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
2. Python Tools for Machine Learning
3. Supervised Machine Learning
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Key Concepts in Machine Learning

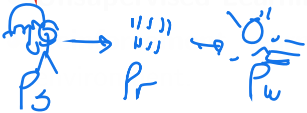
Machine Learning

- **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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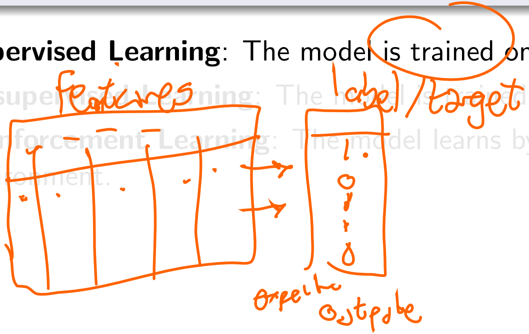

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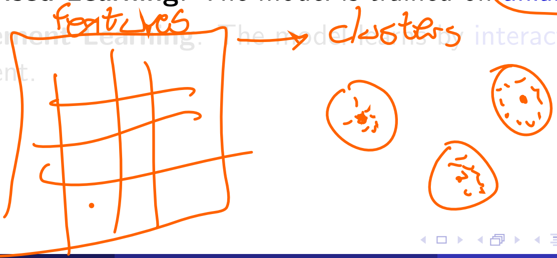

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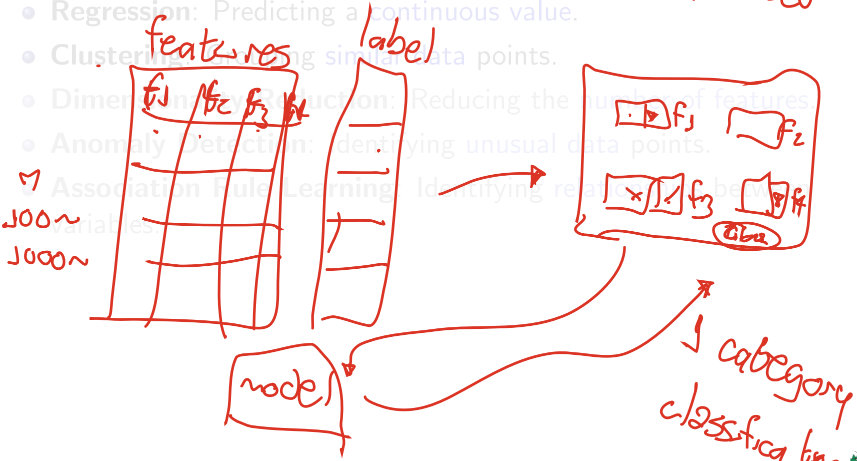
1 step

mult.-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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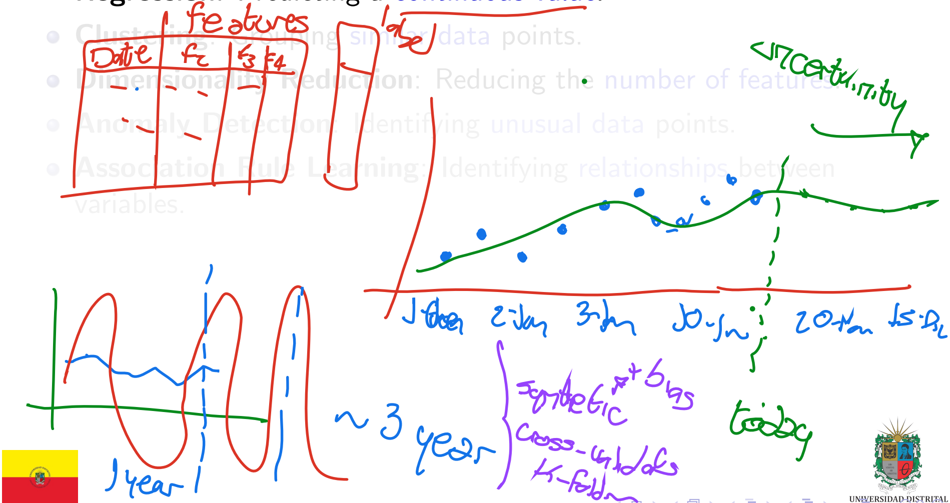

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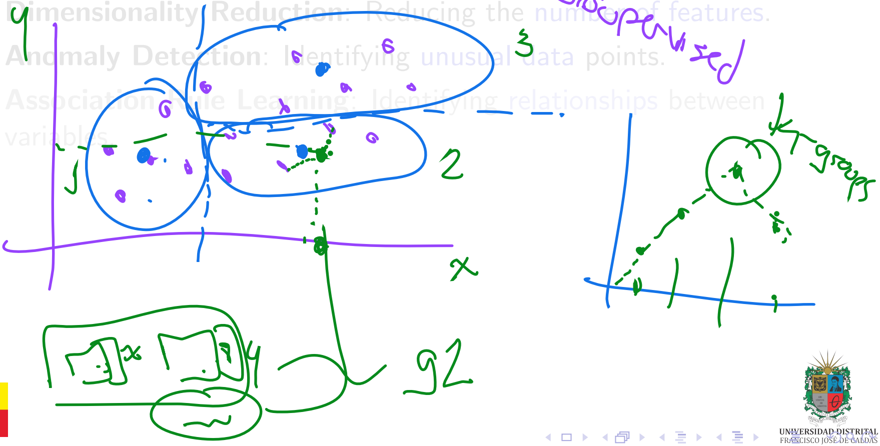
supervised

unsupervised



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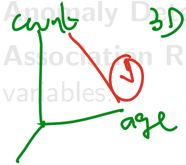
f1 f2 f3

