DataSci 420

Lesson 2

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today's agenda

- historical data vs future data
- why and how we split data into trainig, testing, and validation
- parameters and hyper-parameters
- overfitting and how to avoid it
- what is cross-validation and how to do it
- what is class imbalance and how it affects model evaluation
- common metrics to consider when we have class imbalance

important!

the remaining lectures starting now will only be concerned with **supervised learning**

historical data vs future data

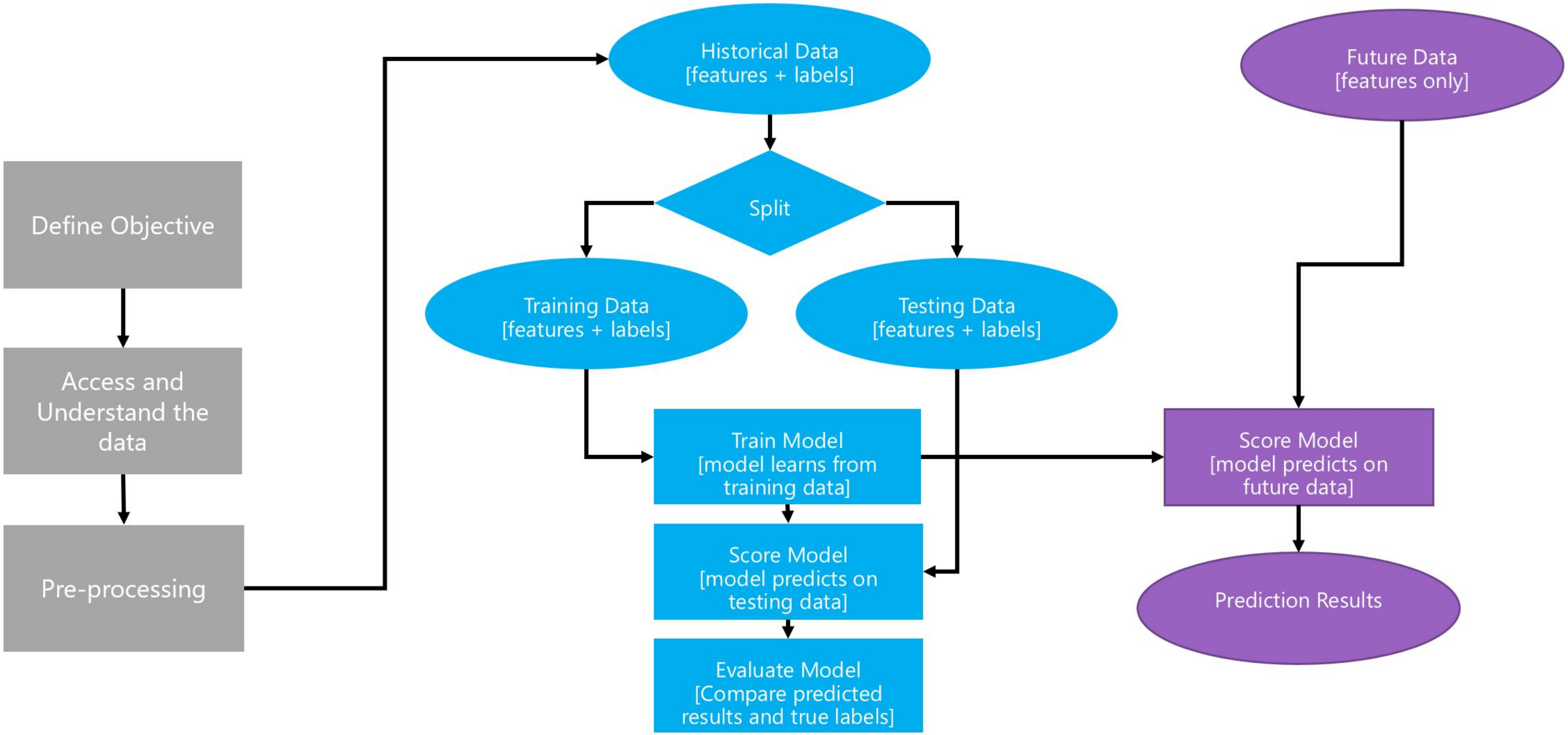
- data we use for modeling is a snapshot, e.g. the last two years
  - we refer to this as **historical data**, and it is labeled
- but we keep collecting data after we train the model
  - we refer to that as **future data**, and it may or may not be labled
- use historical data to create a model
- deploy the model to get predictions on future data, called **scoring**
- but if future data is unlabeled, how do we know if predictions are any good?

