Surprising benefits of ridge regularization for noiseless regression

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Abstract

Numerous recent works show that overparameterization implicitly reduces variance for minimum-norm interpolators, suggesting vanishing benefits for ridge regularization in high dimensions. However, empirical findings suggest that this narrative may not hold true for robust generalization. In this paper we reveal that for overparameterized linear regression, the robust risk is minimized for a positive regularization coefficient even when the training data is noiseless. Hence, we effectively provide, to the best of our knowledge, the first theoretical analysis on the phenomenon of robust overfitting.

1. Introduction

Conventional statistical wisdom suggests that interpolating estimators may overfit on noise and hence achieve sub-optimal prediction performance. For regression on linearized models, *ridge regularization* is commonly used to reduce the effect of noise and consequently obtain an estimator with stronger generalization. In this paper, we study the linear ridge estimate that minimizes the square loss with an λ-weighted ℓ_2 penalty. It has reduced model complexity by paying the price of worse data fit.

This classical rationale is challenged by recent observations on overparameterized models: Very large neural networks, for example, do not sacrifice generalization performance on i.i.d. samples even if they are trained until convergence and exhibit interpolation (Nakkiran et al., 2020). In particular, the benefits of regularization techniques such as early stopping vanish when the neural network is wide enough. This phenomenon is often referred to as double descent (Belkin et al., 2018).

For linear regression without additional prior knowledge, a natural interpolator to study is the *minimum-norm interpolator*: not only is it the ridge estimate when taking $\lambda \to 0$ but it also corresponds to the solution of gradient descent initialized at zero. Motivated by the double descent phenomenon, a plethora of recent papers study generalization properties of minimum-norm interpolators (Dobriban & Wager, 2018; Ghorbani et al., 2021; Hastie et al., 2019; Bartlett et al., 2020; Mei & Montanari, 2019; Muthukumar et al., 2020a;b) and show that the variance decreases as the overparameterization ratio increases. Most works focus on settings where the optimal regularization parameter satisfies $\lambda_{\text{opt}} \leq 0$ (Kobak et al., 2020; Wu & Xu, 2020; Richards et al., 2021), implying that it is redundant or even detrimental to explicitly regularize with $\lambda > 0$.

The narrative that regularization is redundant for large overparameterized models is based on theoretical and experimental findings that analyze the *standard* risk. However, this metric assumes identically distributed training and test data and fails to reflect the prediction performance of a model when the test data has a shifted distribution, is attacked by adversaries, or primarily contains samples from minority groups. In fact, mounting empirical evidence suggests that regularization is indeed helpful for *robust generalization*, even when it *does not* benefit the standard risk (Rice et al., 2020; Sagawa et al., 2020a;b). This phenomenon is sometimes referred to as *robust overfitting*.

In the presence of noise, the following intuition holds true: the robust risk amplifies the estimator variance and hence regularization that reduces the effect of noise can be beneficial for robust generalization (Sanyal et al., 2021). However, we observe that even when the training data is entirely *noiseless*, robust overfitting persists! In particular, we observe in Figure 1 that for high-dimensional feature models, the robust risk of linear minimum ℓ_2-norm interpolators (i.e. $\lambda \to 0$) is larger compared to a ridge estimate with $\lambda > 0$. Further, in contrast to the standard risk, the robust risk benefits from regularization even in the overparameterized regime $d \gg n$ and for noiseless data.

To date, prior work does not predict nor explain our observations in Figure 1 that contradict intuition: if ℓ_2-norm minimization is yielding a bad solution for noiseless data, why would it help to sacrifice data fit and increase the weight of the ridge penalty? In this paper, we show for linear ridge regression with isotropic Gaussian covariates that asymptot-

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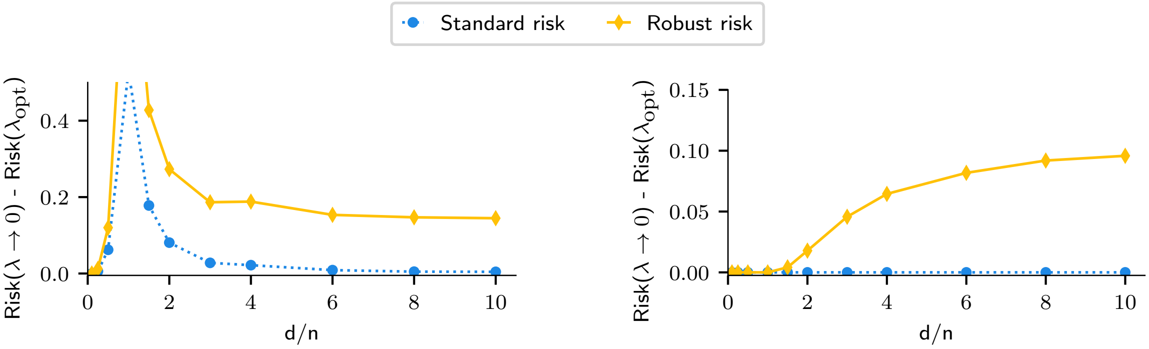


