Chapter 6
Dimension Reduction Methods

Following slides are from the Introduction to Statistical Learning MOOC at Stanford

https://class.stanford.edu/courses/HumanitiesandScience/StatLearning/Winter2015/about

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.

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

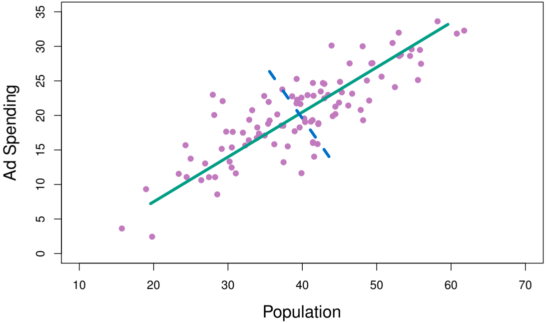
$$\beta_j = \sum_{m=1}^{M} \theta_m \phi_{mj}. \qquad (3)$$

- 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

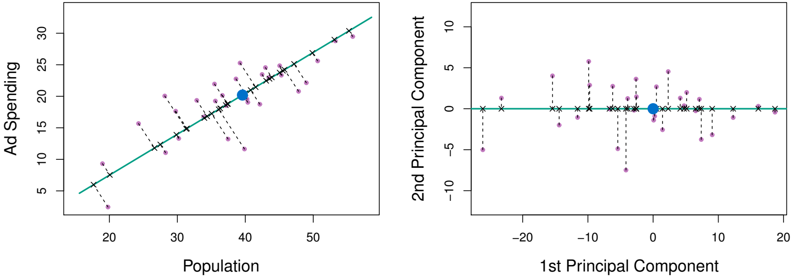
- Here we apply principal components analysis (PCA) (discussed in Chapter 10 of the text) to define the linear combinations of the predictors, for use in our regression.
- The first principal component is that (normalized) linear combination of the variables with the largest variance.
- The second principal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



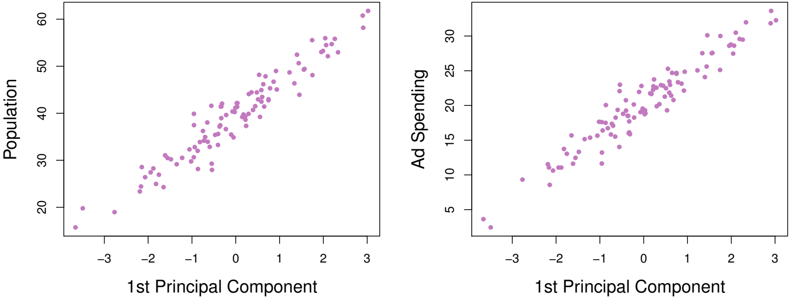
The population size (`pop`) and ad spending (`ad`) for 100 *different cities are shown as purple circles. The green solid line indicates the first principal component, and the blue dashed line indicates the second principal component.*

Pictures of PCA: continued



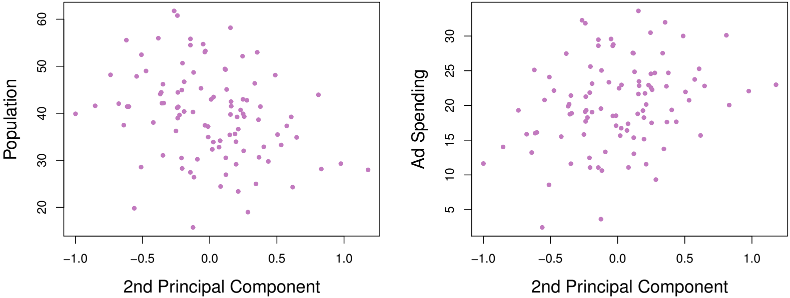
A subset of the advertising data. Left: *The first principal component, chosen to minimize the sum of the squared perpendicular distances to each point, is shown in green. These distances are represented using the black dashed line segments.* Right: *The left-hand panel has been rotated so that the first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

Pictures of PCA: continued



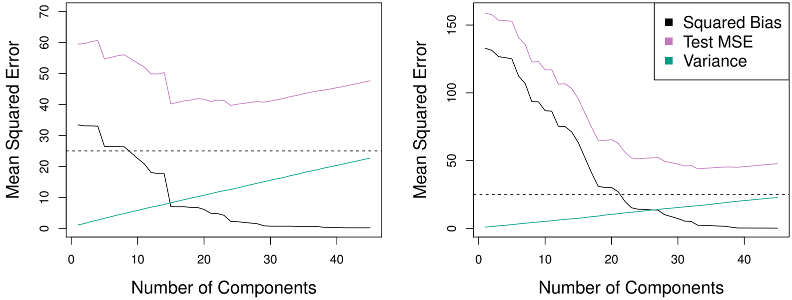
Plots of the first principal component scores z_{i1} *versus* `pop` *and* `ad`*. The relationships are strong.*

Pictures of PCA: continued



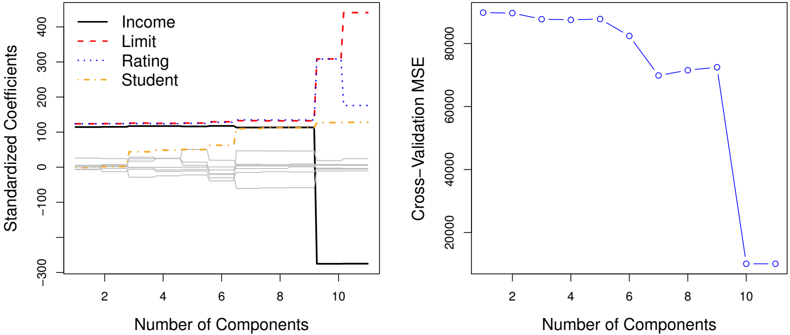
Plots of the second principal component scores z_{i2} *versus* `pop` *and* `ad`*. The relationships are weak.*

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*.

week13: Dimension Reduction

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Principal Components Regression

First, load the libraries and the data.

```
library(pls)
```

```
##
## Attaching package: 'pls'
##
## The following object is masked from 'package:stats':
##
##     loadings
```

```
library(ISLR)
data(Hitters)
Hitters <- na.omit(Hitters)
```