a good model should generalize well

- I repeat: if future data is unlabeled, how do we know if predictions are any good?
- the premise of the question is this: **a model's performance should be measured on data that it hasn't seen during training**
- we say a good model should generalize to out-of-sample data (data not used for training)
- at training time we try to find parameters that minimize error **on the training data**, but there's no guarantee that this will also minimize error on out-of-sample data

the answer: training and test data

- set aside a small **random** portion of historical data and **pretend it's future data**, we call this **test data**
- the remaining portion is called **training data**
- unlike future data, test data is **labeled**, so we can compare predictions with observed, also called **ground truth**
- so we use the training data to train a model
- then we **evaluate** the trained model's performance on the test data (data that the model didn't see at training time)


Define Objective
Access and Understand the data
Pre-processing
Historical Data [features + labels]
Split
Training Data [features + labels]
Testing Data [features + labels]
Train Model [model learns from training data]
Score Model [model predicts on testing data]
Evaluate Model [Compare predicted results and true labels]
Future Data [features only]
Score Model [model predicts on future data]
Prediction Results

break time

lab time

- imagine you need to learn a subject and there's no textbook for it
- all you have is a practice test with the answers included
    - a good analogy is driver's ed test
- you want to study for the upcoming exam and get a good grade
- if you've really studied, you should be able to correctly answer questions you haven't seen before
- how would you could **estimate** your grade in the upcoming exam, so you know if you need to study more or not?

