Elements of Machine Learning & Data Science

Winter semester 2025/26

Lecture 21 – Evaluation I

20.01.2026

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slides by Prof. Holger Hoos

Announcement

Lecture Evaluation

- Please fill out the lecture evaluation form
  - *The evaluation will be open until 27.01.2026*

- We are very interested in your feedback!
  - Tell us what you liked,
    but also what could still be improved.

Empirical Analysis and Performance Evaluation Topics

15. Data Quality and Preprocessing
16. Responsible Data Science
17. **Evaluation**
18. Performance Optimization

Key Questions

- **How good is an ML model?**
  - *Is it "fit for use" (i.e., good enough for deployment)?*
  - *What are its strengths and weaknesses?*
  - *Might anything have gone wrong during training?*

Empirical Analysis and Performance Evaluation Topics

15. Data Quality and Preprocessing
16. Responsible Data Science
17. **Evaluation**
18. Performance Optimization

Key Questions

- **How good is an ML model?**
  - *How do we assess whether it is "fit for use" (i.e., good enough for deployment)?*
  - *How do we assess its strengths and weaknesses?*
  - *How do we detect if anything has gone wrong during training?*

Empirical Analysis and Performance Evaluation Topics

15. Data Quality and Preprocessing
16. Responsible Data Science
17. **Evaluation**
18. Performance Optimization

Key Questions

- **How good could an ML model be?**
  - *Are we using the best possible ML method / model?*
  - *Have we configured and trained it in the best possible way?*
  - *Can we further improve performance?*

Empirical Analysis and Performance Evaluation Topics

15. Data Quality and Preprocessing
16. Responsible Data Science
17. **Evaluation**
18. Performance Optimization

Key Questions

- **How good could an ML model be?**
  - *How can we ensure we are using a good ML method / model?*
  - *How can we configure and train it for optimized performance?*
  - *How can we further improve performance?*

Learning Goals

At the end of this module, students should be able to

- Assess the quality of a model obtained from a supervised machine learning method using widely accepted methods, including standard performance metrics, confusion matrices, ROC curves
- Demonstrate understanding and working knowledge of the problems that can occur when using supervised learning procedures and the models obtained from them
- Explain when and why it is important to distinguish between training, validation and testing data
- Explain standard validation techniques, including k-fold and leave-one-out cross-validation
- Assess performance differences using appropriate statistical techniques
- Explain the problems that can arise from unbalanced data sets and demonstrate understanding as well as working knowledge of methods for addressing these problems

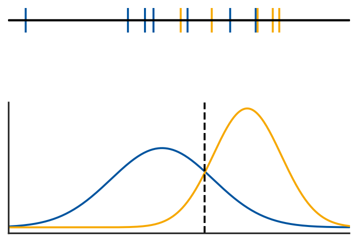
Key Questions for Evaluation

1. **How good is an ML model?**

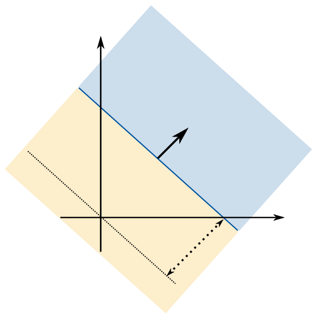
2. How good could an ML model be?

Scenario

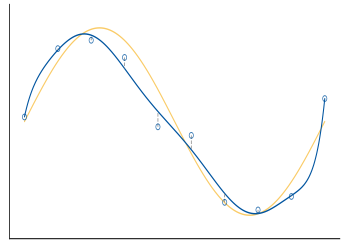
- You have used supervised learning to train a predictive model
- Question: How do you assess the quality of the model?



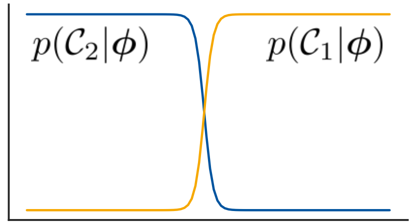
Bayes Classifiers



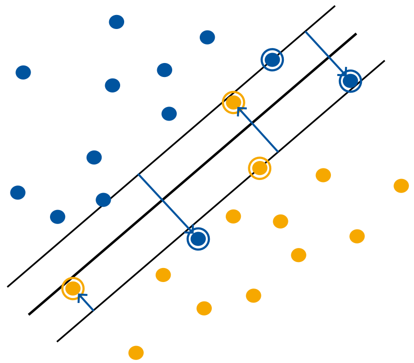
Linear Discriminants



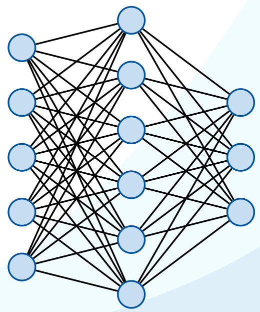
Linear Regression



Logistic Regression

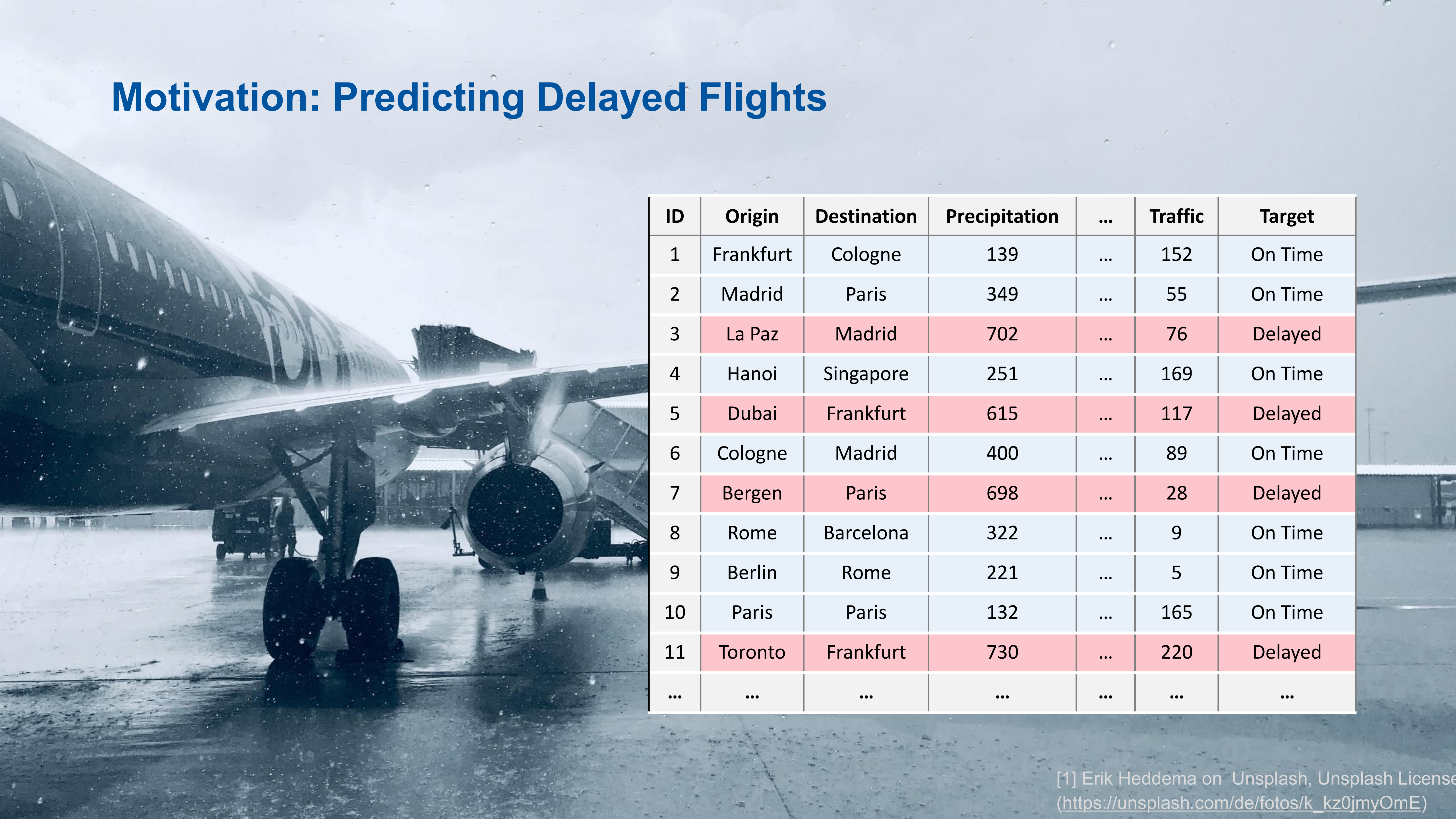


SVMs



Neural Networks

Motivation: Predicting Delayed Flights

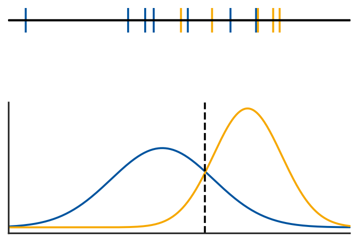


ID	Origin	Destination	Precipitation	...	Traffic	Target
1	Frankfurt	Cologne	139	...	152	On Time
2	Madrid	Paris	349	...	55	On Time
3	La Paz	Madrid	702	...	76	Delayed
4	Hanoi	Singapore	251	...	169	On Time
5	Dubai	Frankfurt	615	...	117	Delayed
6	Cologne	Madrid	400	...	89	On Time
7	Bergen	Paris	698	...	28	Delayed
8	Rome	Barcelona	322	...	9	On Time
9	Berlin	Rome	221	...	5	On Time
10	Paris	Paris	132	...	165	On Time
11	Toronto	Frankfurt	730	...	220	Delayed
...	...	...	...	...	...	...

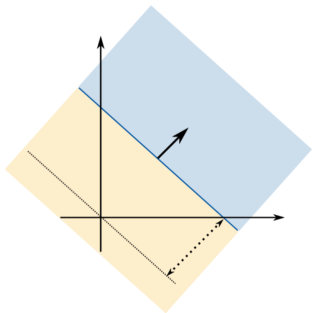
Scenario

- You have used supervised learning to train a predictive model

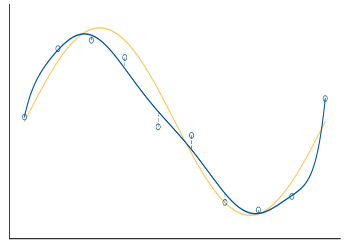
- Question: How do you assess the quality of the model?
  - *Let's collect your ideas here…*



Bayes Classifiers



Linear Discriminants



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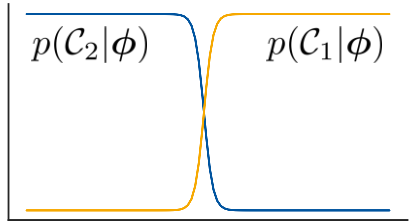
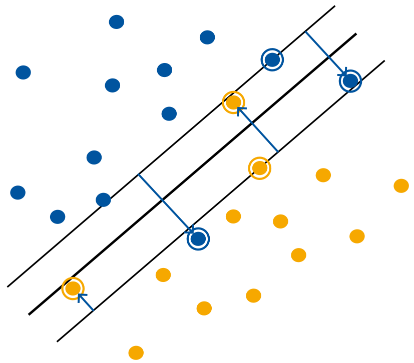
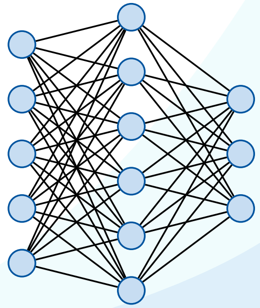


Logistic Regression



SVMs



Neural Networks

Question: How Do You Assess the Quality of the Model?

