Model Evaluation

Classification quality metrics, prediction error, cross-validation

Machine Learning and Data Mining, 2024

Majid Sohrabi
National Research University Higher School of Economics

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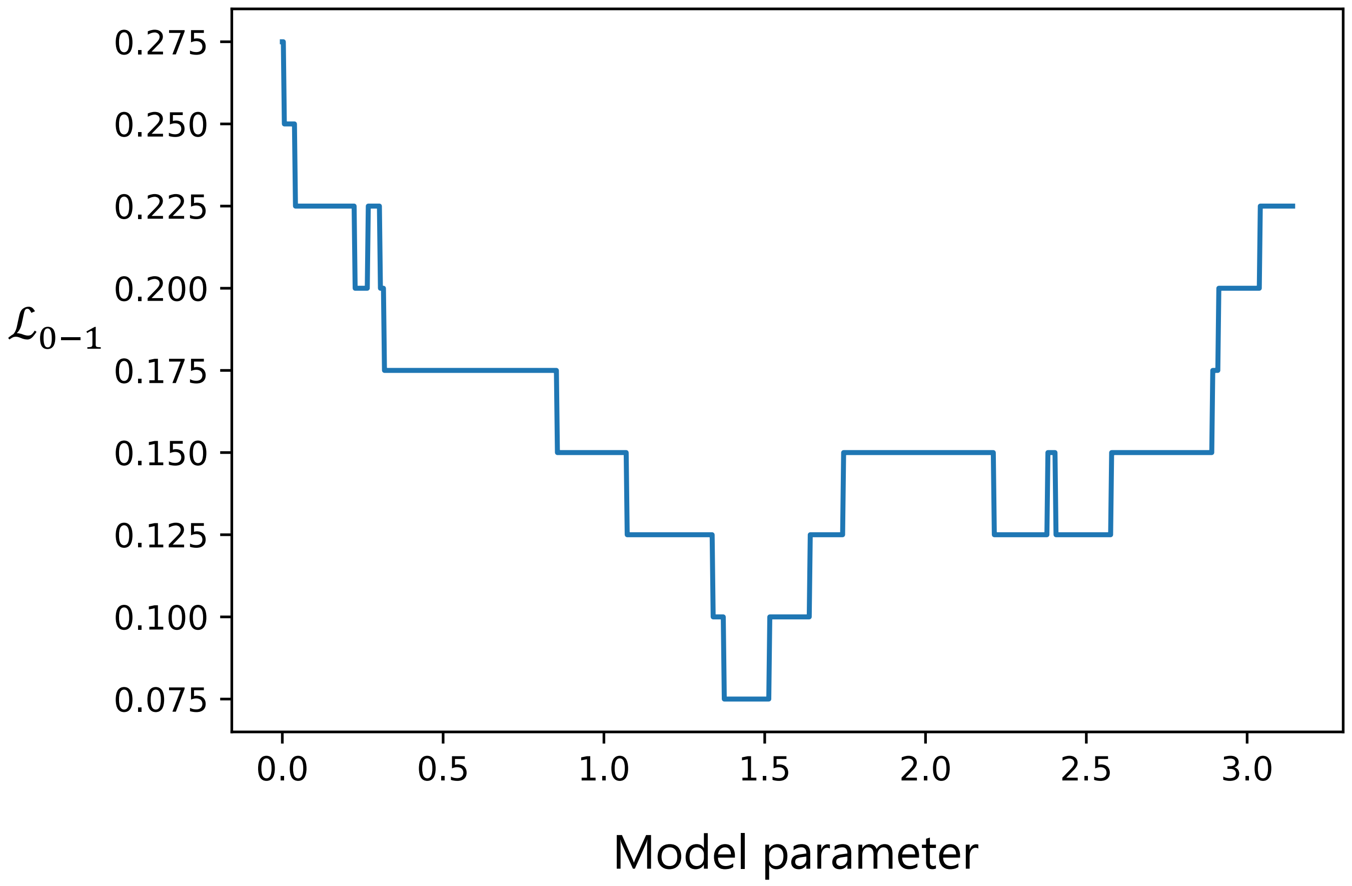
Classification quality metrics

How to evaluate a classifier?

0-1 Loss

Probability of an error (error rate):

$$\mathcal{L}_{0-1} = \frac{1}{N} \sum_{i=1\ldots N} \mathbb{I}(y_i \neq \hat{y}_i)$$



