05 | k-Nearest Neighbors

Ivan Corneillet

Data Scientist

Learning Objectives

After this lesson, you should be able to:

- Define and give examples of classification; implement a simple classifier by hand
- Explain the k-Nearest Neighbors algorithm; build a k-Nearest Neighbors model using *sklearn*
- Understand the fundamentals of evaluating and tuning classifiers; define error metrics for classification problems, goodness of fit, bias, and variance

Classification

k-Nearest Neighbors is a supervised learning algorithm for regression or classification

	Regression (continuous predictions; i.e., how much or how many?)	Classification (categorical predictions; i.e., is this A, B or C?)
Supervised a.k.a., predictive modeling (generalization; make predictions)	k-Nearest Neighbors ✓	k-Nearest Neighbors ✓
Unsupervised *(representation; extract structure)*		

When ❻ BUILD*ing* **a model**, our data needs to be in the form of a **feature matrix $\boldsymbol{X}$** (i.e., the stimuli, e.g., *"ring bell"*) and a **response vector $\boldsymbol{y}$** (i.e., the response, e.g., *"dog salivates"*)

Feature Matrix X

	col0	col1	col2	col3
row0				
row1				
row2				
row3				

Response Vector y

	col
row0	
row1	
row2	
row3	

Response Vector y (or c) (cont.)

Regression

Response vector $\boldsymbol{y}$

	col *e.g. price*
row0	\$1.1M
row1	\$.9M
row2	\$1.5M
row3	…

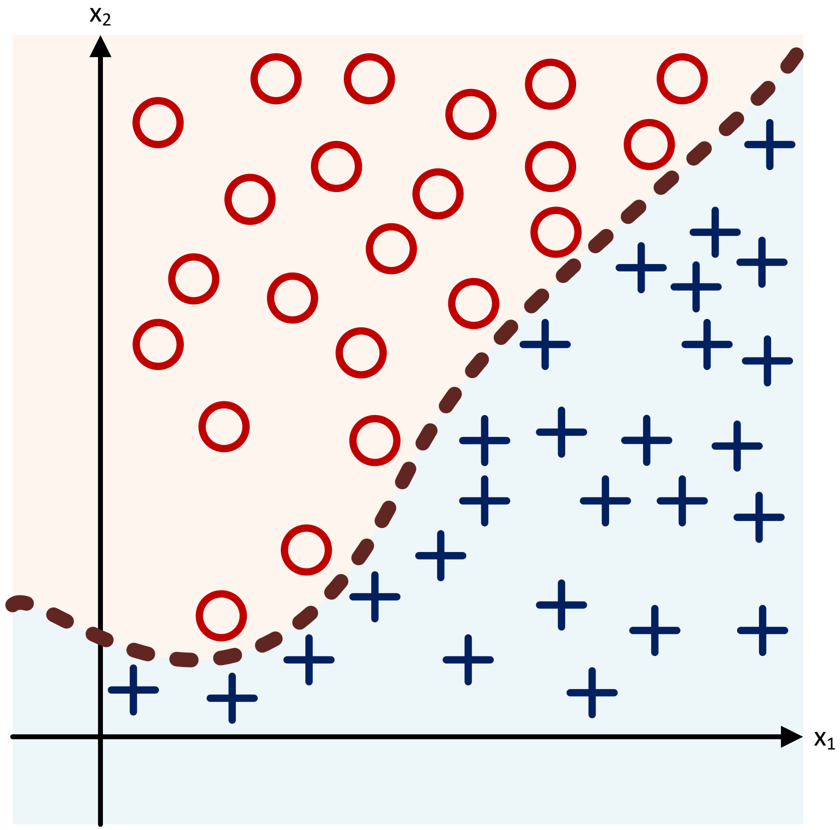
Classification

Response vector $\boldsymbol{c}$

(renamed from y to c for label classes)

	col *e.g., animal*
row0	“dog”
row1	“cat”
row2	“bird”
row3	…

A classifier aims to isolate the response vector y's class label by splitting the feature space modeled by the feature matrix X



The Iris Dataset: 3 class labels of iris plants (*Setosa*, *Versicolor*, and *Virginica*); 50 instances in each class label

