Linear Model Selection and Regularization

1. Subset selection
2. Shrinkage methods
3. Dimension reduction methods (using derived inputs)
4. High dimension data analysis

Feature/variable selection

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QUESTION:

- What is the best?
- Which criterion do we use?

The algorithm of best subset selection

- Step 1. Let $\mathcal{M}_0$ be the *null model*, $Y = \beta_0 + \epsilon$. Which contains no predictors.
- Step 2. For $k = 1, 2, ..., p$,
  - Fit all $\binom{p}{k} = p!/(k!(n-k)!)$ models that contain exactly k predictors.
  - Pick the best model, that with largest R^2, among them and call it $\mathcal{M}_k$.
- Step 3. Select a single best model from $\mathcal{M}_0, ..., \mathcal{M}_p$ by cross validation or AIC or BIC or C_p or adjusted R^2.

Recall: Definitions

- Residue

$$\hat{\epsilon}_i = y_i - \hat{\beta}_0 - \sum_{j=1}^{p} \hat{\beta}_j x_{ij}$$

- Residual Sum of Squares

$$\text{RSS} = \sum_{i=1}^{n} \hat{\epsilon}_i^2 = \sum_{i=1}^{n} (y_i - \hat{\beta}_0 - \sum_{j=1}^{p} \hat{\beta}_j x_{ij})^2$$

- R-squared

$$R^2 = \frac{\text{TSS} - \text{RSS}}{\text{TSS}} = 1 - \frac{\text{RSS}}{\text{TSS}},$$

where $\text{TSS} = \sum_{i=1}^{n} (y_i - \bar{y})^2$.

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- RSS and R^2 are NOT suitable for selecting the best model.
- In order to select the best model with respect to test error, there are two common approaches:
  1. We can *indirectly* estimate test error
     - make an adjustment to the training error to account for the bias due to overfitting.
     - C_p, AIC, BIC, and Adjusted R^2.
  2. We can *directly* estimate the test error,
     - using either a validation set approach or a cross-validation approach.
     - Cross-validation.

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- The *adjusted* R-squared, taking into account of the *degrees of freedom*, is defined as

$$\begin{aligned} \text{adjusted } R^2 &= 1 - \frac{\text{MS}_{error}}{\text{MS}_{total}} \\ &= 1 - \frac{\text{RSS}/(n-p-1)}{\text{TSS}/(n-1)}. \end{aligned}$$

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- With more inputs, the R^2 always not decreasing, but the adjusted R^2 may decrease since more irrelevant inputs are penalized by the smaller degree of freedom of the residuals.
- The adjusted R-squared is preferred over the R-squared in evaluating models.

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- Suppose we use only d of the p covariates with $d \leq p$, for example, $x_{j_1}, \cdots, x_{j_d}$.
- The statistic of Mallow's C_p is defined as (Page 221)

$$C_p = \frac{\text{RSS}(d)}{s_p^2} + 2d - n, \quad \text{or} \quad \frac{1}{n}\left(\text{RSS}(d) + 2ds_p^2\right).$$

  - $\text{RSS}(d) = \sum_{i=1}^{n}(\beta_0 + \beta_{j_1} x_{ij_1} + \cdots \beta_{j_d} z_{ij_d} - y_i)^2$ is the residual sum of squares for the linear model with d inputs.

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  - Mallows' C_p: the smaller it is, the better the model is.

c). AIC.

- AIC stands for *Akaike information criterion*,
- aims at maximizing the predictive likelihood.

$$\text{AIC} = \frac{1}{ns_p^2}\left(\text{RSS}(d) + 2ds_p^2\right),$$

  when Gaussian likelihood is assumed in least square regression.
- The model with the smallest AIC is preferred.

d). BIC.

BIC stands for Schwarz's *Bayesian information criterion*, which is defined as

$$\text{BIC} = \frac{1}{ns_p^2}\left(\text{RSS}(d) + ds_p^2(\log n)\right),$$

for a linear model with p inputs.

- the model with the smallest BIC is perfered.
- The derivation of BIC results from Bayesian statistics and has Bayesian interpretation.
- It replaces $2ds_p^2$ in AIC by $(\log n)ds_p^2$, so for $\log n > 2$ or $n > 7$, BIC penalizes more heavily the models with more number of inputs.

Example

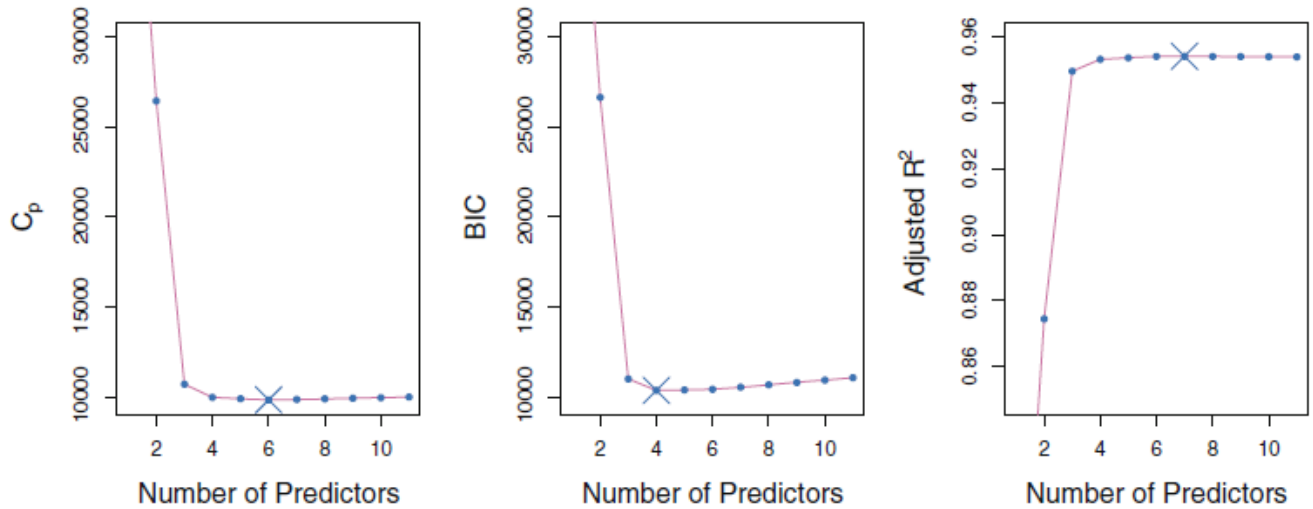

Figure: 6.2. C_p, BIC, and adjusted R^2 are shown for the best models of each size for the Credit data set (the lower frontier in Figure 6.1).

- C_p and BIC are estimates of test MSE.
- In the middle plot we see that the BIC estimate of test error shows an increase after four variables are selected.
- The other two plots are rather flat after four variables are included.

Pros and Cons of best subset selection

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Disadvantages:

- The search space too large (2^p models).
- if $p = 20$, there are $2^{20} > 1000,000$ models.
- Computationally infeasible: too many models to run.

Forward stepwise selection

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- Find the best among all these *best k-variable* models.

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Attention: You should use a suitable criterion for your problem!!!!!

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- Once an input is in, it does not get out.
- Forward stepwise tends to do well in practice, it is not guaranteed to find the best possible model out of all 2^p models containing subsets of the p predictors.

Example: credit dataset

Variables	Best subset	Forward stepwise
1	rating	rating
2	rating, income	rating, income
3	rating, income, student	rating, income, student
4	cards, income, student, limit	rating, income, student, limit

TABLE 6.1. The first four selected models for best subset selection and forward stepwise selection on the Credit data set.

- The first three models are identical,
- the fourth models differ.

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- For $k = p, p-1, \cdots, 1$:
  - (a) Consider all k models that contain all but one of the predictors in Mk, 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.
- Select a single best model from among $\mathcal{M}_0, \cdots, \mathcal{M}_p$ using crossvalidated prediction error, C_p (AIC), BIC, or adjusted R_2.

