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09. Feature Selection

Data Analysis for Networks - DataNets'19

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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

B.2 Giorgos Dimopoulos, Ilias Leontiadis, Pere Barlet-Ros, Konstantina Papagiannaki. "Measuring Video QoE from Encrypted Traffic", IMC '16 Proceedings of the 2016 Internet Measurement Conference Pages 513-526 .

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 Dimensionality Reduction.

Main idea

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☞ 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.

Network example

☞ In [B.2] the authors want to classify Video QoE from encrypted traffic. One of the questions is the quality of stalling

There are potentially many available features to be used (around $p = 70$)

- Only 4-out-of-70 features are actually important factors that correlate with stalling:
  - BDP mean (related to throughput)
  - packet re-transmission max
  - chunk-size min
  - chunk size standard deviation.

❂ In fact chunk size is a very strong indicator, because at the event of stalling, the size of the chunks decrease so that they are reliably transmitting and start filling-up the buffer.

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 we need to perform LSs for all possible combinations for 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.

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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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 Train RSS or high value of R^2.

☞ The model with all the predictors will have the smallest Train RSS.

✴ 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

☞ The training RSS will decrease as more variables are included in the model, but **not the Test RSS** necessarily.

We cannot use Train error to select among models with different numbers of variables.

Adjust the Train error to select the model with best Test prediction:

- **Mallow's 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**: $BIC = \frac{1}{n\hat{\sigma}^2}(RSS + \log(n)d\hat{\sigma}^2)$.
- **Adjusted** $R^2 = 1 - \frac{RSS/(n-d-1)}{TSS/(n-1)}$, where $TSS = \sum(y_i - \bar{y})^2$.

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Understanding Akaike I

The original definition of Akaike reads

$$AIC = \frac{1}{n}\left(2d - 2\log(\hat{L})\right)$$

where $\hat{L}$ is the log-likelihood and d is the number of predictors used. Akaike adds a cost which scales linearly with the number of used predictors.
If the model tested is

$$y = f(x) + \epsilon \Rightarrow \mathbb{E}[y] = f(x),$$

then, the error per data is

$$\epsilon_i = y_i - \mathbb{E}[f(x_i)]$$

Suppose the model describes well the data, so that $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$.

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Understanding Akaike II

The log-likelihood of an error sample is

$$\hat{L}(\mathcal{D}_n) = -\frac{1}{2\sigma^2}\sum_{i=1}^{n}\epsilon_i^2 - \frac{n}{2}\log\sigma^2 - \frac{n}{2}\log(2\pi)$$

The second term changes slowly over σ^2. The third term is constant. Altogether

$$AIC = \frac{1}{n}\left(2d + \frac{1}{\sigma^2}RSS\right)$$

❋ Note that C_p and AIC are proportional to each other!

☞ To estimate the variance we will use (with $TSS = \sum_i (y_i - \bar{y})^2$ the total sum of squares for the response)

$$\hat{\sigma}^2 = \frac{1}{n-1}\sum_{i=1}^{n}(y_i - \bar{y})^2 = \frac{1}{n-1}TSS.$$

Understanding BIC

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Similar to Akaike, but now the cost depends on the $\log(n)$ of the samples

$$BIC = \frac{1}{n}\left(\log(n)d - 2\log(\hat{L})\right),$$

where $\hat{L}$ is the log-likelihood and d is the number of predictors used.

As in AIC

$$BIC = \frac{1}{n}\left(\log(n)d + \frac{1}{\sigma^2}RSS\right).$$

Since $\log(n) > 2$ for $n > 7$ the model places a heavier penalty on models with many features.

We choose the AIC, BIC, C_p model with the **lowest** value!

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Understanding Adjusted R^2

Remember the usual definition of R^2

$$R^2 = 1 - \frac{RSS}{TSS} = \frac{Explained\ \ Variation}{Total\ \ Variation}.$$

☞ The more we add predictors, the more the RSS decreases and the more the Train R^2 increases!

For a least squares model with d features the adjusted R^2 statistic is

$$Adjusted\ R^2 \quad = \quad 1 - \frac{RSS/(n-d-1)}{TSS/(n-1)}.$$

Unlike the other metrics, here a **large value of Adjusted** R^2 indicates a model with a small Test error.

Maximising the Adjusted R^2 is equivalent to minimizing $\frac{RSS}{n-d-1}$.
This statistic also pays a price for inclusion of unnecessary variables.

Overview of adjustment metrics

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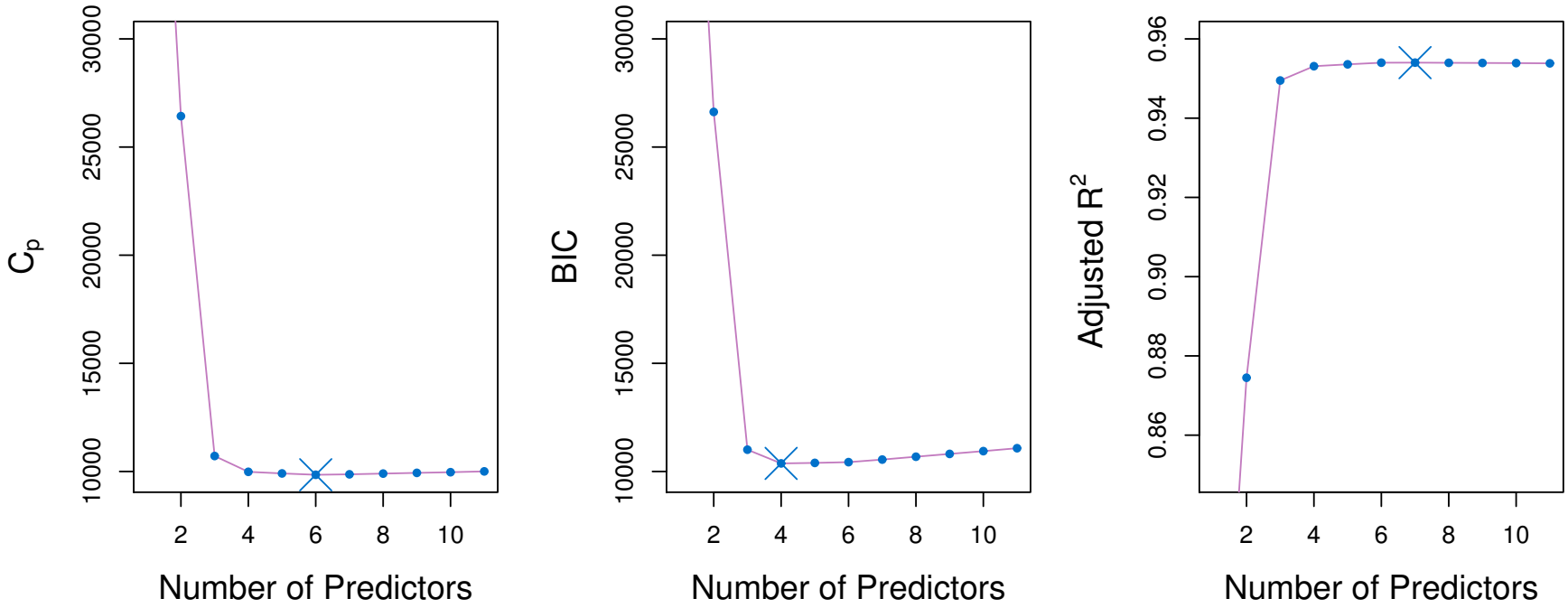