CASE STUDY

Iris Setosa

Iris Versicolor

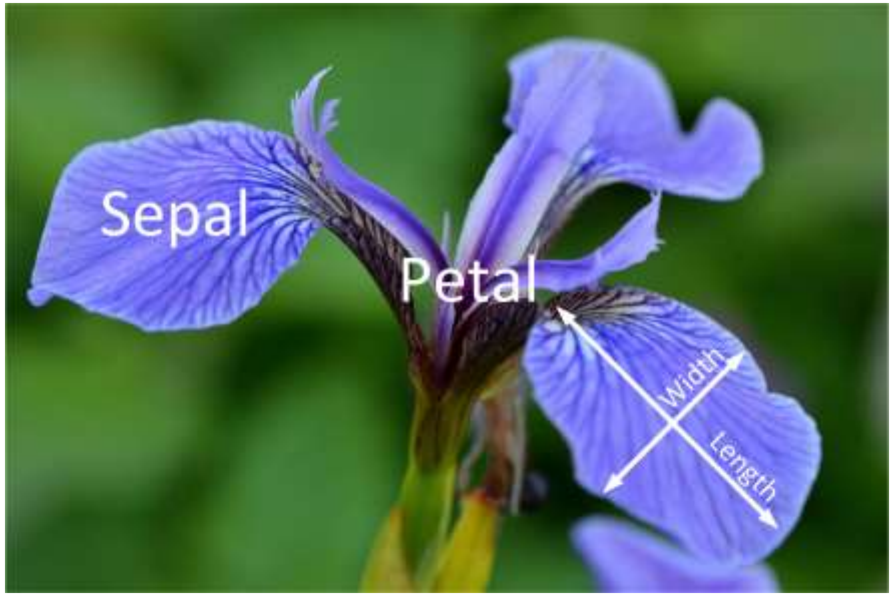
Iris Virginica

Source: Flickr

The Iris Dataset (cont.)

CASE STUDY

- Can we teach a machine to identify the type of iris based on the following four attributes?
  - Sepal length and width
  - Petal length and width



Accuracy and Misclassification Rate

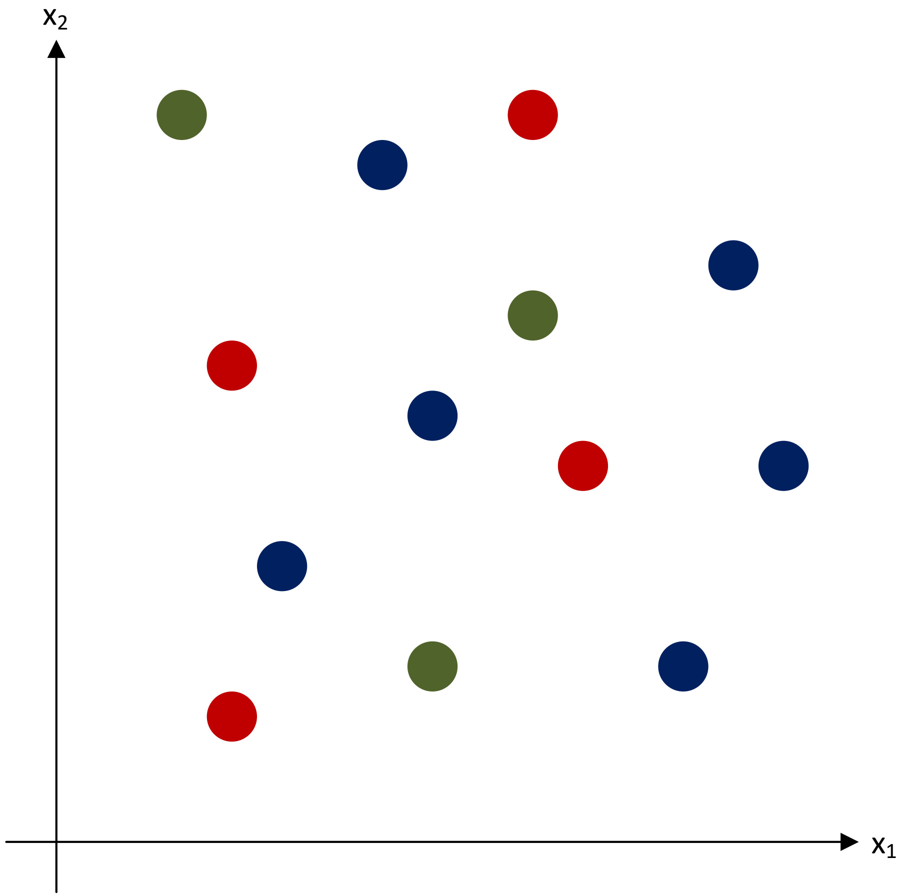
- Accuracy (rate)
  - How many observations that we predicted were correct?
  - This is a value we want as high as possible

- Misclassification rate
  - Of all the observations we predicted, how many were incorrect?
  - This is a value we want as low as possible
  - Directly opposite of accuracy
    - (Pick one or the other; effectively they are the "same")

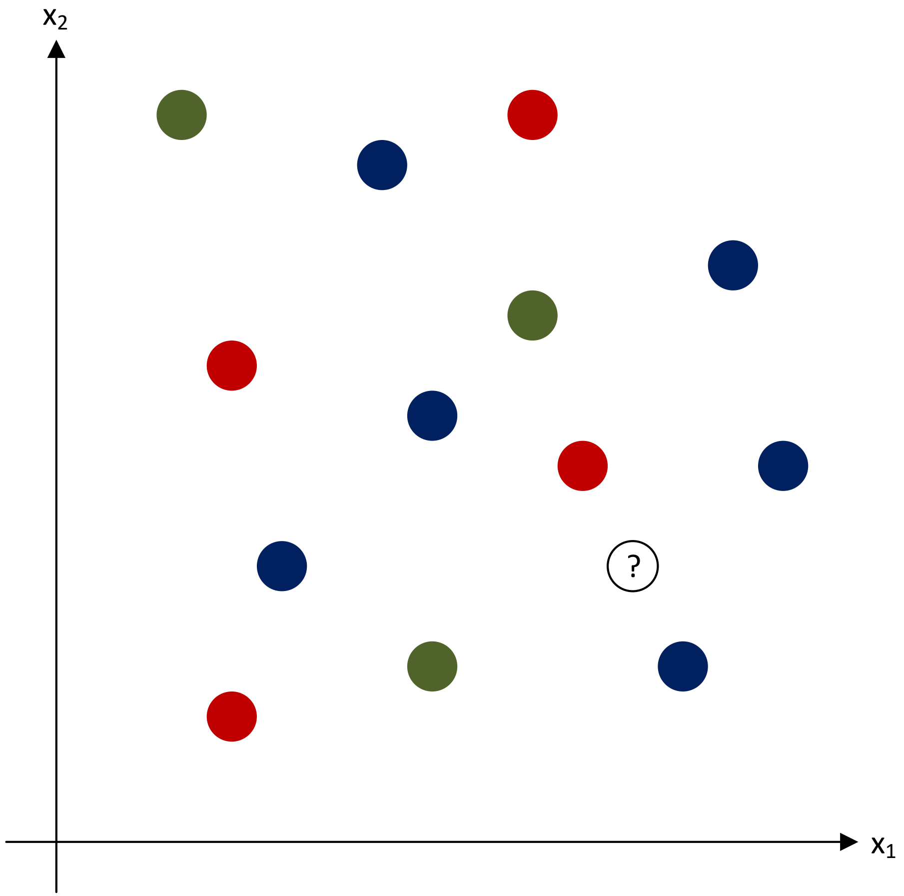
k-Nearest Neighbors

k-Nearest Neighbors

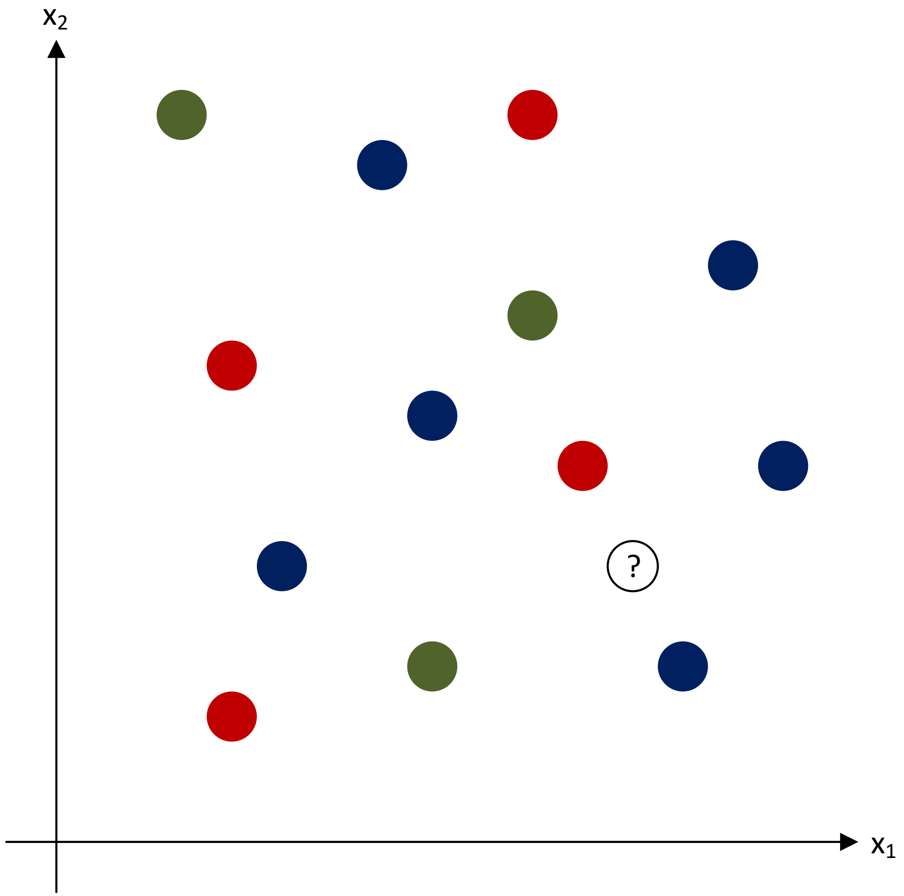
- k-Nearest Neighbors is a classification algorithm that makes a prediction based upon the closest data points



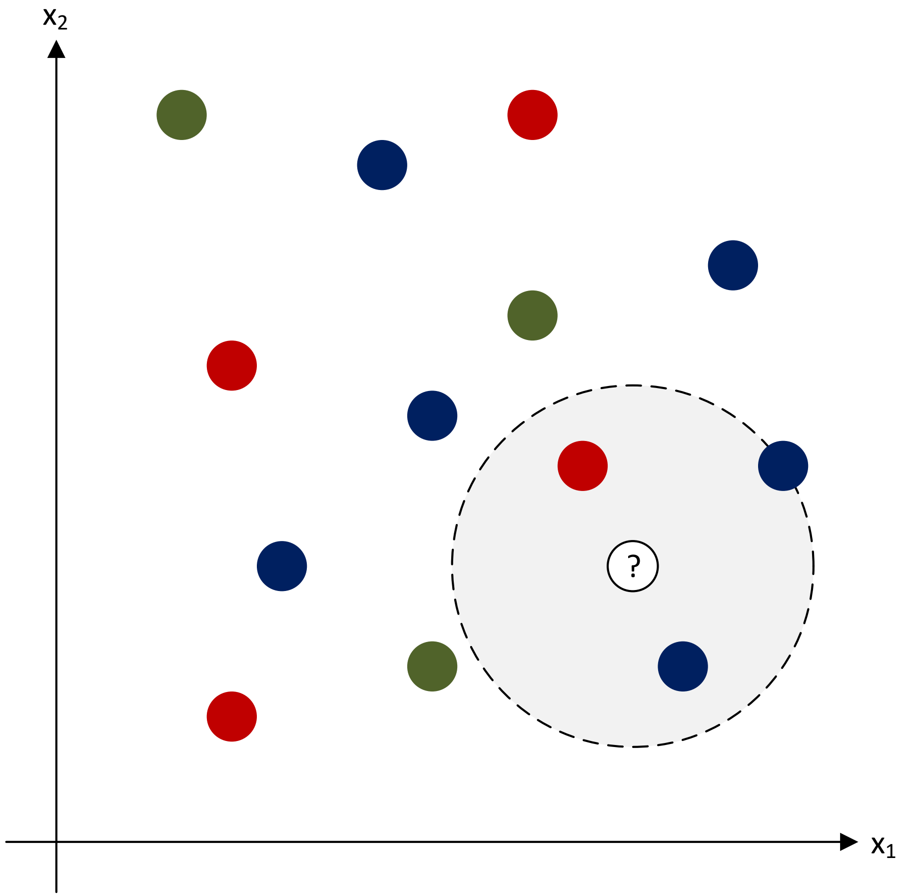
k-Nearest Neighbors | How would you predict the color of the “question mark” point?



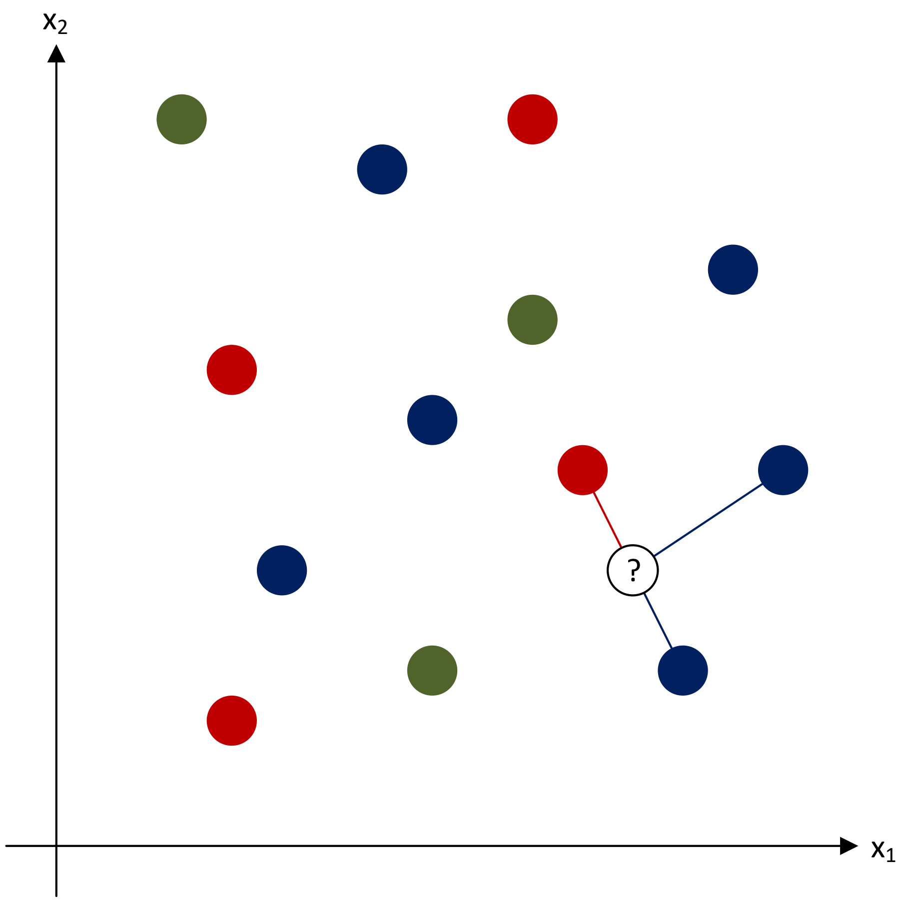
k-Nearest Neighbors | ❶ Pick a value for k, e.g., $k = 3$



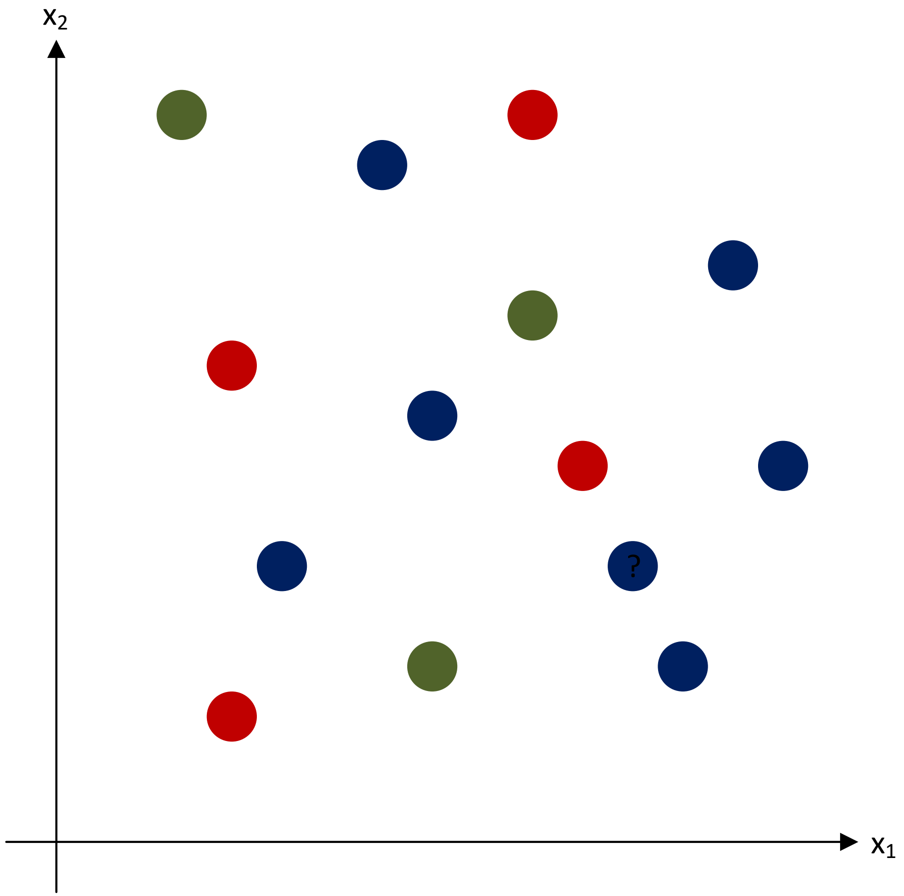
k-Nearest Neighbors | ❷ Calculate the distance to all other points; given those distances, pick the k closest points



k-Nearest Neighbors | ❸ Calculate the probabilities of each class label given those points: $\frac{1}{3}$ "red", $\frac{2}{3}$ "blue"

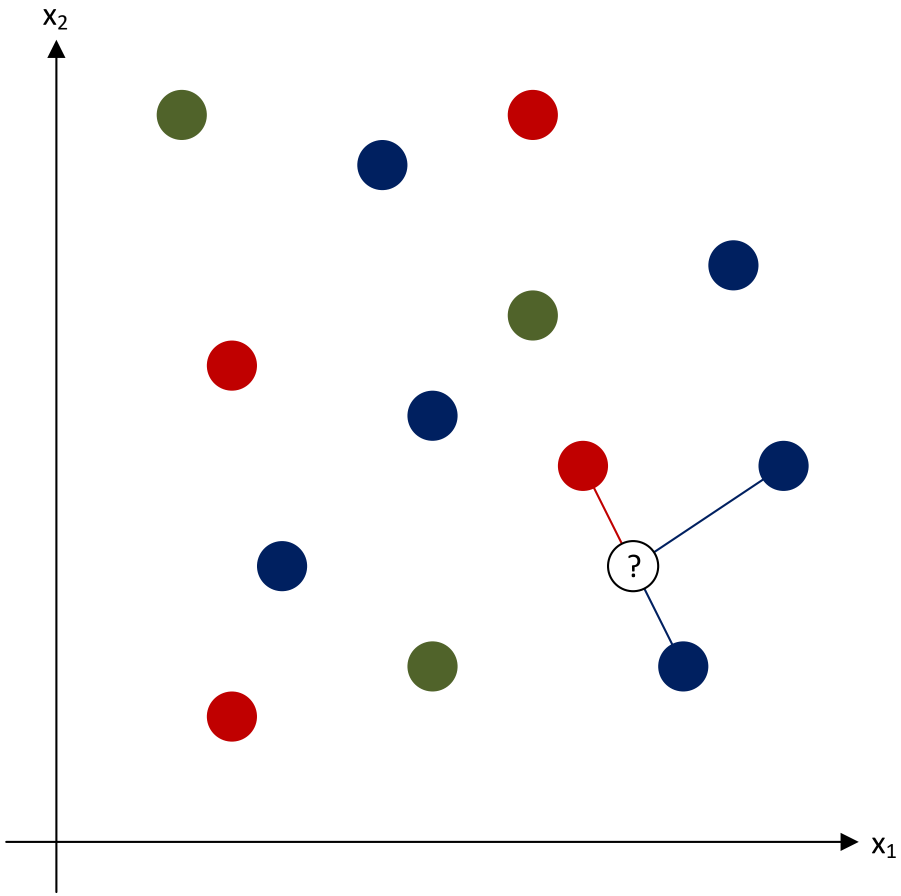


k-Nearest Neighbors | ❹ The original point is classified as the class label with the largest probability (“votes”): “blue”



k-Nearest Neighbors (cont.)

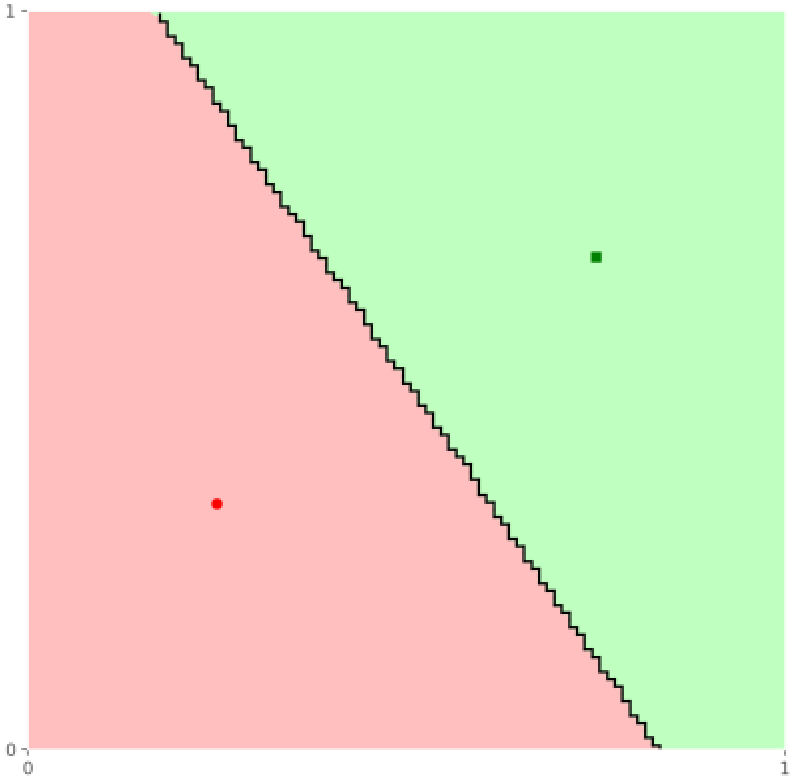
- k-Nearest Neighbors uses distance to predict a class label
- This application of distance is used as a measure of similarity between classifications
  - We are using shared traits to identify the most likely class label



