Introduction to linear regression

(Week 05 lecture notes)

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August 1st 2018

Topics covered in this lecture

- Machine learning the probabilistic way
- Supervised learning problems
- Regression
- Case studies in R and Python

Why and what is machine learning ?

- We are in the era of **big data**: data of massive size and complex nature
  - 40 billion indexed web pages
  - the entire genome of thousands of individuals
  - more than 160 million credit card transactions per hour
- Machine learning provides **automated methods** to process and analyze data
  - automatically detect pattern in data
  - use the pattern to predict future data
  - use the pattern to inform decision making
- Many machine learning approaches rely on tools of probability theory

Types of machine learning

- Supervised learning (or predictive learning)
  - classification (output is categorical)
  - regression (output is continuous)
- Unsupervised learning (or descriptive learning)
  - clustering
  - dimension reduction
  - graph structure
  - matrix completion
- Reinforcement learning (learning to make decisions)

A general setting for supervised learning problems

Suppose we have some inputs X and some outputs y, the goal is to learn a mapping using a set of labelled set of input-output pairs $\{(X_i, y_i)\}_{i=1}^{n}$:

- also called a **training** dataset

To verify the quality of this mapping, we often use

- a **testing** data set containing (sometimes absent) just the inputs $\mathbf{X}_{\text{test}}$

The established mapping provides

- a model that describes the relationship between the inputs and outputs
- a model that can be used to predict outputs in the testing data

Some examples of classification problems

When the outputs are categorical, these are known as the **classification** or **pattern recognition** problems:

- Handwritten digit recognition: postal offices process your letters automatically.
- How likely are you to get a new credit card approved?
- Identifying faces from images.

handwritten digit recognition

handwritten digit recognition

- the data consist of
  - images of handwritten digits from 0 to 9
  - labels identify by a human
- the goal is to process images automatically without humans hand labelling
- the learning algorithm need to achieve “near-human” performance

credit card approval

- given attributes such as
  - age
  - past credit history
  - current financial status
  - number of credit cards owned
  - household income, etc.
- Credit card applications either accepted (+) or rejected (-)

credit card approval

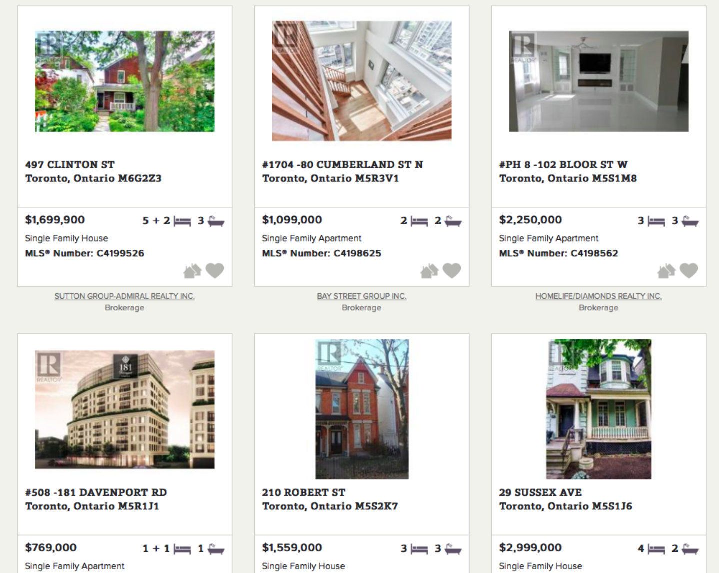
- Data can be found here
- Some analysis in R here
- Some analysis in Python here

Some examples of regression problems

When the outputs are continuous or ordinal, these are known as the **regression** problems:

- How much can your neighbour's house go for in a market like this?
- Predict the trading value of the TSX index tomorrow or in a month given the current market condition and other available information.
- Predict the age of a current subscriber of the Globe and Mail based on their browsing history.
- Predict the amount of pollutant in a given postal code area with weather data, traffic condition and information on industrial activities in the area and nearby.

house price prediction



house price prediction

- the listing price of all other houses in your neigbourhood is public (realtor.ca)
- a number of factors influence the listing price in your neighbourhood
  - house types (detached, semi-detached, etc.)
  - living space (square feet)
  - number of bedrooms
  - number of bathrooms
  - distance to a good public school
  - mortgage policies
  - availability of inventory
  - overall desirability of the neighbourhood
  - other amendities nearby
- How much should your neighbour list their house for in this market?

