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# Feature Selection / Regularization

Data Analysis for Networks - DataNets'19

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February 13, 2019

# Bibliography



B.1 Gareth James, Daniela Witten, Trevor Hastie, Robert Tibshirani. "An introduction to statistical learning: with applications in R". Springer Texts in Statistics. ISBN 978-1-4614-7137-0
Chapter 6
DOI 10.1007/978-1-4614-7138-7

# Intro

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.

# 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

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: $\begin{pmatrix} p \\ 2 \end{pmatrix} = \frac{p(p-1)}{2}$.
- etc.

In total $2^p$ possibilities.

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[1]

**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.

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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]

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# Advantages

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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| # 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.

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# Adjustment of the Train Error

☞ 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 $\lambda \to \infty$ $\beta$'s will approach zero.
- Find the "best" set of parameters $\beta$.

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

**Note 1:** The shrinkage penalty is **not** applied to the intercept $\beta_0$.
**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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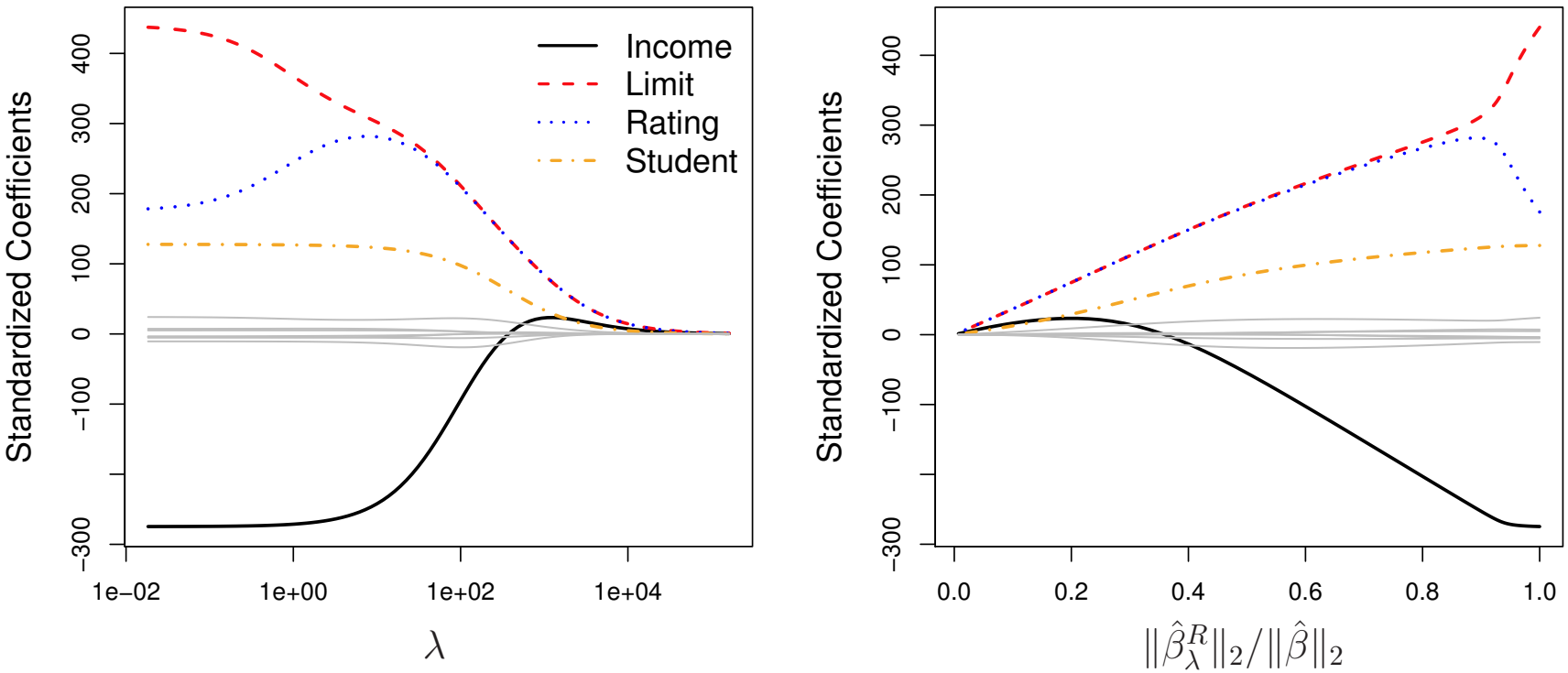


Figure: Change of Ridge Regression coefficients vs $\lambda$.[5]

[5] Source [B.1]

