Introduction to Machine Learning

Systems Sciences Foundations

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Outline

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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`.

- **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 its environment.

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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.

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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.

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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.

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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.

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

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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.

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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 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.
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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.

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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.
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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

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.

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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

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.

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.

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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.

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Model Evaluation & Selection

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

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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.
- **AUC-PR**: The area under the precision-recall 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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Outline

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Thanks!

Questions?

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

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