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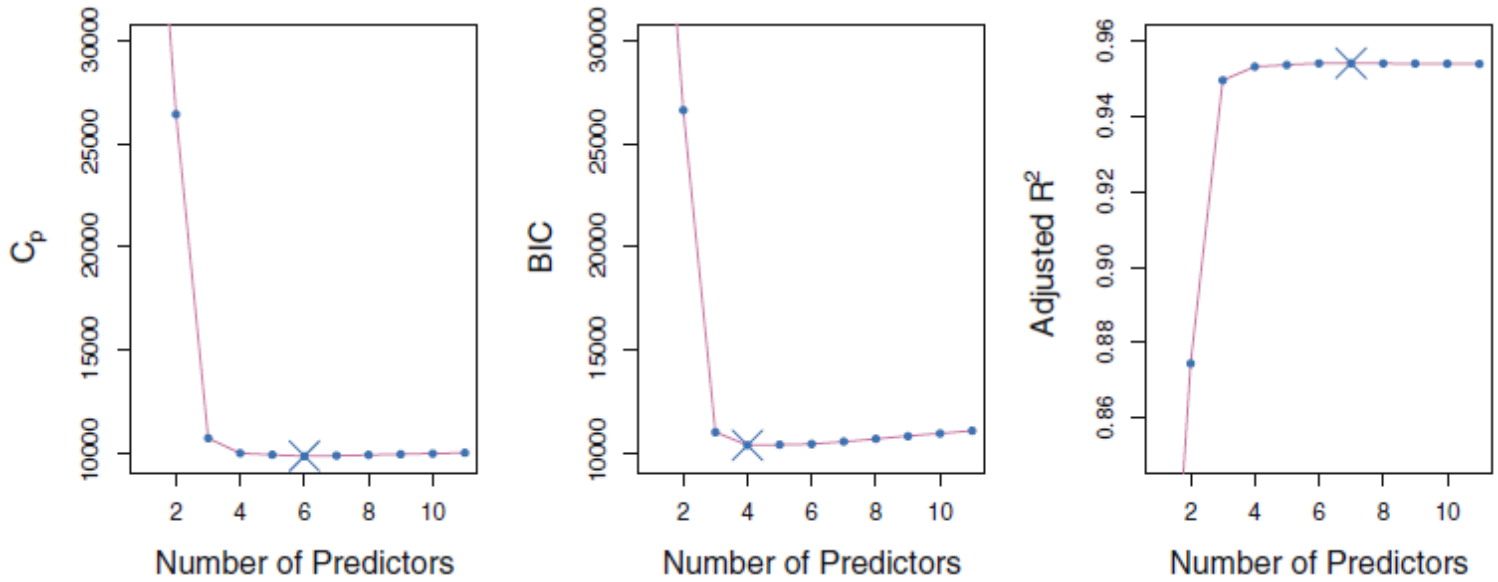

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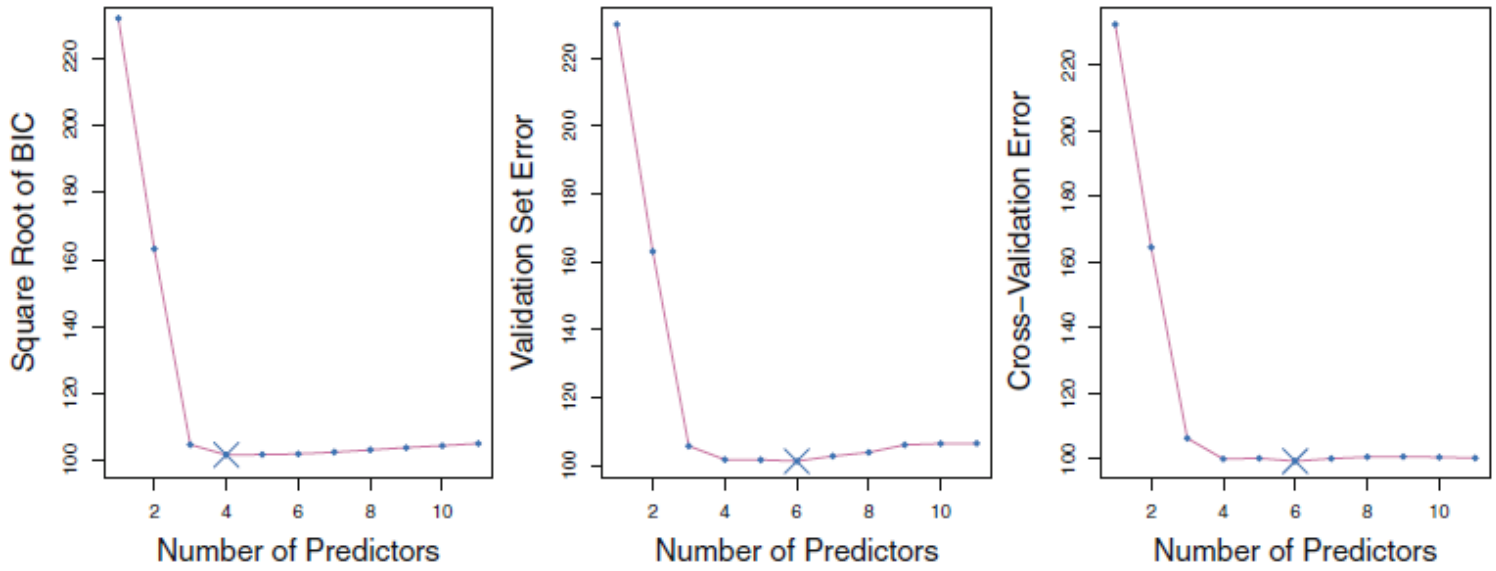

Figure: 6.3. For the Credit data set, three quantities are displayed for the best model containing p predictors, for p ranging from 1 to 11.

- *Left*: Square root of BIC.
- *Center*: Validation set errors (75% training data).
- *Right*: 10-fold Cross-validation errors.
- The overall best model, based on each of these quantities, is shown as a blue cross.

The one standard deviation rule

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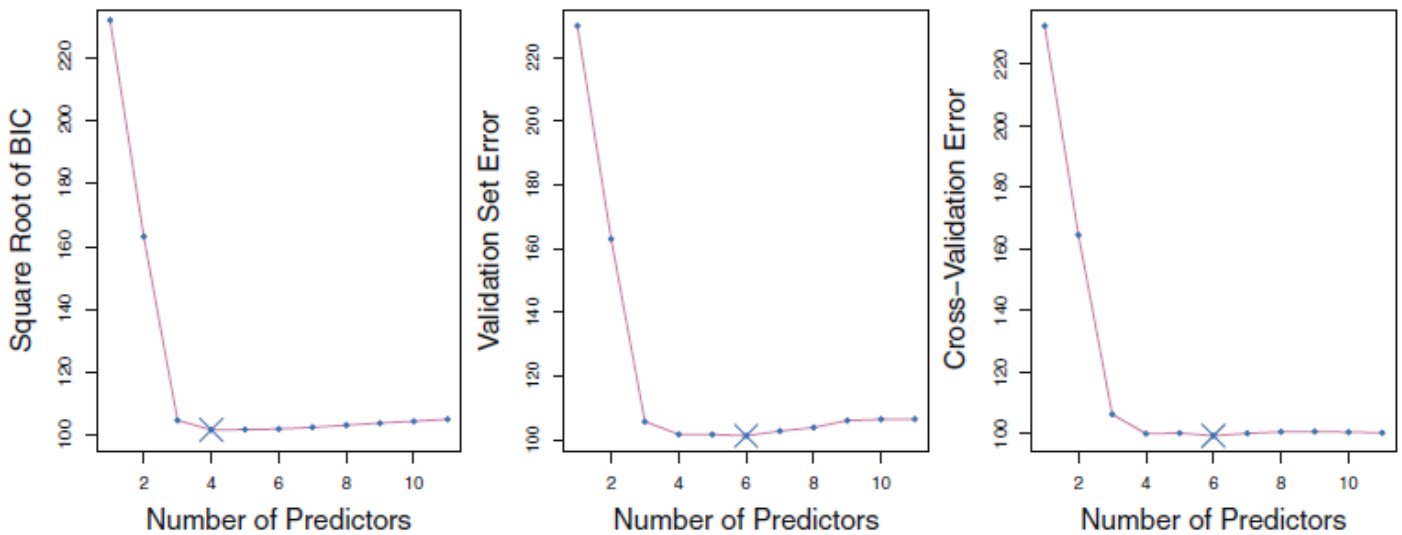

- Model with 6 inputs do not seem to be much better than model with 4 or 3 inputs.

