Chapter 12:

Principal Component Analysis

- §12.1 Introduction
- §12.2 Geometric and algebraic bases of principal components
- §12.4 Plotting of principal components
- §12.5 Principal components from the correlation matrix
- §12.6 Decide how many components to retain
- §12.8 Interpretation of principal components



• Example: We might want to rank students on the basis of their scores on achievement tests in English, mathematics, reading, and so on. An average score would provide a single scale on which to compare the students, but with unequal weights we can spread the students out further on the scale and obtain a better ranking.

- Example: We might want to rank students on the basis of their scores on achievement tests in English, mathematics, reading, and so on. An average score would provide a single scale on which to compare the students, but with unequal weights we can spread the students out further on the scale and obtain a better ranking.
- In *Principal Component Analysis* (PCA), we seek to maximize the variance of a linear combination of p variables from a single sample

$$z = a'y = a_1y_1 + a_2y_2 + \dots + a_py_p$$

- Example: We might want to rank students on the basis of their scores on achievement tests in English, mathematics, reading, and so on. An average score would provide a single scale on which to compare the students, but with unequal weights we can spread the students out further on the scale and obtain a better ranking.
- In *Principal Component Analysis* (PCA), we seek to maximize the variance of a linear combination of p variables from a single sample

$$z = a'y = a_1y_1 + a_2y_2 + \dots + a_py_p$$

• Those linear combinations are called *principal components* (PC). There are totally p such components.

- Example: We might want to rank students on the basis of their scores on achievement tests in English, mathematics, reading, and so on. An average score would provide a single scale on which to compare the students, but with unequal weights we can spread the students out further on the scale and obtain a better ranking.
- In *Principal Component Analysis* (PCA), we seek to maximize the variance of a linear combination of p variables from a single sample

$$z = a'y = a_1y_1 + a_2y_2 + \dots + a_py_p$$

- Those linear combinations are called *principal components* (PC). There are totally p such components.
- The first PC is the linear combination with maximal variance, i.e., a dimension along which the observations are maximally spread out.

- Example: We might want to rank students on the basis of their scores on achievement tests in English, mathematics, reading, and so on. An average score would provide a single scale on which to compare the students, but with unequal weights we can spread the students out further on the scale and obtain a better ranking.
- In *Principal Component Analysis* (PCA), we seek to maximize the variance of a linear combination of p variables from a single sample

$$z = a'y = a_1y_1 + a_2y_2 + \dots + a_py_p$$

- Those linear combinations are called *principal components* (PC). There are totally p such components.
- The first PC is the linear combination with maximal variance, i.e., a dimension along which the observations are maximally spread out.
- The second PC is the linear combination with maximal variance in a direction orthogonal to the first PC, and so on.

