PSY9511: Seminar 4

Model selection, validation and testing

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23.09.24

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Outline

1. Loss functions and performance metrics
2. Strategies for model evaluation
    - Training and validation split
    - (Stratification)
    - (Leave-one-out cross-validation)
    - Cross-validation
    - Bootstrap
3. The theoretical basis for model evaluation
4. Strategies for model selection **and** evaluation
    - Train/validation/test split
    - Nested cross-validation
5. Assignment 4

Motivation

1. Reporting inflated modelling performance due to suboptimal testing practices
2. Using inappropriate measures for model performance (often accuracy)

Motivation

1. Reporting inflated modelling performance due to suboptimal testing practices
2. Using inappropriate measures for model performance (often accuracy)

↓

We believe that our models are better than they actually are, which yields false conclusions

Loss functions and performance metrics

Loss functions versus performance metrics

Commonalities

- Allows us to evaluate the performance of a model
- Typically on the form $f(y, \hat{y})$

Loss functions

- Tailored specifically for mathematical optimization of models

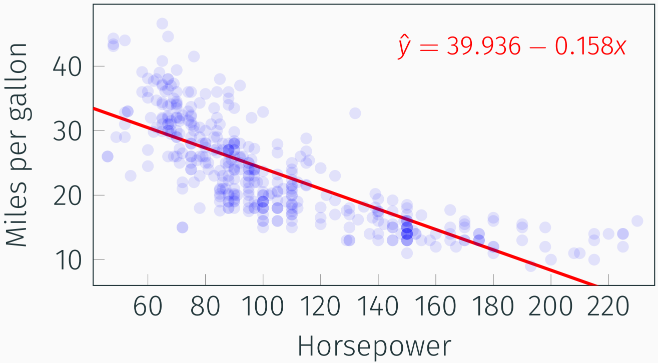
Performance metrics

- Tailored specifically for interpretation of model performance by humans

Loss functions and performance metrics

$$\text{mse}(y, \hat{y}) = \frac{1}{n}\sum_{i=0}^{n}(y_i - \hat{y}_i)^2$$

Loss functions and performance metrics



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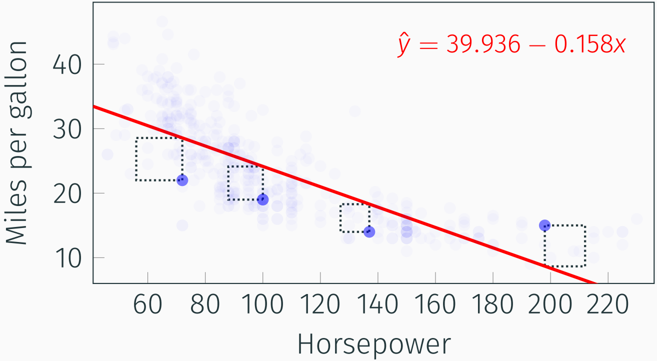

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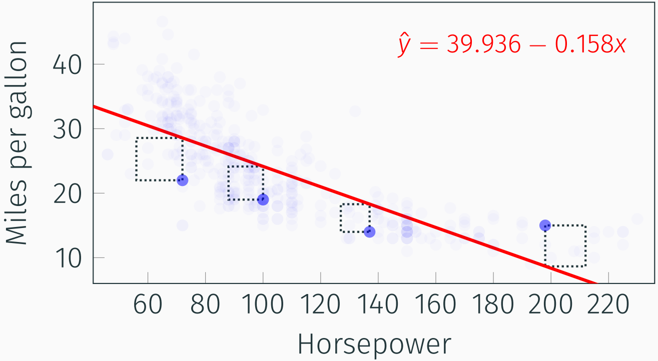
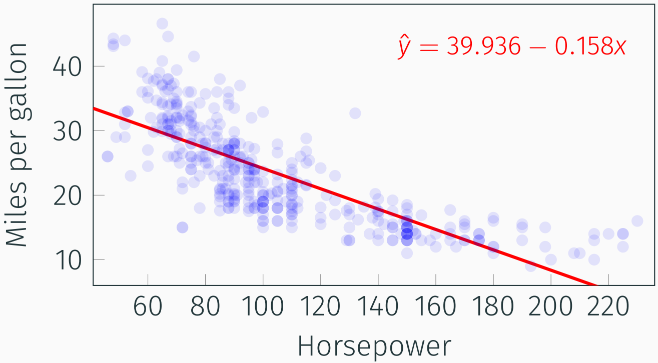


$$\mathrm{mse}(y, \hat{y}) = \frac{1}{n} \sum_{i=0}^{n} (y_i - \hat{y}_i)^2$$

$$= 23.94$$

Loss functions and performance metrics



$$\text{mse}(y, \hat{y}) = \frac{1}{n}\sum_{i=0}^{n}(y_i - \hat{y}_i)^2$$

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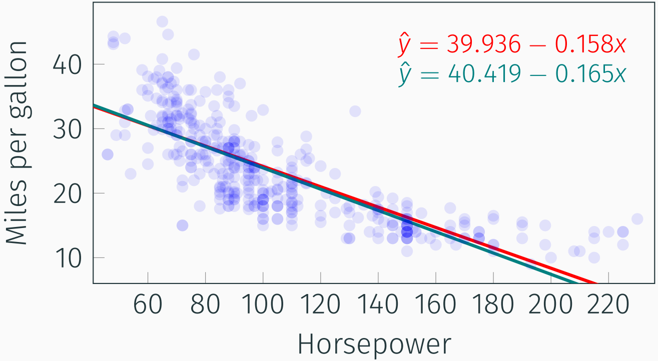
Loss functions and performance metrics



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Loss functions

- Different loss functions measures different properties of the model fit
- Optimizing for different loss functions will yield different parameter estimates

Tolerance-based accuracy:

A prediction is considered correct if it is within a predefined margin of error from the true value

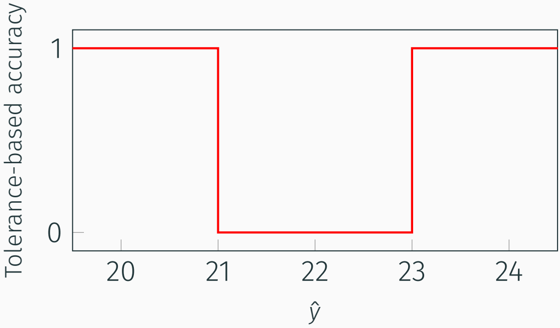
$$\text{accuracy*}(y, \hat{y}) = \begin{cases} 0 & \text{if } |y - \hat{y}| < \text{tol} \\ 1 & \textit{else} \end{cases}$$

Loss functions and performance metrics

mpg	horsepower
22	72

Loss functions and performance metrics

mpg	horsepower
22	72



Loss functions and performance metrics

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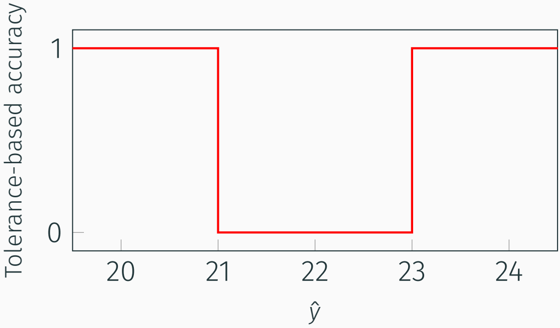

$$\hat{y} = \beta_0 + \beta_1 \times \text{horsepower}$$

Loss functions and performance metrics

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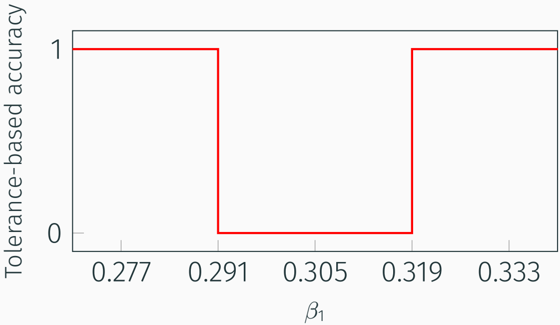

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Loss functions and performance metrics

