Lecture 15: Dimensionality reduction

Reading: Sections 6.3, 6.4

STATS 202: Data mining and analysis

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Shrinkage methods

Ridge regression:

$$\min_{\beta} \ \ \mathsf{RSS}(\beta) + \lambda \sum_{j=1}^{p} \beta_j^2$$

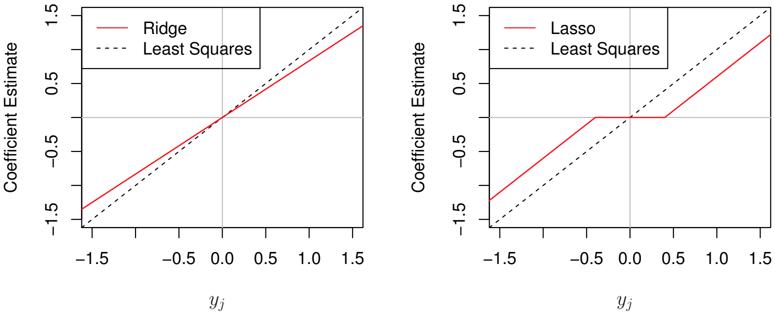
The Lasso:

$$\min_{\beta} \ \ \mathsf{RSS}(\beta) + \lambda \sum_{j=1}^{p} |\beta_j|$$

As we increase λ we increase bias, but reduce variance.

Lasso and Ridge coefficients as a function of λ

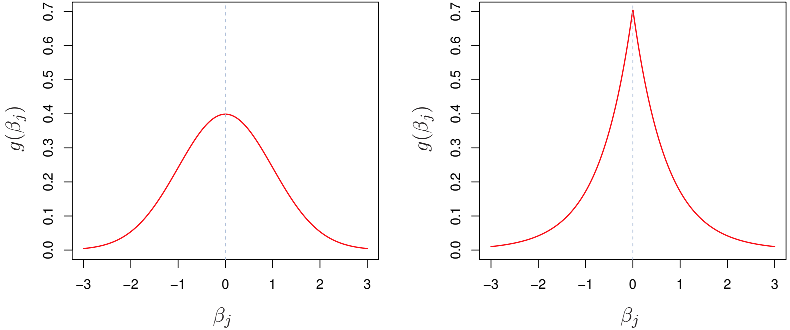
Special case $\mathbf{X} = I$. Each coefficient $\hat{\beta}_j^R$, $\hat{\beta}_j^L$ depends only on y_j.



Bayesian interpretations

Ridge: $\hat{\beta}^R$ is the posterior mean, with a Normal prior on β.

Lasso: $\hat{\beta}^L$ is the posterior mode, with a Laplace prior on β.



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  - Forward and backward stepwise selection
- Shrinkage
  - Ridge regression
  - The Lasso (a form of variable selection)
- Dimensionality reduction:
  - **Idea:** Define a small set of M predictors which *summarize* the information in all p predictors.

Principal Components Regression

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Example. `USArrests` dataset.

Variable	`UrbanPop`	`Murder`	`Assault`	`Rape`
Loading	$\phi_{11} = 0.28$	$\phi_{21} = 0.54$	$\phi_{31} = 0.59$	$\phi_{41} = 0.54$

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Interpretation: The first principal component measures the overall rate of crime.

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$$z_{i1} = \sum_{j=1}^{p} \phi_{j1} x_{ij}$$

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Example. `USArrests` dataset.

Sample	`Alabama`	`Alaska`	...	`Wyoming`
Score	$z_{11} = 172$	$z_{21} = 196$	...	$z_{n1} = 122$

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Score	$z_{11} = 172$	$z_{21} = 196$	...	$z_{n1} = 122$

Interpretation: The scores for the first principal component measure the overall rate of crime in each state.

