Statistics 452: Statistical Learning and Prediction

Chapter 6, Part 3: Dimension Reduction Methods

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Reduced Dimension Regression

- Transform predictors $X_1, \ldots, X_p$ to a lower-dimension set $Z_1, \ldots, Z_M$, for $M < p$.
  - The Z_m's are taken to be linear combinations of the X_j's:

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

- Fit a linear model to $Z_1, \ldots, Z_M$

$$Y = \theta_0 + \sum_{m=1}^{M} \theta_m Z_m + \epsilon.$$

Compare to the linear model

$$Y = \beta_0 + \sum_{j=1}^{p} \beta_m X_m + \epsilon.$$

  - Fewer regression coefficients ($M + 1 < p + 1$).

Lower Dimension, Constraint on β's

- As shown on pages 229,230 of the text, the lower-dimension model implies coefficients in the original model of the form

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

- Thus the p βs are constrained to be functions of M underlying θs.
  - Different form of constraints from those in ridge regression and the lasso (recall the second view of these as constrained maximization).
- Introduction of a constraint is another way to view the bias/variance trade-off:
  - constraints mean lower variance, but higher bias on parameter estimates, which translates into lower variance/higher bias for predictions.

Methods for Dimension Reduction

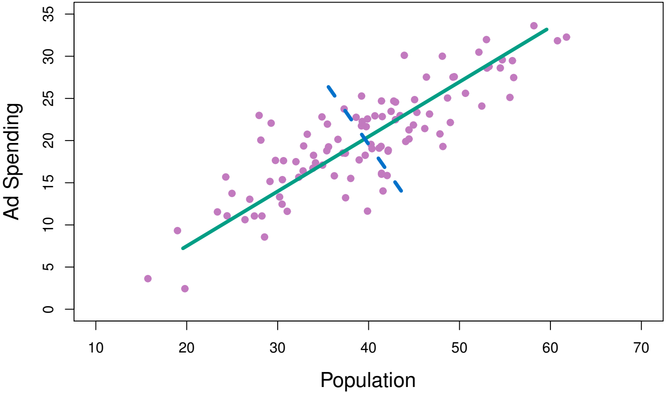
- Principal components – low-rank approximation of the X data matrix
- Partial least squares – explain X by latent variables

Principal Components Analysis (PCA)

- More details on PCA to follow in Chapter 10.
- First centre each variable by subtracting its mean.
- Then, think of principal components (PCs) as new coordinates for the data vectors.
  - The first PC is the direction of greatest variation,
  - The second PC is the direction of second-greatest variation, orthogonal to the first,
  - And so on.

PCs for Advertising Data

- Text Figure 6.14: The green line is the first PC, the blue line the second.



PCs as Linear Combinations of X's

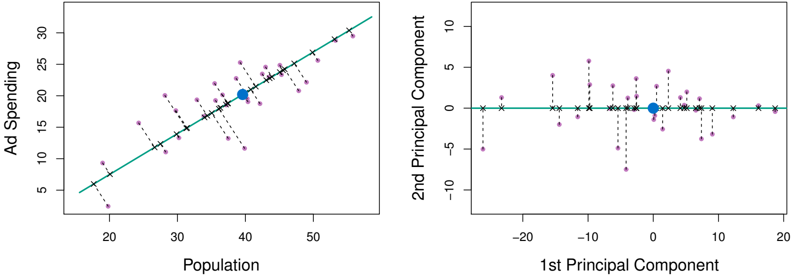
- We won't go into the details of how the linear combinations are derived.
- In the advertising example, the first PC is

$$Z_1 = 0.838X_1 + 0.544X_2$$

  where X_1 is population centred by its mean and X_2 is advertising expenditure centred by its mean.
- The coefficients of the linear combination, $\phi_{11} = 0.838$ and $\phi_{12} = 0.544$, are called the first principal component *loadings*.

