

# INTRODUCTION TO MACHINE LEARNING

## Systems Sciences Foundations

Author: Eng. Carlos Andrés Sierra, M.Sc.  
cavirguezs@udistrital.edu.co

Lecturer  
Department of Computer Engineering  
School of Engineering  
Universidad Distrital Francisco José de Caldas

2025-I



# Outline

- 1 Fundamentals of Machine Learning
- 2 Python Tools for Machine Learning
- 3 Supervised Machine Learning
- 4 Machine Learning Models Evaluation



# Outline

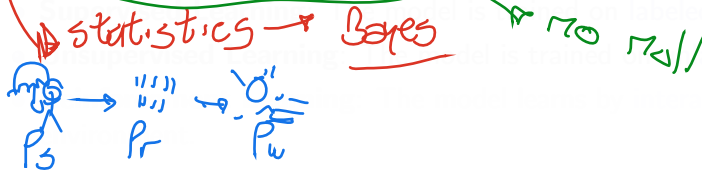
- 1 Fundamentals of Machine Learning
- 2 Python Tools for Machine Learning
- 3 Supervised Machine Learning
- 4 Machine Learning Models Evaluation



# Key Concepts in Machine Learning

## Machine Learning

- **Machine learning** is a method of ~~data~~ analysis that automates analytical model building.
- It is a **branch** of artificial intelligence based on the idea that systems can learn from data, identify patterns and make decisions with minimal human intervention.



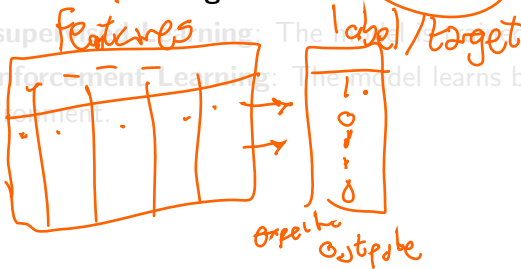
# Key Concepts in Machine Learning

## Machine Learning

- **Machine learning** is a method of data analysis that **automates** analytical model building.
- It is a **branch** of **artificial intelligence** based on the idea that systems can **learn from data**, **identify patterns** and **make decisions** with **minimal human intervention**.

- ① • **Supervised Learning:** The model is trained on labeled data.

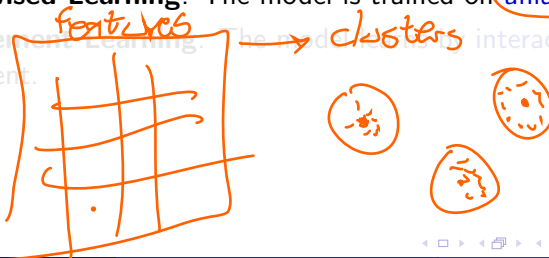
- **Unsupervised Learning:** The model is trained on unlabeled data.
- **Reinforcement Learning:** The model learns by interacting with an environment.



# Key Concepts in Machine Learning

## Machine Learning

- **Machine learning** is a method of data analysis that **automates** analytical model building.
- It is a **branch** of **artificial intelligence** based on the idea that systems can **learn from data**, **identify patterns** and **make decisions** with minimal human intervention.
- **Supervised Learning**: The model is trained on **labeled data**.
- **Unsupervised Learning**: The model is trained on **unlabeled data**.
- **Reinforcement Learning**: The model learns by interacting with an environment.



# Key Concepts in Machine Learning

## Machine Learning

- **Machine learning** is a method of data analysis that **automates** analytical model building.
- It is a **branch** of **artificial intelligence** based on the idea that systems can **learn from data**, **identify patterns** and **make decisions** with minimal human intervention.

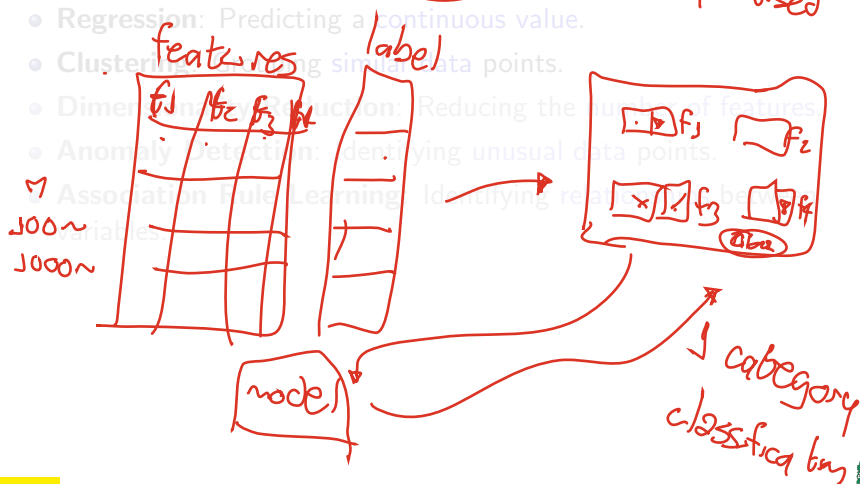
- **Supervised Learning**: The model is trained on **labeled data**.
- **Unsupervised Learning**: The model is trained on **unlabeled data**.
- **Reinforcement Learning**: The model learns by **interacting** with an environment.

*1 step*  
*mult. - step → cybernetics*



# Typical Machine Learning Problems

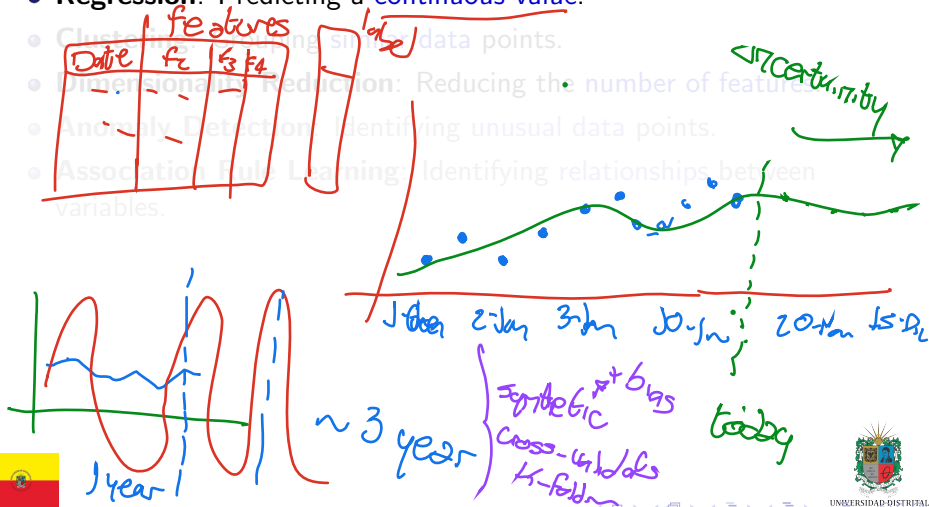
- **Classification:** Predicting a label. *targets → supervised*





# Typical Machine Learning Problems

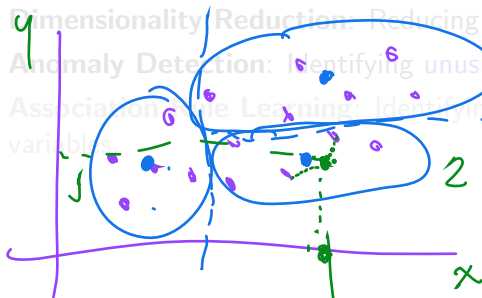
- **Classification:** Predicting a **label**.
- **Regression:** Predicting a **continuous value**.



# Typical Machine Learning Problems

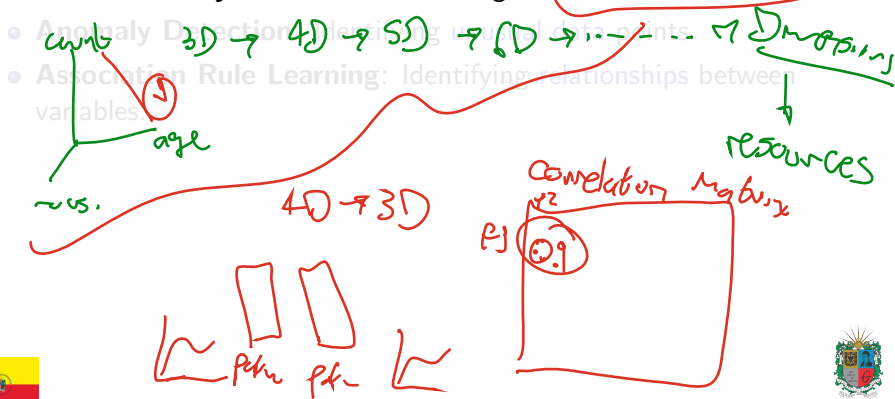
- **Classification:** Predicting a **label**.
- **Regression:** Predicting a **continuous value**.
- **Clustering:** Grouping **similar data** points.
- **Dimensionality Reduction:** Reducing the number of features.
- **Anomaly Detection:** Identifying unusual data points.
- **Association Rule Learning:** Identifying relationships between variables.

supervised  
unsupervised



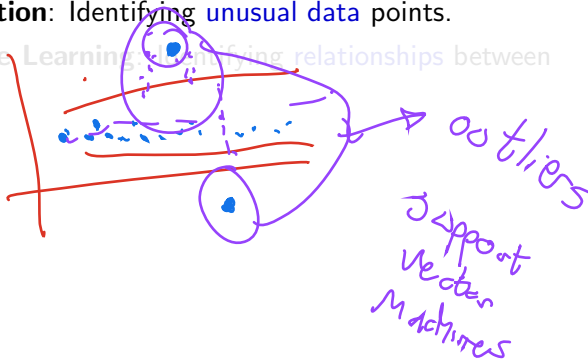
# Typical Machine Learning Problems

- **Classification:** Predicting a **label**.
- **Regression:** Predicting a **continuous value**.
- **Clustering:** Grouping **similar data** points.
- **Dimensionality Reduction:** Reducing the **number of features**.



# Typical Machine Learning Problems

- **Classification:** Predicting a **label**.
- **Regression:** Predicting a **continuous value**.
- **Clustering:** Grouping **similar data** points.
- **Dimensionality Reduction:** Reducing the **number of features**.
- **Anomaly Detection:** Identifying **unusual data** points.
- **Association Rule Learning:** Identifying relationships between variables.



# Typical Machine Learning Problems

- **Classification:** Predicting a **label**.
- **Regression:** Predicting a **continuous value**.
- **Clustering:** Grouping **similar data** points.
- **Dimensionality Reduction:** Reducing the **number of features**.
- **Anomaly Detection:** Identifying **unusual data** points.
- **Association Rule Learning:** Identifying **relationships** between variables.

Language  
↳ words  
sequence

correlation

$f_1$   
 $f_2$  }  $\rightarrow f_3$



# The Machine Learning Workflow

- **Data Collection:** Gathering the data. ①

- **Data Preprocessing:** Cleaning and preparing the data.

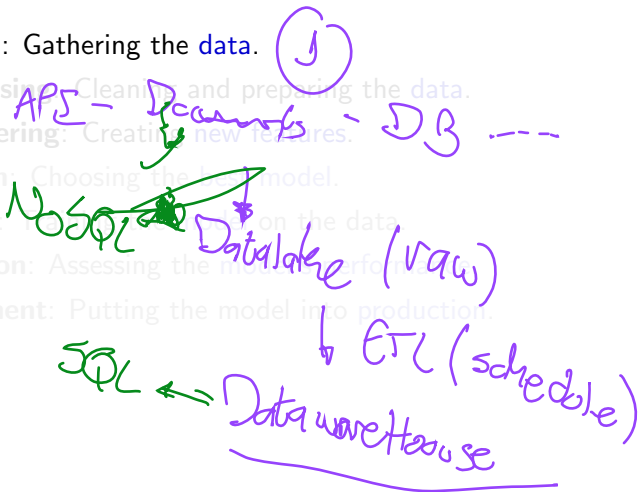
- **Feature Engineering:** Creating new features.

- **Model Selection:** Choosing the best model.

- **Model Training:** Training the model on the data.

- **Model Evaluation:** Assessing the model's performance.

- **Model Deployment:** Putting the model into production.



# The Machine Learning Workflow

- **Data Collection:** Gathering the data.
- **Data Preprocessing:** Cleaning and preparing the data.

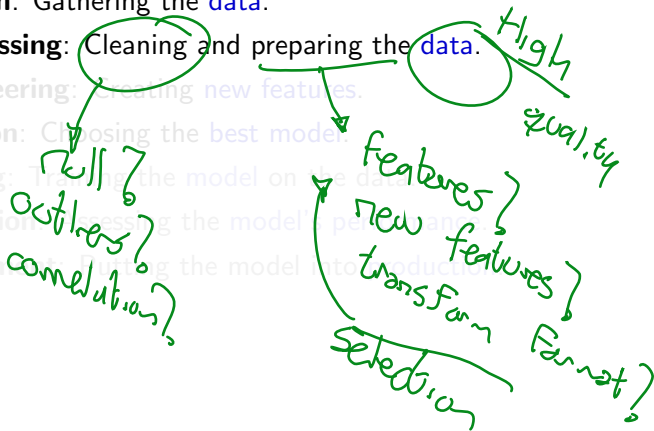
- **Feature Engineering:** Creating new features.

- **Model Selection:** Choosing the best model.

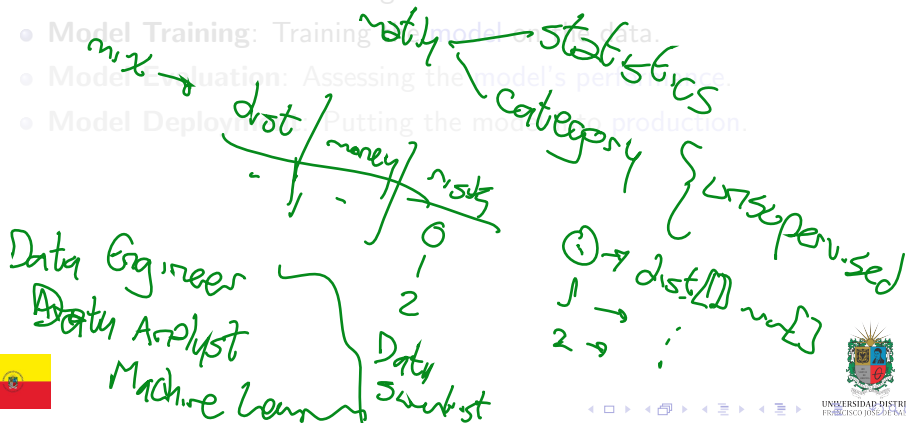
- **Model Training:** Training the model on the data.

- **Model Evaluation:** Assessing the model's performance.

- **Model Deployment:** Putting the model into production.



- Model Selection: Choosing the best model.
  - Model Training: Training the model with data.
  - Model Evaluation: Assessing the model's performance.
  - Model Deployment: Putting the model into production.
- Handwritten notes:
- mix  $\rightarrow$  dot /
  - with  $\rightarrow$  statistics
  - category





# The Machine Learning Workflow

- **Data Collection:** Gathering the data.
- **Data Preprocessing:** Cleaning and preparing the data.
- **Feature Engineering:** Creating new features.
- **Model Selection:** Choosing the best model.

any ~ 50  
108  
202

- **Model Training:** Training the model on the data.
- **Model Evaluation:** Assessing the model's performance.
- **Model Deployment:** Putting the model into production.

Depends on data → Trees

cluster → unsupervised

AutoML



experience



# The Machine Learning Workflow

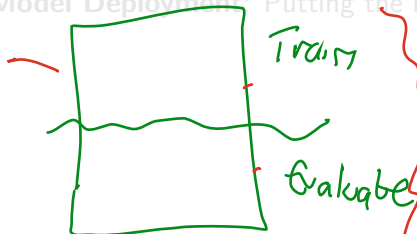
- **Data Collection:** Gathering the data.
- **Data Preprocessing:** Cleaning and preparing the data.
- **Feature Engineering:** Creating new features.
- **Model Selection:** Choosing the best model.
- **Model Training:** Training the model on the data.

one-hot  
encoding



3x3  
2x3  
1x3  
1x3

1m  
2m



Stewart

6 - train  
2 - evaluate

10 groups → groups  
↓  
synthetic  
numeric



3x3=9  
3x4=12

12x3=36  
12x4=48



# The Machine Learning Workflow

- **Data Collection:** Gathering the **data**.
- **Data Preprocessing:** Cleaning and preparing the **data**.
- **Feature Engineering:** Creating **new features**.
- **Model Selection:** Choosing the **best model**.
- **Model Training:** Training the **model** on the data.
- **Model Evaluation:** Assessing the **model's performance**

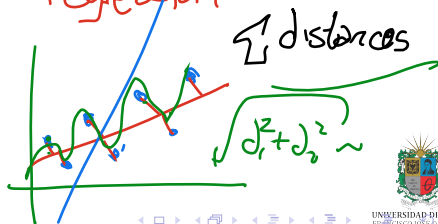
• **Model Deployment:** Putting the model into production.

Metrics  $\Rightarrow$  Error

Classification

Regression

• Matrix Confusion



# The Machine Learning Workflow

- No SW* → *SW* → *SW* → *SW*
- **Data Collection:** Gathering the **data**.
  - **Data Preprocessing:** Cleaning and preparing the **data**.
  - **Feature Engineering:** Creating **new features**.
  - **Model Selection:** Choosing the **best model**.
  - **Model Training:** Training the **model** on the data.
  - **Model Evaluation:** Assessing the **model's** performance.
  - **Model Deployment:** Putting the model into **production**.



*a = ""*  
*b = ""*  
*c = ""*

Notebooks

Docker

Cloud (serverless)

*classes*  
*oop*

*API*  
*Rest*

*direct*  
*Pickle*

*Parameters*

*Features*

*MLOps*



# Examining the Data

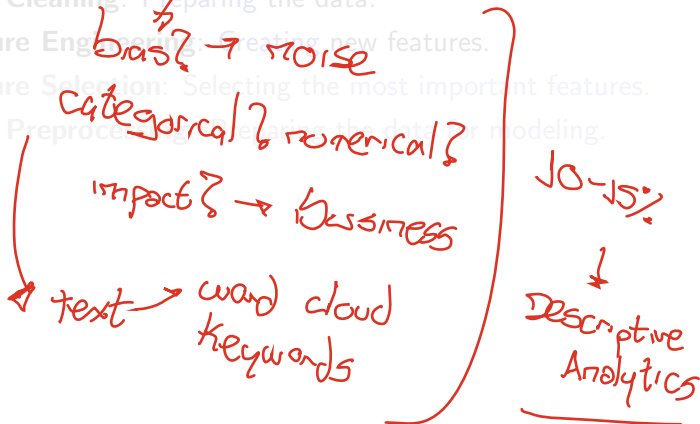
- **Data Exploration:** Understanding the data.

- Data Cleaning: Preparing the data.

- Feature Engineering: Creating new features.

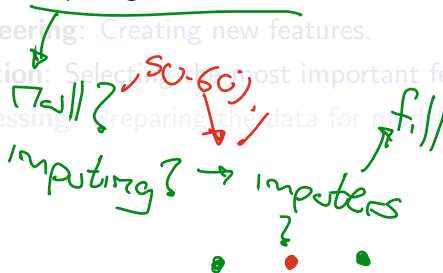
- Feature Selection: Selecting the most important features.

- Data Preprocessing: Preparing the data for modeling.



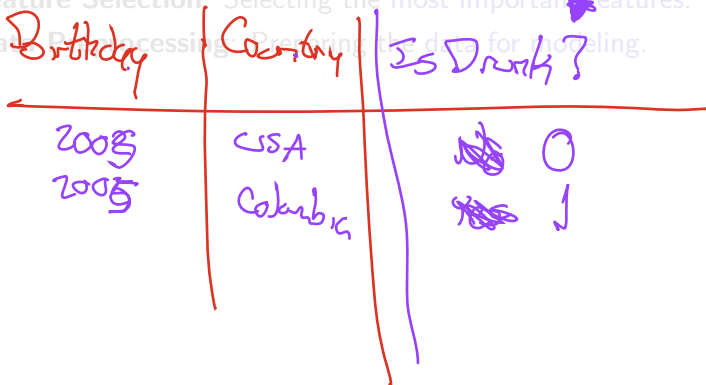
# Examining the Data

- **Data Exploration:** Understanding the data.
- **Data Cleaning:** Preparing the data.
- **Feature Engineering:** Creating new features.
- **Feature Selection:** Selecting the most important features.
- **Data Preprocessing:** Preparing the data for modeling.



# Examining the Data

- **Data Exploration:** Understanding the data.
- **Data Cleaning:** Preparing the data.
- **Feature Engineering:** Creating new features.
- **Feature Selection:** Selecting the most important features.
- **Data Preprocessing:** Preparing the data for modeling.



Birthday	Country	Is Drunk?
2003	USA	<del>1</del> 0
2005	Columbia	<del>0</del> 1



# Examining the Data

- **Data Exploration:** Understanding the data.
- **Data Cleaning:** Preparing the data.
- **Feature Engineering:** Creating new features.
- **Feature Selection:** Selecting the most important features.
- **Data Preprocessing:** Preparing the data for modeling.

features

A	B	C	D	E

Exp. 1. ABC

Exp. 2. ABCDE

Exp. 3. ACE

Exp. 4. BD





# Examining the Data

- **Data Exploration:** Understanding the data.
- **Data Cleaning:** Preparing the data.
- **Feature Engineering:** Creating new features.
- **Feature Selection:** Selecting the most important features.
- **Data Preprocessing:** Preparing the data for modeling.

Categorical  
Text } → Numeric → Vector

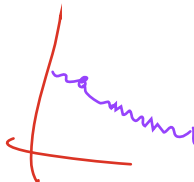


# Algorithmic Bias

- **Algorithmic bias** is a **systematic error** in a model that results in **unfair outcomes**.
- It can be caused by **biased training data**, biased algorithms, or biased **decision-making**.

\$ Families →

Loj	car	codes	inc.
-	-	-	-
+	+	+	+
+	+	+	+
+	+	+	+
+	+	+	+



# Outline

- 1 Fundamentals of Machine Learning
- 2 Python Tools for Machine Learning**
- 3 Supervised Machine Learning
- 4 Machine Learning Models Evaluation



# Python Tools for Machine Learning

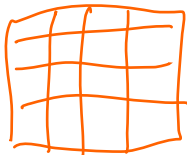
## Python Tools

- NumPy: A library for numerical computing. → Trans-Allyment
- Pandas: A library for data manipulation and analysis.
- Matplotlib: A library for data visualization.
- Scikit-learn: A library for machine learning.

Vectorization → no loops

linear algebra

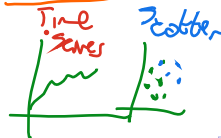
Tabular Data



Dataframe (df)

Analysis

SQL (ORM)



C  
↓  
arrays  
matrix (GPU)  
operations



# Jupyter Notebooks

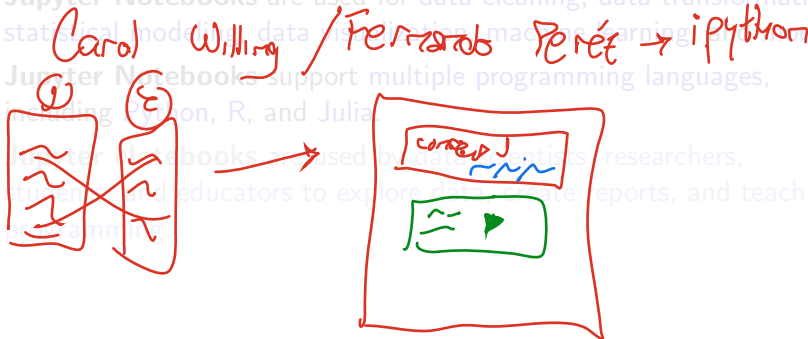
CC LAB

- **Jupyter Notebooks** are a web-based interactive computing environment that allows you to create and share documents that contain live code, equations, visualizations, and narrative text.

- Jupyter Notebooks are used for data cleaning, data transformation, statistical modeling, data visualization, machine learning, etc.

- Jupyter Notebooks support multiple programming languages, including Python, R, and Julia.

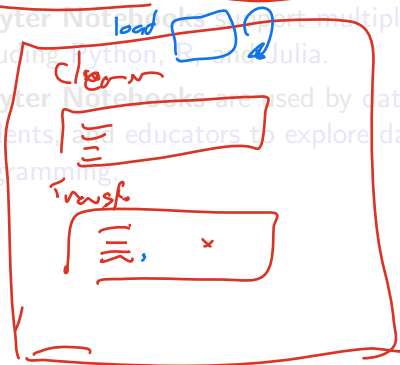
- Jupyter Notebooks are used by data scientists, researchers, students, and educators to explore data, create reports, and teach programming.



# Jupyter Notebooks

- **Jupyter Notebooks** are a **web-based interactive computing environment** that allows you to create and share documents that contain **live code**, **equations**, **visualizations**, and **narrative text**.
- **Jupyter Notebooks** are used for data cleaning, data transformation, statistical modeling, data visualization, machine learning, and more.

- Jupyter Notebooks support multiple programming languages, including Python, R, and Julia.
- Jupyter Notebooks are used by data scientists, researchers, students, and educators to explore data, create reports, and teach programming.



# Jupyter Notebooks

- **Jupyter Notebooks** are a **web-based interactive computing environment** that allows you to create and share documents that contain **live code**, **equations**, **visualizations**, and **narrative text**.
- **Jupyter Notebooks** are used for **data cleaning**, **data transformation**, **statistical modeling**, **data visualization**, **machine learning**, and **more**.
- **Jupyter Notebooks** support **multiple programming languages**, including **Python**, **R**, and **Julia**.
- **Jupyter Notebooks** are used by **scientists**, **researchers**, **students**, and **educators** to **explore data**, **create reports**, and **teach programming**.

Jupyter

Regular — Data Science



# Jupyter Notebooks

- **Jupyter Notebooks** are a **web-based interactive computing environment** that allows you to create and share documents that contain **live code**, **equations**, **visualizations**, and **narrative text**.
- **Jupyter Notebooks** are used for **data cleaning**, **data transformation**, **statistical modeling**, **data visualization**, **machine learning**, and **more**.
- **Jupyter Notebooks** support **multiple programming languages**, including **Python**, **R**, and **Julia**.
- **Jupyter Notebooks** are used by **data scientists**, **researchers**, **students**, and **educators** to **explore data**, **create reports**, and **teach programming**.

*Machine Learning Introduction*





# Lambda Functions

$$f \ x: x+2$$

## Definition

A **lambda function** is a **small** **anonymous** function. A **lambda function** can take any number of **arguments**, but can only have one expression.

lambda arguments: expression

$x = \text{lambda } a: a+2$

$\text{print}(x(10)) \rightarrow 20$

↳ lambda (arguments) {  
    return expression;



$\text{df['adult']} = \text{lambda}$   
 $\text{df['age']}: \text{if } x \geq 18 \text{ else } 0$



# Numerical Python Library — Numpy

- **Numpy** is the core library for scientific computing in Python. It is the fundamental package for scientific computing with Python.
- **Numpy** is a general-purpose array-processing package. It provides a high-performance multidimensional array object, and tools for working with these arrays. *vector*
- **Numpy** was created by Travis Oliphant in 2005, and it is an open-source project. Coming soon, Numpy version 2.0 will be released. *2.1*



# Lineal Algebra with Numpy

- **Numpy** provides a comprehensive set of linear algebra functions.
- **Numpy** provides the functionality to create and manipulate matrices.
- **Numpy** provides the functionality to solve linear systems of equations.
- **Numpy** provides the functionality to calculate the determinant of a matrix.
- **Numpy** provides the functionality to calculate the inverse of a matrix.

$$\begin{bmatrix} - & - & - \\ - & - & - \\ - & - & - \end{bmatrix}$$

Eigen  
Solve Equations

$$\begin{bmatrix} 2 & 1 \\ 3 & 5 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \end{bmatrix}$$



# Lineal Algebra with Numpy

- **Numpy** provides a **comprehensive set** of **linear algebra** functions.
- **Numpy** provides the **functionality** to **create** and **manipulate matrices**.
- **Numpy** provides the functionality to solve linear systems of equations.
- **Numpy** provides the functionality to calculate the determinant of a matrix.
- **Numpy** provides the functionality to calculate the inverse of a matrix.



# Lineal Algebra with Numpy

- **Numpy** provides a **comprehensive set** of **linear algebra** functions.
- **Numpy** provides the **functionality** to **create** and **manipulate matrices**.
- **Numpy** provides the **functionality** to **solve linear systems** of equations.
- **Numpy** provides the **functionality** to **calculate the determinant** of a matrix.
- **Numpy** provides the **functionality** to **calculate the inverse** of a matrix.



# Lineal Algebra with Numpy

- **Numpy** provides a **comprehensive set** of **linear algebra** functions.
- **Numpy** provides the **functionality** to **create** and **manipulate matrices**.
- **Numpy** provides the **functionality** to **solve linear systems** of equations.
- **Numpy** provides the **functionality** to **calculate** the **determinant** of a matrix.
- **Numpy** provides the **functionality** to **calculate** the **inverse** of a matrix.



# Lineal Algebra with Numpy

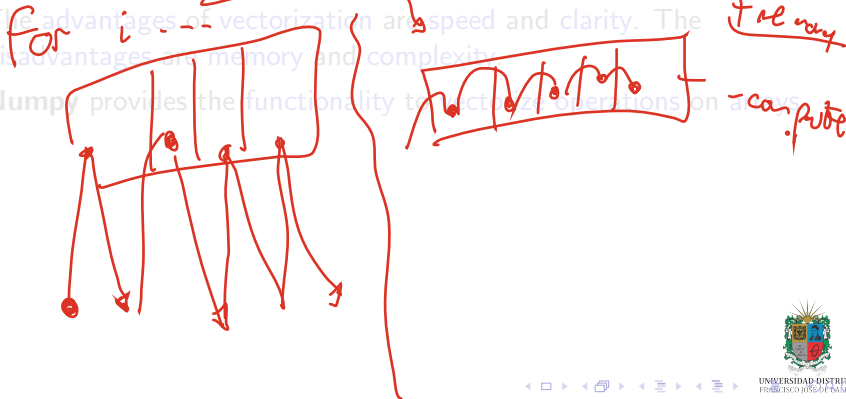
- **Numpy** provides a **comprehensive set** of **linear algebra** functions.
- **Numpy** provides the **functionality** to **create** and **manipulate matrices**.
- **Numpy** provides the **functionality** to **solve linear systems** of equations.
- **Numpy** provides the **functionality** to **calculate** the **determinant** of a matrix.
- **Numpy** provides the **functionality** to **calculate** the **inverse** of a matrix.



# Vectorization with Numpy

- **Vectorization** is the **process** of **converting** an **algorithm** from **operating** on a single value at a time to **operating** on a set of values at one time.
- **Vectorization** is the **process** of **replacing** explicit **loops** with **array expressions** or **matrix operations**.

- The advantages of vectorization are speed and clarity. The disadvantages are memory and complexity.
- Numpy provides the functionality to vectorize operations on arrays.





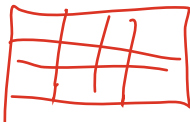
# Vectorization with Numpy

- **Vectorization** is the **process** of **converting** an **algorithm** from **operating** on a single value at a time to **operating** on a set of values at one time.
- **Vectorization** is the **process** of **replacing** explicit **loops** with **array expressions** or **matrix operations**.
- The **advantages** of **vectorization** are **speed** and **clarity**. The **disadvantages** are **memory** and **complexity**.
- **Numpy** provides the **functionality** to **vectorize operations** on **arrays**.



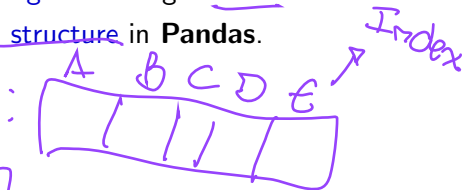
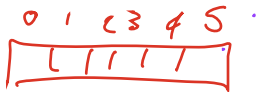
# Introduction to Pandas

- **Pandas** is a fast, powerful, flexible, and easy-to-use open-source data manipulation and data analysis library built on top of the Python programming language.
- **Pandas** is a high-level data manipulation tool developed by Wes McKinney in 2008. → *Polars (Rust)*
- **Pandas** is a fast and efficient data manipulation tool that is built on top of NumPy. → *numerical*
- **Pandas** is one of the most popular and widely-used data manipulation libraries in the world.



# The “Series” Data Structure

- A **Series** is a **one-dimensional array-like object** that contains a **sequence of values** and an **associated array of data labels**, called the **index**.
- The **index** of a **Series** is an **array of labels** that **correspond** to the **values** in the **Series**. The **index** of a **Series** is an **optional parameter** that **defaults** to a **sequence of integers** starting at **zero**.
- The **Series** object is a **core data structure** in **Pandas**.

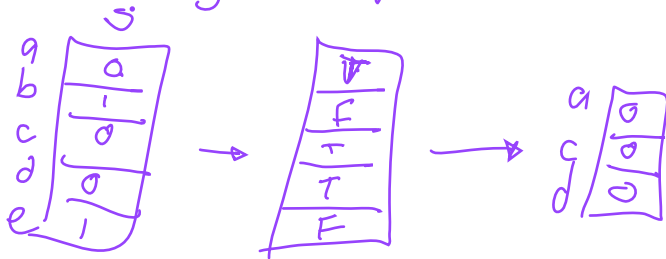


# Querying a Series

- You could query a **Series** using indexing (boolean or fancy).

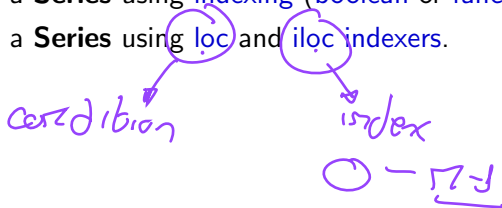
- You could query a Series using loc and ioc indexers.

$$s = s[cond] \rightarrow x=0$$



# Querying a Series

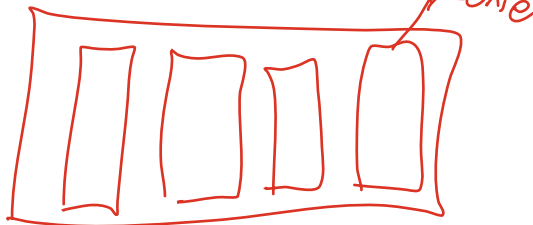
- You could **query** a **Series** using **indexing** (boolean or fancy).
- You could **query** a **Series** using **loc** and **iloc** indexers.


  
 condition
   
 index
   
 0 - 123



# The "DataFrame" Data Structure

- A **DataFrame** is a two-dimensional labeled data structure with columns of potentially different types. *→ matrix*
- A **DataFrame** is a tabular data structure that is similar to a spreadsheet or a SQL table. *→ operations*
- A **DataFrame** is a core data structure in **Pandas**. It is a two-dimensional size-mutable data structure with labeled axes (rows and columns).
- A **DataFrame** is a container for Series objects. *→ serie*



# DataFrame Indexing and Loading

- You could **index** a **DataFrame** using **column names**.
- You could **load** a **DataFrame** from a **CSV** file.
- You could **load** a **DataFrame** from a **JSON** file.
- You could **load** a **DataFrame** from a **SQL** database.



# DataFrame Indexing and Loading

- You could **index** a **DataFrame** using **column names**.
- You could **load** a **DataFrame** from a **CSV file**.
- You could **load** a **DataFrame** from a **JSON file**.
- You could **load** a **DataFrame** from a **SQL database**.





# DataFrame Indexing and Loading

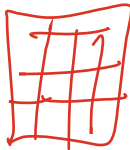
- You could **index** a **DataFrame** using **column names**.
- You could **load** a **DataFrame** from a **CSV file**.
- You could **load** a **DataFrame** from a **JSON file**.
- You could **load** a **DataFrame** from a **SQL database**.

different  
SQL



# DataFrame Indexing and Loading

- You could **index** a **DataFrame** using **column names**.
- You could **load** a **DataFrame** from a **CSV** file.
- You could **load** a **DataFrame** from a **JSON** file.
- You could **load** a **DataFrame** from a **SQL database**.



# DateTime Handling in Pandas

- You could convert a string to a datetime object using the to\_datetime() method.
- You could convert a datetime object to a string using the `strftime()` method.  
*Y-M-D H:M:S*
- You could convert a datetime object to a timestamp using the `timestamp()` method.



# DateTime Handling in Pandas

- You could **convert** a **string** to a **datetime** object using the **to\_datetime()** method.
- You could **convert** a **datetime** object to a **string** using the **strftime()** method.
- You could **convert** a **datetime** object to a **timestamp** using the **timestamp()** method.



# DateTime Handling in Pandas

- You could **convert** a **string** to a **datetime** object using the `to_datetime()` method.
- You could **convert** a **datetime** object to a **string** using the `strftime()` method.
- You could **convert** a **datetime** object to a **timestamp** using the `timestamp()` method.

Handwritten notes illustrating datetime formats and conversions:

Y-M-D H:M:S → Timestamp Y-M-D H:M:S.000 TZ

2025-06-18 10:00:00.000000 (7) → 0 70/10

The diagram shows the structure of a timestamp string, including year, month, day, hour, minute, second, and time zone (TZ). It also shows a specific example of a timestamp string and its conversion to a numerical value.



# Querying a DataFrame

- You could **query** a **DataFrame** using **indexing** (**boolean** or **fancy**).
- You could **query** a **DataFrame** using **loc** and **iloc** indexers.
- You could **query** a **DataFrame** using **query** method.



# Querying a DataFrame

- You could **query** a **DataFrame** using **indexing** (**boolean** or **fancy**).
- You could **query** a **DataFrame** using **loc** and **iloc** indexers.
- You could **query** a **DataFrame** using **query** method.



# Querying a DataFrame

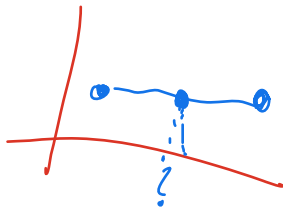
- You could **query** a **DataFrame** using **indexing** (**boolean** or **fancy**).
- You could **query** a **DataFrame** using **loc** and **iloc** indexers.
- You could **query** a **DataFrame** using **query method**.





# Missing Values in a DataFrame

- You could **detect** missing values in a **DataFrame**. The **isnull()** method returns a **Boolean DataFrame** indicating the **presence** of missing values.
  - You could **fill** missing values in a **DataFrame**. The **fillna()** method returns a **DataFrame** with missing values filled.
  - You could **drop** missing values in a **DataFrame**. The **dropna()** method returns a **DataFrame** with missing values dropped.
- Handwritten notes:* "Clean" (above fillna), "Imputer" (above dropna), and "Fill" (with an arrow pointing from dropna to fillna).



# Missing Values in a DataFrame

- You could **detect** missing values in a **DataFrame**. The **isnull()** method returns a **Boolean DataFrame** indicating the **presence** of missing values.
- You could **fill** missing values in a **DataFrame**. The **fillna()** method returns a **DataFrame** with missing values filled.
- You could **drop** missing values in a **DataFrame**. The **dropna()** method returns a **DataFrame** with missing values dropped.

fill → NaN



# Missing Values in a DataFrame

- You could **detect** missing values in a **DataFrame**. The **isnull()** method returns a **Boolean DataFrame** indicating the **presence** of missing values.
- You could **fill** missing values in a **DataFrame**. The **fillna()** method returns a **DataFrame** with missing values filled.
- You could **drop** missing values in a **DataFrame**. The **dropna()** method returns a **DataFrame** with missing values dropped.