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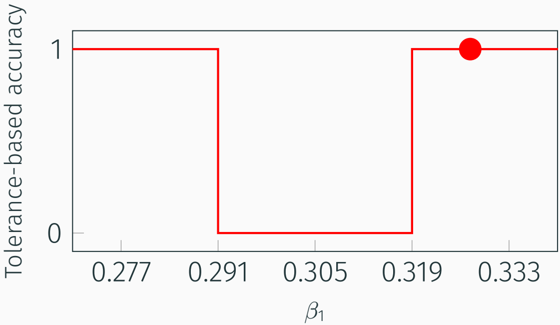

$$\hat{y} = 0 + 0.33 \times \text{horsepower}$$

mpg	horsepower
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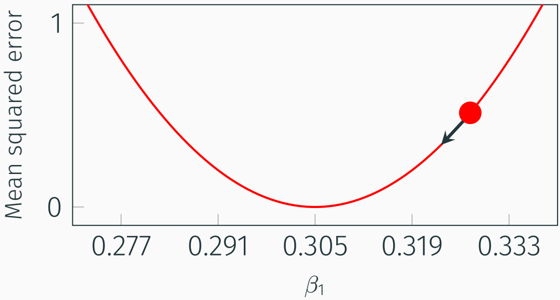


$$\hat{y} = 0 + 0.33 \times \text{horsepower}$$

Loss functions

- Different loss functions measures different properties of the model fit
- Optimizing for different loss functions will yield different parameter estimates
- Should be differentiable to allow for mathematical optimization

Loss functions and performance metrics

$$\text{mse}(y, \hat{y}) = \frac{1}{n} \sum_{i=0}^{n} (y_i - \hat{y}_i)^2$$

OR

$$\text{mae}(y, \hat{y}) = \frac{1}{n} \sum_{i=0}^{n} |y_i - \hat{y}_i|$$

Performance metrics: Regression

$$\frac{1}{n}\sum_{i=0}^{n}(y_i - \hat{y}_i)^2$$

Mean squared error (MSE)

- \+ Can be used as a loss function
- \+ Widely used
- ? Penalizes large errors
- ? Interpretation
- \- Depends on scale

Performance metrics: Regression

$$\sqrt{\frac{1}{n}\sum_{i=0}^{n}(y_i - \hat{y}_i)^2}$$

Root mean squared error (RMSE)

+ Can be used as a loss function
+ More interpretable than MSE, total loss $\approx$ individual errors

? Penalizes large errors

- Depends on scale

$$\frac{1}{n}\sum_{i=0}^{n}|y_i - \hat{y}_i|$$

Mean absolute error (MAE)

+ Can be used as a loss function (but not as suitable as MSE/RMSE)
+ More interpretable than MSE/RMSE, total loss = average error

? Many small errors are as bad as one large error

- Depends on scale

Performance metrics: Regression

$$\frac{\sum_{i=1}^{n}(y_i-\bar{y})(\hat{y}_i-\bar{\hat{y}})}{\sqrt{\sum_{i=1}^{n}(y_i-\bar{y})^2 \sum_{i=1}^{n}(\hat{y}_i-\bar{\hat{y}})^2}}$$

Pearson correlation coefficient (r)

+ Scale independent
? Only suitable for linear relationships
- Should not be used as a loss function
- Does not care about whether the predictions are close to the true values

Performance metrics: Regression

$$1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2}$$

Proportion of variance explained (r^2)

+ Scale independent
+ Interpretable

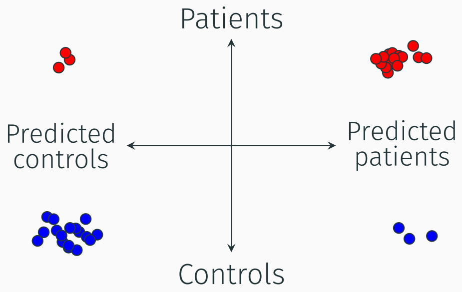
? Only suitable for linear relationships

\- Should not be used as a loss function

Performance metrics: Binary classification

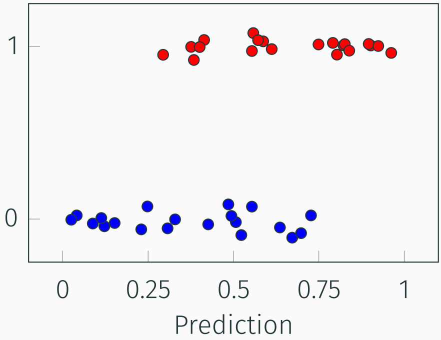
$$y \in \{Patients, Controls\}$$

Performance metrics: Binary classification



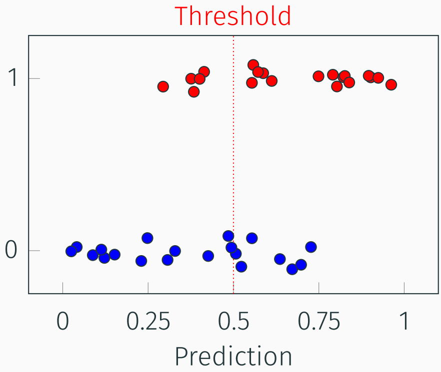
$$y \in \{Patients, Controls\}$$
$$\hat{y} \in \{Patients, Controls\}$$

Performance metrics: Binary classification



$$y \in \{0, 1\}$$
$$\hat{y} \in [0, 1]$$

Performance metrics: Binary classification



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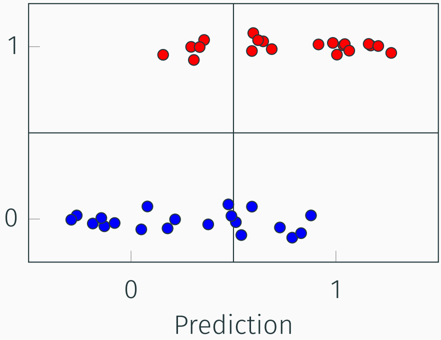
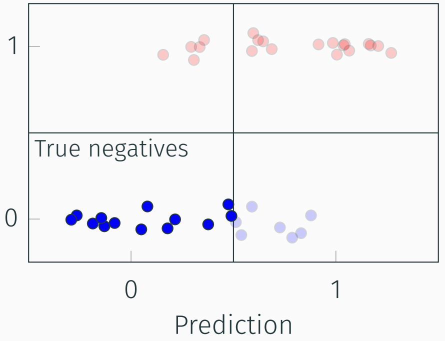
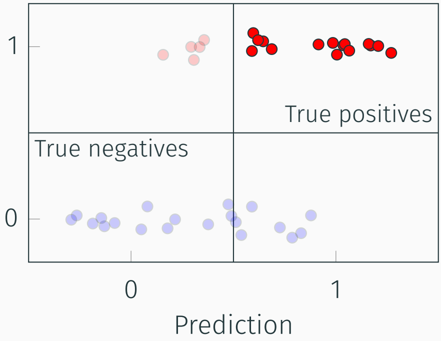


Performance metrics: Binary classification



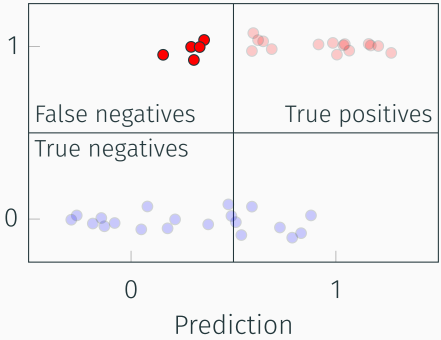
TN	

Performance metrics: Binary classification



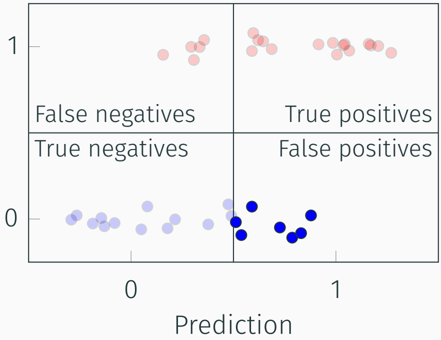
TN	
	TP

Performance metrics: Binary classification



TN	
FN	TP

Performance metrics: Binary classification



TN	FP
FN	TP

Performance metrics: Binary classification

Confusion matrix:

		Predicted 0	Predicted 1
True	0	TN	FP
	1	FN	TP

Performance metrics: Binary classification

Binary classification metrics:

- Many metrics rely on thresholding the predictions to obtain binary predictions.
- Although not a metric per se, the confusion matrix is a very useful tool to understand model behaviour, and should **always** be looked at (and preferably reported).

Performance metrics: Binary classification

$$-(y \log(\hat{y}) + (1 - y) \log(1 - \hat{y}))$$

Logloss

+ Does not rely on thresholding
+ Can be used as a loss function (and very often is)
- Not very interpretable

Performance metrics: Binary classification

$$\frac{TP+TN}{TP+TN+FP+FN}$$

Accuracy

+ Interpretable
- Does not account for different costs of misclassification

Performance metrics: Binary classification

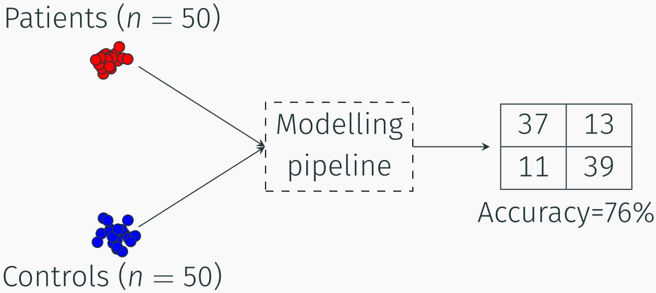
$$\frac{TP+TN}{TP+TN+FP+FN}$$

Accuracy

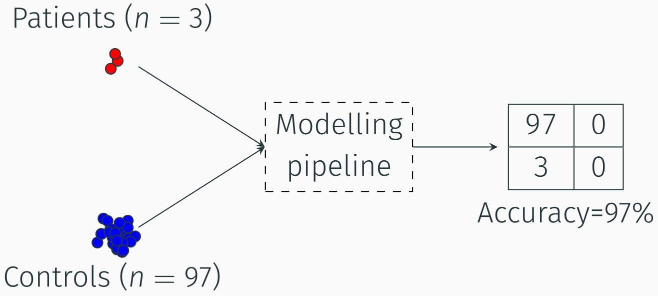
+ Interpretable
- Does not account for different costs of misclassification

What is the major pitfall of accuracy as am metric?

Performance metrics: Binary classification



Performance metrics: Binary classification



Performance metrics: Binary classification

$$\frac{TP+TN}{TP+TN+FP+FN}$$

Accuracy

+ Interpretable
- Does not account for different costs of misclassification
- Does not handle imbalanced classes

Performance metrics: Binary classification

$$\frac{TP}{TP+FN}$$

True positive rate (sensitivity)

- \+ Interpretable, calculates the proportion of cases that are detected
- \+ Useful when the cost of false negatives is high (Population-wide screening for severe disease)
- \- Very one-sided (should be used alongside other metrics)

$$\frac{TN}{TN+FP}$$

True negative rate (specificity)

+ Interpretable, calculates the proportion of controls that are detected
+ Useful when the cost of false positives is high (Intrusive treatment of rare and mild conditions)
- Very one-sided (should be used alongside other metrics)

$$\frac{TP}{TP+FP}$$

Positive predictive value (PPV, precision)

+ Interpretable, calculates the proportion of predicted cases that are actually cases
+ Useful when the cost of false positives is high (Selection of participants for expensive clinical trials)
- Very one-sided (should be used alongside other metrics)

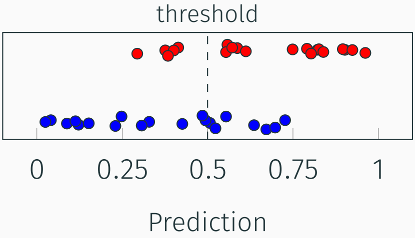
Performance metrics: Binary classification

$$\frac{\frac{TP}{TP+FN}+\frac{TN}{TN+FP}}{2}$$

Balanced accuracy

- + Interpretable, behaves similarly to regular accuracy.
- + Takes into account imbalanced classes

Classification metrics: Area under the curve



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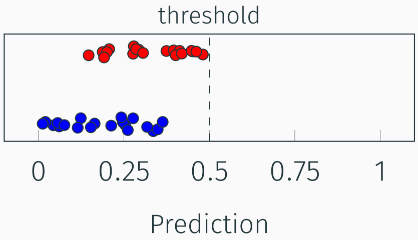

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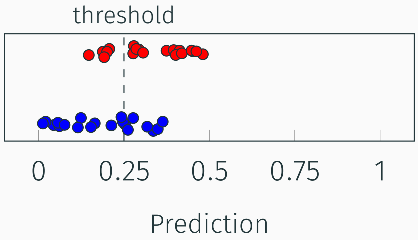

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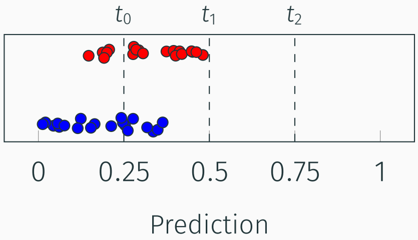

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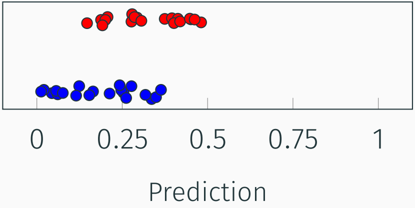
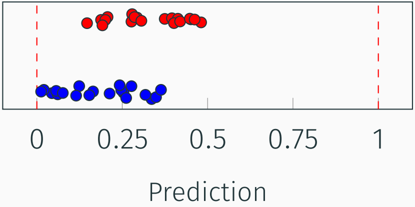


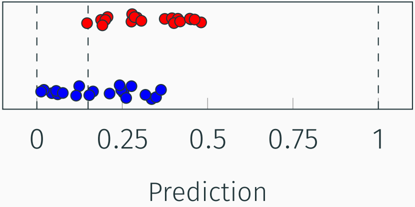
threshold	TPR	FPR

Classification metrics: Area under the curve



threshold	TPR	FPR
0	1	1
1	0	0

Classification metrics: Area under the curve



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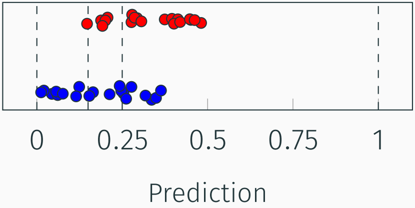
Classification metrics: Area under the curve



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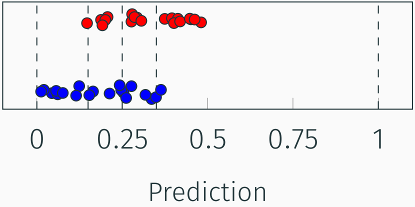

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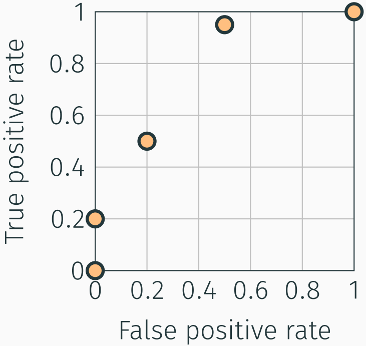

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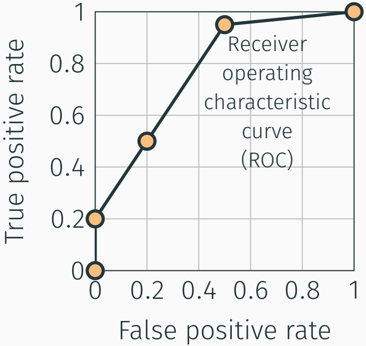

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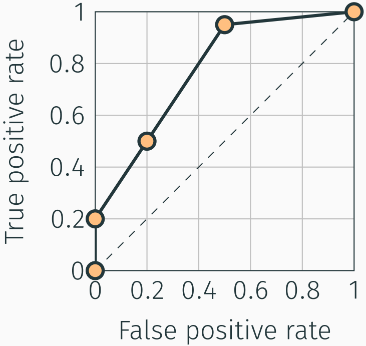

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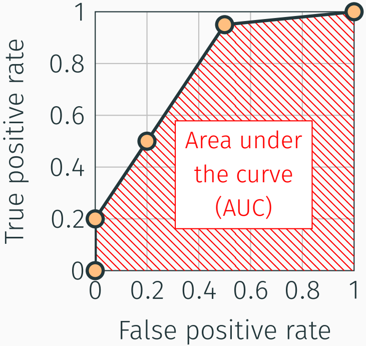