Let's look at this question from different aspects:

- *What do we want to get out of a quality assessment?*
- *How would the output of a quality measure need to look to achieve that?*
- *What do we need in order to measure quality?*
- *How can we make sure the measurement is fair and unbiased?*

Running Example

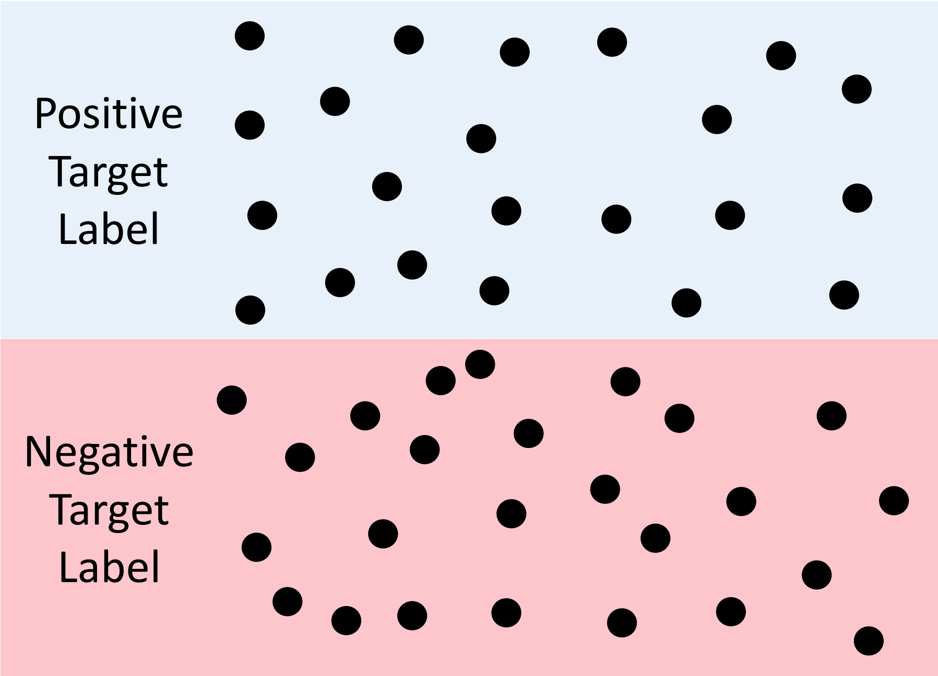
Predicting delayed flights
(set of 20 instances)

- Target Feature:
  On Time (positive),
  Delayed (negative)

ID	Target Label	Prediction
1	On Time	Delayed
2	On Time	Delayed
3	Delayed	Delayed
4	On Time	On Time
5	Delayed	Delayed
6	On Time	On Time
7	Delayed	Delayed
8	On Time	On Time
9	On Time	On Time
10	On Time	On Time

ID	Target Label	Prediction
11	Delayed	Delayed
12	On Time	Delayed
13	Delayed	Delayed
14	Delayed	Delayed
15	Delayed	Delayed
16	Delayed	Delayed
17	Delayed	On Time
18	On Time	On Time
19	Delayed	Delayed
20	Delayed	**On Time**

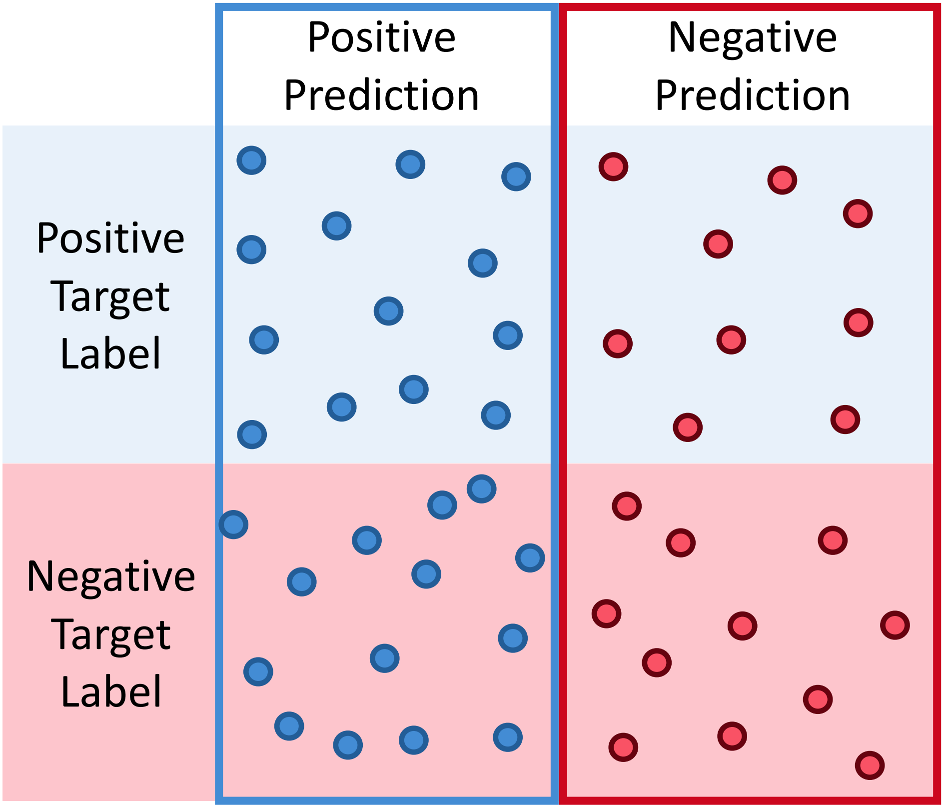
Running Example



ID	Target Label	Prediction
1	On Time	Delayed
2	On Time	Delayed
3	Delayed	Delayed
4	On Time	On Time
5	Delayed	Delayed
6	On Time	On Time
7	Delayed	Delayed
8	On Time	On Time
9	On Time	On Time
10	On Time	On Time

ID	Target Label	Prediction
11	Delayed	Delayed
12	On Time	Delayed
13	Delayed	Delayed
14	Delayed	Delayed
15	Delayed	Delayed
16	Delayed	Delayed
17	Delayed	On Time
18	On Time	On Time
19	Delayed	Delayed
20	Delayed	On Time

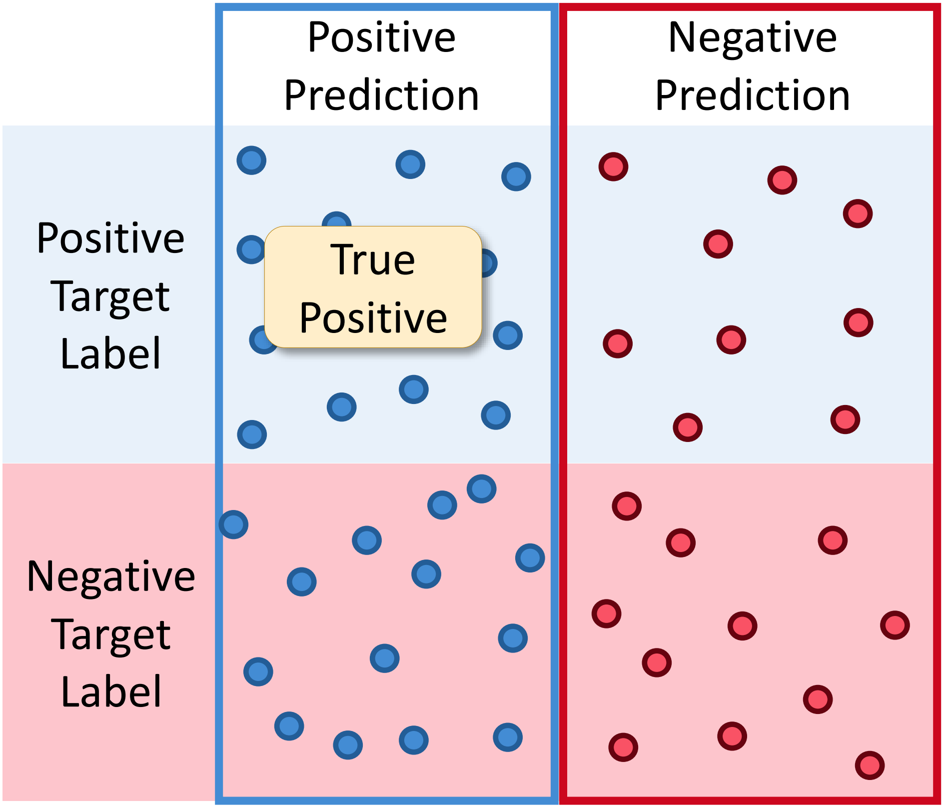
Making Predictions



ID	Target Label	Prediction
1	On Time	Delayed
2	On Time	Delayed
3	Delayed	Delayed
4	On Time	On Time
5	Delayed	Delayed
6	On Time	On Time
7	Delayed	Delayed
8	On Time	On Time
9	On Time	On Time
10	On Time	On Time

ID	Target Label	Prediction
11	Delayed	Delayed
12	On Time	Delayed
13	Delayed	Delayed
14	Delayed	Delayed
15	Delayed	Delayed
16	Delayed	Delayed
17	Delayed	On Time
18	On Time	On Time
19	Delayed	Delayed
20	Delayed	On Time

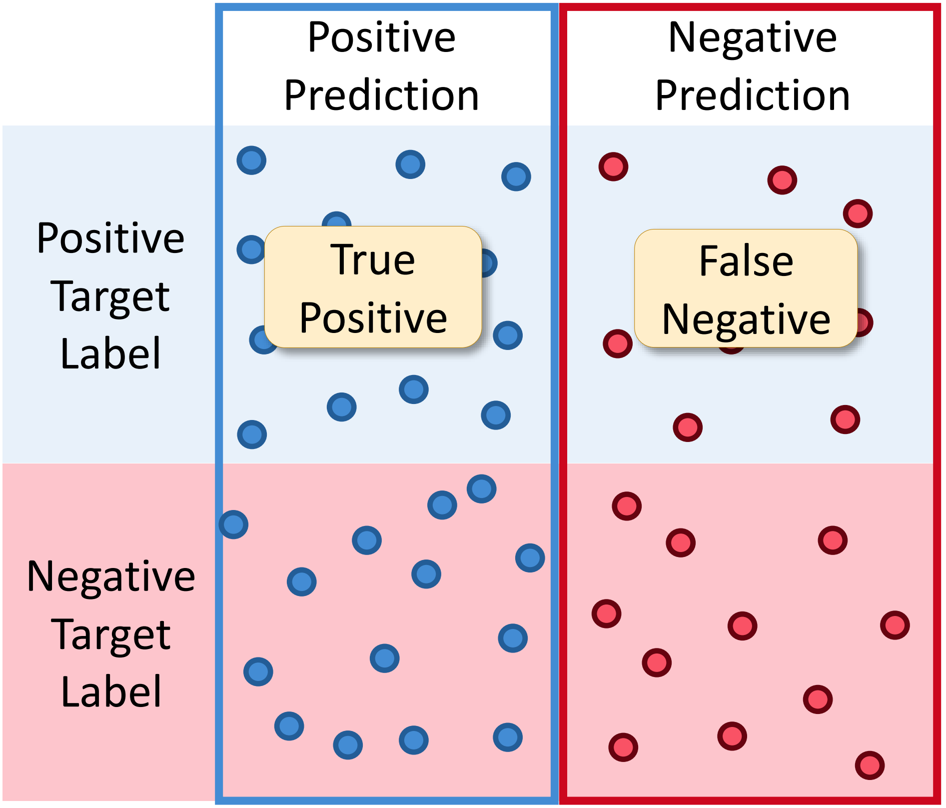
Terminology: True Positives



ID	Target Label	Prediction	
1	On Time	Delayed	
2	On Time	Delayed	
3	Delayed	Delayed	
4	On Time	On Time	**TP**
5	Delayed	Delayed	
6	On Time	On Time	**TP**
7	Delayed	Delayed	
8	On Time	On Time	**TP**
9	On Time	On Time	**TP**
10	On Time	On Time	**TP**

ID	Target Label	Prediction	
11	Delayed	Delayed	
12	On Time	Delayed	
13	Delayed	Delayed	
14	Delayed	Delayed	
15	Delayed	Delayed	
16	Delayed	Delayed	
17	Delayed	On Time	
18	On Time	On Time	**TP**
19	Delayed	Delayed	
20	Delayed	On Time	

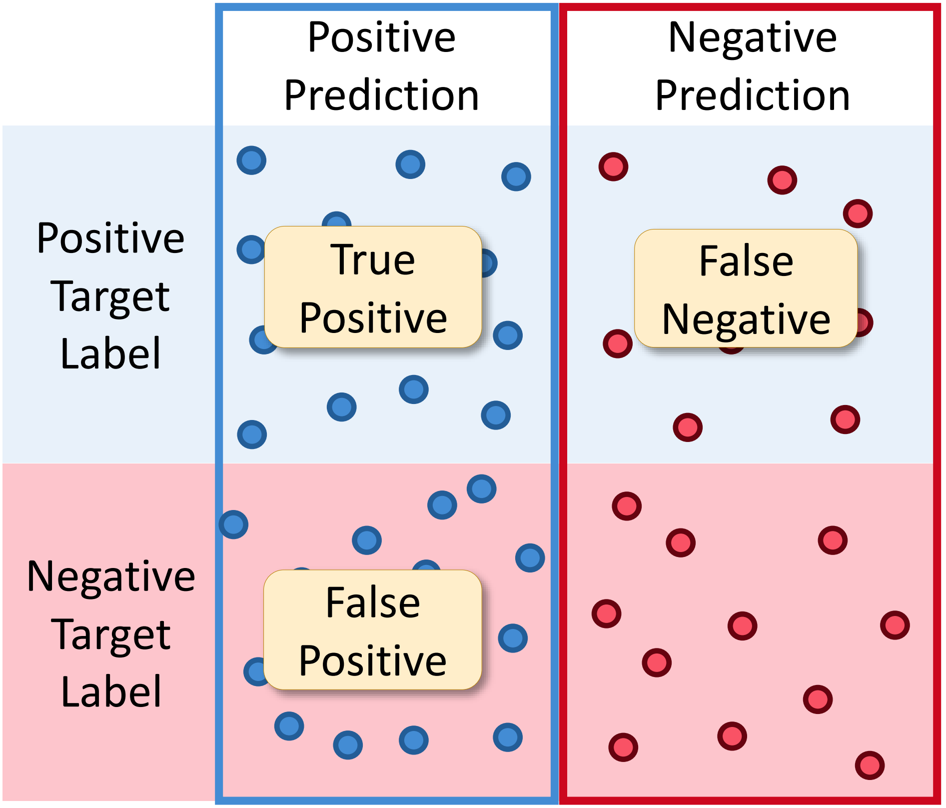
Terminology: False Negatives



ID	Target Label	Prediction	
1	On Time	Delayed	**FN**
2	On Time	Delayed	**FN**
3	Delayed	Delayed	
4	On Time	On Time	**TP**
5	Delayed	Delayed	
6	On Time	On Time	**TP**
7	Delayed	Delayed	
8	On Time	On Time	**TP**
9	On Time	On Time	**TP**
10	On Time	On Time	**TP**

