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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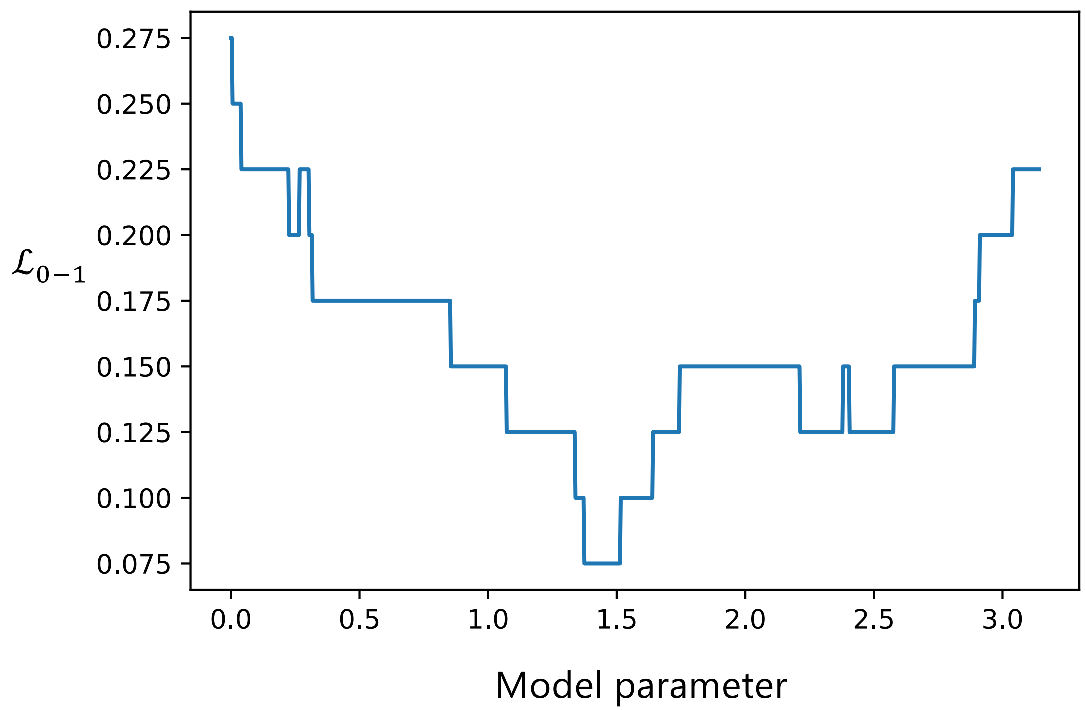
Classification quality metrics

How to evaluate a classifier?

0-1 Loss

Probability of an error (error rate):

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



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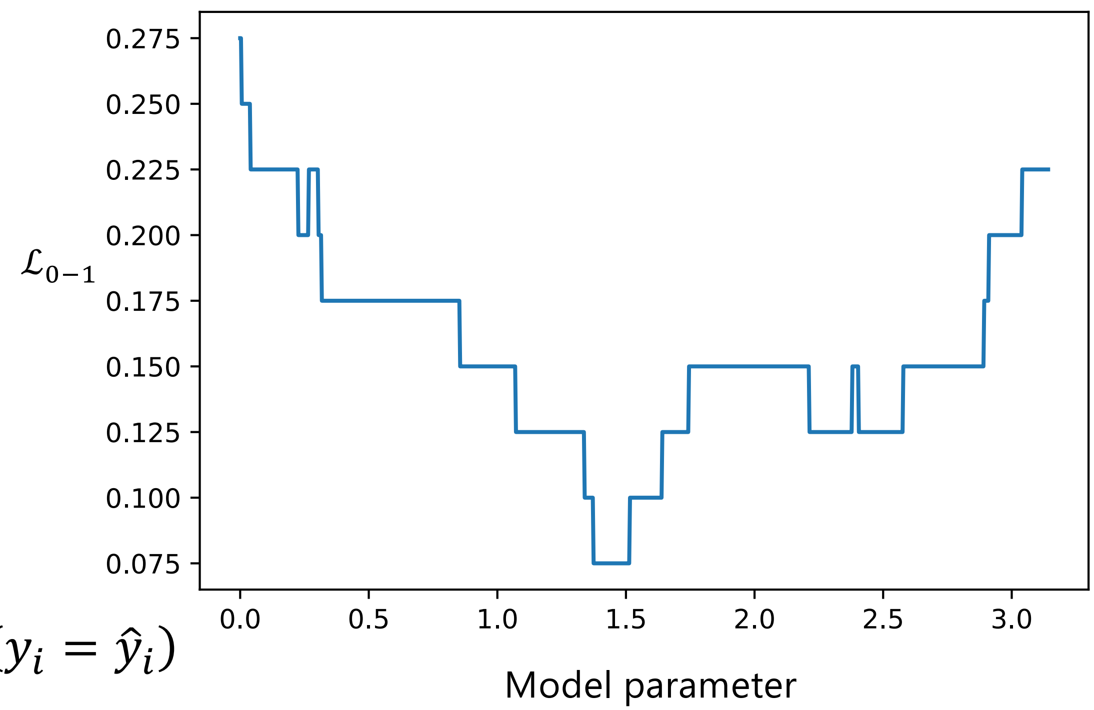
Accuracy:

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



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

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

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$$\text{Precision} = \frac{\text{TP}}{\text{TP+FP}}$$

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

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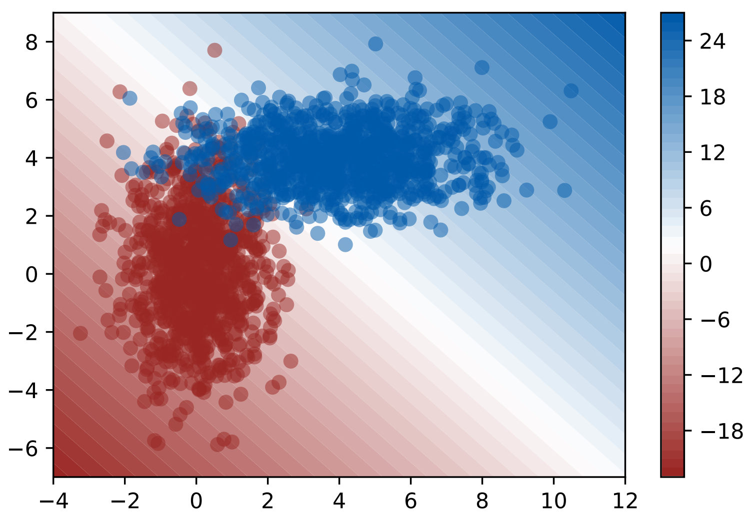
$$F_1\text{-score} = \frac{2 \cdot \mathrm{Precision} \cdot \mathrm{Recall}}{\mathrm{Precision} + \mathrm{Recall}}$$

