



Supervised machine learning

CASA0006: Data Science for Spatial Systems

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Objectives

- Learn the basics of supervised learning
- Develop an intuition of supervised learning
- Understand the analysis workflow of supervised learning
- Be able to choose the metrics for regression and classification

Outline

1. Supervised learning
2. The analysis workflow of SML
3. Cross validation
4. Metrics
5. Randomness in model training



Supervised learning

Supervised learning

- We gave the algorithm a data set where a "right answer" was provided, build a model to predict the output (y) given the input variables (x)

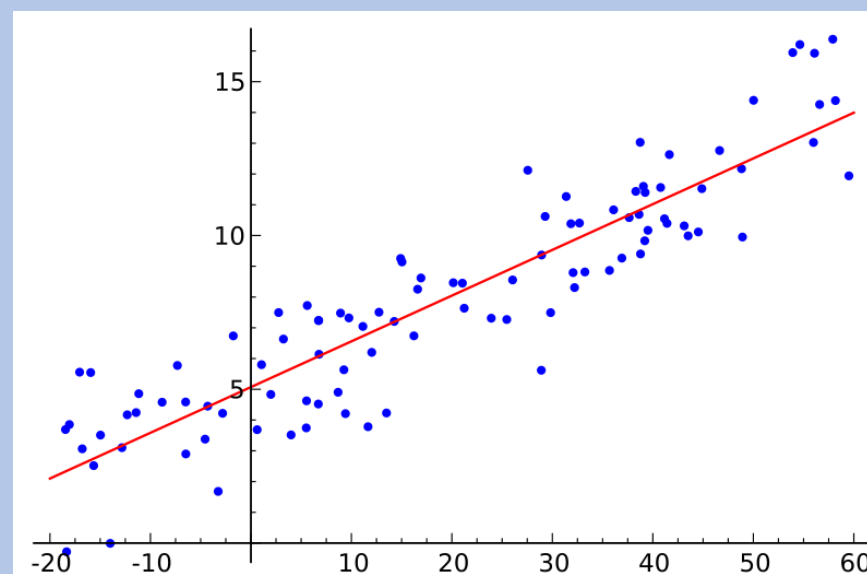
What is the type of Y ?

Continuous (integer/float)

Discrete (categorical)

Regression

- Predicting house price
- Methods include linear regression, tree-based models, neural nets, etc.



Many methods can be used for both tasks

Classification

- Email \rightarrow spam or non-spam
- Methods include logistic regression, tree-based models, neural nets, etc.
- Intuition: *find a boundary between classes*



Challenge of supervised learning: overfitting

- ML is aimed at making accurate predictions for new unseen data.
- The model overfits the data, when the model is fitting the training data too well (accuracy of 100%), but does not generalise to new unseen data
- Overfitting is unavoidable: all machine learning methods tend to overfit, especially the complicated models.
- How to recognise overfitting? Use train-test split
- How to mitigate overfitting? Tune the hyperparameters carefully
- Workflow is crucial!

Example of spam recognition (Is this a spam?)

My name is Aisha Al-Qaddafi the only biological Daughter of late Libyan President (Late Colonel Muammar Al-Qaddafi). i am a Widow with three Children, I'm currently living in Muscat Oman under political asylum protection by the Oman Government. Considering my present condition, i have chosen to contact you after my prayers and I believe you will not betray my trust, but rather take me as your own sister or daughter.

I have investment funds worth \$27,500,000.00 USD

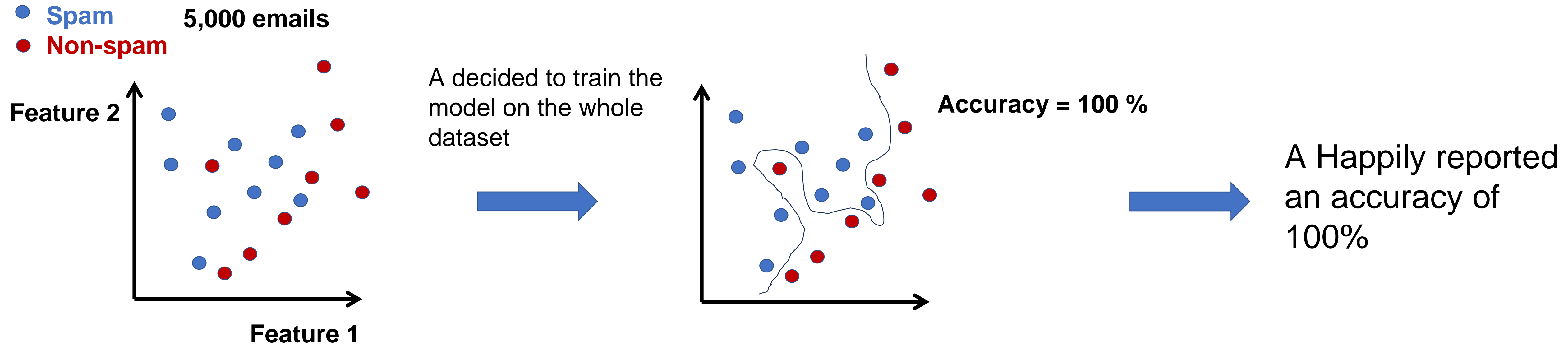
“Twenty Seven Million Five Hundred Thousand United State Dollars” which i want to entrust on you for investment project in your country because of my current refugee status here in Oman. If you are willing to handle this project on my behalf, kindly reply urgently to enable me provide you more information about the investment funds.

..... My husband late Dr. Joe Bronson who died in the year 2020, was a minor at Kruger gold company and trades on gold. **When he was alive he deposited the sum of \$4,800,000 million in a bank in Manama the capital city of Bahrain in Southern Asia.** The money I am willing to give you was income from long years of hard work of my late husband..... I will be going in for an operation surgery soon and I need your urgent answer to know if you will be able to execute this project, and I will give you more information on how the fund will be transferred to your bank account

Is this email a spam?

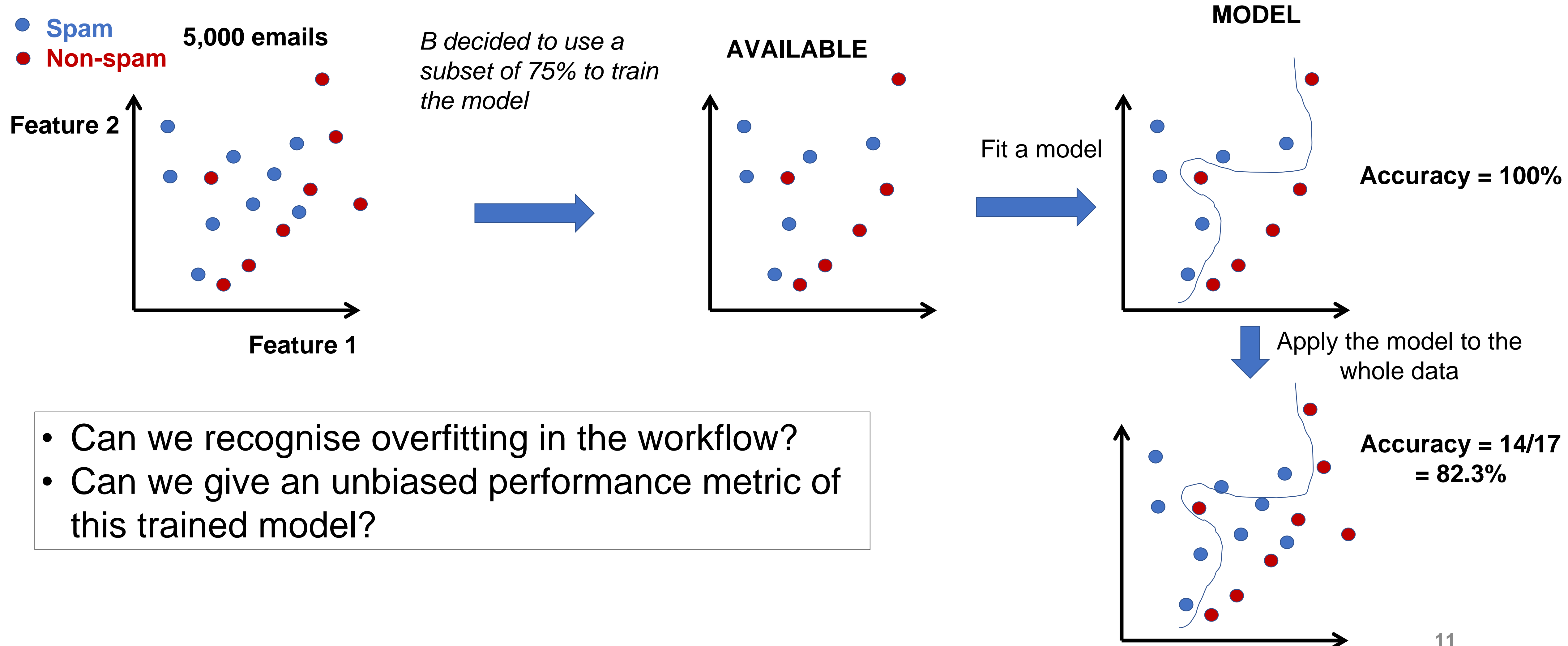
- A data scientist team is asked to develop a spam recognition application using a ML method and 5,000 emails (labelled as spam/non-spam, with two features). The hope is that this application will be used daily in the company.
- Three team members (A, B, C) proposed three different workflow
- You are the team leader, so please think about the following questions
 - Can we recognise overfitting in the workflow?
 - Can we give an unbiased performance metric of this trained model (to the unseen data)?