(a) Noisy observations ($\sigma^2 = 0.2$)

(b) Noiseless observations ($\sigma^2 = 0$)

Figure 1. Decrease of population risks for linear regression when using the ridge estimate ($\lambda_{\text{opt}} > 0$) as opposed to the min-norm interpolator ($\lambda \to 0$) (detailed settings as in Figure 2). While the standard risk only benefits from ridge regularization in the noisy case, the robust risk decreases in the heavily overparameterized setting $d/n \gg 1$ even in the noiseless case.

ically, as $d, n \to \infty$ and $d/n \to \gamma$, a strictly positive ridge penalty leads to a systematic improvement in robust generalization. Our results provide the first rigorous explanation of robust overfitting even in the absence of noise.

2. Risk minimization framework

In this section, we describe the setup for our theoretical analysis of linear regression. We define the data generating process, the standard and robust risks, and formally introduce the estimators that we analyze.

2.1. Problem setting

We consider an observation model with covariates (or features) $x \in \mathbb{R}^d$ drawn from a standard normal distribution with zero mean, i.e., $x \sim \mathbb{P} := \mathcal{N}(0, I_d)$, and with the target variable $y \in \mathbb{R}$ defined as a noisy observation of a linear function $y = \langle \theta^\star, x \rangle + \xi$ with $\xi \sim \mathcal{N}(0, \sigma^2)$. Here, $\theta^\star$ denotes the ground truth vector with unit ℓ_2-norm. As mentioned before, we focus on the noiseless case with $\sigma = 0$ to isolate the effect of finite sampling from observation noise, and include $\sigma > 0$ only for completeness.

The results in this paper are of asymptotic nature and hold when $d/n \to \gamma$ as both the dimensionality d and the number of samples n tend to infinity. This high-dimensional regime is widely studied in the literature (Bühlmann & Van De Geer, 2011; Wainwright, 2019) as it yields precise predictions for many real world problems where both the input dimension and the data set size are large. It is also the predominant setting considered in previous theoretical papers that discuss overparameterized linear models (Dobriban & Wager, 2018; Hastie et al., 2019; Ali et al., 2020; Deng et al., 2021; Javanmard et al., 2020; Javanmard & Soltanolkotabi, 2020; Sur & Candès, 2019).

2.2. Standard and robust risk

We now introduce the standard and robust evaluation metrics for regression. First, we define the standard risk of an estimator θ to be the population mean squared error

$$\mathbf{R}(\theta) := \mathbb{E}_{X \sim \mathbb{P}} \left(\langle \theta, X \rangle - \langle \theta^\star, X \rangle \right)^2, \tag{1}$$

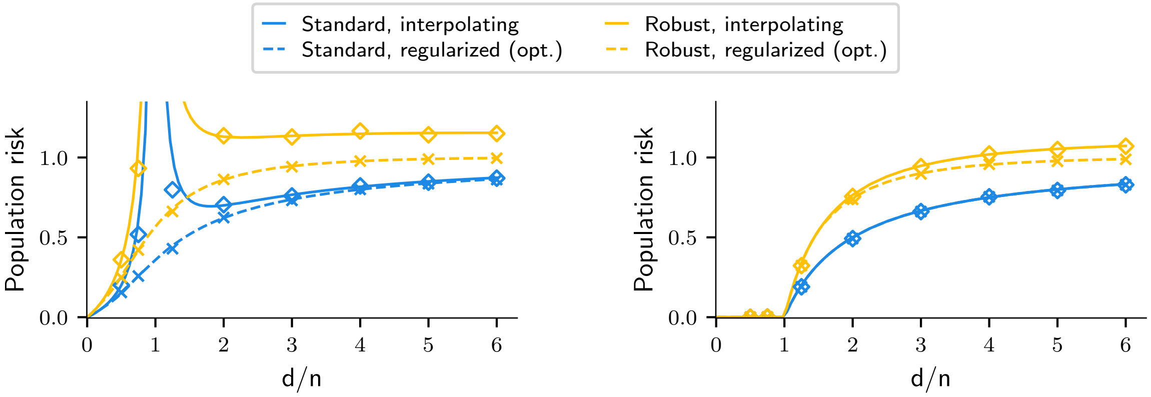
where the expectation is taken over the marginal feature distribution $\mathbb{P}$. Conditioned on the training data, the risk is fixed, and our asymptotic bounds hold almost surely over draws of the training set.

