Why consider alternatives to least squares?

- *Prediction Accuracy:* especially when $p > n$, to control the variance.
- *Model Interpretability:* By removing irrelevant features — that is, by setting the corresponding coefficient estimates to zero — we can obtain a model that is more easily interpreted. We will present some approaches for automatically performing *feature selection*.

Three classes of methods

- *Subset Selection*. We identify a subset of the p predictors that we believe to be related to the response. We then fit a model using least squares on the reduced set of variables.
- *Shrinkage*. We fit a model involving all p predictors, but the estimated coefficients are shrunken towards zero relative to the least squares estimates. This shrinkage (also known as *regularization*) has the effect of reducing variance and can also perform variable selection.
- *Dimension Reduction*. We project the p predictors into a M-dimensional subspace, where $M < p$. This is achieved by computing M different *linear combinations*, or *projections*, of the variables. Then these M projections are used as predictors to fit a linear regression model by least squares.

Subset Selection

Best subset and stepwise model selection procedures

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.

Stepwise Selection

- For computational reasons, best subset selection cannot be applied with very large p.
- Best subset selection may also suffer from statistical problems when p is large:

- an enormous search space can lead to *overfitting* and high variance of the coefficient estimates.
- For both of these reasons, *stepwise* methods, which explore a far more restricted set of models, are attractive alternatives to best subset selection.

Forward Stepwise Selection

- Forward stepwise selection begins with a model containing no predictors, and then adds predictors to the model, one-at-a-time, until all of the predictors are in the model.
- In particular, at each step the variable that gives the greatest *additional* improvement to the fit is added to the model.

In Detail

Forward Stepwise Selection

1. Let $\mathcal{M}_0$ denote the *null* model, which contains no predictors.
2. For $k = 0, \ldots, p-1$:
   - 2.1 Consider all $p - k$ models that augment the predictors in $\mathcal{M}_k$ with one additional predictor.
   - 2.2 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.

Credit data example

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

The first four selected models for best subset selection and forward stepwise selection on the Credit *data set. The first three models are identical but the fourth models differ.*

Backward Stepwise Selection

- Like forward stepwise selection, *backward stepwise selection* provides an efficient alternative to best subset selection.
- However, unlike forward stepwise selection, it begins with the full least squares model containing all p predictors, and then iteratively removes the least useful predictor, one-at-a-time.

More on Backward Stepwise Selection

- Like forward stepwise selection, the backward selection approach searches through only $1 + p(p+1)/2$ models, and so can be applied in settings where p is too large to apply best subset selection
- Like forward stepwise selection, backward stepwise selection is not guaranteed to yield the *best* model containing a subset of the p predictors.
- Backward selection requires that the *number of samples n is larger than the number of variables p* (so that the full model can be fit). In contrast, forward stepwise can be used even when $n < p$, and so is the only viable subset method when p is very large.

Estimating test error: two approaches

- We can indirectly estimate test error by making an *adjustment* to the training error to account for the bias due to overfitting.
- We can *directly* estimate the test error, using either a validation set approach or a cross-validation approach, as discussed in previous lectures.
- We illustrate both approaches next.

C_p, AIC, BIC, and Adjusted R^2

- These techniques adjust the training error for the model size, and can be used to select among a set of models with different numbers of variables.

Now for some details

- *Mallow's C_p*:

$$C_p = \frac{1}{n}\left(\text{RSS} + 2d\hat{\sigma}^2\right),$$

  where d is the total # of parameters used and $\hat{\sigma}^2$ is an estimate of the variance of the error ϵ associated with each response measurement.

- The *AIC* criterion is defined for a large class of models fit by maximum likelihood:

$$\text{AIC} = -2\log L + 2 \cdot d$$

  where L is the maximized value of the likelihood function for the estimated model.

Details on BIC

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

- Like C_p, the BIC will tend to take on a small value for a model with a low test error, and so generally we select the model that has the lowest BIC value.

- Since $\log n > 2$ for any $n > 7$, the BIC statistic generally places a heavier penalty on models with many variables, and hence results in the selection of smaller models than C_p.

Adjusted R^2

- For a least squares model with d variables, the adjusted R^2 statistic is calculated as

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

  where TSS is the total sum of squares.

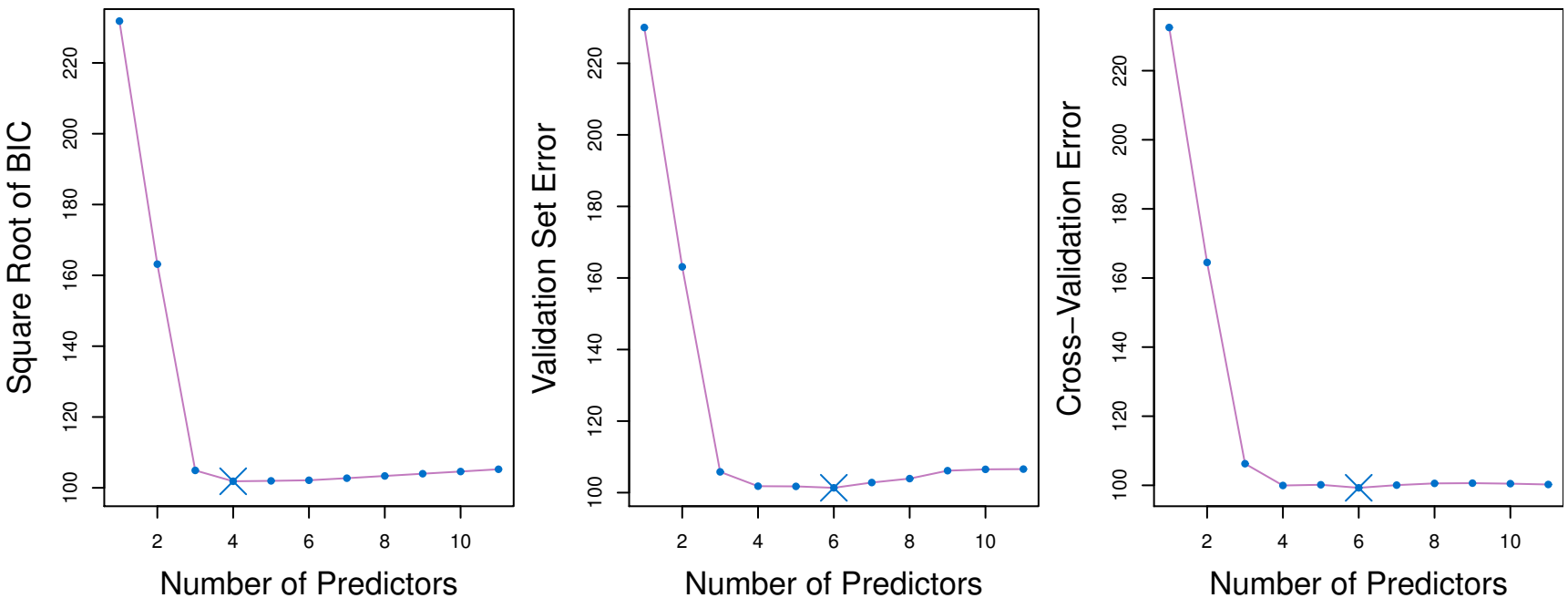
- Maximizing the adjusted R^2 is equivalent to minimizing $\frac{\text{RSS}}{n-d-1}$.

