Lecture 1
Overview

DSA 8070 Multivariate Analysis

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Notes

Agenda

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Introduction

- In many observational or experimental studies, measurements are collected simultaneously on more than one variable on each unit

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> head(Boston)
     crim zn indus chas   nox    rm  age    dis rad tax ptratio  black lstat medv
1 0.00632 18  2.31    0 0.538 6.575 65.2 4.0900   1 296    15.3 396.90  4.98 24.0
2 0.02731  0  7.07    0 0.469 6.421 78.9 4.9671   2 242    17.8 396.90  9.14 21.6
3 0.02729  0  7.07    0 0.469 7.185 61.1 4.9671   2 242    17.8 392.83  4.03 34.7
4 0.03237  0  2.18    0 0.458 6.998 45.8 6.0622   3 222    18.7 394.63  2.94 33.4
5 0.06905  0  2.18    0 0.458 7.147 54.2 6.0622   3 222    18.7 396.90  5.33 36.2
6 0.02985  0  2.18    0 0.458 6.430 58.7 6.0622   3 222    18.7 394.12  5.21 28.7
```

- Multivariate analysis is the collection of statistical methods that can be used to (jointly) analyze these multiple measurements
  $\Rightarrow$ *some are extensions of familiar methods (t-test, ANOVA, Linear Regression, ...) while others are unique to multivariate analysis (PCA, CCA, Factor Analysis, ...)*

- The idea is to exploit potential "correlations" among the multiple measurements to improve inference

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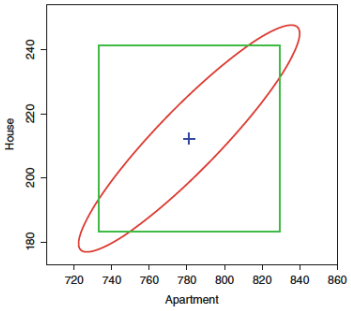
Importance of Multivariate Analysis

- If all the variables are independent, one can't do better than analyze each variable's behavior by using histograms or box plots, looking at the means, medians, variances and other 'one dimensional statistics'
- However if some of the variables are acting together, either that they are positively correlated or that they inhibit each other, one will miss a lot of important information by slicing the data up into those column vectors and studying them separately
- Thus important connections between variables are only available to us if we consider the data as a whole.

Notes

Using Multivariate Methods Could Lead to Sharper Inference



Source: Fig. 1.1 of Applied Multivariate Statistics with R by Zelterman

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Objectives of Multivariate Analysis

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Dimensionality Reduction or Structural Simplification

- Goal: to reduce the "dimensionality" by considering a small number of (linear) combinations of a large number of measurements without losing important information
- Examples:
  - A single index of patient reaction to radiotherapy can be constructed from measurements on several response variables
  - Wildlife ecologists can construct a few indices of habitat preference from measurements of dozens of features of nesting sites selected by a certain bird species
- Techniques:
  - **Principal Component Analysis** (Week 9)
  - **Factor Analysis** (Week 10)
  - **Multidimensional Scaling** (Week 14)

Notes

Grouping or Classification

- Goal: to **identify** groups of "similar" units or to **classify** units into previously defined groups
- Examples:
  - Using the concentration of elements (copper, silver, tin, antimony) in the lead alloy used in bullets, the FBI **identifies** 'similar' bullets that may be used to infer whether bullets were produced from the same batch of lead
  - The US IRS uses data collected from tax returns (income, amount withheld, deductions, ...) to **classify** taxpayers into two groups: those who will be audited and those who will not
- Techniques:
  - **Classification Analysis** (Week 12)
  - **Cluster Analysis** (Week 13)

Notes

Dependence among Variables and Prediction

- Goal: to estimate the relationship among variables and to predict the value of some of them given information on the others
- Examples:
  - The associations between measures of risk-taking propensity and measures of socioeconomic characteristics for top-level business executives were used to assess the relation between risk-taking behavior and performance
  - The association between test scores, and several college performance variables were used to develop predictors of success in college
- Techniques:
  - **Multivariate Regression** (Week 7)
  - **Repeated Measures Analysis** (Week 8)
  - **Canonical Correlation Analysis** (Week 11)

Notes

Hypothesis Testing

- Goal: to test if differences in sets of response mean vectors for two or more groups large enough to be distinguished from sampling variation
- Examples:
  - A transportation company wants to know if means for gasoline mileage, repair costs, downtime due to repairs differ for different truck models
  - An insurance company wants to know if changing case management practices leads to changes in mean length of hospital stay, mean infection rates, and mean costs
- Techniques:
  - **Hotelling's T^2 and MAVONA** (Week 5 and Week 6)

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Useful Concepts/Tools for Multivariate Analysis

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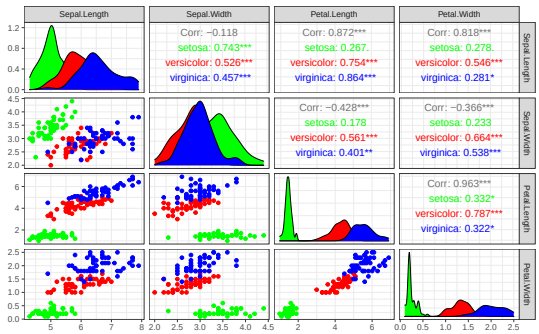
Exploratory Data Analysis [EDA, Tukey 1977]



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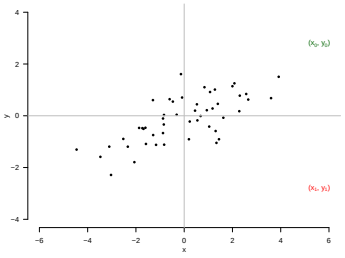
Statistical Distance

Multivariate methods rely on "distances" between data points: clustering (group units that are "close"); classification (allocate each unit to the "closest" group)



Question: which one ((x_0, y_0) or (x_1, y_1)) is closer the center of the observations? ⇒ We will learn **Mahalanobis distance** to formally answer this question

Notes

Matrix Algebra (Week 3)

The study of multivariate methods is greatly facilitated by the use of matrix algebra

- Many operations performed on multivariate data are presented using vector/matrix notation, e.g., $\boldsymbol{X}_{n\times p}$ (Data matrix); $\hat{\boldsymbol{\mu}}_{p\times 1}$ (estimated mean vector); $\hat{\boldsymbol{\Sigma}}_{p\times p}$ (estimated covaraince matrix)
- The computation of eigenvalues and eigenvectors (i.e., the **spectral decomposition**) plays an important role in multivariate analysis
- We will use R to perform the needed matrix operations

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Multivariate Normal Distribution (Week 4)

- We will often assume the joint distribution of $\boldsymbol{X} = (X_1, X_2, \cdots, X_p)^{\mathrm{T}}$ follows a multivariate normal distribution with the probability density function:

$$f(\boldsymbol{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{\frac{d}{2}}\det(\boldsymbol{\Sigma})^{\frac{1}{2}}} \exp\left[-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu})\right]$$

- The multivariate normal assumption is often appropriate:
  - Variables can sometimes be assumed to be multivariate normal (perhaps after transformation)
  - Central limit theorem tells us that distribution of many **multivariate sample statistics** is approximately normal, regardless of the form of the population distribution

Notes

Data Mining, Machine Learning, and Multivariate Analysis

- Data Mining is the process of extracting and discovering patterns (e.g., unexpected structures or relationships, trends, clusters, and outliers) in **massive data sets**
- Supervised learning and unsupervised learning are two most common problems in machine learning
- Data mining/machine learning applications usually involve many variables, often related in complex ways, hence techniques from multivariate analysis play an important role

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