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Abstract
We compare the risk of ridge regression to a simple variant of ordinary least squares, in which one simply projects the data onto a finite dimensional subspace (as specified by a principal component analysis) and then performs an ordinary (un- regularized) least squares regression in this subspace. This note shows that the risk of this ordinary least squares method (PCA-OLS) is within a constant factor (namely 4) of the risk of ridge regression (RR).

Keywords
risk inflation, ridge regression, pca

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A Risk Comparison of Ordinary Least Squares vs Ridge Regression

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Abstract

We compare the risk of ridge regression to a simple variant of ordinary least squares, in which one simply projects the data onto a finite dimensional subspace (as specified by a principal component analysis) and then performs an ordinary (un-regularized) least squares regression in this subspace. This note shows that the risk of this ordinary least squares method (PCA-OLS) is within a constant factor (namely 4) of the risk of ridge regression (RR).

Keywords: risk inflation, ridge regression, pca

1. Introduction

Consider the fixed design setting where we have a set of n vectors $\mathcal{X} = \{X_i\}$, and let $\mathbf{X}$ denote the matrix where the i^{th} row of $\mathbf{X}$ is X_i. The observed label vector is $Y \in \mathbb{R}^n$. Suppose that:

$$Y = \mathbf{X}\beta + \varepsilon,$$

where ε is independent noise in each coordinate, with the variance of ε_i being σ^2.

The objective is to learn $\mathbb{E}[Y] = \mathbf{X}\beta$. The expected loss of a vector β estimator is:

$$L(\beta) = \frac{1}{n}\mathbb{E}_{\mathbb{Y}}[\|Y - \mathbf{X}\beta\|^2],$$

Let $\hat{\beta}$ be an estimator of β (constructed with a sample Y). Denoting

$$\mathbf{\Sigma} := \frac{1}{n}\mathbf{X}^T\mathbf{X},$$

we have that the risk (i.e., expected excess loss) is:

$$\text{Risk}(\hat{\beta}) := \mathbb{E}_{\hat{\beta}}[L(\hat{\beta}) - L(\beta)] = \mathbb{E}_{\hat{\beta}}\|\hat{\beta} - \beta\|^2_{\mathbf{\Sigma}},$$

where $\|x\|_{\mathbf{\Sigma}} = x^\top \mathbf{\Sigma} x$ and where the expectation is with respect to the randomness in Y.

We show that a simple variant of ordinary (un-regularized) least squares always compares favorably to ridge regression (as measured by the risk). This observation is based on the following bias variance decomposition:

$$\text{Risk}(\hat{\beta}) = \underbrace{\mathbb{E}\|\hat{\beta} - \bar{\beta}\|^2_{\mathbf{\Sigma}}}_{\text{Variance}} + \underbrace{\|\bar{\beta} - \beta\|^2_{\mathbf{\Sigma}}}_{\text{Prediction Bias}}, \tag{1}$$

where $\bar{\beta} = \mathbb{E}[\hat{\beta}]$.

1.1 The Risk of Ridge Regression (RR)

Ridge regression or Tikhonov Regularization (Tikhonov, 1963) penalizes the ℓ_2 norm of a parameter vector β and "shrinks" it towards zero, penalizing large values more. The estimator is:

$$\hat{\beta}_\lambda = \underset{\beta}{\text{argmin}}\{\|Y - \mathbf{X}\beta\|^2 + \lambda\|\beta\|^2\}.$$

The closed form estimate is then:

$$\hat{\beta}_\lambda = (\mathbf{\Sigma} + \lambda\mathbf{I})^{-1}\left(\frac{1}{n}\mathbf{X}^T Y\right).$$

Note that

$$\hat{\beta}_0 = \hat{\beta}_{\lambda=0} = \underset{\beta}{\text{argmin}}\{\|Y - \mathbf{X}\beta\|^2\},$$

is the ordinary least squares estimator.

Without loss of generality, rotate $\mathbf{X}$ such that:

$$\mathbf{\Sigma} = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_p),$$

where the λ_i's are ordered in decreasing order.

To see the nature of this shrinkage observe that:

$$[\hat{\beta}_\lambda]_j := \frac{\lambda_j}{\lambda_j + \lambda}[\hat{\beta}_0]_j,$$

where $\hat{\beta}_0$ is the ordinary least squares estimator.

Using the bias-variance decomposition, (Equation 1), we have that:

Lemma 1

$$\text{Risk}(\hat{\beta}_\lambda) = \frac{\sigma^2}{n}\sum_j \left(\frac{\lambda_j}{\lambda_j + \lambda}\right)^2 + \sum_j \beta_j^2 \frac{\lambda_j}{(1 + \frac{\lambda_j}{\lambda})^2}.$$

The proof is straightforward and is provided in the appendix.