- Unlike the R^2 statistic, the adjusted R^2 statistic *pays a price* for the inclusion of unnecessary variables in the model.

Validation and Cross-Validation

- Each of the procedures returns a sequence of models $\mathcal{M}_k$ indexed by model size $k = 0, 1, 2, \ldots$. Our job here is to select $\hat{k}$. Once selected, we will return model $\mathcal{M}_{\hat{k}}$
- We compute the validation set error or the cross-validation error for each model $\mathcal{M}_k$ under consideration, and then select the k for which the resulting estimated test error is smallest.
- This procedure has an advantage relative to AIC, BIC, C_p, and adjusted R^2, in that it provides a direct estimate of the test error, and *doesn't require an estimate of the error variance* σ^2.

Credit data example



Shrinkage Methods

Ridge regression and *Lasso*

- The subset selection methods use least squares to fit a linear model that contains a subset of the predictors.
- As an alternative, we can fit a model containing all p predictors using a technique that *constrains* or *regularizes* the coefficient estimates, or equivalently, that *shrinks* the coefficient estimates towards zero.

Ridge regression

- Recall that the least squares fitting procedure estimates $\beta_0, \beta_1, \ldots, \beta_p$ using the values that minimize

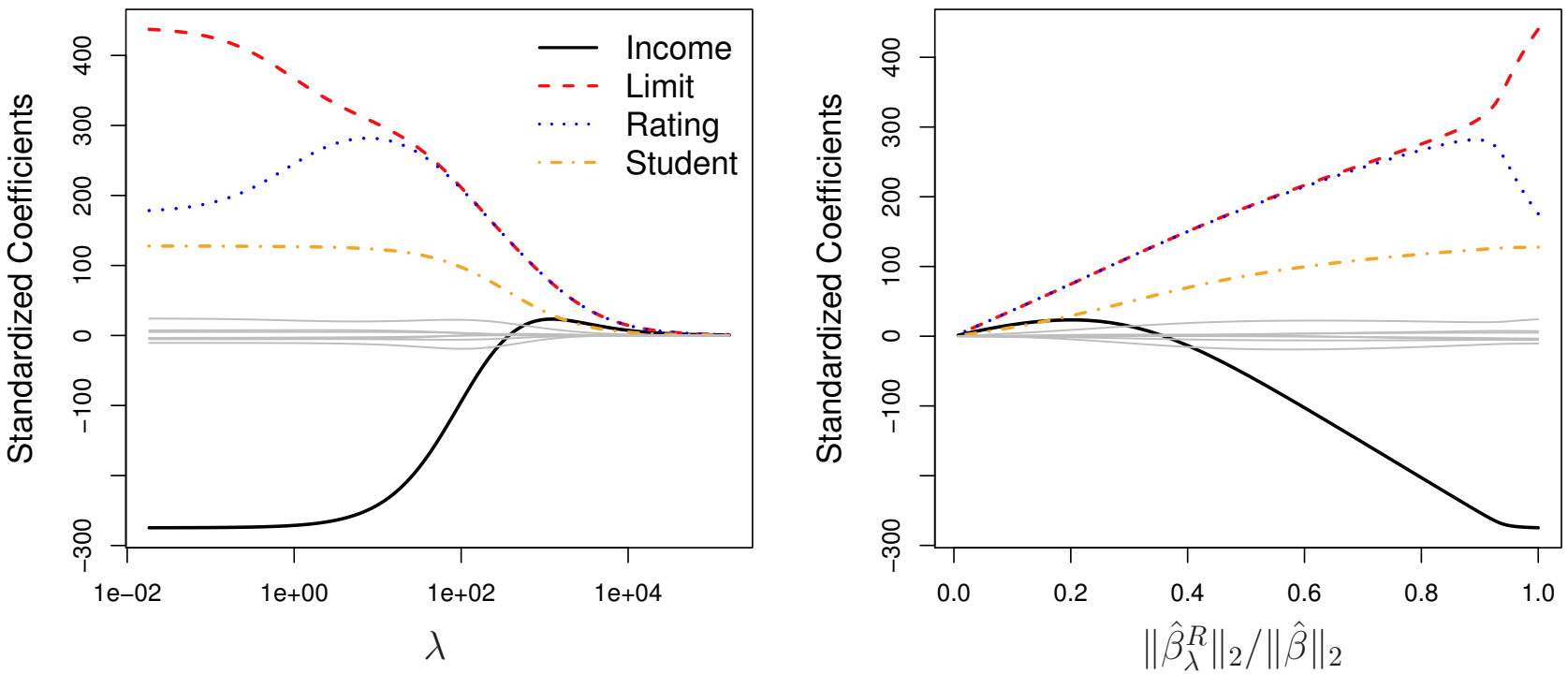
$$\text{RSS} = \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 .$$

- In contrast, the ridge regression coefficient estimates $\hat{\beta}^R$ are the values that minimize

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

where $\lambda \geq 0$ is a *tuning parameter*, to be determined separately.

Credit data example



Ridge regression: scaling of predictors

- The standard least squares coefficient estimates are *scale equivariant*:

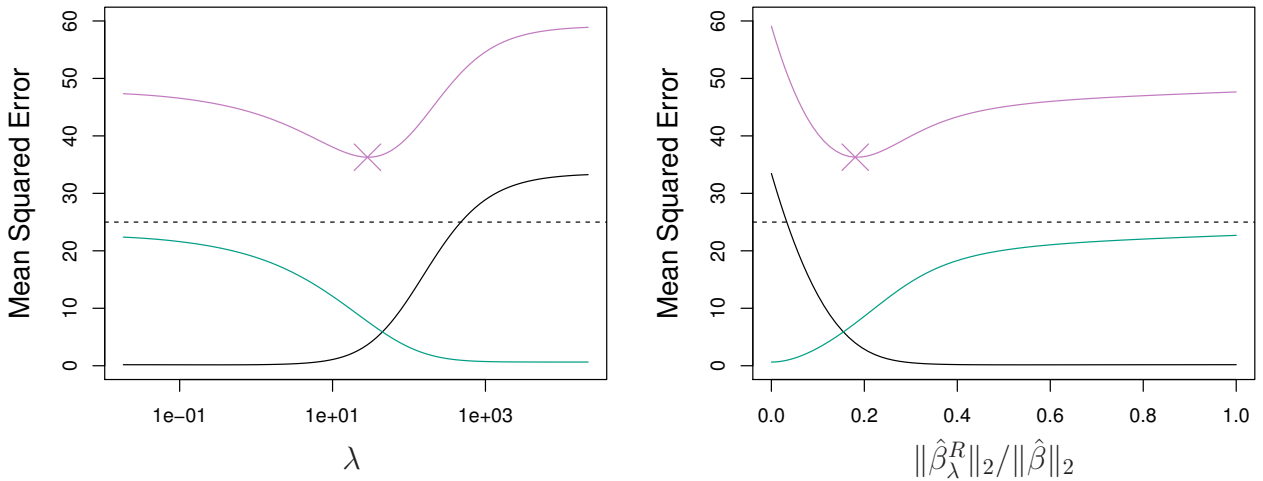
- In contrast, the ridge regression coefficient estimates can change *substantially* when multiplying a given predictor by a constant

- Therefore, it is best to apply ridge regression after *standardizing the predictors*, using the formula

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

Why Does Ridge Regression Improve Over Least Squares?