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# Improvement over LSs

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

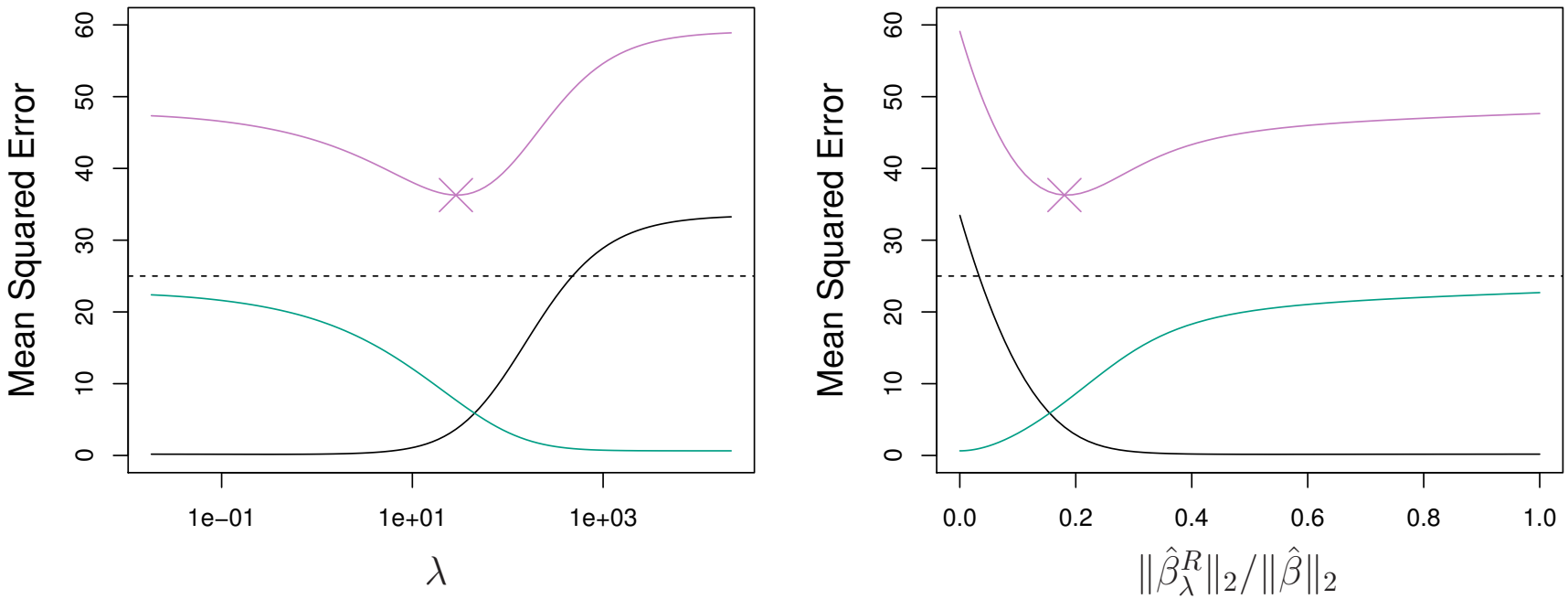


Figure: Bias vs Variance tradeoff and Test MSE.[6]

[6] Source [B.1]

# The Lasso

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Similar to Ridge Regression, the Lasso solves a different problem

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

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 $\ell_1$-norm instead of $\ell_2$).

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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 $\rightarrow$ performs Variable Selection.
- Lasso's models are sparse involving a subset of variables.
- Simple, more interpretable models.

# Example Lasso

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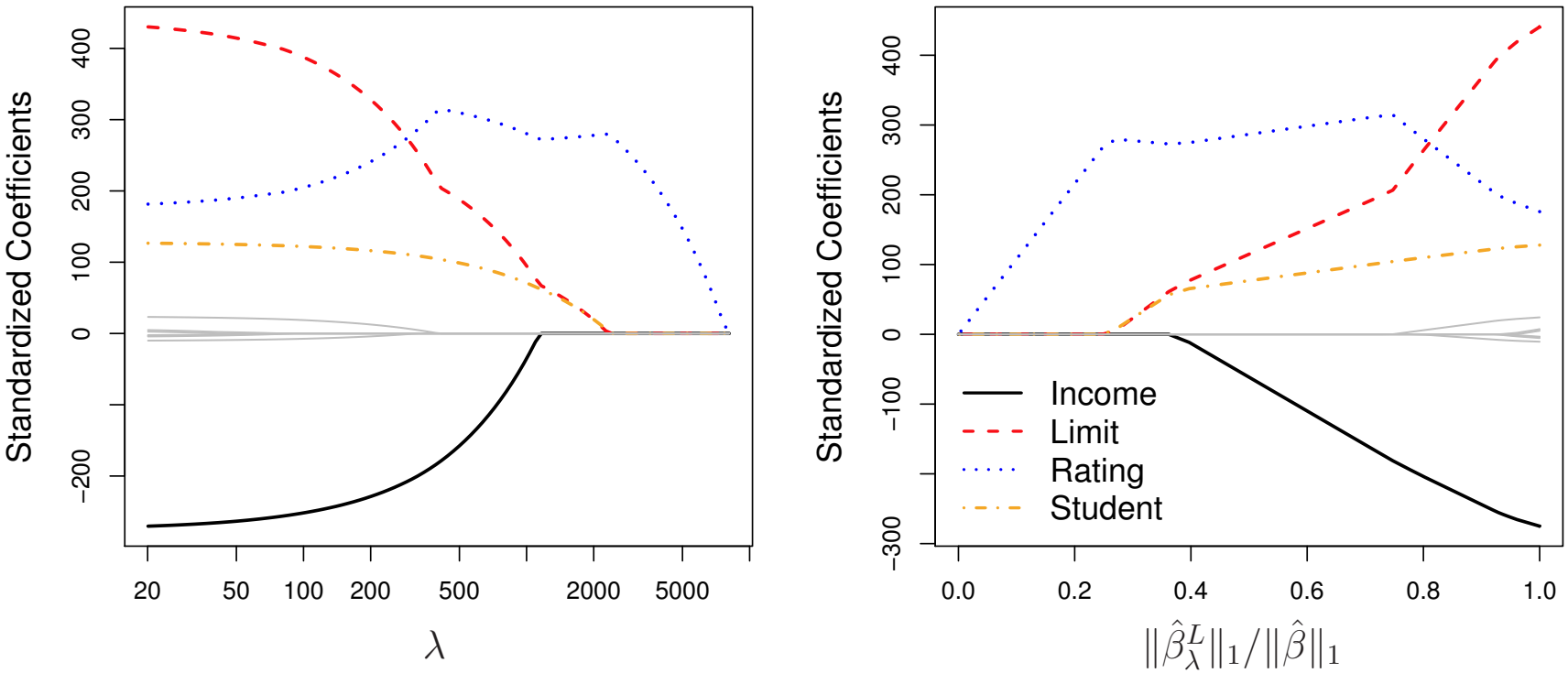