Figure: Feature selection from different metrics.[5]

[5] Source [B.1]

Comparison with Validation and CV tests

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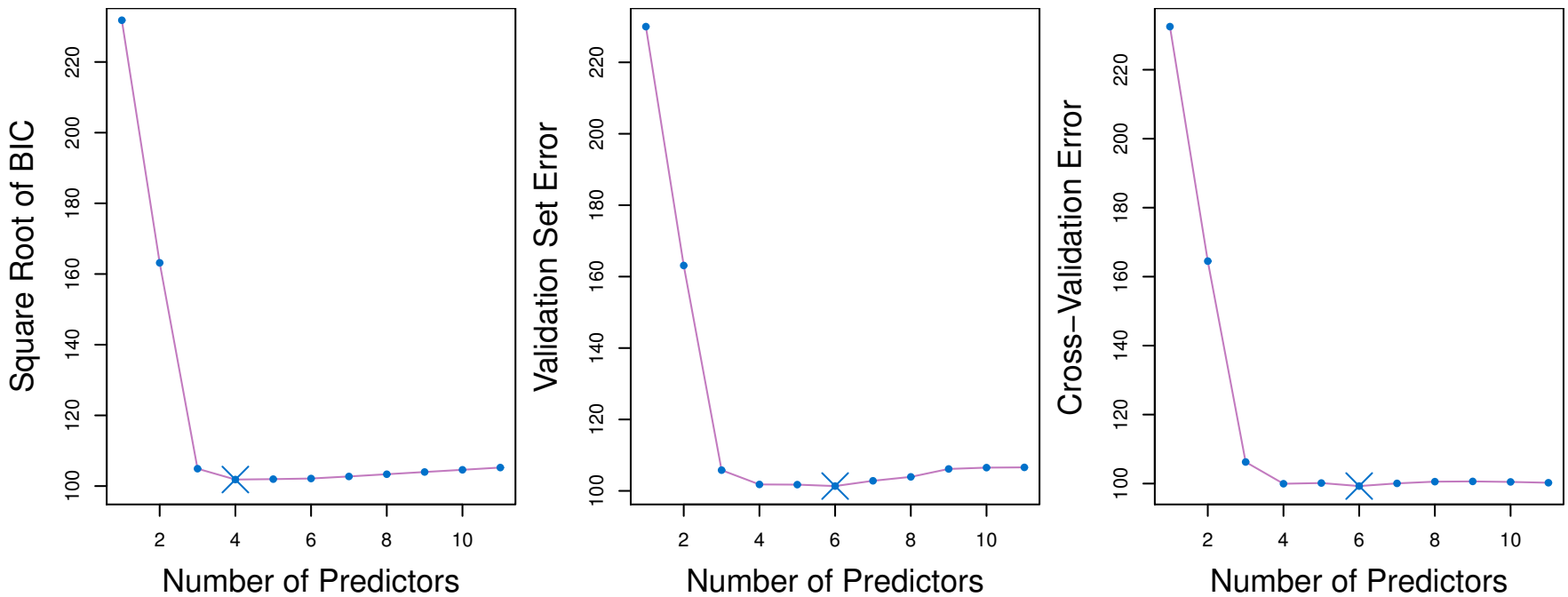

Figure: CV used to be computationally expensive, not any more.[6]

[6] Source [B.1]

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 $\lambda \to \infty$ 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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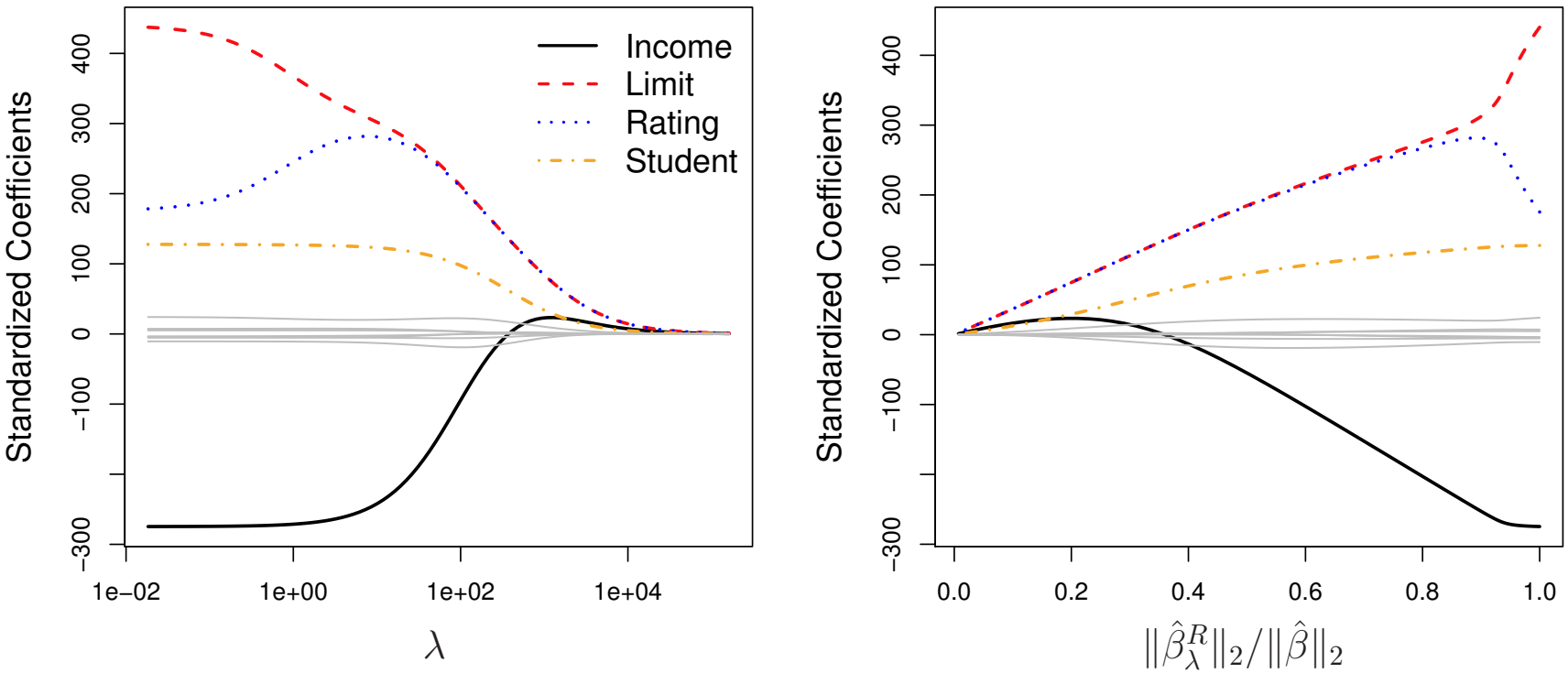