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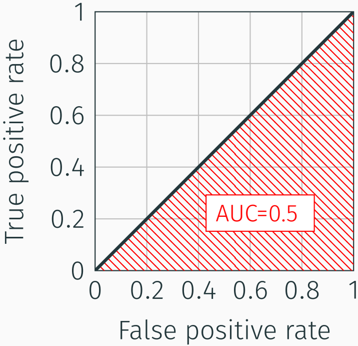

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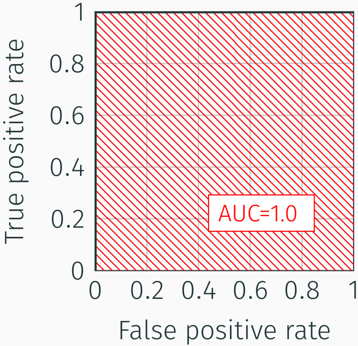

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Area under the receiver operating characteristic curve (AUC/AUROC)

- A performance metric that does not rely on a correct classification threshold
- Measures whether the predictions are ranked correctly (e.g. patients have a higher prediction than controls)
- **Handles class imbalance (relatively well)** and is commonly reported in the literature

Loss functions and performance metrics: Summary

Performance metrics and loss functions measure the performance of a predictive model

- There is a range of alternatives that can be used, each capturing a different aspect of a model's performance
- It is good practice to report more than one metric
- For regression, **MSE** is a common loss function with nice mathematical properties and **MAE** is an intuitive performance metric
- For classification, **log-loss** is the most common loss function for probabilistic classifiers and **AUC** is a widely used metric that is easy to interpret, handles class imbalance (to some degree), and is not reliant on the choice of classification threshold

Loss functions and performance metrics: Summary

http://localhost:8888/notebooks/notebooks%2FClassification%20metrics.ipynb

Strategies for model evaluation

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Model evaluation: Rationale

Statistical inference:

Goal: In-sample quantification

Predictive modelling:

Goal: Out-of-sample generalization

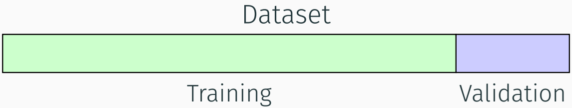
Model evaluation: Rationale

How can we test how good our model is on **unseen data** and **be certain that this predictive performance holds if we present even more new data**

Model evaluation: Validation set

Dataset

Model evaluation: Validation set



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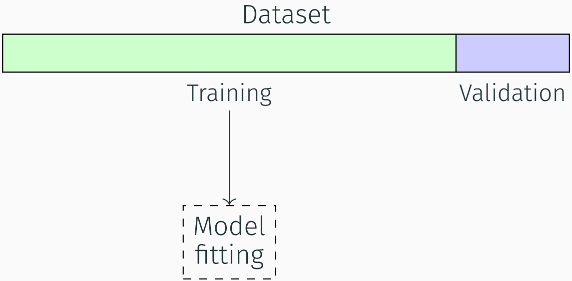

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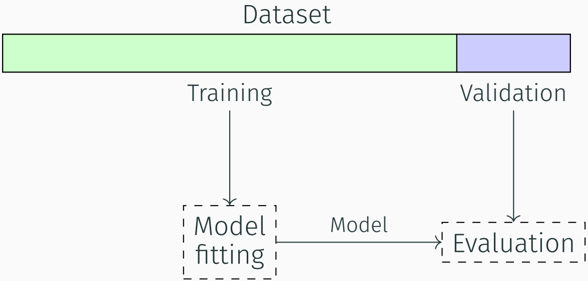

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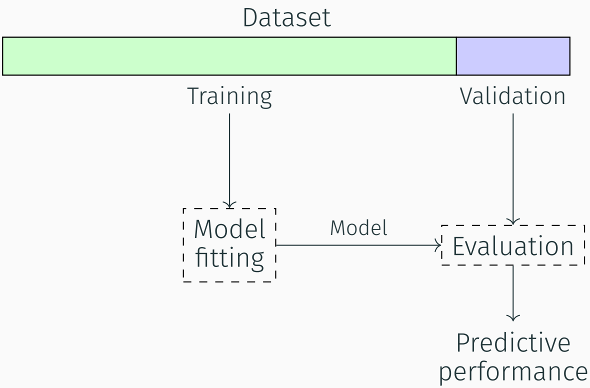
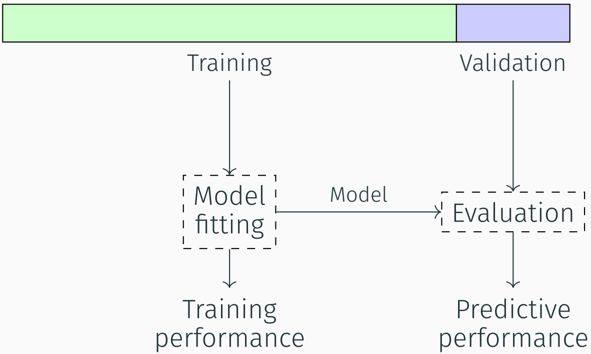


Model evaluation: Validation set

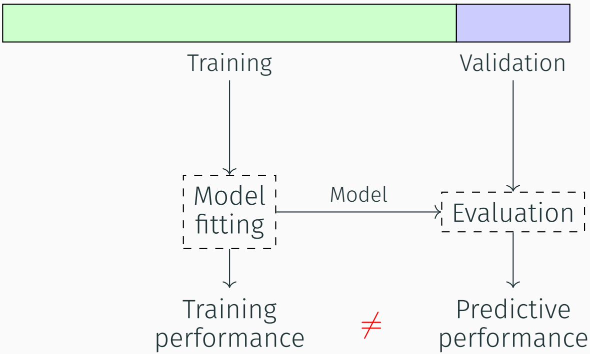
In the validation set approach we split the dataset into two subsets (commonly ∼80%/20%), use the first for training the model and the second to test its performance.

+ Accurate estimate of out-of-sample error
+ Simple
- Variable results depending on the exact split
- Only uses a subset of data for training models
- Gives a point estimate of the error, without confidence intervals

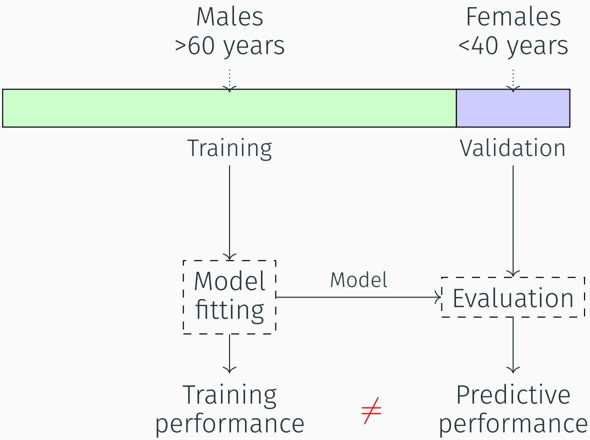
Model evaluation: Validation set



Model evaluation: Validation set



Model evaluation: Validation set



Model evaluation: Stratification

<u>Stratification:</u>

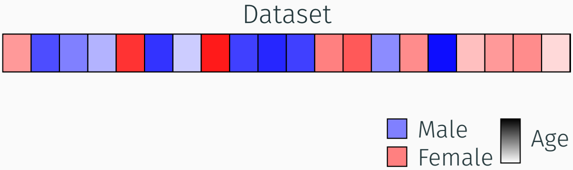
Ensuring all folds of the dataset are similar with respect to some given characteristics.

