Advanced Data Analysis with Python

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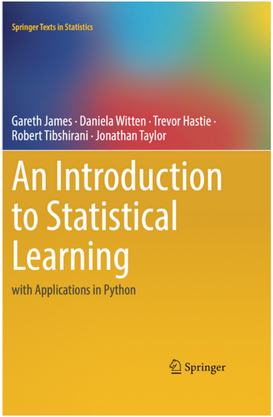
Resources for this class



An Introduction to Statistical Learning

- This class follows **Chapters 4 and 8** of this book
- Refer to the book if you want to deepen today's topic
- It is a bit more mathematically intensive than this class!

Homework Correction

Course recap

What is expected from you

Project Description

Due: November 3, 2025, 23:59

What to upload: PDF with project proposal (2-3 research questions, planned pipeline) and group members' names

Final Project

Due: December 20, 2025, 23:59

What to upload: Complete project report in form of a paper (5-8 pages), commented code

Deadline cannot be delayed!

Resources for scientific writing

- Writing a scientific paper (ETH Zurich, 2019)
- Writing a scientific article: A step-by-step guide for beginners
- How to write your first research paper (NIH 2011)
- ... and many others!

Project checklist

- **Code**:
  - Comment each function to explain to me what it does
  - Upload the code on **GitHub** and share the repository with me
  - Document your repository structure in the **README** file

If you do not know how to use GitHub, you can refer to the guide I uploaded on Moodle.

Project checklist

- **Paper**:
  - 5-8 pages in English
  - Structured as a **research paper**:
    - **Introduction**: introduce your research questions (RQs) and their motivation
    - **Related Work**: ground in the literature your choice of RQs and methods
    - **Methods**: explain your pipeline and how you implemented it
    - **Discussion**: present your results (e.g. in form of graphs or tables) and interpret them **qualitatively** and **quantitatively**
    - **Conclusion**: sum up your work

Statistical Modeling Foundations

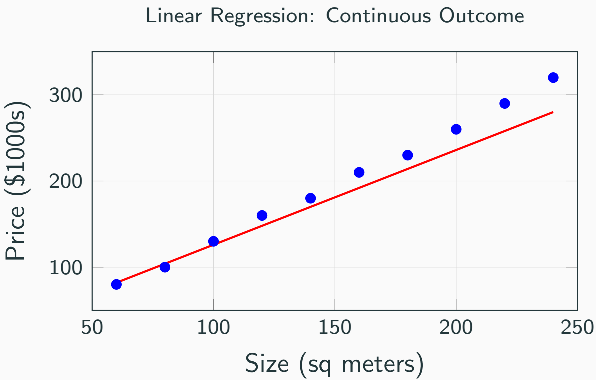
What is a statistical model?

Definition (Statistical Model)

A statistical model is a mathematical model that embodies a set of statistical assumptions concerning the generation of sample data (and similar data from a larger population).

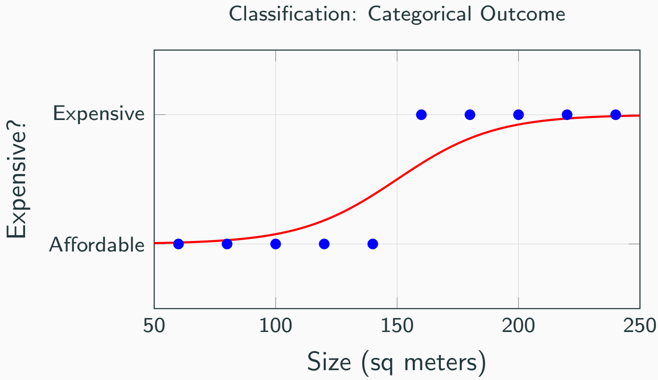
Source: Wikipedia

Linear Regression Example: Predicting House Prices



- Continuous outcome: house price ($1000s)
- Red line: regression line through the data
- Blue points: actual house prices (data points)

Classification Example: Predicting Expensive Houses



- Categorical outcome: affordable vs expensive
- Red curve: probability of being expensive
- Blue points: observed house labels

Classification

Classification problem

Definition

Classification involves assigning a label to a set of data (**categorical variables)**.

- Example:

$$EmploymentSector \in \{"Healthcare", "Hospitality", "Manufacturing"\}$$

Difference with Linear Regression

Why not linear regression?

