PSY9511: Seminar 4

Model selection, validation and testing

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Outline

1. Assignment 3
2. Loss functions and 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

Assigment 3

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Assignment 3

Loss functions and performance metrics

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Loss functions and performance metrics

Commonalities

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

Loss functions

- Tailored specifically for mathematical optimization of models

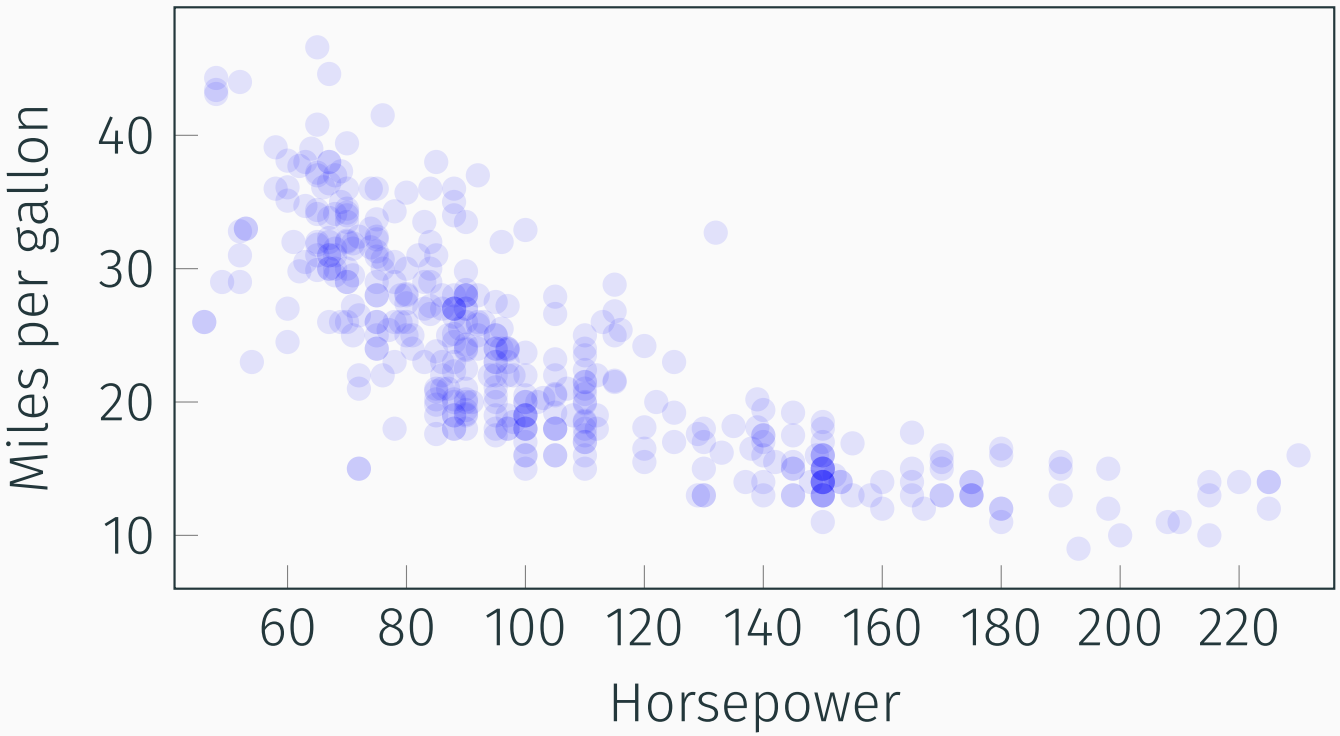
Performance metrics

- Tailored specifically for interpretation of model performance by humans

Loss functions and performance metrics

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

Loss functions and performance metrics



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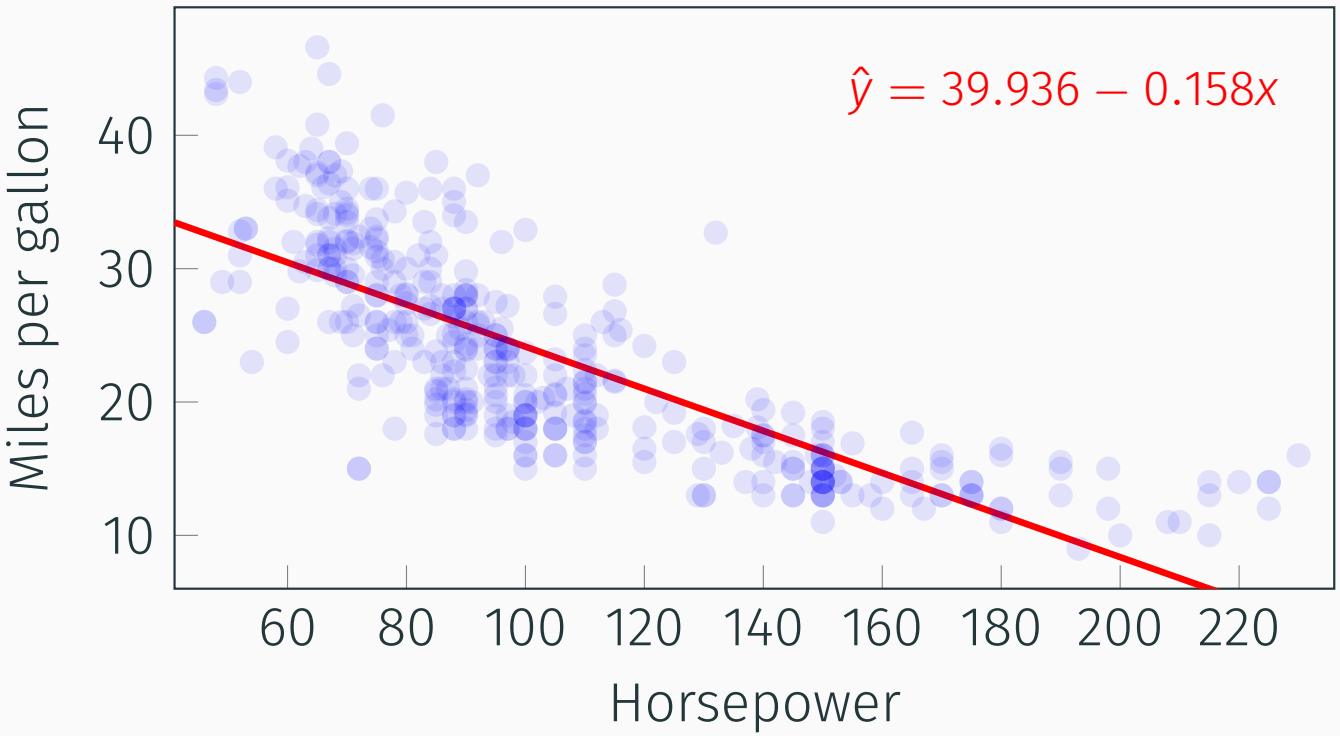
Loss functions and performance metrics



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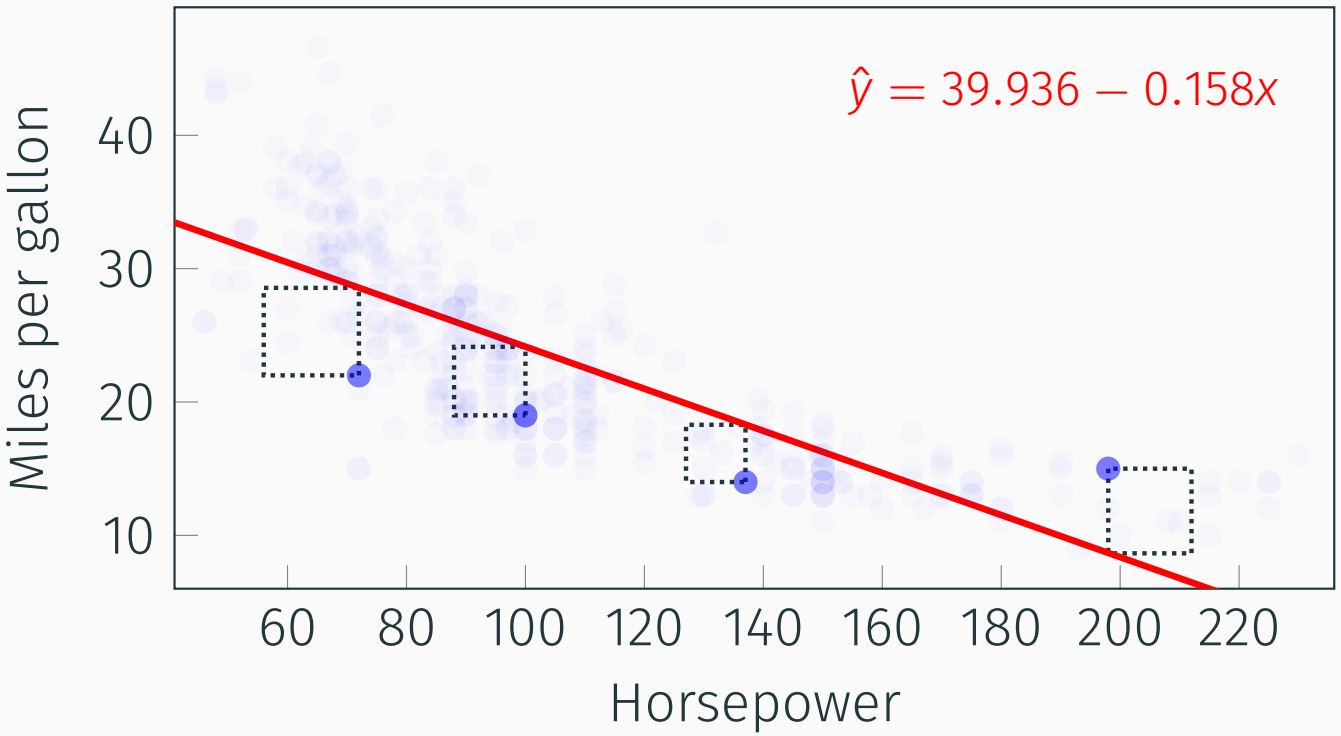
Loss functions and performance metrics



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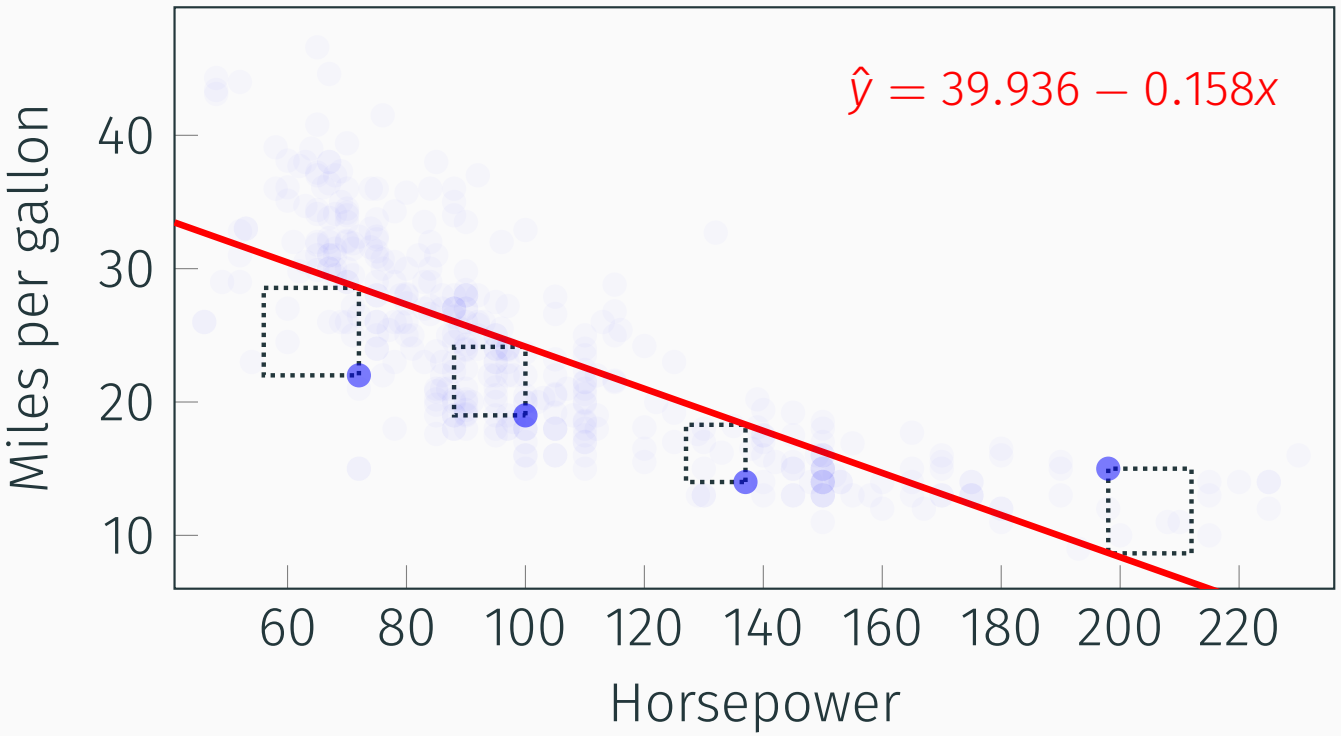
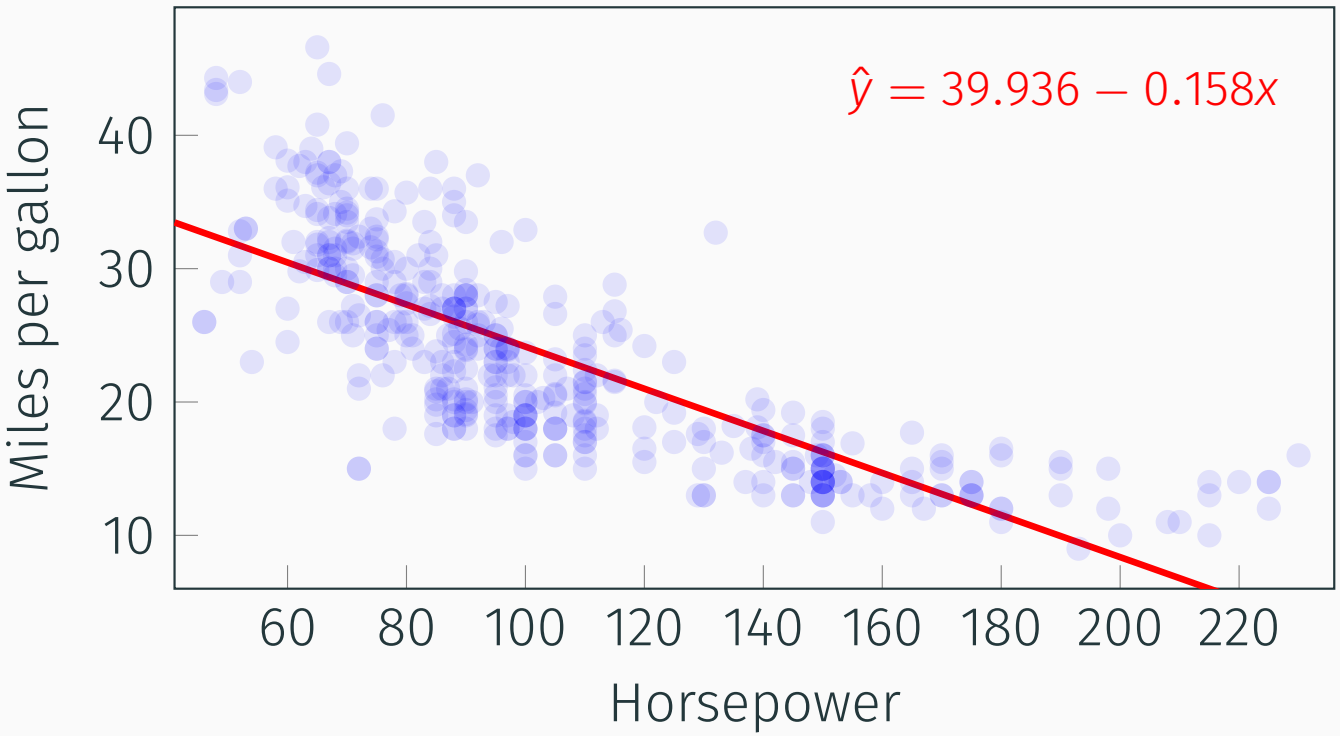
Loss functions and performance metrics



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

$$= 23.94$$

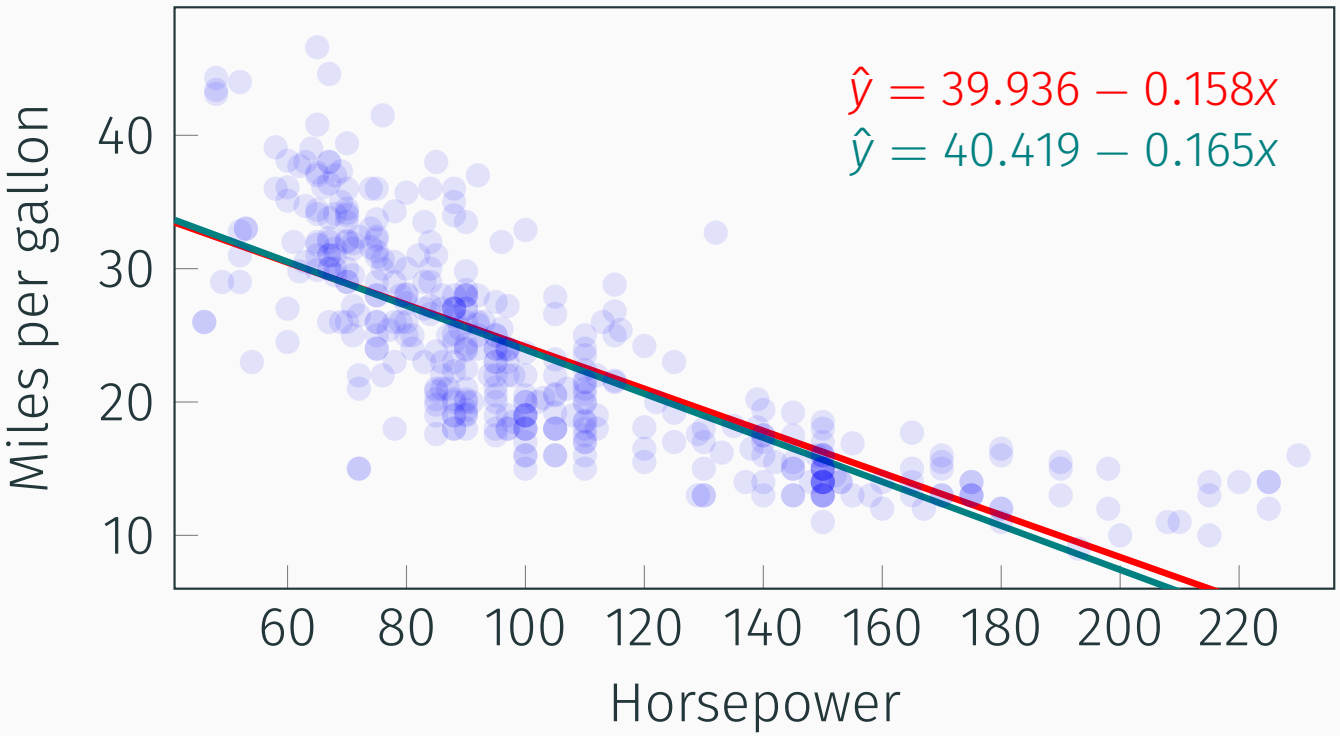
Loss functions and performance metrics



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

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

Loss functions and performance metrics



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Loss functions and performance metrics

Loss functions

- Different loss functions measures different properties of the model fit
- Optimizing for them gives different parameter estimates

Loss functions and performance metrics

Tolerance-based accuracy:

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

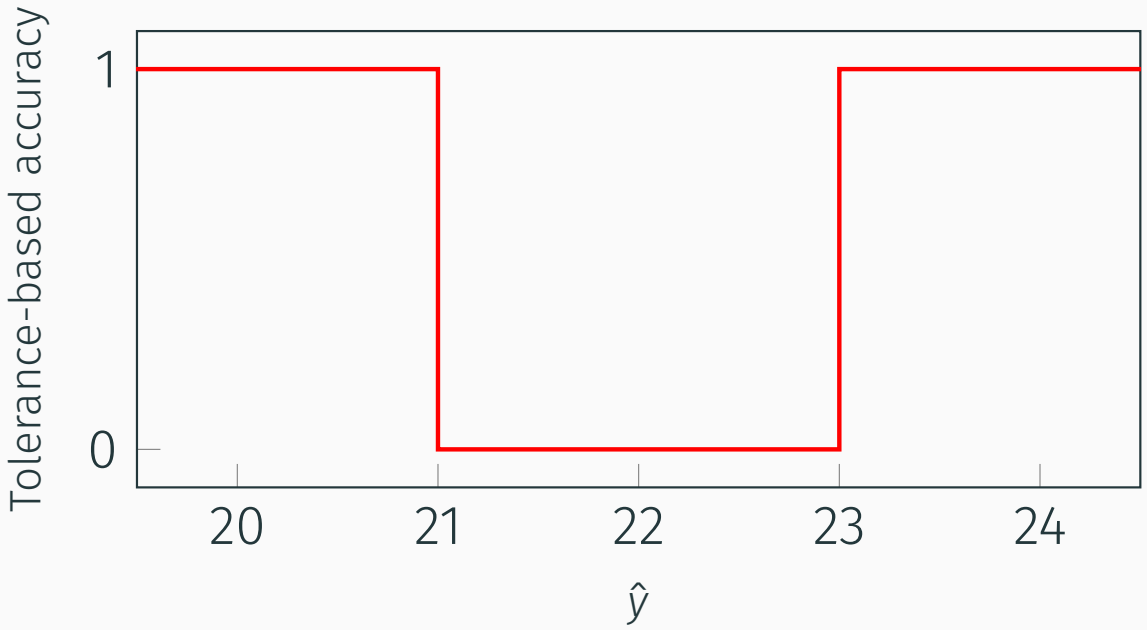
$$\text{accuracy*}(y, \hat{y}) = \begin{cases} 0 & \text{if } |y - \hat{y}| < \text{tol} \\ 1 & \textit{else} \end{cases}$$

Loss functions and performance metrics

mpg	horsepower
22	72

Loss functions and performance metrics

mpg	horsepower
22	72



Loss functions and performance metrics

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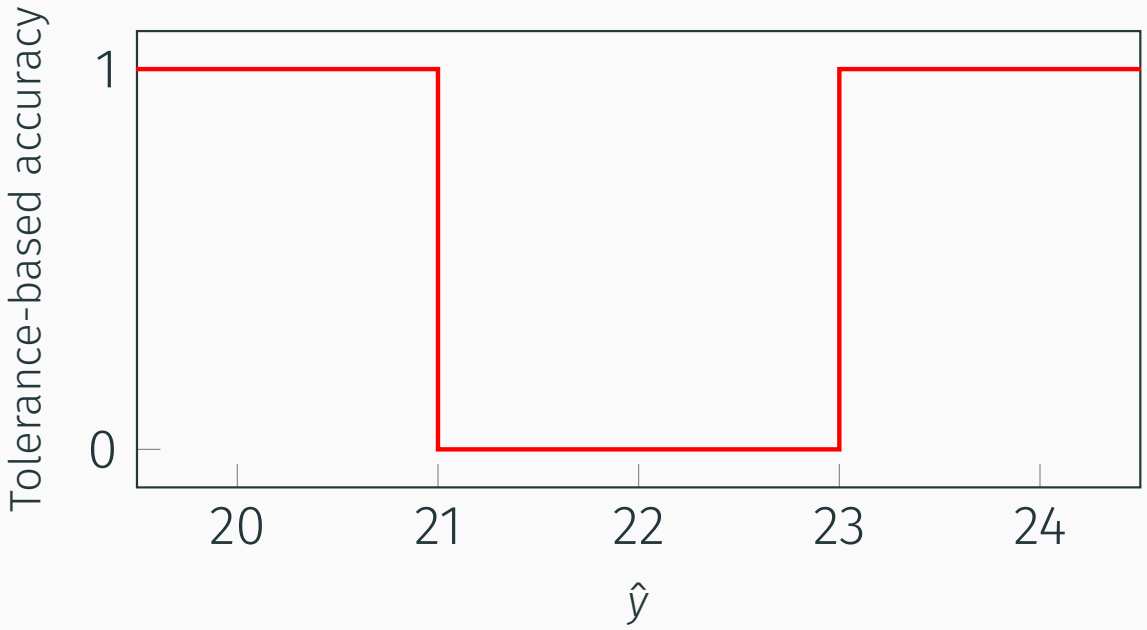

$$\hat{y} = \beta_0 + \beta_1 \times \text{horsepower}$$

Loss functions and performance metrics

mpg	horsepower
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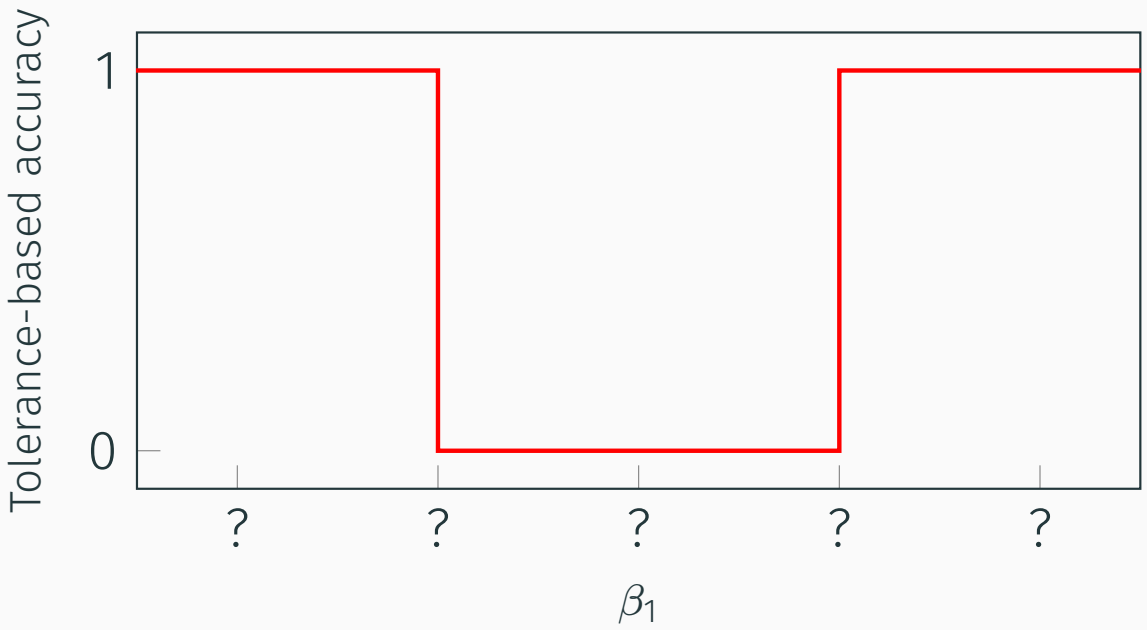

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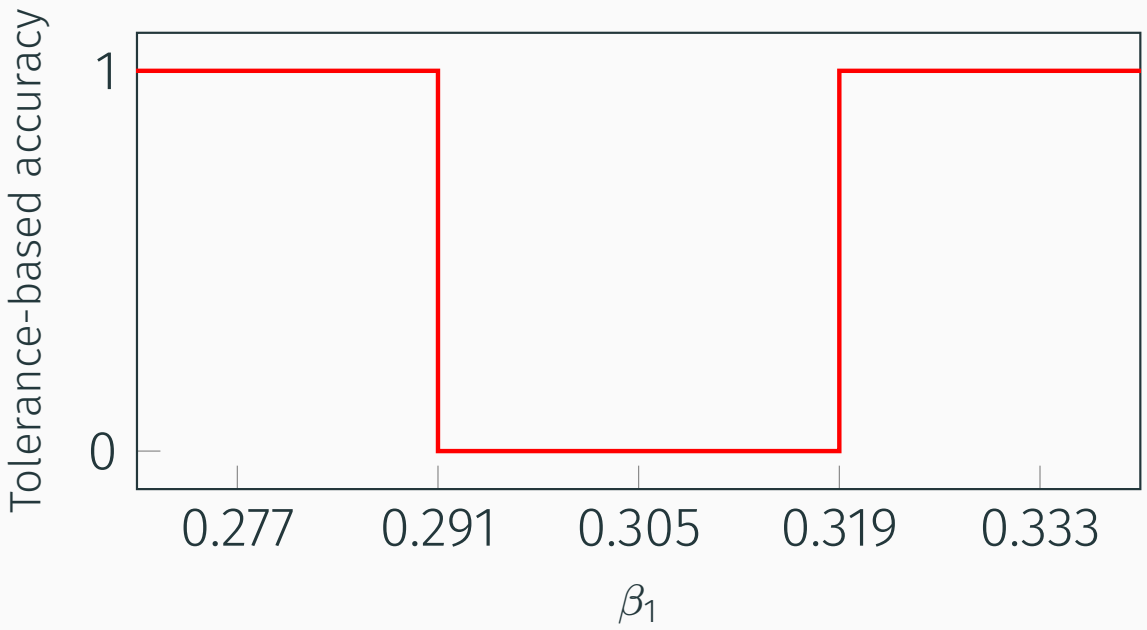
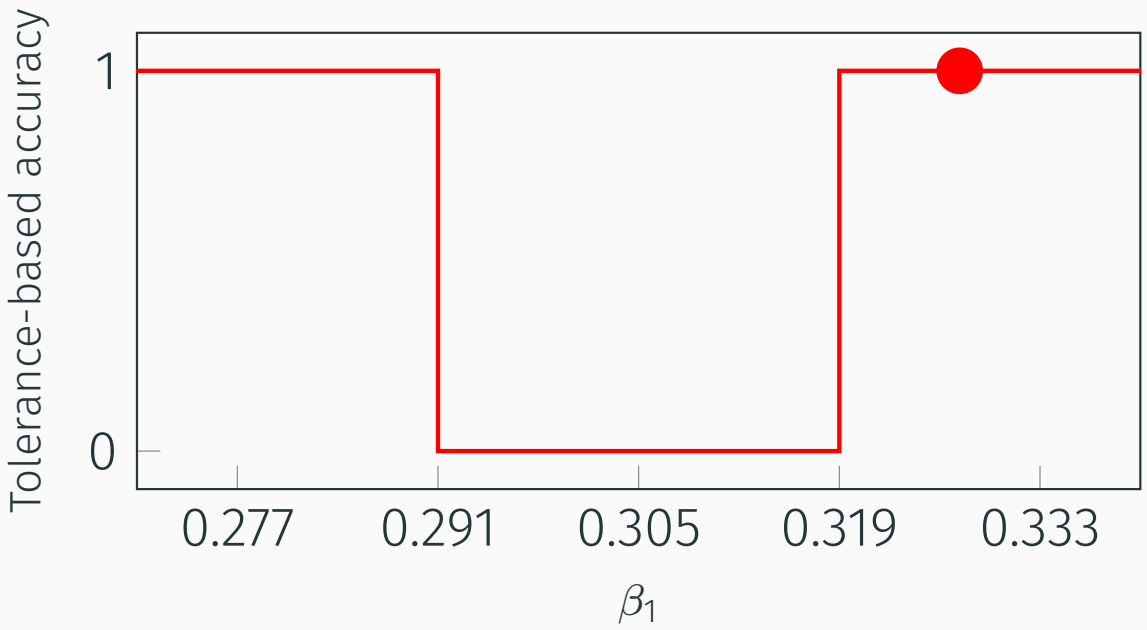
Loss functions and performance metrics



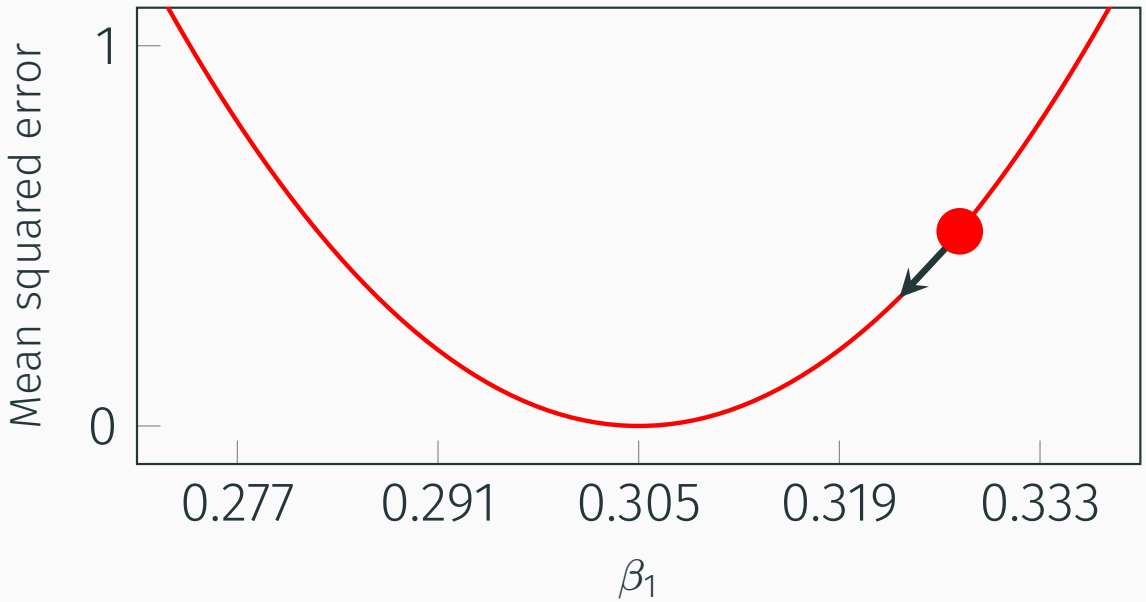
$$\hat{y} = 0 + \beta_1 \times \text{horsepower}$$

Loss functions and performance metrics



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

Loss functions and performance metrics



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

Loss functions and performance metrics

Loss functions

- Different loss functions measures different properties of the model fit
- Optimizing for them gives different parameter estimates
- Must be differentiable to allow for mathematical optimization

Loss functions and performance metrics

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

OR

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

Performance metrics: Regression

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

Mean squared error (MSE)

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

Performance metrics: Regression

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

Root mean squared error (RMSE)

- \+ Can be used as a loss function
- \+ Intuitive
- \+ Penalizes large errors
- \+ More interpretable than MSE, total loss $\approx$ individual loss
- \- Depends on scale

Performance metrics: Regression

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

Mean absolute error (MAE)

+ Can be used as a loss function
+ More interpretable than MSE/RMSE, total loss = average error
- Feels a bit off
- Depends on scale

Performance metrics: Regression

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

Pearson correlation coefficient (r)

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

Performance metrics: Regression

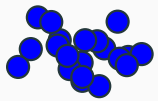
$$1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2}$$

Proportion of variance explained (r^2)

+ Scale independent
+ Interpretable
? Captures linear correlation
- Should not be used as a loss function
- Does not care about whether the predictions are close to the true values

Performance metrics: Binary classification

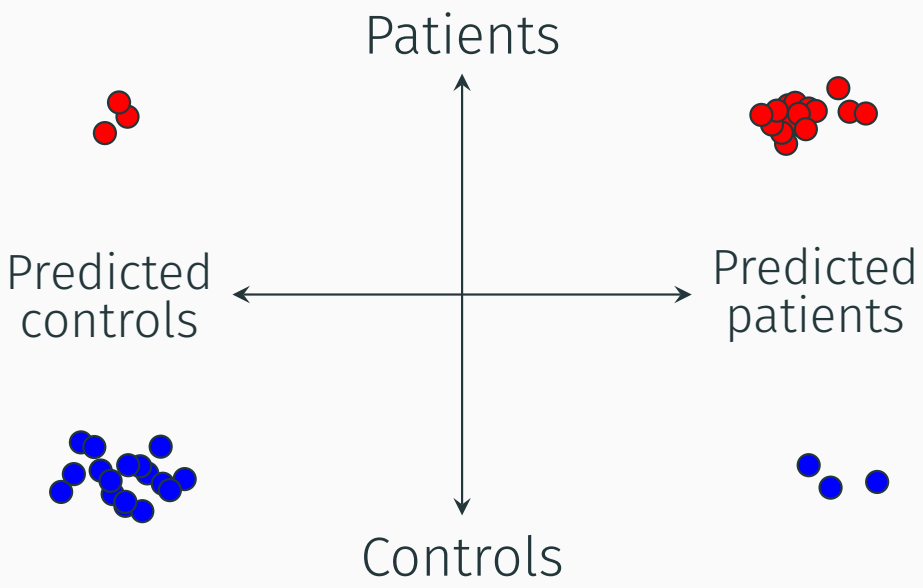
Patients



Controls

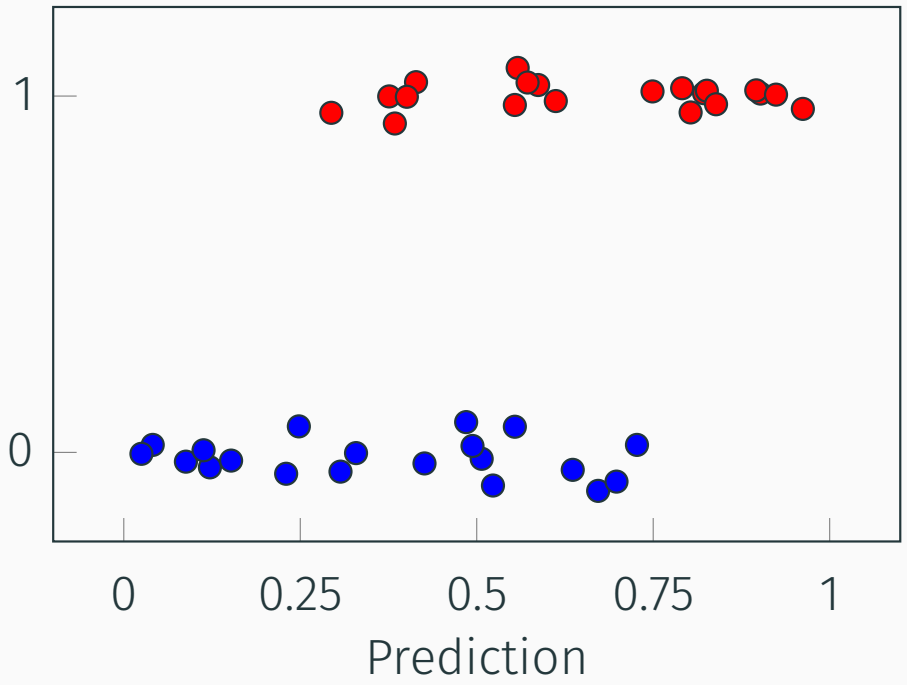
$$y \in \{Patients, Controls\}$$

Performance metrics: Binary classification



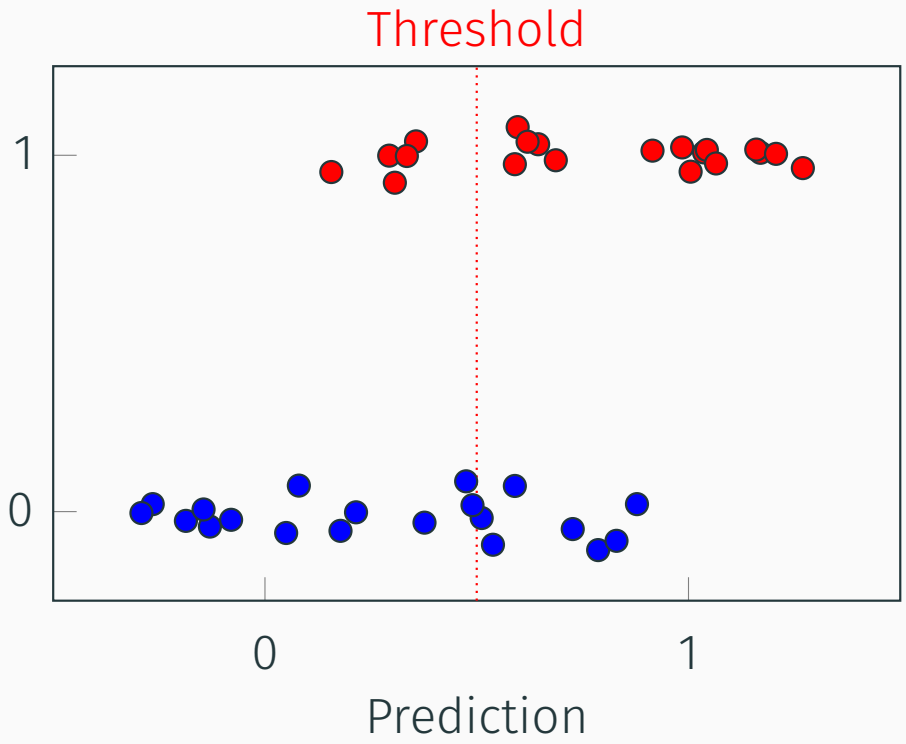
$$y \in \{Patients, Controls\}$$
$$\hat{y} \in \{Patients, Controls\}$$

Performance metrics: Binary classification



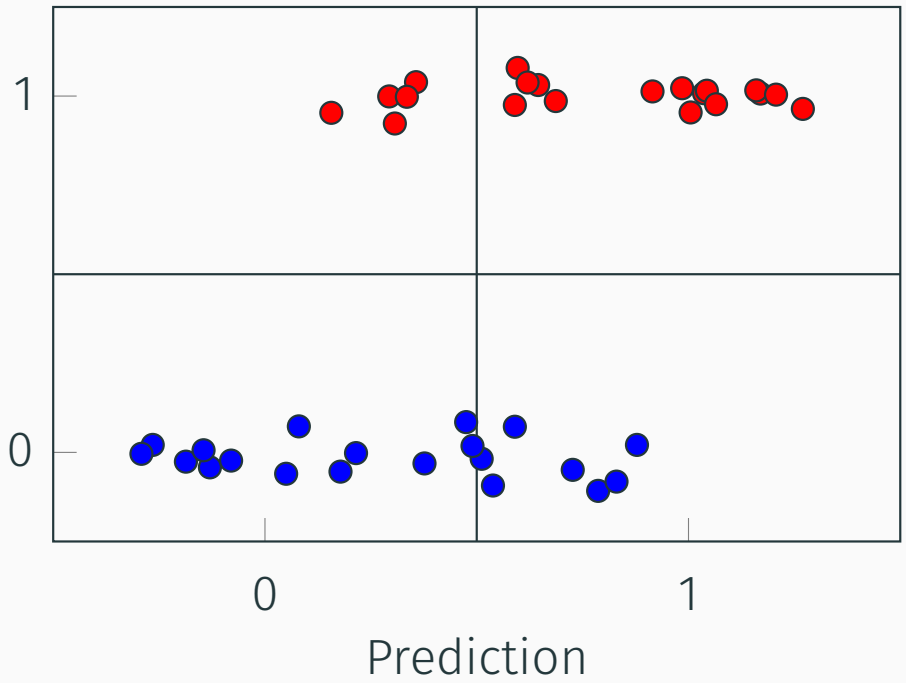
$$y \in \{0, 1\}$$
$$\hat{y} \in [0, 1]$$

Performance metrics: Binary classification

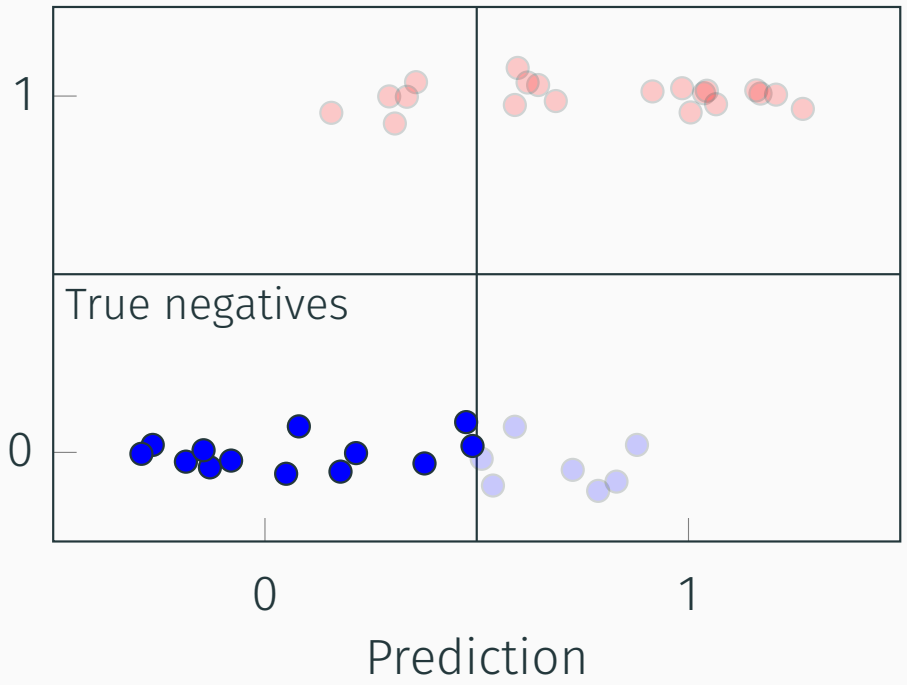


$$y \in \{0, 1\}$$
$$\hat{y} \in \{0, 1\}$$

Performance metrics: Binary classification

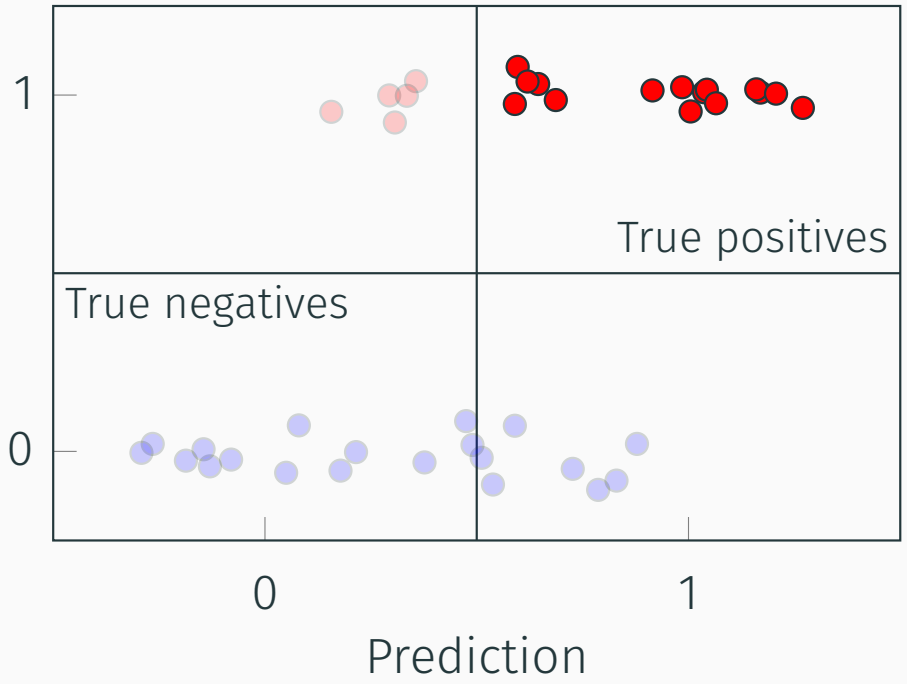


Performance metrics: Binary classification



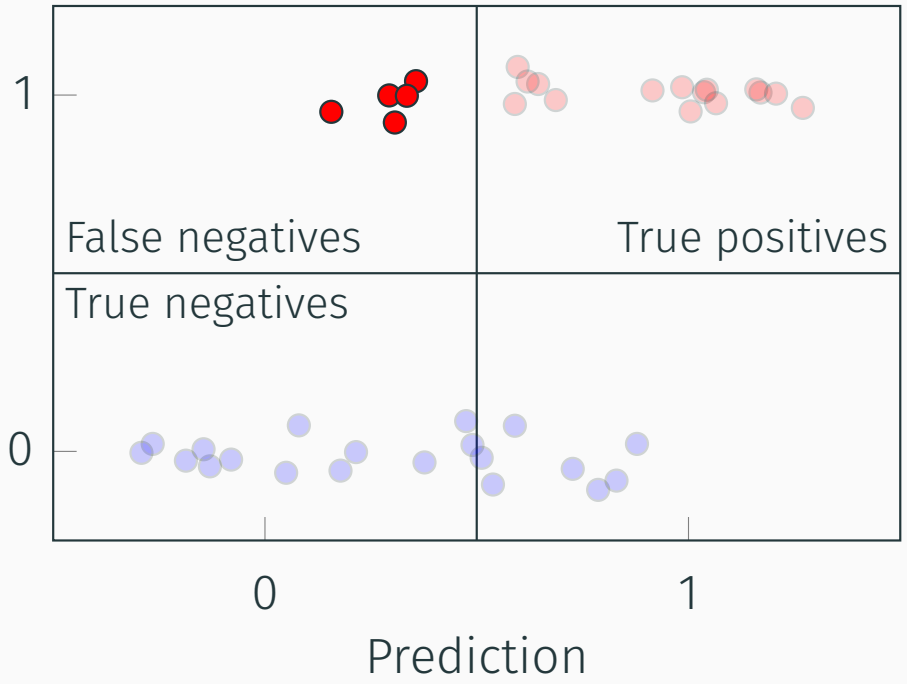
TN	

Performance metrics: Binary classification



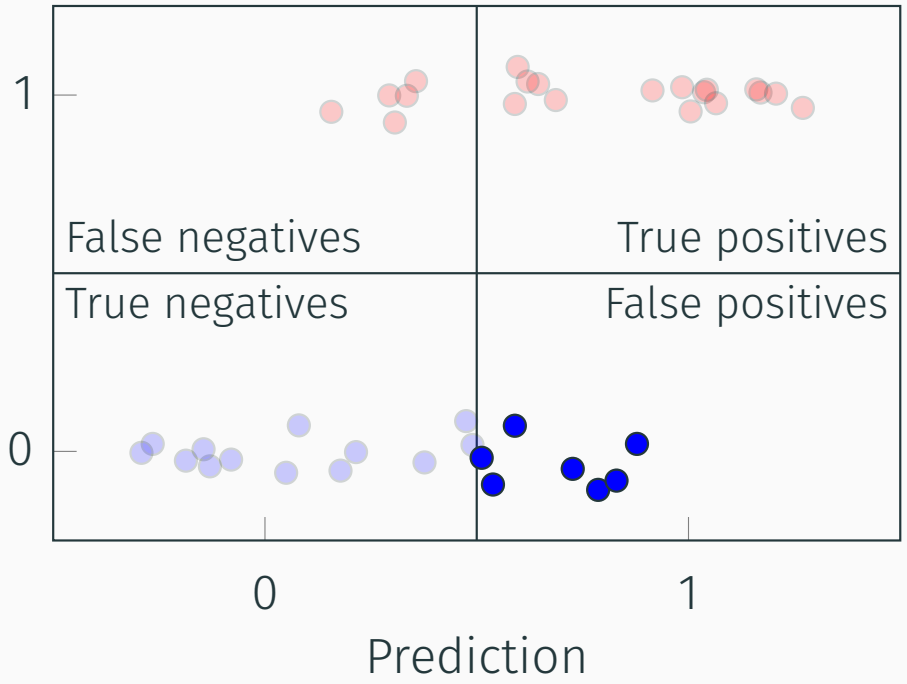
TN	
	TP

Performance metrics: Binary classification



TN	
FN	TP

Performance metrics: Binary classification



TN	FP
FN	TP

Performance metrics: Binary classification

Confusion matrix:

		Predicted 0	Predicted 1
True	0	TN	FP
	1	FN	TP

Performance metrics: Binary classification

Binary classification metrics:

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

Performance metrics: Binary classification

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

Accuracy

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

Performance metrics: Binary classification

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

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

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

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

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

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)

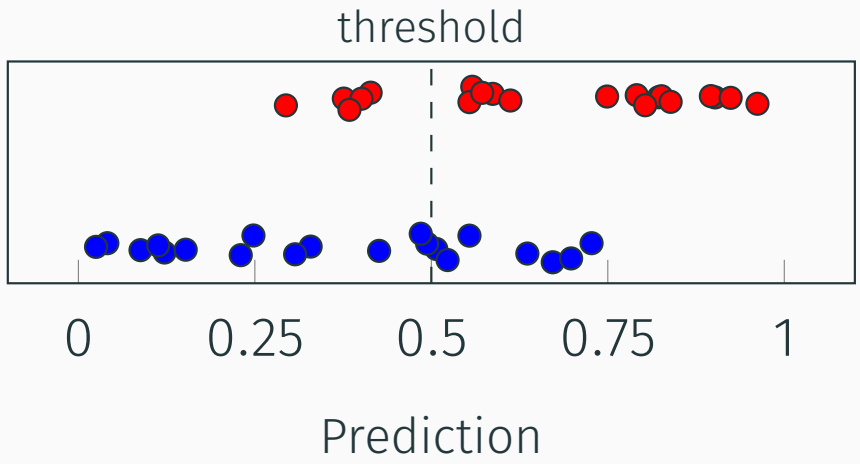
Performance metrics: Binary classification

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

Balanced accuracy

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

Classification metrics: Area under the curve



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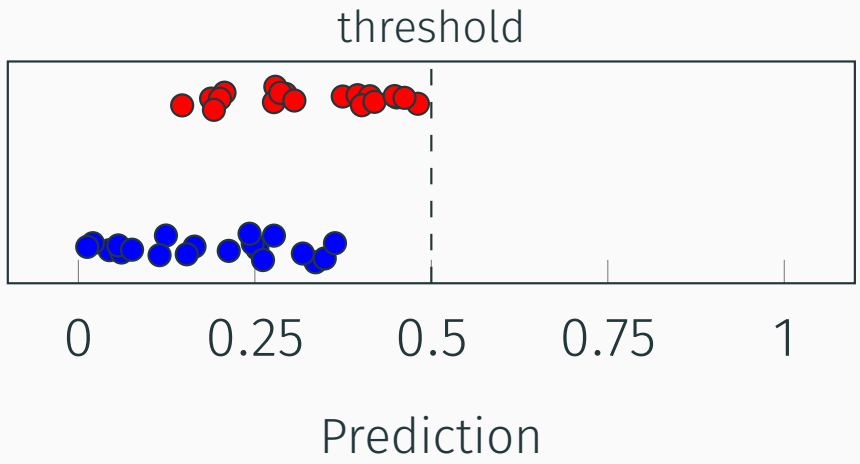

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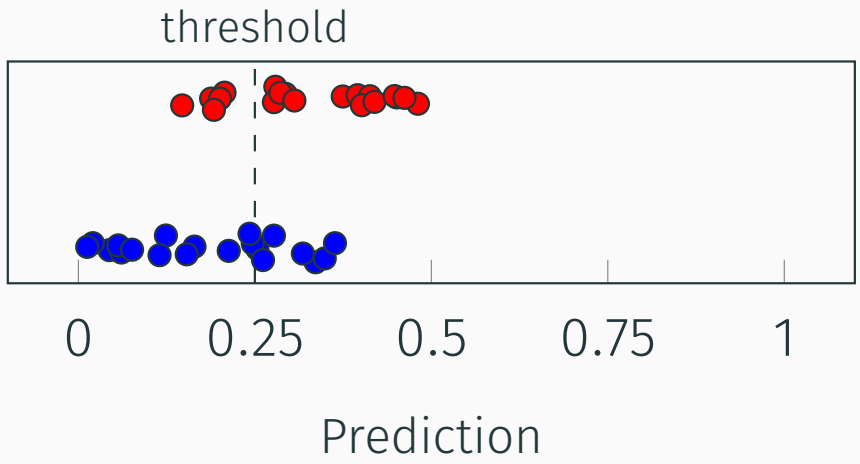

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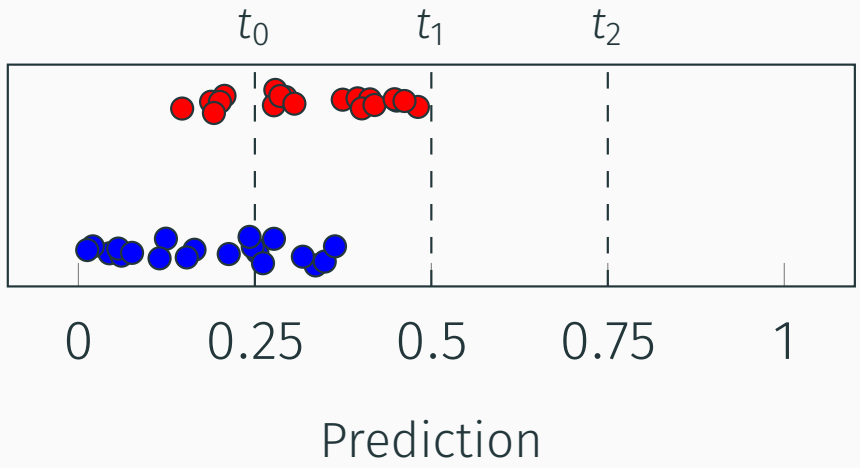

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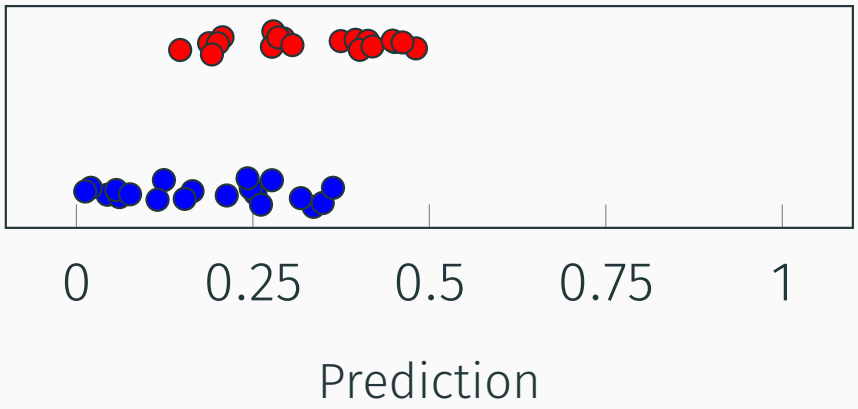
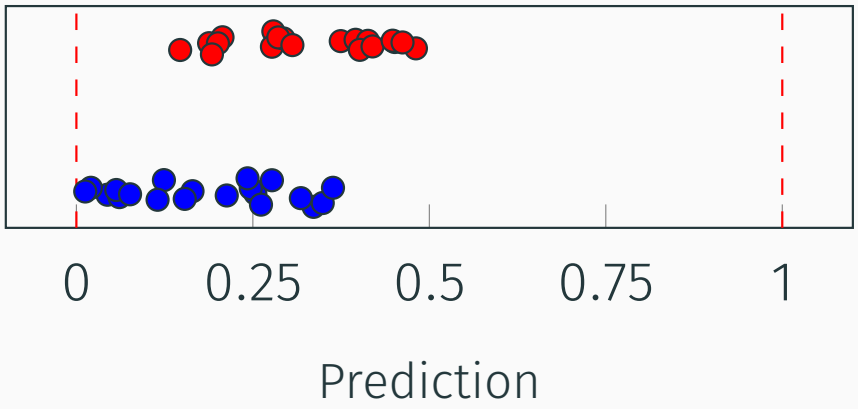


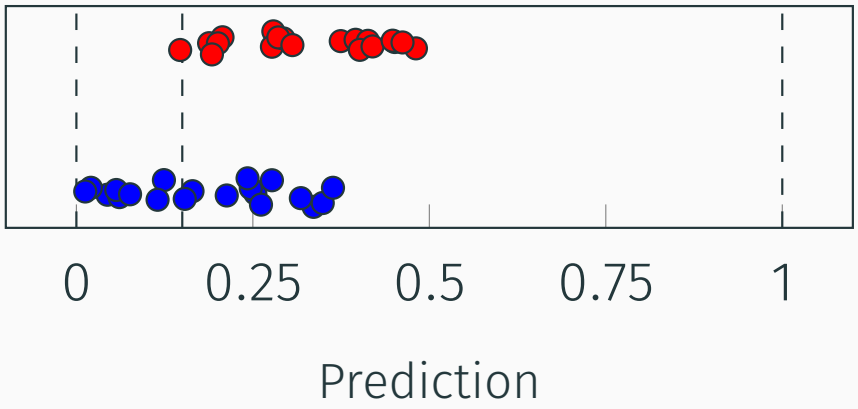
threshold	TPR	FPR

Classification metrics: Area under the curve



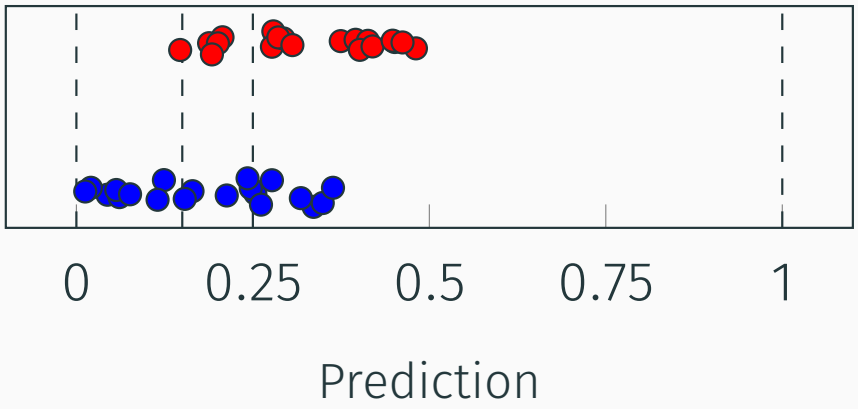
threshold	TPR	FPR
0	1	1
1	0	0

Classification metrics: Area under the curve



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

Classification metrics: Area under the curve



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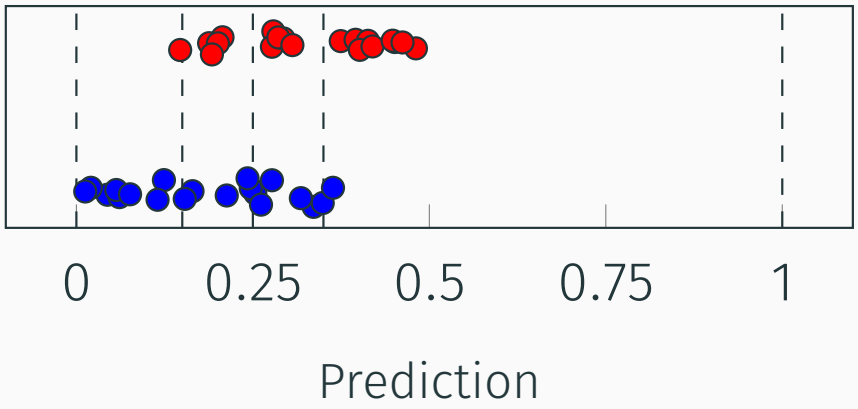
Classification metrics: Area under the curve



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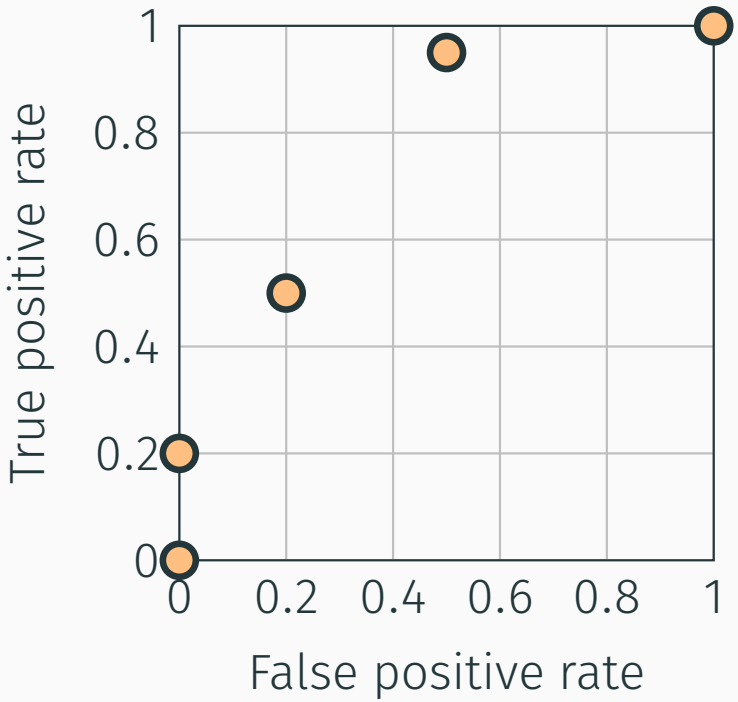

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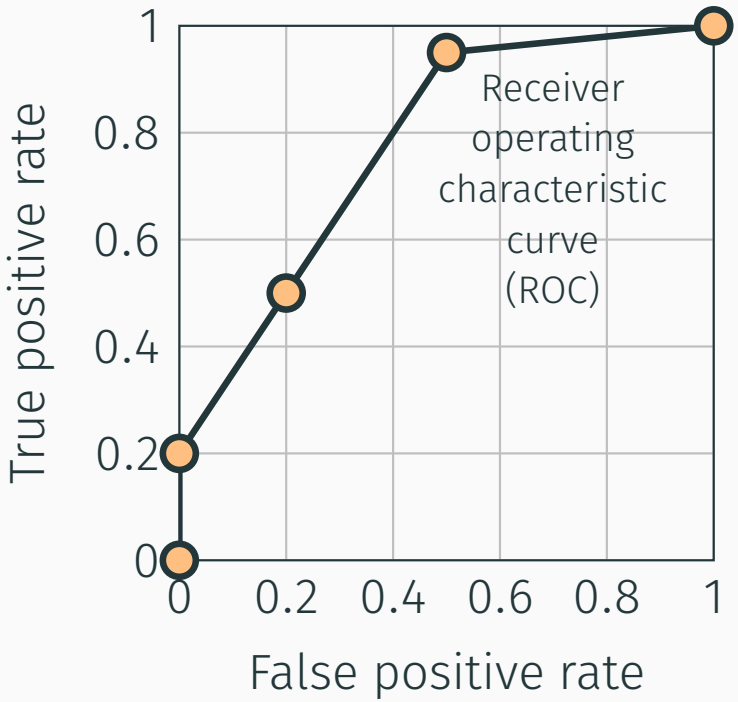

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Classification metrics: Area under the curve

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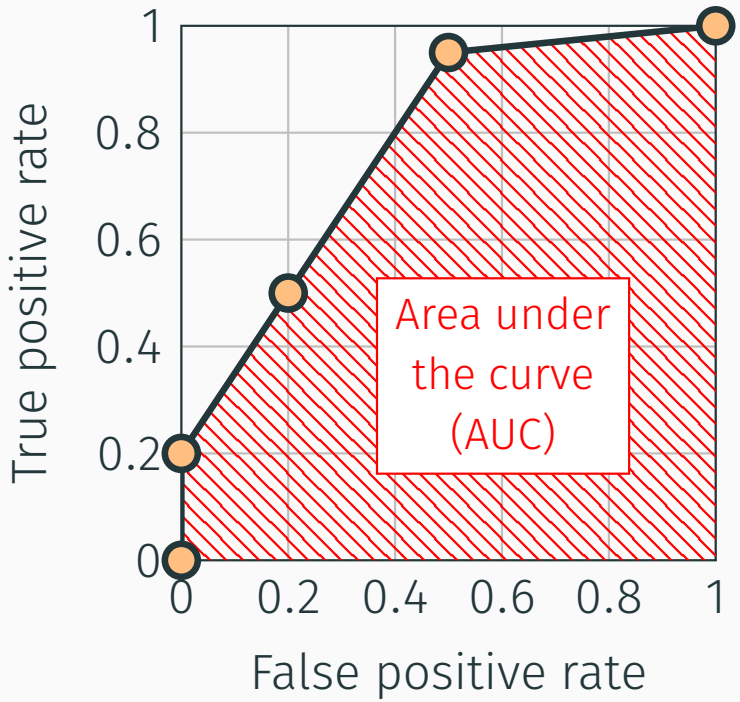

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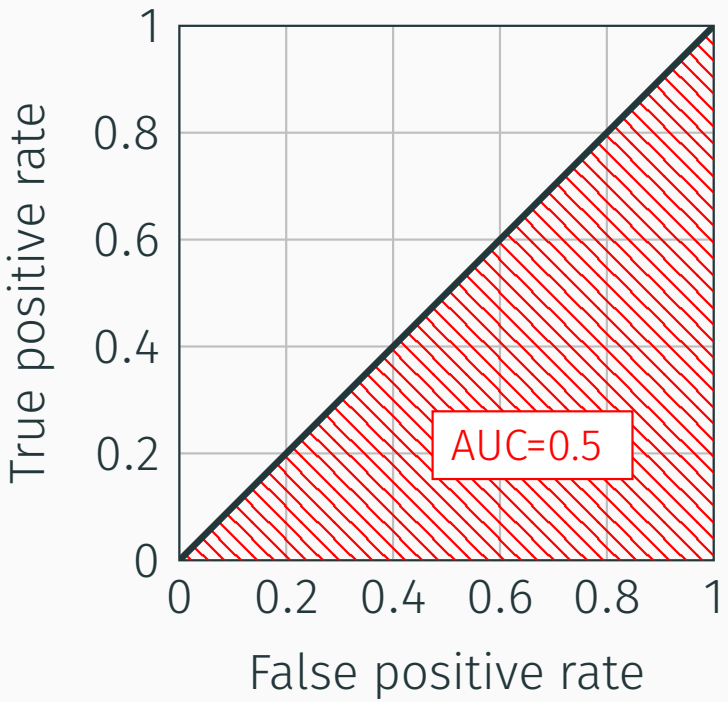

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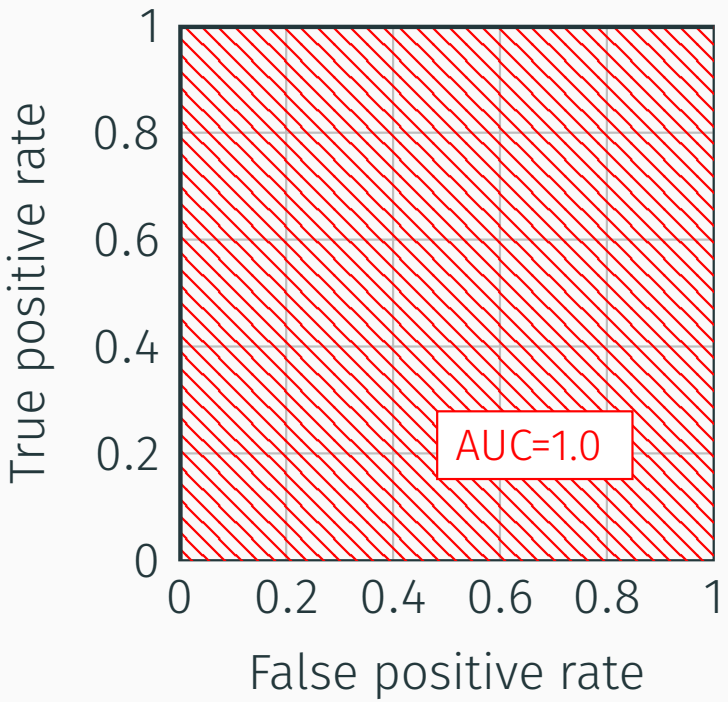

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Classification metrics: Area under the curve

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

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

Loss functions and performance metrics: Summary

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

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

Loss functions and performance metrics: Summary

http://localhost:8889/notebooks/notebooks%2FClassification%20metrics.ipynb

Strategies for model evaluation

UNIVERSITETET
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Model evaluation: Rationale

Statistical inference:

Goal: In-sample quantification

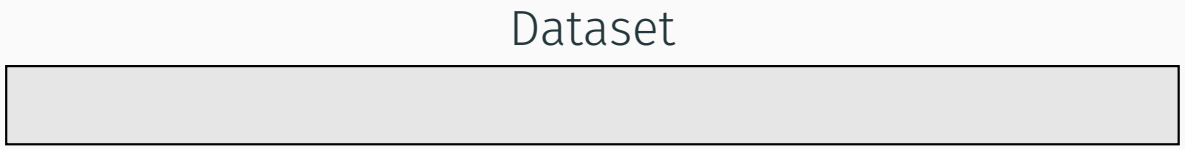
Predictive modelling:

Goal: Out-of-sample generalization

Model evaluation: Rationale

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

Model evaluation: Validation set



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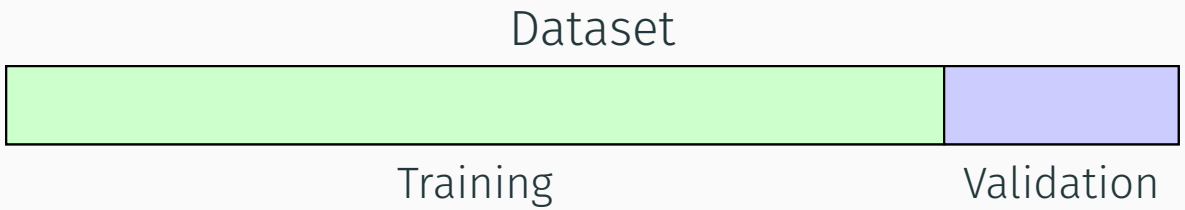

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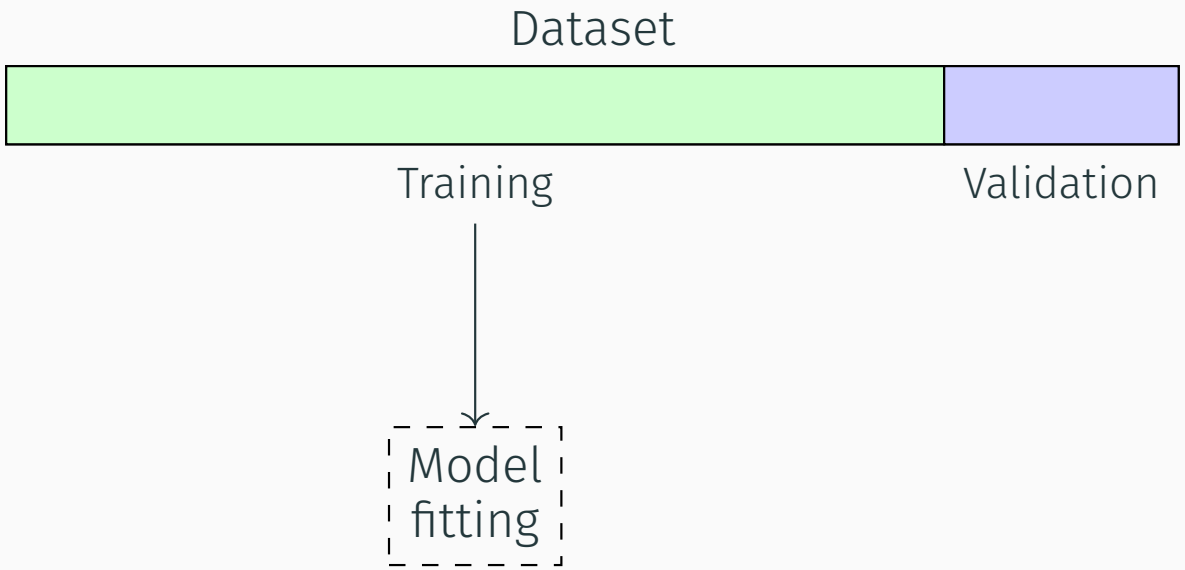

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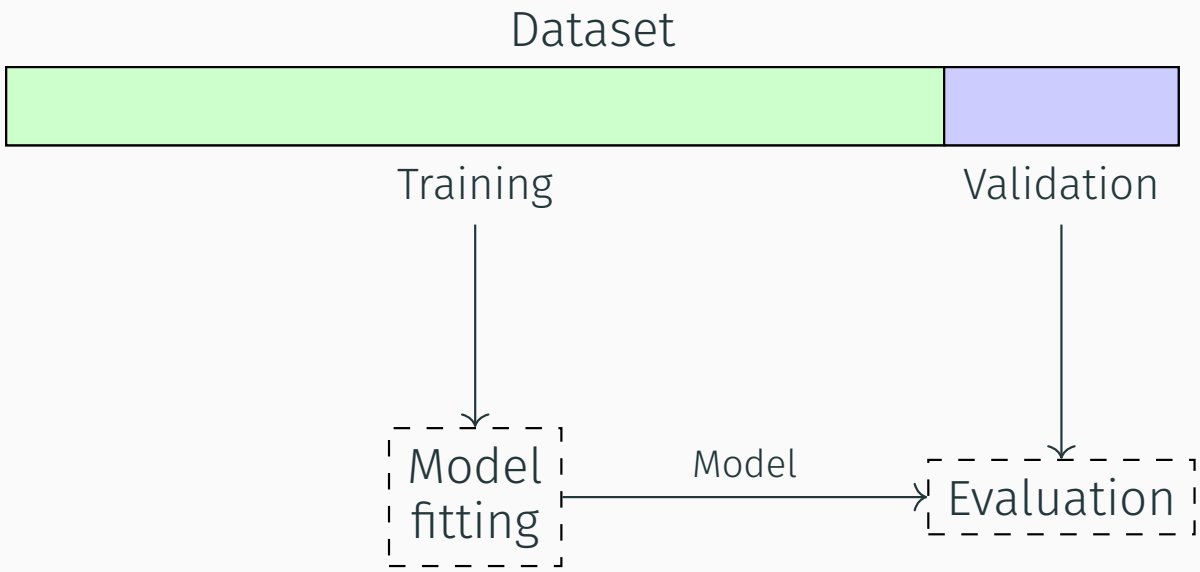

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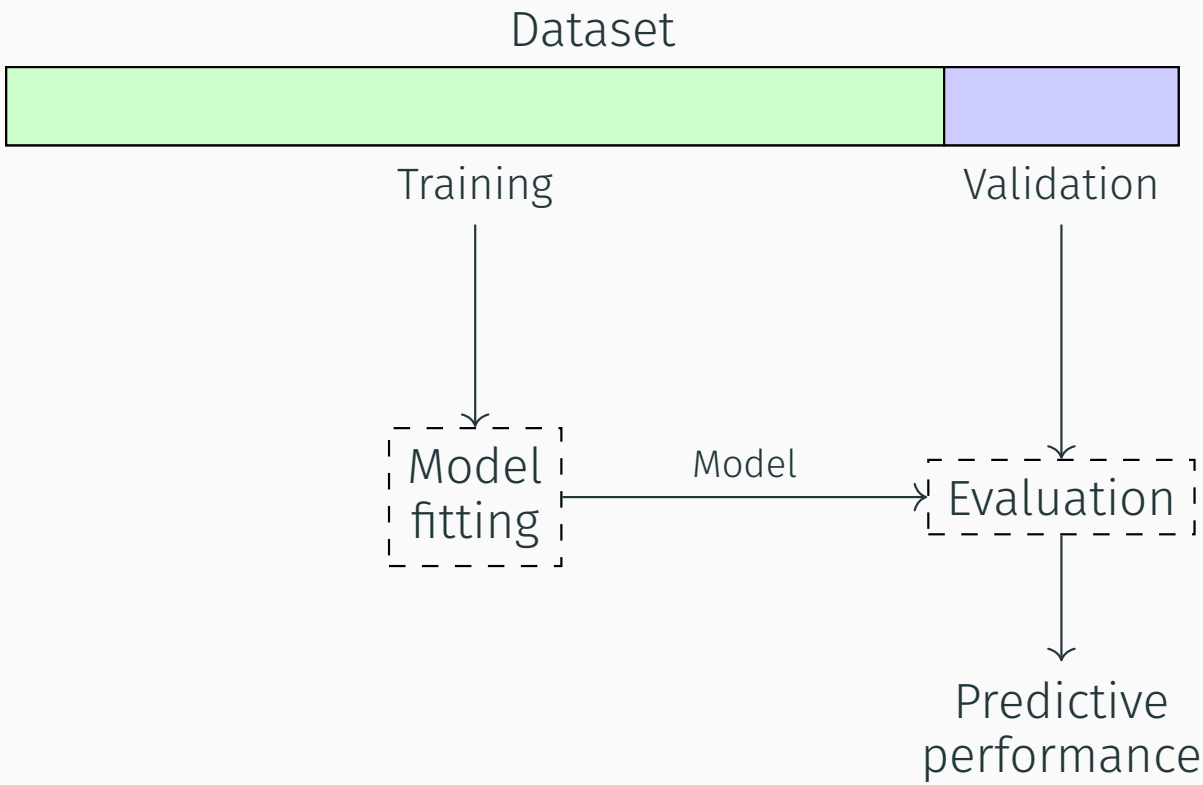
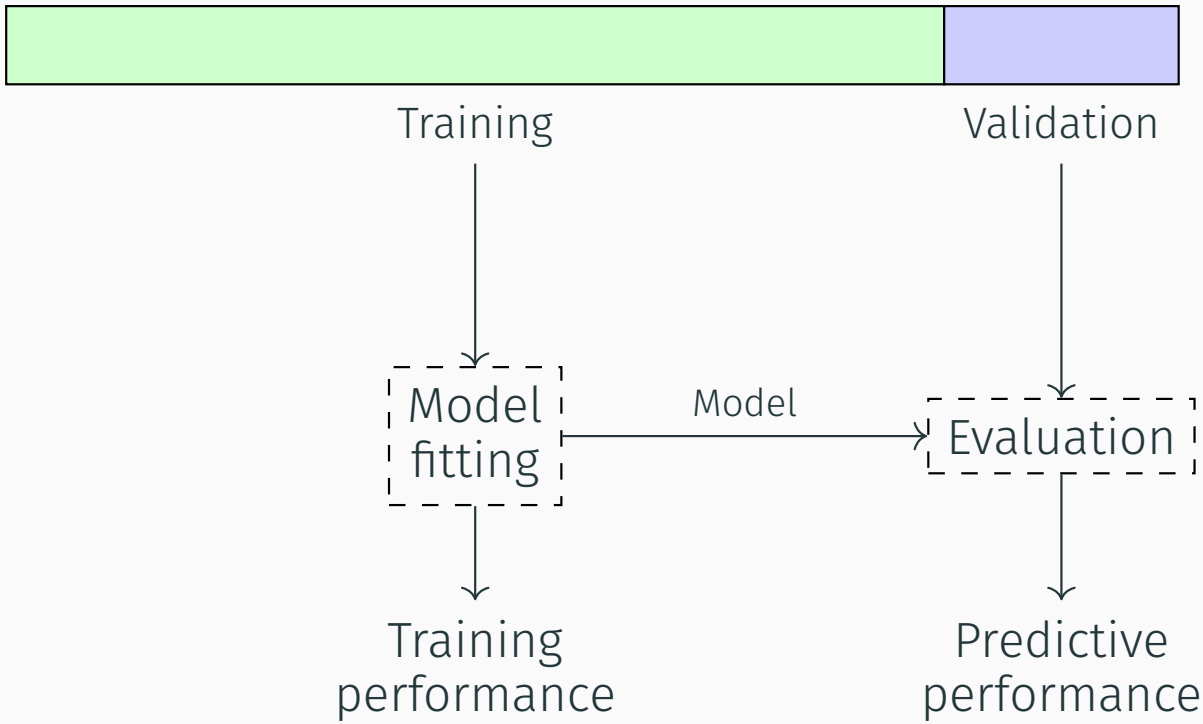


Model evaluation: Validation set

In the validation set approach we split the dataset into two subsets (commonly ∼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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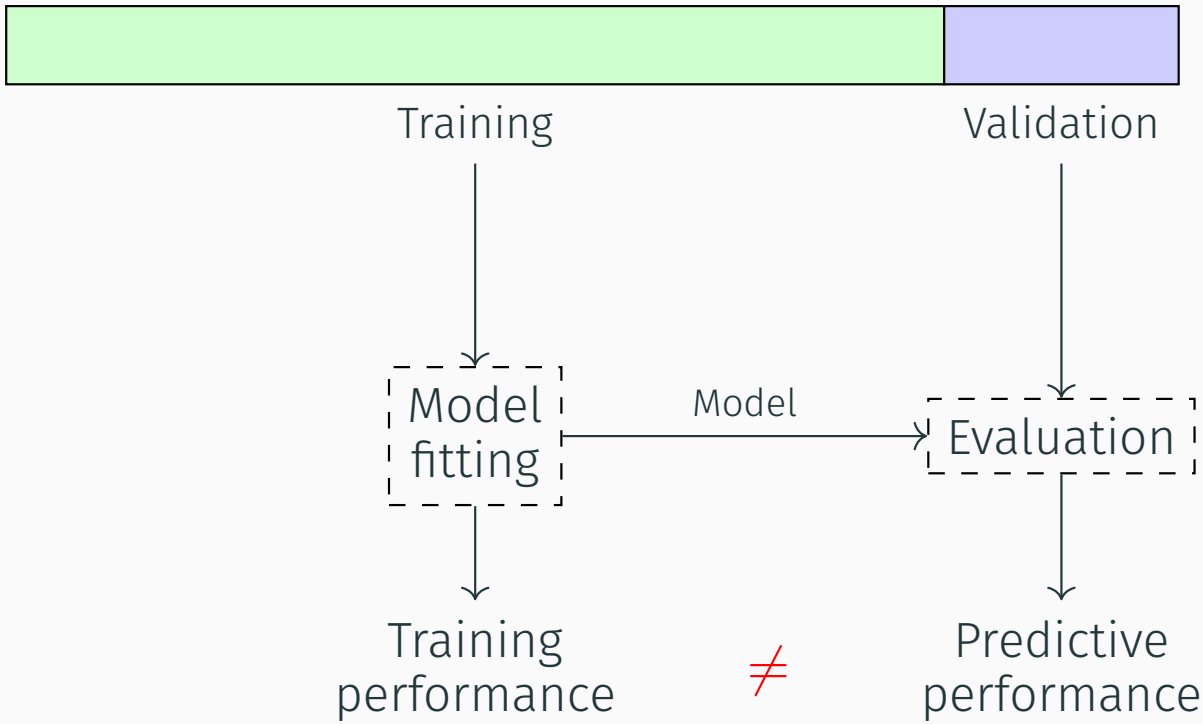
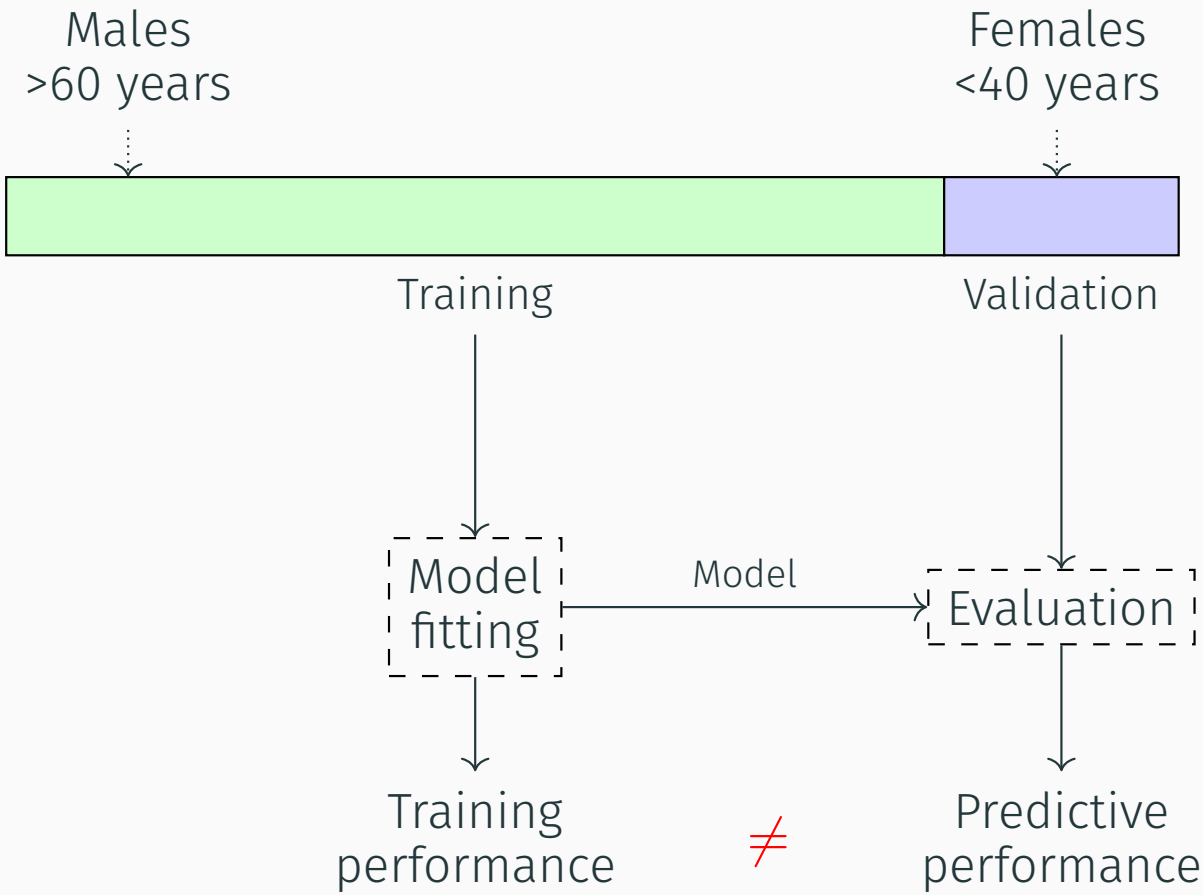


Model evaluation: Validation set



Model evaluation: Stratification

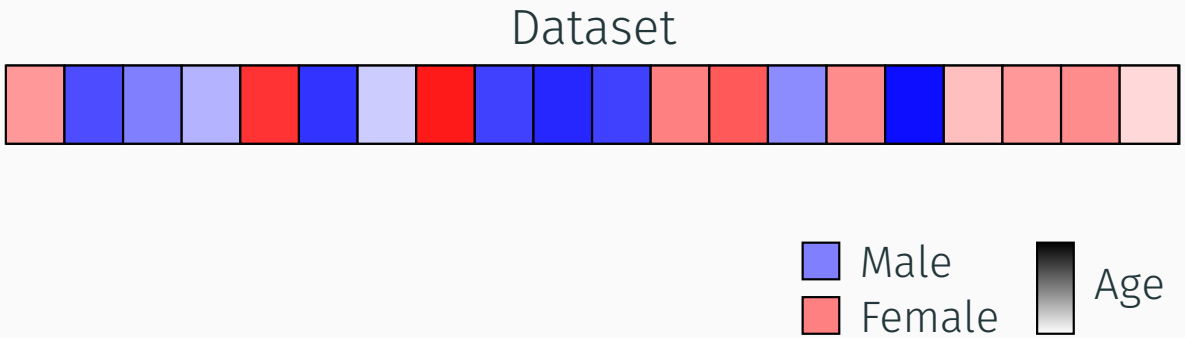
Stratification:

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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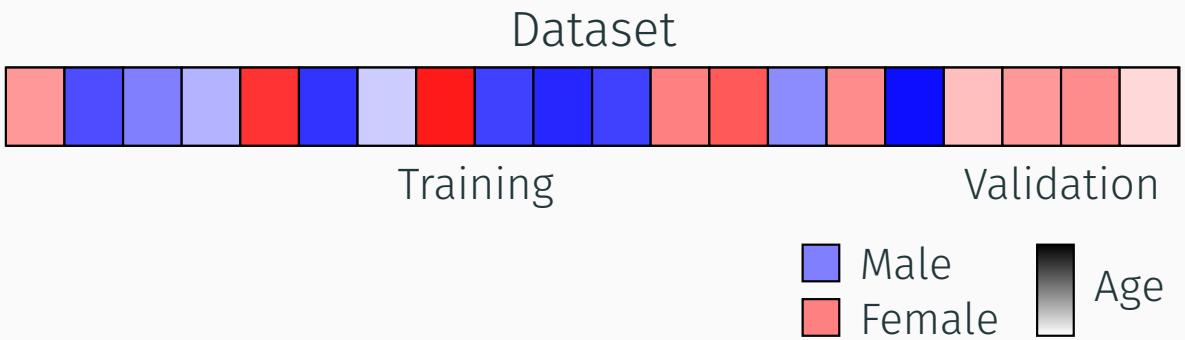
Model evaluation: Stratification

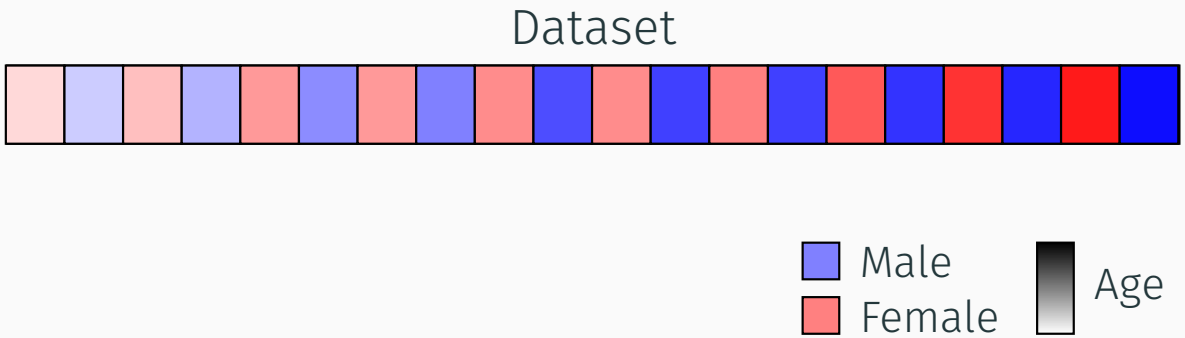


In[1]:

```
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'])
```

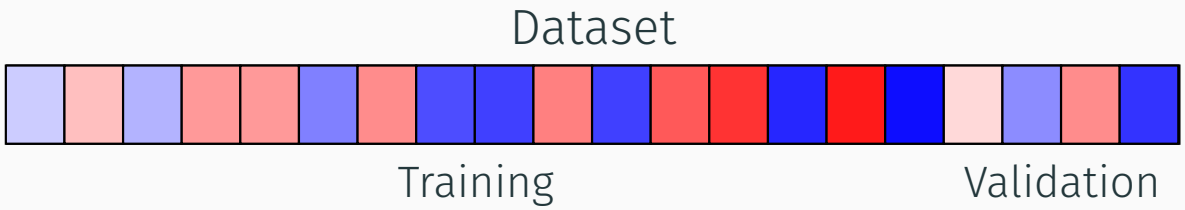
Model evaluation: Stratification

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



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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

In[1]:
```python
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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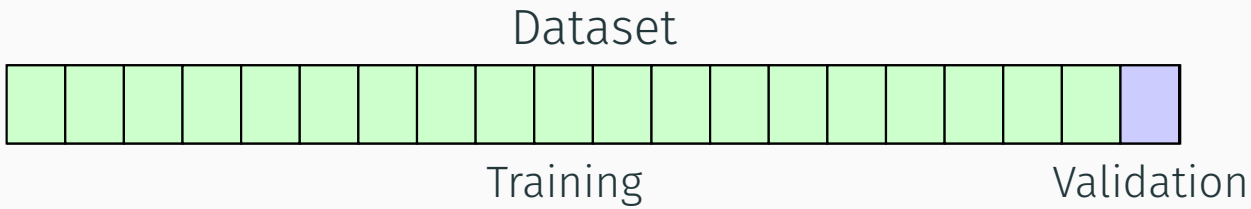

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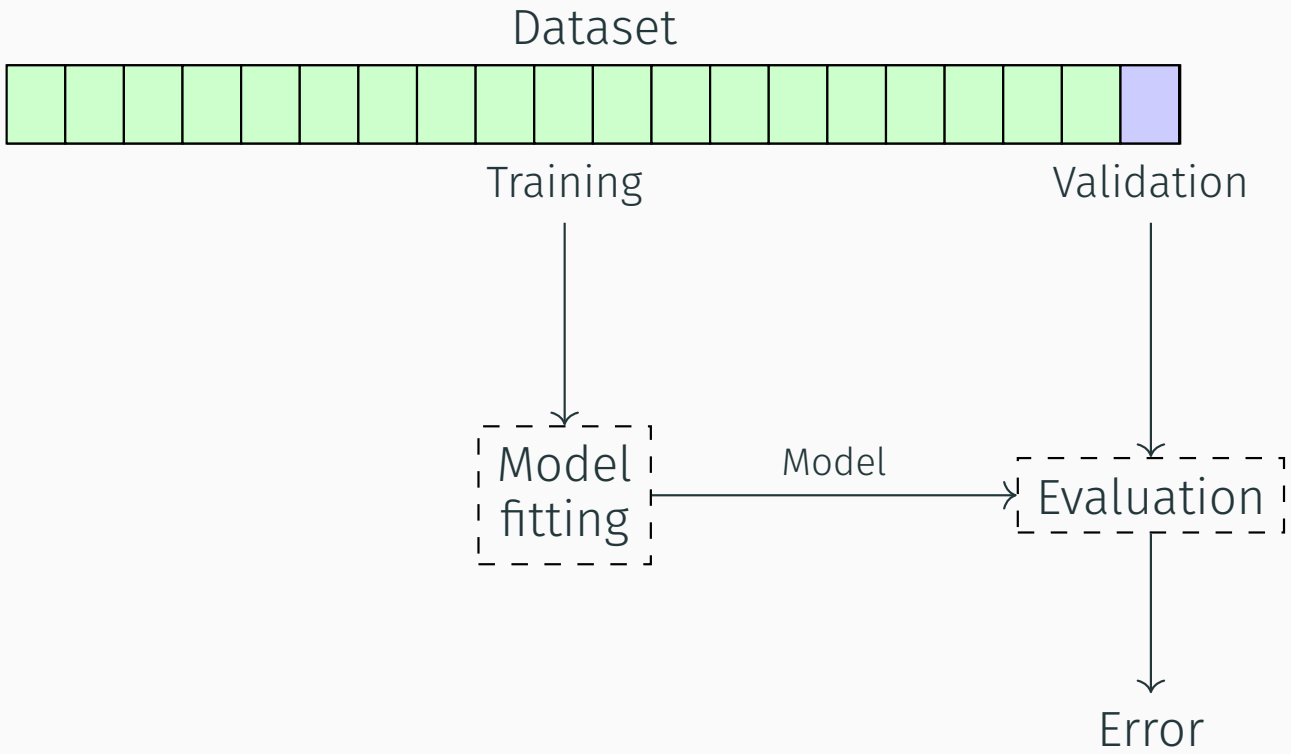

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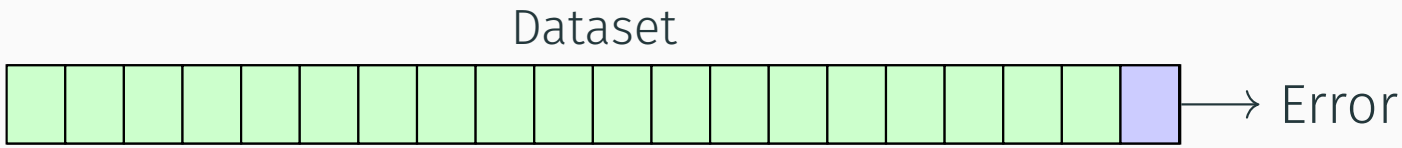

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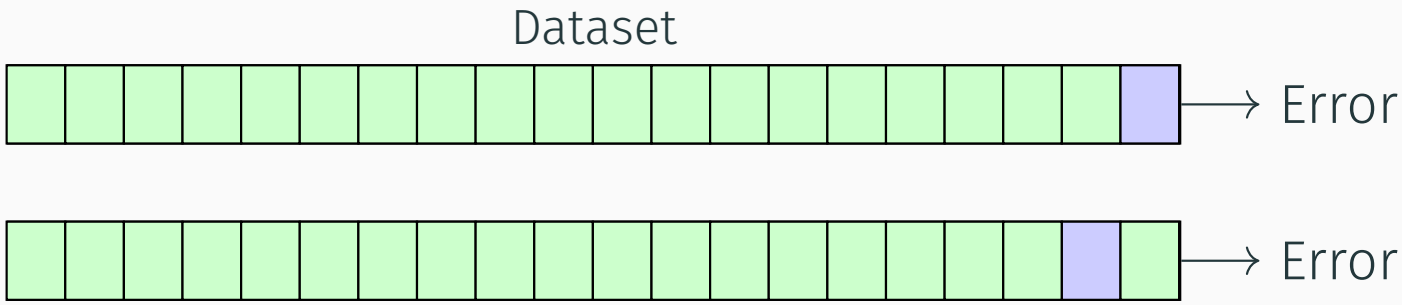

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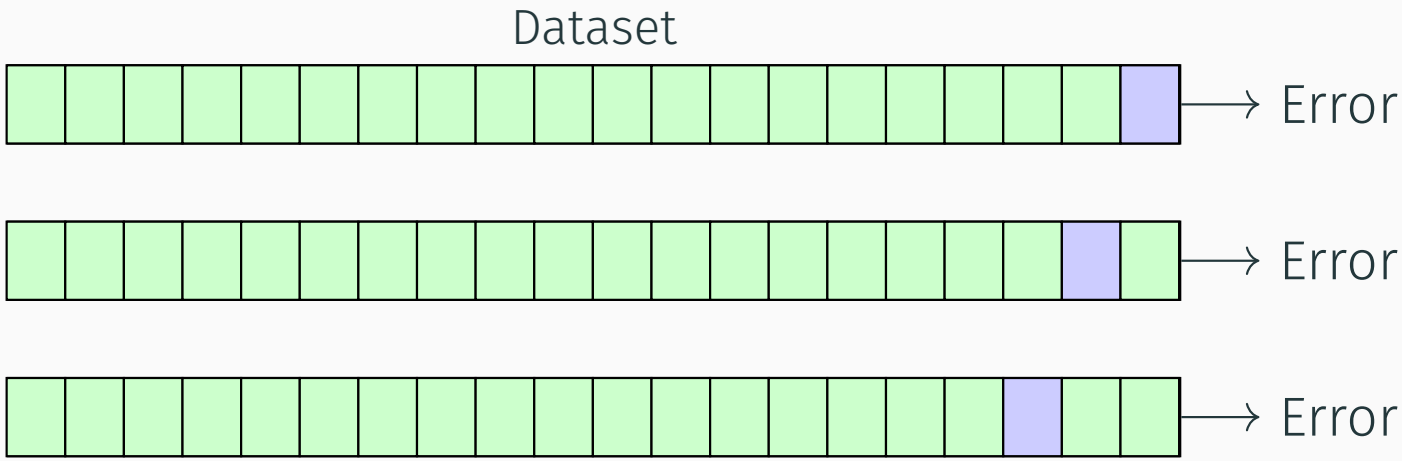

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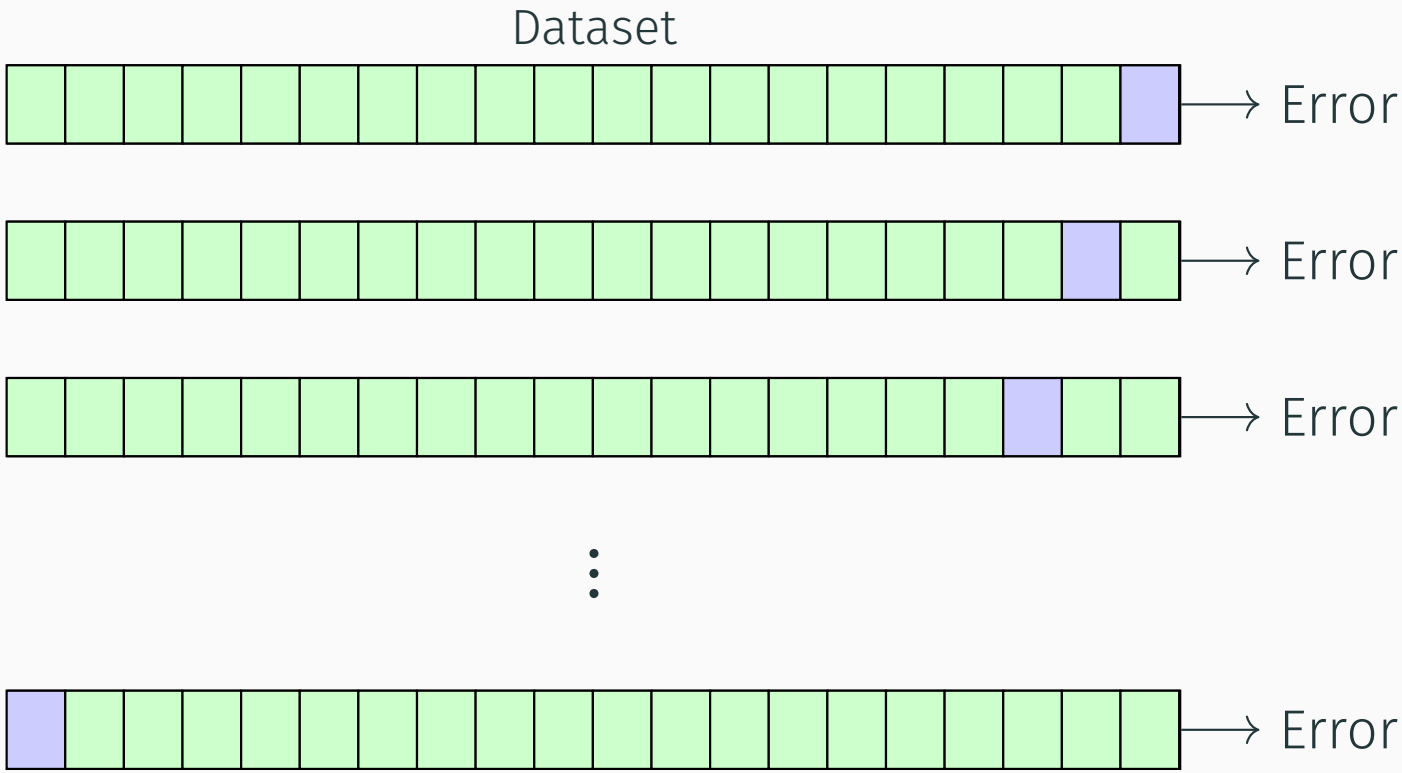

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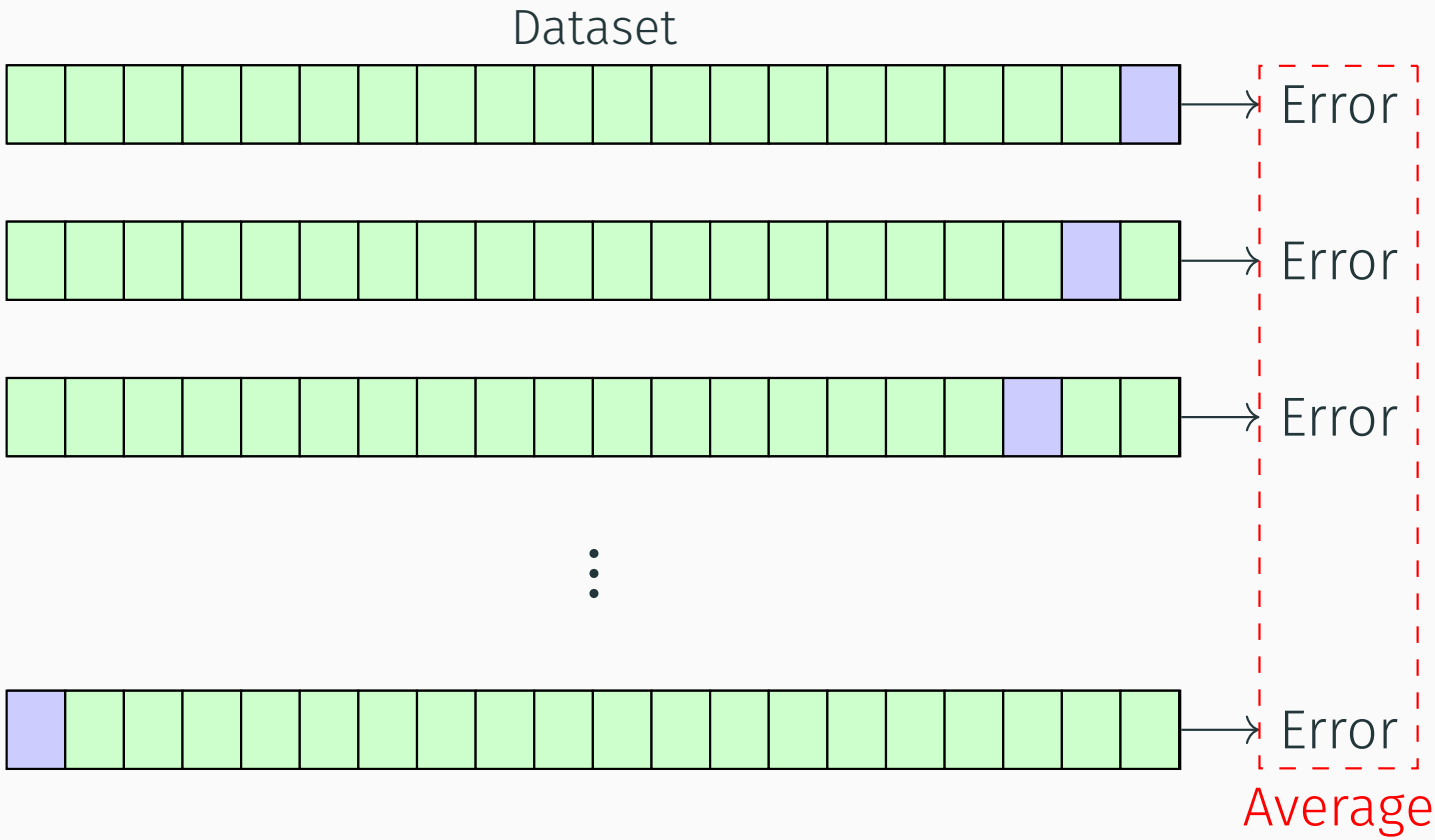

Model evaluation: Leave-one-out cross-validation

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

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

Model evaluation: Cross-validation

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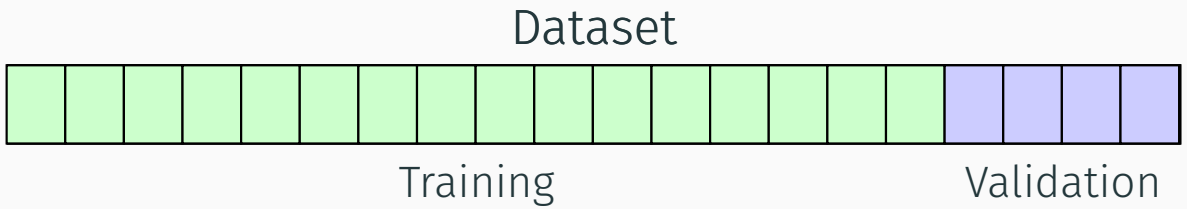

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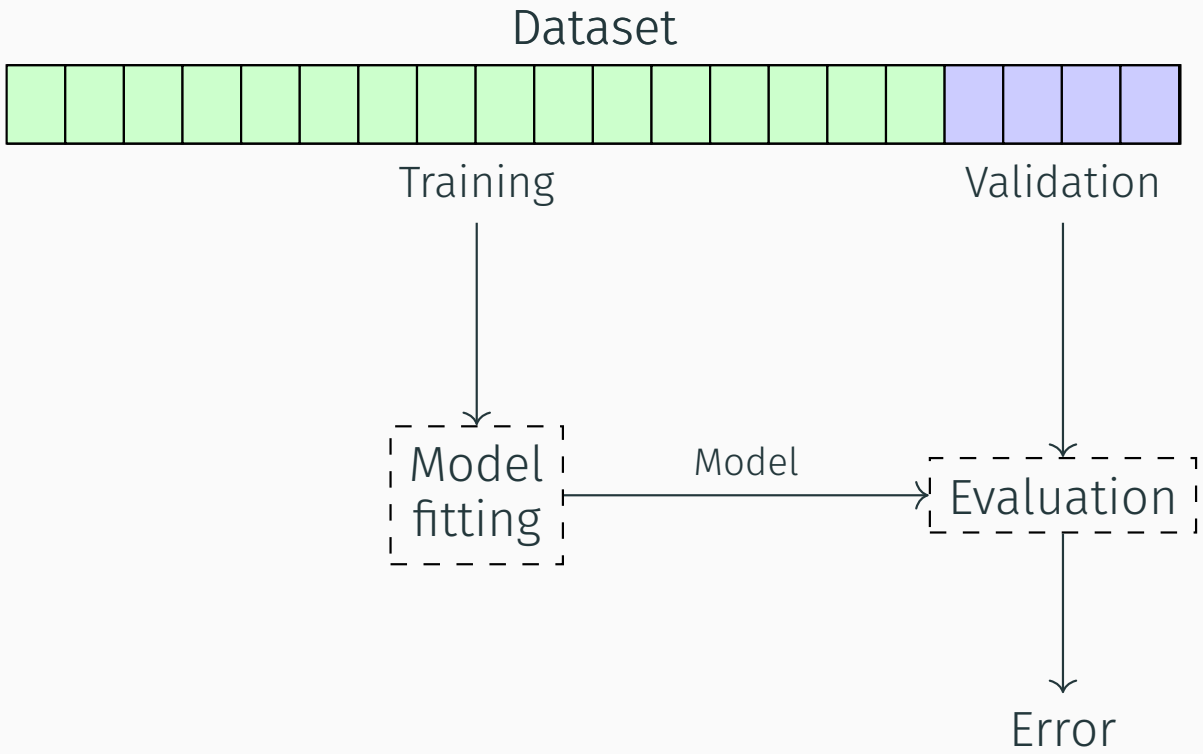

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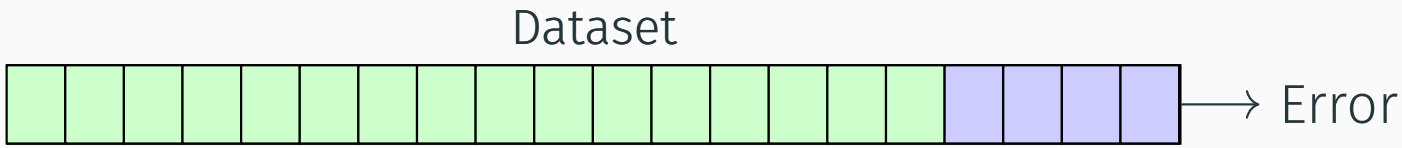

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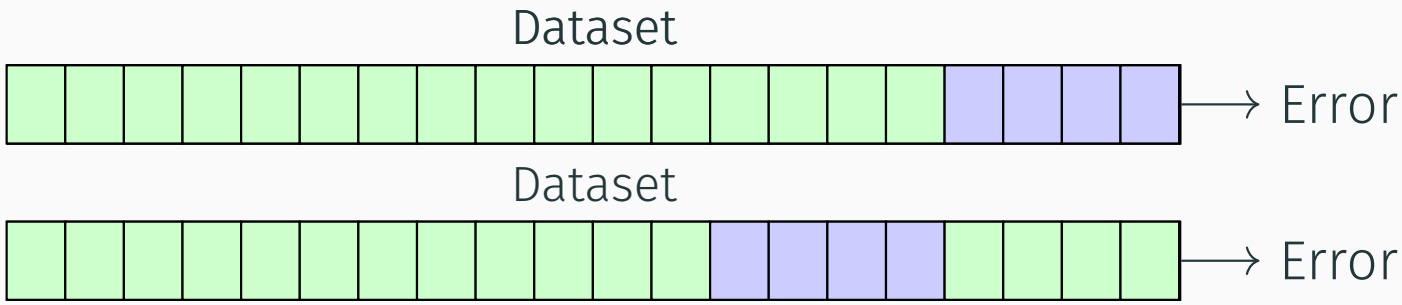

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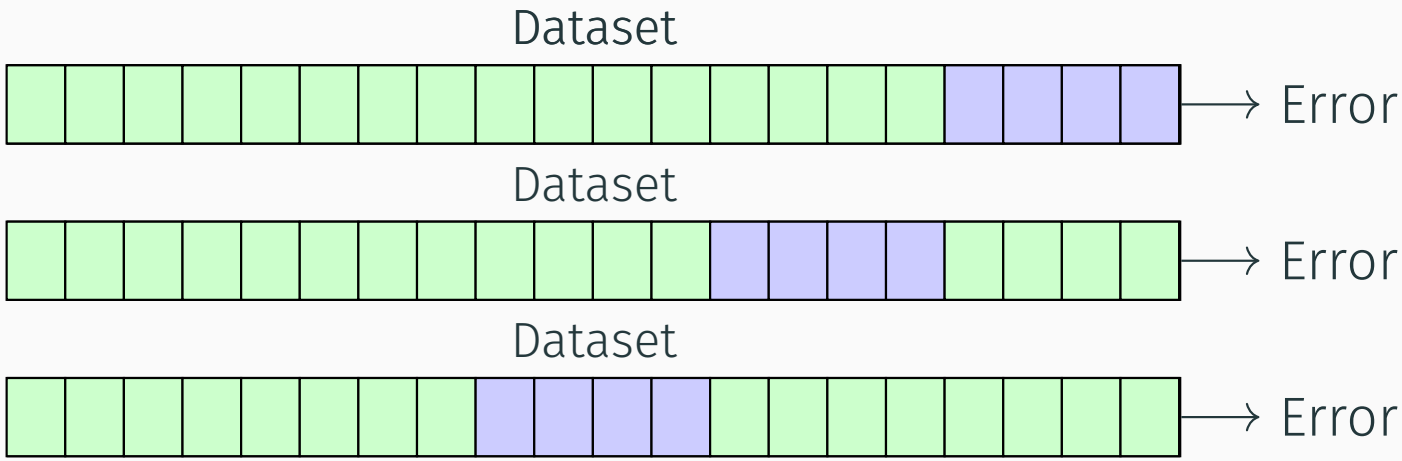

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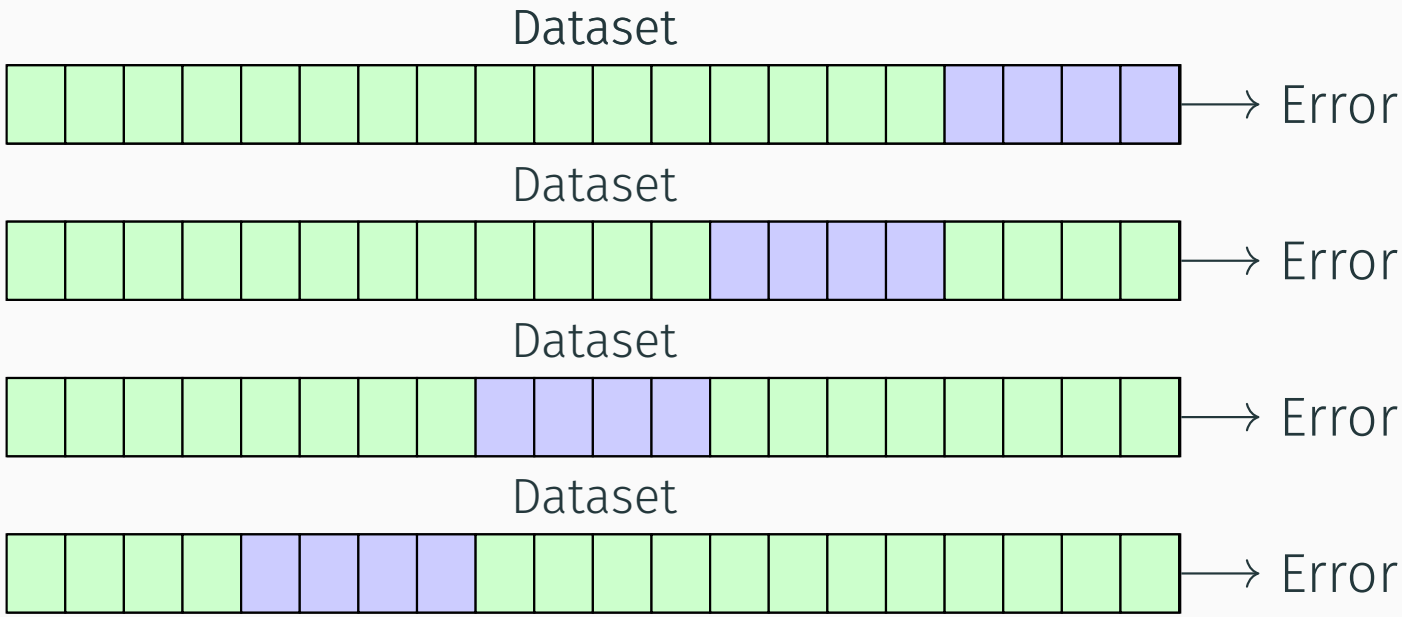

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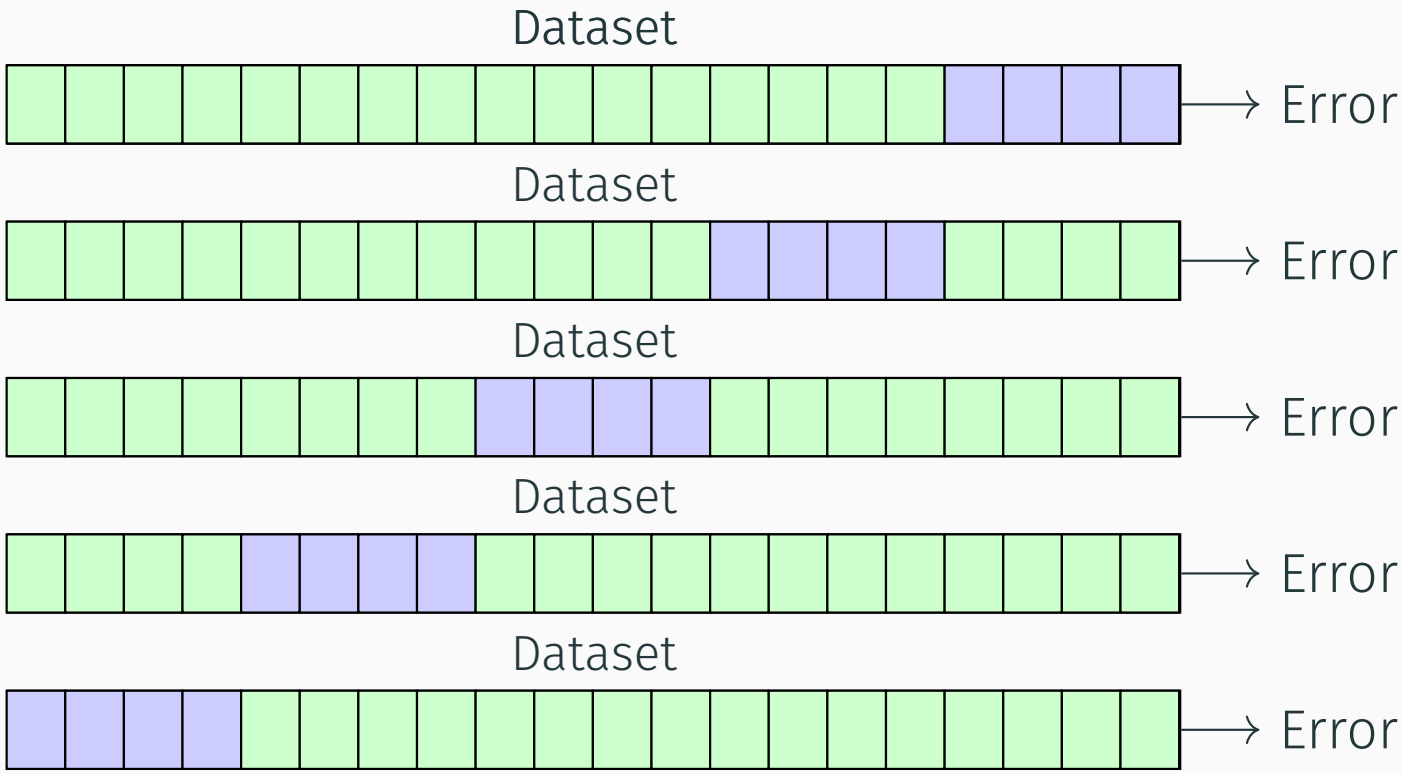

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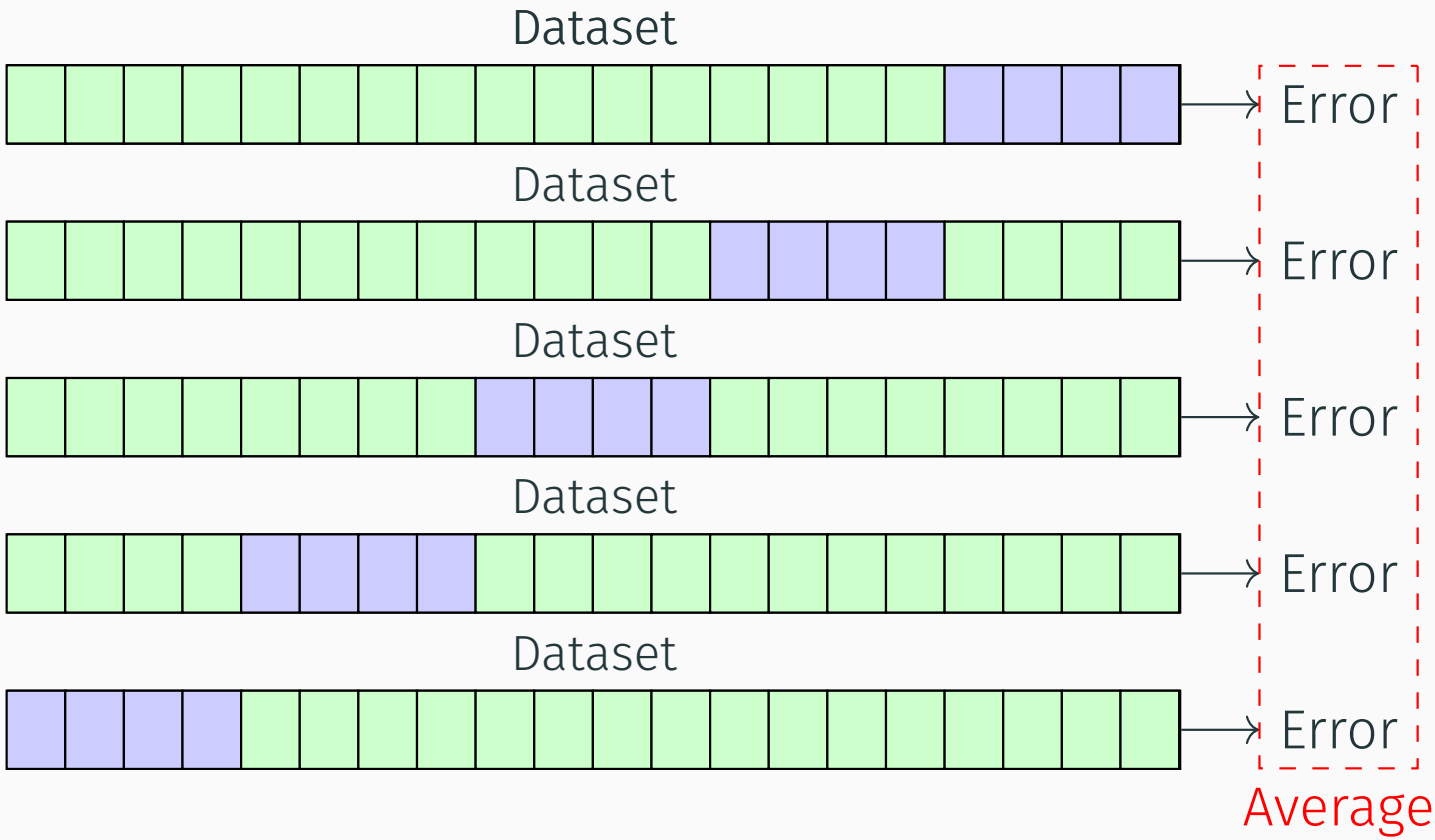

Model evaluation: Cross-validation

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

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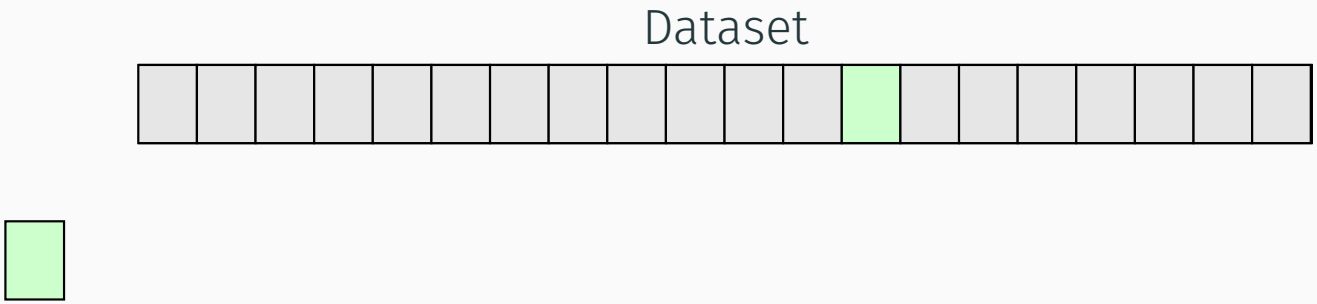

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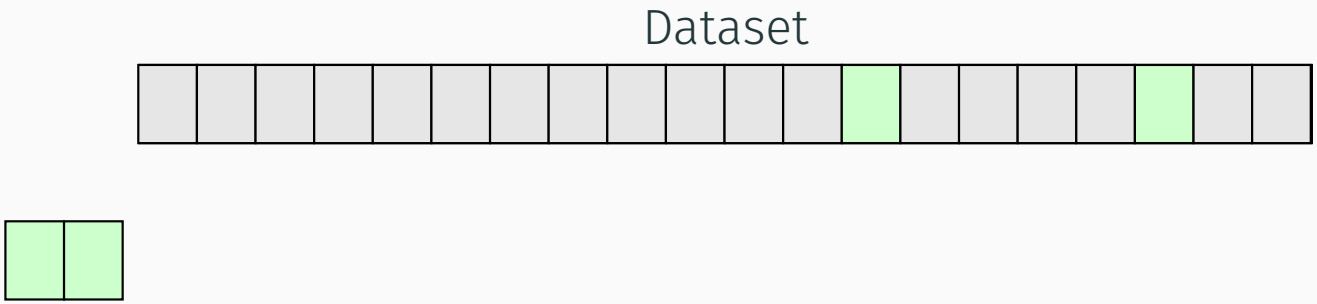

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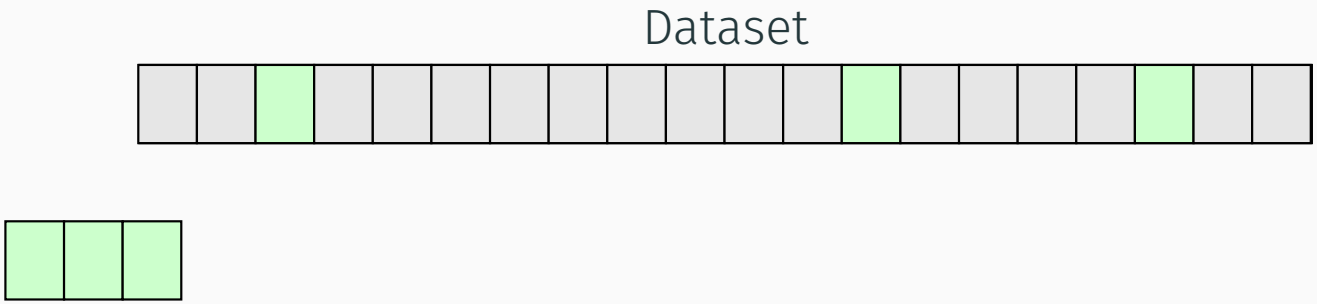

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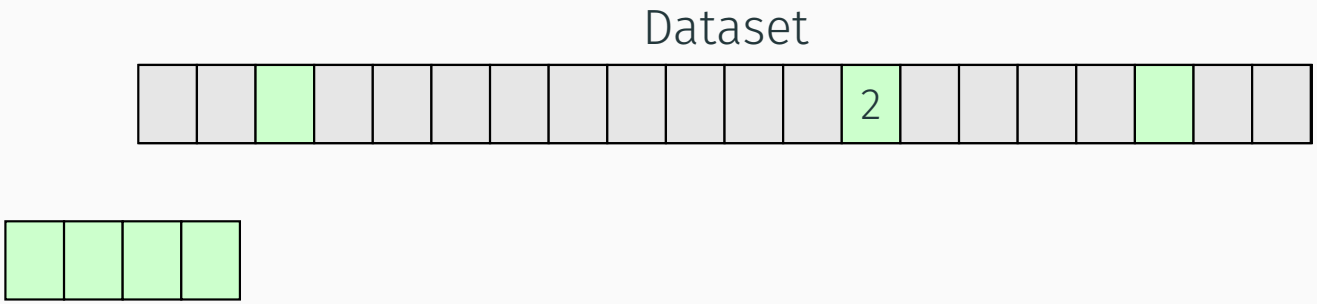

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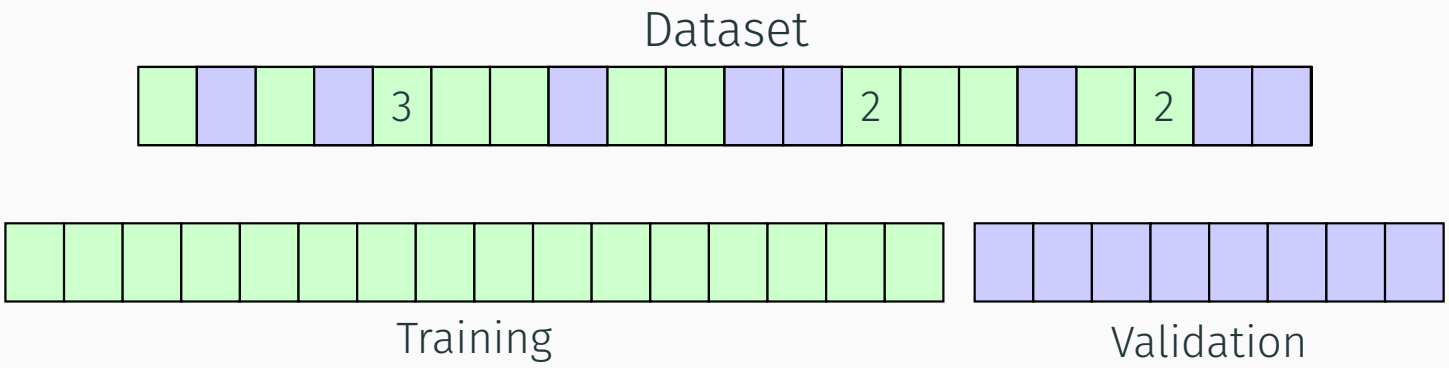

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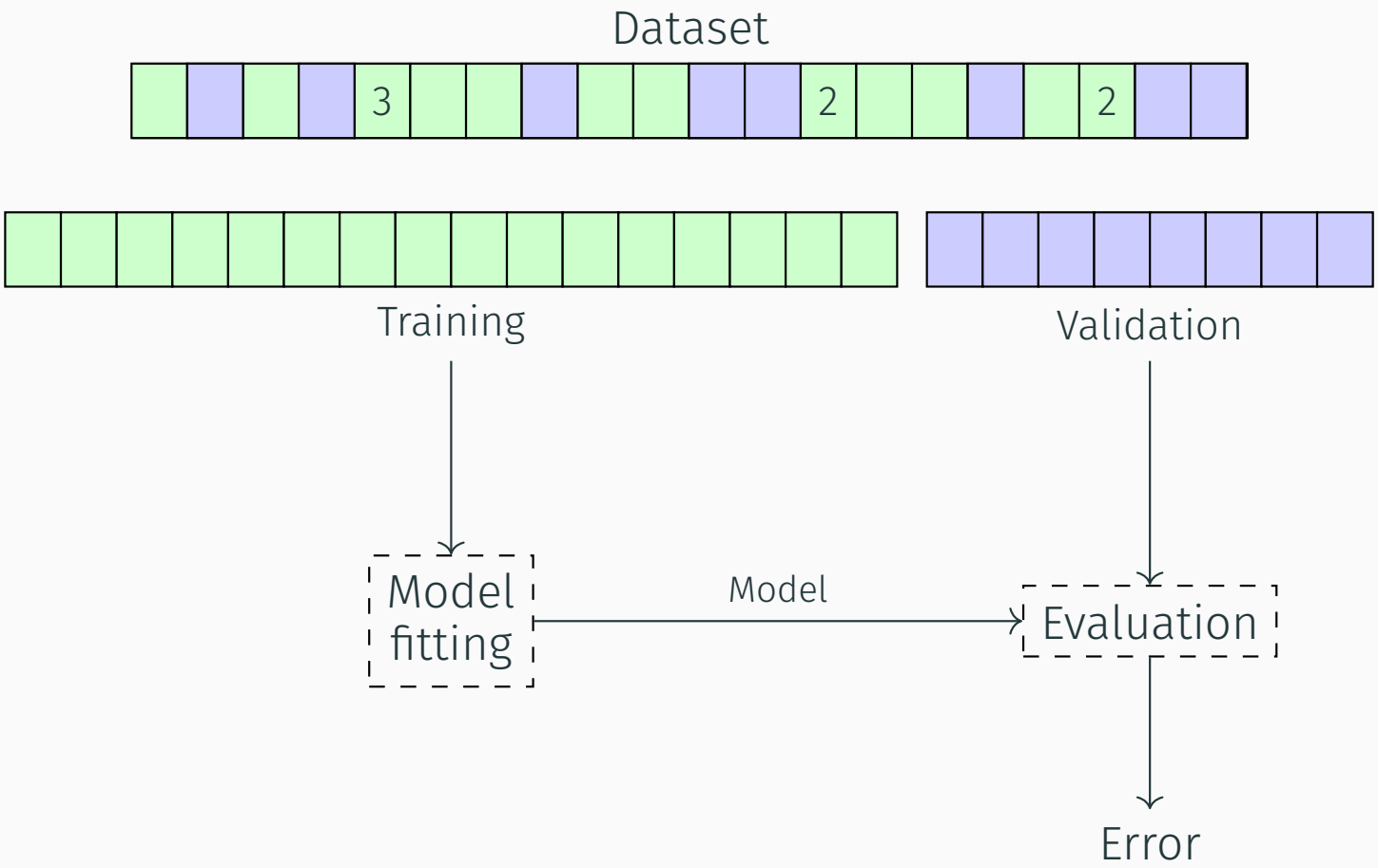

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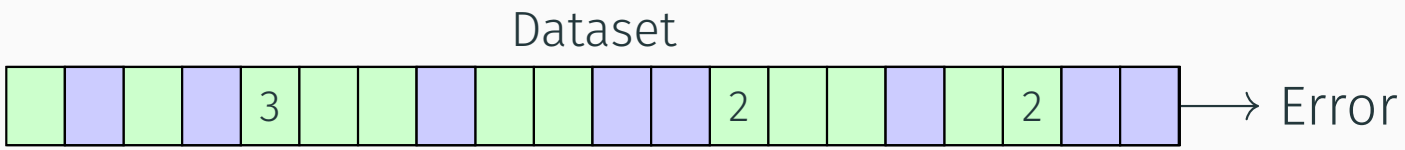

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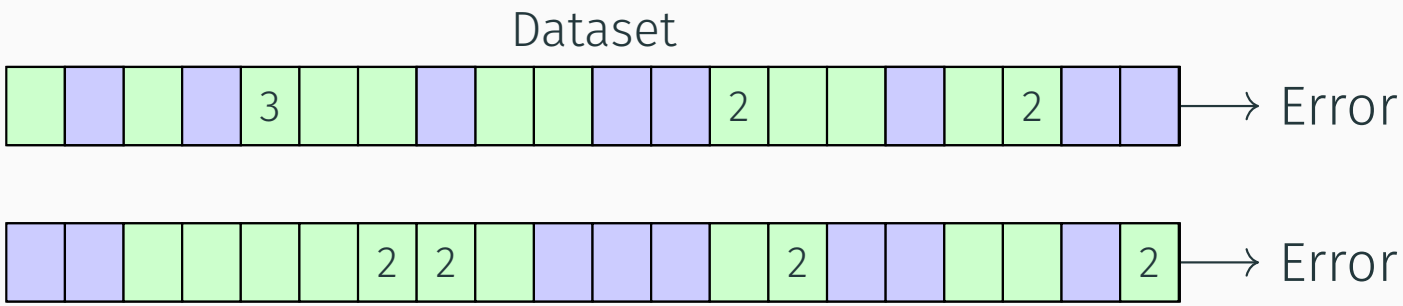

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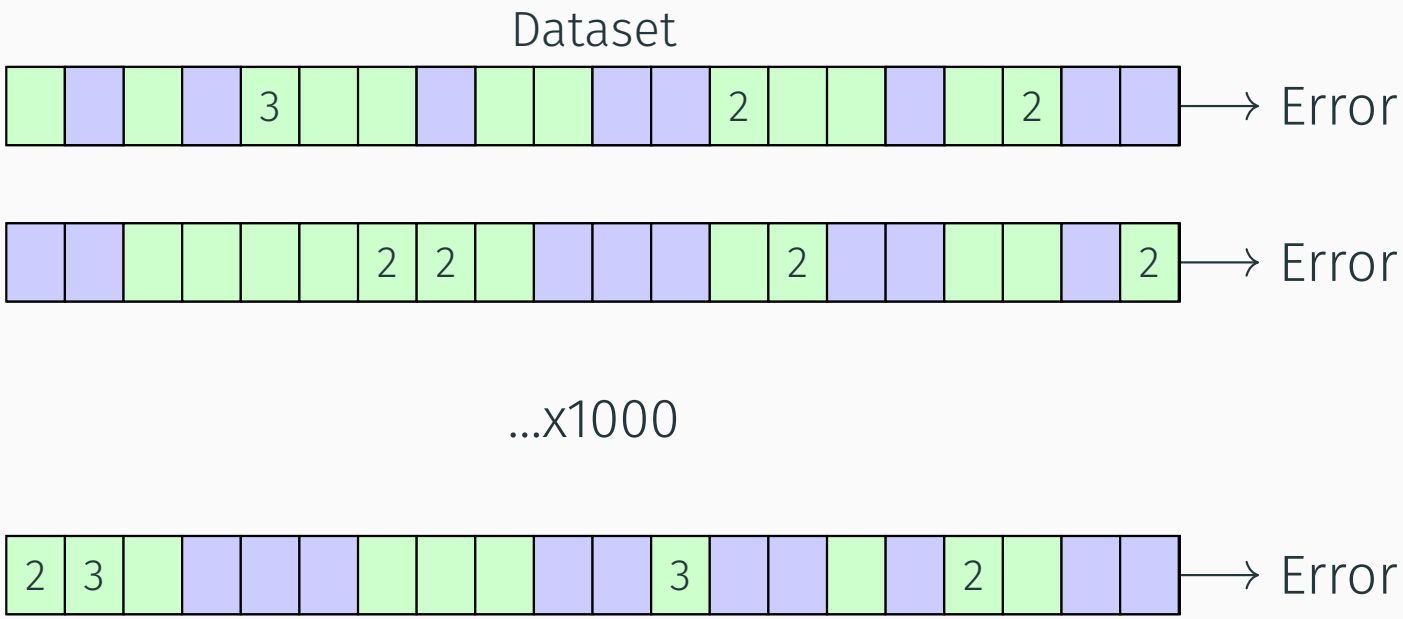

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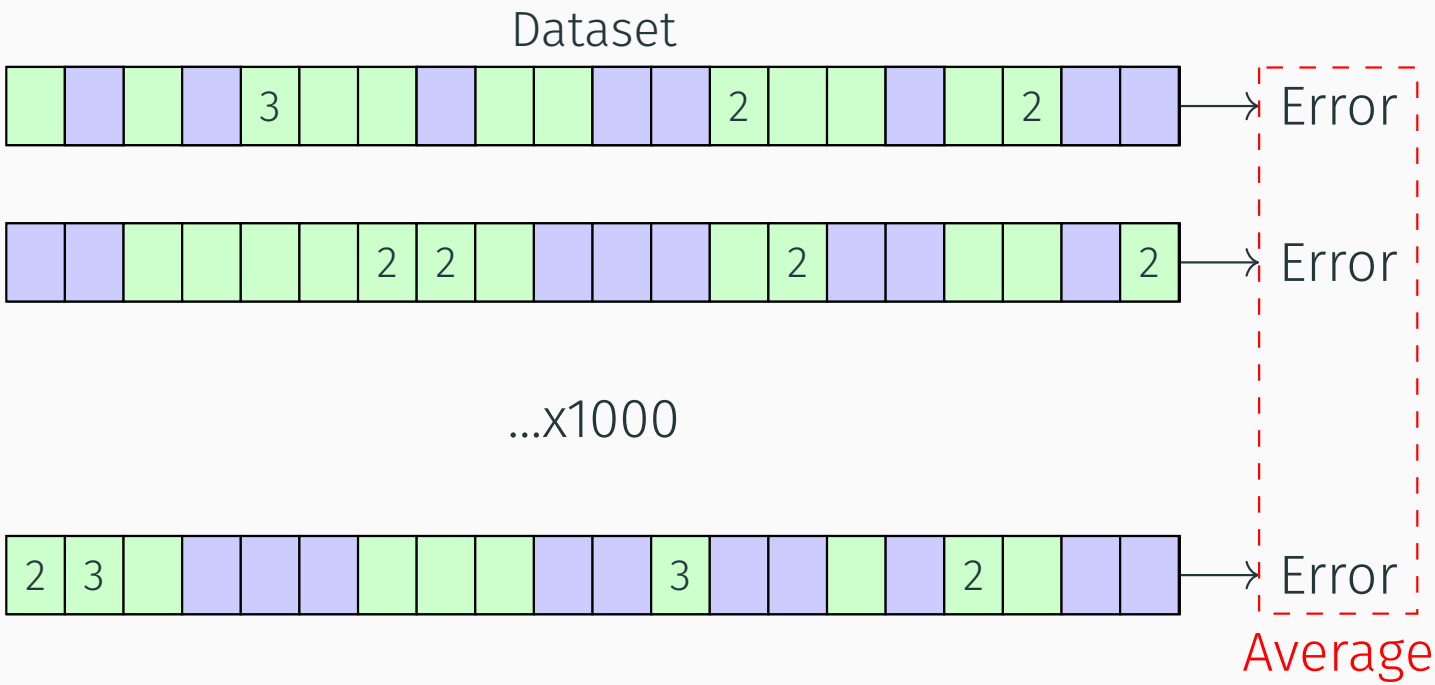
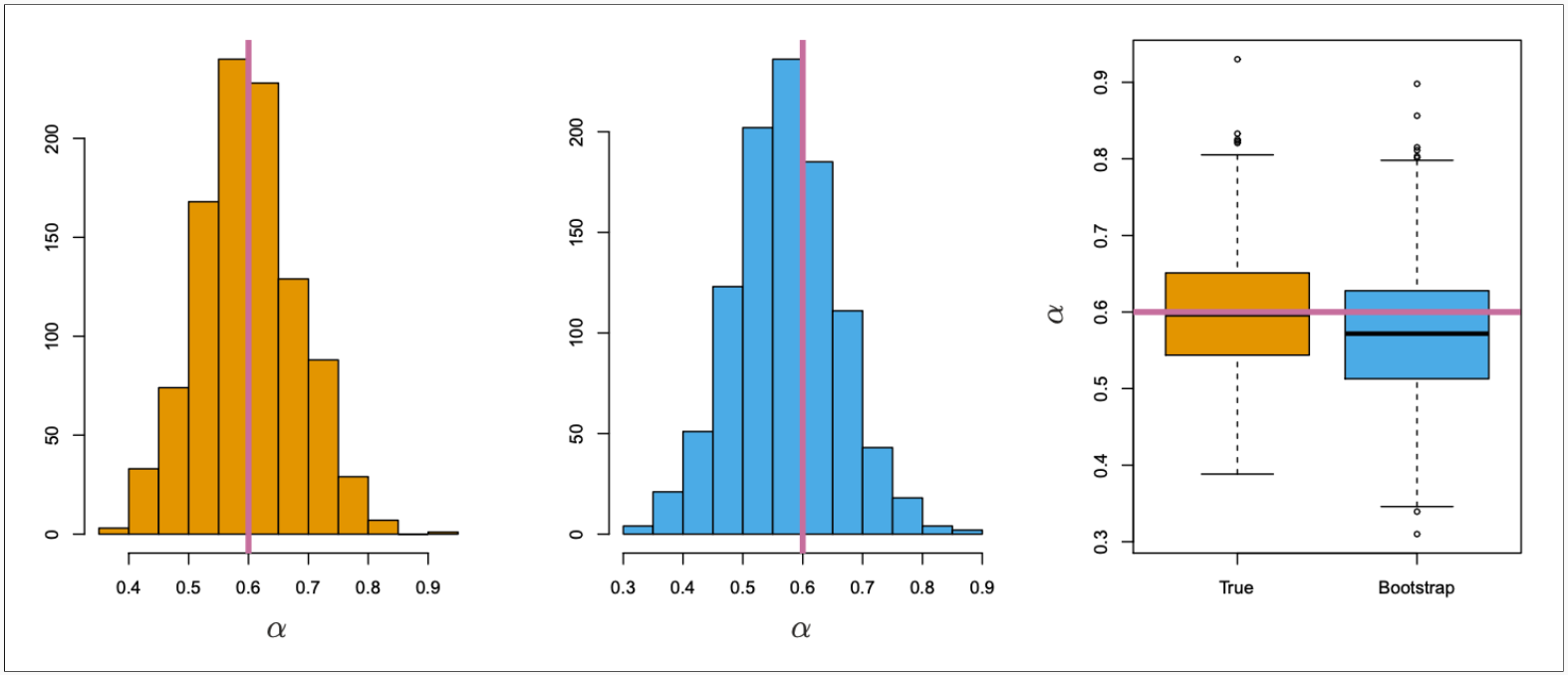


Model evaluation: Bootstrapping

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

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

Model evaluation: Bootstrapping



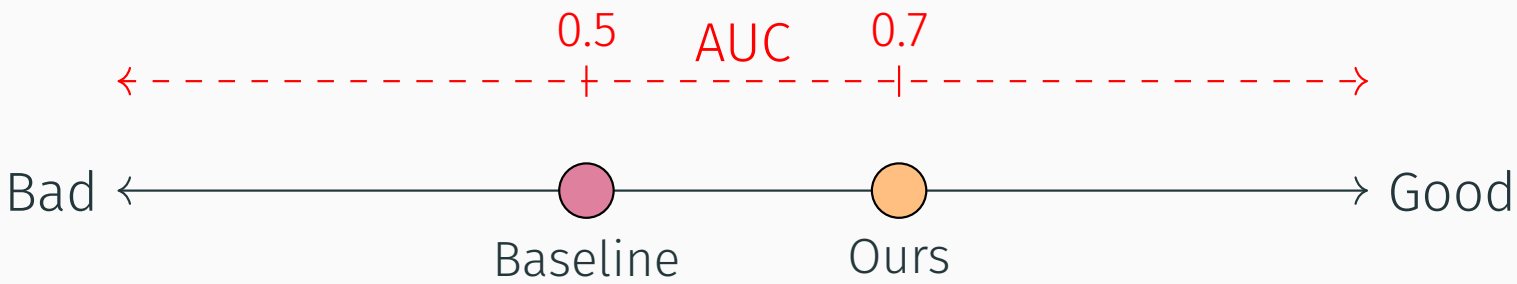
Model evaluation: Comparison

Why do we want to evaluate our model?

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

Model evaluation: Comparison

Model evaluation: Comparison



Model evaluation: Comparison

http://localhost:8890/notebooks/notebooks%2FModel%20variability.ipynb

Model evaluation: Comparison

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

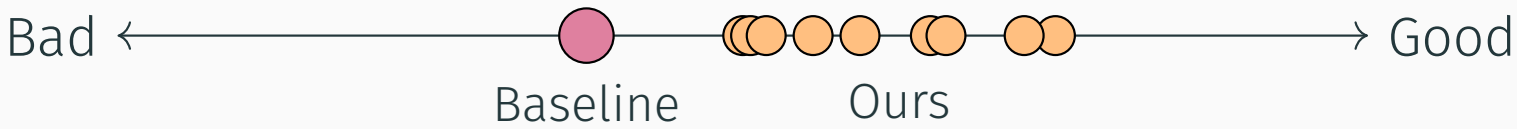
Is our model significantly better?

Model evaluation: Comparison

Approach 1:

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

Model evaluation: Comparison



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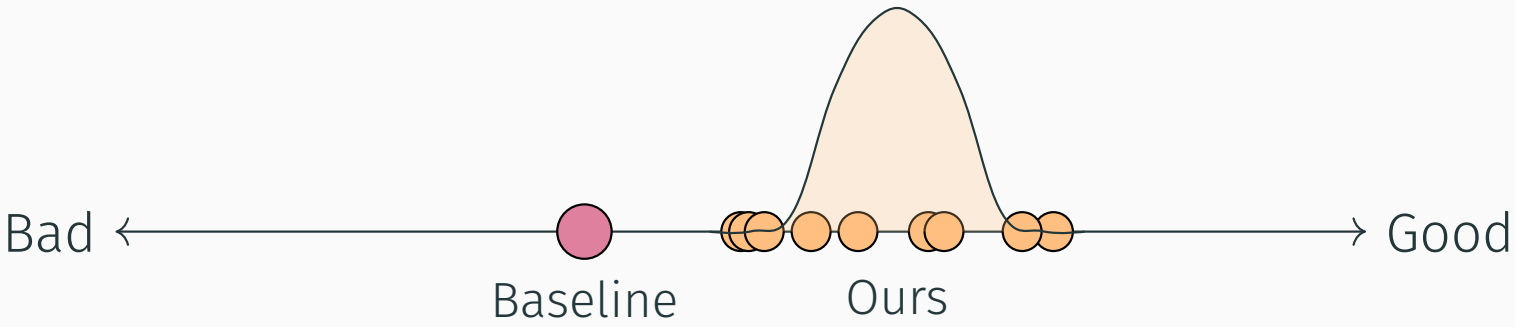


Approach 1:

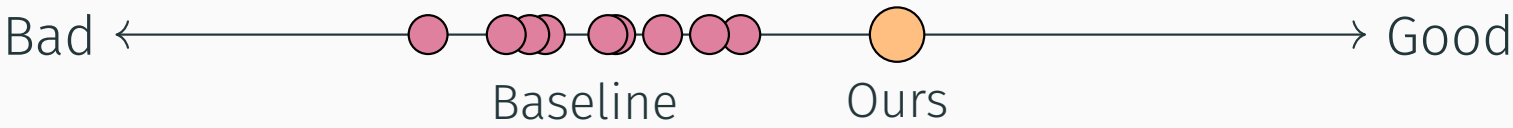
Is the mean of the distribution of performances from our model (with regards to variability that is **unrelated** to efficacy) significantly higher than the point-estimate baseline?

Model evaluation: Comparison

Approach 2:

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

Model evaluation: Comparison



Approach 2:

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

Model evaluation: Comparison

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

Model evaluation: Comparison

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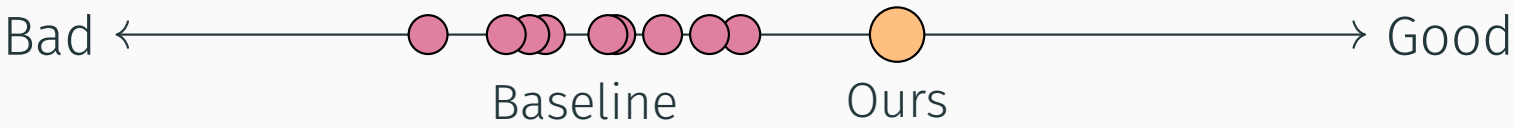
52	Female	-0.32	0
31	Male	0.91	1
48	Female	-0.15	1

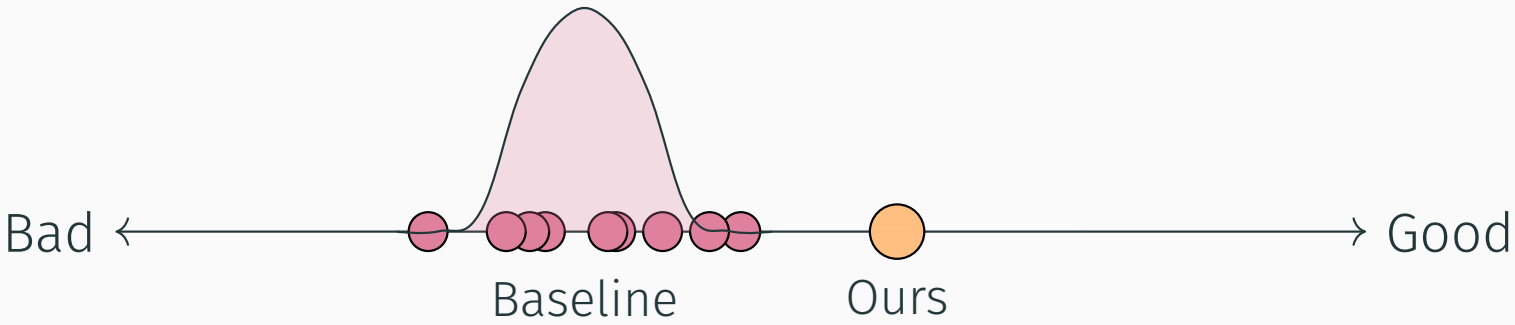
Model evaluation: Comparison



Approach 2:

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

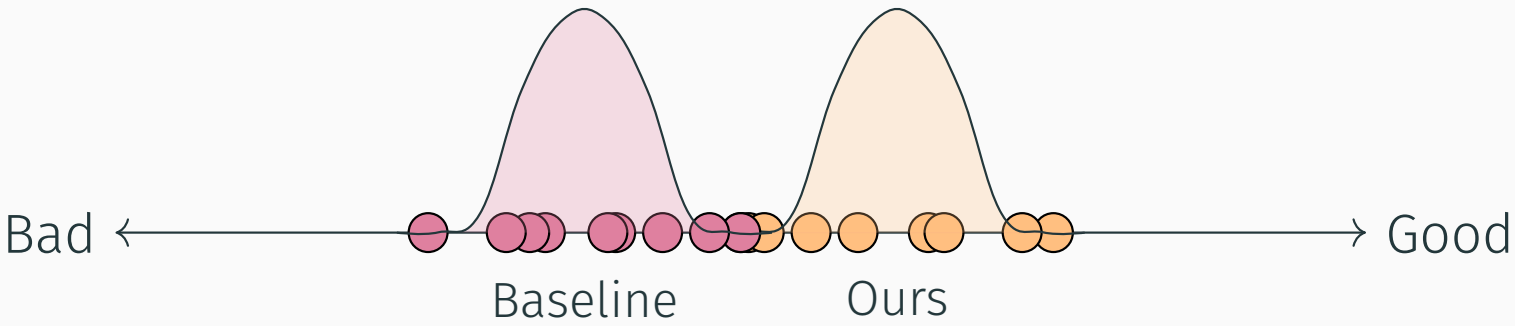
Model evaluation: Comparison



Approach 2:

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

Model evaluation: Comparison



Approach 3:

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

Model evaluation: 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 performance **and parameters**
- Cross-validation (or bootstrapping) will produce a distribution of model performances (although caution the correlation)
- Permutation testing will produce a distribution of baseline performances
- Compare models across folds using Wilcoxon signed-rank test **(ensure the folds are the same!)**