Introduction to Classification

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Learning Objectives

After this lesson, you should be able to:

- Define class label and classification
- Build a K-Nearest Neighbors using the scikit-learn library
- Evaluate and tune model by using metrics such as classification accuracy/error

Outline

- **Final Project 1 Presentations ☺**
- Review
- Types of machine learning problems
- What is classification?
- What is binary classification?
- Iris dataset and exploratory analysis
- Hand-coded classifiers
- Classification metrics
- K-Nearest Neighbors (KNN)
- High dimensionality
- What is the best value for k?
- Validation and cross-validation
- Advantages and disadvantages of KNN
- Lab
- Review
- Assigned
  - Final Project 2 (due in 3 weeks)
- In-flight
  - **Unit Project 3 (due next session on 3/24)**

Pre-Work

Pre-Work

Before this lesson, you should already be able to:

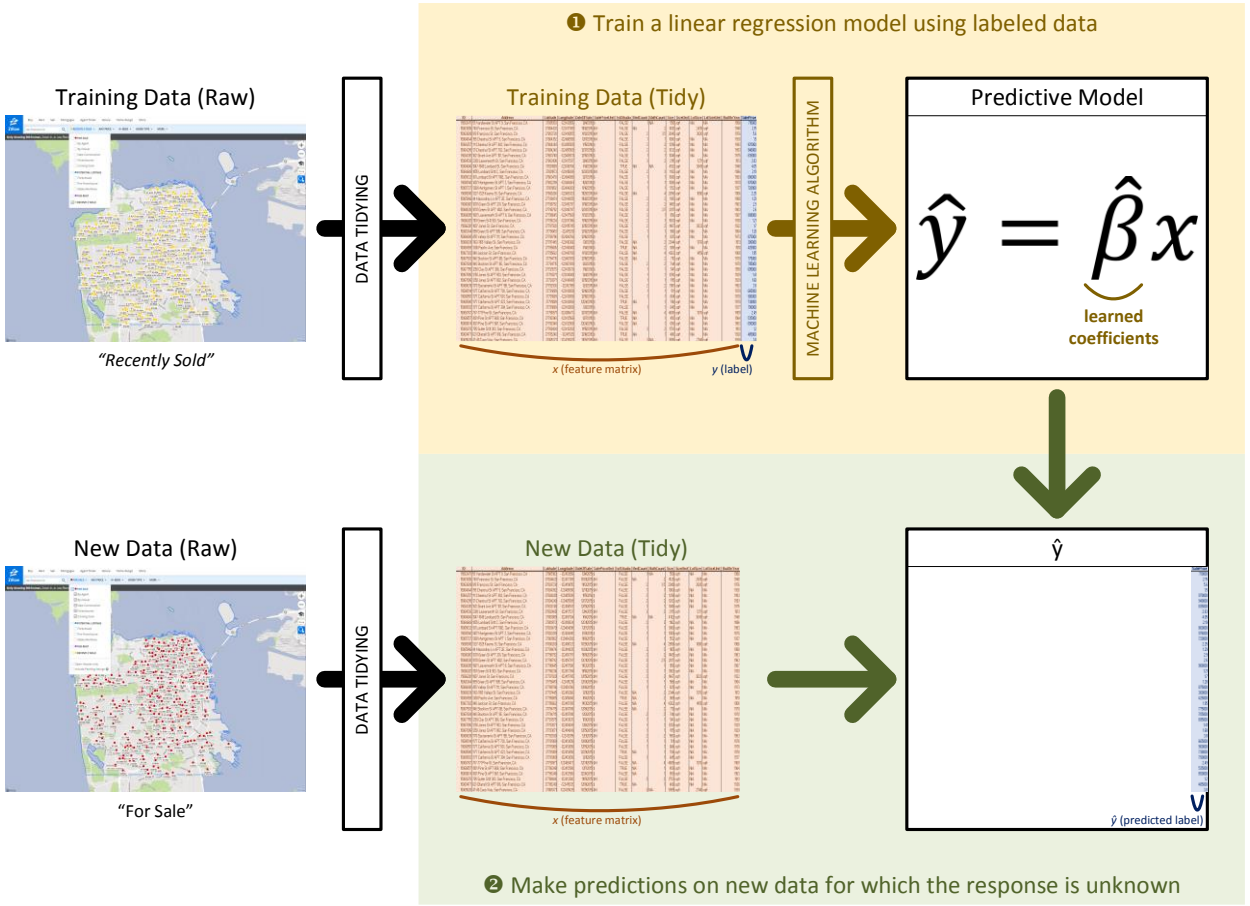
- Understand how to optimize for error in a model
- Understand the concept of iterations to solve problems
- Measure basic probability

Review

Linear Regression Review

- Linear regression assumes that the dependence of y (your response variable) on x (your input variables) is linear. Linear regressions are:
  - Highly interpretable and simple to explain
  - Model training and prediction are fast
  - No tuning is required (excluding regularization)
  - (Input) Features don't need scaling
  - Can perform well with a small number of observations
  - Well-understood

Linear regression is a simple approach to supervised learning



Linear regression is a simple approach to supervised learning (cont.)

- A supervised machine learning model learns the relationship between the feature variables and the response variable (also called the labeled data)
- The primary goal of supervised learning is to build a model that "generalizes" so as to accurately predicts the future (rather than the past)

- We've focused so far on predicting a continuous set of values
  - That means that we've been able to use distance to measure how accurate our predictions are
- However, for other problems, we need to predict binary responses. E.g., Will a loan default? Is an email spam or ham?

Types of Machine Learning Problems

Types of Machine Learning Problems

	Continuous	Categorical
Supervised (a.k.a., predictive modeling)	Linear Regression (sessions 6 & 7)	K-Nearest Neighbors (session 8) Logistic Regression (session 9)
Unsupervised	A machine learning model that doesn't use labeled data is called unsupervised. It extract structure from the data. Goal is "representation"	

What is Classification?

What is classification?

- Classification is a machine learning problem for solving a set of categorical values (y; the response variable) given the knowledge we have about these values (x; the feature matrix)
  - E.g., what if you are predicting whether an image is of a *human*, *dog*, or *cat*?
- The possible values of the response variable are called *class labels*
  - E.g., *"human"*, *"dog"*, and *"cat"*

What is binary classification?

- Binary classification is the simplest form of classification
  - I.e., the response is a *boolean* value (true/false)
- Many classification problems are binary in nature
  - E.g., we may be using patient data (medical history) to predict whether a patient smokes or not

- At first, many problems don't appear to be binary; however, you can usually transform them into binary problems
  - E.g., what if you are predicting whether an image is of a *"human"*, *"dog"*, or *"cat"*?
  - You can transform this non-binary problem into three binary problems
    - 1. Will it be *"human"* or *"not human"*?
    - 2. Will it be *"dog"* or *"not dog"*?
    - 2. Will it be *"cat"* or *"not cat"*?
- This is similar to the concept of dummy variables

Iris Dataset

The Iris dataset contains 3 classes of 50 instances each, each class referencing a type of iris plant (Setosa, Versicolor, or Virginica)

Iris Setosa

Iris Versicolor

Iris Virginica

Source: Flickr

Iris dataset (cont.)

- Can you identify the type of iris based on the following four attributes?
  - Sepal length and width
  - Petal length and width

Source: Flickr

Codealong & Activity – Part A Iris Dataset Exploratory Analysis

Activity: Iris Dataset Exploratory Analysis

EXERCISE

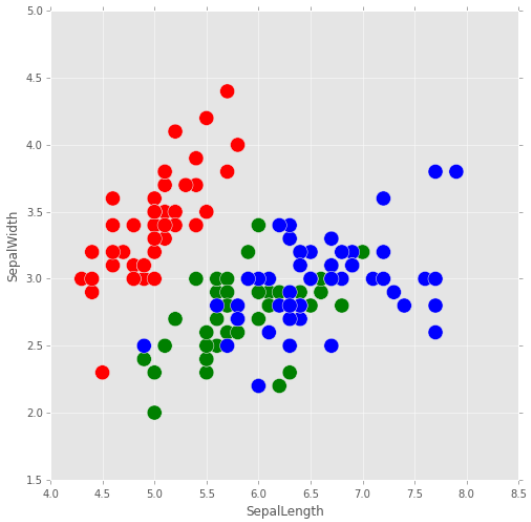
ANSWER THE FOLLOWING QUESTIONS (10 minutes)

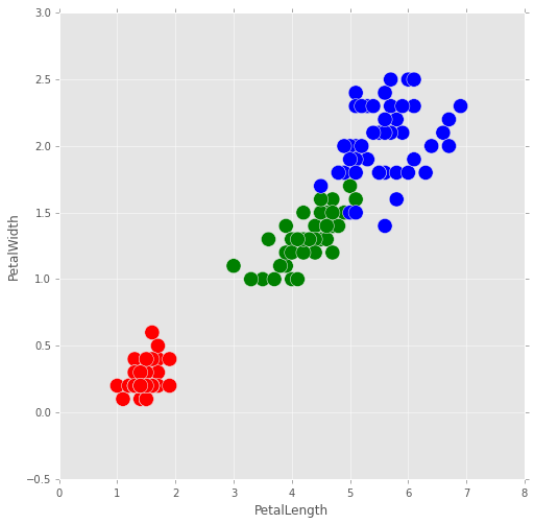
1. Using the Iris dataset (`iris.csv` in the `datasets` folder), perform exploratory analysis between *SepalLength*, *SepalWidth*, *PetalLength*, and *PetalWidth* (the *feature* variables) and *Species* (the *class* variable). How can you use these features to separate one species from the other two?
2. When finished, share your answers with your table