Null → NaN → row at least 1  
nan → gone



# Merging DataFrames

- You could **merge** two **DataFrames** using the **merge()** method.
- You could **concatenate** two **DataFrames** using the **concat()** method.
- You could **join** two **DataFrames** using the **join()** method.

Join  
concatenations



# Merging DataFrames

- You could **merge** two **DataFrames** using the **merge()** method.
- You could **concatenate** two **DataFrames** using the **concat()** method.
- You could ~~join~~ two **DataFrames** using the **join()** method.



# Merging DataFrames

- You could **merge** two **DataFrames** using the **merge()** method.
- You could **concatenate** two **DataFrames** using the **concat()** method.
- You could **join** two **DataFrames** using the **join()** method.



# GroupBy in Pandas

- You could **group** a **DataFrame** using the **groupby()** method.
- You could **aggregate** a **DataFrame** using the **agg()** method.
- You could **transform** a **DataFrame** using the **transform()** method.
- You could **filter** a **DataFrame** using the **filter()** method.



# GroupBy in Pandas

- You could **group** a **DataFrame** using the **groupby()** method.
- You could **aggregate** a **DataFrame** using the **agg()** method.
- You could **transform** a **DataFrame** using the **transform()** method.
- You could **filter** a **DataFrame** using the **filter()** method.





# GroupBy in Pandas

- You could **group** a **DataFrame** using the `groupby()` method.
- You could **aggregate** a **DataFrame** using the `agg()` method.
- You could **transform** a **DataFrame** using the `transform()` method.
- You could **filter** a **DataFrame** using the `filter()` method.



# GroupBy in Pandas

- You could **group** a **DataFrame** using the `groupby()` method.
- You could **aggregate** a **DataFrame** using the `agg()` method.
- You could **transform** a **DataFrame** using the `transform()` method.
- You could **filter** a **DataFrame** using the `filter()` method.



# Outline

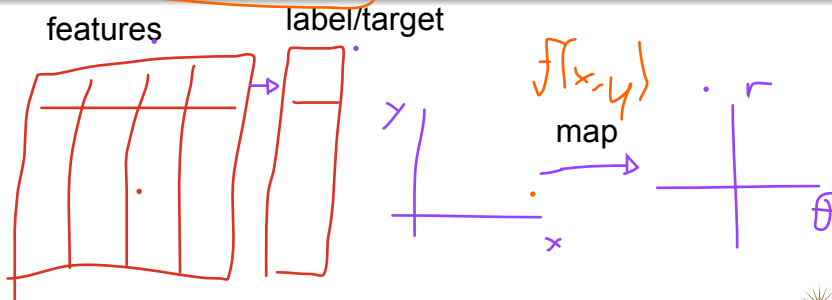
- 1 Fundamentals of Machine Learning
- 2 Python Tools for Machine Learning
- 3 Supervised Machine Learning
- 4 Machine Learning Models Evaluation



# Introduction to Supervised Machine Learning

## Definition

- **Supervised learning** is a type of **machine learning** where the model is trained on **labeled data**.
- It involves training a model to **map** **input data** to **output data** based on example **input-output pairs**.



# Overfitting and Underfitting

## Overfitting

**Overfitting** occurs when a model learns the training data too well and performs poorly on new data.

## Underfitting

**Underfitting** occurs when a model is too simple to capture the underlying structure of the data.



# Overfitting and Underfitting

## Overfitting

**Overfitting** occurs when a model learns the training data too well and performs poorly on new data.

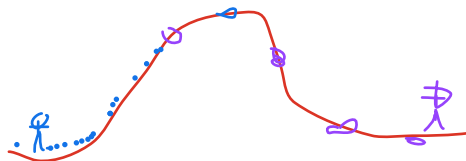
## Underfitting

**Underfitting** occurs when a model is too simple to capture the underlying structure of the data.

Iterations

Hill Climbing

Learning Rate



# Supervised Learning Datasets

- **Training Dataset:** The data used to **train the model**.

- **Validation Dataset:** The data used to **tune the model hyperparameters**.

- **Test Dataset:** The data used to **evaluate the model performance**.  
Learning a pattern to map  
features -> label

80-70  
9



# Supervised Learning Datasets

- **Training Dataset:** The data used to **train the model**.
- **Validation Dataset:** The data used to **tune** the model **hyperparameters**.
- **Test Dataset:** The data used to **evaluate** the model **performance**.

model setup

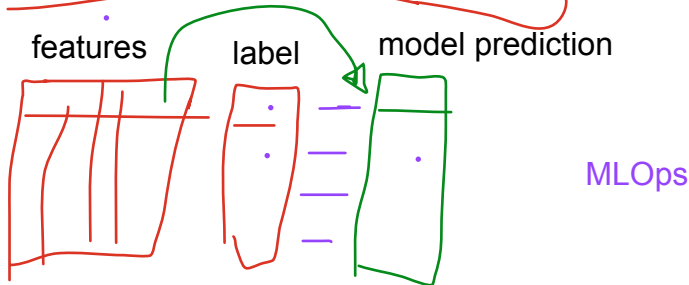
- \* iterations
- \* learning rate
- \* optimization metric (error)





# Supervised Learning Datasets

- **Training Dataset:** The data used to **train the model**.
- **Validation Dataset:** The data used to **tune** the model **hyperparameters**.
- **Test Dataset:** The data used to **evaluate** the model **performance**.



# Cross-Validation

- **Cross-validation** is a technique for assessing the performance of a model.
- It involves splitting the data into multiple subsets, training the model on some subsets, and evaluating it on others.
- Common cross-validation **techniques** include k-fold cross-validation and leave-one-out cross-validation. JL 4
- Cross-validation helps to reduce overfitting and provides a more accurate estimate of the model's performance.



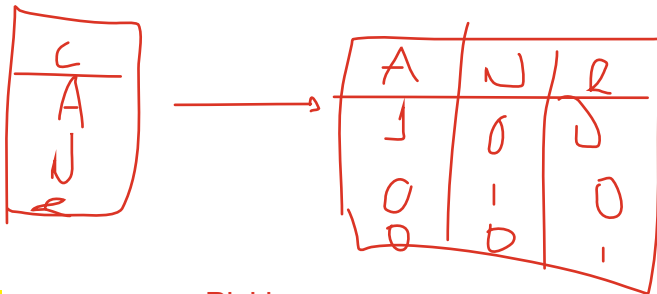
Training 1: 1234    Testing: 5  
 • Training 2: 1235    Testing: 4



# One-Hot Encoding

## One-Hot Encoding

- One-hot encoding is a technique for converting categorical variables into numerical variables.
- It creates a binary vector for each category, with a 1 for the *category* and 0s for all other categories.

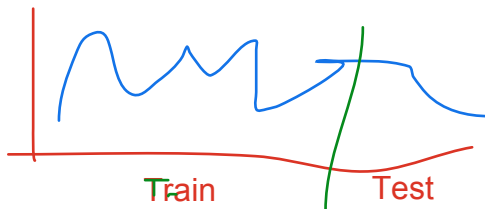


Pickle •



# Data Leakage

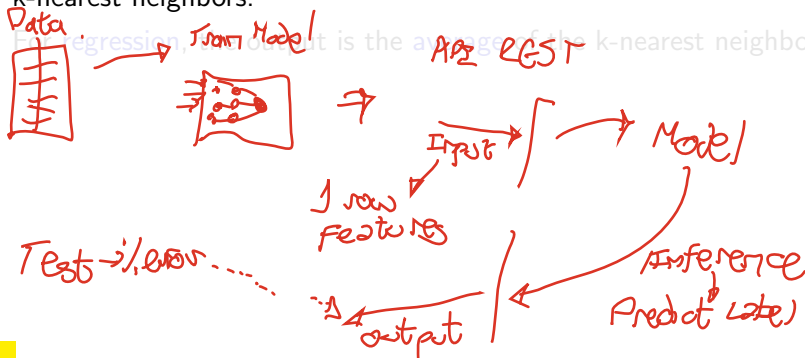
- **Data leakage** occurs when information from the test set is inadvertently used to train the model.
- It can lead to overfitting and inflated performance metrics.
- Common sources of **data leakage** include target leakage, train-test contamination, and information leakage.
- To prevent **data leakage**, it is important to carefully separate the training and test data and avoid using information from the test set during training.



# K-Nearest Neighbors: Classification and Regression

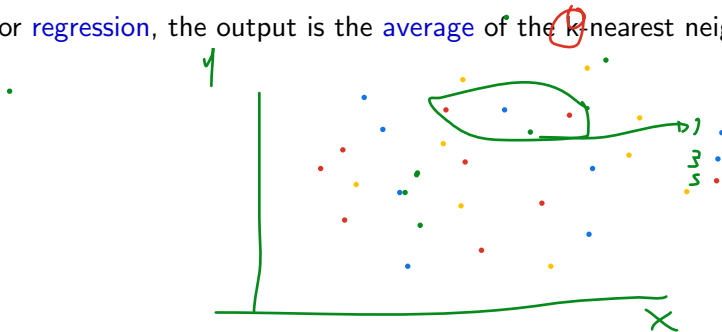
- **K-Nearest Neighbors (KNN)** is a simple algorithm that stores all available cases and classifies new cases based on a **similarity measure**.
- It can be used for both **classification** and **regression** tasks.
- For **classification**, the output is the **class label** of the majority of the k-nearest neighbors.

- For **regression**, the output is the **average** of the k-nearest neighbors.



# K-Nearest Neighbors: Classification and Regression

- **K-Nearest Neighbors (KNN)** is a simple algorithm that stores all available cases and classifies new cases based on a similarity measure.
- It can be used for both **classification** and **regression** tasks.
- For **classification**, the output is the **class label** of the majority of the k-nearest neighbors.
- For **regression**, the output is the **average** of the **k**-nearest neighbors.



# Linear Regression with Least Squares

## Linear Regression

- **Linear regression** is a type of regression analysis used for predicting the value of a continuous dependent variable.
- It works by finding the line that best fits the data.

## Least Squares

Least squares is a method for finding the best-fitting line by minimizing the sum of the squared differences between the predicted and actual values.



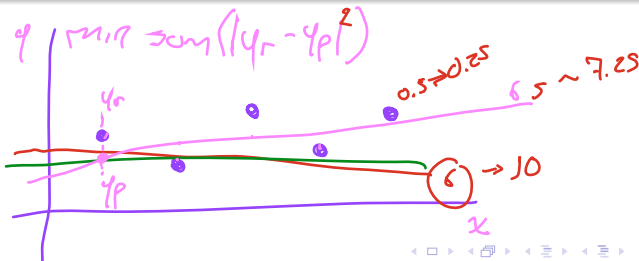
# Linear Regression with Least Squares

## Linear Regression

- **Linear regression** is a type of **regression analysis** used for predicting the value of a **continuous dependent variable**.
- It works by finding the **line that best fits the data**.

## Least Squares

**Least squares** is a method for finding the **best-fitting line** by **minimizing the sum** of the squared differences between the **predicted** and **actual** values.



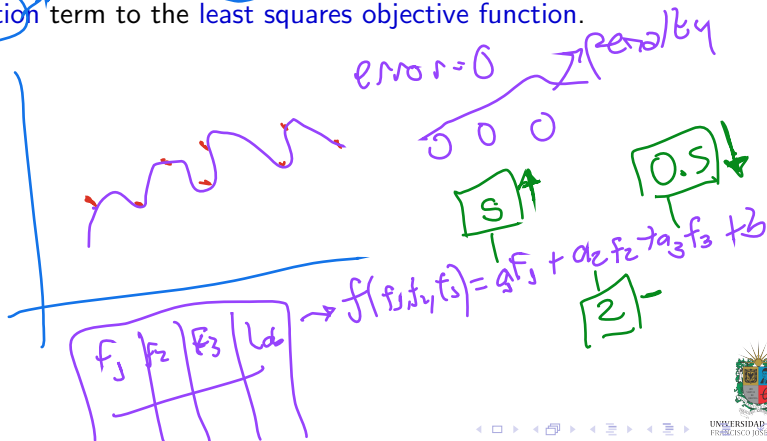


# Ridge & Lasso

L1 → overfitting

L2 → feature importance

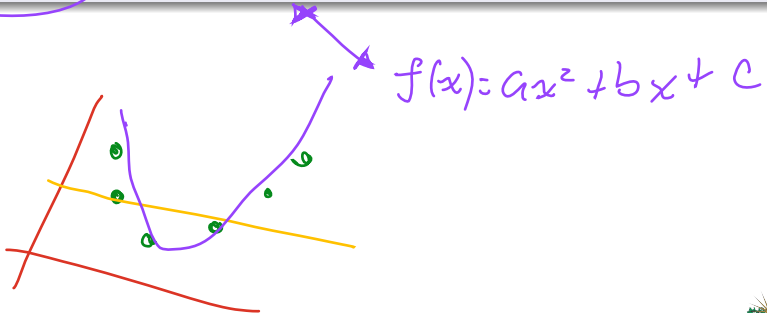
**Ridge regression** & **Lasso regression** are a type of linear regression that includes a penalty term to prevent overfitting. It works by adding a regularization term to the least squares objective function.



# Polynomial Regression

## Polynomial Regression

- **Polynomial regression** is a type of regression analysis that models the relationship between the independent and dependent variables as an  $n$ th-degree polynomial.
- It can capture non-linear relationships between the variables.



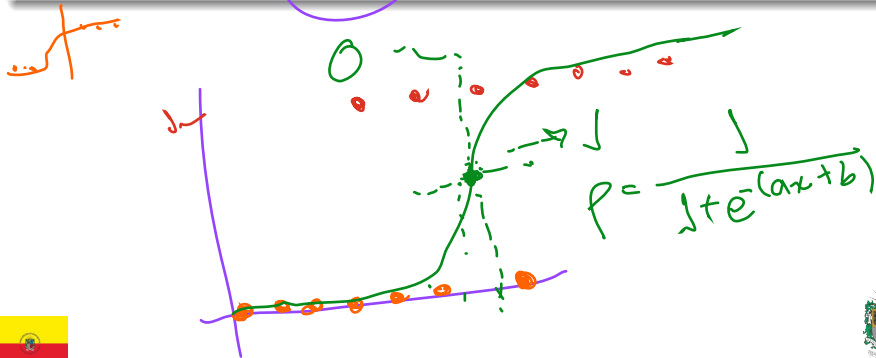
$$f(x) = ax^2 + bx + c$$



# Logistic Regression

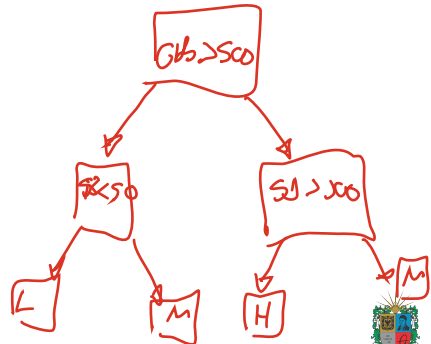
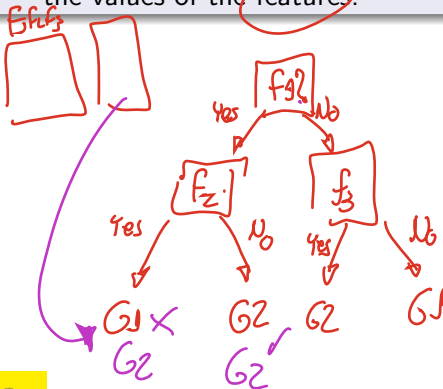
## Logistic Regression

- **Logistic regression** is a type of regression analysis used for predicting the outcome of a categorical dependent variable.
- It is used for binary classification tasks, where the output is a probability between 0 and 1.



# Decision Trees

- **Decision trees** are a type of **machine learning model** that can be used for both **classification** and **regression** tasks.
- They work by recursively **partitioning** the data into **subsets** based on the values of the features.