Model TSX index

Model TSX index

- Index Characteristics such as constituents
- a number of economic factors influence the index
  - labor costs
  - interest rates
  - government policy
  - taxes
  - etc.
- recent news or economic developments
- Can you provide a one-day or one-month forecast for the TSX composite index?

How to approach these problems?

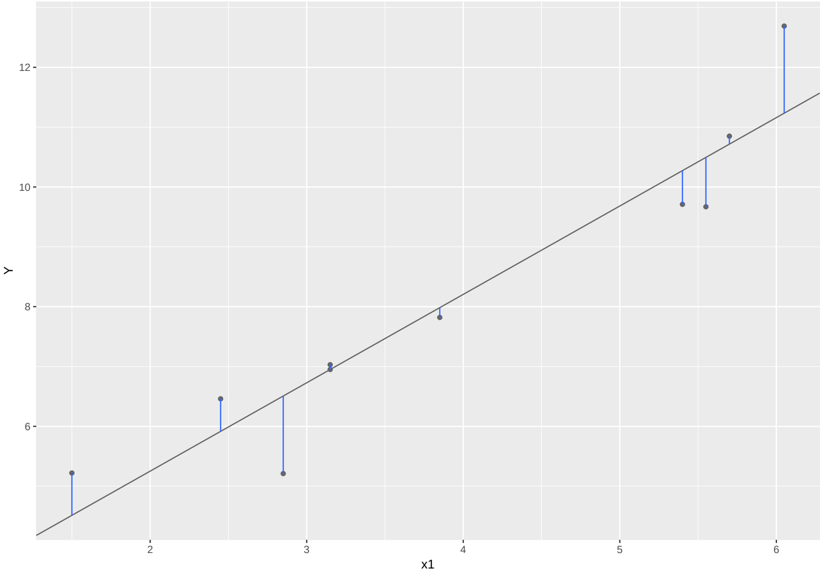
What does data look like?

For the simplest case, we look at a dataset with one input vector.

i	X	Y
1	3.2	6.95
2	1.5	5.22
3	2.4	6.46
4	3.2	7.03
5	5.4	9.71
6	5.5	9.67
7	6.1	12.69
8	5.7	10.85
9	2.8	5.21
10	3.9	7.82

For example, the third observation is $(X_3, Y_3) = (2.4, 6.46)$. For real data, usually you don't have the index i column as given in the table.

Visualize the data with a scatterplot



Observing the scatterplot

- Most data seem to fall near a line
- For bigger values of X, Y seems to be bigger as well
- In other words, X and Y seem to be positively related
- How can we find the line that "best" describes the relationship between X and Y?

A simple linear regression

- the output: an **outcome** variable Y
- one input: a **predictor** variable X
- We want to find a simple linear function of $X = (x_1, \ldots, x_n)$ that approximates $Y = (y_1, \ldots, y_n)$:
  - A simple linear function has the form $f(X) = a + bX$
  - "best" fit for a data point (i) is measured by a small distance $r_i = y_i - f(x_i)$
  - How do we aggregate the residuals (r_i) to find the line of best fit?
- **Least squares method**

$$\text{argmin}_{a,b} \sum_{i=1}^{n} r_i^2 = \text{argmin}_{a,b} \sum_{i=1}^{n} (y_i - a - bx_i)^2$$

