11 - Principal Components Analysis

Junvie Pailden

SIUE, F2017, Stat 589

September 25, 2017

General Objectives

- Explaining the variance-covariance structure of a set of variables through a few linear combinations of these variables.
 - 1. Data Reduction
 - 2. Interpretation
- Although p components are required to reproduce the total system variability, often much of this variability can be accounted for by a small number of k of the principal components.

- If so, there is as much information in the k components as there is in the original p variables.
- The k principal components can then replace the initial p variables, and the original data set, consisting of n measurements on p variables, is reduced to a data set consisting of n measurements on k principal components.

Population Principal Components

- Principal components are particular linear combinations of the p random variables X_1, X_2, \ldots, X_p .
- Geometrically, these linear combinations represent the selection of a new coordinate system obtained by rotating the original system with X_1, X_2, \ldots, X_p as the coordinate axes.
- The new axes represent the directions with maximum variability and provide a simpler and more parsimonious description of the covariance structure.
- Principal components depend solely on the covariance matrix Σ (or the correlation matrix ρ) of X_1, X_2, \ldots, X_p .
- NO Multivariate Normal Assumption Required

Population Principal Components: Notation

- Let the random vector $\mathbf{X}' = [X_1, X_2, \dots, X_p]$ have the covariance matrix Σ with eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p \geq 0$.
- Consider the linear combinations

$$Y_{1} = \mathbf{a}_{1}'\mathbf{X} = a_{11}X_{1} + a_{12}X_{2} + \dots + a_{1p}X_{p}$$

$$Y_{2} = \mathbf{a}_{2}'\mathbf{X} = a_{21}X_{1} + a_{22}X_{2} + \dots + a_{2p}X_{p}$$

$$\vdots$$

$$Y_{p} = \mathbf{a}_{p}'\mathbf{X} = a_{p1}X_{1} + a_{p2}X_{2} + \dots + a_{pp}X_{p}$$

We obtain

$$Var(Y_i) = \mathbf{a}_i' \mathbf{\Sigma} \mathbf{a}_i \quad i = 1, 2, \dots, p$$

 $Cov(Y_i, Y_k) = \mathbf{a}_i' \mathbf{\Sigma} \mathbf{a}_k \quad i, k = 1, 2, \dots, p$

• The principal components are those uncorrelated linear combinations Y_1, Y_2, \ldots, Y_p whose variances in $Var(Y_i)$ are as large as possible.

First principal component = linear combination $\mathbf{a}_1'\mathbf{X}$ that maximizes $Var(\mathbf{a}_1'\mathbf{X})$ subject to $\mathbf{a}_1'\mathbf{a}_1=1$

Second principal component = linear combination $\mathbf{a}_2'\mathbf{X}$ that maximizes $Var(\mathbf{a}_2'\mathbf{X})$ subject to $\mathbf{a}_2'\mathbf{a}_2=1$ $Cov(\mathbf{a}_1'\mathbf{X},\mathbf{a}_2'\mathbf{X})=0$

At the ith step, $ith \ \text{principal component} = \text{linear combination } \mathbf{a}_i'\mathbf{X} \ \text{that maximizes}$ $Var(\mathbf{a}_i'\mathbf{X}) \ \text{subject to } \mathbf{a}_i'\mathbf{a}_i = 1 \ \text{and}$ $Cov(\mathbf{a}_i'\mathbf{X}, \mathbf{a}_k'\mathbf{X}) = 0 \ \text{ for } \ k < i$

Result 8.1

Let Σ be the covariance matrix associated with the random vector $\mathbf{X}' = [X_1, X_2, \dots, X_p]$. Let Σ have the eigenvalue-eigenvector pairs $(\lambda_1, \mathbf{e}_2), (\lambda_1, \mathbf{e}_2), \dots, (\lambda_p, \mathbf{e}_p)$ where $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p \geq 0$.