The broad application of ML models in real-world decision-making processes increases requirements on their robustness. For example, for the image domain, robust classifiers should yield the same prediction when an image is attacked via an additive imperceptible ℓ_p-perturbation that do not change the ground truth label. In this case, the estimator which has zero standard population risk also achieves zero robust population risk. Transferred to linear regression, such additive *consistent* perturbations need to be orthogonal to $\theta^\star$. In particular, we study the adversarially robust risk of a parameter θ with respect to consistent ℓ_2-perturbations

$$\begin{aligned}\mathbf{R}_\epsilon(\theta) &:= \mathbb{E}_{X \sim \mathbb{P}} \max_{\delta \in \mathcal{U}_2(\epsilon)} \left(\langle \theta, X + \delta \rangle - \langle \theta^\star, X \rangle \right)^2 \qquad (2) \\ &= \|\theta^\star - \theta\|_2^2 + \sqrt{\frac{8\epsilon^2}{\pi}} \|\Pi_\perp \theta\|_2 \|\theta^\star - \theta\|_2 + \epsilon^2 \|\Pi_\perp \theta\|_2^2,\end{aligned}$$

where $\mathcal{U}_2(\epsilon) := \{\delta \in \mathbb{R}^d : \|\delta\|_2 \leq \epsilon \text{ and } \langle \theta^\star, \delta \rangle = 0\}$ and $\Pi_\perp$ is the orthogonal projection onto the ground truth vector $\theta^\star$. The proof for the second equality can be found in Appendix A.1.

In many scientific applications, security against adversarial attacks may not be the dominating concern and one may instead require estimators that are robust against small distribution shifts. Earlier work (Sinha et al., 2018) points



(a) Noisy observations ($\sigma^2 = 0.2$)

(b) Noiseless observations ($\sigma^2 = 0$)

Figure 2. Asymptotic theoretical predictions for $d, n \to \infty$ (curves) and experimental results with finite d, n (markers) for the robust (yellow, $\epsilon = 0.4$) and standard (blue) risk of the min-norm solution (solid, *interpolating*) and the ridge regression estimate with optimal λ (dashed, *regularized*) for noisy (left) and noiseless data (right). The experiments use $n = 1000$ samples of the model described in Section 2.1. We observe that the gap between the robust risk of the interpolating and optimally regularized estimator persists even in the noiseless case.

out that distribution shift robustness and adversarial robustness are equivalent for losses that are convex in the parameter θ. In our setting, adversarial robustness against consistent ℓ_p-perturbations implies distributional robustness against ℓ_p mean shifts in the covariate distribution $\mathbb{P}$ (see Appendix A.2).

2.3. Interpolating and regularized estimator

We study the minimizer of standard linear ridge regression

$$\hat{\theta}_\lambda = \arg\min_\theta \frac{1}{n}\sum_{i=0}^{n}(y_i - \langle\theta, x_i\rangle)^2 + \lambda\|\theta\|_2^2 \qquad (3)$$

that we call the ridge estimate. For $\lambda > 0$, we obtain a regularized predictor $\hat{\theta}_\lambda$. As $\lambda \to 0$, we obtain the minimum norm interpolator

$$\hat{\theta}_0 = \arg\min_\theta \|\theta\|_2 \;\text{ such that }\; \langle\theta, x_i\rangle = y_i \;\text{ for all } i. \quad (4)$$

For linear regression on isotropic features there exists a well-known correspondence between the optimization path of zero-initialized gradient descent and the regularization path of the ridge regression estimator (see for example (Ali et al., 2019; 2020)). Hence, the results presented in this paper for ridge regularization directly translate to early stopped gradient descent on the mean squared loss.

3. Main results for ridge regression

In this section, we prove that preventing interpolation on noiseless samples via ridge regularization (3) with $\lambda > 0$ improves the robust risk relative to an un-regularized, interpolating predictor. We further provide an explanation for why regularization is beneficial for the robust risk even when it does not improve the standard risk.

3.1. Main result

The following theorem provides a precise asymptotic description of the consistent ℓ_2 robust risk for the ridge regression estimate in (3) as $d/n \to \gamma$ and $d, n \to \infty$. The proof uses techniques from (Hastie et al., 2019; Knowles & Yin, 2014) and can be found in Appendix B.

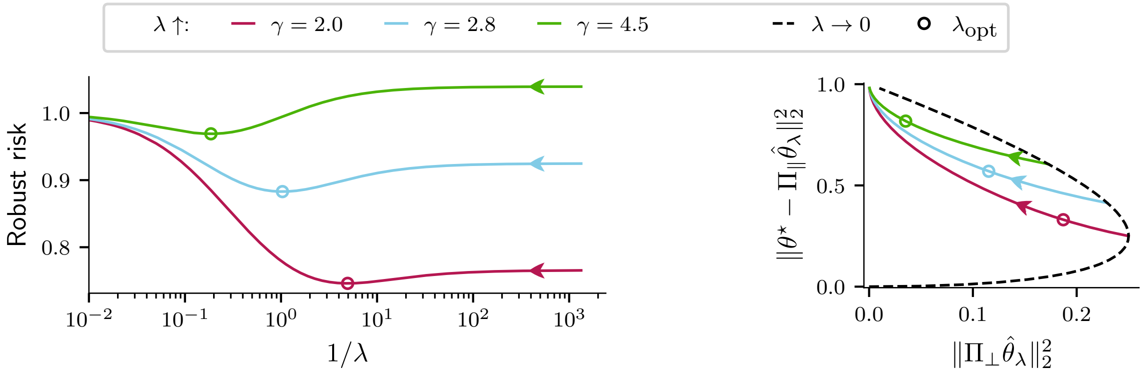
Theorem 3.1. *Assume isotropic Gaussian covariates, i.e., $\mathbb{P}_X = \mathcal{N}(0, I_d)$). Then, for $d, n \to \infty$ with $d/n \to \gamma$ and for any $\lambda \geq 0$, the robust risk of the estimators $\hat{\theta}_\lambda$ defined in Equations (3), (4) converges to*