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$$y_i = \theta_0 + \theta_1 z_{i1} + \theta_2 z_{i2} + \cdots + \theta_M z_{iM}$$

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$$
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Equivalent to a linear regression onto $X_1, \ldots, X_p$, with coefficients:

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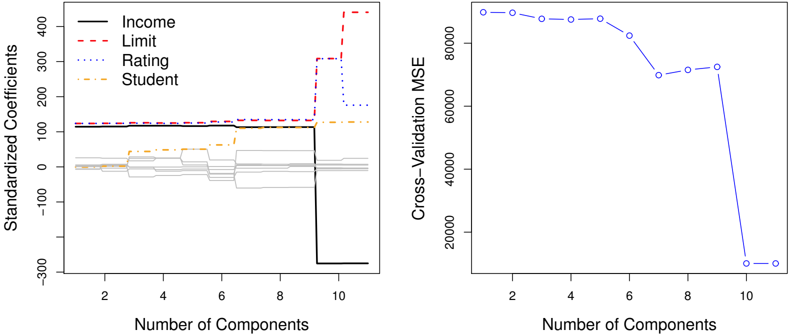
This constraint in the form of β_j introduces *bias*, but it can lower the *variance* of the model.

Application to the Credit dataset



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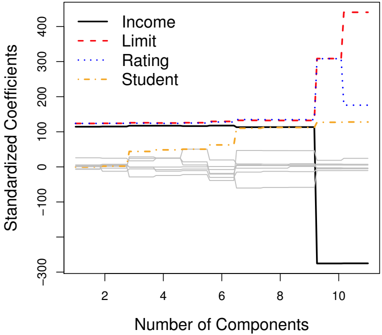

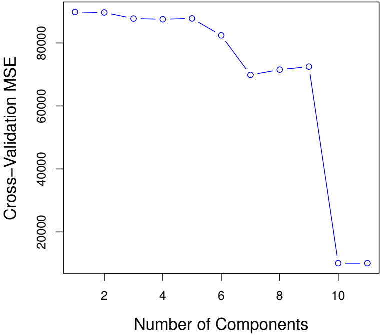

- A model with 11 components is equivalent to least-squares regression

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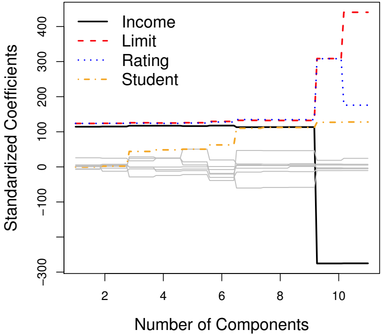

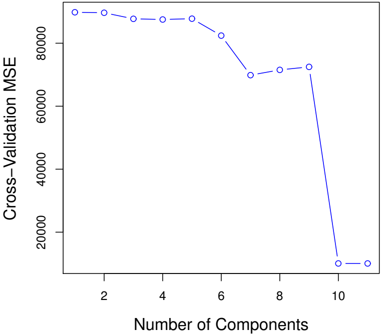

- A model with 11 components is equivalent to least-squares regression
- Best error is achieved with 10 components (almost no dimensionality reduction)

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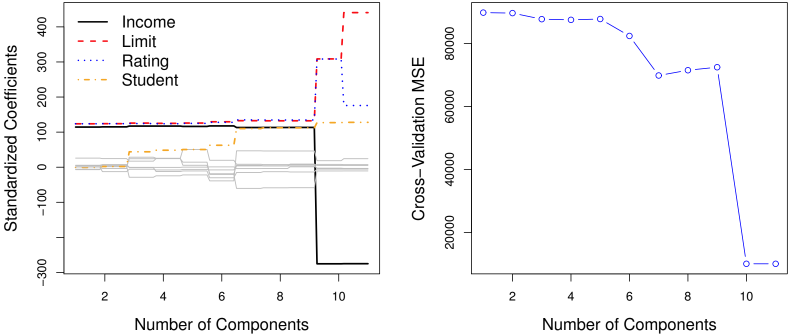

The left panel shows the coefficients β_j estimated for each M.
The coefficients shrink as we decrease M!