Workflow of A

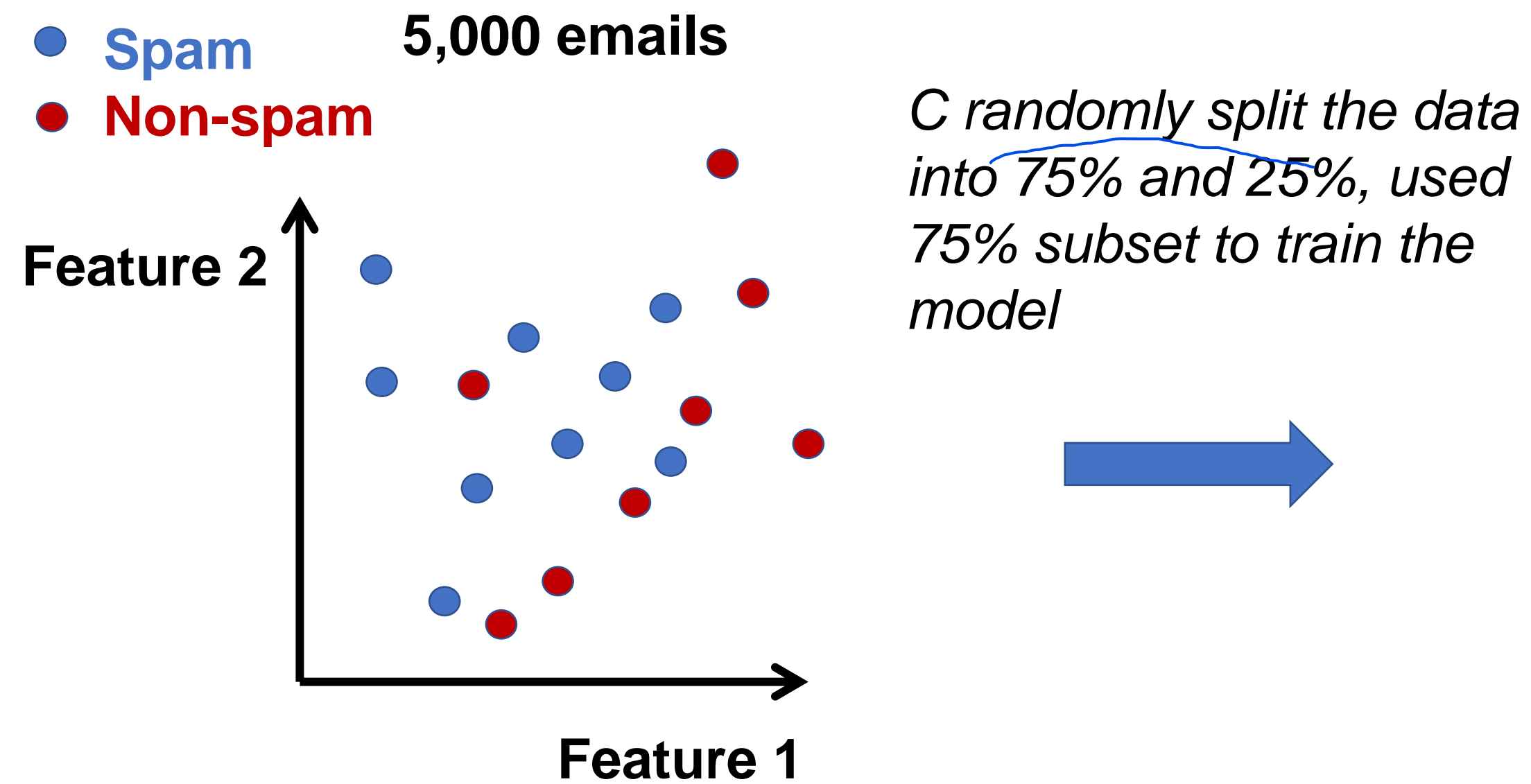


- Can we recognise overfitting in the workflow?
- Can we give an unbiased performance metric of this trained model?

Workflow of B



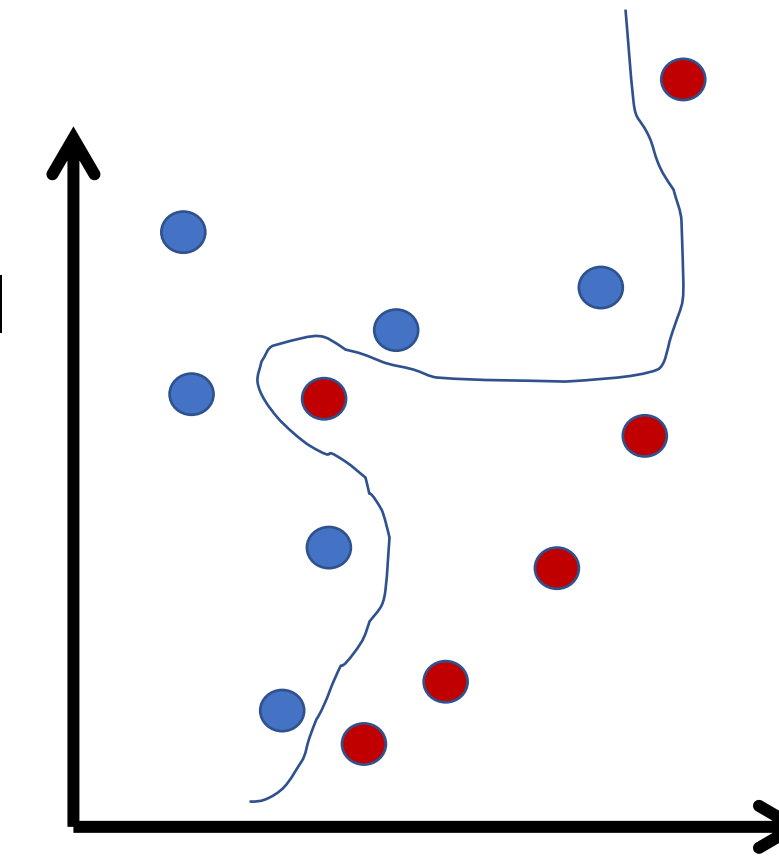
Workflow of C



Fit a model



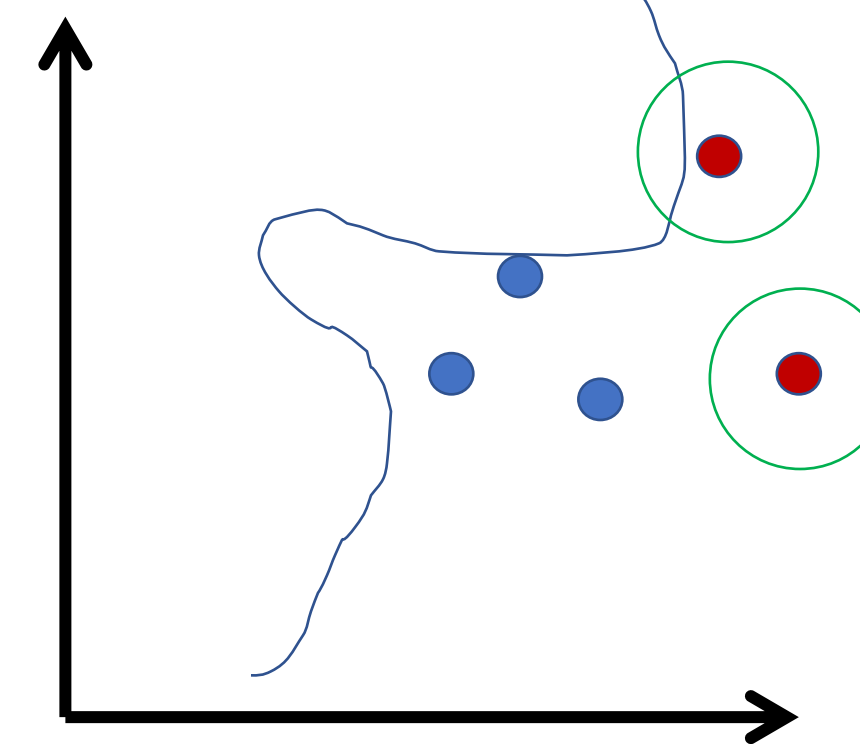
MODEL



Accuracy = 100%



Apply the model to the rest 25%



Accuracy = 40%

- Can we recognise overfitting in the workflow?
- Can we give an unbiased performance metric of this trained model?

Summary – which workflow is the best?

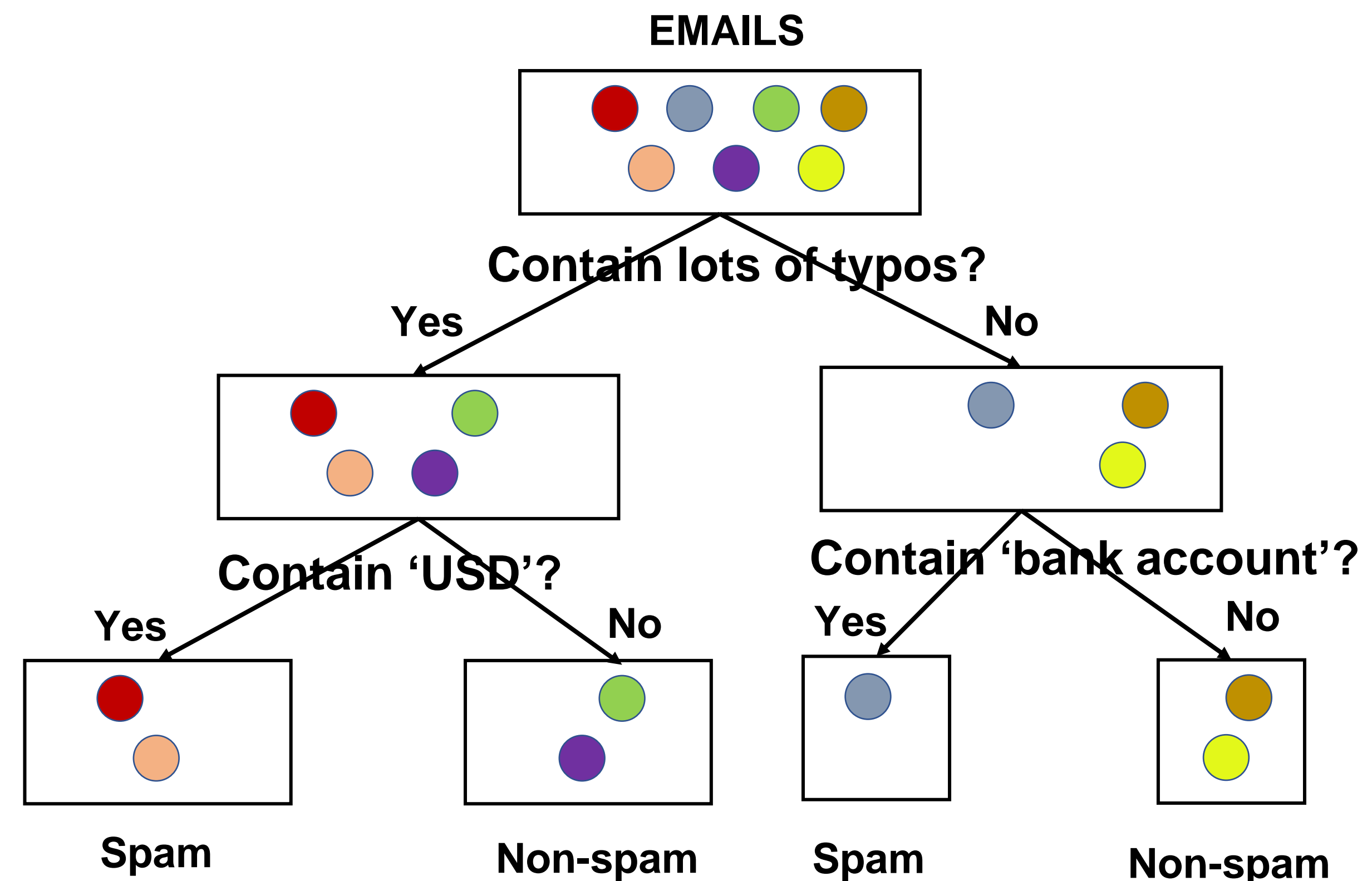


Analysis workflow of supervised learning

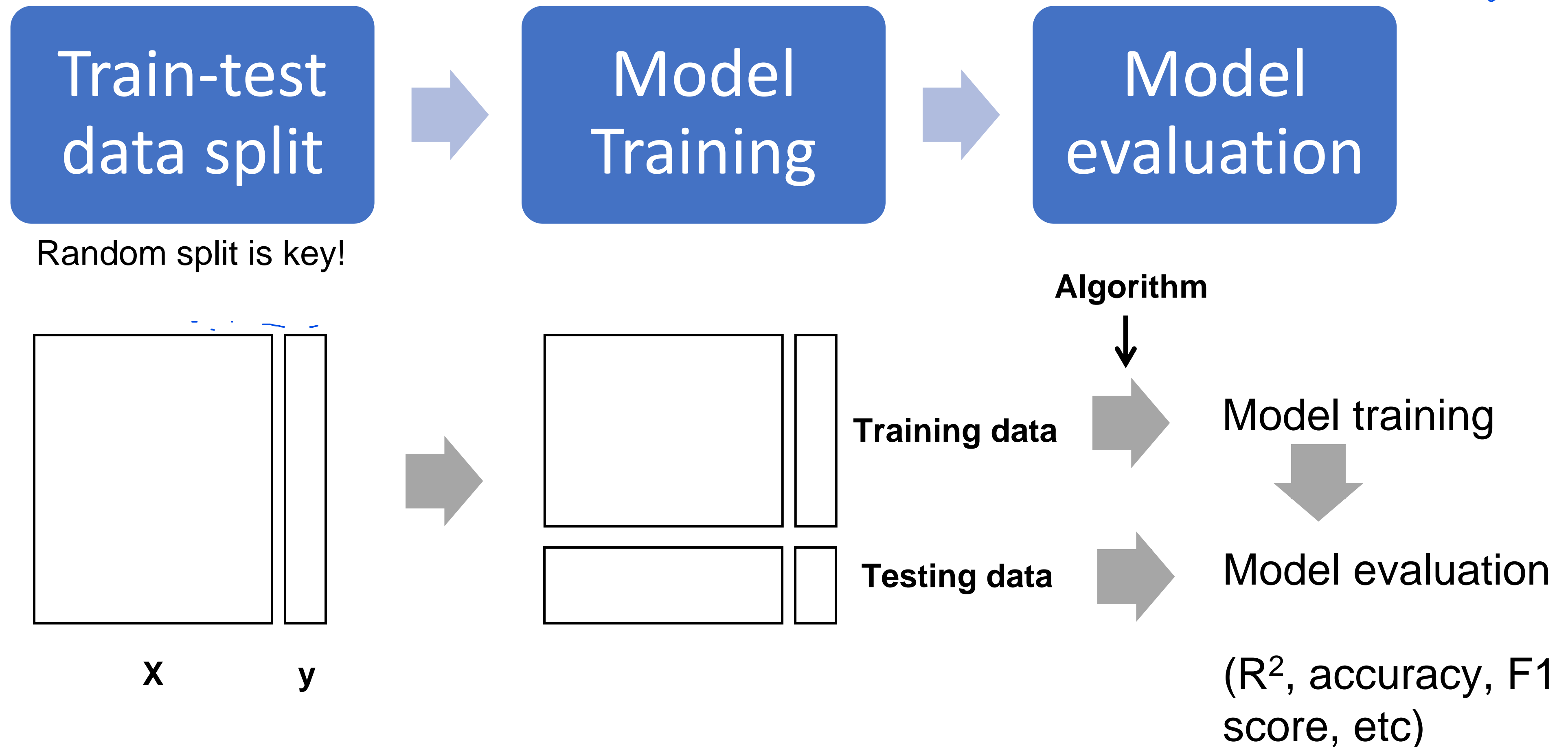
Terminology (decision tree for spam detection)

- Decision tree = a flow diagram or a 'tree' of decisions about the x variables of a dataset

- Algorithm: decision tree
- Model: a trained decision tree (with many splits)
- Model training: to find the optimal 'criteria' to split data points
- Prediction: given a new sample, is it spam?



Analysis workflow (v1; train-test split)



Train-test data split

- Usually, 75% for training and 25% for testing
- A random split: the data is randomly shuffled before split. This is to avoid selection bias and guarantee that the training and testing data are independently and identically distributed (i.i.d)
- But, the random split introduces randomness in model training and evaluation – will discuss randomness later.
- This technique is called hold-out validation in statistics.



Train-test data split

- The testing data should be not used in any stages of model training.
- If the testing data is used in model training, this caused data leakage.
- Sometimes, data leakage is subtle and not easy to identify.



Is this workflow perfect?

- Problem solved
 - Providing an unbiased evaluation of model performance
 - Diagnosing overfitting (overfitting occurs, if training accuracy >> testing accuracy)
- New challenges
 - How can we compare performance of multiple algorithms for one task – random forest, SVM, and neural networks?
 - *We can't compare these algorithms without tuning their hyperparameters. This requires more complicated workflow.*

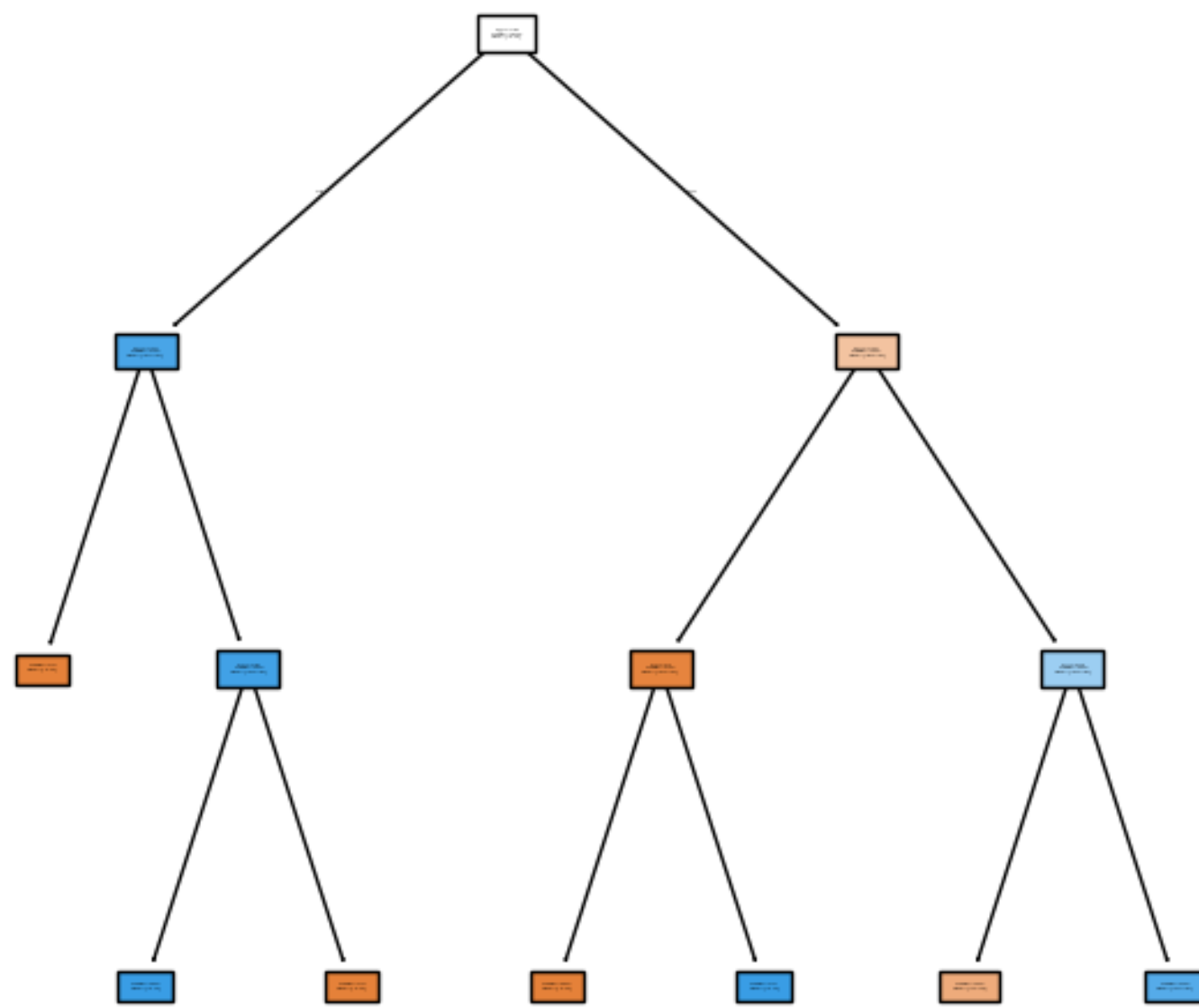
Hyperparameter tuning

- **Hyperparameters:** the algorithm settings predefined by the user, e.g. max tree height (range: 3,4,5)
- **Hyperparameter tuning:** to find the optimal hyperparameters for the algorithm
- A common approach is to predefine the range of each hyperparameter, and empirically find the optimal combination of these values.
- For simple algorithms (linear/logistic regression), hyperparameter tuning is not needed (as there are no hyperparameters)

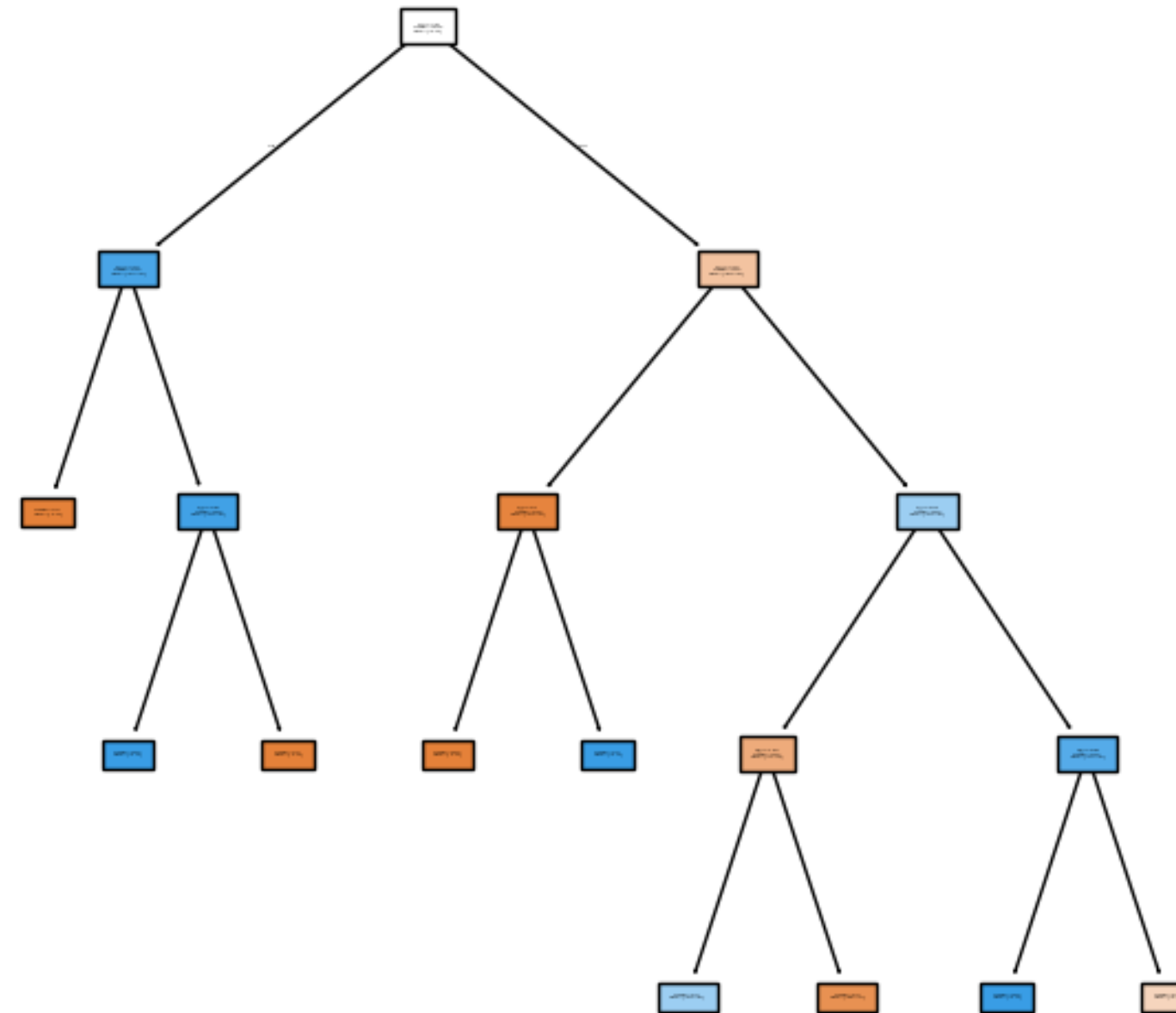
Hyperparameter tuning

With different hyperparameter settings, an algorithm will lead to multiple models

