Model Evaluation

Classification quality metrics, prediction error, cross-validation

Machine Learning and Data Mining, 2021

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LAMBDA • HSE

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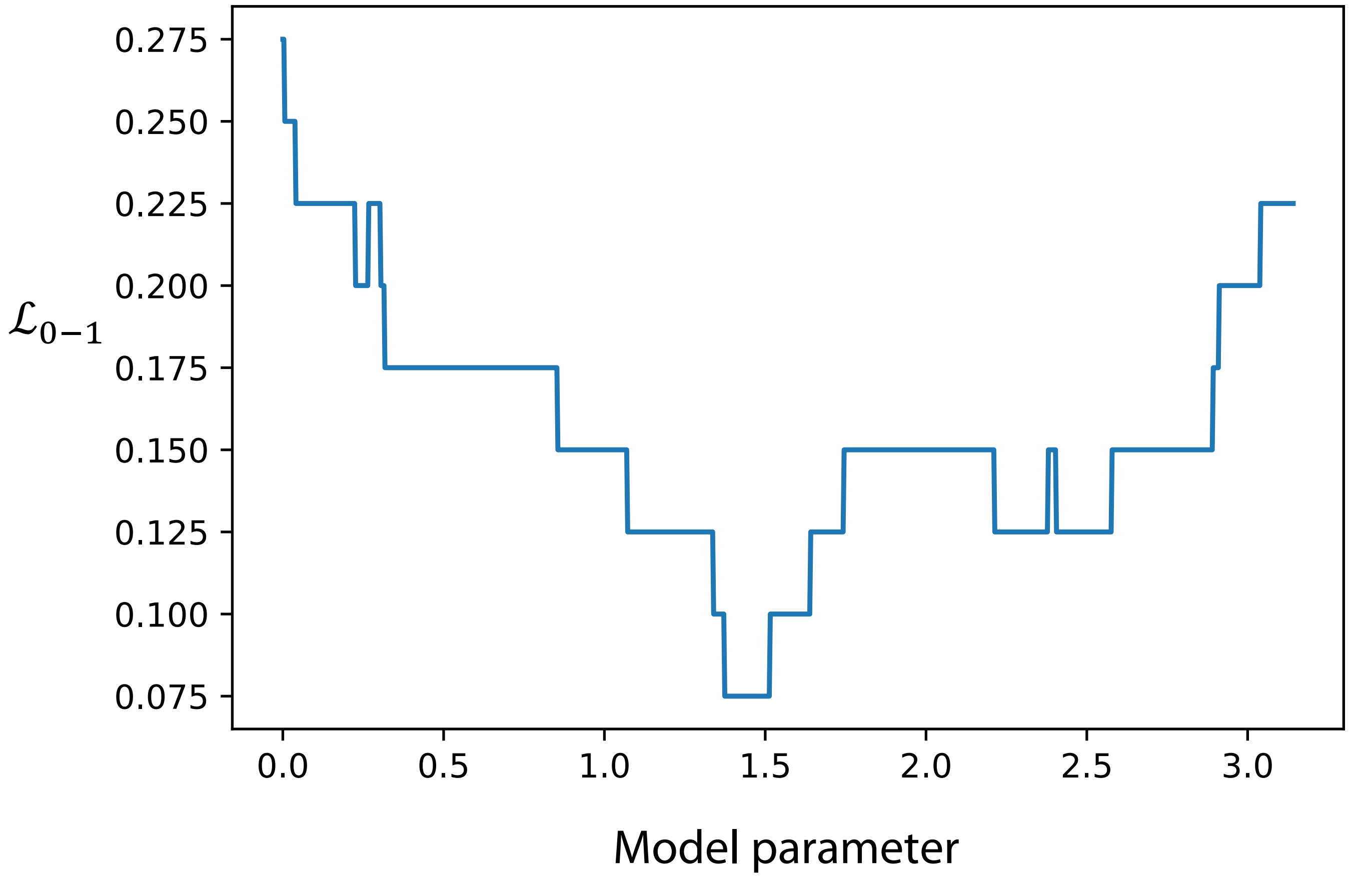
Classification quality metrics