0-1 Loss

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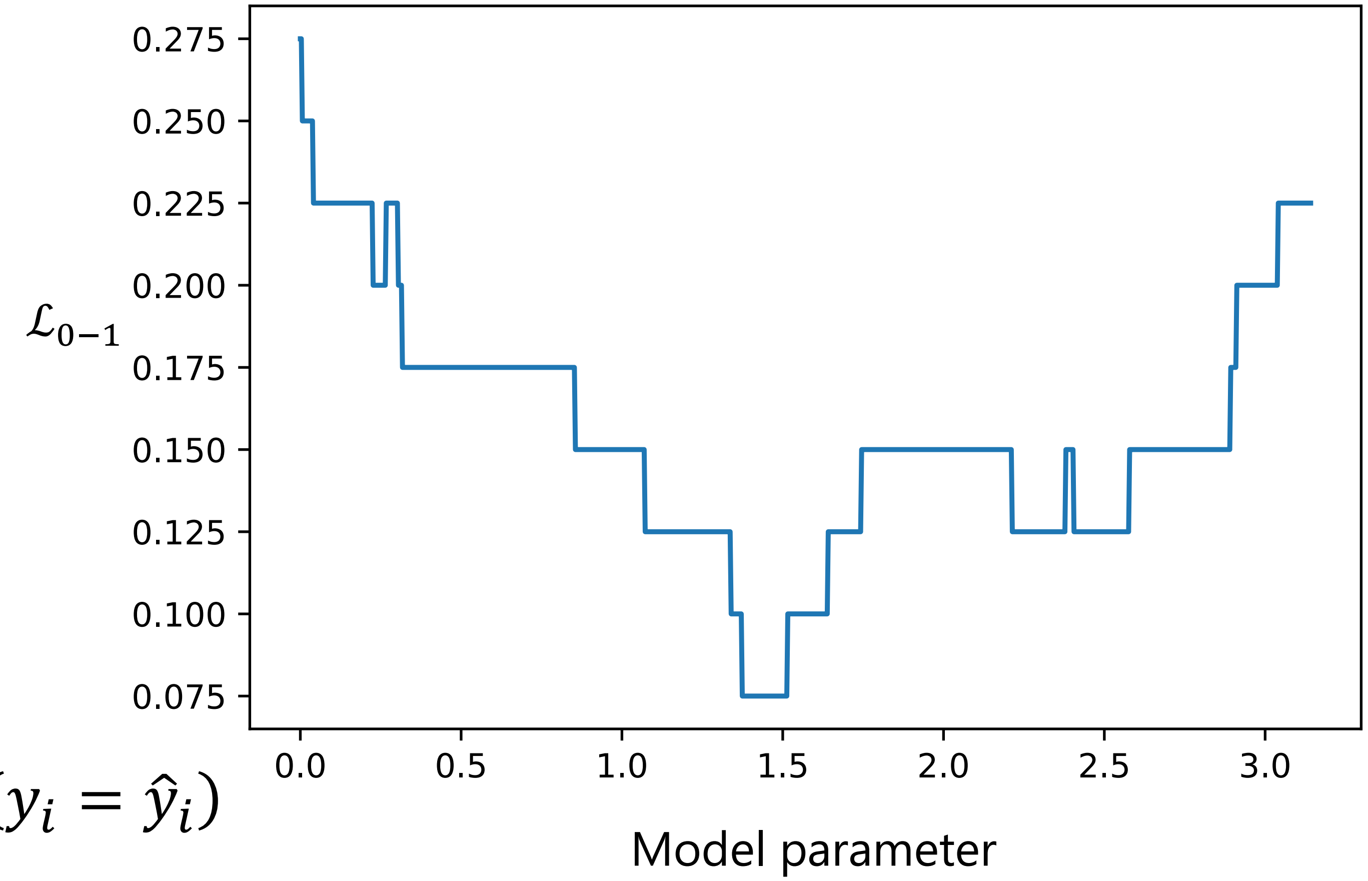
Accuracy:

$$accuracy = 1 - \mathcal{L}_{0-1} = \frac{1}{N} \sum_{i=1\ldots N} \mathbb{I}(y_i = \hat{y}_i)$$

Not always a good quality measure

- E.g. when classes are imbalanced



Confusion matrix

Actual class

$$\begin{array}{c|cccc}
 & 1 & 2 & \cdots & C \\
\hline
1 & n_{11} & n_{12} & \cdots & n_{1C} \\
2 & n_{21} & n_{22} & \cdots & n_{2C} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
C & n_{C1} & n_{C2} & \cdots & n_{CC}
\end{array}$$

Predicted class

n_{ij} – number of objects of class j, that were predicted as class i

Diagonal elements – correct classifications

Off-diagonal elements – incorrect classifications

Binary case

		Actual class	
		+	−
Predicted class	+	**TP** (True Positives)	**FP** (False Positives)
	−	**FN** (False Negatives)	**TN** (True Negatives)

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

Binary case

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

Binary case

Predicted class \ Actual class	+	−
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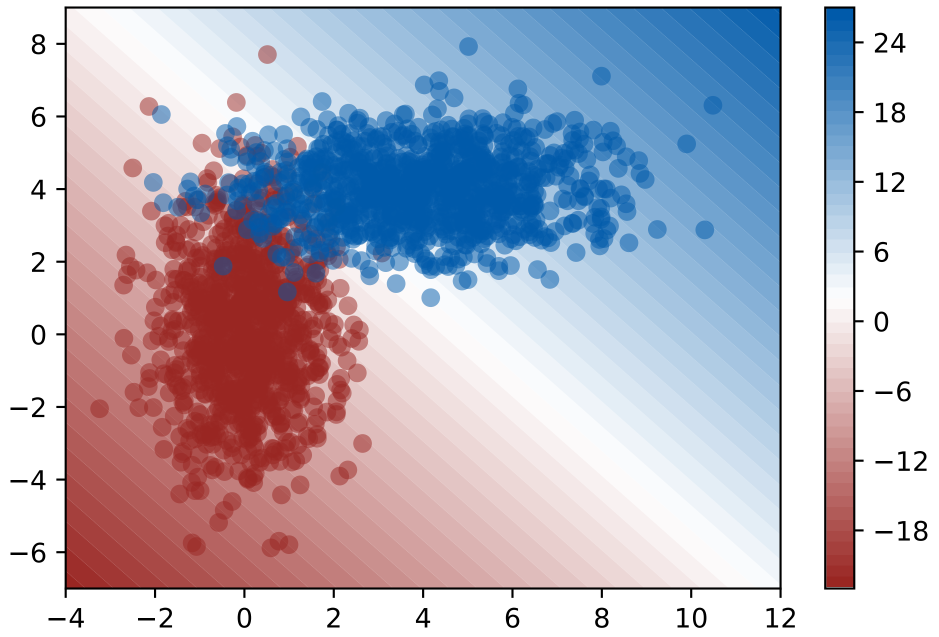
$$\text{Recall} = \frac{\text{TP}}{\text{TP+FN}}$$