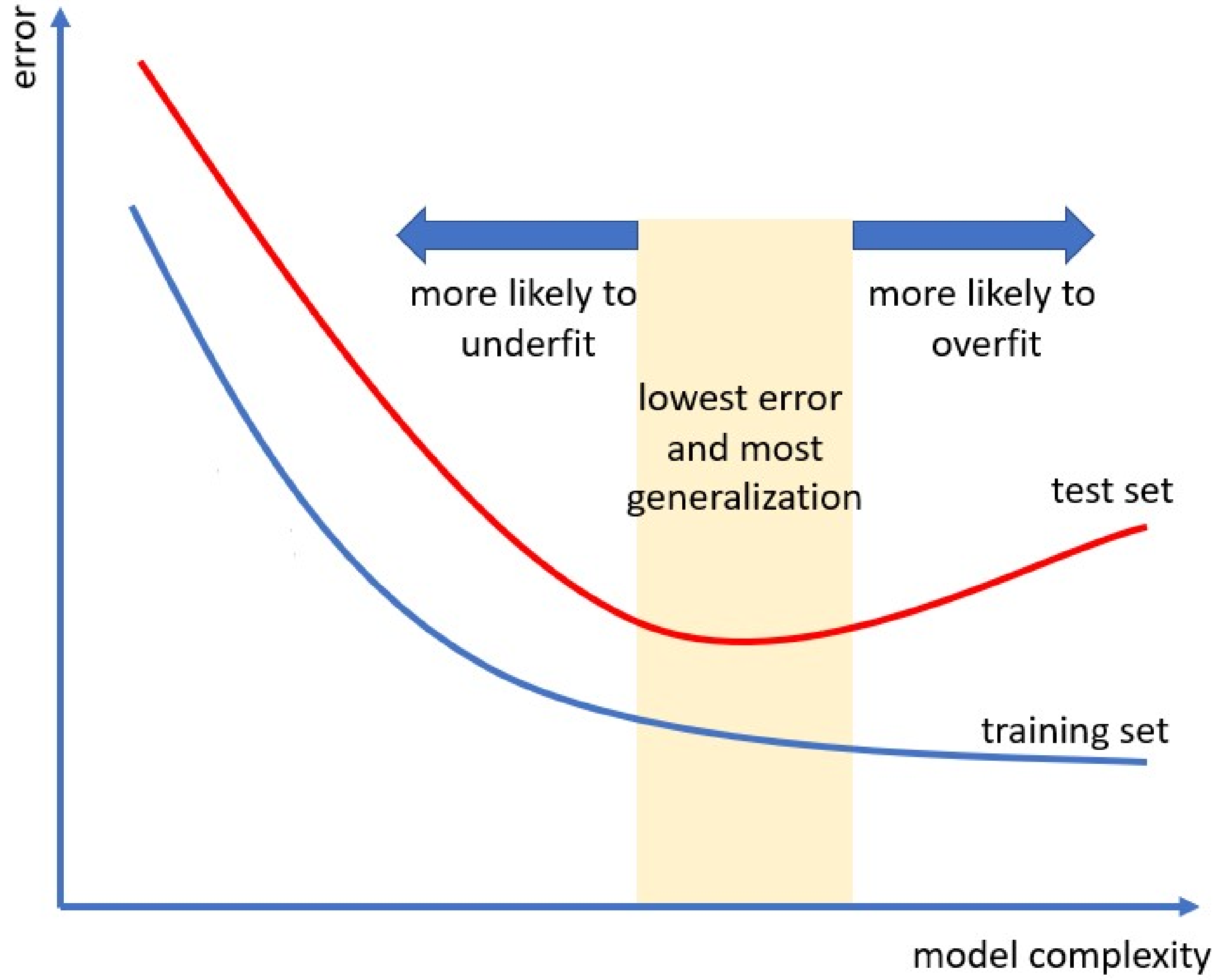
underfitting and overfitting

- *fitting* means learning: remember calling the `.fit()` method
- if a model performs poorly on the training data, then it almost certainly will perform poorly on the test data as well: we say the model is **underfitting** (not learning enough)
- if a model performs well on the training data, but poorly on the test data: we say the model is **overfitting** (it's learning the signal but also "learning" the noise in the training data, and hence fails to generalize)
- a good model is one that neither underfits nor overfits

overfitting and complexity

- more simple models tend to underfit, because they are more likely to oversimplify (not pick up enough signal)
  - analogy: models can be prejudiced too, we call it **bias**
- more complex models tend to overfit, because they are so eager to pick up any signal that they also grab noise disguised as signal
  - analogy: people who **read too much into** a literary passage
- the trick is to find the happy median

> *Everything should be made as simple as possible, but not simpler.*
> **Albert Einstein** (also look up **okam's razor**)


error
more likely to underfit
more likely to overfit
lowest error and most generalization
test set
training set
model complexity

break time

what are hyper-parameters?

- choosing a model isn't just about choosing the right ML algorithm
- almost all algorithm have ways they can be "tuned" through different **hyper-parameter** choices
- some hyper-parameters are very generic, such as the **learning rate**
- most hyper-parameters are algorithm-specific, such as
  - for tree-based algorithms: tree depth, min leaf size
- ML algorithms **cannot** directly learn optimal hyper-parameter values during training
- if we don't specify them, they usuall default to "reasonable" values

model selection and validation

- so how do we know what hyper-parameter values to pick?
  - mostly through trial and error, though we call it **model selection**
- if we want to tune our hyper-parameters, we also need a **validation data** in addition to training and testing

1. train many models, each with a different set of hyper-parameters, and evaluate their performance on the validation data
2. select the model which performs best on the validation data as the winner
3. check how the winner model performs on the test data

lab time

the answer to this question is not at all straight-forward, but it's good to take some time to think about this:

- why don't we just use the test data as the validation data?

in other words

1. train many models, each with a different set of hyper-parameters, and evaluate their performance on the test data
2. select the model which performs best on the test

test data vs validation data

- so why not combine test data and validation data?
  - because the test data is used **once** with the **final model** to get an **unbiased estimate** of preformance (prediction error)
  - the validation data is used **many times** so we can compare the performance of models trained with different sets of hyper-parameters, a.k.a. **hyper-parameter tuning**
  - if we also use the test data to tune hyper-parameters, we are over-using it and its estimate of performance will not be so unbiased anymore

recap

- we use a **training set** to estimates model's **parameters**
- we use a **validation set** when we (optionally) want to tune the model's **hyper-parameters** by training and evaluating **many times**
- the **test set** is used **once** to evaluate the model's performance so we can have an unbiased estimate of its prediction error, where **unbiased** here means
  - test data didn't infulence model's parameters (during training)
  - test data didn't influence model's hyper-parameters (during validation)

break time

lab time

consider how knowing the following information about your data should inflence how you split the data in trainig and test sets:

1. let's say you have class imbalance in your data, meaning some classes very sparse
2. most data is **cross-sectional**, meaning it's a single snapshot (or close) and every example (row) is **independent** of the rest, but data can also be **time-series**, meaning that the order matters because the past can influence the future, so our examples are **dependent** and the order is represented by a **time-stamp**

more on class imbalance

- also sometimes referred to as **rate events** scenaro
- class imbalance is very common in many use-cases:
  - fraud detection (binary classification)
  - medical diagnosis (binary classification)
- class imbalance usually implies that not all errors (misclassification) should have the same importance
  - looking at accuracy (percent misclassifications) can be optimistic
  - instead we look at other metrics, like precision, recall, or AUC

the confusion matrix

- it's really not that confusing!

	predicted positive	predicted negative
actually positve	true positive TP	false negative FN
actually negative	false positive FP	true negative TN