Solving the least squares problem

$$\frac{\partial \sum_{i=1}^n r_i^2}{\partial a} = 2\sum_{i=1}^n r_i \frac{\partial r_i}{\partial a} = 0$$

and

$$\frac{\partial \sum_{i=1}^n r_i^2}{\partial b} = 2\sum_{i=1}^n r_i \frac{\partial r_i}{\partial b} = 0$$

Plug in $r_i = y_i - f(x_i) = y_i - a - bx_i$ and solve the two equations simultaneiously to obtain the least squares solutions.

$$\hat{a} = \bar{y} - \hat{b}\bar{x}$$

and

$$\hat{b} = \frac{\sum_{i=1}^n - \frac{1}{n}\sum_{i=1}^n x_i \sum_{i=1}^n y_i}{\sum_{i=1}^n x_i^2 - \frac{1}{n}(\sum_{i=1}^n x_i)^2}$$

Regression coefficients

The output is approximated by a simple linear function has the form $f(X) = a + bX$

- a is the **intercept** (i.e. the value of the function when $X = 0$)
- b is the **slope** (the strength of the positive or negative relationship between input and output)

The regression coefficients obtained using the least squares method:

- $\hat{a}$ is the estimated intercept
- $\hat{b}$ is the estimated slope

Directions of association

- If the linear relationship is absent, then $\hat{b}$ should be fairly close to 0
- If $\hat{b} > 0$, a positive relationship is possible
- If $\hat{b} > 0$, a negative relationship is possible

Strength of association

- The strength of association between the input and output can be captured by **Pearson's correlation coefficient** *if* the input has only one variable (e.g. a simple linear regression model)
  - the correlation coefficient in a sample is denoted by $r \in [-1, 1]$
  - the closer $|r|$ is to 1, the stronger the relationship
  - between $(-0.2, 0.2)$
- The strength of association between the input and output can be captured by **Pearson's correlation coefficient** *if* the input has only one variable (e.g. a simple linear regression model)
  - usually we square it and use r^2
  - intepreted as the porportion of variance in Y that is explained by X

Regression in statistical software programs

The objective of the remaining lecture is to solve real prediction problems using statistical programming. You should be able to:

- Setup the regression problem
- Produce initial visualization of data
- Obtain an estimated linear regression model in either R or Python
- Read the outputs from R or Python
- Make prediction or interpret the results

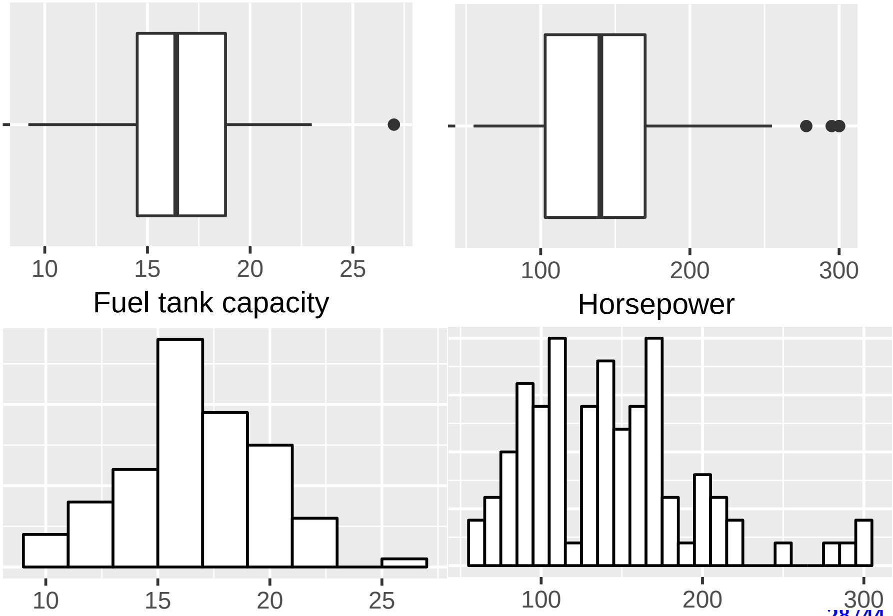
Case study of regression in R and Python

- Data "Cars93" from the MASS library (appeared in lecture 1)
- Use data to answer the question:
  - Does car with a bigger fule tank capacity necessarily have more horsepower?
  - For a car with fuel tank capacity of 27 US gallons, what is the maximum horsepower roughly?
  - What about a car with 9 US gallons?
  - What about a car with 16 gallons?