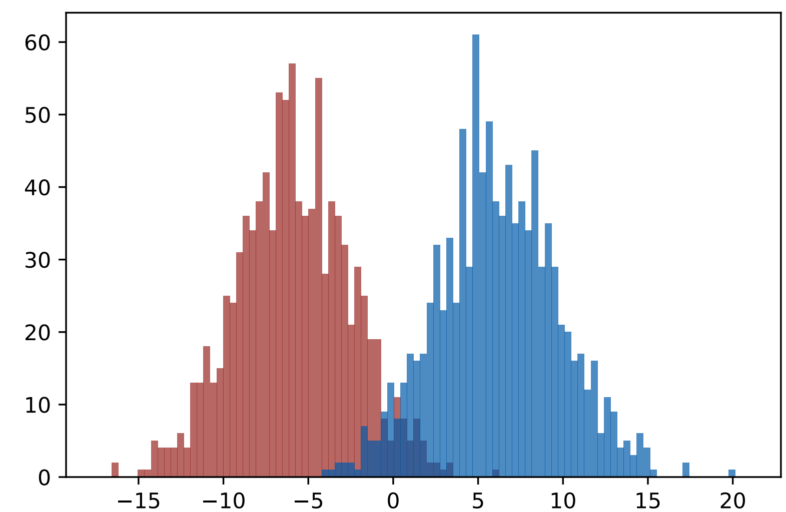
Continuous predictions

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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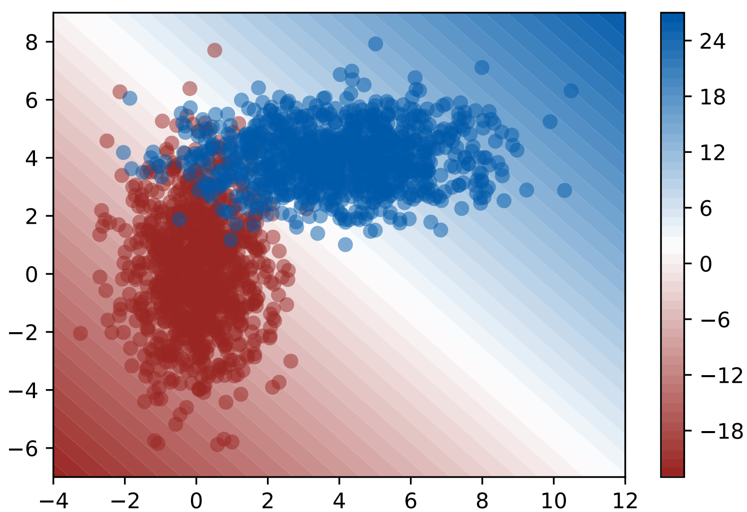

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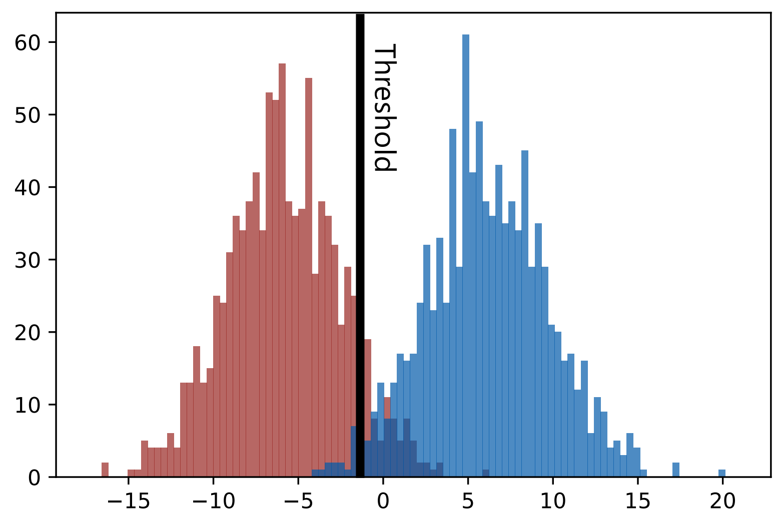
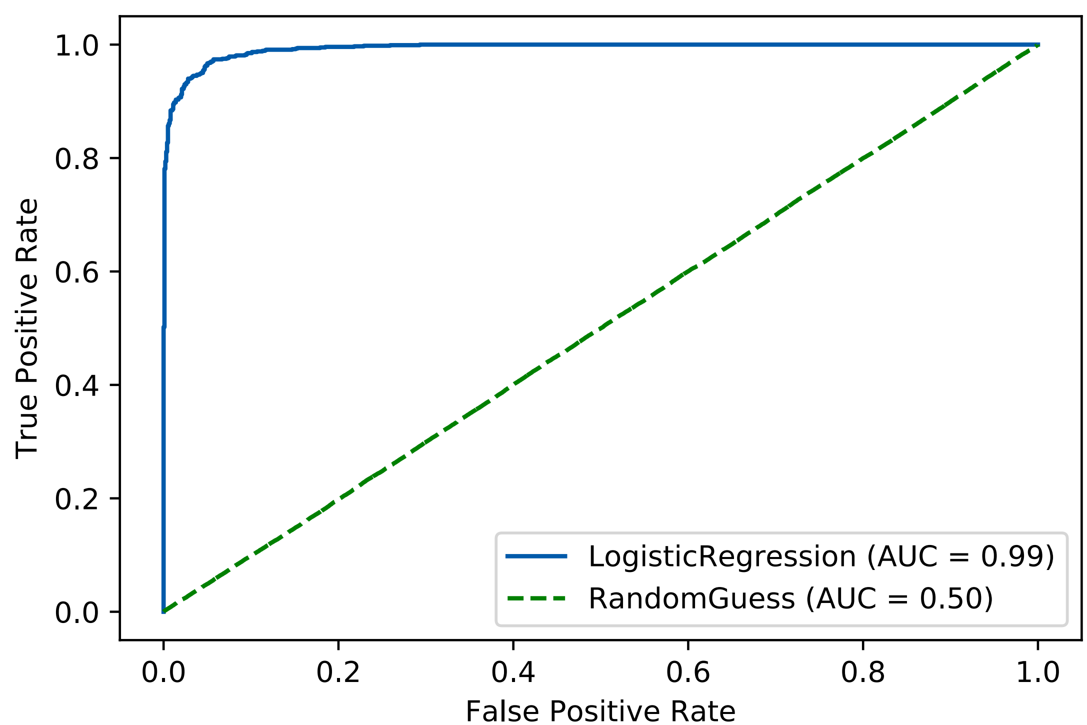