$$\boldsymbol{R}_\epsilon(\hat{\theta}_\lambda) \xrightarrow{a.s.} \mathcal{B} + \mathcal{V} + \epsilon^2\mathcal{P} + \sqrt{\frac{8\epsilon^2}{\pi}\mathcal{P}(\mathcal{B} + \mathcal{V})} \qquad (5)$$

where $\mathcal{P} = \mathcal{B} + \mathcal{V} - \lambda^2(m(-\lambda))^2$ and $\mathcal{B} = \lambda^2 m'(-\lambda)$, $\mathcal{V} = \sigma^2\gamma(m(-\lambda) - \lambda m'(-\lambda))$ are the asymptotic bias and variance. The function $m(z)$ is given by $m(z) = \frac{1-\gamma-z-\sqrt{(1-\gamma-z)^2-4\gamma z}}{2\gamma z}$ and m' is the derivative of m. Furthermore, the standard risk $\boldsymbol{R}(\hat{\theta}_\lambda) \xrightarrow{a.s.} \mathcal{B} + \mathcal{V}$.

We plot the precise asymptotic risks of the ridge estimate with optimal regularization parameter λ_{opt} and the minimum-norm interpolator $\lambda = 0$ in Figure 2.[1] For the robust risk we use $\epsilon = 0.4$. Firstly, Figure 2a reveals that ridge regularization reduces the robust risk even for $d/n \gg 1$ well

[1] Here we choose λ using the population risk oracle, in practice one would resort to standard tools such as cross-validation techniques that also enjoy theoretical guarantees (see e.g. (Patil et al., 2021)).



(a) Robust risk as λ increases

(b) Orthogonal and parallel parameter error

Figure 3. Theoretical curves for the robust risk with $\epsilon = 0.4$ (a) and decomposed terms (b) as λ increases (arrow direction) for different choices of the overparameterization ratio $d/n \to \gamma$. In (b) we observe for large $\gamma > 1$ that, as λ increases, the orthogonal error $\|\Pi_\perp\hat{\theta}_\lambda\|_2$ decreases, whereas the parallel error $\|\theta^\star - \Pi_{\|}\hat{\theta}_\lambda\|_2$ increases. For $\epsilon > 0$, the optimal λ is large enough to prevent interpolation.

beyond the interpolation threshold where previous works show that the variance is negligible.

Moreover, Figure 2b shows that the beneficial effect of ridge regularization persists even for noiseless data, that is when $\mathcal{V} = 0$. This supports our statement that regularization not only helps to reduce variance, but also reduces the part of the robust risk that is unaffected by noise in the overparameterized regime. Furthermore, we show that experiments run with finite d and n (depicted by the markers in Figure 2) closely match the predictions in Theorem 3.1 for $d, n \to \infty$ and $d/n \to \gamma$. This indicates that the high-dimensional asymptotic regime indeed correctly predicts and characterizes the high-dimensional non-asymptotic regime. Finally, even though Theorem 3.1 assumes isotropic Gaussian covariates ($\Sigma_d = I_d$), we can extend the result to more general covariance matrices following the same argument as in (Hastie et al., 2019) based on random matrix theory (Knowles & Yin, 2014).

3.2. Intuitive explanations and discussion

We now shed light on the phenomena revealed by Theorem 3.1 and Figure 2. In particular, we discuss why regularization can reduce the robust risk even in a noiseless setting and why the effect is not noticeable for the standard risk.

For this purpose, we examine the robust risk as a function of λ, depicted in Figure 3a for different overparameterization ratios $\gamma > 1$ and $\epsilon = 0.4$. The arrow points in the direction of increasing λ. We observe how the minimal robust risk is achieved for a λ_{opt} bounded away from zero and how the optimum increases with the overparameterization ratio $d/n \to \gamma$.