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

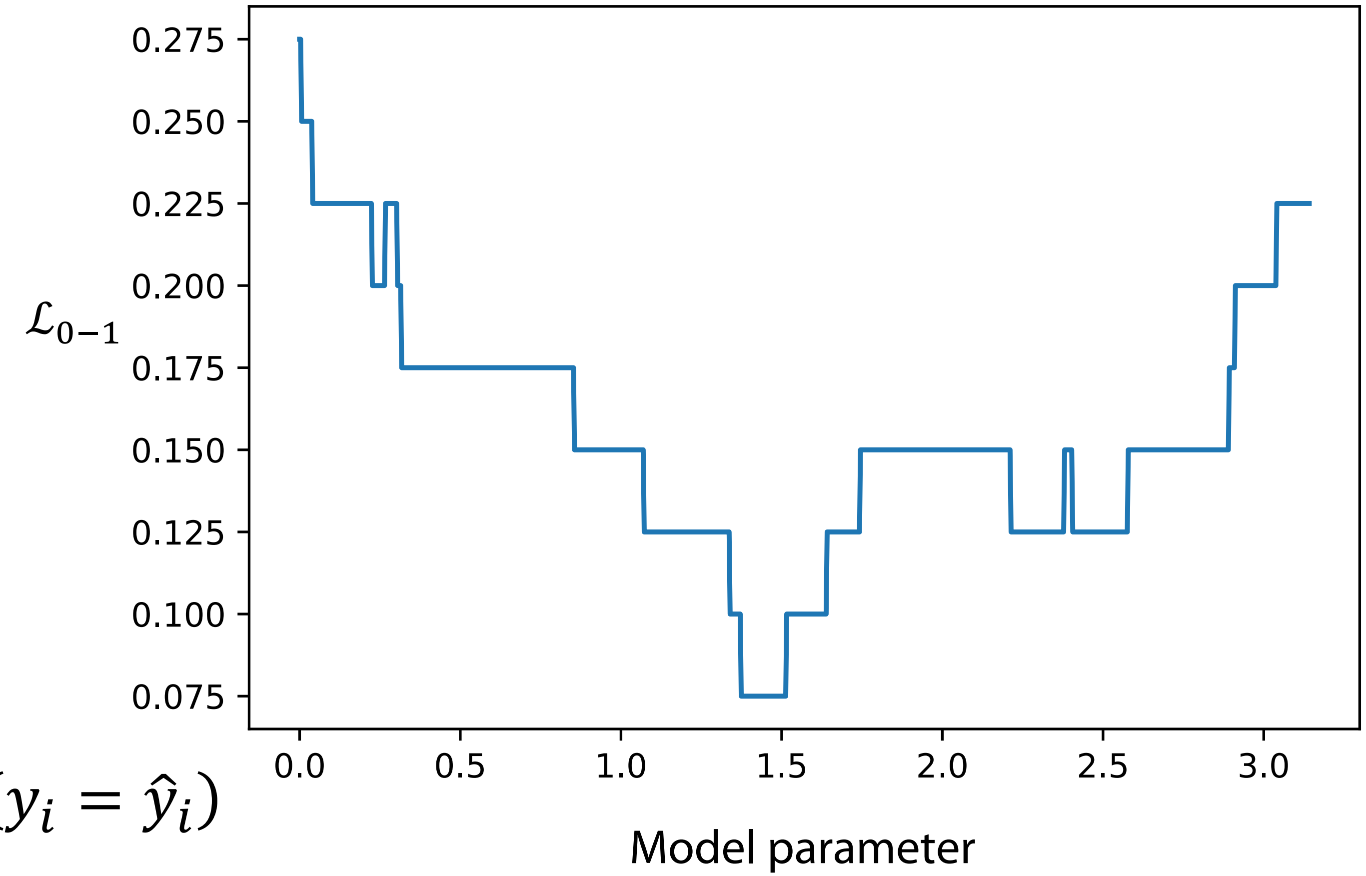
- Probability of an error (error rate):

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

- 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

Predicted class

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

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

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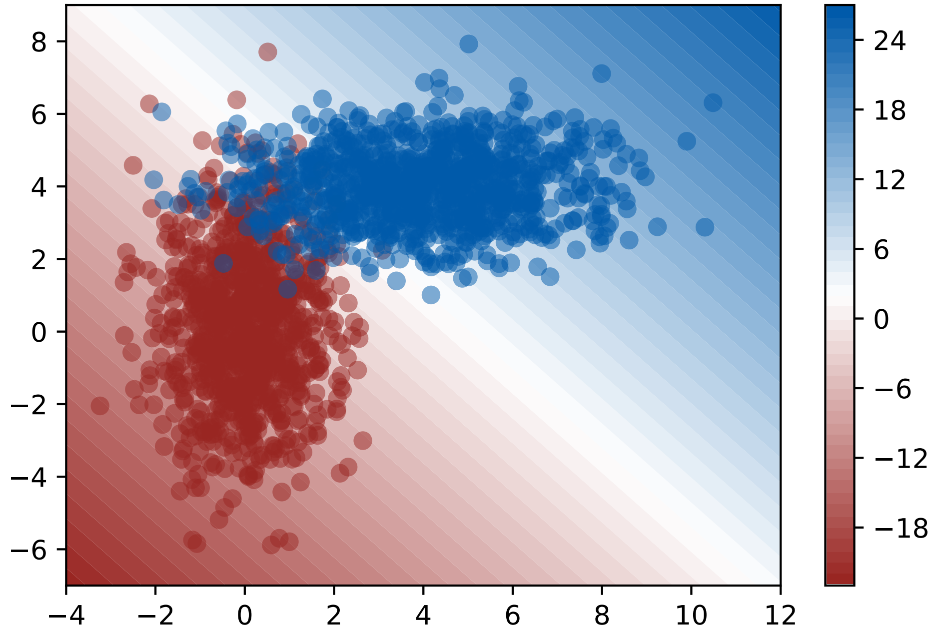
$$\text{Precision} = \frac{\mathrm{TP}}{\mathrm{TP+FP}}$$

