Multivariate Statistical Analysis

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Outline

- Introduction
- Organization of Data
- Data Displays and Pictorial Representations
- Distances
- Reading Assignments

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Questions

- What is a model?
- How to model Nature?
- What is statistics?

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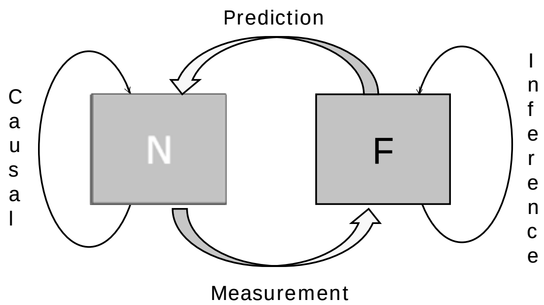
How to Model Nature?



R. Rosen, Life Itself, Columbia Univ. Press, 1991

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Questions

- What is univariate statistics?
- What is multivariate statistics?
- Why to learn multivariate analysis?
- What are major uses and applications of multivariate analysis?
- What will be covered in this course?
- What are required to this course?
- How to handle the term project?

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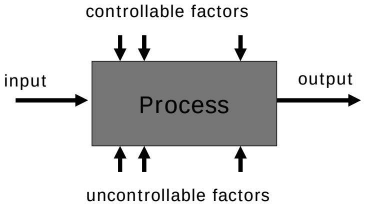
What Is Multivariate Analysis?

- Statistical methodology to analyze data with measurements on many variables



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Why to Learn Multivariate Analysis?

- Explanation of a social or physical phenomenon must be tested by gathering and analyzing data
- Complexities of most phenomena require an investigator to collect observations on many different variables

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Major Uses of Multivariate Analysis

- Data reduction or structural simplification
- Sorting and grouping
- Investigation of the dependence among variables
- Prediction
- Hypothesis construction and testing

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Application Examples

- Is one product better than the other?
- Which factor is the most important to determine the performance of a system?
- How to classify the results into clusters?
- What are the relationships between variables?

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Course Outline

- Introduction
- Matrix Algebra and Random Vectors
- Sample Geometry and Random Samples
- Multivariate Normal Distribution
- Inference about a Mean Vector
- Comparison of Several Multivariate Means
- Multivariate Linear Regression Models

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Course Outline

- Principal Components
- Factor Analysis and Inference for Structured Covariance Matrices
- Canonical Correlation Analysis*
- Discrimination and Classification*
- Clustering, Distance Methods, and Ordination*

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Important Multivariate Techniques Not Included

- Structural Equation Models
- Classification
- Experiment Design

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Feature of This Course

- Uses matrix algebra to introduce theories and practices of multivariate statistical analysis

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Text Book and Website

- R. A. Johnson and D. W. Wichern, Applied Multivariate Statistical Analysis, 6th ed., Pearson Education, 2007. (雙葉)
- http://cc.ee.ntu.edu.tw/~skjeng/MultivariateAnalysis2012.htm

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References

- 林震岩, 多變量分析-SPSS的操作與應用, 智勝, 2007
- J. F. Hair, Jr., B. Black, B. Babin, R. E. Anderson, and R. L. Tatham, Multivariate Data Analysis, 6th ed., Prentice Hall, 2006. (華泰)
- D. C. Montgomery, Design and Analysis of Experiments, 6th ed., John Wiley, 2005. (歐亞)

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References

- D. Salsberg著, 葉偉文譯, *統計,改變了世界*, 天下遠見, 2001.
- 張碧波，*推理統計學*，三民，1976.
- 張輝煌編譯，*實驗設計與變異分析*，建興，1986.