Is it possible to map the variables to integers and perform linear regression?

Difference with Linear Regression

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- Suppose we have a **binary classification question**: "Is this person in favour of the adoption of a new policy for public transportation?"

$$Y = \begin{cases} 0 & \text{if No} \\ 1 & \text{if Yes} \end{cases}$$

$$\bar{Y} > 0.5 = Yes$$

Difference with Linear Regression

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$$\bar{Y} > 0.5 = Yes$$

Linear regression can work as a **binary classifier**, but it can output probabilities bigger than 0 or smaller than 1.

Important:

In the above mentioned case, you can easily demonstrate that **if you flip the two variables, the output does not change.**

Difference with Linear Regression

- Multiclass question:

$$\mathit{EmploymentSector} = \begin{cases} 1 & \text{if Healthcare} \\ 2 & \text{if Hospitality} \\ 3 & \text{if Manufacturing} \end{cases}$$

This mapping implies:

- Order between the three variables
- Same relation between healthcare and hospitality and hospitality and manufacturing

Both assumptions are not necessarily real.

Logistic Regression

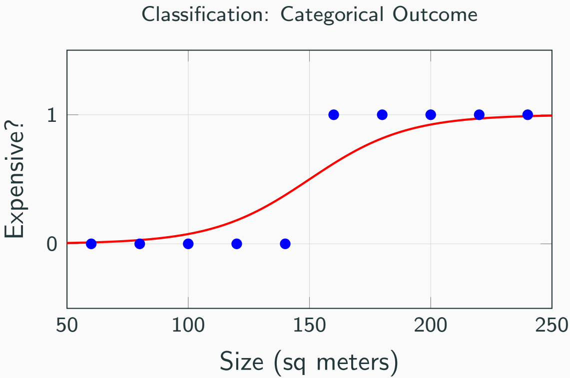
The logistic regression model is displayed here:

$$\Pr(Y = 1 \mid X) = \frac{e^{\beta_0+\beta_1 X}}{1 + e^{\beta_0+\beta_1 X}}$$

where:

- $e = 2.71828$ is a constant (Euler's number)
- $(Y = 1 \mid X)$ is the conditional probability that $Y = 1$ given X
- β_0 is the intercept.
- β_1 measures the effect of X on Y.

It is easy to see that the results will always be between 0 and 1.



Logistic regression ensures that the estimated values lie between 0 and 1.

Adapted from: An Introduction to Statistical Learning.

Estimating the parameters: Maximum Likelihood

- For clarity, let $p(x_i) = P(Y = 1 \mid X = x_i)$
- The **parameters** β_0 and β_1 are estimated based on **maximum likelihood**:

$$(\beta_0, \beta) = \prod_{i:y_i=1} p(x_i) \prod_{i:y_i=0} \big(1 - p(x_i)\big)$$

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- Gives **the probability of the observed 0s and 1s** in the data
- β_0 and β_1 picked so that $\hat{p}(x_i)$ is as close as possible to the actual data
  - **Maximizing** the **likelihood**
  - Example: when predicting if a house will sell (1) or not (0), trying to predict a number as close as possible to 1 if the house was sold, and to 0 if it was not

Housing Dataset

- Binary outcome: **Sold (Yes/No)**
- Predictor: **House Price (in €100k)**
- Example records:

House Price	Sold
1.2	Yes
2.5	No
1.8	Yes
3.0	No

Goal: Predict probability of selling based on house price.

Logistic Regression Model

Equation

$$\log \frac{\Pr(Y = 1 \mid \mathit{Price})}{1 - \Pr(Y = 1 \mid \mathit{Price})} = \beta_0 + \beta_1 \cdot \text{Price}$$

- Parameters estimated using Maximum Likelihood

Estimated Model

$$\hat{P}(Y = 1 \mid \text{Price}) = \frac{1}{1 + e^{-(-2.5 + 0.8 \cdot \text{Price})}}$$

Results: Predicted Probabilities

House Price	Observed Sale	Predicted P(Sales)
1.2	Yes	0.18
2.5	No	0.47
1.8	Yes	0.28
3.0	No	0.62

