Feature Selection / Regularization

Data Analysis for Networks - DataNets'19
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Bibliography

A. Giovanidis 2019

B.1 Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani.
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Chapter 6
DOI 10.1007/978-1-4614-7138-7

Intro

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In the multiple-regression setting, we assumed that the linear model with additive noise:

$$Y = \beta_0 + \beta_1 X_1 + \ldots + \beta_p X_p + \epsilon$$

describes the relationship between a response Y and a set of $p \geq 1$ predictor variables $X_1, X_2, \ldots, X_p$.
- The model fit uses least squares (LSs) to estimate the $\hat{\beta}_i$'s.

But, is it always a good fit? Are there any ways to improve this fit?

☞ Feature Selection, Regularization, and Dimension Reduction.

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Main idea

☞ Either shrink the coefficients for some feature variables or remove them completely!

Why?

- Prediction Accuracy: If $n >> p$ then LSs do have low variance. But when e.g. $n \leq p$ the model is highly variable!
- Model Interpretability: Some variables used as predictors may not be relevant with the response. Better remove them to reduce model complexity.

Methods

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We will present three main methods that modify the LSs:

- Subset Selection: Identify a subset of the original p predictors to be relevant (say $p_s < p$). Then apply LSs fit.
- Shrinkage: Fit the model with all p features, but shrink some coefficients even to zero.
  $\rightarrow$ This method reduces variance.
- Dimension Reduction: This method projects the p predictors to an $M < p$ dimensional space, through M different linear combinations. Then apply LSs fit.

Best subset selection

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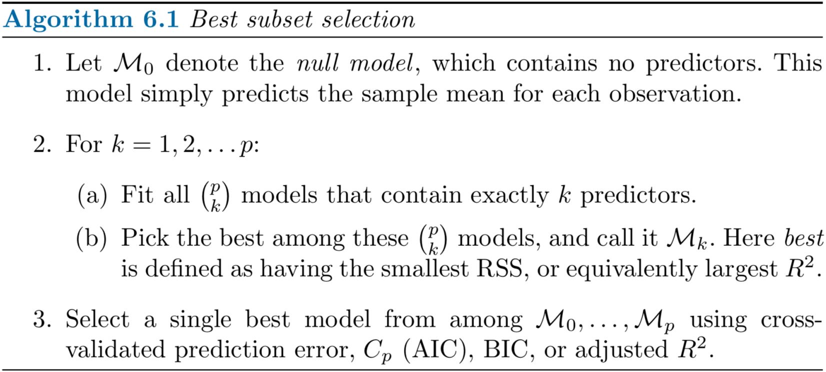
To find the best set one needs to perform LSs for all possible combinations fo the p predictors:

- All models with 1 predictor: p.
- All models with 2 predictors: $\left(\begin{array}{c} \mathrm{p} \\ 2 \end{array} \right) = \frac{p(p-1)}{2}$.
- etc.

In total 2^p possibilities.

[1] A. Giovanidis 2019



Algorithm 6.1 *Best subset selection*

```
1. Let $\mathcal{M}_0$ denote the null model, which contains no predictors. This
   model simply predicts the sample mean for each observation.
2. For $k = 1, 2, \ldots p$:
   (a) Fit all $\binom{p}{k}$ models that contain exactly $k$ predictors.
   (b) Pick the best among these $\binom{p}{k}$ models, and call it $\mathcal{M}_k$. Here best
       is defined as having the smallest RSS, or equivalently largest $R^2$.
3. Select a single best model from among $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using cross-
   validated prediction error, $C_p$ (AIC), BIC, or adjusted $R^2$.
```

☞ Pick models with smallest Train RSS, Select with smallest Test RSS.

[1] Source [B.1]

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Many possibilities to test...

The method needs to test too many feature combinations:

- for $p = 10$, approx $1,000$ models,
- for $p = 20$, over $1,000,000$ possibilities!
- etc.

The Best subset selection becomes computationally infeasible for large sets of features.

☞ We need to find other ways to select good subsets stepwise.