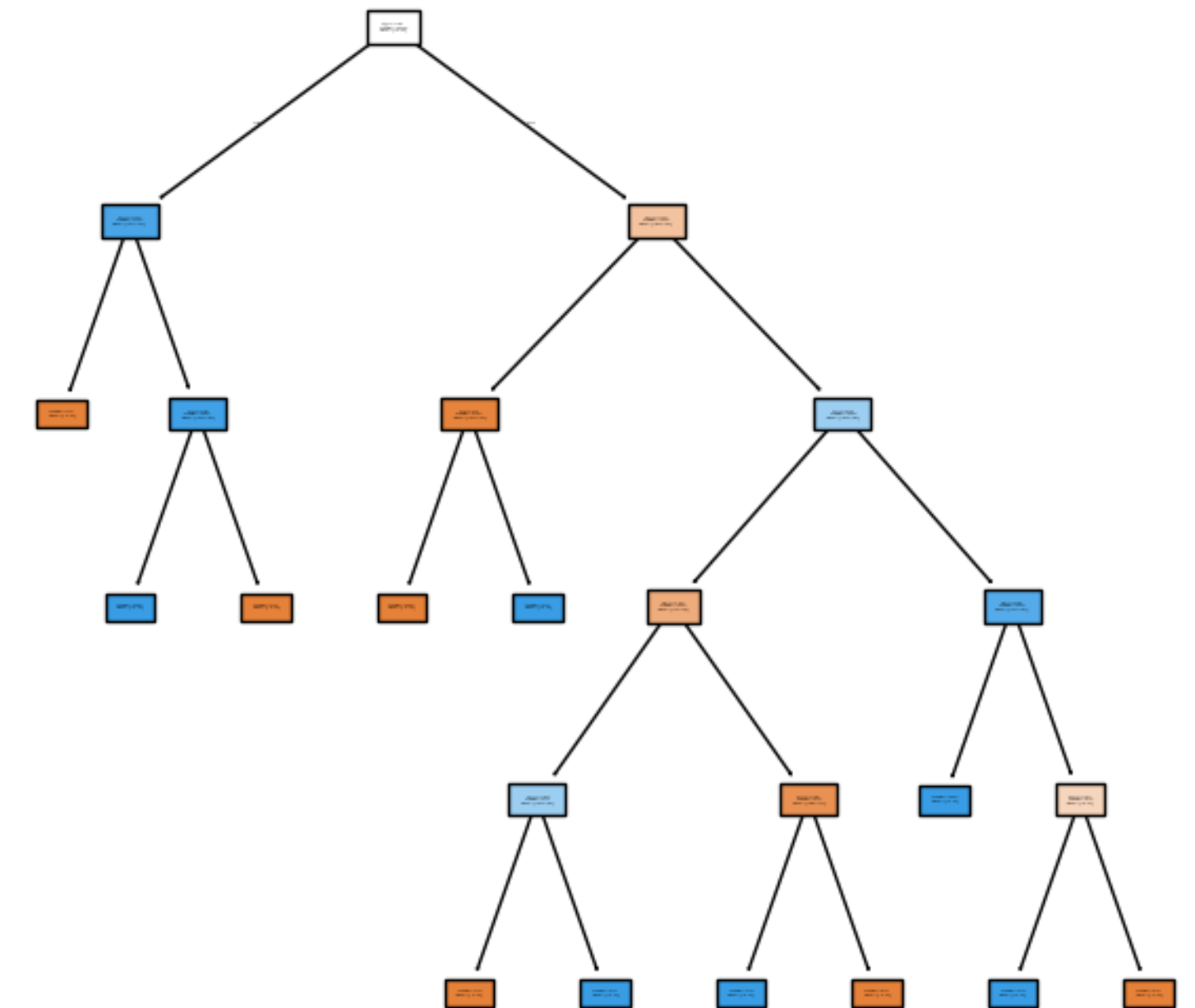
Decision Tree (Max Depth = 3)



Decision Tree (Max Depth = 4)



Decision Tree (Max Depth = 5)



Comparing algorithms

- How can we compare performance of multiple algorithms for one task
– random forest, SVM, and neural networks? (*We can't simply compare all possible models of these algorithms*)
- Two-stage process

Stage 1: hyperparameter tuning

Stage 2: compare tuned models

Confirmed 2024 presidential candidates

As of March 6, 2024

Confirmed Suspended campaign

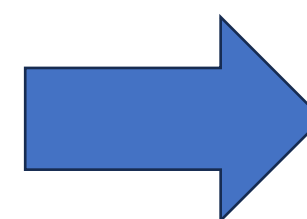
Republican



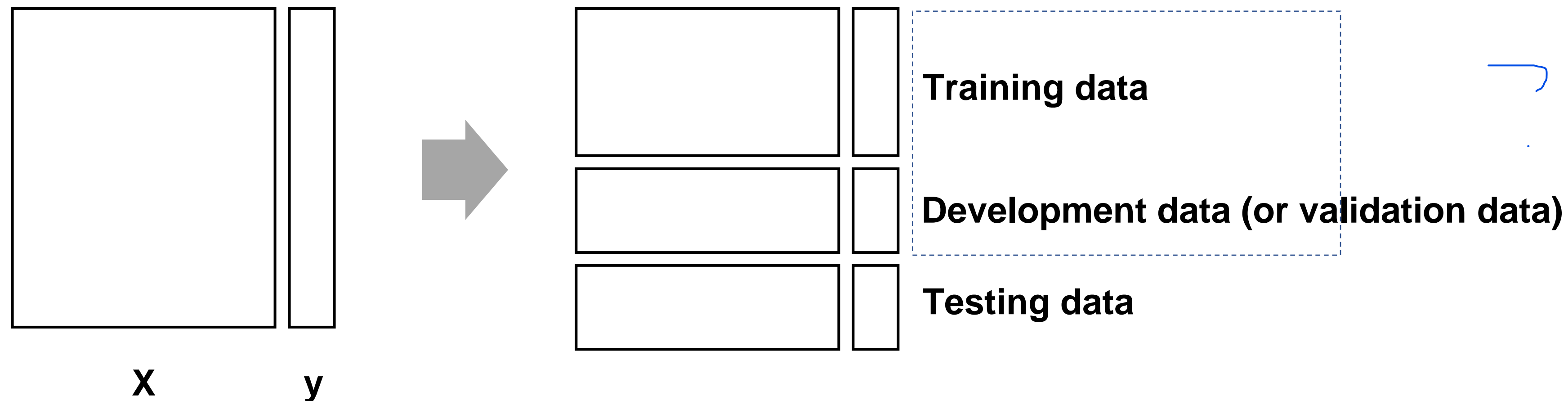
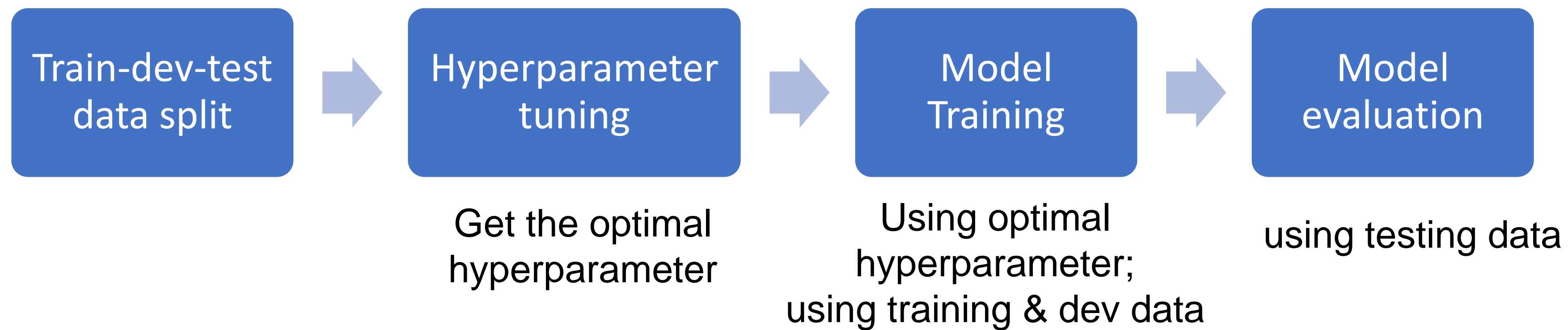
Democrat



Independent



Analysis workflow (v2, hold-out validation)



Hyperparameter tuning

Example: to find the optimal tree heights (range: 5, 10, 15), we split the data into training/dev/testing sets and trained three model (using only training data) with height=5,10,15.

Model	1	2	3
Tree heights	5	10	15
Accuracy on training data	90%	92%	95%
Accuracy on dev data	83%	87%	70%
Accuracy on testing data	80%	75%	66%



Tree height = 10 is the optimal. So, the model #2 is adopted and testing accuracy of 75% from model #2 is reported as performance of decision tree.

The problem is – we only use training data to train the model, and the hyperparameter selection is influenced by the split of training/dev set, so it is not very accurate.

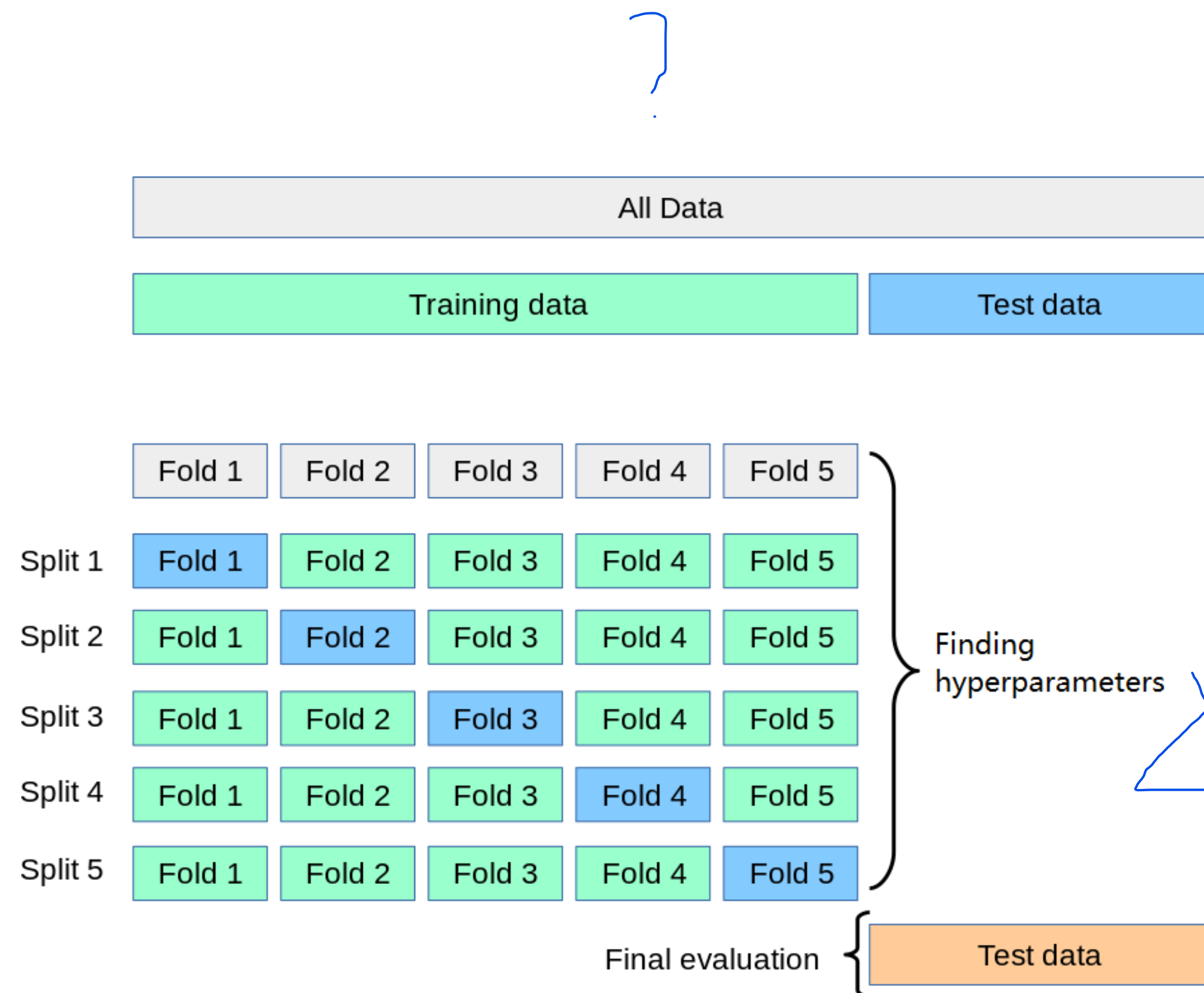
However, hold-out validation is computationally efficient for large set, when compared to cross validation.

Cross validation

Problem of workflow v2

Problem with Train-dev-test split: only limited data is used for model training, which is a problem when data are sparse; subject to the split between train and dev data

Solution - Cross validation: more sufficient use of data for model training (*default approach*)



Example: to find the optimal tree heights (TH, range: 5, 10, 15) using 5-fold CV.

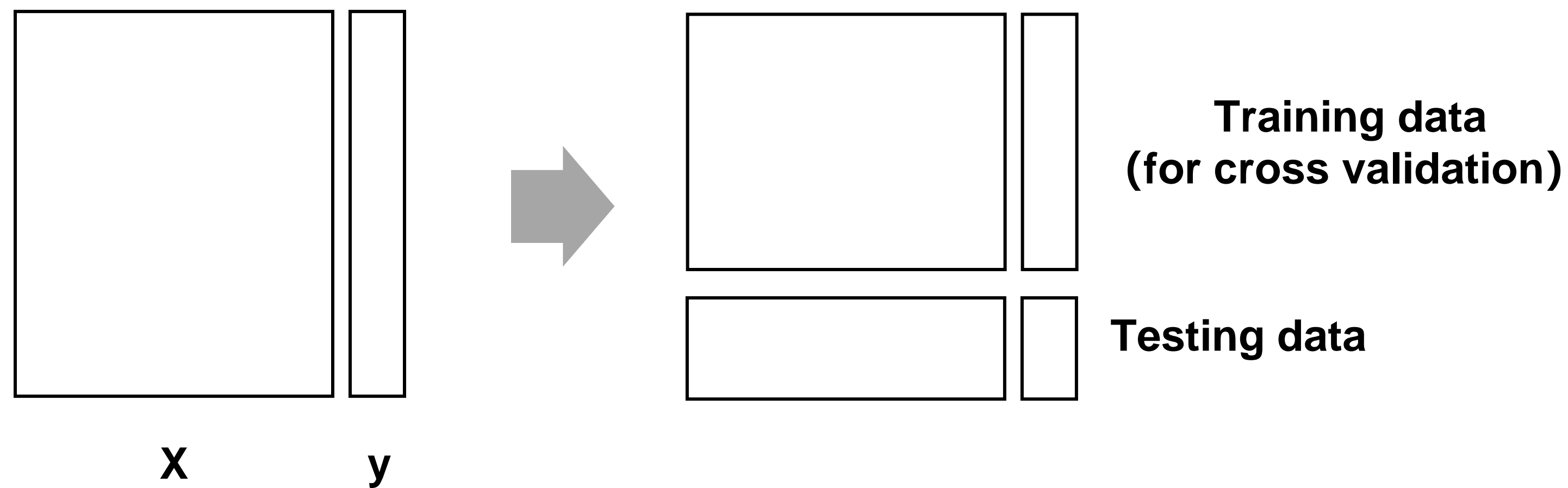
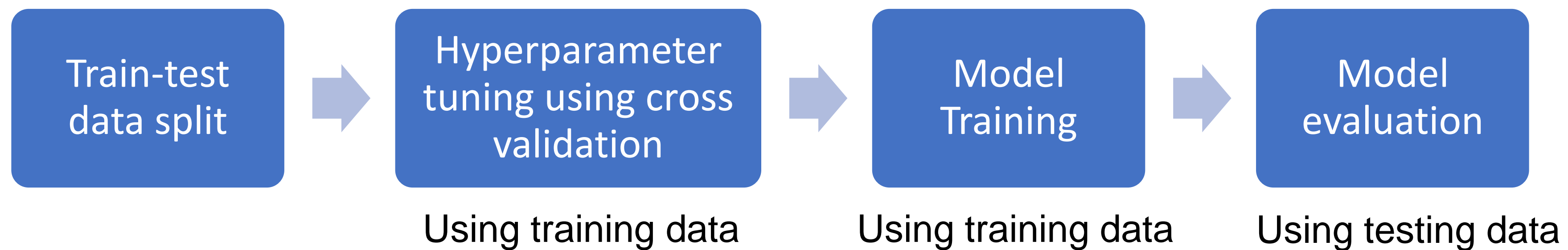
- To get performance of TH=5: 5 models are trained.

Model	1	2	3	4	5
Training	Fold 2/3/4/5	Fold 1/3/4/5	Fold 1/2/4/5	Fold 1/2/3/5	Fold 1/2/3/4
Evaluation	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5

Performance of TH=5: average of these five models

Pick up TH with best performance, then train a model using this TH on the whole training data

Analysis workflow (v3)