In order to understand the overfitting phenomenon better, we decompose the ridge estimate $\hat{\theta}_\lambda$ into its projection $\Pi_{\|}$ on the ground-truth direction $\theta^\star$ and its projection $\Pi_\perp$ onto its orthogonal complement, i.e., $\hat{\theta}_\lambda = \Pi_{\|}\hat{\theta}_\lambda + \Pi_\perp\hat{\theta}_\lambda$. For the noiseless setting ($\sigma^2 = 0$), substituting the decomposition into Equation (2) yields the following closed-form expression of the robust risk

$$\begin{aligned}\mathbf{R}_\epsilon(\hat{\theta}_\lambda) = \|\theta^\star - \Pi_{\|}\hat{\theta}_\lambda\|_2^2 + (1+\epsilon^2)\|\Pi_\perp\hat{\theta}_\lambda\|_2^2 \\ + \sqrt{\frac{8\epsilon^2}{\pi}\|\Pi_\perp\hat{\theta}_\lambda\|_2^2(\|\theta^\star - \Pi_{\|}\hat{\theta}_\lambda\|_2^2 + \|\Pi_\perp\hat{\theta}_\lambda\|_2^2)}.\end{aligned} \tag{6}$$

that now involves the parallel error $\|\theta^\star - \Pi_{\|}\hat{\theta}_\lambda\|_2^2$ and the orthogonal error $\|\Pi_\perp\hat{\theta}_\lambda\|_2^2$. The proof can be found in Appendix A.1.

Figure 3b shows that, as λ increases, the orthogonal error decreases faster than the parallel error increases. Since by Equation (6), the orthogonal error is weighted more heavily for large enough perturbation strength ϵ, some nonzero ridge coefficient yields the best trade-off. On the other hand, the standard risk with $\epsilon = 0$ weighs both errors equally, resulting in an optimum at $\lambda = 0$.

4. Conclusions

In this paper we prove that high-dimensional ridge regression achieves lower robust risk for a strictly positive ridge penalty as opposed to minimum-norm interpolation, even for the highly overparameterized regime $d/n \to \gamma \gg 1$ and noiseless observations. Our results put into perspective the modern narrative that interpolating overparameterized models yield good performance without explicit regularization and motivate the use of ridge regularization and early stopping for improved robust generalization.

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A. Setting

In Section A.1 we give a closed form expression for the robust risk. Furthermore, Section A.2 discusses that the robust risk (2) upper-bounds the worst case risk under distributional mean shifts.

A.1. Closed form solution of robust risk

Lemma A.1. *Assume that $\mathbb{P}_X$ is the isotropic Gaussian distribution, and let $\Pi_\perp$ be the orthonormal projection onto the ground truth vector $\theta^\star$. Then, the robust risk (2) with respect to ℓ_2 perturbations is given by*

$$\boldsymbol{R}_\epsilon(\theta) = \|\theta^\star - \theta\|_2^2 + 2\epsilon\sqrt{2/\pi}\|\Pi_\perp\theta\|_2\|\theta^\star - \theta\|_2 + \epsilon^2\|\Pi_\perp\theta\|_2^2. \tag{7}$$

Proof. A similar result for inconsistent attacks has already been shown before (Lemma 3.1. in (Javanmard et al., 2020)). Define $\tilde{y}_i = y_i - \langle x_i, \theta\rangle$, and note that using similar arguments as in Section 6.2. (Javanmard et al., 2020)

$$\begin{aligned}\max_{\delta_i\in\mathcal{U}_2(\epsilon)} (\tilde{y}_i - \langle\delta_i, \theta\rangle)^2 &= (\max_{\delta_i\in\mathcal{U}_2(\epsilon)} |\tilde{y}_i - \langle\delta_i,\theta\rangle|)^2 \\ &= (|\tilde{y}_i| + \max_{\|\delta_i\|_2\leq\epsilon, \delta_i\perp\theta^\star} |\langle\delta_i,\theta\rangle|)^2 \\ &= (|\tilde{y}_i| + \epsilon\|\Pi_\perp\theta\|_2)^2.\end{aligned}$$

With this characterization, we can derive a convenient expression for the robust risk:

$$\begin{aligned}\mathbf{R}_\epsilon(\theta) &= \mathbb{E}_X(|\langle X, \theta^\star - \theta\rangle| + \epsilon\|\Pi_\perp\theta\|_q)^2 \\ &= \mathbb{E}_X(\langle X, \theta^\star - \theta\rangle)^2 + 2\epsilon\mathbb{E}_X|\langle X, \theta^\star - \theta\rangle|\|\Pi_\perp\theta\|_2 + \epsilon^2\|\Pi_\perp\theta\|_2^2.\end{aligned} \tag{8}$$

Since we assume isotropic Gaussian features, that is $\mathbb{P}_X = \mathcal{N}(0, I)$, we can further simplify

$$\mathbf{R}_\epsilon(\theta) = \|\theta - \theta^*\|_2^2 + 2\epsilon\sqrt{2/\pi}\|\Pi_\perp\theta\|_2\|\theta - \theta^*\|_2 + \epsilon^2\|\Pi_\perp\theta\|_2^2$$

which concludes the proof. □

A.2. Distribution shift robustness and consistent adversarial robustness

In this section we rigorously introduce distribution shift robustness and show the relation to consistent ℓ_p adversarial robustness for certain types of distribution shifts.