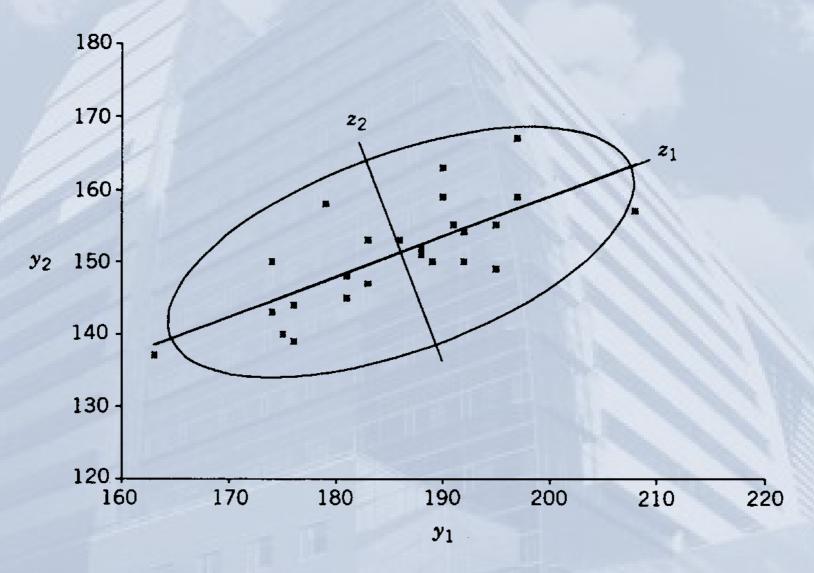
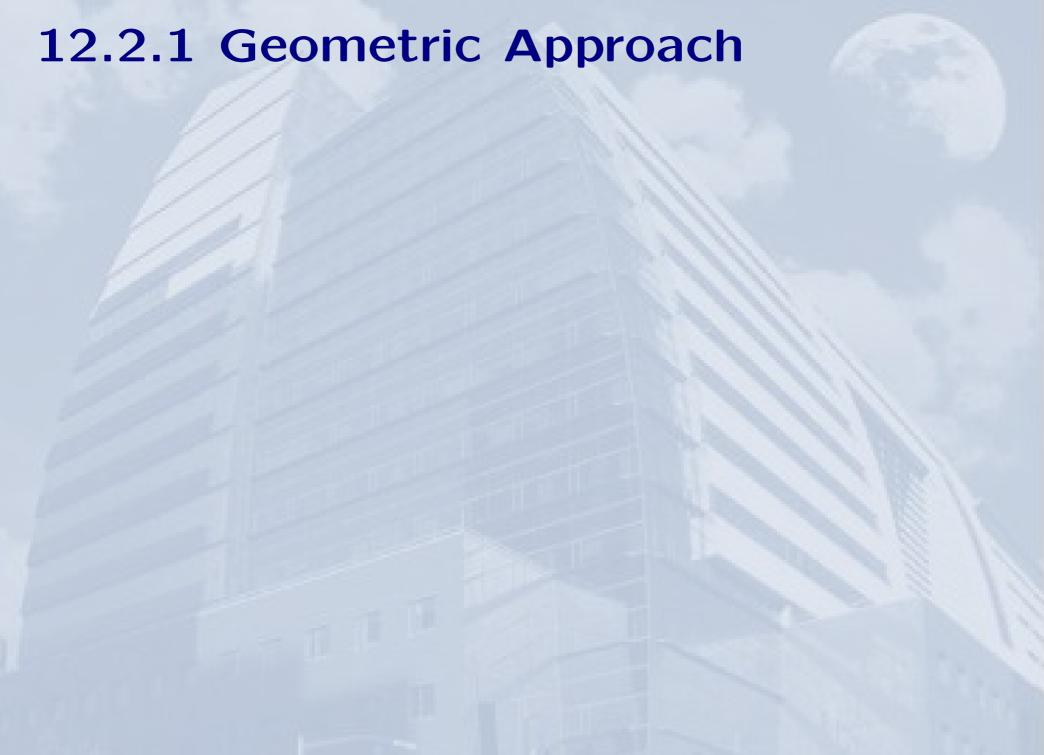


Figure 12.1. Principal component transformation for the sons data.



• Let y_1, \ldots, y_n be a p-dimmensional multivariate sample.

- Let y_1, \ldots, y_n be a p-dimmensional multivariate sample.
- Center the data $\mathbf{y}_i \bar{\mathbf{y}}$ to make $\bar{\mathbf{y}}_{new} = \mathbf{0}$ ($\bar{\mathbf{y}}$ at origin).

- Let y_1, \ldots, y_n be a p-dimmensional multivariate sample.
- Center the data $\mathbf{y}_i \bar{\mathbf{y}}$ to make $\bar{\mathbf{y}}_{new} = \mathbf{0}$ ($\bar{\mathbf{y}}$ at origin).
- Rotate axes to find a new coordinate system, where the data are maximally spread out along new directions.

