Lecture 2

Characterizing and Displaying Multivariate Data

DSA 8070 Multivariate Analysis

Whitney Huang
Clemson University

Agenda

1. Descriptive Statistics
2. Graphs and Visualization

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

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

Organization of Data and Notation

- 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: Sample Mean & Variance

- The sample mean of the k-th 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 k-th 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: Sample Covariance

- 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

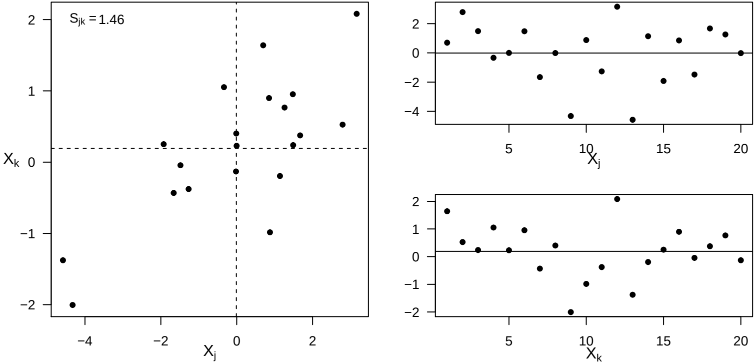
$$s_{jk} = \frac{1}{n-1}\sum_{i=1}^{n}(x_{ij} - \bar{x}_j)(x_{ik} - \bar{x}_k)$$

- 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[, 2])
```

```
[1] -0.1508848
```

Sample Covariance



Descriptive Statistics: Sample Correlation

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

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

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

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 $r_{jk} = 0$
- The sample correlation (r_{ij}) will vary about the value of the population correlation (ρ_{ij})

Matrix Representation of Sample Statistics

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

- $\bar{\boldsymbol{x}} = [\bar{x}_1, \bar{x}_2, \cdots, \bar{x}_p]^{\mathrm{T}}$ is the $p \times 1$ vector of sample means
- $\boldsymbol{S} = \begin{bmatrix} s_{11} & s_{12} & \cdots & s_{1p} \\ s_{21} & s_{22} & \cdots & s_{2p} \\ \vdots & \cdots & \cdots & \cdots \\ s_{p1} & s_{p2} & \cdots & s_{pp} \end{bmatrix}$ is the $p \times p$ symmetric matrix of variance (on the diagonal) and covariances (the off-diagonal elements)
- $\boldsymbol{R} = \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1p} \\ r_{21} & r_{22} & \cdots & r_{2p} \\ \vdots & \cdots & \cdots & \cdots \\ r_{p1} & r_{p2} & \cdots & r_{pp} \end{bmatrix}$ 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

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

- Sample mean vector is:

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

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

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

Generalized Variance

- The generalized variance is a scalar value which generalizes variance for multivariate random variables
- The generalized variance is defined as the determinant of the (sample) covariance matrix $\boldsymbol{S}$, $\det(\boldsymbol{S})$
- **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
```

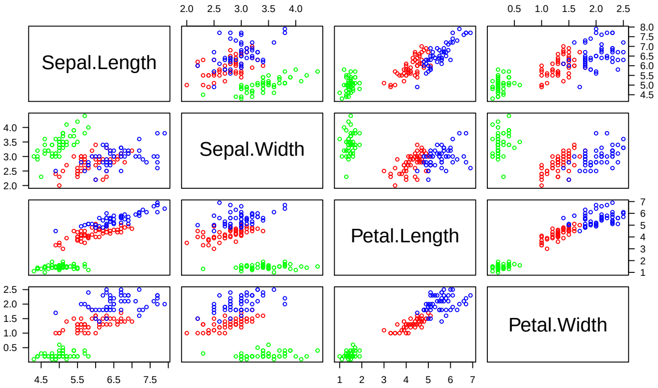
Graphs and Visualization

Graphs and Visualization

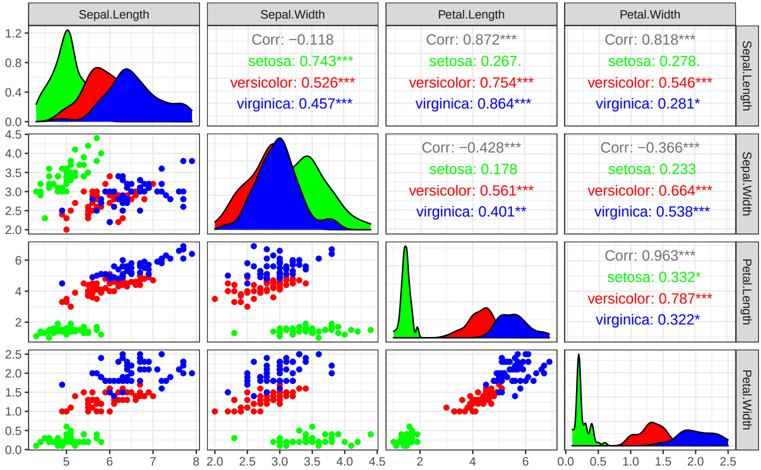
- Graphs convey information about associations between variables and also about unusual observations
- One difficulty with multivariate data is their visualization, in particular when $p > 3$.
- At the very least, we can construct pairwise scatter plots of variables