When learned models are deployed in the wild, the i.i.d. assumption does not always hold. That is, the test loss might be evaluated on samples from a slightly different distribution. Shifts in the mean of the covariate distribution is a standard intervention studied in the invariant causal prediction literature (Bühlmann et al., 2020; Chen & Bühlmann, 2020). For mean shifts in the null space of the ground truth $\theta^\star$ we define an alternative evaluation metric that we refer to as the *distributionally robust risk* defined as follows:

$$\begin{aligned}\tilde{\mathbf{R}}_\epsilon(\theta) &:= \max_{\mathbb{Q}\in\mathcal{V}_q(\epsilon;\mathbb{P})} \mathbb{E}_{X\sim\mathbb{Q}}\ell_{\text{test}}(\langle\theta, X + \delta\rangle, \langle\theta^\star, X\rangle), \quad \text{with} \\ \mathcal{V}_p(\epsilon;\mathbb{P}) &:= \{\mathbb{Q}\in\mathcal{P} : \|\mu_\mathbb{P} - \mu_\mathbb{Q}\|_p \leq \epsilon \text{ and } \langle\mu_\mathbb{P} - \mu_\mathbb{Q}, \theta^\star\rangle = 0\}\end{aligned}$$

where $\mathcal{V}_p$ is the neighborhood of mean shifted probability distributions and ℓ_{test} is a convex loss function.

A duality between distribution shift robustness and adversarial robustness has been established in earlier work such as (Sinha et al., 2018) for general convex, continuous losses ℓ_{test}. For our setting, the following lemma holds.

Lemma A.2. *For any $\epsilon \geq 0$ and θ, we have $\tilde{\boldsymbol{R}}_\epsilon(\theta) \leq \boldsymbol{R}_\epsilon(\theta)$.*

Proof. The proof follows directly from the definition and consistency of the perturbations $\mathcal{U}_p(\epsilon)$ and orthogonality of the mean shifts for the neighborhood $\mathcal{V}_p$. By defining the random variable $w = x - \mu_\mathbb{P}$ for $x \sim \mathbb{P}$ we have the distributional equivalence

$$x' = \mu_\mathbb{P} + \delta + w \overset{d}{=} x + \delta$$

for $x' \sim \mathbb{Q}$ and $x \sim \mathbb{P}$ with $\mu_{\mathbb{Q}} - \mu_{\mathbb{P}} = \delta$ and hence

$$\begin{aligned}\tilde{\mathbf{R}}_\epsilon(\theta) = \max_{\mathbb{Q}\in\mathcal{V}_p(\epsilon)} \mathbb{E}_{x\sim\mathbb{Q}}\ell_{\text{test}}(\langle\theta, x\rangle, \langle\theta^\star, x\rangle) &= \max_{\|\delta\|_p\leq\epsilon, \delta\perp\theta^\star} \mathbb{E}_{x\sim\mathbb{P}}\ell_{\text{test}}(\langle\theta, x+\delta\rangle, \langle\theta^\star, x\rangle) \\ &\leq \mathbb{E}_{x\sim\mathbb{P}} \max_{\|\delta\|_p\leq\epsilon, \delta\perp\theta^\star} \ell_{\text{test}}(\langle\theta, x+\delta\rangle, \langle\theta^\star, x\rangle) = \mathbf{R}_\epsilon(\theta)\end{aligned}$$

where the first line follows from orthogonality of the mean-shift to $\theta^\star$. □

B. Proof of Theorem 3.1

In this section, we provide a proof of Theorem 3.1, which characterizes the asymptotic risk of the linear regression estimator $\hat{\theta}_\lambda$ defined in Equation (3).

We first introduce some notation and give the standard closed form solution for the ridge regression estimate $\hat{\theta}_\lambda$. Denoting the input data matrix by $\mathrm{X} \in \mathbb{R}^{d\times n}$, the observation vector $y \in \mathbb{R}^n$ reads $y = \mathrm{X}^\top\theta^\star + \xi$ with $\xi \sim \mathcal{N}(0, I)$ the noise vector. the noise vector containing i.i.d. zero-mean σ^2-variance Gaussian noise as entries. Defining the empirical covariance matrix as $\widehat{\Sigma} = \frac{1}{n}\mathrm{X}^\top\mathrm{X}$ yields the ridge estimate

$$\begin{aligned}\hat{\theta}_\lambda &= \frac{1}{n}(\lambda I_d + \widehat{\Sigma})^{-1}\mathrm{X}^\top y \\ &= (\lambda I_d + \widehat{\Sigma})^{-1}\widehat{\Sigma}\theta^\star + \frac{1}{n}(\lambda I_d + \widehat{\Sigma})^{-1}\mathrm{X}^\top\xi. \end{aligned} \tag{9}$$

For $\lambda \to 0$, we obtain the min-norm interpolator

$$\hat{\theta}_0 = \lim_{\lambda\to 0}\hat{\theta}_\lambda = (\lambda I_d + \widehat{\Sigma})^{-1}\mathrm{X}^\top y = \widehat{\Sigma}^\dagger \mathrm{X}^\top y$$

where $\widehat{\Sigma}^\dagger$ denotes the Moore-Penrose pseudo inverse.