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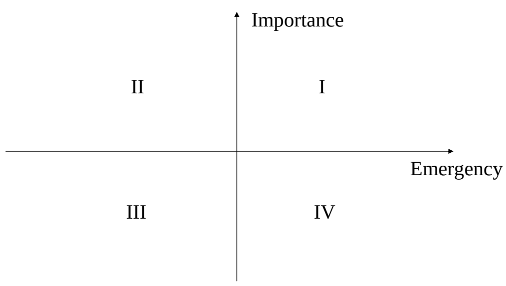
Time Management



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Some Important Laws

- First things first
- 80 – 20 Law
- Fast prototyping and evolution
- 物有本末，事有始终，知所先後，則近道矣。

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Questions

- How to represent the measurement data for multivariate analysis?
- How to summarize the measurement data?
- How to determine if two variables are related?

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Array of Data

$$\mathbf{x} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1k} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2k} & \cdots & x_{2p} \\ \vdots & \vdots & & \vdots & & \vdots \\ x_{j1} & x_{j2} & \cdots & x_{jk} & \cdots & x_{jp} \\ \vdots & \vdots & & \vdots & & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nk} & \cdots & x_{np} \end{bmatrix}$$

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Descriptive Statistics

- Summary numbers to assess the information contained in data
- Basic descriptive statistics
  - Sample mean
  - Sample variance
  - Sample standard deviation
  - Sample covariance
  - Sample correlation coefficient

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Sample Mean and Sample Variance

$$\bar{x}_k = \frac{1}{n}\sum_{j=1}^{n} x_{jk}$$

$$s_k^2 = s_{kk} = \frac{1}{n}\sum_{j=1}^{n}\left(x_{jk} - \bar{x}_k\right)^2$$

$$k = 1, 2, \cdots, p$$

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Sample Covariance and Sample Correlation Coefficient

$$s_{ik} = \frac{1}{n}\sum_{j=1}^{n}\left(x_{ji} - \bar{x}_i\right)\left(x_{jk} - \bar{x}_k\right)$$

$$r_{ik} = \frac{s_{ik}}{\sqrt{s_{ii}}\sqrt{s_{kk}}} = \frac{\sum_{j=1}^{n}\left(x_{ji} - \bar{x}_i\right)\left(x_{jk} - \bar{x}_k\right)}{\sqrt{\sum_{j=1}^{n}\left(x_{ji} - \bar{x}_i\right)^2}\sqrt{\sum_{j=1}^{n}\left(x_{jk} - \bar{x}_k\right)^2}}$$

$$i = 1, 2, \cdots, p; \quad k = 1, 2, \cdots, p$$

$$s_{ik} = s_{ki}, \quad r_{ik} = r_{ki}$$

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Standardized Values (or Standardized Scores)

- Centered at zero
- Unit standard deviation
- Sample correlation coefficient can be regarded as a sample covariance of two standardized variables

$$\frac{x_{jk} - \bar{x}_k}{\sqrt{s_{kk}}}$$

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Properties of Sample Correlation Coefficient

- Value is between -1 and 1
- Magnitude measure the strength of the linear association
- Sign indicates the direction of the association
- Value remains unchanged if all x_{ji}'s and x_{jk}'s are changed to $y_{ji} = a\, x_{ji} + b$ and $y_{jk} = c\, x_{jk} + d$, respectively, provided that the constants a and c have the same sign

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Arrays of Basic Descriptive Statistics

$$\bar{\mathbf{x}} = \begin{bmatrix} \bar{x}_1 \\ \bar{x}_2 \\ \vdots \\ \bar{x}_p \end{bmatrix}, \quad \mathbf{S}_n = \begin{bmatrix} s_{11} & s_{12} & \cdots & s_{1p} \\ s_{21} & s_{22} & \cdots & s_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ s_{p1} & s_{p2} & \cdots & s_{pp} \end{bmatrix}$$

$$\mathbf{R} = \begin{bmatrix} 1 & r_{12} & \cdots & r_{1p} \\ r_{21} & 1 & \cdots & r_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ r_{p1} & r_{p2} & \cdots & 1 \end{bmatrix}$$