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

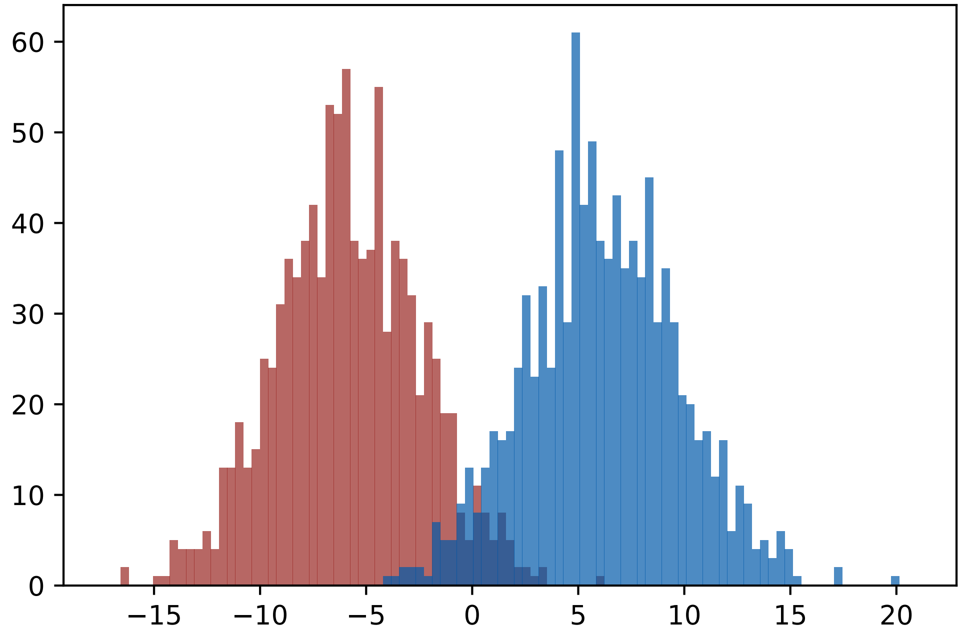
$$F_1\text{-score} = \frac{2 \cdot \mathrm{Precision} \cdot \mathrm{Recall}}{\mathrm{Precision} + \mathrm{Recall}}$$

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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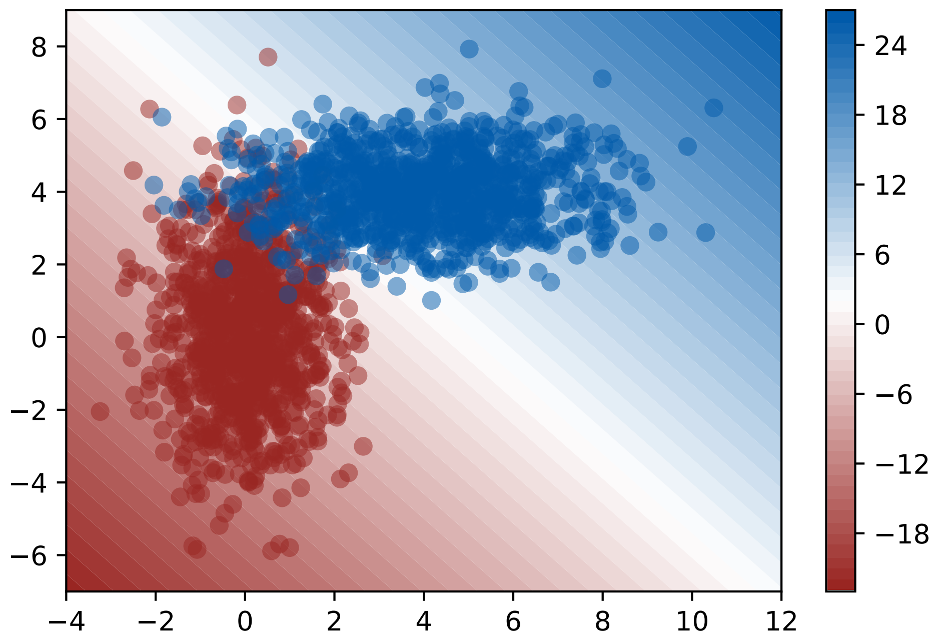

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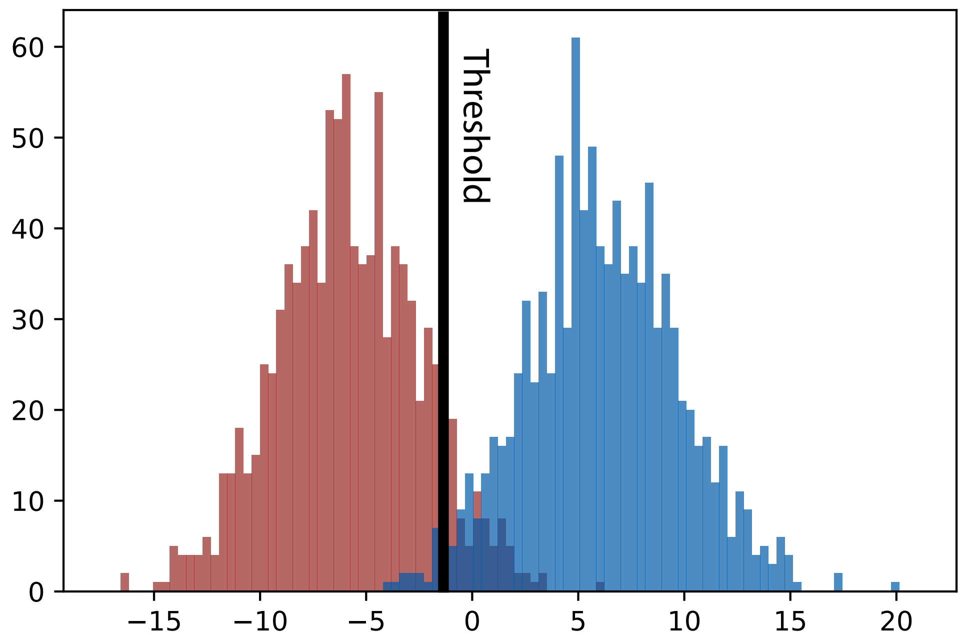
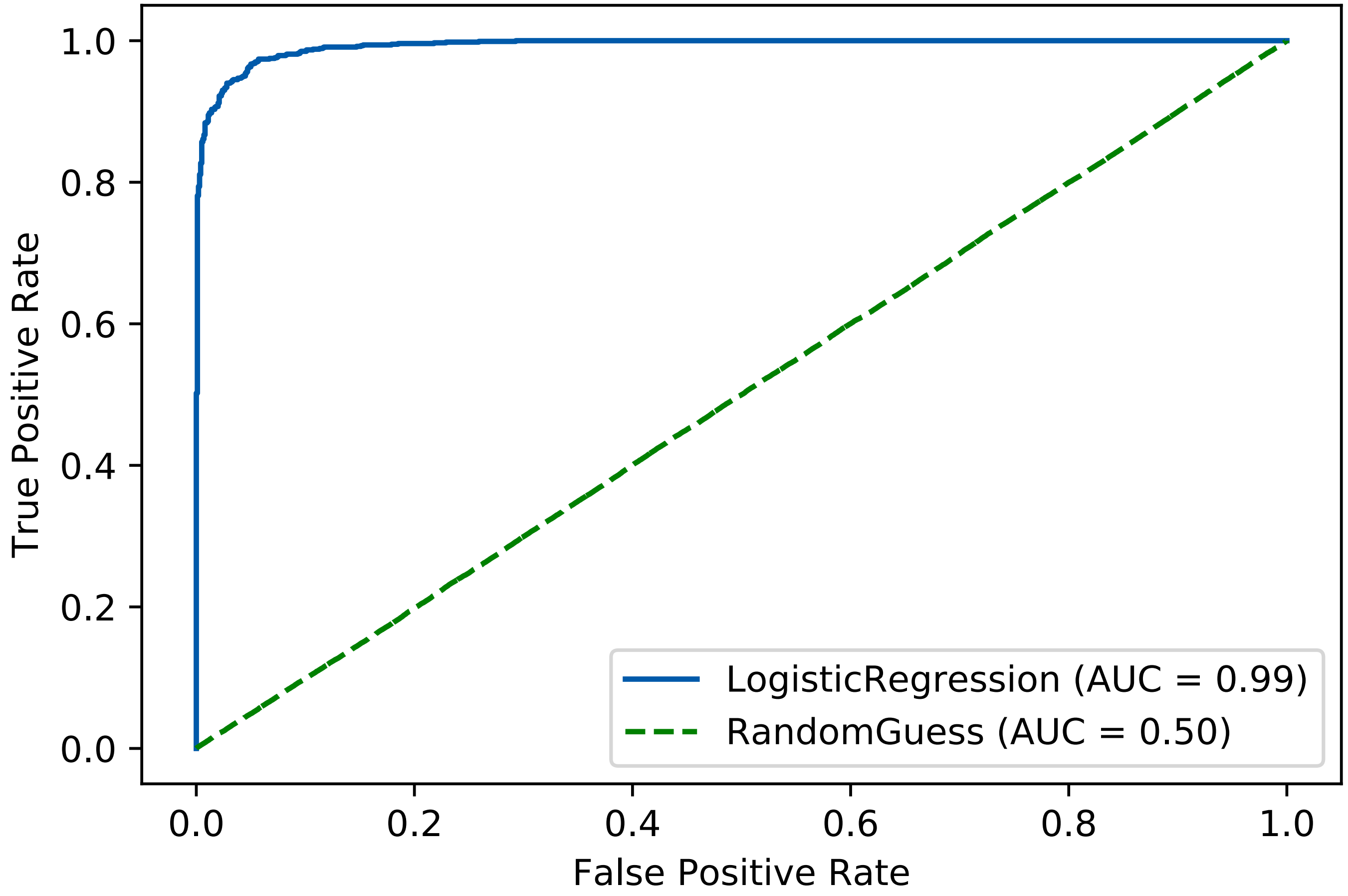