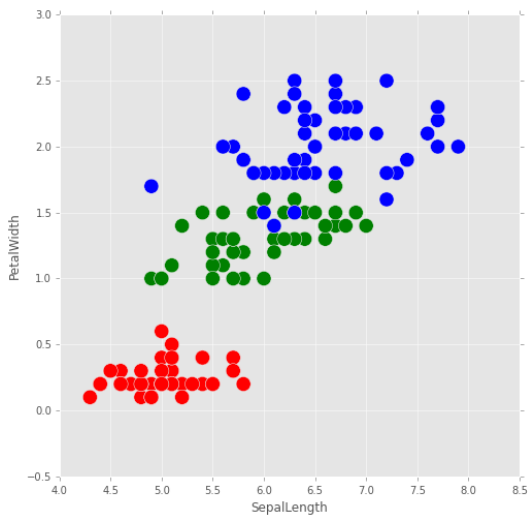
DELIVERABLE

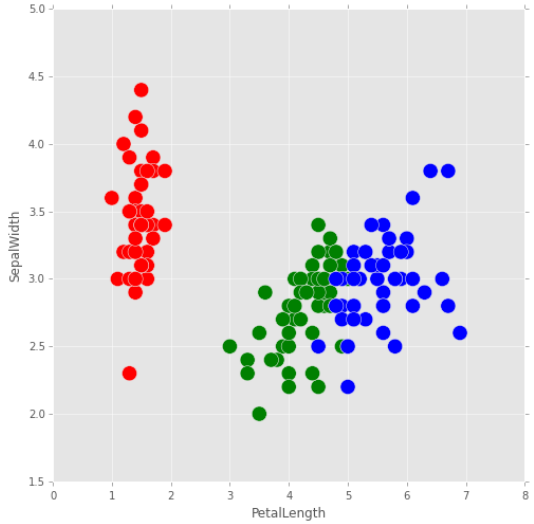
Answers to the above questions

Iris Dataset Exploratory Analysis

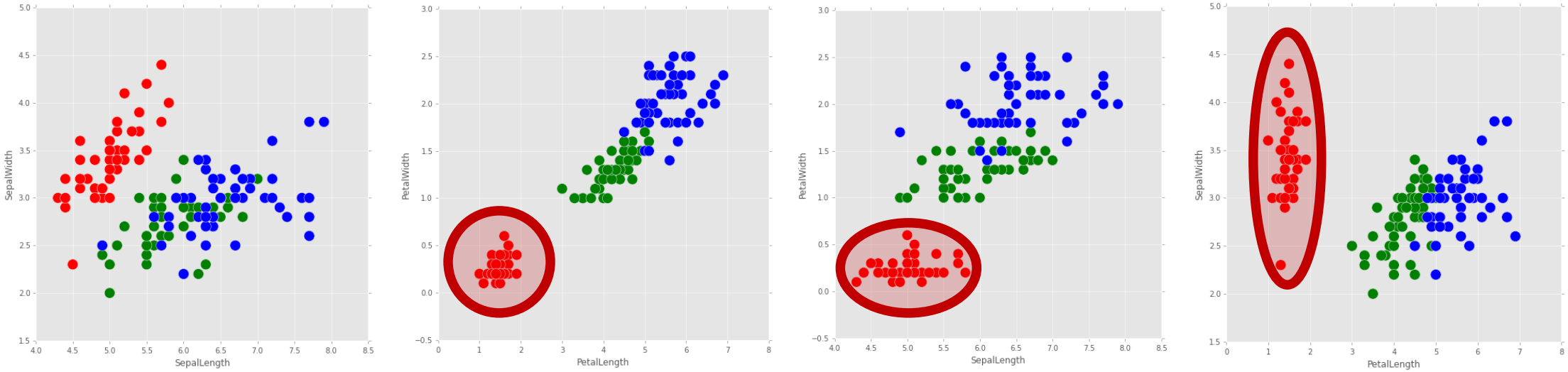






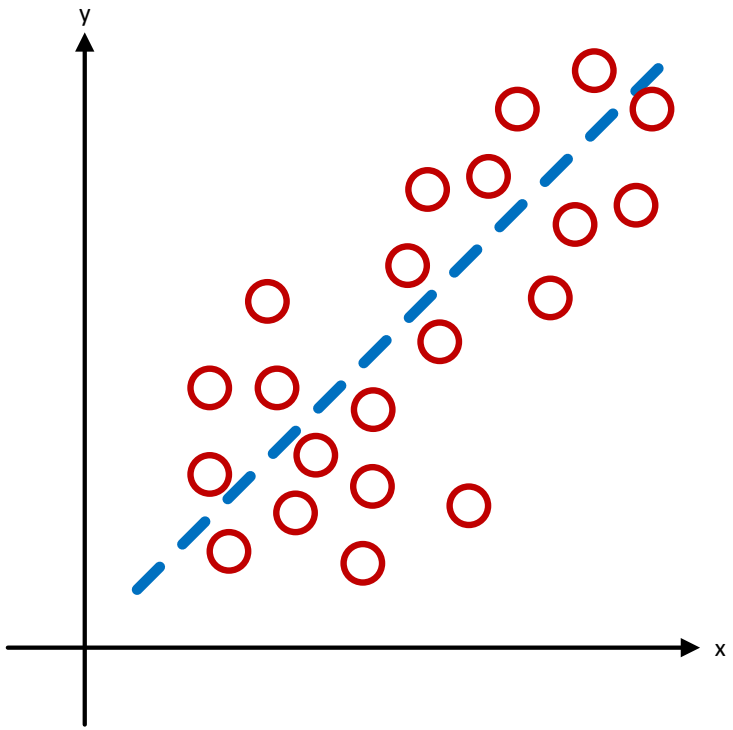


The setosa class is linearly separable from the other two

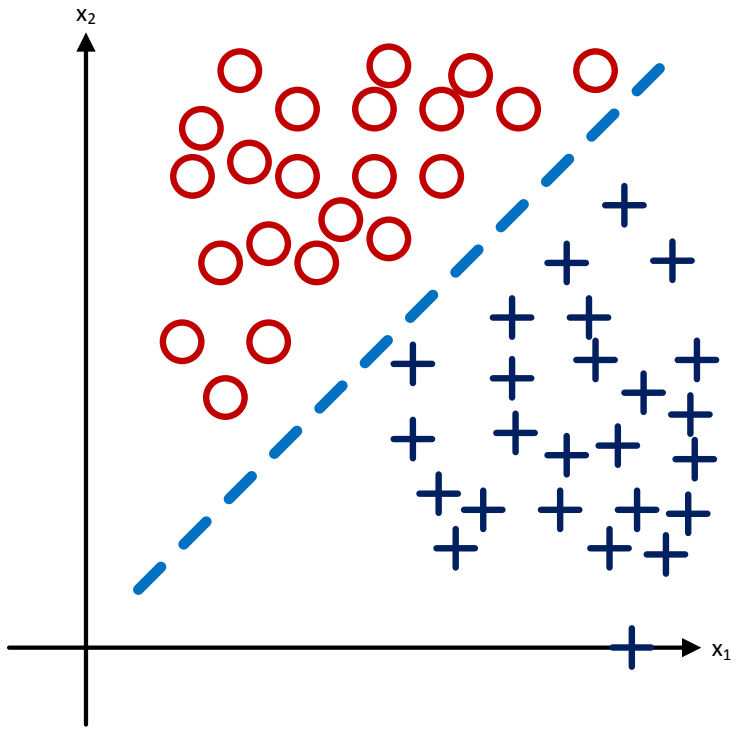


Classification and regression differ in what they are trying to predict

Regression



Classification



Codealong – Part B
First Hand-Coded Classifier

Classification Metrics

Classification Metrics

- The metrics we've used for regressions do not apply for classification
  - We could measure distance between the probability of a given class and an item being in the class. E.g., guessing .6 for a 1 is a .4 error, while guessing .99 for 1 is .01 error…
  - but this overly complicates our current goal: understanding binary classifications, like whether something is right or wrong

Classification Metrics (cont.)

- Instead, let's start with two new metrics, which are inverses of each other: accuracy and misclassification rate
- Since they are opposite of each other, you can pick one or the other; effectively they will be the same. But when coding, do make sure that you are using a classification metric when solving a classification problem!
- *sklearn* will not intuitively understand if you are doing classification or regression, and accidentally using mean squared error for classification, or accuracy for regression, is a common programming pitfall

- Accuracy
  - How many observations that we predicted were correct? This is a value we'd want to increase (like R^2)

- Misclassification rate
  - Directly opposite of accuracy
  - Of all the observations we predicted, how many were incorrect? This is a value we'd want to decrease (like the mean squared error)

Codealong – Part C
Classification Metrics

Codealong & Activity – Part D Second Hand-Coded Classifier

Activity: Second hand-coded classifier

EXERCISE

ANSWER THE FOLLOWING QUESTIONS (10 minutes)

1. Improve the first hand-coded classifier to further separate the remaining classes of iris
2. When finished, share your answers with your table