Then the *ith principal component* is given by

$$Y_i = \mathbf{e}_i' \mathbf{X} = e_{i1} X_1 + e_{i2} X_2 + \dots + e_{ip} X_p, \ i = 1, 2, \dots, p$$

With these choices,

$$Var(Y_i) = \mathbf{e}_i' \Sigma \mathbf{e}_i = \lambda_i \quad i = 1, 2, \dots, p$$
$$Cov(Y_i, Y_k) = \mathbf{e}_i' \Sigma \mathbf{e}_k = 0 \quad i \neq k$$

Result 8.1 (cont)

If some λ_i are equal, the choices of the corresponding coefficient vectors, ${\bf e}_i$ and hence Y_i are not unique.

Result 8.1, the principal components are uncorrelated and have variances equal to the eigenvalues of Σ .

Result 8.2

Let $\mathbf{X}' = [X_1, X_2, \dots, X_p]$ have covariance matrix Σ , with eigenvalue-eigenvector pairs $(\lambda_1, \mathbf{e}_1), (\lambda_2, \mathbf{e}_2), \dots, (\lambda_p, \mathbf{e}_p)$ where $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_p \geq 0$. Let $Y_1 = \mathbf{e}_1'\mathbf{X}$, $Y_2 = \mathbf{e}_2'\mathbf{X}, \dots, Y_p = \mathbf{e}_p'\mathbf{X}$ be the principal components. Then

$$\sigma_{11} + \sigma_{22} + \dots + \sigma_{pp} = \sum_{i=1}^{p} Var(X_i) = \lambda_1 + \lambda_2 + \dots + \lambda_p = \sum_{i=1}^{p} Var(Y_i)$$

Result 8.2 says that

Total population variance =
$$\sigma_{11} + \sigma_{22} + \cdots + \sigma_{pp}$$

= $\lambda_1 + \lambda_2 + \cdots + \lambda_p$

Result 8.2 (cont)

and, the proportion of total variance due to (explained by) the $k{\rm th}$ principal component is

$$\left(\begin{array}{c} \text{Proportion of total} \\ \text{population variance} \\ \text{due to } kth \text{ principal} \\ \text{component} \end{array}\right) = \frac{\lambda_k}{\lambda_1 + \lambda_2 + \dots + \lambda_p}$$

- If most (for instance, 80 to 90%) of the total population variance, for large p, can be attributed to the first one, two, or three components, then these components can "replace" the original p variables without much of loss of information. Each component of the coefficient vector $\mathbf{e}_i' = [e_{i1}, \dots, e_{ik}, \dots, e_{ip}]$
- The magnitude of e_{ik} measures the importance of the kth variable to the ith principal component, irrespective of the other variables. In particular, e_{ik} is proportional to the correlation coefficient between Y_i and X_k .

also merits inspection.

Result 8.3

If $Y_1 = \mathbf{e}_1' \mathbf{X}$, $Y_2 = \mathbf{e}_2' \mathbf{X}$,..., $Y_p = \mathbf{e}_p' \mathbf{X}$ are the principal components obtained from the covariance matrix Σ , then

$$\rho_{Y_i, X_k} = \frac{e_{ik}\sqrt{\lambda_i}}{\sqrt{\sigma_{kk}}} \quad i, k = 1, 2, \dots, p$$

are the correlation coefficients between the components Y_i and the variables X_k .