The Bias-Variance tradeoff



Simulated data with $n = 50$ observations, $p = 45$ predictors, all having nonzero coefficients. Squared bias (black), variance (green), and test mean squared error (purple) for the ridge regression predictions on a simulated data set, as a function of λ and $\|\hat{\beta}^R_\lambda\|_2/\|\hat{\beta}\|_2$

The Lasso

- Ridge regression does have one obvious disadvantage: unlike subset selection, which will generally select models that involve just a subset of the variables, ridge regression will include all p predictors in the final model
- The *Lasso* is a relatively recent alternative to ridge regression that overcomes this disadvantage. The lasso coefficients, $\hat{\beta}_\lambda^L$, minimize the quantity

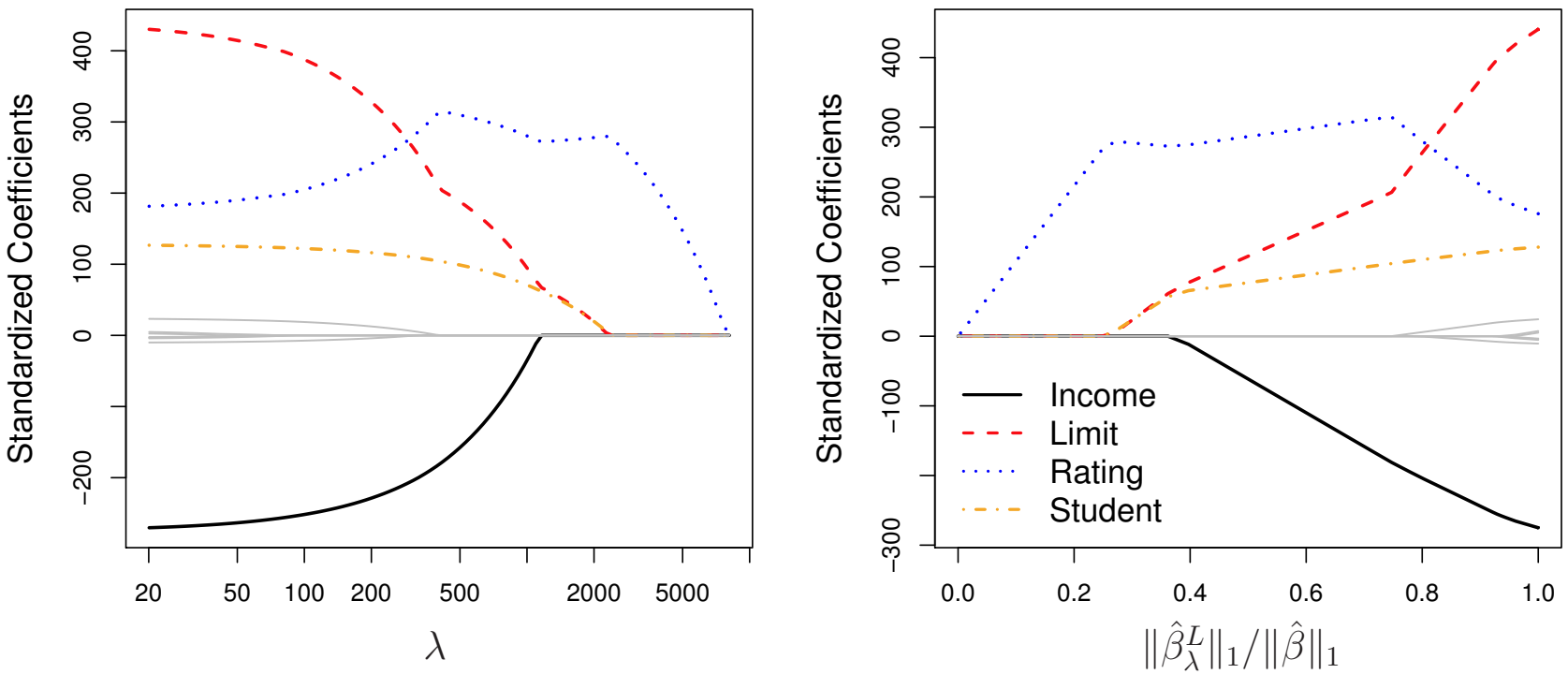
$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}|\beta_j| \;= \text{RSS} + \lambda\sum_{j=1}^{p}|\beta_j|.$$

The Lasso: continued

- As with ridge regression, the lasso shrinks the coefficient estimates towards zero.
- However, in the case of the lasso, the 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.

- We say that the lasso yields *sparse* models — that is, models that involve only a subset of the variables.

Example: Credit dataset



The Variable Selection Property of the Lasso

Why is it that the lasso, unlike ridge regression, results in coefficient estimates that are exactly equal to zero?

One can show that the lasso and ridge regression coefficient estimates solve the problems