Scoring function values on data

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:

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

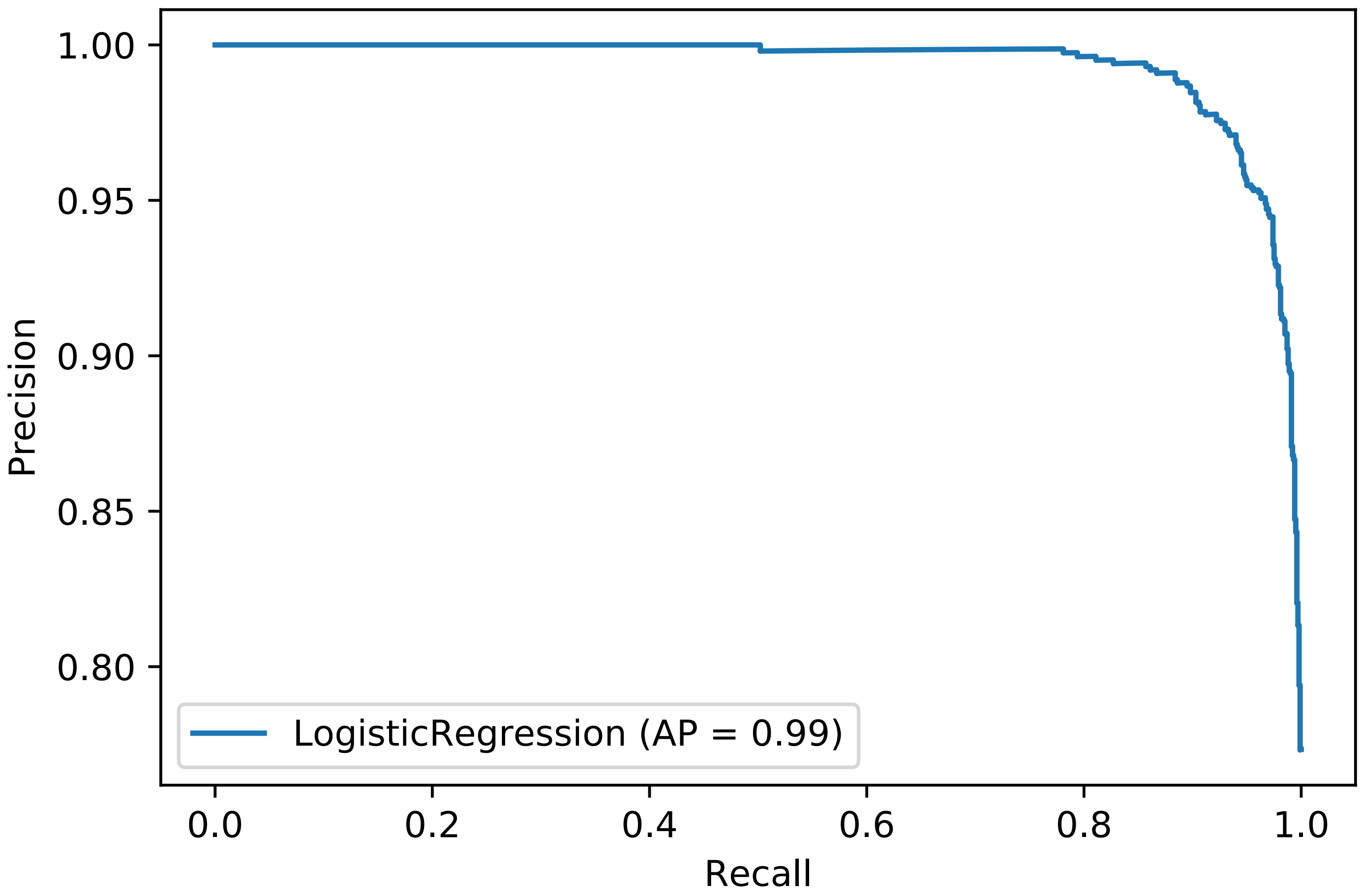
$$\hat{f}(x)\colon\ \mathbb{R}^d \to \mathbb{R}$$ – classifier scoring function

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 $P(x \mid y = 1)$

Precision-recall curve



Prediction error
vs
expected prediction error

Two scenarios

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A:

- Trained a model $\widehat{f_\tau}(x)$ on a particular dataset τ
- Want to know, how well this particular $\widehat{f_\tau}(x)$ will perform on new data

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

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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?