- Higher house price = higher predicted probability of selling

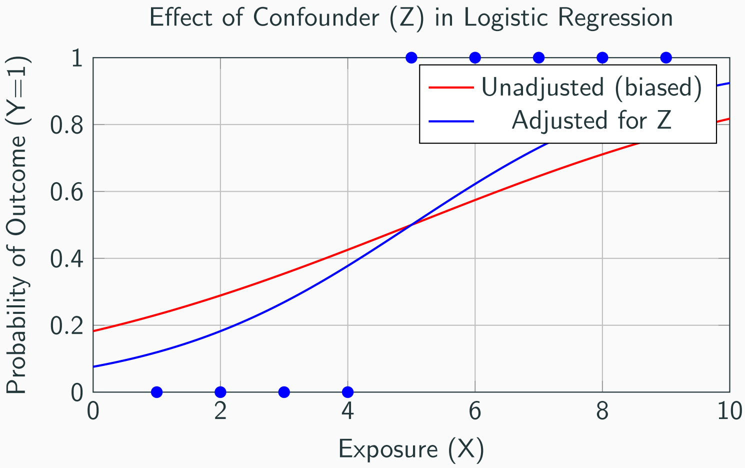
Caveat: Confounding

Problem: We plot the relationship between **credit card balance** and **default** (setting: US). The statistics reveal that students have a higher credit card balances, but for each balance, they tend to default less. This means that depending on the analysis we conduct, we apparently get contradictory results.

- **Student** and **Balance** are correlated
- **Balance** has an effect on the output (**Default**) as well
- Consequence: **confounding**
- (One possible) solution: **Multiple Logistic Regression**

Source of example: An Introduction to Statistical Learning - Chapter 4

Frame Title



Effect of Confounder (Z) in Logistic Regression
Probability of Outcome (Y=1)
Exposure (X)
0
0.2
0.4
0.6
0.8
1
0
2
4
6
8
10
Unadjusted (biased)
Adjusted for Z

Multiple Logistic Regression

- Same as simple, but with more than one predictor:

$$\log \frac{P(Y = 1 \mid X)}{1 - P(Y = 1 \mid X)} = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_k X_k$$

Multinomial Logistic Regression

- Used for **multiclass classification problems**

$$\Pr(Y = k \mid X) = \frac{e^{\beta_{0k}+\beta_{1k}X_1+\cdots+\beta_{pk}X_p}}{\sum_{j=1}^{K} e^{\beta_{0j}+\beta_{1j}X_1+\cdots+\beta_{pj}X_p}}$$

- Approach: Model the distribution of X in each class **separately**, and deduct $\Pr(Y \mid X)$

We will only focus on **normal distribution** in this class.

Binary Example: Housing

We want to predict whether a house will **sell within 30 days** (Yes $= 1$, No $= 0$) based on its characteristics:

- **Price**
- **Size**
- **Bedrooms**

Question: Given a house with 200000, 3 bedrooms, and 100 m², what is the probability it sells within 30 days?

Logistic Regression Formula

The probability a house sells is estimated as:

$$P(\text{Sold} = 1) = \frac{e^{\beta_0 + \beta_1 \text{Price} + \beta_2 \text{Size} + \beta_3 \text{Bedrooms}}}{1 + e^{\beta_0 + \beta_1 \text{Price} + \beta_2 \text{Size} + \beta_3 \text{Bedrooms}}}$$

- β_0: baseline probability (intercept)
- $\beta_1, \beta_2, \beta_3$: coefficients showing effect of each feature

Example Houses and Predicted Probability

House	Price ($k)	Size (m^2)	Bedrooms	Probability Sold	Sold?
A	100	80	2	0.3	No
B	150	100	3	0.6	Yes
C	200	120	4	0.8	Yes

Logistic regression predicts probabilities, not just yes/no.

When Logistic Regression isn't enough?

1. The classes are well separated
2. The distribution of the predictors X is approximately normal in each of the classes and the sample size is small

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Instead: **Linear Discriminant Analysis (LDA)**.

- LDA is also more popular **when we have more than 2 response classes**.

Discriminative and Generative Models

Discriminative Models

- Model the **conditional distribution** $p(Y|X)$ directly
- Focus on assigning labels to the data
- Examples: Logistic Regression, SVM, Neural Networks
- Usually better for classification accuracy

Generative Models

- Model the **joint distribution** $p(X, Y)$
- Learn $p(X|Y)$ and $p(Y)$
- Examples: Naive Bayes, LDA, QDA

Tree-based methods

Decision trees

- **Decision trees** model the classification problem in a tree structure
- They break down the problem into smaller and smaller subsets
- A tree is incrementally built from these smaller subsets
- **Decision nodes** (two branches or more) and **leaf nodes** (last nodes, correspond to classification)
- Uppest node is the **root**
- Applied to both **regression** and **classification**

Decision trees: Classification example (simplified)

Is the price $>=$ 500k?