Figure: Change of Lasso coefficients vs $\lambda$.[7]

[7] Source [B.1]

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# Equivalent Problems

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

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

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

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

# Illustrative Explanation

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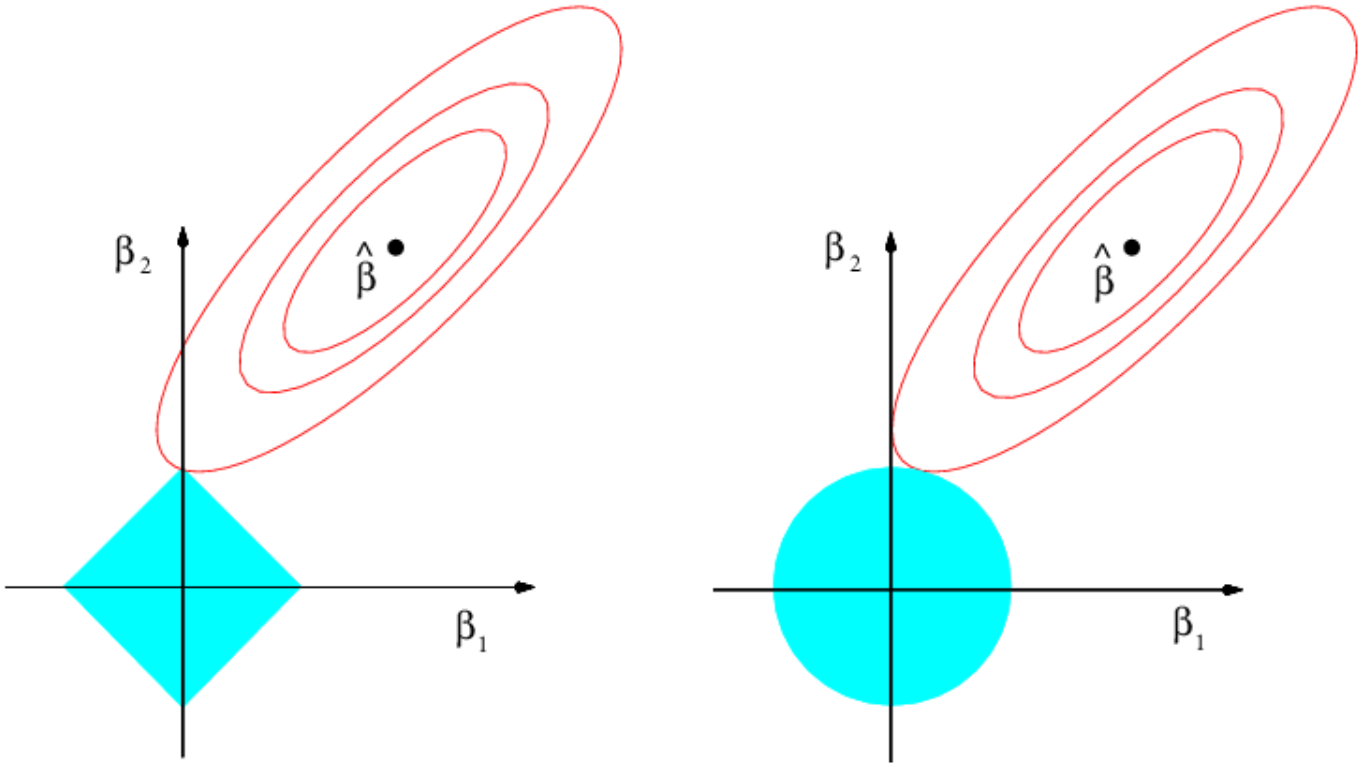


Figure: Why does Lasso lead to estimates equal to 0?[8]

[8] Source [B.1]

# Ridge > Lasso

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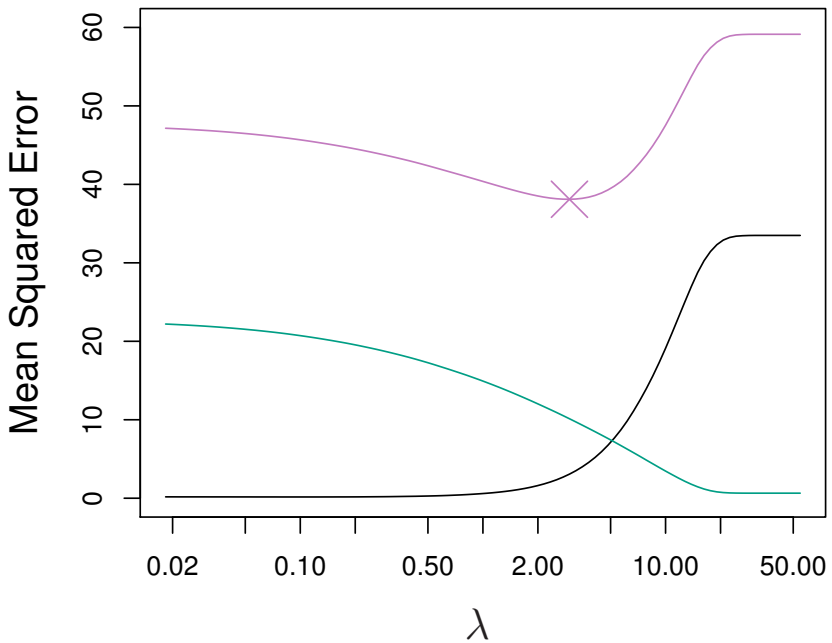
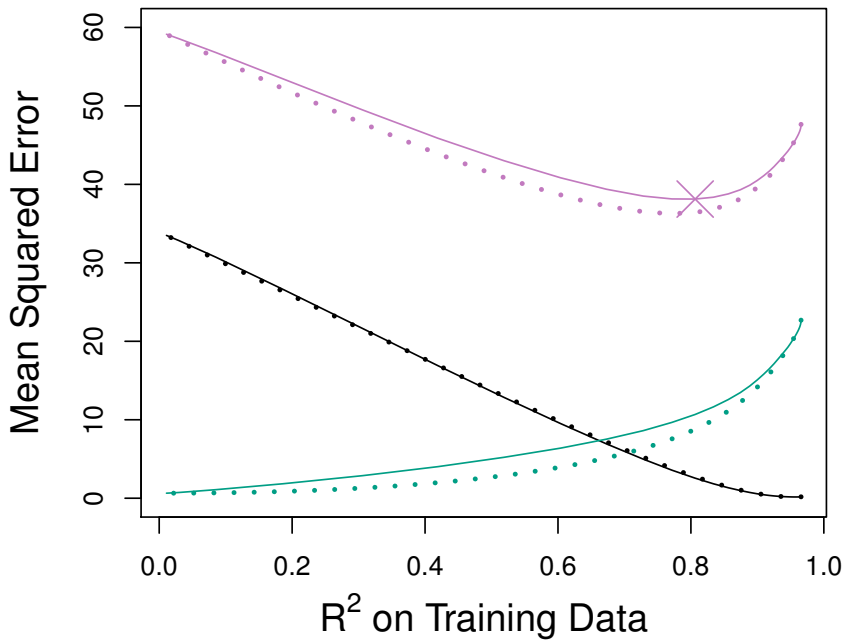
Here: Ridge needs all 45 coefficients $\neq 0$. Lasso chose 2-out-of-45 features.[9]