Shrinkage methods

- The least squares estimator $\hat{\beta}$ is minimizing

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  where $\lambda \geq 0$ is a tuning parameter.
- The first term measures goodness of fit, the smaller the better.
- The second term $\lambda\mathcal{R}(\beta_1, \cdots, \beta_p)$ is called *shrikage penalty*, which shrinks $\beta_j, j = 1, \cdots, p$ towards 0.
- Note that β_0 is NOT penalized.

Ridge

- Ridge: $\mathcal{R}(\beta_1, \cdots, \beta_p) = \sum_{j=1}^{p} \beta_j^2$.

$$\min_{\beta_0, \cdots, \beta_p} \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij})^2 + \lambda \sum_{j=1}^{p} \beta_j^2.$$

- The solution is

$$\hat{\beta}_\lambda^R = (\mathbf{X}^T \mathbf{X} + \lambda I)^{-1} \mathbf{X}^T \mathbf{y},$$

where $I = \text{diag}([0, 1, 1, ..., 1])$ is $(p+1)$-by-$(p+1)$ diagnal matrix.

The lasso

- The lasso $\mathcal{R}(\beta_1, \cdots, \beta_p) = \|\beta\|_1 = \sum_{j=1}^{p} |\beta_j|$, which is the l_1 norm.
- Lasso stands for *Least Absolute Shrinkage and Selection Operator*.
- The Lasso estimator $\hat{\beta}_\lambda^L$ is the minimizer of

$$\min_{\beta_0, \cdots, \beta_p} \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij})^2 + \lambda \sum_{j=1}^{p} |\beta_j|. \tag{1}$$

which is equivalent to

$$\min_{\beta_0, \cdots, \beta_p, \alpha_1, \cdots, \alpha_p} \sum_{i=1}^{n} (y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij})^2 + \lambda \sum_{j=1}^{p} |\alpha_j| + \frac{\rho}{2} \sum_{i=1}^{p} (\alpha_i - \beta_i)^2.$$

We can solve it by alternating minimization.

- Solve $\beta_0, \cdots, \beta_p$ with $\alpha_1, \cdots, \alpha_p$ fixed:

$$\min_{\beta_0,\cdots,\beta_p} \sum_{i=1}^{n}(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij})^2 + \frac{\rho}{2}\sum_{i=1}^{p}(\alpha_i - \beta_i)^2,$$

- Solve $\alpha_1, \cdots, \alpha_p$ with $\beta_0, \cdots, \beta_p$ fixed:

$$\min_{\alpha_1,\cdots,\alpha_p} \lambda\sum_{j=1}^{p}|\alpha_j| + \frac{\rho}{2}\sum_{i=1}^{p}(\alpha_i - \beta_i)^2.$$

- For the first one, we can solve by least squares.
- For the second one, we can use soft thresholding.

$$\alpha_i = \begin{cases} \beta_i - \lambda/\rho, & \beta_i \geq \lambda/\rho, \\ 0, & |\beta_i| < \lambda/\rho, \\ \beta_i + \lambda/\rho, & \beta_i \leq -\lambda/\rho, \end{cases}$$

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- Ridge has closed form solution. Lasso generally does not have closed form solution.

Standardize the inputs.

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$$X_j\hat{\beta}_j = (cX_j)(\hat{\beta}_j/c).$$

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- Shrinkage method is affected by λ as well as the scale of the inputs.
- Suggest to apply standardization before trying regression with penalties.
- For j-th input X_j with observations: $(x_{1j}, ..., x_{nj})$, standardize it as

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

to get rid of the scale of X_j.

Example

- Consider the simple model $y_i = \beta_i + \epsilon_i$, $i = 1, ..., n$ and $n = p$.
  Then,
  The least squares $\hat{\beta}_j = y_j$; the ridge $\hat{\beta}_j^R = y_j/(1 + \lambda)$
  The Lasso $\hat{\beta}_j^L = \text{sign}(y_j)(|y_j| - \lambda/2)_+$.

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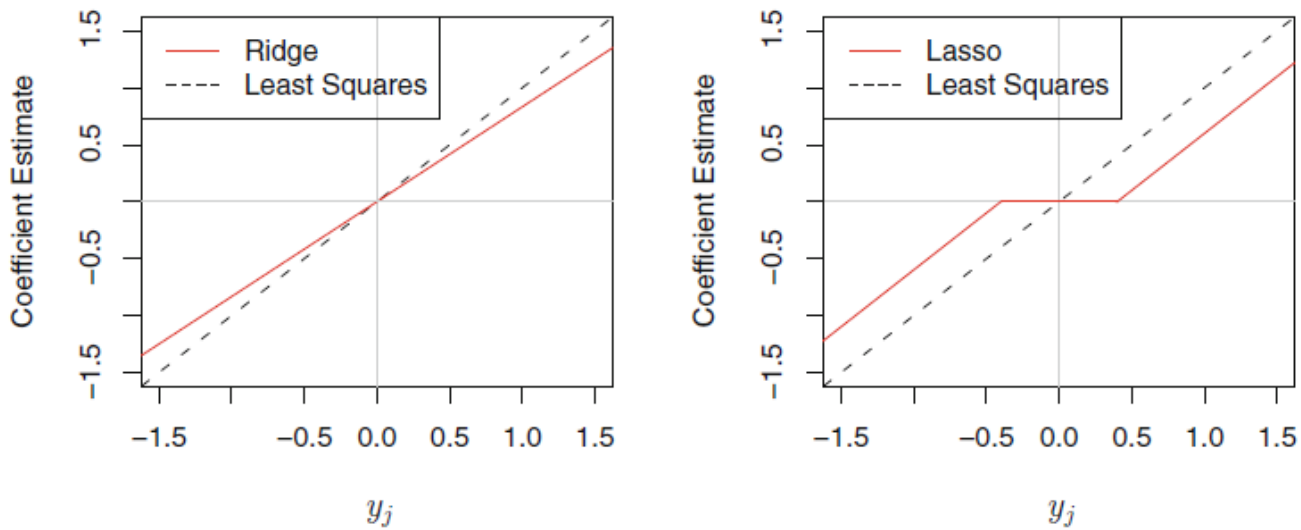

- *Left*: The ridge regression coefficient estimates are shrunken proportionally towards zero, relative to the least squares estimates.
- *Right*: Lasso coefficient estimates are soft-thresholded towards 0.

Another formulation

- For Lasso: Minimize

$$\sum_{i=1}^{n}(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij})^2 \text{ subject to } \sum_{j=1}^{p}|\beta_j| \leq s$$

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$$\sum_{i=1}^{n}(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij})^2 \text{ subject to } \sum_{j=1}^{p}\beta_j^2 \leq s$$

- For l_0: Minimize

$$\sum_{i=1}^{n}(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij})^2 \text{ subject to } \sum_{j=1}^{p}I(\beta \neq 0) \leq s$$

l_0 method penalizes number of non-zero coefficients. A difficult (NP-hard) problem for optimization.

