

데이터분석방법론(1)

# Analysis of Collinear Data

통계·데이터과학과장영재교수





- Collinearity
- 2 Introduction to PCA
- 3 Example of PCA



01

### Collinearity



#### 1. Collinearity

- A perfect linear relationship among the regressors in a linear model implies that the least-squares coefficients are not uniquely defined.
- A strong, but less than perfect, linear relationship among the X's causes the leastsquares coefficients to be unstable:
  - Coefficient standard errors are large, reflecting the imprecision of estimation of the  $\beta$ 's; consequently confidence intervals for the  $\beta$ 's are broad.

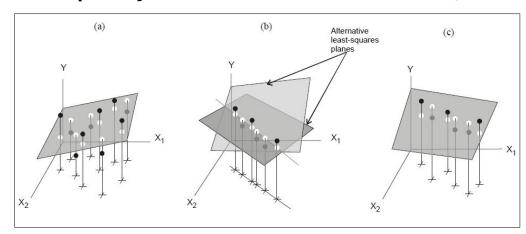


Figure 1. (a) Low correlation between  $X_1$  and  $X_2$  – regression plane well supported; (b) perfect correlation beten  $X_1$  and  $X_2$ , showing two of the infinite number of least-squares planes; (c) high but not perfect correlation between  $X_1$  and  $X_2$  – regression plane not well supported.

#### 2. Detecting Collinearity

A perfect linear relationship among the X's

$$c_1 X_{i1} + c_2 X_{i2} + \cdots + c_k X_{ik} = c_0$$

where  $c_1, c_2, ..., c_k$  are not all 0:

- When some predictors are linear combinations of others, then X'X
  is singular, and we have (exact) collinearity.
- The least-squares normal equations do not have a unique solution.
- The sampling variances of the regression coefficients are infinite.

#### 2. Detecting Collinearity

- A less than perfect collinearity:
  - The sampling variance of the least-squares slope coefficient  $B_i$  is

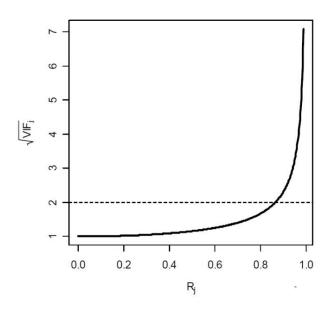
$$V(B_j) = \frac{1}{1 - R_j^2} \times \frac{\sigma_{\varepsilon}^2}{(n - 1)S_j^2}$$

#### where

- $R_j^2$  is the squared multiple correlation for the regression of  $X_j$  on the other X's, and  $S_j^2 = \sum (X_{ij} \bar{X}_j)^2/(n-1)$  is the variance of  $X_j$ .
- The term  $1/(1 R_i^2)$ : the variance-inflation factor (VIF)
  - : the impact of collinearity on the precision of  $B_i$ .
- The width of the confidence interval for  $\beta_i$ 
  - : proportional to the square root of the VIF
- Collinearity leads to imprecise estimate of  $\beta$ .
- If  $VIF_j > 5\sim 10$ , we conclude that there is a collinearity.

#### 2. Detecting Collinearity

• Figure 2 shows that the precision of estimation experiences a significant degradation when Rj approaches .9.



```
> rj= seq(0,1, length=100)
> vifj = 1/(1-rj^2)
> rvifj=sqrt(vifj)
> plot(rj, rvifj, ylab="sqrt(vifj)", type="l")
> abline(h=2, lty=2)
```

Figure 2. The square root of the variance-inflation factor as a function of the multiple correlation for the regression of  $X_i$  on the other X's.

Data: Seat position, size and age of 38 drivers (Univ. of Michigan)

- > library(faraway)
- > data(seatpos)
- > seatpos[c(1:10),]

```
> seatpos[c(1:10),]
  Age Weight HtShoes
                                 Arm Thigh Leg hipcenter
                       Ht Seated
               187.2 184.9
                           95.2 36.1 45.3 41.3
                                                 -206.300
              167.5 165.5
   31
         175
                           83.8 32.9
                                       36.5 35.9
                                                 -178.210
   23
         100
              153.6 152.2
                           82.9 26.0
                                       36.6 31.0
                                                  -71.673
   19
         185
              190.3 187.4
                           97.3 37.4
                                       44.1 41.0
                                                 -257.720
   23
         159
               178.0 174.1
                           93.9 29.5
                                       40.1 36.9
                                                 -173.230
         170
              178.7 177.0
                          92.4 36.0
                                       43.2 37.4
                                                 -185.150
         137
              165.7 164.6
                          87.7 32.5 35.6 36.2
                                                -164.750
   28
         192
              185.3 182.7 96.9 35.8 39.9 43.1
                                                 -270.920
   23
              167.6 165.0
         150
                          91.4 29.4 35.5 33.4
                                                 -151.780
              161.2 158.7 85.2 26.6 31.0 32.8 -113.880
   29
         120
```