Forward Stepwise Selection

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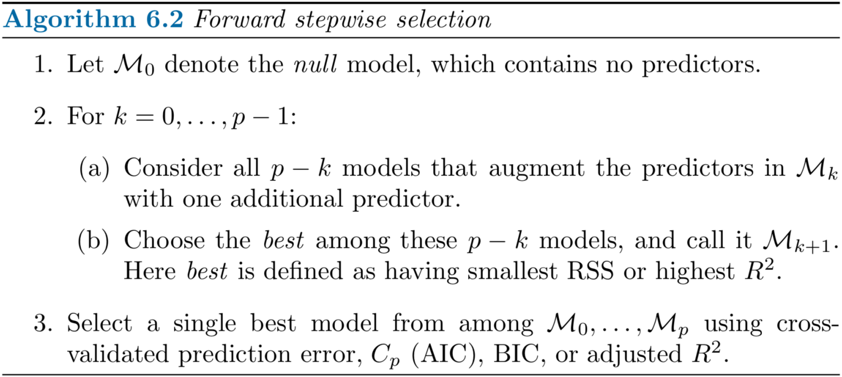
The method:

- Begins with a model without predictors,
- adds predictors to the model one-at-a-time,
- until all predictors are in the model.

At each step the variable that gives the greatest additional improvement to the fit is added.

[2]



Algorithm 6.2 *Forward stepwise selection*

```
1. Let $\mathcal{M}_0$ denote the *null* model, which contains no predictors.
2. For $k = 0, \ldots, p-1$:
    (a) Consider all $p-k$ models that augment the predictors in $\mathcal{M}_k$
        with one additional predictor.
    (b) Choose the *best* among these $p-k$ models, and call it $\mathcal{M}_{k+1}$.
        Here *best* is defined as having smallest RSS or highest $R^2$.
3. Select a single best model from among $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using cross-
   validated prediction error, $C_p$ (AIC), BIC, or adjusted $R^2$.
```

☞ Pick models with smallest Train RSS, Select with smallest Test RSS.

[2] Source [B.1]

Advantages

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The method is computationally advantageous compared to Best selection:

- Instead of 2^p fitting models, it needs to compute only $1 + \sum_{k=0}^{p-1}(p-k) = 1 + p(p+1)/2$ models.
- e.g. for $p = 20$, fit 211 models instead of $1,048,576$!
- Can be used also when $n < p$ (stops at n features)

It is not guaranteed to find the best possible model out of the 2^p.

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[3]

# Variables	Best subset	Forward stepwise
One	rating	rating
Two	rating, income	rating, income
Three	rating, income, student	rating, income, student
Four	cards, income, student, limit	rating, income, student, limit

[3] Source [B.1]

Backward Stepwise Selection

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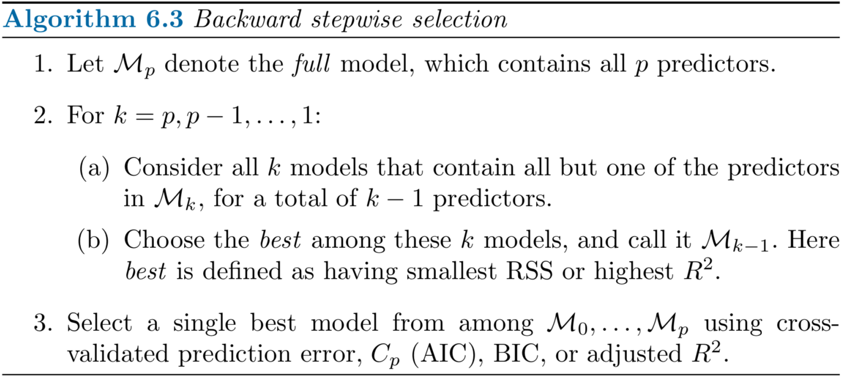
[4]



Algorithm 6.3 *Backward stepwise selection*

1. Let $\mathcal{M}_p$ denote the *full* model, which contains all p predictors.
2. For $k = p, p-1, \ldots, 1$:
   - (a) Consider all k models that contain all but one of the predictors in $\mathcal{M}_k$, for a total of $k-1$ predictors.
   - (b) Choose the *best* among these k models, and call it $\mathcal{M}_{k-1}$. Here *best* is defined as having smallest RSS or highest R^2.
3. Select a single best model from among $\mathcal{M}_0, \ldots, \mathcal{M}_p$ using cross-validated prediction error, C_p (AIC), BIC, or adjusted R^2.

[4] Source [B.1]

Choosing the Optimal Model

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All methods hand-pick a small number of models based on a small value of Test RSS or high value of R^2.

To choose exactly one model among these, we need to find the one with smallest Test error. To do so we can:

- Estimate the Test Error, by adjusting the Train Error to account for Bias.
- Directly estimate the Test Error using a validation set or cross-validation.

Adjustment of the Train Error

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☞ We already know the Cross-Validation concept.

We can also adjust the Train error to select the model with best Test prediction:

- C_p-estimate: $C_p = \frac{1}{n}\left(RSS + 2d\hat{\sigma}^2\right)$.
- Akaike Information Criterion: $AIC = \frac{1}{n\hat{\sigma}^2}(RSS + 2d\hat{\sigma}^2)$.
- Bayesian Information Criterion: $BIC = \frac{1}{n\hat{\sigma}^2}(RSS + \log(n)d\hat{\sigma}^2)$.
- Adjusted $R^2 = 1 - \frac{RSS/(n-d-1)}{TSS/(n-1)}$, where $TSS = \sum(y_i - \bar{y})^2$.

Shrinkage

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We have seen methods to optimally select a subset of appropriate features, leaving the rest out.

☞ As an alternative, we can keep all p features, but use a technique that constraints or regularizes the coefficient estimates.

Estimates can be shrunk towards zero! This technique can significantly reduce variance.

Ridge Regression and the Lasso.

Ridge Regression

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Similar to LSs fit, the Ridge Regression solves

$$\min_{\beta} \quad \sum_{i=1}^{n}\left(y_i-\beta_0-\sum_{j=1}^{p}\beta_j x_{ij}\right)^2+\lambda\sum_{j=1}^{p}\beta_j^2$$

where the lefthand side is just the RSS, and $\lambda \geq 0$ is a tuning parameter, to be determined.

The second term is called shrinkage penalty.

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Properties

- When $\lambda = 0$: it is just the Least-Squares fit.
- When $\lambda \rightarrow \infty$ β's will approach zero.
- Find the "best" set of parameters β.

☞ Each choice of λ produces a different set of estimates $\hat{\beta}_\lambda$.

Note 1: The shrinkage penalty is **not** applied to the intercept β_0.
Note 2: Best apply ridge-regression after standardizing the predictors (all on the same scale / standard deviation 1)

$$\tilde{x}_{ij} = \frac{x_{ij}}{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij} - \bar{x}_j)^2}}.$$

Ridge Example

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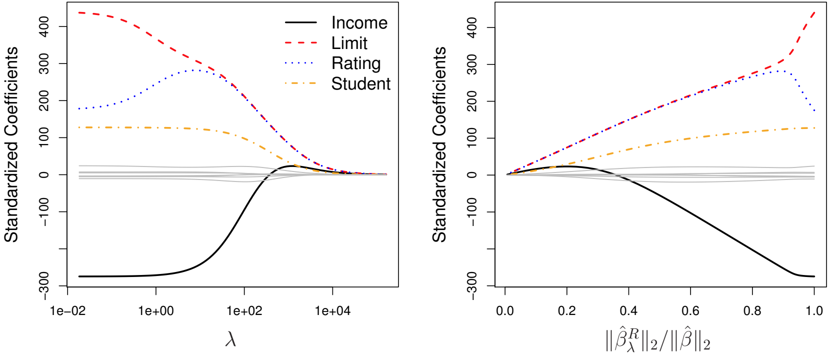

Figure: Change of Ridge Regression coefficients vs λ.[5]

[5] Source [B.1]

Improvement over LSs

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☞ As λ increases, the flexibility of the ridge regression fit decreases: decreased variance but increased Bias.

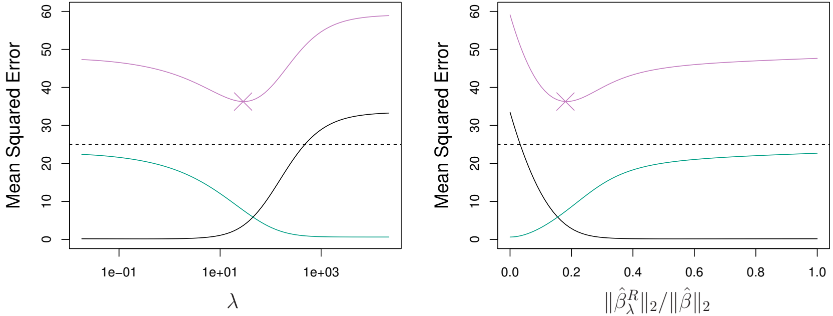

Figure: Bias vs Variance tradeoff and Test MSE.[6]

[6] Source [B.1]

The Lasso

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Similar to Ridge Regression, the Lasso solves a different problem

$$\min_\beta \qquad \sum_{i=1}^{n}\left(y_i-\beta_0-\sum_{j=1}^{p}\beta_j x_{ij}\right)^2+\lambda\sum_{j=1}^{p}|\beta_j|$$

where the lefthand side is just the RSS, and $\lambda \geq 0$ is again a tuning parameter, to be determined.

The second term is the lasso penalty (uses ℓ_1-norm instead of ℓ_2).

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Advantages

As formulation, the Lasso is similar to Ridge Regression, with a penalty that uses a different norm.

What is new here?

- The Lasso penalty can force some estimates to be exactly zero → performs Variable Selection.
- Lasso's models are sparse involving a subset of variables.
- Simple, more interpretable models.

Example Lasso

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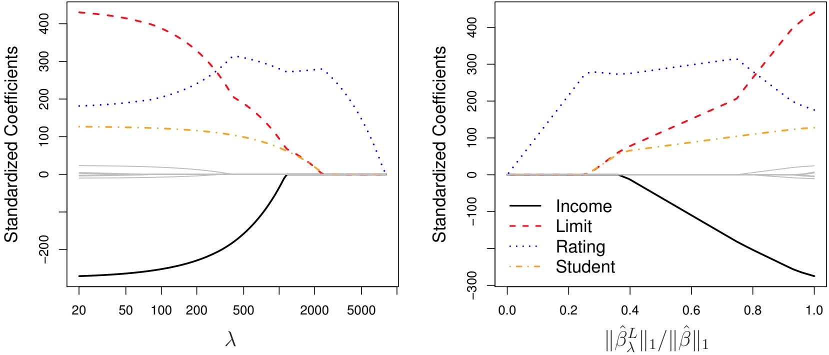

Figure: Change of Lasso coefficients vs λ.[7]

[7] Source [B.1]

Equivalent Problems

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The Ridge, Lasso, and Best subset selection are each equivalent to:

$$\min_\beta \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \right\} \quad s.t. \quad \sum_{j=1}^{p} \beta_j^2 \leq s \quad (\textit{Ridge})$$

$$\min_\beta \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \right\} \quad s.t. \quad \sum_{j=1}^{p} |\beta_j| \leq s \quad (\textit{Lasso})$$

$$\min_\beta \left\{ \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \right\} \quad s.t. \quad \sum_{j=1}^{p} \mathbf{1}\left(\beta_j \neq 0\right) \leq s \quad (\textit{Best}).$$

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Illustrative Explanation

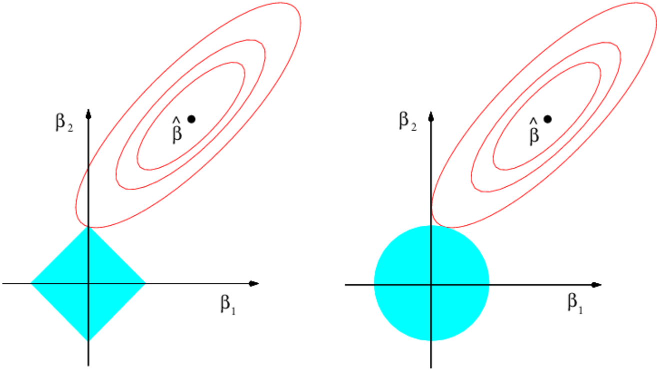

Figure: Why does Lasso lead to estimates equal to 0?[8]

[8] Source [B.1]

Ridge > Lasso

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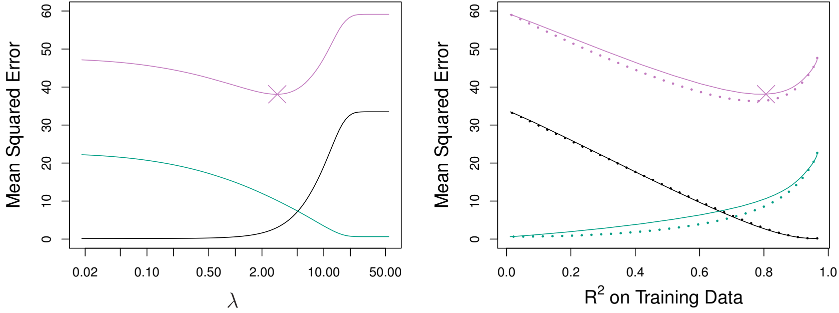
Here: Ridge needs all 45 coefficients $\neq 0$. Lasso chose 2-out-of-45 features.[9]