Model evaluation: Stratification

Dataset

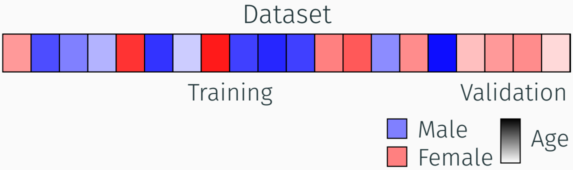
In[1]:
```
df = ...
```

Model evaluation: Stratification



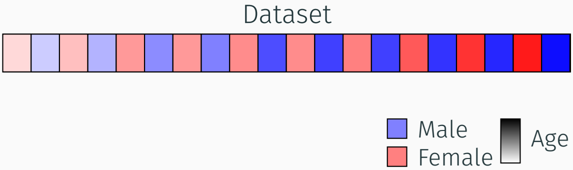
In[1]:
```
df = ...
```

Model evaluation: Stratification



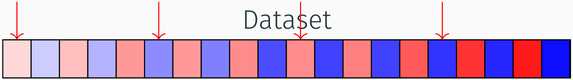
In[1]:
```python
df = ...

train = df.iloc[:int(len(df) * 0.8)]
validation = df.iloc[int(len(df) * 0.8):]
```

Model evaluation: Stratification



In[1]:
```
df = ...
df = df.sort_values(['sex', 'age'])
```

Model evaluation: Stratification



In[1]:

```
df = ...
df = df.sort_values(['sex', 'age'])

df['fold'] = np.arange(len(df)) % (1 / 0.2)
train = df[df['fold'] != 0]
val = df[df['fold'] == 0]
```

Model evaluation: Stratification

In[1]:
```
df = ...
df = df.sort_values(['sex', 'age'])

df['fold'] = np.arange(len(df)) % (1 / 0.2)
train = df[df['fold'] != 0]
val = df[df['fold'] == 0]
```

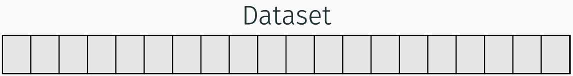
<u>Stratification:</u>
Ensuring all folds of the dataset are similar with respect to some given characteristics.

- Helps alleviate the risk of training performance $\gg$ validation performance
- **Always** stratify on target variable first
- Also good idea to stratify on other core characteristics, e.g. sex and age

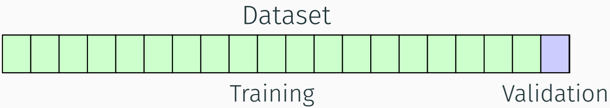
In[1]:
```
from sklearn.model_selection import  train_test_split
```

```
library(splitstackshape)
stratified(data, columns, split)
```

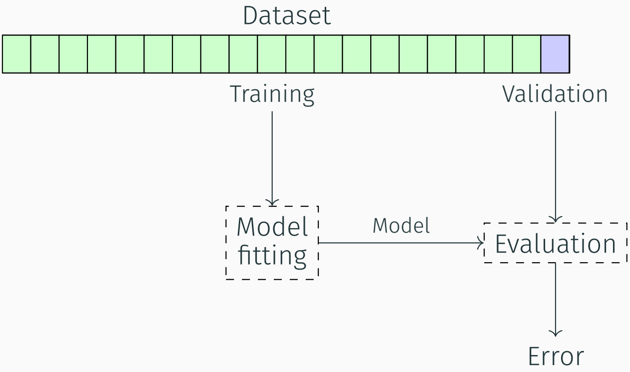
Model evaluation: Leave-one-out cross-validation



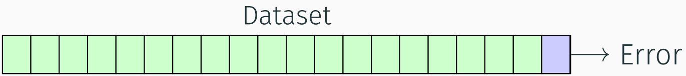
Model evaluation: Leave-one-out cross-validation



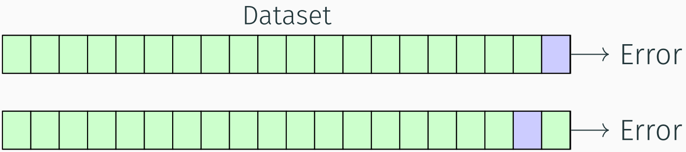
Model evaluation: Leave-one-out cross-validation



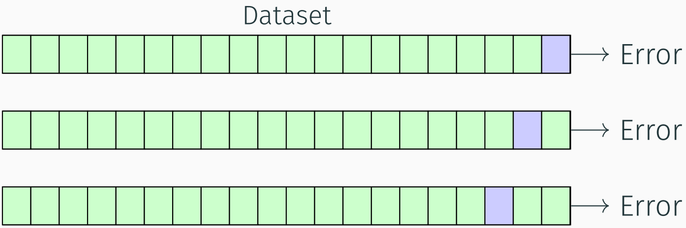
Model evaluation: Leave-one-out cross-validation



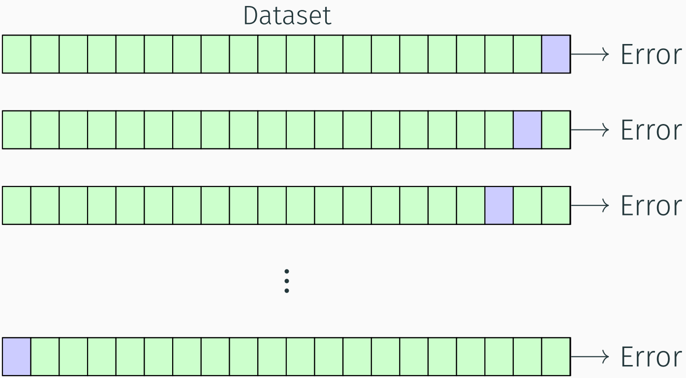
Model evaluation: Leave-one-out cross-validation



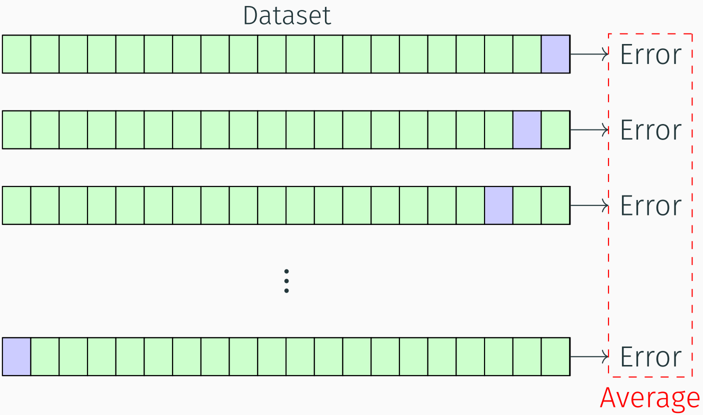
Model evaluation: Leave-one-out cross-validation



Model evaluation: Leave-one-out cross-validation



Model evaluation: Leave-one-out cross-validation



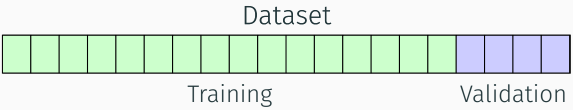
Model evaluation: Leave-one-out cross-validation

Fits n models for n datapoints, each time leaving a single datapoint out for testing.

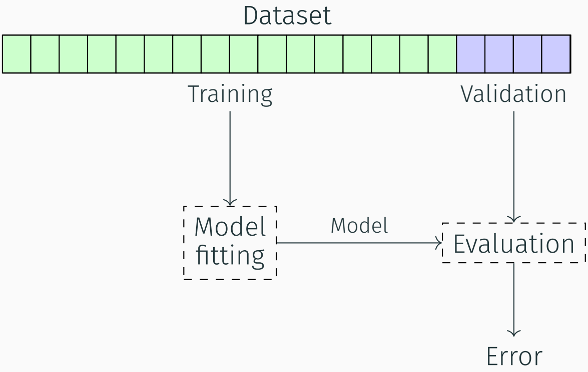
+ Uses all data to train models
+ Not dependent on arbitrary data splits
+ Unbiased (with regards to the full dataset)
- Computationally expensive
- Effectively gives a point estimate of the error
- All models are going to be trained on $> 99\%$ overlapping data $\rightarrow$ highly correlated