- > g = Im(hipcenter~., seatpos)
- > summary(g)

```
> g = lm(hipcenter~ ., seatpos)
> summary(g)
Call:
lm(formula = hipcenter ~ ., data = seatpos)
Residuals:
   Min
            10 Median
                                 Max
-73.827 -22.833 -3.678 25.017 62.337
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
                                       0.0138 *
(Intercept) 436.43213 166.57162
                               2.620
Age
            0.77572 0.57033 1.360
                                       0.1843
           0.02631 0.33097 0.080
                                      0.9372
Weight
           -2.69241 9.75304 -0.276
HtShoes
                                      0.7845
           0.60134 10.12987 0.059 0.9531
           0.53375 3.76189 0.142 0.8882
Seated
           -1.32807 3.90020 -0.341 0.7359
Arm
           -1.14312 2.66002 -0.430 0.6706
Thigh
           -6.43905 4.71386 -1.366 0.1824
Leg
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 37.72 on 29 degrees of freedom
Multiple R-squared: 0.6866,
                          Adjusted R-squared: 0.6001
F-statistic: 7.94 on 8 and 29 DF, (p-value: 1.306e-05)
```

p-value for the F-statistics is very small, but none of the individual predictors is significant. This models shows the signs of collinearity.

Take a look at the pairwise correlations.

#### > round(cor(seatpos),3)

```
> round(cor(seatpos),3)
            Age Weight HtShoes
                                                     Thigh
                        -0.079 -0.090 -0.170
                                              0.360
                                                                       0.205
Age
                                                                     -0.640
                                              0.698
Weight
           0.081 1.000
                         0.828
                                0.829
                                                                     -0.797
HtShoes
          -0.079 0.828
                         1.000
                                0.998
                                       0.930
                                              0.752
                                              0.752
                                                                     -0.799
          -0.090
                0.829
                         0.998
                                1.000
                                       0.928
                                0.928
                                       1.000
                                                                     -0.731
Seated
          -0.170 0.776
                         0.930
                                              0.625
                                                                     -0.585
          0.360 0.698
                                              1.000
Arm
                         0.752 0.752
                                       0.625
                                                                     -0.591
                         0.725
Thigh
          0.091 0.573
                                0.735 0.607
                                              0.671
                                                                     -0.787
          -0.042 0.784
                         0.908
                                0.910
                                       0.812
                                              0.754
hipcenter 0.205 -0.640 -0.797 -0.799 -0.731 -0.585 -0.591 -0.787
                                                                      1.000
```

: There are several large correlation between predictors.

Take a look at the pairwise correlations.

: Much VIF in HtShoes and Ht.

One cure for collinearity

Examine the full correlation matrix and consider just the correlations of the length variables.

> round(cor(x[,3:8]), 2)

```
> round(cor(x[,3:8]),2)
       HtShoes
                Ht Seated Arm Thigh Leg
          1.00 1.00 0.93 0.75 0.72 0.91
HtShoes
         1.00 1.00 0.93 0.75 0.73 0.91
Ht
Seated
         0.93 0.93 1.00 0.63 0.61 0.81
         0.75 0.75 0.63 1.00 0.67 0.75
Arm
Thigh
         0.72 0.73 0.61 0.67 1.00 0.65
          0.91 0.91
                     0.81 0.75 0.65 1.00
Leg
```

: These six variables are strongly correlated each other – any one of them might do a good job of representing the other.

```
> g2 = lm(hipcenter~Age+Weight+Ht, seatpos)
> summary(g2)
Call:
lm(formula = hipcenter ~ Age + Weight + Ht, data = seatpos)
Residuals:
   Min
            1Q Median
-91.526 -23.005 2.164 24.950 53.982
Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) 528.297729 135.312947 3.904 0.000426 ***
            0.519504 0.408039 1.273 0.211593
Age
            0.004271 0.311720 0.014 0.989149
Weight
            -4.211905 0.999056 -4.216 0.000174 ***
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
Residual standard error: 36.49 on 34 degrees of freedom
Multiple R-squared: 0.6562, Adjusted R-squared: 0.6258
F-statistic: 21.63 on 3 and 34 DF, p-value: 5.125e-08
```

- : The fit is very similar to the original one in terms of  $\mathbb{R}^2$ , but with much fewer predictors
- : To keep all variables, we can use ridge regression.

