PSY9511: Seminar 4

Testing, resampling, and splitting

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Outline

1. Coding tips
   - Loops
   - Functions
2. Performance metrics
3. Strategies for model assessment
   - Training and validation split
   - (Stratification)
   - (Leave-one-out cross-validation)
   - Cross-validation
   - Bootstrap
   - Model comparison
4. Strategies for model selection **and** assessment
   - Train/validation/test split
   - Nested cross-validation

Coding tips

Coding tips

In[1]:

```
import numpy as np
import pandas as pd

df = pd.read_csv('Auto.csv')
df = df.replace('?', np.nan)
train = df.iloc[:200].copy()
test = df.iloc[300:].copy()

test['cylinders'] = (test['cylinders'] - train['cylinders'].mean()) / train['cylinders'].std()
train['cylinders'] = (train['cylinders'] - train['cylinders'].mean()) / train['cylinders'].std()
test['weight'] = (test['weight'] - train['weight'].mean()) / train['weight'].std()
train['weight'] = (train['weight'] - train['weight'].mean()) / train['weight'].std()
test['year'] = (test['year'] - train['year'].mean()) / train['year'].std()
train['year'] = (train['year'] - train['year'].mean()) / train['year'].std()
```

Coding tips: Live coding

[Live coding]

Coding tips: Python

In[1]:

```
import numpy as np
import pandas as pd

df = pd.read_csv('Auto.csv')
df = df.replace('?', np.nan)
train = df.iloc[:200].copy()
test = df.iloc[300:].copy()

test['cylinders'] = (test['cylinders'] - train['cylinders'].mean()) / train['cylinders'].std()
train['cylinders'] = (train['cylinders'] - train['cylinders'].mean()) / train['cylinders'].std()
test['weight'] = (test['weight'] - train['weight'].mean()) / train['weight'].std()
train['weight'] = (train['weight'] - train['weight'].mean()) / train['weight'].std()
test['year'] = (test['year'] - train['year'].mean()) / train['year'].std()
train['year'] = (train['year'] - train['year'].mean()) / train['year'].std()
```

In[2]:

```
import numpy as np
import pandas as pd

df = pd.read_csv('Auto.csv')
df = df.replace('?', np.nan)
train = df.iloc[:200].copy()
test = df.iloc[300:].copy()

def standardize(train: pd.DataFrame, test: pd.DataFrame, column: str):
    train = train.copy()
    test = test.copy()

    test[column] = (test[column] - train[column].mean()) / train[column].std()

    return train, test

for column in ['cylinders', 'displacement', 'weight']:
    train, test = standardize(train, test, column=column)
```

Coding tips: R

```r
data <- read.csv('Auto.csv')
data[] <- lapply(data, function(x) replace(x, x == '?', NA))

train <- data[1:200,]
test <- data[200:nrow(data),]

test$cylinders <- (test$cylinders - mean(train$cylinders)) / sd(train$cylinders)
train$cylinders <- (train$cylinders - mean(train$cylinders)) / sd(train$cylinders)
test$weight <- (test$weight - mean(train$weight)) / sd(train$weight)
train$weight <- (train$weight - mean(train$weight)) / sd(train$weight)
test$year <- (test$year - mean(train$year)) / sd(train$year)
train$year <- (train$year - mean(train$year)) / sd(train$year)
```


```r
data <- read.csv('Auto.csv')
data[] <- lapply(data, function(x) replace(x, x == '?', NA))

train <- data[1:200,]
test <- data[200:nrow(data),]

test$cylinders <- (test$cylinders - mean(train$cylinders)) / sd(train$cylinders)
train$cylinders <- (train$cylinders - mean(train$cylinders)) / sd(train$cylinders)
test$weight <- (test$weight - mean(train$weight)) / sd(train$weight)
train$weight <- (train$weight - mean(train$weight)) / sd(train$weight)
test$year <- (test$year - mean(train$year)) / sd(train$year)
train$year <- (train$year - mean(train$year)) / sd(train$year)
```

Coding tips: Minimal, complete scripts

Ctrl+Shift+Enter

Performance metrics

Performance metrics: Regression

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

Performance metrics: Regression

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

Mean squared error (MSE)

+ Widely used
+ Intuitive
+ Penalizes large errors

? Interpretation

- Depends on scale

Performance metrics: Regression

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

Performance metrics: Regression

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

Root mean squared error (RMSE)

+ Intuitive
+ Penalizes large errors
+ More interpretable than MSE, total loss $\approx$ individual loss
- Depends on scale

Performance metrics: Regression

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

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

Mean absolute error (MAE)

- + More interpretable than MSE/RMSE, total loss = average error
- – Feels a bit off
- – Depends on scale

Performance metrics: Regression

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

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
- Captures linear correlation
- Does not care about whether the predictions are close to the true values

Performance metrics: Regression

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

Performance metrics: Regression

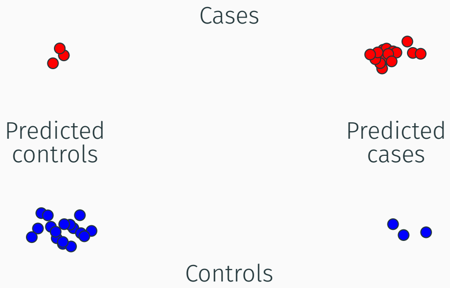
$$1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2}$$

Proportion of variance explained (r^2)

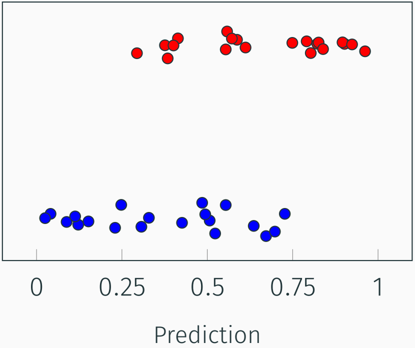
- \+ Scale independent
- \+ Interpretable
- \- Captures linear correlation
- \- Does not care about whether the predictions are close to the true values

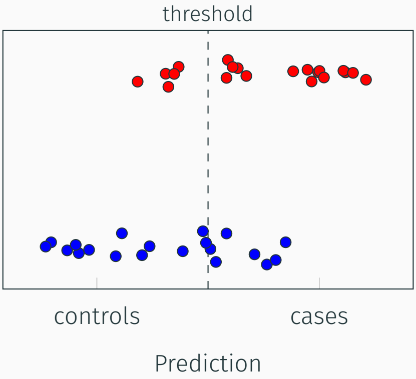
Performance metrics: Binary classification