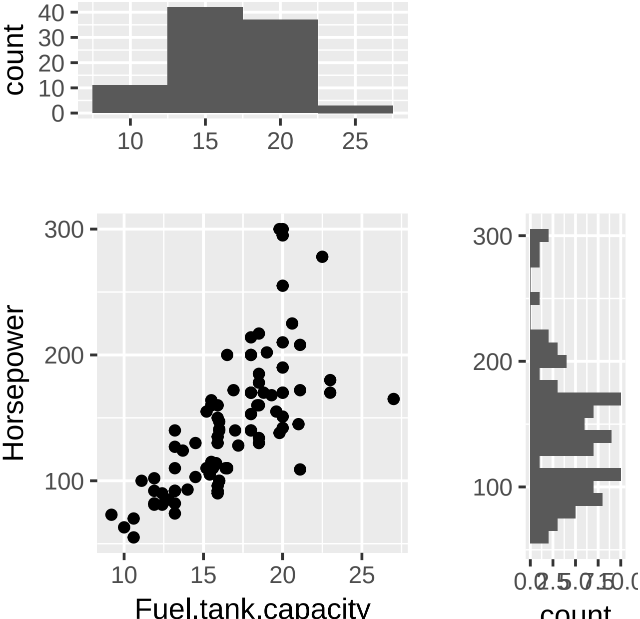
About the dataset

- Data from 93 Cars on Sale in the USA in 1993
- Input variable is "Fuel tank capacity" in US gallon
- Output variable is "Horsepower" (maximum horsepower)
- Randomly choose 10 cars/observations to be the testing data
- The remaining 83 cars will be used to build the linear model

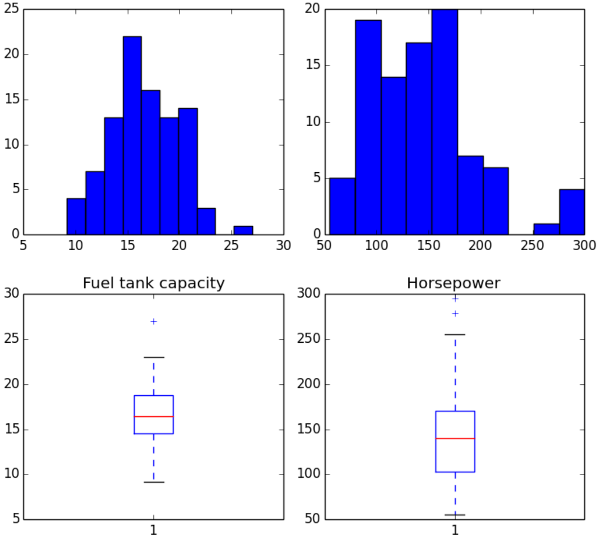
Data visualization (R)



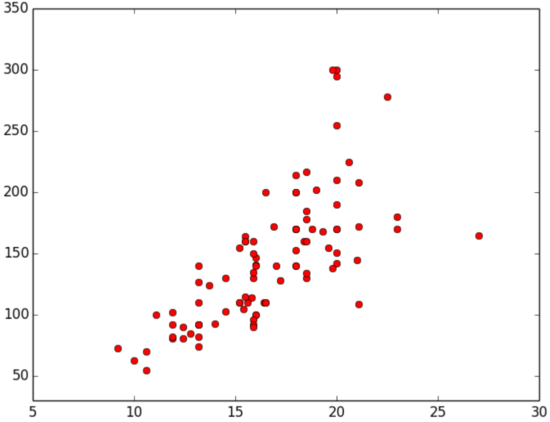
Data visualization (R)