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Example

- Four receipts from a university bookstore
- Variable 1: dollar sales
- Variable 2: number of books

$$\mathbf{X} = \begin{bmatrix} 42 & 4 \\ 52 & 5 \\ 48 & 4 \\ 58 & 3 \end{bmatrix}$$

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Arrays of Basic Descriptive Statistics

$$\bar{\mathbf{x}} = \begin{bmatrix} 50 \\ 4 \end{bmatrix}, \quad \mathbf{S}_n = \begin{bmatrix} 34 & -1.5 \\ -1.5 & 0.5 \end{bmatrix}$$

$$\mathbf{R} = \begin{bmatrix} 1 & -0.36 \\ -0.36 & 1 \end{bmatrix}$$

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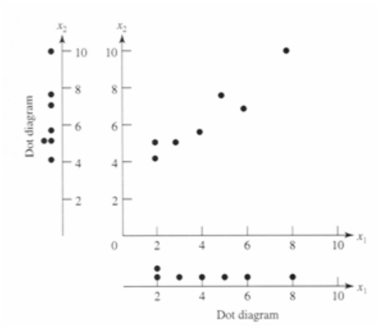
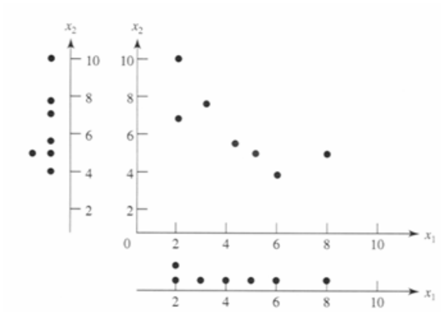
Questions

- How to visually represent multivariate data?
- What are the advantages of data plots?

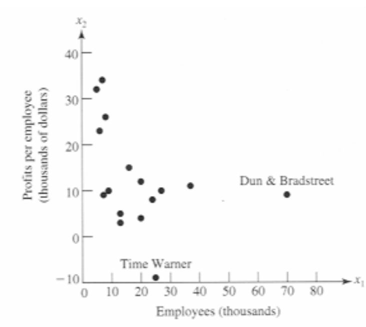
Scatter Plot and Marginal Dot Diagrams



Scatter Plot and Marginal Dot Diagrams for Rearranged Data



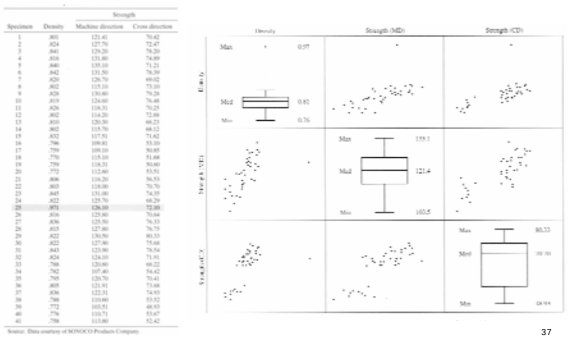
Effect of Unusual Observations



Effect of Unusual Observations

$$r_{12} = \begin{cases} -0.39 & \text{for all 16 firms} \\ -0.56 & \text{for all firms but Dun \& Bradstreet} \\ -0.39 & \text{for all firms but Time Warner} \\ -0.50 & \text{for all firms but Dun \& Bradstreet and Time Warner} \end{cases}$$