Model evaluation: Cross-validation

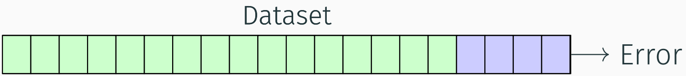
Model evaluation: Cross-validation



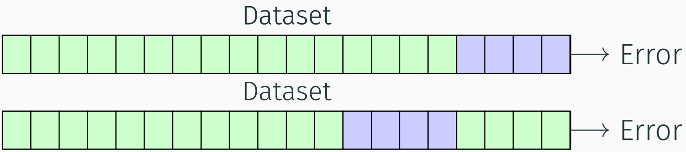
Model evaluation: Cross-validation



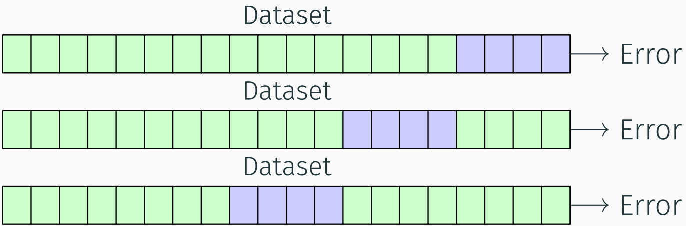
Model evaluation: Cross-validation



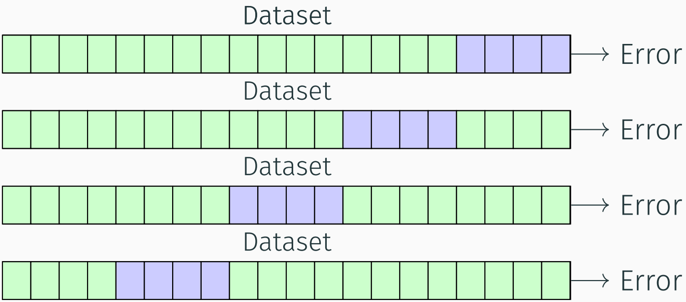
Model evaluation: Cross-validation



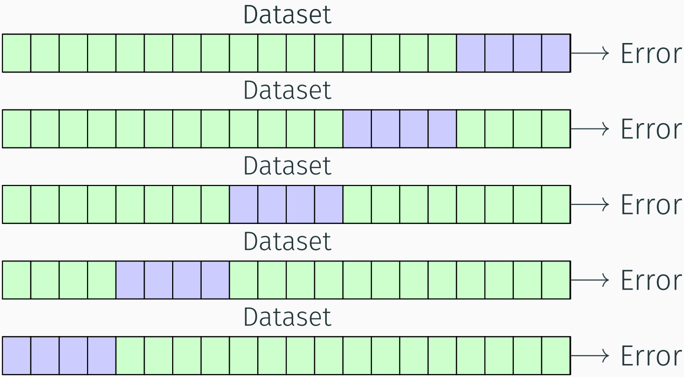
Model evaluation: Cross-validation



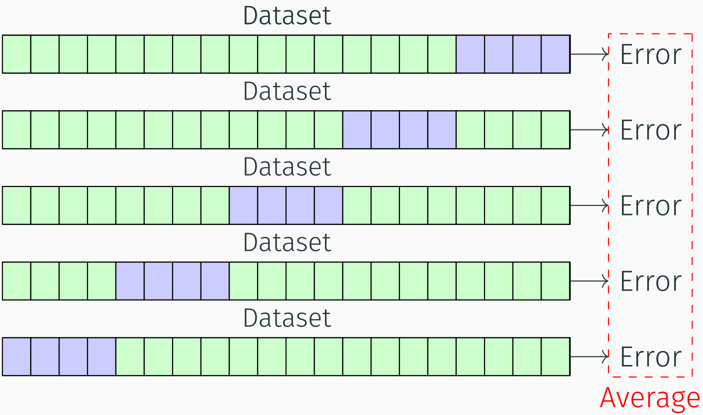
Model evaluation: Cross-validation



Model evaluation: Cross-validation



Model evaluation: Cross-validation



Model evaluation: Cross-validation

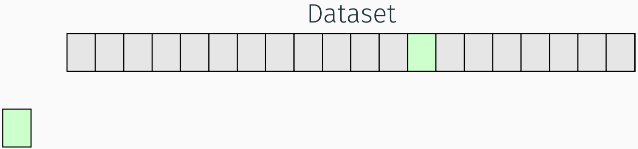
Fits k (usually $k \in \{5, 10\}$) models for $n > k$ datapoints, each leaving n/k datapoints for out-of-sample testing.

- \+ Uses all data to train models
- \+ Yields multiple estimates of out-of-sample error
- \- Different choices of k (and exact splits) yields different results
- \- **No longer a single model from which information (e.g. parameter estimates and p-values) can be derived**