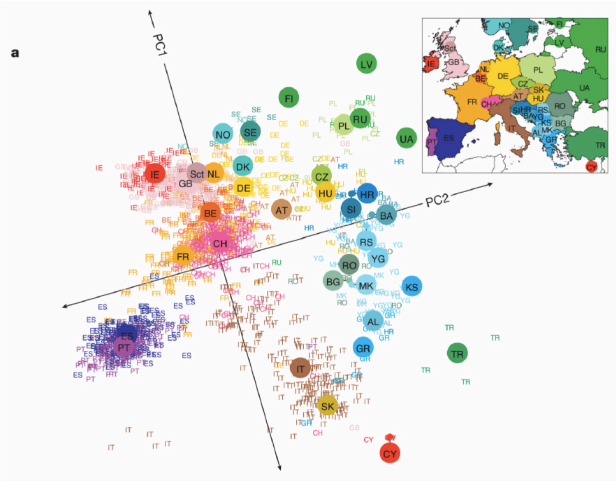
Principal Component Scores

- Projecting each point onto the PCs gives the PC scores.
  - Projecting a data vector onto a line means finding the point on the line closest to the vector.
- Text Figure 6.15: Black x's are the first PC score for each observation, distance of each purple dot from the green line is the second PC score.



High-Dimensional Example: Genes Reflect Geography

- First 2 PCs from 197,146 genetic markers on 1,387 European individuals (Novembre *et al.* 2008)



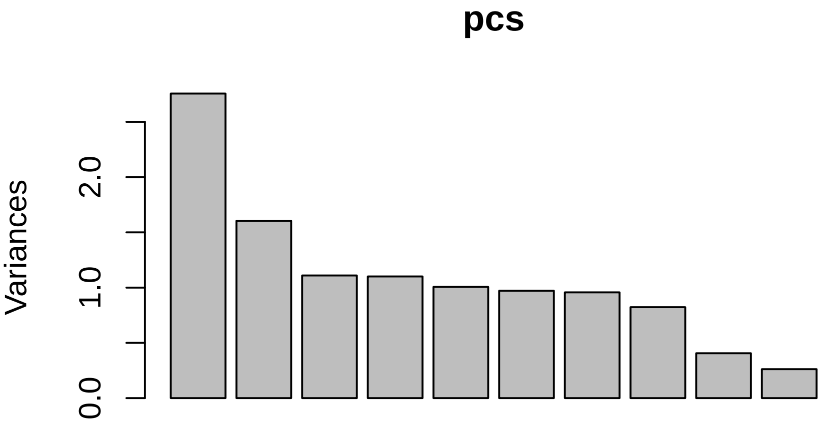
PCs and PC Scores for the Credit Data

```r
uu <- url("http://faculty.marshall.usc.edu/gareth-james/ISL/Credit.csv")
Credit <- read.csv(uu,row.names=1)
head(Credit,n=3)
```

```
##    Income Limit Rating Cards Age Education Gender Student Married
## 1  14.891  3606    283     2  34        11   Male      No     Yes
## 2 106.025  6645    483     3  82        15 Female     Yes     Yes
## 3 104.593  7075    514     4  71        11   Male      No      No
##   Ethnicity Balance
## 1 Caucasian     333
## 2     Asian     903
## 3     Asian     580
```

```r
X <- model.matrix(Balance ~ ., data=Credit)
X <- X[,-1] # Remove intercept
X <- scale(X) # Centre and scale
pcs <- prcomp(X)
```

```r
plot(pcs)
```

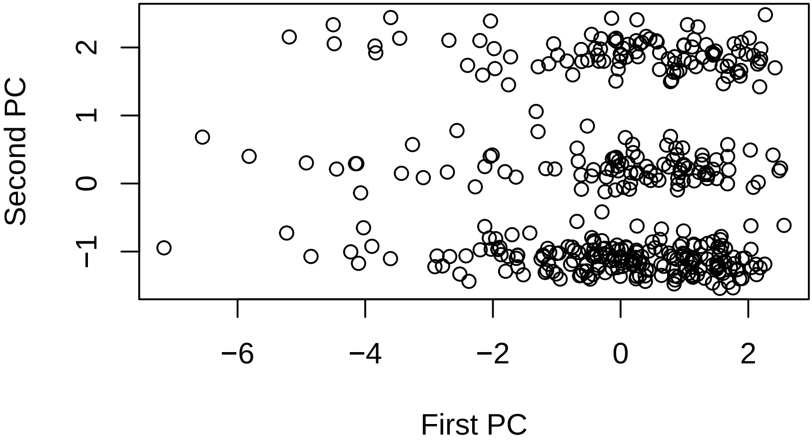


Loadings for First Two PCs

```
pcs$rotation[,1:2]
```

```
##                           PC1          PC2
## Income            -0.542206953  0.029036783
## Limit             -0.586332930  0.017502630
## Rating            -0.586751867  0.014971105
## Cards             -0.019086978 -0.008549632
## Age               -0.122783390 -0.071116603
## Education          0.026797471  0.096557225
## GenderMale         0.002519860 -0.052811098
## StudentYes         0.002276904  0.125422970
## MarriedYes        -0.026218561  0.094278214
## EthnicityAsian     0.032769895  0.696759512
## EthnicityCaucasian -0.004070799 -0.686505857
```

```
plot(pcs$x[,1],pcs$x[,2],xlab="First PC",ylab="Second PC")
```