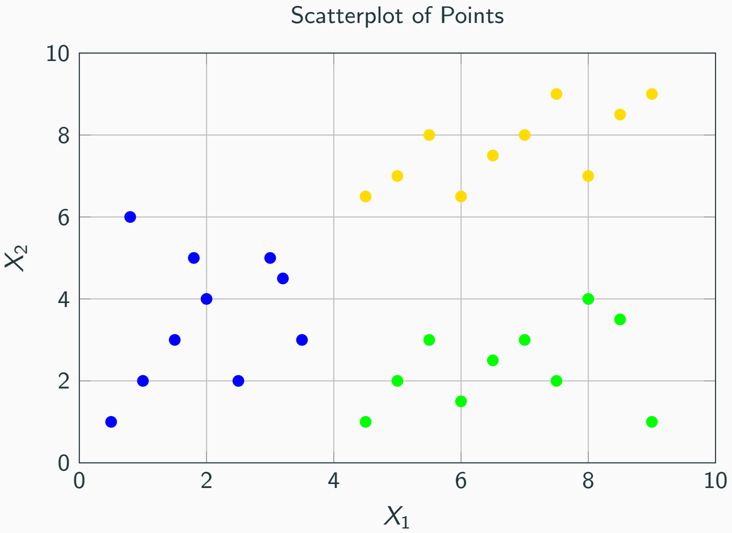
- **Yes**
  - **Expensive**
- **No**
  - **Affordable**

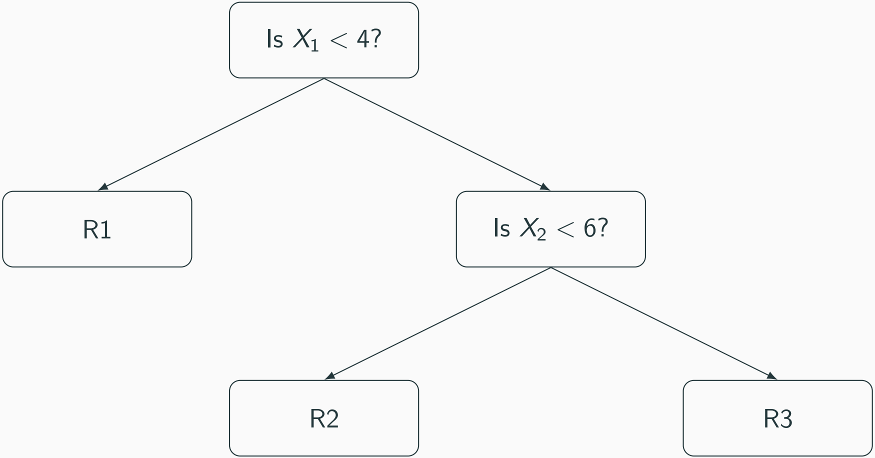
Decision trees: Classification example (simplified)

- **Is the price $>=$ 500k?**
  - **Yes**
    - **Expensive**
  - **No**
    - **Is the surface $>=$ 100 m^2?**
      - **Yes**
        - **Suitable choice.**
      - **No**
        - **Non-suitable choice.**

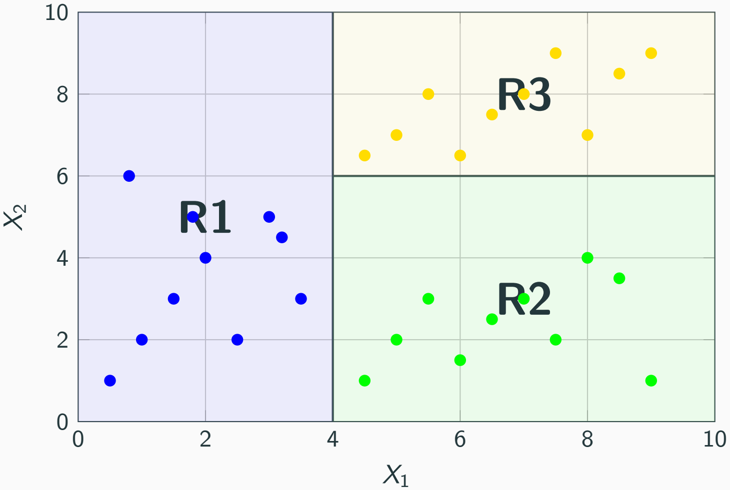
(Clearly not in Paris.)