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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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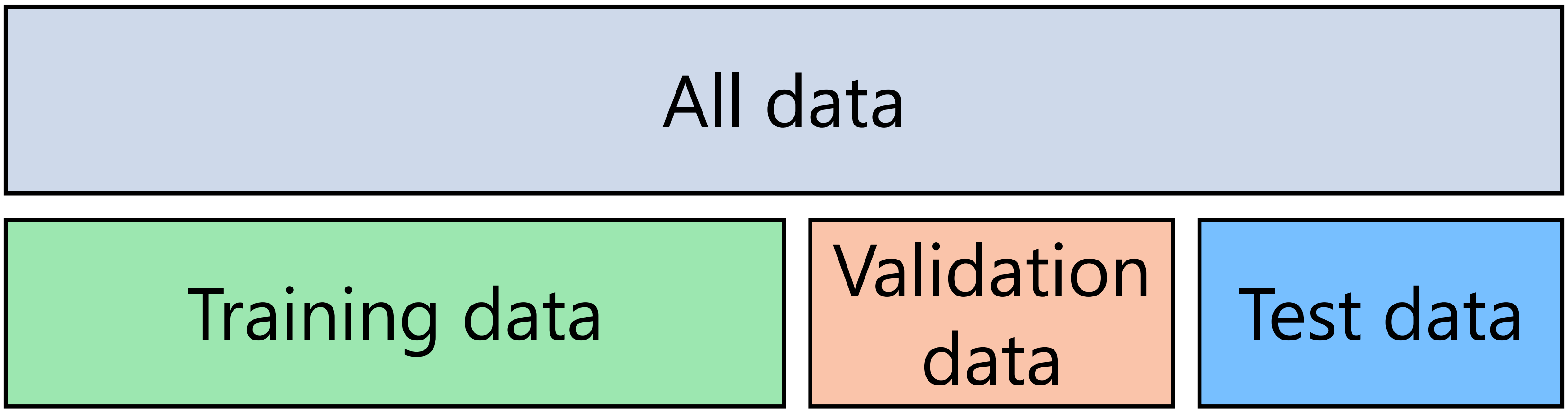

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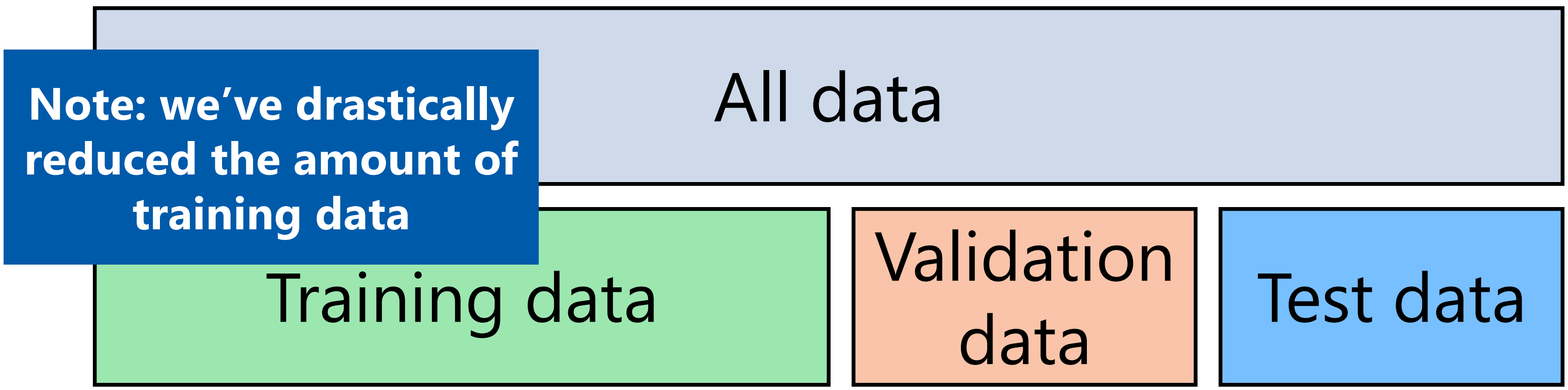


Cross-validation

How to estimate the expected prediction error?