[9] Source [B.1]

# Ridge $<$ Lasso

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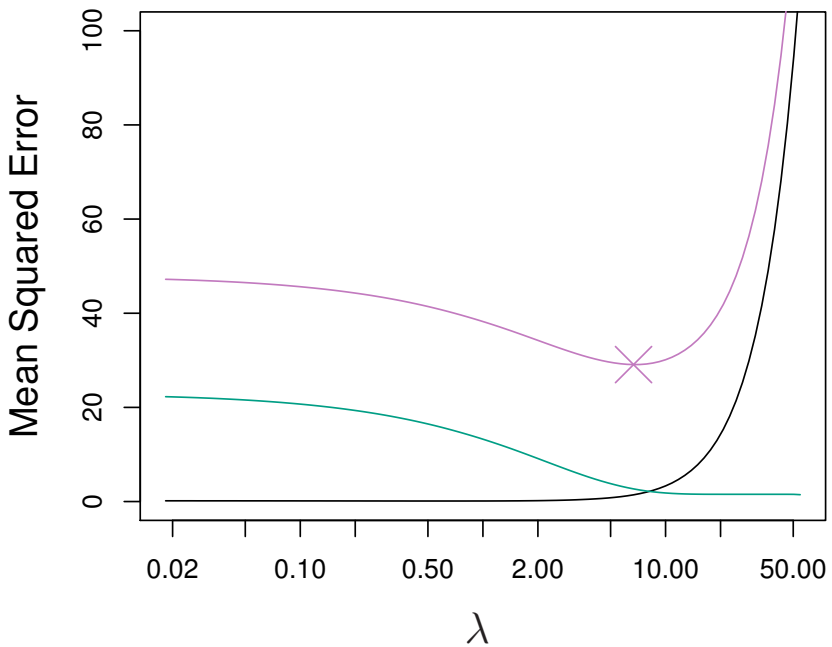
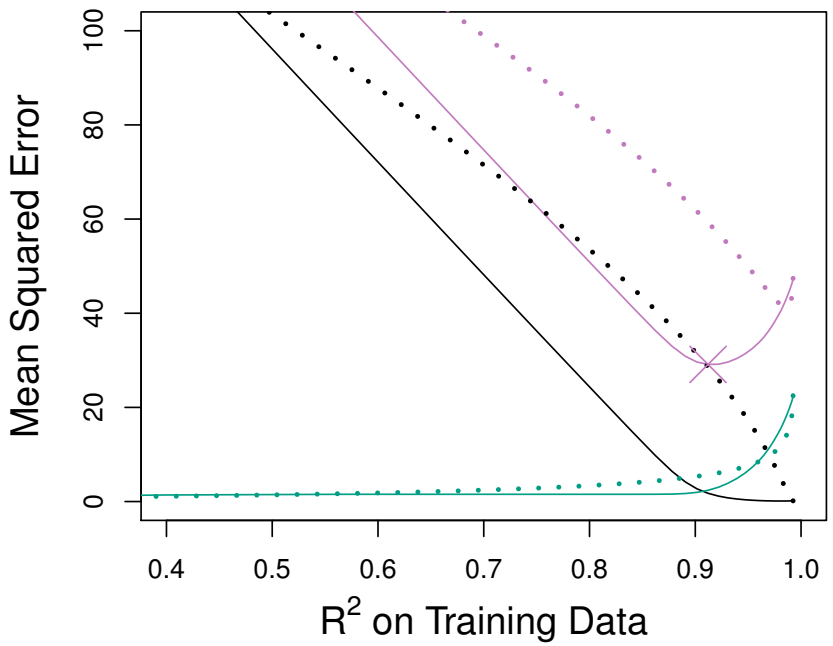
Here: True response is a function of only 2 predictors and the rest are irrelevant. Ridge needs again all 45 coefficients $\neq 0$. Lasso chose 2-out-of-45 features.[10]




[10] Source [B.1]