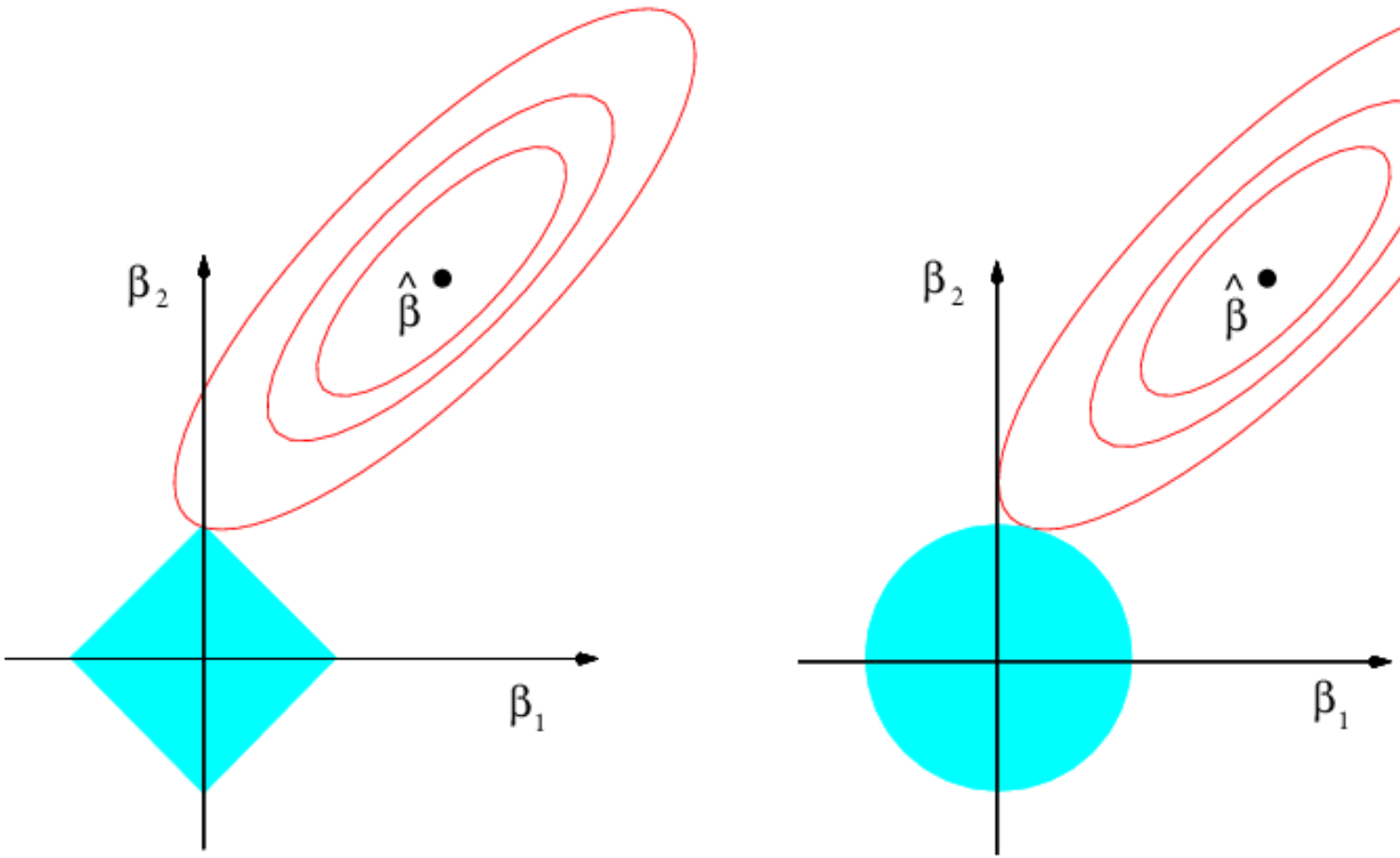
$$\underset{\beta}{\text{minimize}} \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \quad \text{subject to} \quad \sum_{j=1}^{p} |\beta_j| \leq s$$

and

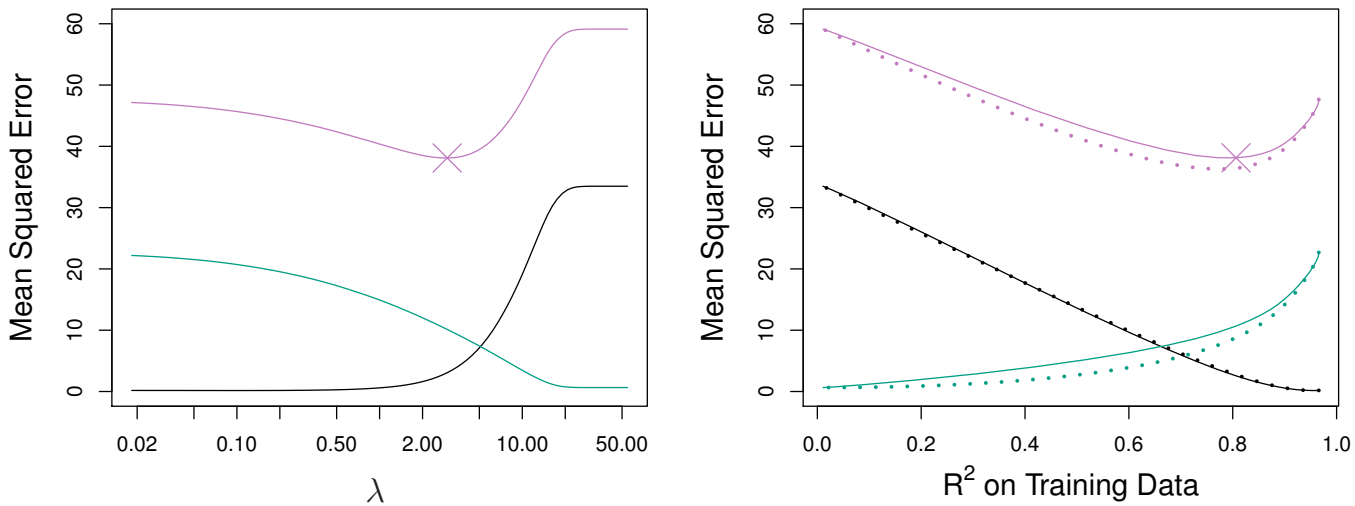
$$\underset{\beta}{\text{minimize}} \sum_{i=1}^{n} \left(y_i - \beta_0 - \sum_{j=1}^{p} \beta_j x_{ij} \right)^2 \quad \text{subject to} \quad \sum_{j=1}^{p} \beta_j^2 \leq s,$$

respectively.