Set a seed and fit the PCR

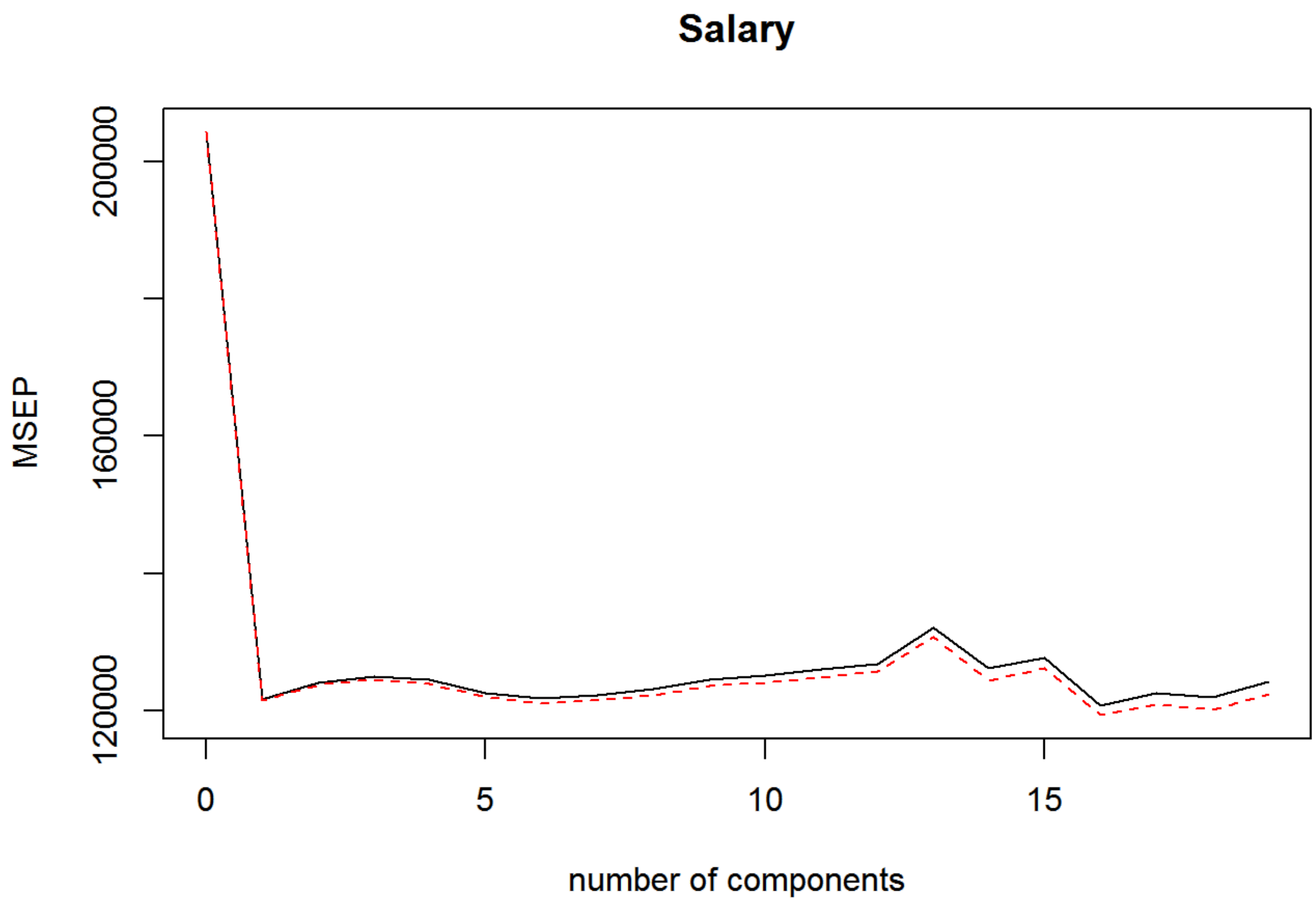
```
set.seed(2)
pcr.fit <- pcr(Salary~., data=Hitters, scale=TRUE, validation="CV")
```

Prediction Mean Squared Error Plot

```
summary(pcr.fit)
```

```
## Data:    X dimension: 263 19
##  Y dimension: 263 1
## Fit method: svdpc
## Number of components considered: 19
##
## VALIDATION: RMSEP
## Cross-validated using 10 random segments.
##        (Intercept)  1 comps  2 comps  3 comps  4 comps  5 comps  6 comps
## CV             452    348.9    352.2    353.5    352.8    350.1    349.1
## adjCV          452    348.7    351.8    352.9    352.1    349.3    348.0
##        7 comps  8 comps  9 comps  10 comps  11 comps  12 comps  13 comps
## CV       349.6    350.9    352.9     353.8     355.0     356.2     363.5
## adjCV    348.5    349.8    351.6     352.3     353.4     354.5     361.6
##        14 comps  15 comps  16 comps  17 comps  18 comps  19 comps
## CV        355.2     357.4     347.6     350.1     349.2     352.6
## adjCV     352.8     355.2     345.5     347.6     346.7     349.8
##
## TRAINING: % variance explained
##         1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps
## X         38.31    60.16    70.84    79.03    84.29    88.63    92.26
## Salary    40.63    41.58    42.17    43.22    44.90    46.48    46.69
##         8 comps  9 comps  10 comps  11 comps  12 comps  13 comps  14 comps
## X         94.96    96.28     97.26     97.98     98.65     99.15     99.47
## Salary    46.75    46.86     47.76     47.82     47.85     48.10     50.40
##         15 comps  16 comps  17 comps  18 comps  19 comps
## X          99.75     99.89     99.97     99.99    100.00
## Salary     50.55     53.01     53.85     54.61     54.61
```

```
validationplot(pcr.fit, val.type="MSEP")
```


Salary
MSEP
120000
160000
200000
0
5
10
15
number of components