2. Ordinary Least Squares with PCA (PCA-OLS)

Now let us construct a simple estimator based on λ. Note that our rotated coordinate system where Σ is equal to $diag(\lambda_1, \lambda_2, \dots, \lambda_p)$ corresponds the PCA coordinate system.

Consider the following ordinary least squares estimator on the "top" PCA subspace — it uses the least squares estimate on coordinate j if $\lambda_j \geq \lambda$ and 0 otherwise

$$[\hat{\beta}_{PCA,\lambda}]_j = \begin{cases} [\hat{\beta}_0]_j & \text{if } \lambda_j \geq \lambda \\ 0 & \text{otherwise} \end{cases} .$$

The following claim shows this estimator compares favorably to the ridge estimator (for every λ)– no matter how the λ is chosen, for example, using cross validation or any other strategy.

Our main theorem (Theorem 2) bounds the Risk Ratio/Risk Inflation[1] of the PCA-OLS and the RR estimators.

Theorem 2 *(Bounded Risk Inflation) For all $\lambda \geq 0$, we have that:*

$$0 \leq \frac{\text{Risk}(\hat{\beta}_{PCA,\lambda})}{\text{Risk}(\hat{\beta}_\lambda)} \leq 4,$$

and the left hand inequality is tight.

Proof Using the bias variance decomposition of the risk we can write the risk as:

$$\text{Risk}(\hat{\beta}_{PCA,\lambda}) = \frac{\sigma^2}{n} \sum_j \mathbb{1}_{\lambda_j \geq \lambda} + \sum_{j:\lambda_j < \lambda} \lambda_j \beta_j^2.$$

The first term represents the variance and the second the bias.

The ridge regression risk is given by Lemma 1. We now show that the j^{th} term in the expression for the PCA risk is within a factor 4 of the j^{th} term of the ridge regression risk. First, let's consider the case when $\lambda_j \geq \lambda$, then the ratio of j^{th} terms is:

$$\frac{\frac{\sigma^2}{n}}{\frac{\sigma^2}{n}\left(\frac{\lambda_j}{\lambda_j+\lambda}\right)^2 + \beta_j^2 \frac{\lambda_j}{(1+\frac{\lambda_j}{\lambda})^2}} \leq \frac{\frac{\sigma^2}{n}}{\frac{\sigma^2}{n}\left(\frac{\lambda_j}{\lambda_j+\lambda}\right)^2} = \left(1 + \frac{\lambda}{\lambda_j}\right)^2 \leq 4.$$

Similarly, if $\lambda_j < \lambda$, the ratio of the j^{th} terms is:

$$\frac{\lambda_j \beta_j^2}{\frac{\sigma^2}{n}\left(\frac{\lambda_j}{\lambda_j+\lambda}\right)^2 + \beta_j^2 \frac{\lambda_j}{(1+\frac{\lambda_j}{\lambda})^2}} \leq \frac{\lambda_j \beta_j^2}{\frac{\lambda_j \beta_j^2}{(1+\frac{\lambda_j}{\lambda})^2}} = \left(1 + \frac{\lambda_j}{\lambda}\right)^2 \leq 4.$$

Since, each term is within a factor of 4 the proof is complete. ■

It is worth noting that the converse is not true and the ridge regression estimator (RR) can be arbitrarily worse than the PCA-OLS estimator. An example which shows that the left hand inequality is tight is given in the Appendix.

1. Risk Inflation has also been used as a criterion for evaluating feature selection procedures (Foster and George, 1994).

3. Experiments

First, we generated synthetic data with $p = 100$ and varying values of n= {20, 50, 80, 110}. The data was generated in a fixed design setting as $Y = \mathbf{X}\beta + \varepsilon$ where $\varepsilon_i \sim \mathcal{N}(0,1) \;\; \forall i = 1,\ldots,n$. Furthermore, $\mathbf{X}_{n\times p} \sim MVN(\mathbf{0},\mathbf{I})$ where MVN($\mu,\mathbf{\Sigma}$) is the Multivariate Normal Distribution with mean vector μ, variance-covariance matrix $\mathbf{\Sigma}$ and $\beta_j \sim \mathcal{N}(0,1) \;\; \forall j = 1,\ldots,p$.

The results are shown in Figure 1. As can be seen, the risk ratio of PCA (PCA-OLS) and ridge regression (RR) is never worse than 4 and often its better than 1 as dictated by Theorem 2.