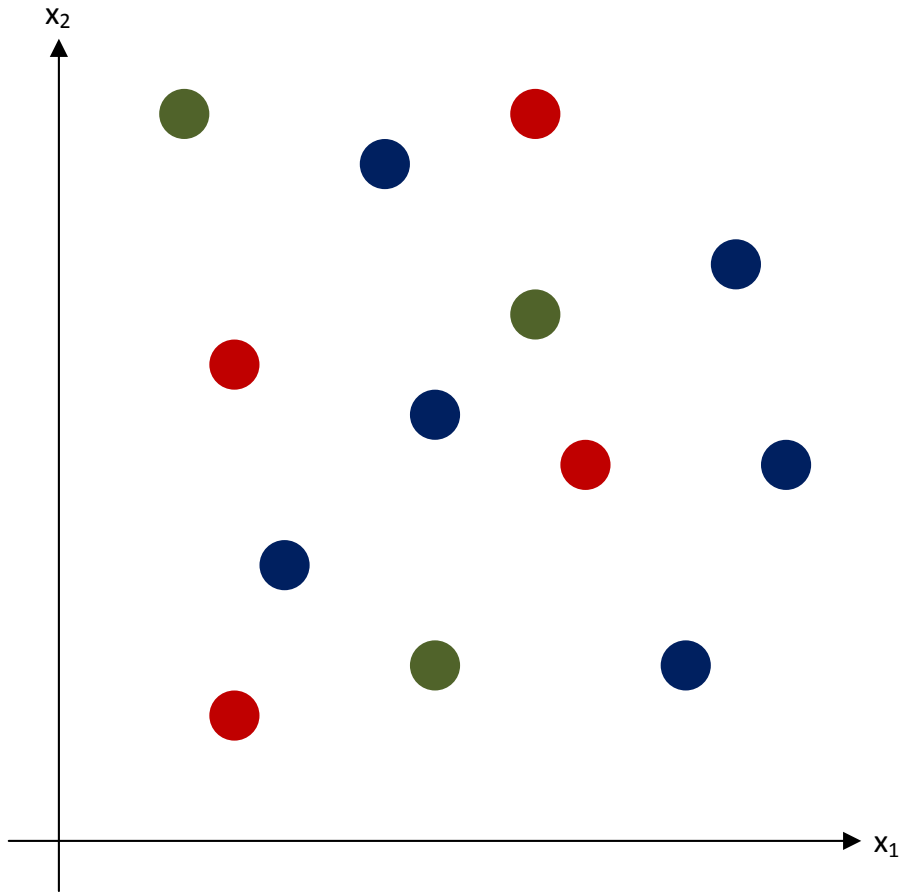
DELIVERABLE

Answers to the above questions

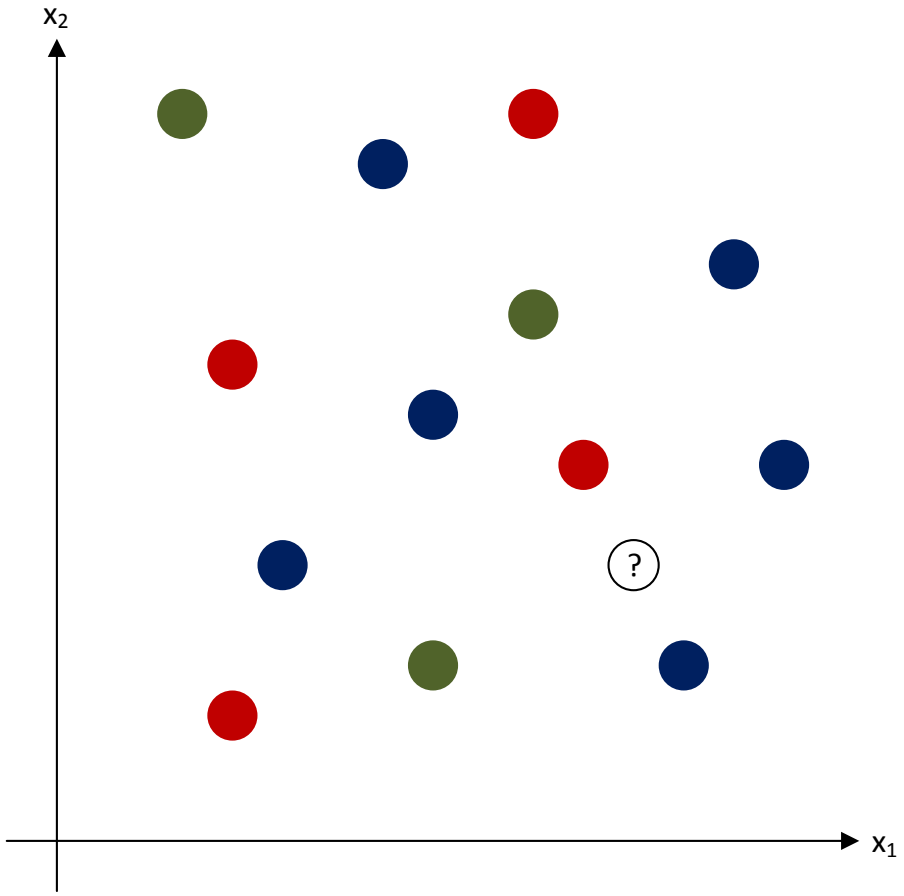
K-Nearest Neighbors (KNN)

K-Nearest Neighbors

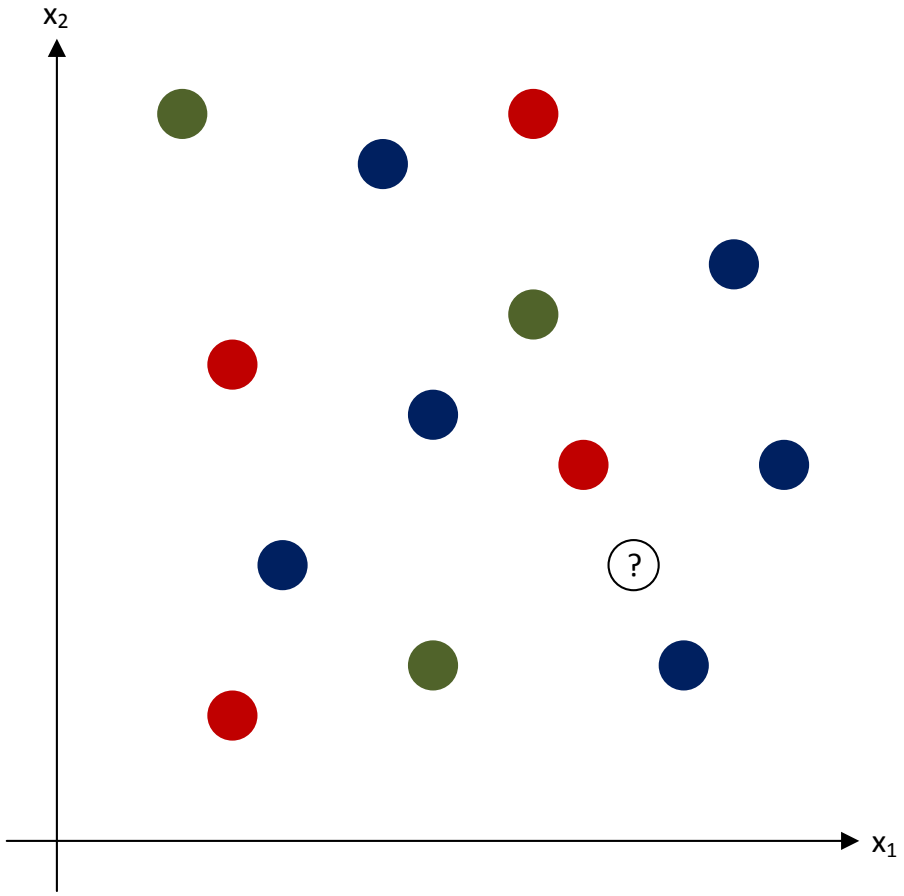
- K-Nearest Neighbors (KNN) is a classification algorithm that makes a prediction based upon the closest data points



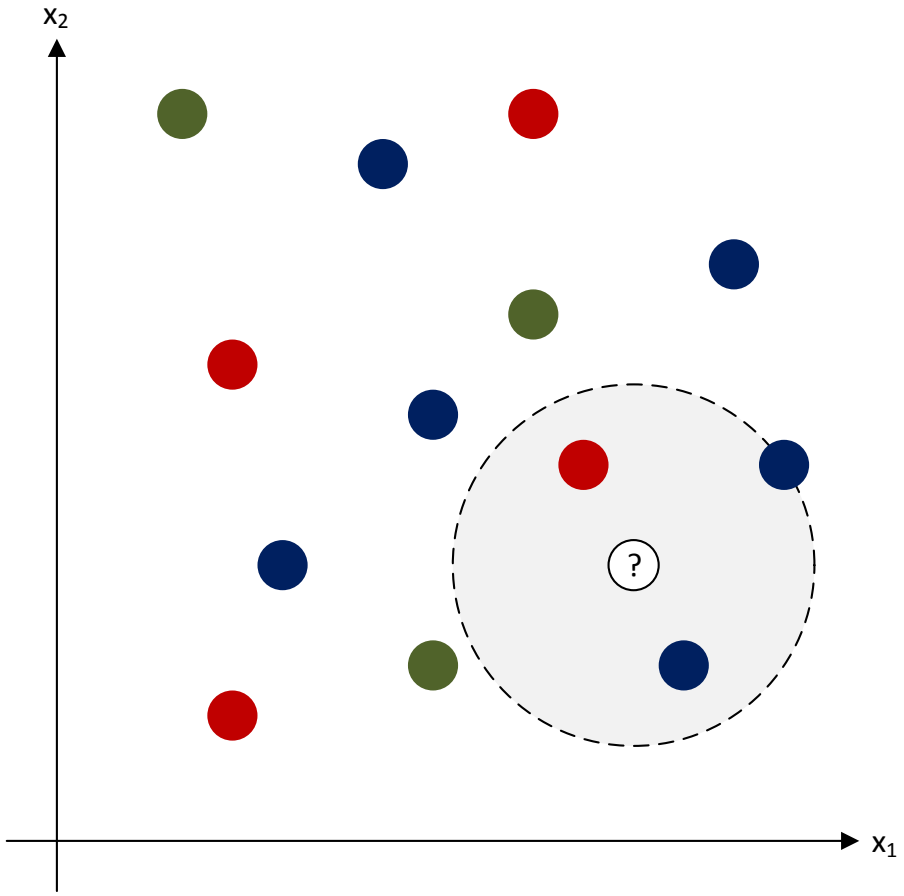
How would you predict the color of the "question mark" point?