[9] Source [B.1]

Ridge < Lasso

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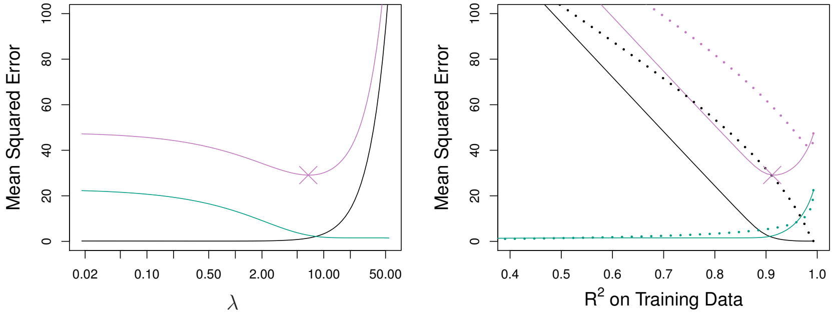
Here: True response is a function of only 2 predictors and the rest are irrelevant. Ridge needs again all 45 coefficients $\neq 0$. Lasso chose 2-out-of-45 features.[10]



[10] Source [B.1]

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Special Case $n = p$

☞ Data centred around $\bar{x}$, no need for intercept.

- Least Squares: $\min \sum_{j=1}^{p}(y_j - \beta_j)^2$. Solution:

$$\hat{\beta}_j = y_j.$$

- Ridge Regression: $\min \sum_{j=1}^{p}(y_j - \beta_j)^2 + \lambda \sum_{j=1}^{p} \beta_j^2$. Solution:

$$\hat{\beta}_j^{(R)} = y_j/(1 + \lambda).$$

- Lasso: $\min \sum_{j=1}^{p}(y_j - \beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j|$. Solution:

$$\hat{\beta}_j^{(L)} = \begin{cases} y_j - \lambda/2, & \text{if } y_j > \lambda/2 \\ y_j + \lambda/2, & \text{if } y_j < -\lambda/2 \\ 0, & \text{if } |y_j| \leq \lambda/2 \end{cases}$$

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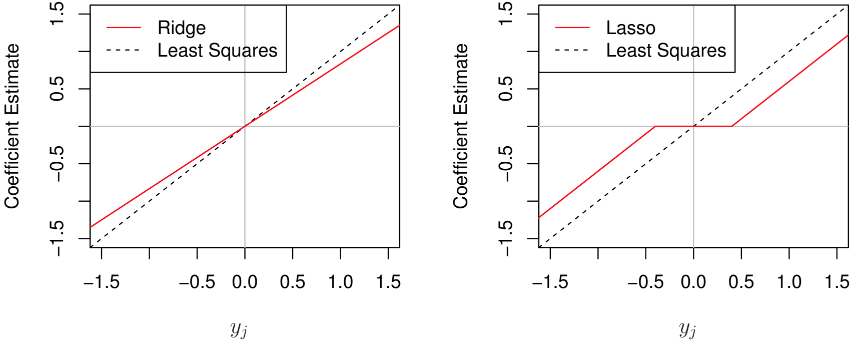

Figure: Ridge and Lasso coefficients over λ, compared to LSs.[11]

[11] Source [B.1]

How to select parameter λ?

For both Ridge and Lasso the tuning parameter λ (equivalently s) needs to be determined.
☞Again find the minimum Test MSE using Cross-Validation!

- Choose a grid of λ values.
- Compute the cross-validation error for each value of λ.
- Select the tuning parameter value with minimum CV error.
- Finally, re-fit the model using all observations and the chosen λ.

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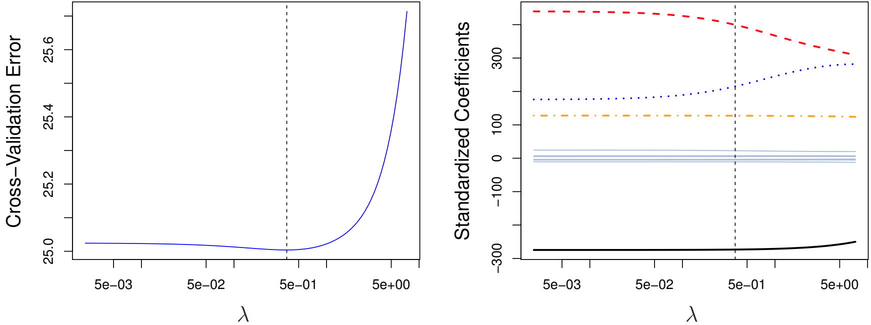

Figure: Ridge parameter tuning and comparison with LSs.[12]

[12] Source [B.1]

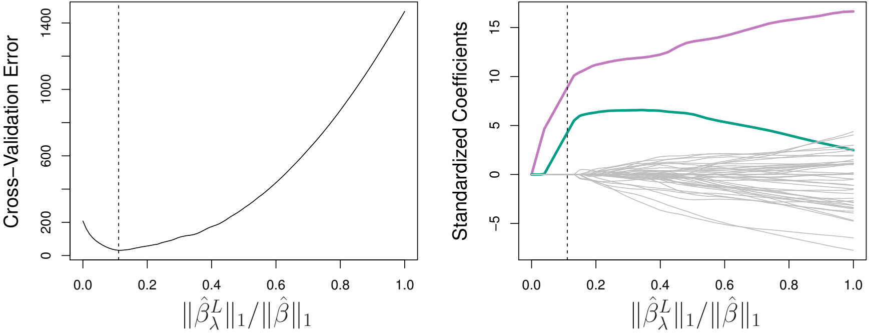

Figure: Lasso parameter tuning and comparison with LSs.[13]

[13] Source [B.1]

Dimension Reduction

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Until here, methods control variance in 2 ways. From the original $X_1, \ldots, X_p$ predictors,

- either choose a subset of the original variables, or
- shrink some of their coefficients to zero.

☞ A new method!

1. first, Transform the predictors to a lower dimension $Z_1, \ldots, Z_M$, with $M < p$,
2. then Fit the LS model using the M predictors.

Dimension Reduction cont'd

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$Z_1, Z_2, \ldots, Z_M$: linear combinations ($M \leq p$) of our original p predictors.

$$Z_m \quad = \quad \sum_{j=1}^{p} \phi_{j,m} X_j.$$

Unknowns: $\phi_{1,m}, \ldots, \phi_{p,m}$, for $m = 1, \ldots, M$

Then we can fit the linear regression model:

$$y_i \quad = \quad \theta_0 + \sum_{m=1}^{M} \theta_m z_{i,m} + \epsilon_i, \quad i = 1, \ldots, n$$

using the Least Squares. The method can outperform simple LSs!

Dimension Reduction cont'd II

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We need not estimate the $p+1$ coefficients: $\beta_0, \beta_1, \ldots, \beta_p$, but rather the less $M+1$ coefficients: $\theta_0, \theta_1, \ldots, \theta_M$.

$$\begin{aligned} \sum_{m=1}^{M} \theta_m z_{i,m} &= \sum_{m=1}^{M} \theta_m \sum_{j=1}^{p} \phi_{j,m} x_{i,j} \\ &= \sum_{j=1}^{p} \sum_{m=1}^{M} \theta_m \phi_{j,m} x_{i,j} = \sum_{j=1}^{p} \beta_j x_{i,j}. \end{aligned}$$

so that, the β_j's need to take the form:

$$\beta_j := \sum_{m=1}^{M} \theta_m \phi_{j,m}.$$

☞ Works well when p is large compared to n data available.

Principal Components Regression (PCR)

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Steps of the PCR Method:

1. Standardise $X_j/\sqrt{Var(X_j)}$ and then centre $(X_j - \bar{X}_j)$ all p features.
2. Choose a number $M \leq p$ for the components.
3. Using Principal Component Analysis (PCA) define $Z_1, \ldots, Z_M$ using the coefficients $\phi_{j,m}$, $j = 1, \ldots, p$.
4. Use $Z_1, \ldots, Z_M$ as the predictors in a linear regression model that is fit using LSs.
5. Using different number of components M choose the model which minimises the Test MSE.

☞ The PCR is not a feature selection method!
(uses linear combinations of all p original features)

What is Principal Components Analysis?

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PCA is a technique to reduce the dimension of a $(n \times p)$ data matrix $\mathbf{X}$:

$$\mathbf{X} \quad = \quad \mathbf{UDV}^T$$

where $\mathbf{U}$ is $(n \times p)$, $\mathbf{V}$ is $(p \times p)$ and $\mathbf{D}$ is a $p \times p$ diagonal matrix, with diagonal entries $d_1 \geq d_2 \geq \ldots \geq d_p \geq 0$, called the singular values of $\mathbf{X}$.

