Introduction to Machine Learning

Systems Sciences Foundations

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2025-I

Outline

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

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1. Fundamentals of Machine Learning
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Key Concepts in Machine Learning

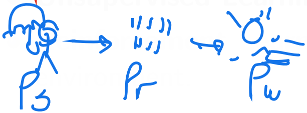
Machine Learning

- **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`.

statistics → Bayes

mo [illegible]

- 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.



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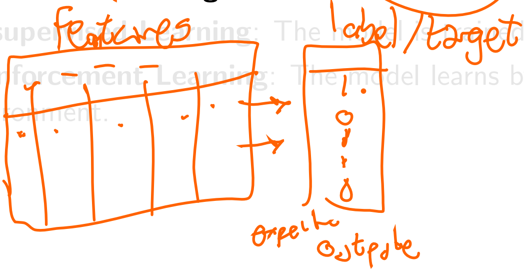

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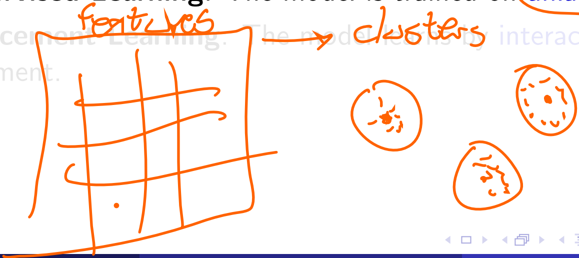

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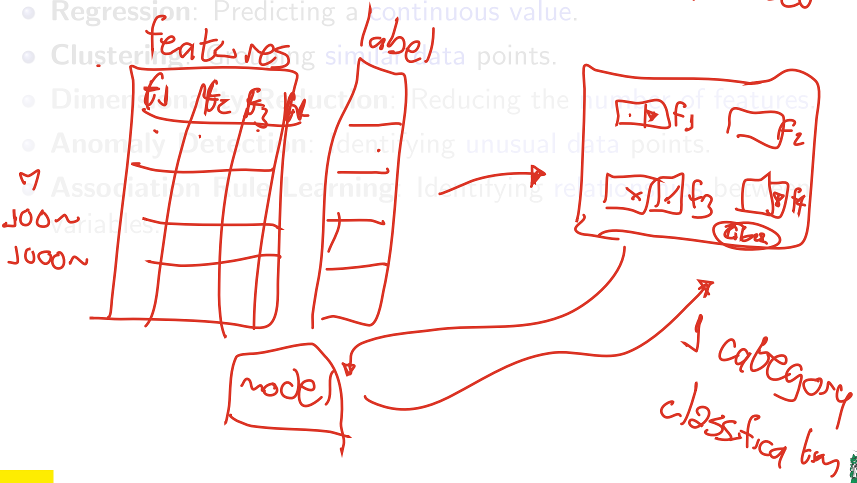
step

- **Reinforcement Learning**: The model learns by interacting with an environment.

multi-step → cybernetics

Typical Machine Learning Problems

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



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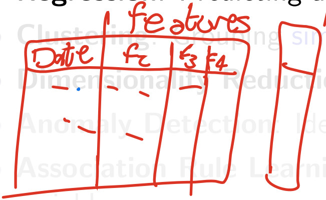