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

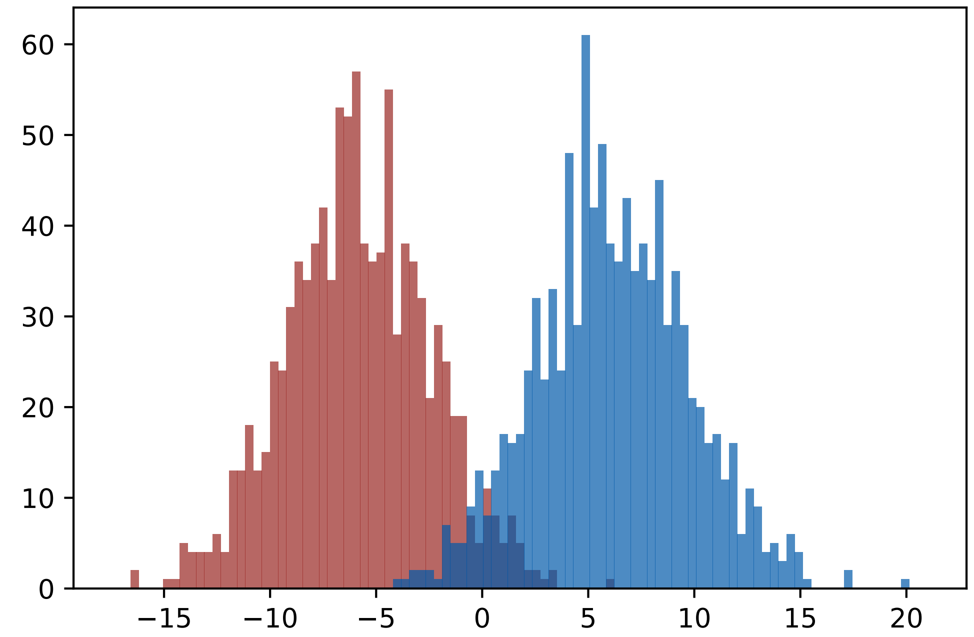
Continuous predictions

Many classification algorithms work with continuous scoring functions

- E.g. log odds in Logistic Regression, or scoring function of an SVM model



Model prediction



Scoring function values on data

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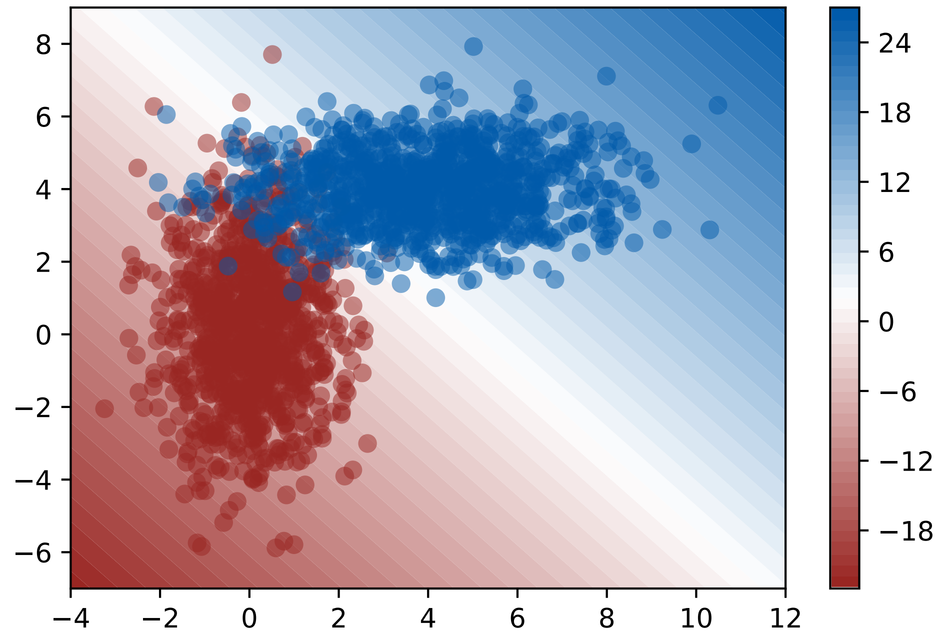

