Lecture 2

Characterizing and Displaying Multivariate Data

DSA 8070 Multivariate Analysis August 23-27, 2021

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Notes			

Agenda

- Descriptive Statistics
- 2 Graphs and Visualization



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Organization of Data and Notation

- ullet 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.
- $\bullet \ \mbox{ If } p=1,$ 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

 $(x_{i1}, x_{i2}, \cdots, x_{ip})$



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Organization of Data and Notation

ullet 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).

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Descriptive Statistics

Descriptive Statistics: Sample Mean & Variance

 \bullet The sample mean of the kth variable ($k=1,\cdots,p)$ 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

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



Descriptive Statistics

Graphs and

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Descriptive Statistics: Sample Covariance

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

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

 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

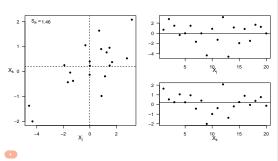
{r}										
dat <- mvrnorm(n =	50,	mu	= c(0,	0),	Sigma	= matrix(c(1,	0,	0,	1),	2))
cov(dat[, 1], dat[. 27)								



Descriptive Statistics Graphs and

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Sample Covariance



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Descriptive Statistics: Sample Correlation

• The sample correlation between variables k and j is defined as

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

- ullet r_{jk} is between -1 and 1
- $r_{jk} = r_{kj}$



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Sample Correlation

- The sample correlation is equal to the sample covariance if measurements are standardized (i.e., $s_{kk} = s_{jj} = 1)$
- Covariance and correlation measure linear association. Other non-linear dependencies may exist among variables even if $r_{jk}=0$
- \bullet The sample correlation (r_{ij}) will vary about the value of the population correlation (ρ_{ij})



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Matrix Representation of Sample Statistics

Sample statistics of a *p*-dimnesional multivariate data can be organized as vectors and matrices:

 $oldsymbol{ar{x}}=[ar{x}_1,ar{x}_2,\cdots,ar{x}_p]^{\mathrm{T}}$ is the p imes 1 vector of sample means

$$\bullet \ \ S = \begin{bmatrix} s_{11} & s_{12} & \cdots & s_{1p} \\ s_{21} & s_{22} & \cdots & s_{2p} \\ \vdots & \cdots & \cdots & \ddots \\ s_{p1} & s_{p2} & \cdots & s_{pp} \end{bmatrix} \text{ is the } p \times p \text{ symmetric}$$

matrix of variance (on the diagonal) and covariances (the off-diagonal elements)

$$\bullet \ \, \boldsymbol{R} = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1p} \\ r_{21} & r_{22} & \cdots & r_{2p} \\ \vdots & \cdots & \cdots & \ddots \\ r_{p1} & r_{p2} & \cdots & r_{pp} \end{bmatrix} \text{ is the } p \times p \text{ symmetric}$$

 $\mbox{\it matrix}$ of sample correlations. Diagonal elements are all equal to 1

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Descriptive Statistics

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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

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

Sample mean vector is:

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



Descriptive Statistics Graphs and

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Example: Bivariate Data

• 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

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

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Descriptive Statistics Graphs and Visualization

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Generalized Variance

- The generalized variance is a scalar value which generalizes variance for multivariate random variables
- \bullet The generalized variance is defined as the determinant of the (sample) covariance matrix $S, \det(S)$
- Example:

```
'``{r}
data(mtcars)
vars <- which(names(mtcars) %in% c("mpg", "disp", "hp", "drat", "wt"))
car <- mtcars[, vars]; S <- cov(car)
(genVar <- det(S))

[1] 3951786
```



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Graphs and Visualization



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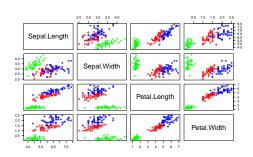
Graphs and Visualization

- Graphs convey information about associations between variables and also about unusual observations
- $\bullet \ \, \hbox{One difficulty with multivariate data is their} \\ \hbox{visualization, in particular when} \ p>3.$
- At the very least, we can construct pairwise scatter plots of variables

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Example: Fisher's Iris Data

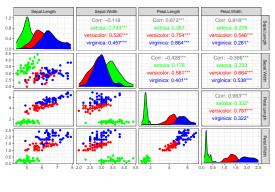
5 variables (sepal length and width, petal length and width, species (setosa, versicolor, and virginica), 50 flowers from each of 3 species $\Rightarrow p=4, n=50\times 3=150$





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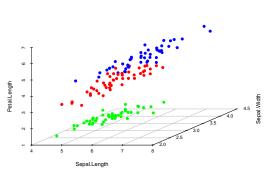
Plotting Iris Data using ggpairs





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3D Scatter Plot





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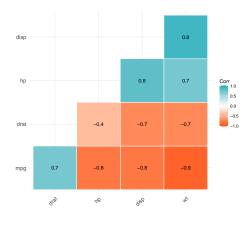
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Visualizing Summary Statistics





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