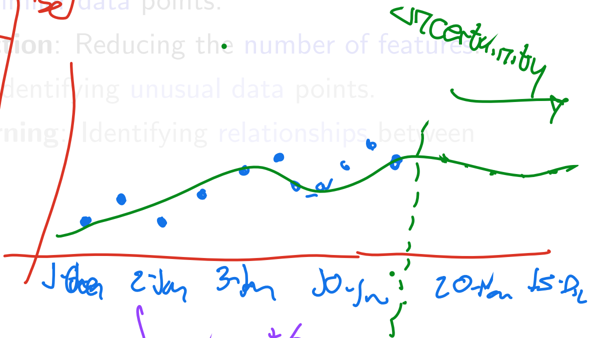

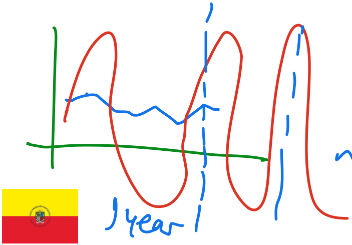

~3 years
synthetic + bias
cross-validate
K-fold

today

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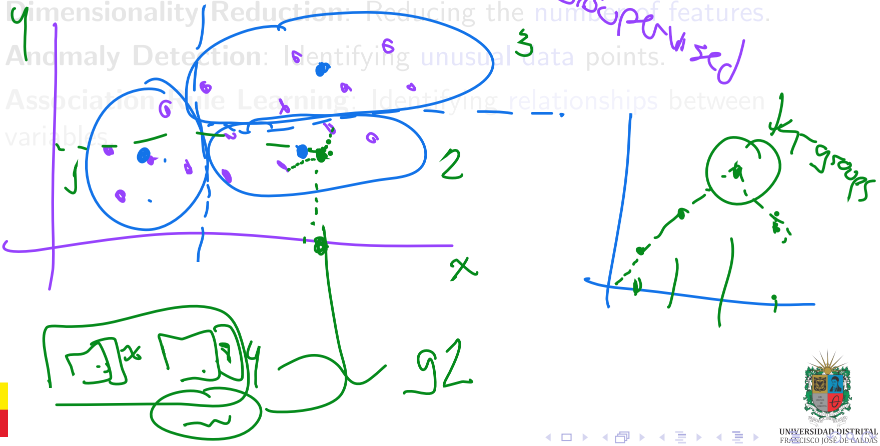
supervised

unsupervised



Typical Machine Learning Problems

f1 f2 f3

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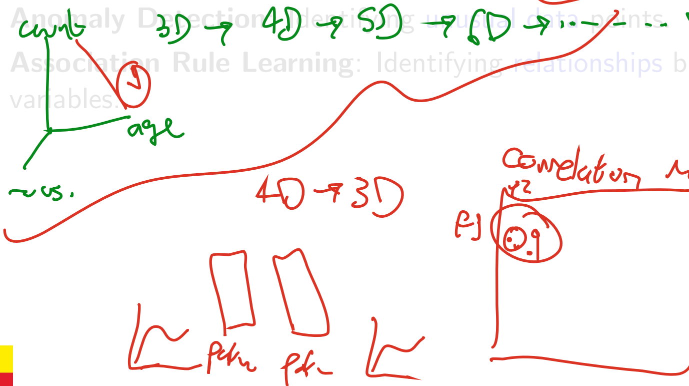
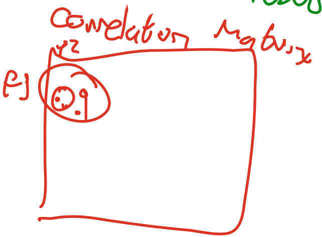
3D → 4D → 5D → 6D → ... → ∞ Dimensions

↓

resources





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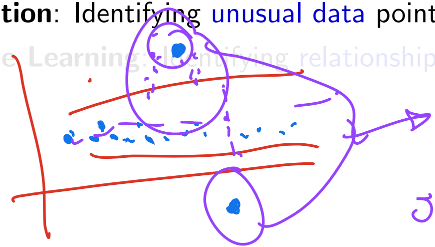

outliers

Support Vector Machines

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language

↳ a words sequence

correlation

$$\left.\begin{matrix} f_1 \\ f_2 \end{matrix}\right\} \rightarrow f_3$$

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.
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J

APIs - Documents - DB ----

NoSQL

Datalake (raw)

ETL (schedule)

SQL

DataWareHouse

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High quality

Null?

Outliers?

correlation?

features?

new features?

transform

selection

Format?

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mix →

math ← statistics

category

dist

money

risks

0

1

2

{ unsupervised

i → dist[]

1 →

2 →

⋮

[]

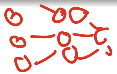
Data Engineer

Data Analyst

Machine Learning

Data Scientist

The Machine Learning Workflow



ax+b → 50
100
200

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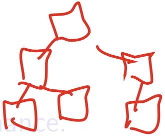
Depends on data → Trees



cluster → unsupervised

AutoML

experience

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onehot encoding

$$\begin{pmatrix} M \\ R \\ G \end{pmatrix} \rightarrow \begin{array}{ccc} M & R & G \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{array}$$

8 - train

2 - evaluate

Stewart

8k

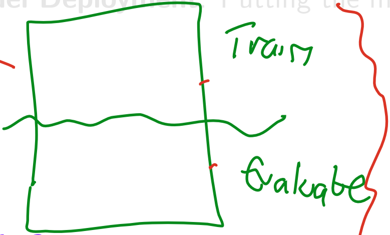
2k

1k

k.

1m

2m.



10 6003 → groups

syntetic

%≈%

numeric

3x3=9

3x4=12

12987x 4532=

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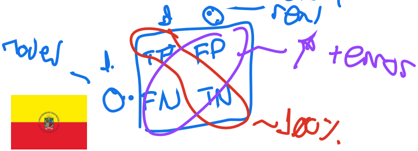
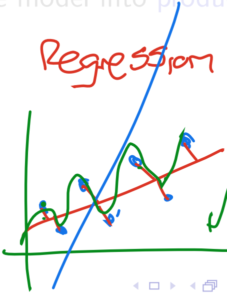
Metrics => Error

Classification

- Matrix Cofusion



Regression



↑ distances

$\sqrt{d_1^2+d_2^2}$ ~

The Machine Learning Workflow

Do SW

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

Notebook → classes → OOP → API Rest → Pickle

object

Docker → Cloud (serverless) → MLOps

Parameters → Features

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.

bias? → noise

categorical? numerical?

impact? → business

text → word cloud

keywords

10-15%

↓

Descriptive Analytics

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null?

