

Machine Learning in Python

Supervised Learning - Classification and Metrics

Cristian A. Marocico, A. Emin Tatar

Center for Information Technology
University of Groningen

Friday, July 4th 2025

Outline

- 1 Introduction to Classification
- 2 Classification Basics
- 3 Evaluation Metrics

Introduction to Classification

Classification	Definition

Introduction to Classification

Classification

Definition

Classification is a type of supervised learning where the model learns from labeled data to predict the class of new observations based on past data.

Introduction to Classification

Classification

Definition

Classification is a type of supervised learning where the model learns from labeled data to predict the class of new observations based on past data.

Classification vs. Regression is a key distinction in supervised learning:

- In **classification**, the target variable is categorical (e.g., "spam" or "not spam").

Introduction to Classification

Classification

Definition

Classification is a type of supervised learning where the model learns from labeled data to predict the class of new observations based on past data.

Classification vs. Regression is a key distinction in supervised learning:

- In **classification**, the target variable is categorical (e.g., "spam" or "not spam").
- In **regression**, the target variable is continuous (e.g., predicting a price).

Classification Types

Classification Types	Definition

Classification Types

Classification Types

Definition

Classification can be broadly divided into two types:

- **Binary Classification:** The target variable has two classes (e.g., "yes" or "no", "spam" or "not spam"). Numerically, this can always be represented as 0 and 1.

Classification Types

Classification Types

Definition

Classification can be broadly divided into two types:

- **Binary Classification:** The target variable has two classes (e.g., "yes" or "no", "spam" or "not spam"). Numerically, this can always be represented as 0 and 1.
- **Multiclass Classification:** The target variable has more than two classes (e.g., "cat", "dog", "weasel"). In this case, the model predicts one of several possible categories.

Classification Algorithms

Classification Algorithms

Definition

Classification Algorithms

Classification Algorithms

Definition

Classification algorithms are designed to learn from labeled data and make predictions about the class of new, unseen data. Some common algorithms include:

- **Logistic Regression**: Despite its name, it is used for binary classification. It models the probability that a given input belongs to a particular class.

Classification Algorithms

Classification Algorithms

Definition

Classification algorithms are designed to learn from labeled data and make predictions about the class of new, unseen data. Some common algorithms include:

- **Logistic Regression**: Despite its name, it is used for binary classification. It models the probability that a given input belongs to a particular class.
- **k-Nearest Neighbors (k-NN)**: A non-parametric method that classifies a data point based on the classes of its nearest neighbors in the feature space.

Classification Algorithms

Classification Algorithms

Definition

Classification algorithms are designed to learn from labeled data and make predictions about the class of new, unseen data. Some common algorithms include:

- **Logistic Regression**: Despite its name, it is used for binary classification. It models the probability that a given input belongs to a particular class.
- **k-Nearest Neighbors (k-NN)**: A non-parametric method that classifies a data point based on the classes of its nearest neighbors in the feature space.
- **Decision Trees**: A tree-like model that splits the data into subsets based on feature values, leading to a decision about the class label.

Classification Algorithms

Classification Algorithms

Definition

Classification algorithms are designed to learn from labeled data and make predictions about the class of new, unseen data. Some common algorithms include:

- **Logistic Regression**: Despite its name, it is used for binary classification. It models the probability that a given input belongs to a particular class.
- **k-Nearest Neighbors (k-NN)**: A non-parametric method that classifies a data point based on the classes of its nearest neighbors in the feature space.
- **Decision Trees**: A tree-like model that splits the data into subsets based on feature values, leading to a decision about the class label.
- **Support Vector Machines (SVM)**: A method that finds the hyperplane that best separates the classes in the feature space.

Classification Algorithms

Classification Algorithms

Definition

Classification algorithms are designed to learn from labeled data and make predictions about the class of new, unseen data. Some common algorithms include:

- **Logistic Regression**: Despite its name, it is used for binary classification. It models the probability that a given input belongs to a particular class.
- **k-Nearest Neighbors (k-NN)**: A non-parametric method that classifies a data point based on the classes of its nearest neighbors in the feature space.
- **Decision Trees**: A tree-like model that splits the data into subsets based on feature values, leading to a decision about the class label.
- **Support Vector Machines (SVM)**: A method that finds the hyperplane that best separates the classes in the feature space.
- More advanced algorithms like **Random Forests**, **Gradient Boosting**, and **Neural Networks**.

Logistic Regression

Logistic Regression

Definition

Logistic Regression

Logistic Regression

Definition

Logistic Regression models the probability that the target variable y belongs to a particular class. The **logistic function (sigmoid)** is used to map predicted values to probabilities between 0 and 1. The decision boundary is determined by the threshold (commonly 0.5) for classifying observations into different classes.

