

Ch11-A Principal Component Analysis

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11A Subsections

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A.1 Principal Component Analysis

- Unsupervised Learning
- Can be part of exploratory data analysis
- No way to check your work
- Dimensionality reduction technique
- Ex.
 - Cancer researcher might look at gene expression levels in 100 patients
 - Online Shopping site

A.2 Princial Component

- Low-dimentional representation of data
- Can't see all paired scatterplot
- Which low-dimentional plot will make the observations most distinctive?
- The first principal component of i th observation is

$$Z_{i1} = \phi_{11}X_{i1} + \phi_{21}X_{i2} + \cdots + \phi_{p1}X_{ip}$$

- normalized: $\sum_{j=1}^p \phi_{j1}^2 = 1$.
- loadings: $\phi_{11}, \dots, \phi_{p1}$
- orthogonal: $\sum_{j=1}^p \phi_{j1}\phi_{j2} = 0$.

A.3 Computing 1st PC

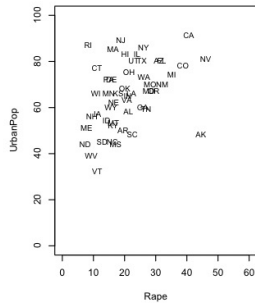
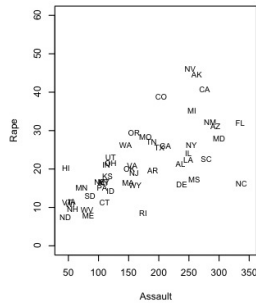
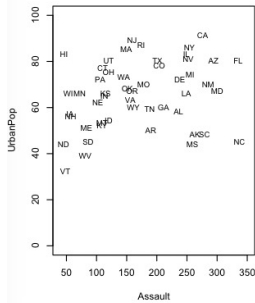
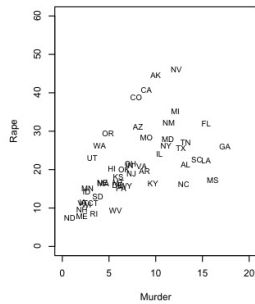
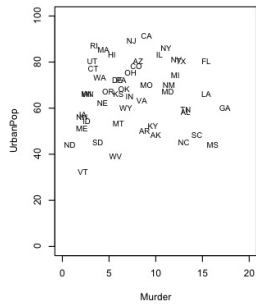
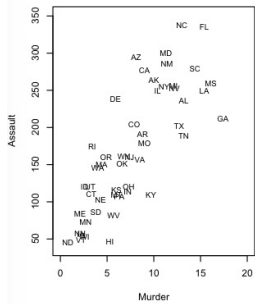
- Low-dimensional representation of data
- Can't see all paired scatterplot
- Which low-dimensional plot will make the observations most distinctive?
- The first principal component

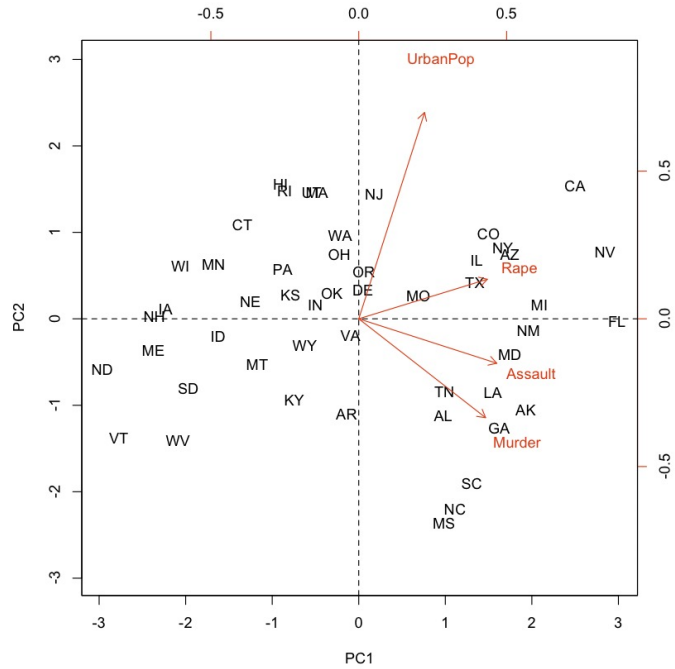
$$\text{Maximize}_{\phi_{11}, \dots, \phi_{p1}} \left\{ \frac{1}{n} \sum_{i=1}^n \left\{ \sum_{j=1}^p \phi_{j1} x_{ij} \right\}^2 \right\} \quad \text{subject to} \quad \sum_{h=1}^p \phi_{h1}^2 = 1.$$

- It's maximizing average of Z_{i1}^2 .
- Same as maximizing variance of Z_{i1}
- PC1 is the direction that the data varies the most.