Relationship between PCR and Ridge regression

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Solve the singular value decomposition: $\mathbf{X} = UD^{1/2}V^T$, where $D^{1/2} = \text{diag}(\sqrt{d_1}, \ldots, \sqrt{d_p})$; then

$$(\mathbf{X}^T \mathbf{X})^{-1} = VD^{-1}V^T$$

where $D^{-1} = \text{diag}(1/d_1, 1/d_2, \ldots, 1/d_p)$.

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Predictions of least squares regression:

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The projection of y onto a principal component is shrunk toward zero. The smaller the principal component, the larger the shrinkage.

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Predictions of PCR:

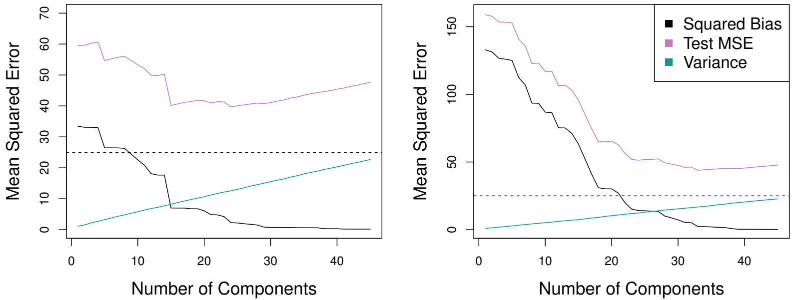
$$\hat{y} = \mathbf{X}\hat{\beta}^{\mathsf{PC}} = \sum_{j=1}^{p} u_j \mathbf{1}(j \leq M) u_j^T y$$

The projections onto small principal components are shrunk to zero.

Simulated example

In each case $n = 50$, $p = 45$.

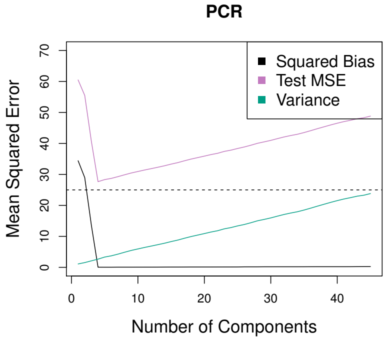
- **Left:** Response is a function of all the predictors.
- **Right:** Response is a function of 2 predictors (good for Lasso).

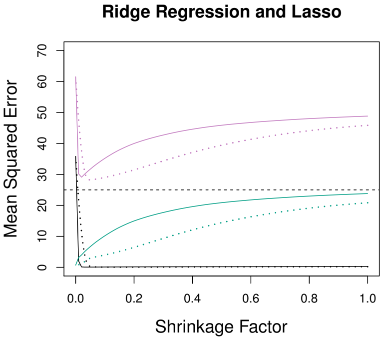


Simulated example

Again, $n = 50$, $p = 45$.

The response is a function of the first 5 principal components.





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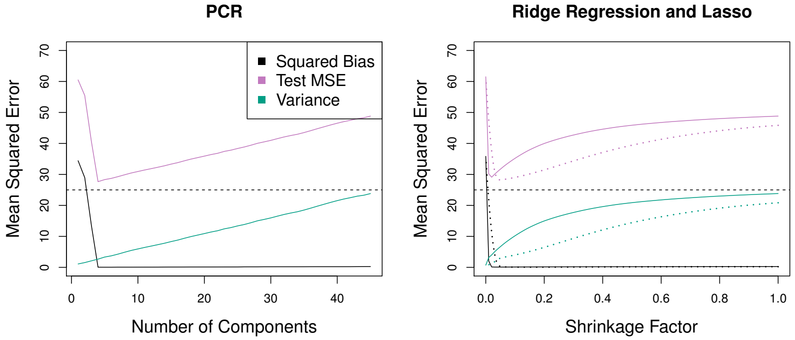

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5. ...

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- At each step, we try to find the linear combination of predictors that is highly correlated to the response (the highest correlation is the least squares fit).

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- After each step, we transform the predictors such that they are *uncorrelated* from the linear combination chosen.
- Compared to PCR, partial least squares has less bias and more variance (a stronger tendency to overfit).