#### 4. Coping With Collinearity

- $\bullet$  When  $X_1$  and  $X_2$  are strongly collinear
  - The data contain little information about the impact of X1 on Y holding X2 constant, because there is little variation in X1 when X2 is fixed.
  - Of course, the same is true for  $X_2$  fixing  $X_1$ .
- Strategies for dealing with collinear data
- None magically extracts nonexistent information from the data.
- Rather, the research problem is redefined, often subtly and implicitly.
- Sometimes the redefinition is reasonable; usually it is not.
- The ideal solution to the problem of collinearity
  - To collect new data in such a manner that the problem is avoided, for example, by experimental manipulation of the X's
    - : This solution is rarely practical.

02

### Introduction to PCA



#### 1. The model

◆ The regression model is

$$Y = X\beta + \varepsilon$$
 (1)

- Y is an  $n \times 1$  vector of observations on the response variable,
- $X = (X_{(1)}, \dots, X_{(p)})$  is an  $n \times p$  matrix of n observations on p explanatory variables
- $\beta$  is a  $p \times 1$  vector
- Assumption :

$$E(\varepsilon) = 0, E(\varepsilon'\varepsilon) = \sigma^2 I$$

X and Y have been centered and scaled so that X'X and X'Y are matrices of correlation coefficients.

#### 2. Principal components

There exists a matrix, C, satisfying

$$C'(X'X)C = \Lambda$$
 and  $C'C = CC' = I$  (2)

- $\Lambda$  is a diagonal matrix with the ordered eigenvalues of X'X on the diagonal.
- The eigenvalues are denoted by  $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_p$ .
- The columns of C are the normalized eigenvectors corresponding to  $\lambda_1, \dots, \lambda_p$ .
- C may be used to calculate a new set of explanatory variables, namely C may be used to calculate a new set of explanatory variables, namely

$$(W_{(1)}, W_{(2)}, \dots, W_{(p)}) = W = XC = (W_{(1)}, \dots, W_{(p)})C$$
 (3)

That are linear functions of the original explanatory variables. The W's are referred to as principal components.

#### 3. The model in terms of principal components

◆ The regression model of Equation (1) can be restated in terms of the principal components as

$$Y = W\alpha + u \tag{4}$$

where W=XC and  $\alpha=C'\beta$ .

- $W'_{(i)}W_{(j)}=0$  for  $i\neq j$  and  $W'_{(i)}W_{(i)}=\lambda_i$ . The  $\lambda's$  may be viewed as sample variances of the principal components
- When  $\lambda_i = 0$ , an exact linear dependence exists among the explanatory variables, and when  $\lambda_i$  is small (approximately equal to zero) there is an approximate linear relationship among the explanatory variables.

# 03

## Example of PCA



#### 1. R Example of PCA

Data

에) heptathlon in R "HSAUR" Package.
Records of athletes in 1988 Seoul Olympics in hurdles(110m), highjump(high jump), shot(투포환), run200m(200m), longjump(long jump), javelin(창던지기), run800m(800m), score