The Lasso Picture



Comparing the Lasso and Ridge Regression

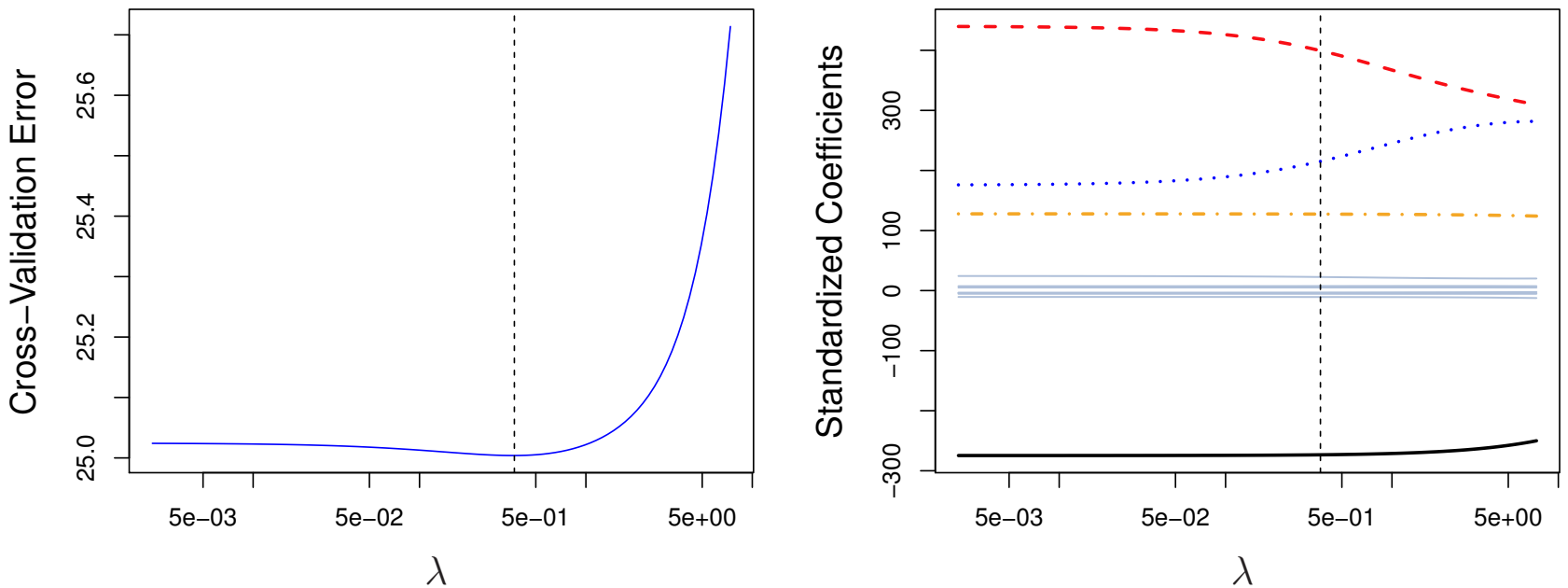


Left: *Plots of squared bias (black), variance (green), and test MSE (purple) for the lasso on simulated data set of Slide 32.* *Right:* *Comparison of squared bias, variance and test MSE between lasso (solid) and ridge (dashed). Both are plotted against their R^2 on the training data, as a common form of indexing. The crosses in both plots indicate the lasso model for which the MSE is smallest.*

Conclusions

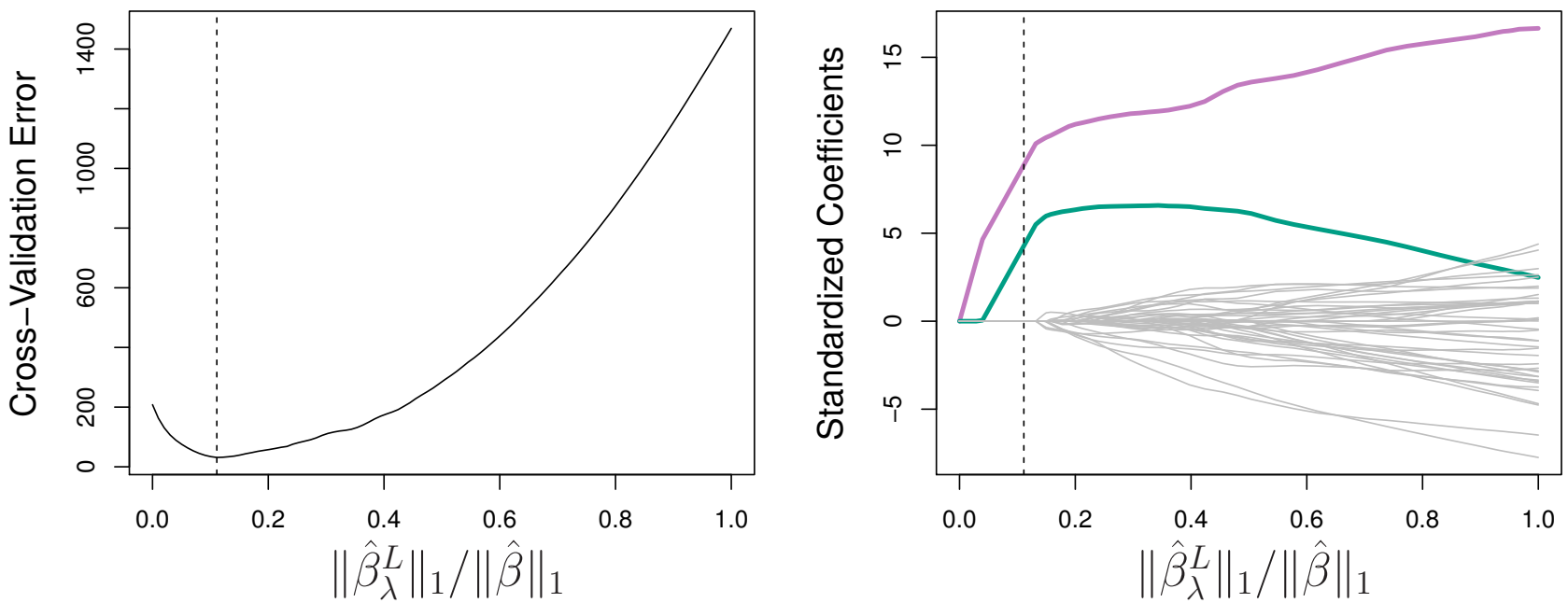
- In general, one might expect the lasso to perform better when the response is a function of only a relatively small number of predictors.
- However, the number of predictors that is related to the response is never known *a priori* for real data sets.
- A technique such as cross-validation can be used in order to determine which approach is better on a particular data set.

Credit data example



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

Simulated data example



Left: *Ten-fold cross-validation MSE for the lasso, applied to the sparse simulated data set from Slide 39.* 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 methods that we have discussed so far in this chapter have involved fitting linear regression models, via least squares or a shrunken approach, using the original predictors, $X_1, X_2, \ldots, X_p$.
- We now explore a class of approaches that *transform* the predictors and then fit a least squares model using the transformed variables. We will refer to these techniques as *dimension reduction* methods.

Dimension Reduction Methods: details

- Let $Z_1, Z_2, \ldots, Z_M$ represent $M < p$ *linear combinations* of our original p predictors. That is,

$$Z_m = \sum_{j=1}^{p} \phi_{mj} X_j \tag{1}$$

  for some constants $\phi_{m1}, \ldots, \phi_{mp}$.
- We can then fit the linear regression model,

$$y_i = \theta_0 + \sum_{m=1}^{M} \theta_m z_{im} + \epsilon_i, \quad i = 1, \ldots, n, \tag{2}$$

  using ordinary least squares.
- Note that in model (2), the regression coefficients are given by $\theta_0, \theta_1, \ldots, \theta_M$. If the constants $\phi_{m1}, \ldots, \phi_{mp}$ are chosen wisely, then such dimension reduction approaches can often outperform OLS regression.