Example 8.1 Calculation the population principal components I

Let X_1 , X_2 , and X_3 have the covariance matrix

```
(Sigma <- matrix(c(1,-2,0,-2,5,0,0,0,2), nrow=3, byrow=T))

# [,1] [,2] [,3]

# [1,] 1 -2 0

# [2,] -2 5 0

# [3,] 0 0 2
```

```
eigen.Sigma <- eigen(Sigma)
(lambda <- eigen.Sigma$values)</pre>
```

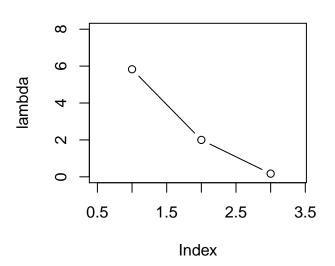
```
# [1] 5.83 2.00 0.17
```

Example 8.1 Calculation the population principal components II

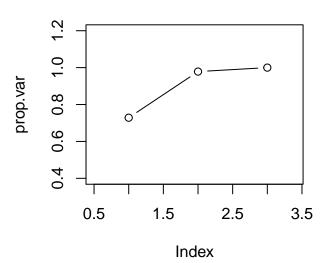
```
(eigen.Sigma$vectors)
# [,1] [,2] [,3]
# [1,] -0.38 0 0.92
 [2,] 0.92 0 0.38
# [3,] 0.00 1 0.00
(prop.var <- cumsum(lambda)/sum(lambda) )</pre>
# [1] 0.73 0.98 1.00
```

Plots

Eigenvalues of Sigma



Proportion of Variation



Principal Components Obtained from Standardized Variables

Principal components may also be obtained for the standardized variables

$$Z_1 = \frac{(X_1 - \mu_1)}{\sqrt{\sigma_{11}}}, \ Z_2 = \frac{(X_2 - \mu_2)}{\sqrt{\sigma_{22}}}, \dots, Z_p = \frac{(X_p - \mu_p)}{\sqrt{\sigma_{pp}}}$$

In matrix notation,

$$\begin{split} \mathbf{Z} &= (\mathbf{V}^{1/2})^{-1}(\mathbf{X} - \mu), \\ E(\mathbf{Z}) &= 0, \text{and} \ , \ Cov(Z) = (\mathbf{V}^{1/2})^{-1} \mathbf{\Sigma} (\mathbf{V}^{1/2})^{-1} = \pmb{\rho}, \end{split}$$

where ${f V}^{1/2}$ is the diagonal standard deviation matrix.

Result 8.4

The *i*th principal component of the standardized variables $\mathbf{Z}' = [Z_1, Z_2, \dots, Z_p]_{\text{with}} Cov(\mathbf{Z}) = \boldsymbol{\rho}$, is given by

$$Y_i = e_i' Z = e_i' (\mathbf{V}^{1/2})^{-1} (\mathbf{X} - \mu), \ i = 1, 2, \dots, p$$

Moreover.

$$\sum_{i=1}^{p} Var(Y_i) = \sum_{i=1}^{p} Var(Z_i) = p$$

and

$$\rho_{Y_i,Z_k} = e_{ik}\sqrt{\lambda_i} \quad i,k = 1,2,\ldots,p.$$

$$\left(\begin{array}{c} \text{Proportion of (standardized)} \\ \text{population variance} \\ \text{due to } kth \text{ principal} \\ \text{component} \end{array}\right) = \frac{\lambda_k}{p}, \ \ k=1,2,\dots,p$$

Summarizing Sample Variation by Principal Components

- Suppose the data $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n$ represent n independent drawings from some p-dimensional population with mean vector $\boldsymbol{\mu}$ and covariance matrix $\boldsymbol{\Sigma}$.
- These data yield the sample mean vector $\bar{\mathbf{x}}$, the sample covariance matrix \mathbf{S} , and the sample correlation matrix \mathbf{R} .
- Our objective in this section will be to construct uncorrelated linear combinations of the measured characteristics that account for much of the variation in the sample.
- The uncorrelated combinations with the largest variances will be called the *sample principal components*.

ullet Recall that the n values of any linear combination

$$\mathbf{a}_{1}'\mathbf{x} = a_{11}x_{j1} + a_{12}x_{j2} + \dots + a_{1p}x_{jp}, \quad j = 1, 2, \dots, n$$

have the sample mean $\mathbf{a}_1'\bar{\mathbf{x}}$ and sample variance $\mathbf{a}_1'\mathbf{S}\mathbf{a}_1.$

• Also, the pairs of values $(\mathbf{a}_1'\mathbf{x}_j, \mathbf{a}_2'\mathbf{x}_j)$ have sample covariance $\mathbf{a}_1'\mathbf{S}\mathbf{a}_2$.