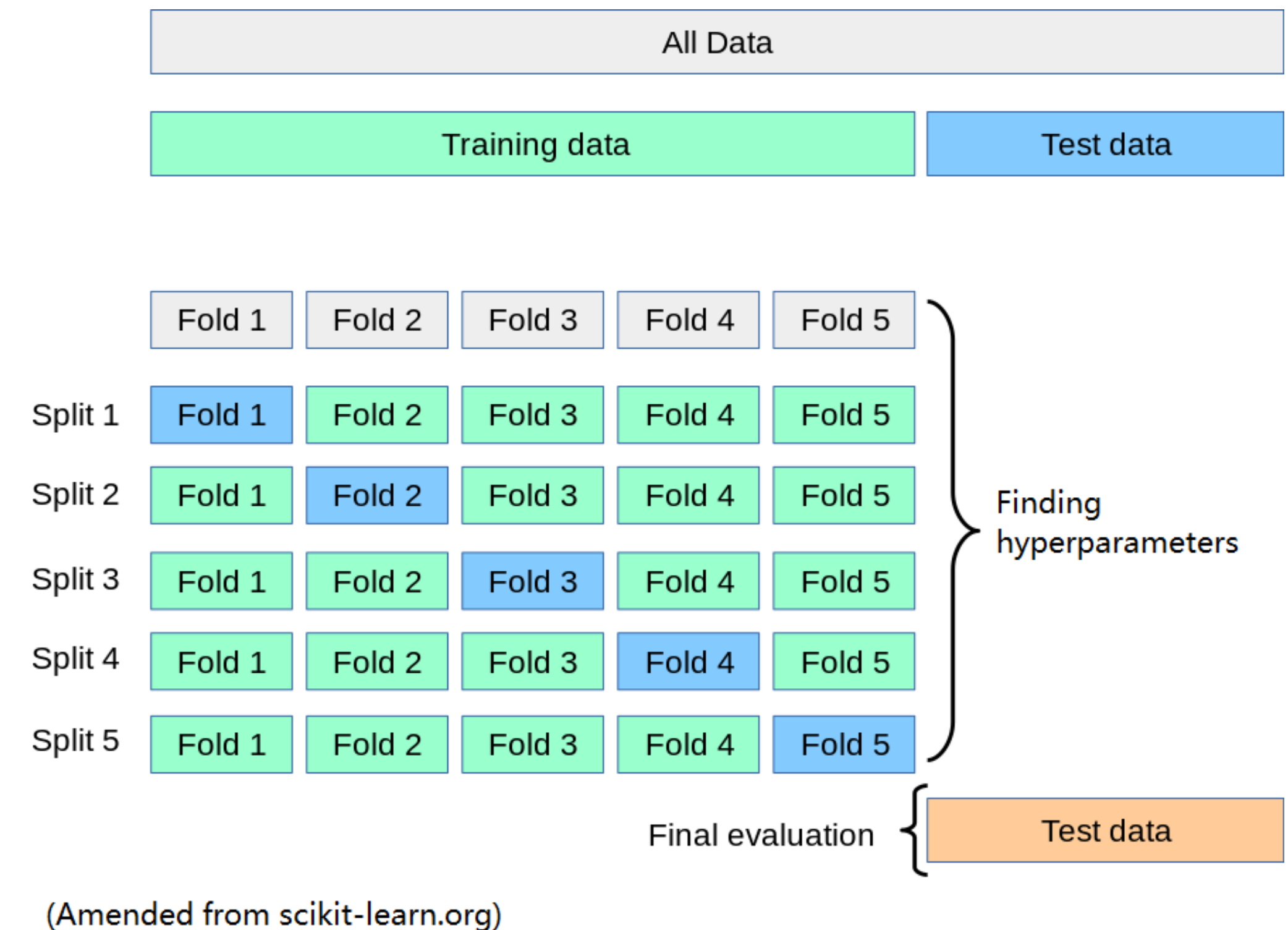


Cross validation

Cross validation is default workflow for most machine learning tasks.

- Pros: sufficient use of training data; less subject to random split (using average performance); accurate results
- Cons: time-consuming for big datasets

Common: 5-fold or 10-fold CV



Metrics

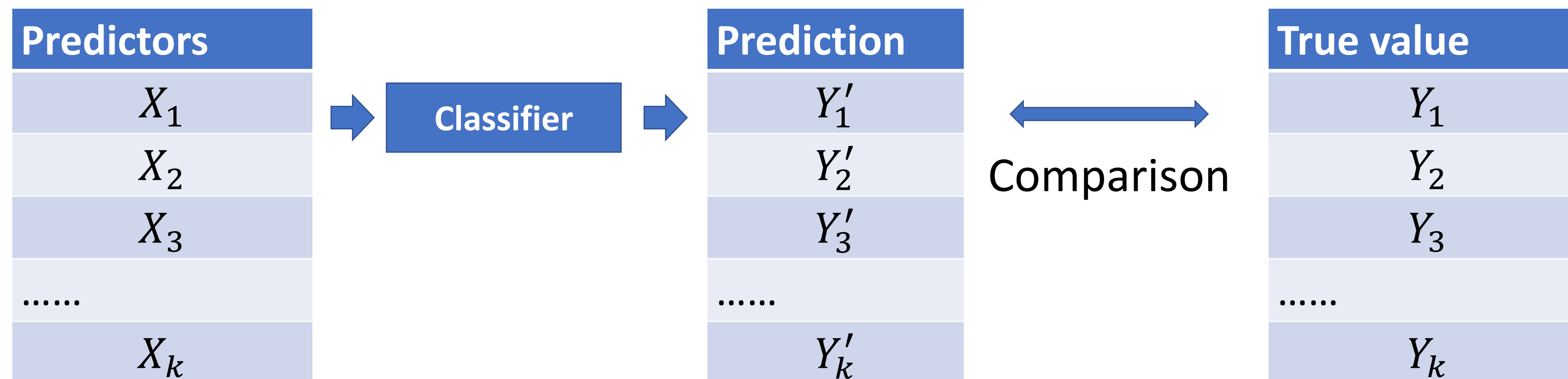
Metrics for regression

	Definition	Range	Direction
R Squared	$R^2 = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2}$	$(-\text{Inf}, 1]$	The higher R^2 , the higher accuracy
RMSE	$\frac{\sqrt{\sum (y_i - \hat{y}_i)^2}}{n}$	$[0, \text{Inf})$	The smaller RMSE, the higher accuracy

1. According to the definition, R^2 is not the square of a value.
2. Two possibilities of a negative R^2 : the prediction algorithm is not suitable or not well tuned; the input variables are not related to y variable.
3. A special case of R^2 is that linear regression has a R^2 in the range of $[0,1]$.

Metrics for classification

Example: given travel survey data, predict travel modes as one of four modes



How accurate are the predictions?

- For a single record: the prediction is TRUE or FALSE
- For many records: confusion matrix

<https://towardsdatascience.com/accuracy-precision-recall-or-f1-331fb37c5cb9>

Performance metrics

Confusion Matrix: comparing predicted against observed classes

Two-class (e.g. Driving vs. Not-driving)

		Actual Values	
		Positive (1)	Negative (0)
Predicted Values	Positive (1)	TP	FP
	Negative (0)	FN	TN

Performance metrics

Comparing predicted against observed classes

		Actual Values	
		Positive (1)	Negative (0)
Predicted Values	Positive (1)	TP	FP
	Negative (0)	FN	TN

Confusion Matrix

Classification Accuracy

Proportion correctly classified

$$\frac{\text{Correct}}{\text{Correct} + \text{Incorrect}} = \frac{\#tp + \#tn}{\#tp + \#tn + \#fp + \#fn}$$

Range of [0,1]

Precision

How many positive predictions are correctly classified?

$$\frac{\#tp}{\#tp + \#fp}$$

Range of [0,1]

Recall

How many positive classes are correctly classified?

$$\frac{\#tp}{\#tp + \#fn}$$

Range of [0,1]

F1

A balance between precision and recall, takes beta attribute which weights precision or recall (usually beta = 1)

$$(1 + \beta^2) \frac{\text{precision} * \text{recall}}{\beta^2 \text{precision} + \text{recall}}$$

Range of [0,1]

Performance metrics

Q1: What is the conflict between precision and recall?

In many cases, improving one of them would lead to degrading of the other.

*S1: predict most as 'negative' –
maximise prec*

Actual	Predicted	
	Positive	Negative
	Positive	Negative
Positive	1	99
Negative	0	100

Precision = 1
Recall = 0.01

*S2: predict most as 'positive' –
maximise recall*

Actual	Predicted	
	Positive	Negative
	Positive	Negative
Positive	100	0
Negative	99	1

Precision = 0.5
Recall = 1

Performance metrics

Q2: why is F1 score a tradeoff between prec and recall?

F1 score combines these two metrics into a single metric; It has a value between $\min(\text{prec}, \text{recall})$ and $\max(\text{prec}, \text{recall})$.