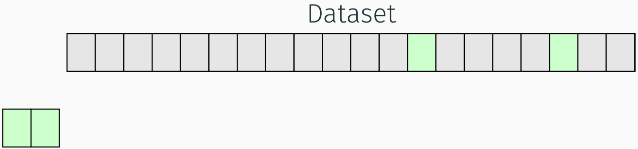
Model evaluation: Bootstrapping

Dataset

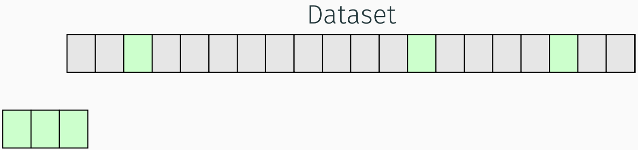
Model evaluation: Bootstrapping



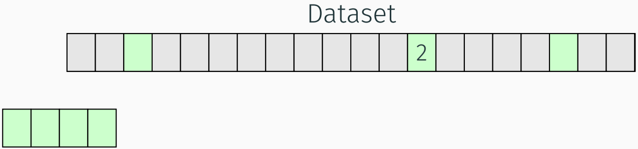
Model evaluation: Bootstrapping



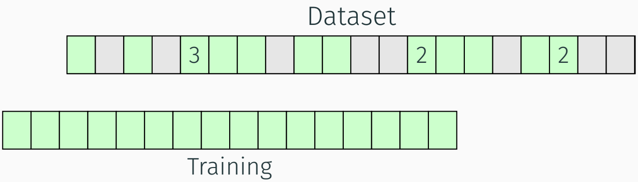
Model evaluation: Bootstrapping



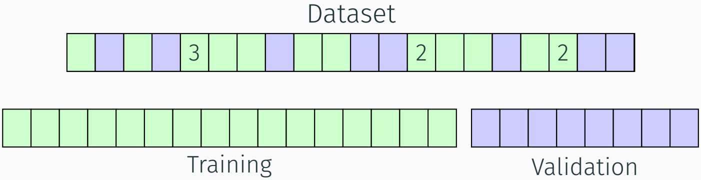
Model evaluation: Bootstrapping



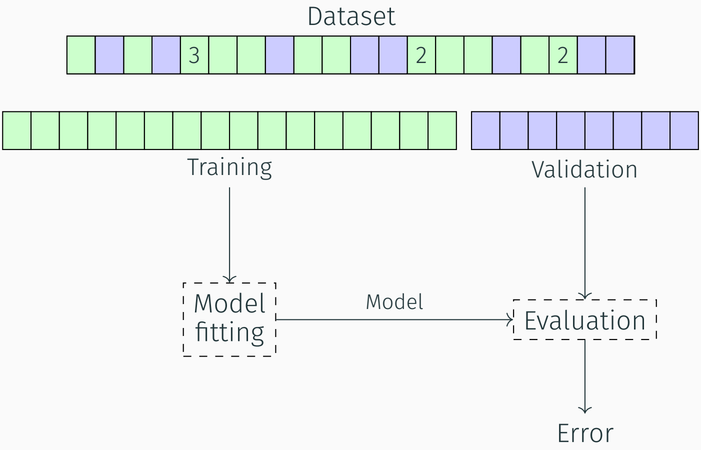
Model evaluation: Bootstrapping



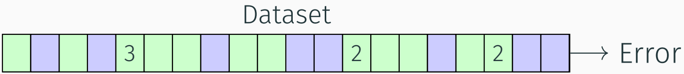
Model evaluation: Bootstrapping



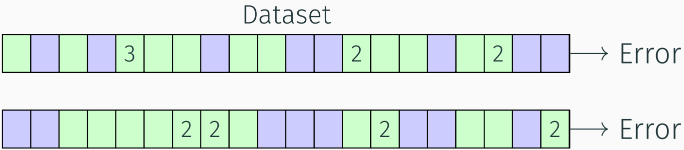
Model evaluation: Bootstrapping

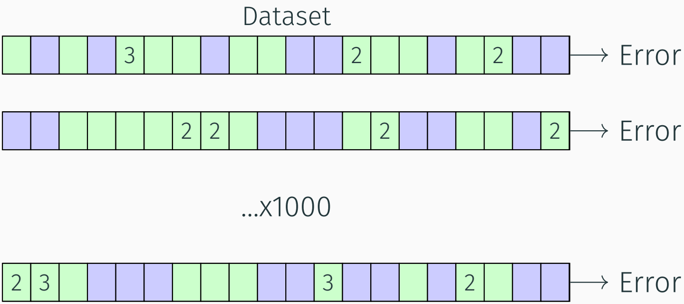


Model evaluation: Bootstrapping

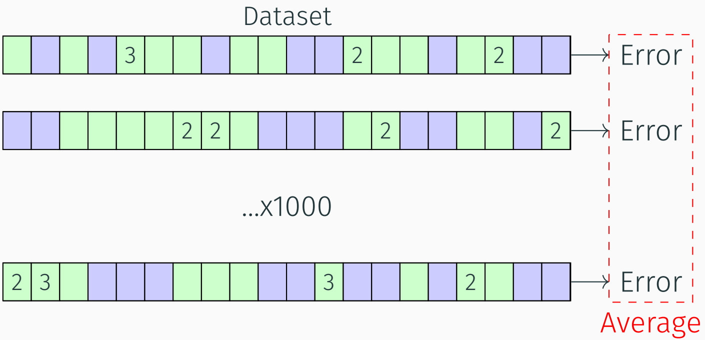


Model evaluation: Bootstrapping




Dataset
3
2
2
Error
2
2
2
2
Error
...x1000
2
3
3
2
Error

Model evaluation: Bootstrapping

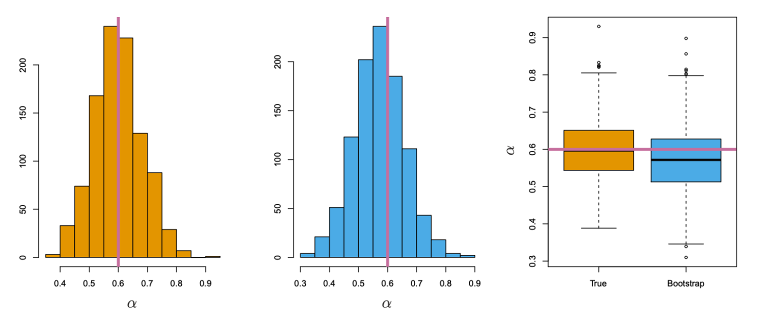


Model evaluation: Bootstrapping

Fits b models with m datapoints (typically $m < n$), sampled from the original dataset **with replacement**.

- \+ Uses all data to train models
- \+ Provides a dense distribution of model performances
- \+ **Versatile: Can be used for other things, e.g. getting a confidence interval for model parameters**
- \- Different choices of b (and exact splits) yields different results

Model evaluation: Bootstrapping

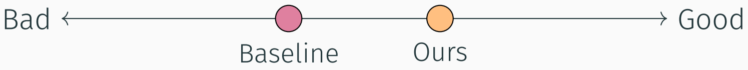


Model evaluation: Comparison

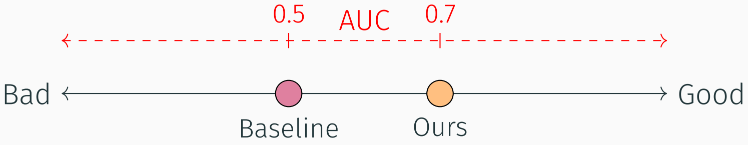
Why do we want to evaluate our model?

1. We want to show that our model is better than random guessing
2. We want to show that our model is better than another model

Model evaluation: Comparison



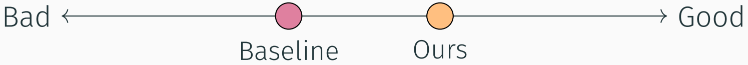
Model evaluation: Comparison



Model evaluation: Comparison

http://localhost:8888/notebooks/notebooks%2FModel%20variability.ipynb

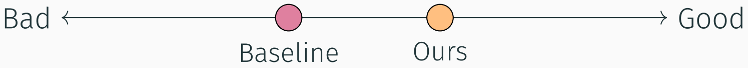
Model evaluation: Comparison



There is going to be variability in our model's performance (and possibly the baseline).

Is our model significantly better?

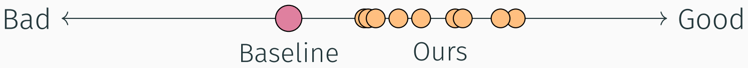
Model evaluation: Comparison



Approach 1:

Is the mean of the distribution of performances from our model (with regards to variability that is **unrelated** to efficacy) significantly higher than the point-estimate baseline?

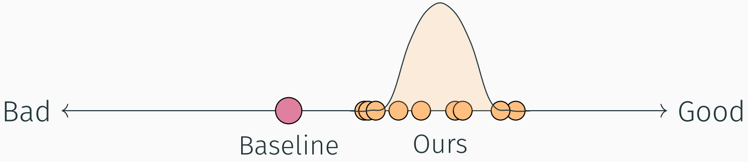
Model evaluation: Comparison



Approach 1:

Is the mean of the distribution of performances from our model (with regards to variability that is **unrelated** to efficacy) significantly higher than the point-estimate baseline?

Model evaluation: Comparison



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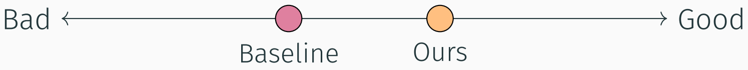
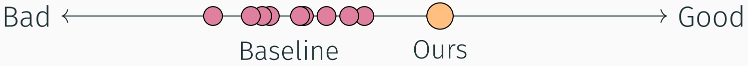
Model evaluation: Comparison



Approach 2:

Is the point-estimate performance of our model significantly higher than the mean of the baseline distribution?

Model evaluation: Comparison



Approach 2:

Is the point-estimate performance of our model significantly higher than the mean of the baseline distribution?

Model evaluation: Comparison

Age	Sex	Feature	Outcome
25	Male	0.53	1
38	Female	-0.76	1
45	Male	0.89	1
33	Female	-0.21	1
29	Male	0.12	1
41	Female	-0.68	0
56	Male	0.45	0
52	Female	-0.32	0
31	Male	0.91	0
48	Female	-0.15	0

→ Modelling pipeline → Error

Model evaluation: Comparison

Age	Sex	Feature	Outcome
25	Male	0.53	1
38	Female	-0.76	1
45	Male	0.89	1
33	Female	-0.21	1
29	Male	0.12	1
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56	Male	0.45	0
52	Female	-0.32	0
31	Male	0.91	0
48	Female	-0.15	0

$\longrightarrow$ Modelling pipeline $\longrightarrow$ 0.70

Model evaluation: Comparison

Age	Sex	Feature	Outcome
25	Male	0.53	1
38	Female	-0.76	0
45	Male	0.89	1
33	Female	-0.21	0
29	Male	0.12	1
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56	Male	0.45	1
52	Female	-0.32	0
31	Male	0.91	1
48	Female	-0.15	0

→ Modelling pipeline → 0.50

Model evaluation: Comparison

Age	Sex	Feature	Outcome
25	Male	0.53	0
38	Female	-0.76	0
45	Male	0.89	0
33	Female	-0.21	0
29	Male	0.12	0
41	Female	-0.68	1
56	Male	0.45	1
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→ Modelling pipeline → 0.50 0.45

Model evaluation: Comparison

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25	Male	0.53	0
38	Female	-0.76	1
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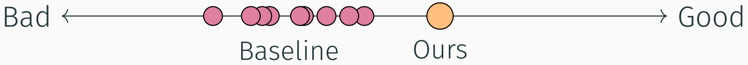
→ Modelling pipeline →

0.50
0.45
0.55

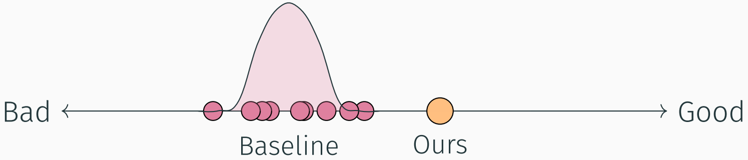
Model evaluation: Comparison



Approach 2:

Is the point-estimate performance of our model significantly higher than the mean of the baseline distribution?

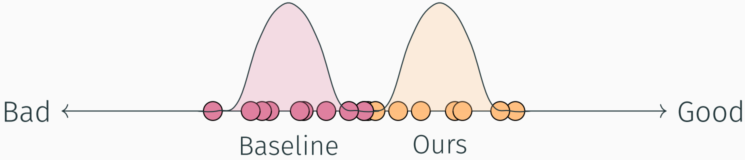
Model evaluation: Comparison



Approach 2:

Is the point-estimate performance of our model significantly higher than the mean of the baseline distribution?

Model evaluation: Comparison



Approach 3:

Is the mean of the distribution of performances from our model significantly higher than the mean of the distribution of baseline performances?