If $\mathbf{S} = \{s_{ik}\}$ is the $p \times p$ sample covariance matrix with eigenvalue-eigenvector pairs $(\hat{\lambda}_1, \hat{\mathbf{e}}_1), (\hat{\lambda}_2, \hat{\mathbf{e}}_2), \dots, (\hat{\lambda}_p, \hat{\mathbf{e}}_p)$, the ith sample principal component is given by

$$\hat{y}_i = \hat{\mathbf{e}}'_i = \hat{e}_{i1}x_1 + \hat{e}_{i2}x_2 + \dots + \hat{e}_{ip}x_p, \quad i = 1, 2, \dots, p$$

where $\hat{\lambda}_1 \geq \hat{\lambda}_2 \geq \cdots \geq \hat{\lambda}_p \geq 0$ and \mathbf{x} is any observation on the variables X_1, X_2, \ldots, X_p . Also,

Sample variance
$$(\hat{y}_k) = \hat{\lambda}_k, \ k = 1, 2, \dots, p$$

Sample covariance $(\hat{y}_i, \hat{y}_k) = 0, \ i \neq k$

In addition,

Total sample variance
$$=\sum_{i=1}^p s_{ii}=\hat{\lambda}_1+\hat{\lambda}_2+\cdots+\hat{\lambda}_p$$

$$r_{\hat{y_i},x_k}=\frac{\hat{e}_{ik}\sqrt{\hat{\lambda}_i}}{\sqrt{s_{kk}}},\quad i,k=1,2,\ldots,p$$

Sample Variation by Principal Components

- We shall denote the sample principal components by $\hat{y}_1, \hat{y}_2, \dots, \hat{y}_p$.
- The observations x_i are often "centered" by subtracting \bar{x} .
- This has no effect on the sample covariance matrix ${f S}$ and gives the ith principal component

$$\hat{y}_i = \hat{\mathbf{e}}'_i(x - \bar{x}), \quad i = 1, 2, \dots, p$$

for any observation vector \mathbf{x} .

• If we consider the values of the *i*th component

$$\hat{y}_{ii} = \hat{\mathbf{e}}'_i(\mathbf{x}_i - \bar{\mathbf{x}}), \quad j = 1, 2, \dots, n$$

generating by substituting each observation \mathbf{x}_j for the arbitrary \mathbf{x}_j , then

$$\hat{y}_i = \frac{1}{n} \sum_{j=1}^n \hat{\mathbf{e}}_i'(\mathbf{x}_j - \bar{\mathbf{x}}) = \frac{1}{n} \hat{\mathbf{e}}_i' \left(\sum_{j=1}^n (\mathbf{x}_j - \bar{\mathbf{x}}) \right) = \frac{1}{n} \hat{\mathbf{e}}_i' \mathbf{0} = 0$$

The Number of Principal Components

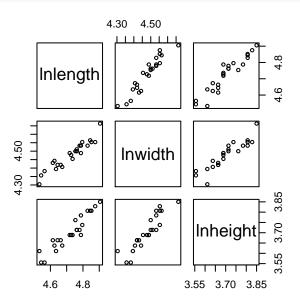
- There is always the question of how many components to retain.
- A useful visual aid to determining an appropriate number of principal components is a scree plot.
- With the eigenvalues ordered from largest to smallest, a scree plot is a plot of $\hat{\lambda}_i$ versus i the magnitude of an eigenvalue versus its number.
- To determine the appropriate number of components, we look for an elbow (bend) in the scree plot.
- The number of components is taken to be the point at which the remaining eigenvalues are relatively small and all about the same size.