Principal Components Regression (PCR)

- Take $Z_1, \ldots, Z_M$ to be the first M PC scores.
  - M can be chosen by cross-validation to minimize estimated test set error.
- The idea is that a handful of PCs might explain the variation in X **and** the relationship between X and Y.

PCR on the Credit Data

```r
library(pls) # install.packages("pls")
set.seed(123)
cfit <- pcr(Balance ~ ., data=Credit,scale=TRUE,
            validation="CV")
```

Summary

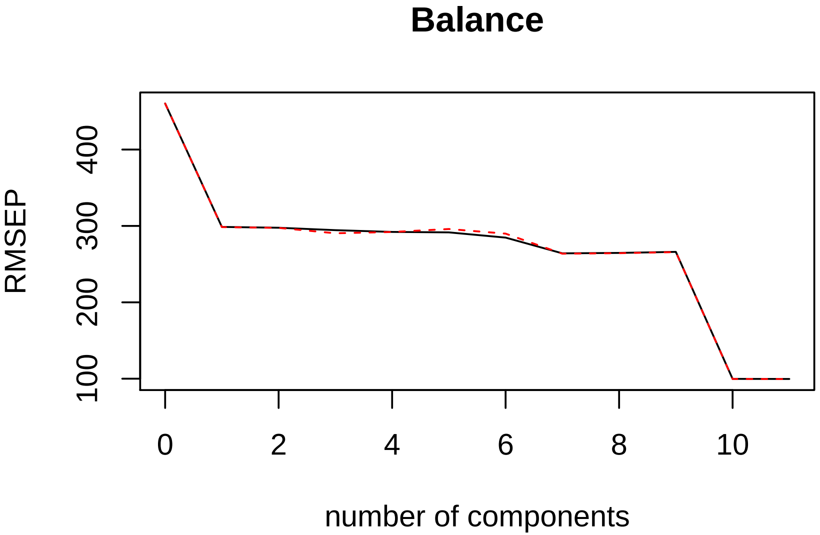
```r
summary(cfit)
```

```
## Data:    X dimension: 400 11
##  Y dimension: 400 1
## Fit method: svdpc
## Number of components considered: 11
##
## VALIDATION: RMSEP
## Cross-validated using 10 random segments.
##        (Intercept)  1 comps  2 comps  3 comps  4 comps  5 comps  6 comps
## CV           460.3    298.7    297.6    294.5    292.2    291.6    284.7
## adjCV        460.3    298.5    297.5    290.4    292.1    296.0    289.9
##        7 comps  8 comps  9 comps  10 comps  11 comps
## CV       264.1    264.7    266.0     99.75     99.65
## adjCV    263.6    264.3    265.7     99.64     99.53
##
## TRAINING: % variance explained
##          1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps
## X          25.05    39.64    49.73    59.74    68.89    77.73    86.43
## Balance    58.07    58.37    60.78    60.90    61.46    63.11    68.70
##          8 comps  9 comps  10 comps  11 comps
## X          93.91    97.60     99.98    100.00
## Balance    68.71    68.72     95.47     95.51
```

- Note: `RMSEP` is root mean squared error of prediction, the square root of the MSE.

Plot the Root MSE of Prediction

```r
validationplot(cfit)
```



Extract $\hat{\beta}$'s

- These are the estimates of the coefficients of the X's,

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

```r
coef(cfit,ncomp=10)
```

```
## , , 10 comps
##
##                          Balance
## Income               -275.334437
## Limit                 308.685448
## Rating                308.331638
## Cards                  18.588390
## Age                   -10.700222
## Education              -2.758126
## GenderMale              5.354857
## StudentYes            127.056873
## MarriedYes             -5.131238
## EthnicityAsian          8.004166
## EthnicityCaucasian      5.143306
```