Model evaluation: Summary

- Model evaluation should **always** happen out-of-sample
- If n is big (≥ 10000), a train/validation split can be sufficient
- For smaller samples, k-fold cross-validation with $5 \leq k \leq 10$ is a good trade-off between bias and variance
- The bootstrap is an effective way of getting confidence intervals for model performance **and parameters**
- Cross-validation (or bootstrapping) will produce a distribution of model performances (although caution the correlation)
- Permutation testing can produce a distribution of baseline performances

Model selection and evaluation

Model selection and evaluation: Rationale

- Model evaluation via cross-validation is sufficient if we want to estimate the out-of-sample error of a **known model**.
- Very often we want to know whether a set of predictors are informative for an outcome **given the best possible model**.
- In that case, we have to both **choose the best model**, and **estimate its performance**.
- If we choose the model based on regular cross-validation, the performance estimate will (likely) be inflated

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- In that case, we have to both **choose the best model**, and **estimate its performance**.
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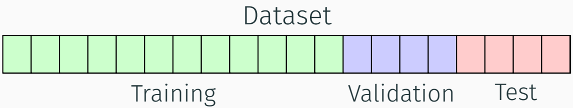
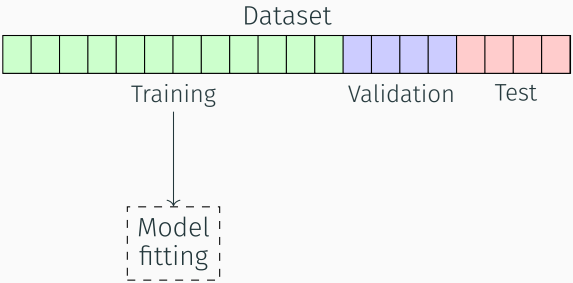
→ We need a more advanced strategy

Model selection and evaluation: Train/validation/test

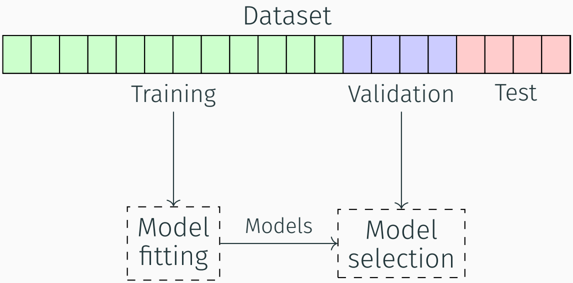
Model selection and evaluation: Train/validation/test



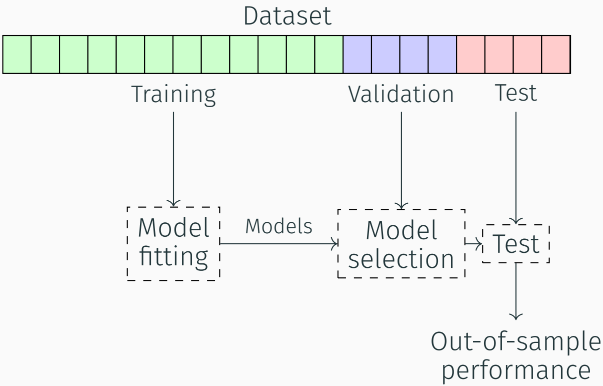
Model selection and evaluation: Train/validation/test



Model selection and evaluation: Train/validation/test



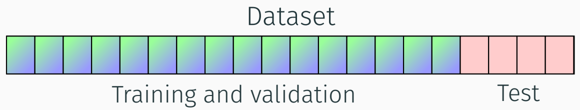
Model selection and evaluation: Train/validation/test



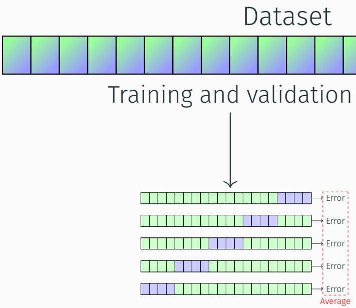
Model selection and evaluation: Nested cross-validation

Dataset

Model selection and evaluation: Nested cross-validation



Model selection and evaluation: Nested cross-validation



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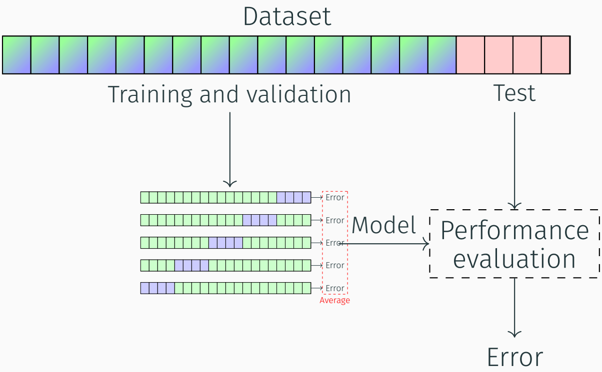
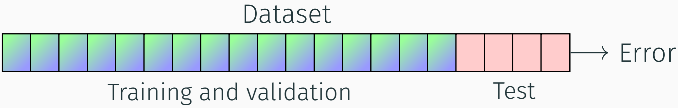
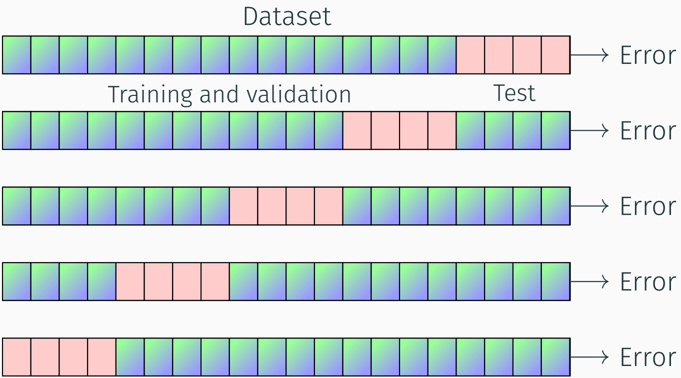


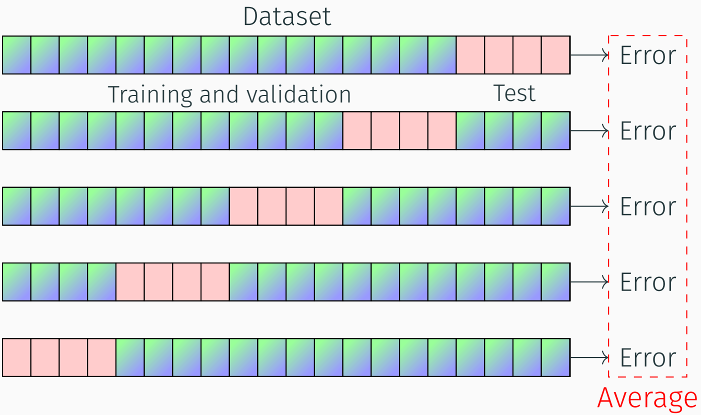
Model selection and evaluation: Nested cross-validation



Model selection and evaluation: Nested cross-validation



Model selection and evaluation: Nested cross-validation



Model selection and evaluation: Nested cross-validation

Performs k outer cross-validations, each performing $k-1$ inner cross validations, and uses the best models from the inner loop to predict in the outer loop.

+ Uses all data to train models
+ **Unbiased estimate of out-of-sample error**
- **Very** computationally expensive
- Hard to interpret beyond performance: We now have either k, or k^2 models that might behave in different ways

Model selection and evaluation: Summary

- Whenever a modelling choice is made on the basis of performance in a dataset, **we have to assume the performance achieved by the chosen model is inflated**
- If n is big (≥ 10000), a single train/validation/test split is often sufficient
- When possible, use nested cross-validation to select the best model and estimate the out-of-sample error

Model selection and evaluation: Summary

!!!!!

- Whenever a modelling choice is made on the basis of performance in a dataset, **we have to assume the performance achieved by the chosen model is inflated**
- If n is big (≥ 10000), a single train/validation/test split is often sufficient
- When possible, use nested cross-validation to select the best model and estimate the out-of-sample error

Assignment 4

1. Download the Heart-dataset from the book
2. Fit and validate a model using a train/validation split
3. Fit and validate multiple models using cross-validation
4. (Optional): Fit and validate multiple models using the bootstrap