Stat 501: Introduction to Multivariate Statistical Analysis

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Introduction

- In many observational or designed studies, observations are collected simultaneously on more than one variable on each experimental unit.
- Multivariate analysis is the collection of methods that can be used to collectively analyze these multiple measurements.
- Idea is to exploit potential correlations among the multiple measurements to improve inference.
- Most multivariate techniques rely on an underlying probability model
  - For the continuous variables, the most common model is the *multivariate normal* distribution, but other models are also possible.
  - For discrete cases, the multinomial probability distribution is commonly used for frequency data from multiple categories when assumptions allow.
  - There are also techniques that are “model-free” and do not follow any distribution.

Objectives of Multivariate Analysis

- *Dimensionality Reduction*: Can we reduce the dimensionality of the problem by considering a small number of (linear) combinations of a large number of measurements without losing important information?
- *Grouping*: Identify groups of 'similar' units using a common set of measured traits.
- *Classification*: Classify units into previously defined groups using a common set of measured traits.
- *Dependence among variables*: What is the nature of associations among variables?
- *Prediction*: If variables are associated, then we might be able to predict the value of some of them given information on the others.
- *Hypothesis testing*: Are differences in sets of response means for two or more groups large enough to be distinguished from sampling variation?

Examples – Dimensionality Reduction

- Running times over 10 km intervals of participants in 100 km ultra-marathon. Of interest is to see if a few times characterize their performances.
- Carapace length, width and height of tortoises. Of interest is to see if there is a single combination of these carapace measurements which can characterize aspects of tortoises
- In metabolomic profiling chemical compounds (about 500 compounds) are generated from samples using gas chromatography mass spectrometer (GC-MS). Of interest is to see if there are a few (say, two or three) major chemical compounds which can explan the profiles. It may well be that a few (say 2-3) linear combinations of these compounds may be enough to characterize these profiles: in this case, it is of interest to understand which compounds are the major contributors in these linear combincations.
- An index of consumer satisfaction with new car ownership can be constructed from dozens of questions on a survey.
- 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.

Examples – Classification and Grouping

- The US IRS uses data collected from tax returns (income, amount withheld, deductions, contributions to charity, age) to classify taxpayers into two groups: those who will be audited and those who will not.
- Using the concentration of elements (copper, silver, tin, antimony) in the lead alloy used in bullets, the FBI identifies 'compositional groups' of 'similar' bullets that may be used to infer whether bullets were produced from the same batch of lead.
- The USPS reads zipcodes via Optical Character Recognition (OCR) using features and a classification algorithm to sort mail.
- An insurance company wants to group customers with respect to products purchased and demographic variables to target marketing efforts at different groups
- A marketing company examines traits of people who respond or fail to respond to a mass mailing.
- An entomologist uses measurements on various physical characteristics to group insects into categories representing subspecies.

Examples – Hypothesis Testing

- 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, mean costs, measures of patient satisfaction, ...
- Water quality monitors want to know if different tillage practices lead to different patterns of nitrate concentrations in nearby waterways?
- A designed computer experiment evaluates several competing methods on the same simulated datasets for each setting. (Think of evaluating performance of several methods.) Of interest is to find out different aspects of the performance of these methods at different settings. The performance measures of these methods on a simulation dataset can not be assumed to be independent or uncorrelated because they are all evaluated on the same dataset and so the linear regression model with appropriate design matrix and homoscedastic independent univariate errors is not going to be correct or adequate.

Organization of Data and Notation

- We will use n to denote the number of individuals or units in our sample and use p to denote the number of variables measured on each unit.
- If $p = 1$, then we are back in the usual univariate setting.
- x_{ik} is the value of the k-th measurement on the i-th unit. For the i-th unit we have measurements

$$x_{i1}, x_{i2}, ..., x_{ip}$$

- We often collect all measurements taken on the i-th unit into a column vector. If five measurements are taken on the i-th unit, we would have

$$\boldsymbol{x}_i = \begin{bmatrix} x_{i1} \\ x_{i2} \\ x_{i3} \\ x_{i4} \\ x_{i5} \end{bmatrix}$$

- We often display measurements from a sample of n units in matrix form:

$$X_{n\times p} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix}$$

is a matrix with n rows (one for each unit) and p columns (one for each measured trait or variable).