Variable selection property for Lasso

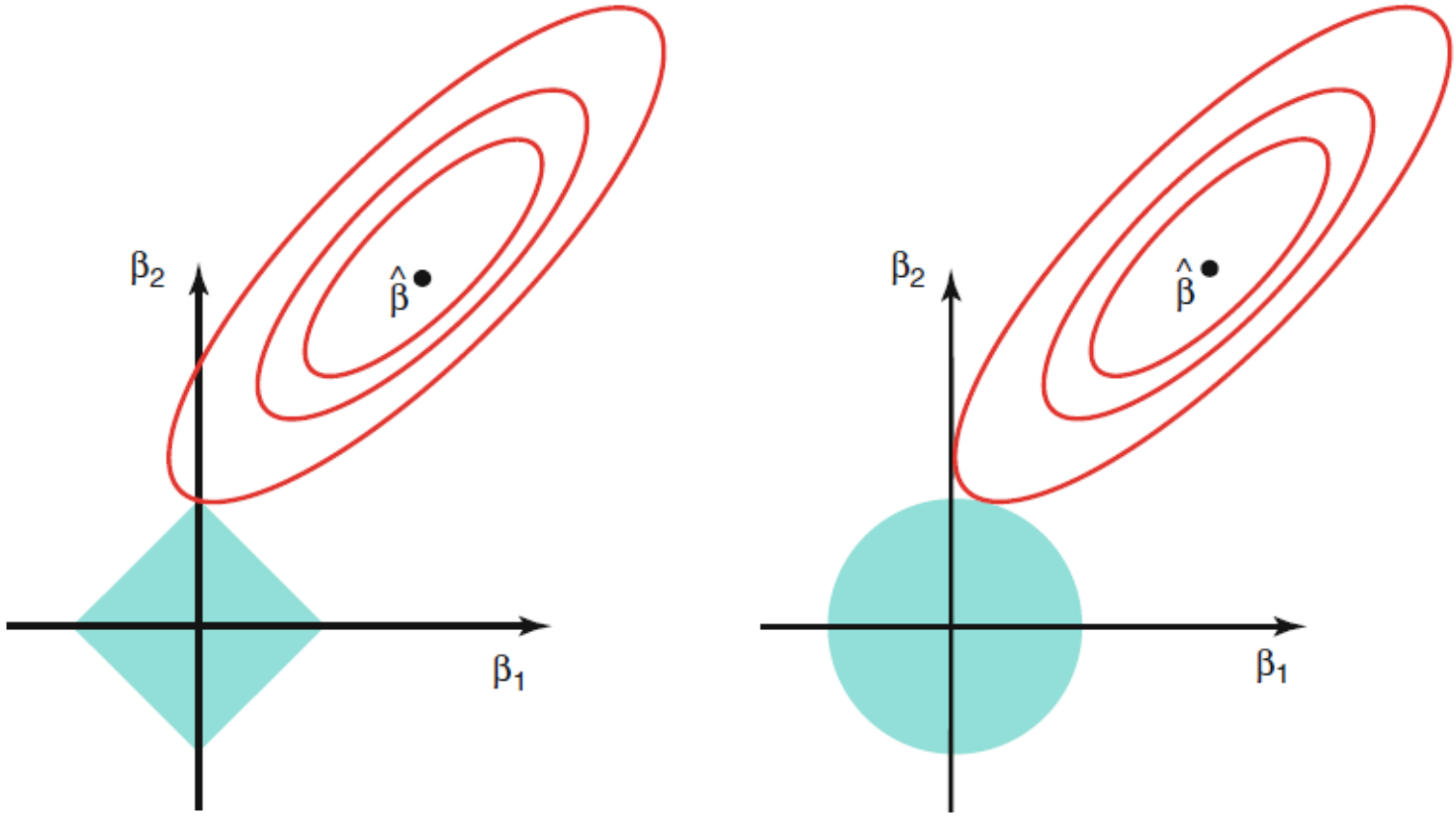

Figure: 6.7. Contours of the error and constraint functions for the lasso (left) and ridge regression (right). The solid blue areas are the constraint regions, $|\beta_1| + |\beta_2| \leq s$ and $\beta_1^2 + \beta_2^2 \leq s$, while the red ellipses are the contours of the RSS.

- l_1 penalty has the effect of forcing some of the coefficient estimates to be exactly equal to zero when the tuning parameter λ is sufficiently large.
- This is not the case for ridge.
- It performs variable selection, and yields sparse models.

- l_1 penalty has the effect of forcing some of the coefficient estimates to be exactly equal to zero when the tuning parameter λ is sufficiently large.
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- It performs variable selection, and yields sparse models.

Why we set $\mathcal{R}(\beta_1, \cdots, \beta_p)$, which is not related to β_0?

Tuning parameter λ.

- $\lambda = 0$: no penalty, $\hat{\beta}_0^R = \hat{\beta}_0^L = \hat{\beta}$.
- $\lambda = \infty$: infinity penalty, $\hat{\beta}_\infty^R = \hat{\beta}_\infty^L = 0$.
- Large λ: heavy penalty, more shrinkage of the estimator.

Example: ridge.

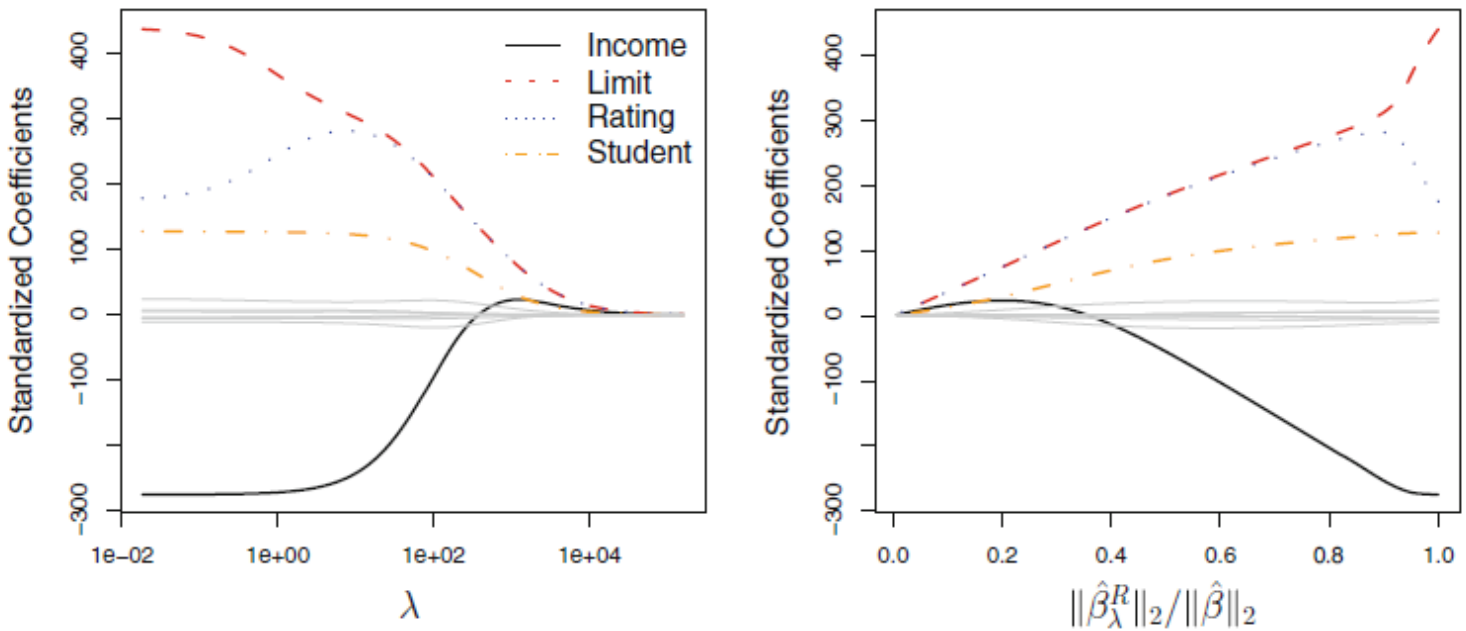

Figure: 6.4. The standardized ridge regression coefficients are displayed for the Credit data set, as a function of λ and $\|\hat{\beta}^R_\lambda\|_2/\|\hat{\beta}\|_2$. Here $\|\mathbf{a}\|_2 = \sqrt{\sum_{j=1}^{p} a_j^2}$.

Example: lasso.