Figure: Change of Ridge Regression coefficients vs λ.[7]

[7] Source [B.1]

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Improvement over LSs

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

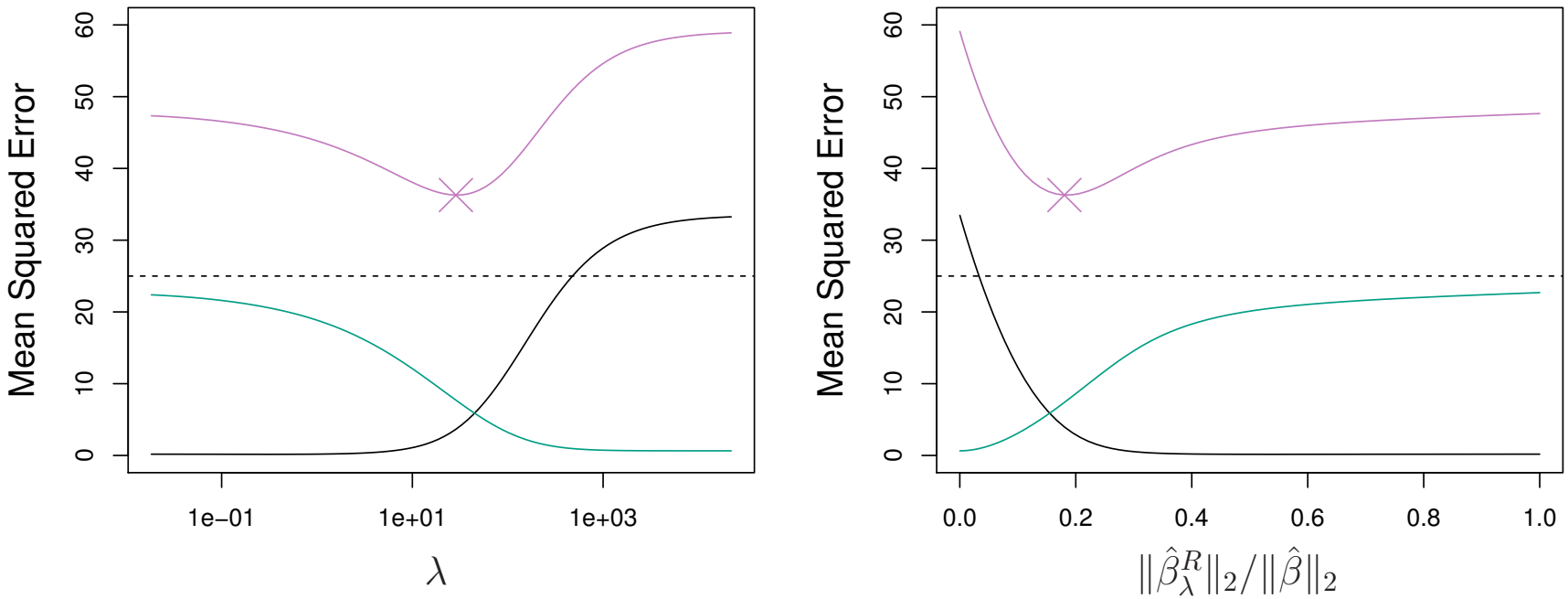

Figure: Bias vs Variance tradeoff and Test MSE.[8]

[8] 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 ℓ_1-norm instead of ℓ_2).

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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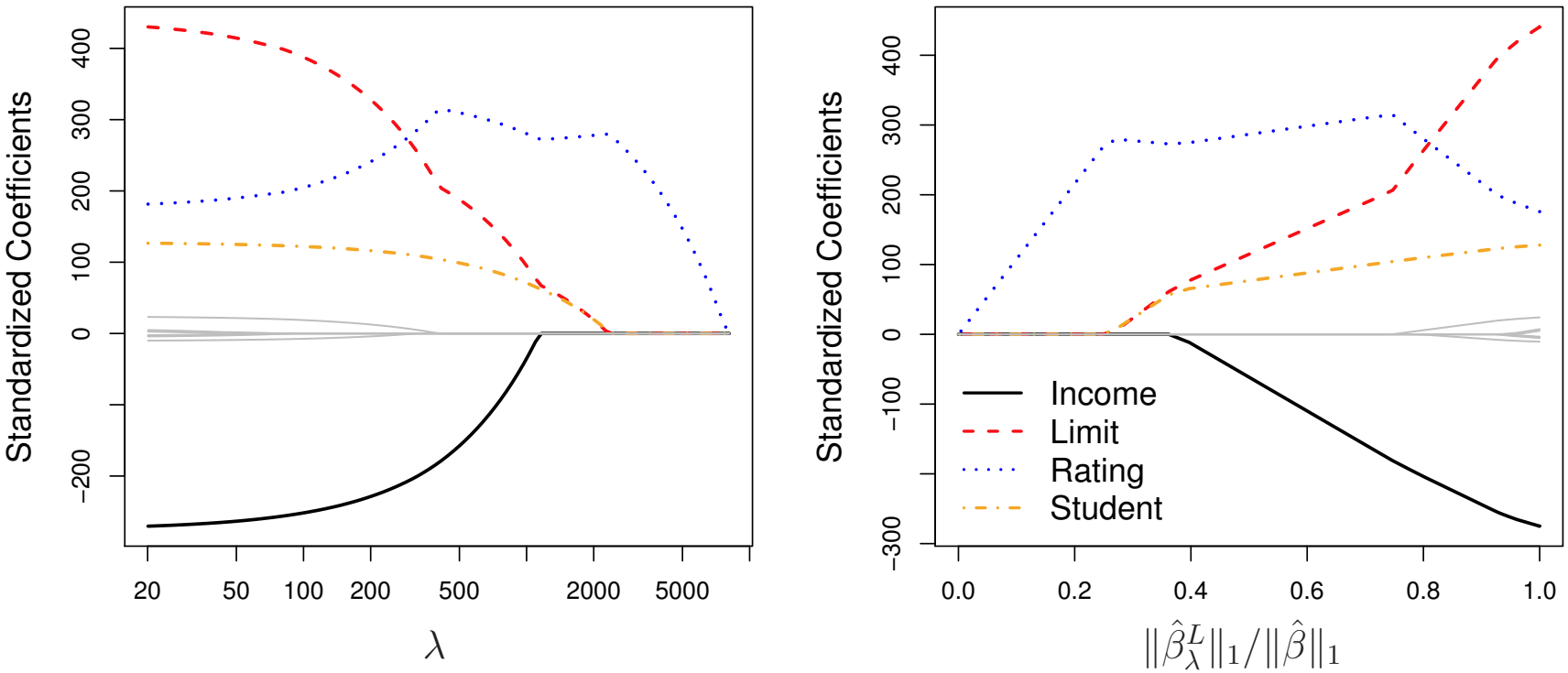

