for either the \( f \) or \( q \) moments the algorithm proceeds as previously described with the given choice of \( \hat{g}(\cdot) \).

**JM-style method** For the real data experiments the \( \lambda_w \) for the JM-style estimator was selected by constructing a logarithmically-spaced grid of 100 values of \( \lambda_w \) between \( 10^{-7} \) and \( 10^2 \) and selecting the smallest value of \( \lambda_w \) for which the convex program in Eq. (3) was feasible.

**Datasets** All regression datasets, in this paper were downloaded from the publicly available UCI dataset repository [14]. The triazines dataset was randomly split in an 80/20 train-test split and
selected since $n_{\text{train}} \approx p$ for it. The other 4 datasets were selected due to the fact they can be naturally induced to have distributional shift. The Parkinsons and Wine datasets were selected exactly as in Chen et al. [10]. The Parkinsons dataset, where the task is to predict a jitter index, was split into train and test as in Chen et al. [10], by splitting on the "age" feature of patients: $\leq 60 \rightarrow$ train and $> 60 \rightarrow$ test. The task for prediction in the Wine dataset, as in Chen et al. [10], is to predict the acidity levels of wine but given training data comprised only of red wines with a test set comprised only of white wines. In the fertility dataset, where the task is to predict the fertility of a sample, we split into train and test by splitting upon the binary feature of whether patients were in the $18 - 36$ age group ($\rightarrow$ train) or not ($\rightarrow$ test). Finally, for the Forest Fires dataset, where the task it to predict the burned area of forest fires that occurred in Portugal during a roughly year-long period, we split into train/test based on the "month" feature of the fire: those occurring before the month of September ($\rightarrow$ train) and those after the month of September ($\rightarrow$ test).

Note in all the cases the feature that was split upon was not used as a covariate in the prediction task. In Table 2 we include further information these datasets,

| Dataset     | $n_{\text{train}}$ | $n_{\text{test}}$ | $p$ | Distrib. Shift? |
|-------------|---------------------|-------------------|----|------------------|
| Fertility   | 69                  | 31                | 8  | Yes              |
| Forest Fires| 320                 | 197               | 10 | Yes              |
| Parkinson   | 1877                | 3998              | 17 | Yes              |
| Wine        | 4898                | 1599              | 11 | Yes              |
| Triazines   | 139                 | 47                | 60 | No               |

Table 2: Information on Real Datasets.