*S1: predict most as 'negative' –
maximise prec*

Actual	Predicted	
	Positive	Negative
Positive	1	99
Negative	0	100

Precision = 1
Recall = 0.01
F1 = 0.02

*S2: predict most as 'positive' –
maximise recall*

Actual	Predicted	
	Positive	Negative
Positive	100	0
Negative	99	1

Precision = 0.5
Recall = 1
F1 = 0.67

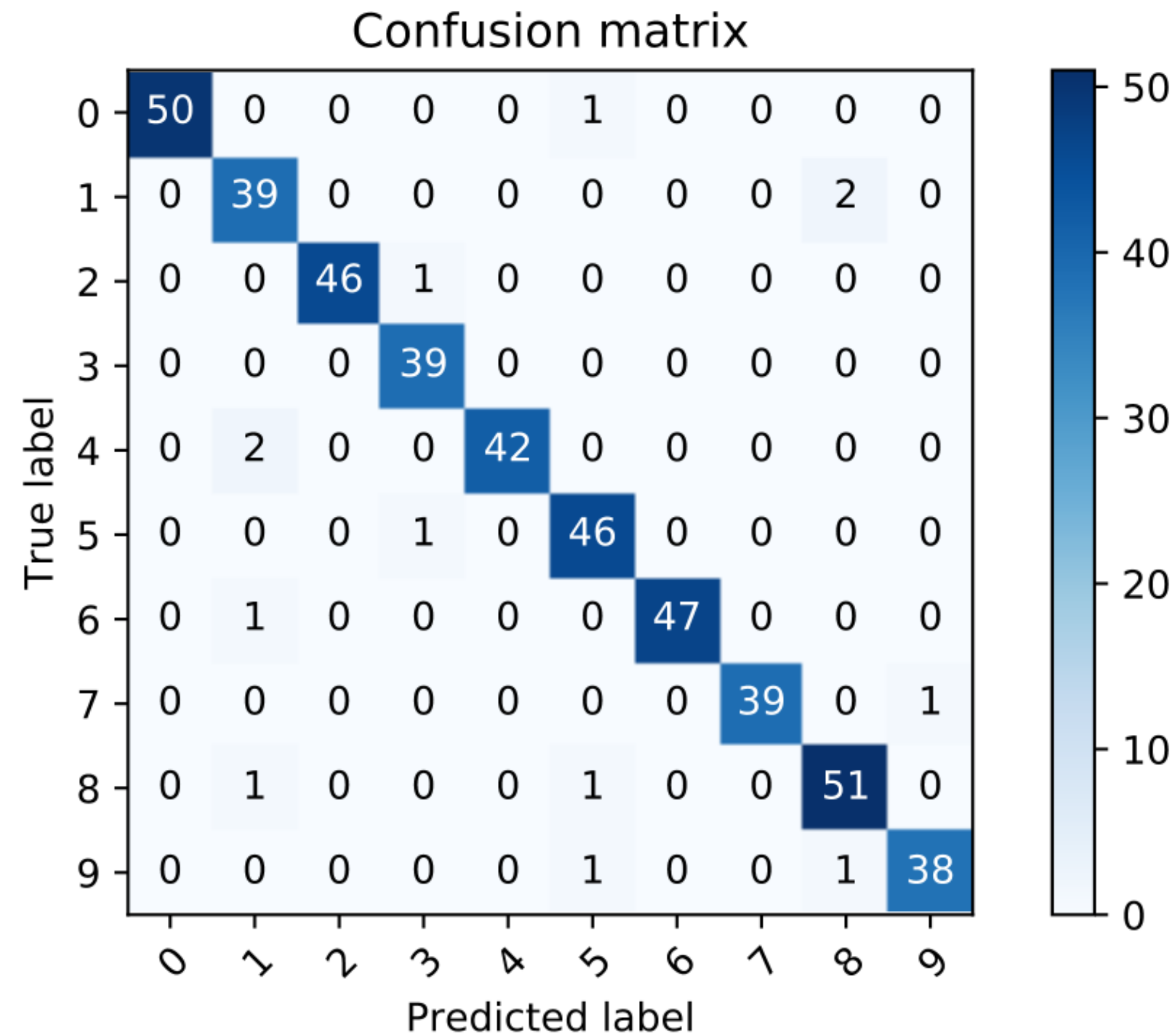
Performance metrics

Q3: What is the problem of accuracy (or why are other metrics needed?)

Accuracy paradox: Accuracy might be not useful when the class distribution is highly imbalanced. For example, when predicting mode with actual 99% driving and 1% cycling, a 'trivial' predictor that simply predicts 'driving' will have very high accuracy, but this predictor is not useful.

Suggestion: when presenting classification results, you could present both accuracy and F1 score.

Performance metrics



- Numbers on the diagonal line are the TP for each class
- n_{ij} is the number of instances with actual class i that are classified as class j .
- When reading a confusion matrix, it is important to know meaning of rows and columns (rows as true or predicted label?)

Performance metrics

Multiple-class problem (K classes)
→ **K confusion matrices**

Classification Accuracy $\frac{\sum_i n_{ii}}{\sum_i \sum_j n_{ij}}$

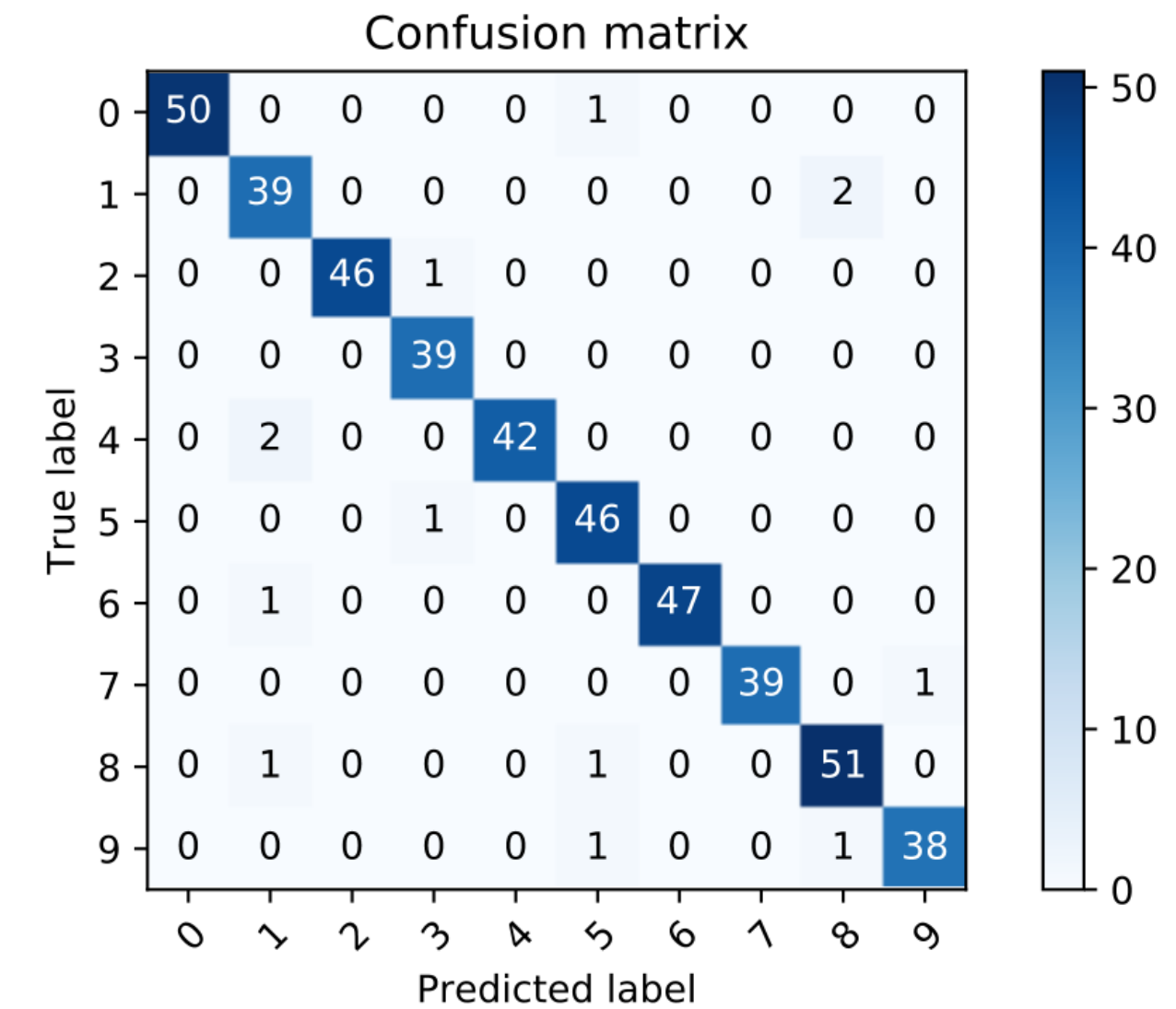
Precision* $\text{average}(Prec_1, Prec_2, \dots, Prec_K)$

Recall* $\text{average}(Rec_1, Rec_2, \dots, Rec_K)$

F1* $\text{average}(F1_1, F1_2, \dots, F1_K)$

This is called macro average of precision/recall/F1.

Other ways of calculating these scores include 'micro' and 'weighted'. See [here](#).



An aerial photograph of a tropical island. The island has a dense green forest in the center, surrounded by a wide, light grey beach. The water around the island is a deep blue, with some lighter blue areas near the shore. The text "Randomness in machine learning" is overlaid on the left side of the image in a large, white, sans-serif font.

Randomness in machine learning

Randomness

There are multiple sources of randomness in model training and testing.

- Random data split
- Random seeds used by models (almost all modes using random seeds)
- Model optimisation (may be subject to local optimum)

Ways to mitigate randomness

- Get sufficient data (>50 data samples, preferably > 100)
- Use robust methods
- Multiple runs using different random seeds and report average and standard deviation of performance

Summary

- Basics of supervised learning: regression, classification, model generalisation
- The analysis workflow of supervised learning: train-test split, hold-out validation, cross validation (default)
- Metrics for regression: R^2 , RMSE
- Metrics for classification: accuracy, F1 score
- Randomness in machine learning

Workshop