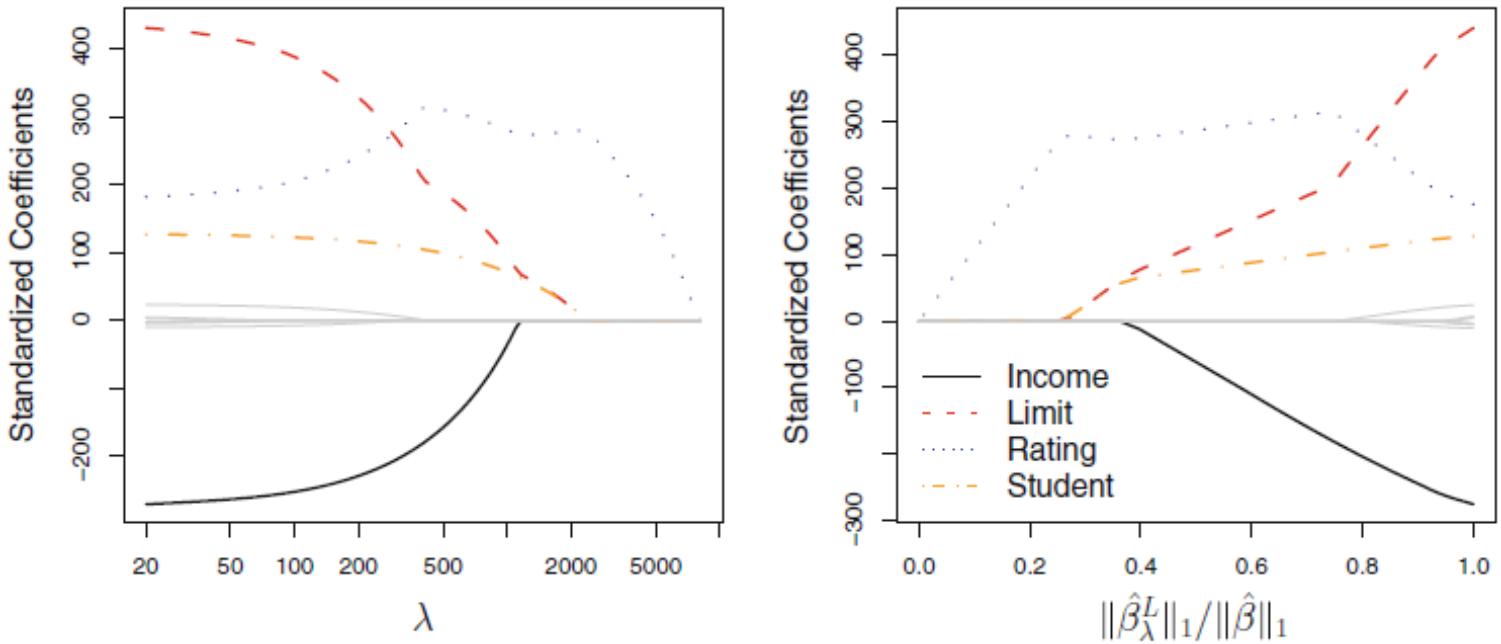

Figure: 6.6. The standardized lasso coefficients on the Credit data set are shown as a function of λ and $\|\hat{\beta}^L_\lambda\|_1/\|\hat{\beta}\|_1$.

Bias-variance tradeoff (why ridge improves over LSE)

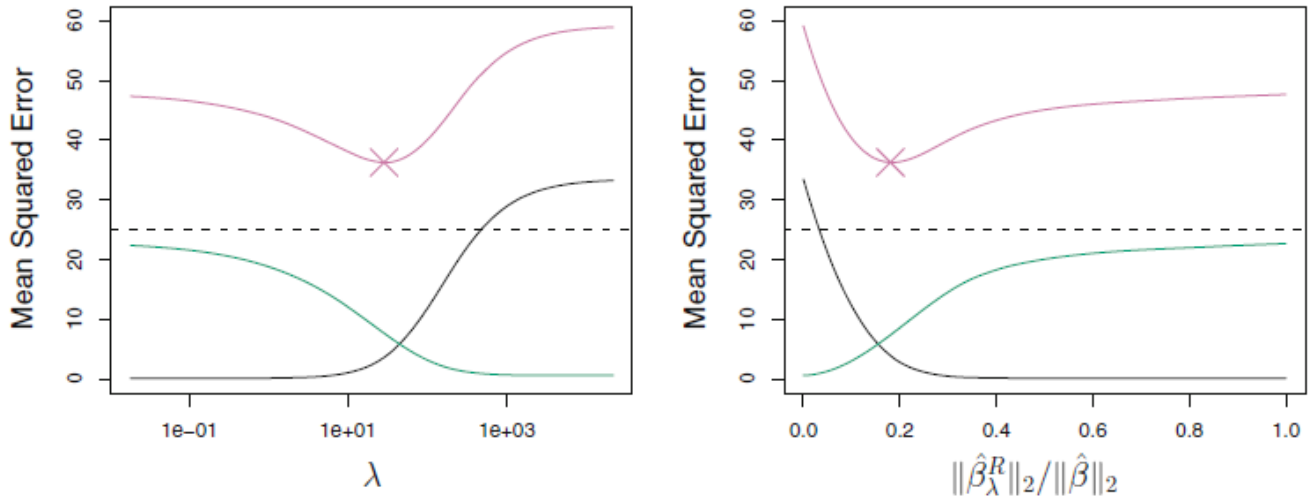

Figure: Simulated data ($p = 45, n = 50$).

- Squared bias (black), variance (green), and test mean squared error (purple) for the ridge regression predictions.
- The horizontal dashed lines indicate the minimum possible MSE.
- Purple crosses – ridge regression models with smallest MSE.

Bayesian interpretation

- Suppose $\beta = (\beta_0, ..., \beta_p)$ are random variables with a prior distribution $p(\cdot)$.
- Given β and the input X, Y has conditional density $f(y|X, \beta)$.
- The posterior distribution of the parameter β is

$$p(\beta|X, Y) \propto f(Y|X, \beta)p(\beta|X) = f(Y|X, \beta)p(\beta)$$

The proporionality means a constant (not related with β) multiplier. (β and X are independent.)

Bayesian interpretation

- Now consider the linear regression model, $Y = \beta_0 + X_1\beta_1 + ... + X_p\beta_p + \epsilon$, with ϵ conditioning on X follows $N(0, \sigma^2)$.
- If the β has the normal prior, the prior of β following normal distribution with mean 0 then the posterior mode for β is ridge estimator.
- If the β has the double exponential prior:

$$f(t) = \lambda e^{-\lambda|t|}/2$$

the prior of β following a double-exponential (Laplace) distribution with mean zero, then it follows that the posterior mode for β is the lasso solution.

The Gaussian and double expoential curves

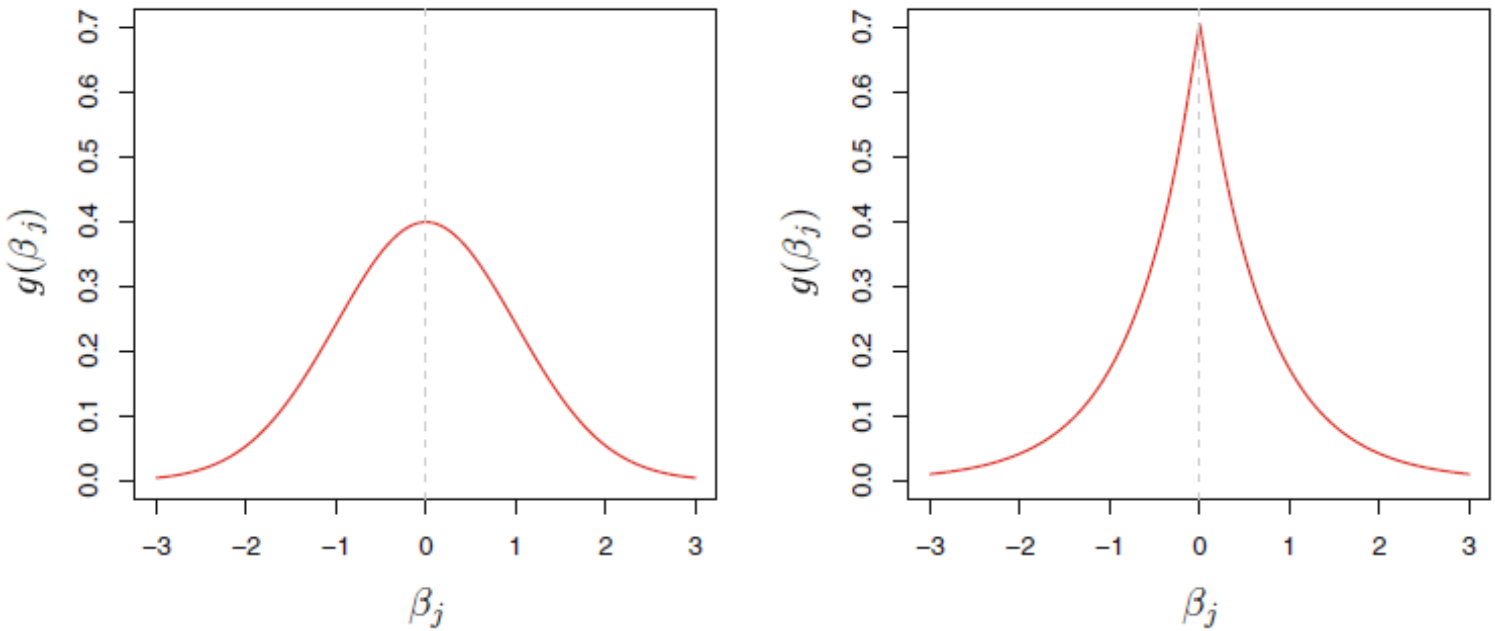

Figure: 6.11. Left: Ridge regression is the posterior mode for β under a Gaussian prior. Right: The lasso is the posterior mode for β under a double-exponential prior.

Tuning parameter selection by cross-validation: Credit data

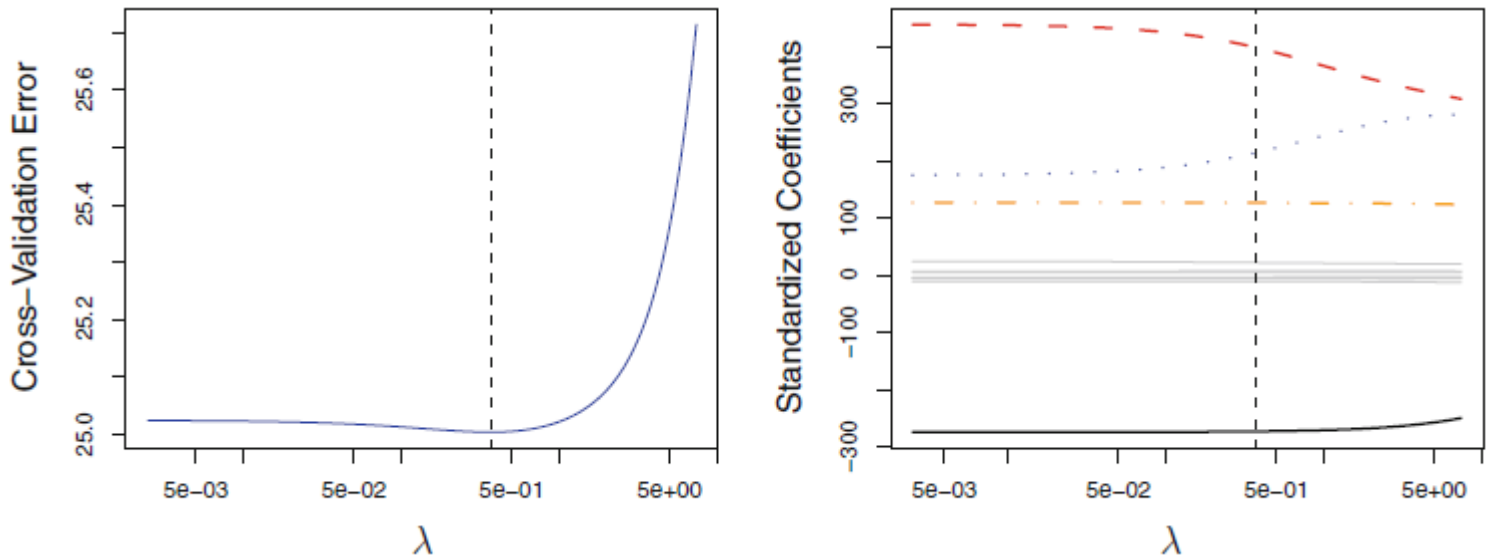

Figure: 6.12. Left: Cross-validation errors that result from applying ridge regression to the Credit data set with various value of λ. Right: The coefficient estimates as a function of λ. The vertical dashed lines indicate the value of λ selected by cross-validation.

Example

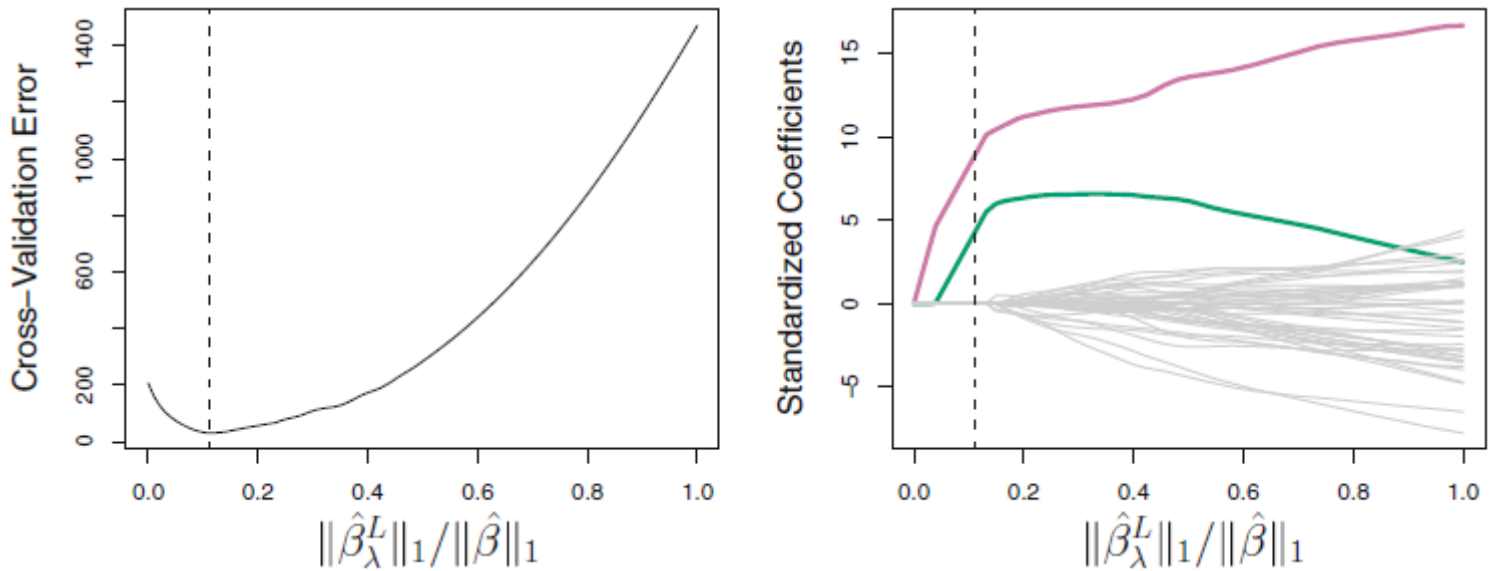

Figure: 6.13. Left: Ten-fold cross-validation MSE for the lasso, applied to the sparse simulated data set from Figure 6.9. Right: The corresponding lasso coefficient estimates are displayed. The vertical dashed lines indicate the lasso fit for which the cross-validation error is smallest.

Dimension reduction methods.

- The linear regression

$$y_i = \beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p + \epsilon_i, \ \ i = 1, \cdots, n.$$

- Our idea: when p is large,
  - transform the predictors
  - fit a least squares model using the transformed variables.
  - it is called *dimension reduction* methods.
- That is,
  - $Z_1, Z_2, \cdots, Z_M$ represent $M \ll p$ linear combinations of $X_1, ..., X_p$.

$$Z_m = \sum_{j=1}^{p} \phi_{jm} X_j. \tag{2}$$

  - We regress on $Z_1, ..., Z_M$ with $M < p$.

$$y_i = \theta_0 + \sum_{m=1}^{M} \theta_m Z_m + \epsilon_i, \ \ i = 1, ..., n. \tag{3}$$

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$$y_i = \theta_0 + \sum_{m=1}^{M} \theta_m Z_m + \epsilon_i, \ \ i = 1, ..., n. \tag{3}$$

- Plug (2) into (3) and compare with the original linear regression, we have

$$\beta_j = \sum_{m=1}^{M} \theta_m \phi_{jm}.$$

- Dimension reduction serves to constrain the estimated β_j coefficients.
- For Dimension reduction, a key step is how to determine the linear combination.
- Choose $Z_1, .., Z_M$ as the first M principle components.

Principal Component Analysis

- PCA is a technique for reducing the dimension of data matrix.
- The first principal component direction of the data is that along which the observations *vary the most*.
- The second principal component direction of the data is that along which the observations *vary the second most*.
- and so on...