Performance metrics: Binary classification

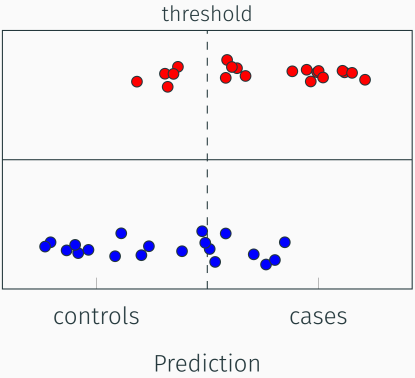


Performance metrics: Binary classification

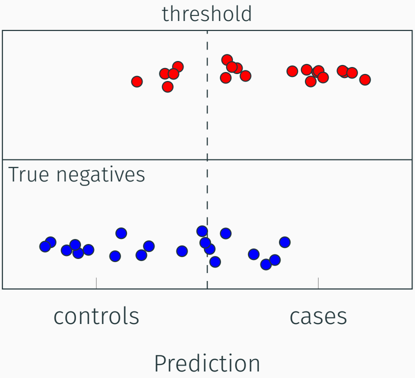



threshold
controls
cases
Prediction

Performance metrics: Binary classification

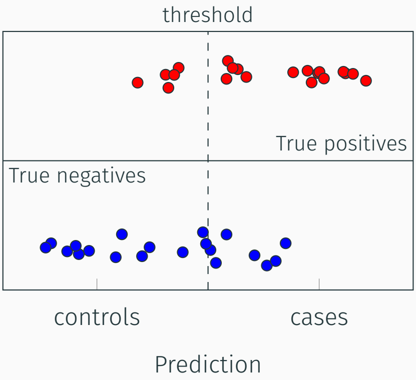


Performance metrics: Binary classification



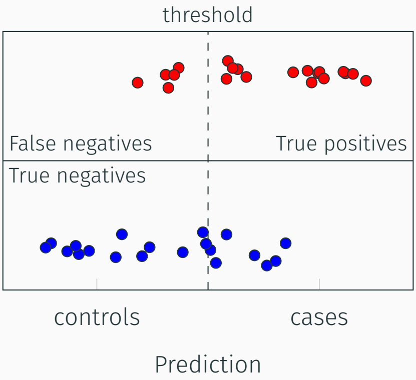
	TN

Performance metrics: Binary classification



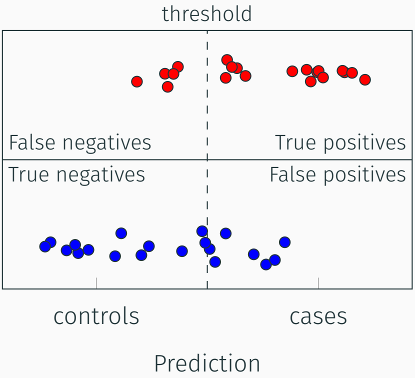
TP	
	TN

Performance metrics: Binary classification



TP	FN
	TN

Performance metrics: Binary classification



TP	FN
FP	TN

Performance metrics: Binary classification

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

Performance metrics: Binary classification

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

Accuracy

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

Performance metrics: Binary classification

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

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)

Performance metrics: Binary classification

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

Performance metrics: Binary classification

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

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 benign condition)

Performance metrics: Binary classification

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

Performance metrics: Binary classification

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

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)

Performance metrics: Binary classification

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

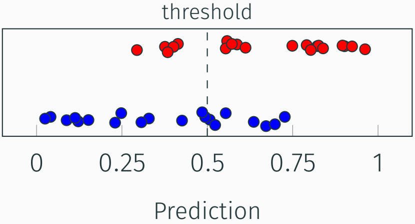
Performance metrics: Binary classification

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

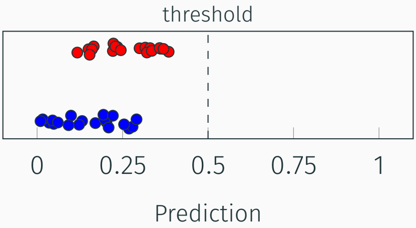
Balanced accuracy

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

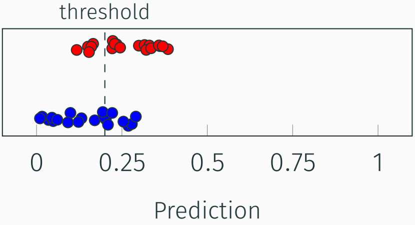
Performance metrics: Binary classification



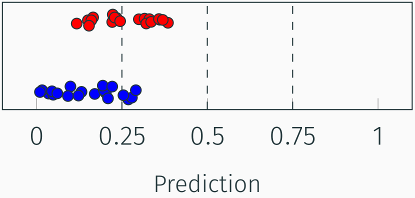
Performance metrics: Binary classification



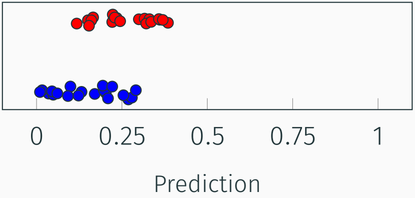
Performance metrics: Binary classification



Performance metrics: Binary classification

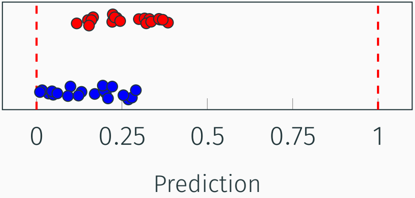


Performance metrics: Binary classification



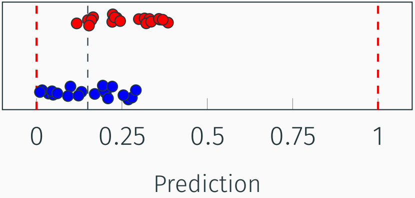
threshold	TPR	FPR

Performance metrics: Binary classification



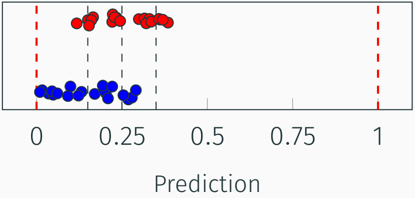
threshold	TPR	FPR
0	1	1
1	0	0

Performance metrics: Binary classification



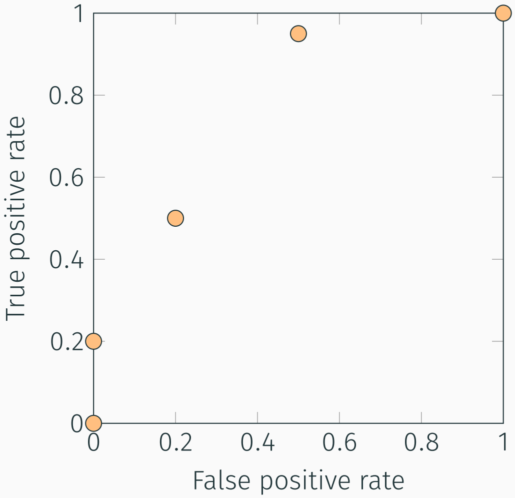
threshold	TPR	FPR
0	1	1
0.15	0.95	0.5
1	0	0

Performance metrics: Binary classification

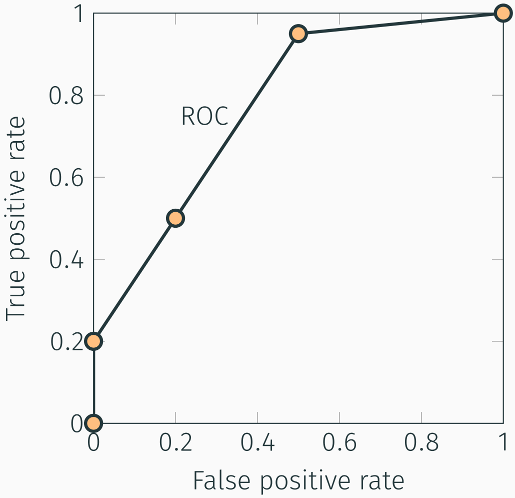


threshold	TPR	FPR
0	1	1
0.15	0.95	0.5
0.25	0.5	0.2
0.35	0.2	0.0
1	0	0

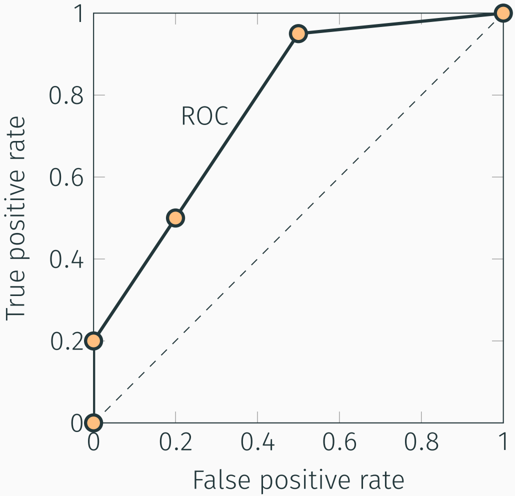
Performance metrics: Binary classification



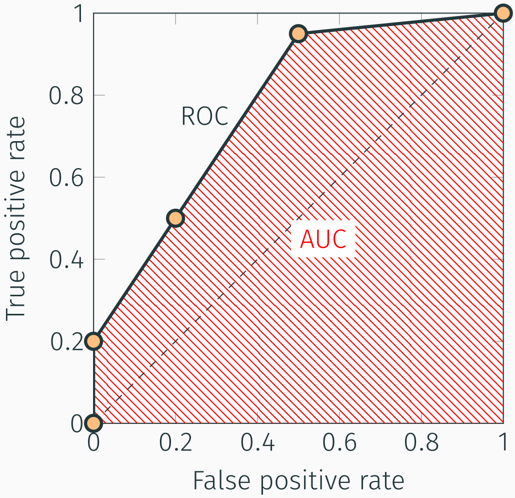
Performance metrics: Binary classification



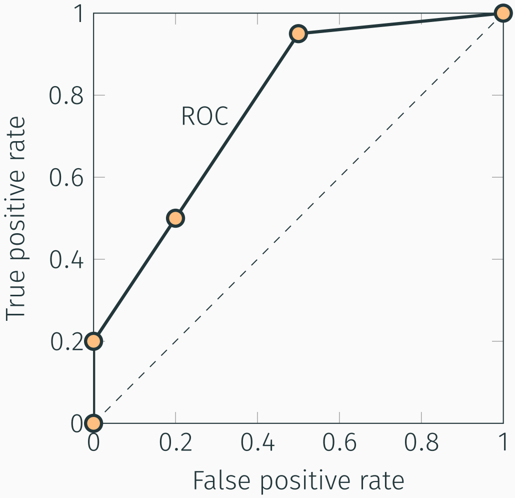
Performance metrics: Binary classification



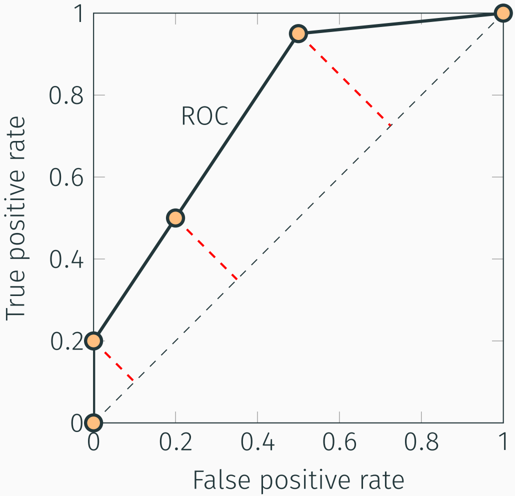
Performance metrics: Binary classification



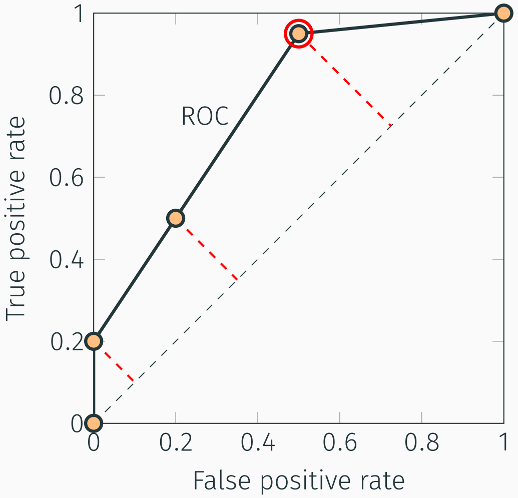
Performance metrics: Binary classification



Performance metrics: Binary classification



Performance metrics: Binary classification



Performance metrics: Summary

- There is a range of metrics that can be used, each capturing a different aspect of a model's performance
- If possible, it is my personal preference is to evaluate a model using a different model than the one that was used for training
- It is good practice to report more than one metric
- For regression, MAE provides a good, intuitive summary of model performance
- For classification, AUC is a widely used metric that is easy to interpret, not reliant on the choice of classification threshold, and handles class imbalance

Strategies for model assessment

Model assessment: Rationale

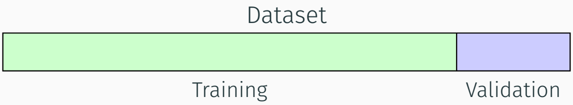
Statistical inference:
In-sample quantification

Predictive modelling:
Out-of-sample prediction (generalization)

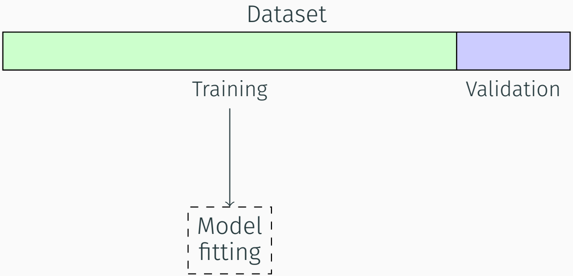
Model assessment: Validation set

Dataset

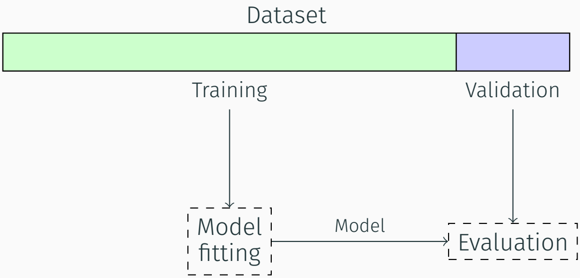
Model assessment: Validation set



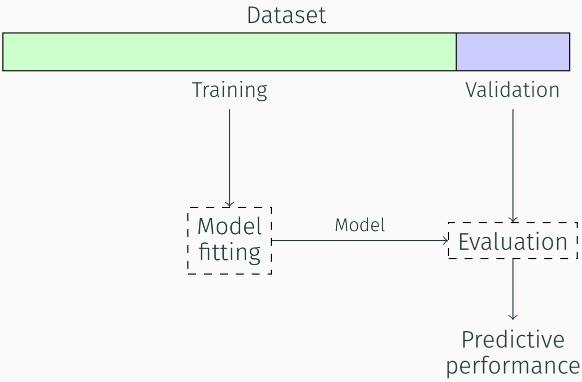
Model assessment: Validation set



Model assessment: Validation set



Model assessment: Validation set

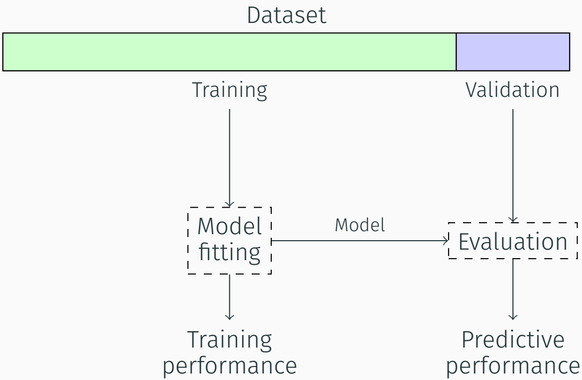


Model assessment: Validation set

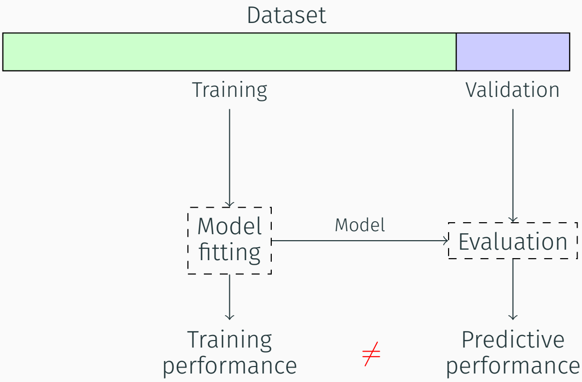
In the validation set approach we split the dataset into two subsets, and use for training the model and the other for testing performance.

- \+ Accurate estimate of out-of-sample error
- \+ Simple
- \- Highly variable, depends on the exact split
- \- Only uses a subset of data for training models
- \- Gives a point estimate of the error, without confidence intervals

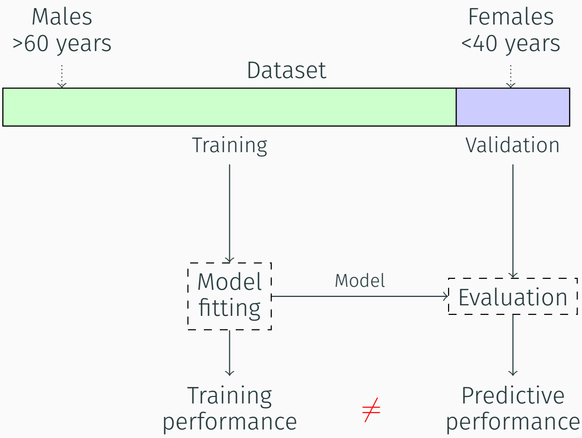
Model assessment: Validation set



Model assessment: Validation set



Model assessment: Validation set



Model assessment: Stratification

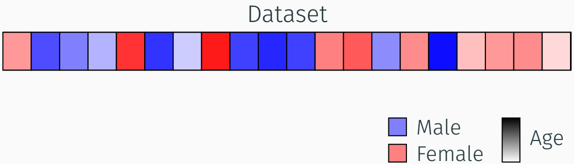
Stratification:

Ensuring all folds of the dataset are similar in terms of some given characteristics.

Model assessment: Stratification

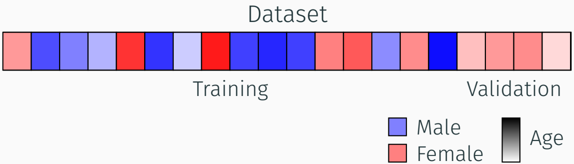

```
In[1]: df = ...
```

Model assessment: Stratification



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

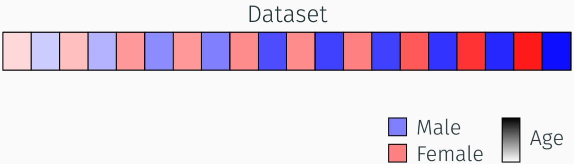
Model assessment: Stratification



In[1]:

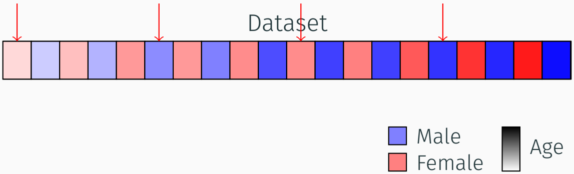
```
df = ...

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

Model assessment: Stratification



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

Model assessment: 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 assessment: Stratification

Stratification:

Ensuring all folds of the dataset are similar in terms of 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

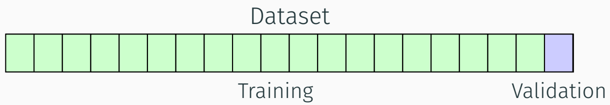
In[1]:
```python
from sklearn.model_selection import  train_test_split
```

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

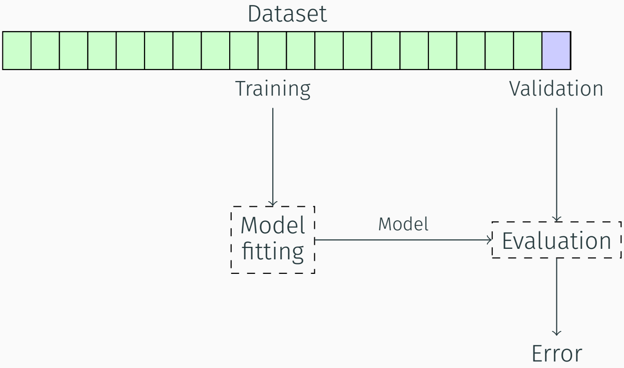
Model assessment: Leave-one-out cross-validation

Model assessment: Leave-one-out cross-validation

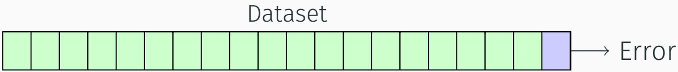
Model assessment: Leave-one-out cross-validation



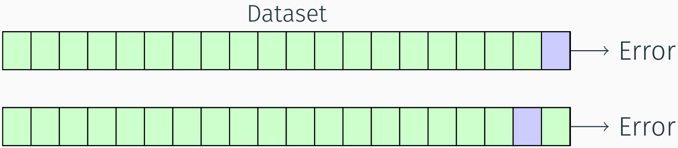
Model assessment: Leave-one-out cross-validation



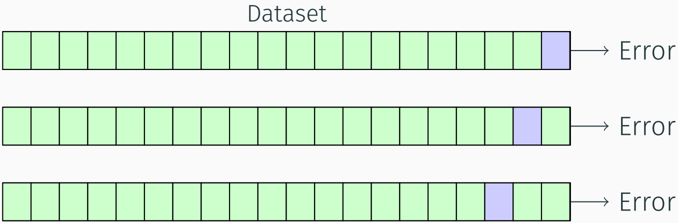
Model assessment: Leave-one-out cross-validation



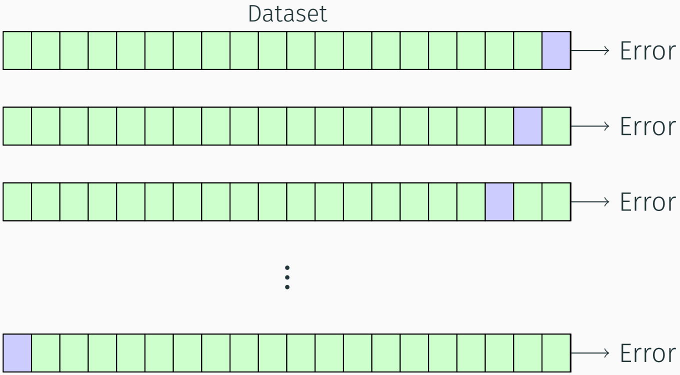
Model assessment: Leave-one-out cross-validation



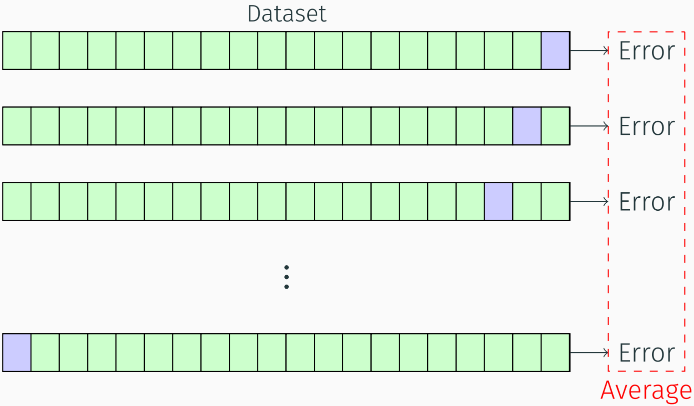
Model assessment: Leave-one-out cross-validation



Model assessment: Leave-one-out cross-validation



Model assessment: Leave-one-out cross-validation



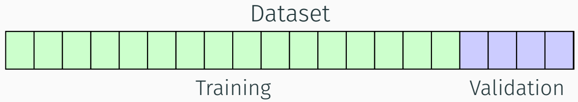
Model assessment: Leave-one-out cross-validation

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

+ Uses all data to train models
+ Not dependent on arbitrary data splits
- Computationally expensive
- Effectively gives a point estimate of the error

Model assessment: Cross-validation

Model assessment: Cross-validation



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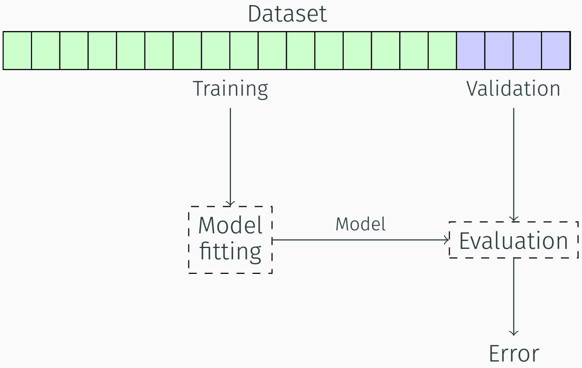
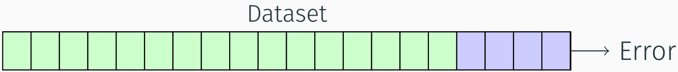


Model assessment: Cross-validation



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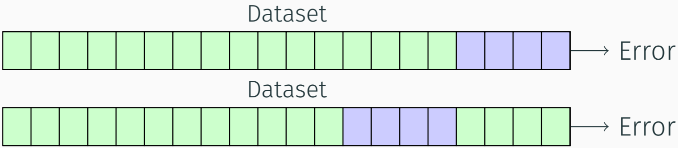

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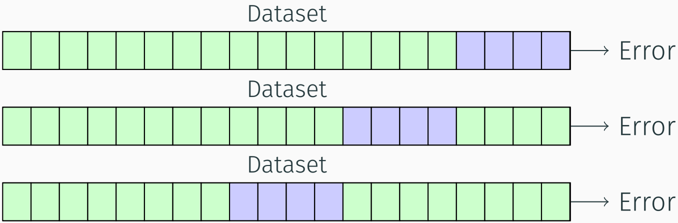

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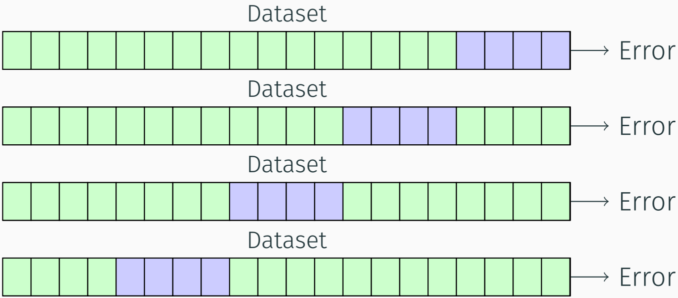

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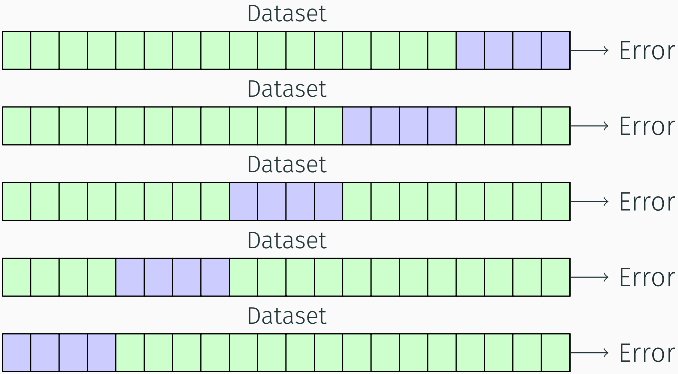
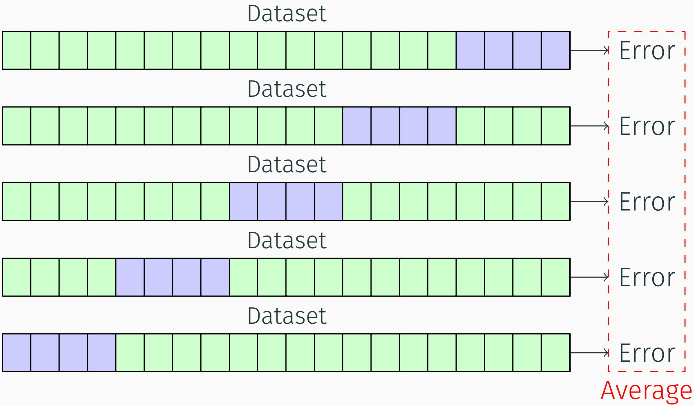


Model assessment: Cross-validation



Model assessment: Cross-validation

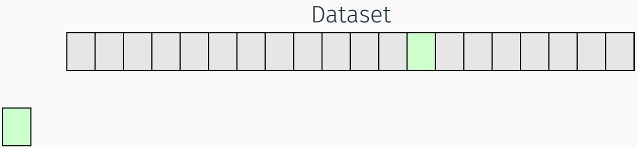
Fits k models for $n > k$ datapoints, each leaving n/k datapoints out for testing.

- \+ 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 assessment: The bootstrap

Dataset

Model assessment: The bootstrap



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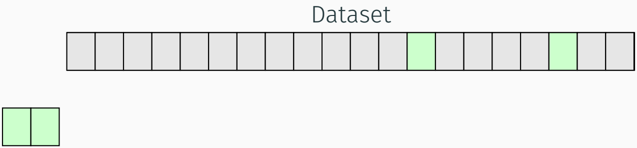

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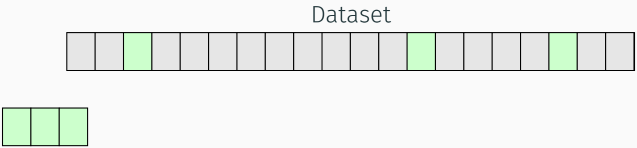

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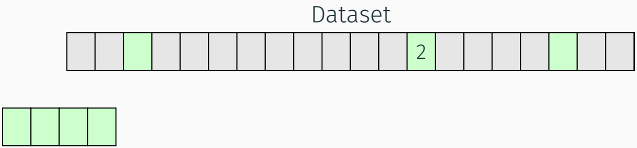

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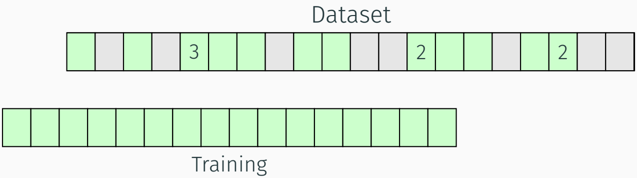

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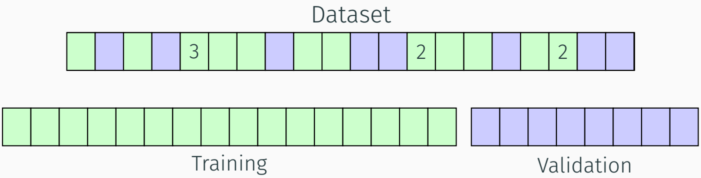

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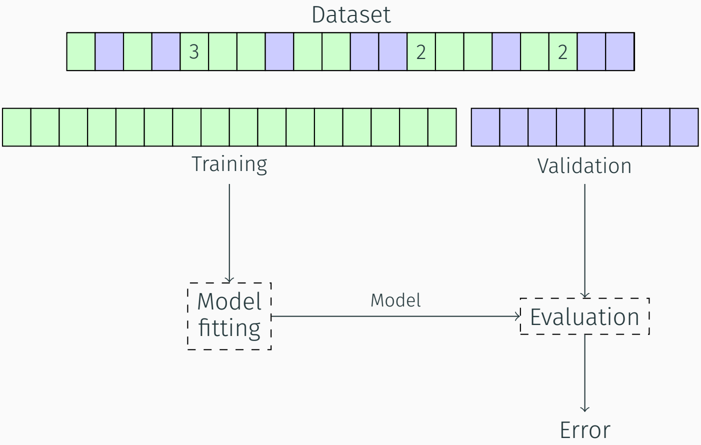

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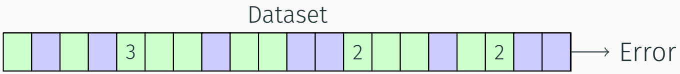

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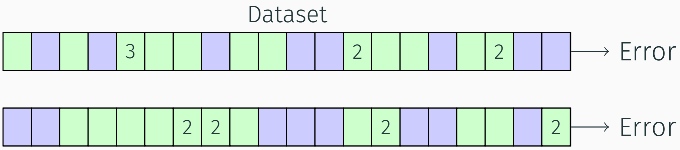
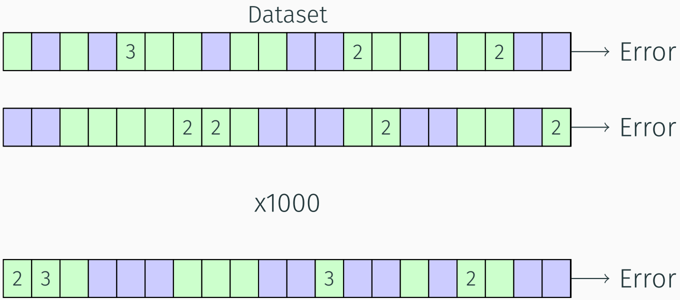


Model assessment: The bootstrap



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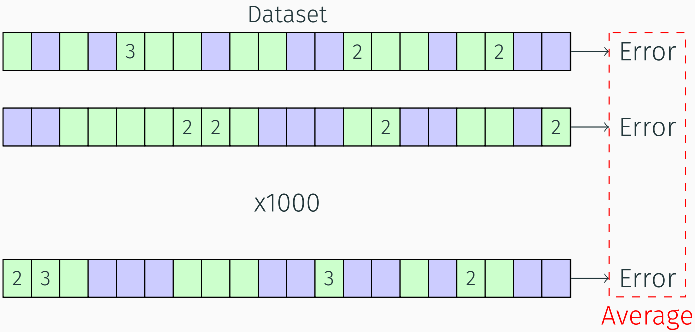


Model assessment: The bootstrap

Fits x models with m datapoints each, sampled from the original dataset with replacement.

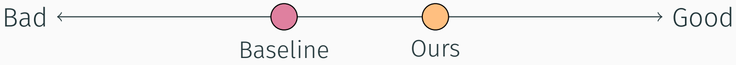
- \+ Uses all data to train models
- \+ Provides a smooth distribution of model performance
- \+ **Versatile: Can be used for other things, e.g. getting a confidence interval for model parameters**
- \- Different choices of k (and exact splits) yields different results

Model assessment: Comparison

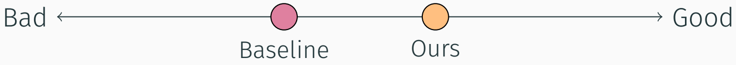
Why do we want to assess our model?

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 assessment: Comparison



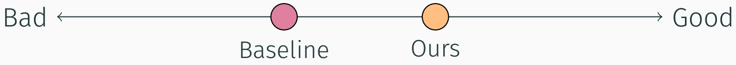
Model assessment: Comparison



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

Is our model significantly better?

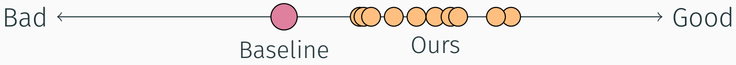
Model assessment: Comparison



Approach 1:

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

Model assessment: Comparison



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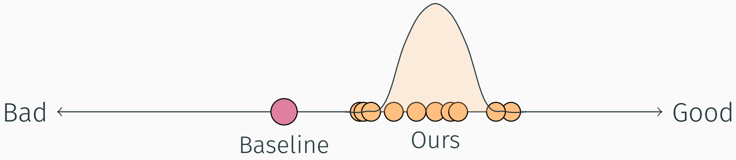

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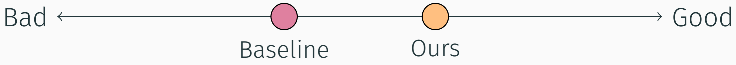

Approach 2:

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

Model assessment: 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

$\rightarrow$ Pipeline $\rightarrow$ Error

Model assessment: Comparison

Age	Sex	Feature	Outcome
25	Male	0.53	1
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48	Female	-0.15	0

→ Pipeline → 0.75

Model assessment: 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
41	Female	-0.68	0
56	Male	0.45	1
52	Female	-0.32	0
31	Male	0.91	1
48	Female	-0.15	0

→ Pipeline → 0.50

Model assessment: 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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→ Pipeline → 0.50
0.45

Model assessment: Comparison

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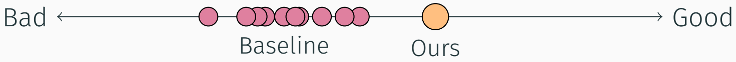
31	Male	0.91	1
48	Female	-0.15	1

→ Pipeline → 0.50, 0.45, 0.55

Model assessment: Comparison



Approach 2:

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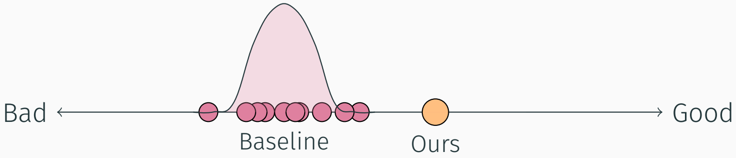
Model assessment: Comparison



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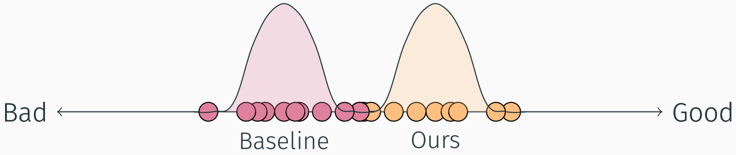

Approach 3:

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

Model assessment: Comparison

Fold	Ours	Baseline
1	0.75	0.71
2	0.62	0.55
3	0.58	0.57
4	0.87	0.81
5	0.65	0.63
6	0.98	0.97
7	0.55	0.52
8	0.69	0.52
9	0.91	0.85
10	0.88	0.81

The small gain of our model will disappear in the noise between the folds using a non-paired statistical test. Use a paired test, e.g. Wilcoxon signed-rank test

Model assessment: Summary

- Model assessment should **always** happen out-of-sample
- If n is big (≥ 10000), a single train/validation split is often 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 parameters
- We can use the results from cross-validation (or bootstrap) to produce a distribution of performances (although caution the correlation)
- We can use a permutation test to produce a distribution of baseline performances
- Compare models using Wilcoxon signed-rank test

Model selection and assessment

Model selection and assessment

- Model assessment 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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$\rightarrow$ We need a more advanced strategy

Model selection and assessment: Train/validation/test

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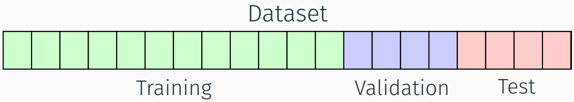
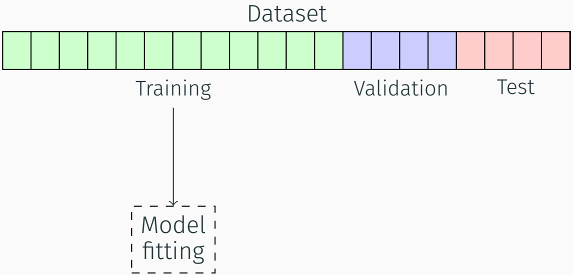


Model selection and assessment: Train/validation/test



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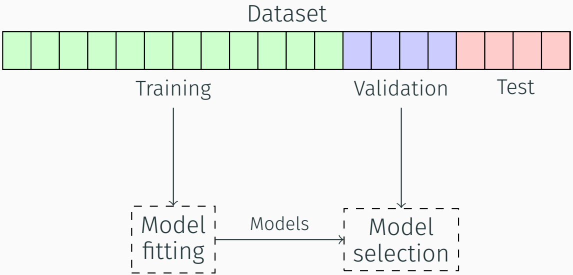
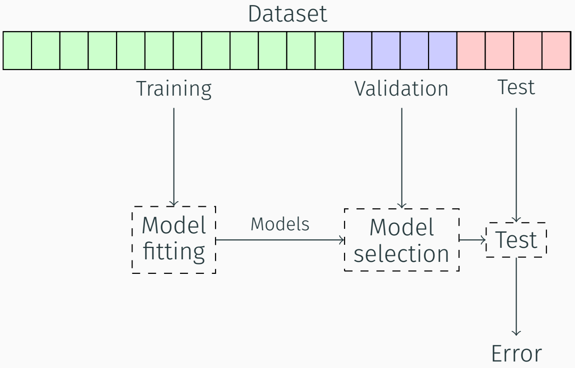
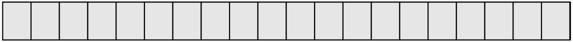


Model selection and assessment: Train/validation/test

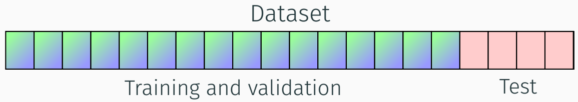


Model selection and assessment: Neste cross-validation

Dataset



Model selection and assessment: Nested cross-validation



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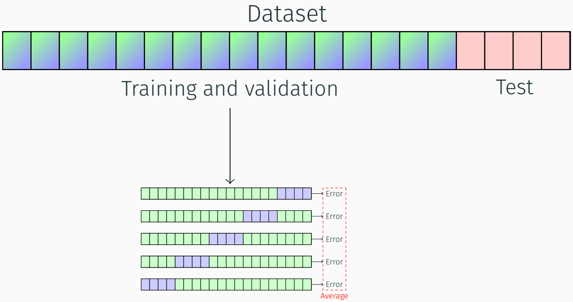

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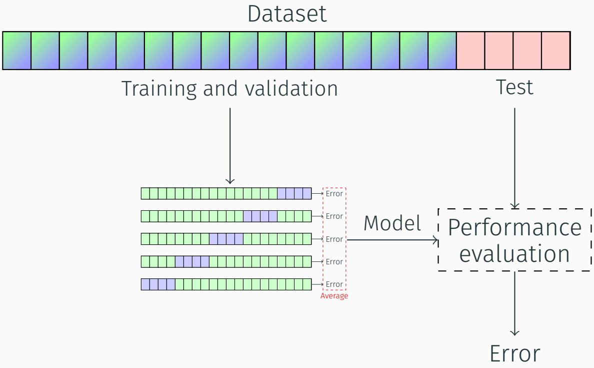

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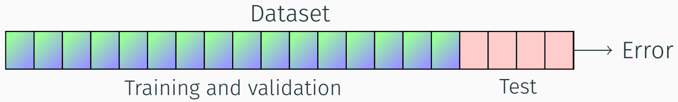

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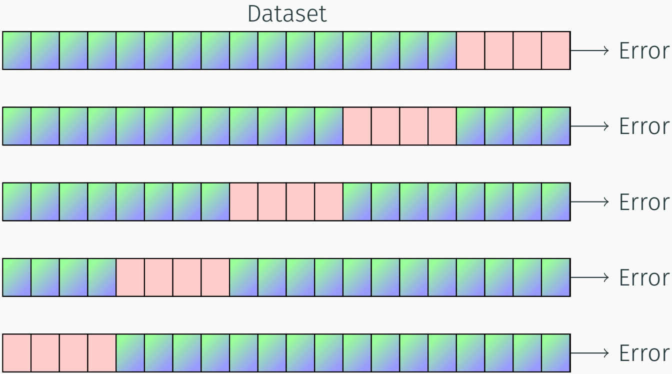

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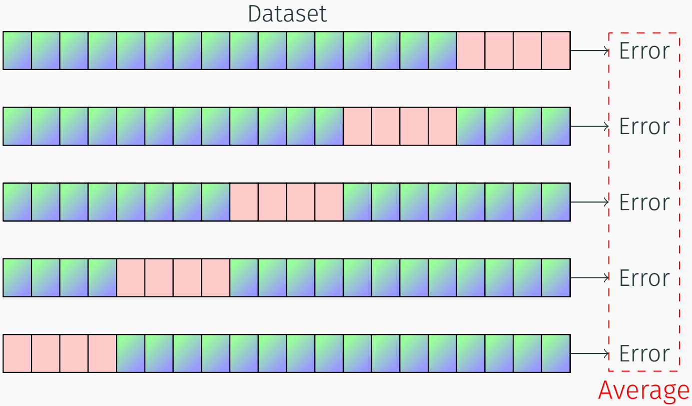

Model selection and assessment: Summary

- Whenever a choice is made on the basis of performance in a dataset, the performance of the chosen model on that dataset is going to be biased.
- If n is big (≥ 10000), a single train/validation/test split is often sufficient
- If possible, use nested cross-validation to select the best model *and* estimate the out-of-sample error