# 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:

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

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

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

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

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

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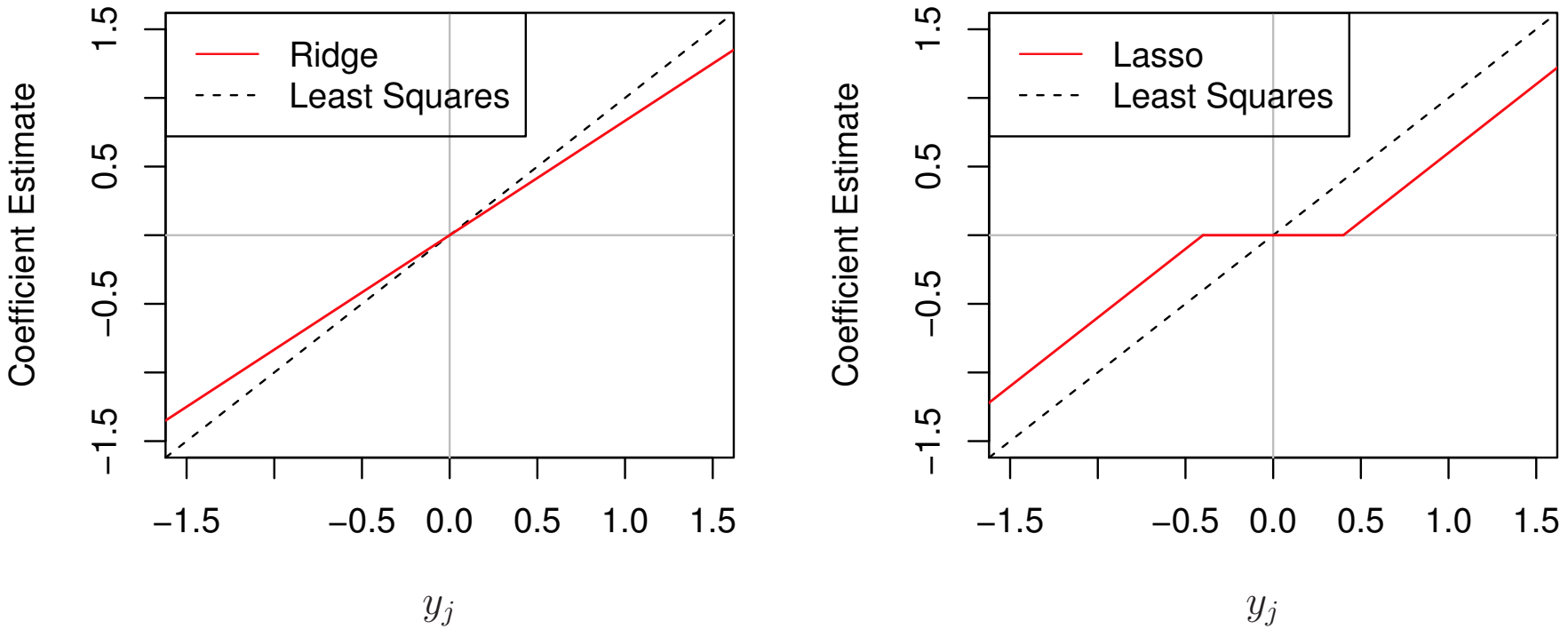


Figure: Ridge and Lasso coefficients over $\lambda$, compared to LSs.[11]

[11] Source [B.1]

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# How to select parameter $\lambda$?

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

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

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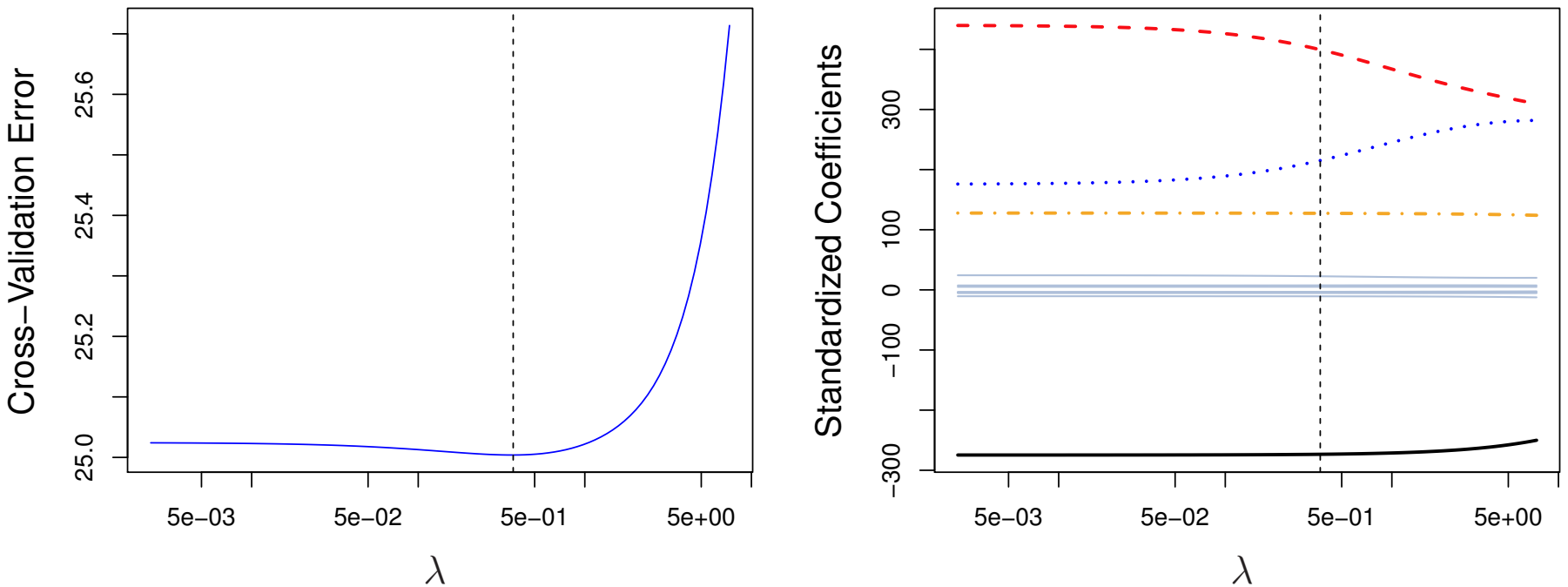