Figure: Change of Lasso coefficients vs λ.[9]

[9] 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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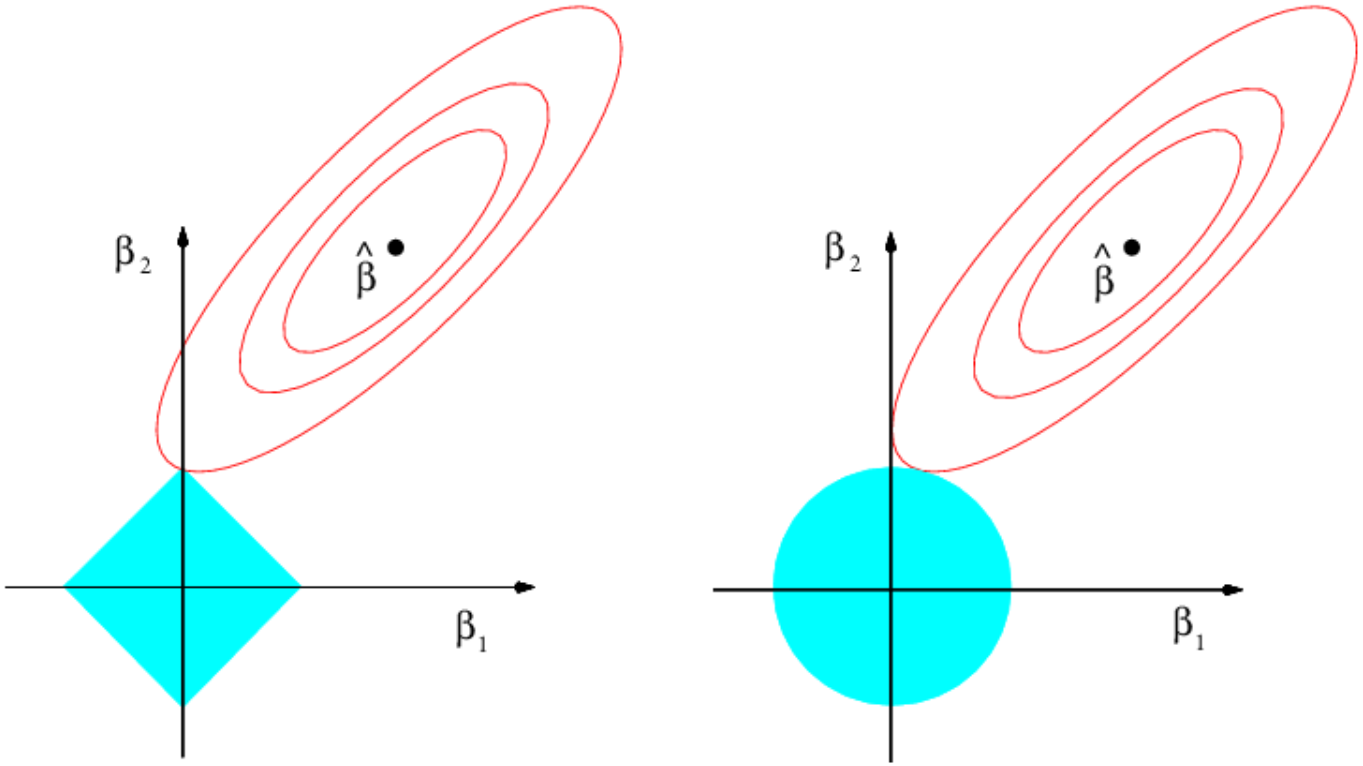

Figure: Why does Lasso lead to estimates equal to 0?[10]

[10] Source [B.1]