Example 8.4: Summarizing the data with one sample principal component

In a study of size and relationships for painted male turtles, Joicoeur and Moistmann measured carapace length, width, and height. The authors suggests a logarithmic transformation in studies of size-and-shape relationships. Perform a principal component analysis.

```
turtles <- read.table("T6-9.DAT", header=F)[25:48,-4]
X <- log(as.matrix(turtles))
colnames(X) <- c("lnlength", "lnwidth", "lnheight")</pre>
```

Make plots of data: pairs(X, cex = 0.7)



```
# Compute means and covariance matrix
colMeans(X)
```

```
# lnlength lnwidth lnheight
# 4.7 4.5 3.7
```

```
(S \leftarrow cov(X))
```

```
# Inlength lnwidth lnheight
# lnlength 0.0111 0.0080 0.0082
# lnwidth 0.0080 0.0064 0.0060
# lnheight 0.0082 0.0060 0.0068
```

Compute principal components for original data. Use prcomp built-in function in R

```
(turtles.pcomp <- prcomp(X))</pre>
# Standard deviations (1, .., p=3):
# [1] 0.153 0.024 0.019
#
# Rotation (n \times k) = (3 \times 3):
#
          PC1 PC2 PC3
# lnlength 0.68 -0.16 0.71
# lnwidth 0.51 -0.59 -0.62
# lnheight 0.52 0.79 -0.32
```

```
# eigenvalues
turtles.pcomp$sdev^2
```

[1] 0.02330 0.00060 0.00036

summary(turtles.pcomp)

```
# Importance of components%s:

# PC1 PC2 PC3

# Standard deviation 0.153 0.0245 0.0190

# Proportion of Variance 0.961 0.0247 0.0148

# Cumulative Proportion 0.961 0.9852 1.0000
```

Checking

Check calculations of principal components by computing eigenvalues/eigenvectors and proportion explained from the original data. Use the covariance matrix S

```
eigen.turtles <- eigen(S)
eigen.turtles$values</pre>
```

```
# [1] 0.02330 0.00060 0.00036
```

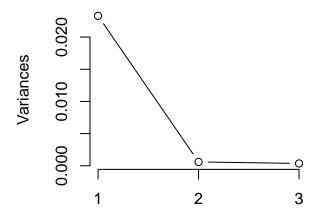
```
cumsum(eigen.turtles$values)/sum(eigen.turtles$values)
```

```
# [1] 0.96 0.99 1.00
```

Screeplot order eigenvalues from largest to smallest

```
screeplot(turtles.pcomp, type="lines")
```

turtles.pcomp



eigen.turtles\$vectors

```
# [,1] [,2] [,3]
# [1,] 0.68 -0.16 0.71
# [2,] 0.51 -0.59 -0.62
# [3,] 0.52 0.79 -0.32
```

Turtle Measurements via Principal Components

- The scree plot in the previous slide has a very distinct elbow that occurs at i=2. There is clearly a dominant principal component.
- The first principal component, which explains 96% of the total variance, has an interesting subject-matter interpretations.

$$\begin{split} \hat{y}_1 &= .68 \ln(\mathsf{length}) + .51 \ln(\mathsf{width}) + .52 \ln(\mathsf{height}) \\ &= \ln\left[(\mathsf{length})^{.68} \times (\mathsf{width})^{.51} \times (\mathsf{height})^{.52} \right] \end{split}$$

- The first principal component \hat{y}_1 may be viewed as the *volume* of a box with adjusted dimensions.
- For instance, the adjusted height, (height).⁵², can account (in some sense) for the rounded shape of the carapace.
- The values of the first principal component can be computed as

$$\hat{\mathbf{y}}_1 = \begin{bmatrix} y_{11} \\ \hat{y}_{21} \\ \vdots \\ \hat{y}_{n1} \end{bmatrix} = \mathbf{X}\hat{\mathbf{e}}_1 = \mathbf{X}[.68, .51, .52]$$

```
#
     0.68
             0.51
                     0.52
PC1 <- X%*%ev1
summary(PC1)
#
       V1
#
  Min. :7.2
# 1st Qu.:7.3
#
  Median:7.5
#
 Mean :7.4
# 3rd Qu.:7.6
```