Descriptive Statistics – Mean and Variance

- The sample mean of the kth variable ($k = 1, ..., p$) is computed as

$$\bar{x}_k = \frac{1}{n} \sum_{i=1}^{n} x_{ik}$$

- The sample variance of the kth variable is usually computed as

$$s_k^2 = \frac{1}{n-1} \sum_{i=1}^{n} (x_{ik} - \bar{x}_k)^2$$

  and the sample standard deviation is given by

$$s_k = \sqrt{s_k^2}$$

- Sometimes the variance is defined with a denominator of n instead of $n - 1$, and this will be clear from the notation. In this case, either the mean is known or the variance estimator will be biased.

Descriptive Statistics – Covariance and Correlation

- We often use s_{kk} to denote the sample variance for the k-th variable. Thus,

$$s_k^2 = s_{kk}$$

- The sample covariance between variable k and variable j is computed as

$$s_{jk} = \frac{1}{n-1} \sum_{i=1}^{n} (x_{ij} - \bar{x}_j)(x_{ik} - \bar{x}_k)$$

- If variables k and j are independent, the population covariance will be exactly zero, but the sample covariance will vary about zero.
- The sample correlation between variables k and j is defined as

$$r_{jk} = \frac{s_{jk}}{\sqrt{s_{jj}}\sqrt{s_{kk}}}$$

Descriptive Statistics – Properties of Sample Correlation

- r_{jk} is between -1 and 1.
- $r_{jk} = r_{kj}$
- The sample correlation is the same whether n or $n-1$ is used as the divisor in evaluating sample variances and covariances. (This is because it is a dimensionless and scale-free quantity.)
- The sample correlation is equal to the sample covariance if measurements are standardized.
- Covariance and correlation measure *linear association*. Other non-linear dependencies may exist among variables even if $r_{jk} = 0$.
- A population correlation of zero means *no linear association* but it does not necessarily imply independence
- The sample correlation (r_{ij}) will vary about the value of the population correlation (ρ_{ij})

Descriptive Statistics

- Sums of squares and cross-products:

$$a_{kk} = \sum_{i=1}^{n}(x_{ik} - \bar{x}_k)^2, \qquad k = 1, ..., p$$

$$a_{jk} = \sum_{i=1}^{n}(x_{ij} - \bar{x}_j)(x_{ik} - \bar{x}_k), \qquad k, j = 1, ..., p$$

- Sample statistics can be organized as vectors and matrices:
  - $\bar{\boldsymbol{x}}$ is the $p \times 1$ vector of sample means.
  - $\boldsymbol{S}$ is the $p \times p$ symmetric matrix of variances (on the diagonal) and covariances (the off-diagonal elements).
  - $\boldsymbol{R}$ is the $p \times p$ symmetric matrix of sample correlations. Diagonal elements are all equal to 1.

Example: Bivariate Data

- Data consist of $n = 5$ receipts from a bookstore. On each receipt we observe the total amount of the sale ($) and the number of books sold ($p = 2$). Then

$$\boldsymbol{X}_{5\times 2} = \begin{bmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \\ x_{31} & x_{32} \\ x_{41} & x_{42} \\ x_{51} & x_{52} \end{bmatrix} = \begin{bmatrix} 42 & 4 \\ 52 & 5 \\ 88 & 7 \\ 58 & 4 \\ 60 & 5 \end{bmatrix}$$

- Sample mean vector is :

$$\bar{\boldsymbol{x}} = \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \end{bmatrix} = \begin{bmatrix} 60 \\ 5 \end{bmatrix}$$

- Sample covariance matrix is

$$\boldsymbol{S} = \begin{bmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{bmatrix} = \begin{bmatrix} 294.0 & 19.0 \\ 19.0 & 1.5 \end{bmatrix}$$

