

PCA example I

Stock data

STAT 32950-24620

Spring 2023 (3/23, wk1)

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Stock price data

Data: Weekly rates of return for five stocks

```
stock = read.table("T8-4.DAT")
colnames(stock) =
  c("JPMorgan", "Citibank", "WellsFargo", "Shell", "Exxon")
attach(stock)
```

```
str(stock)
```

```
## 'data.frame':    103 obs. of  5 variables:
## $ JPMorgan : num  0.01303 0.00849 -0.01792 0.02156 0.0...
## $ Citibank  : num  -0.00784 0.01669 -0.00864 -0.00349 0.0...
## $ WellsFargo: num  -0.00319 -0.00621 0.01004 0.01744 -0.0...
## $ Shell     : num  -0.0448 0.012 0 -0.0286 0.0292 ...
## $ Exxon     : num  0.00522 0.01349 -0.00614 -0.00695 0.0...
```

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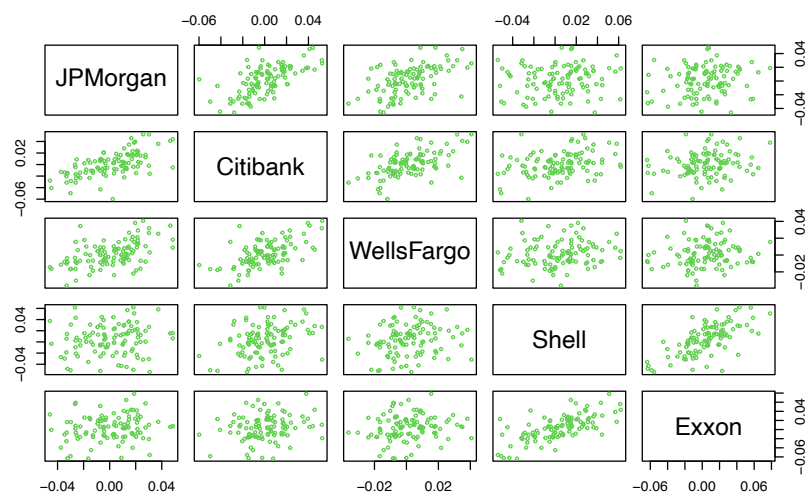
```
summary(stock[,1:3]);summary(stock[,4:5])
```

##	JPMorgan	Citibank	WellsFargo
##	Min. :-0.04587	Min. :-0.059792	Min. :-0.03621
##	1st Qu.: -0.01356	1st Qu.: -0.013241	1st Qu.: -0.00809
##	Median : 0.00336	Median : 0.001734	Median : 0.00033
##	Mean : 0.00106	Mean : 0.000655	Mean : 0.00162
##	3rd Qu.: 0.01680	3rd Qu.: 0.014029	3rd Qu.: 0.01001
##	Max. : 0.04848	Max. : 0.052527	Max. : 0.04069
##	Shell	Exxon	
##	Min. :-0.05395	Min. :-0.06360	
##	1st Qu.: -0.01447	1st Qu.: -0.01254	
##	Median : 0.00634	Median : 0.00522	
##	Mean : 0.00405	Mean : 0.00404	
##	3rd Qu.: 0.02224	3rd Qu.: 0.02162	
##	Max. : 0.06199	Max. : 0.07842	

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Plot raw data

```
pairs(stock,cex=.5,col=3)
```



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Sample variance-covariance matrix S

```
cov(stock) # same as var(stock)
```

```
##           JPMorgan  Citibank WellsFargo  Shell
## JPMorgan  4.3327e-04 0.00027567 1.5903e-04 6.4119e-05
## Citibank  2.7567e-04 0.00043872 1.7997e-04 1.8145e-04
## WellsFargo 1.5903e-04 0.00017997 2.2397e-04 7.3413e-05
## Shell     6.4119e-05 0.00018145 7.3413e-05 7.2250e-05
## Exxon     8.8966e-05 0.00012326 6.0546e-05 5.0828e-05
```

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To have a sense of relative magnitudes: $S \times 10^5$

```
round(cov(stock)*10^5);
```

```
##           JPMorgan  Citibank WellsFargo  Shell  Exxon
## JPMorgan      43      28      16      6      9
## Citibank      28      44      18      18     12
## WellsFargo    16      18      22      7      6
## Shell         6      18      7      72     51
## Exxon         9      12      6      51     77
```

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Sample correlation matrix R

```
cor(stock)
```

```
##           JPMorgan  Citibank WellsFargo  Shell  Exxon
## JPMorgan  1.00000  0.63229   0.51050  0.11460  0.15446
## Citibank  0.63229  1.00000   0.57414  0.32229  0.21267
## WellsFargo 0.51050  0.57414   1.00000  0.18250  0.14621
## Shell     0.11460  0.32229   0.18250  1.00000  0.68338
## Exxon     0.15446  0.21267   0.14621  0.68338  1.00000
```

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Better view:

```
round(cor(stock),2)
```

```
##           JPMorgan  Citibank WellsFargo  Shell  Exxon
## JPMorgan      1.00      0.63      0.51  0.11  0.15
## Citibank      0.63      1.00      0.57  0.32  0.21
## WellsFargo    0.51      0.57      1.00  0.18  0.15
## Shell         0.11      0.32      0.18  1.00  0.68
## Exxon         0.15      0.21      0.15  0.68  1.00
```

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Eigenvalues and eigenvectors of S

```
eigen(cov(stock))

## eigen() decomposition
## $values
## [1] 0.00136768 0.00070116 0.00025380 0.00014260 0.000118
##
## $vectors
##      [,1]      [,2]      [,3]      [,4]      [,5]
## [1,] 0.22282 0.62523 0.326112 0.66276 0.117660
## [2,] 0.30729 0.57039 -0.249590 -0.41409 -0.588608
## [3,] 0.15481 0.34450 -0.037639 -0.49705 0.780304
## [4,] 0.63897 -0.24795 -0.642497 0.30887 0.148455
## [5,] 0.65090 -0.32185 0.645861 -0.21638 -0.093718
```

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Principal Component Analysis on original data (using S)

```
summary(princomp(stock),loading=T)

## Importance of components:
##                               Comp.1   Comp.2   Comp.3   Comp.4
## Standard deviation      0.036802 0.026351 0.015854 0.0118
## Proportion of Variance  0.529261 0.271333 0.098216 0.055
## Cumulative Proportion  0.529261 0.800594 0.898809 0.953
##
## Loadings:
##                               Comp.1 Comp.2 Comp.3 Comp.4 Comp.5
## JPMorgan      0.223  0.625  0.326  0.663  0.118
## Citibank      0.307  0.570 -0.250 -0.414 -0.589
## WellsFargo    0.155  0.345          -0.497  0.780
## Shell         0.639 -0.248 -0.642  0.309  0.148
## Exxon         0.651 -0.322  0.646 -0.216
```

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Comparison: PCA and Eigen-Analysis

Eigenvalues of covariance matrix S :

```
round(eigen(cov(stock))$values,4)

## [1] 0.0014 0.0007 0.0003 0.0001 0.0001
```

Standard deviations of Principal Component variables:

```
round(princomp(stock)$sdev,4)

## Comp.1 Comp.2 Comp.3 Comp.4 Comp.5
## 0.0368 0.0264 0.0159 0.0119 0.0109
```

Variance of PC variables:

```
round(princomp(stock)$sdev^2,4)

## Comp.1 Comp.2 Comp.3 Comp.4 Comp.5
## 0.0014 0.0007 0.0003 0.0001 0.0001
```

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Eigenvalue of S and PC variance

$$\lambda_i = \text{Var}(Y_i), \quad i = 1, \dots, p$$

Proportions of variation:

$$\frac{\lambda_i}{\sum_j \lambda_j} = \frac{\text{Var}(Y_i)}{\sum_j \text{Var}(Y_j)}, \quad i = 1, \dots, p$$

```
round(princomp(stock)$sdev^2/sum(princomp(stock)$sdev^2),3)

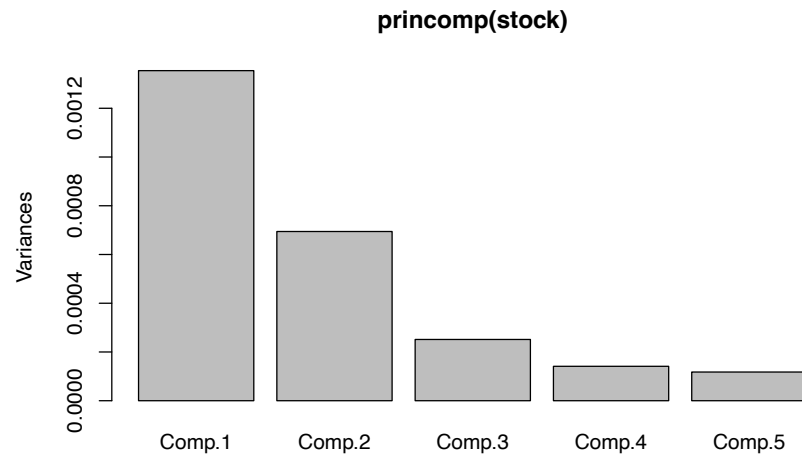
## Comp.1 Comp.2 Comp.3 Comp.4 Comp.5
## 0.529 0.271 0.098 0.055 0.046
```

