Advanced Data Analysis with Python

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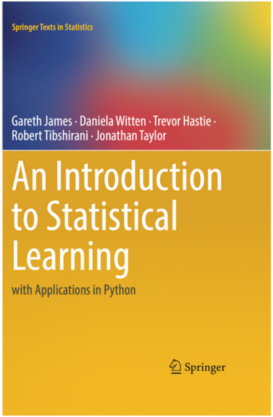
Resources for this class



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

Example: Regression

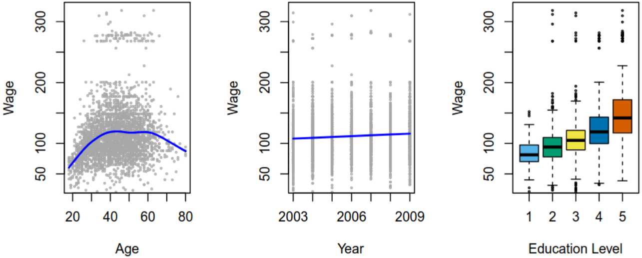


FIGURE 1.1. `Wage` *data, which contains income survey information for men from the central Atlantic region of the United States.* Left: `wage` *as a function of* `age`. *On average,* `wage` *increases with* `age` *until about* 60 *years of age, at which point it begins to decline.* Center: `wage` *as a function of* `year`. *There is a slow but steady increase of approximately* \$10,000 *in the average* `wage` *between* 2003 *and* 2009. Right: *Boxplots displaying* `wage` *as a function of* `education`, *with* 1 *indicating the lowest level (no high school diploma) and* 5 *the highest level (an advanced graduate degree). On average,* `wage` *increases with the level of education.*

Source: *An Introduction to Statistical Learning with Applications in Python.*

Example: Classification

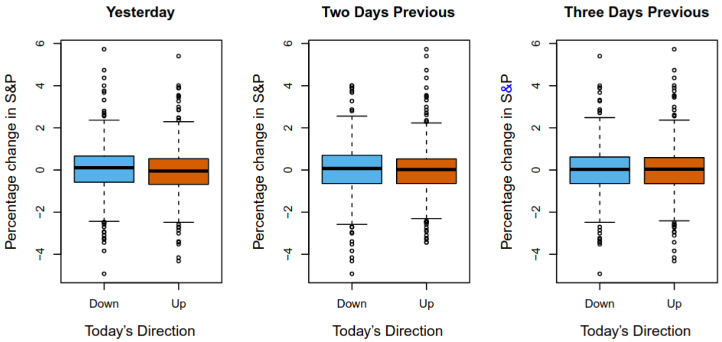


FIGURE 1.2. Left: *Boxplots of the previous day's percentage change in the S&P index for the days for which the market increased or decreased, obtained from the* `Smarket` *data.* Center and Right: *Same as left panel, but the percentage changes for 2 and 3 days previous are shown.*

Source: *An Introduction to Statistical Learning with Applications in Python.*

Example: Classification

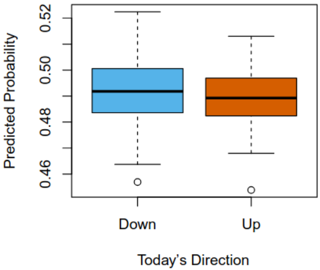


FIGURE 1.3. *We fit a quadratic discriminant analysis model to the subset of the* `Smarket` *data corresponding to the 2001–2004 time period, and predicted the probability of a stock market decrease using the 2005 data. On average, the predicted probability of decrease is higher for the days in which the market does decrease. Based on these results, we are able to correctly predict the direction of movement in the market 60% of the time.*

Source: *An Introduction to Statistical Learning with Applications in Python.*

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

- 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

Why not linear regression?

