INTRODUCTION TO MACHINE LEARNING

Measuring model performance or error

Is our model any good?

- Context of task
  - Accuracy
  - Computation time
  - Interpretability
- 3 types of tasks
  - Classification
  - Regression
  - Clustering

Classification

- **Accuracy** and **Error**
- System is **right** or **wrong**
- Accuracy goes **up** when Error goes **down**

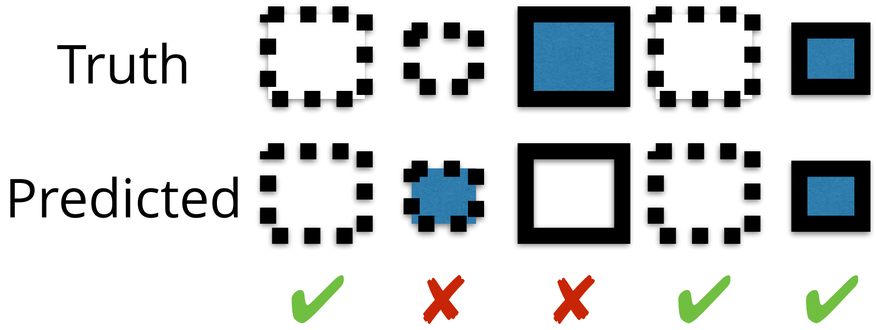
$$\textbf{Accuracy} = \frac{\text{correctly classified instances}}{\text{total amount of classified instances}}$$

Error = 1 - Accuracy

Example

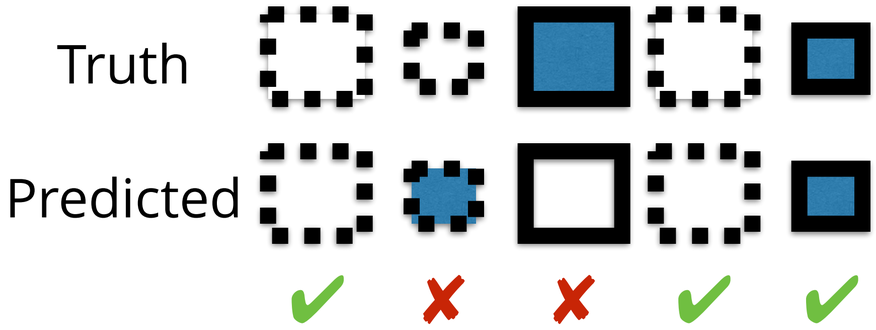
- Squares with 2 features: small/big and solid/dotted
- Label: colored/not colored
- Binary classification problem

Example



$$\frac{\checkmark\ \checkmark\ \checkmark}{\checkmark\ \checkmark\ \checkmark\ \times\ \times} = \frac{3}{5} = 60\%$$

Example



$$\frac{\checkmark\ \checkmark\ \checkmark}{\checkmark\ \checkmark\ \checkmark\ \times\ \times} = \frac{3}{5} = 60\%$$

Limits of accuracy

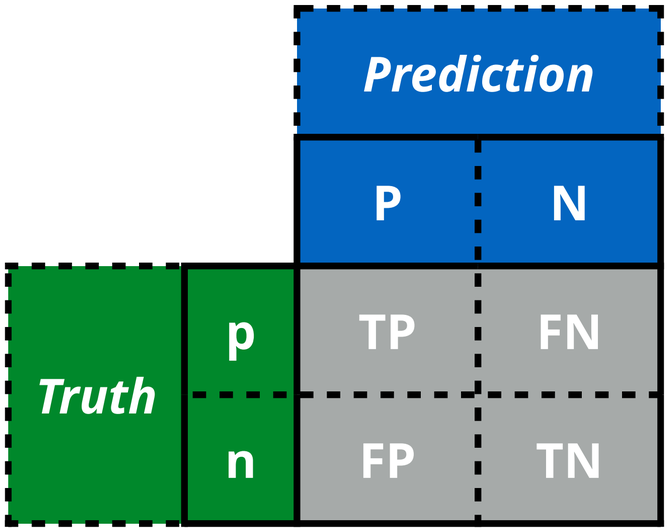
- Classifying very rare heart disease
- Classify all as negative (not sick)
- Predict 99 correct (not sick) and miss 1
- Accuracy: 99%
- Bogus... you miss every positive case!

Confusion matrix

- Rows and columns contain all available labels
- Each cell contains frequency of instances that are classified in a certain way

Confusion matrix

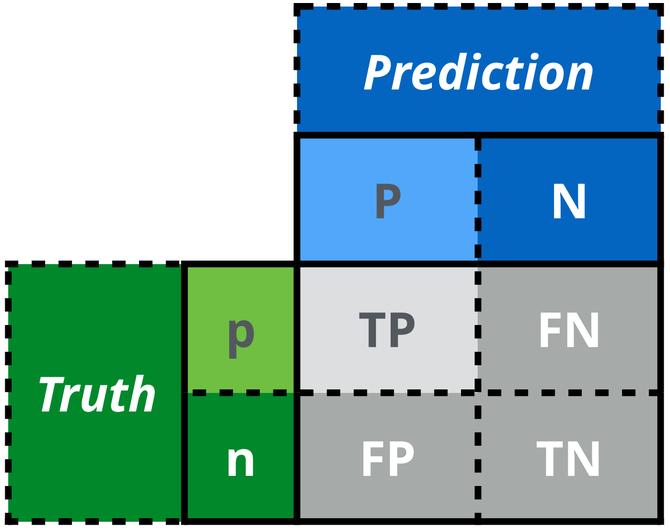
- Binary classifier: positive or negative (1 or 0)



Confusion matrix

- Binary classifier: positive or negative (1 or 0)

True Positives
Prediction: P
Truth: P



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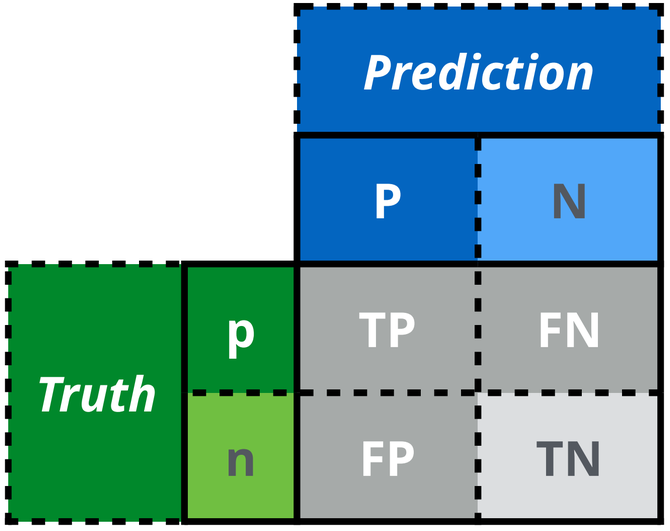

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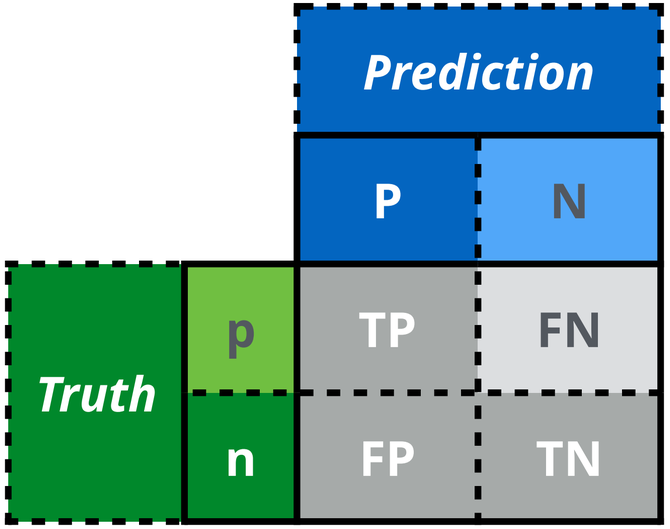

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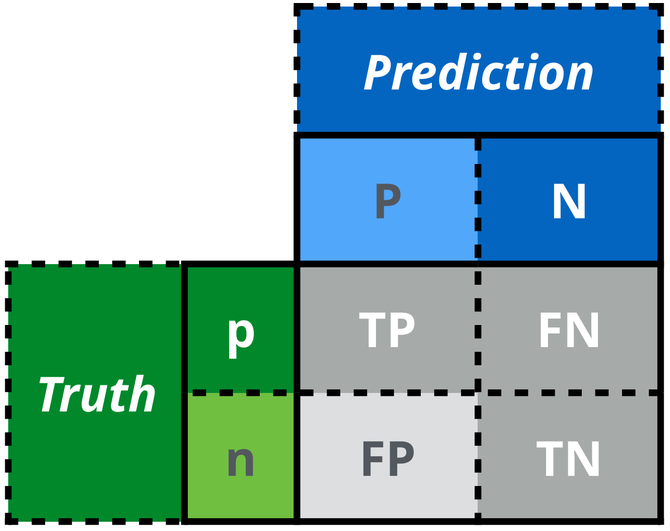
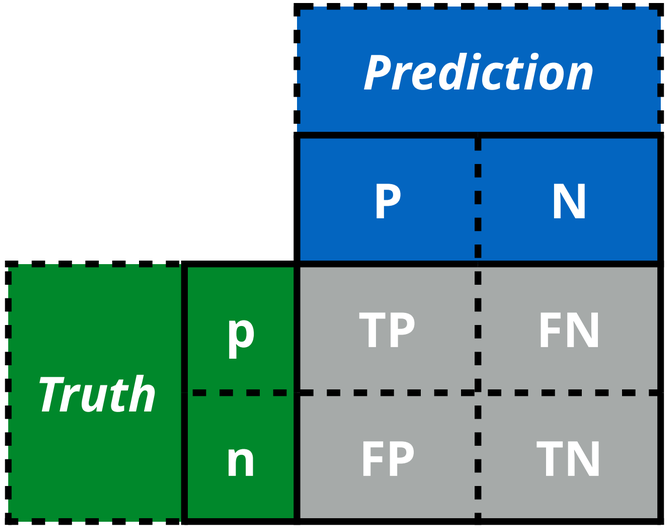


Ratios in the confusion matrix

- Accuracy
- Precision
- Recall



Ratios in the confusion matrix

- Accuracy
- Precision
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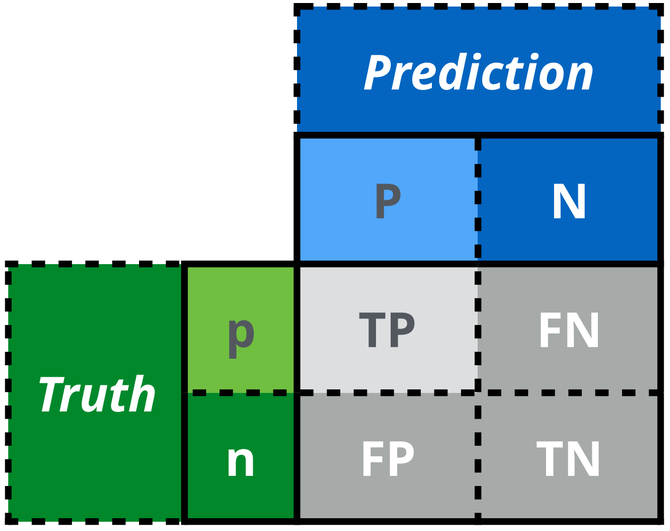
Precision
TP/(TP+FP)