#### 2. Descriptive statistics

```
> library(HSAUR)
> data(heptathlon)
> head(heptathlon)
                   hurdles highjump shot run200m longjump javelin run800m score
                                                            45.66 128.51 7291
Joyner-Kersee (USA)
                     12.69
                               1.86 15.80
                                           22.56
                                                     7.27
John (GDR)
                     12.85
                              1.80 16.23
                                           23.65
                                                     6.71
                                                            42.56 126.12
                                                                          6897
Behmer (GDR)
                     13.20
                              1.83 14.20
                                           23.10
                                                     6.68
                                                            44.54 124.20
                                                                          6858
Sablovskaite (URS)
                     13.61
                              1.80 15.23
                                           23.92
                                                     6.25
                                                            42.78 132.24
                                                                          6540
Choubenkova (URS)
                     13.51
                              1.74 14.76
                                           23.93
                                                     6.32
                                                            47.46 127.90
                                                                          6540
Schulz (GDR)
                     13.75
                               1.83 13.50
                                           24.65
                                                     6.33
                                                            42.82 125.79 6411
> summary (heptathlon)
   hurdles
                   highjump
                                     shot
                                                  run200m
                                                                  longjump
       :12.69
                                      :10.00
                                                      :22.56
                                                               Min. :4.880
                Min.
                       :1.500
                                               Min.
 Min.
                                Min.
                                                              1st Qu.:6.050
 1st Qu.:13.47
                1st Qu.:1.770
                               1st Qu.:12.32
                                               1st Qu.:23.92
 Median :13.75
                Median :1.800
                               Median :12.88
                                               Median :24.83
                                                              Median :6.250
 Mean :13.84
                Mean :1.782
                               Mean :13.12
                                                    :24.65
                                               Mean
                                                              Mean :6.152
                                                              3rd Qu.:6.370
 3rd Qu.:14.07
                3rd Qu.:1.830
                               3rd Qu.:14.20
                                               3rd Qu.:25.23
 Max.
      :16.42
                Max.
                       :1.860
                                Max.
                                      :16.23
                                               Max.
                                                      :26.61
                                                               Max. :7.270
                   run800m
   javelin
                                   score
       :35.68
                       :124.2
                                      :4566
 Min.
                Min.
                                Min.
 1st Qu.:39.06
                1st Ou.:132.2
                               1st Qu.:5746
                Median :134.7
 Median:40.28
                               Median:6137
      :41.48
                Mean :136.1
                               Mean :6091
 Mean
 3rd Qu.:44.54
                3rd Qu.:138.5
                               3rd Qu.:6351
                Max. :163.4
                               Max. :7291
 Max. :47.50
>
```

#### 3. Need to transform the data

#### Transformation

For hurdles, run200m, and run800m, transform the data because the smaller the value, the better the score.

```
> heptathlon$hurdles = max(heptathlon$hurdles) - heptathlon$hurdles
> heptathlon$run200m = max(heptathlon$run200m) - heptathlon$run200m
> heptathlon$run800m = max(heptathlon$run800m) - heptathlon$run800m
> heptathlon
                    hurdles highjump shot run200m longjump javelin run800m score
                       3.73
                                1.86 15.80
                                              4.05
                                                       7.27
                                                              45.66
                                                                      34.92
Joyner-Kersee (USA)
                                                                      37.31 6897
John (GDR)
                       3.57
                                1.80 16.23
                                              2.96
                                                       6.71
                                                              42.56
                                1.83 14.20
Behmer (GDR)
                       3.22
                                              3.51
                                                       6.68
                                                              44.54
                                                                      39.23
                                                                             6858
                                1.80 15.23
                                              2.69
                                                       6.25
                                                              42.78
                                                                      31.19
Sablovskaite (URS)
                       2.81
Choubenkova (URS)
                       2.91
                                1.74 14.76
                                              2.68
                                                       6.32
                                                              47.46
                                                                      35.53
                                                                             6540
                       2.67
                                1.83 13.50
                                              1.96
                                                              42.82
                                                                      37.64
Schulz (GDR)
                                                       6.33
                                                                             6411
                      3.04
                                1.80 12.88
                                              3.02
                                                       6.37
                                                              40.28
                                                                      30.89
Fleming (AUS)
                                              2.13
Greiner (USA)
                       2.87
                                1.80 14.13
                                                       6.47
                                                              38.00
                                                                      29.78
                       2.79
                                1.83 14.28
                                              1.75
                                                              42.20
                                                                      27.38
                                                                             6252
Lajbnerova (CZE)
                                                       6.11
Bouraga (URS)
                       3.17
                                1.77 12.62
                                              3.02
                                                       6.28
                                                              39.06
                                                                      28.69
                       2.67
                                1.86 13.01
                                              1.58
                                                              37.86
                                                                      31.94
Wijnsma (HOL)
                                                       6.34
Dimitrova (BUL)
                       3.18
                                1.80 12.88
                                              3.02
                                                              40.28
                                                                      30.89
                                                                             6171
Scheider (SWI)
                       2.57
                                1.86 11.58
                                              1.74
                                                       6.05
                                                              47.50
                                                                      28.50
                                                                             6137
Braun (FRG)
                       2.71
                                1.83 13.16
                                              1.83
                                                       6.12
                                                              44.58
                                                                      20.61 6109
                                1.80 12.32
                                                                      26.37
Ruotsalainen (FIN)
                       2.49
                                1.86 14.21
                                              1.61
                                                       6.40
                                                              38.60
                                                                      16.76
Yuping (CHN)
                       2.95
                                1.80 12.75
                                              1.14
                                                                      24.95
Hagger (GB)
                                                       6.34
                                                              35.76
                                                                             5975
                       2.35
                                1.83 12.69
                                              1.78
                                                              44.34
                                                                      17.00
                                                                             5972
Brown (USA)
Mulliner (GB)
                       2.03
                                1.71 12.68
                                              1.69
                                                       6.10
                                                              37.76
                                                                      25.41
                       2.38
                                1.77 11.81
                                              1.00
                                                       5.99
                                                              35.68
                                                                      29.53
                                                                             5734
Hautenauve (BEL)
                       2.11
                                1.77 11.66
                                              0.92
                                                              39.48
                                                                             5686
Kytola (FIN)
                                                       5.75
                                                                      30.08
Geremias (BRA)
                       2.19
                                1.71 12.95
                                              1.11
                                                       5.50
                                                              39.64
                                                                      19.41
```