Data visualization (Python)



Data visualization (Python)



Summarizing the data (R)

```r
mean(Cars93[["Fuel.tank.capacity"]])
```

```
## [1] 16.66452
```

```r
median(Cars93[["Fuel.tank.capacity"]])
```

```
## [1] 16.4
```

```r
sd(Cars93[["Fuel.tank.capacity"]])
```

```
## [1] 3.27937
```

```r
mean(Cars93[["Horsepower"]])
```

```
## [1] 143.828
```

```r
median(Cars93[["Horsepower"]])
```

```
## [1] 140
```

```r
sd(Cars93[["Horsepower"]])
```

```
## [1] 52.37441
```

```r
round(cor(Cars93[["Fuel.tank.capacity"]],Cars93[["Horsepower"]]),3)
```

```
## [1] 0.712
```

Summarizing the data (Python)

```
import pandas
```

```
## /Library/Frameworks/Python.framework/Versions/3.5/lib/python3.5/importlib/_bootstrap.py:2
##   return f(*args, **kwds)
```

```
Cars93 = pandas.read_csv("Cars93.csv")
import scipy
from scipy.stats.stats import pearsonr
```

```
## /Library/Frameworks/Python.framework/Versions/3.5/lib/python3.5/importlib/_bootstrap.py:2
##   return f(*args, **kwds)
```

```
Cars93[["Fuel.tank.capacity"]].mean()
Cars93[["Fuel.tank.capacity"]].median()
Cars93[["Fuel.tank.capacity"]].std()
```

```
import pandas
Cars93 = pandas.read_csv("Cars93.csv")
Cars93[["Horsepower"]].mean()
Cars93[["Horsepower"]].median()
Cars93[["Horsepower"]].std()
```

```
import pandas
Cars93 = pandas.read_csv("Cars93.csv")
from scipy.stats.stats import pearsonr
pearsonr(Cars93[["Fuel.tank.capacity"]],Cars93[["Horsepower"]])
```

Estimated linear model in R

```r
summary(lm(Horsepower~Fuel.tank.capacity, data = Cars93))
```

```
##
## Call:
## lm(formula = Horsepower ~ Fuel.tank.capacity, data = Cars93)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -96.321 -21.915  -5.349  14.863 120.528
##
## Coefficients:
##                    Estimate Std. Error t value Pr(>|t|)
## (Intercept)         -45.613     19.968  -2.284   0.0247 *
## Fuel.tank.capacity   11.368      1.176   9.667 1.27e-15 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 36.99 on 91 degrees of freedom
## Multiple R-squared:  0.5066, Adjusted R-squared:  0.5012
## F-statistic: 93.45 on 1 and 91 DF,  p-value: 1.268e-15
```

Estimated linear model in Python

```
import pandas
import numpy as np
import stats
Cars93 = pandas.read_csv("Cars93.csv")
x = np.array(Cars93[["Fuel.tank.capacity"]])
y = np.array(Cars93[["Horsepower"]])
x.reshape((len(x), 1))
y.reshape((len(y), 1))
from sklearn.linear_model import LinearRegression
```

```
## /Library/Frameworks/Python.framework/Versions/3.5/lib/python3.5/impo
##   return f(*args, **kwds)
## /Library/Frameworks/Python.framework/Versions/3.5/lib/python3.5/impo
##   return f(*args, **kwds)
```

```
regression_model = LinearRegression()
regression_model.fit(x, y)
```

```
## /Library/Frameworks/Python.framework/Versions/3.5/lib/python3.5/site
##   linalg.lstsq(X, y)
```

```
intercept = regression_model.intercept_[0]
```