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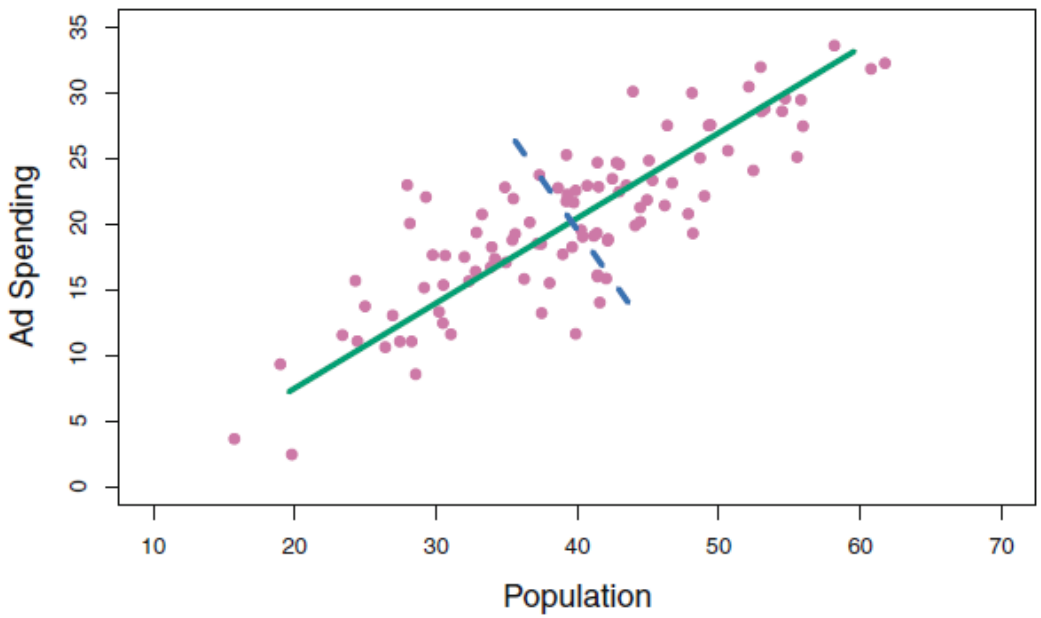

- Let X be the random vector (sample) of p dimension,
- $\mathbf{a}$ be the vector the sample varies the most.
- The variation can be measured by $Z_1 = \mathbf{a}^T(X - \mathbb{E}(X))$.
- The variation of a one dimensional random variable X can be quantified by its variance. Then

$$\text{var}(Z_1) = \mathbf{a}^T \text{var}(X)\mathbf{a}.$$

- $\mathbf{a}$ should be the leading eigenvector of $\text{var}(X)$.

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- The variation can be measured by $Z = A^T(X - \mathbb{E}(X))$.
- For a p-dimension random vector, its variation, fully described by its covariance matrix Σ. Then

$$\text{var}(Z) = A^T \text{var}(X) A = A^T \Sigma A.$$

- A will be the eigenvectors corresponding to the the largest M eigenvalues when we solve A by maximizing $\text{var}(Z)$.

Principal Components as major statistical methodology

- Let X be the random vector of p dimension that we are concerned with and Σ be the covariance matrix of X.

$$X = \begin{pmatrix} X_1 \\ \vdots \\ X_p \end{pmatrix}, \Sigma = \text{var}(X) = \begin{pmatrix} \sigma_{11} & \cdots & \sigma_{1p} \\ \vdots & \vdots & \vdots \\ \sigma_{p1} & \cdots & \sigma_{pp} \end{pmatrix}.$$

  where $\sigma_{kl} = \text{cov}(X_k, X_l)$.
- We assume here $E(X) = 0$ for convenience, since the mean of X plays no role in PCs.

Principal Component Analysis (PCA).

- By matrix singular value decomposition, we know

$$\Sigma = \mathbf{e}\Lambda\mathbf{e}'$$

where

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_p \end{pmatrix}, \ \mathbf{e} = (\mathbf{e}_1 \vdots \cdots \vdots \mathbf{e}_p) = \begin{pmatrix} e_{11} & \cdots & e_{1p} \\ \vdots & \vdots & \vdots \\ e_{p1} & \cdots & e_{pp} \end{pmatrix}$$

with $\lambda_1 \geq \cdots \geq \lambda_p > 0$ and $\mathbf{e}\mathbf{e}' = I_p$.

- $(\lambda_k, \mathbf{e}_k)$, $k = 1, ..., p$, are the eigenvalue-eigenvector pairs of the matrix Σ.

- *The first P.C:* $Z_1 = \mathbf{e}_1^T X$ *– the most important.*

$$\text{var}(Z_1) = \lambda_1 = \max\{\text{var}(b'X) : \|b\| = 1,\ b \in R^p\}.$$

The fraction of total variation of X explained by Z_1 is

$$\frac{\text{var}(Z_1)}{\text{var}(Z_1) + \cdots + \text{var}(Z_p)} = \frac{\lambda_1}{\lambda_1 + \cdots + \lambda_p}.$$

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$$\frac{\text{var}(Z_1)}{\text{var}(Z_1) + \cdots + \text{var}(Z_p)} = \frac{\lambda_1}{\lambda_1 + \cdots + \lambda_p}.$$

- ...
- *The k-th P.C:* $Z_k = \mathbf{e}_k^T X$ – *the k-th important.*

$$\text{var}(Z_k) = \lambda_k = \max_{b \in R^p}\{\text{var}(b'X) : \|b\| = 1,\ b'X \perp Z_i, i = 1, \cdots, k-1\},$$

Here and throughout, $\perp$ means 0 correlation. The fraction of total variation of X explained by Z_k is

$$\frac{\text{var}(Z_k)}{\text{var}(Z_1) + \cdots \text{var}(Z_p)} = \frac{\lambda_k}{\lambda_1 + \cdots \lambda_p}.$$

A summary table of PCs

		eigenvalue (variance)	eigenvector (combination coefficient)	percent of variation explained	P.C.s as linear combination of $X - \mu$
1st	Z_1	λ_1	$u\mathbf{e}_1$	$\lambda_1 / \sum_{j=1}^{p} \lambda_j$	$Z_1 = u_1'(X - \mu)$
2nd	Z_2	λ_2	bfe_2	$\lambda_2 / \sum_{j=1}^{p} \lambda_j$	$Z_2 = u_2'(X - \mu)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
p-th	Z_p	λ_p	$\mathbf{e}_p$	$\lambda_p / \sum_{j=1}^{p} \lambda_j$	$Z_1 = u_p'(X - \mu)$

- The population P.C.s are only theoretical,
- in data analysis, we need to work with the sample P.C.s.
- Suppose there are n observations of p variables presented as

$$\mathbf{X} = \left(X_{(1)} \vdots X_{(2)} \vdots \cdots \vdots X_{(p)}\right) = \begin{pmatrix} x_{11} & \cdots & x_{1p} \\ \vdots & \vdots & \vdots \\ x_{n1} & \cdots & x_{np} \end{pmatrix}_{n \times p}.$$

  Then $X_{(k)}$, an n-vector, contains all n observations of the k-th variable.
- We compute the sample variance matrix, denoted as $\mathbf{S}$ and do eigenvalue decomposition,

$$\mathbf{S} = \hat{\mathbf{e}}\hat{\Lambda}\hat{\mathbf{e}}'.$$

A summary of sample P.C.s

		eigenvalue (variance)	eigenvector (combination coefficient)	percent of variation explained	P.C.s as linear combination of $X - \mu$
1st	$Z_{(1)}$	$\hat{\lambda}_1$	$\hat{\mathbf{e}}_1$	$\hat{\lambda}_1 / \sum_{j=1}^{p} \hat{\lambda}_j$	$Z_{(1)} = \sum_{j=1}^{p} \hat{e}_{j1}(X_{(j)} - \bar{X}_1)$
2nd	$Z_{(2)}$	$\hat{\lambda}_2$	$\hat{\mathbf{e}}_2$	$\hat{\lambda}_1 / \sum_{j=1}^{p} \hat{\lambda}_j$	$Z_{(2)} = \sum_{j=1}^{p} \hat{e}_{j2}(X_{(j)} - \bar{X}_1)$
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
p-th	$Z_{(p)}$	$\hat{\lambda}_p$	$\hat{\mathbf{e}}_1$	$\hat{\lambda}_p / \sum_{j=1}^{p} \hat{\lambda}_j$	$Z_{(p)} = \sum_{j=1}^{p} \hat{e}_{jp}(X_{(j)} - \bar{X}_1)$

Principal component regression (PCR).

- Key assumption: a small number of principal components suffice to explain most of the variability in the data, as well as the relationship with the response.
- the directions in which $X_1, \cdots, X_p$ show the most variation are the directions that are associated with Y.

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- the directions in which $X_1, \cdots, X_p$ show the most variation are the directions that are associated with Y.
- Set $Z_i, i = \mathbf{e}_i, i = 1, \cdots, M$.
- fit a least squares model to $Z_1, \cdots, Z_M$.

Principal component regression (PCR).

- Key assumption: a small number of principal components suffice to explain most of the variability in the data, as well as the relationship with the response.
- the directions in which $X_1, \cdots, X_p$ show the most variation are the directions that are associated with Y.
- Set $Z_i, i = \mathbf{e}_i, i = 1, \cdots, M$.
- fit a least squares model to $Z_1, \cdots, Z_M$.
- If assumption holds, the fitting will lead a good result.

Partial least squares approach

- Principal components are designed to explain variation within X, not the relation of X with Y.
- The *key* assumption with principal components regression may NOT hold.
- Partial least squares approach avoids this shortcoming.

Partial least squares approach (PLS).

Like PCR, PLS is a dimension reduction method,

- first identifies squares a new set of features $Z_1, \cdots, Z_M$ that are linear combinations of the original features,
- fits a linear model via least squares using these M new features.

Partial least squares approach (PLS).

Like PCR, PLS is a dimension reduction method,

- first identifies squares a new set of features $Z_1, \cdots, Z_M$ that are linear combinations of the original features,
- fits a linear model via least squares using these M new features.

Unlike PCR, PLS identifies these new features in a supervised way

- it makes use of the response Y in order to identify new features that not only approximate the old features well,
- but also that are related to the response.

Partial least squares approach

- standardize each input $\mathbf{x}_j$ to have mean 0 and variance 1.
- Set $\hat{\mathbf{y}}^{(0)} = \bar{y}\mathbf{1}$ and $\mathbf{x}_j^{(0)} = \mathbf{x}_j, j = 1, \cdots, M$.
- For $m = 1, 2, \cdots, M$,
  $\mathbf{z}_m = \sum_{j=1}^{p} \hat{\phi}_{mj}\mathbf{x}_j^{(m-1)}$, where $\hat{\phi}_{mj} = \mathbf{y}^T\mathbf{x}_j^{(m-1)}$.
  $\hat{\theta}_m = \mathbf{z}_m^T\mathbf{y}/\mathbf{z}_m^T\mathbf{z}_m$
  $\hat{\mathbf{y}}^{(m)} = \hat{\mathbf{y}}^{(m-1)} + \hat{\theta}_m\mathbf{z}_m$.
  $\mathbf{x}_j^{(m)} = \mathbf{x}_j^{(m-1)} - s_{jm}\mathbf{z}_m$, where $s_{jm} = \mathbf{z}_m^T\mathbf{x}_j^{(m-1)}/\mathbf{z}_m^T\mathbf{z}_m$
- Output the sequence of fitted vectors $\{\hat{y}^{(m)}\}_1^p$. Since the $\{z_l\}_1^m$ are linear in the original $\mathbf{x}_j$, so is $\hat{y}^{(m)} = X\hat{\beta}^{\text{pls}}(m)$. These linear coefficients can be recovered from the sequence of PLS transformations.

Example

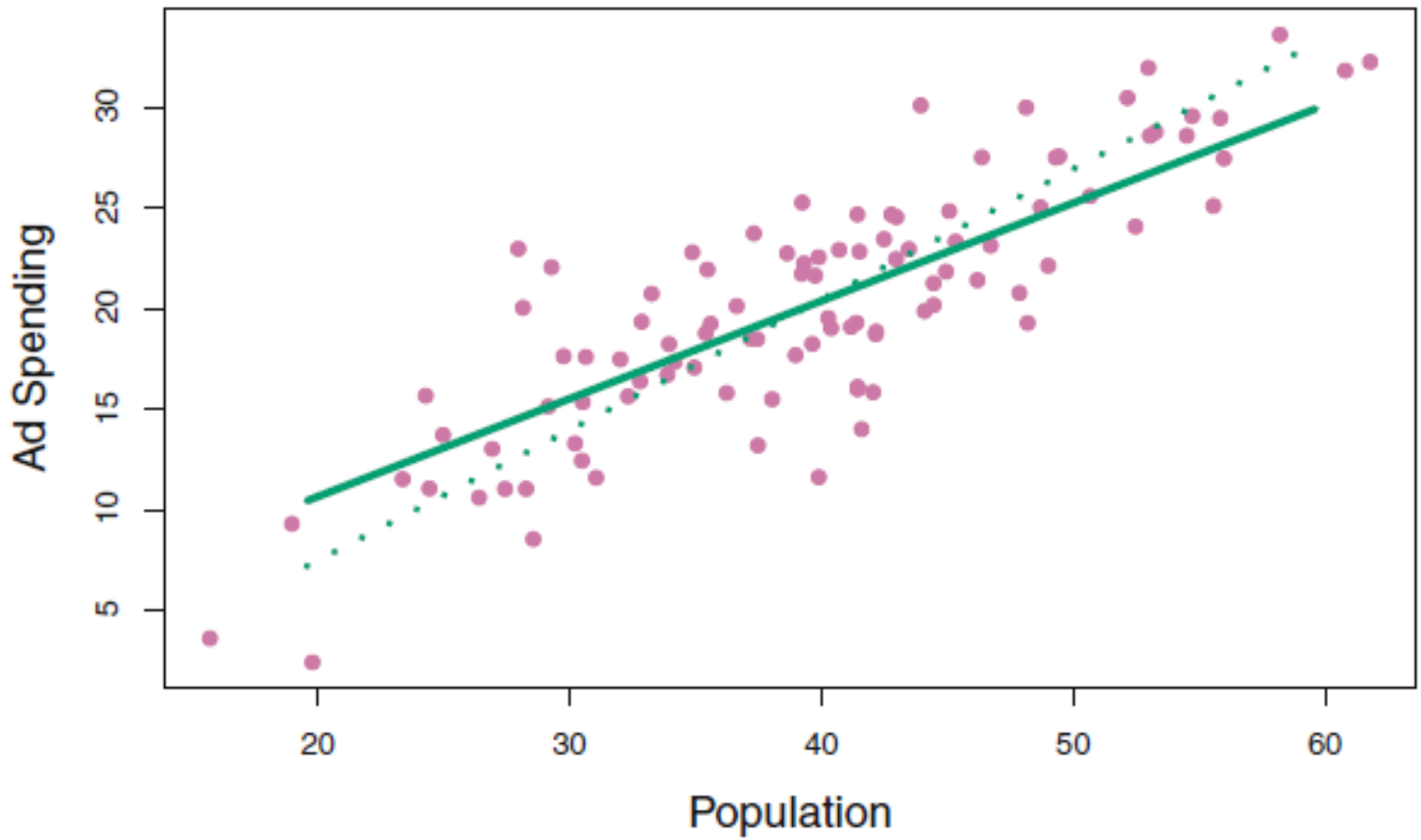

Figure: 6.21. For the advertising data, the first PLS direction (solid line) and first PCR direction (dotted line) are shown.

Partial least squares approach

- Partial least squares puts more weights on the variables with higher correlation with the response.
- It seeks the directions that have high variance and have high correlation with the reposne (while PCR only seeks those direction with high variance.)
- When the relationship between response and predictors is strong, PLS is better.
- Popular in chemometrics.

High dimension data

- Digitization of the society brings big data.
- Many of the datasets contain large number of varaibles.
- It is common that $p \gg n$, which is called the *curse of dimensionality*.
- Example: predition of blood pressure.
  Response: blood pressure.
  Inputs: SNPs; (Individual DNA mutations).
  n may be of hundreds, but p can be of millions.

The trouble

- Large p makes our linear regression model too flexible (or too large).
- If $p > n$, the LSE is not even uniquely determined.
- It can easily lead to overfit.
- A common phenomenon: small training error, but large test error.

Deal with high dimensional data

- Fit less flexible models to avoid overfit.
- feature selction:
  - forward stepwise selection,
  - ridge regression,
  - the lasso,
  - principal components regression.