Partial Least Squares (PLS) versus PCR

- Statistical learning methods that use the response are said to be "supervised", while those that do not are "unsupervised".
- PCR does unsupervised selection of the transformed features $Z_1, \ldots, Z_M$.
- By contrast, PLS is supervised (sketch of details below).
- No clear winner between PCR and PLS.
  - Supervised dimension reduction may reduce bias by identifying features that are truly related to Y.
  - However, supervising "... has the potential to increase variance," (text, page 238)

PLS Directions

- The loadings for the first PLS direction, Z_1 are the coefficients from the simple linear regression of Y on each X_j.
- The loadings for the second PLS direction are coefficients from the simple linear regression of the *adjusted* variable $Y - \hat{Y}$ on the adjusted $X_j - \hat{X}_j$, where $\hat{Y}$ and $\hat{X}_j$ are from regressions on Z_1.
  - The residuals are the information in the variables not explained by Z_1.
- The loadings for the third PLS direction are coefficients from the simple linear regression of the adjusted variable $Y - \hat{Y}$ on the adjusted $X_j - \hat{X}_j$, where $\hat{Y}$ and $\hat{X}_j$ are from regressions on Z_1 **and** Z_2.
  - The residuals are the information in the variables not explained by Z_1 and Z_2.
- And so on.

PLS on the Credit Data

```r
cfit <- plsr(Balance ~ ., data=Credit,scale=TRUE,
             validation="CV")
```

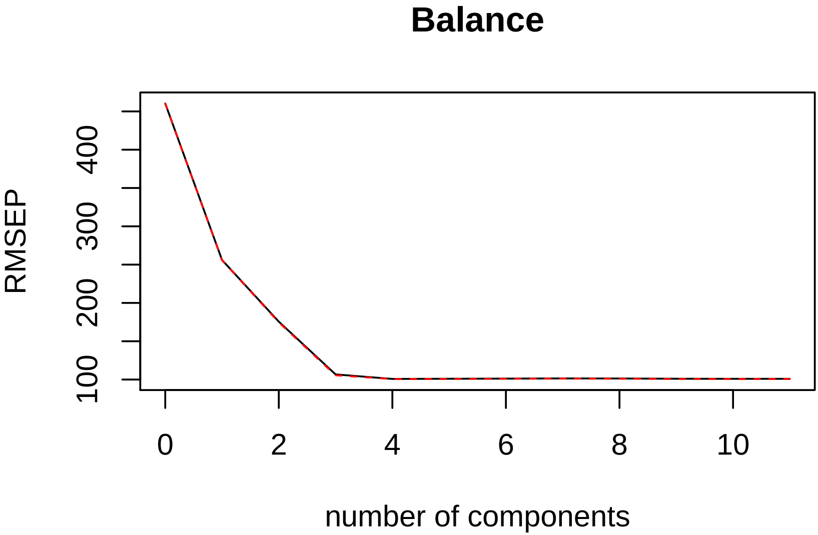
Summary

```r
summary(cfit)
```

```
## Data:    X dimension: 400 11
##  Y dimension: 400 1
## Fit method: kernelpls
## Number of components considered: 11
##
## VALIDATION: RMSEP
## Cross-validated using 10 random segments.
##        (Intercept)  1 comps  2 comps  3 comps  4 comps  5 comps  6 comps
## CV           460.3    256.1    175.6    106.7    100.8    101.0    101.2
## adjCV        460.3    255.8    174.7    105.6    100.6    100.8    101.0
##        7 comps  8 comps  9 comps  10 comps  11 comps
## CV       101.5    101.4    101.0     101.0     101.0
## adjCV    101.2    101.1    100.8     100.8     100.8
##
## TRAINING: % variance explained
##          1 comps  2 comps  3 comps  4 comps  5 comps  6 comps  7 comps
## X          24.58    32.53    37.84    50.55    60.80    65.92    73.20
## Balance    69.67    86.53    94.95    95.46    95.48    95.48    95.48
##          8 comps  9 comps  10 comps  11 comps
## X          76.45    81.33     90.76    100.00
## Balance    95.50    95.51     95.51     95.51
```

Plot the Root MSE of Prediction

```r
validationplot(cfit)
```



Extract $\hat{\beta}$'s

```r
coef(cfit,ncomp=4)
```

```
## , , 4 comps
##
##                        Balance
## Income             -274.942446
## Limit               310.143749
## Rating              306.656366
## Cards                22.106900
## Age                 -11.915766
## Education            -4.175268
## GenderMale            7.683003
## StudentYes          125.944486
## MarriedYes           -3.676939
## EthnicityAsian       10.377071
## EthnicityCaucasian    5.060771
```