50-60;

imputing? → imputes

fill

?

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Birthday	Country	IsDrunk?
2008	USA	0
2005	Colombia	1

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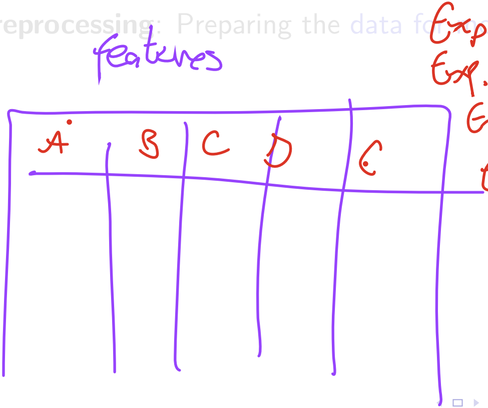

Exp 1.	ABC
Exp. 2.	ABCDE
Exp. 3	ACE
Exp 4	BD

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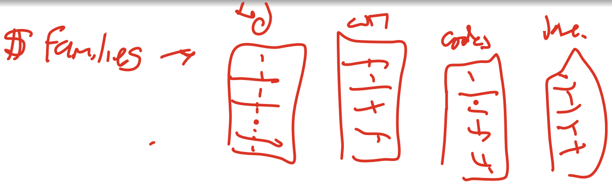
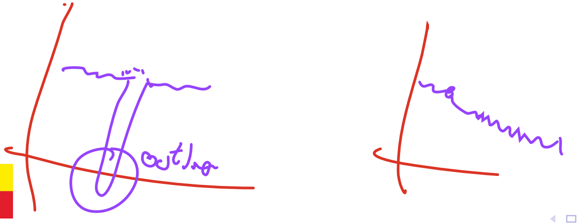
Categoric
Text } → Numeric → Vector

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.





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Python Tools for Machine Learning

~97

Guido Von Rossum

Python Tools

- **NumPy**: A library for numerical computing. → Travis Oliphant
- **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

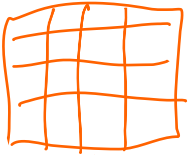
C

arrays

matriz (GPU)

→ operations

Tabular Data



Dataframe (df)

→ Analysis

SQL (ORM)

Time Series

Scatter

Jupyter Notebooks

COLAB

- **Jupyter Notebooks** are a web-based interactive computing environment that allows you to create and share documenmts 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.

Carol Willing / Fernando Peréz → ipython

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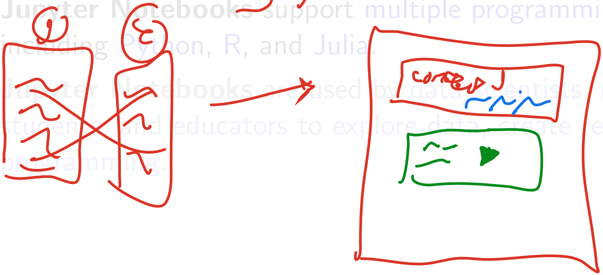
- **Jupyter Notebooks** are used by data scientists, researchers, students, and educators to explore data, create reports, and teach programming.



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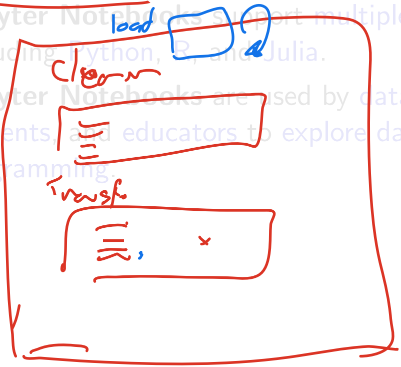

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Jupyter

Popular — Data Science

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Machine learning Introduction

Lambda Functions

f x: x+2

Definition

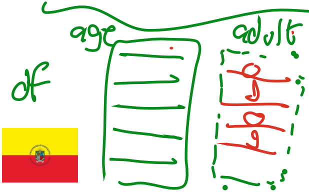
A **lambda function** is a small anonymous function. A **lambda function** can take any number of arguments, but can only have one expression.

lambda arguments : expression

↳ lambda (arguments){
return expression;
}

x = lambda a: a*2

print(x(10)) → 20



df['adult'] = lambda df['age']: 1 if x≥18 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.

vectors

- **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.