☞ Intuition: the right matrix $\mathbf{V}$ and the square of the singular value matrix $\mathbf{D}^2$ also determine the eigen-decomposition of the sample covariance matrix $\mathbf{S} = \mathbf{X}^T\mathbf{X}/n$,

$$\begin{aligned}
\mathbf{X}^T\mathbf{X} \quad &= \quad (\mathbf{UDV}^T)^T(\mathbf{UDV}^T) \\
&= \quad \mathbf{VDU}^T\mathbf{UDV}^T \\
&\overset{\mathbf{U}^T\mathbf{U}=\mathbf{I}_p}{=} \quad \mathbf{VD}^2\mathbf{V}^T
\end{aligned}$$

PCA cont'd

A. Giovanidis 2019

The principal components directions of $\mathbf{X}$ are the columns of $\mathbf{V}$.

☞ The first principal component direction has the property that $\mathbf{Z_1} = \mathbf{X} v_1$ has the largest sample variance, equal to d_1^2/n.

- This practically means that along the direction v_1, the data vary the most (if projected).
- Also, this direction defines the line which is as close as possible to the data!

PCA Example

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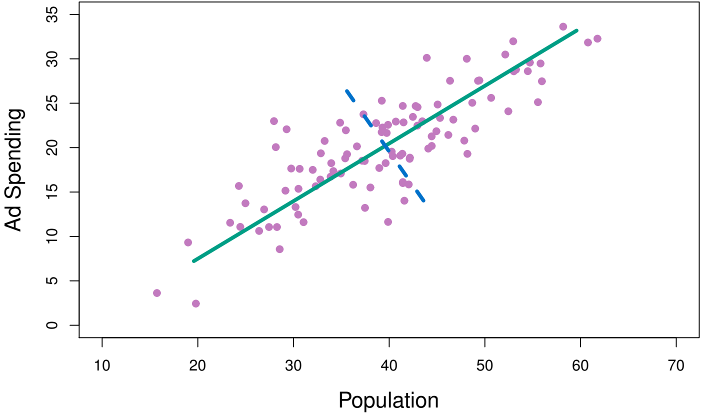

Figure: Principal components directions for $p = 2$.[14]

[14] Source [B.1]

PCA Example cont'd

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The two PCA directions are:

$$
\begin{aligned}
Z_1 &= 0.839 \times (pop - \overline{pop}) + 0.544 \times (ad - \overline{ad}) \\
Z_2 &= 0.544 \times (pop - \overline{pop}) - 0.839 \times (ad - \overline{ad})
\end{aligned}
$$

- With $p = 2$, we can construct at most $M = 2$ linear combinations.
- The directions $(0.839,\ 0.544)$ and $(0.544,\ -0.839)$ are orthogonal!
- For the Regression using PCA, we need to choose the sets $\{Z_1\}$ and $\{Z_1,\ Z_2\}$ and find which one leads to smallest Test MSE.

PCR vs Ridge and Lasso

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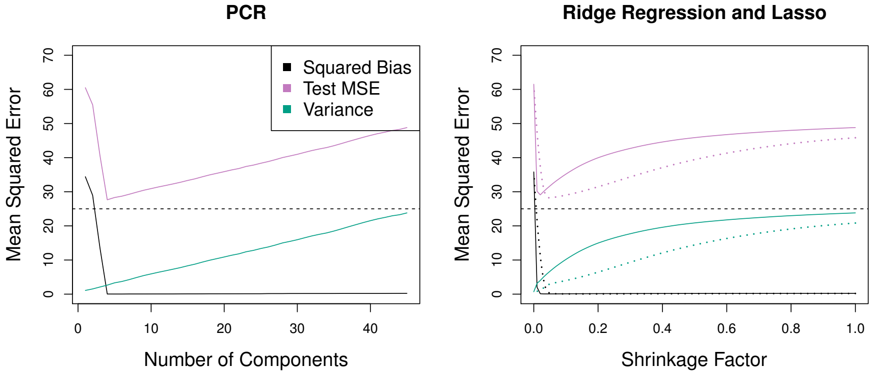

Figure: $p = 45$ features: PCR vs Lasso (solid) and Ridge (dotted).[15]

[15] Source [B.1]

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END