#### 4. Principal Component Analysis

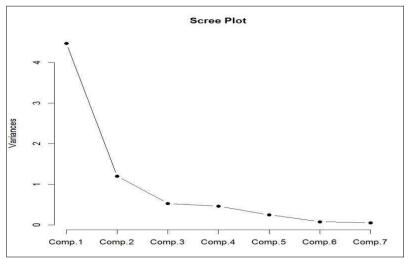
```
> library(stats)
> hep.data = heptathlon[,-8]
> heptathlon.pca = princomp(hep.data, cor=T, scores=T)
> names (heptathlon.pca)
[1] "sdev"
            "loadings" "center" "scale"
                                              "n.obs"
> heptathlon.pca
Call:
princomp(x = hep.data, cor = T, scores = T)
Standard deviations:
                     Comp.3 Comp.4 Comp.5
  Comp.1
            Comp. 2
                                                   Comp.6
2.1119364 1.0928497 0.7218131 0.6761411 0.4952441 0.2701029 0.2213617
   variables and 25 observations.
>
```

```
> summary(heptathlon.pca)
Importance of components:
                                               Comp.3
                                                          Comp. 4
                                    Comp.2
Standard deviation
                       2.1119364 1.0928497 0.72181309 0.67614113 0.49524412 0.27010291
Proportion of Variance 0.6371822 0.1706172 0.07443059 0.06530955 0.03503811 0.01042223
Cumulative Proportion 0.6371822 0.8077994 0.88222998 0.94753952 0.98257763 0.99299986
                            Comp.7
Standard deviation
                       0.221361710
Proportion of Variance 0.007000144
Cumulative Proportion 1.000000000
> eig.val = heptathlon.pca$sdev^2
> eig.val
    Comp.1
              Comp.2
                          Comp.3
                                     Comp. 4
                                                Comp.5
                                                           Comp.6
                                                                       Comp. 7
4.46027516 1.19432056 0.52101413 0.45716683 0.24526674 0.07295558 0.04900101
```

#### 4. Principal Component Analysis

Scree plot and coefficients of principal components

A scree plot is drawn in order of the size of the eigenvalues of the principal components using the screeplot() function. It can be seen that there are two principal components with eigenvalues greater than 1.



#### 4. Principal Component Analysis

#### First and Second Principal components

```
\begin{split} PC_1 = & -0.453 \times hurdles - 0.377 \times highjump - 0.363shot + ... - 0.075 \times javelin - 0.375 \times run800m \\ PC_2 = & 0.158 \times hurdles + 0.248 \times highjump - 0.289shot ... - 0.842 \times javelin + 0.224 \times run800m \end{split}
```

- Considering that the absolute values of all variables except javelin(창던지기) have large absolute values, the first principal component can be said to be a component that represents the overall level of physical strength.
- The second principal component can be identified as a component closely related to javelin, given that the coefficient of javelin(창던지기) has a relatively large absolute value compared to other variables.

다음시간 안내

12

# Selection of Variables in Regression Equation

