

# Introduction to Machine Learning

## Evaluation: Simple Measures for Classification

|           |   | True Class $y$      |                     |
|-----------|---|---------------------|---------------------|
|           |   | +                   | -                   |
| Pred.     | + | True Positive (TP)  | False Positive (FP) |
| $\hat{y}$ | - | False Negative (FN) | True Negative (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:

- ❶ Class labels  $\rightarrow \hat{h}(\mathbf{x}) = \hat{y}$
- ❷ Class probabilities  $\rightarrow \hat{\pi}_k(\mathbf{x})$

$\rightarrow$  We evaluate based on those

# LABELS: MCE

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

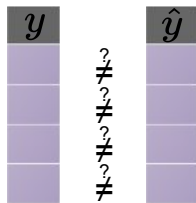
$$MCE = \frac{1}{n} \sum_{i=1}^n [y^{(i)} \neq \hat{y}^{(i)}] \in [0; 1]$$

Accuracy is defined in a similar fashion for correct classifications:

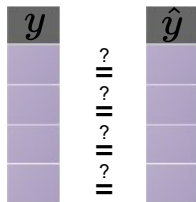
$$ACC = \frac{1}{n} \sum_{i=1}^n [y^{(i)} = \hat{y}^{(i)}] \in [0; 1]$$

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

**MCE**



**ACC**



# LABELS: CONFUSION MATRIX

Much better than simply 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 and true) and where errors occur.

|                      |            | True classes |            |           |       |     |
|----------------------|------------|--------------|------------|-----------|-------|-----|
|                      |            | setosa       | versicolor | virginica | error | $n$ |
| Predicted<br>classes | setosa     | 50           | 0          | 0         | 0     | 50  |
|                      | versicolor | 0            | 46         | 4         | 4     | 50  |
|                      | virginica  | 0            | 4          | 46        | 4     | 50  |
|                      | error      | 0            | 4          | 4         | 8     | -   |
| $n$                  |            | 50           | 50         | 50        | -     | 150 |

# LABELS: CONFUSION MATRIX

## In binary classification

|           |   | True Class $y$         |                        |
|-----------|---|------------------------|------------------------|
|           |   | +                      | -                      |
| Pred.     | + | True Positive<br>(TP)  | False Positive<br>(FP) |
| $\hat{y}$ | - | False Negative<br>(FN) | True Negative<br>(TN)  |

e.g.,

- **True Positive** (TP) means that an instance is classified as positive which is also positive (true prediction).
- **False Negative** (FN) means that an instance is classified as negative which is actually positive (false prediction).

# LABELS: COSTS

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

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

Example: [@BB Elkan Paper! Confusion matrix discussion](#)

Depending on certain features (age, income, profession, ...) a bank wants to decide, if it grants a 10,000 EUR loan.

Predict if a person is solvent (yes / no).

Should a bank give her/him a loan?

## Exemplary costs:

Loan cannot be repaid: 10,000 EUR

Interest paid for the loan: 100 EUR

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

# LABELS: COSTS

Cost matrix

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

Confusion matrix

|                   |             | True classes |             |
|-------------------|-------------|--------------|-------------|
|                   |             | solvent      | not solvent |
| Predicted classes | solvent     | 70           | 3           |
|                   | not solvent | 7            | 20          |

- If the bank gives every person a credit, the costs are at:

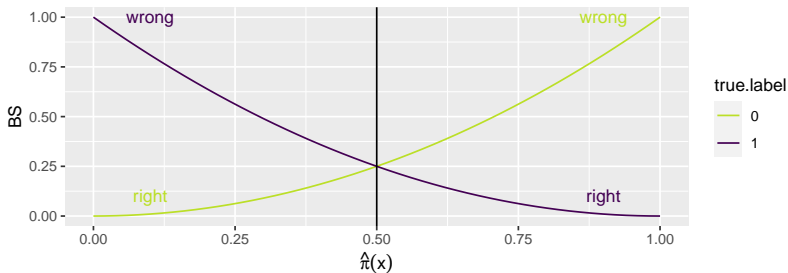
$$\begin{aligned} \text{Costs} &= \frac{1}{n} \sum_{i=1}^n C[y^{(i)}, \hat{y}^{(i)}] \\ &= \frac{1}{100} (-37 \cdot 7 + 0 \cdot 0 + 3 \cdot 93 + 0 \cdot 0) = 0.2 \end{aligned}$$

# PROBABILITIES: BRIER SCORE

Measures squared distances of probabilities from the true class labels:

$$BS1 = \frac{1}{n} \sum_{i=1}^n \left( \hat{\pi}(\mathbf{x}^{(i)}) - y^{(i)} \right)^2$$

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





# PROBABILITIES: BRIER SCORE

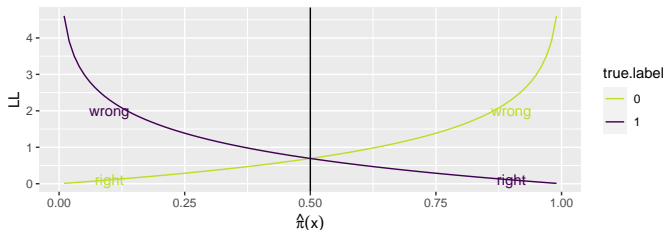
$$BS2 = \frac{1}{n} \sum_{i=1}^n \sum_{k=1}^g \left( \hat{\pi}_k(\mathbf{x}^{(i)}) - o_k^{(i)} \right)^2$$

- Original by Brier, works also for multiple classes
- $o_k^{(i)} = [y^{(i)} = k]$  is a 0-1-one-hot coding for labels
- For the binary case, BS2 is twice as large as BS1, because in BS2 we sum the squared difference for each observation regarding class 0 **and** class 1, not only the true class.

# PROBABILITIES: LOG-LOSS

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

$$LL = \frac{1}{n} \sum_{i=1}^n \left( -y^{(i)} \log(\hat{\pi}(\mathbf{x}^{(i)})) - (1 - y^{(i)}) \log(1 - \hat{\pi}(\mathbf{x}^{(i)})) \right)$$



- Optimal value is 0, “confidently wrong” is penalized heavily
- Multiclass version:  $LL = -\frac{1}{n} \sum_{i=1}^n \sum_{k=1}^g o_k^{(i)} \log(\hat{\pi}_k(\mathbf{x}^{(i)}))$