# Naive Bayes Classifier

- The **naive Bayes classifier** is a simple probabilistic **classifier** based on **Bayes' theorem**.
- It assumes that the features are **conditionally independent** given the class label.

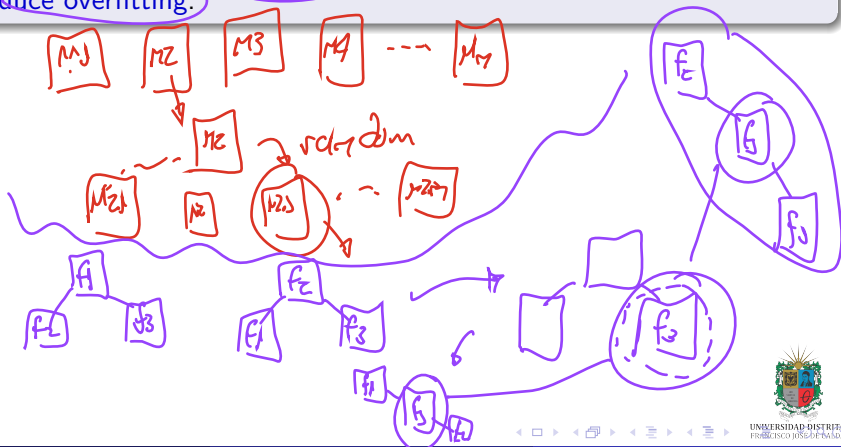
$P_{\text{rain}} \rightarrow P_{\text{wind}} \rightarrow P_{\text{sun}} \rightarrow P_{\text{dependent}}$

Baseline / performance



# Random Forest

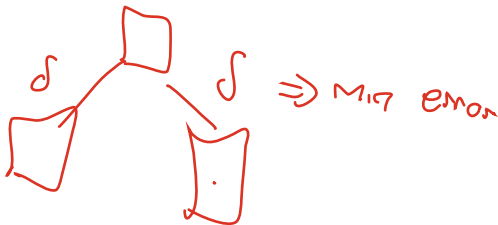
- **Random forest** is an **ensemble learning** method that combines **multiple decision trees** to create a strong predictive model.
- It works by building **multiple trees** and averaging their predictions to reduce overfitting.



# Gradient Boosted Decision Trees

- **Gradient boosted decision trees** are an ensemble learning method that combines multiple decision trees and gradient descent optimization to create a strong predictive model.
- They work by building trees sequentially, with each tree correcting the errors of the previous trees.

Bagging



# Neural Networks

- **Neural networks** are a type of **machine learning model** inspired by the **human brain**.
- They consist of **layers** of interconnected nodes that process **input data** and produce **output data**.





# Outline

- 1 Fundamentals of Machine Learning
- 2 Python Tools for Machine Learning
- 3 Supervised Machine Learning
- 4 Machine Learning Models Evaluation**



# Model Evaluation & Selection

- **Model Evaluation:** Assessing the **performance** of a model.
- **Model Selection:** Choosing the **best model** for the task.



# Confusion Matrices

## Definition

- A **confusion matrix** is a **table** that summarizes the **performance** of a **classification model**.
- It shows the number of **true positives**, **true negatives**, **false positives**, and **false negatives**.



# Basic Evaluation Metrics

- **Accuracy:** The proportion of correct predictions.
- **Precision:** The proportion of true positives among all positive predictions.
- **Recall:** The proportion of true positives among all actual positives.
- **F1 Score:** The harmonic mean of precision and recall.



# Basic Evaluation Metrics

- **Accuracy:** The proportion of correct predictions.
- **Precision:** The proportion of true positives among all positive predictions.
- **Recall:** The proportion of true positives among all actual positives.
- **F1 Score:** The harmonic mean of precision and recall.



# Basic Evaluation Metrics

- **Accuracy:** The proportion of correct predictions.
- **Precision:** The proportion of true positives among all positive predictions.
- **Recall:** The proportion of true positives among all actual positives.
- **F1 Score:** The harmonic mean of precision and recall.



# Basic Evaluation Metrics

- **Accuracy:** The proportion of correct predictions.
- **Precision:** The proportion of true positives among all positive predictions.
- **Recall:** The proportion of true positives among all actual positives.
- **F1 Score:** The harmonic mean of precision and recall.



# Classifier Metrics

- **ROC Curve:** A plot of the true positive rate against the false positive rate.
- Precision-Recall Curve: A plot of precision against recall.
- AUC-ROC: The area under the ROC curve.
- AUC-PR: The area under the precision-recall curve.





# Classifier Metrics

- **ROC Curve:** A plot of the true positive rate against the false positive rate.
- **Precision-Recall Curve:** A plot of precision against recall.
- **AUC-ROC:** The area under the ROC curve.
- **AUC-PR:** The area under the precision-recall curve.



# Classifier Metrics

- **ROC Curve:** A plot of the true positive rate against the false positive rate.
- **Precision-Recall Curve:** A plot of precision against recall.
- **AUC-ROC:** The area under the ROC curve.
- **AUC-PR:** The area under the precision-recall curve.



# Classifier Metrics

- **ROC Curve:** A plot of the true positive rate against the false positive rate.
- **Precision-Recall Curve:** A plot of precision against recall.
- **AUC-ROC:** The area under the ROC curve.
- **AUC-PR:** The area under the precision-recall curve.



# Regression Metrics

- **Mean Squared Error:** The **average** of the **squared differences** between the predicted and actual values.
- **Mean Absolute Error:** The **average** of the **absolute differences** between the predicted and actual values.
- **R-Squared:** The **proportion** of the **variance** in the dependent variable that is predictable from the independent variables.
- **Adjusted R-Squared:** A modified version of R-squared that adjusts for the **number of predictors** in the model.
- **Root Mean Squared Error:** The **square root** of the **mean squared error**.



# Regression Metrics

- **Mean Squared Error:** The **average** of the **squared differences** between the predicted and actual values.
- **Mean Absolute Error:** The **average** of the **absolute differences** between the predicted and actual values.
- **R-Squared:** The **proportion** of the **variance** in the dependent variable that is predictable from the independent variables.
- **Adjusted R-Squared:** A modified version of R-squared that adjusts for the **number of predictors** in the model.
- **Root Mean Squared Error:** The **square root** of the mean squared error.



# Regression Metrics

- **Mean Squared Error:** The **average** of the **squared differences** between the predicted and actual values.
- **Mean Absolute Error:** The **average** of the **absolute differences** between the predicted and actual values.
- **R-Squared:** The **proportion** of the **variance** in the dependent variable that is predictable from the independent variables.
- **Adjusted R-Squared:** A modified version of R-squared that adjusts for the **number of predictors** in the model.
- **Root Mean Squared Error:** The **square root** of the mean squared error.



# Regression Metrics

- **Mean Squared Error:** The **average** of the **squared differences** between the predicted and actual values.
- **Mean Absolute Error:** The **average** of the **absolute differences** between the predicted and actual values.
- **R-Squared:** The **proportion** of the **variance** in the dependent variable that is predictable from the independent variables.
- **Adjusted R-Squared:** A modified version of R-squared that adjusts for the **number of predictors** in the model.
- **Root Mean Squared Error:** The **square root** of the mean squared error.



# Regression Metrics

- **Mean Squared Error:** The **average** of the **squared differences** between the predicted and actual values.
- **Mean Absolute Error:** The **average** of the **absolute differences** between the predicted and actual values.
- **R-Squared:** The **proportion** of the **variance** in the dependent variable that is predictable from the independent variables.
- **Adjusted R-Squared:** A modified version of R-squared that adjusts for the **number of predictors** in the model.
- **Root Mean Squared Error:** The **square root** of the mean squared error.





# Outline

- 1 Fundamentals of Machine Learning
- 2 Python Tools for Machine Learning
- 3 Supervised Machine Learning
- 4 Machine Learning Models Evaluation



# Thanks!

## Questions?



Repo: <https://github.com/EngAndres/ud-public/tree/main/courses/systems-sciences-foundations>

