

# Statistical Data Modelling

Monash University

#### **About this Unit**

- Moodle contains
  - Unit Orientation, Assessments and Discussion Forums
  - links to Lecture Notes, recommended videos & readings, Alexandria material

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- 3. probability cheat sheet, print out now in colour!
- 4. using R in Jupyter Notebook. Alternatives:
  - install RStudio, <a href="https://www.rstudio.com">https://www.rstudio.com</a>, on your own computer
  - or use https://jupyterhub.erc.monash.edu/
  - ▶ or use MoVE
  - Short R Reference Card and Base R Cheat Sheet, print out now in colour!

- ► FIT5197M1: Introduction to Modelling for Data Science in Alexandria
- videos

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- watch videos & read background material between classes
- bring a device to lectures to participate in quizzes
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#### 4. Want to learn more yourself?

- work through Ross chapters 1-10; answers to questions available
- in particular, work through the proofs he gives to better understand the why's

#### **Assessment**

	Week due	Content	Percent
Assign. 1	1a:4,1b:5,1c:7,	Hand written	6 x 2.5% per
	1d:8,1e:9,1f:12,	MCQ and SAQ	sub-part = 15%
		(6 sub-parts)	
Assign. 2	6	R program stats	20%
Assign. 3	10	R program model	15%
Exam	TBD	MCQ and SAQ	50%

- Exam is closed book but you have the formula sheet included, and can bring in non-programmable calculator.
- Assignments 1 (each of the 6 sub-parts) due back marked after 1 week.
- Assignments 2 and 3 due back marked after 2 weeks.
- No R in exam.

## **Academic Integrity**

Monash University is committed to upholding standards of academic integrity and honesty. Monash students are therefore required to:

- undertake studies and research responsibly and with honesty and integrity;
- ensure that academic work is in no way falsified;
- seek permission to use the work of others, where required;
- acknowledge appropriately the work of others; and
- take reasonable steps to ensure that other students are unable to copy or misuse their work.

see Student Academic Integrity Policy



#### Contacts

#### Need help?

- 1. ask questions during tutorials and lectures
  - please interrupt me with questions!
  - am happy to work through proofs in Ross

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#### Need help?

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- 2. check for relevant Discussions Forum on Moodle
  - note in particular the "Assessments" discussion threads
  - but do NOT post your solutions to assignments ;-)
- attend the consultation hour of the tutors or the lecturer
  - consultation hours in Moodle
- 4. send email to tutor or lecturer
- contact Levin Kuhlmann (levin.kuhlmann@monash.edu) for special consideration

#### Content of the Unit

- technical overview of basic principles of probability and data analysis
- exposure to some common analytic models
- basic experience with R

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- technical overview of basic principles of probability and data analysis
- exposure to some common analytic models
- basic experience with R
- students wanting more in depth machine learning after FIT5197:
  - work through the relevant chapters of Ross fully
  - I'll present various additional pointers during class
  - learn to use and learn from Wikipedia

#### Motivation for the Unit

• technologies in data science are constantly evolving

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  - despite what the popular press may tell you, deep neural networks also builds on these principles

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- technologies in data science are constantly evolving
- one thing that will never change is the importance of probability, statistics and modelling
  - despite what the popular press may tell you, deep neural networks also builds on these principles
- understand this and you can then read the important text books and pick up on the new technologies for machine learning, etc.
  - consider <u>"gradient boosting machines"</u>: look at Wikipedia or Medium.com entry
  - Google's <u>Tensor Flow Probability talk</u> at Al Conference by O'Reilly.

#### Unit Schedule: Modules

Module	Week	Content	Ross
1.	1	Introduction to modelling for data sci-	1,2
		ence and to R	
2.	2	Probabilities	3
	3	Expectations	4
	4	Distributions	5
3.	5	Statistical inference	6&7
	6	Hypothesis testing	7&8
4.	7	Dependence and linear regression	9
	8	classification and clustering	
5.	9	Comparing means	10
	10	Random number generation and sim-	
		ulation	
6.	11	Validation and complexity	15
	12	Modelling	

## Any Other Questions?

... before we get started?