Eigen

Soli Equations

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

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Vectorization with Numpy

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- **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.

for i - - -
+memory
-compute

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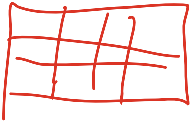
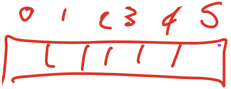
Introduction to Pandas

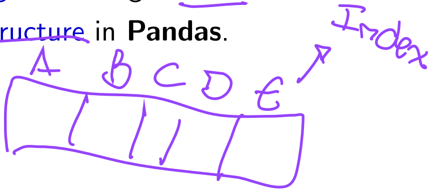
- **Pandas** is a fast, powerful, flexible, and easy-to-use open-source data manipulation and data analysis library built on top of the Python programming language.
- **Pandas** is a high-level data manipulation tool developed by Wes McKinney in 2008. → Polars (Rust)
- **Pandas** is a fast and efficient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

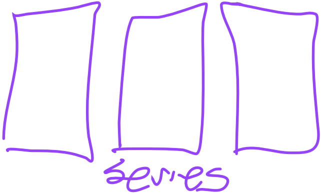


The "Series" Data Structure

- 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**.



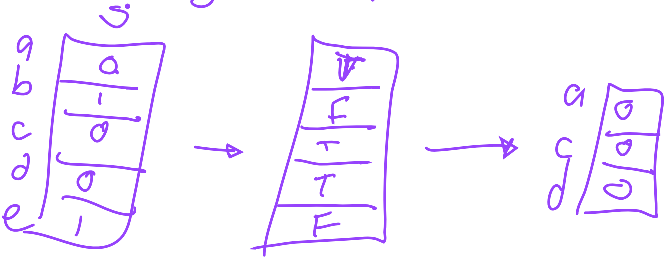




Querying a Series

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

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



Querying a Series

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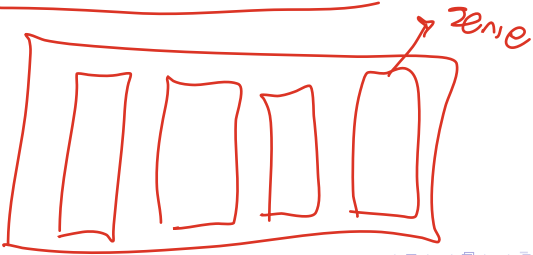
condition

index

0 - [n-1]

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.



DataFrame Indexing and Loading

- You could index a **DataFrame** using column names.
- You could load a **DataFrame** from a CSV file.
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different

null

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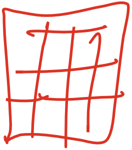

DateTime Handling in Pandas

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

Y-M-d H:M:S

- You could convert a datetime object to a string using the strftime() method.
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Timestamp

ms

Y-M-d H:M:S → Y-M-d H:M:S.000 TZ

2025-06-18 10:00:00.000 Z → 0

Zulu

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.

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- You could detect missing values in a **DataFrame**. The isnull() method returns a Boolean **DataFrame** indicating the presence of missing values.

Clear

- You could fill missing values in a **DataFrame**. The fillna() method returns a **DataFrame** with missing values filled.

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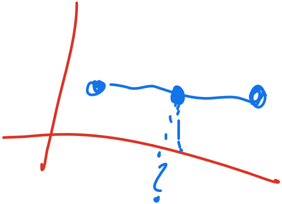
Imputer → fill



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Null → NaN

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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

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Outline

1. Fundamentals of Machine Learning

2. Python Tools for Machine Learning

3. Supervised Machine Learning

4. Machine Learning Models Evaluation

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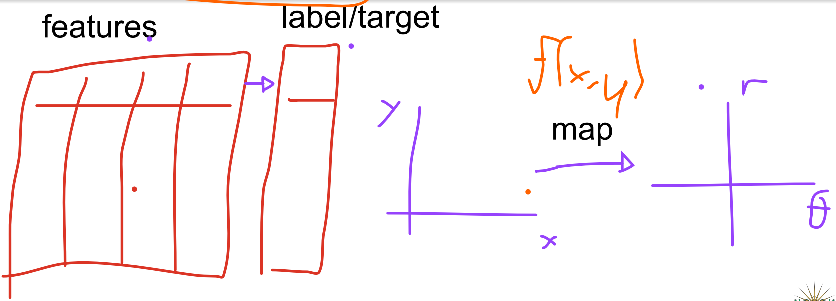
FRANCISCO JOSÉ DE CALDAS

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

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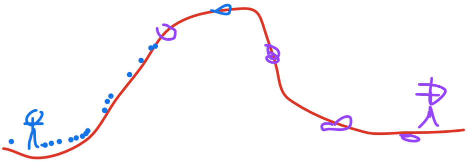
Iterations

Learning Rate

Hill Climbing



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.

