Linear Model Selection and Regularization

- Recall the linear model

$$Y = \beta_0 + \beta_1 X_1 + \cdots + \beta_p X_p + \epsilon.$$

- In the lectures that follow, we consider some approaches for extending the linear model framework. In the lectures covering Chapter 7 of the text, we generalize the linear model in order to accommodate *non-linear*, but still *additive*, relationships.
- In the lectures covering Chapter 8 we consider even more general *non-linear* models.

In praise of linear models!

- Despite its simplicity, the linear model has distinct advantages in terms of its *interpretability* and often shows good *predictive performance*.
- Hence we discuss in this lecture some ways in which the simple linear model can be improved, by replacing ordinary least squares fitting with some alternative fitting procedures.

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.

Choosing the Optimal Model

- The model containing all of the predictors will always have the smallest RSS and the largest R^2, since these quantities are related to the training error.
- We wish to choose a model with low test error, not a model with low training error. Recall that training error is usually a poor estimate of test error.
- Therefore, RSS and R^2 are not suitable for selecting the best model among a collection of models with different numbers of predictors.

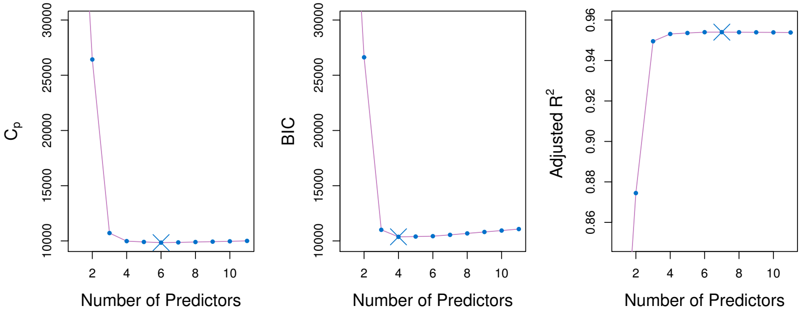
Estimating test error: two approaches

- 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.
- The next figure displays C_p, BIC, and adjusted R^2 for the best model of each size produced by best subset selection on the `Credit` data set.

Credit data example



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.

- In the case of the linear model with Gaussian errors, maximum likelihood and least squares are the same thing, and C_p and AIC are equivalent. *Prove this.*

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.
- Notice that BIC replaces the $2d\hat{\sigma}^2$ used by C_p with a $\log(n)d\hat{\sigma}^2$ term, where n is the number of observations.
- 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. See Figure on slide 19.

Adjusted R^2

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

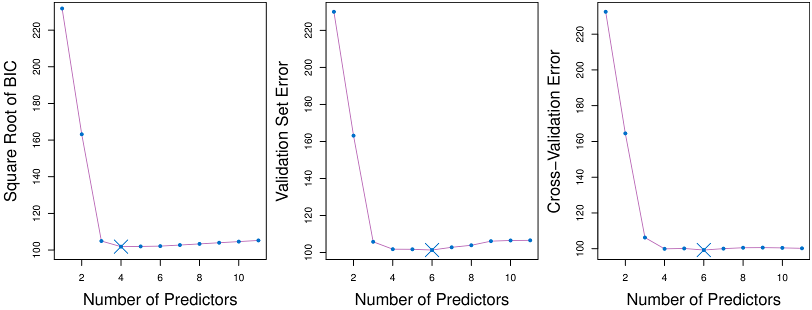
$$\text{Adjusted } R^2 = 1 - \frac{\text{RSS}/(n-d-1)}{\text{TSS}/(n-1)}.$$

  where TSS is the total sum of squares.
- Unlike C_p, AIC, and BIC, for which a *small* value indicates a model with a low test error, a *large* value of adjusted R^2 indicates a model with a small test error.
- Maximizing the adjusted R^2 is equivalent to minimizing $\frac{\text{RSS}}{n-d-1}$. While RSS always decreases as the number of variables in the model increases, $\frac{\text{RSS}}{n-d-1}$ may increase or decrease, due to the presence of d in the denominator.
- Unlike the R^2 statistic, the adjusted R^2 statistic *pays a price* for the inclusion of unnecessary variables in the model. See Figure on slide 19.

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*.
- It can also be used in a wider range of model selection tasks, even in cases where it is hard to pinpoint the model degrees of freedom (e.g. the number of predictors in the model) or hard to estimate the error variance σ^2.

Credit data example



Details of Previous Figure

- The validation errors were calculated by randomly selecting three-quarters of the observations as the training set, and the remainder as the validation set.
- The cross-validation errors were computed using $k = 10$ folds. In this case, the validation and cross-validation methods both result in a six-variable model.
- However, all three approaches suggest that the four-, five-, and six-variable models are roughly equivalent in terms of their test errors.
- In this setting, we can select a model using the *one-standard-error rule*. We first calculate the standard error of the estimated test MSE for each model size, and then select the smallest model for which the estimated test error is within one standard error of the lowest point on the curve. *What is the rationale for this?*