- Let y_1, \ldots, y_n be a p-dimmensional multivariate sample.
- Center the data $\mathbf{y}_i \bar{\mathbf{y}}$ to make $\bar{\mathbf{y}}_{new} = \mathbf{0}$ ($\bar{\mathbf{y}}$ at origin).
- Rotate axes to find a new coordinate system, where the data are maximally spread out along new directions.
- For each observation y, find p principal components

$$z_1 = \mathbf{a}_1' \mathbf{y}, \quad z_2 = \mathbf{a}_2' \mathbf{y}, \quad \dots \quad , z_p = \mathbf{a}_p' \mathbf{y}$$

- Let y_1, \ldots, y_n be a p-dimmensional multivariate sample.
- Center the data $\mathbf{y}_i \bar{\mathbf{y}}$ to make $\bar{\mathbf{y}}_{new} = \mathbf{0}$ ($\bar{\mathbf{y}}$ at origin).
- Rotate axes to find a new coordinate system, where the data are maximally spread out along new directions.
- For each observation y, find p principal components

$$z_1 = \mathbf{a}_1' \mathbf{y}, \quad z_2 = \mathbf{a}_2' \mathbf{y}, \quad \dots \quad , z_p = \mathbf{a}_p' \mathbf{y}$$

$$- \operatorname{Var}(z_1) > \operatorname{Var}(z_2) > \cdots > \operatorname{Var}(z_p)$$

- Let y_1, \ldots, y_n be a p-dimmensional multivariate sample.
- Center the data $\mathbf{y}_i \bar{\mathbf{y}}$ to make $\bar{\mathbf{y}}_{new} = \mathbf{0}$ ($\bar{\mathbf{y}}$ at origin).
- Rotate axes to find a new coordinate system, where the data are maximally spread out along new directions.
- For each observation y, find p principal components

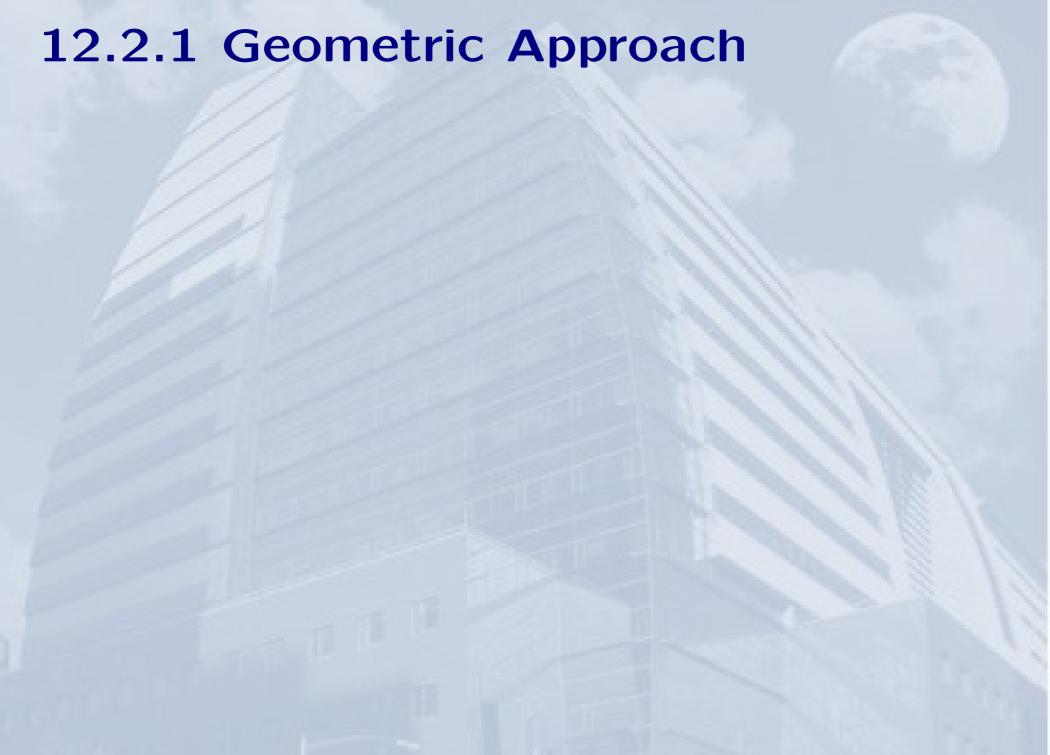
$$z_1 = \mathbf{a}_1' \mathbf{y}, \quad z_2 = \mathbf{a}_2' \mathbf{y}, \quad \dots \quad , z_p = \mathbf{a}_p' \mathbf{y}$$