- Notice that from definition (1),

$$\sum_{m=1}^{M} \theta_m z_{im} = \sum_{m=1}^{M} \theta_m \sum_{j=1}^{p} \phi_{mj} x_{ij} = \sum_{j=1}^{p} \sum_{m=1}^{M} \theta_m \phi_{mj} x_{ij} = \sum_{j=1}^{p} \beta_j x_{ij},$$

  where

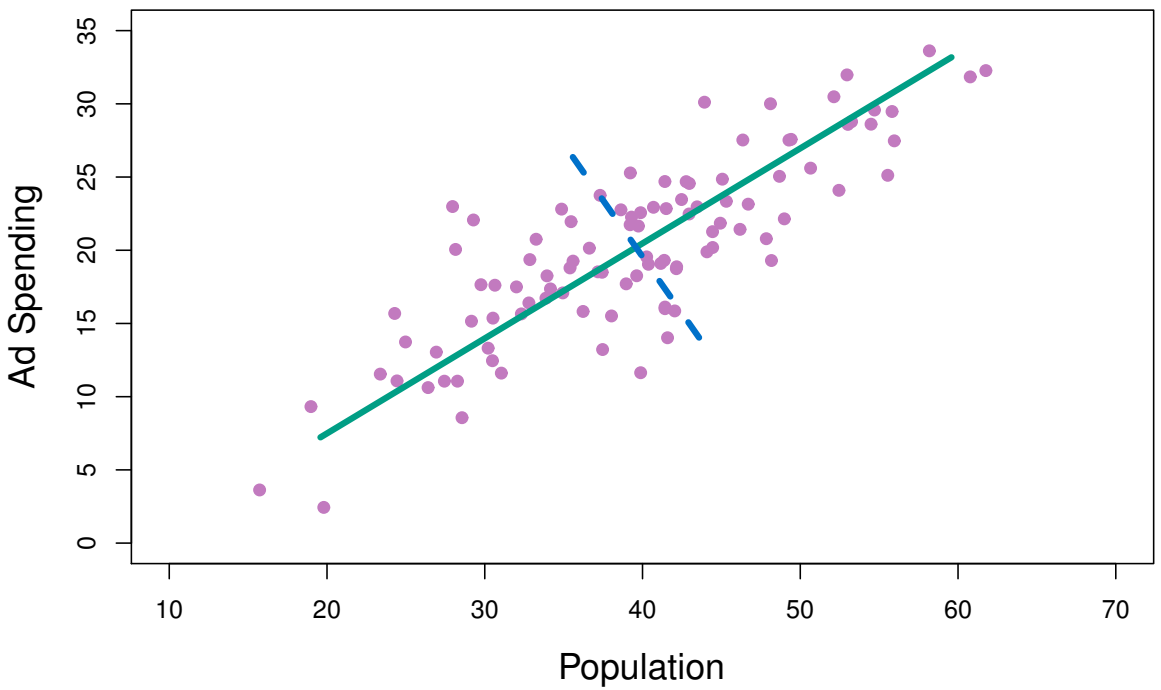
$$\beta_j = \sum_{m=1}^{M} \theta_m \phi_{mj}. \tag{3}$$

- Hence model (2) can be thought of as a special case of the original linear regression model.
- Dimension reduction serves to constrain the estimated β_j coefficients, since now they must take the form (3).
- Can win in the bias-variance tradeoff.

Principal Components Regression

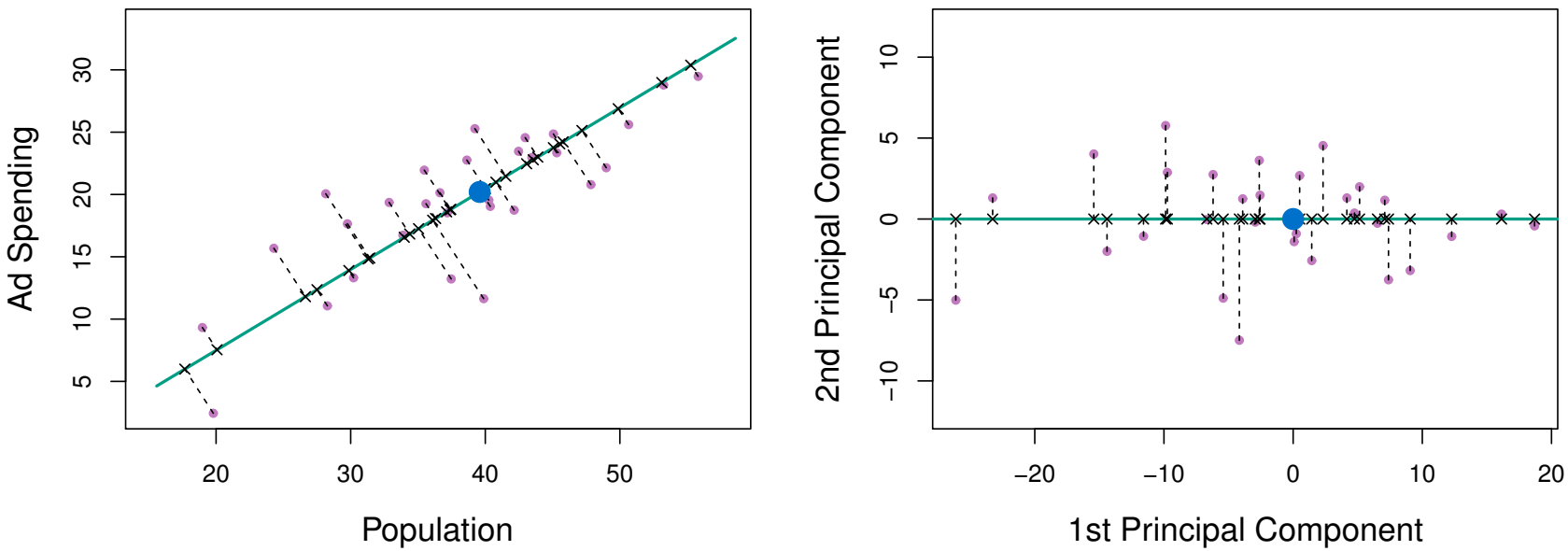
- Here we apply principal components analysis (PCA) (discussed in Chapter 10 of the text) to define the linear combinations of the predictors, for use in our regression.
- The first principal component is that (normalized) linear combination of the variables with the largest variance.
- The second principal component has largest variance, subject to being uncorrelated with the first.
- And so on.
- Hence with many correlated original variables, we replace them with a small set of principal components that capture their joint variation.