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

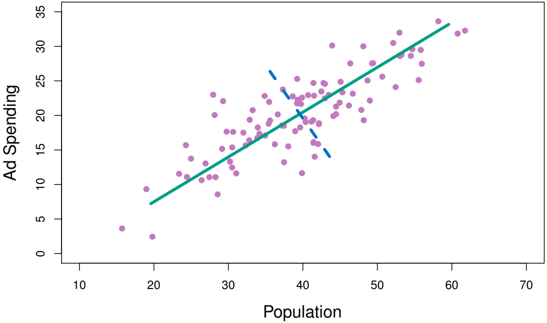
$$\beta_j = \sum_{m=1}^{M} \theta_m \phi_{mj}. \tag{3}$$

- 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

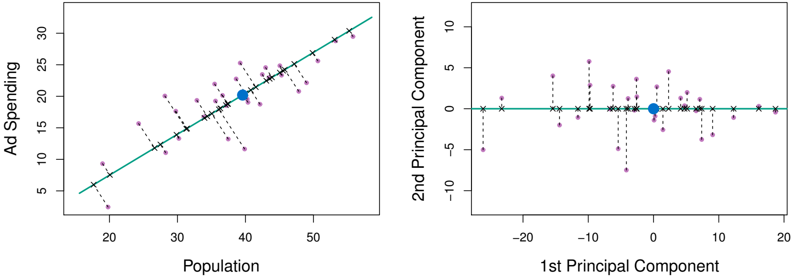
- Here we apply principal components analysis (PCA) (discussed in Chapter 10 of the text) to define the linear combinations of the predictors, for use in our regression.
- The first principal component is that (normalized) linear combination of the variables with the largest variance.
- The second principal 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



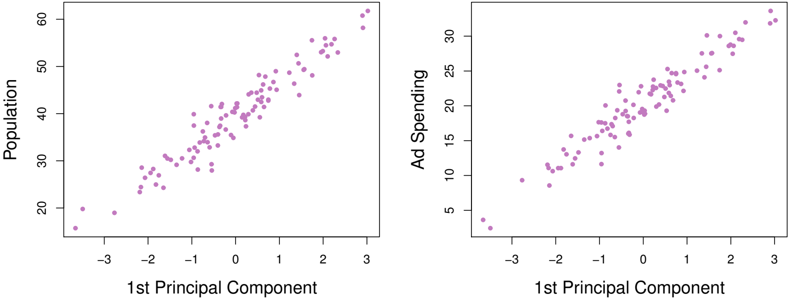
The population size (`pop`) and ad spending (`ad`) for 100 *different cities are shown as purple circles. The green solid line indicates the first principal component, and the blue dashed line indicates the second principal component.*

Pictures of PCA: continued



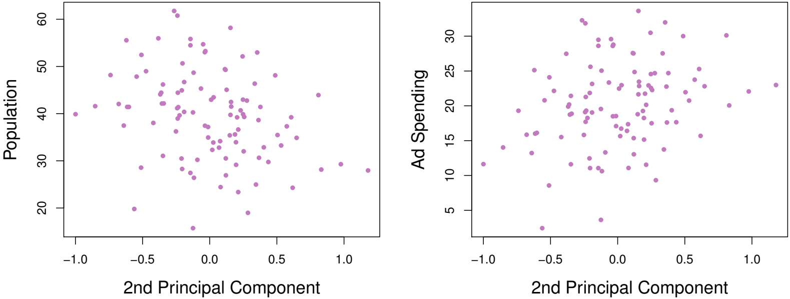
A subset of the advertising data. Left: *The first principal component, chosen to minimize the sum of the squared perpendicular distances to each point, is shown in green. These distances are represented using the black dashed line segments.* Right: *The left-hand panel has been rotated so that the first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

Pictures of PCA: continued



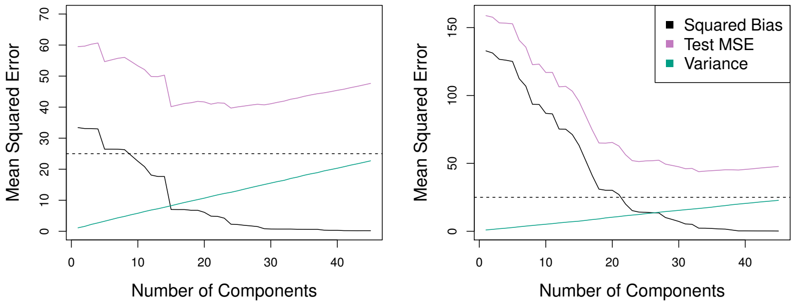
Plots of the first principal component scores z_{i1} versus `pop` *and* `ad`*. The relationships are strong.*

Pictures of PCA: continued



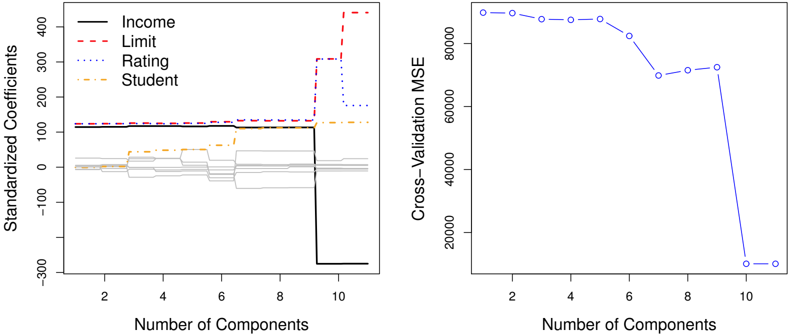
Plots of the second principal component scores z_{i2} versus `pop` *and* `ad`*. The relationships are weak.*

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*.