We now compute the adversarial risk of this estimator. By Equation (7), the adversarial risk depends on the estimator only via the two terms $\|\hat{\theta}_\lambda - \theta^\star\|_2$ and $\|\Pi_\perp\hat{\theta}_\lambda\|_2$. To characterize the asymptotic risk, we hence separately derive asymptotic expressions for each of both terms. The following convergence results hold almost surely with respect to the draws of the train dataset, with input features X and observations y, as $n, d \to \infty$.

Step 1: Characterizing $\|\hat{\theta}_\lambda - \theta^\star\|_2^2$. Here, we show that

$$\|\hat{\theta}_\lambda - \theta^\star\|_2^2 \to \mathcal{B} + \mathcal{V}. \tag{10}$$

where $\mathcal{B} = \lambda^2 m'(-\lambda)$, $\mathcal{V} = \sigma^2\gamma(m(-\lambda) - \lambda m'(-\lambda))$ are the asymptotic bias and variance as in the Theorem and Theorem 5 of (Hastie et al., 2019), whre the authors shows that $\mathbb{E}_\xi\|\hat{\theta}_\lambda - \theta^\star\|_2^2 \to \mathcal{B} + \mathcal{V}$ and the expectation is taken over the observation noise ξ in the train dataset. In this paper, we define the population risks without the expectation over the noise. Hence, in a first step, the goal is to extend Theorem 5 (Hastie et al., 2019) for the standard risk $\mathbf{R}(\hat{\theta}_\lambda) = \|\hat{\theta}_\lambda - \theta^\star\|_2^2$ such that (10) holds almost surely over the draws of the training data.

Using Equation (9) we can rewrite

$$\begin{aligned}\|\hat{\theta}_\lambda - \theta^\star\|_2^2 &= \|\left(I_d - (\lambda I_d + \widehat{\Sigma})^{-1}\widehat{\Sigma}\right)\theta^\star + \frac{1}{n}(\lambda I_d + \widehat{\Sigma})^{-1}\mathrm{X}^\top\xi\|_2^2 \\ &= \underbrace{\|\left(I_d - (\lambda I_d + \widehat{\Sigma})^{-1}\widehat{\Sigma}\right)\theta^\star\|_2^2}_{T_1} + \underbrace{\langle\frac{\xi}{\sqrt{n}}, (\lambda I_d + \widehat{\Sigma})^{-2}\widehat{\Sigma}\frac{\xi}{\sqrt{n}}\rangle}_{T_2} \\ &\quad + \underbrace{\left\langle\frac{\mathrm{X}^\top}{\sqrt{n}}(\lambda I_d + \widehat{\Sigma})^{-1}\left(I_d - (\lambda I_d + \widehat{\Sigma})^{-1}\widehat{\Sigma}\right)\theta^\star, \frac{\xi}{\sqrt{n}}\right\rangle}_{T_3},\end{aligned}$$

where we used for the second term that $\langle\frac{\xi}{\sqrt{n}}, \frac{X}{\sqrt{n}}(\lambda I_d + \widehat{\Sigma})^{-2}\frac{X^\top}{\sqrt{n}}\frac{\xi}{\sqrt{n}}\rangle = \langle\frac{\xi}{\sqrt{n}}, (\lambda I_d + \widehat{\Sigma})^{-2}\widehat{\Sigma}\frac{\xi}{\sqrt{n}}\rangle$.

The first term $T_1 \to \mathcal{B}$ directly via Theorem 5 (Hastie et al., 2019). We next show that $T_2 \to \mathcal{V}$ and $T_3 \to 0$ almost surely, which establishes Equation 10.

Proof that $T_2 \to \mathcal{V}$: While Theorem 5 (Hastie et al., 2019) also shows that $\mathbb{E}_\xi \operatorname{tr}\left(\frac{1}{n}\xi\xi^\top\widehat{\Sigma}(\lambda I_d + \widehat{\Sigma})^{-2}\right) \to \mathcal{V}$, we require the convergence almost surely over a single draw of ξ. In fact, this directly follows from the same argument as used for the proof of Theorem 5 (Hastie et al., 2019) and the fact that $\|\frac{\xi}{\sqrt{n}}\|_2^2 \to \sigma^2$. Hence $\langle \frac{\xi}{\sqrt{n}}, (\lambda I_d + \widehat{\Sigma})^{-2}\widehat{\Sigma}\frac{\xi}{\sqrt{n}}\rangle \to \mathcal{V}$ almost surely over the draws of ξ.