Scoring function values on data

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:

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

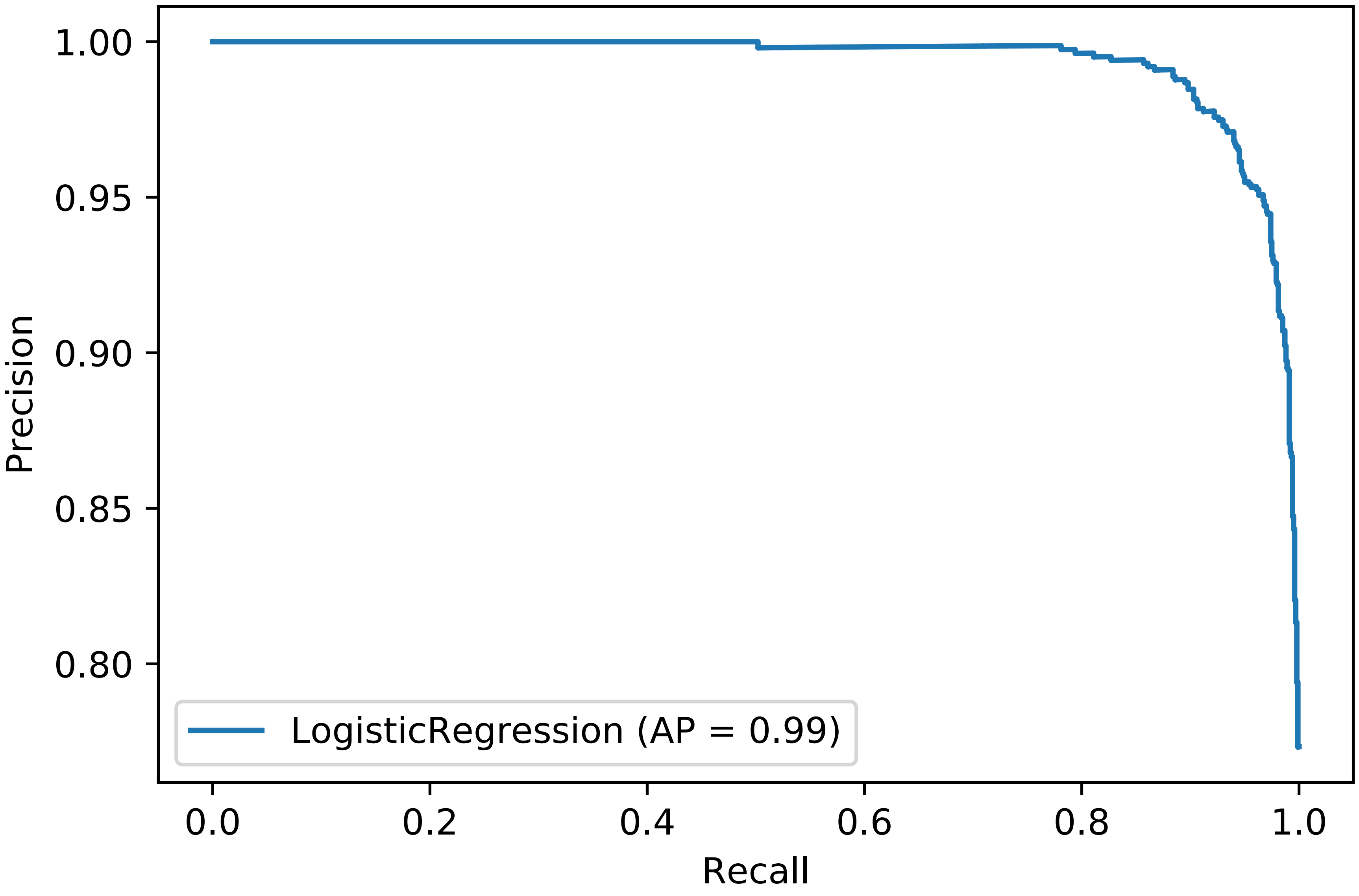
$\hat{f}(x)\colon\ \mathbb{R}^d \to \mathbb{R}$ – classifier scoring function