- $\operatorname{Var}(z_1) > \operatorname{Var}(z_2) > \cdots > \operatorname{Var}(z_p)$
- $-\operatorname{Cov}(z_i,z_j)=0$ for $i\neq j$

- Let y_1, \ldots, y_n be a p-dimmensional multivariate sample.
- Center the data $\mathbf{y}_i \bar{\mathbf{y}}$ to make $\bar{\mathbf{y}}_{new} = \mathbf{0}$ ($\bar{\mathbf{y}}$ at origin).
- Rotate axes to find a new coordinate system, where the data are maximally spread out along new directions.
- For each observation y, find p principal components

$$z_1 = a'_1 y, \quad z_2 = a'_2 y, \quad \dots \quad , z_p = a'_p y$$

- $Var(z_1) > Var(z_2) > \cdots > Var(z_p)$
- $-\operatorname{Cov}(z_i, z_j) = 0$ for $i \neq j$
- The p PCs are uncorrelated, but not necessarily independent (need normality assumption).



• Let **S** be the single sample covariance matrix.

- Let S be the single sample covariance matrix.
- Recall eigen-decomposition: S = CDC', where D is a diagonal matrix of eigenvalues $\lambda_1, \ldots, \lambda_p$ and C is an orthogonal matrix of corresponding eigenvectors.

- Let S be the single sample covariance matrix.
- Recall eigen-decomposition: S = CDC', where D is a diagonal matrix of eigenvalues $\lambda_1, \ldots, \lambda_p$ and C is an orthogonal matrix of corresponding eigenvectors.
- We take a_i to be the *i*th eigenvector of S, then

$$Var(z_i) = Var(\mathbf{a}_i'\mathbf{y}) = \lambda_i$$

 $Cov(z_i, z_j) = Cov(\mathbf{a}_i'\mathbf{y}, \mathbf{a}_j'\mathbf{y}) = 0$

- Let S be the single sample covariance matrix.
- Recall eigen-decomposition: S = CDC', where D is a diagonal matrix of eigenvalues $\lambda_1, \ldots, \lambda_p$ and C is an orthogonal matrix of corresponding eigenvectors.
- We take a_i to be the *i*th eigenvector of S, then

$$Var(z_i) = Var(\mathbf{a}_i'\mathbf{y}) = \lambda_i$$

 $Cov(z_i, z_j) = Cov(\mathbf{a}_i'\mathbf{y}, \mathbf{a}_j'\mathbf{y}) = 0$

• The z_1 has the largest variance λ_1 , followed by z_2 , z_3 , etc.

- Let S be the single sample covariance matrix.
- Recall eigen-decomposition: S = CDC', where D is a diagonal matrix of eigenvalues $\lambda_1, \ldots, \lambda_p$ and C is an orthogonal matrix of corresponding eigenvectors.
- We take a_i to be the *i*th eigenvector of S, then

$$Var(z_i) = Var(\mathbf{a}_i'\mathbf{y}) = \lambda_i$$

 $Cov(z_i, z_j) = Cov(\mathbf{a}_i'\mathbf{y}, \mathbf{a}_j'\mathbf{y}) = 0$

- The z_1 has the largest variance λ_1 , followed by z_2 , z_3 , etc.
- We represent the p-dimmentional data with first k principal components that account for a large proportion of the total variation.