Paper Quality Measurements



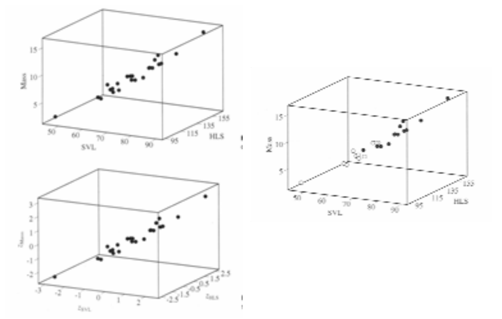
Lizard Size Data

Lizard	Mass	SVL	HLS	Lizard	Mass	SVL	HLS
1	5.526	59.0	113.5	14	10.067	73.0	136.5
2	10.401	75.0	142.0	15	10.091	73.0	135.5
3	9.213	69.0	124.0	16	10.888	77.0	139.0
4	8.953	67.5	125.0	17	7.610	61.5	118.0
5	7.063	62.0	129.5	18	7.733	66.5	133.5
6	6.610	62.0	123.0	19	12.015	79.5	150.0
7	11.273	74.0	140.0	20	10.049	74.0	137.0
8	2.447	47.0	97.0	21	5.149	59.5	116.0
9	15.493	86.5	162.0	22	9.158	68.0	123.0
10	9.004	69.0	126.5	23	12.132	75.0	141.0
11	8.199	70.5	136.0	24	6.978	66.5	117.0
12	6.601	64.5	116.0	25	6.890	63.0	117.0
13	7.622	67.5	135.0				

Source: Data courtesy of Kevin E. Bonine.

***SVL: snout-vent length; HLS: hind limb span**

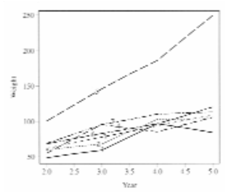
3D Scatter Plots of Lizard Data



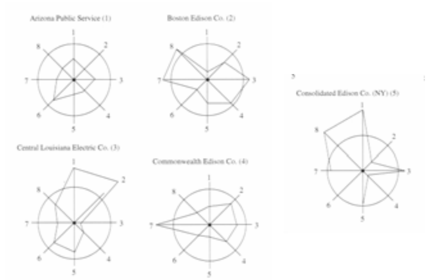
Female Bear Data and Growth Curves

Bear	Wt2	Wt3	Wt4	Wt5	Lngth 2	Lngth 3	Lngth 4	Lngth 5
1	48	59	95	82	141	157	168	183
2	59	68	102	102	140	168	174	170
3	61	77	93	107	145	162	172	177
4	54	43	104	104	146	159	176	171
5	100	145	185	247	150	158	168	175
6	68	82	95	118	142	140	178	189
7	68	95	109	111	139	171	176	175

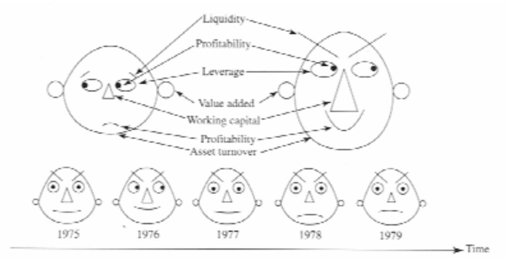
Source: Data courtesy of H. Roberts.



Utility Data as Stars



Chernoff Faces over Time



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- How to determine if two multivariate data are close?
- How to deal with the case that two variables are correlated?

Euclidean Distance

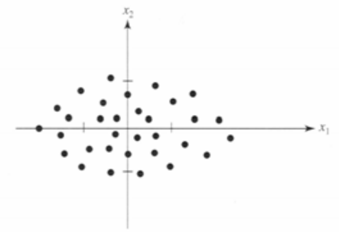
- Each coordinate contributes equally to the distance

$$P(x_1, x_2, \cdots, x_p), \quad Q(y_1, y_2, \cdots, y_p)$$

$$d(P,Q) = \sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2 + \cdots + (x_p - y_p)^2}$$

Statistical Distance

- Weight coordinates subject to a great deal of variability less heavily than those that are not highly variable



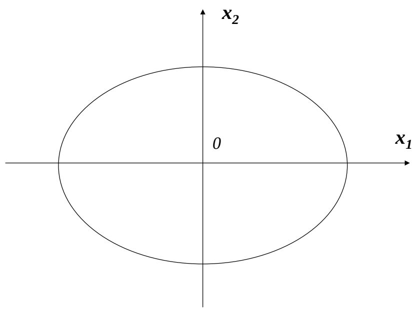
Statistical Distance for Uncorrelated Data

$$P(x_1, x_2), \quad O(0,0)$$

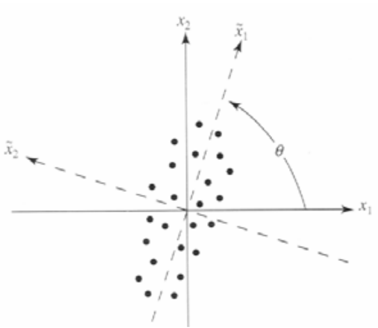
$$x_1^* = x_1 / \sqrt{s_{11}}, \quad x_2^* = x_2 / \sqrt{s_{22}}$$

$$d(O,P) = \sqrt{(x_1^*)^2 + (x_2^*)^2} = \sqrt{\frac{x_1^2}{s_{11}} + \frac{x_2^2}{s_{22}}}$$

Ellipse of Constant Statistical Distance for Uncorrelated Data



Scattered Plot for Correlated Measurements



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Statistical Distance under Rotated Coordinate System

$$O(0,0), \quad P(\tilde{x}_1, \tilde{x}_2)$$

$$d(O,P) = \sqrt{\frac{\tilde{x}_1^2}{\tilde{s}_{11}} + \frac{\tilde{x}_2^2}{\tilde{s}_{22}}}$$

$$\tilde{x}_1 = x_1 \cos\theta + x_2 \sin\theta$$

$$\tilde{x}_2 = -x_1 \sin\theta + x_2 \cos\theta$$

$$d(O,P) = \sqrt{a_{11}x_1^2 + 2a_{12}x_1x_2 + a_{22}x_2^2}$$

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General Statistical Distance

$$P(x_1, x_2, \cdots, x_p), \quad O(0,0,\cdots,0), \quad Q(y_1, y_2, \cdots, y_p)$$

$$d(O,P) = \sqrt{\begin{array}{l}[a_{11}x_1^2 + a_{22}x_2^2 + \cdots + a_{pp}x_p^2 + \\ 2a_{12}x_1x_2 + 2a_{13}x_1x_3 + \cdots + 2a_{p-1,p}x_{p-1}x_p]\end{array}}$$

$$d(P,Q) = \sqrt{\begin{array}{l}[a_{11}(x_1-y_1)^2 + a_{22}(x_2-y_2)^2 + \cdots + \\ a_{pp}(x_p-y_p)^2 + \\ 2a_{12}(x_1-y_1)(x_2-y_2) + 2a_{13}(x_1-y_1)(x_3-y_3) \\ + \cdots + 2a_{p-1,p}(x_{p-1}-y_{p-1})(x_p-y_p)]\end{array}}$$

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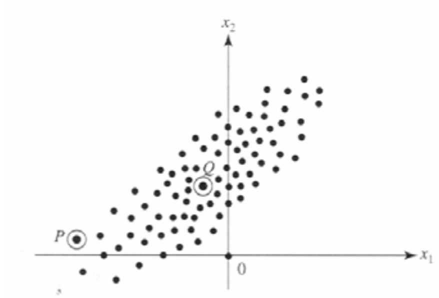
Necessity of Statistical Distance



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Necessary Conditions for Statistical Distance Definitions

$$d(P,Q) = d(Q,P)$$

$$d(P,Q) > 0 \text{ if } P \neq Q$$

$$d(P,Q) = 0 \text{ if } P = Q$$

$$d(P,Q) \leq d(P,R) + d(R,Q)$$

(Triangle inequality)

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Reading Assignments

- Text book
  - pp. 49-59 (Sections 2.1~2.2)
  - pp. 82-96 (Supplement 2A)

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