# Introduction to Machine Learning

# Evaluation Simple Measures for Classification

		True Class y			
		+	-		
Pred.	+	True Positive	False Positive		
		(TP)	(FP)		
ŷ	-	False Negative	True Negative		
		(FN)	(TN)		

### Learning goals

- Know the definitions of misclassification error rate (MCE) and accuracy (ACC)
- Understand the entries of a confusion matrix
- Understand the idea of costs
- Know definitions of Brier score and log loss



### LABELS VS PROBABILITIES

In classification we predict:



Class labels:

$$\boldsymbol{F} = \left(\hat{\boldsymbol{o}}_{k}^{(i)}\right)_{i \in \{1, \dots, m\}, k \in \{1, \dots, g\}} \in \mathbb{R}^{m \times g},$$

where  $\hat{o}_{k}^{(i)} = [\hat{y}^{(i)} = k], k = 1, ..., g$  is the one-hot-encoded class label prediction.

Class probabilities: 2

$$\boldsymbol{F} = \left(\hat{\pi}_{k}^{(i)}\right)_{i \in \{1, \dots, m\}, k \in \{1, \dots, g\}} \quad \in [0, 1]^{m \times g}$$

 $\rightarrow$  These form the basis for evaluation.



Х  $\times \times$ 

### LABELS: MCE & ACC

The **misclassification error rate (MCE)** counts the number of incorrect predictions and presents them as a rate:

$$ho_{MCE} = rac{1}{m} \sum_{i=1}^m [y^{(i)} 
eq \hat{y}^{(i)}] \in [0,1].$$

Accuracy (ACC) is defined in a similar fashion for correct classifications:

$$\rho_{ACC} = \frac{1}{m} \sum_{i=1}^{m} [y^{(i)} = \hat{y}^{(i)}] \in [0, 1].$$



MCE



× 0 0 × 0 × ×

- If the data set is small this can be brittle.
- MCE says nothing about how good/skewed predicted probabilities are.
- Errors on all classes are weighted equally, which is often inappropriate.

## LABELS: CONFUSION MATRIX

Much better than reducing prediction errors to a simple number is tabulating them in a **confusion matrix**:

- true classes in columns,
- predicted classes in rows.

We can nicely see class sizes (predicted/true) and where errors occur.

× 0 0 × × ×

		setosa	versicolor	virginica	error	n
Predicted classes	setosa	50	0	0	0	50
	versicolor	0	46	4	4	50
	virginica	0	4	46	4	50
	error	0	4	4	8	-
	п	50	50	50	-	150

True classes

## LABELS: CONFUSION MATRIX

- In binary classification, we typically call one class "positive" and the other "negative".
- The positive class is the more important, often smaller one.



× 0 0 × 0 × ×

e.g.,

- **True Positive** (TP) means that an instance is classified as positive that is really positive (correct prediction).
- False Negative (FN) means that an instance is classified as negative that is actually positive (incorrect prediction).

### LABELS: COSTS

We can also assign different costs to different errors via a cost matrix.

Costs = 
$$\frac{1}{n} \sum_{i=1}^{n} C[y^{(i)}, \hat{y}^{(i)}]$$

Example: Depending on certain features (age, income, profession, ...) a bank wants to decide whether to grant a 10,000 EUR loan.

Predict if a person is solvent (yes / no). Should the bank lend them the money?

### Examplary costs:

Loss in event of default: 10,000 EUR Income through interest paid: 100 EUR

	True classes		
	solvent	not solvent	
Predicted solvent	0	10,000	
classes not solvent	100	0	



### LABELS: COSTS

1

#### Cost matrix

#### Confusion matrix

True classes				True	classes
	solvent	not solvent		solvent	not so
Predicted solvent	0	10,000	Predicted solvent	70	3
classes not solvent	100	0	classes not solvent	7	2

Х  $\times \times$ 

• If the bank gives everyone a credit, who was predicted as *solvent*, the costs are at:

$$Costs = \frac{1}{n} \sum_{i=1}^{n} C[y^{(i)}, \hat{y}^{(i)}]$$
$$= \frac{1}{100} (100 \cdot 7 + 0 \cdot 70 + 10.000 \cdot 3 + 0 \cdot 20) = 307$$

• If the bank gives everyone a credit, the costs are at:

$$Costs = \frac{1}{100} \left( 100 \cdot 0 + 0 \cdot 77 + 10.000 \cdot 23 + 0 \cdot 0 \right) = 2.300$$

not solvent 3 20

### **PROBABILITIES: BRIER SCORE**

Measures squared distances of probabilities from the true class labels:

$$\rho_{BS} = \frac{1}{m} \sum_{i=1}^{m} \left( \hat{\pi}^{(i)} - y^{(i)} \right)^2$$

- Fancy name for MSE on probabilities.
- Usual definition for binary case;  $y^{(i)}$  must be encoded as 0 and 1.



× 0 0 × 0 × ×

### PROBABILITIES: BRIER SCORE / 2

$$\rho_{BS,MC} = \frac{1}{m} \sum_{i=1}^{m} \sum_{k=1}^{g} \left( \hat{\pi}_{k}^{(i)} - o_{k}^{(i)} \right)^{2}$$

- Original by Brier, works also for multiple classes.
- $o_k^{(i)} = [y^{(i)} = k]$  marks the one-hot-encoded class label.
- For the binary case, ρ<sub>BS,MC</sub> is twice as large as ρ<sub>BS</sub>: in ρ<sub>BS,MC</sub>, we sum the squared difference for each observation regarding both class 0 and class 1, not only the true class.

× 0 0 × 0 × × ×

## **PROBABILITIES: LOG-LOSS**

m

Logistic regression loss function, a.k.a. Bernoulli or binomial loss,  $y^{(i)}$  encoded as 0 and 1.

$$\rho_{LL} = \frac{1}{m} \sum_{i=1}^{m} \left( -y^{(i)} \log \left( \hat{\pi}^{(i)} \right) - \left( 1 - y^{(i)} \right) \log \left( 1 - \hat{\pi}^{(i)} \right) \right).$$



- Optimal value is 0, "confidently wrong" is penalized heavily.
- Multi-class version:  $\rho_{LL,MC} = -\frac{1}{m} \sum_{i=1}^{m} \sum_{k=1}^{g} o_k^{(i)} \log\left(\hat{\pi}_k^{(i)}\right)$ .