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... otherwise, use the discussion board!

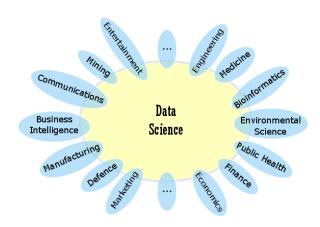
# FIT5197 Statistical Data Modelling Module 1 Introduction to modelling for data science and to R

2020 Lecture 1

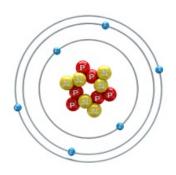
Monash University

# Introduction to Modelling (ePub sections 1.2, 1.3, 1.4, 1.5,1.7, Ross Ch. 1)

#### **Data Science Views**

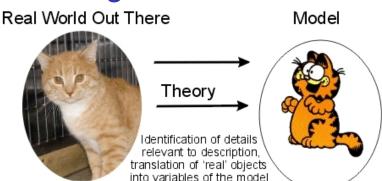


#### What Are Models?



- representation of a real world problem/object/process
- allows explanation, analysis and inference
- for us, usually a probabilistic model

### Modelling



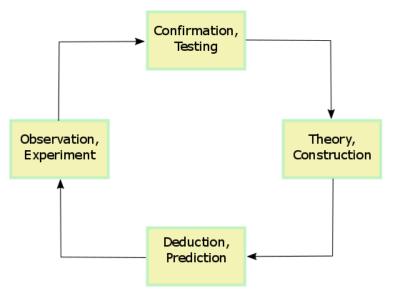
from the BackReaction blog by Sabine Hossenfelder

#### George Box (renowned statistician)

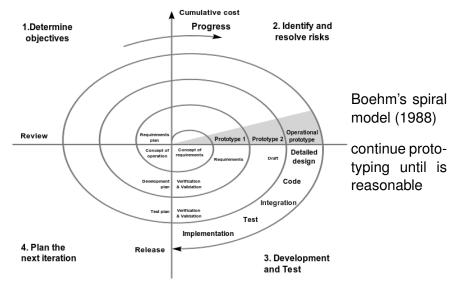
"Essentially, all models are wrong, but some are useful"



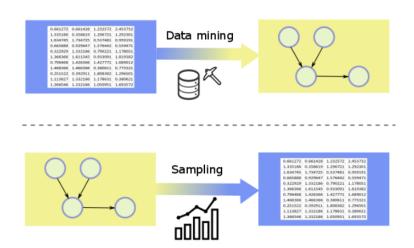
#### What is the Scientific Method?



## How to Build Complex Systems



#### Data to Models and Back



### Concepts for Data

Quantitative data: numerical values, always given to a fixed precision, including vectors, etc.

Qualitative data: categorical values, including structured data

Object: thing about which data is measured

Population: set of all objects of interest

Sample: data from a subset of the population

Inference: estimate properties of the population based on

properties of the sample

Prediction: predict/guess of properties given a new set of

sample

## Inference/Prediction Examples

- Book-seller: how many copies of this popular book will I sell this month?
- Electicity company: what's the maximum kWhs needed at any one time to meet consumer demand in Clayton over summer?
- Oncologist: how does this drug affect female patients with stage 3 bowel cancer who are over 60 years of age?
- Hospital administrator: what sorts of patient cohorts are there for cardiology patients in the Intensive Care Unit so I can organise staff and treatment?

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**Warning:** the traditional scientific method only tests very specific questions; in general in data analysis we can ask broader questions.

# Where Does the Data Come From?

- To do inference we need a sample.
  - ▶ But where does it come from?

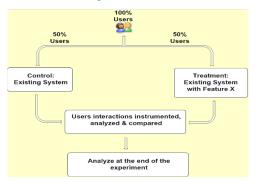
# Where Does the Data Come From?

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- *Controlled Experiments*: gather data that best supports inference about the questions under consideration.
  - ► A/B testing
  - Randomised control trial (RCT)
  - can be used to assess cause and effect

# Where Does the Data Come From?

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- Controlled Experiments: gather data that best supports inference about the questions under consideration.
  - ► A/B testing
  - Randomised control trial (RCT)
  - can be used to assess cause and effect
- Use observational data or survey data.
  - see convenience sampling
  - see participation bias
  - see observational study
    - •

## **Controlled Experiments**



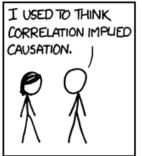
- Random allocation of treatment and control group
- Blinding: participants, administers, outcome accessors or data analyst were blinded of the allocation
- Attrition: loss to follow up

#### Observational studies

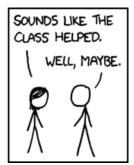
- <u>Case-control study</u>: compares those who with and without outcome of interest, and looks back retrospectively to identify risk factors for the outcome.
- <u>Cross-sectional study</u>: using data collection from a population at one specific point in time
- <u>Longitudinal study</u>: correlational research study that involves repeated observations of the same variables over long periods of time (i.e. <u>Cohort study</u>)
  - Longitudinal data
  - Time series data
  - Survival data

#### Causal Inference

#### Association or Correlation ≠ Causation







https://xkcd.com/552/

#### Causal Inference

#### Criteria for causal relationship by Sir Austin Bradford Hill

- Strength: strong associations more likely to be causal, but weak association does not rule out a causal connection
- Consistency: reproducibility
- Temporality: The effect has to occur after the cause
- Dose resonse relationship
- Plausibility: plausible mechanism between cause and effect
- Specificity, Coherence, Experiment and Analogy

Making causal inferences requires judgment about quality and quantity of evidence. Strong causal evidence:

Systematic literature review and RCT



#### **Data Problems**

- Missing data
- Confounders
- Bias
- Outliers
- ...

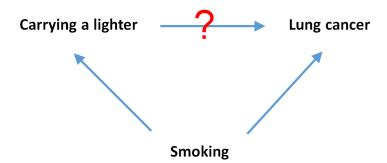
## Missing Data

- Missing completely at random (MCAR): the missing data are just a random subset of the data
  - Complete cases analysis normal approach, unbiased and conservative
  - Single value imputation underestimation of standard errors
- Missing at random (MAR): "missingness" is random given (i.e. conditional on) observed information
  - Complete cases analysis biased
  - Single value imputation underestimation of standard errors
  - Advanced methods: multiple imputation (MI), EM etc.
- Missing not at random (NMAR):responders differ from non-responders, even after accounting for the observed information:
  - imputation methods such as MI and EM will not work
  - investigate missing mechanisms...



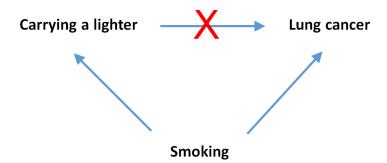
## **Dealing with Confounders**

Confounding variable (confounders): variable that influences both the dependent variable and independent variable causing a spurious association.



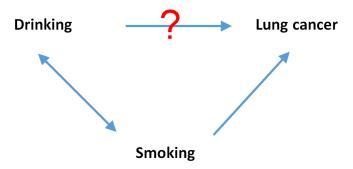
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**Confounding variable** (confounders): variable that influences both the dependent variable and independent variable causing a spurious association.



- stratified sampling
- or justification (include as a covariance)

#### Bias

**Bias**: influence in the collection/analyses of data which results in systematically inaccurate estimates of population values.

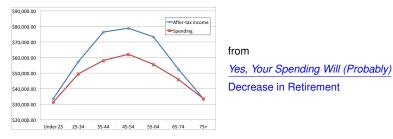
- Selection or participation bias: members of a population are not selected uniformly randomly.
  - ► 1936 US presidential election (The Literary Digest poll)
- Instrument bias: systematic bias in measurements
  - there is a true NASA story along these lines!
  - but they don't mention the data censoring done by NASA that caused the issue to not be discovered by NASA instead
- Statistical or inductive bias: bias inherent in a statistical or data mining tool



#### Statistical or Inductive Bias

When the model restricts the class of functions/fits one allows:

- predicting income from age using a linear model
  - there will be a negative bias at the end when the person retires
- predicting income from age using a piecewise linear model
  - you can make small linear pieces to fit the "true" function



#### **Outliers**

Outliers are data points that lie well beyond the bulk of samples for a variable on one or more dimensions. Outliers be:

- legitimate data points
- due to measurement error
- from a heavy-tailed distribution

How to deal with outliers?