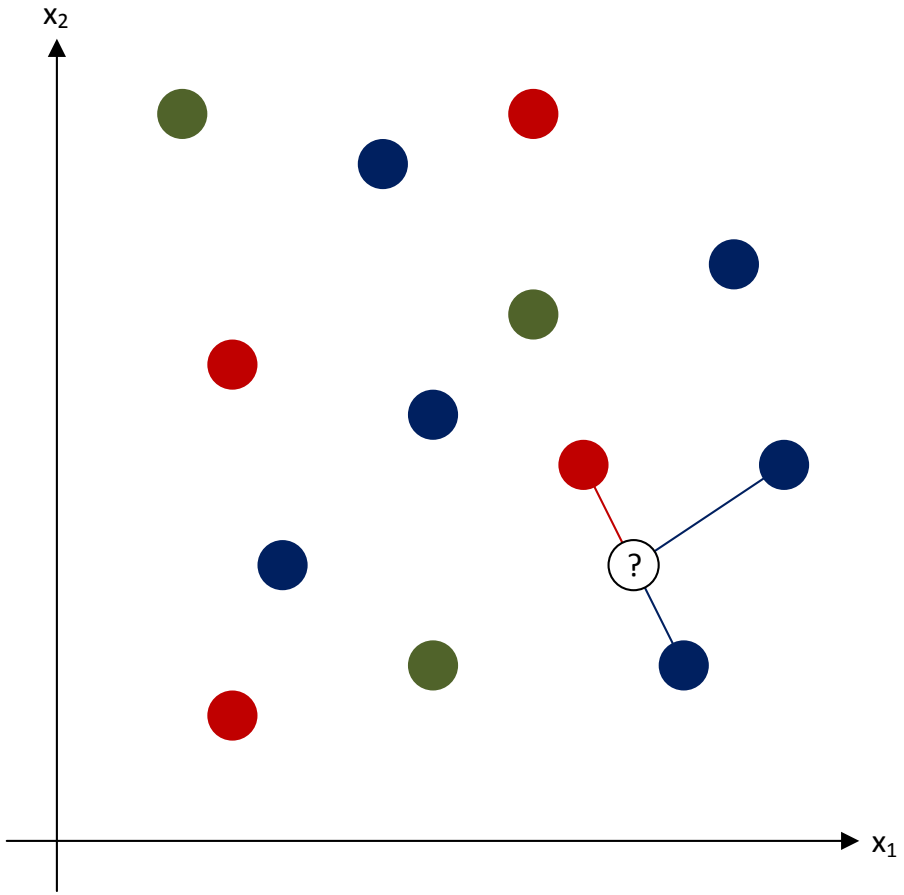
❶ Pick a value for k, e.g., $k = 3$



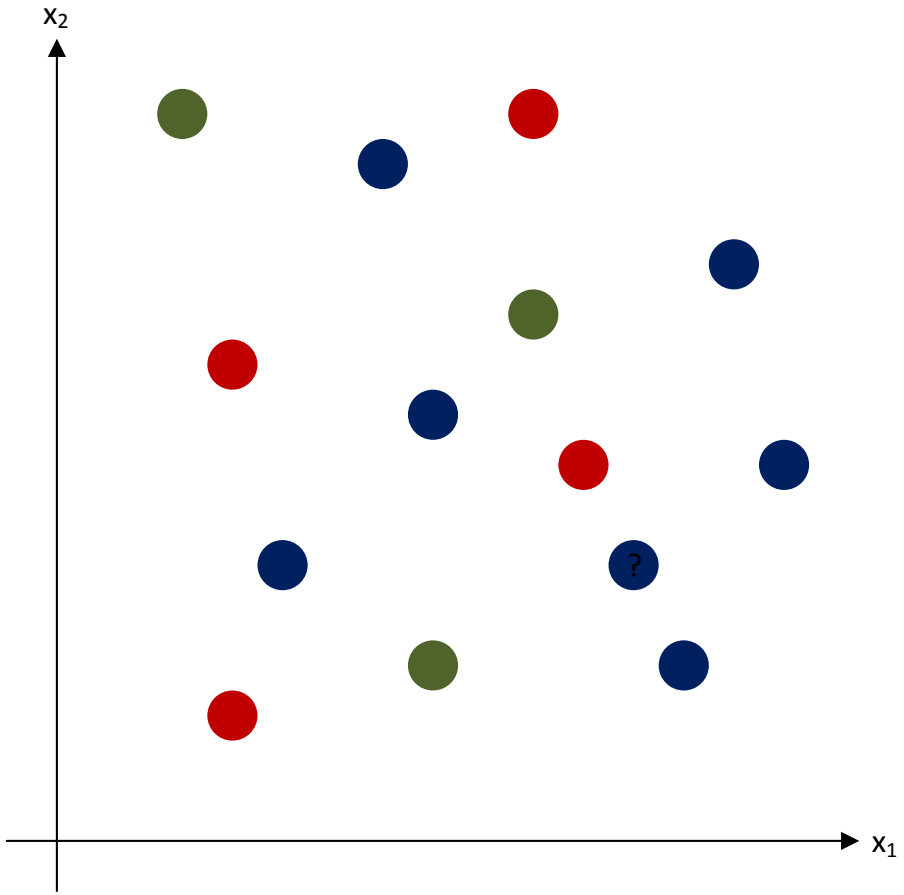
❷ Calculate the distance to all other points; given those distances, pick the k closest points



❸ Calculate the probabilities of each class label given those points: $\frac{1}{3}$ “red”, $\frac{2}{3}$ “blue”

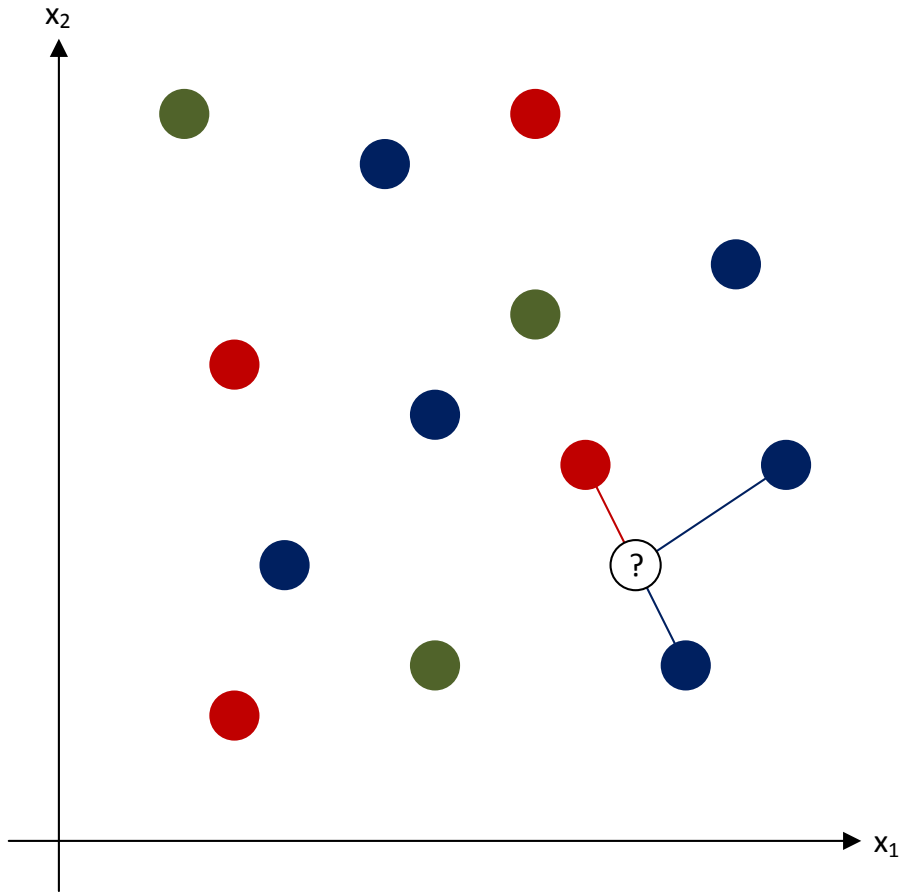


❹ The original point is classified as the class label with the largest probability (“votes”): “blue”



K-Nearest Neighbors (cont.)

- KNN uses distance to predict a class label
- This application of distance is used as a measure of similarity between classifications
  - We are using shared traits to identify the most likely class label



What happens if two classes get the same number of votes?

- *Scikit-learn* will choose the class it first saw in the training set

- We could also implement a weight, taking into account the distance between a point and its neighbors
- This can be done in *sklearn* by changing the *weights* parameter to *'distance'*

Codealong – Part E
K-Nearest Neighbors

High Dimensionality

What happens in high dimensionality?

- Since KNN works with distance, higher dimensionality of data (i.e., more features) requires significantly more samples in order to have the same predictive power
  - With more dimensions, all points slowly start averaging out to be equally distant; this causes significant issues for KNN

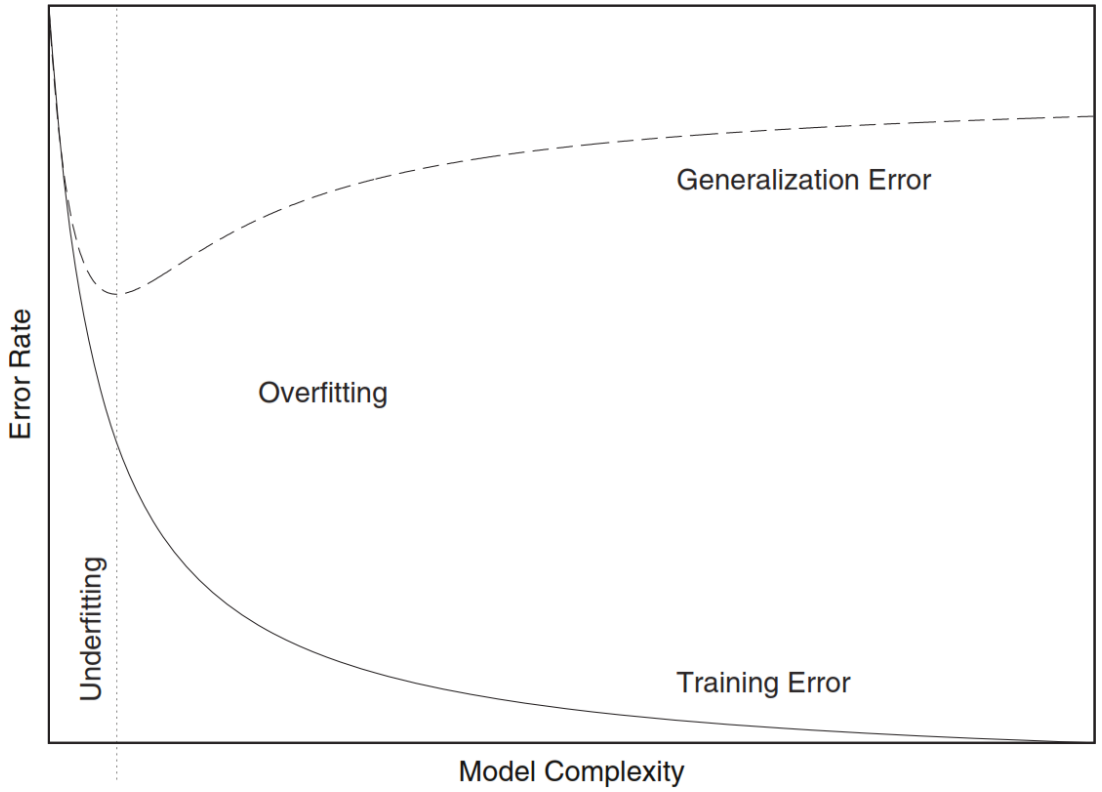
- Keep the feature space limited and KNN will do well; exclude extraneous features when using KNN

Codealong – Part F
What is the best value for k?

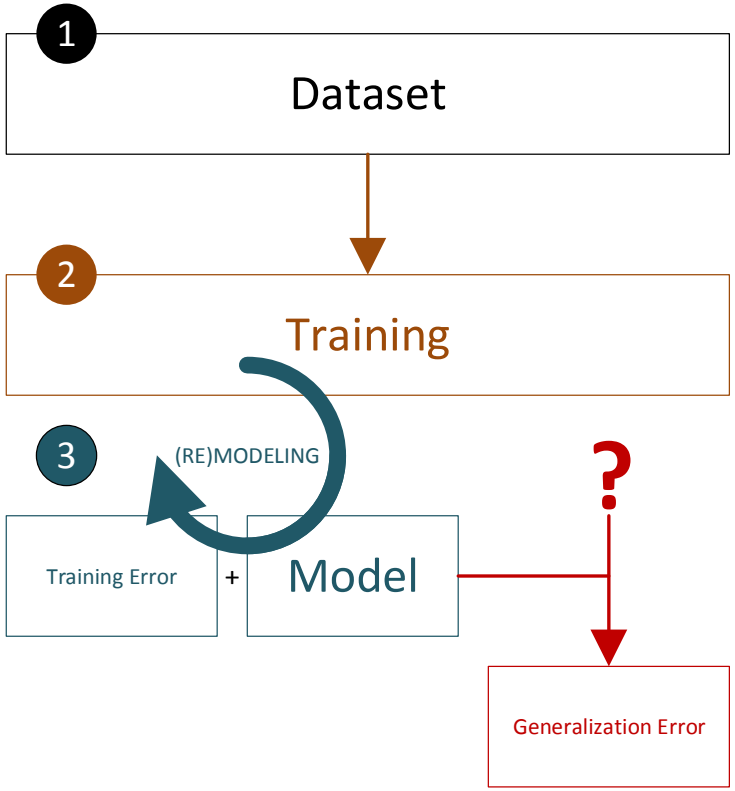
What is the best value for k?

Validation

So far, we used the entire dataset to train the models. How can we estimate the generalization error?

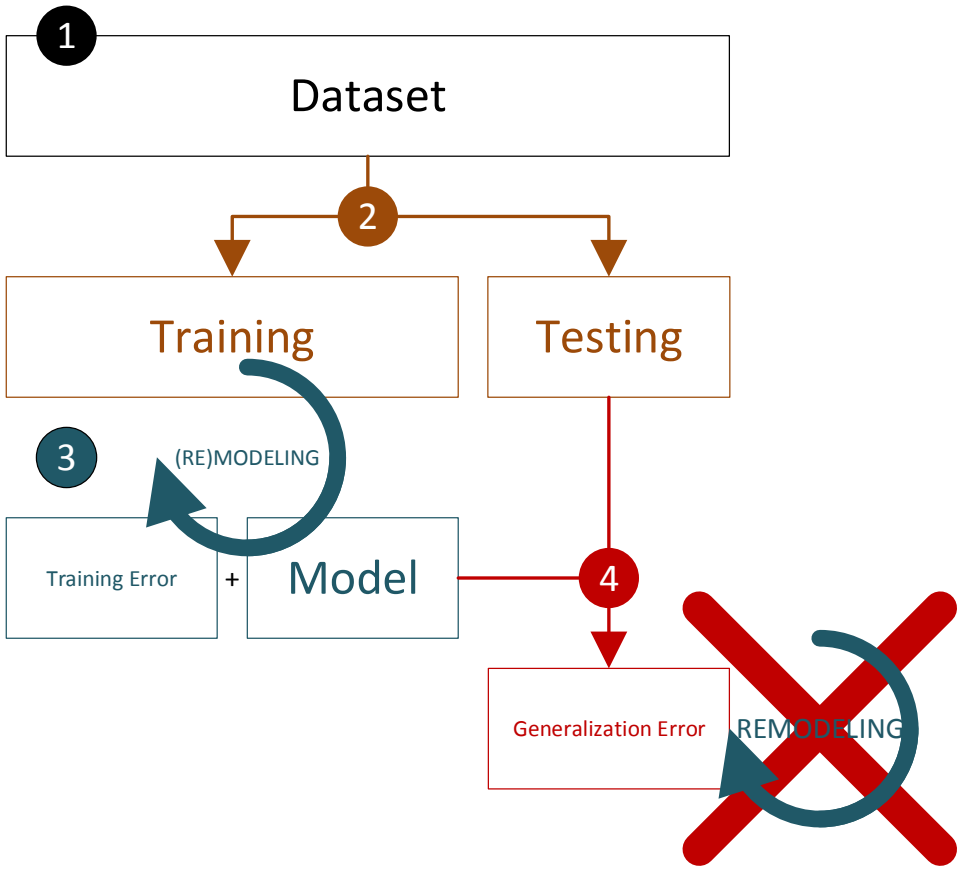


Source: Data Analysis with Open Source Tools



Validation is an answer

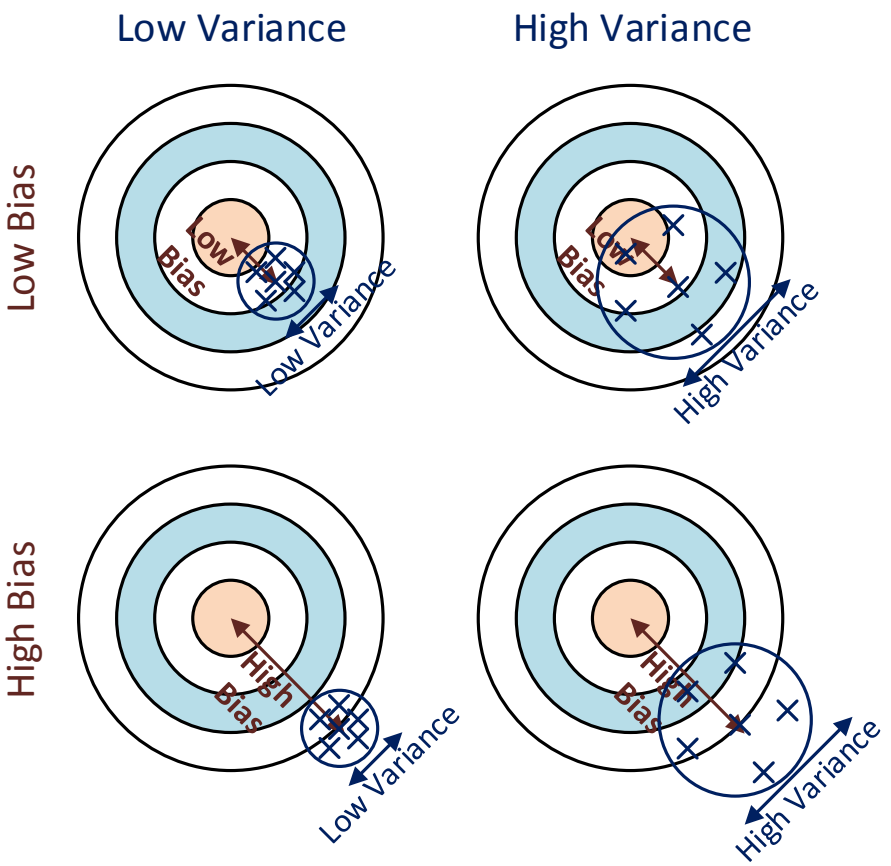
- Answer: (Randomly) divide the dataset into a training set and a testing set
  - Set aside the testing set; don't look at it
- Train the models with the training set
  - Compute the training set and remodel as needed
- Once you are happy with your model, use the testing set to compute the generalization error
  - But you cannot go back and remodel; otherwise these previously unknown data points are not longer unseen



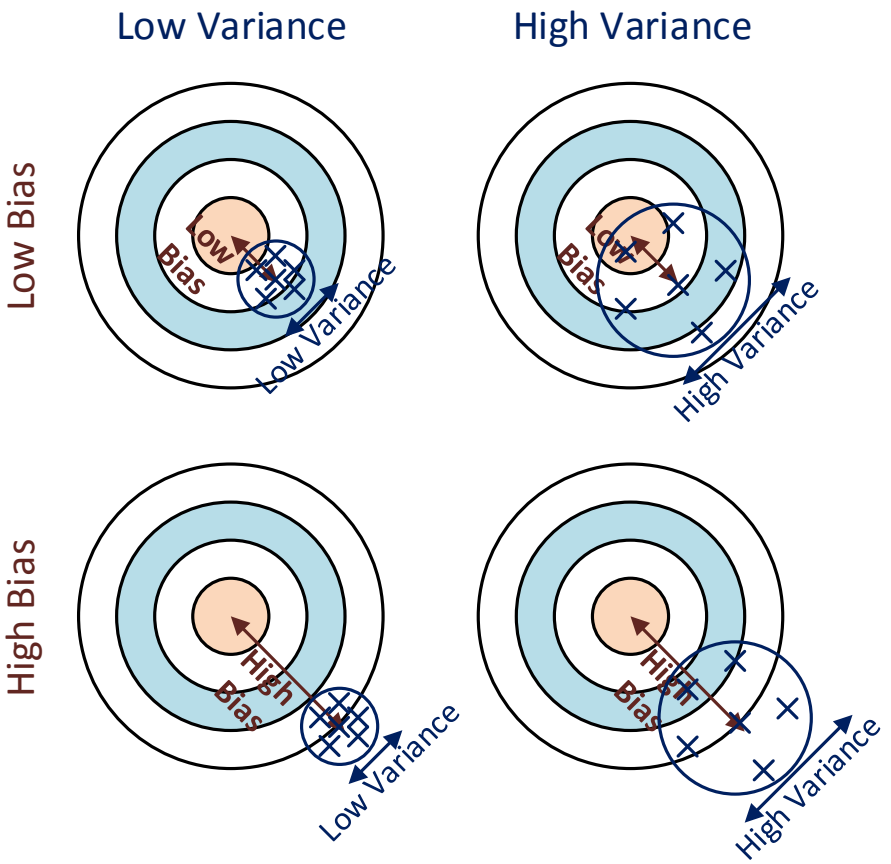
Codealong – Part G Validation

Cross-Validation

Recall our conversation about bias and variance, a.k.a., *systematic* and *random* errors? (session 3)

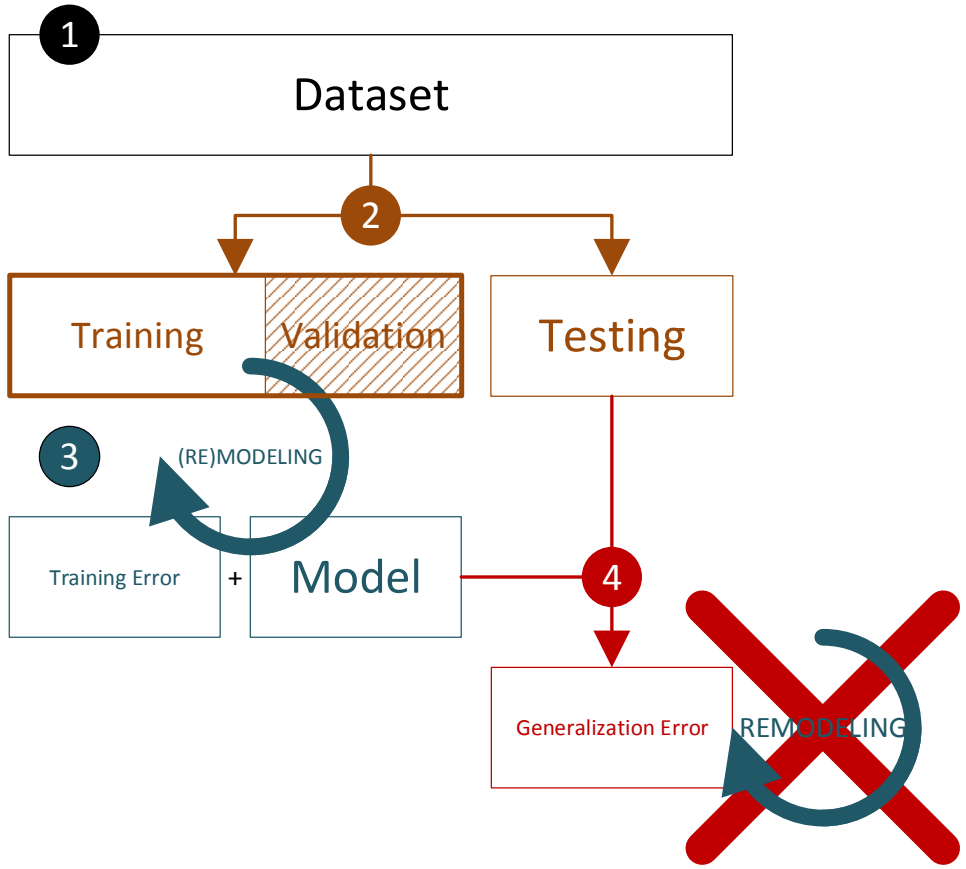


The generalization error has a bias component (systematic; non-random) and a variance component (idiosyncratic; random). Can we lower the bias error?



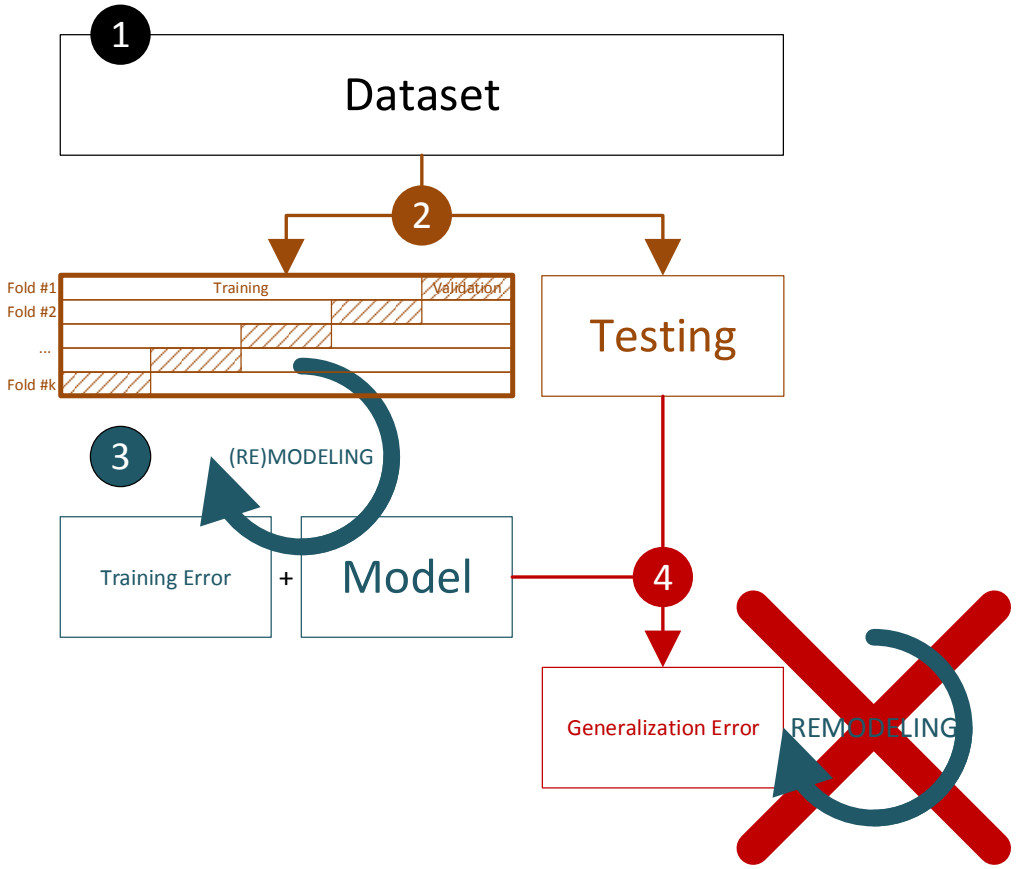
Cross-validation (CV) is a technique to lower the bias error

- Cross-validation
  - Another technique to validate models
  - Used to estimate how accurately the model generalize to unseen data
  - You can iterate as much as you want with the data
  - You then build a final model that uses all the data (cross-validation is used for model checking, not model building)
- [You still create an unseen testing set to estimate how well your model generalize to unseen data (and you stop there; no remodeling)]



(k-fold) cross-validation

- k-fold cross-validation
  - Quite popular
  - Typically, $k = 5$ or 10 with each sample being used both for training ($k - 1$ times) and validation (1 time)
  - The training error is the average training error of all folds
  - Again, after selecting the model that minimize the training error, you then build a final model that uses all the data
- You still create an unseen testing set to estimate how well your model generalize to unseen data (and you stop there; no remodeling)



Codealong – Part H
Cross-Validation

Advantages and Disadvantages of KNN

Advantages and disadvantages of KNN

Advantages

- Simple to understand and explain
- Model training phase is fast
- Non-parametric (does not presume a “form” of the “decision boundary”)

Disadvantages

- Prediction phase can be slow when n is large
- Sensitive to irrelevant features
- Very sensitive to feature scaling

Review

Review

- What are class labels? What does it mean to classify?
- How is a classification problem different from a regression problem? How are they similar?
- How does the KNN algorithm work?
- What primary parameters are available for tuning a KNN estimator?
- How do you define accuracy and misclassification?

Review (cont.)

You should now be able to:

- Define class label and classification
- Build a K-Nearest Neighbors using the scikit-learn library
- Evaluate and tune model by using metrics such as classification accuracy/error

Pre-Work

Pre-Work

Before the next lesson, you should already be able to:

- Implement a linear model (`LinearRegression`) with *scikit-learn*
- Define the concept of coefficients
- Recall metrics for accuracy and misclassification
- Recall the differences between L1 and L2 regularization

Q & A

Exit Ticket

Don’t forget to fill out your exit ticket here