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Scree plot

PCA on raw data (no scaling, using the covariance matrix)

```
par(mfrow=c(1,1)); screeplot(princomp(stock))
```



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Relation between PCs and original variables

PC of the raw data (using covariance matrix)

The first principal component: $Y_1 = a_1'X$

$$\lambda_1 = 0.00136 = V(Y_1)$$

$$Y_1 = .22(JPM) + .31(Citibk) + .15(WellsF) + .64(Shell) + .65(Exxon)$$

Interpretations?

Y_1 could be viewed as " **Market component** "

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Relation between PCs and original variables (cont.)

The Second principal component: $Y_2 = a_2'X$

$$\lambda_2 = 0.000701 = V(Y_2)$$

$$Y_2 = .63(JPM) + .57(Citibk) + .34(WellsF) - .25(Shell) - .32(Exxon)$$

Interpretations:

Y_2 could be viewed as " **Industry component** "

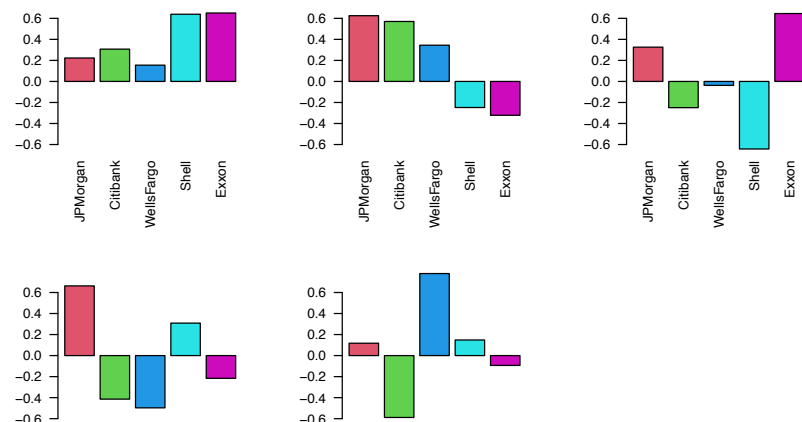
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PC loadings by original variables -Code

```
par(mfrow=c(2,3));
barplot(princomp(stock)$loadings[,1],
        las=2,ylim=c(-.6,.6),col=2:6)
barplot(princomp(stock)$loadings[,2],
        las=2,ylim=c(-.6,.6),col=2:6)
barplot(princomp(stock)$loadings[,3],
        las=2,ylim=c(-.6,.6),col=2:6)
barplot(princomp(stock)$loadings[,4],
        las=2,ylim=c(-.6,.6),axisnames = F,col=2:6)
barplot(princomp(stock)$loadings[,5],
        las=2,ylim=c(-.6,.6),axisnames = F,col=2:6)
```

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PC loadings by original variables - Plots



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PC variance proportions

Other components:

$$\hat{\lambda}_3 = 0.000253 = \hat{V}(Y_3) \approx 9.8\% \text{ of } \sum_{i=1}^5 V(Y_i)$$

$$\hat{\lambda}_4 = 0.000143 = \hat{V}(Y_4) \approx \text{of } 5.5\% \sum_{i=1}^5 V(Y_i)$$

$$\hat{\lambda}_5 = 0.000119 = \hat{V}(Y_5) \approx 4.6\% \text{ of } \sum_{i=1}^5 V(Y_i)$$

Compared with

$$\hat{V}(Y_2) \approx 27.1\% \text{ of } \sum_{i=1}^5 V(Y_i), \quad \hat{V}(Y_1) \approx 52.9\% \text{ of } \sum_{i=1}^5 V(Y_i)$$

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Eigenvalues and eigenvectors of correlation matrix

```
eigen(cor(stock))
```

```
## eigen() decomposition
## $values
## [1] 2.43727 1.40701 0.50051 0.40003 0.25517
##
## $vectors
##      [,1]      [,2]      [,3]      [,4]      [,5]
## [1,] -0.46908  0.36801 -0.604315  0.36302  0.384122
## [2,] -0.53241  0.23646 -0.136106 -0.62921 -0.496188
## [3,] -0.46516  0.31518  0.771828  0.28897  0.071169
## [4,] -0.38735 -0.58504  0.093362 -0.38125  0.594664
## [5,] -0.36068 -0.60585 -0.108826  0.49341 -0.497552
```

