# PSY9511: Seminar 4

## Testing, resampling, and splitting

Esten H. Leonardsen

26.10.23

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# Outline

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

[Live coding]

# Coding tips: Python

In[1]:

```python
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]:

```python
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('~/Downloads/Auto.csv')
data[] <- lapply(data, function(x) replace(x, x == '?', NA))

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

standardize <- function(train, test, column)
train <- copy(train)
test <- copy(test)

test[,column] <- (test[column] - mean(train[,column])) / sd(train[,column])
train[,column] <- (train[column] - mean(train[,column])) / sd(train[,column])

return(list(train=train, test=test))


for (column in c('cylinders', 'weight', 'year'))
result <- standardize(train, test, column)
train <- result$train
test <- result$test
```

# Coding tips: Minimal, complete scripts

Ctrl+Shift+Enter

# Performance metrics

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# 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

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

# Performance metrics: Regression

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

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

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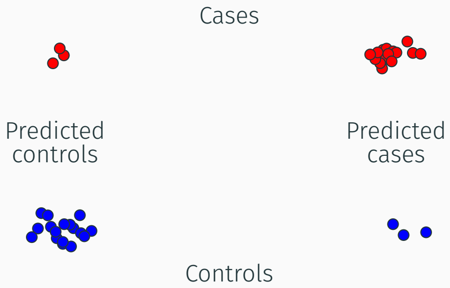
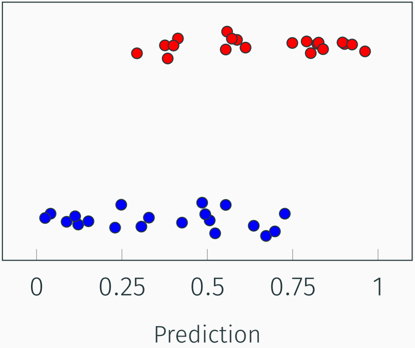


# Performance metrics: Binary classification



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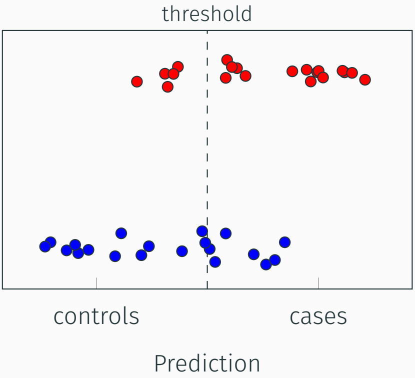

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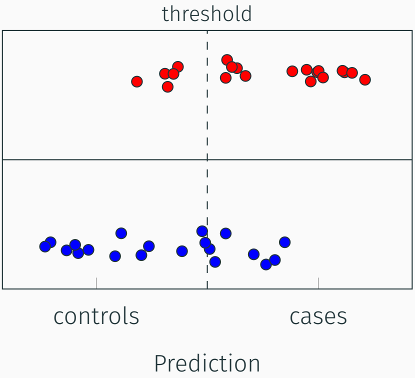


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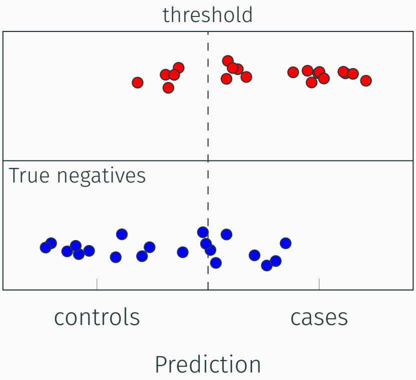
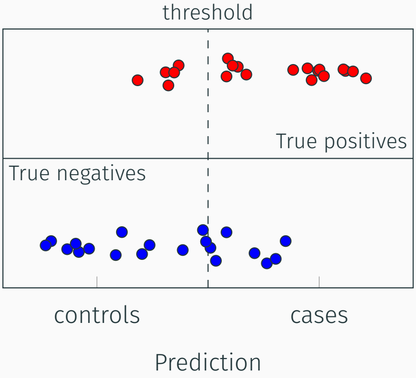


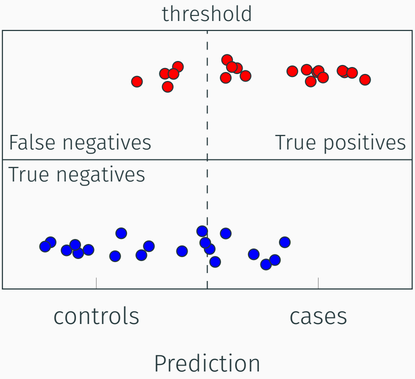

| | |
|---|---|
| TN | |
| | |

# Performance metrics: Binary classification



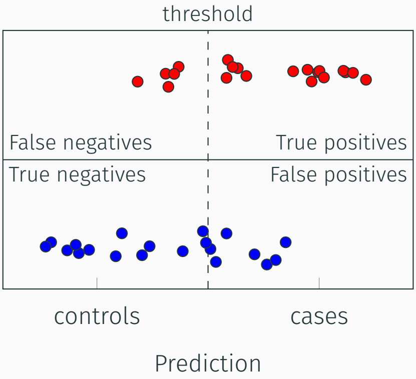

| | |
|---|---|
| TN | |
| | TP |

# Performance metrics: Binary classification




| | |
|---|---|
| TN | |
| FN | TP |

# Performance metrics: Binary classification




| | |
|---|---|
| TN | FP |
| FN | TP |

# Performance metrics: Binary classification

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

# Performance metrics: Binary classification

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

Accuracy

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

# Performance metrics: Binary classification

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

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

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 mild conditions)

# 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

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

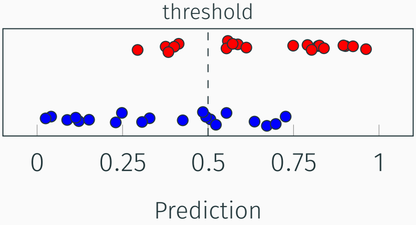
# Performance metrics: Binary classification

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

Balanced accuracy

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

# Performance metrics: Binary classification



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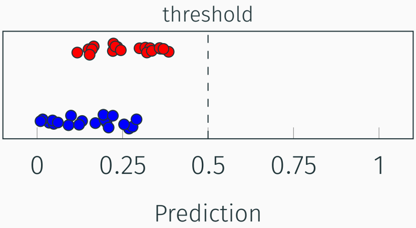

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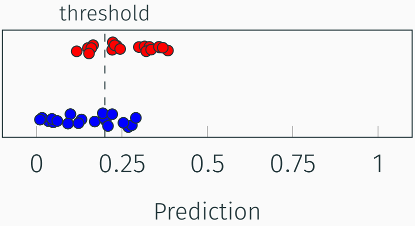

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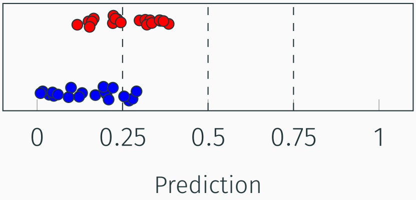

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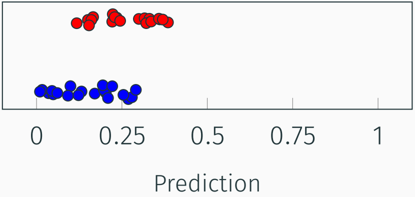


| threshold | TPR | FPR |
|---|---|---|
| | | |
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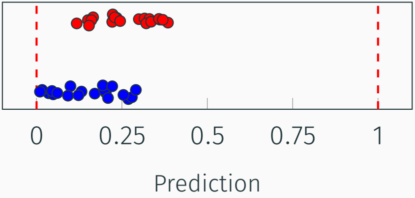
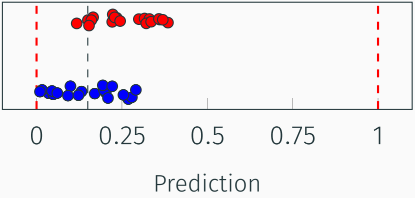
| | | |
| | | |
| | | |

# Performance metrics: Binary classification



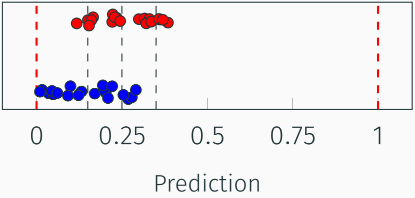

| threshold | TPR | FPR |
|---|---|---|
| 0 | 1 | 1 |
| | | |
| | | |
| | | |
| 1 | 0 | 0 |

# Performance metrics: Binary classification



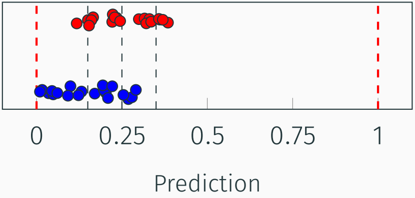

| threshold | TPR | FPR |
|---|---|---|
| 0 | 1 | 1 |
| 0.15 | 0.95 | 0.5 |
| | | |
| | | |
| 1 | 0 | 0 |

# Performance metrics: Binary classification



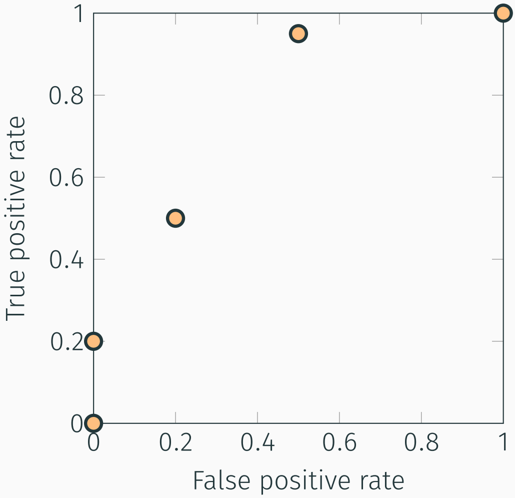

| threshold | TPR | FPR |
|---|---|---|
| 0 | 1 | 1 |
| 0.15 | 0.95 | 0.5 |
| 0.25 | 0.5 | 0.2 |
| 0.35 | 0.2 | 0.0 |
| 1 | 0 | 0 |

# Performance metrics: Binary classification




| 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



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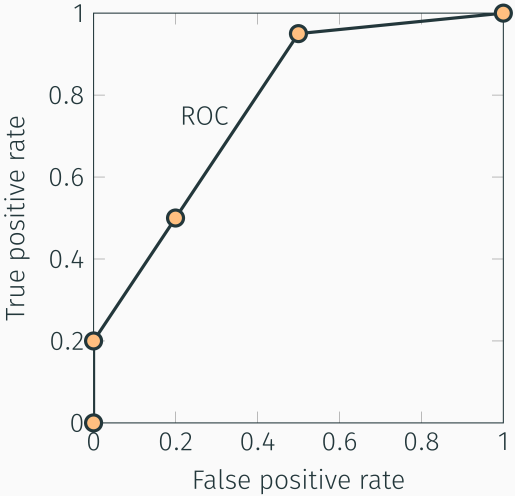

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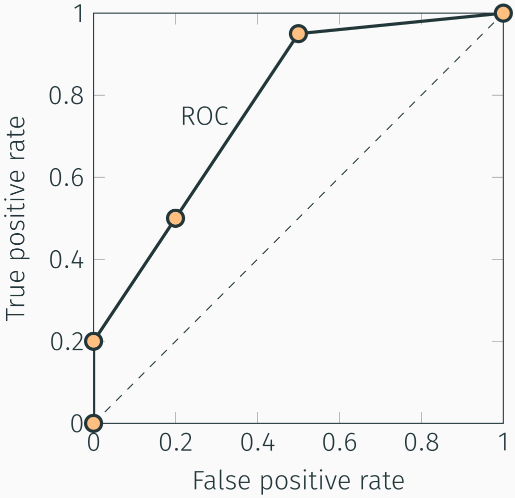

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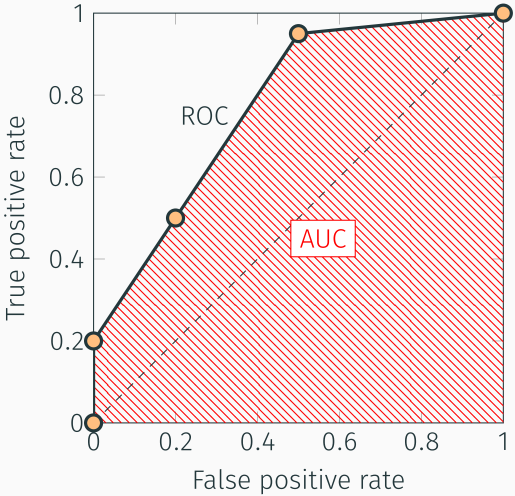

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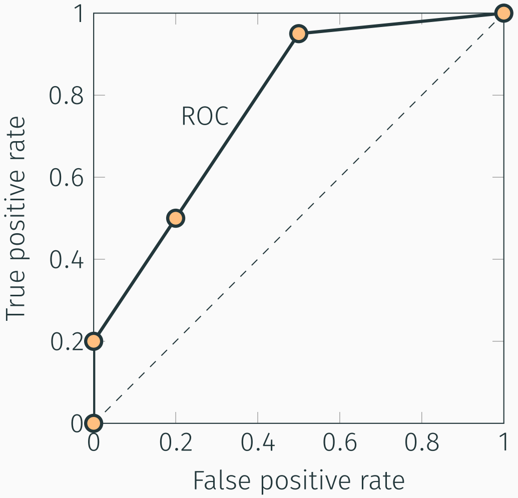

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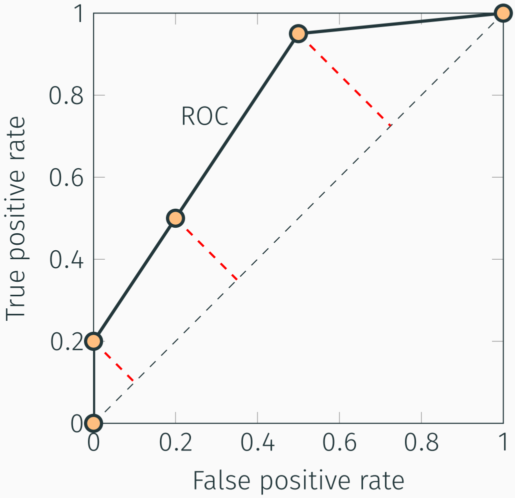

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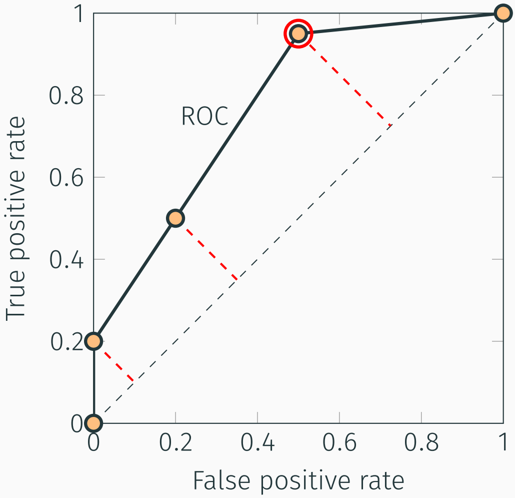

# Performance metrics: Summary

- 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 to) evaluate a model using a different metric 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, handles class imbalance (to some degree), and is not reliant on the choice of classification threshold

# 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: Validation set

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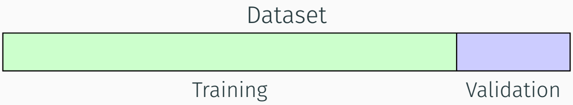

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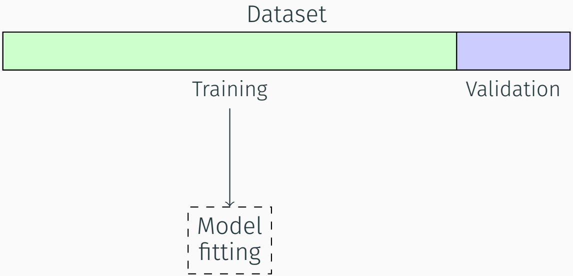

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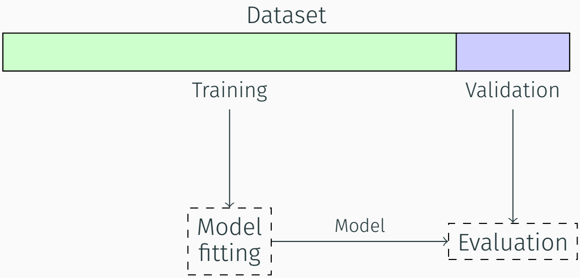

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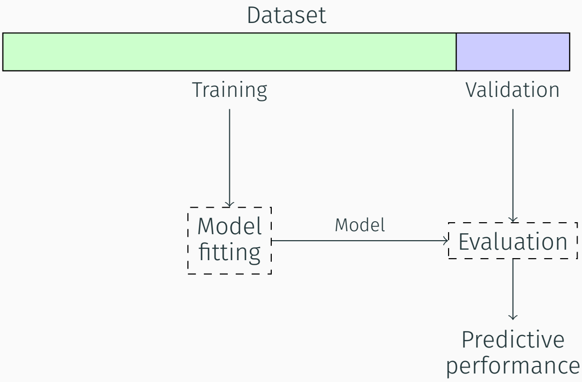
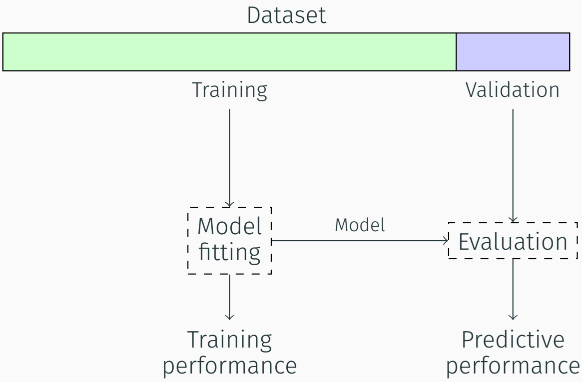


# Model evaluation: Validation set

In the validation set approach we split the dataset into two subsets (commonly $\sim$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



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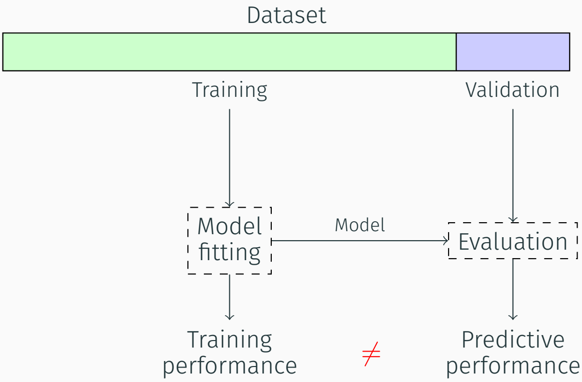
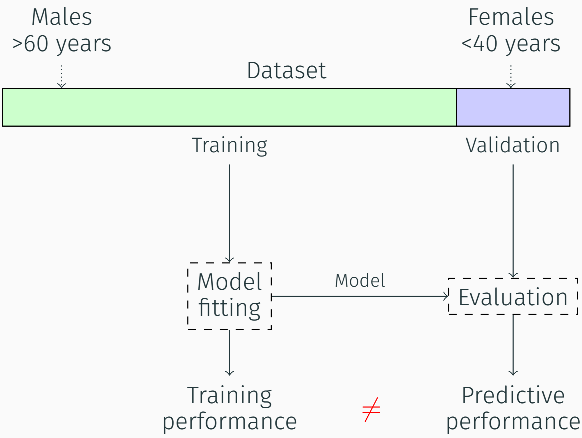


# Model evaluation: Validation set



# Model evaluation: Stratification

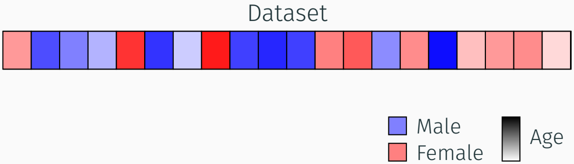
<u>Stratification:</u>
Ensuring all folds of the dataset are similar with respect to some given characteristics.

# Model evaluation: Stratification


In[1]:

```
df = ...
```

# Model evaluation: Stratification

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```
df = ...
```

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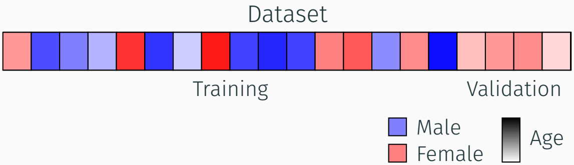
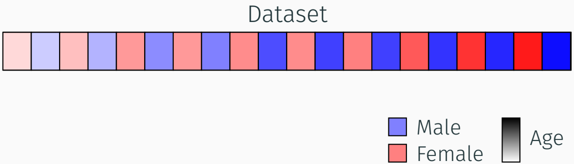


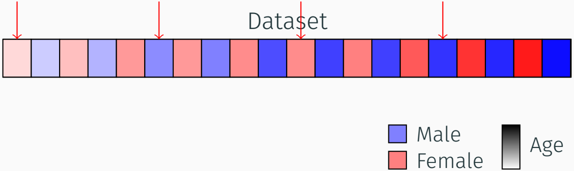

In[1]:
```
df = ...

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

**Stratification:**

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

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

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

# Model evaluation: Leave-one-out cross-validation

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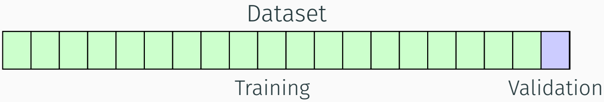

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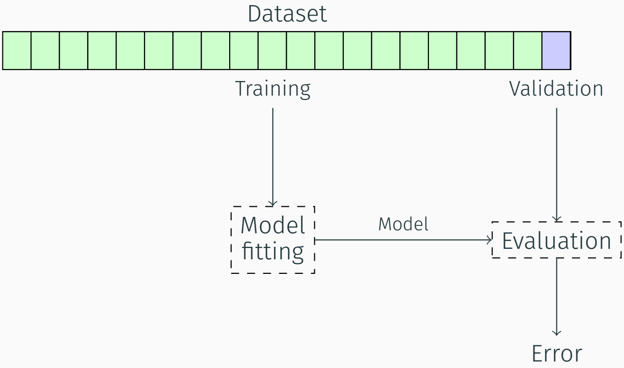

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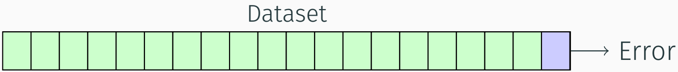
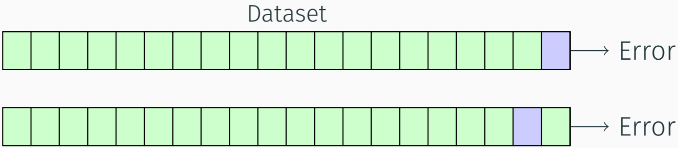
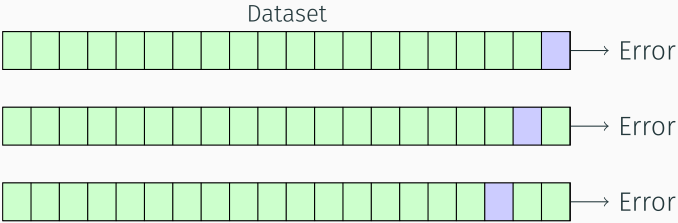


# Model evaluation: Leave-one-out cross-validation



# Model evaluation: Leave-one-out cross-validation



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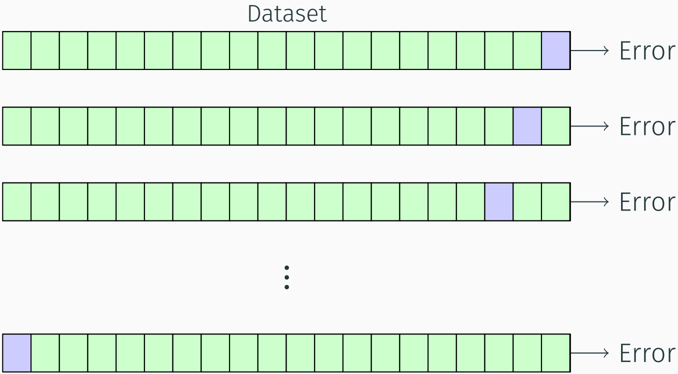
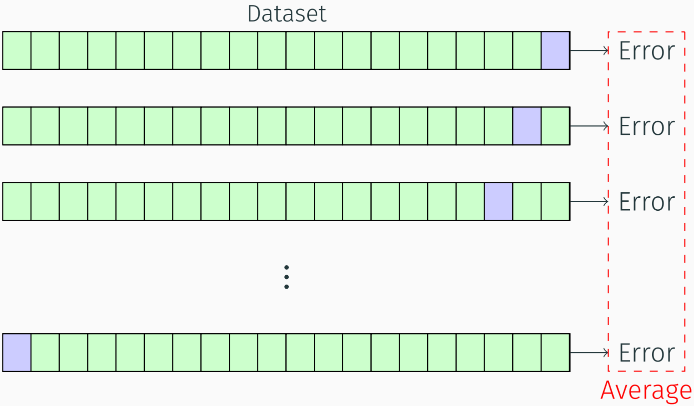


# Model evaluation: Leave-one-out cross-validation



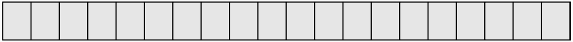
# Model evaluation: Leave-one-out cross-validation

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

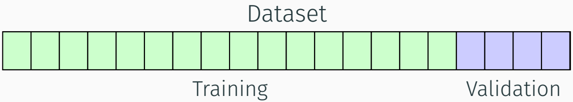
+ Uses all data to train models
+ Not dependent on arbitrary data splits
+ Unbiased (with regards to the full dataset)
- Computationally expensive
- Effectively gives a point estimate of the error
- All models are going to be trained on $> 99\%$ overlapping data $\rightarrow$ highly correlated

# Model evaluation: Cross-validation

Dataset



# Model evaluation: Cross-validation



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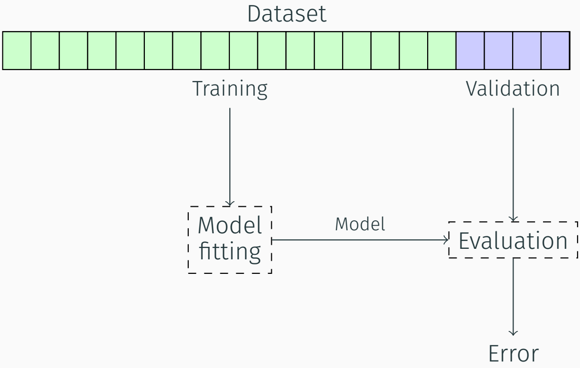

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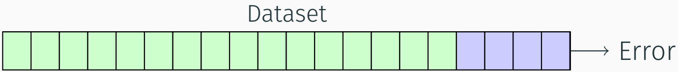
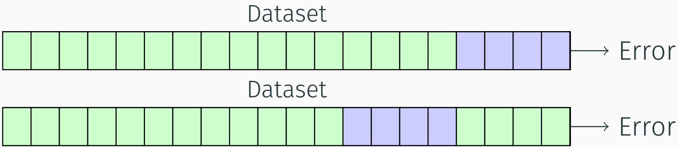


# Model evaluation: Cross-validation



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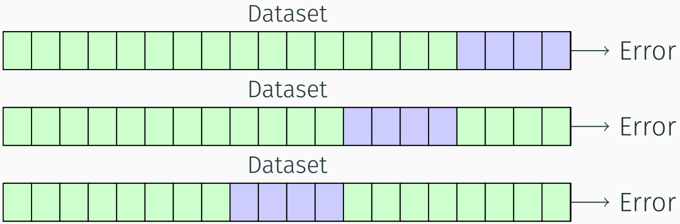

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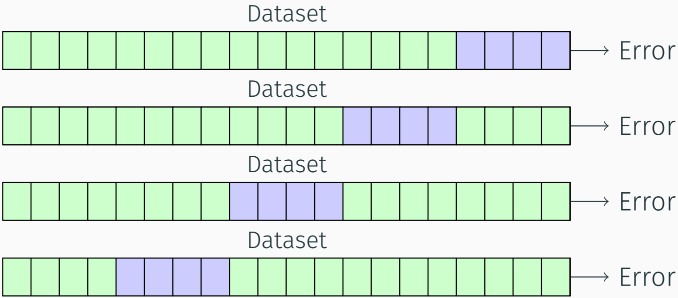

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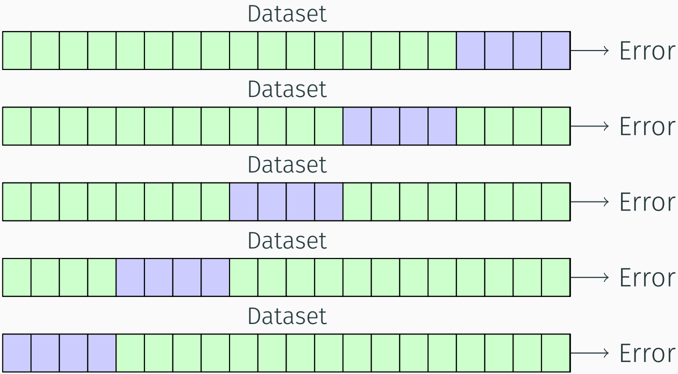

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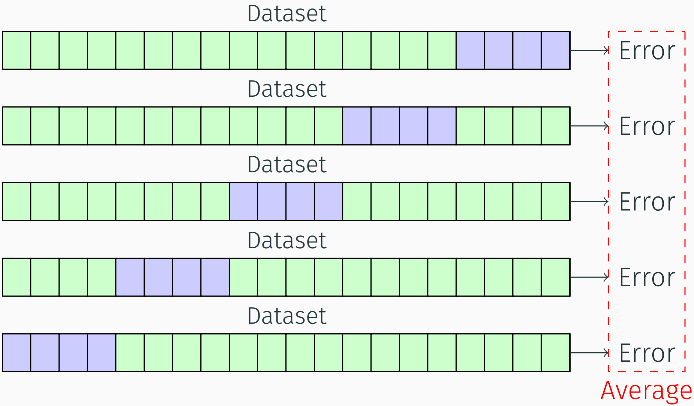


# Model evaluation: Cross-validation

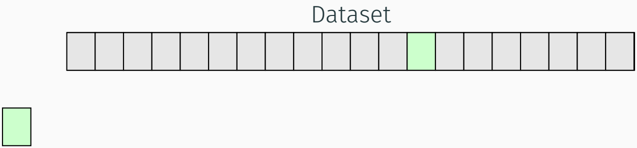
Fits $k$ (usually $k \in \{5, 10\}$) models for $n > k$ datapoints, each leaving $n/k$ datapoints for out-of-sample testing.

- \+ 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



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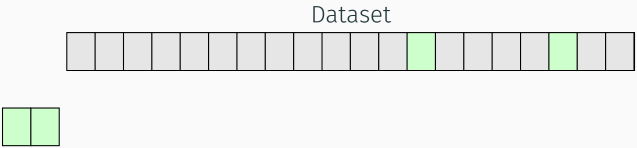

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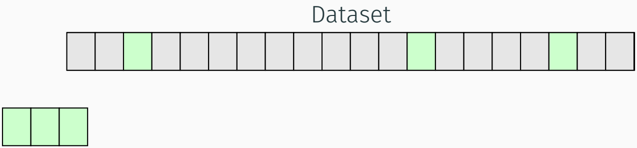

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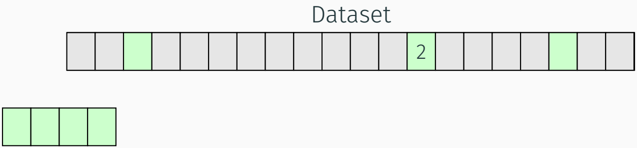

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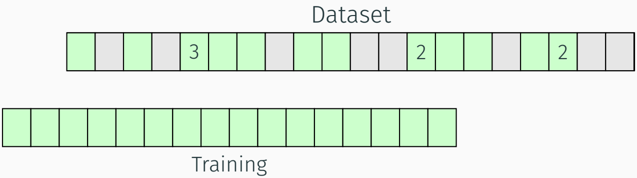

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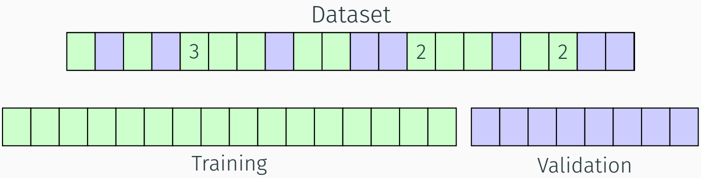

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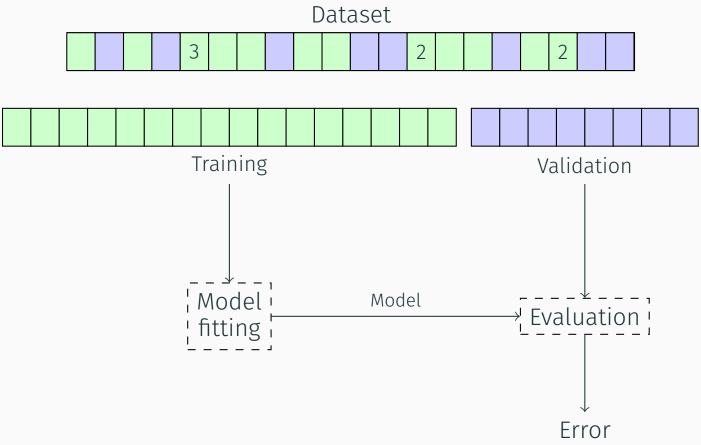

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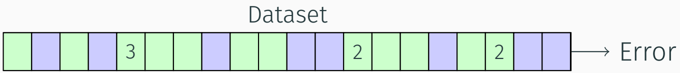

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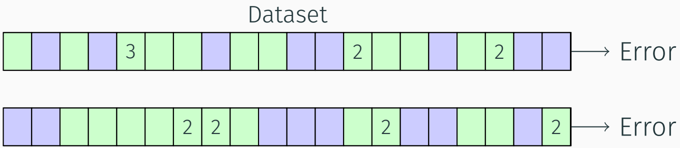

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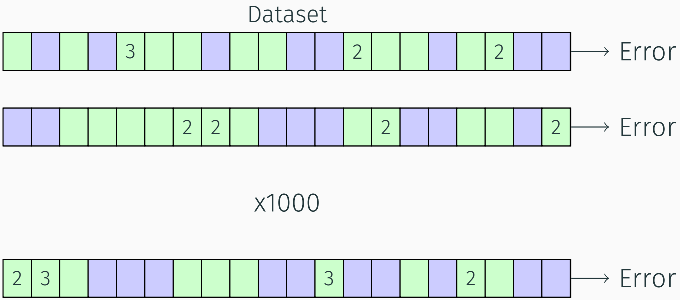
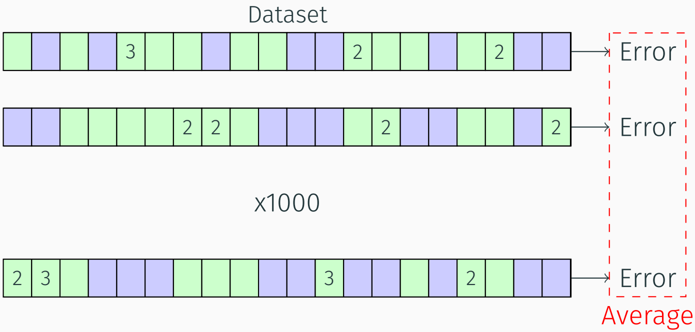


# Model evaluation: Bootstrapping

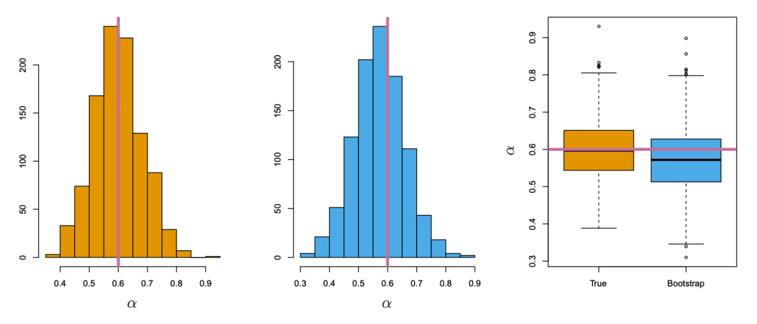


# Model evaluation: Bootstrapping

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

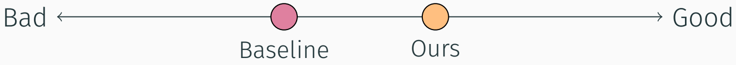


# Model evaluation: Comparison

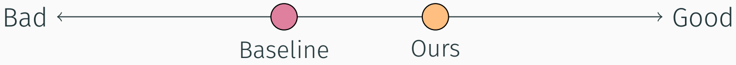
Why do we want to evaluate our model?

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



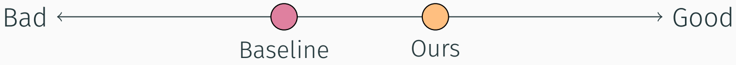
# Model evaluation: Comparison




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

**Is our model significantly better?**

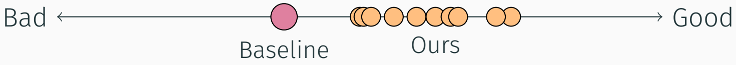
# Model evaluation: Comparison




Approach 1:

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

# Model evaluation: Comparison

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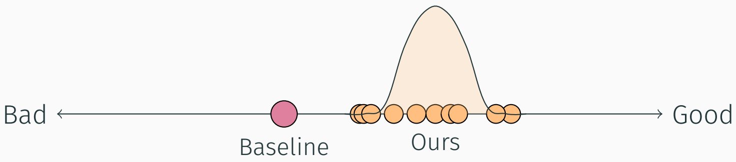


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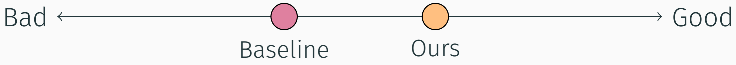


Approach 2:

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

# Model 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 |

→ Pipeline → Error

# Model evaluation: Comparison

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|---|---|---|---|
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| 56 | Male | 0.45 | 0 |
| 52 | Female | -0.32 | 0 |
| 31 | Male | 0.91 | 0 |
| 48 | Female | -0.15 | 0 |

→ Pipeline → 0.75

# 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 |
| 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 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 |
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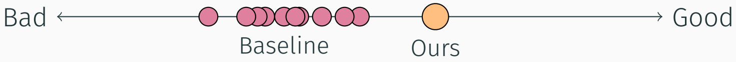
Pipeline

0.50
0.45
0.55

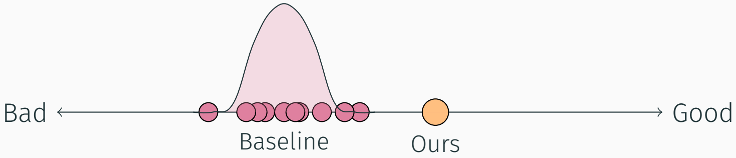
# Model evaluation: Comparison




Approach 2:

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

# Model evaluation: Comparison

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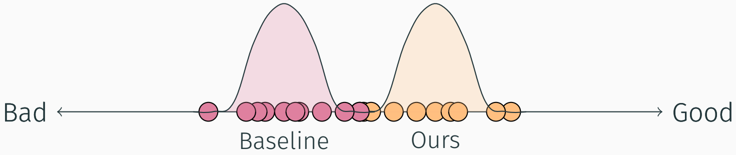


Approach 3:

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

# Model evaluation: 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 evaluation: Summary

- Model evaluation should **always** happen out-of-sample
- If n is big ($\geq 10000$), 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 bootstrapping) 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 across folds using Wilcoxon signed-rank test **(ensure the folds are the same!)**

# Model selection and evaluation

# Model selection and evaluation

- 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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→ We need a more advanced strategy

# Model selection and evaluation: Train/validation/test

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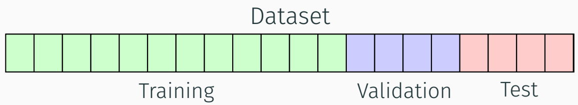
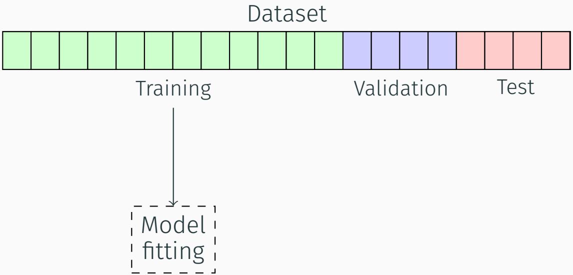


# Model selection and evaluation: Train/validation/test



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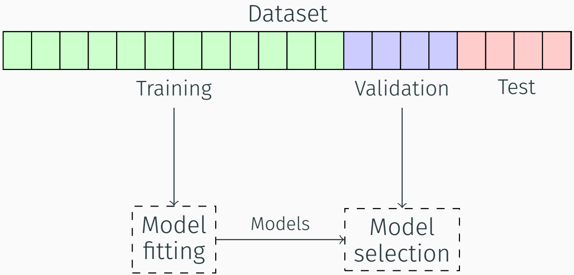
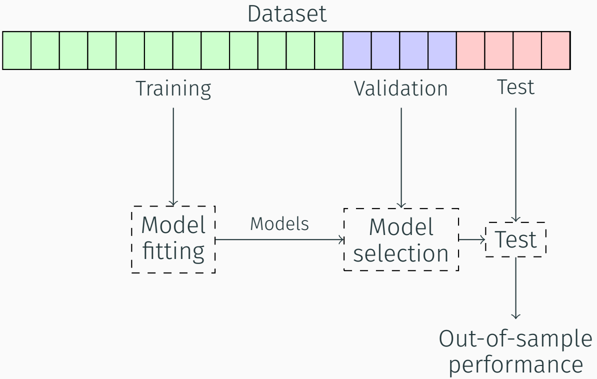
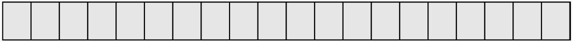


# Model selection and evaluation: Train/validation/test



# Model selection and evaluation: Nested cross-validation

Dataset



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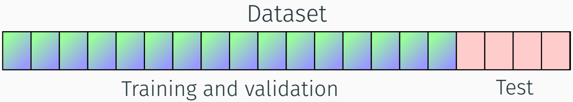

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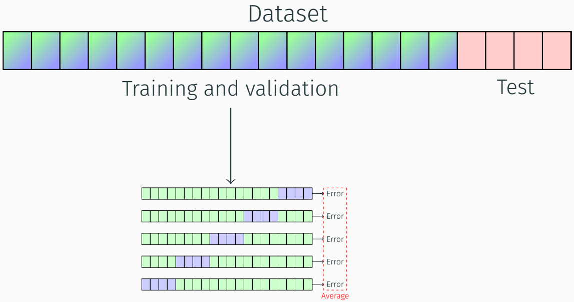

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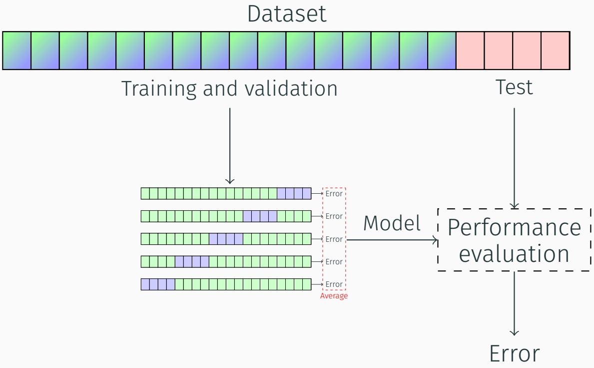

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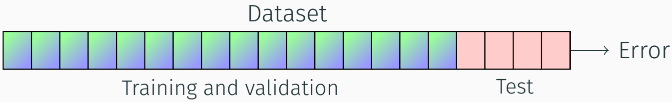

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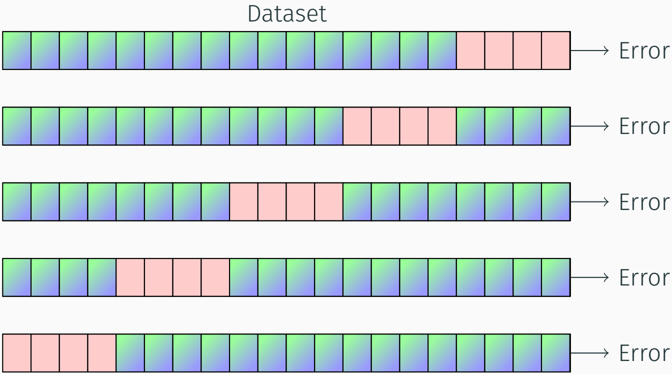

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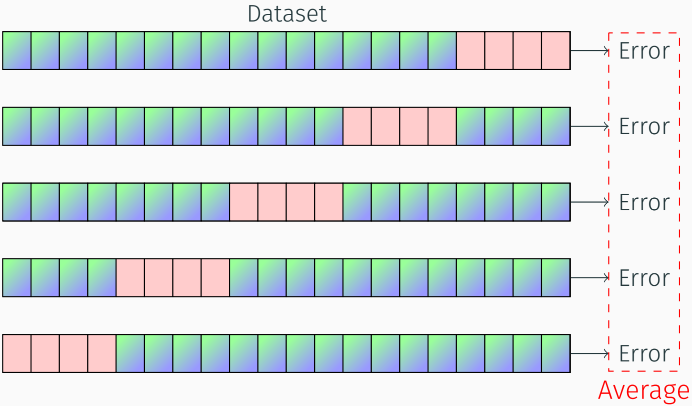

# Model selection and evaluation: Summary

- Whenever a 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 ($\geq 10000$), 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