- delete
- correct the measurement error
- keep in the analysis

The choice of how to deal with an outlier should depend on the cause, type of analysis and the research question



 How do we infer properties of the entire population from a small sample?

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- How do we infer properties of the entire population from a small sample?
- What sorts of models would we use for the population?
- How would inference be done?
- How can we best predict when the new data arrived?

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largely recipe driven, (covered in Module 3)

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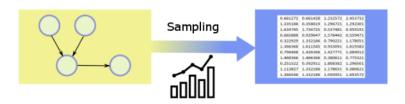
Diagnostics: "debugging" a model or an algorithm

- is your model suitable for the problem?
- is the algorithm working?

- Hypothesis Testing: main tool for all of empirical science
  - largely recipe driven, (covered in Module 3)
  - Modelling: build a "model" for a domain problem
    - to be used for prediction, "understanding," planning, (covered in Module 4)
- Diagnostics: "debugging" a model or an algorithm
  - is your model suitable for the problem?
  - is the algorithm working?
- Algorithm Analysis and Design: techniques and issues
  - don't have to "do", but should be aware of
  - building up from parts,
  - model "fitting", MLE, minimum cost
  - bias-variance

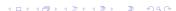


#### Generative Models

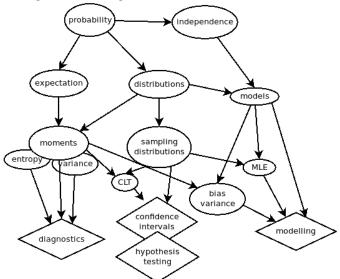


A generative model gives probabilities for every data point:

- thus probabilities for every sample
- thus lets us compare typical versus rare samples
- thus lets us test whether the model is reasonable or unreasonable for the sample
- is the basis for hypothesis testing (covered in Module 3)



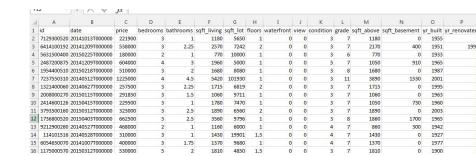
## Concept Map for This Unit



# Exploratory Data Analysis (ePub section 1.7, Ross Ch. 2)

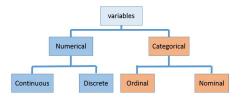
practical for this will be done in tutorial of Week 2

# Data Matrix, Observations and Variables



#### **Variables**

- a <u>variable</u> is any characteristic, number, or quantity that can be measured or counted
- there are different types of variables based on the ways they are studied, measured and represented:
- Numerical (quantitative)
  - Continuous
  - Discrete
- Categorical (qualitative)
  - Ordinal
  - Nominal



## Variables, cont

Numerical (quantitative)

Have values that describe a measurable quantity as a number, like 'how many' or 'how much'. It is meaningful to do arithmetic.

Continuous: Observations can take any value between

two specified values.

Discrete: Observations can take a value based on a

count from a set of distinct values

Categorical (qualitative)

Have values that describe a 'quality' or 'characteristic' of a data unit, like 'what type' or 'which category'

Ordinal: Observations can take a value that can be

logically ordered or ranked

Nominal: Observations can take a value that is not able

to be organized in a logical sequence

## Examples

#### Variables:

Age, sex, business income and expenses, country of birth, capital expenditure, class grades, eye colour, vehicle type

- Continuous (how much)
   Height, time, age, and temperature
- Discrete (how many)
   Number of registered cars, number of business locations, and number of children in a family
- Ordinal (has order)
   Academic grades (e.g., A, B, C), clothing size (e.g., small, medium, large, extra large), attitudes (e.g., strongly agree, agree, disagree, strongly disagree), dates
- Nominal (no order)
   Gender, business type, eye colour, religion and brand