ID	Target Label	Prediction	
11	Delayed	Delayed	
12	On Time	Delayed	**FN**
13	Delayed	Delayed	
14	Delayed	Delayed	
15	Delayed	Delayed	
16	Delayed	Delayed	
17	Delayed	On Time	
18	On Time	On Time	**TP**
19	Delayed	Delayed	
20	Delayed	On Time	

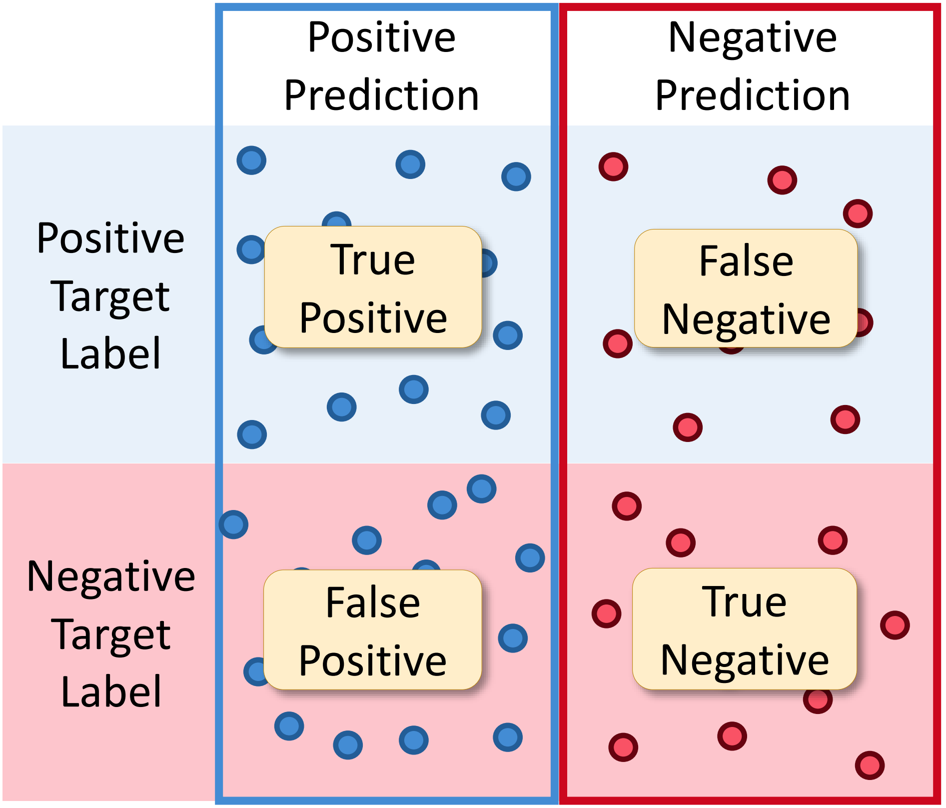
Terminology: False Positives



ID	Target Label	Prediction	
1	On Time	Delayed	**FN**
2	On Time	Delayed	**FN**
3	Delayed	Delayed	
4	On Time	On Time	**TP**
5	Delayed	Delayed	
6	On Time	On Time	**TP**
7	Delayed	Delayed	
8	On Time	On Time	**TP**
9	On Time	On Time	**TP**
10	On Time	On Time	**TP**

ID	Target Label	Prediction	
11	Delayed	Delayed	
12	On Time	Delayed	**FN**
13	Delayed	Delayed	
14	Delayed	Delayed	
15	Delayed	Delayed	
16	Delayed	Delayed	
17	Delayed	On Time	**FP**
18	On Time	On Time	**TP**
19	Delayed	Delayed	
20	Delayed	On Time	**FP**

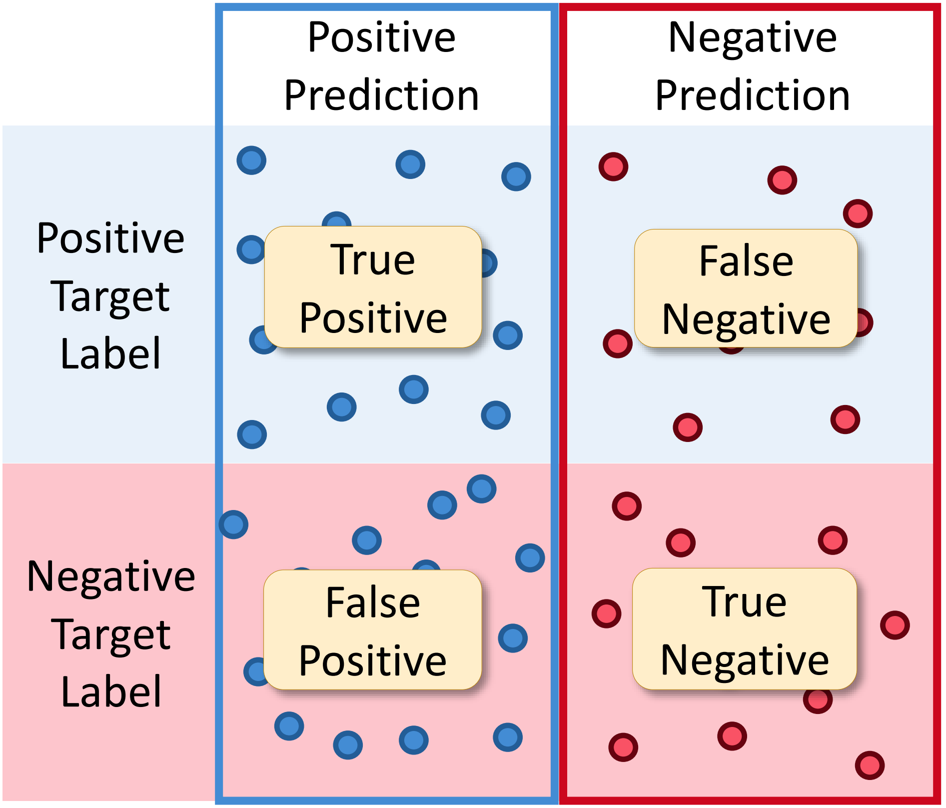
Terminology: True Negatives



ID	Target Label	Prediction	
1	On Time	Delayed	**FN**
2	On Time	Delayed	**FN**
3	Delayed	Delayed	**TN**
4	On Time	On Time	**TP**
5	Delayed	Delayed	**TN**
6	On Time	On Time	**TP**
7	Delayed	Delayed	**TN**
8	On Time	On Time	**TP**
9	On Time	On Time	**TP**
10	On Time	On Time	**TP**

ID	Target Label	Prediction	
11	Delayed	Delayed	**TN**
12	On Time	Delayed	**FN**
13	Delayed	Delayed	**TN**
14	Delayed	Delayed	**TN**
15	Delayed	Delayed	**TN**
16	Delayed	Delayed	**TN**
17	Delayed	On Time	**FP**
18	On Time	On Time	**TP**
19	Delayed	Delayed	**TN**
20	Delayed	On Time	**FP**

Confusion Matrix



ID	Target Label	Prediction	
1	On Time	Delayed	**FN**
2	On Time	Delayed	**FN**
3	Delayed	Delayed	**TN**
4	On Time	On Time	**TP**
5	Delayed	Delayed	**TN**
6	On Time	On Time	**TP**
7	Delayed	Delayed	**TN**
8	On Time	On Time	**TP**
9	On Time	On Time	**TP**
10	On Time	On Time	**TP**

ID	Target Label	Prediction	
11	Delayed	Delayed	**TN**
12	On Time	Delayed	**FN**
13	Delayed	Delayed	**TN**
14	Delayed	Delayed	**TN**
15	Delayed	Delayed	**TN**
16	Delayed	Delayed	**TN**
17	Delayed	On Time	**FP**
18	On Time	On Time	**TP**
19	Delayed	Delayed	**TN**
20	Delayed	On Time	**FP**

Confusion Matrix

	Positive Prediction	Negative Prediction
Positive Target Label	**TP** (number of true positives)	**FN** (number of false negatives)
Negative Target Label	**FP** (number of false positives)	**TN** (number of true negatives)

ID	Target Label	Prediction	
1	On Time	Delayed	**FN**
2	On Time	Delayed	**FN**
3	Delayed	Delayed	**TN**
4	On Time	On Time	**TP**
5	Delayed	Delayed	**TN**
6	On Time	On Time	**TP**
7	Delayed	Delayed	**TN**
8	On Time	On Time	**TP**
9	On Time	On Time	**TP**
10	On Time	On Time	**TP**

ID	Target Label	Prediction	
11	Delayed	Delayed	**TN**
12	On Time	Delayed	**FN**
13	Delayed	Delayed	**TN**
14	Delayed	Delayed	**TN**
15	Delayed	Delayed	**TN**
16	Delayed	Delayed	**TN**
17	Delayed	On Time	**FP**
18	On Time	On Time	**TP**
19	Delayed	Delayed	**TN**
20	Delayed	On Time	**FP**

Confusion Matrix

	Positive Prediction	Negative Prediction
Positive Target Label	**6**	**3**
Negative Target Label	**2**	**9**

ID	Target Label	Prediction		ID	Target Label	Prediction	
1	On Time	Delayed	**FN**	11	Delayed	Delayed	**TN**
2	On Time	Delayed	**FN**	12	On Time	Delayed	**FN**
3	Delayed	Delayed	**TN**	13	Delayed	Delayed	**TN**
4	On Time	On Time	**TP**	14	Delayed	Delayed	**TN**
5	Delayed	Delayed	**TN**	15	Delayed	Delayed	**TN**
6	On Time	On Time	**TP**	16	Delayed	Delayed	**TN**
7	Delayed	Delayed	**TN**	17	Delayed	On Time	**FP**
8	On Time	On Time	**TP**	18	On Time	On Time	**TP**
9	On Time	On Time	**TP**	19	Delayed	Delayed	**TN**
10	On Time	On Time	**TP**	**20**	Delayed	On Time	**FP**

Defining a Performance Measure

- You have used supervised learning to train a predictive model
  - And you have computed a confusion matrix based on the predictions on a given set of data

- Question: How can we assess performance with a single number?
  - *Let's collect your ideas here…*

	Positive Prediction	Negative Prediction
Positive Target Label	**6**	**3**
Negative Target Label	**2**	**9**

Confusion Matrix ➜ Performance Measures

	Positive Prediction	Negative Prediction
Positive Target Label	**TP=6**	**FN=3**
Negative Target Label	**FP=2**	**TN=9**

True Positive Rate: $TPR = \frac{TP}{TP+FN}$

False Negative Rate: $FNR = \frac{FN}{TP+FN}$

False Positive Rate: $FPR = \frac{FP}{FP+TN}$

True Negative Rate: $TNR = \frac{TN}{FP+TN}$

Classification Accuracy: $\frac{TP+TN}{TP+TN+FP+FN}$

Misclassification Rate: $\frac{FP+FN}{TP+TN+FP+FN}$

Confusion Matrix ➜ Performance Measures

	Positive Prediction	Negative Prediction
Positive Target Label	**TP=6**	**FN=3**
Negative Target Label	**FP=2**	**TN=9**

True Positive Rate: $TPR = \frac{TP}{TP+FN}$

False Negative Rate: $FNR = \frac{FN}{TP+FN}$

False Positive Rate: $FPR = \frac{FP}{FP+TN}$

True Negative Rate: $TNR = \frac{TN}{FP+TN}$

Recall: $recall = \frac{TP}{TP+FN} = TPR$

Precision: $precision = \frac{TP}{TP+FP}$

F_1: $F_1 = 2 \cdot \frac{precision \cdot recall}{precision + recall}$

Confusion Matrix → Performance Measures

	Positive Prediction	Negative Prediction
Positive Target Label	**TP=6**	**FN=3**
Negative Target Label	**FP=2**	**TN=9**

$TPR + FNR = 1$

True Positive Rate: $TPR = \frac{TP}{TP+FN} = \frac{6}{6+3} = \frac{2}{3}$

False Negative Rate: $FNR = \frac{FN}{TP+FN} = \frac{3}{6+3} = \frac{1}{3}$

False Positive Rate: $FPR = \frac{FP}{FP+TN} = \frac{2}{2+9} = \frac{2}{11}$

True Negative Rate: $TNR = \frac{TN}{FP+TN} = \frac{9}{2+9} = \frac{9}{11}$

$FPR + TNR = 1$

Classification Accuracy:

Misclassification Rate:

Recall:

Precision:

F_1:

Confusion Matrix ➜ Performance Measures

	Positive Prediction	Negative Prediction
Positive Target Label	**TP=6**	**FN=3**
Negative Target Label	**FP=2**	**TN=9**

True Positive Rate: $TPR = \frac{TP}{TP+FN} = \frac{6}{6+3} = \frac{2}{3}$

False Negative Rate: $FNR = \frac{FN}{TP+FN} = \frac{3}{6+3} = \frac{1}{3}$

False Positive Rate: $FPR = \frac{FP}{FP+TN} = \frac{2}{2+9} = \frac{2}{11}$

True Negative Rate: $TNR = \frac{TN}{FP+TN} = \frac{9}{2+9} = \frac{9}{11}$

Classification Accuracy: $\frac{TP+TN}{TP+TN+FP+FN} = \frac{6+9}{6+9+2+3} = \frac{15}{20}$

Misclassification Rate: $\frac{FP+FN}{TP+TN+FP+FN} = \frac{2+3}{6+9+2+3} = \frac{5}{20}$

$\text{Classification Accuracy} + \text{Misclassification Rate} = 1$

Recall:

Precision:

F_1:

Confusion Matrix → Performance Measures

	Positive Prediction	Negative Prediction
Positive Target Label	**TP=6**	**FN=3**
Negative Target Label	**FP=2**	**TN=9**

True Positive Rate: $TPR = \frac{TP}{TP+FN} = \frac{6}{6+3} = \frac{2}{3}$

False Negative Rate: $FNR = \frac{FN}{TP+FN} = \frac{3}{6+3} = \frac{1}{3}$

False Positive Rate: $FPR = \frac{FP}{FP+TN} = \frac{2}{2+9} = \frac{2}{11}$

True Negative Rate: $TNR = \frac{TN}{FP+TN} = \frac{9}{2+9} = \frac{9}{11}$

Classification Accuracy: $\frac{TP+TN}{TP+TN+FP+FN} = \frac{6+9}{6+9+2+3} = \frac{15}{20}$

Misclassification Rate: $\frac{FP+FN}{TP+TN+FP+FN} = \frac{2+3}{6+9+2+3} = \frac{5}{20}$

Recall: $recall = \frac{TP}{TP+FN} = TPR = \frac{2}{3} \approx 0.67$

Precision: $precision = \frac{TP}{TP+FP} = \frac{6}{6+2} = \frac{3}{4} = 0.75$

F_1: $F_1 = 2 \cdot \frac{precision \cdot recall}{precision + recall} = \frac{2 \cdot \frac{3}{4} \cdot \frac{2}{3}}{\frac{3}{4}+\frac{2}{3}} = \frac{12}{17} \approx 0.71$

Scenario

- You have used supervised learning to train a predictive model
  - And you have computed a confusion matrix based on the predictions on a given set of data

- Question: Which measure should we use to assess performance? And why?
  - *Let's collect your ideas here…*

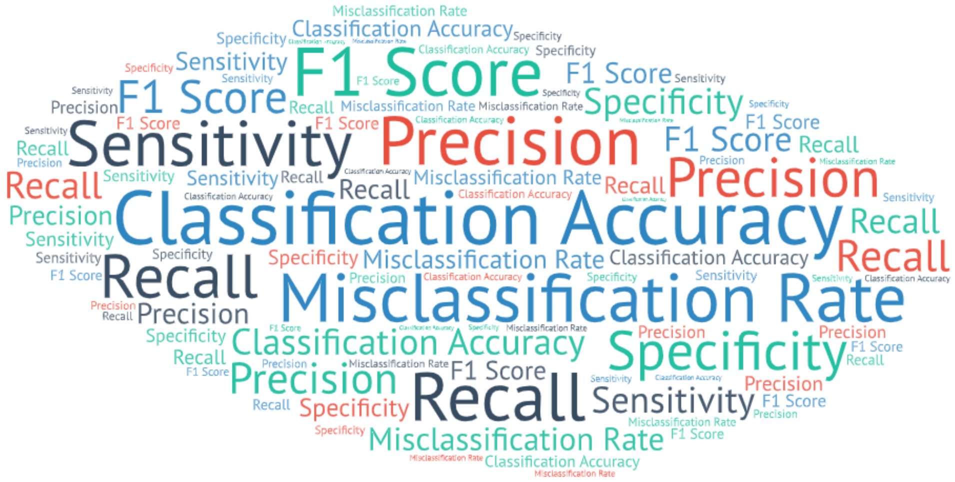
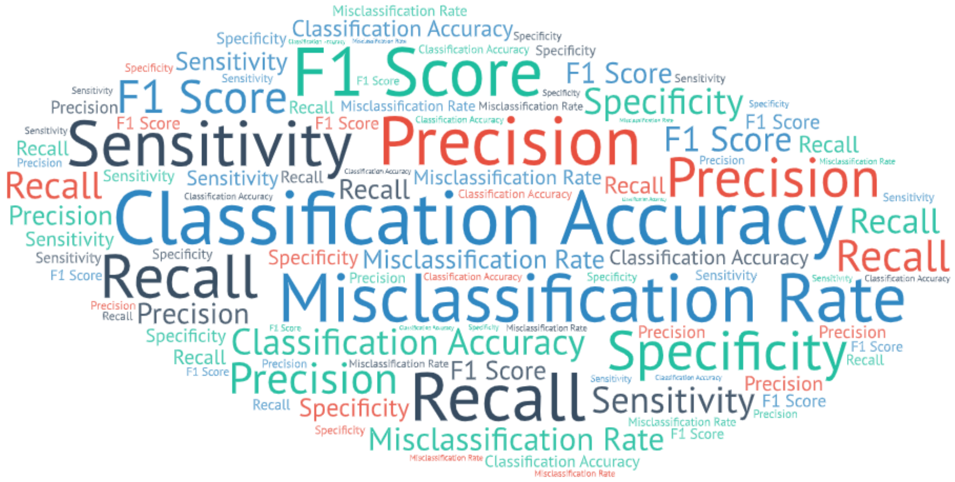


Image generated with https://wordart.com/create

Scenario

- You have used supervised learning to train a predictive model
  - And you have computed a confusion matrix based on the predictions on a given set of data



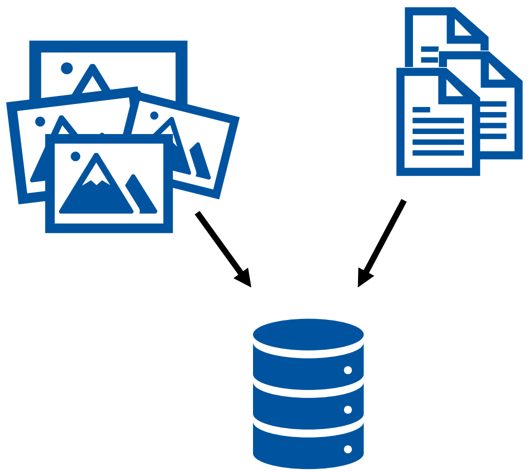
- Question: Which measure should we use to assess performance? And why?
  - *Let's collect your ideas here…*

It depends – often a single measure is not enough.

Image generated with https://wordart.com/create

Practical Aspects

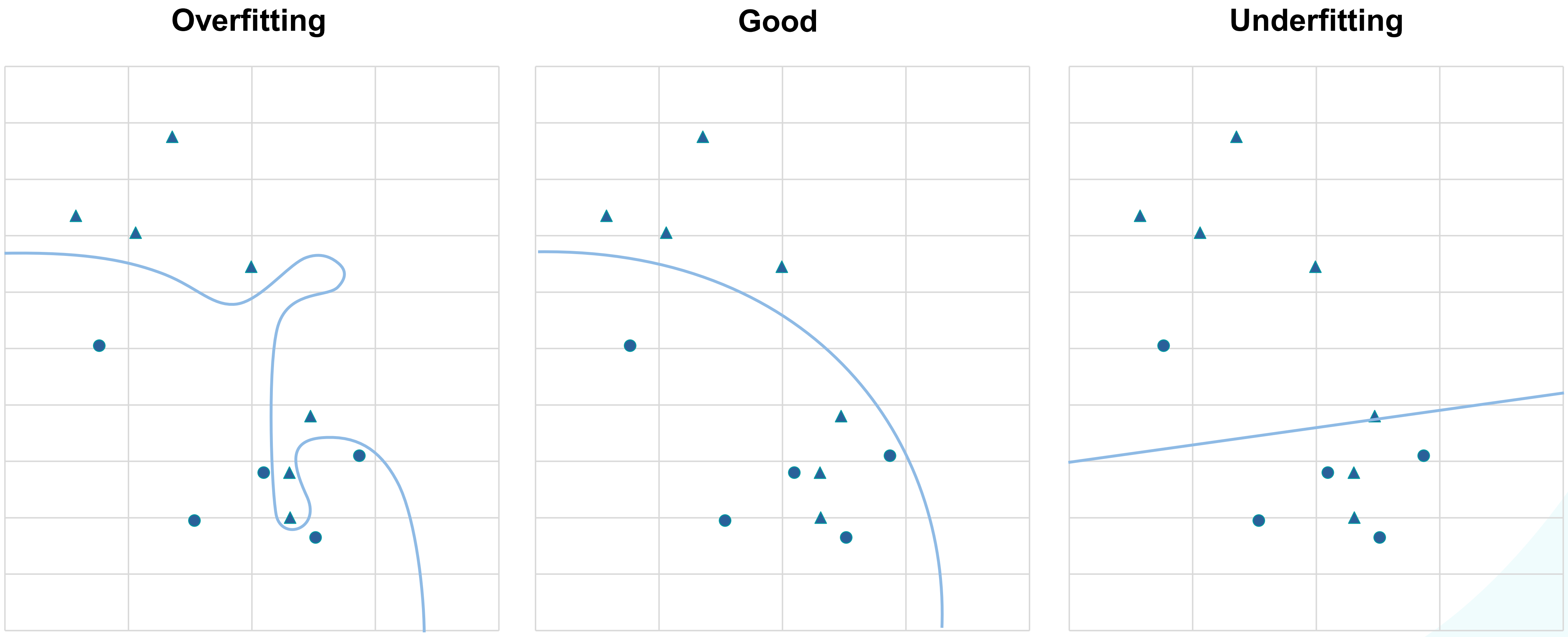
- You have used supervised learning to train a predictive model
  - And you have computed a confusion matrix based on the predictions on a given set of data



- Question: What set of data instances should we use as the basis for assessing performance?
  - *Let's collect your ideas here…*

  Let's use training instances. What could go wrong?

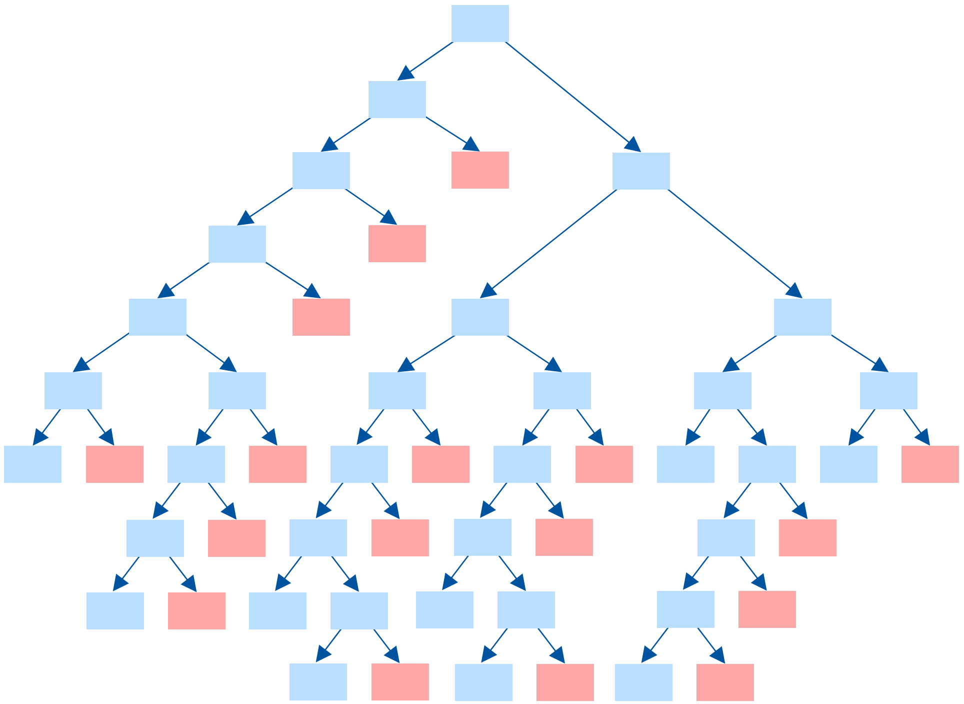
Remember Overfitting and Underfitting



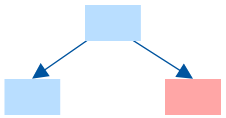
Remember Overfitting and Underfitting

Flight Classification (Running Example)

Overfitting



Underfitting



ID	Target
1	On Time
2	On Time
3	Delayed
4	On Time
5	Delayed
6	On Time
7	Delayed
8	On Time
9	On Time
10	On Time
11	Delayed
…	…

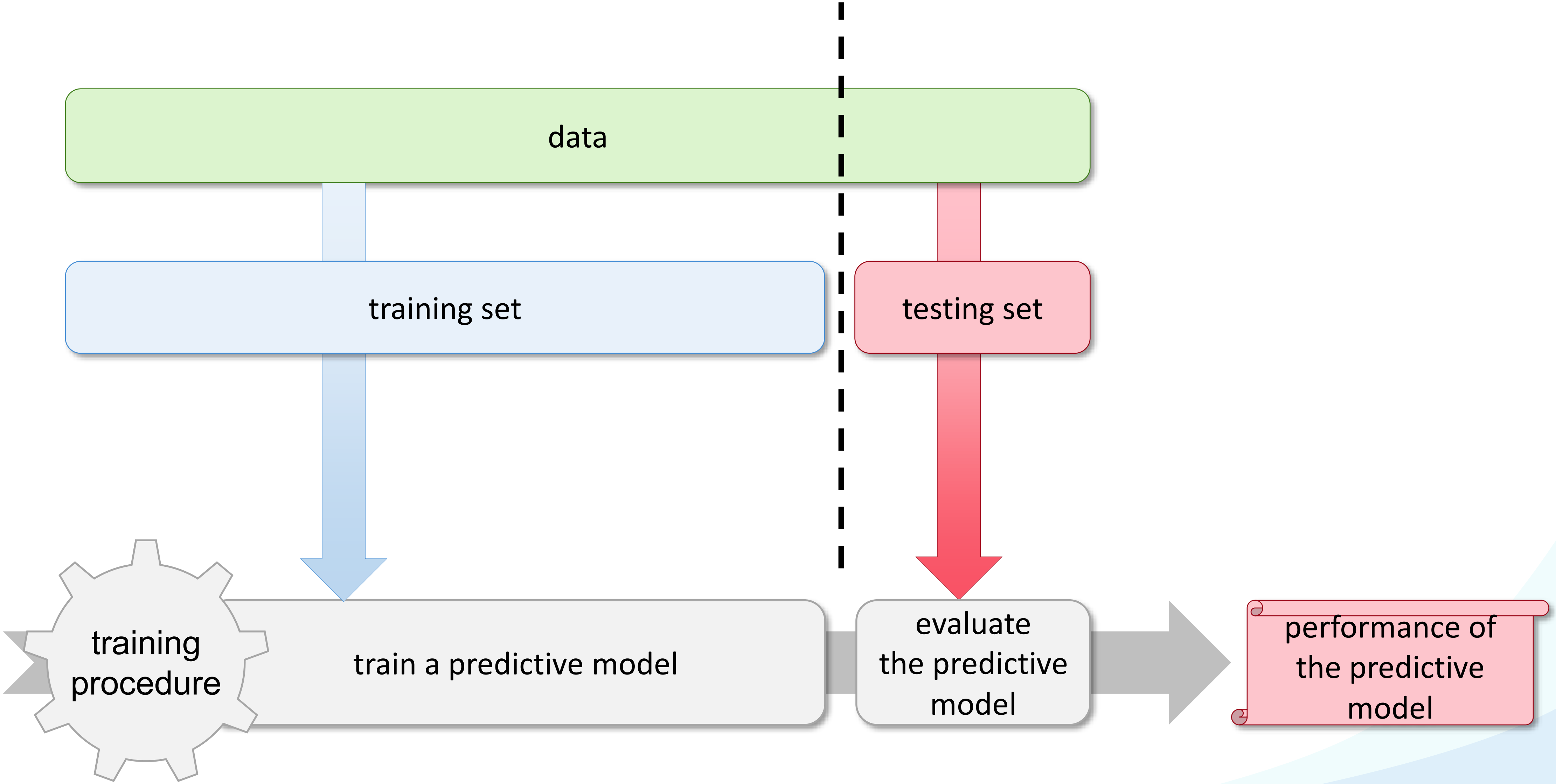
Practical Aspects

- You have used supervised learning to train a predictive model
  - And you have computed a confusion matrix based on the predictions on a given set of data

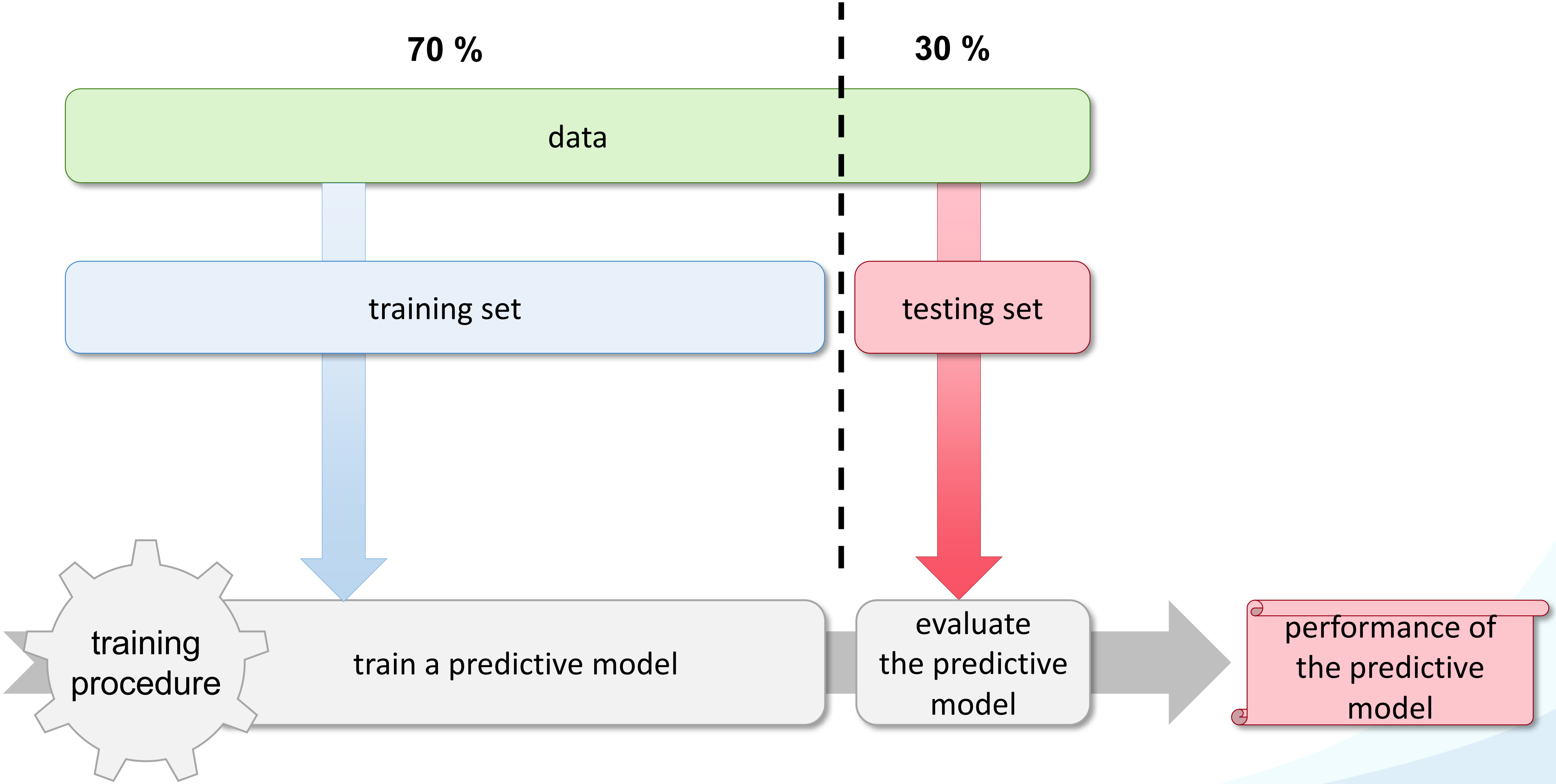
- Question: What set of data instances should we use as the basis for assessing performance?
  - *Let's collect your ideas here…*

- Key Issue: Generalization to new data
  - *Don't assess performance based on training data!*

Training & Testing Data



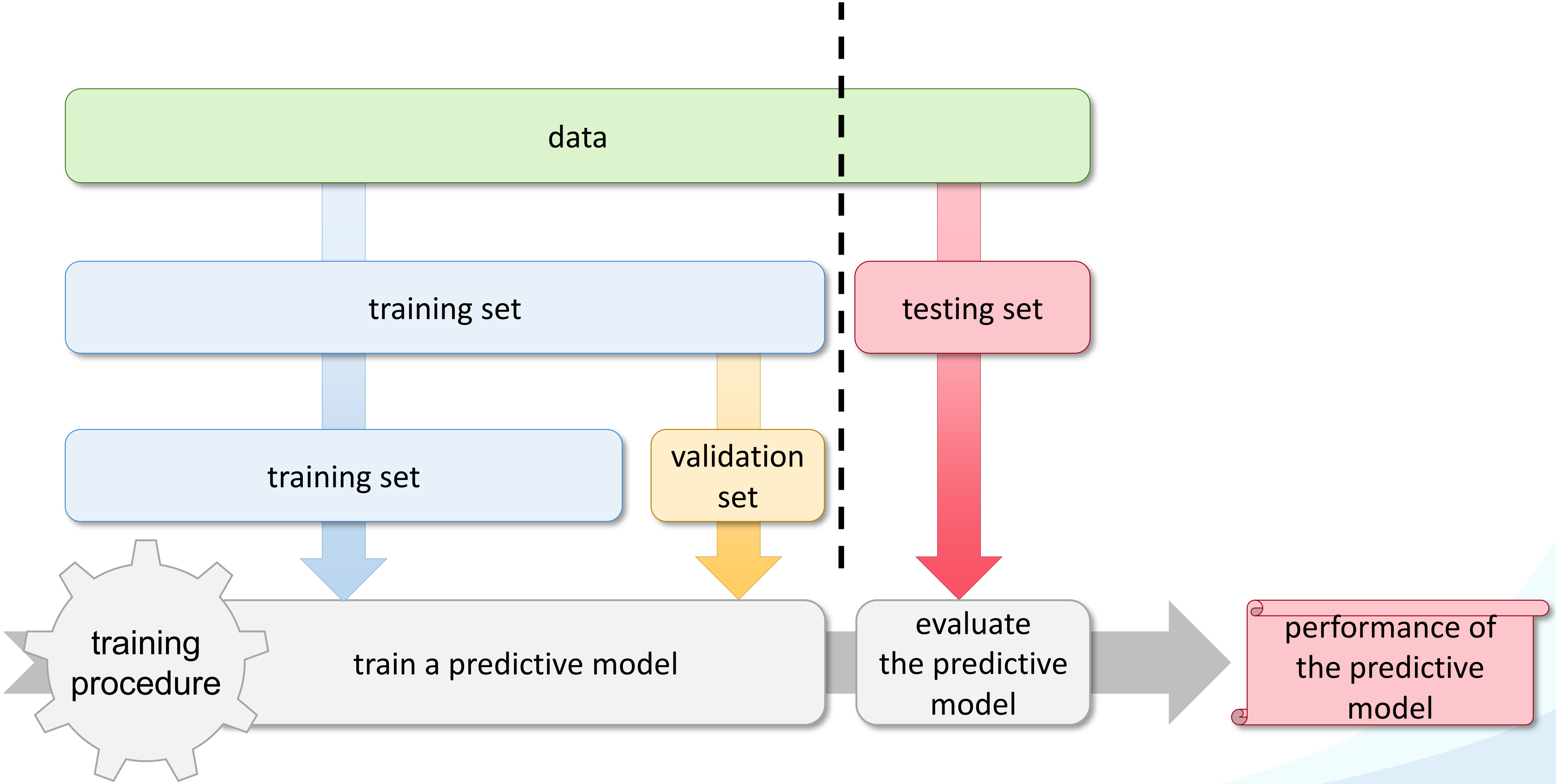
Training & Testing Data



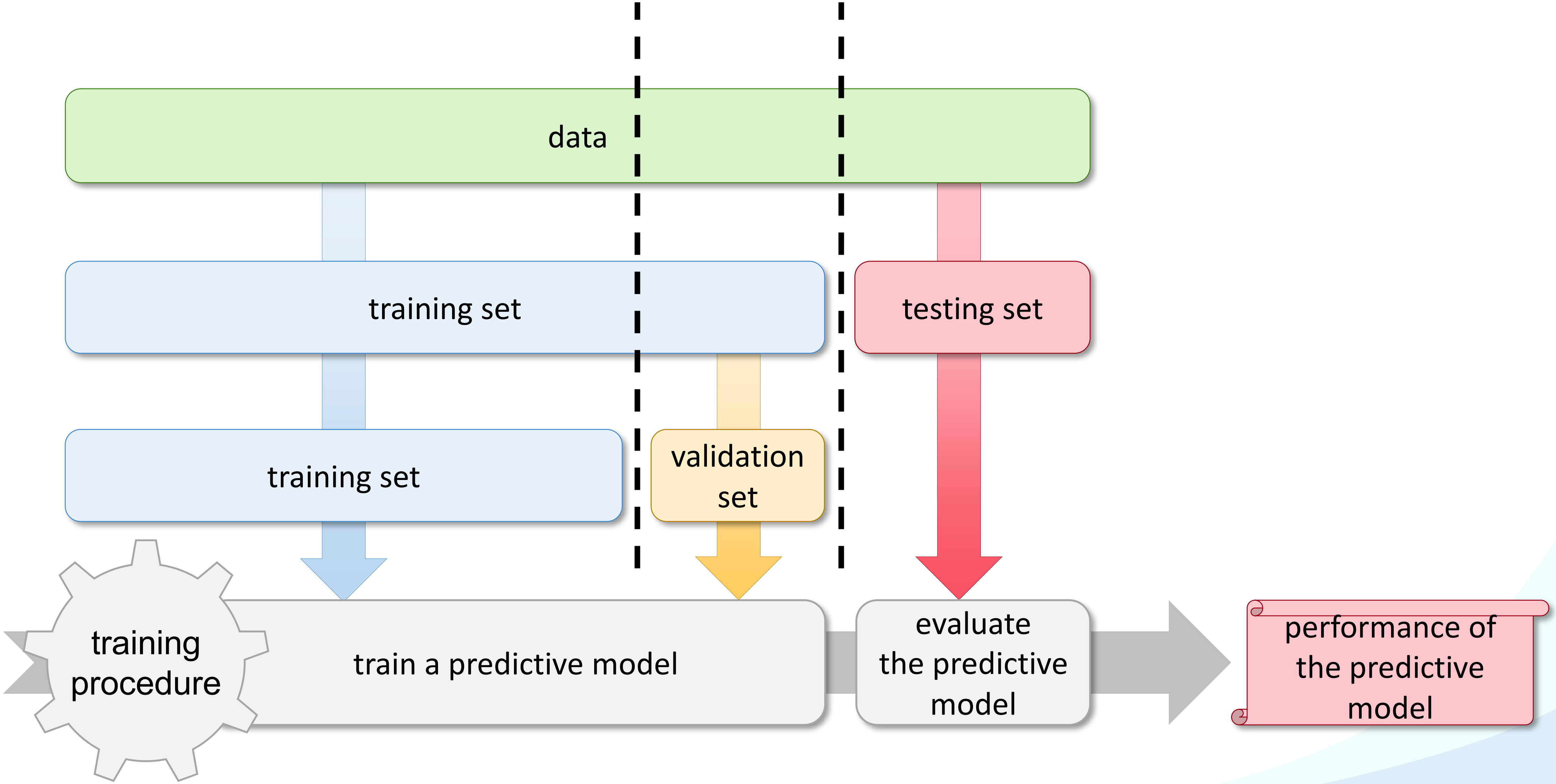
Validation Set

- Training a predictive model is often done iteratively (e.g., regression, neural networks)
- The model is fitted closer and closer to the training data
- The validation set can be used to avoid overfitting the training data
- Often used for parameter selection or hyperparameter tuning

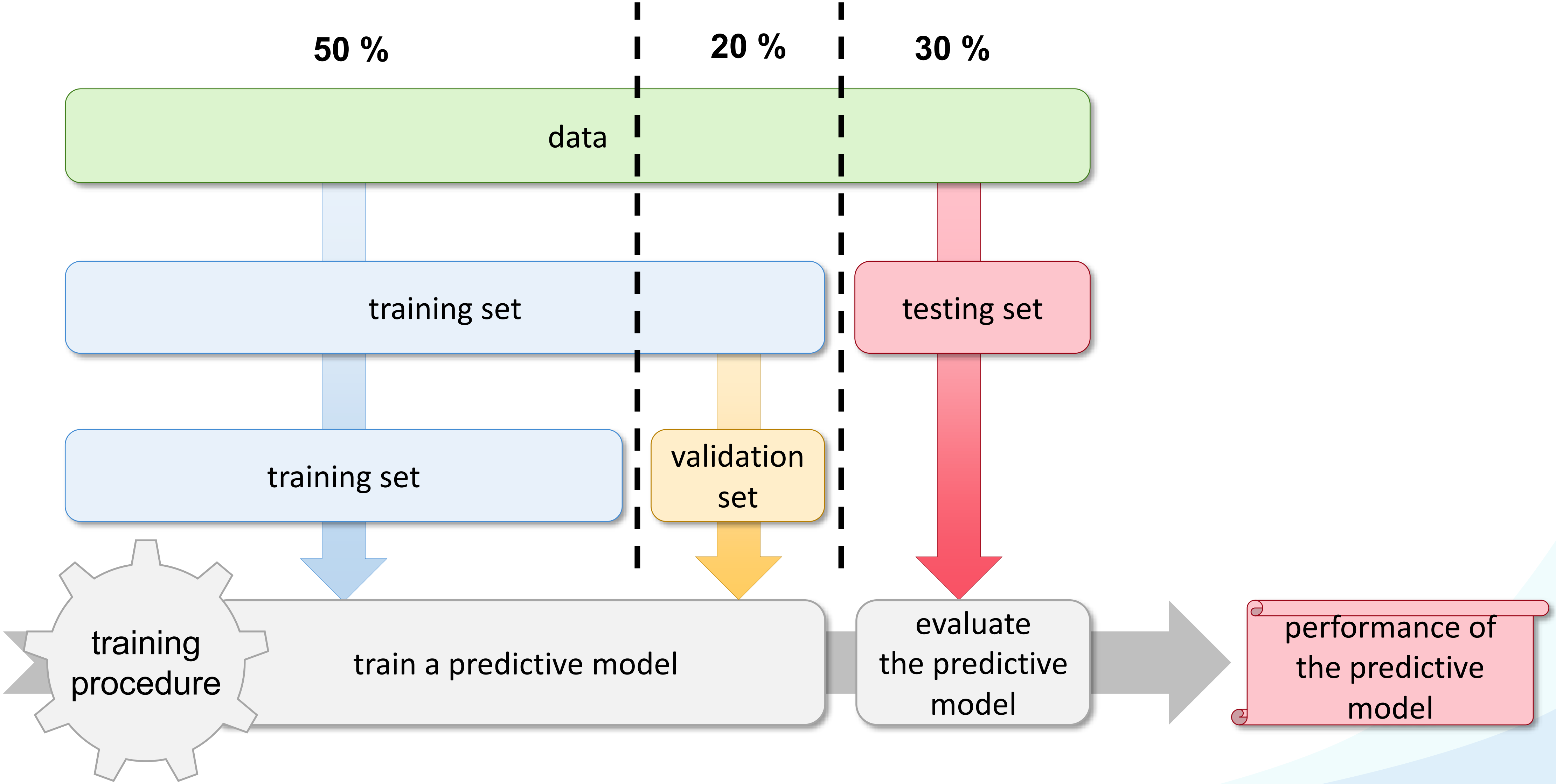
Training & Testing Data



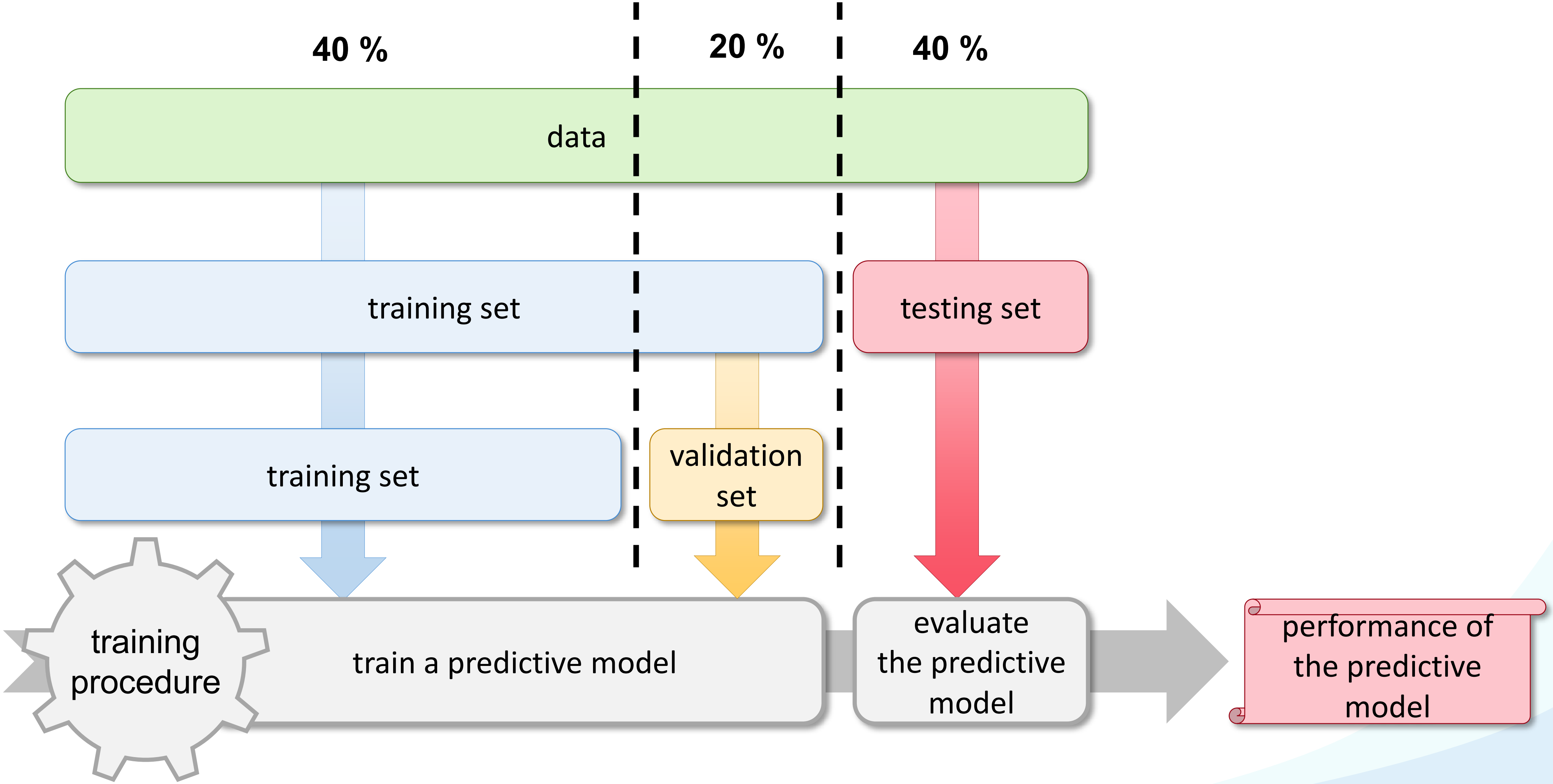
Training & Testing Data



Training & Testing Data



Training & Testing Data



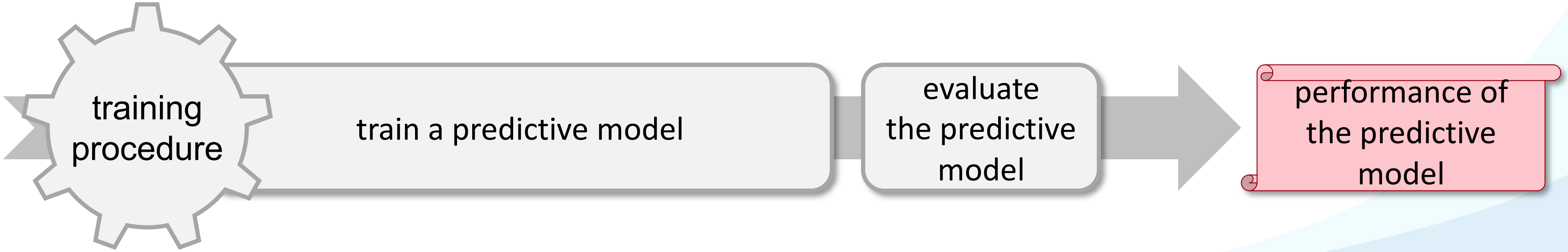
Practical Aspects

- You have used supervised learning to train a predictive model
  - And you have computed a confusion matrix based on the predictions on a given set of data