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

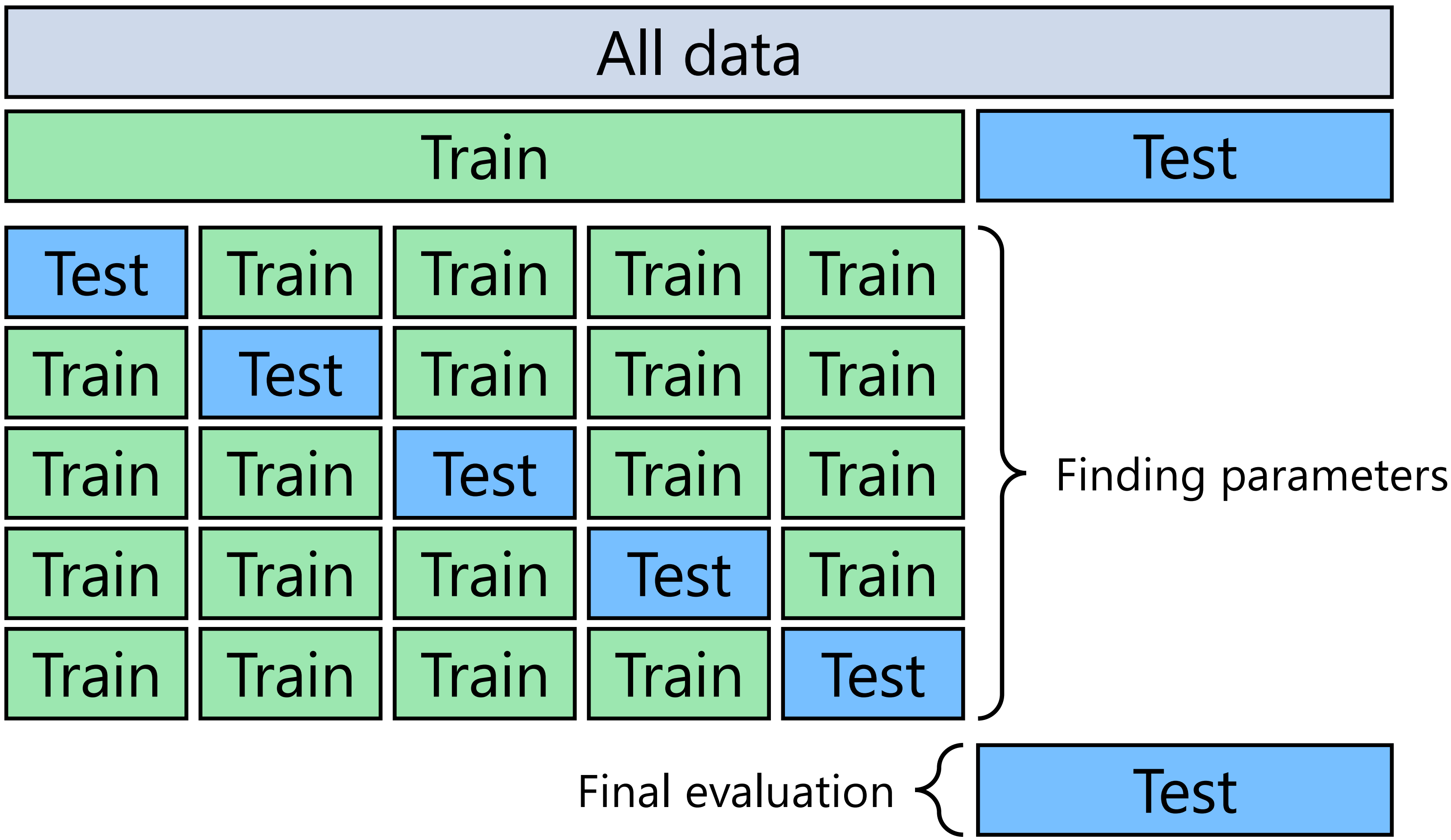
We can't just sample new training sets!
(unless there's **really** a lot of data available to us)

Note: Err_τ is by itself an estimate of Err,
but since it's just a single observation we
know nothing about its variance

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



Thank you!

Majid Sohrabi

msohrabi@hse.ru