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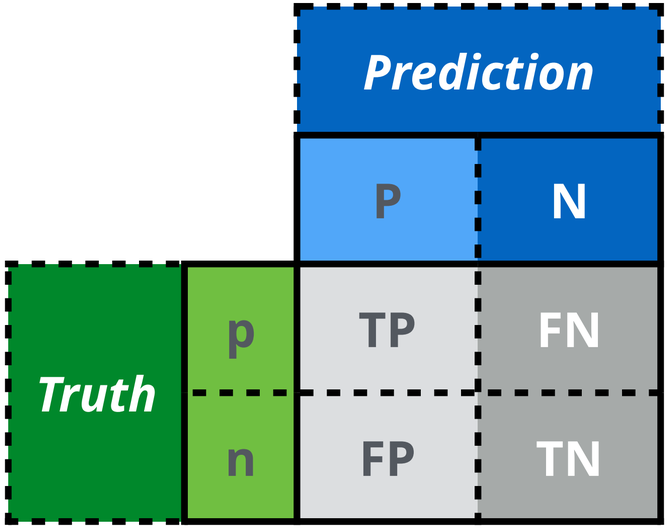

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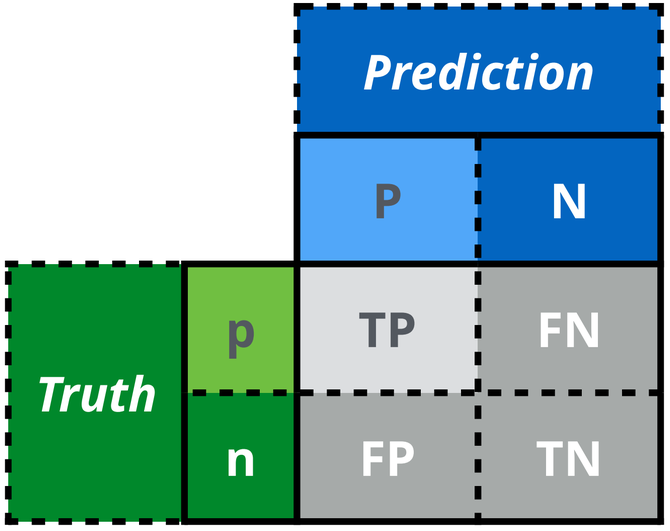

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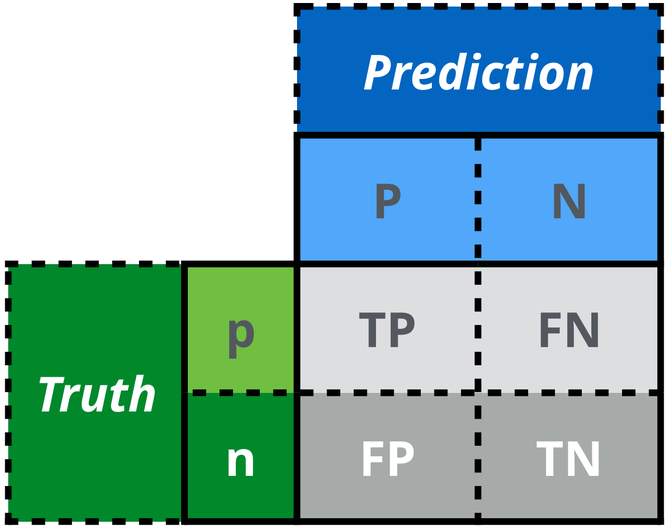
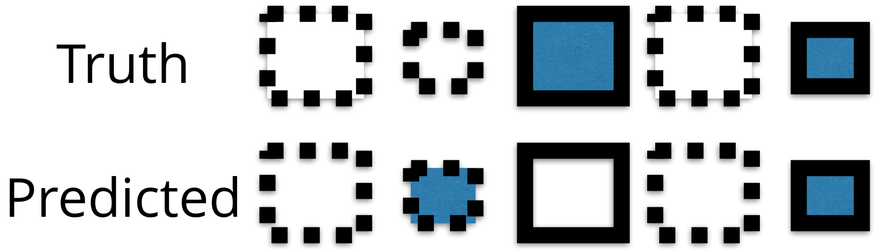
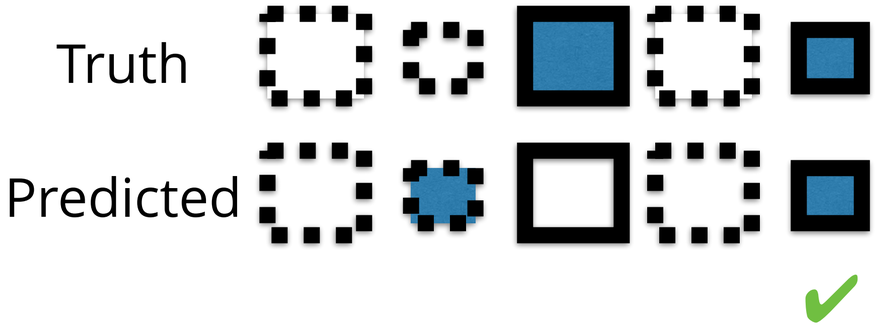


Back to the squares



		Prediction: P	Prediction: N
Truth: p		1	1
Truth: n		1	2

Back to the squares



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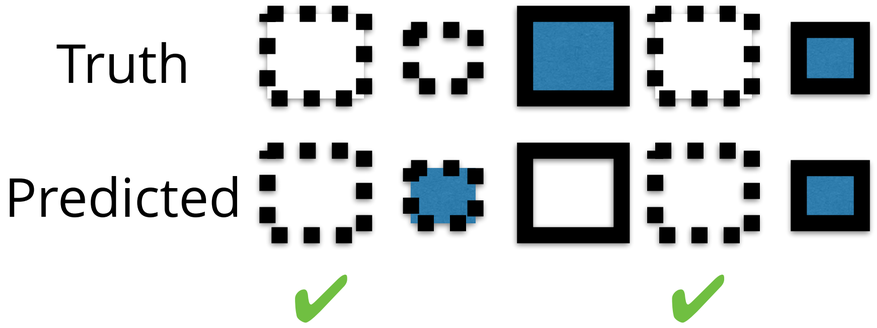

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Truth	p	1	1
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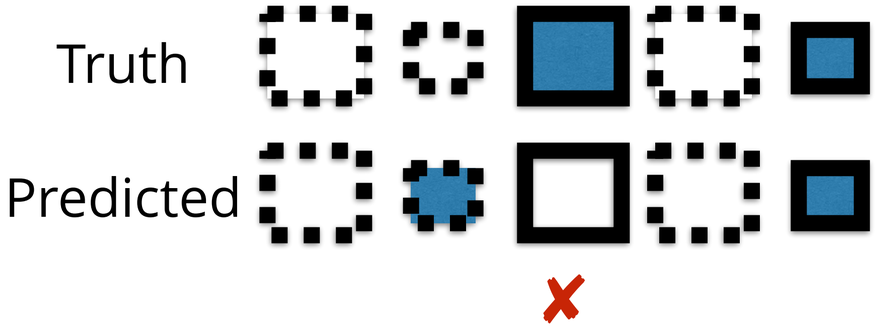

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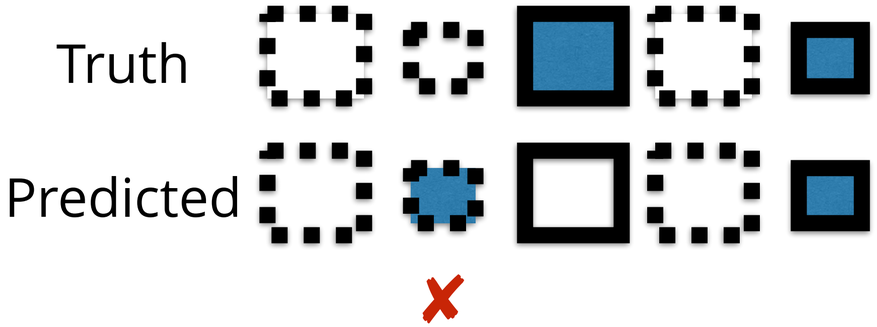

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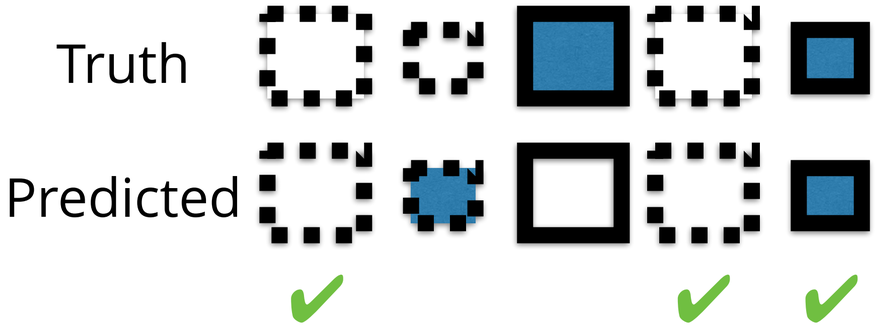
Back to the squares

- Accuracy: (TP+TN)/(TP+FP+FN+TN) = (1+2)/(1+2+1+1) = 60%
- Precision: TP/(TP+FP) = 1/(1+1) = 50%
- Recall: TP/(TP+FN) = 1/(1+1) = 50%



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		P	N
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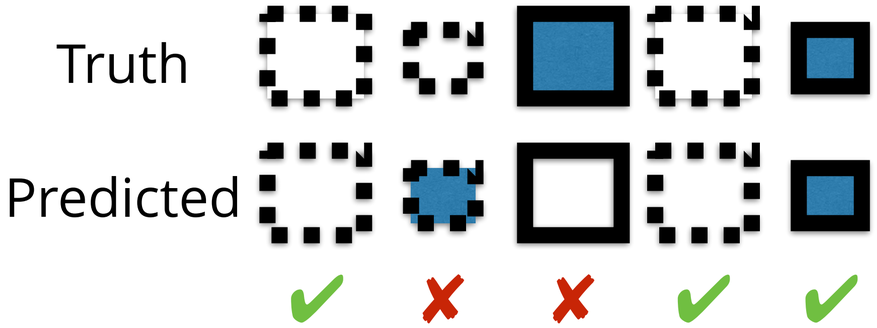

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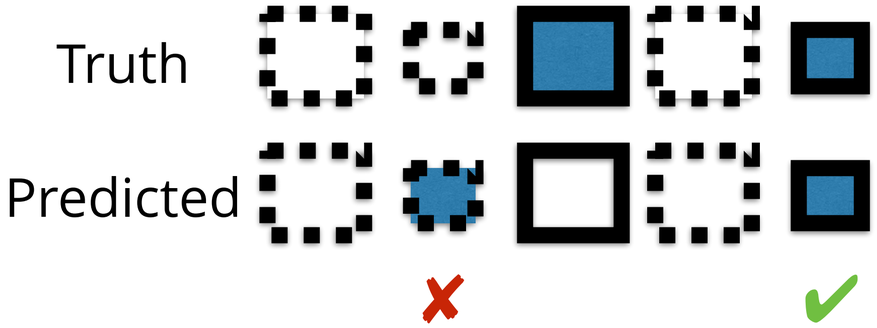

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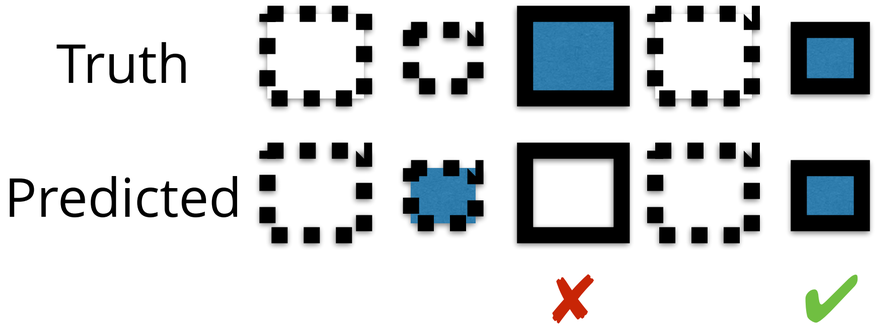


		Prediction	
		P	N
Truth	p	1	1
	n	1	2

Rare heart disease

- Accuracy: 99/(99+1) = 99%
- Recall: 0/1 = 0%
- Precision: undefined — no positive predictions

		Prediction	
		P	**N**
Truth	**p**	**0**	**1**
	n	**0**	**99**

Regression: RMSE

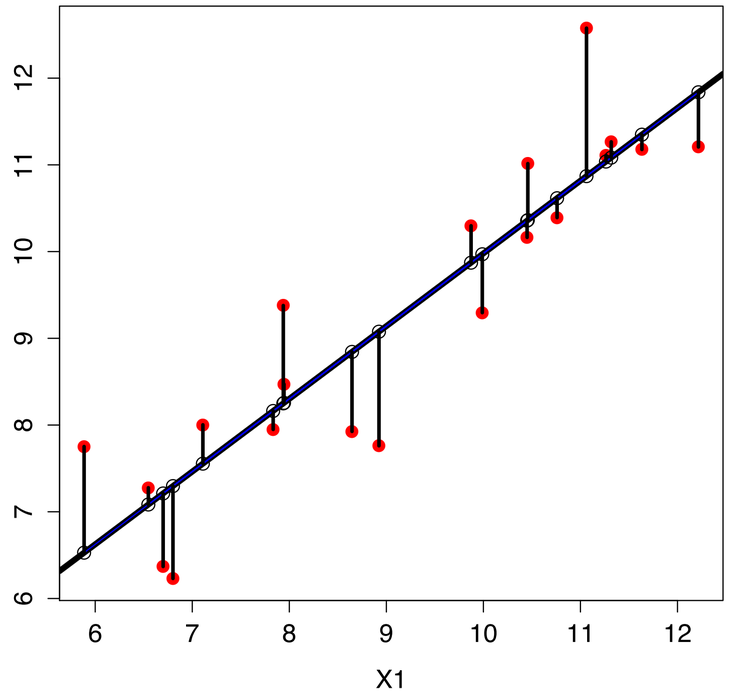
- Root Mean Squared Error (RMSE)
- Mean distance between estimates and regression line

$$\text{RMSE} = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}$$

y_i : actual outcome for obs. i

$\hat{y}_i$: predicted outcome for obs. i

N : Number of observations



Clustering

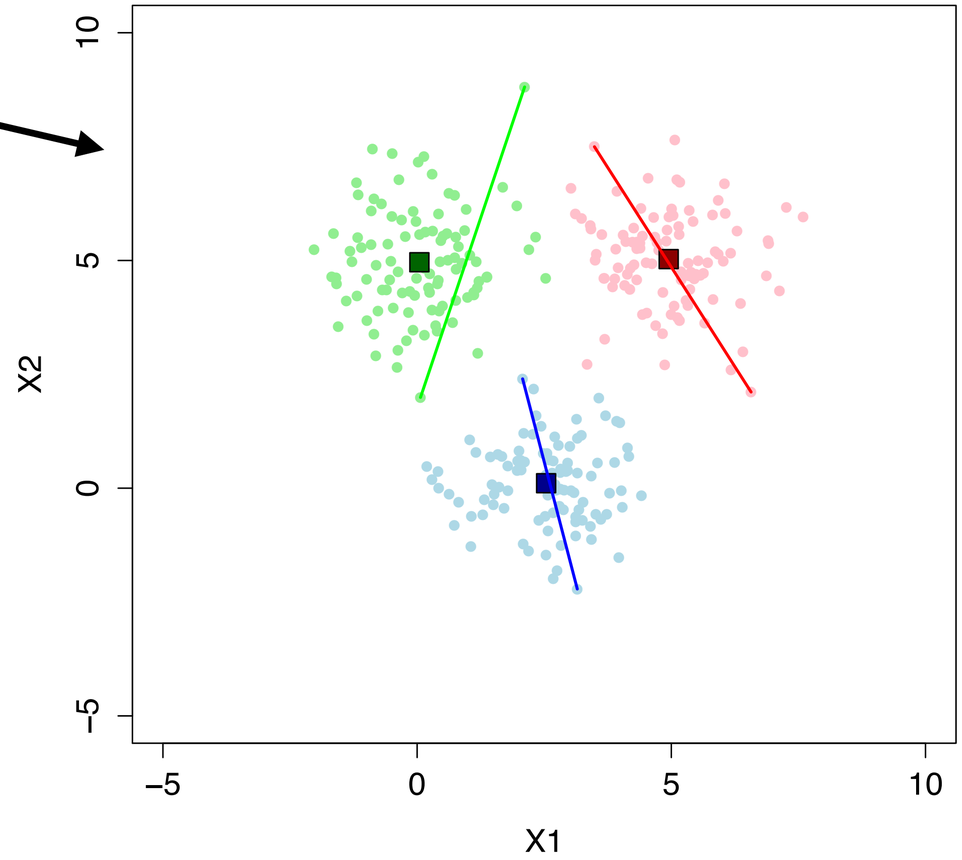
- No label information
- Need distance metric between points

Clustering

- Performance measure consists of 2 elements
  - Similarity within each cluster ↑
  - Similarity between clusters ↓

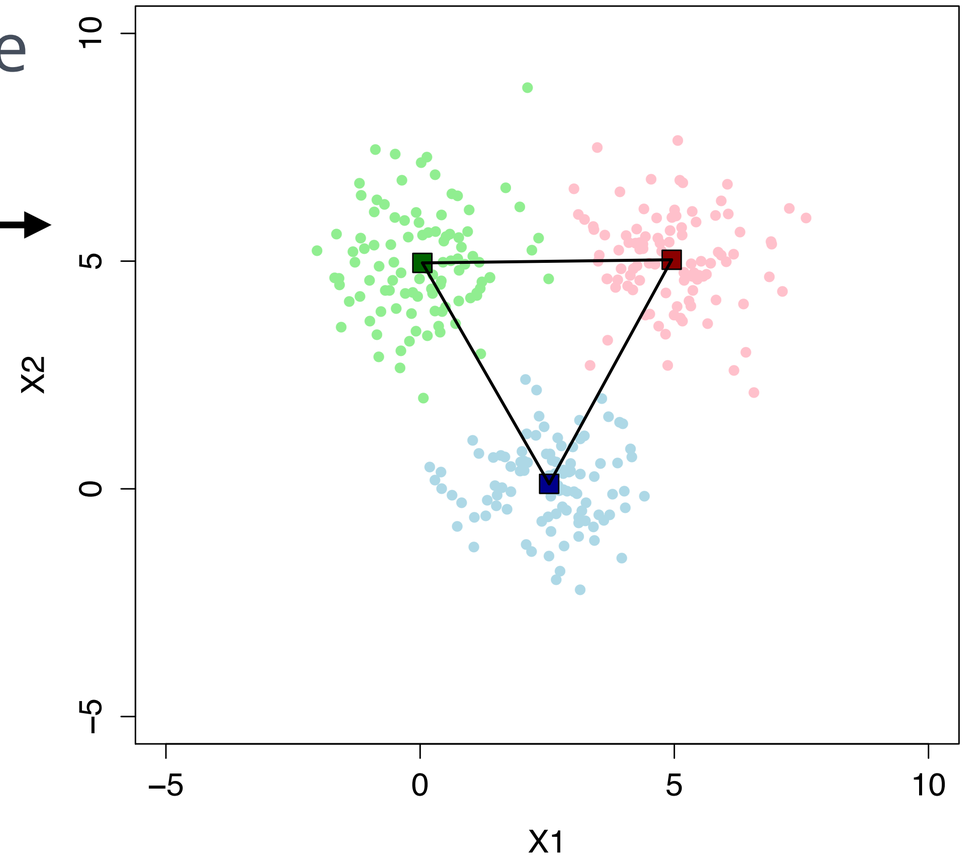
Within cluster similarity

- Within sum of squares (WSS)
- Diameter
- **Minimize**



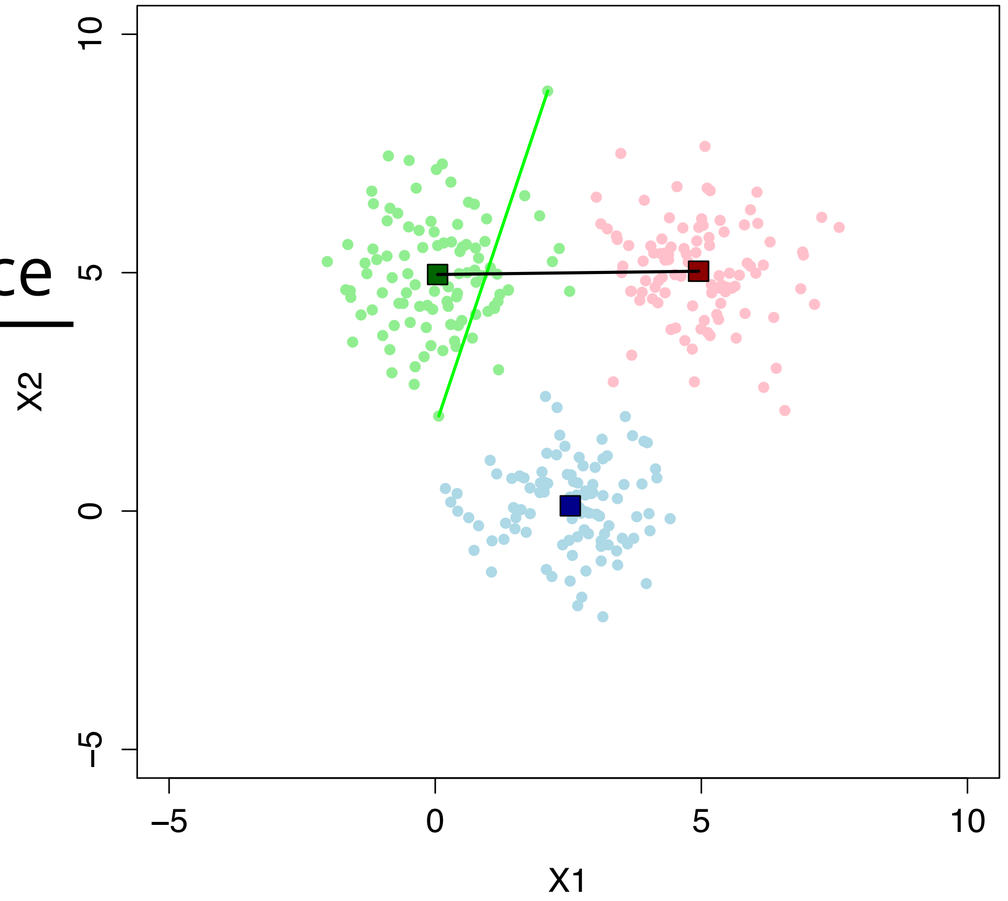
Between cluster similarity

- Between cluster sum of squares (BSS)
- Intercluster distance
- **Maximize**



Dunn's index

$$\frac{\text{minimal intercluster distance}}{\text{maximal diameter}}$$



INTRODUCTION TO MACHINE LEARNING

Let’s practice!

INTRODUCTION TO MACHINE LEARNING

Training set and test set

Machine learning - statistics

- Predictive power vs. descriptive power
- **Supervised learning:** model must predict
  - unseen observations
- **Classical statistics:** model must fit data
  - explain or describe data

Predictive model

- **Training**
  - **not** on complete dataset
  - **training set**
- **Test set** to evaluate performance of model
- Sets are **disjoint**: **NO OVERLAP**
- Model tested on **unseen** observations
  -> Generalization!

Split the dataset

- N instances (=observations): **X**
- K features: **F**
- Class labels: **y**

	f_1	f_2	...	f_K	y
x_1	$x_{1,1}$	$x_{1,2}$	...	$x_{1,K}$	y_1
x_2	$x_{2,1}$	$x_{2,2}$	...	$x_{2,K}$	y_2
...	...	...	...	...	...
x_r	$x_{r,1}$	$x_{r,2}$	...	$x_{r,K}$	y_r
x_{r+1}	$x_{r+1,1}$	$x_{r+1,2}$	...	$x_{r+1,K}$	y_{r+1}
x_{r+2}	$x_{r+2,1}$	$x_{r+2,2}$	...	$x_{r+2,K}$	y_{r+2}
...	...	...	...	...	...
x_N	$x_{N,1}$	$x_{N,2}$	...	$x_{N,K}$	y_N

Training set

Test set

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...	...	...	...	...	...
x_r	$x_{r,1}$	$x_{r,2}$	...	$x_{r,K}$	y_r
x_{r+1}	$x_{r+1,1}$	$x_{r+1,2}$	...	$x_{r+1,K}$	y_{r+1}
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...	...	...	...	...	...
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Training set

Test set

Use to predict y: $\hat{y}$

Split the dataset

	f_1	f_2	...	f_K	y
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...	...	...	...	...	...
x_N	$x_{N,1}$	$x_{N,2}$	...	$x_{N,K}$	y_N

Training set

Test set

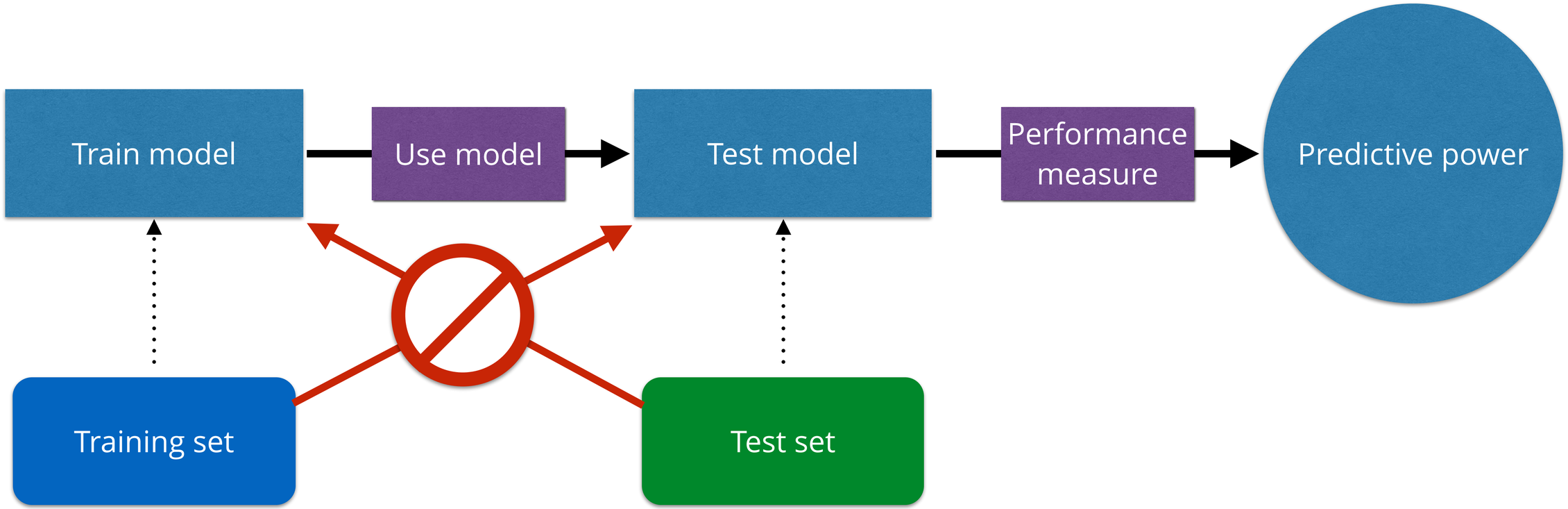
Use to predict y: $\hat{y}$ ⟷ real y

compare them

When to use training/test set?

- Supervised learning
- **Not** for unsupervised (clustering)
    - Data not labeled

Predictive power of model



How to split the sets?

- Which **observations** go where?
- Training set larger test set
- Typically about 3/1
- Quite arbitrary
- **Generally:** more data = better model
- Test set not too small

Distribution of the sets

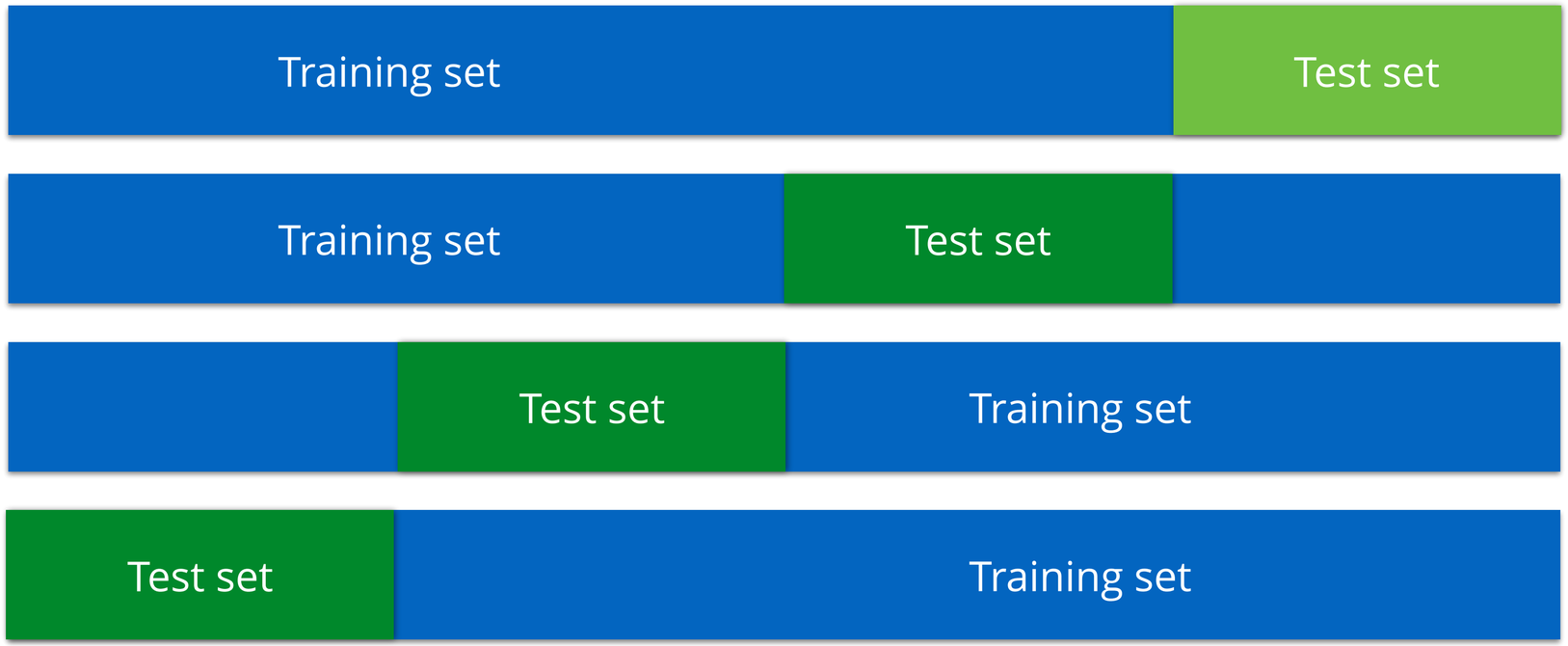
- **Classification**
  - classes must have similar distributions
  - avoid a class not being available in a set
- **Classification & regression**
  - shuffle dataset before splitting

Effect of sampling

- Sampling can affect performance measures
- Add **robustness** to these measures: **cross-validation**
- **Idea:** sample multiple times, with different seperations

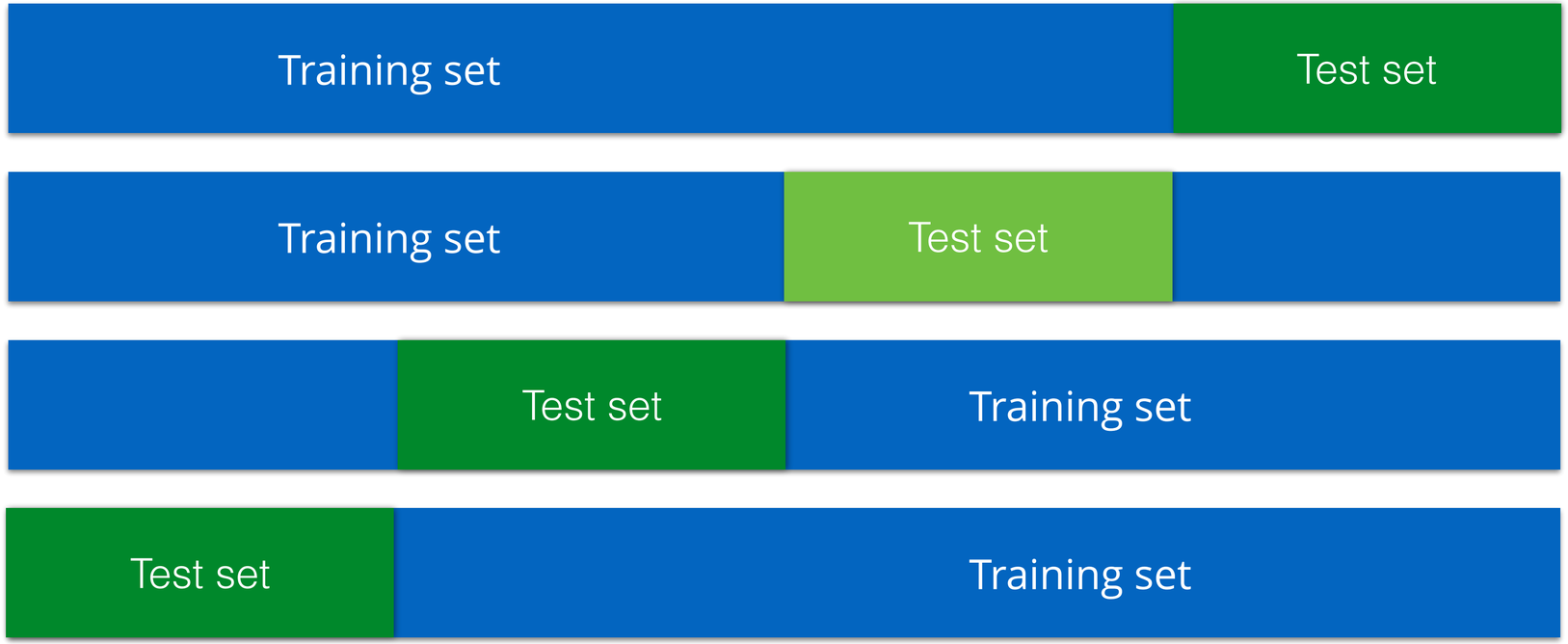
Cross-validation

- E.g.: 4-fold cross-validation



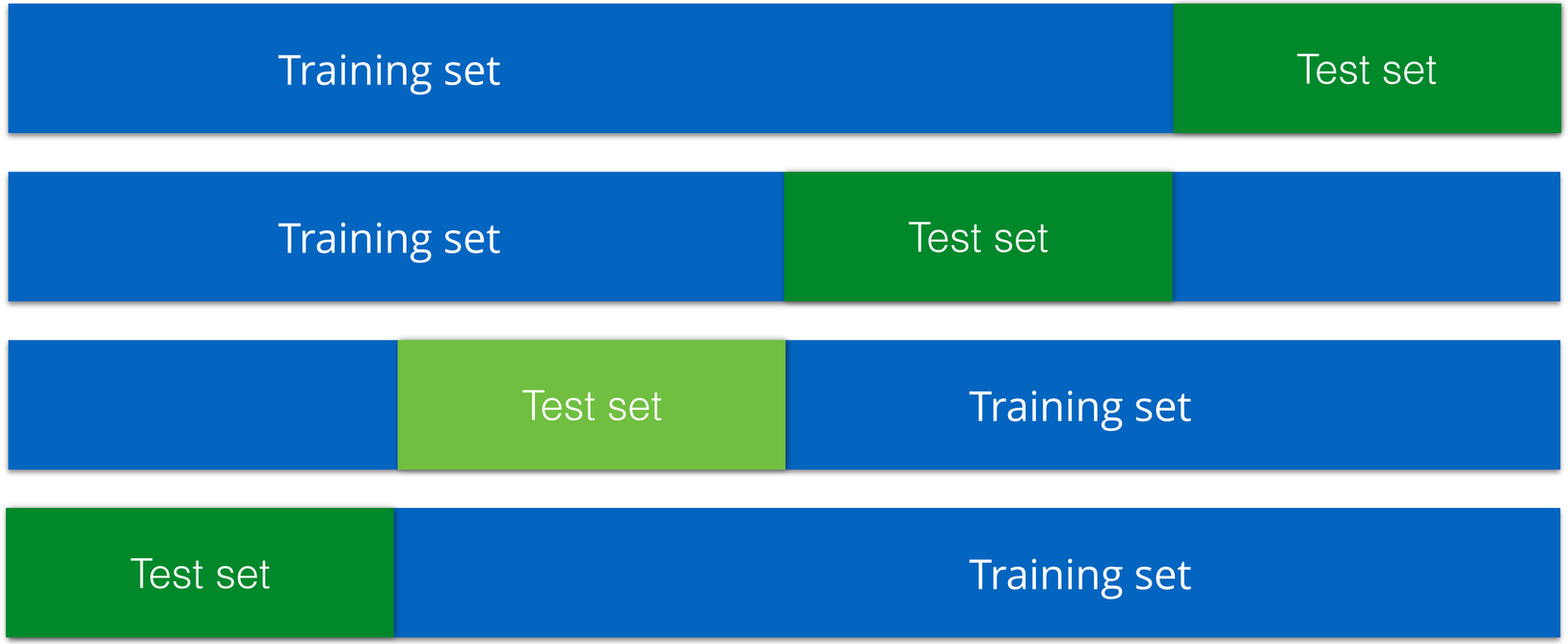
Cross-validation

- E.g.: 4-fold cross-validation



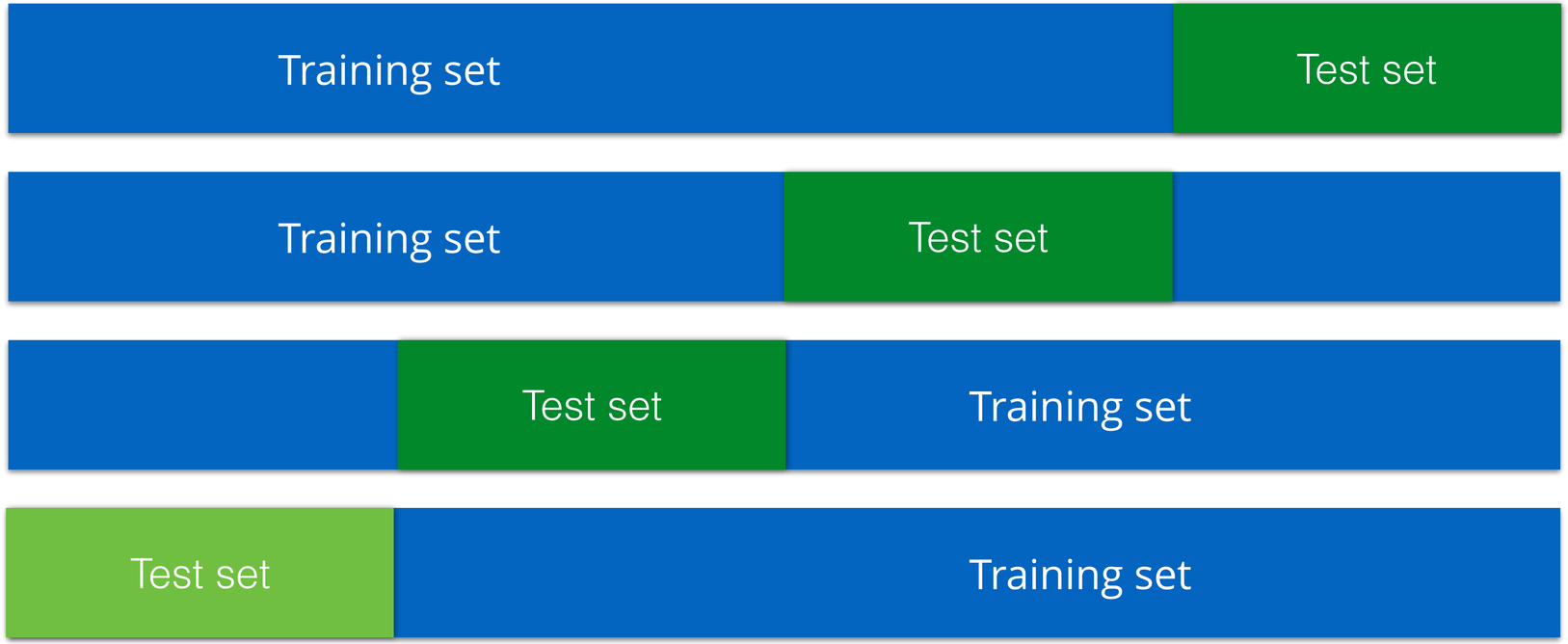
Cross-validation

- E.g.: 4-fold cross-validation



Cross-validation

- E.g.: 4-fold cross-validation



aggregate results for robust measure

n-fold cross-validation

- Fold test set over dataset **n** times
- Each test set is **1/n** size of total dataset

INTRODUCTION TO MACHINE LEARNING

Let’s practice!

INTRODUCTION TO MACHINE LEARNING

Bias and Variance

What you've learned?

- Accuracy and other performance measures
- Training and test set

Knitting it all together

- Effect of splitting dataset (train/test) on accuracy
- Over- and underfitting

Introducing

BIAS **VARIANCE**

Bias and Variance

- Main goal of supervised learning: **prediction**
- **Prediction error** ~ reducible + irreducible error

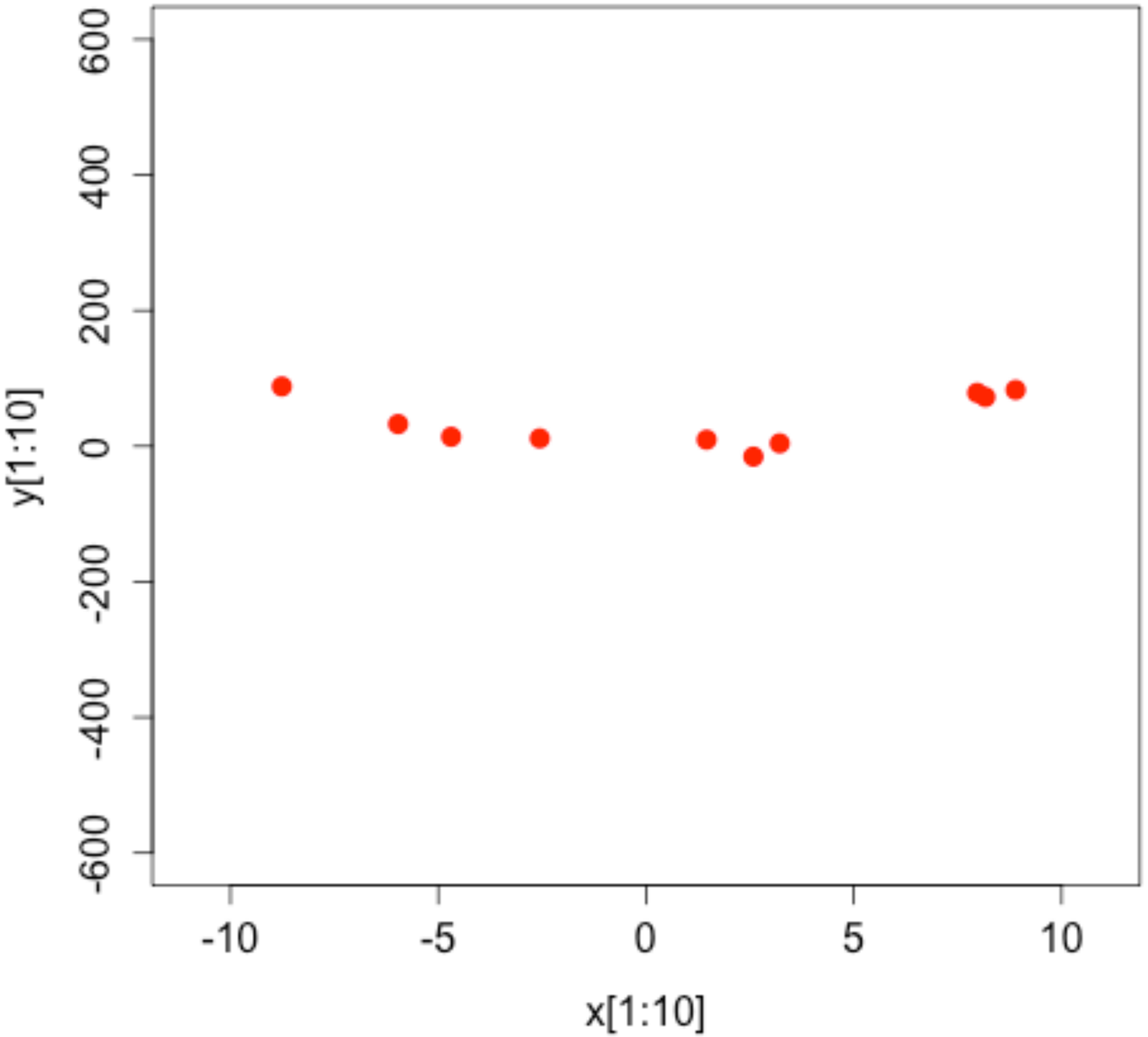
Irreducible - reducible error

- **Irreducible:** noise — **don't minimize**
- **Reducible:** error due to unfit model — **minimize**
- **Reducible error** is split into **bias** and **variance**

Bias

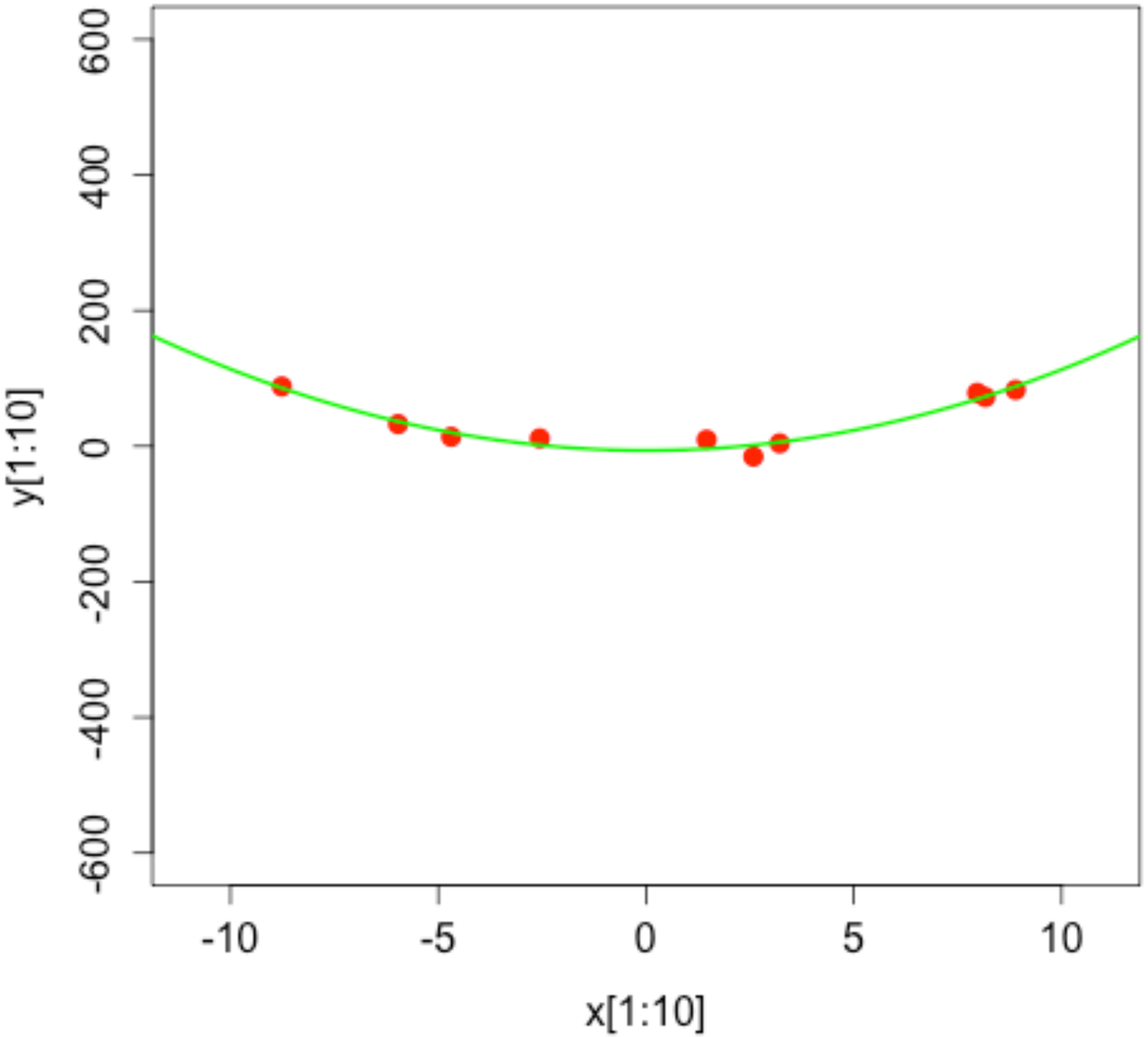
- Error due to **bias**: wrong **assumptions**
- Difference **predictions** and **truth**
  - using models trained by specific **learning algorithm**

Example



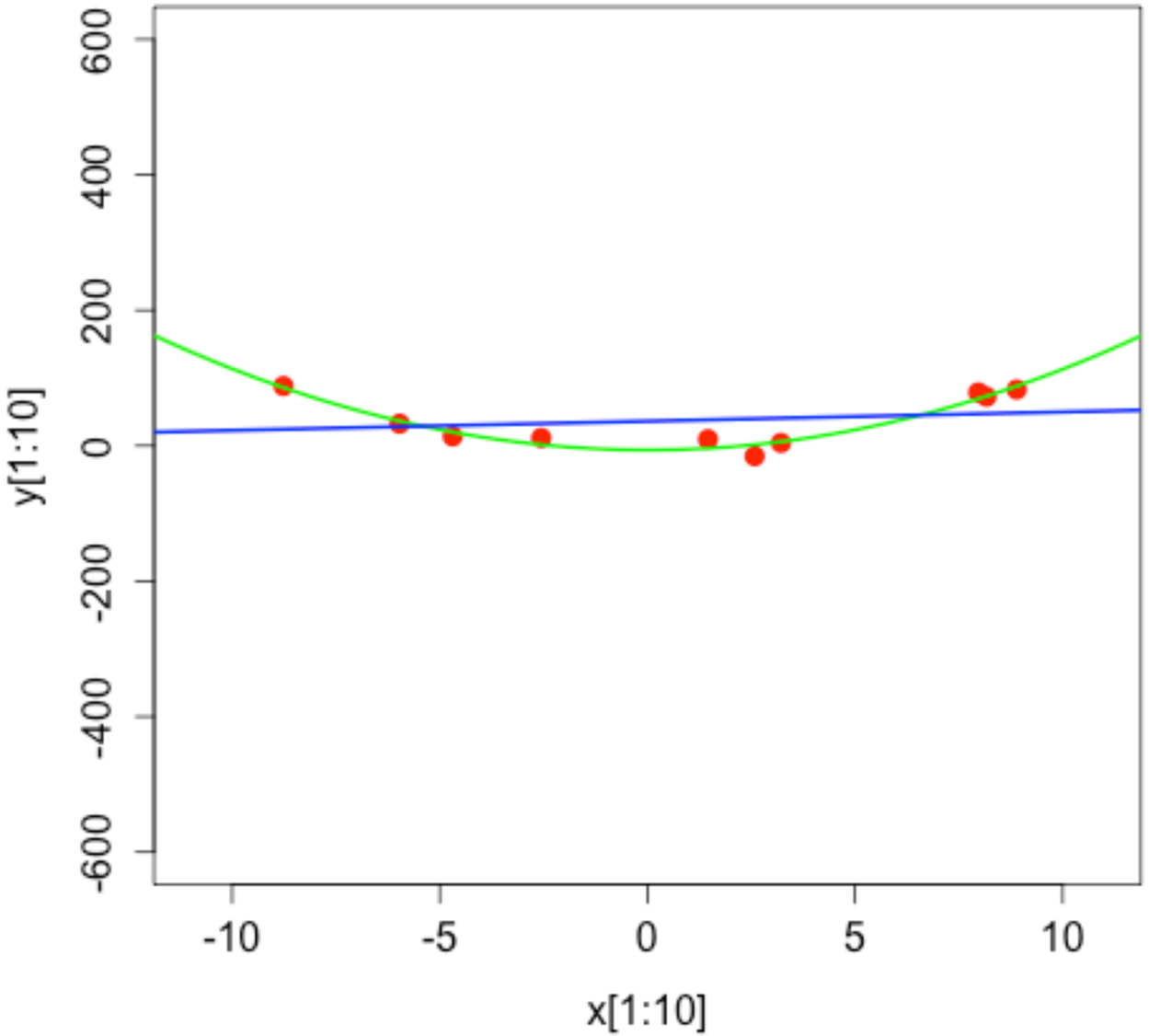
Example

- **Quadratic** data



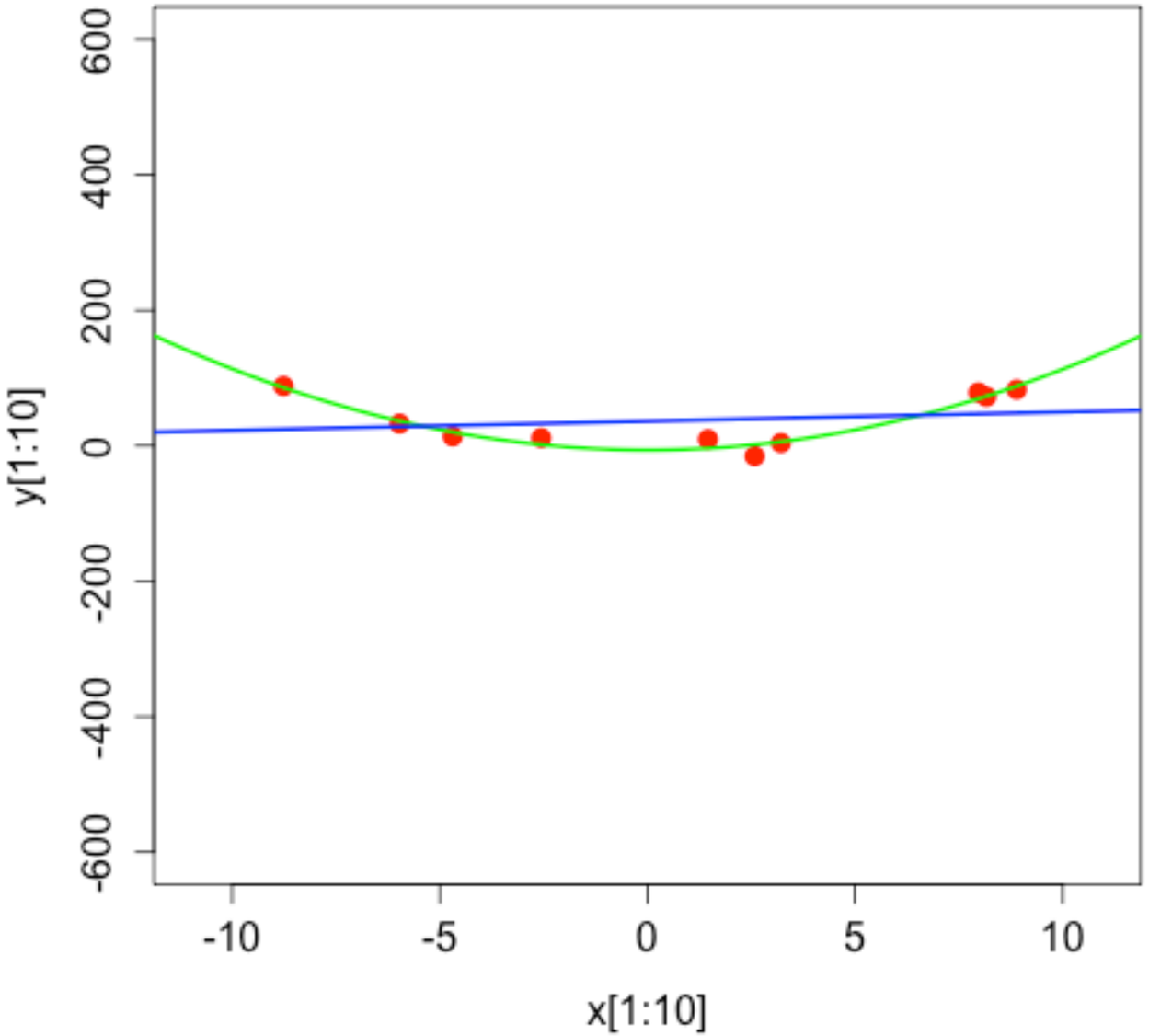
Example

- **Quadratic** data
- **Assumption**: data is **linear** — use linear regression



Example

- **Quadratic** data
- **Assumption**: data is **linear** — use linear regression
- Error due to **bias** is high: more restrictions on model



Bias

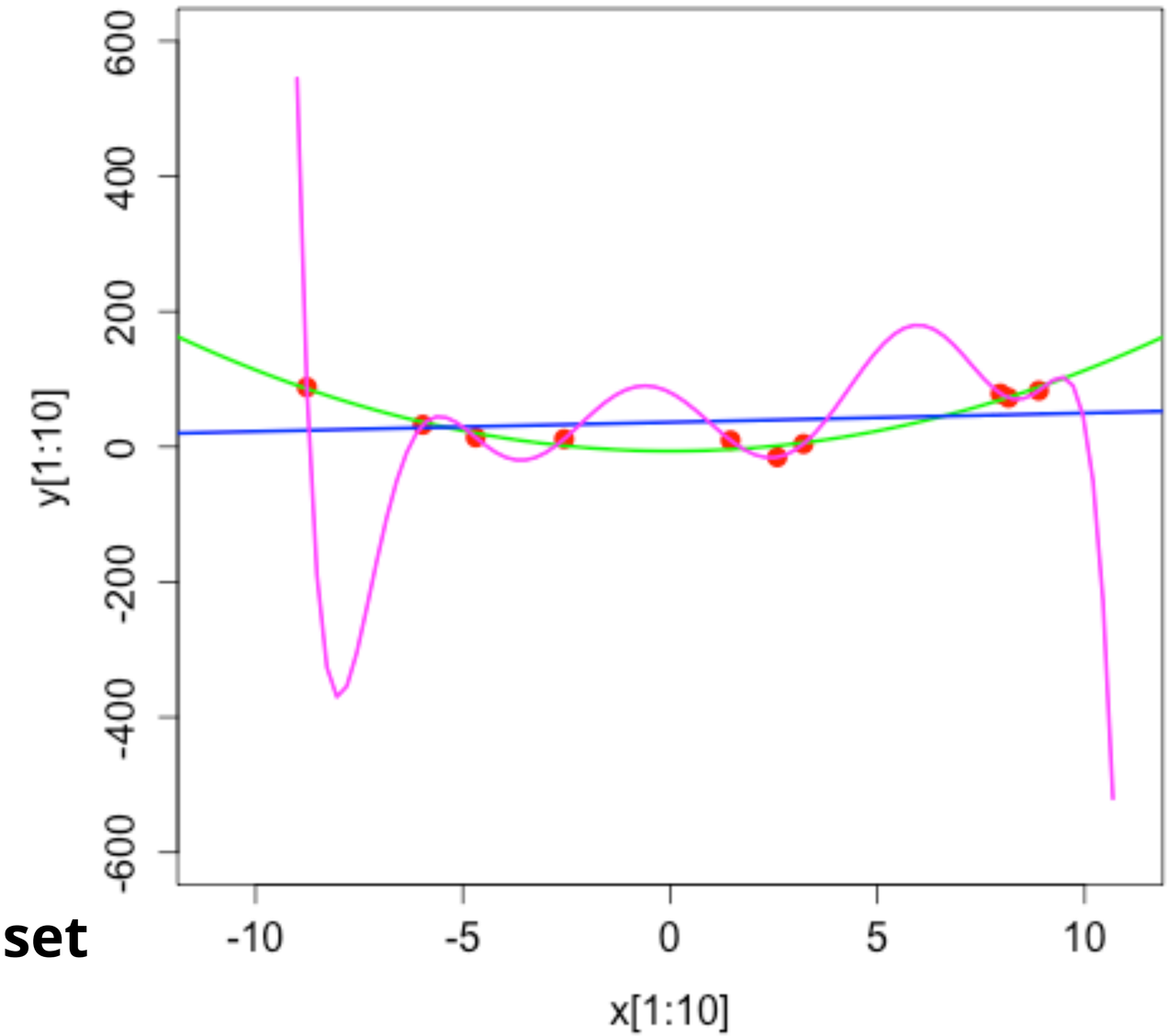
- Complexity of model
- More restrictions lead to high **bias**

Variance

- Error due to **variance**: error due too the sampling of the **training set**
- Model with high **variance** fits **training set** closely

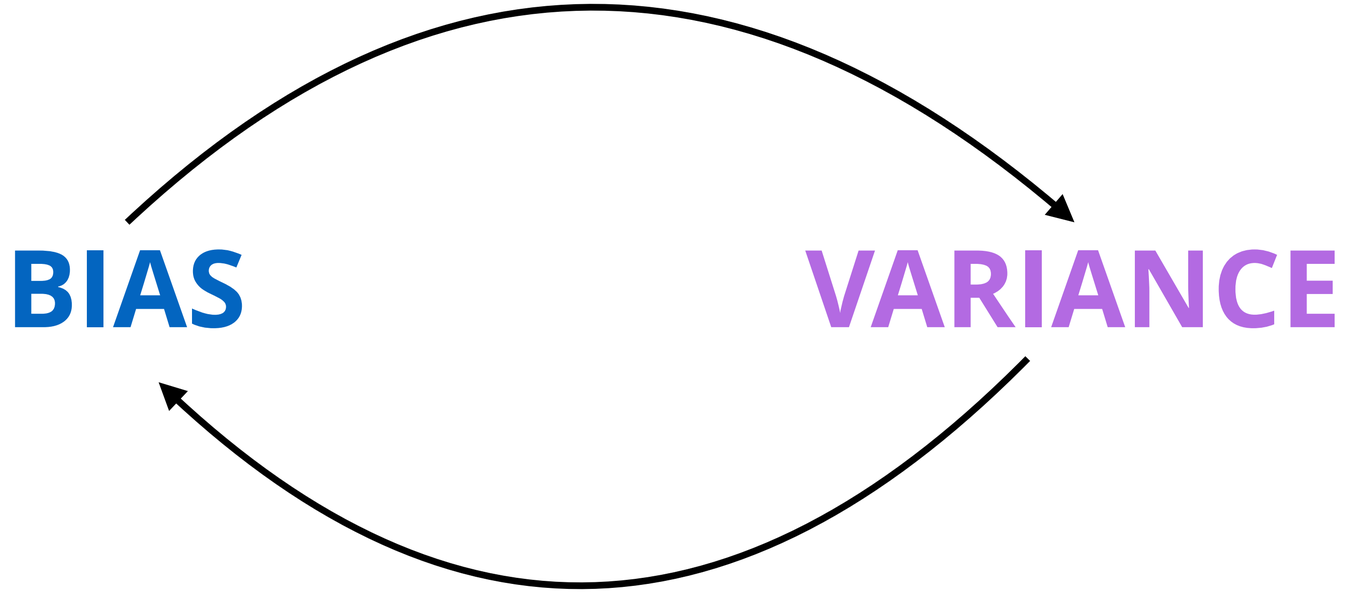
Example

- **Quadratic** data
- **Few** restrictions: fit **polynomial** perfectly through **training set**
- If you **change** training set, model will **change** completely



high **variance**: generalizes bad to **test set**

Bias-variance tradeoff



low **bias** - high **variance**

low **variance** - high **bias**

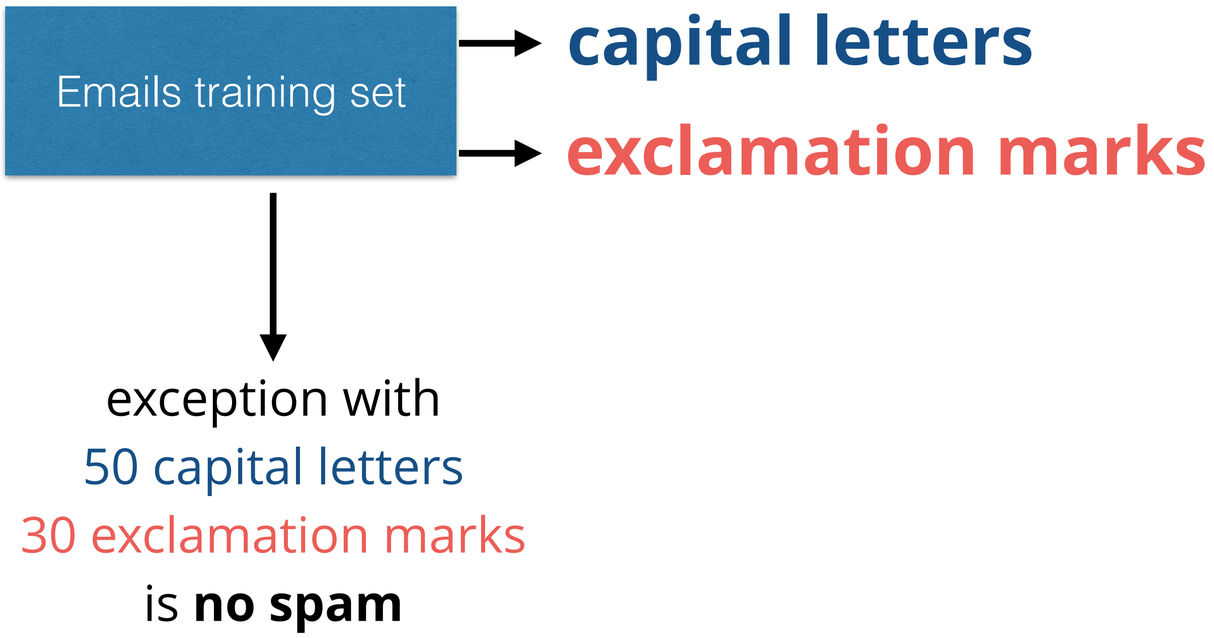
Overfitting

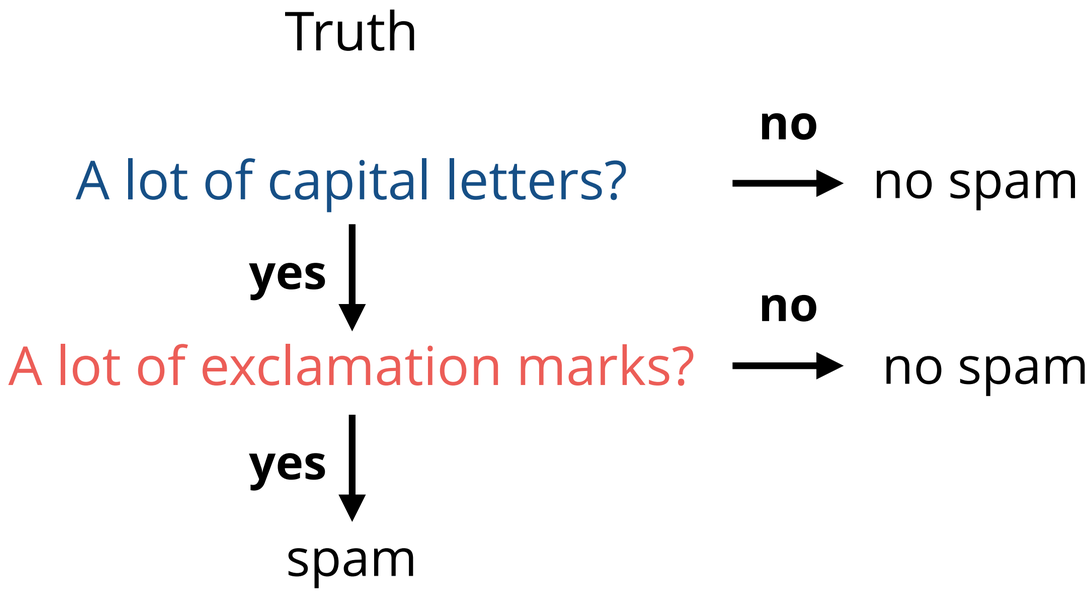
- **Accuracy** will depend on dataset **split** (train/test)
- High **variance** will **heavily** depend on **split**
- **Overfitting** = model fits **training set** a lot better than **test set**
- Too **specific**

Underfitting

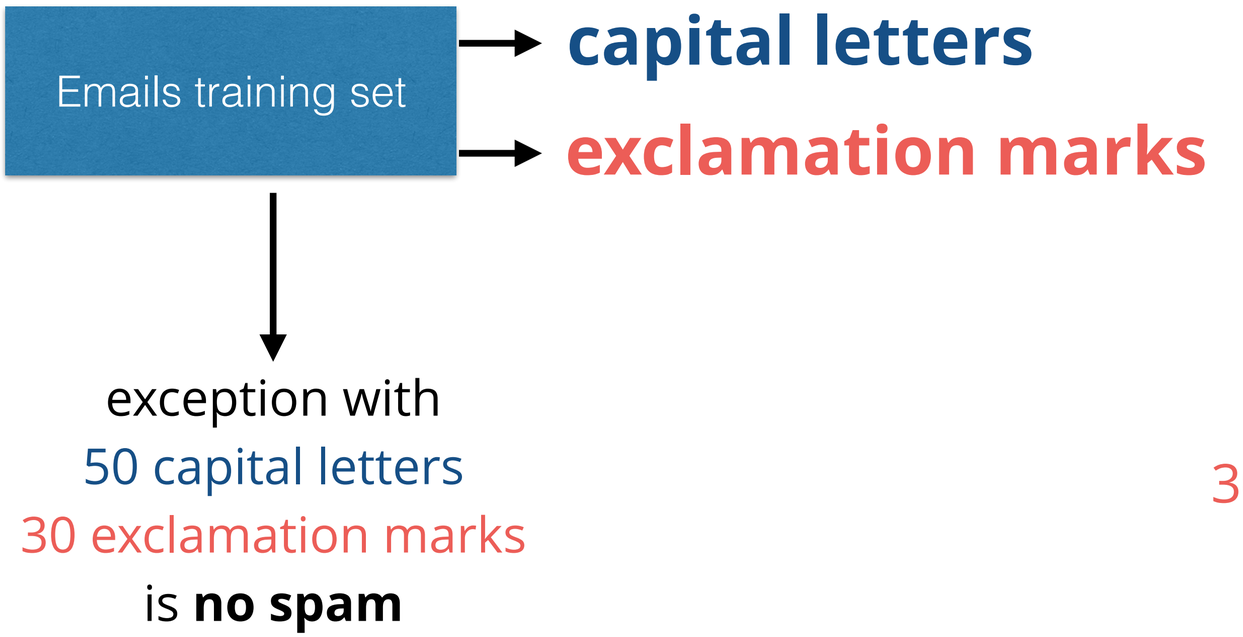
- Restricting your model **too much**
- High **bias**
- Too **general**

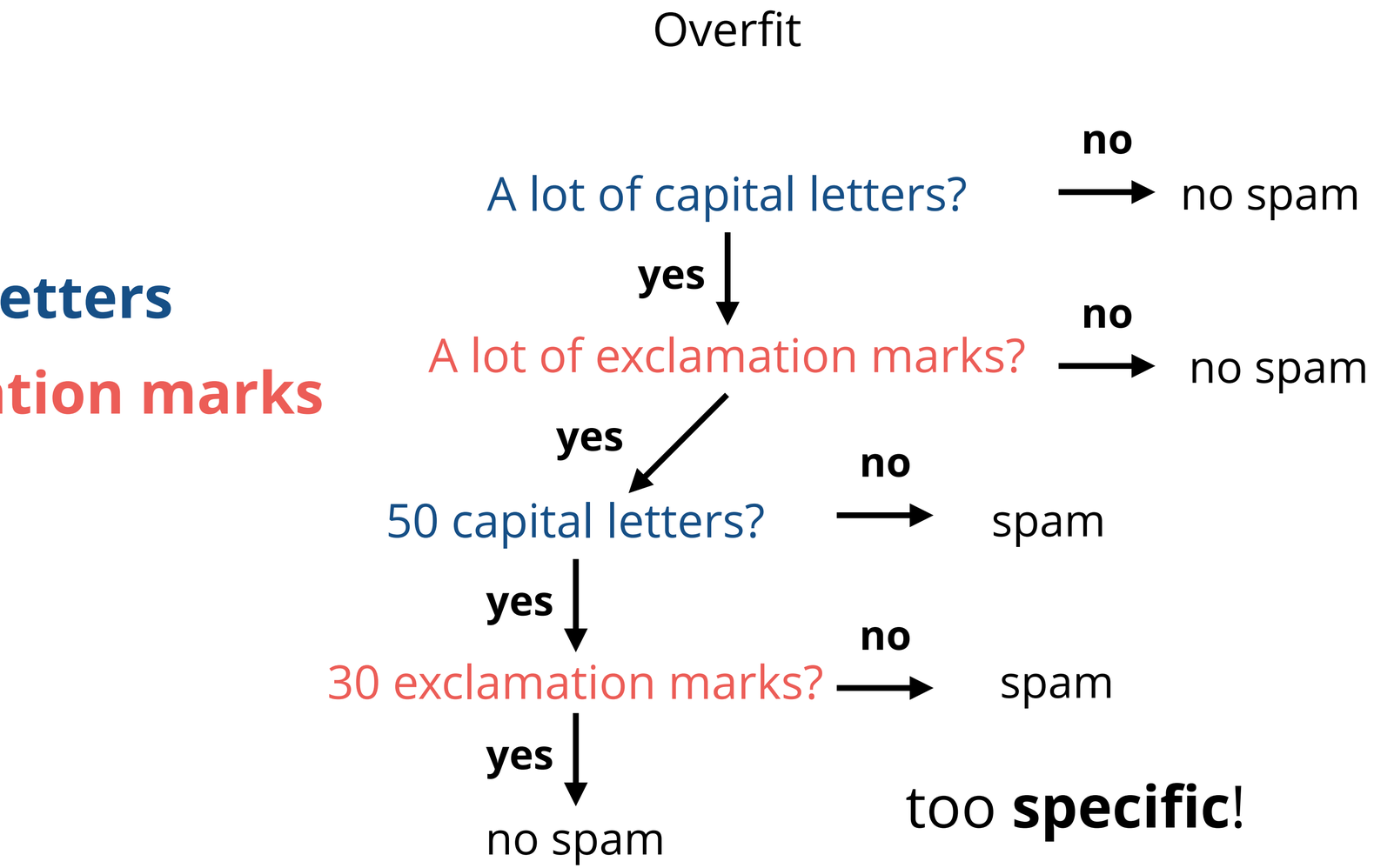
Example - spam or not?





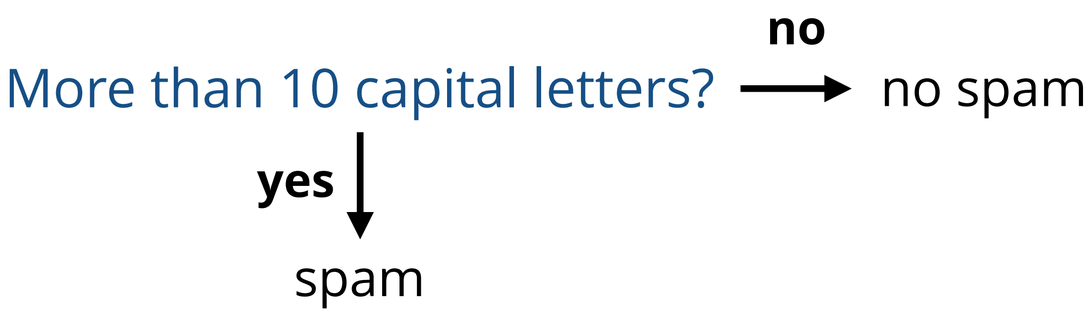
Example - spam or not?





Example - spam or not?

Underfit



too **general**!

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