- Sample correlation matrix is

$$\boldsymbol{R} = \begin{bmatrix} r_{11} & r_{12} \\ r_{21} & r_{22} \end{bmatrix} = \begin{bmatrix} 1 & 0.90476 \\ 0.90476 & 1 \end{bmatrix}$$

Data on Colleges and Universities

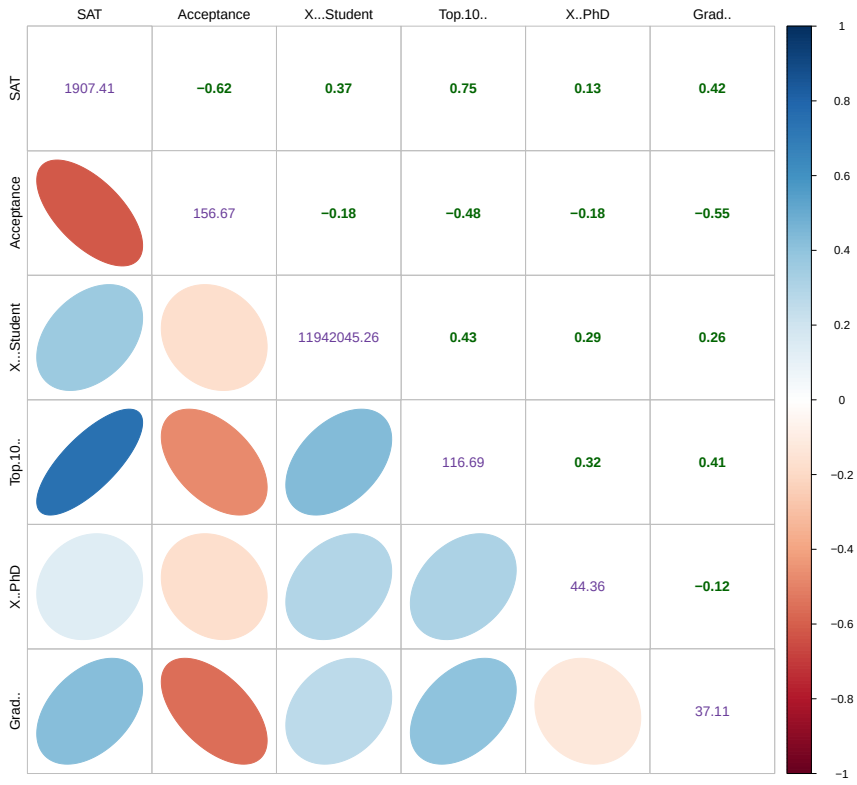
- Data in `Colleges.txt` collected from 25 top liberal arts colleges and 25 top research universities. There are 50 cases on 8 variables. Source: unknown.
- Variable Names:
  - School: Contains the name of each school
  - School_Type: Coded 'LibArts' for liberal arts and 'Univ' for university
  - SAT: Median combined Math and Verbal SAT score of students
  - Acceptance: % of applicants accepted
  - $/Student: Money spent per student in dollars
  - Top 10%: % of students in the top 10% of their h.s. graduating class
  - %PhD: % of faculty at the institution that have PhD degrees
  - Grad%: % of students at institution who eventually graduate
- **Objective:** Display variances and correlations using code in `plotcorr.R`

```
colleges <- read.table(file = "Colleges.txt", sep = "\t", header = T)

plotcorr(xx = colleges[colleges$School_Type == "Lib\ Arts", - c(1,2)])

plotcorr(xx = colleges[colleges$School_Type == "Univ", - c(1,2)])
```

Display Correlations and Variances



Liberal Arts Colleges

Universities

- Correlations are broadly similar, but not all the variances for the two groups.