Logistic Regression

Logistic Regression

Definition

Logistic Regression models the probability that the target variable y belongs to a particular class. The **logistic function (sigmoid)** is used to map predicted values to probabilities between 0 and 1. The decision boundary is determined by the threshold (commonly 0.5) for classifying observations into different classes.

The sigmoid function is defined as:

$$\sigma(z) = \frac{1}{1 + e^{-z}}$$

where z is a linear combination of the input features.

Evaluation Metrics for Classification

Confusion Matrix

Definition

Evaluation Metrics for Classification

Confusion Matrix

Definition

The **confusion matrix** summarizes the performance of a classification algorithm by comparing predicted and actual labels.

Evaluation Metrics for Classification

Confusion Matrix

Definition

The **confusion matrix** summarizes the performance of a classification algorithm by comparing predicted and actual labels.

	Predicted = 1	Predicted = 0
Actual = 1	True Positive (TP)	False Negative (FN)
Actual = 0	False Positive (FP)	True Negative (TN)

From these four numbers we obtain the core metrics summarized next.

Accuracy (Overall Success Rate)

Accuracy (Overall Success Rate)

Definition

Accuracy is a measure of how often the classifier is correct across all predictions. It answers the question: "What fraction of **all** predictions are correct?"

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

Despite its simplicity, accuracy can be misleading, especially in imbalanced datasets where one class dominates.

Precision (Positive Predictive Value)

Precision (Positive Predictive Value)

Definition

Precision is a measure of the accuracy of positive predictions. It answers the question: "When the classifier predicts 1, how often is it correct?"

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

High precision indicates that when the model predicts a positive class, it is likely correct, but it does not account for false negatives.

Recall (Sensitivity, True-Positive Rate)

Recall (Sensitivity, True-Positive Rate)

Definition

Recall is a measure of the model's ability to capture all positive instances. It answers the question: "Of all the actual 1 cases, how many did we catch?"

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

High recall indicates that the model is good at identifying positive cases, but it does not consider false positives.

F1-Score

F1-Score

Definition

F1-Score is the harmonic mean of precision and recall, providing a balance between the two metrics:

$$F_1 = 2 \cdot \frac{\text{Precision} \times \text{Recall}}{\text{Precision} + \text{Recall}}$$

It is particularly useful when the class distribution is imbalanced, as it considers both false positives and false negatives. High F1-Score indicates a good balance between precision and recall, while a low F1-Score suggests that either precision or recall (or both) are low.

Precision-Recall Trade-off

Precision-Recall Trade-off

Definition

The **Precision-Recall Trade-off** illustrates the inverse relationship between precision and recall:

Precision-Recall Curve

Definition

Precision-Recall Trade-off

Precision-Recall Trade-off

Definition

The **Precision-Recall Trade-off** illustrates the inverse relationship between precision and recall:

- Increasing the threshold for classifying a positive instance will **increase precision** but **decrease recall**.

Precision-Recall Curve

Definition

Precision-Recall Trade-off

Precision-Recall Trade-off

Definition

The **Precision-Recall Trade-off** illustrates the inverse relationship between precision and recall:

- Increasing the threshold for classifying a positive instance will **increase precision** but **decrease recall**.
- Decreasing the threshold will **increase recall** but **decrease precision**.

Precision-Recall Curve

Definition

Precision-Recall Trade-off

Precision-Recall Trade-off

Definition

The **Precision-Recall Trade-off** illustrates the inverse relationship between precision and recall:

- Increasing the threshold for classifying a positive instance will **increase precision** but **decrease recall**.
- Decreasing the threshold will **increase recall** but **decrease precision**.

Precision-Recall Curve

Definition

Precision-Recall Trade-off

Precision-Recall Trade-off

Definition

The **Precision-Recall Trade-off** illustrates the inverse relationship between precision and recall:

- Increasing the threshold for classifying a positive instance will **increase precision** but **decrease recall**.
- Decreasing the threshold will **increase recall** but **decrease precision**.

Precision-Recall Curve

Definition

Precision-Recall Curve is a graphical representation of the trade-off between precision and recall for different threshold values.

Receiver Operating Characteristic (ROC) Curve

Receiver Operating Characteristic (ROC) Curve

Definition

ROC Curve is a graphical representation of a classifier's performance across different thresholds. It plots the true positive rate (recall) against the false positive rate (FPR) at various threshold settings.

Area Under the Curve (AUC)

Area Under the Curve (AUC)

Definition

Area Under the Curve (AUC)

Area Under the Curve (AUC)

Definition

Area Under the Curve (AUC) is a single scalar value that summarizes the performance of a classifier across all possible thresholds. It is calculated as the area under the ROC curve. AUC provides an aggregate measure of performance across all classification thresholds, making it useful for comparing different classifiers.