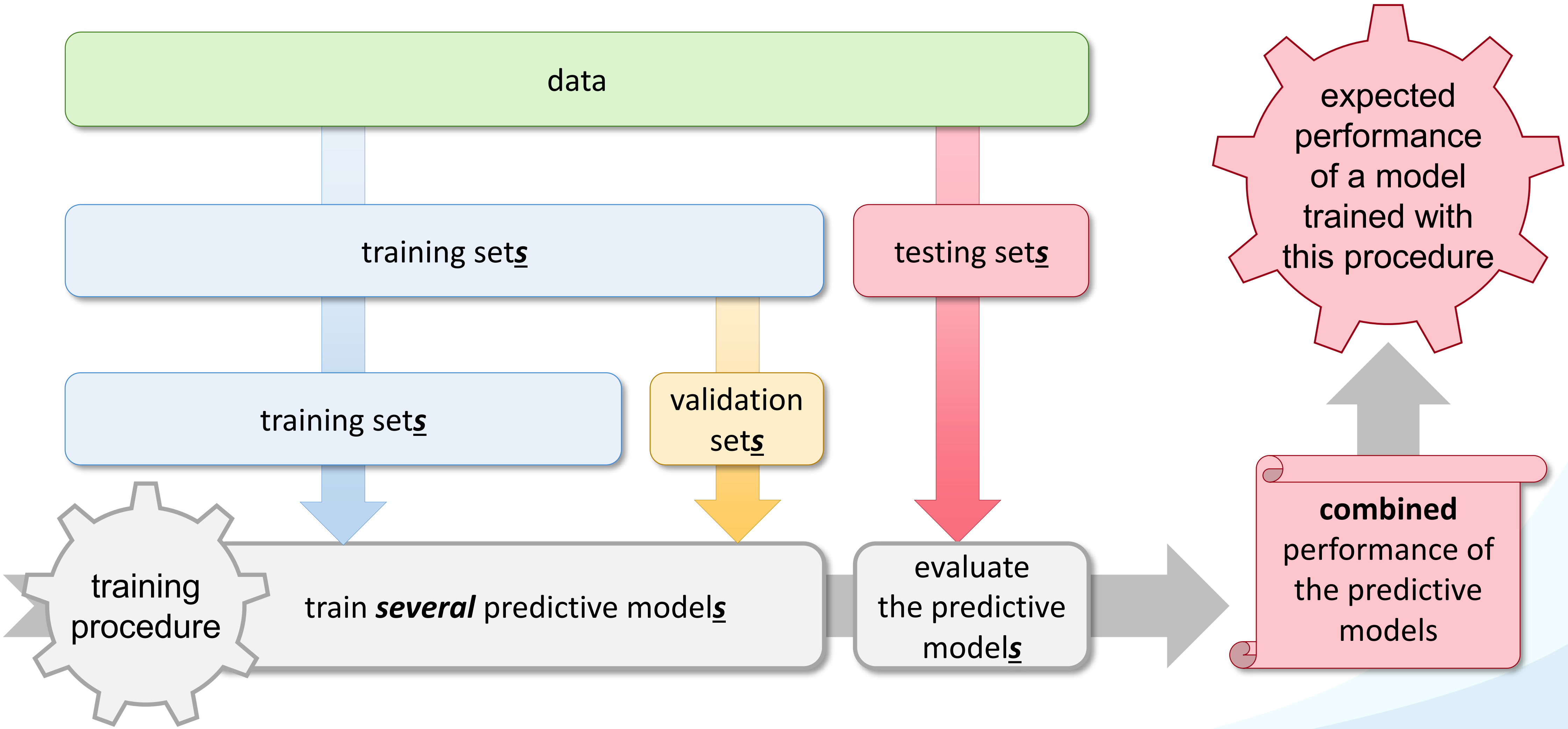
- Question: How to split the data into training, validation and testing sets if there are only 20 instances?
  - *Any ideas?*

Dealing with Small datasets:

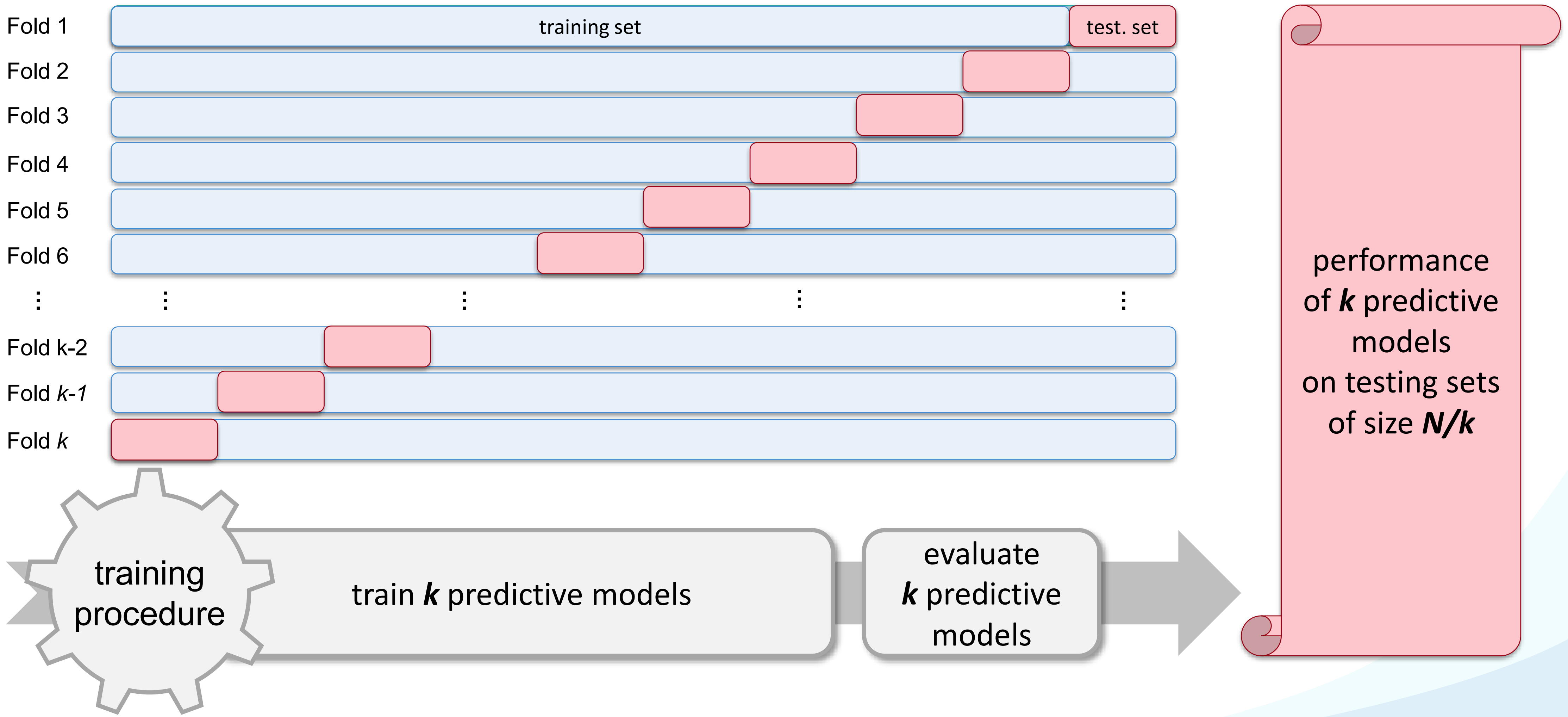
- Splitting into **one** training and **one** testing set is reliable only for sufficiently large data sets
- On small data sets the training, validation or testing set become too small
- Small data set increases danger of a ‘lucky split’ (with most easy instances in the testing set)



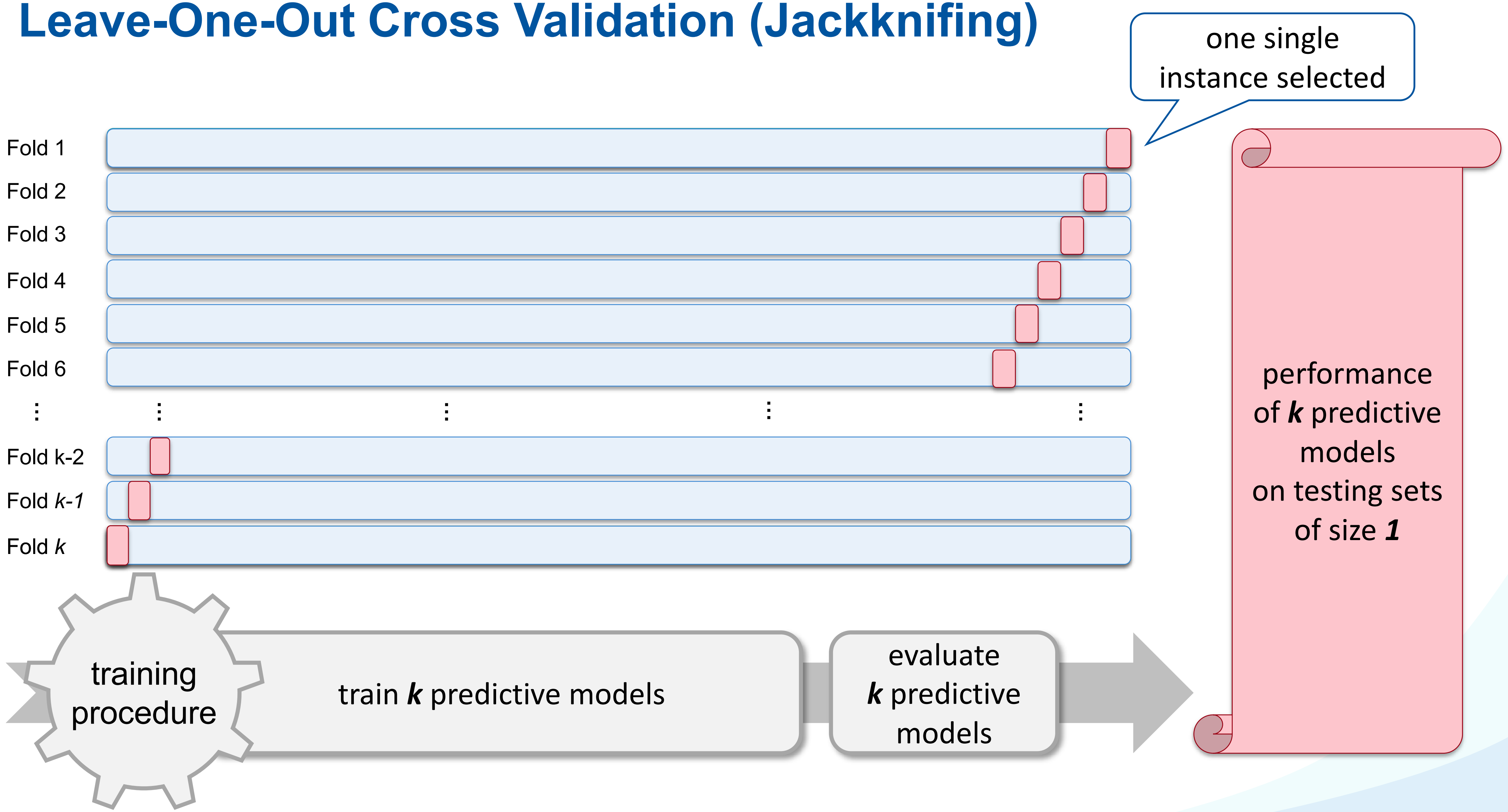
Motivation


data
training sets
testing sets
training sets
validation sets
training procedure
train several predictive models
evaluate the predictive models
combined performance of the predictive models
expected performance of a model trained with this procedure

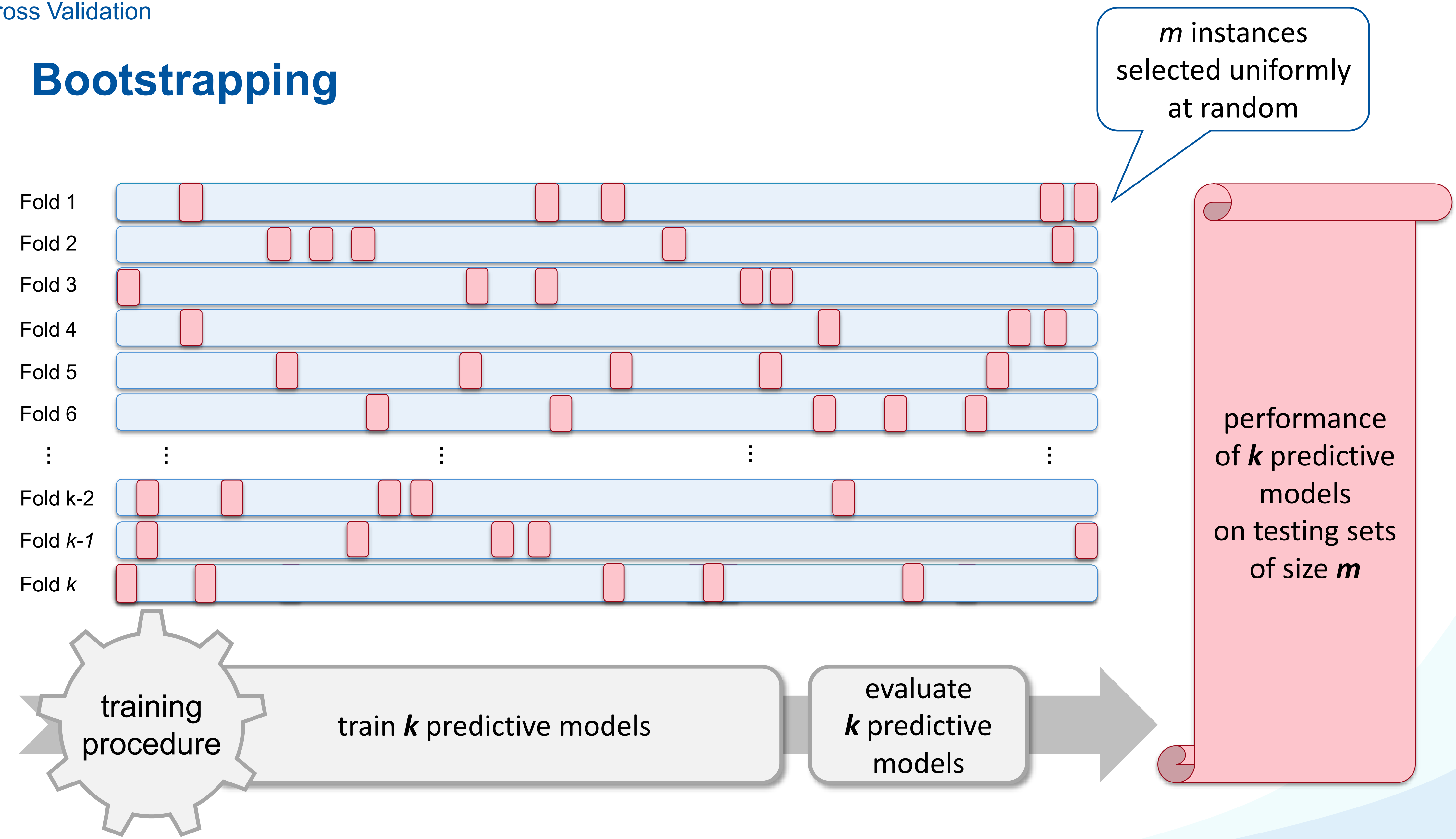
k-Fold Cross Validation



Leave-One-Out Cross Validation (Jackknifing)



Bootstrapping



What problem could arise?