Descriptive Statistics – Distance

- Multivariate methods rely on distances between units.
  - Clustering: group units that are 'closest' in some sense.
  - Classification: allocate each unit to the 'closest' group.
  - Distance can be defined in different ways.
- There are several kinds of distances:
  - Euclidean, Mahalanobis, Manhattan, etc
- Mathematically, distances have to satisfy three properties:
  1. Nonnegativity:

$$d(\boldsymbol{x}, \boldsymbol{y}) \geq 0 \quad \forall \quad \boldsymbol{x}, \boldsymbol{y} \quad \text{with equality holding for } \boldsymbol{x} = \boldsymbol{y}.$$

  2. Symmetry:

$$d(\boldsymbol{x}, \boldsymbol{y}) = d(\boldsymbol{y}, \boldsymbol{x}).$$

  3. Triangle inequality:

$$d(\boldsymbol{x}, \boldsymbol{y}) \leq d(\boldsymbol{x}, \boldsymbol{z}) + d(\boldsymbol{z}, \boldsymbol{y}) \quad \forall \quad \boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}.$$

Euclidean Distance

- Straight-line distance from a point $\boldsymbol{x} = \{x_1, x_2, ..., x_p\}'$ in p dimensions to the origin $\mathbf{0}$ is

$$d(\mathbf{0}, \boldsymbol{x}) = \sqrt{x_1^2 + x_2^2 + ... + x_p^2}$$

- All points $\boldsymbol{x}$ at an equal squared distance c^2 from the origin satisfy:

$$d^2(\mathbf{0}, \boldsymbol{x}) = x_1^2 + x_2^2 + ... + x_p^2 = \sum_{j=1}^{p} x_j^2 = \boldsymbol{x}'\boldsymbol{x} = c^2,$$

  which defines a hypersphere centered at $\mathbf{0}$.
- Euclidean distance between two arbitrary points: $\boldsymbol{x} = (x_1, x_2, \ldots, x_p)'$ and $\boldsymbol{y} = (y_1, y_2, \ldots, y_p)'$ is

$$d(\boldsymbol{x}, \boldsymbol{y}) = \sqrt{\sum_{j=1}^{p} (x_j - y_j)^2}$$

- Even though p variables may be observed with different precision, Euclidean distance gives equal weight to all.
- All points $\boldsymbol{x}$ at an equal squared distance c^2 from Q satisfy:

$$d^2(\boldsymbol{x}, \boldsymbol{y}) = \sum_{j=1}^{p} (x_j - y_j)^2 = c^2,$$

  a hypersphere centered at $\boldsymbol{y}$.

Standardized Distance

- Suppose that the variability in each of the p dimensions (variables) is different.
- We want to give more weight in the distance calculation to those dimensions (variables) that are measured more precisely.
- Weights are inversely proportional to the standard deviation in the measurements:

$$d(\boldsymbol{x}, \boldsymbol{y}) = \sqrt{\sum_{j=1}^{p} \left(\frac{x_j - y_j}{s_j} \right)^2}$$

- If we define $\boldsymbol{x} = (x_1, x_2, \ldots, x_p)'$, $\boldsymbol{y} = (y_1, y_2, \ldots, y_p)'$ and $D = diag\{s_{jj}\}$, then

$$d(\boldsymbol{x}, \boldsymbol{y}) = \sqrt{(\boldsymbol{x} - \boldsymbol{y})' \boldsymbol{D}^{-1} (\boldsymbol{x} - \boldsymbol{y})}$$

- This measure of distance does not account for correlations among variables: $\boldsymbol{D}$ is a diagonal matrix with all covariances set equal to zero.
- All points $\boldsymbol{x}$ at the same standardized distance c from the origin satisfy:

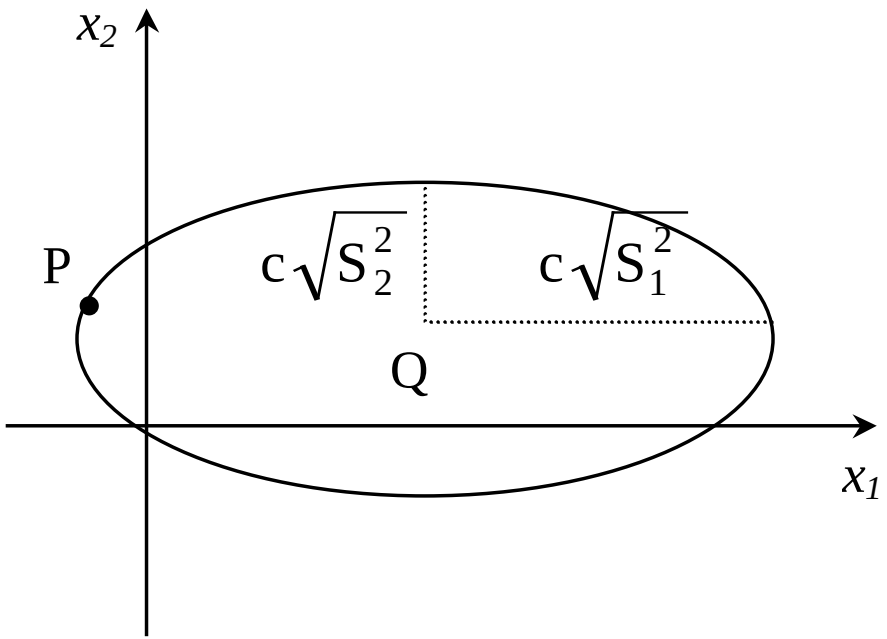
$$(\boldsymbol{x} - \boldsymbol{0})' \boldsymbol{D}^{-1} (\boldsymbol{x} - \boldsymbol{0}) = \boldsymbol{x}' \boldsymbol{D}^{-1} \boldsymbol{x} = c^2,$$

Standardized Distance

- Any $\boldsymbol{P} \equiv \boldsymbol{x}$ at a standarized distance c from $\boldsymbol{Q} \equiv \boldsymbol{y}$ satisfies

$$(\boldsymbol{P} - \boldsymbol{Q})' \boldsymbol{D}^{-1} (\boldsymbol{P} - \boldsymbol{Q}) = c^2$$

- This defines a hyper-ellipsoid centered at $\boldsymbol{Q}$, with axes parallel to the coordinates axes. The half-length of the axis parallel to the j-th coordinate axis is equal to $c\sqrt{s_{jj}}$



Other Distance Measures

- Suppose now that the various measurements do not vary independently.
- What is a reasonable distance measure when the variability in each direction is different and the variables are correlated?
- A general distance measure is

$$d(P, Q) = \sqrt{(P - Q)' A (P - Q)}$$

where A is a symmetric *positive definite* matrix, a matrix with entries $a_{jk} = a_{kj}$ such that the distances are always non-negative.

- For $p = 2$,

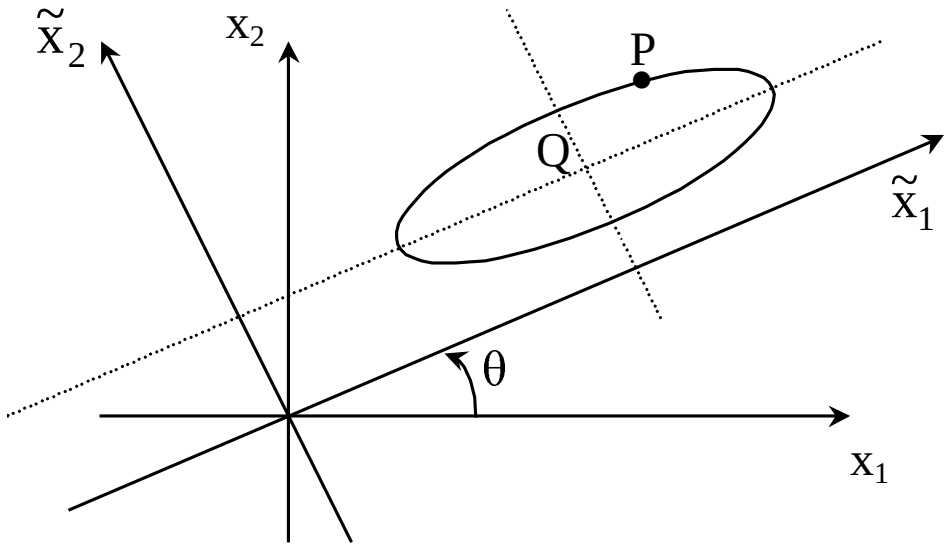
$$d(P, Q) = \sqrt{[(x_1 - y_1)^2 a_{11} + 2(x_1 - y_1)(x_2 - y_2) a_{12} + (x_2 - y_2)^2 a_{22}]}$$