- Let S be the single sample covariance matrix.
- Recall eigen-decomposition: S = CDC', where D is a diagonal matrix of eigenvalues $\lambda_1, \ldots, \lambda_p$ and C is an orthogonal matrix of corresponding eigenvectors.
- We take a_i to be the *i*th eigenvector of S, then

$$Var(z_i) = Var(\mathbf{a}_i'\mathbf{y}) = \lambda_i$$

 $Cov(z_i, z_j) = Cov(\mathbf{a}_i'\mathbf{y}, \mathbf{a}_j'\mathbf{y}) = 0$

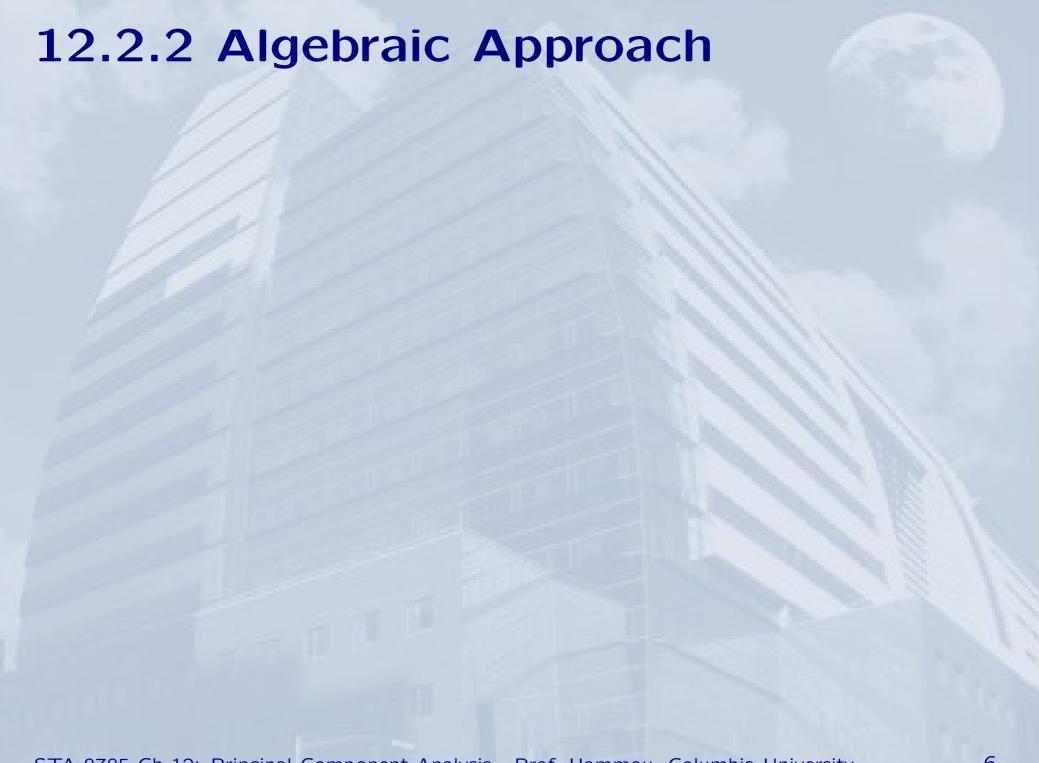
- The z_1 has the largest variance λ_1 , followed by z_2 , z_3 , etc.
- We represent the p-dimmentional data with first k principal components that account for a large proportion of the total variation.
- PCA can be applied to any distribution of y.

- Let S be the single sample covariance matrix.
- Recall eigen-decomposition: S = CDC', where D is a diagonal matrix of eigenvalues $\lambda_1, \ldots, \lambda_p$ and C is an orthogonal matrix of corresponding eigenvectors.
- We take a_i to be the *i*th eigenvector of S, then

$$Var(z_i) = Var(\mathbf{a}_i'\mathbf{y}) = \lambda_i$$

 $Cov(z_i, z_j) = Cov(\mathbf{a}_i'\mathbf{y}, \mathbf{a}_j'\mathbf{y}) = 0$

- The z_1 has the largest variance λ_1 , followed by z_2 , z_3 , etc.
- We represent the p-dimmentional data with first k principal components that account for a large proportion of the total variation.
- PCA can be applied to any distribution of y.
- Show Example 12.2.1 (p.384).