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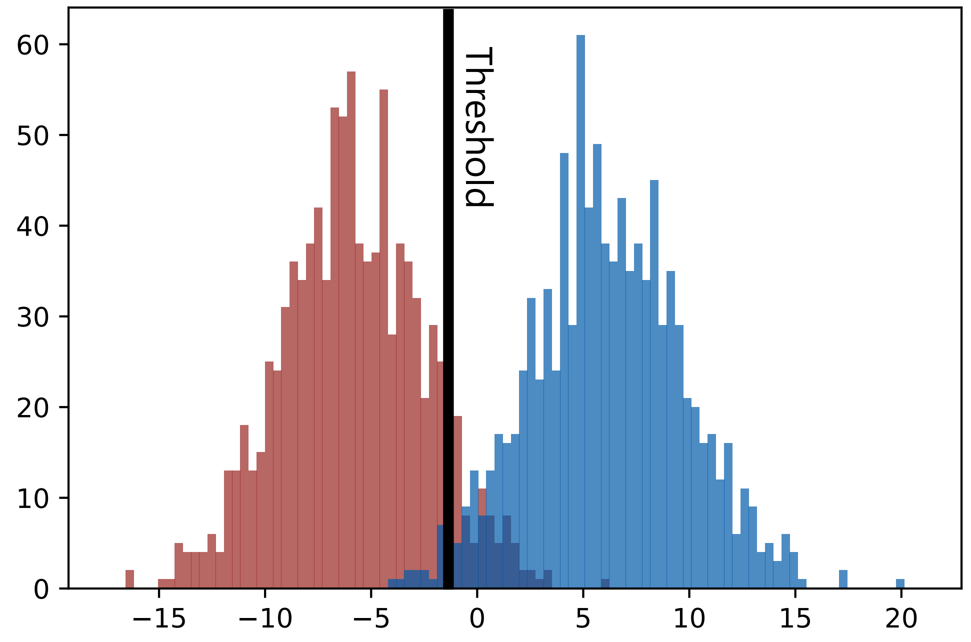
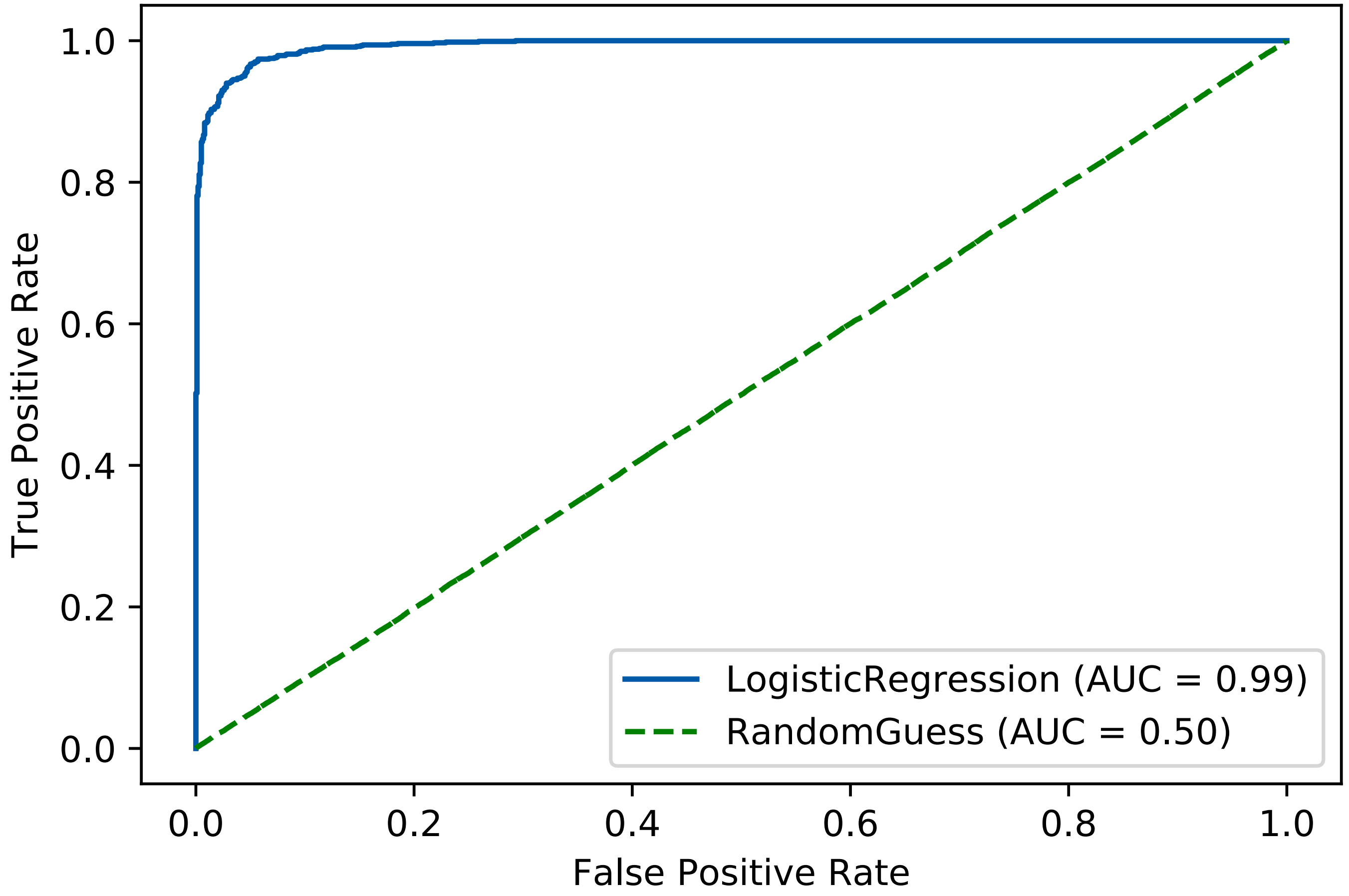
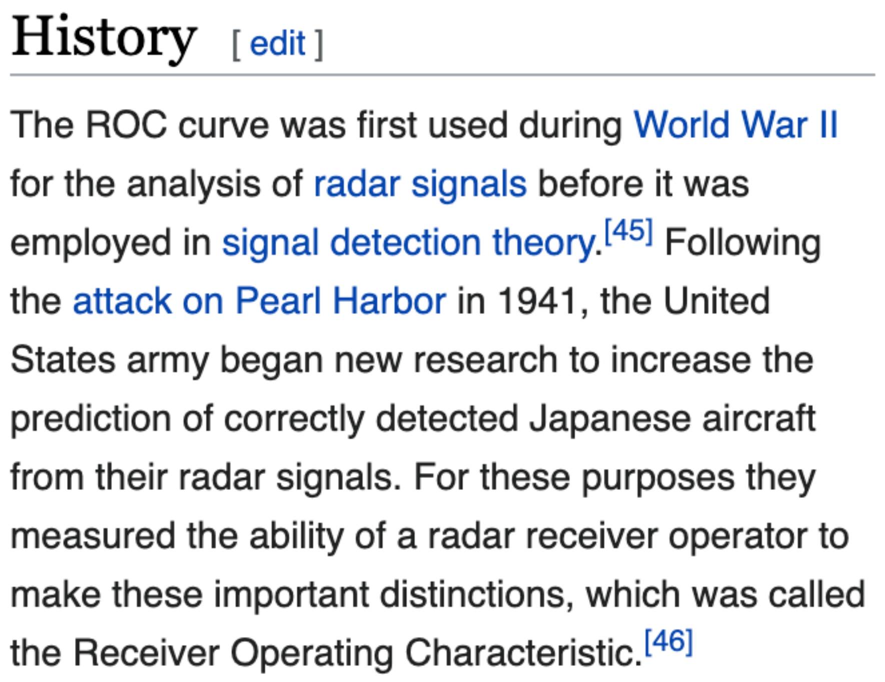