Next , we chose two real world data sets, namely USPS (n=1500, p=241) and BCI (n=400, p=117).[2]

Since we do not know the true model for these data sets, we used all the n observations to fit an OLS regression and used it as an estimate of the true parameter β. This is a reasonable approximation to the true parameter as we estimate the ridge regression (RR) and PCA-OLS models on a small subset of these observations. Next we choose a random subset of the observations, namely $0.2\times p$, $0.5\times p$ and $0.8\times p$ to fit the ridge regression (RR) and PCA-OLS models.

The results are shown in Figure 2. As can be seen, the risk ratio of PCA-OLS to ridge regression (RR) is again within a factor of 4 and often PCA-OLS is better, that is, the ratio < 1.

4. Conclusion

We showed that the risk inflation of a particular ordinary least squares estimator (on the "top" PCA subspace) is within a factor 4 of the ridge estimator. It turns out the converse is not true — this PCA estimator may be arbitrarily better than the ridge one.

Appendix A.

Proof of Lemma 1. We analyze the bias-variance decomposition in Equation 1. For the variance,

$$\begin{aligned}
\mathbb{E}_Y\|\hat{\beta}_\lambda - \bar{\beta}_\lambda\|^2_{\Sigma} &= \sum_j \lambda_j \mathbb{E}_Y([\hat{\beta}_\lambda]_j - [\bar{\beta}_\lambda]_j)^2 \\
&= \sum_j \frac{\lambda_j}{(\lambda_j+\lambda)^2}\frac{1}{n^2}\mathbb{E}\left[\sum_{i=1}^n (Y_i - \mathbb{E}[Y_i])[X_i]_j \sum_{i'=1}^n (Y_i' - \mathbb{E}[Y_i'])[X_i']_j\right] \\
&= \sum_j \frac{\lambda_j}{(\lambda_j+\lambda)^2}\frac{\sigma^2}{n}\sum_{i=1}^n Var(Y_i)[X_i]_j^2 \\
&= \sum_j \frac{\lambda_j}{(\lambda_j+\lambda)^2}\frac{\sigma^2}{n}\sum_{i=1}^n [X_i]_j^2 \\
&= \frac{\sigma^2}{n}\sum_j \frac{\lambda_j^2}{(\lambda_j+\lambda)^2}.
\end{aligned}$$

2. The details about the data sets can be found here: `http://olivier.chapelle.cc/ssl-book/benchmarks.html`.

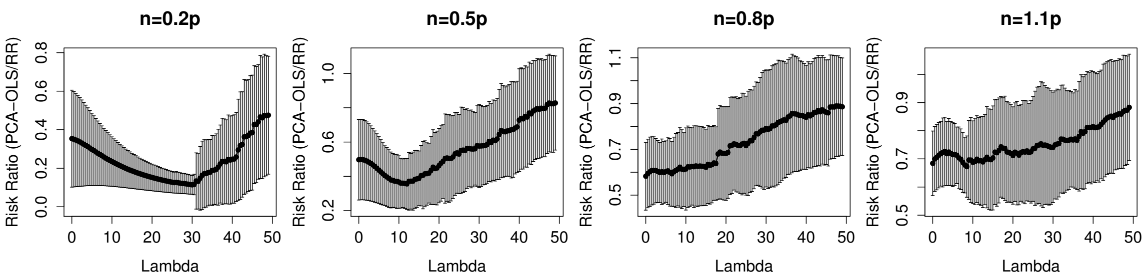

Figure 1: Plots showing the risk ratio as a function of λ, the regularization parameter and n, for the synthetic data set. p=100 in all the cases. The error bars correspond to one standard deviation for 100 such random trials.

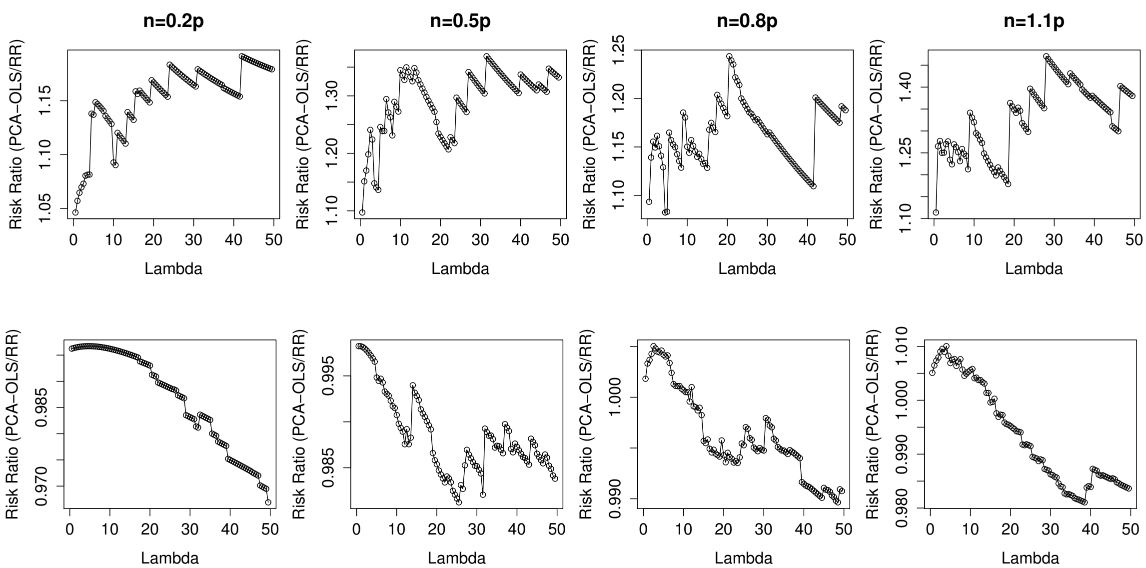

Figure 2: Plots showing the risk ratio as a function of λ, the regularization parameter and n, for two real world data sets (BCI and USPS–top to bottom).

Similarly, for the bias,

$$
\begin{aligned}
\|\bar{\beta}_\lambda - \beta\|^2_{\Sigma} &= \sum_j \lambda_j([\bar{\beta}_\lambda]_j - [\beta]_j)^2 \\
&= \sum_j \beta_j^2 \lambda_j \left(\frac{\lambda_j}{\lambda_j+\lambda} - 1\right)^2 \\
&= \sum_j \beta_j^2 \frac{\lambda_j}{(1+\frac{\lambda_j}{\lambda})^2},
\end{aligned}
$$

which completes the proof. ■

The risk for RR can be arbitrarily worse than the PCA-OLS estimator.

Consider the standard OLS setting described in Section 1 in which $\mathbf{X}$ is $n \times p$ matrix and Y is a $n \times 1$ vector.

Let $\mathbf{X} = diag(\sqrt{1+\alpha}, 1, \ldots, 1)$, then $\mathbf{\Sigma} = \mathbf{X}^\top \mathbf{X} = diag(1+\alpha, 1, \ldots, 1)$ for some $(\alpha > 0)$ and also choose $\beta = [2+\alpha, 0, \ldots, 0]$. For convenience let's also choose $\sigma^2 = n$.

Then, using Lemma 1, we get the risk of RR estimator as

$$
\text{Risk}(\hat{\beta}_\lambda) = \left(\underbrace{\left(\frac{1+\alpha}{1+\alpha+\lambda}\right)^2}_{\text{I}} + \underbrace{\frac{(p-1)}{(1+\lambda)^2}}_{\text{II}} \right) + \underbrace{(2+\alpha)^2 \times \frac{(1+\alpha)}{(1+\frac{1+\alpha}{\lambda})^2}}_{\text{III}}.
$$

Let's consider two cases

- **Case 1:** $\lambda < (p-1)^{1/3} - 1$, then $II > (p-1)^{1/3}$.
- **Case 2:** $\lambda > 1$, then $1 + \frac{1+\alpha}{\lambda} < 2+\alpha$, hence $III > (1+\alpha)$.

Combining these two cases we get $\forall\lambda$, $\text{Risk}(\hat{\beta}_\lambda) > min((p-1)^{1/3}, (1+\alpha))$. If we choose p such that $p-1 = (1+\alpha)^3$, then $\text{Risk}(\hat{\beta}_\lambda) > (1+\alpha)$.

The PCA-OLS risk (From Theorem 2) is:

$$
\text{Risk}(\hat{\beta}_{PCA,\lambda}) = \sum_j \mathbb{1}_{\lambda_j \geq \lambda} + \sum_{j:\lambda_j<\lambda} \lambda_j \beta_j^2.
$$

Considering $\lambda \in (1, 1+\alpha)$, the first term will contribute 1 to the risk and rest everything will be 0. So the risk of PCA-OLS is 1 and the risk ratio is

$$
\frac{\text{Risk}(\hat{\beta}_{PCA,\lambda})}{\text{Risk}(\hat{\beta}_\lambda)} \leq \frac{1}{(1+\alpha)}.
$$

Now, for large α, the risk ratio ≈ 0.

References

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