Proof that $T_3 \to 0$: This follows straight forwardly from sub-Gaussian concentration inequalities and from the fact that

$$\left\| \frac{\mathrm{X}}{\sqrt{n}}(\lambda I_d + \widehat{\Sigma})^{-1}\left(I_d - (\lambda I_d + \widehat{\Sigma})^{-1}\widehat{\Sigma}\right)\theta^\star \right\|_2 = O(1),$$

which is a direct consequence of the Bai-Yin theorem (Bai & Yin, 1993), stating that for sufficiently large n, the non zero eigenvalues of $\widehat{\Sigma}$ can be almost surely bounded by $(1+\sqrt{\gamma})^2 \geq \lambda_{\max}(\widehat{\Sigma}) \geq \lambda_{\min}(\widehat{\Sigma}) \geq (1-\sqrt{\gamma})^2$. Hence we can conclude the first part of the proof.

Step 2: Characterizing $\|\Pi_\perp \hat{\theta}_\lambda\|_2$. Here, we show that

$$\|\Pi_\perp \hat{\theta}_\lambda\|_2^2 \to \mathcal{B} + \mathcal{V} - \lambda^2(m(-\lambda))^2 =: \mathcal{P}. \tag{11}$$

We assume without loss of generality that $\|\theta^\star\|_2 = 1$ and hence $\Pi_\perp = I_d - \theta^\star(\theta^\star)^\top$. It follows that

$$\begin{aligned}
\|\Pi_\perp \hat{\theta}_\lambda\|_2^2 &= \|\hat{\theta}_\lambda\|_2^2 - \left(\langle \hat{\theta}_\lambda, \theta^\star\rangle\right)^2 \\
&= \|\theta^\star - \hat{\theta}_\lambda - \theta^\star\|_2^2 - \left(1 - \langle \theta^\star - \hat{\theta}_\lambda, \theta^\star\rangle\right)^2 \\
&= \|\theta^\star - \hat{\theta}_\lambda\|_2^2 - 2\langle \theta^\star - \hat{\theta}_\lambda, \theta^\star\rangle + 1 - \left(1 - \langle \theta^\star - \hat{\theta}_\lambda, \theta^\star\rangle\right)^2 \\
&= \|\theta^\star - \hat{\theta}_\lambda\|_2^2 - \left(\langle \theta^\star - \hat{\theta}_\lambda, \theta^\star\rangle\right)^2.
\end{aligned}$$

The convergence of the first term is already known form step 1. Hence, it is only left to find an asymptotic expression for $\langle \theta^\star - \hat{\theta}_\lambda, \theta^\star\rangle$. Inserting the closed form expression from Equation (9), we obtain:

$$\langle \theta^\star - \hat{\theta}_\lambda, \theta^\star\rangle = \langle I_d - \left(\lambda I_d + \widehat{\Sigma})^{-1}\widehat{\Sigma}\right)\theta^\star, \theta^\star\rangle - \langle (\lambda I_d + \widehat{\Sigma})^{-1}\frac{\mathrm{X}^\top\xi}{n}, \theta^\star\rangle. \tag{12}$$

Note that $\langle (\lambda I_d + \widehat{\Sigma})^{-1}\frac{\mathrm{X}\xi}{n}, \theta^\star\rangle$ vanishes almost surely over the draws of ξ using the same reasoning as in the first step. Hence, we only need to find an expression for the first term on the RHS of Equation (12). Note that we can use Woodbury's matrix identity to write:

$$\langle I_d - \left(\lambda I_d + \widehat{\Sigma})^{-1}\widehat{\Sigma}\right)\theta^\star, \theta^\star\rangle = \lambda\langle (\lambda I_d + \widehat{\Sigma})^{-1}\theta^\star, \theta^\star\rangle.$$

However, the expression on the RHS appears exactly in the proof of Theorem 1 (Hastie et al., 2019) (Equation 116), which shows that $\lambda\langle(\lambda I_d + \widehat{\Sigma})^{-1}\theta^\star, \theta^\star\rangle \to \lambda m(-\lambda)$ with $m(z)$ as in Theorem 3.1. Hence the proof of almost sure convergence (11) of $\|\Pi_\perp \hat{\theta}_\lambda\|_2$ is complete.

Substituting Equations (10) and (11) into robust risk (7) expression yields:

$$\mathbf{R}_\epsilon(\hat{\theta}_\lambda) \overset{\text{a.s.}}{\longrightarrow} \mathcal{B} + \mathcal{V} + \epsilon^2\mathcal{P} + \sqrt{\frac{8\epsilon^2}{\pi}\mathcal{P}(\mathcal{B} + \mathcal{V})},$$

and the proof is complete.