#### Have a Look at iris Data

- The iris dataset has been used for classification
- Consists of 50 samples from each of three classes of iris flowers
- Use str() to compactly display the structure of an arbitrary R object

```
> str(iris)
'data.frame': 150 obs. of 5 variables:
$ Sepal.Length: num 5.1 4.9 4.7 4.6 5 5.4 4.6 5 4.4 4.9 ...
$ Sepal.Width: num 3.5 3 3.2 3.1 3.6 3.9 3.4 3.4 2.9 3.1 ...
$ Petal.Length: num 1.4 1.4 1.3 1.5 1.4 1.7 1.4 1.5 1.4 1.5 ...
$ Petal.Width: num 0.2 0.2 0.2 0.2 0.2 0.4 0.3 0.2 0.2 0.1 ...
$ Species : Factor w/ 3 levels "setosa", "versicolor", ..: 1 1 1 1 1
```

#### Have a Look at iris Data

- The first or last rows of data can be retrieved with head() or tail()
- We can also retrieve the values of a single column

```
> head(iris)
> tail(iris)
> iris[1:5,]
  Sepal.Length Sepal.Width Petal.Length Petal.Width Species
1
           5.1
                        3.5
                                      1.4
                                                  0.2 setosa
           4.9
                        3.0
                                      1.4
                                                  0.2 setosa
           4.7
                        3.2
                                      1.3
                                                  0.2 setosa
4
           4.6
                                      1.5
                        3.1
                                                  0.2 setosa
           5.0
                        3.6
                                      1.4
                                                  0.2 setosa
> iris[1:10, "Sepal.Length"]
[1] 5.1 4.9 4.7 4.6 5.0 5.4 4.6 5.0 4.4 4.9
> iris$Sepal.Length[1:10]
[1] 5.1 4.9 4.7 4.6 5.0 5.4 4.6 5.0 4.4 4.9
```

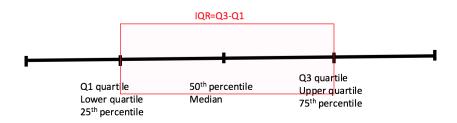
### Statistics on variables

- Measure of centre
  - Mean,  $\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$
  - Median
    - Order the data
    - Find the mid-point or average of two mid-points
- Measure of spread
  - ► Variance, var =  $s_x^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i \bar{x})^2$
  - Standard deviation,  $s_x = \sqrt{\text{var}}$ 
    - also called sd, s.d., std dev, etc.
  - $Range = \max_{i=1}^{n} x_i \min_{i=1}^{n} x_i$
  - ightharpoonup (inter-quartile range)  $IQR = Q_3 Q_1$
- Robust statistics: extreme observations have little effect
  - Median is more robust than mean
  - IQR more robust than range, variance and std
  - They are usually better for skewed data



### Quartiles

- For sorted data
- Quartiles are 3 points that divide into 4 equal groups
- Each group is a quarter of data



```
> x < -c(0:10, 50)
> xm < -mean(x)
> xm
Г17 8.75
> median(1:4)
[1] 2.5
> median(1:5)
Г17 3
> median(c(1:3, 100, 1000))
Г1] 3
> c(median(1:4), mean(1:4))
[1] 2.5 2.5
> c(median(1:5), mean(1:5))
Г1] 3 3
> c(median(c(1:3, 100, 1000)), mean(c(1:3, 100, 1000)))
[1] 3.0 221.2
> var(1:20)
Г1] 35
> sd(1:20)
Γ1 5.91608
> sqrt(var(1:20)) == sd(1:20)
[1] TRUE
```

```
> range(3:10)
[1] 3 10
> diff(range(3:10))
[1] 7
> IQR(c(3:10, 100, 1000))
[1] 4.5
> c(IQR(c(3:10, 100, 1000)), diff(range(c(3:10, 100, 1000))))
[1] 4.5 997.0
> boxplot(c(3:100, 150, 200))
```

## Summary of Variables

- Distribution of every variable can be checked with function summary()
- it returns the min, max, mean, median, and the first (25%) and third (75%) quartiles.
- For factors (or categorical variables), it shows the frequency of every level.