Ridge > Lasso

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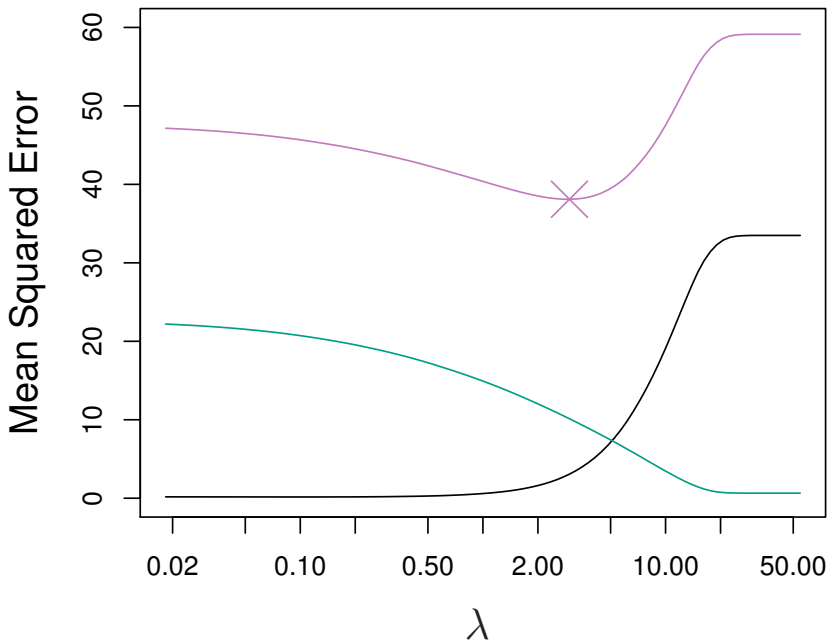
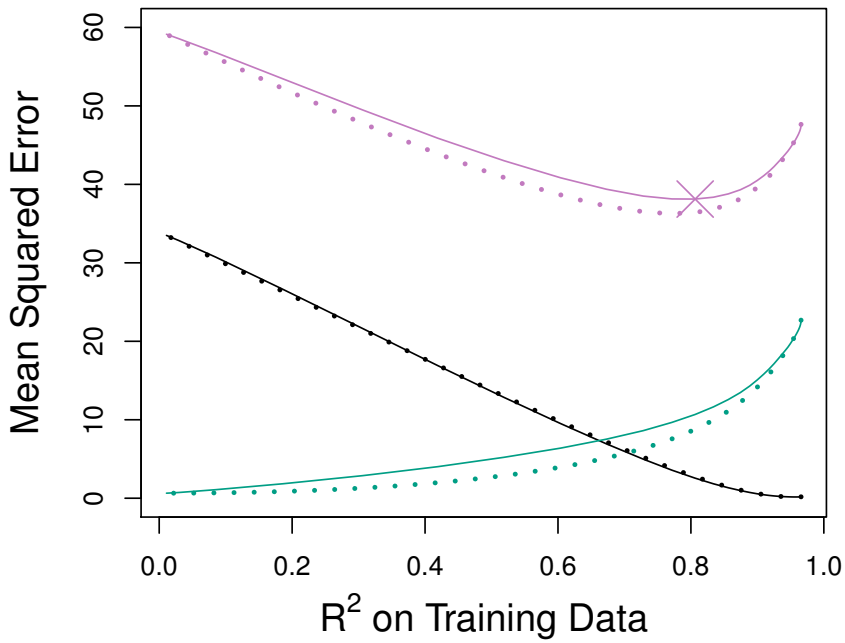
Here: Ridge needs all 45 coefficients $\neq 0$. Lasso chose 2-out-of-45 features.[11]





[11] Source [B.1]

Ridge $<$ Lasso

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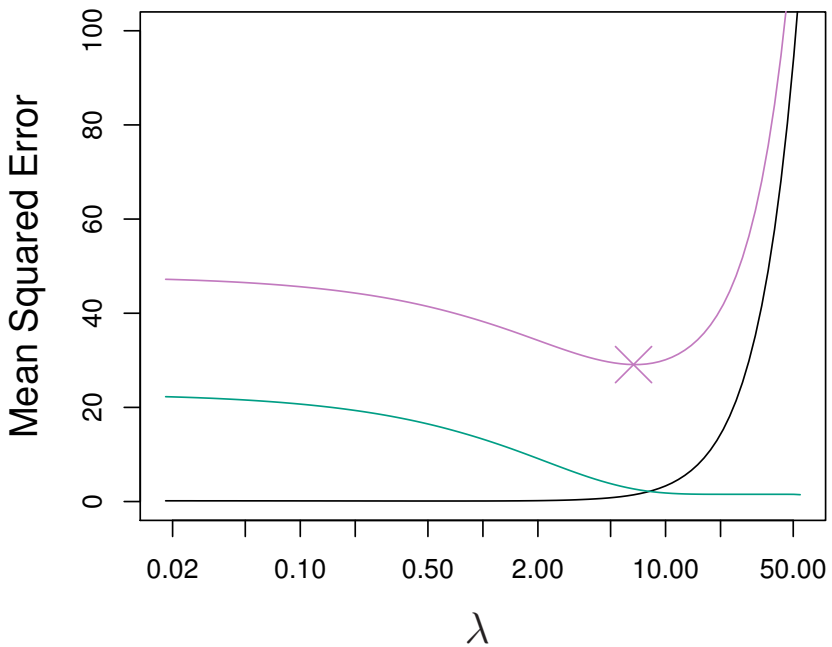
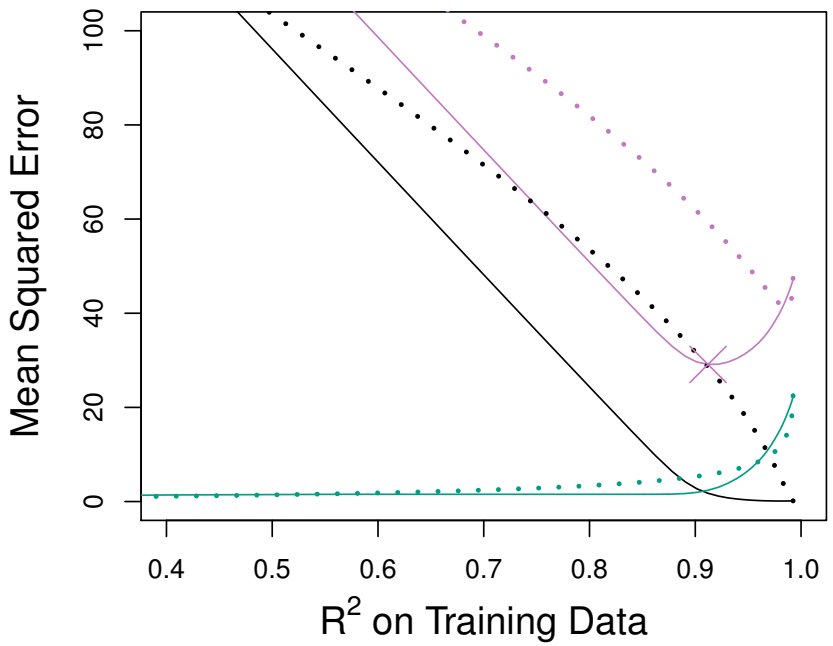
Here: True response is a function of only 2 predictors and the rest are irrelevant. Ridge needs again all 45 coefficients $\neq 0$. Lasso chose 2-out-of-45 features.[12]





[12] 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:

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

- 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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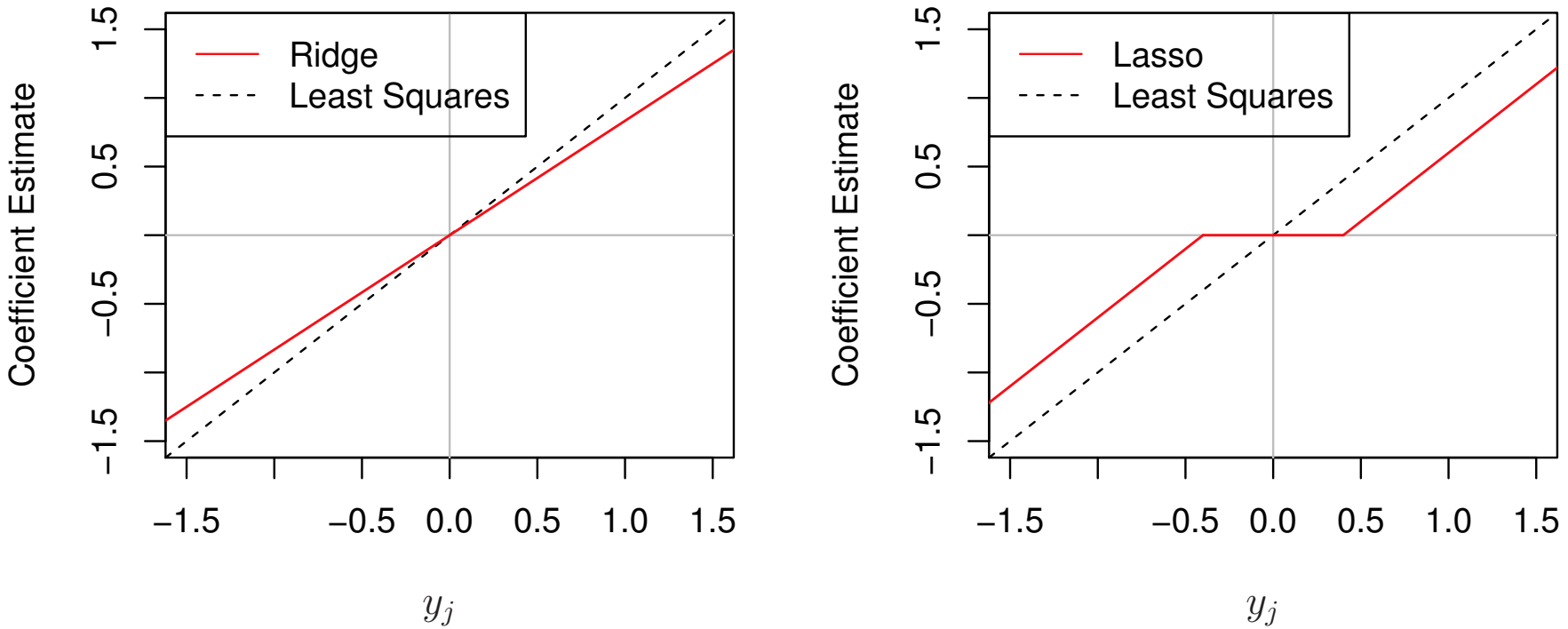

Figure: Ridge and Lasso coefficients over λ, compared to LSs.[13]

[13] Source [B.1]

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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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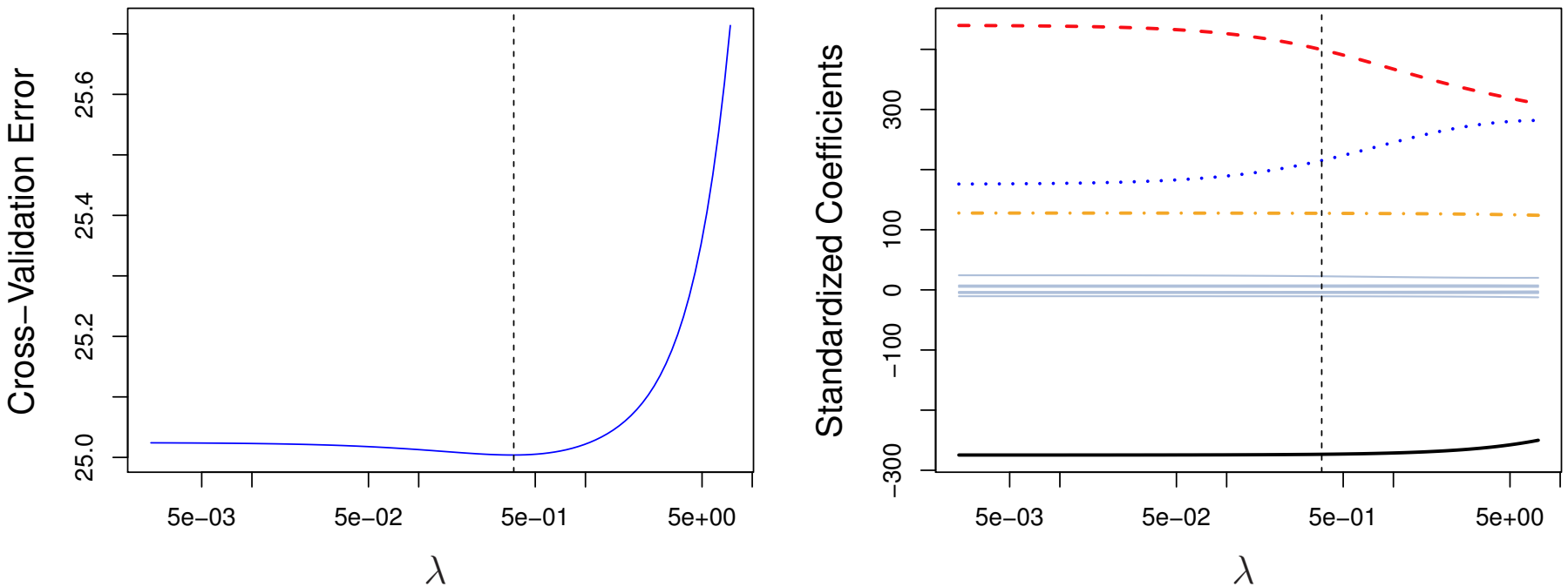

Figure: Ridge parameter tuning and comparison with LSs.[14]

[14] Source [B.1]