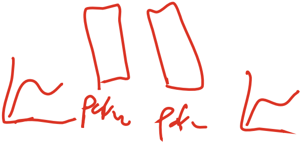
3D → 4D → 5D → 6D → . . . - - - . . ↑ Dimensions

↓

resources



4D → 3D



Correlation Matrix

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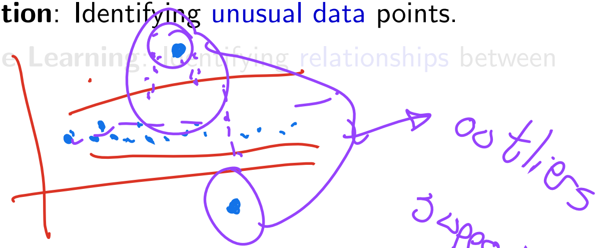

Support Vector Machines

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correlation

language

↳ a words sequence

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

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

J

APIs - Documents - DB ......

NoSQL

Datalake (raw)

ETL (schedule)

SQL ← Data wareHouse

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High quality

Null?
outliers?
correlation?

features?
new features?
transform
selection
Format?

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mix →

with ← statistics

category

dist / money / risk

0

1

2

{ unsupervised

(1) → dist[][] → [ ]

1 →

2 →

⋮

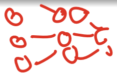
Data Engineer

Data Analyst

Machine Learn

Data Scientist

The Machine Learning Workflow



a+b → 50
100
200

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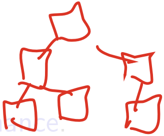
Depends on data → Trees



cluster → unsupervised

AutoML

experience

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onehot encoding

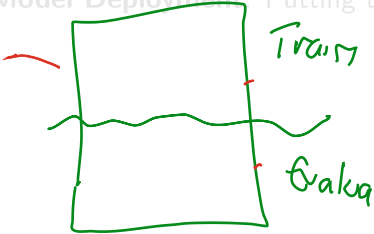
$$\begin{array}{c}M\\R\\G\end{array} \rightarrow \begin{array}{ccc}M & R & G\\ \hline 1 & 0 & 0\\ 0 & 1 & 0\\ 0 & 0 & 1\end{array}$$

8 { 6 - train
2 - evaluate

Stewart

3x
2x
1x
x.

1m
2m.



10 bars

6 bars → groups

syntetic

%≈%

numeric

3x3=9
3x4=32

12697x 4532=

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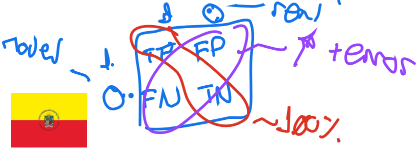
Metrics => Errors

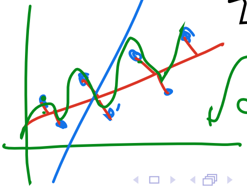
Classification

- Matrix Confusion



Regression

↑ distances



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

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

Notebook

classes

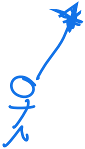
OOP

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? → imputers ?

fill

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Birthday	Country	Is Drunk?
2008	USA	0
2005	Colombia	1

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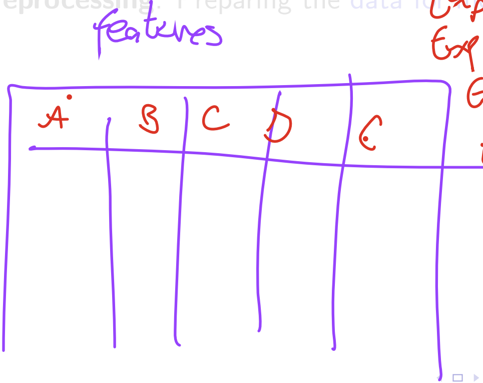

Exp 1.	ABC
Exp. 2.	ABCDE
Exp. 3	ACE
Exp 4	BD

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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

Python Tools

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

Jupyter Notebooks

- **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.
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Lambda Functions

Definition

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

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.
- **Numpy** was created by Travis Oliphant in 2005, and it is an open-source project. Coming soon, Numpy version 2.0 will be released.

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.
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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.
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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.
- **Pandas** is a fast and efficient data manipulation tool that is built on top of NumPy.
- **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.

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The “DataFrame” Data Structure

- A **DataFrame** is a two-dimensional labeled data structure with columns of potentially different types.
- A **DataFrame** is a tabular data structure that is similar to a spreadsheet or a SQL table.
- 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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DateTime Handling in Pandas

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- 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.

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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

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

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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.

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

One-Hot Encoding

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- **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.

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.

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

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 nth-degree polynomial.
- It can capture non-linear relationships between the variables.

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.

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 descedent optimization to create a `strong predictive model`.
- They work by building trees sequentially, with each tree correcting the errors of the previous trees.

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.

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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.
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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.

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Thanks!

Questions?

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