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PCA using scaled data of variable variance = 1

That is, **PCA using correlation matrix**.

```
summary(princomp(stock,cor=T),loading=T)
```

```
## Importance of components:
##                Comp.1  Comp.2  Comp.3  Comp.4
## Standard deviation    1.56118  1.18618  0.70747  0.632481
## Proportion of Variance 0.48745  0.28140  0.10010  0.080006
## Cumulative Proportion 0.48745  0.76886  0.86896  0.948966
##
## Loadings:
##                Comp.1  Comp.2  Comp.3  Comp.4  Comp.5
## JPMorgan      0.469   0.368   0.604   0.363   0.384
## Citibank       0.532   0.236   0.136  -0.629  -0.496
## WellsFargo     0.465   0.315  -0.772   0.289
## Shell          0.387  -0.585           -0.381  0.595
## Exxon          0.361  -0.606   0.109   0.493  -0.498
```

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Correlation of PC and original variables

For PCA on scaled data (using correlation matrix):

The correlation between
the i th PC variable Y_i and the (scaled) k th variable X_k is

$$\rho_{Y_i, X_k} = a_{ik} \sqrt{\lambda_i}$$

For PCA on raw data (using covariance matrix):

$$\rho_{Y_i, X_k} = a_{ik} \sqrt{\lambda_i / \sigma_{kk}}$$

(both ignoring the presence of other X_j variables)

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PCA vs eigen-analysis on correlation matrix R

Eigenvalues of correlation matrix R :

```
round(eigen(cor(stock))$values,4)
```

```
## [1] 2.4373 1.4070 0.5005 0.4000 0.2552
```

Standard deviations of PC variables (scaled data):

```
round(princomp(stock,cor=T)$sdev,4)
```

```
## Comp.1 Comp.2 Comp.3 Comp.4 Comp.5
```

```
## 1.5612 1.1862 0.7075 0.6325 0.5051
```

Variance of PC variables (scaled data):

```
round(princomp(stock,cor=T)$sdev^2,4)
```

```
## Comp.1 Comp.2 Comp.3 Comp.4 Comp.5
```

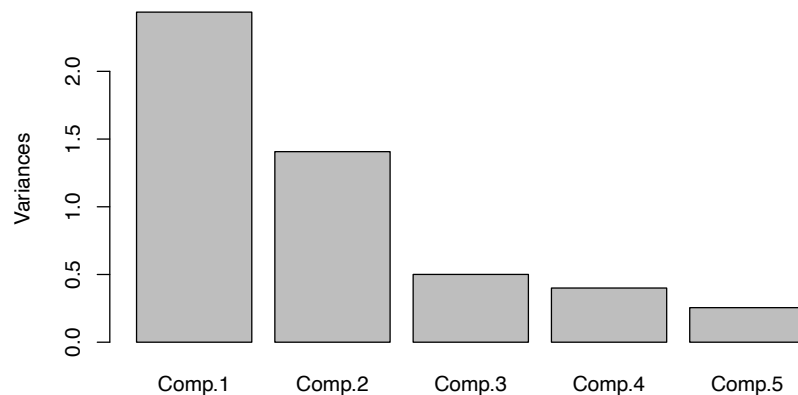
```
## 2.4373 1.4070 0.5005 0.4000 0.2552
```

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Scree plot (scaled, using correlation matrix)

```
par(mfrow=c(1,1))
screeplot(princomp(stock,cor=T))
```

princomp(stock, cor = T)

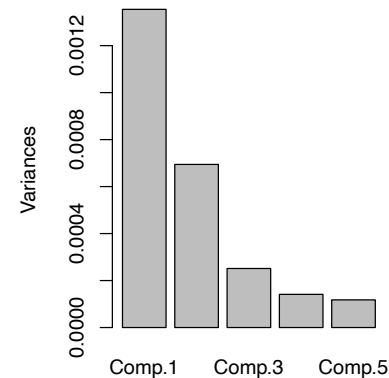


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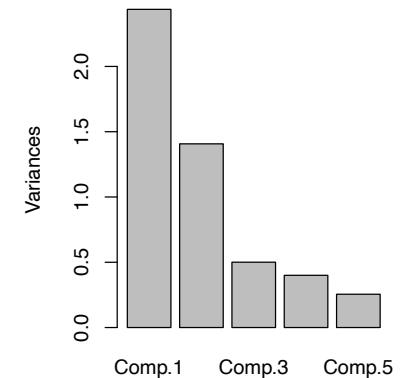
Scree plots (scaled vs not scaled)

```
par(mfrow=c(1,2))
screeplot(princomp(stock));screeplot(princomp(stock,cor=T))
```

princomp(stock)