ID	Target Label	Prediction
1	On Time	
2	On Time	
3	On Time	
4	On Time	
5	On Time	
6	On Time	
7	On Time	
8	On Time	
9	On Time	
10	On Time	

ID	Target Label	Prediction
11	On Time	
12	On Time	
13	On Time	
14	On Time	
15	On Time	
16	On Time	
17	On Time	
18	On Time	
19	Delayed	
20	Delayed	

What problem could arise?

ID	Target Label	Prediction	ID	Target Label	Prediction
1	On Time	On Time	11	On Time	On Time
2	On Time	On Time	12	On Time	On Time
3	On Time	On Time	13	On Time	On Time
4	On Time	On Time	14	On Time	On Time
5	On Time	On Time	15	On Time	On Time
6	On Time	On Time	16	On Time	On Time
7	On Time	On Time	17	On Time	On Time
8	On Time	On Time	18	On Time	On Time
9	On Time	On Time	19	Delayed	On Time
10	On Time	On Time	**20**	Delayed	On Time

Imbalanced Data

	On Time Prediction	Delayed Prediction
On Time Target Label	**18**	**0**
Delayed Target Label	**2**	**0**

Motivational Example

- A test set with many (18) positive instances and few (2) negative instances
- A model that always predicts positive

ID	Target Label	Prediction	ID	Target Label	Prediction
1	On Time	On Time	11	On Time	On Time
2	On Time	On Time	12	On Time	On Time
3	On Time	On Time	13	On Time	On Time
4	On Time	On Time	14	On Time	On Time
5	On Time	On Time	15	On Time	On Time
6	On Time	On Time	16	On Time	On Time
7	On Time	On Time	17	On Time	On Time
8	On Time	On Time	18	On Time	On Time
9	On Time	On Time	19	Delayed	On Time
10	On Time	On Time	20	Delayed	On Time

Imbalanced Data

	On Time Prediction	Delayed Prediction
On Time Target Label	**18**	**0**
Delayed Target Label	**2**	**0**

Motivational Example

- A test set with many (18) positive instances and few (2) negative instances
- A model that always predicts positive (= On Time)

Recall:

$$recall = \frac{TP}{TP+FN} = \frac{18}{18+0} = 1.0$$

Precision:

$$precision = \frac{TP}{TP+FP} = \frac{18}{18+2} = \frac{18}{20} = 0.9$$

ID	Target Label	Prediction	ID	Target Label	Prediction
1	On Time	On Time	11	On Time	On Time
2	On Time	On Time	12	On Time	On Time
3	On Time	On Time	13	On Time	On Time
4	On Time	On Time	14	On Time	On Time
5	On Time	On Time	15	On Time	On Time
6	On Time	On Time	16	On Time	On Time
7	On Time	On Time	17	On Time	On Time
8	On Time	On Time	18	On Time	On Time
9	On Time	On Time	19	Delayed	On Time
10	On Time	On Time	20	Delayed	On Time

Imbalanced Data

	On Time Prediction	Delayed Prediction
On Time Target Label	**18**	**0**
Delayed Target Label	**2**	**0**

Average Class Accuracy

Average recall over the elements in the set of possible target feature values $C = \{\text{Delayed}, \text{On Time}\}$

ID	Target Label	Prediction	ID	Target Label	Prediction
1	On Time	On Time	11	On Time	On Time
2	On Time	On Time	12	On Time	On Time
3	On Time	On Time	13	On Time	On Time
4	On Time	On Time	14	On Time	On Time
5	On Time	On Time	15	On Time	On Time
6	On Time	On Time	16	On Time	On Time
7	On Time	On Time	17	On Time	On Time
8	On Time	On Time	18	On Time	On Time
9	On Time	On Time	19	Delayed	On Time
10	On Time	On Time	20	Delayed	On Time

Imbalanced Data

	On Time Prediction	Delayed Prediction
On Time Target Label	**18**	**0**
Delayed Target Label	**2**	**0**

$$recall = \frac{TP}{TP+FN} = \frac{18}{18+0} = 1.0$$

	Delayed Prediction	On Time Prediction
Delayed Target Label	**0**	**2**
On Time Target Label	**0**	**18**

$$recall = \frac{TP}{TP+FN} = \frac{0}{0+2} = 0.0$$

Average Class Accuracy

Average recall over the elements in the set of possible target feature values $C = \{\text{Delayed, On Time}\}$

ID	Target Label	Prediction	ID	Target Label	Prediction
1	On Time	On Time	11	On Time	On Time
2	On Time	On Time	12	On Time	On Time
3	On Time	On Time	13	On Time	On Time
4	On Time	On Time	14	On Time	On Time
5	On Time	On Time	15	On Time	On Time
6	On Time	On Time	16	On Time	On Time
7	On Time	On Time	17	On Time	On Time
8	On Time	On Time	18	On Time	On Time
9	On Time	On Time	19	Delayed	On Time
10	On Time	On Time	20	Delayed	On Time

Imbalanced Data

	On Time Prediction	Delayed Prediction
On Time Target Label	**18**	**0**
Delayed Target Label	**2**	**0**

$$recall = \frac{TP}{TP+FN} = \frac{18}{18+0} = 1.0$$

	Delayed Prediction	On Time Prediction
Delayed Target Label	**0**	**2**
On Time Target Label	**0**	**18**

$$recall = \frac{TP}{TP+FN} = \frac{0}{0+2} = 0.0$$

Average Class Accuracy

Average recall over the elements in the set of possible target feature values $C = \{\text{Delayed, On Time}\}$

- arithmetic mean: $\frac{1}{|C|}\sum_{c \in C} recall_c$
- harmonic mean: $\frac{1}{\frac{1}{|C|}\sum_{c \in C}\frac{1}{recall_c}}$

ID	Target Label	Prediction	ID	Target Label	Prediction
1	On Time	On Time	11	On Time	On Time
2	On Time	On Time	12	On Time	On Time
3	On Time	On Time	13	On Time	On Time
4	On Time	On Time	14	On Time	On Time
5	On Time	On Time	15	On Time	On Time
6	On Time	On Time	16	On Time	On Time
7	On Time	On Time	17	On Time	On Time
8	On Time	On Time	18	On Time	On Time
9	On Time	On Time	19	Delayed	On Time
10	On Time	On Time	20	Delayed	On Time

Imbalanced Data

	On Time Prediction	Delayed Prediction
On Time Target Label	18	0
Delayed Target Label	2	0

$$recall = \frac{TP}{TP+FN} = \frac{18}{18+0} = 1.0$$

	Delayed Prediction	On Time Prediction
Delayed Target Label	0	2
On Time Target Label	0	18

$$recall = \frac{TP}{TP+FN} = \frac{0}{0+2} = 0.0$$

Average Class Accuracy

Average recall over the elements in the set of possible target feature values $C = \{\text{Delayed}, \text{On Time}\}$

- arithmetic mean:

$$\frac{1}{|C|}\sum_{c \in C} recall_c = \frac{1}{2}(1+0) = 0.5$$

- harmonic mean:

$$\frac{1}{\frac{1}{|C|}\sum_{c \in C}\frac{1}{recall_c}} = \frac{1}{\frac{1}{2}\left(\frac{1}{1}+\frac{1}{0}\right)} = 0.0$$

$\frac{1}{0} = \infty$ in the limit

ID	Target Label	Prediction	ID	Target Label	Prediction
1	On Time	On Time	11	On Time	On Time
2	On Time	On Time	12	On Time	On Time
3	On Time	On Time	13	On Time	On Time
4	On Time	On Time	14	On Time	On Time
5	On Time	On Time	15	On Time	On Time
6	On Time	On Time	16	On Time	On Time
7	On Time	On Time	17	On Time	On Time
8	On Time	On Time	18	On Time	On Time
9	On Time	On Time	19	Delayed	On Time
10	On Time	On Time	20	Delayed	On Time

Practical Aspects

- You have used supervised learning to train a predictive model
  - And you have computed a confusion matrix based on the predictions on a given set of data

- Question: *What is worse – Predicting a flight to be delayed and having it arrive on time, or predicting it to be on time and find it to be delayed?*

- Does the self-driving car need to stop?
- Should the patient be tested for a severe disease?

→ **FP**s and **FN**s can have (very) different cost!

Profit (Utility) Matrix

Example Flight Classification

- Correctly inform customers about a delay:
  - Customers can plan to arrive later
  - ***A little*** 'profit' from less unhappy customers
- Incorrectly inform customers about a delay:
  - Customers arrive too late
  - ***Huge*** loss of 'profit' by unnecessarily delayed flight

- Incorrectly predicting 'Delayed' (FN) costs more than incorrectly predicting 'On Time' (FP)

Profit Matrix		Prediction: On Time	Prediction: Delay
Target Label	On Time	**0**	**-80**
Target Label	Delay	**-10**	**20**

Profit (Utility) Matrix

M_1		Prediction: On Time	Prediction: Delay
Target Label	On Time	**6**	**3**
	Delay	**2**	**9**

M_2		Prediction: On Time	Prediction: Delay
Target Label	On Time	**5**	**0**
	Delay	**9**	**6**

Profit Matrix		Prediction: On Time	Prediction: Delay
Target Label	On Time	**0**	**-80**
	Delay	**-10**	**20**

Profit (Utility) Matrix

M_1 (Confusion matrix)

Target Label	Prediction: On Time	Prediction: Delay
On Time	6	3
Delay	2	9

M_2 (Confusion matrix)

Target Label	Prediction: On Time	Prediction: Delay
On Time	5	0
Delay	9	6

Profit Matrix

Target Label	Prediction: On Time	Prediction: Delay
On Time	0	-80
Delay	-10	20

M_1 (Profit)

Target Label	Prediction: On Time	Prediction: Delay
On Time	0	-240
Delay	-20	180
Profit	-80	

M_2 (Profit)

Target Label	Prediction: On Time	Prediction: Delay
On Time	0	0
Delay	-90	120
Profit	30	

Profit (Utility) Matrix

M_1

		Prediction: On Time	Prediction: Delay
Target Label	On Time	6	3
	Delay	2	9

M_2

		Prediction: On Time	Prediction: Delay
Target Label	On Time	5	0
	Delay	9	6

Profit Matrix

		Prediction: On Time	Prediction: Delay
Target Label	On Time	0	-80
	Delay	-10	20

M_1

		Prediction: On Time	Prediction: Delay
Target Label	On Time	0	-240
	Delay	-20	180
	Profit	-80	

M_2

		Prediction: On Time	Prediction: Delay
Target Label	On Time	0	0
	Delay	-90	120
	Profit	30	

$$\begin{aligned} \mathit{profit} &= \mathbf{FP} \cdot \mathbf{FP}_{\text{profit}} + \mathbf{TP} \cdot \mathbf{TP}_{\text{profit}} \\ &+ \mathbf{FN} \cdot \mathbf{FN}_{\text{profit}} + \mathbf{TN} \cdot \mathbf{TN}_{\text{profit}} \end{aligned}$$

Key Concepts Covered Today

- Confusion matrix
- Performance measures for binary classification
- Training, testing and validation sets
- *k*-fold cross validation
- Leave-one-out cross validation (jackknife)
- Bootstrap sampling validation
- Imbalanced data, average class accuracy
- Profit (utility) matrix

Homework for Next Monday

Think and discuss about the following questions:

- **How to assess predictive models for multi-class classification?**
  (> 2 target classes, *e.g.*, on time, mildly delayed, severely delayed)

- **How to assess predictive models for regression tasks?**
  (predictions = numbers, *e.g.*, minutes of delay)