Figure: Ridge parameter tuning and comparison with LSs.[12]

[12] Source [B.1]

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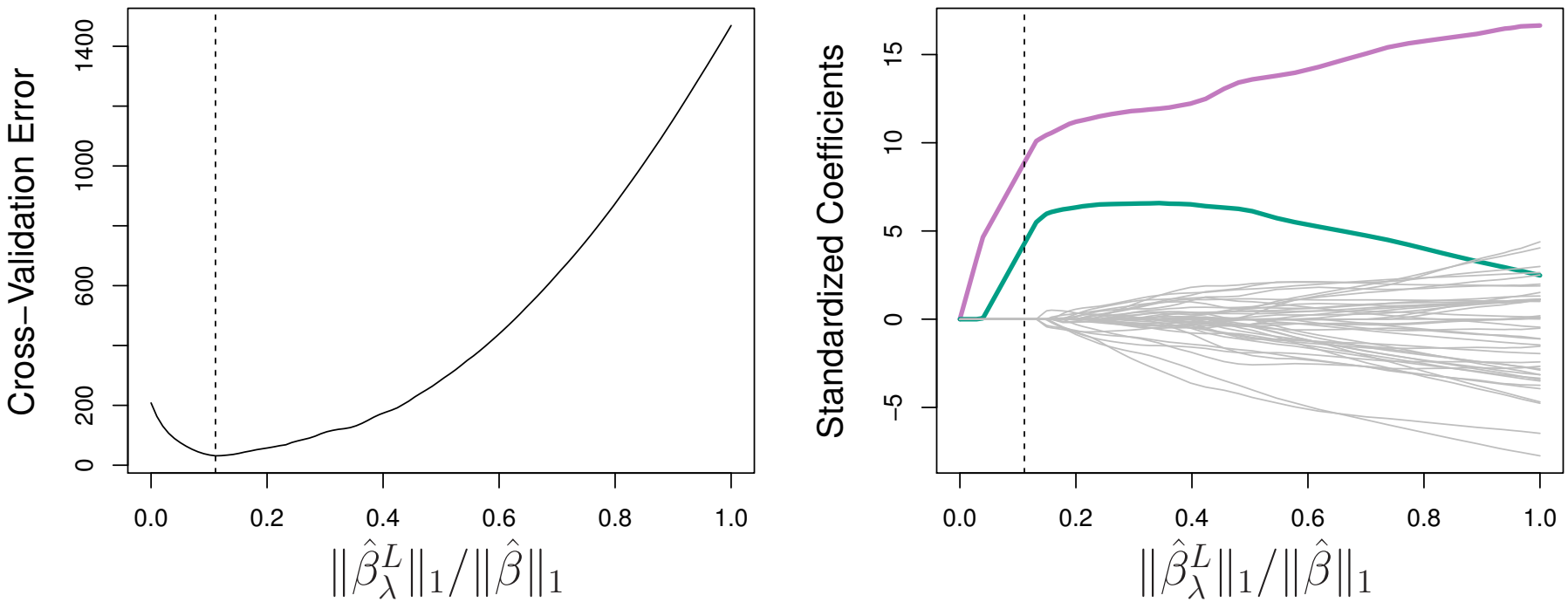


Figure: Lasso parameter tuning and comparison with LSs.[13]

[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.

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

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

Then we can fit the linear regression model:

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

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: $\theta_0, \theta_1, \ldots, \theta_M$.

$$\sum_{m=1}^{M} \theta_m z_{i,m} = \sum_{m=1}^{M} \theta_m \sum_{j=1}^{p} \phi_{j,m} x_{i,j}$$

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

so that, the $\beta_j$'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.

# Partial Least Squares (PLS)

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PLS is a dimension reduction method:

1. First, identifies a new set of features $Z_1, \ldots, Z_M$, $M < p$ in a supervised way,
2. then fits a linear model via LSs using the $M$ features.

Supervised way: means uses the response $Y$ to identify new features, related to the response.

# PLS cont'd

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PLS steps:

- Standardise and centre the $p$ predictors.
- $Z_1$: Do LSs for all pairs $(X_j, Y) \rightarrow$ use $\phi_{\mathbf{j,1}} := \beta_{\mathbf{j,1}}$, $i = 1, \ldots, p$.

  In $Z_1 = \sum_{j=1}^{p} \phi_{j,1} X_1$, PLS places the highest weight on the variables most strongly related to the response $Y$.
- $Z_2$: Do LSs for all pairs $(X_j, Z_1)$ and find new $X_j^{(2)} = X_j - \gamma_{j,1} Z_1$.
  Then do LSs for all pairs $(X_j^{(2)}, Y) \rightarrow$ use $\phi_{\mathbf{j,1}} := \beta_{\mathbf{j,1}}^{\mathbf{(2)}}$, $i = 1, \ldots, p$.
- $Z_3$: ...

The PLS seeks directions that have high variance and high correlation with the response.