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

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

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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

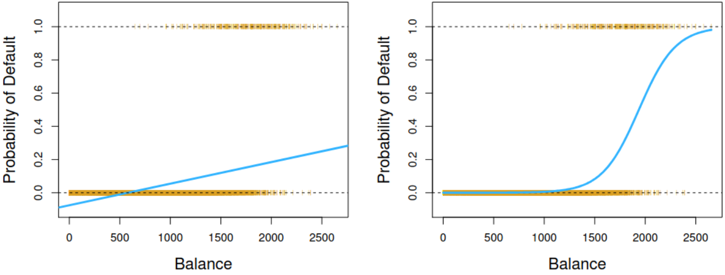
The logistic regression model is displayed in equation 1:

$$\Pr(Y = 1 \mid X) = \frac{e^{\beta_0 + \beta_1 X}}{1 + e^{\beta_0 + \beta_1 X}} \xrightarrow{\textit{becoming}} \log\left(\frac{\Pr(Y = 1 \mid X)}{1 - \Pr(Y = 1 \mid X)}\right) = \beta \quad (1)$$

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 our estimate for $p(X)$ lies between 0 and 1.

Source: An Introduction to Statistical Learning with Applications in Python

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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- β_0 and β_1 picked so that $\hat{p}(x_i)$ is as close as possible to the actual data

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

House Price	Default
1.2	Yes
2.5	No
1.8	Yes
3.0	No

Goal: Predict probability of default 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

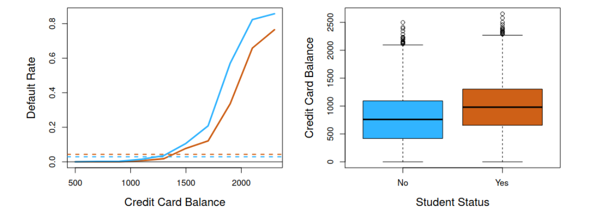
$$\hat{P}(Y = 1 \mid \text{Price}) = \frac{1}{1 + e^{-(-2.5 + 0.8 \cdot \text{Price})}}$$

Results: Predicted Probabilities

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

- Higher house price $\Rightarrow$ higher predicted probability of default
- Predictions may not perfectly match observations

Caveat: Confounding



- **Student** and **Balance** are correlated (see figure on the right)
- **Balance** has an effect on the output (**Default**) as well
- Consequence: **confounding**
- Solution: **Multiple Logistic Regression**

Source: An Introduction to Statistical Learning - Chapter 4

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 \$200,000, 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
- Can generate new data

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

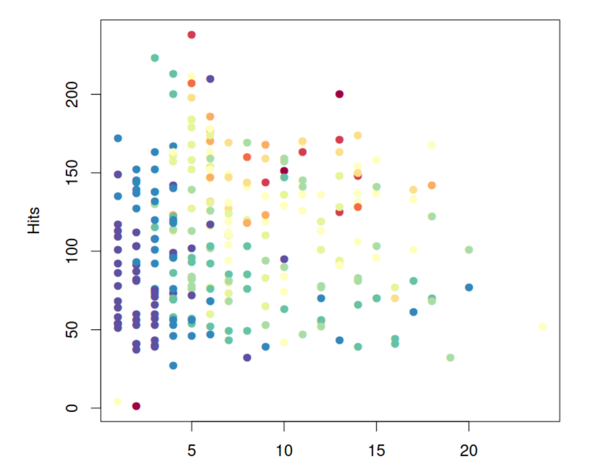

Figure 1: Example salary data of baseball players in relation to years of experience and hits.

Source: An Introduction to Statistical Learning.

Decision trees: Regression example

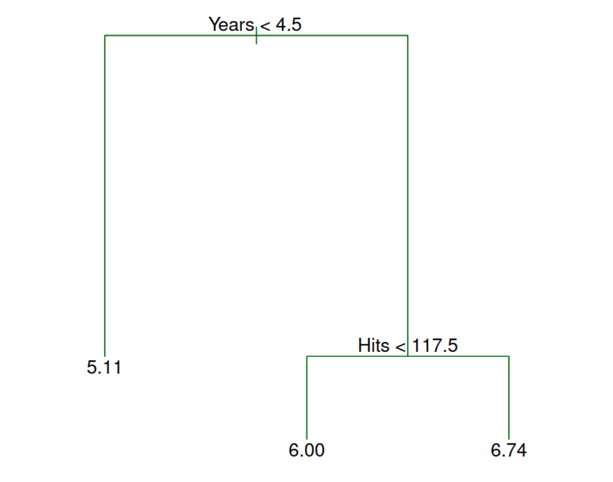

Figure 2: Decision tree for the baseball salary example.