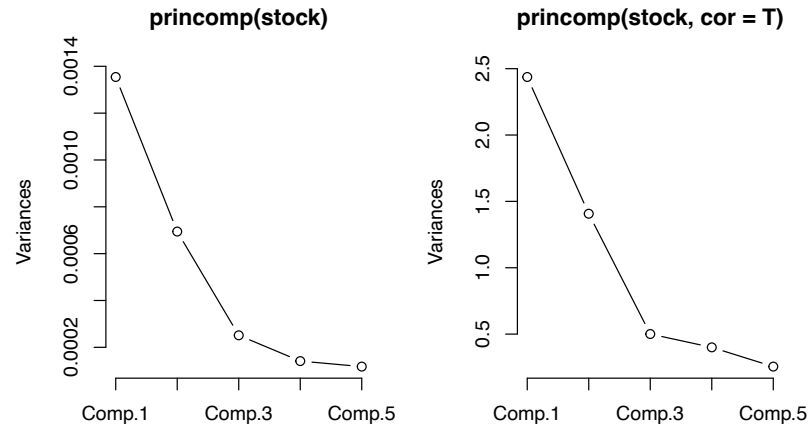
princomp(stock, cor = T)



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To scale or not to scale?

```
par(mfrow=c(1,2))
screepplot(princomp(stock),type="l")
screepplot(princomp(stock, cor=T),type="l")
```



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Proportion of total variation explained

- Of sample covariance matrix S

```
cumsum((princomp(stock)$sdev)^2)/sum((princomp(stock)$sdev,
```

```
## Comp.1 Comp.2 Comp.3 Comp.4 Comp.5
## 0.52926 0.80059 0.89881 0.95399 1.00000
```

- Of sample correlation matrix R

```
cumsum((princomp(stock,cor=T)$sdev)^2)/5
```

```
## Comp.1 Comp.2 Comp.3 Comp.4 Comp.5
## 0.48745 0.76886 0.86896 0.94897 1.00000
```

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Sum of eigenvalues

- Of covariance matrix S

```
sum(eigen(cov(stock))$values)
```

```
## [1] 0.0025841
```

- Of correlation matrix R

```
sum(eigen(cor(stock))$values)
```

```
## [1] 5
```

- Comparison: What is the dimension of variables?

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Scale sizes

Scale = Using sample correlation matrix R

```
princomp(stock,cor=T)$scale
```

```
## JPMorgan Citibank WellsFargo Shell Exxon
## 0.020714 0.020844 0.014893 0.026748 0.027536
```

- What should the values of the "scale" be?
- Should scaling make a significant difference for this dataset?

No re-scale = Using original sample covariance matrix S

```
princomp(stock)$scale
```

```
## JPMorgan Citibank WellsFargo Shell Exxon
## 1 1 1 1 1
```

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Using correlation matrix

Relation between principal components and original variables

$$\hat{\lambda}_1 = 2.437$$

$$Y_1 = .469(JPMorgan) + .532(Citibank) + .465(WellsFargo) \\ + .387(Shell) + .361(Exxon)$$

Y_1 : " **Market component** " (or similar interpretations)

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(Using correlation matrix)

$$\hat{\lambda}_2 = 1.407$$

$$Y_2 = .368(JPMorgan) + .236(Citibank) + .315(WellsFargo) \\ - .585(Shell) - .606(Exxon)$$

Y_2 : " **Industry component** "

$$\hat{\lambda}_3 = 0.501 > \hat{\lambda}_4 = 0.400 > \hat{\lambda}_5 = 0.255$$

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Observed values vs PC values

Data:

n measurements of the original random vector (X_1, \dots, X_p) :

$$\begin{matrix} x_{11} & \cdots & x_{1p} \\ \vdots & \cdots & \vdots \\ x_{n1} & \cdots & x_{np} \end{matrix}$$

PC scores

n "measurements" of principal components (Y_1, \dots, Y_p) :

$$\begin{matrix} y_{11} & \cdots & y_{1p} \\ \vdots & \cdots & \vdots \\ y_{n1} & \cdots & y_{np} \end{matrix}$$

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Weekly rate of returns of the original five stocks

```
head(stock,3)
```

```
##      JPMorgan  Citibank WellsFargo      Shell      Exxon
## 1  0.0130338 -0.0078431 -0.0031889 -0.044769  0.0052151
## 2  0.0084862  0.0166886 -0.0062100  0.011956  0.0134890
## 3 -0.0179153 -0.0086393  0.0100360  0.000000 -0.0061428
```

```
tail(stock)
```

```
##      JPMorgan  Citibank WellsFargo      Shell      Exxon
## 98  0.0217449  0.0229645  0.0291983  0.0084395  0.03192
## 99  0.0033740 -0.0153061 -0.0238245 -0.0016738 -0.01722
## 100 0.0033626  0.0029016 -0.0030507 -0.0012193 -0.00970
## 101 0.0170147  0.0095061  0.0181994 -0.0161758 -0.00756
## 102 0.0103929 -0.0026612  0.0044290 -0.0024818 -0.01645
## 103 -0.0127948 -0.0143678 -0.0187402 -0.0049759 -0.01637
```

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Weekly data of five "PC stocks" (using correlation matrix)

```
head(princomp(stock,cor=T)$scores,3)
```

```
##          Comp.1   Comp.2   Comp.3   Comp.4   Comp.5
## [1,] -0.78790  1.056230  0.71834  1.089819 -0.7052807
## [2,]  0.57118 -0.232923  0.73713 -0.449297 -0.2764345
## [3,] -0.59651  0.047938 -1.07632 -0.013571  0.0034684
```

```
tail(princomp(stock,cor=T)$scores)
```

```
##          Comp.1   Comp.2   Comp.3   Comp.4   Comp.5
## [98,]  2.32830  0.494367 -0.584970  0.661200 -0.422135
## [99,] -1.51171 -0.085575  1.218117 -0.270965  0.558224
## [100,] -0.29287  0.384882  0.288229 -0.289340  0.097955
## [101,]  0.66015  1.432133 -0.310988  0.414374 -0.075710
## [102,] -0.14883  0.781089  0.047103  0.043971  0.490387
## [103,] -1.73173 -0.201152  0.503933 -0.421642  0.171508
```

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$Y_k = a'_k X$ relates PC scores and data

```
stock[33,]
```

```
##      JPMorgan Citibank WellsFargo      Shell      Exxon
## 33 0.027618 0.016832  0.010498 0.0004153 0.00433
```

```
princomp(stock,cor=T)$scores[33,]
```

```
##      Comp.1   Comp.2   Comp.3   Comp.4   Comp.5
## 1.242857 0.916126 0.434434 0.206232 0.063711
```

```
princomp(stock)$scores[33,]
```

```
##          Comp.1   Comp.2   Comp.3   Comp.4   Cor
## 1.0129e-02  2.9694e-02  6.8116e-03  5.3063e-03 -4.1301e-04
```

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PC score correlation property

```
dim(stock); dim(princomp(stock,cor=T)$scores) # 103 5
```

```
## [1] 103  5
```

```
## [1] 103  5
```

```
round(cor(princomp(stock,cor=T)$scores),3)
```

```
##          Comp.1   Comp.2   Comp.3   Comp.4   Comp.5
## Comp.1      1      0      0      0      0
## Comp.2      0      1      0      0      0
## Comp.3      0      0      1      0      0
## Comp.4      0      0      0      1      0
## Comp.5      0      0      0      0      1
```

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Un-correlatedness of PCs is true regardless of scaling

```
round(cor(princomp(stock)$scores),3)
```

```
##          Comp.1   Comp.2   Comp.3   Comp.4   Comp.5
## Comp.1      1      0      0      0      0
## Comp.2      0      1      0      0      0
## Comp.3      0      0      1      0      0
## Comp.4      0      0      0      1      0
## Comp.5      0      0      0      0      1
```

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PC score covariance property

```
round(cov(princomp(stock,cor=T)$scores),2)
```

```
##          Comp.1 Comp.2 Comp.3 Comp.4 Comp.5
## Comp.1    2.46  0.00  0.00   0.0  0.00
## Comp.2    0.00  1.42  0.00   0.0  0.00
## Comp.3    0.00  0.00  0.51   0.0  0.00
## Comp.4    0.00  0.00  0.00   0.4  0.00
## Comp.5    0.00  0.00  0.00   0.0  0.26
```

Note the diagonal patterns.

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Observations using PC scores as coordinates - Code

PC scores can be used as coordinates of data observation points

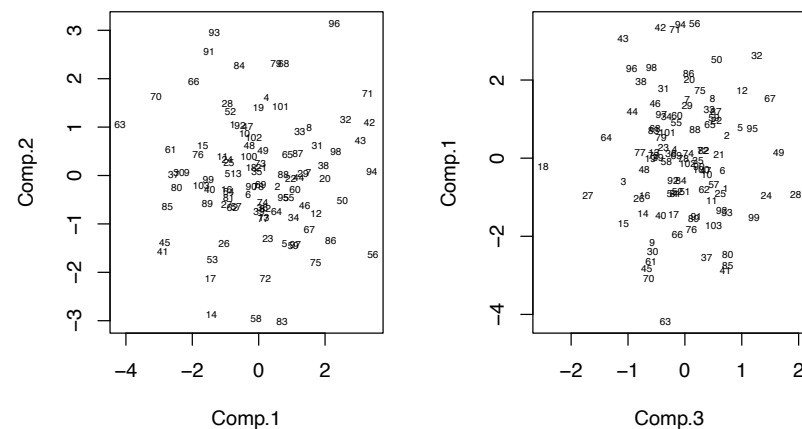
```
par(mfrow=c(1,2));
plot(princomp(stock,cor=T)$score[,1:2],
     type="n",main="Stock obs(wks) in PC scores")
text(princomp(stock,cor=T)$score[,1:2],
     labels=row.names(stock),cex=.5)
plot(princomp(stock,cor=T)$score[,c(3,1)],type="n")
text(princomp(stock,cor=T)$score[,c(3,1)],
     labels=row.names(stock),cex=.5)
```

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Observations using PC scores as coordinates - Plots

The plots may reveal interesting data patterns sometimes (not here).

Stock obs(wks) in PC scores



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Variables using PC loading as coordinates - Code

PC loadings (a_{ij}) can be used as coordinates of original variables.

```
par(mfrow=c(1,1))
plot(princomp(stock,cor=T)$loading[,1:2],
     xlim=c(0,.6),ylim=c(-.7,.6),type="n")
title(main="Original stock variables in PC loadings")
text(princomp(stock,cor=T)$loading[,1:2],
     labels=(colnames(stock)),cex=.8,col=c(4,4,4,2,2))

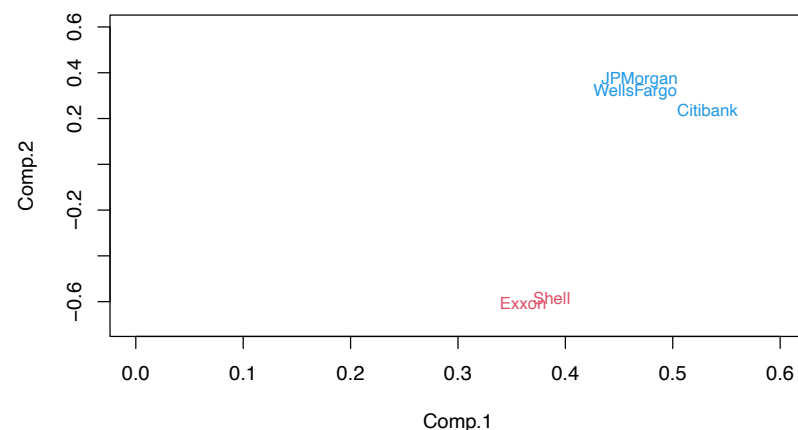
par(mfrow=c(1,2))
barplot(princomp(stock,cor=T)$loadings[,1],
        las=2,ylim=c(-.6,.6),col=2:6,cex.names=.7)
barplot(princomp(stock,cor=T)$loadings[,2],
        las=2,ylim=c(-.6,.6),col=2:6,cex.names=.7)
```

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Variables using PC loading as coordinates - Plot

The plot may reveal interesting variable patterns.

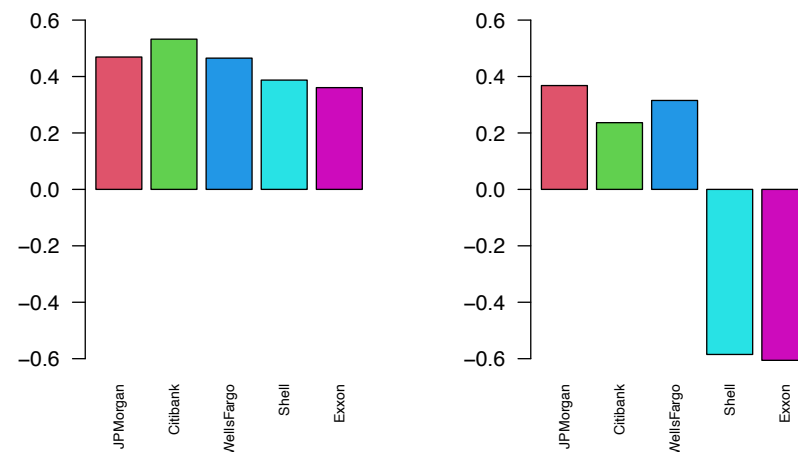
Original stock variables in PC loadings



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Variable loading a_{ij} 's of top PCs

$$Y_1 = a_1'X, \quad Y_2 = a_2'X$$



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Norm-one property of PC loadings

In the derivation of PC variables,

$$Y_k = a_k'X, \quad \|a_k\| = 1, \quad a_i'a_k = 0, \quad i \neq k, \quad i, k = 1, \dots, p.$$

- The p -vector a_i 's are restricted to be of length 1.
- The loading vectors of different PCs are mutually orthogonal.
- The loading coefficients should form an orthogonal matrix.