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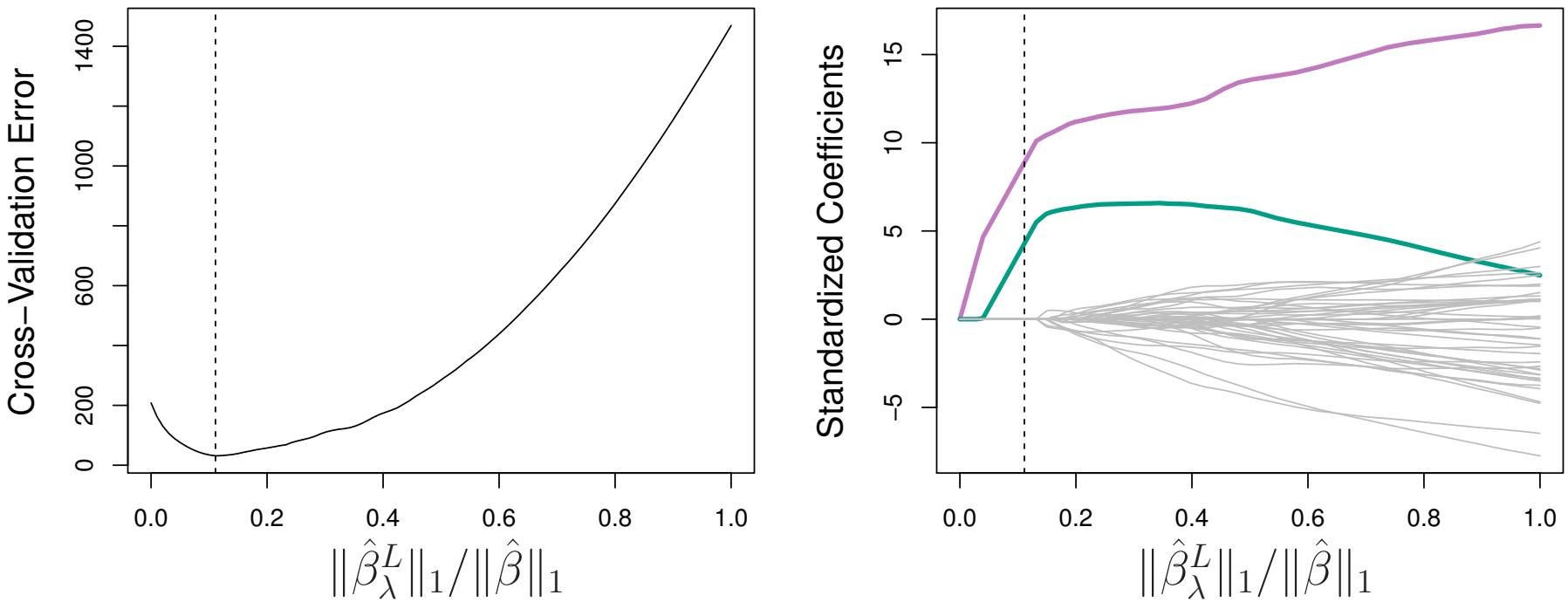

Figure: Lasso parameter tuning and comparison with LSs.[15]

[15] 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 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.

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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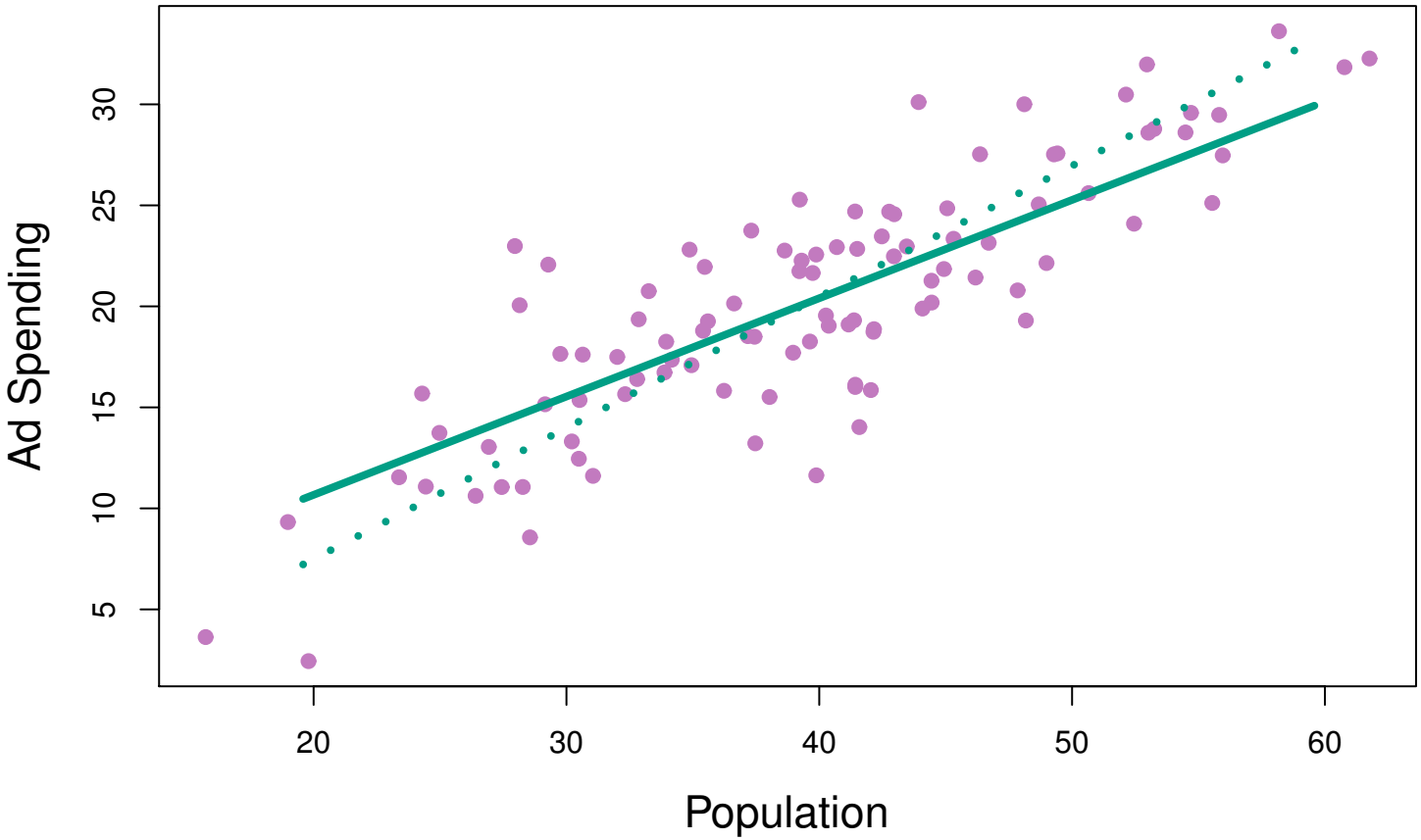

Figure: PCR direction Z_1 for $p = 2$.[16]

[16] 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 $\mathbf{X}$:

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

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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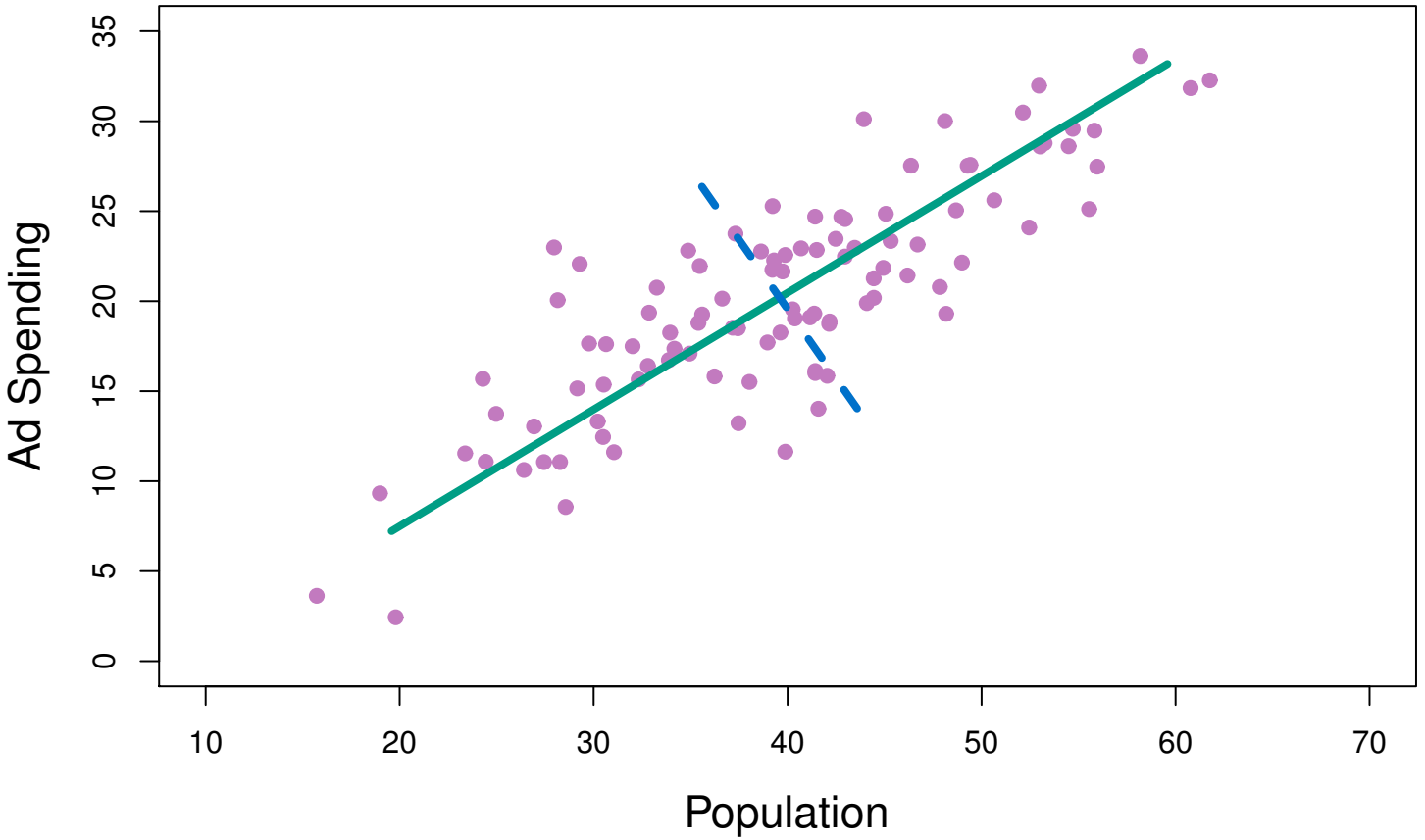

Figure: Principal components directions for $p = 2$.[17]

[17] 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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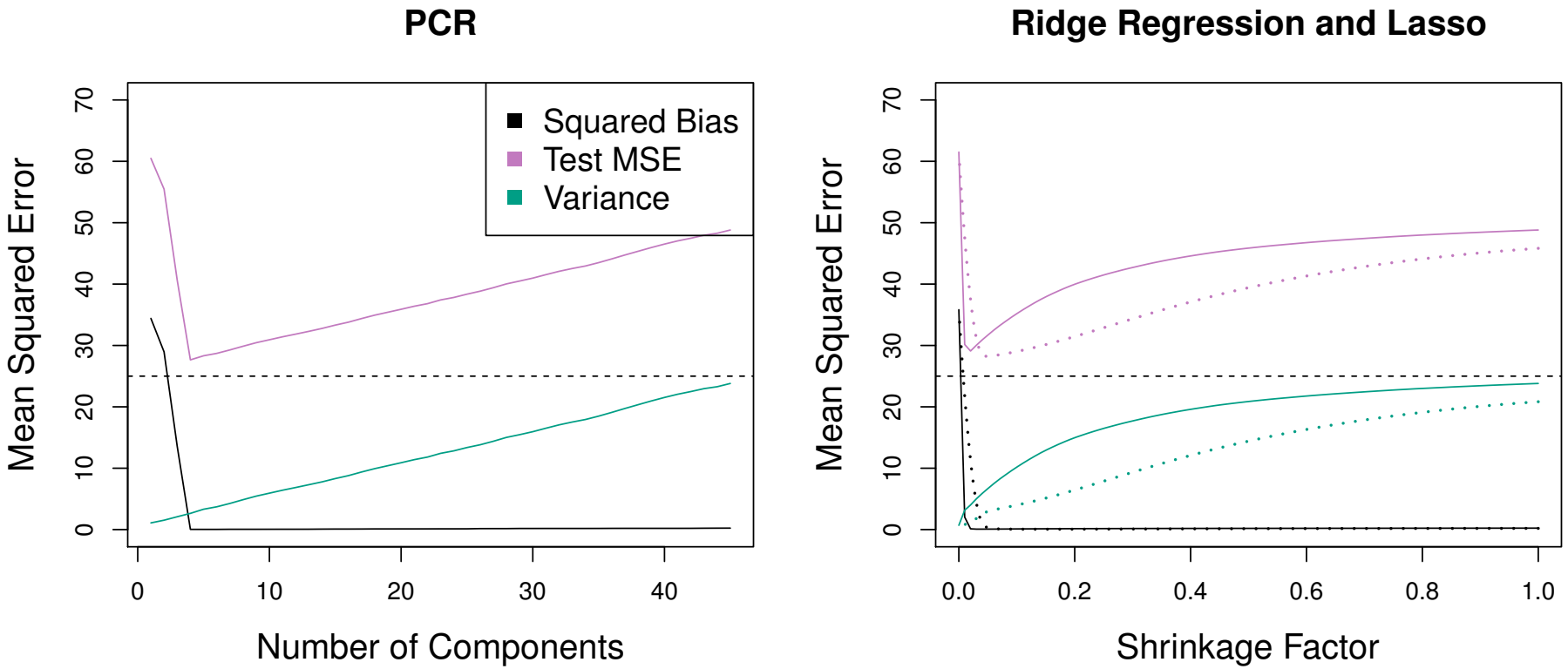

Figure: $p = 45$ features: PCR vs Lasso (solid) and Ridge (dotted).[18]

[18] Source [B.1]

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END