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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  - **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)
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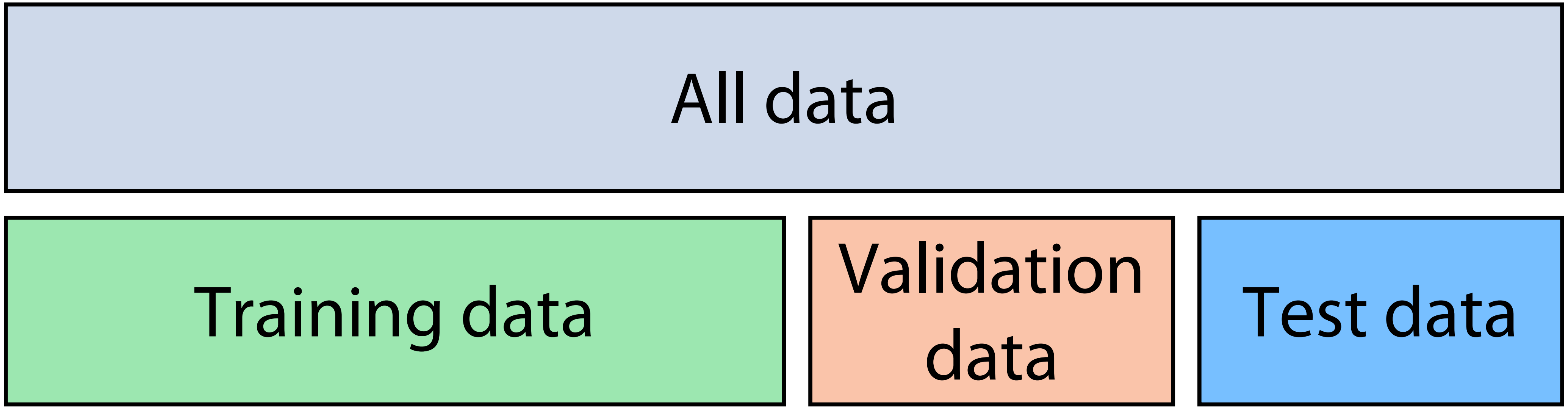

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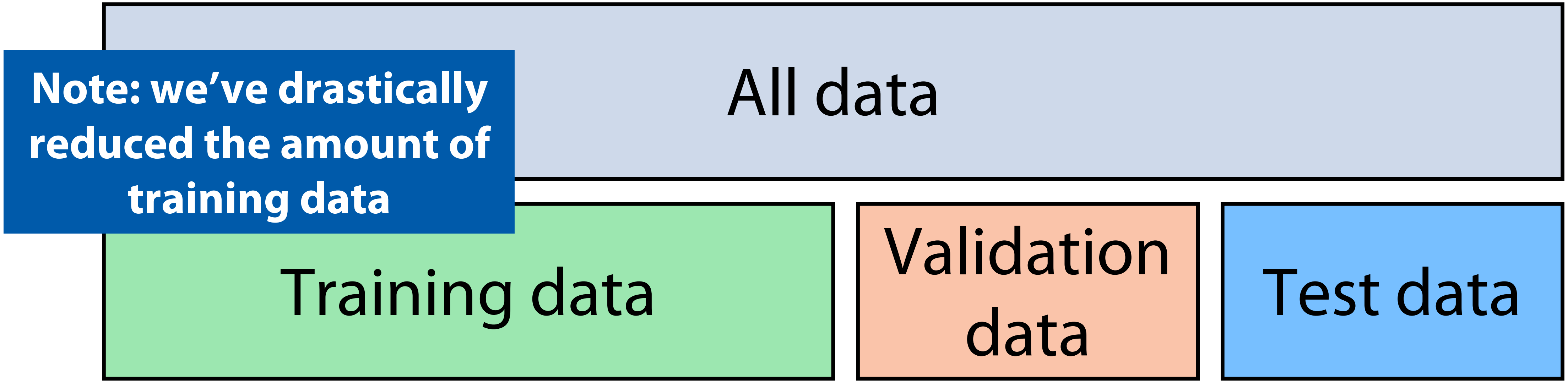


Cross-validation

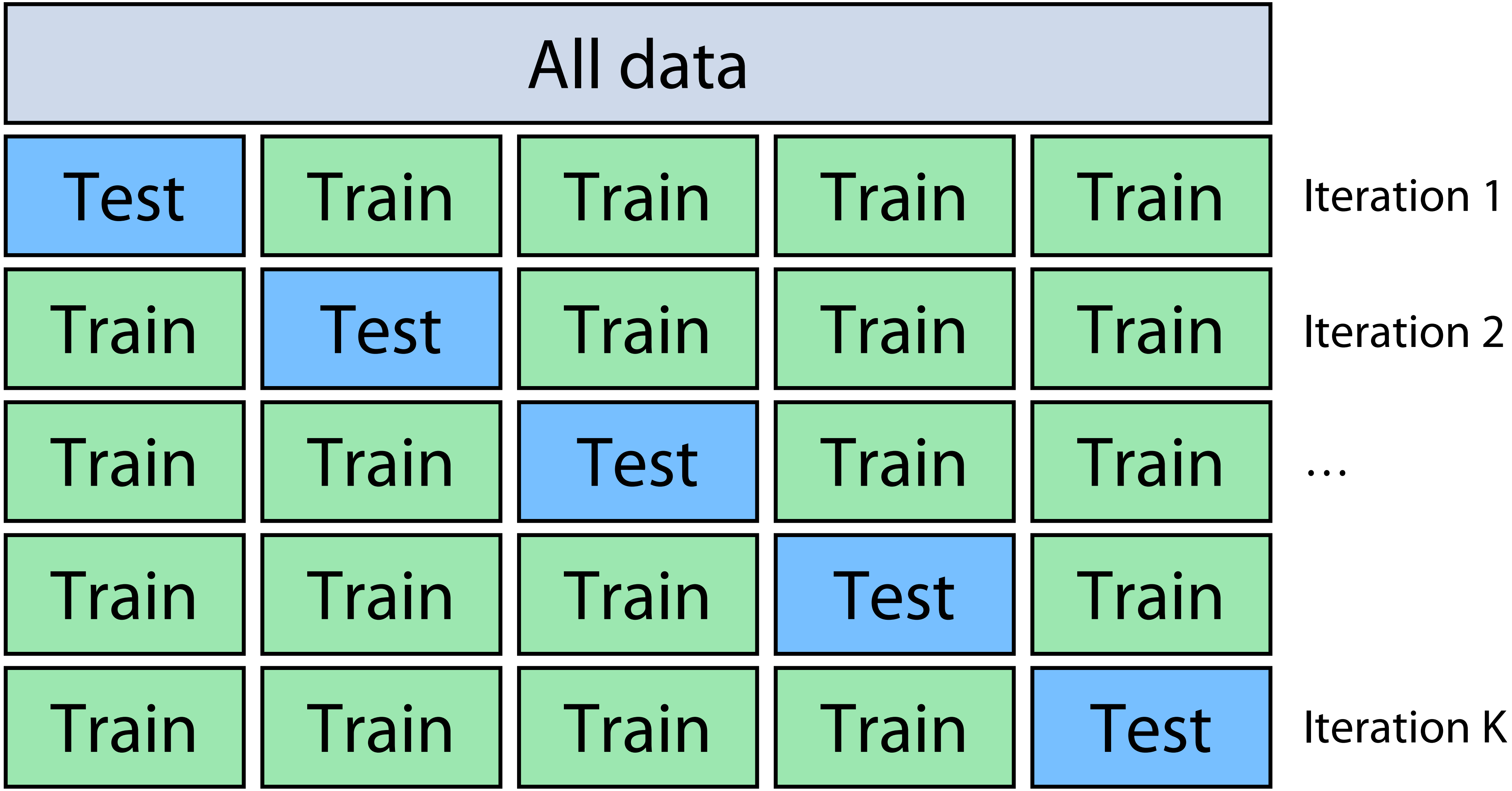
How to estimate the expected prediction error?