Pictures of PCA



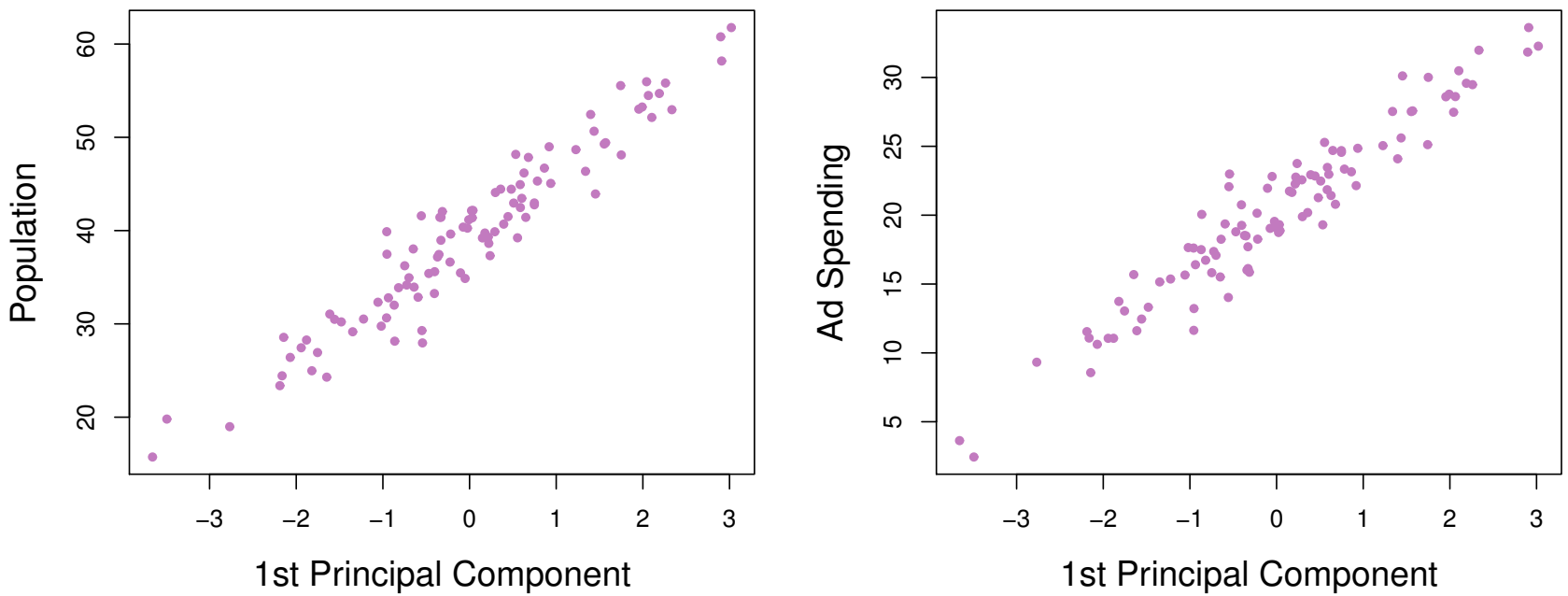
*The population size (*pop*) and ad spending (*ad*) for* 100 *different cities are shown as purple circles. The green solid line indicates the first principal component, and the blue dashed line indicates the second principal component.*

Pictures of PCA: continued



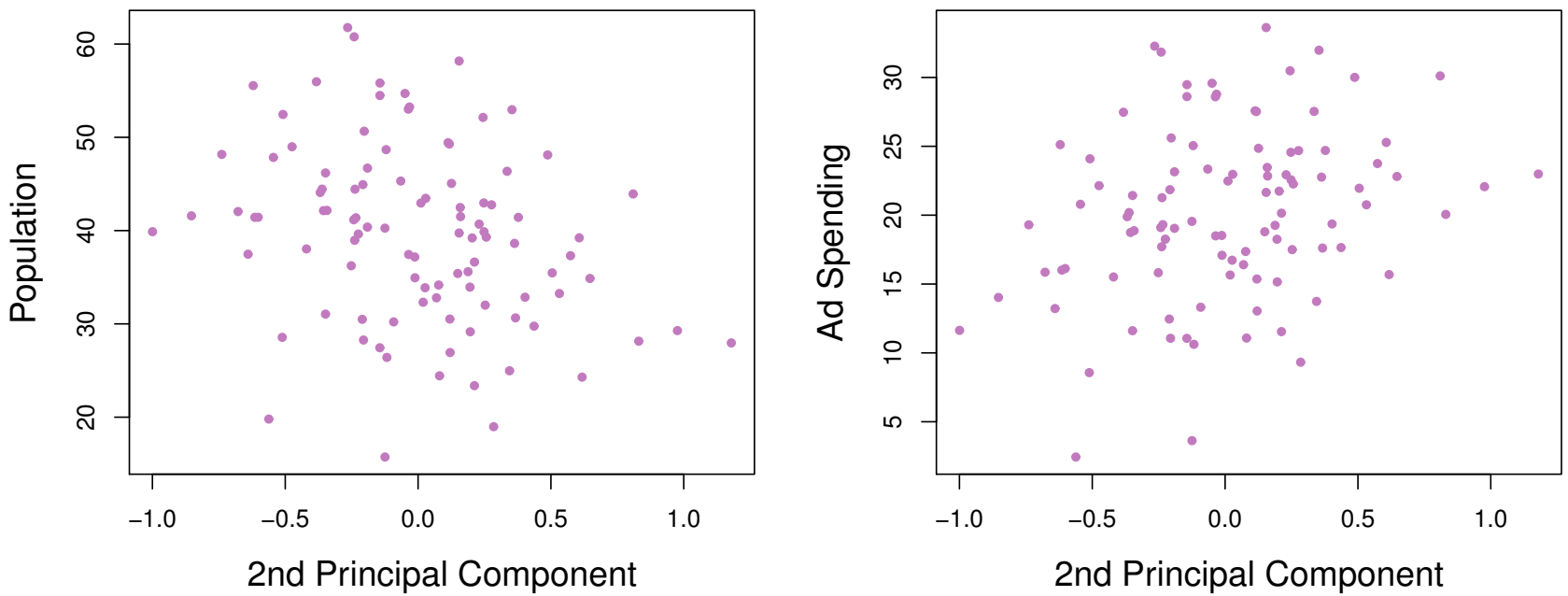
A subset of the advertising data. Left: *The first principal component, chosen to minimize the sum of the squared perpendicular distances to each point, is shown in green. These distances are represented using the black dashed line segments.* Right: *The left-hand panel has been rotated so that the first principal component lies on the x-axis.*

Pictures of PCA: continued



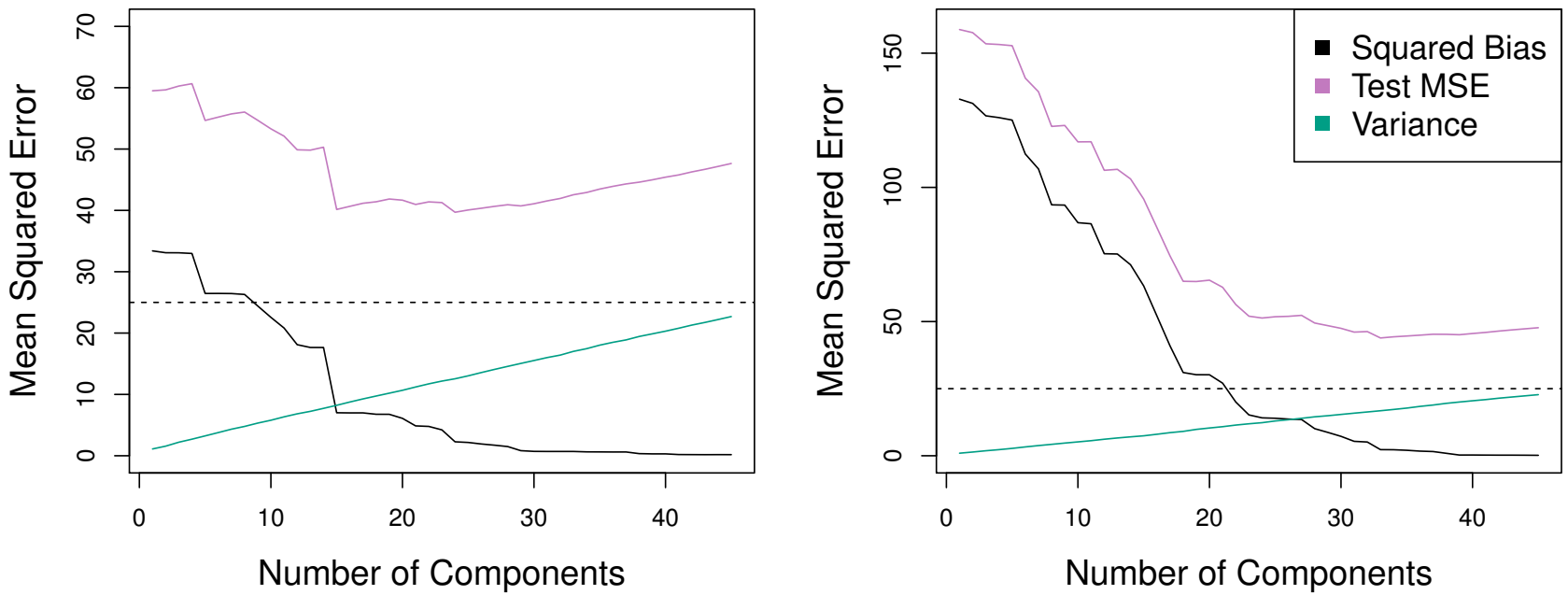
Plots of the first principal component scores z_{i1} *versus* pop *and* ad. *The relationships are strong.*