Decision trees: Regression Example




Is $X_1 < 4$?
R1
Is $X_2 < 6$?
R2
R3

Visualization of the "splitting" in different areas done by tree-based methods.



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How to build a decision tree

- **Divide the predictor space into** N **non-overlapping regions** $R_1, R_2, ..., R_n$

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- Goal: Find the best regions R_1 to R_n according to an optimization criterium
    - **Regression: Minimize RSS**
    - **Classification: Gini or entropy**

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  - **Regression: Minimize RSS**
  - **Classification: Gini or entropy**
- Make predictions in leaves
  - **Regression**: **mean** of the response values for the training observations in R_n
  - **Classification**: **majority class** in the leaf

Regression tree

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Regression tree

- **Divide the predictor space into** N **non-overlapping regions** $R_1, R_2, ..., R_n$
- For each observation in region R_n, make the same predictions: **mean of the response values for the training observations in** R_n
- Goal: Find regions R_1 to R_n so to minimize the Residual Sum of Squares (RSS)

Regression tree

Problem: it is infeasible to compute RSS for every possible partition of the space in n regions.

Solution: **top-down, greedy approach.**

- **top-down**: begins **at the top** of the tree and then successively splits the predictor space.
- **greedy**: at each step of the tree-building process, the best split is made **at that particular step**.

Classification Trees

- Same as regression, but for **qualitative values**

For a classification tree, we predict that each observation belongs to the most commonly occurring class of training observations in the region to which it belongs.

- The measures for the binary splits are **GIni index** and **entropy**

Source: An Introduction to Statistical Learning.

Classification trees

1. Gini Index:

Measures the total variance across the classes.

$$G = \sum_{k=1}^{K} \hat{p}_{mk}\left(1 - \hat{p}_{mk}\right)$$

- p_i = proportion of training observations in the mth region that are from the kth class i
- K = number of classes

Classification Trees

2. **Entropy:** An alternative measure to Gini.

$$D = -\sum_{k=1}^{K} \hat{p}_{mk} \left(\log(\hat{p}_{mk})\right)$$

Lower Gini or entropy = predominantly observations from a single class (node "purity") = better

Considerations on decision trees

- **Pro:** easy to compute, represent, and interpret
- **Contra:** accuracy is way lower; oversimplification

> The risk of **overfitting** is particularly high. This means that the model performs **well on the training set, but poorly on the test set.** One common approach to reduce overfitting is **pruning**. An alternative is also **random forest**, a learning method that is more accurate and reduces overfitting, but is also more complicated to implement.

Evaluation

Confusion Matrix

- Visualization of **True Positives (TP)**, **True Negatives (TN)**, **False Positives (FP)** and **False Negatives (FN)** values

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	Predicted	Predicted
Actual	4 TN	1 FP
Actual	2 FN	3 TP

Accuracy

- Ratio between **correctly predicted values** and **all values**.

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- Accuracy $= \frac{TP+TN}{TP+TN+FP+FN}$

Precision

- Ratio between **correctly predicted positive values** and **all predicted positive values**.

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- Ratio between **correctly predicted positive values** and **all predicted positive values**.
- Precision $= \frac{TP}{TP+FP}$

Recall

- Ratio between **correctly predicted positive values** and **all actual positive values**.
- Recall $= \frac{TP}{TP+FN}$

F1 score

- F1 Score $= 2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}}$

ROC curve

- **ROC (Receiver Operating Characteristic)**: plots *True Positive Rate* (TPR = recall) vs *False Positive Rate*
  - **TPR =** $\frac{TP}{TP + FN}$
  - **FPR =** $\frac{FP}{FP + TN}$

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- **AUC (Area Under Curve)**: probability a randomly selected positive ranks above a randomly selected negative.
- **Interpretation:**
  - AUC $= 0.5$: random guessing (diagonal).
  - AUC close to 1: perfect!
  - AUC < 0.5: predictions inverted.

ROC curve: example