# 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)

# PCR example

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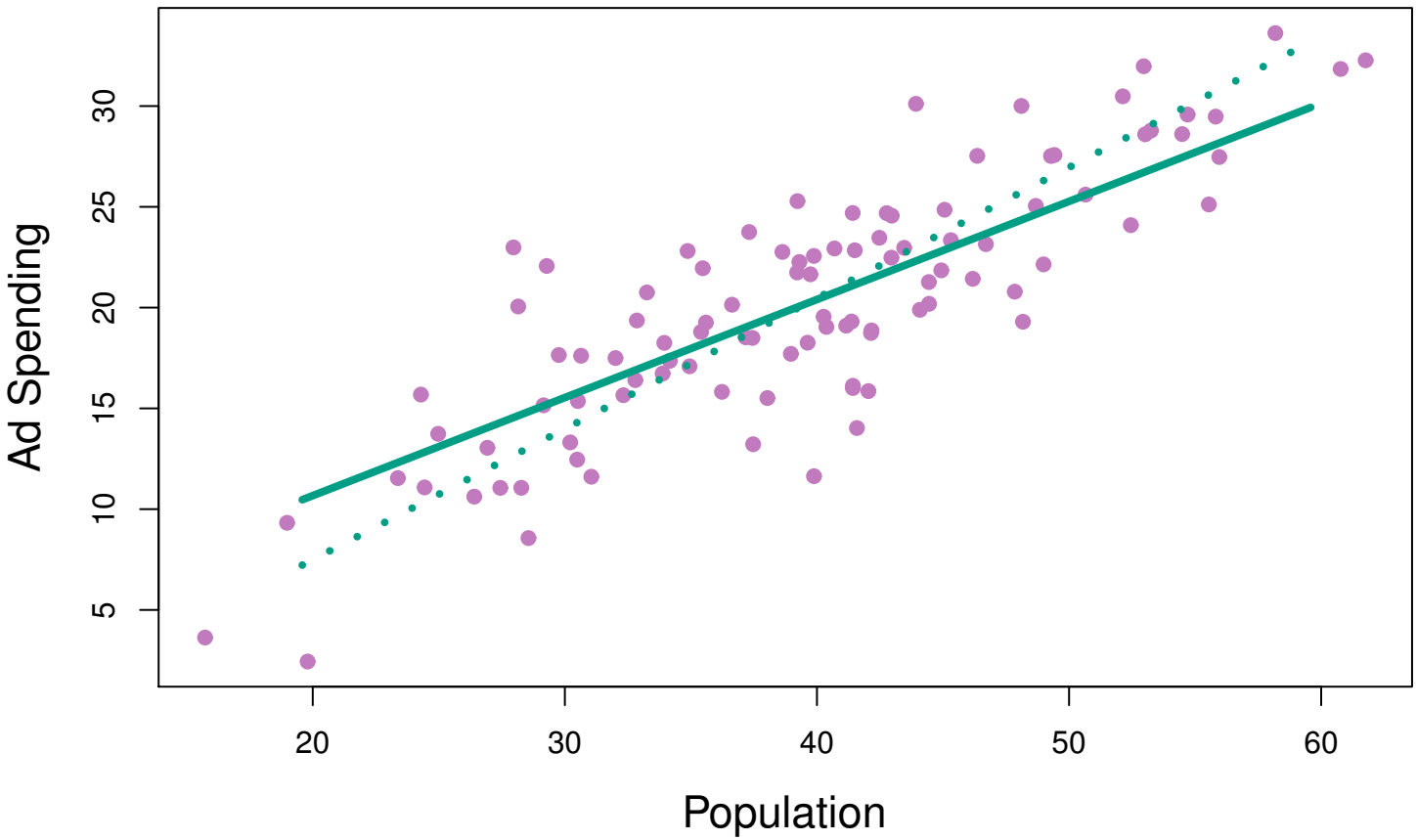


Figure: PCR direction $Z_1$ for $p = 2$.[14]

[14] Source [B.1]

# What is Principal Components Analysis?

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

$$\mathbf{X} \quad = \quad \mathbf{U}\mathbf{D}\mathbf{V}^T$$

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 $\mathbf{S} = \mathbf{X}^T\mathbf{X}/n$,

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

# PCA cont'd

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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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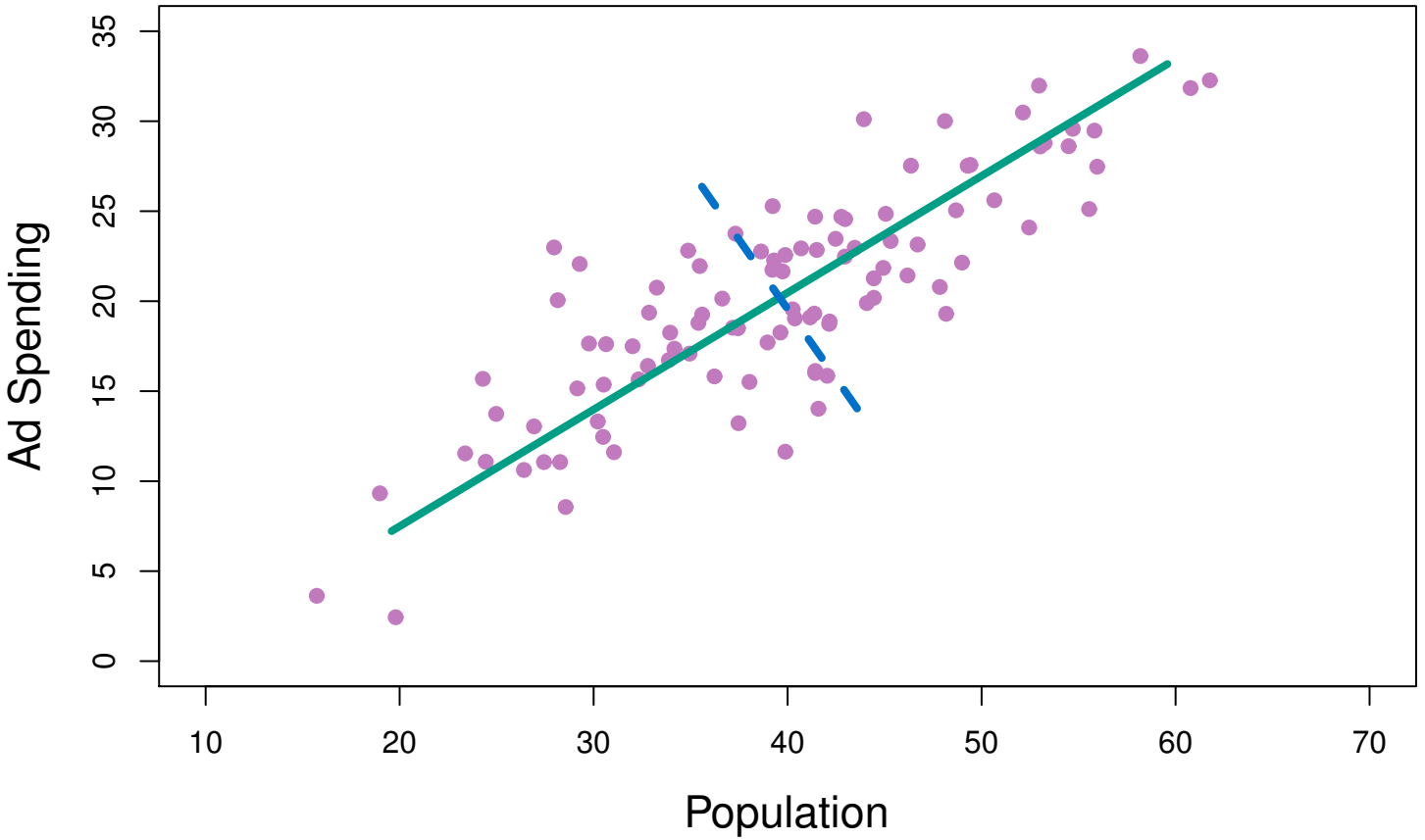