Pictures of PCA: continued



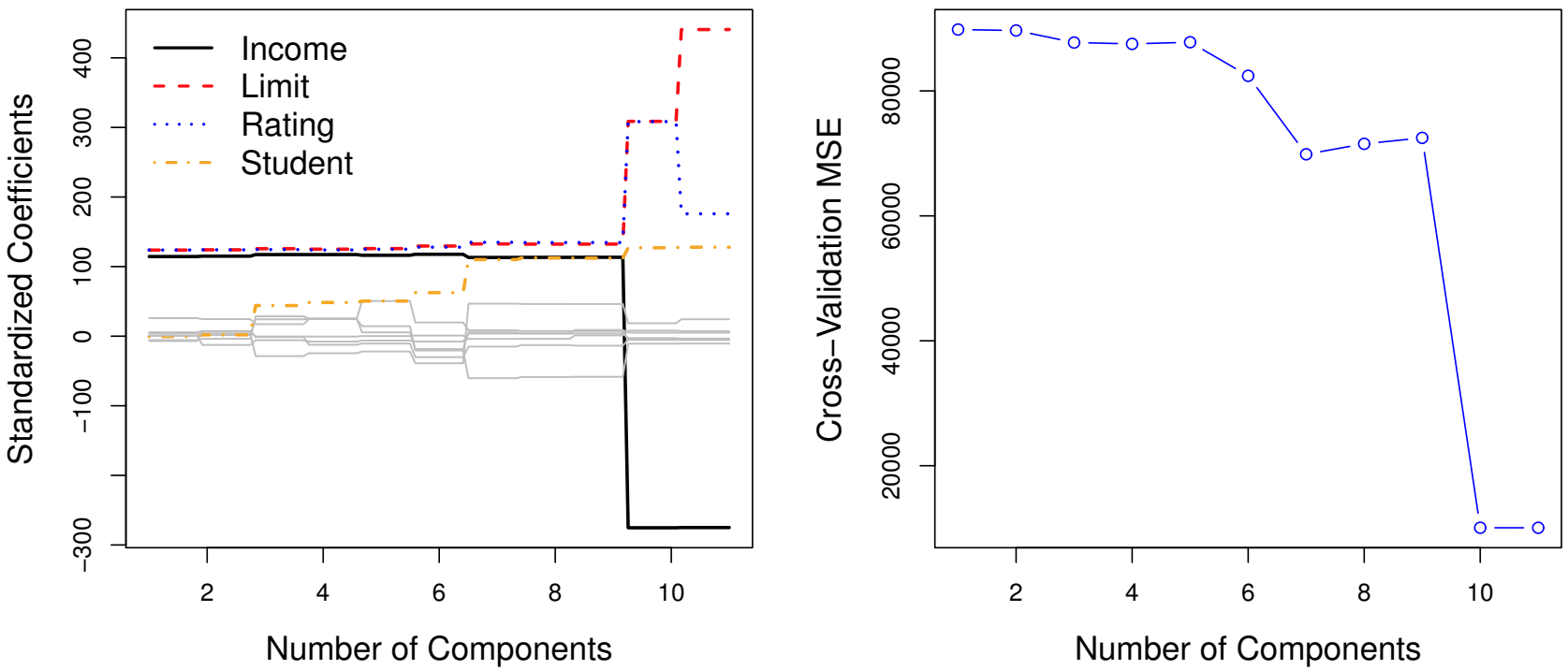
Plots of the second principal component scores z_{i2} versus `pop` *and* `ad`*. The relationships are weak.*

Application to Principal Components Regression



PCR was applied to two simulated data sets. The black, green, and purple lines correspond to squared bias, variance, and test mean squared error, respectively. Left: *Simulated data from slide 32.* Right: *Simulated data from slide 39.*

Choosing the number of directions M



Left: *PCR standardized coefficient estimates on the* `Credit` *data set for different values of* M. Right: *The* 10*-fold cross validation MSE obtained using PCR, as a function of* M.

Partial Least Squares

- PCR identifies linear combinations, or *directions*, that best represent the predictors $X_1, \ldots, X_p$.
- These directions are identified in an *unsupervised* way, since the response Y is not used to help determine the principal component directions.
- That is, the response does not *supervise* the identification of the principal components.
- Consequently, PCR suffers from a potentially serious drawback: there is no guarantee that the directions that best explain the predictors will also be the best directions to use for predicting the response.

Partial Least Squares: continued

- Like PCR, PLS is a dimension reduction method, which first identifies a new set of features $Z_1, \ldots, Z_M$ that are linear combinations of the original features, and then fits a linear model via OLS using these M new features.
- But unlike PCR, PLS identifies these new features in a supervised way – that is, 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*.
- Roughly speaking, the PLS approach attempts to find directions that help explain both the response and the predictors.

Details of Partial Least Squares

- After standardizing the p predictors, PLS computes the first direction Z_1 by setting each ϕ_{1j} in (1) equal to the coefficient from the simple linear regression of Y onto X_j.
- One can show that this coefficient is proportional to the correlation between Y and X_j.
- Hence, in computing $Z_1 = \sum_{j=1}^{p} \phi_{1j} X_j$, PLS places the highest weight on the variables that are most strongly related to the response.
- Subsequent directions are found by taking residuals and then repeating the above prescription.

Summary

- Model selection methods are an essential tool for data analysis, especially for big datasets involving many predictors.
- Research into methods that give *sparsity*, such as the *lasso* is an especially hot area.
- Later, we will return to sparsity in more detail, and will describe related approaches such as the *elastic net*.