Source: An Introduction to Statistical Learning.

Decision trees: Regression example

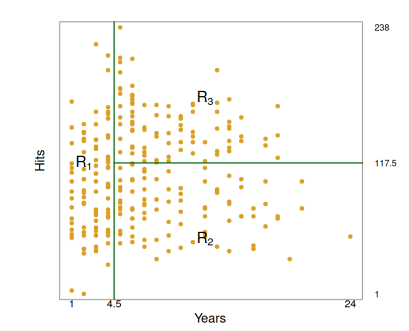

Figure 3: Visualization of the "splitting" in different areas done by tree-based methods. In this case, the data is split as follows:

$$R_1 = \{X \mid \text{Years} < 4.5\},\ R_2 = \{X \mid \text{Years} \geq 4.5,\ \text{Hits} < 117.5\},$$

$$R_3 = \{X \mid \text{Years} \geq 4.5,\ \text{Hits} \geq 117.5\}$$

.

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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    - **Classification: Gini or entropy**

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- **Divide the predictor space into** N **non-overlapping regions** $R_1, R_2, ..., R_n$
- Goal: Find the best regions R_1 to R_n according to an optimization criterium
  - **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

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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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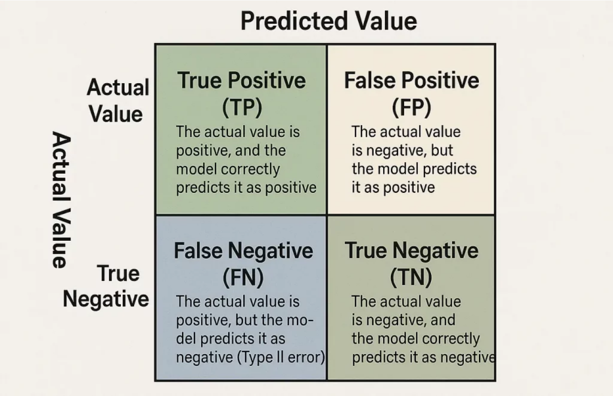

Figure 4: Confusion Matrix explanation.

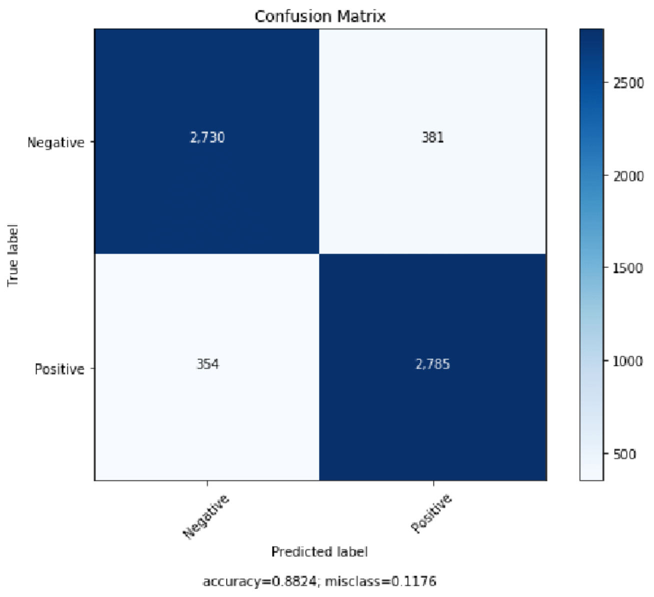

Figure 5: Confusion Matrix with real data

Source:ResearchGate

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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- Precision $= \frac{TP}{TP+FP}$

Recall

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

F1 score

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

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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  - **TPR =** $\dfrac{TP}{TP + FN}$
  - **FPR =** $\dfrac{FP}{FP + TN}$
- **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