The variance of a PC is

$$Var(z) = Var(a'y) = a'Sa.$$

The variance of a PC is

$$Var(z) = Var(a'y) = a'Sa.$$

• The $z_1 = \mathbf{a}_1' \mathbf{y}$ can be obtained by maximizing

$$\lambda = \frac{a'Sa}{a'a}.$$

The variance of a PC is

$$Var(z) = Var(a'y) = a'Sa.$$

• The $z_1 = \mathbf{a}_1' \mathbf{y}$ can be obtained by maximizing

$$\lambda = \frac{a'Sa}{a'a}.$$

• It can be shown that maximum $\lambda = largest eigenvalue of S$, and a_1 is the corresponding eigenvector.

The variance of a PC is

$$Var(z) = Var(a'y) = a'Sa.$$

• The $z_1 = \mathbf{a}_1' \mathbf{y}$ can be obtained by maximizing

$$\lambda = \frac{a'Sa}{a'a}.$$

- It can be shown that maximum $\lambda = \text{largest eigenvalue}$ of S, and a_1 is the corresponding eigenvector.
- Unlike discriminant analysis or canonical correlation, S can be singular (S^{-1} does not exist) in PCA, and zero eigenvalues and their eigenvectors can be ignored.

The variance of a PC is

$$Var(z) = Var(a'y) = a'Sa.$$

• The $z_1 = \mathbf{a}_1' \mathbf{y}$ can be obtained by maximizing

$$\lambda = \frac{a'Sa}{a'a}.$$

- It can be shown that maximum $\lambda = largest eigenvalue of S$, and a_1 is the corresponding eigenvector.
- Unlike discriminant analysis or canonical correlation, S can be singular (S^{-1} does not exist) in PCA, and zero eigenvalues and their eigenvectors can be ignored.
- Show Example 12.2.2 (p.386)

Motivation

Motivation

 Generally, extracting components from S rather than R remains closer to the spirit and intent of PCA, especially if the components are to be used in further computations.

Motivation

- Generally, extracting components from S rather than R remains closer to the spirit and intent of PCA, especially if the components are to be used in further computations.
- In some cases, the PCs will be more interpretable if R is used.

Motivation

- Generally, extracting components from S rather than R remains closer to the spirit and intent of PCA, especially if the components are to be used in further computations.
- In some cases, the PCs will be more interpretable if R is used.
- For example, if the variances differ widely or if the measurement units are not commensurate, the PCs of S will be dominated by the variables with large variances. The other variables will contribute very little. For a more balanced representation in such cases, the PCs of R may be used.

Properties

Properties

• The R has different eigenvalues than S.

- The R has different eigenvalues than S.
- The PCs from R differ from those obtained from S.

- The R has different eigenvalues than S.
- The PCs from R differ from those obtained from S.
- The percent of variance accounted for by each PC of R will differ from the percent for S.

- The R has different eigenvalues than S.
- The PCs from R differ from those obtained from S.
- The percent of variance accounted for by each PC of R will differ from the percent for S.
- The PCs from R are scale invariant.

- The R has different eigenvalues than S.
- The PCs from R differ from those obtained from S.
- The percent of variance accounted for by each PC of R will differ from the percent for S.
- The PCs from R are scale invariant.
- Different R matrices may produce the same PCs.

- The R has different eigenvalues than S.
- The PCs from R differ from those obtained from S.
- The percent of variance accounted for by each PC of R will differ from the percent for S.
- The PCs from R are scale invariant.
- Different R matrices may produce the same PCs.
- Show example on page 397.

• Retain as many components as needed to achieve a pre-specified percentage of variance, say 80%.

- Retain as many components as needed to achieve a pre-specified percentage of variance, say 80%.
- Retain components with eigenvalues above the average.

- Retain as many components as needed to achieve a pre-specified percentage of variance, say 80%.
- Retain components with eigenvalues above the average.
- Use *scree graph*, a plot of λ_i versus i, and look for a natural break between the OlargeÓ eigenvalues and the OsmallÓ eigenvalues.