- Second PC is same, but maximizing variance of Z_{i2} that is uncorrelated with Z_{i1} .
- PC2 will be orthogonal to PC1.

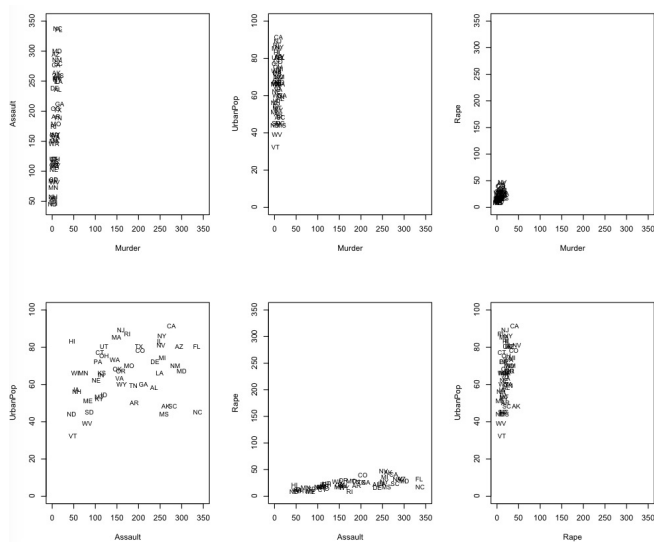
A.4 Example:





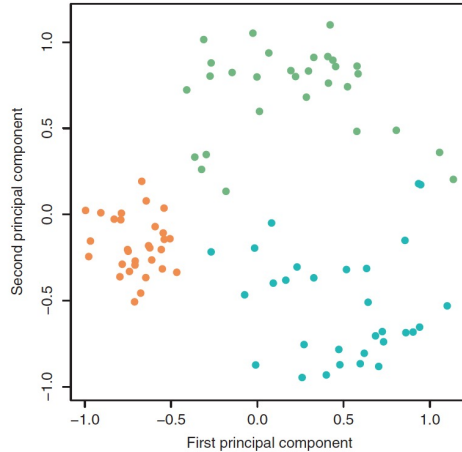
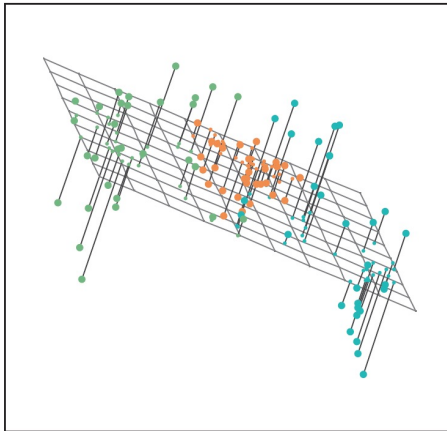
A.5 Scaling

- Scaling is important



A.6 Another Interpretation

- First two PC makes up a linear surface that is CLOSEST to obs.



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A.7 PVE

- Proportion of Variation Explained
- Total variance in the data

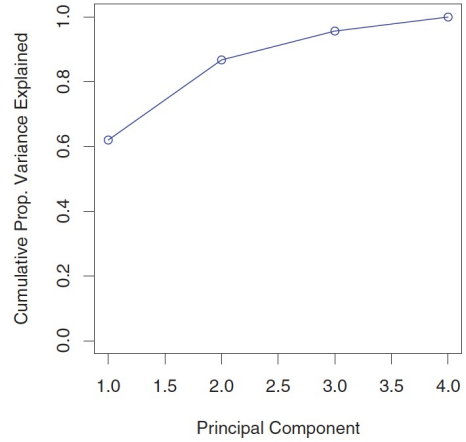
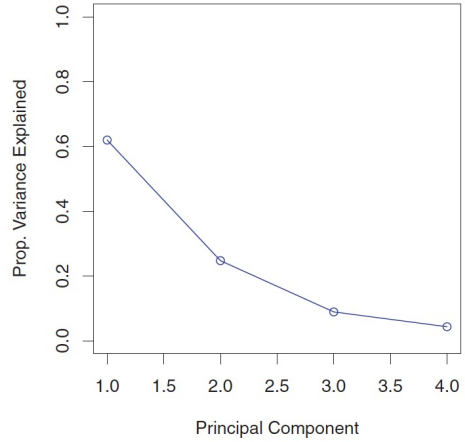
$$\sum_{j=1}^p \text{Var}(X_j) = \sum_{j=1}^p \frac{1}{n} \sum_{i=1}^n x_{ij}^2$$

- Variance explained by the m th PC is

$$\frac{1}{n} \sum_{i=1}^n Z_{im}^2$$

- PVE

$$\frac{\sum_{i=1}^n Z_{im}^2}{\sum_{j=1}^p \sum_{i=1}^n x_{ij}^2}$$



Some of the figures in this presentation are taken from "An Introduction to Statistical Learning, with applications in R" (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani