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
4. Strategies for model selection **and** assessment
    - Train/validation/test split
    - Nested cross-validation

Coding tips

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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]:

```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('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

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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

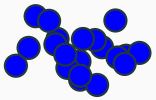
$$1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2}$$

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

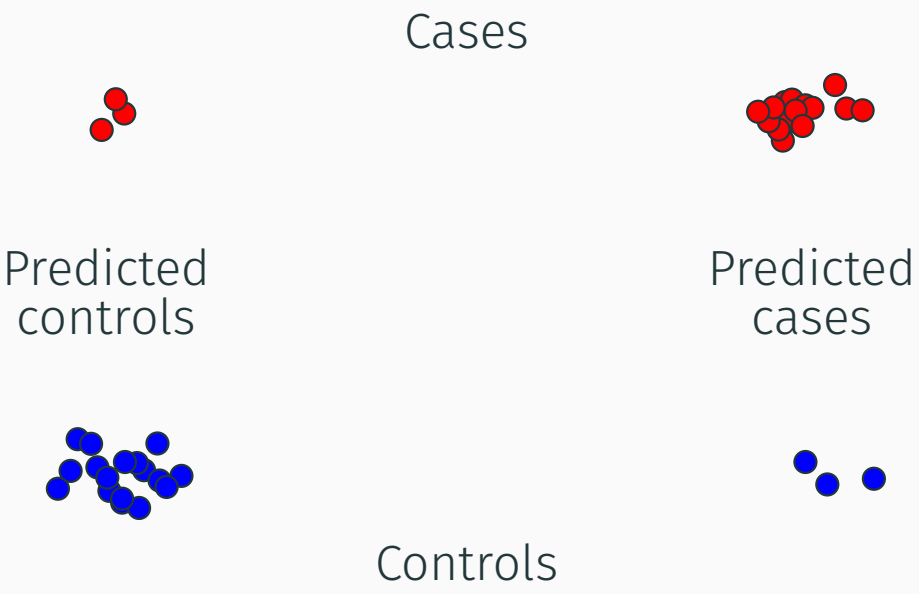
Performance metrics: Binary classification

Cases

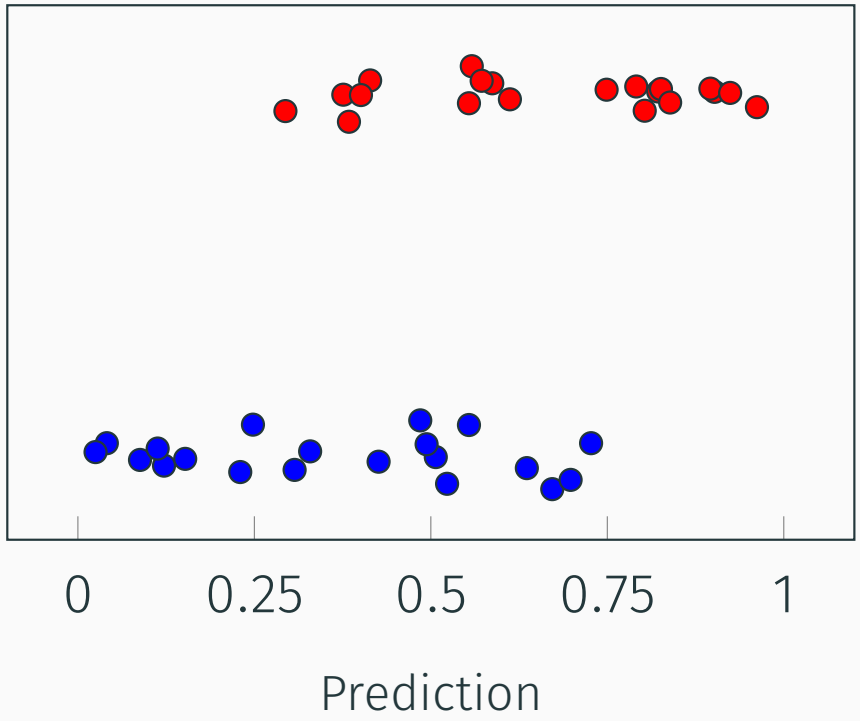


Controls

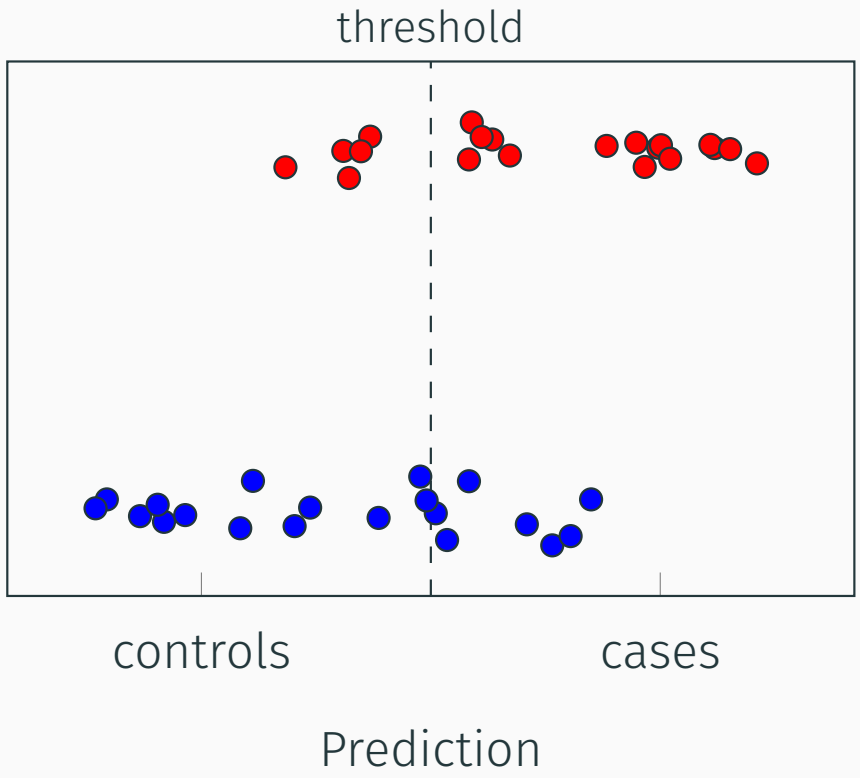
Performance metrics: Binary classification



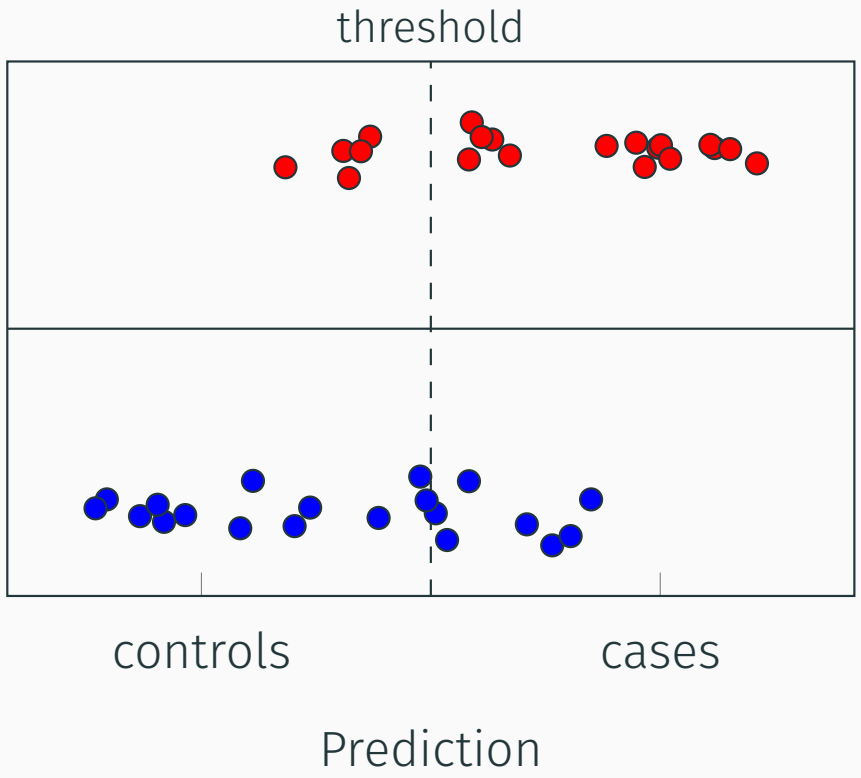
Performance metrics: Binary classification



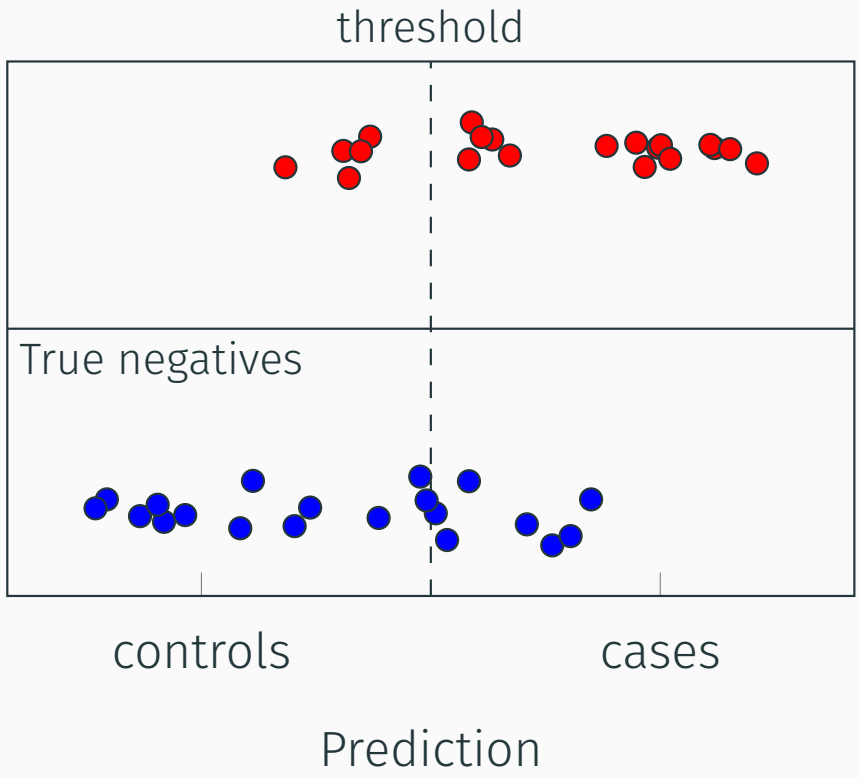
Performance metrics: Binary classification



Performance metrics: Binary classification

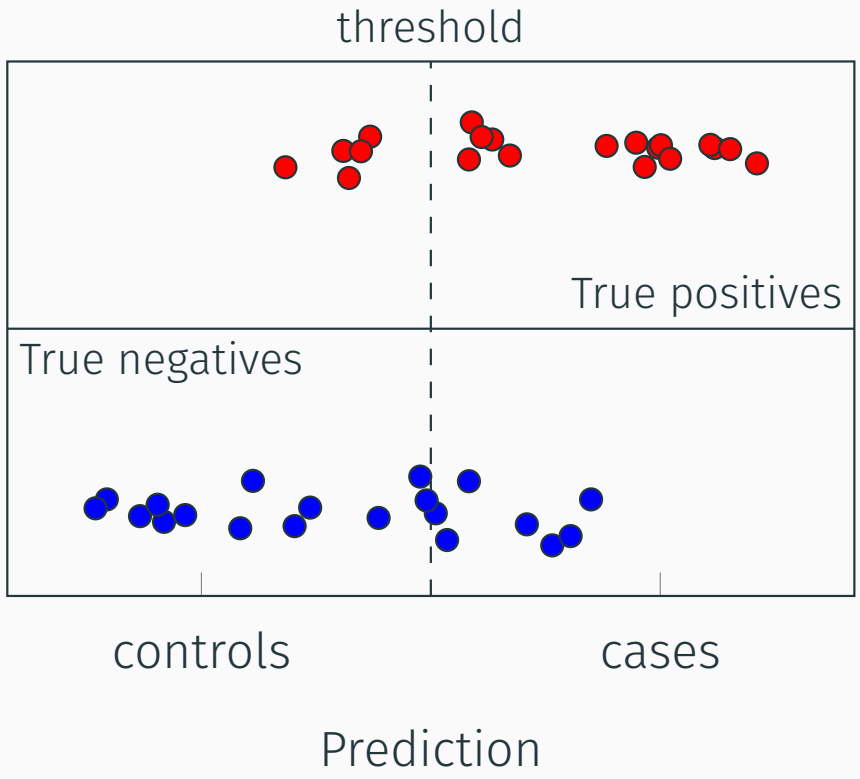


Performance metrics: Binary classification



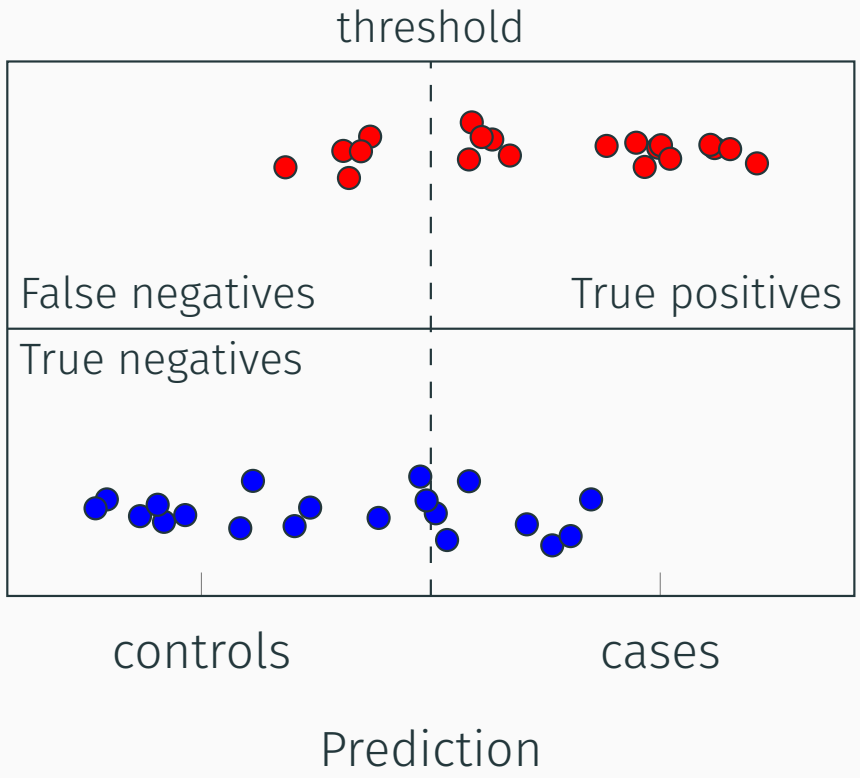
	TN

Performance metrics: Binary classification



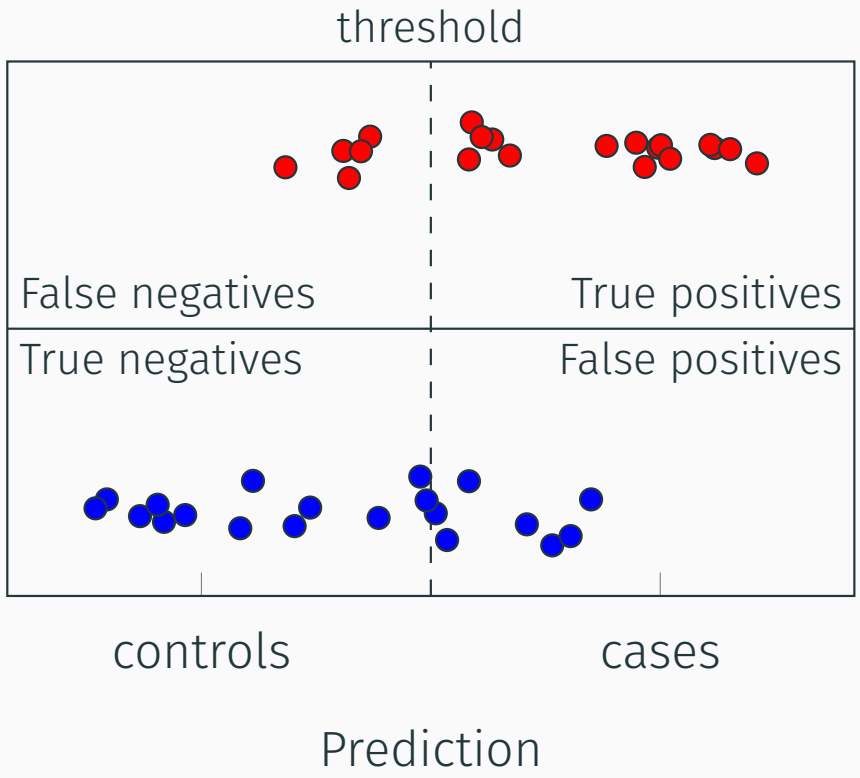
TP	
	TN

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

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

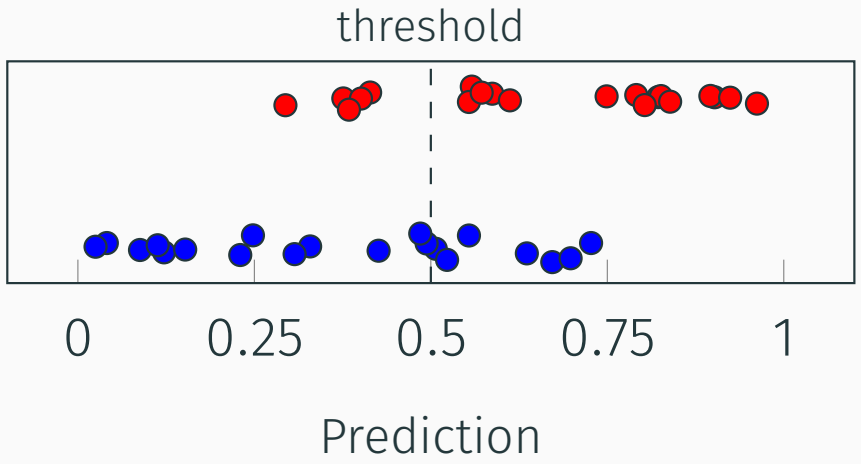
Performance metrics: Binary classification

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

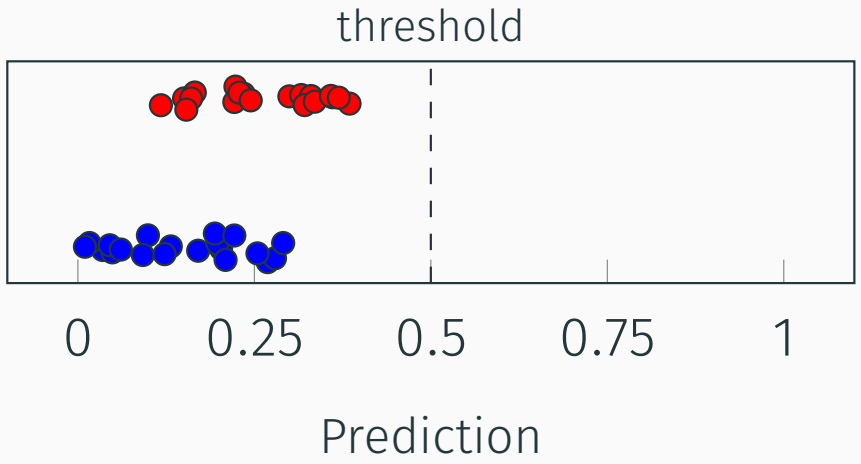
Balanced accuracy

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

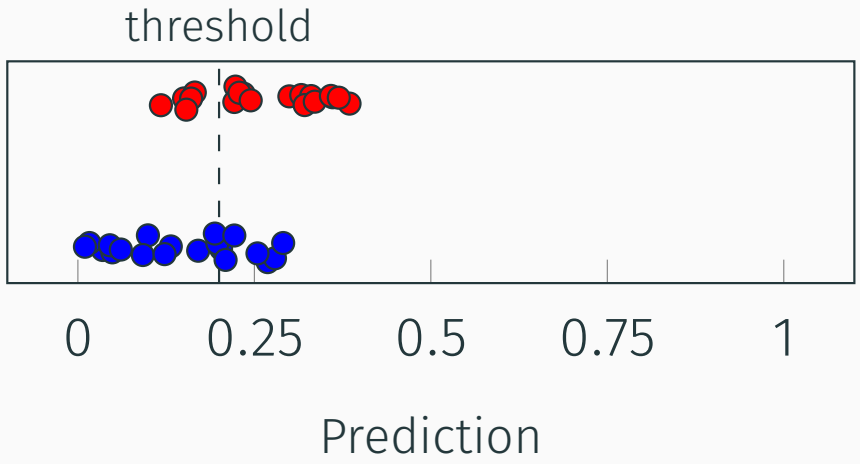
Performance metrics: Binary classification



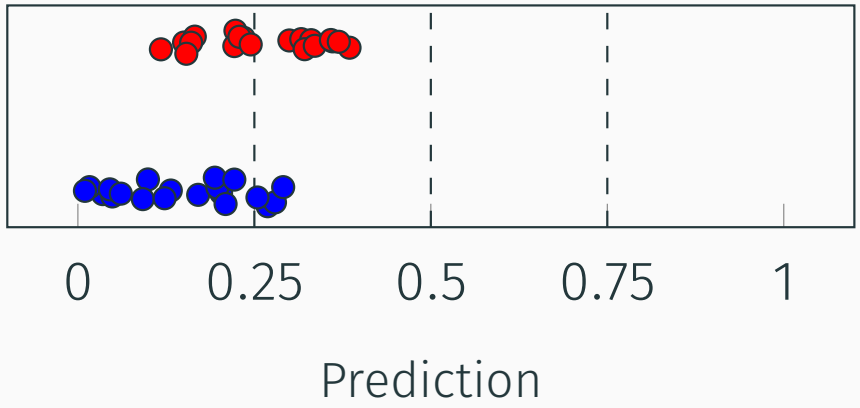
Performance metrics: Binary classification



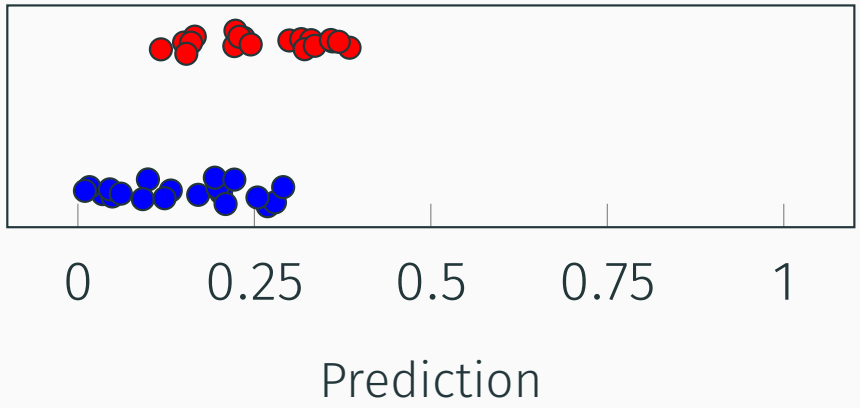
Performance metrics: Binary classification



Performance metrics: Binary classification

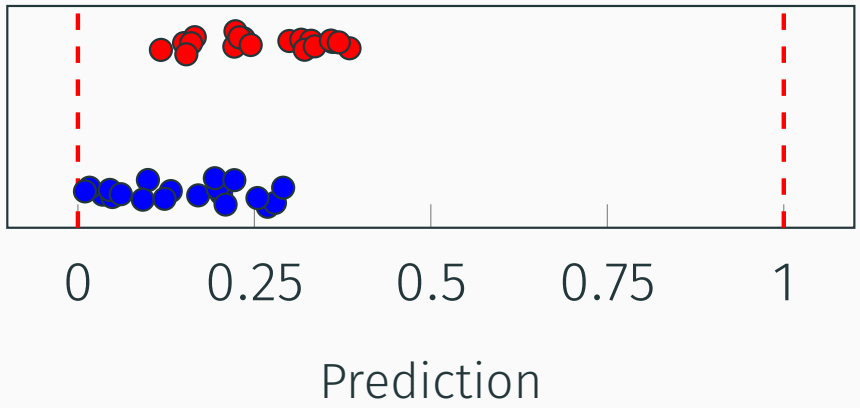


Performance metrics: Binary classification



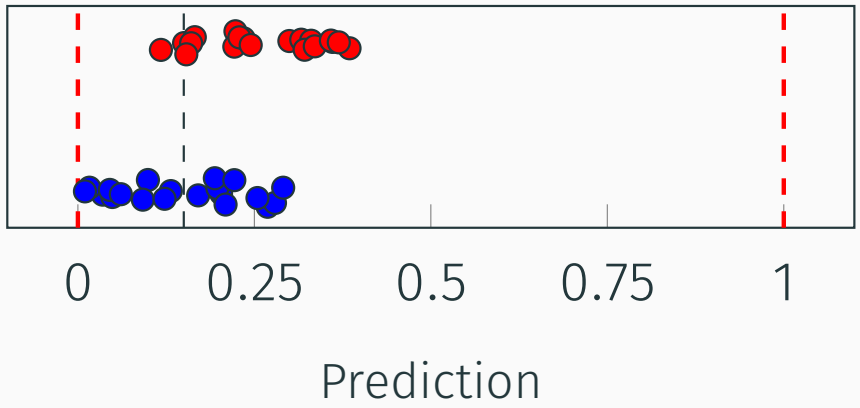
threshold	TPR	FPR

Performance metrics: Binary classification



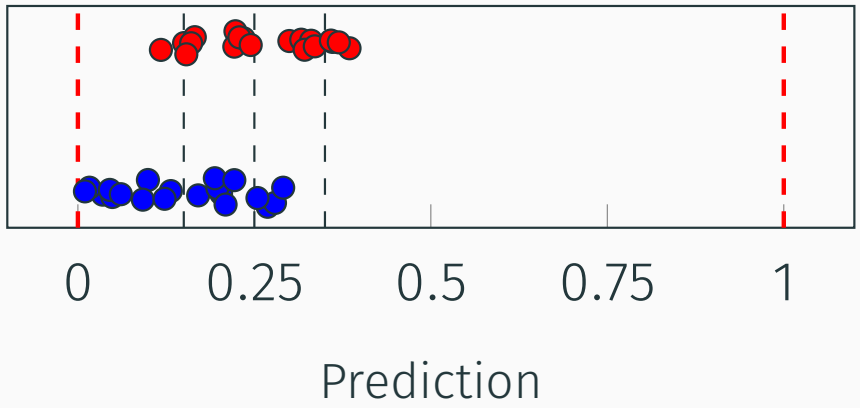
threshold	TPR	FPR
0	0	0
1	1	1

Performance metrics: Binary classification



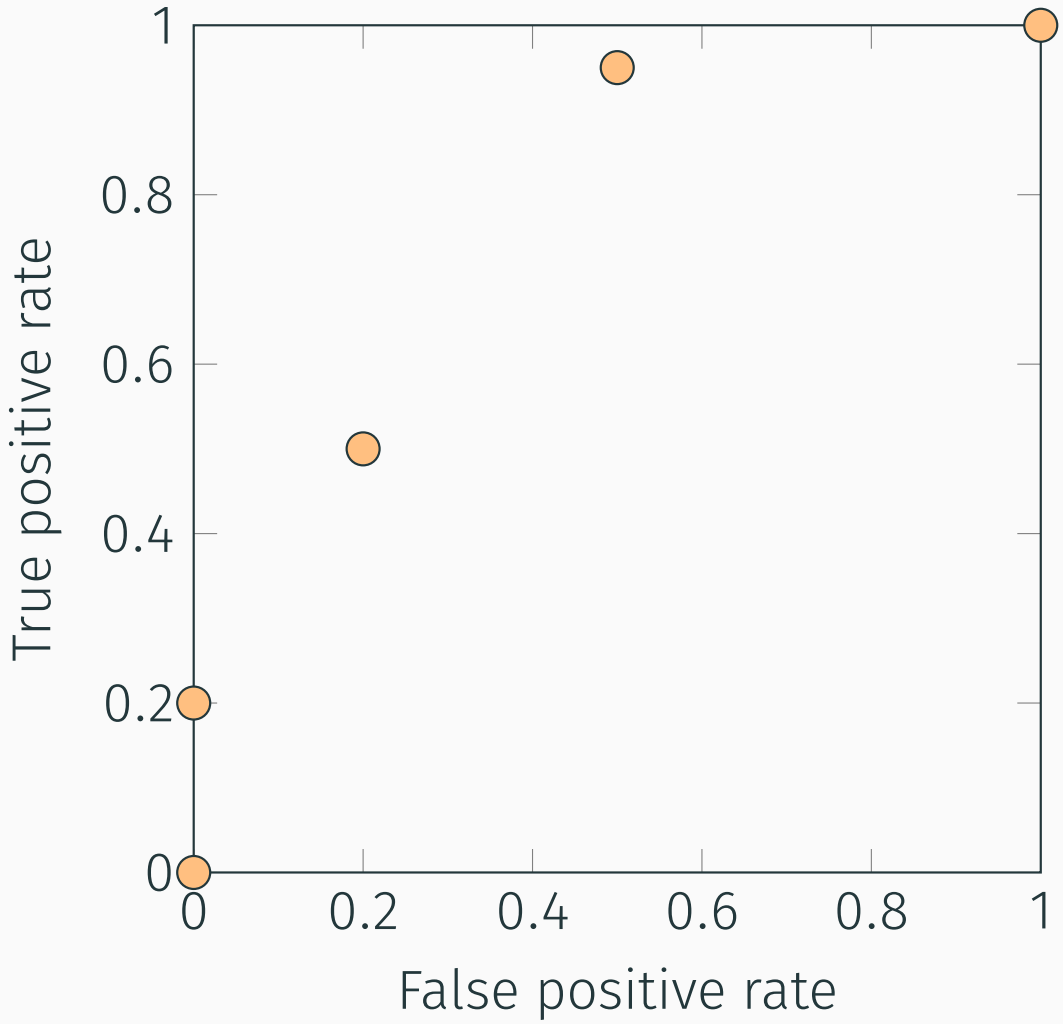
threshold	TPR	FPR
0	0	0
0.15	0.95	0.5
1	1	1

Performance metrics: Binary classification

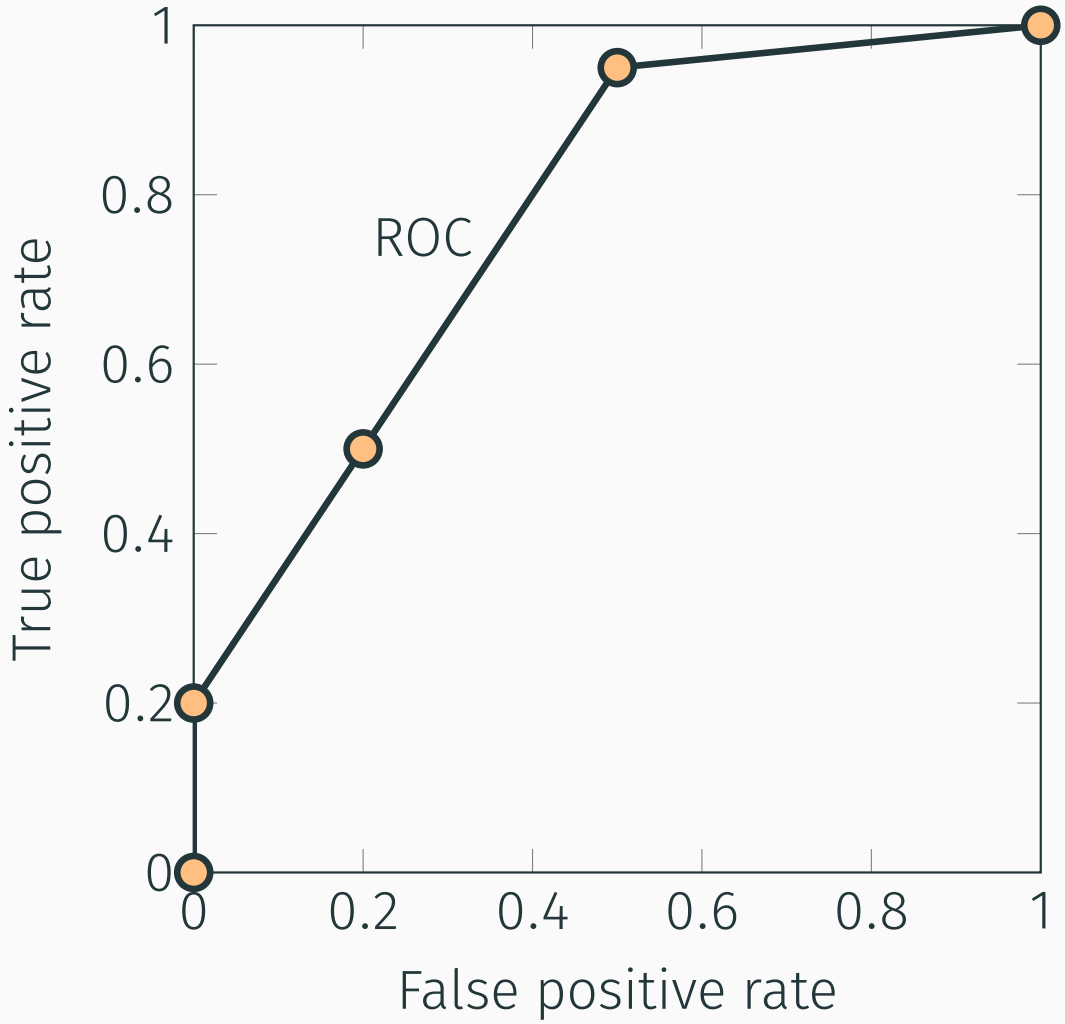


threshold	TPR	FPR
0	1	1
0.15	0.95	0.5
0.25	0.5	0.2
0.35	0.2	0.0
1	0	0

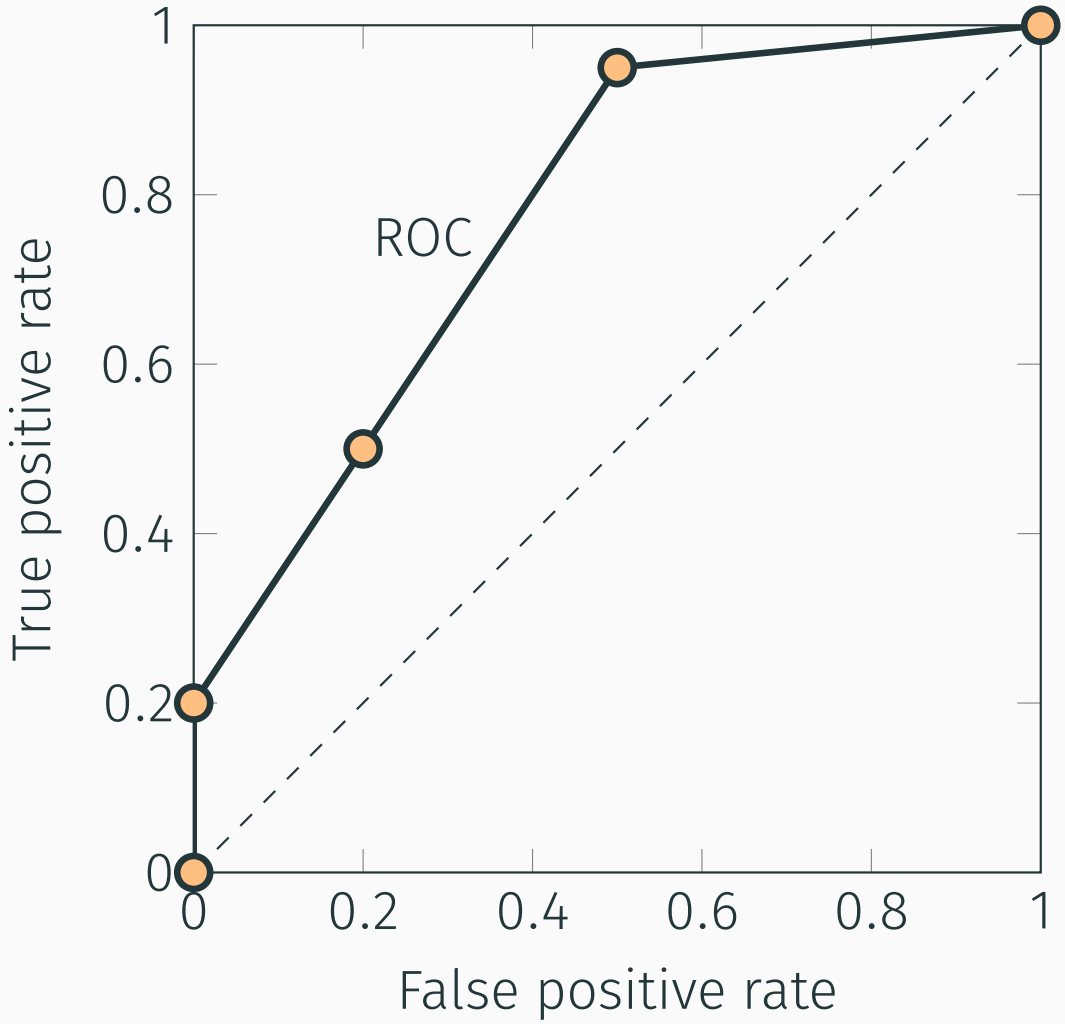
Performance metrics: Binary classification



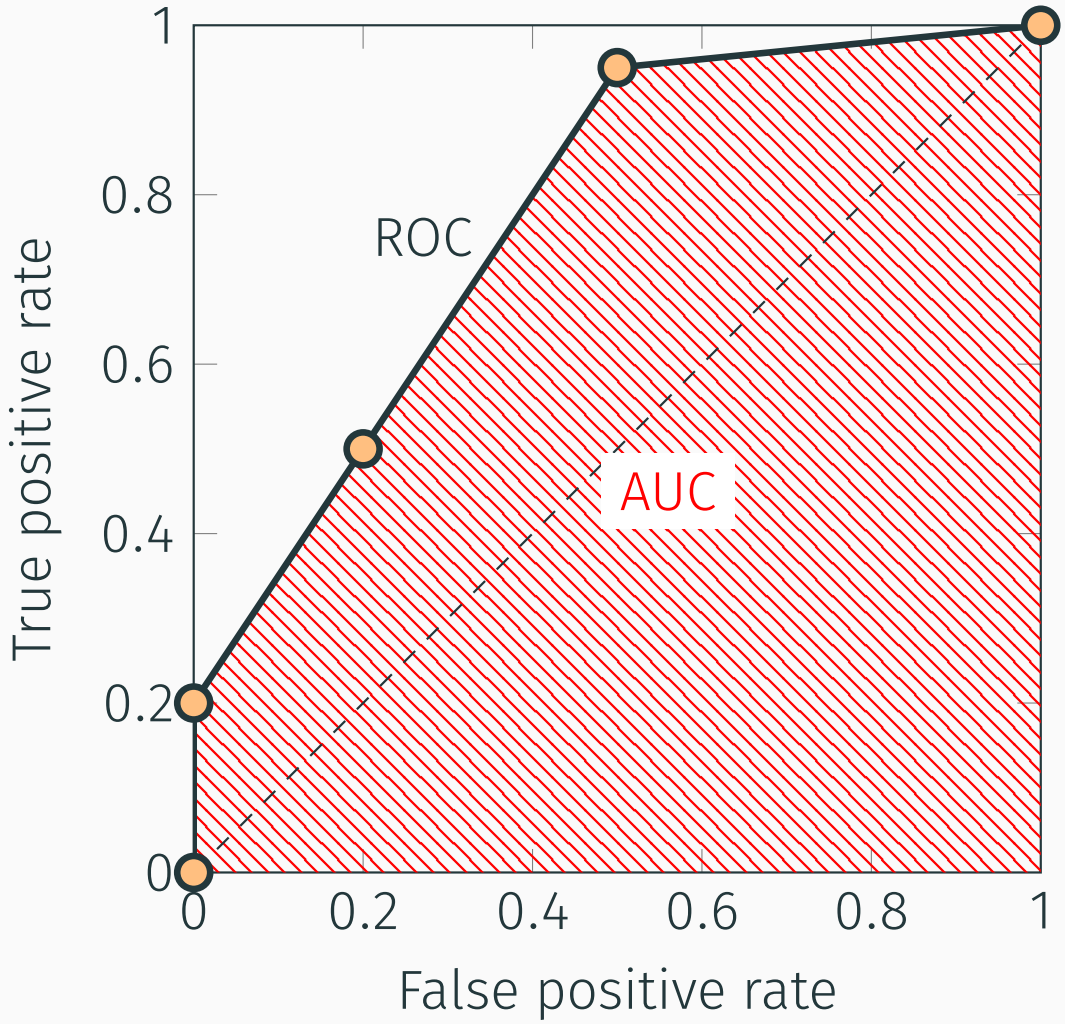
Performance metrics: Binary classification



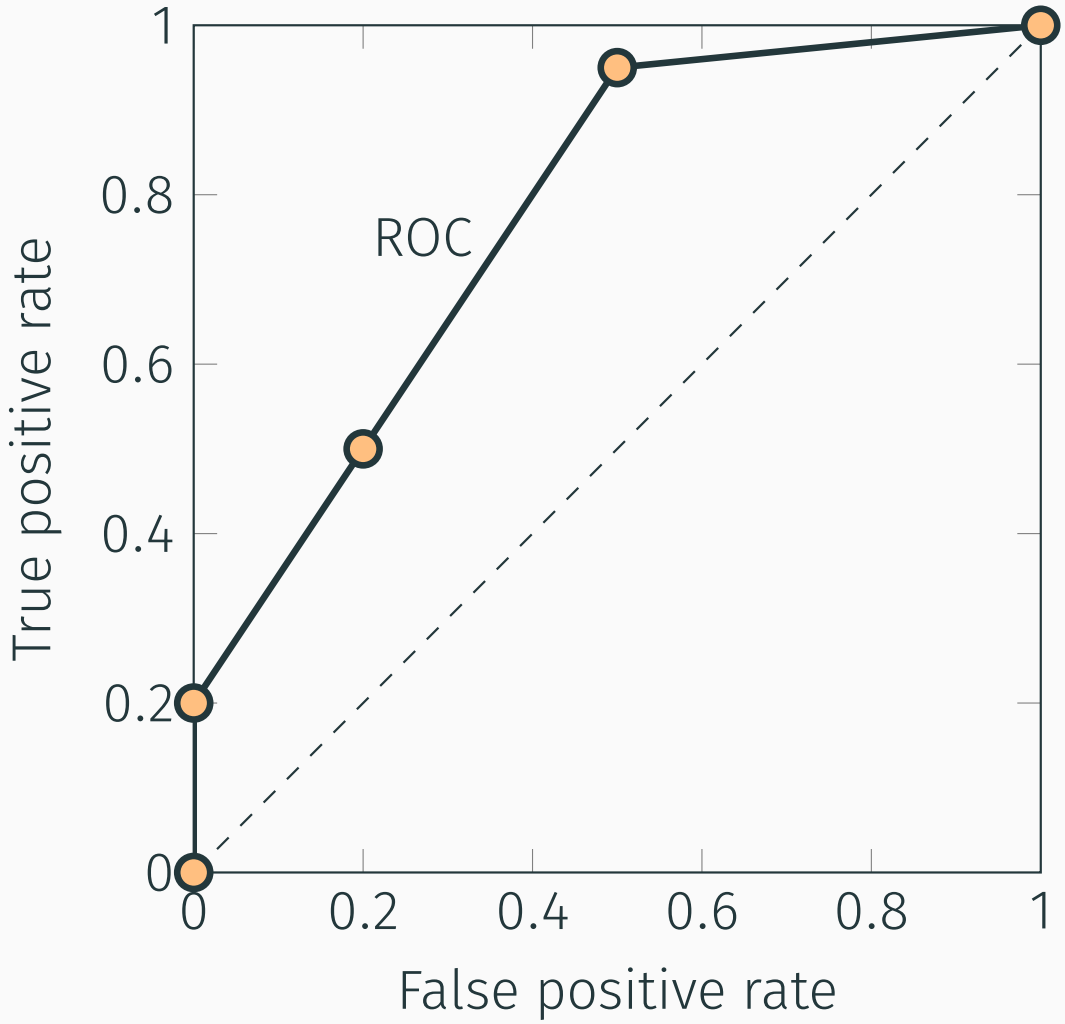
Performance metrics: Binary classification



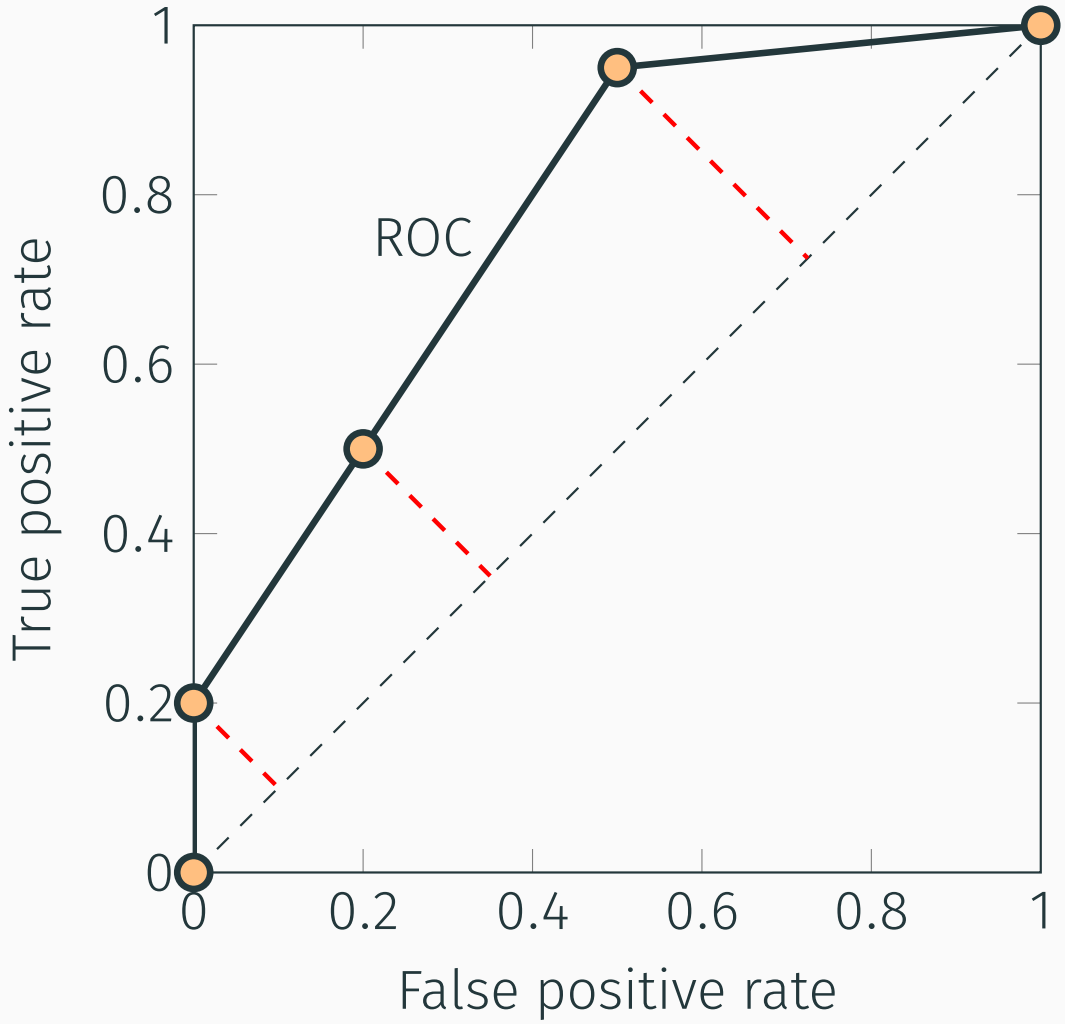
Performance metrics: Binary classification



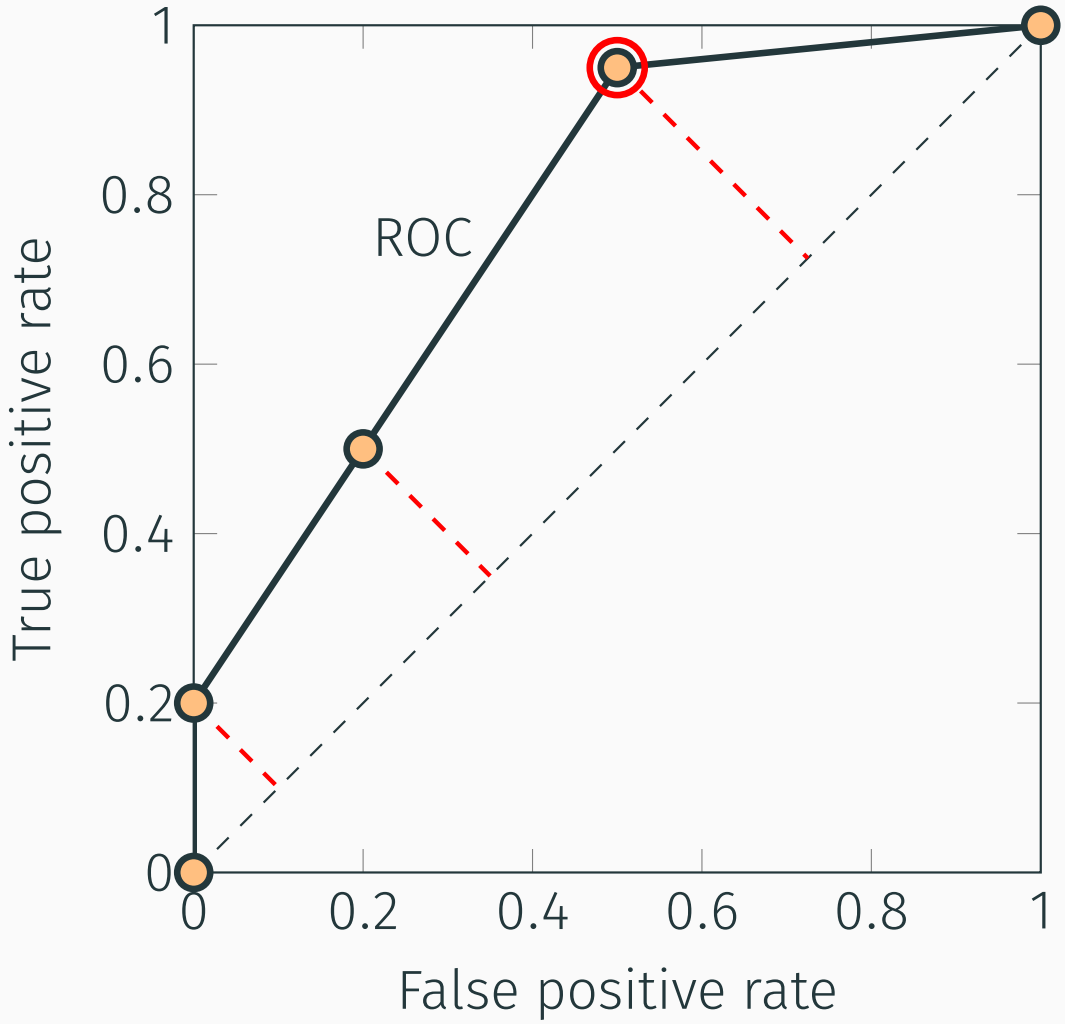
Performance metrics: Binary classification



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

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Model assessment: Rationale

Statistical inference:

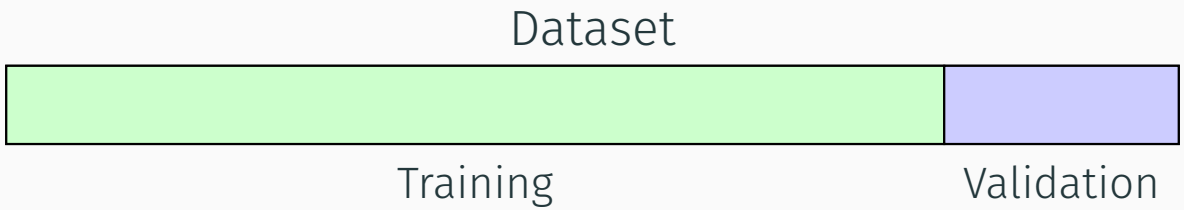
asdf

Predictive modelling:

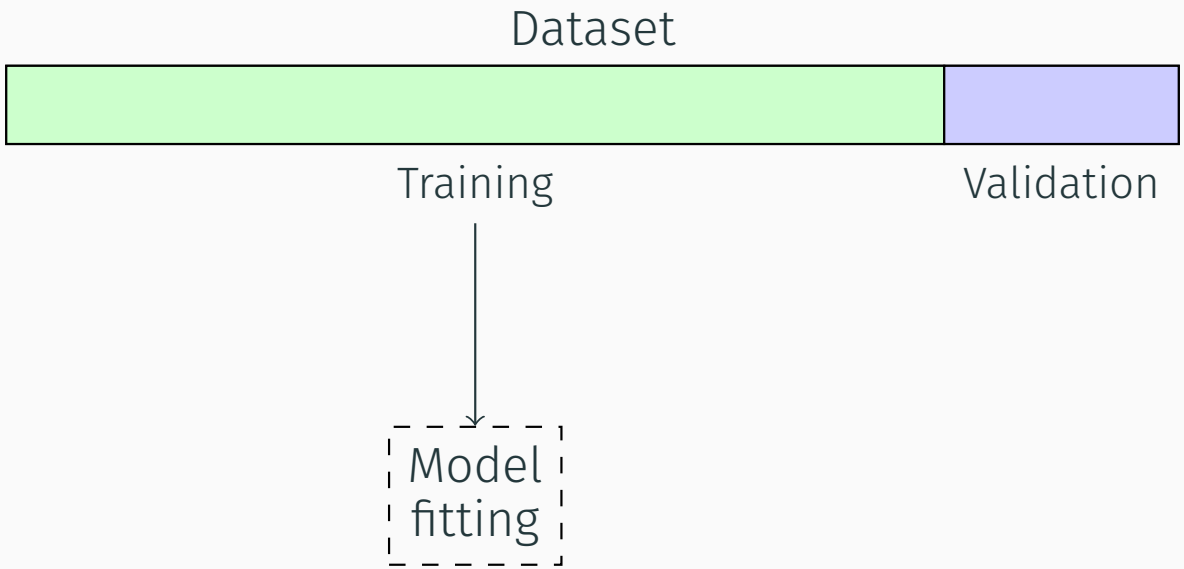
asdf

Model assessment: Validation set

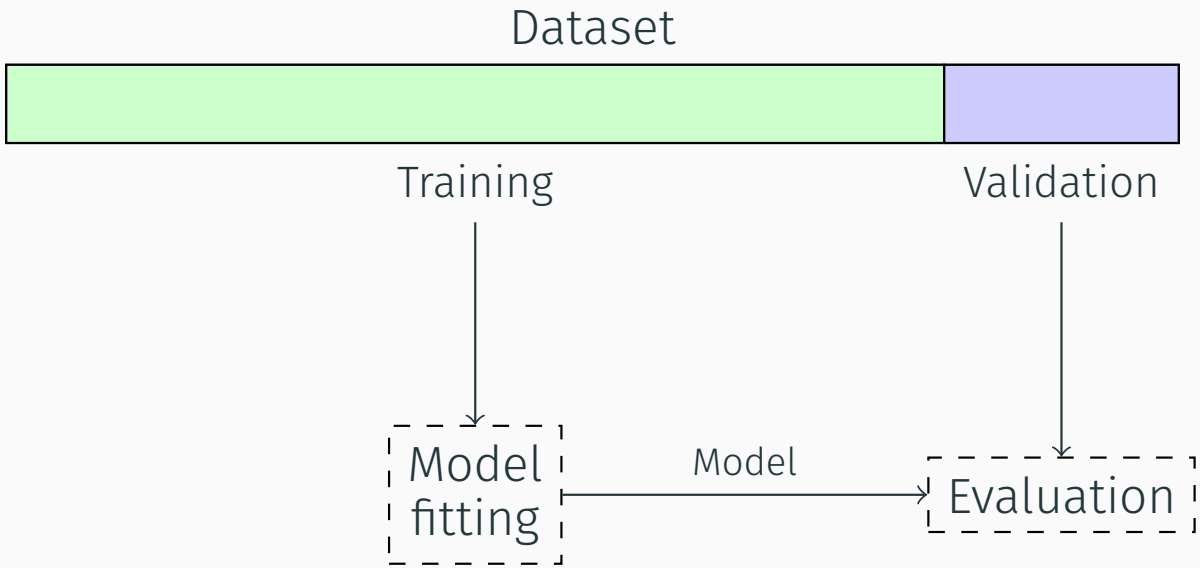
Model assessment: Validation set



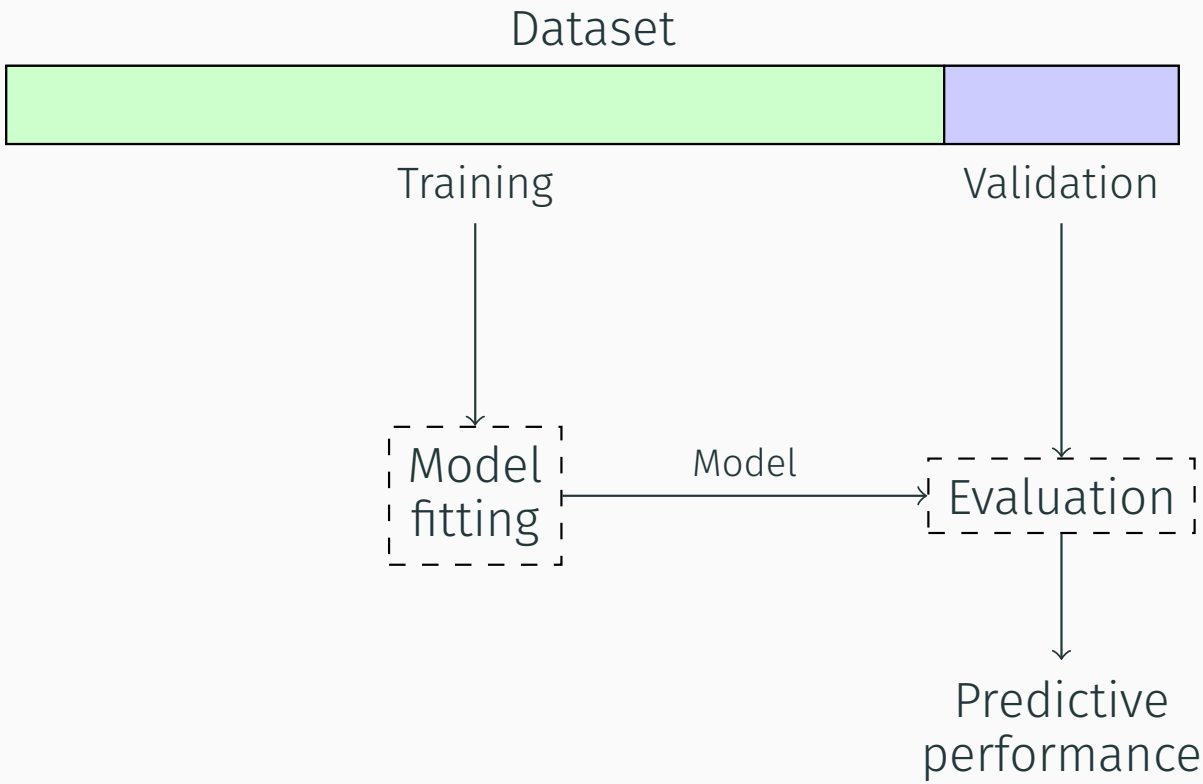
Model assessment: Validation set



Model assessment: Validation set



Model assessment: Validation set

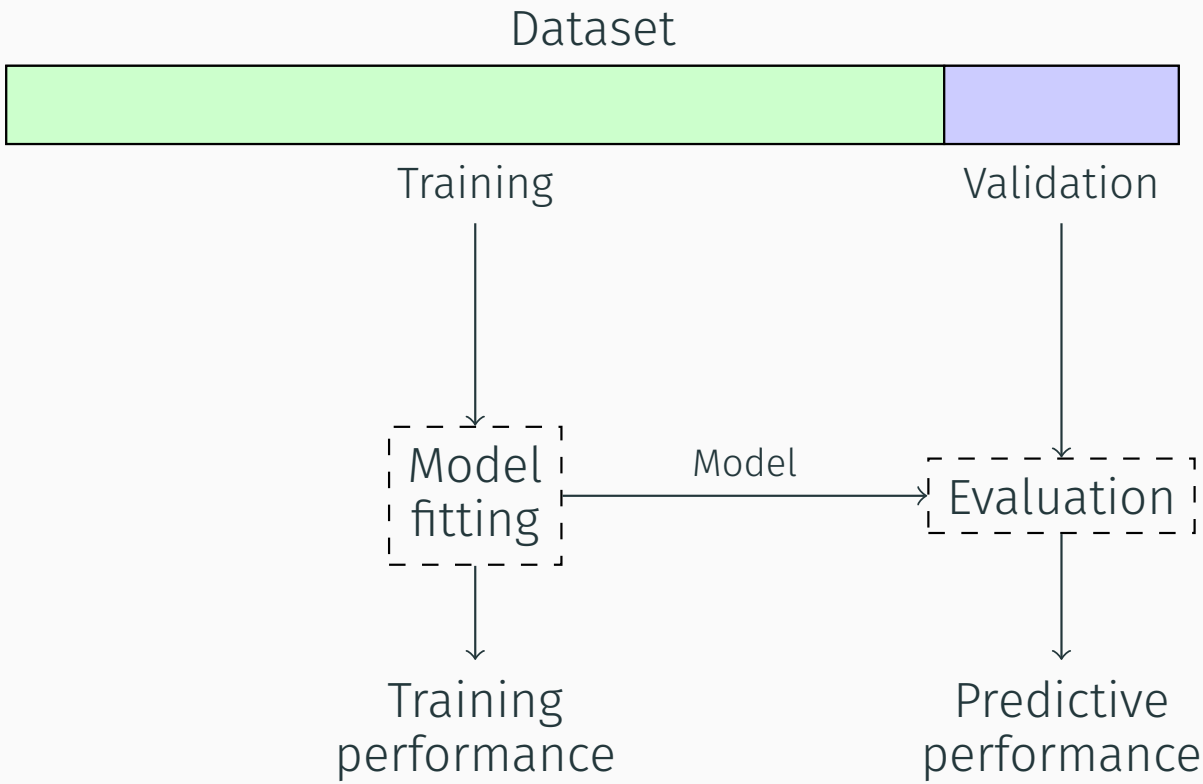


Model assessment: Validation set

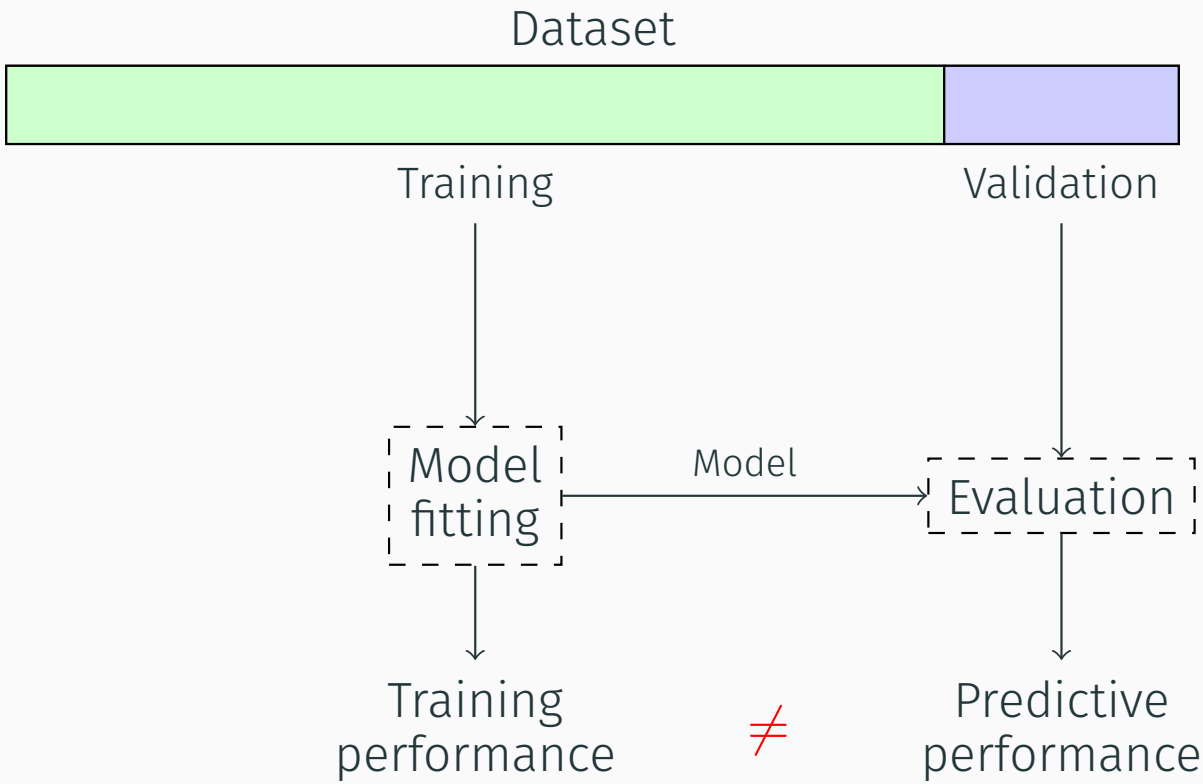
In the validation set approach we split the dataset into two subsets, and use for training the model and the other for testing performance.

+ 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

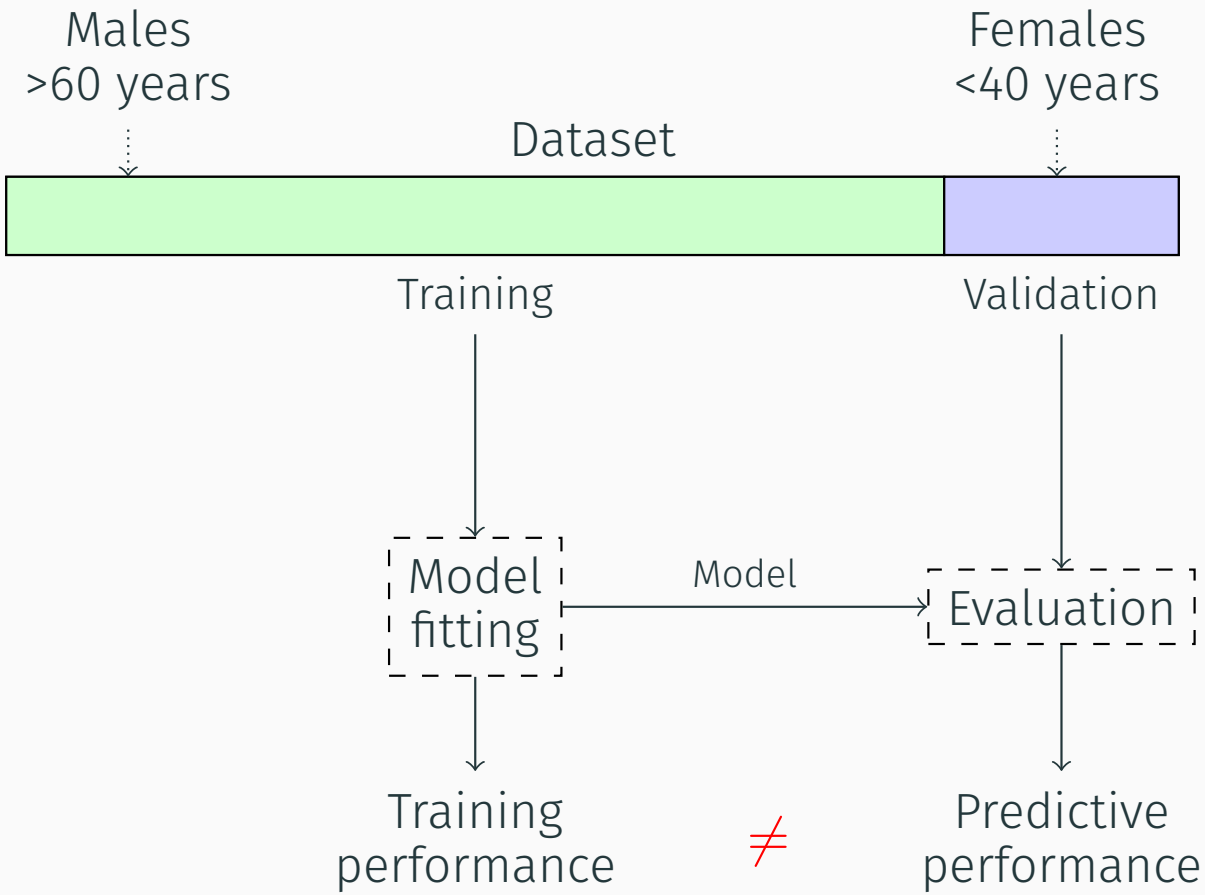
Model assessment: Validation set



Model assessment: Validation set



Model assessment: Validation set



Model assessment: Stratification

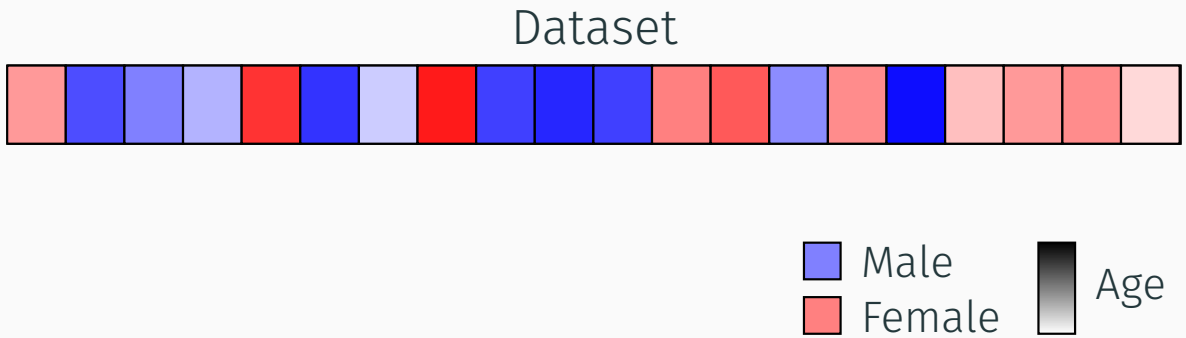
Stratification:

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

Model assessment: Stratification

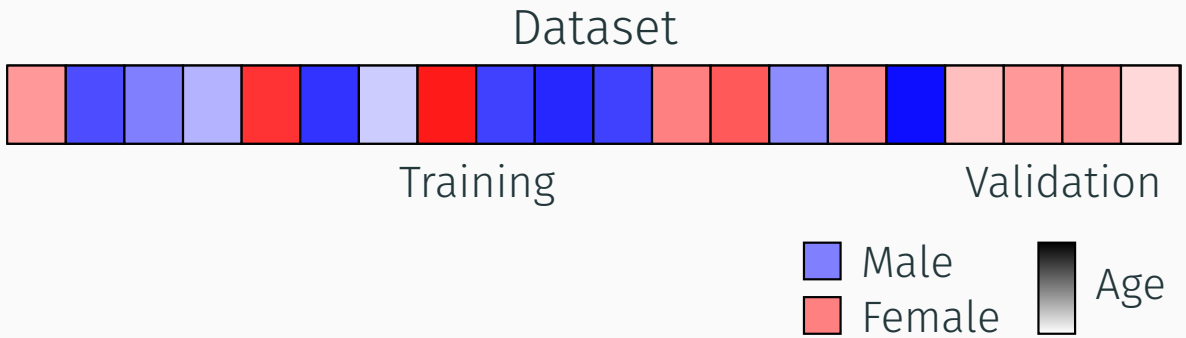
In[1]:
```
df = ...
```

Model assessment: Stratification



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

Model assessment: Stratification

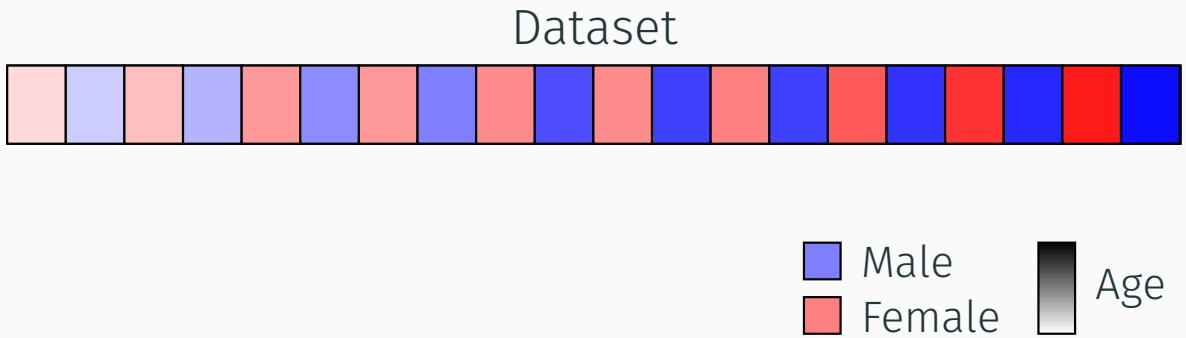


In[1]:

```
df = ...

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

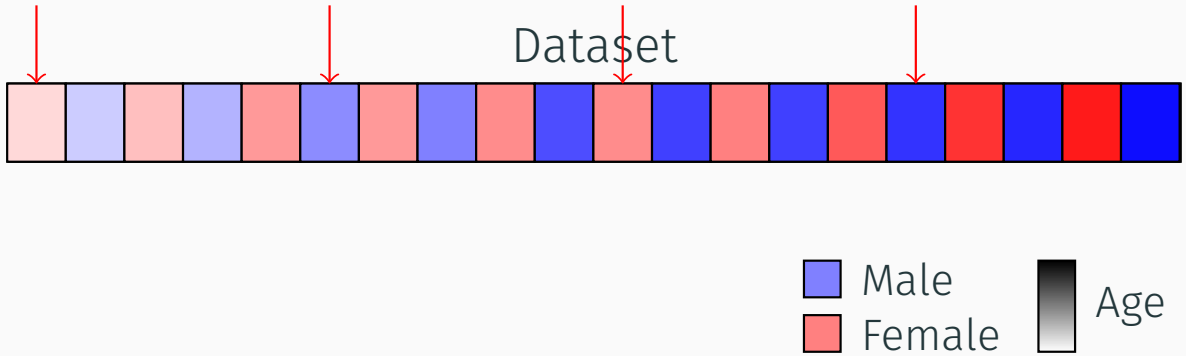
Model assessment: Stratification



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.

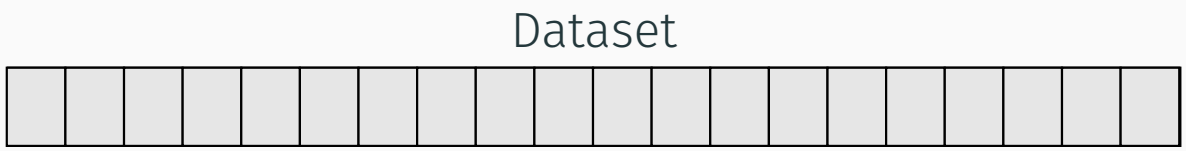
- Helps alleviate the risk of training performance $\gg$ validation performance
- **Always** stratify on target variable first
- Also good idea to stratify on other core characteristics, e.g. sex and age

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

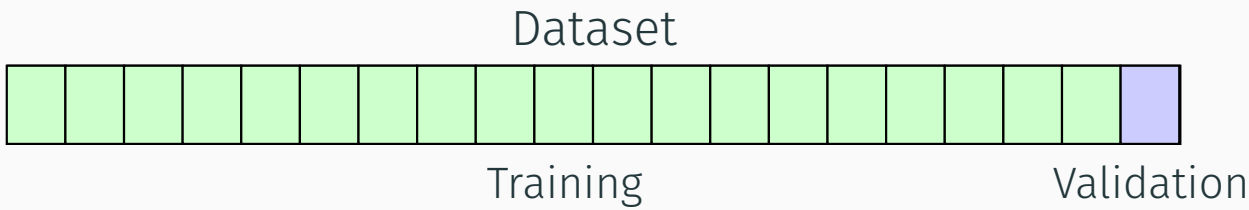
```r
library(splitstackshape)
stratified(data, columns, split)
```

Model assessment: Leave-one-out cross-validation

Model assessment: Leave-one-out cross-validation



Model assessment: Leave-one-out cross-validation



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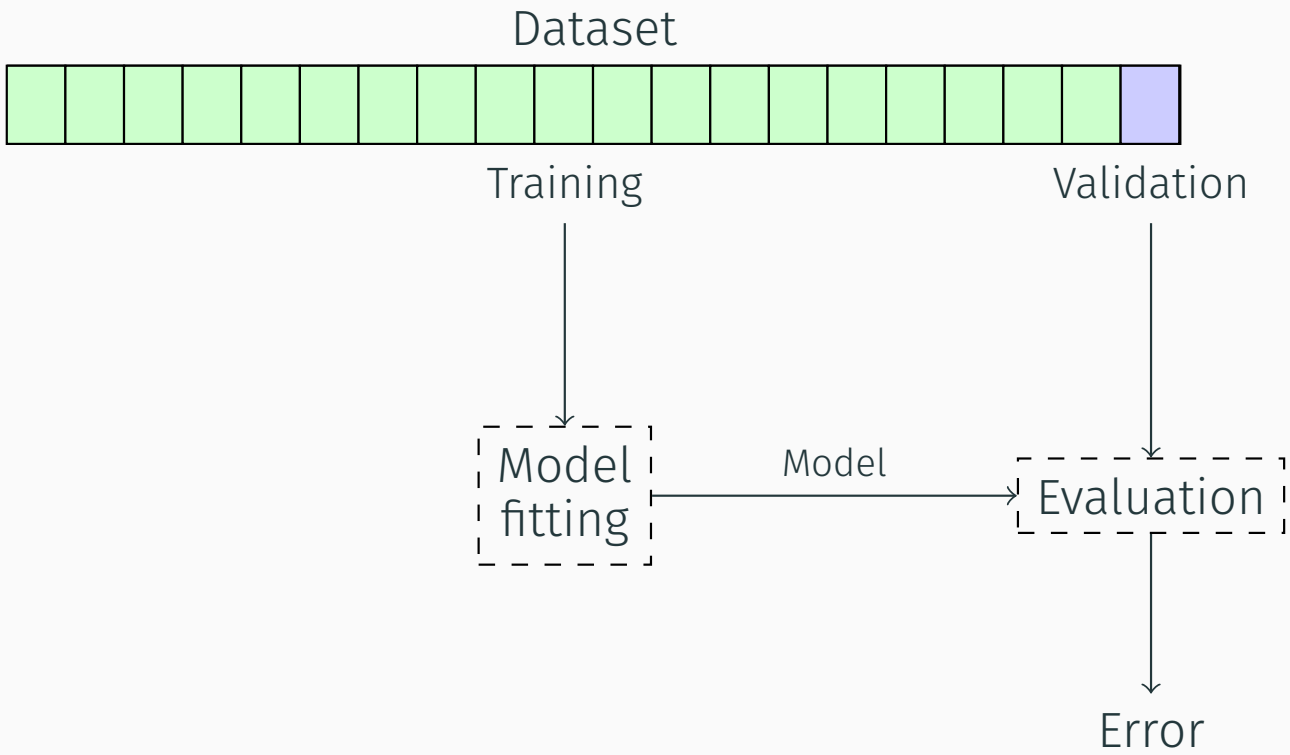

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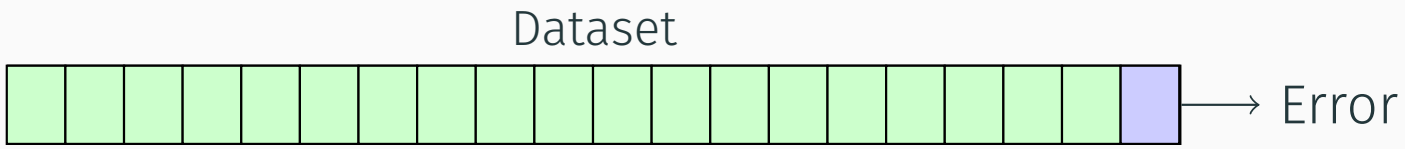

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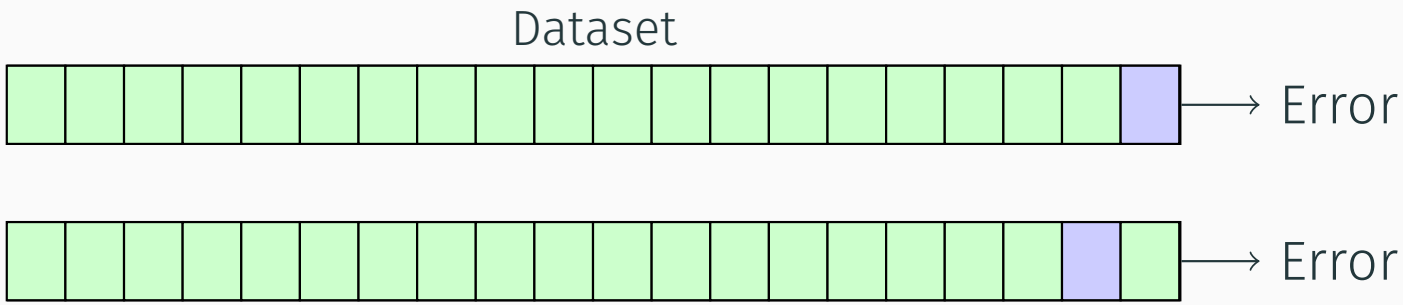

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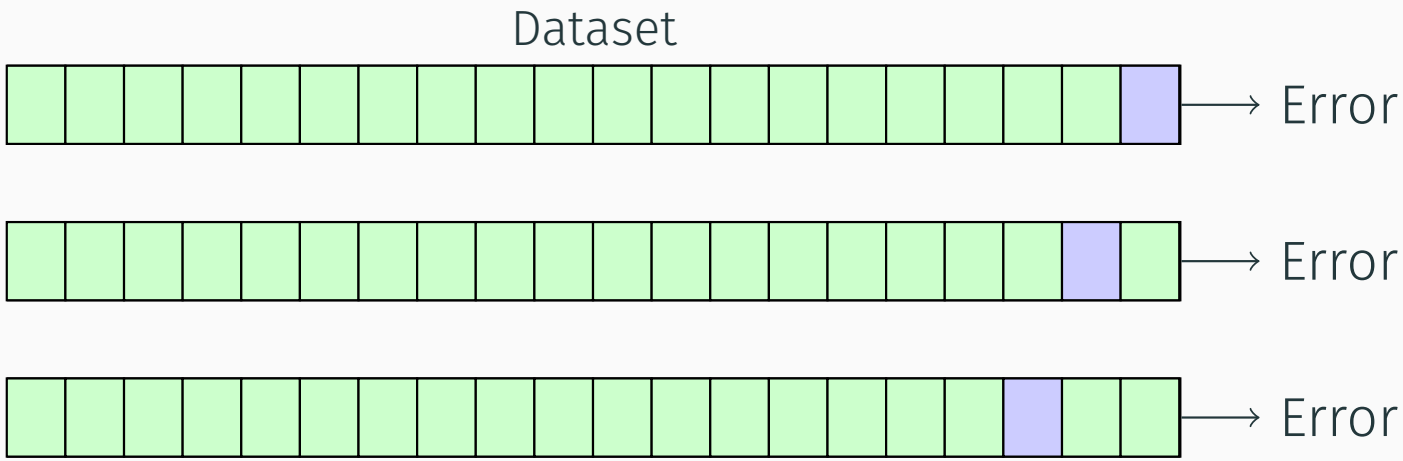

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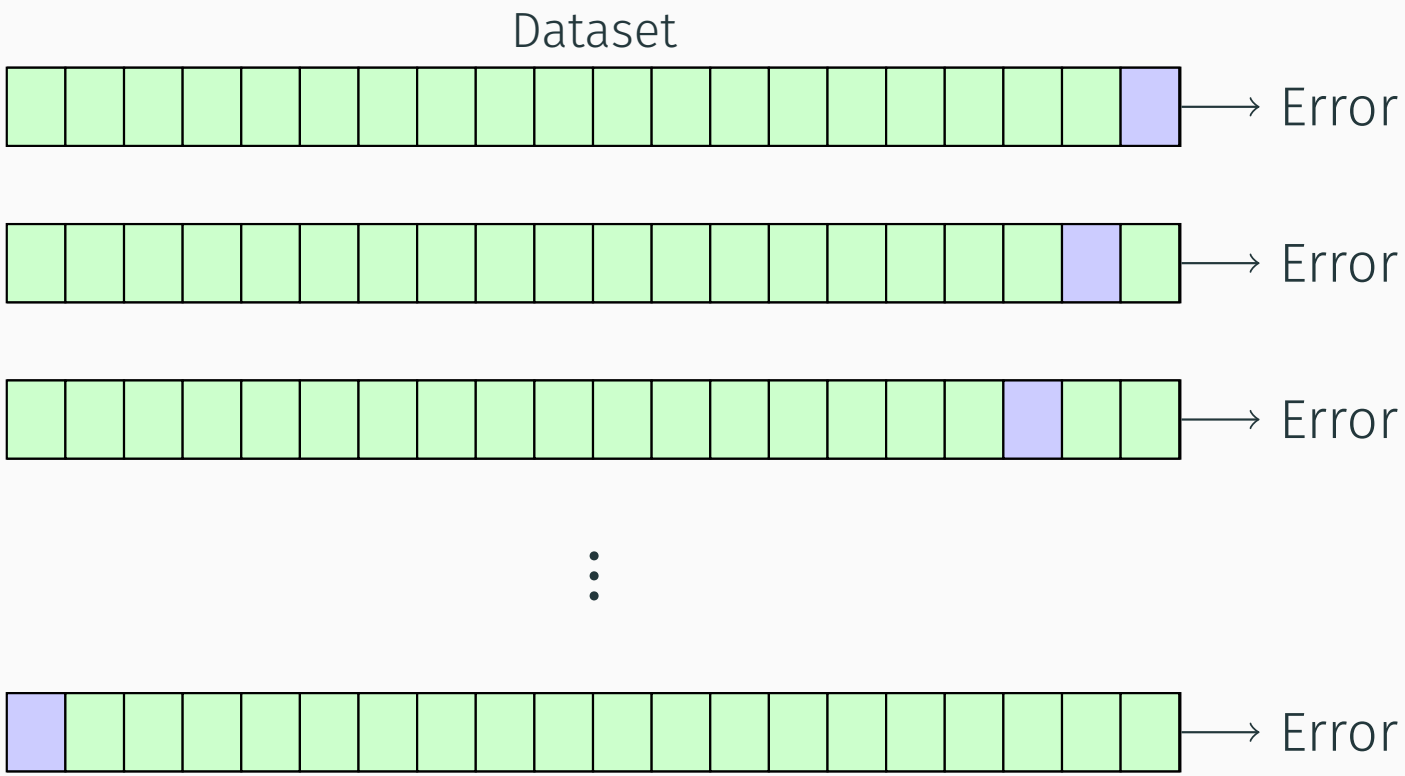

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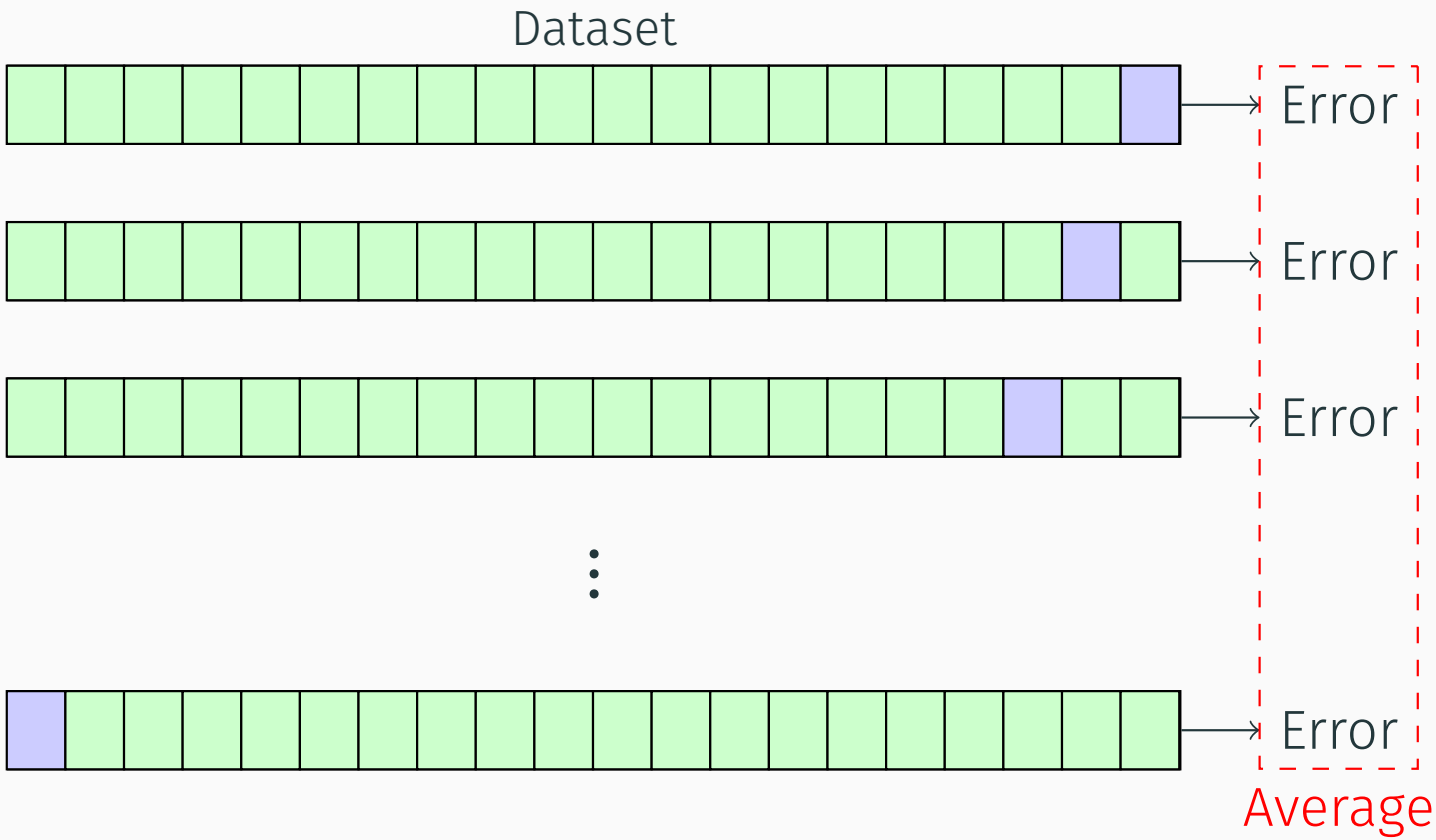
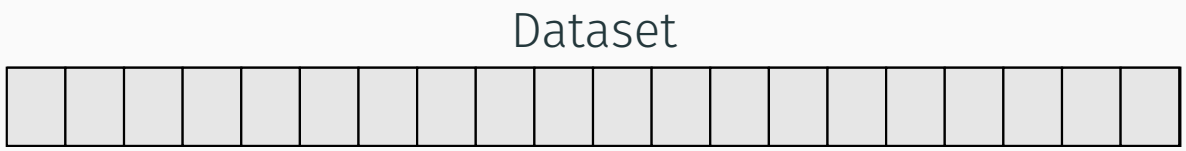


Model assessment: Leave-one-out cross-validation

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



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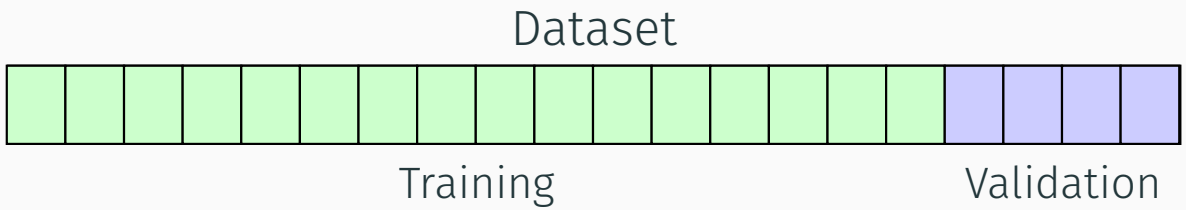

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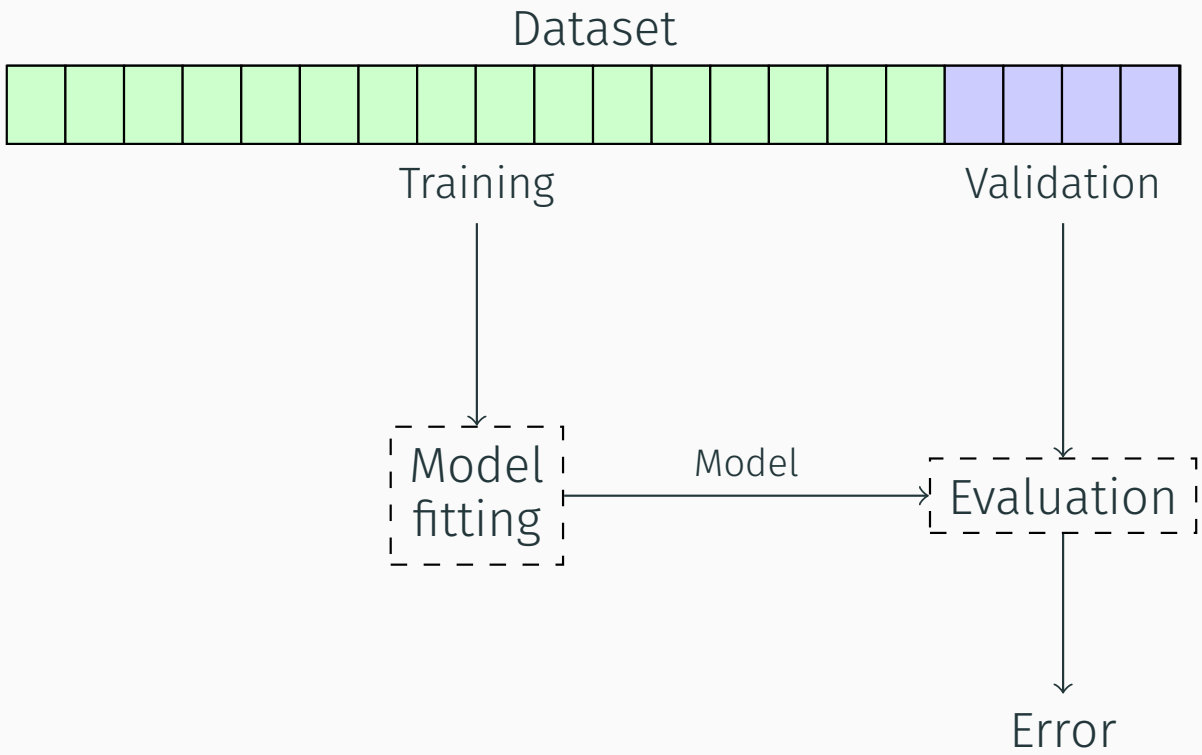

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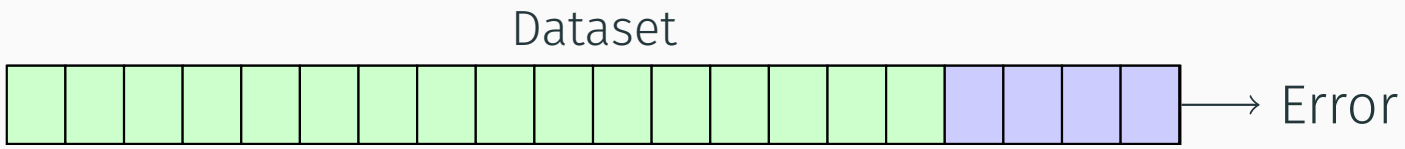

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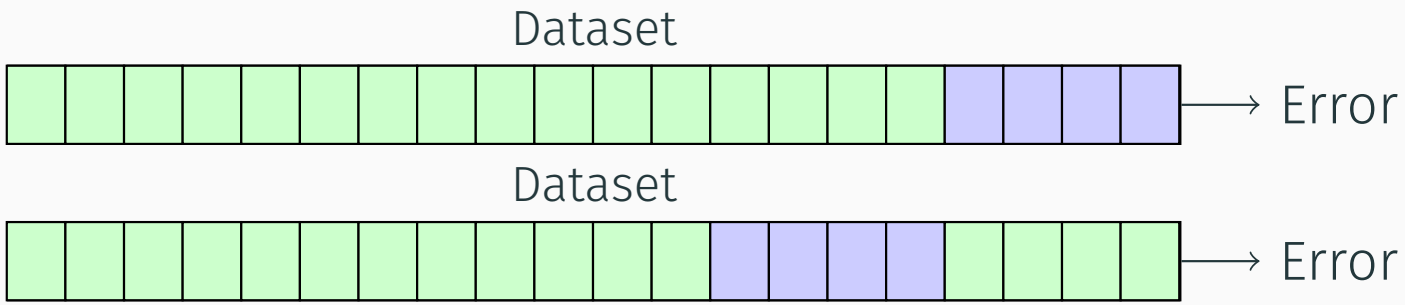

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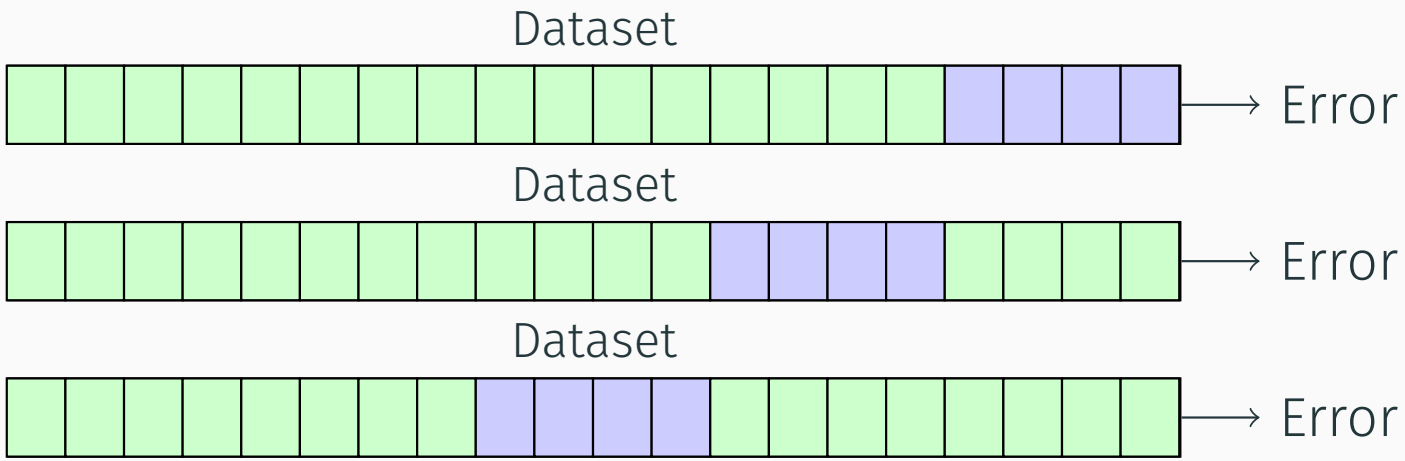
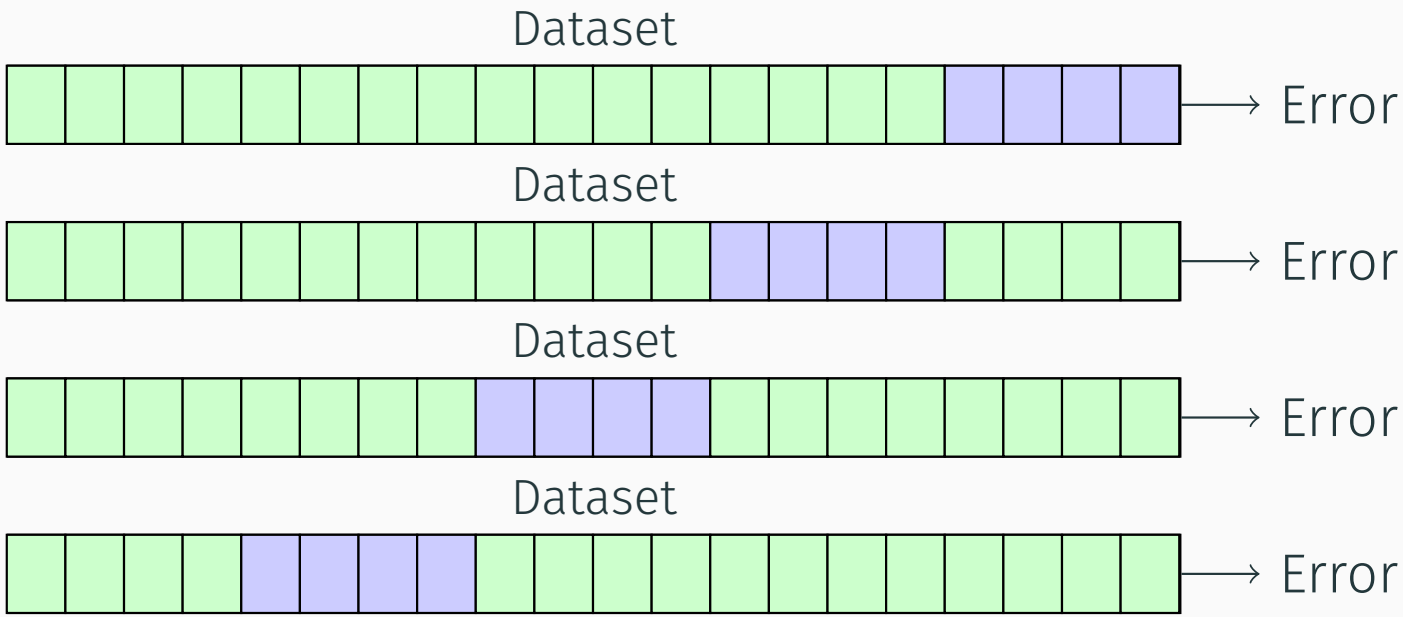


Model assessment: Cross-validation



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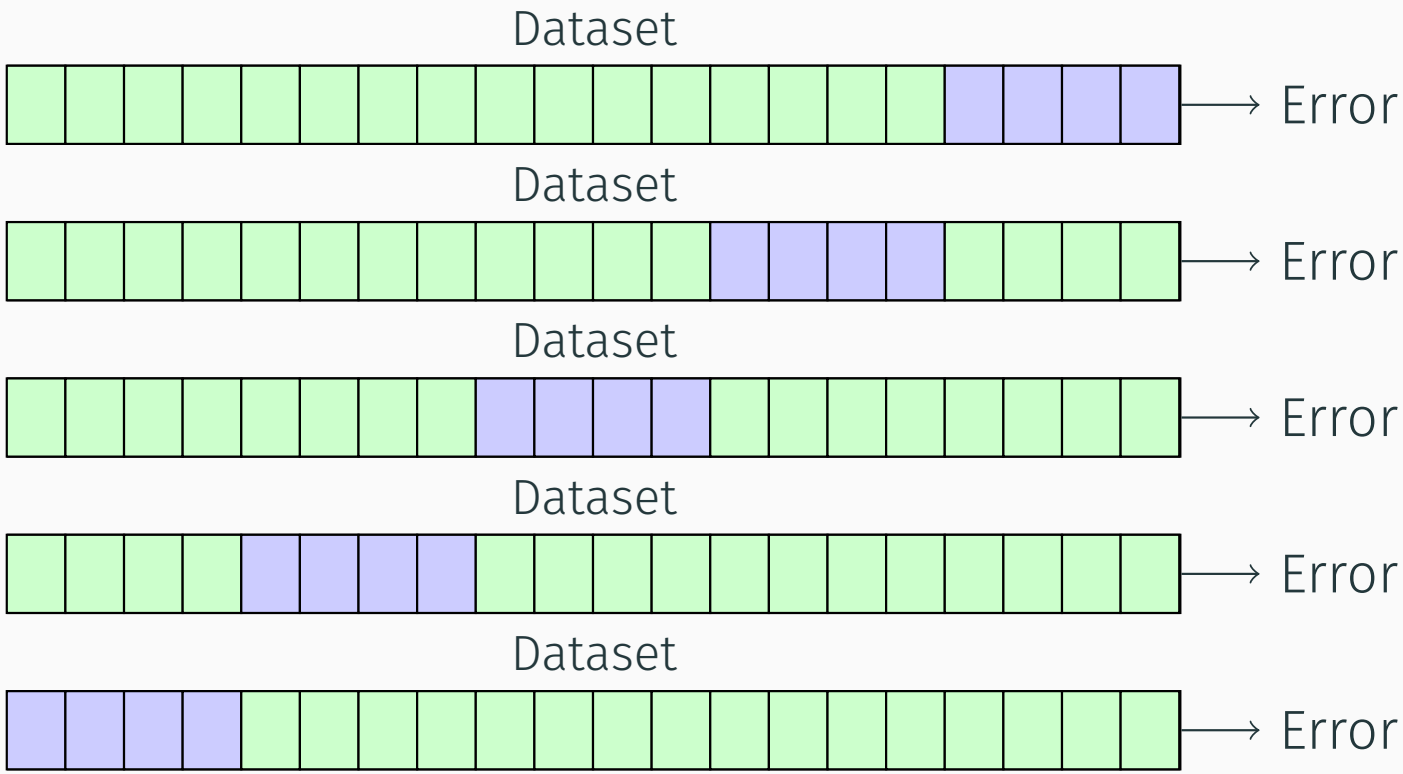

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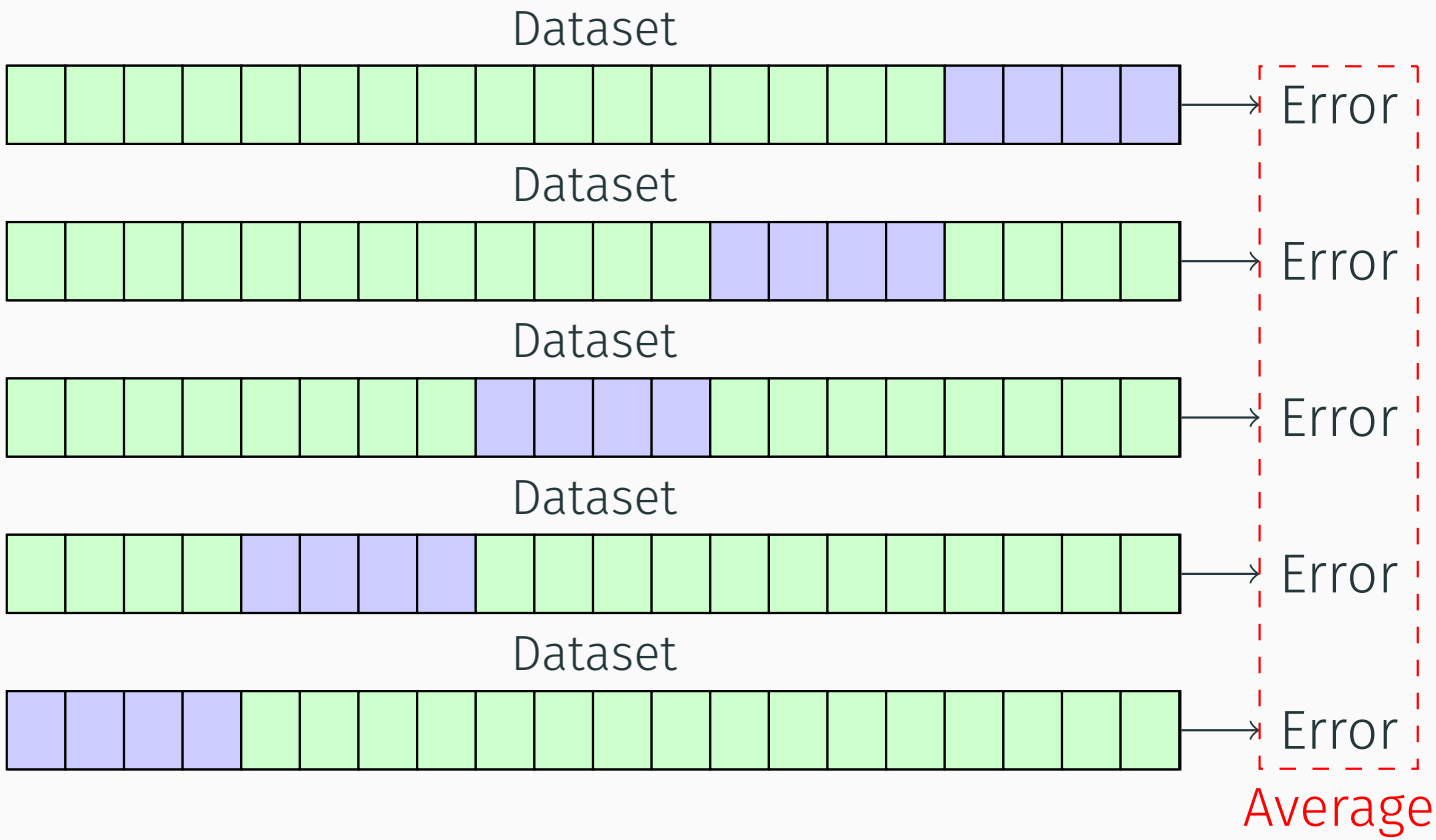

Model assessment: Cross-validation

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

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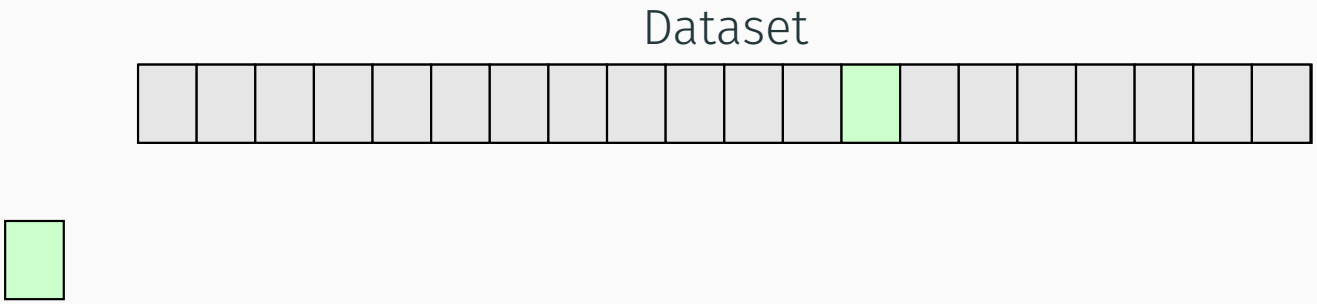

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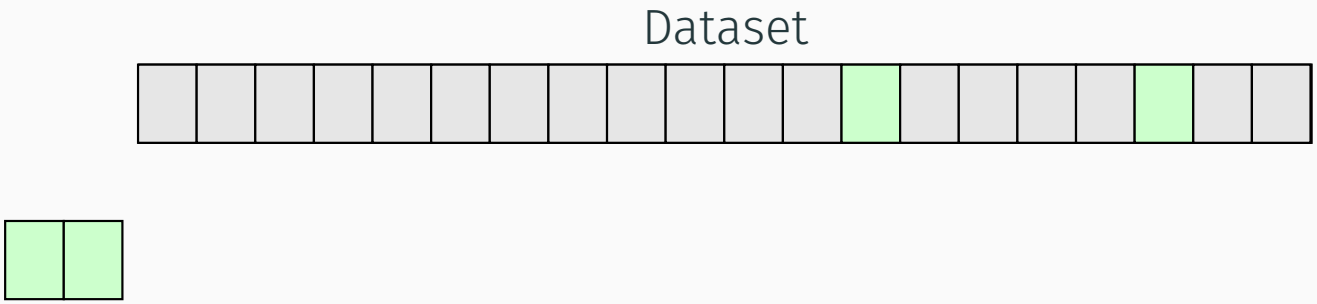

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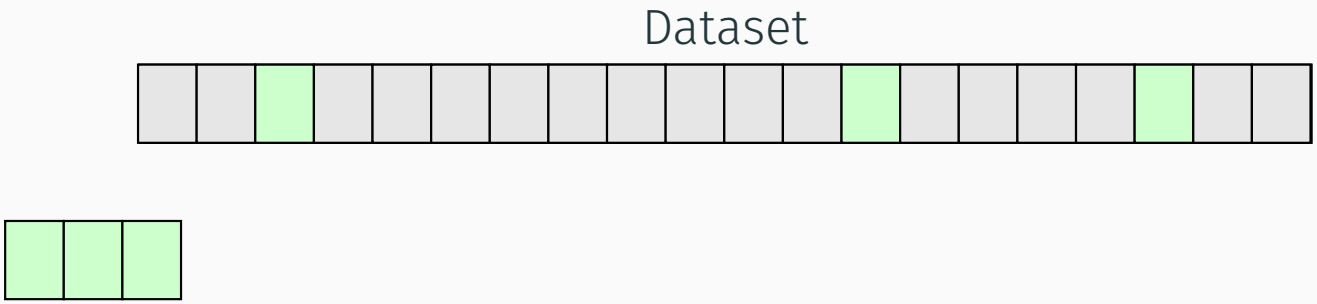

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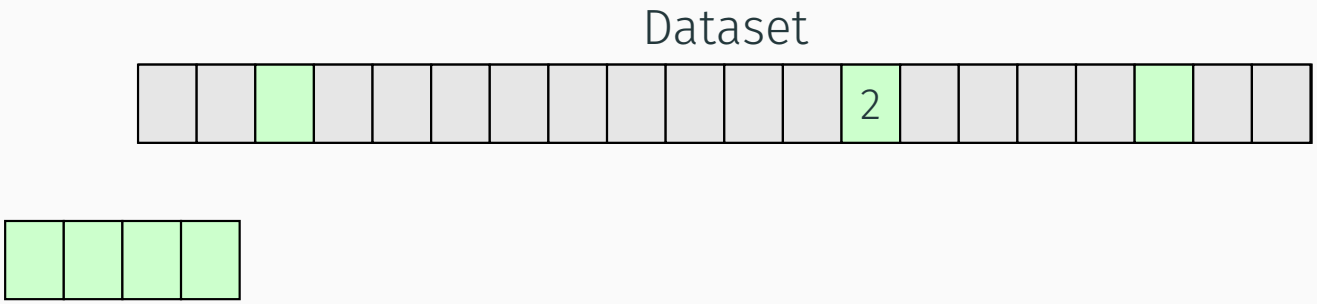

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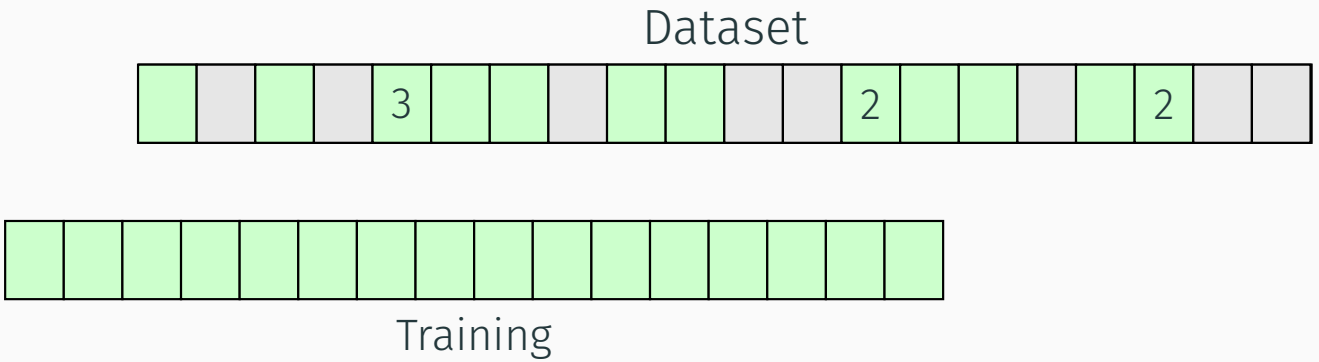

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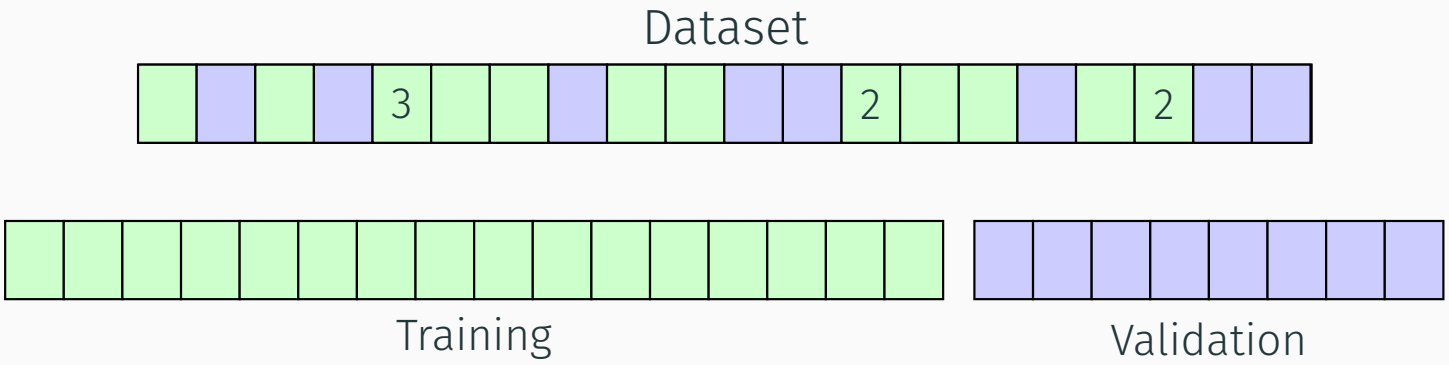

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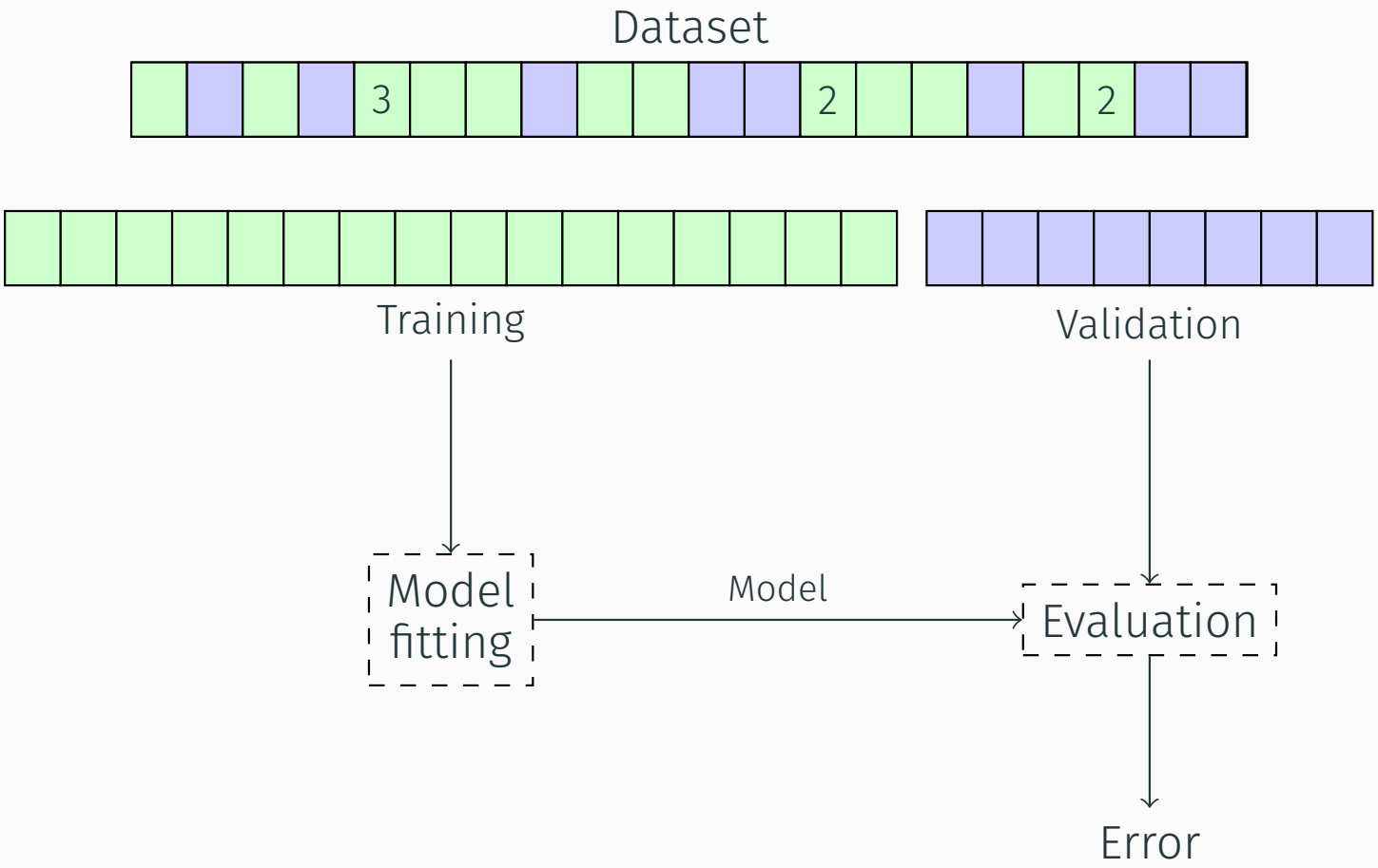

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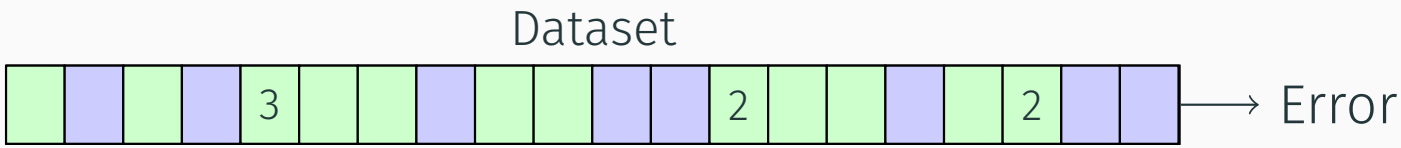

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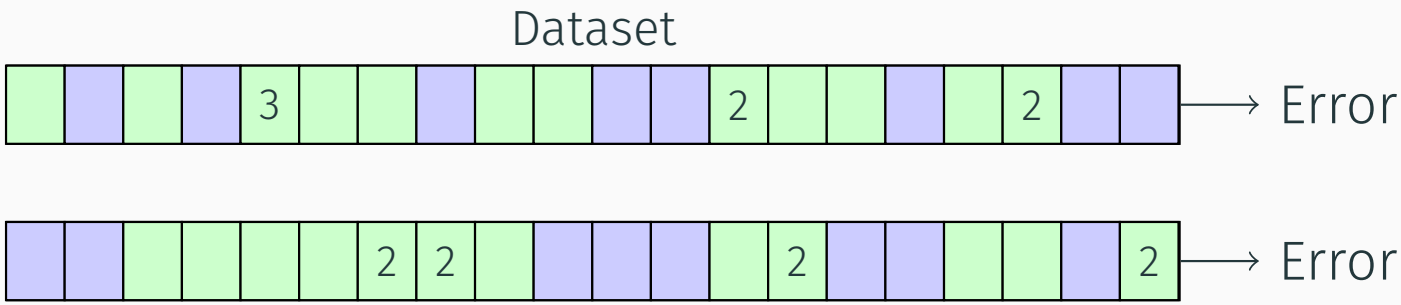

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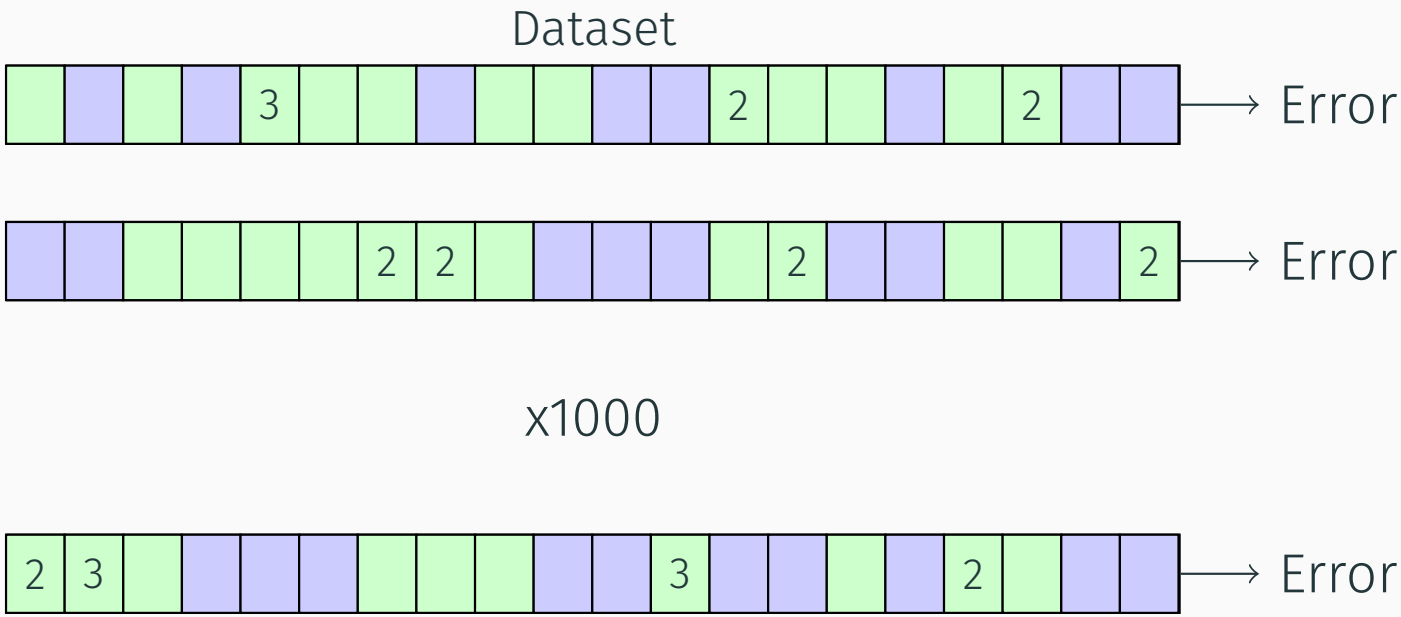
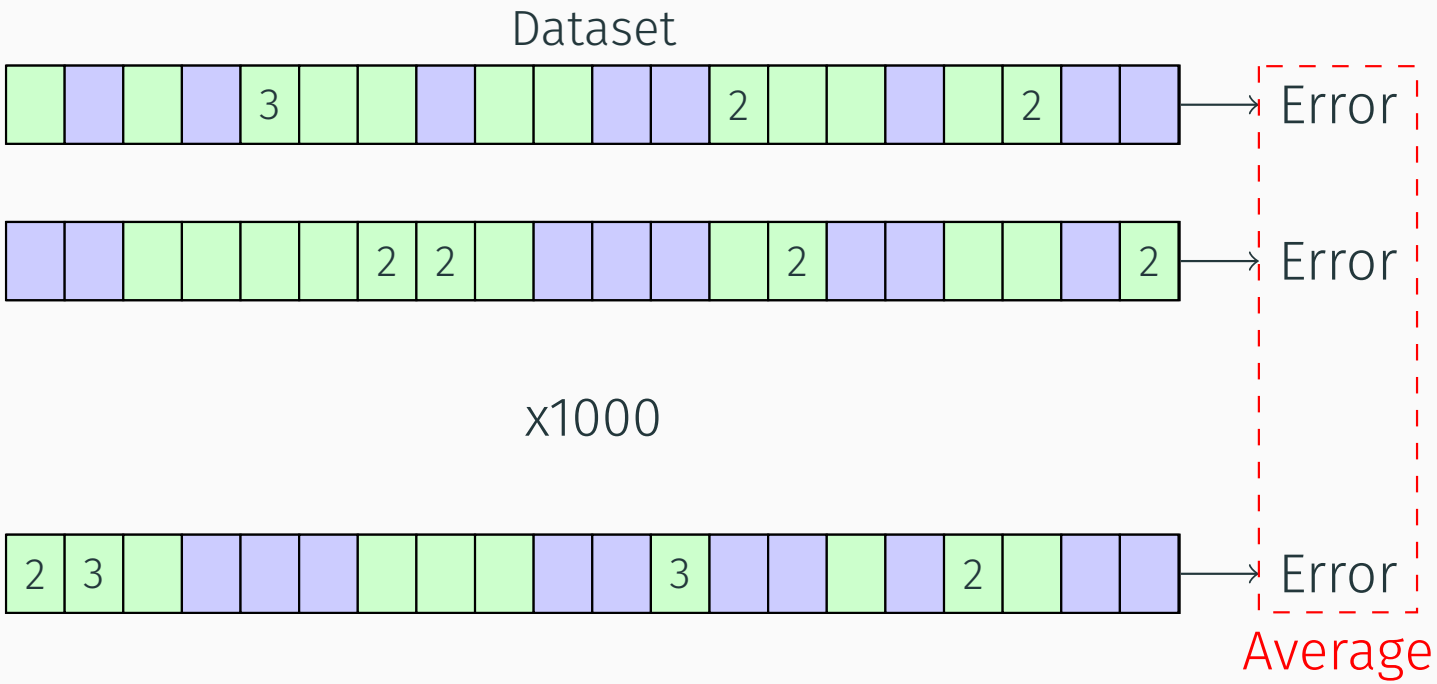


Model assessment: The bootstrap



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: Summary

- Model assessment 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

Model selection and assessment

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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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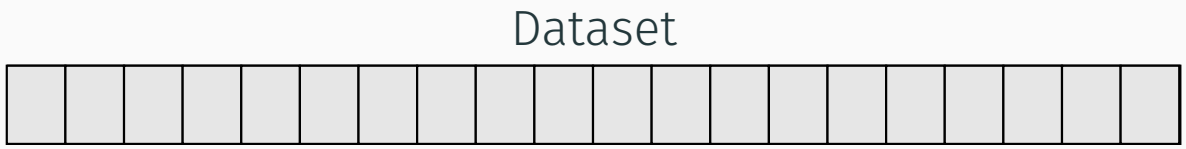
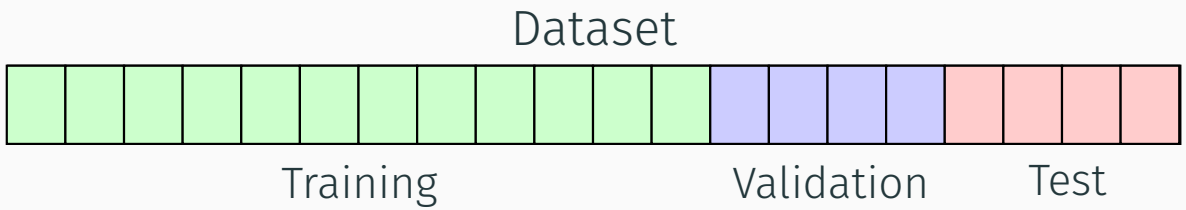
$\rightarrow$ We need a more advanced strategy

Model selection and assessment: Train/validation/test



Model selection and assessment: Train/validation/test



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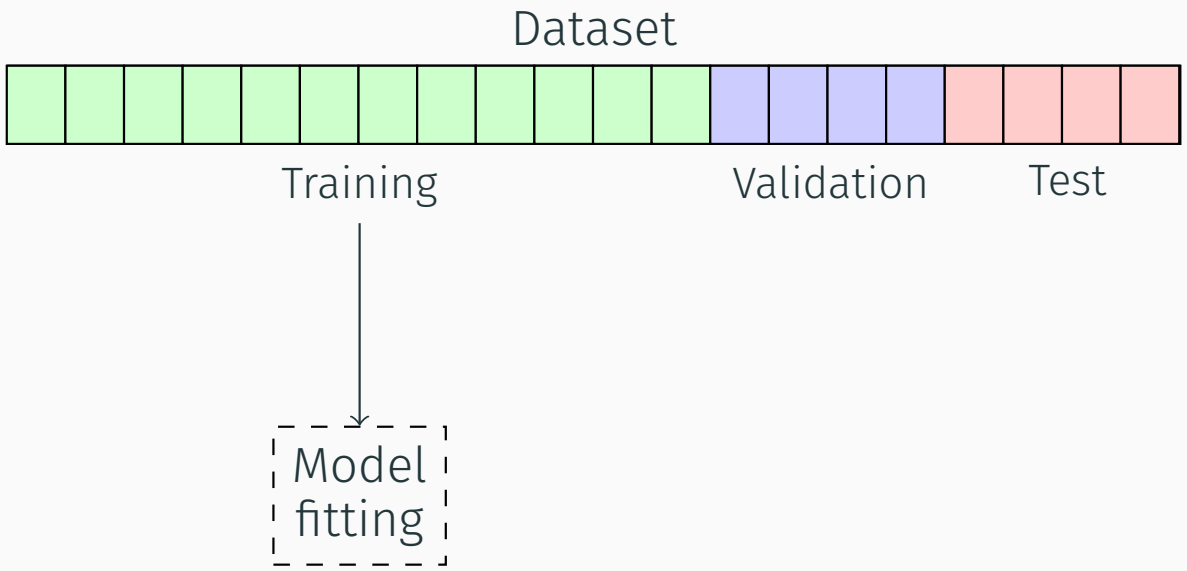

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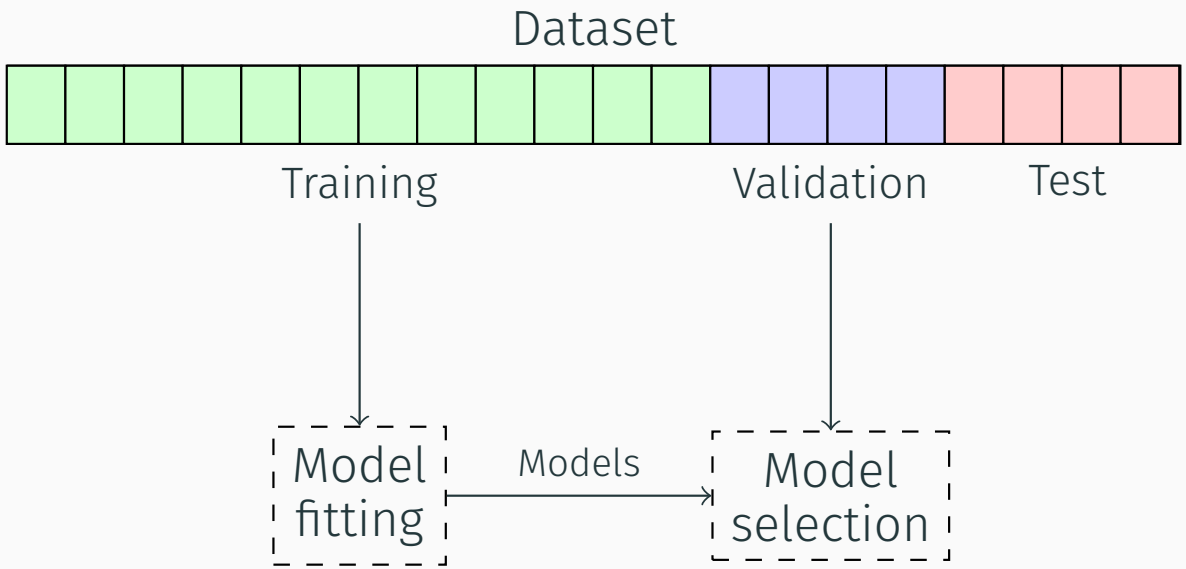

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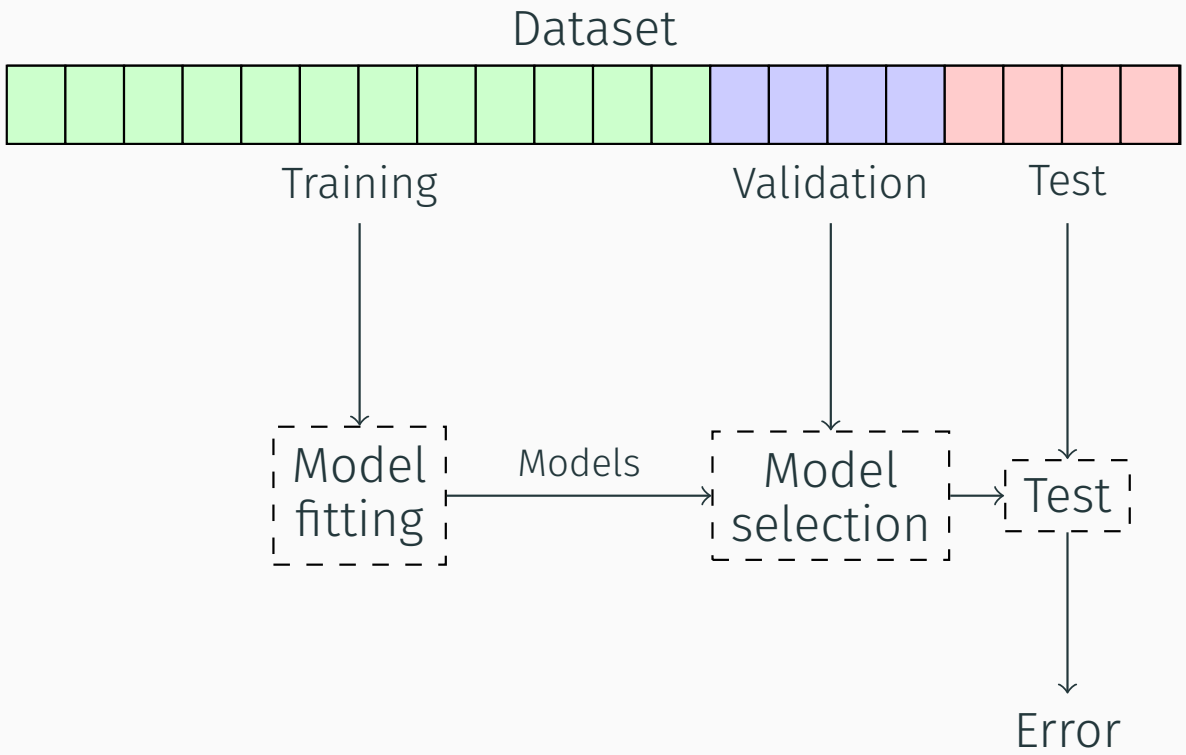
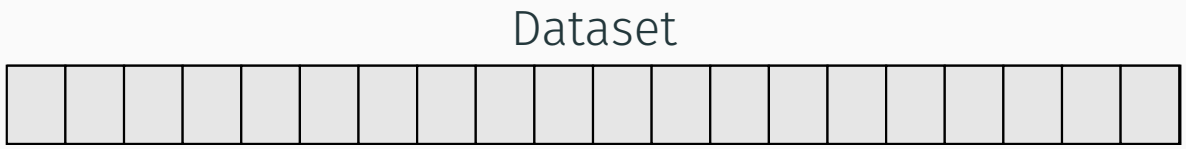
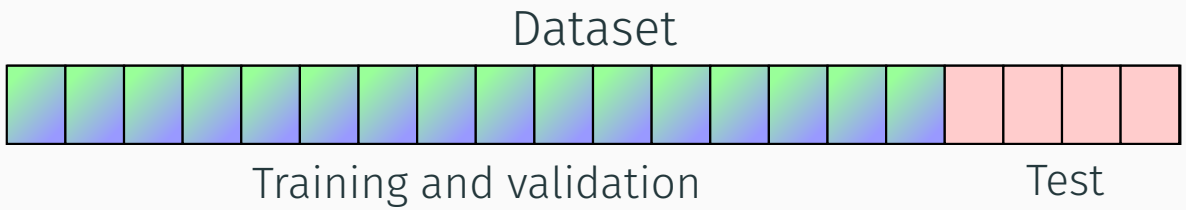


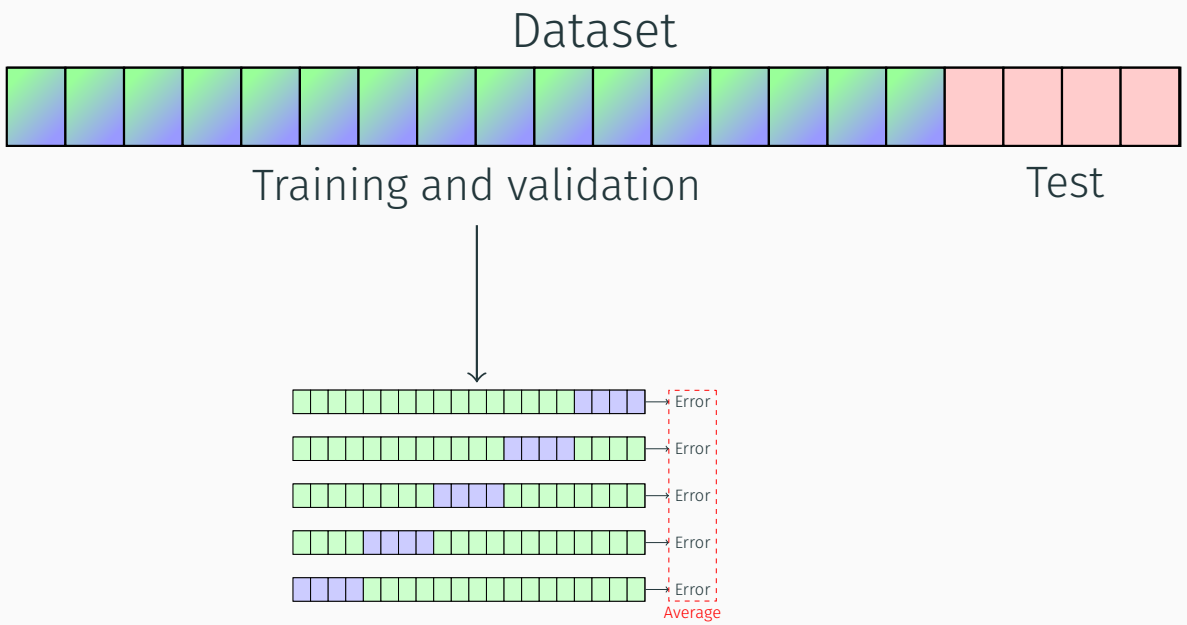
Model selection and assessment: Neste cross-validation



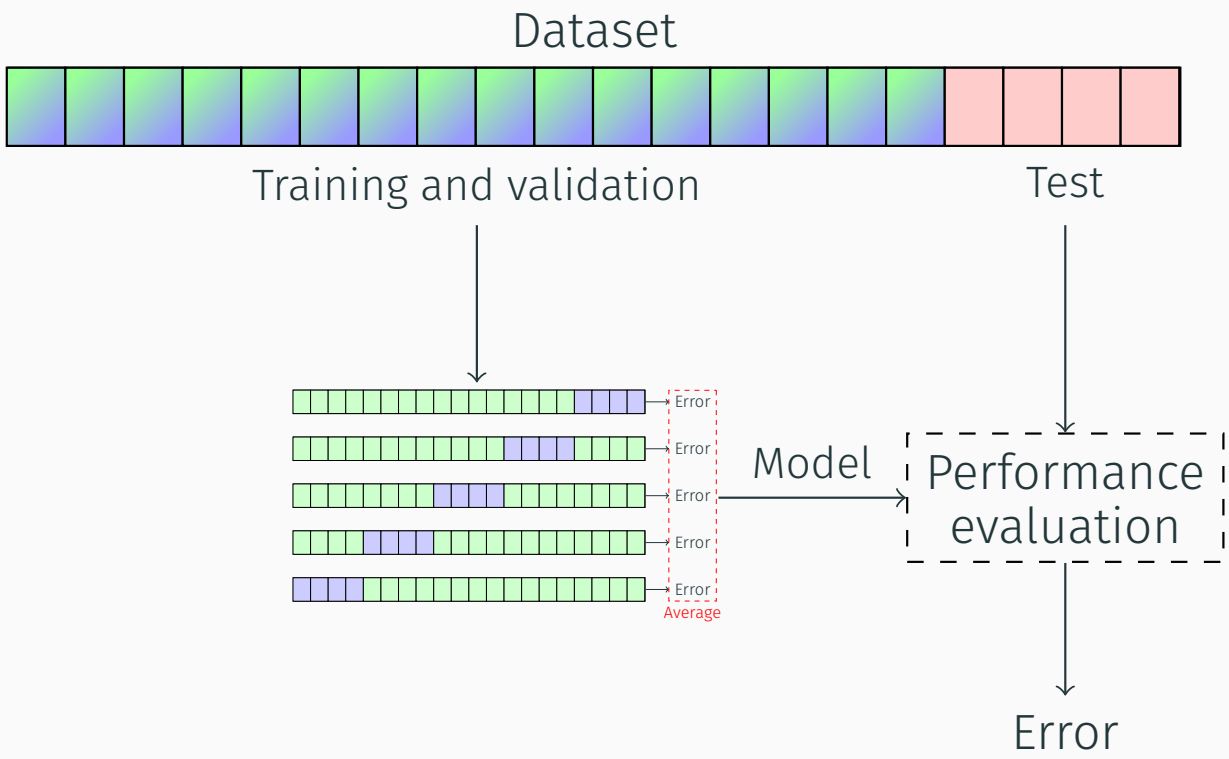
Model selection and assessment: Nested cross-validation



Model selection and assessment: Nested cross-validation



Model selection and assessment: Nested cross-validation



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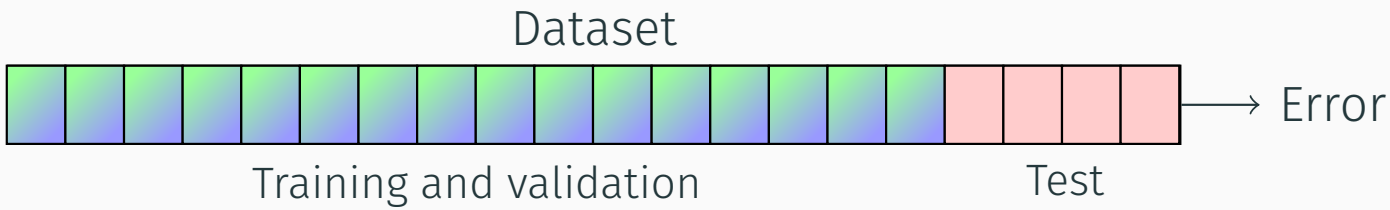

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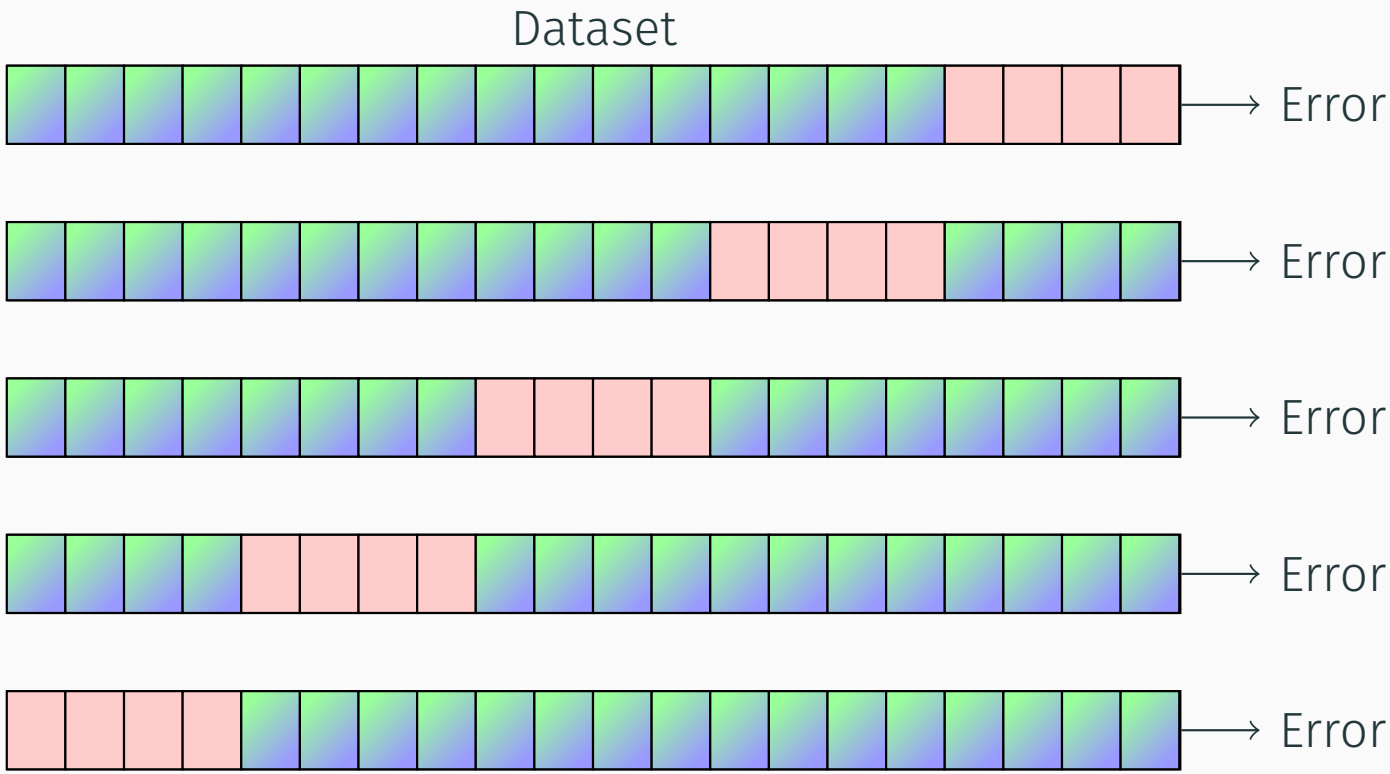

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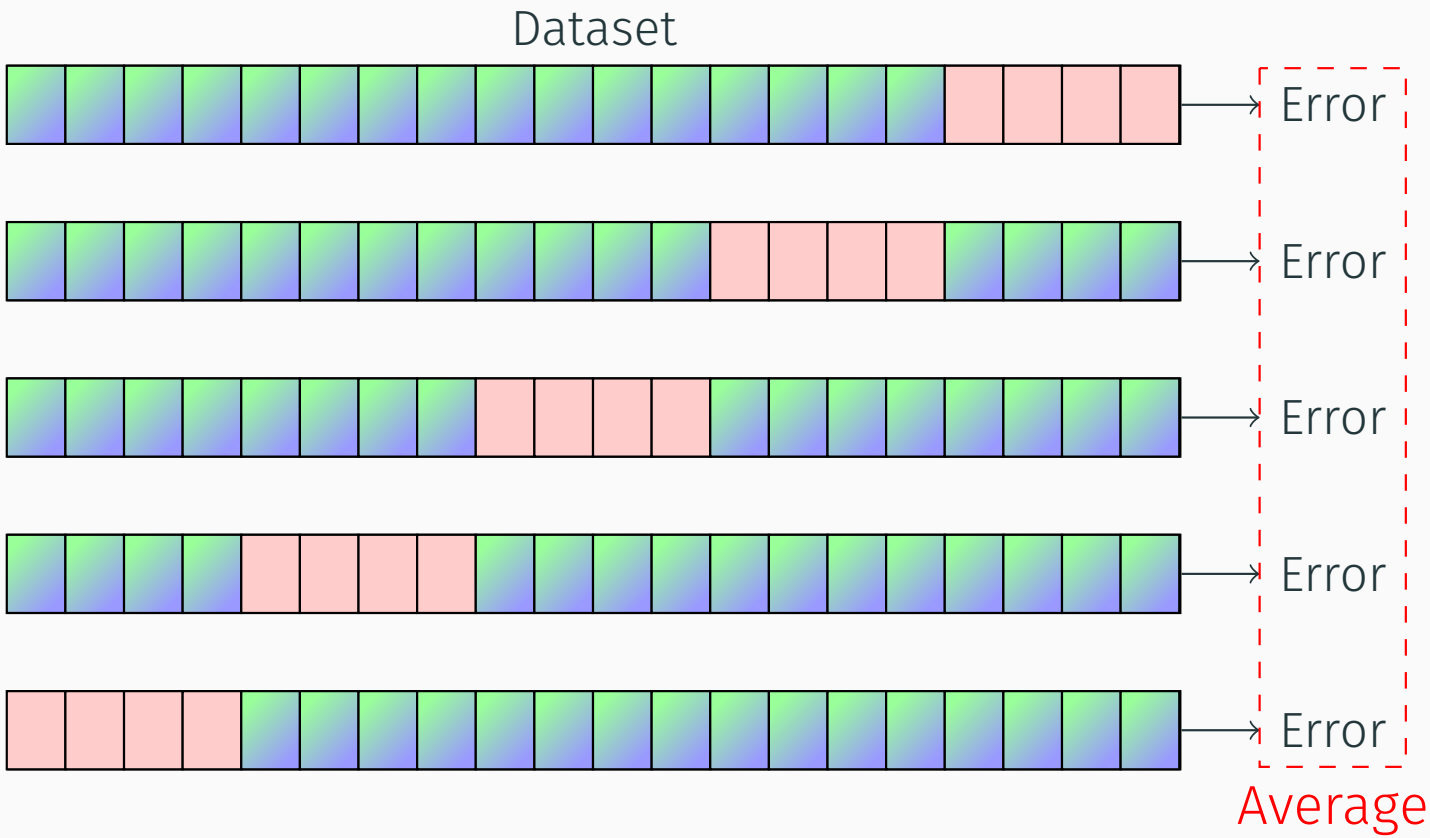

Model selection and assessment: Summary

- 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 ($\geq$ 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