Example: Fisher's Iris Data

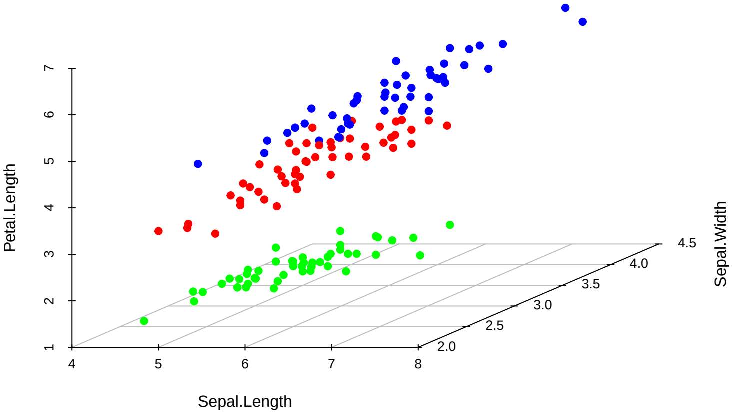
5 variables (sepal length and width, petal length and width, species (setosa, versicolor, and virginica), 50 flowers from each of 3 species $\Rightarrow p = 4, n = 50 \times 3 = 150$



Plotting Iris Data using *ggpairs*

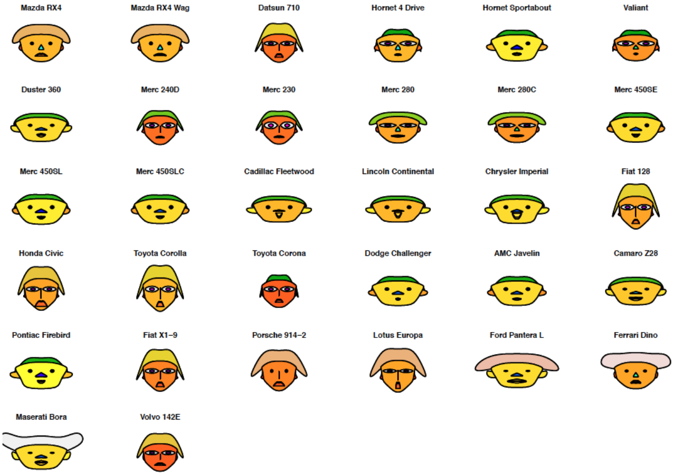


3D Scatter Plot

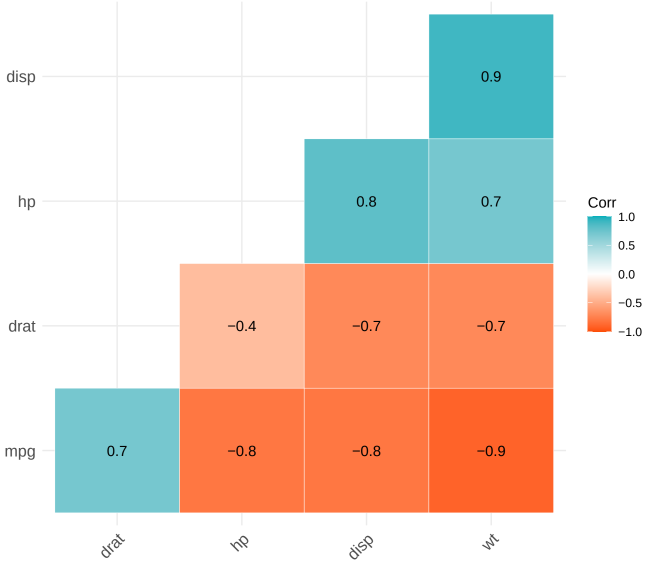


Chernoff Faces

```
> head(mtcars)
                   mpg cyl disp  hp drat    wt  qsec vs am gear carb
Mazda RX4         21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
Mazda RX4 Wag     21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
Datsun 710        22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
Hornet 4 Drive    21.4   6  258 110 3.08 3.215 19.44  1  0    3    1
Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2
Valiant           18.1   6  225 105 2.76 3.460 20.22  1  0    3    1
```



Visualizing Summary Statistics



Summary

In this lecture, we learned

- Summarizing multivariate data numerically
- Summarizing multivariate data graphically

In the next lecture, I will give a short review of Matrix Algebra