- Retain as many components as needed to achieve a pre-specified percentage of variance, say 80%.
- Retain components with eigenvalues above the average.
- Use *scree graph*, a plot of λ_i versus i, and look for a natural break between the OlargeO eigenvalues and the OsmallO eigenvalues.

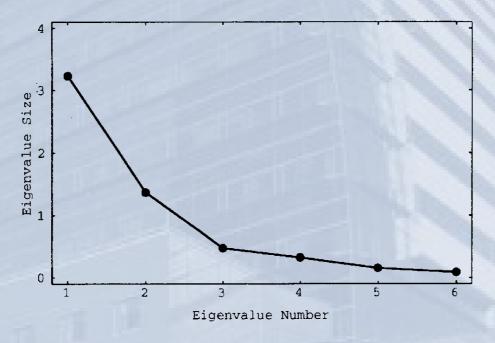


Figure 12.8. Scree graph for eigenvalues of modified football data.

- Retain as many components as needed to achieve a pre-specified percentage of variance, say 80%.
- Retain components with eigenvalues above the average.
- Use scree graph, a plot of λ_i versus i, and look for a natural break between the OlargeO eigenvalues and the OsmallO eigenvalues.

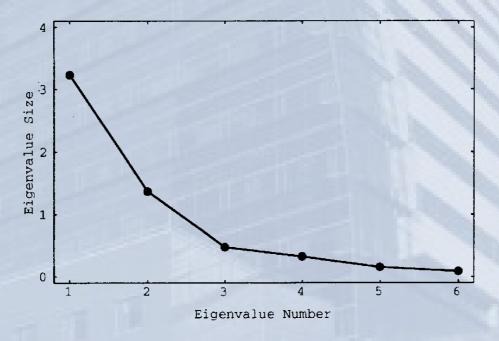


Figure 12.8. Scree graph for eigenvalues of modified football data.

• Show Example 12.6 (p.400).



 The PC's from S and R are NOT compatible, and will have different interpretations.

- The PC's from S and R are NOT compatible, and will have different interpretations.
- The absolute value of a coefficient in PC shows the contribution of corresponding variable.

- The PC's from S and R are NOT compatible, and will have different interpretations.
- The absolute value of a coefficient in PC shows the contribution of corresponding variable.
- If one variable has a much larger variance than other variables, this variable will dominate the first component, which will account for most of the variance.

- The PC's from S and R are NOT compatible, and will have different interpretations.
- The absolute value of a coefficient in PC shows the contribution of corresponding variable.
- If one variable has a much larger variance than other variables, this variable will dominate the first component, which will account for most of the variance.
- A component will duplicate a variable when the variable is uncorrelated with the other variables, i.e., $z_i = \mathbf{a}_i' \mathbf{y} = y_i, \ i = 1, \dots, p$.

- The PC's from S and R are NOT compatible, and will have different interpretations.
- The absolute value of a coefficient in PC shows the contribution of corresponding variable.
- If one variable has a much larger variance than other variables, this
 variable will dominate the first component, which will account for
 most of the variance.
- A component will duplicate a variable when the variable is uncorrelated with the other variables, i.e., $z_i = \mathbf{a}_i' \mathbf{y} = y_i, \ i = 1, \dots, p$.
- All elements of the first eigenvector a₁ are positive if all correlations or covariances are positive.

- The PC's from S and R are NOT compatible, and will have different interpretations.
- The absolute value of a coefficient in PC shows the contribution of corresponding variable.
- If one variable has a much larger variance than other variables, this
 variable will dominate the first component, which will account for
 most of the variance.
- A component will duplicate a variable when the variable is uncorrelated with the other variables, i.e., $z_i = \mathbf{a}_i' \mathbf{y} = y_i, \ i = 1, \dots, p$.
- All elements of the first eigenvector a₁ are positive if all correlations or covariances are positive.
- Show Example 12.8.1 (p.403).