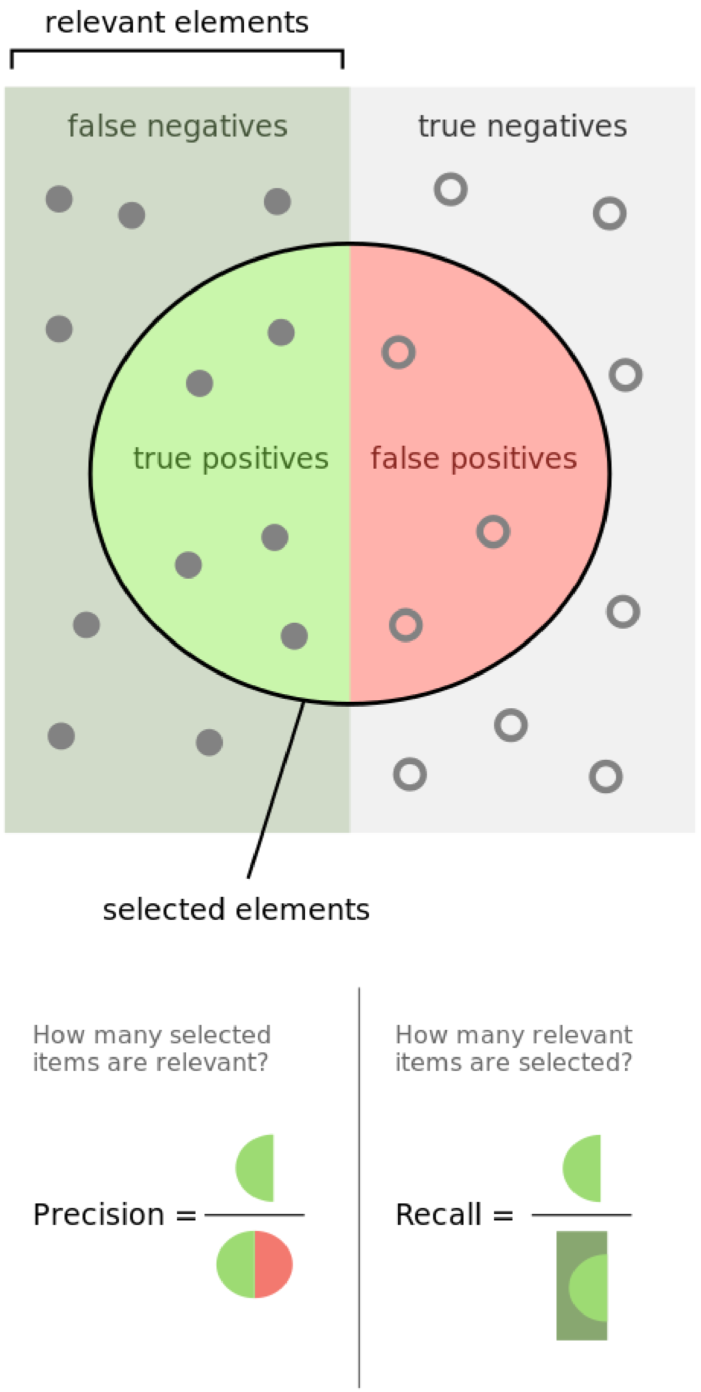
- for TP / FP / TN / FN
  - the second letter indicates what the prediction was, and
  - the first letter indicates if the prediction was right or not

lab time

- we saw there a binary classification model can make two kinds of errors: `FP` and `FN`
- for the following scenarios, say what kind of error is more costly (use common sense)
  - **credit card fraud detection**: someone impersonates you to use your credit card
  - **medical diagnosis**: finding out who has a disease
  - **information retrieval**: finding relevant web pages based on a search query

precision and recall

- **accuracy** is just the misclassification rate
- **precision** is the percentage of positive predictions that were actually positive
- **recall** is the percentage of positive cases that we correctly predicted as such
- image source: [wikipedia]



accuracy, precision and recall

- accuracy $= \dfrac{TP + TN}{TP + FP + TN + FN}$
- precision $= \dfrac{TP}{TP + FP}$
- recall $= \dfrac{TP}{TP + FN}$
- notice that neither precision nor recall have `TN` in it, but accuracy has it both in the numerator and denominator
- for rare events usually `TN` far exceeds `TP`, `FN`, or `FP`

lab time

here's an analogy that to why we should evaluate a classification model's accuracy using **both** precision and recall:

- when you stand witness in a court of law, you are asked to tell the truth:
  - **the whole truth**: no lie of omission
  - **nothing but the truth**: no lies
- relate the above two statements to precision and recall

the end