60-70%

Learning a pattern to map
features -> label

Supervised Learning Datasets

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

~10%

- **Test Dataset**: The data used to evaluate the model performance.

model setup
* iterations
* learning rate
* optimization metric (error)

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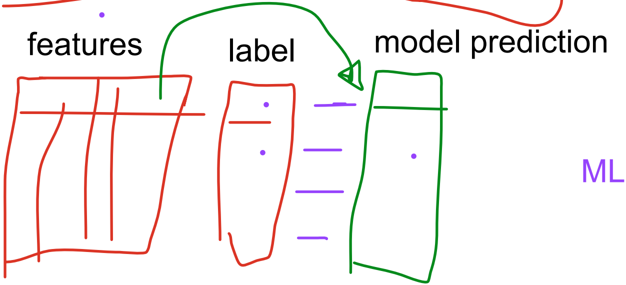
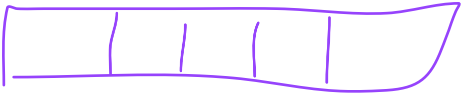


MLOps

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. 123 4
- Cross-validation helps to reduce overfitting and provides a more accurate estimate of the model's performance.



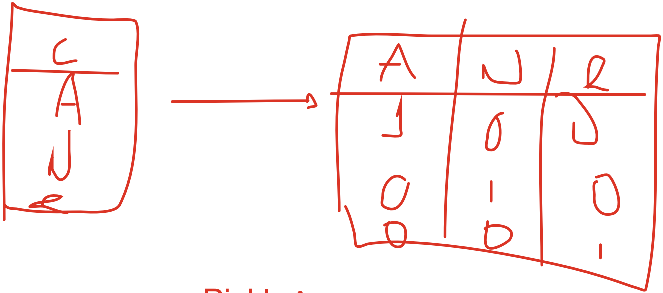
Training 1: 1234 Testing: 5

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.



C
A
J
R

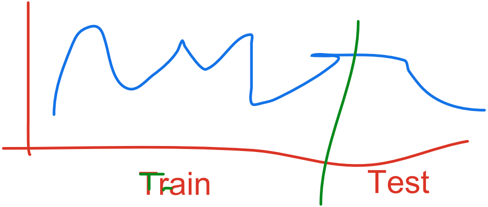
→

A	J	R
1	0	0
0	1	0
0	0	1

Pickle

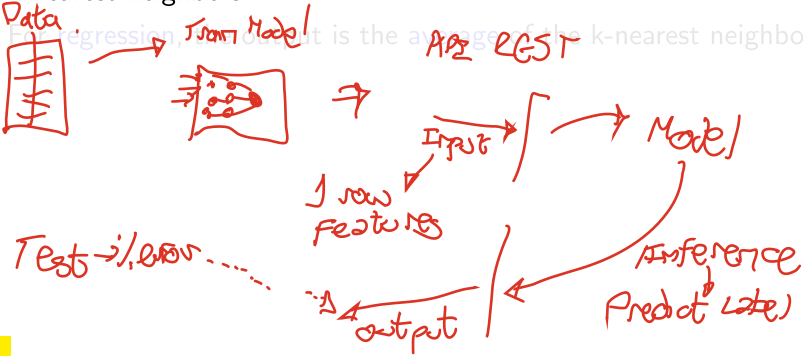
Data Leakage

- **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.



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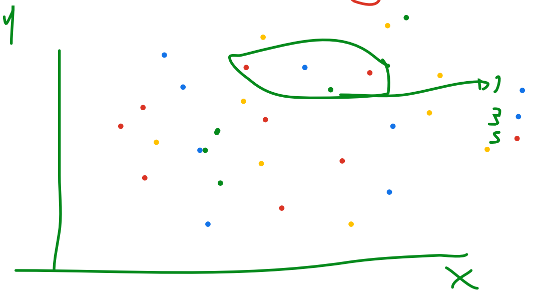


Linear Regression with Least Squares

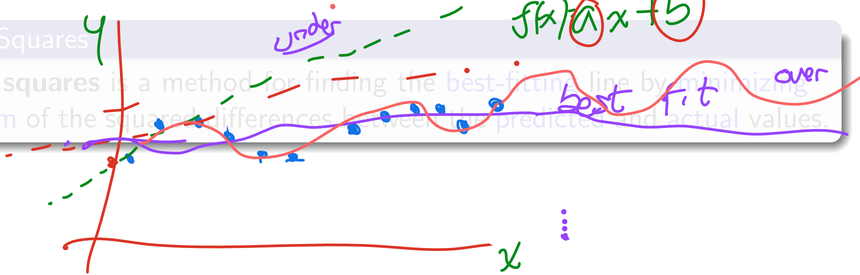
Linear Regression

- **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.

$f(x)=\boxed{a}x+\boxed{b}$

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.



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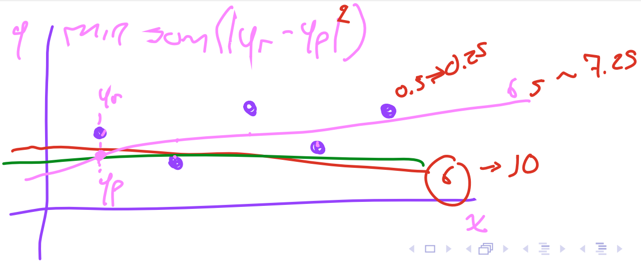


Ridge & Lasso

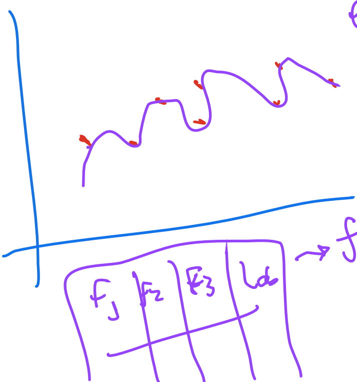
L1 → overfitting

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.

error = 0

penalty



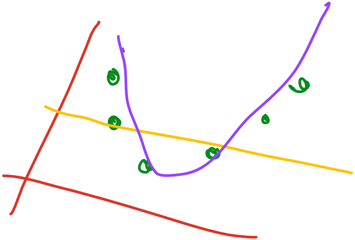
$$\rightarrow f(f_1,f_2,f_3) = \overset{\boxed{5}\uparrow}{a_1} f_1 + \underset{\boxed{2}}{a_2} f_2 + \overset{\boxed{0.5}\downarrow}{a_3} f_3 + b$$

Polynomial Regression

Polynomial Regression

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

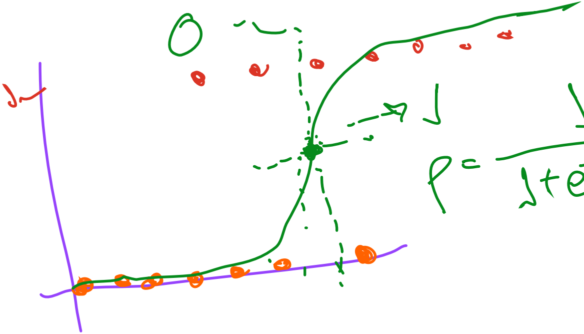
$f(x) = ax^2 + bx + c$



Logistic Regression

Logistic Regression

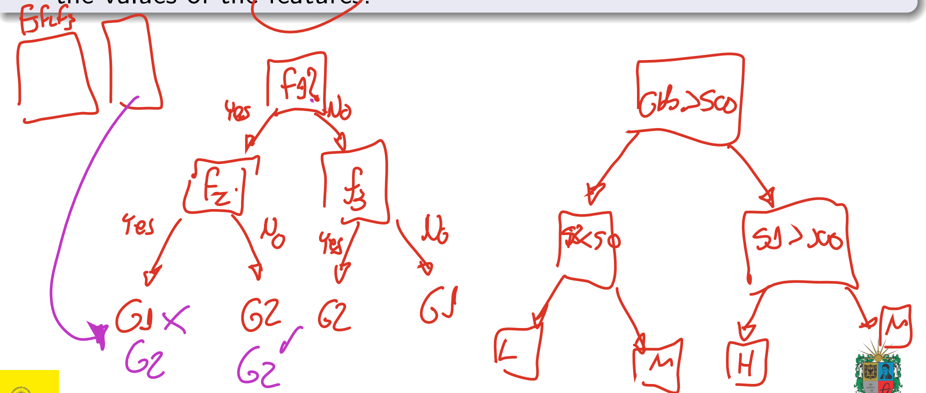
- **Logistic regression** is a type of regression analysis used for predicting the outcome of a categorical dependent variable.
- It is used for binary classification tasks, where the output is a probability between 0 and 1.



$$p = \frac{1}{1+e^{-(ax+b)}}$$

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

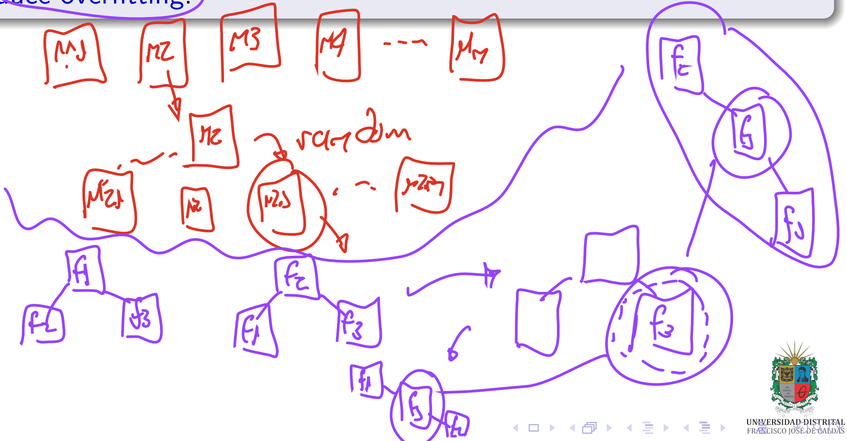
- The **naive Bayes classifier** is a simple probabilistic classifier based on Bayes' theorem.
- It assumes that the features are conditionally independent given the class label.

$P_{rain} \rightarrow P_{wind} \rightarrow P_{sun} \rightarrow P_{Abenpent}.$

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.



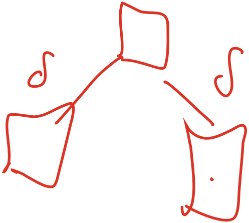
Gradient Boosted Decision Trees

- **Gradient boosted decision trees** are an ensemble learning method that combines multiple decision trees and gradient descendent optimization to create a strong predictive model.

random Forest

- They work by building trees sequentially, with each tree correcting the errors of the previous trees.

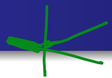
Bagging



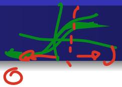
⇒ Min error

Neural Networks

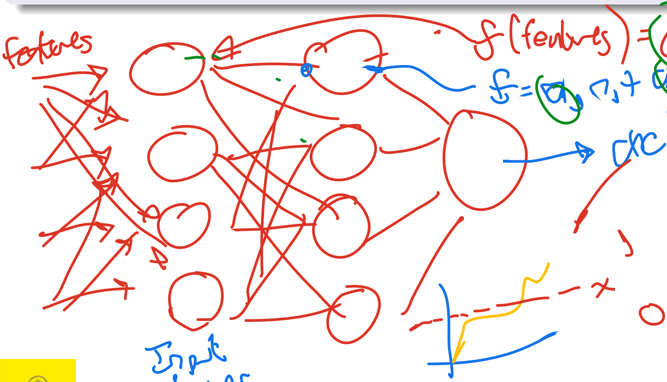
ReLu



Softmax



- **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.



$f(\text{features}) = a_1 f_1 + a_2 f_2 + a_n f_n + b$

$f = a_1 n_1 + a_2 n_2 + a_n n_n + b$

activation function

parameters

Outline

1. Fundamentals of Machine Learning
2. Python Tools for Machine Learning
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Model Evaluation & Selection

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

	M1		M 2	
	error 1	error 2	error 1	error 2
Dataset 1	x_1	y_1	x_2	y_2
Dat. 2	x_3	y_3	x_4	y_4
Dat. 3	x_5	y_5	x_6	y_6

S-10 ⇒ average

error

predict vs expected

Confusion Matrices

↳ Classification

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.

		real (expected)	
		1	0
Predicted	1	True Positives → 1.0	False Positive → 0.0
	0	False Negative → 0.0	True Negatives → 1.0

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.

TP	FP
FN	TN

→ 100%

$$\to \text{Accuracy} = \frac{TP + TN}{TP + FP + FN + TN} \approx 1.0$$

→ Total samples test

Basic Evaluation Metrics

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1

TP	FP
FN	TN

→ Precision = $\frac{TP}{TP + FP}$

FP → great

↳ TP less

↳ Pre ⇒ 0

small

$\frac{N_1}{N_2}$ smaller

Pre ⇒ 1

Basic Evaluation Metrics

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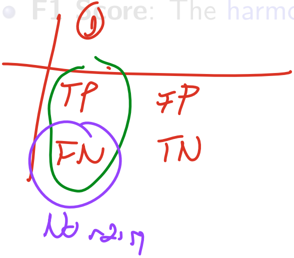

$$\text{recall} = \frac{TP}{TP + FN}$$

$$\downarrow$$

1.0

Basic Evaluation Metrics

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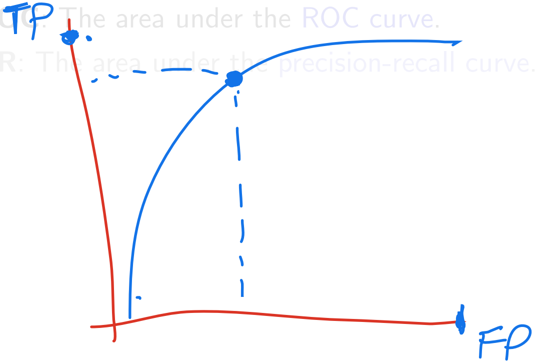
$\Rightarrow 2_x = 1$

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

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.



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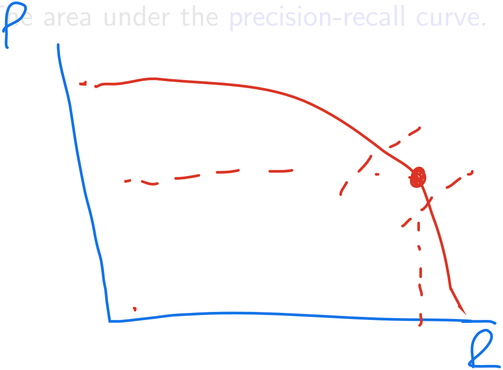

Classifier Metrics

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parameter → auc-roc

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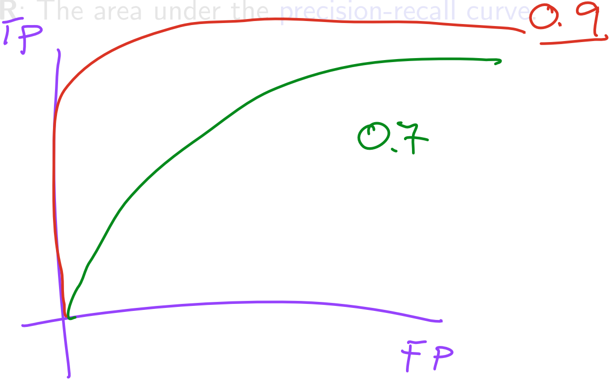
~ >0.75



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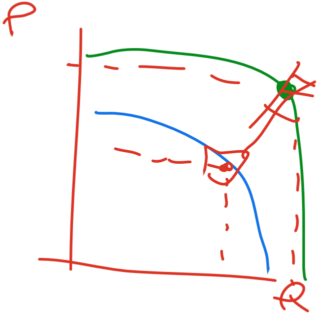
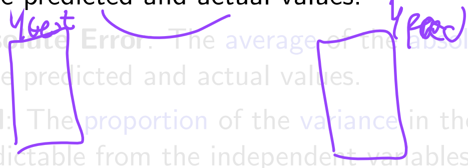


Regression Metrics

- **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.

$$MSE = \frac{(y_i^{pred} - y_i^{test})^2}{len(y)}$$

Regression Metrics

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$$mae = \frac{|y_{pred} - y_{test}|}{len(y)}$$

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features

y pred

Var (features)

(num range)

→ var (y pred)

→ corr

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features most significance

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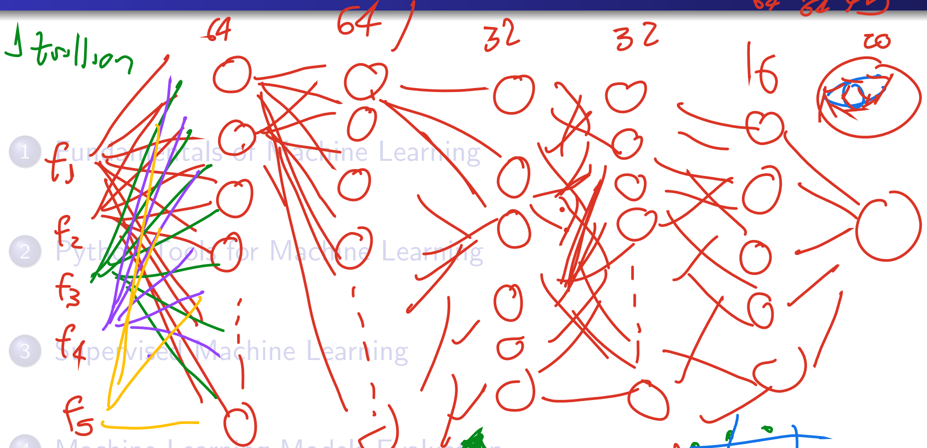
- **Mean Absolute Error**: The average of the absolute differences between the predicted and actual values.
- **R-Squared**: The proportion of the variance in the dependent variable that is predictable from the independent variables.
- **Adjusted R-Squared**: A modified version of R-squared that adjusts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

$$rmse = \sqrt{\frac{\sum_{i=0}^{m} \left(y_i^{pred} - y_i^{test}\right)^2}{m}}$$

$\downarrow$ 0

Outline

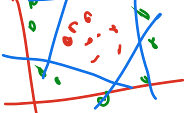
$f() = a_1 x_1 + a_2 x_2 + \dots + a_{64} x_{64} + b$



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

$f = a_1 f_1 + a_2 f_2 + a_3 f_3 + a_4 f_4 + a_5 f_5 + C$

LLM 7B



7000000000

Thanks!

Questions?

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