Scoring function values on data

ROC-curve

Receiver operating characteristic = TPR as a function of FPR





History [edit]

The ROC curve was first used during World War II for the analysis of radar signals before it was employed in signal detection theory.[45] Following the attack on Pearl Harbor in 1941, the United States army began new research to increase the prediction of correctly detected Japanese aircraft from their radar signals. For these purposes they measured the ability of a radar receiver operator to make these important distinctions, which was called the Receiver Operating Characteristic.[46]

https://en.wikipedia.org/wiki/Receiver_operating_characteristic

Nice demo: http://arogozhnikov.github.io/2015/10/05/roc-curve.html

ROC AUC probabilistic interpretation

ROC AUC = area under the ROC curve

For the population distribution:

$$P(x, y), \qquad x \in \mathbb{R}^d, \qquad y \in \{0, 1\}$$

$\hat{f}(x)\colon\ \mathbb{R}^d \rightarrow \mathbb{R}$ – classifier scoring function

ROC AUC also equals the probability that

$$P\left[\hat{f}(x_0) < \hat{f}(x_1)\right]$$

for x_0 sampled from $P(x \mid y = 0)$, and x_1 sampled from $P(x \mid y = 1)$

Prediction error
vs
expected prediction error

Two scenarios

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- Trained a model $\widehat{f_\tau}(x)$ on a particular dataset τ
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$$\mathrm{Err}_\tau = \mathop{\mathbb{E}}_{x,y}\left[L\left(y, \widehat{f}_\tau(x)\right)\right]$$

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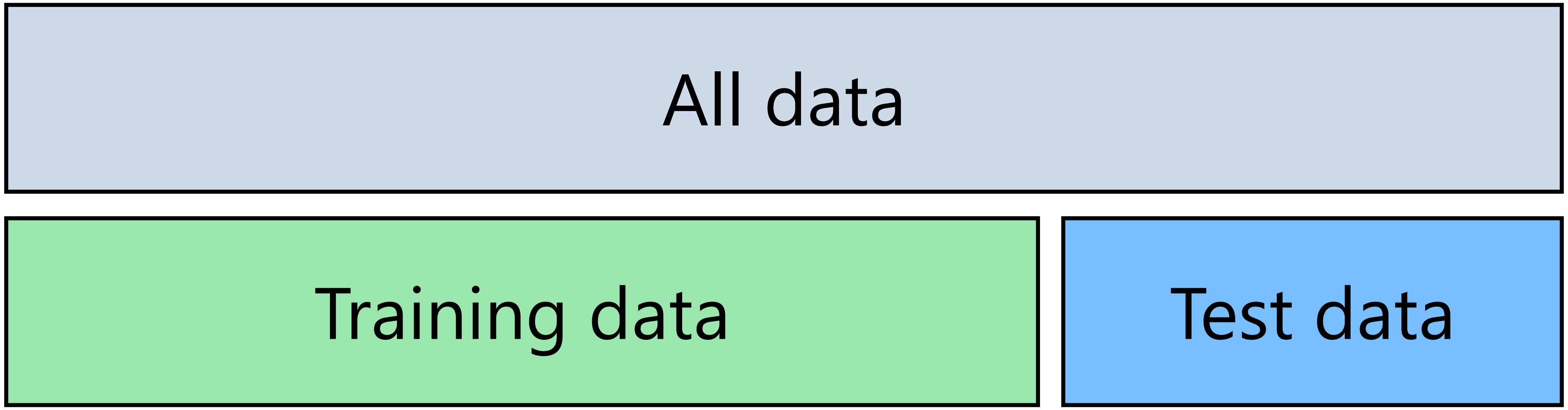
- **Expected prediction error**:

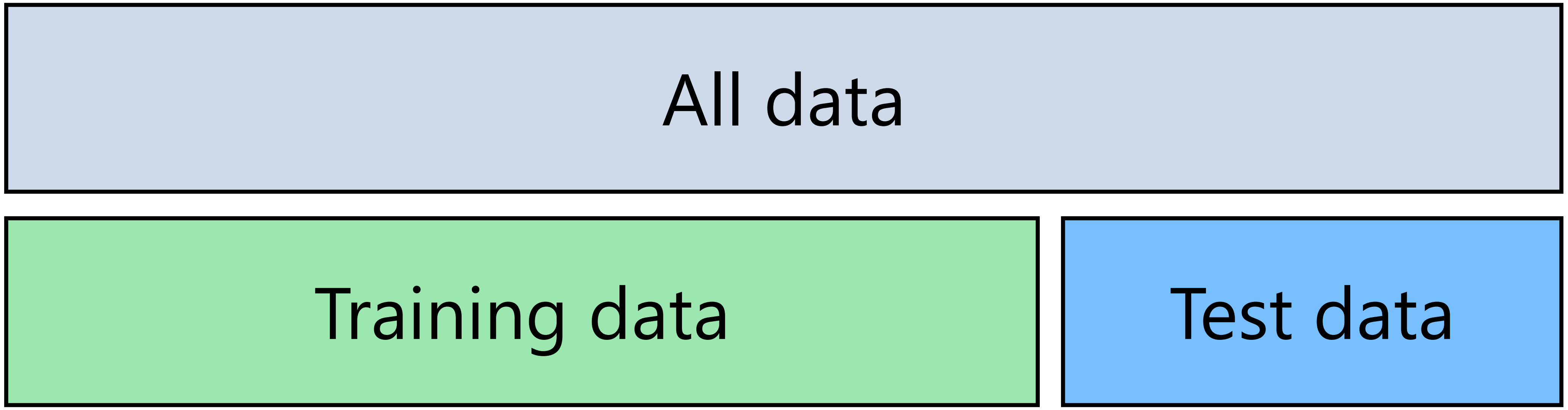
$$\mathrm{Err} = \mathop{\mathbb{E}}_{x,y,\tau}\left[L\left(y, \widehat{f}_\tau(x)\right)\right] = \mathop{\mathbb{E}}_{\tau}[\mathrm{Err}_\tau]$$

Splitting to train and test



What kind of error do we estimate here?

Splitting to train and test



What kind of error do we estimate here?

How to estimate its variance?

Splitting to train, validation and test

When we do model selection, we use the left-out data to estimate the prediction error and minimize it (e.g., wrt the hyperparameters)

May ‘overfit to test’, so the resulting minimized error is not a good estimate of the prediction error

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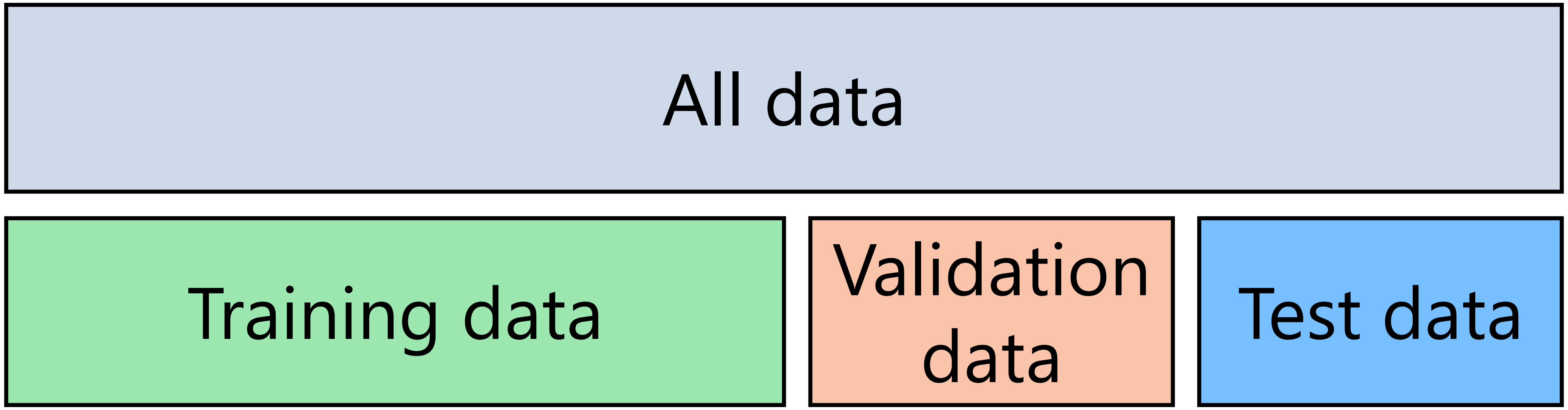