Interpreting the results

- The model is written as "Horsepower~Fuel.tank.capacity"
- **Regression Coefficients**:

Predictors	Estimate	Std. Error	t value	Pr(>
(Intercept)	-45.613	19.968	-2.284	0.0247 *
Fuel.tank.capacity	11.368	1.176	9.667	1.27e-15 ***

- **Significance codes**:

Extremely Strong	Strong	Moderate	Weak	No evidence against H_o
0 ***	0.001 **	0.01 *	0.05 .	0.1-1

Interpreting the results - Cont'd

- Residual standard error: 36.99 on 91 degrees of freedom
- R-squared
  - Multiple R-squared: **0.5066**
  - Adjusted R-squared: 0.5012
- F-statistic: 93.45 on 1 and 91 DF,
- **p-value**: 1.268e-15

What additional information do you observe?

Back to the question

Does car with a bigger fuel tank capacity (FTC) necessarily have more horsepower?

- There is extremely strong evidence of a car with larger FTC having more horsepower.
- For one US gallon increase in fuel tank capacity, the maximum horsepower increases by 11 on average.

Prediction problems:

- For a car with fuel tank capacity of 27 US gallons, what is the maximum horsepower roughly?
- What about a car with 9 US gallons?
- What about a car with 16 gallons?

Prediction in R

```r
new <- data.frame("Fuel.tank.capacity" = c(27, 9, 16))
predict(lm(Horsepower~Fuel.tank.capacity, data = Cars93),
        newdata = new)
```

```
##         1         2         3
## 261.32084  56.69841 136.27380
```

Prediction in Python

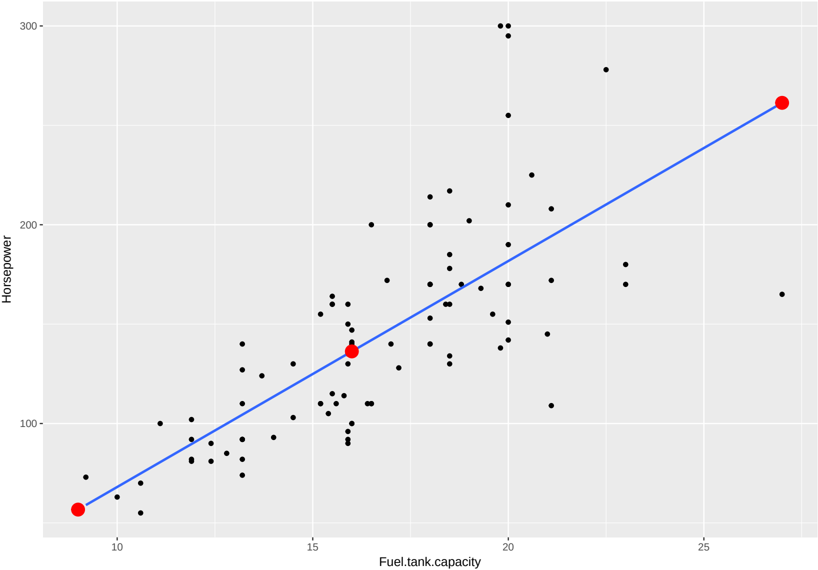
```
x_new = [[27], [9], [16]]
y_predict = regression_model.predict(x_new)
print(y_predict)
```

```
## [[261.32083648]
##  [ 56.69840591]
##  [136.27379557]]
```

Interpret the results

- For a car with fuel tank capacity of 27 US gallons, the *predicted* maximum horsepower is roughly 261.
- For a car with fuel tank capacity of 9 US gallons, the *predicted* maximum horsepower is roughly 57
- For a car with fuel tank capacity of 16 US gallons, the *predicted* maximum horsepower is roughly 136

Are these results trustworthy?



Next class

- Linear regression as a statistical model
- Classic assumptions of linear regression
- More examples of linear regression
- Tests for equality of means as a special case of a simple linear regression
- Extending to multiple predictors in R