Figure: Principal components directions for $p = 2$.[15]

[15] Source [B.1]

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# PCA Example cont'd

The two PCA directions are:

$$Z_1 = 0.839 \times (pop - \overline{pop}) + 0.544 \times (ad - \overline{ad})$$

$$Z_2 = 0.544 \times (pop - \overline{pop}) - 0.839 \times (ad - \overline{ad})$$

- 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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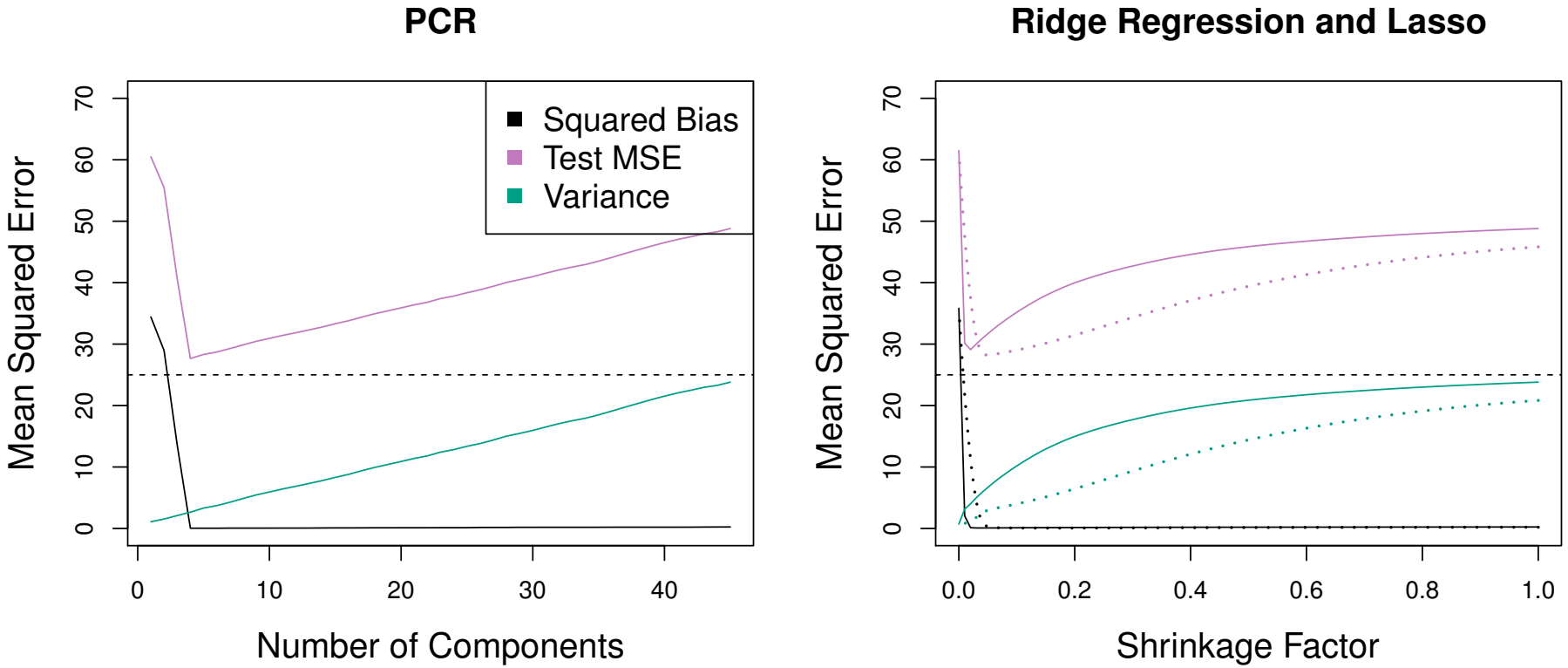


Figure: $p = 45$ features: PCR vs Lasso (solid) and Ridge (dotted).[16]

[16] Source [B.1]

# END