Machine Learning Metrics

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Given a set of data points $\{x^{(1)}, \ldots, x^{(m)}\}$, where each $x^{(i)}$ has n features, associated with a set of outcomes $\{y^{(1)}, \ldots, y^{(m)}\}$, we aim to assess a given classifier that learns how to predict y from x.

1 Classification Metrics

In the context of classification, various metrics help evaluate the performance of a model's predictions. These metrics are essential for understanding the strengths and weaknesses of the model.

1.1 Confusion Matrix

The confusion matrix summarizes the predicted and actual class labels. It serves as a foundation for calculating other metrics.

	Predicted class	
Actual class	True Positives	False Negatives
	False Positives	True Negatives

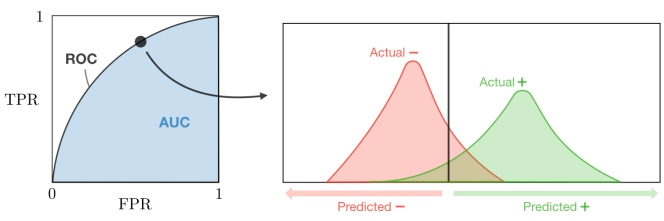
1.2 Main Classification Metrics

Metric	Formula
Accuracy	$\frac{TP+TN}{TP+TN+FP+FN}$
Precision	$\frac{TP}{TP+FP}$
Recall (Sensitivity)	$\frac{TP}{TP+FN}$
Specificity	$\frac{TN}{TN+FP}$
F1 Score	$\frac{2TP}{2TP+FP+FN}$

1.3 ROC and AUC

The Receiver Operating Characteristic (ROC) curve plots True Positive Rate (TPR) against False Positive Rate (FPR). The Area Under the ROC Curve (AUC) quantifies model performance.

Metric	Formula	Equivalent
True Positive Rate	$\text{TPR} = \frac{TP}{TP+FN}$	Recall, Sensitivity
False Positive Rate	$\text{FPR} = \frac{FP}{TN+FP}$	$1 -$ Specificity



2 Regression Metrics

For regression tasks, metrics assess how well the model's predicted values match the actual values. Let y_i represents the actual observed value of the dependent variable for the i-th data point. and $\hat{y}_i$ represents the predicted value of the dependent variable for the i-th data point.

2.1 Mean Absolute Error (MAE)

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|$$

2.2 Mean Squared Error (MSE)

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

2.3 Root Mean Squared Error (RMSE)

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}$$

2.4 R-squared (R^2) Score

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}$$

3 Model Selection

When selecting a model, we distinguish three different parts of the data that we have as follows:

Data Split	Description
Training Set	Model is trained. Usually 80% of the dataset.
Validation Set	Model is assessed. Usually 20% of the dataset.
Testing Set	Model gives predictions. Unseen data.

Once the model has been chosen, it is trained on the entire dataset and tested on the unseen test set. These are represented in the figure below: