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:

1. Class labels:

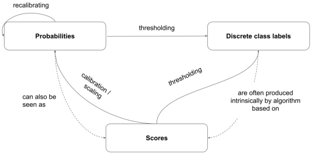
$$\boldsymbol{F} = \left(\hat{o}_k^{(i)}\right)_{i \in \{1,\ldots,m\}, k \in \{1,\ldots,g\}} \quad \in \mathbb{R}^{m \times g},$$

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

2. Class probabilities:

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

$\rightarrow$ These form the basis for evaluation.

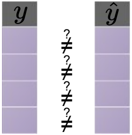


LABELS: MCE & ACC

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

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

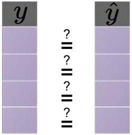
MCE



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

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

ACC



- 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.

		True classes				
		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	-
	n	50	50	50	-	150

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.

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

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 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 everyone a credit, who was predicted as *solvent*, the costs are at:

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

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

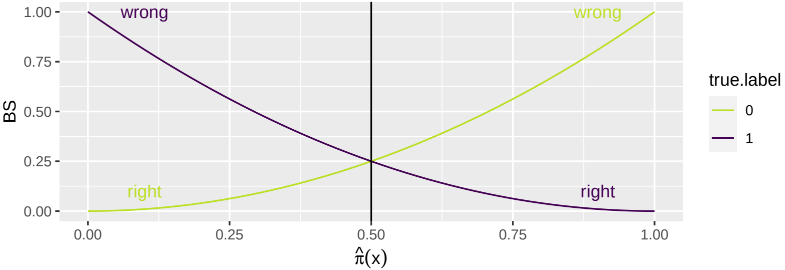
$$Costs = \frac{1}{100}\left(100 \cdot 0 + 0 \cdot 77 + 10.000 \cdot 23 + 0 \cdot 0\right) = 2.300$$

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.



PROBABILITIES: BRIER SCORE

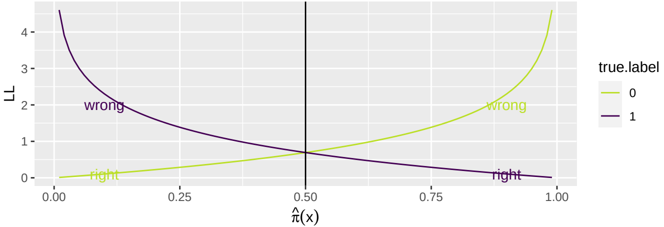
$$\rho_{BS,MC} = \frac{1}{m} \sum_{i=1}^{m} \sum_{k=1}^{g} \left(\hat{\pi}_k^{(i)} - o_k^{(i)} \right)^2$$

- 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, $\rho_{BS,MC}$ is twice as large as ρ_{BS}: in $\rho_{BS,MC}$, we sum the squared difference for each observation regarding both class 0 **and** class 1, not only the true class.

PROBABILITIES: LOG-LOSS

Logistic regression loss function, a.k.a. Bernoulli or binomial loss, $y^{(i)}$ 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: $\rho_{LL,MC} = -\frac{1}{m}\sum_{i=1}^{m}\sum_{k=1}^{g} o_k^{(i)}\log\left(\hat{\pi}_k^{(i)}\right).$