(ev1 <- turtles.pcomp\$rotation[, 1])</pre>

lnlength lnwidth lnheight

#

Max. :7.7

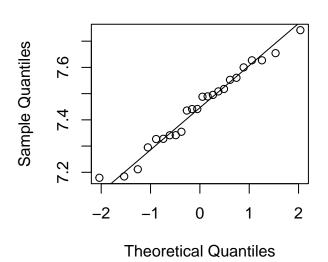
```
#
# The decimal point is 1 digit(s) to the left of the |
# 70 | 88
# 72 | 1933445
# 74 | 4449901256
```

```
qqnorm(PC1)
qqline(PC1)
```

76 | 03354

#

Normal Q-Q Plot



Standardizing the Sample Principal Components

- Sample principal components are, in general, not invariant with respect to changes in scale.
- Variables measured on different scales or on a common scale with widely differing ranges are often standardized.
- For $j=1,2,\ldots,n$, the standardized observation of the jth observation in the sample is

$$\mathbf{z}_{j} = \mathbf{D}^{-1/2}(\mathbf{x}_{j} - \bar{\mathbf{x}}) = \begin{bmatrix} \frac{x_{j1} - x_{1}}{\sqrt{s_{11}}} \\ \frac{x_{j2} - \bar{x}_{2}}{\sqrt{s_{22}}} \\ \vdots \\ \frac{x_{jp} - \bar{x}_{p}}{\sqrt{s_{pp}}} \end{bmatrix} = \begin{bmatrix} z_{j1} \\ z_{j2} \\ \vdots \\ z_{jp} \end{bmatrix}$$

Standardizing the Sample Principal Components

• The $n \times p$ data matrix of standardized observations

$$\mathbf{Z} = \left[egin{array}{c} \mathbf{z}'_1 \ \mathbf{z}'_2 \ dots \ \mathbf{z}'_n \end{array}
ight] = \left[egin{array}{cccc} z_{11} & z_{12} & \cdots & z_{1p} \ z_{21} & z_{22} & \cdots & z_{2p} \ dots & dots & \ddots & dots \ z_{n1} & z_{n2} & \cdots & z_{np} \end{array}
ight]$$

- Verify that $\bar{\mathbf{z}} = \frac{1}{n} (\mathbf{1}'\mathbf{Z})' = \frac{1}{n} \mathbf{Z}' \mathbf{1} = \mathbf{0}$ and $\mathbf{S}_z = \mathbf{R}$, where \mathbf{R} is the correlation matrix.
- The *i*th principal component, i = 1, 2, ..., p, is

$$\hat{y}_i=\hat{\mathbf{e}}_i'\mathbf{z}=\hat{e}_{i1}z_1+\hat{e}_{i2}z_2+\cdots+\hat{e}_{ip}z_p$$
 Sample variance $(\hat{y}_i)=\hat{\lambda}_i$

Sample covariance $(\hat{y}_i, \hat{y}_k) = 0, i \neq k$

where $(\hat{\lambda}_i, \hat{\mathbf{e}}_i)$ is the ith eigenvalue-eigenvector pair of \mathbf{R} with $\hat{\lambda}_1 \geq \hat{\lambda}_2 \geq \cdots \geq \hat{\lambda}_p \geq 0$.