Other Distance Measures

- All points $P = (x_1, x_2, ..., x_p)'$ a constant distance c^2 from some fixed point $Q = (y_1, y_2, ..., y_p)'$ satisfy

$$d^2(P, Q) = (P - Q)'A(P - Q) = c^2$$

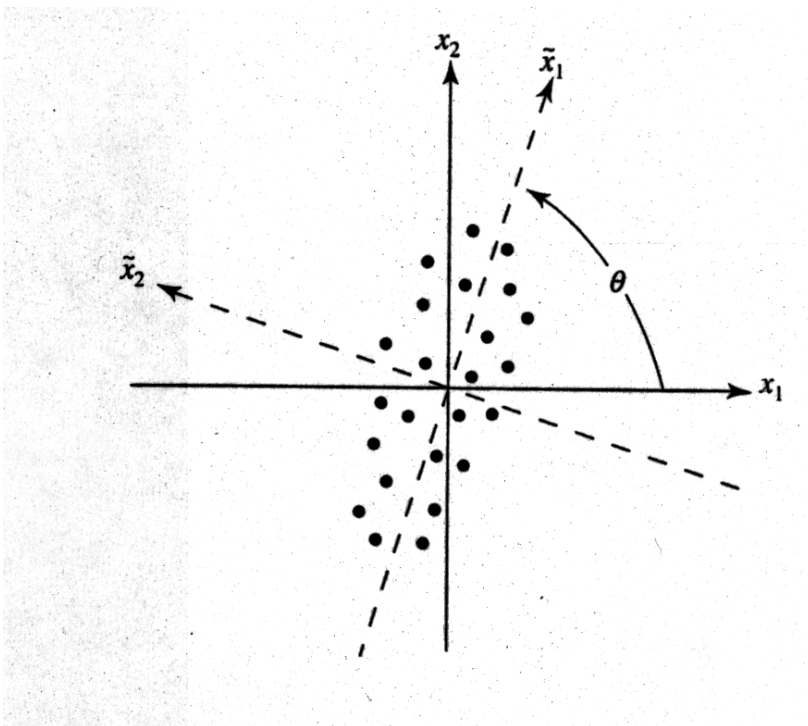
  which is the equation of an ellipse.
- The axes of the ellipse are parallel to the set of new axes $(\tilde{x}_1, \tilde{x}_2)$ obtained by rotating the original axes by an angle θ.



Statistical Distance

- When the measurements are correlated, we can construct a *statistical distance* that accounts for correlations and unequal variances by:
  - First rotating the axes to be paralell to the axes of the ellipsoid
  - Then using the expression for a standardized distance
- We can re-express any point with respect to the rotated coordinates. For $P = (x_1, x_2)'$, we have

$$\begin{aligned} \tilde{x}_1 &= x_1 \cos(\theta) + x_2 \sin(\theta) \\ \tilde{x}_2 &= -x_1 \sin(\theta) + x_2 \cos(\theta). \end{aligned}$$



Mahalanobis Distance

- A distance measure that automatically does this is obtained by choosing A as the inverse of the covariance matrix.
- The squared *statistical distance* between $P = (x_1, x_2, ..., x_p)'$ and $Q = (y_1, y_2, ..., y_p)'$ is

$$d^2(P, Q) = (P - Q)' S^{-1} (P - Q)$$

- This is also called the squared Mahalnobis distance
- When measurements are uncorrelated this becomes the standardized distance