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

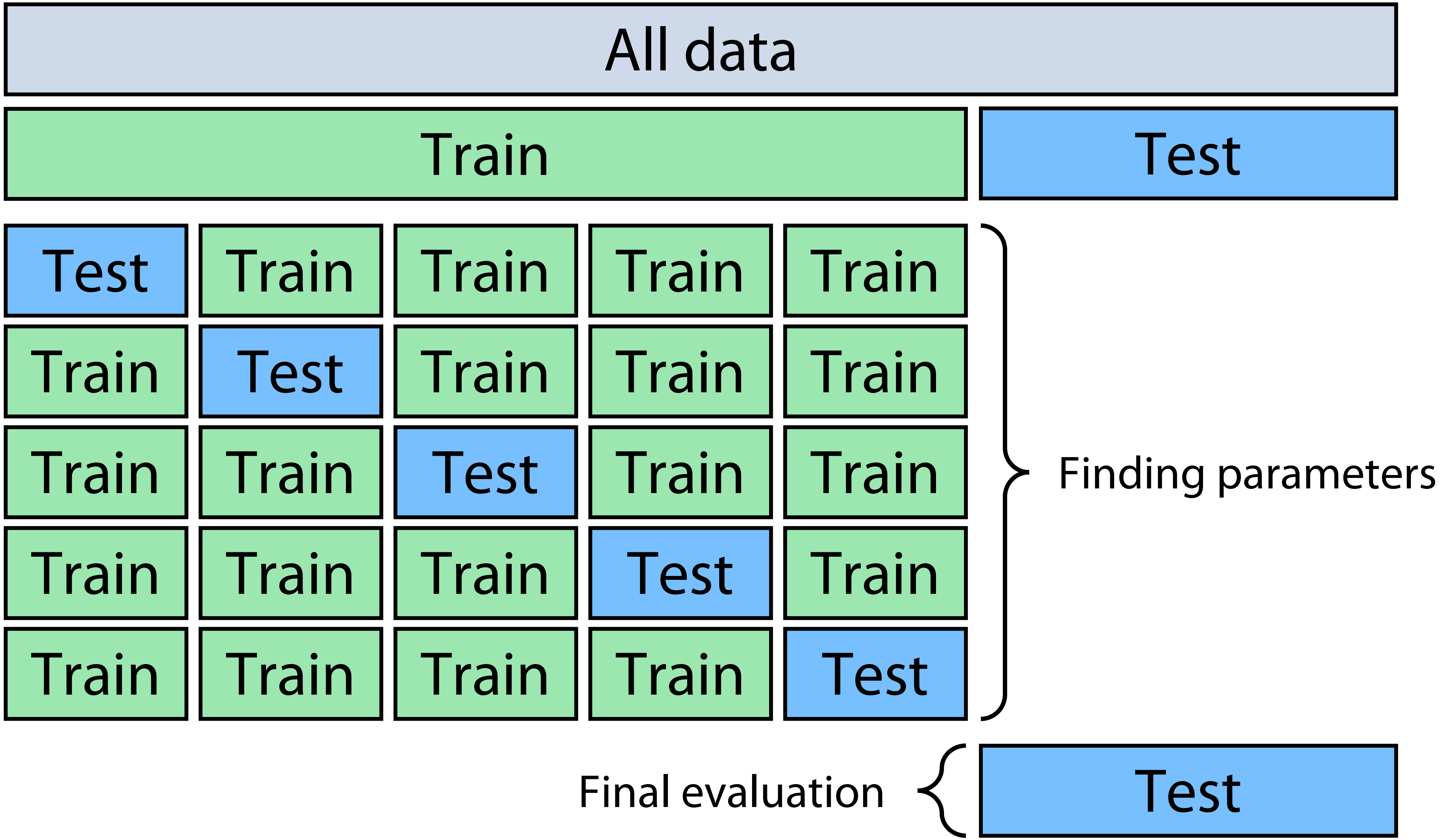
We can't just sample new training sets!
(unless there's **really** a lot of data available to us)

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



Hyperparameter tuning



K-fold cross-validation

- Note: K-fold CV estimate of the expected prediction error is unbiased
- Though the variance estimate is biased!

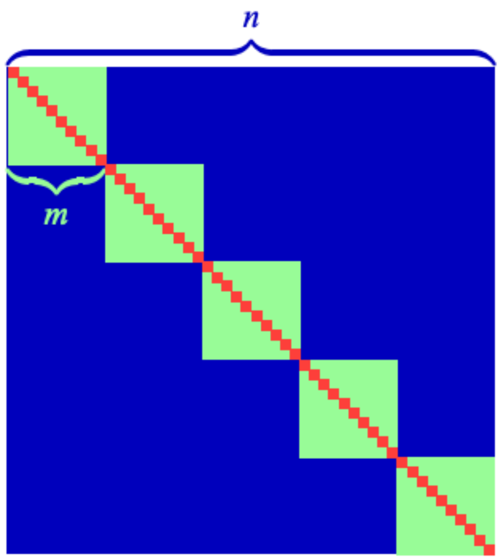


Figure 2: Structure of the covariance matrix.

- For more details see: https://www.jmlr.org/papers/v5/grandvalet04a.html

Thank you!

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