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Loading coefficients are norm-1: $Y_k = a_k'X, \|a_k\| = 1$

```
round(princomp(stock)$loading[,1:5],3)
```

```
##           Comp.1 Comp.2 Comp.3 Comp.4 Comp.5
## JPMorgan    0.223  0.625  0.326  0.663  0.118
## Citibank    0.307  0.570 -0.250 -0.414 -0.589
## WellsFargo  0.155  0.345 -0.038 -0.497  0.780
## Shell       0.639 -0.248 -0.642  0.309  0.148
## Exxon       0.651 -0.322  0.646 -0.216 -0.094
```

```
a1 = princomp(stock,cor=T)$loading[,1]; round(a1,3)
```

```
##      JPMorgan  Citibank WellsFargo      Shell      Exxon
##      0.469      0.532      0.465      0.387      0.361
```

```
sum(a1^2)
```

```
## [1] 1
```

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Orthogonality of PC loadings $Y_k = a'_k X$, $a'_i a_k = 0, i \neq k$

```
a2 = princomp(stock,cor=T)$loading[,2]; round(a2,3)
```

```
##      JPMorgan      Citibank WellsFargo      Shell      Exxon
##      0.368      0.236      0.315      -0.585      -0.606
```

```
a1%*%a2;
```

```
##           [,1]
## [1,] 1.9429e-16
```

```
round(a1%*%a2,3)
```

```
##           [,1]
## [1,] 0
```

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Loading coefficients form an orthogonal matrix

```
L=as.matrix(princomp(stock,cor=T)$loading,5,5);
round(L%*%t(L),3)
```

```
##           JPMorgan Citibank WellsFargo Shell Exxon
## JPMorgan           1         0         0         0         0
## Citibank           0         1         0         0         0
## WellsFargo         0         0         1         0         0
## Shell              0         0         0         1         0
## Exxon              0         0         0         0         1
```

$$L^{-1} = L^T, \quad L^T L = L L^T = I_p$$

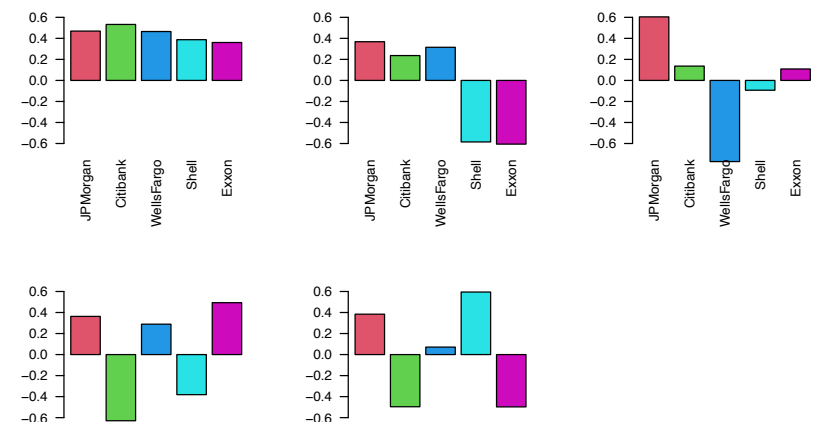
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PC loadings by original variables (scaled data) - Code

```
par(mfrow=c(2,3))
barplot(princomp(stock,cor=T)$loadings[,1],
        las=2,ylim=c(-.6,.6),col=2:6)
barplot(princomp(stock,cor=T)$loadings[,2],
        las=2,ylim=c(-.6,.6),col=2:6)
barplot(princomp(stock,cor=T)$loadings[,3],
        las=2,ylim=c(-.6,.6),col=2:6)
barplot(princomp(stock,cor=T)$loadings[,4],
        las=2,ylim=c(-.6,.6),axisnames = F,col=2:6)
barplot(princomp(stock,cor=T)$loadings[,5],
        las=2,ylim=c(-.6,.6),axisnames = F,col=2:6)
```

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PC loadings by original variables (scaled data) - Plots



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