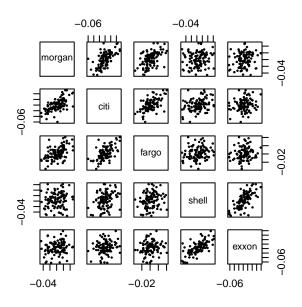
Principal Components for stock return data - Exercise 8.10

The weekly rates of return for five stocks listed on the New York Stock Exchange are given in T8-4.DAT.

- Construct the sample covariance matrix S, and find the sample principal components.
- Determine the proportion of the total sample variance explained by the first three principal components. Interpret the components.
- Given the results, do you feel that the stock rates-of-terun data can be summarized in fewer than five dimensions? Explain.

```
# morgan citi fargo shell exxon
# 0.00106 0.00066 0.00163 0.00405 0.00404
```

pairs(stock, cex = 0.3)



Compute principal components for standardized data scale = TRUE will result in all variables being scaled to have unit variance (i.e. a variance of 1, and hence a standard deviation of 1).

```
# Standard deviations (1, .., p=5):
# [1] 1.56 1.19 0.71 0.63 0.51
#
# Rotation (n \times k) = (5 \times 5):
#
          PC1 PC2 PC3 PC4 PC5
# morgan -0.47 0.37 -0.604 0.36 0.384
# citi -0.53 0.24 -0.136 -0.63 -0.496
# fargo -0.47 0.32 0.772 0.29 0.071
# shell -0.39 -0.59 0.093 -0.38 0.595
\# exxon = -0.36 - 0.61 - 0.109 = 0.49 - 0.498
```

(stock.pcomp <- prcomp(stock, scale = T))</pre>

eigenvalues
stock.pcomp\$sdev^2

Checking

Check calculations of principal components by computing eigenvalues/eigenvectors and proportion explained from the standardized data

```
(R <- cor(stock))
```

```
# morgan citi fargo shell exxon
# morgan 1.00 0.63 0.51 0.11 0.15
# citi 0.63 1.00 0.57 0.32 0.21
# fargo 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
```

```
eigen.stock <- eigen(R)
eigen.stock$values</pre>
```

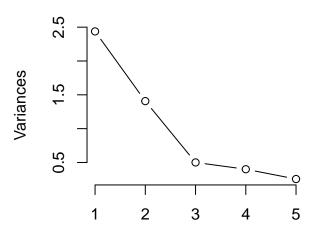
```
# [1] 2.44 1.41 0.50 0.40 0.26
```

Screeplot - Stocks Data

Screeplot order eigenvalues from largest to smallest.

```
screeplot(stock.pcomp, npcs = 5, type = "lines")
```

stock.pcomp



Stock Data via Principal Components

Using the standardized variables, the first two sample principal components

$$\hat{y}_1 = \hat{\mathbf{e}}_1 \mathbf{z} = .469z_1 + .532z_2 + .465z_3 + .387z_4 + .361z_5$$

$$\hat{y}_2 = \hat{\mathbf{e}}_2 \mathbf{z} = -.368z_1 - .236z_2 - .315z_3 + .585z_4 + .606z_5$$

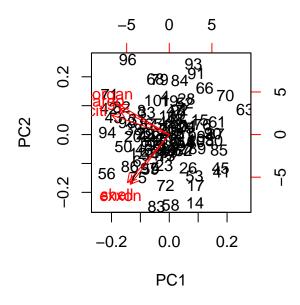
These components account for

$$\left(\frac{\hat{\lambda}_1 + \hat{\lambda}_2}{p}\right) 100\% = \left(\frac{2.437 + 1.407}{5}\right) 100\% = 77\%$$

of the total (standardized) sample variance.

 The first component is a roughly equally weighted sum, or "index" of the five stocks. This component might be called a market component.

biplot(stock.pcomp)



- The second component represents a contrast between the banking stocks (JP Morgan, Citibank, Wells Fargo) and the oil stocks (Royal Dutch Shell, Exxon-Mobil). It might be called an industry component.
- We see that most of the variation in these stock returns is due to market activity and uncorrelated industry activity.