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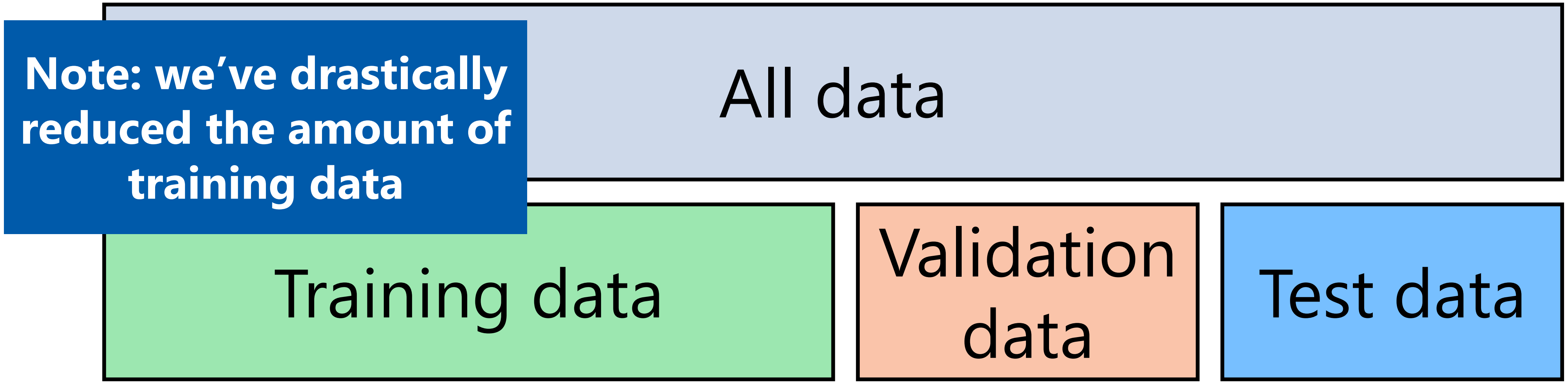
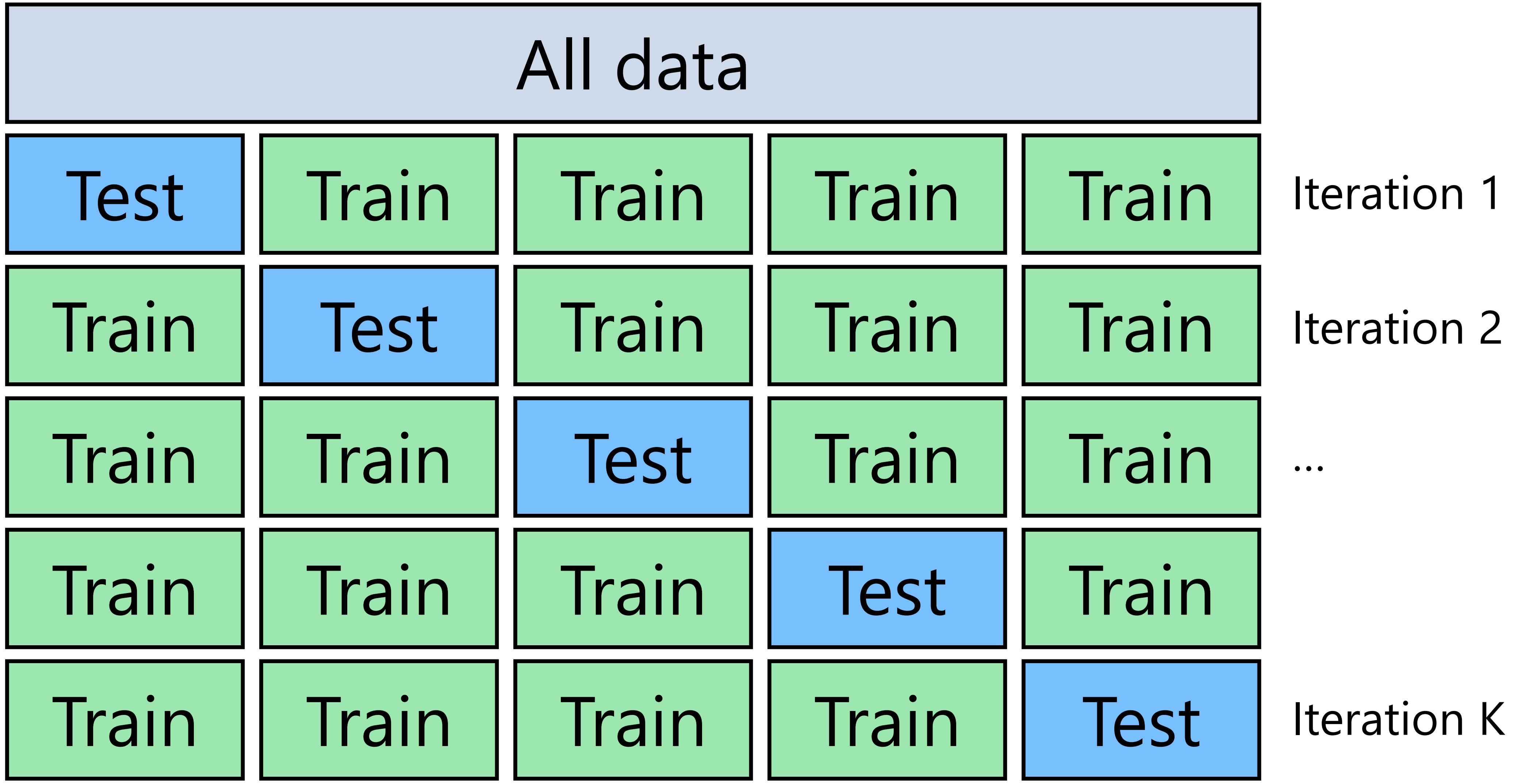
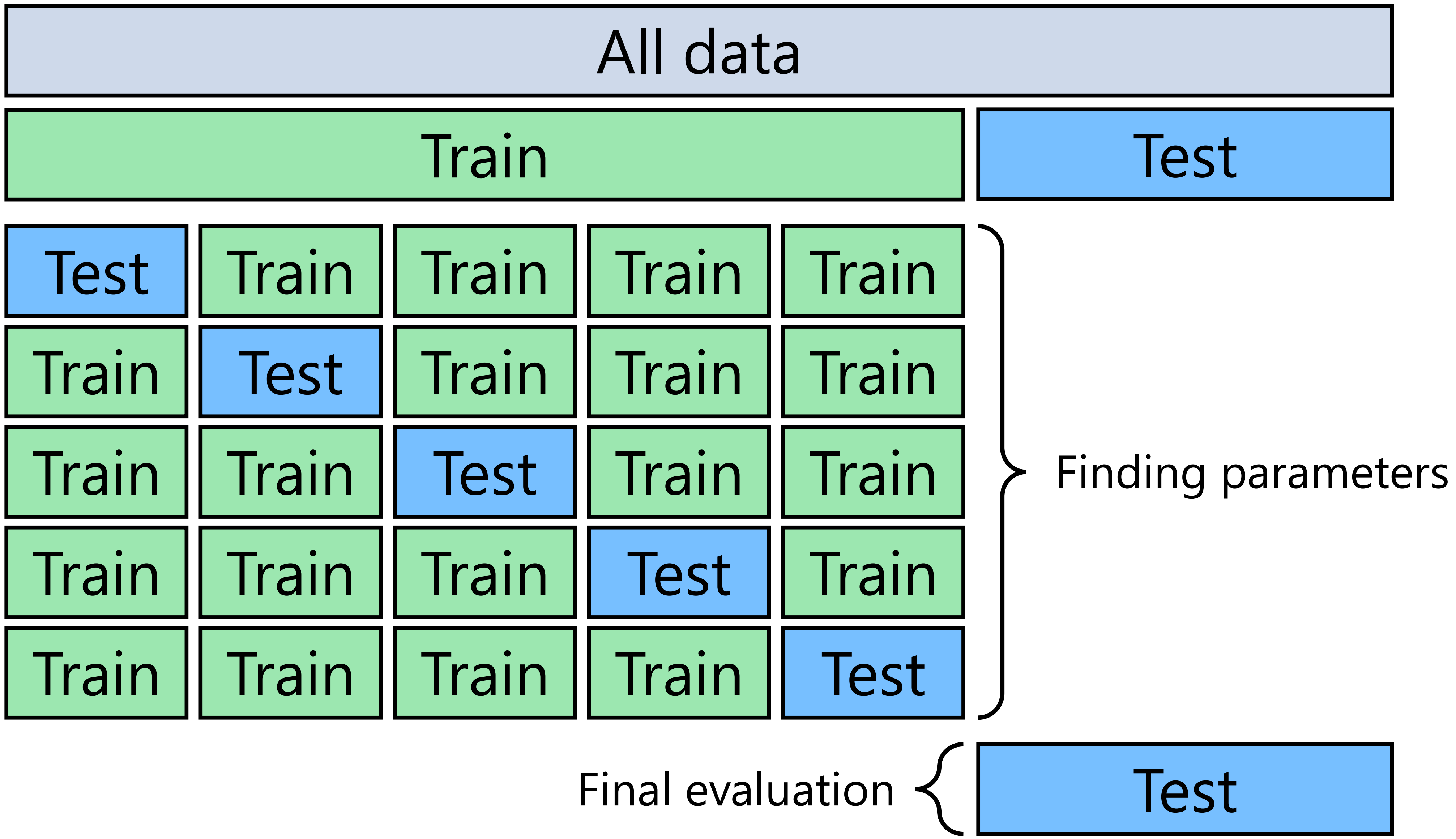


Cross-validation

K-fold cross-validation


All data
Test Train Train Train Train
Iteration 1
Train Test Train Train Train
Iteration 2
Train Train Test Train Train
…
Train Train Train Test Train
Train Train Train Train Test
Iteration K

Hyperparameter tuning


All data
Train
Test
Test Train Train Train Train
Train Test Train Train Train
Train Train Test Train Train
Train Train Train Test Train
Train Train Train Train Test
Finding parameters
Final evaluation
Test

Thank you!

Majid Sohrabi

msohrabi@hse.ru