## Summary of Variables

- The mean, median and range can also be obtained with functions with mean(), median() and range()
- Quartiles and percentiles are supported by function quantile()
- Use var() to check variance

```
> quantile(iris$Sepal.Length)
0% 25% 50% 75% 100%
4.3 5.1 5.8 6.4 7.9
> quantile(iris$Sepal.Length, c(.1, .3, .65))
10% 30% 65%
4.80 5.27 6.20
> var(iris$Sepal.Length)
[1] 0.6856935
```

## Further Summary of Variables

```
> summary(cars)
    speed
                dist
Min. : 4.0 Min. : 2.00
1st Qu.:12.0 1st Qu.: 26.00
Median: 15.0 Median: 36.00
Mean : 15.4 Mean : 42.98
3rd Qu.:19.0 3rd Qu.: 56.00
Max. :25.0 Max. :120.00
> fivenum(cars$speed) # min, lower hinge, median, upper hinge, max.
[1] 4 12 15 19 25
> boxplot.stats(cars$speed) # Boxplot stats: fivenum (as above: min, lower hin
               # upper hinge, max), n, confidence interval (CI) of the median
$stats
Γ17 4 12 15 19 25
$n
Γ17 50
$conf
Γ17 13.43588 16.56412
$out
numeric(0)
```

### **Graphical Representations**

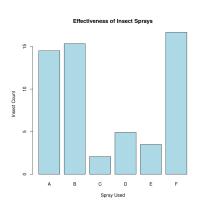
- To understand the properties of data
- To find possible pattern in data
- To guide us in choosing better and more suitable models
- To communicate the outcome with others

	Single variable	Two variables	Categorical
Numerical	Histogram	Scatter plot	Side-by-side box plo
	Box plot		
Categorical	Pie chart	segmented bar plot	
	Bar plot	Mosaic plot	

#### Data exploration choices

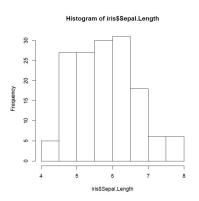


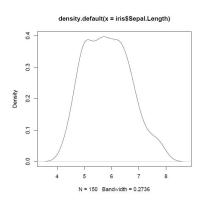
## Single Categorical: Bar Chart and Pie Chart





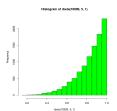
### **Explore Individual Variables**

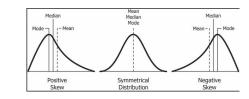


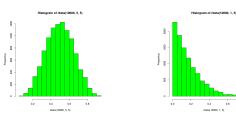


#### Visual Attributes of Distrib.s

- Shape of skewness
  - Symmetric
  - Left skewed
  - Right Skewed





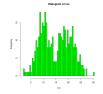


rbeta/10000, 1, 5/

#### Visual Attributes of Distrib.s

- Modality
  - Unimodal
  - Bimodal
  - Uniform
  - Multimodal



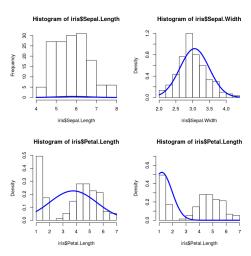






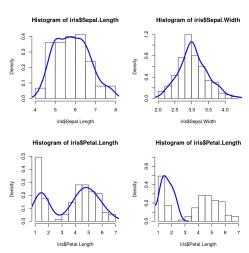
## Histogram and Density

curve(dnorm(x, mean = mean(iris\$Petal.Width), sd = sd(iris\$Petal.Width)), add = TRUE)



## Histogram and Density

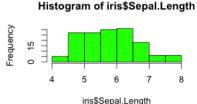
lines(density(iris\$Petal.Width), col = "blue", lwd = 3)

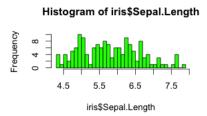


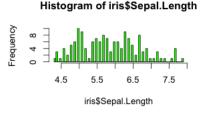
#### Different Number of Bars



iris\$Sepal.Length

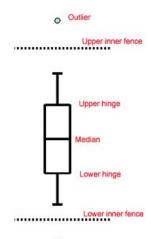






## Boxplot for R

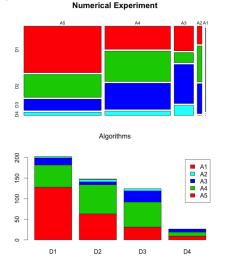
- introduced by John W. Tukey
- represent numerical data through quartiles (lower hinge is Q<sub>1</sub>, upper is Q<sub>3</sub>)
- whiskers indicating variability outside the upper and lower quartiles
- lower inner fence is  $Q1 1.5 \times IQR$
- upper inner fence is  $Q3 + 1.5 \times IQR$
- whiskers at min/max data values inside fences
- highlights outliers outside fences





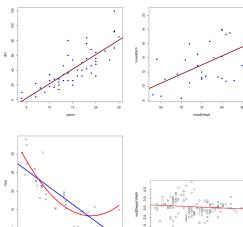
(there are many versions of layouts for a boxplot, and the default in R (seems) to be the Tukey boxplot, see *boxplot types*)

## Segmented Bar Chart and Mosaic Plot



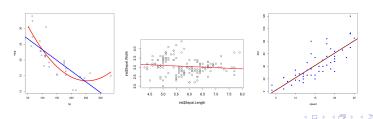
## Relationship Between Two Numerical Variables

- Direction of relationship
  - Increasing
  - Decreasing
- Shape
  - Linear
  - Nonlinear
- Strength
  - Strong
  - Weak



#### Covariance and Correlation

- <u>Covariance</u> of two random variables shows how they are related:
  - Positive covariance, then they are positively related
  - Negative covariance, then they are negatively related
- The <u>correlation coefficient</u> of two random variables is covariance divided by the product of their standard deviations:
  - it shows how the two random variable are linearly related
  - if close to 1, then they are positively linearly related
  - ▶ if close to −1, then they are negatively linearly related
  - if close to 0, then they are weakly related



## Covariance and Correlation, cont.

• Sample covariance

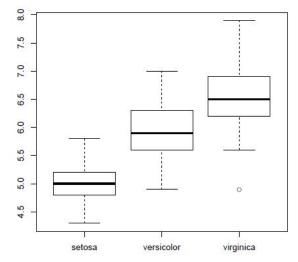
$$q_{xy} = \frac{1}{n-1} \sum_{i=1}^{n} (x_i - \bar{x})(y_i - \bar{y})$$

• Sample correlation coefficient

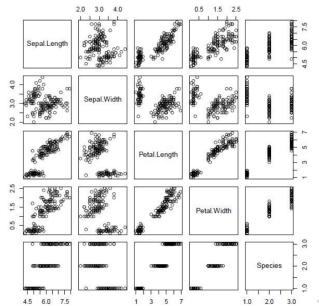
$$r_{xy} = \frac{q_{xy}}{s_x s_y} = \frac{\sum_{i=1}^n (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^n (x_i - \bar{x})^2 \sum_{i=1}^n (y_i - \bar{y})^2}}$$

See Ross for details.

# Exploring categorical against numerical variables



#### Multivariate Scatter Plots



### Data Exploration Recipe

 Find variables and decide if they are numerical or categorical. str(), attributes()

- Numerical: Continuous and Discrete
- Categorical: Ordinal and Nominal
- Find statistics of each variable
  - Quantitative:Find summary(), fivenum(), boxplot.stats()
  - Qualitative: Find frequencies. table() or prob.table()
- 3. Perform pictorial representation of each single variable
  - Quantitative: Histograms or box plots. hist(), boxplot()
  - Qualitative: Bar or pie charts. plot(), barplot(), pie()
- 4. Be aware of outliers and robust statistics
- Association between variables
  - scatterplot() to compare two numerical variables
  - Side-by-side boxplots for categorical and numerical vars
  - pairs() for a matrix of scatter plots of all variables
  - cor(), cov() for correlation and covariance between vars

#### End of Week 1