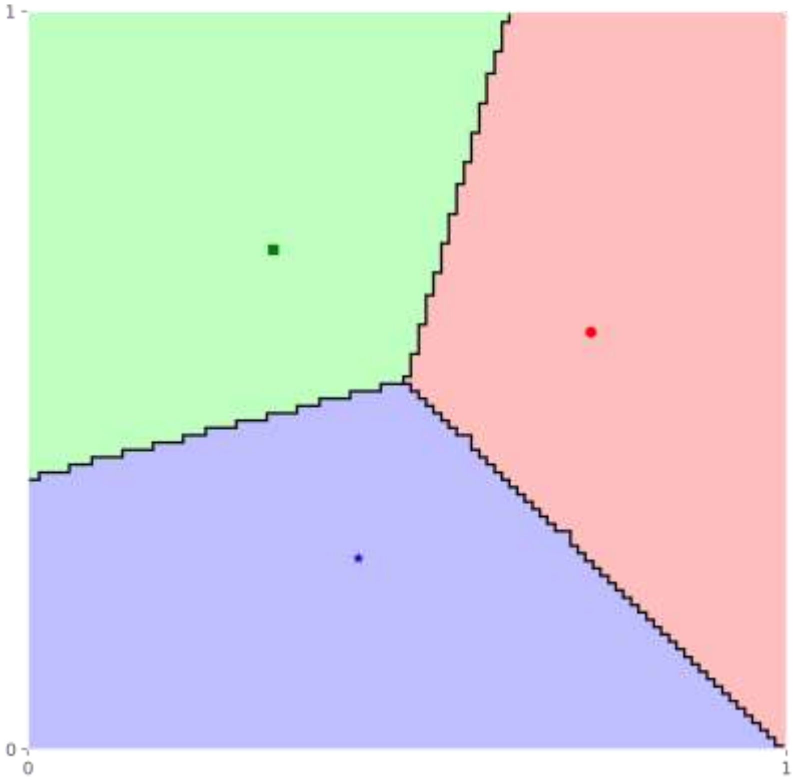
1-Nearest Neighbors

EXAMPLE

$n = 2$



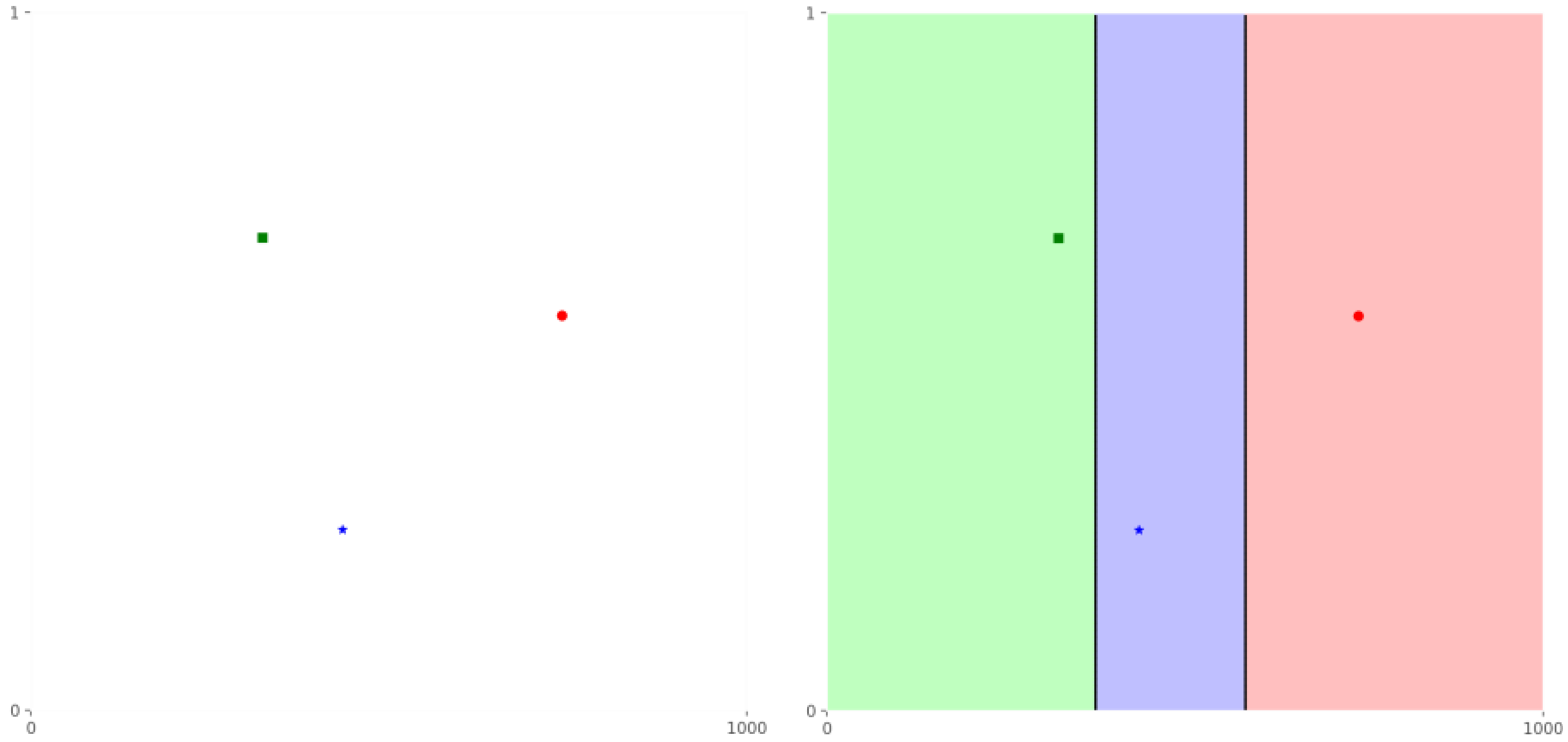
$n = 3$



Feature Normalization

Non-Normalized Features with k-Nearest Neighbors (cont.)

EXAMPLE



Feature Normalization with k-Nearest Neighbors

- k-Nearest Neighbors uses the Euclidean distance to find the closest neighbors:

$$d(A,B) = \sqrt{\left(x_1^A - x_1^B\right)^2 + \left(x_2^A - x_2^B\right)^2}$$

- Let's assume that x_1 and x_2 are not normalized so we have $x_2 \ll x_1$, e.g., x_1 in \$M and x_2 in \$

- In many cases the differences $x_1^A - x_1^B$ is also in \$B and $x_2^A - x_2^B$ in \$ so $\left|x_2^A - x_2^B\right| \ll \left|x_1^A - x_1^B\right|$ or $\left|\frac{x_2^A - x_2^B}{x_1^A - x_1^B}\right| \ll 1$

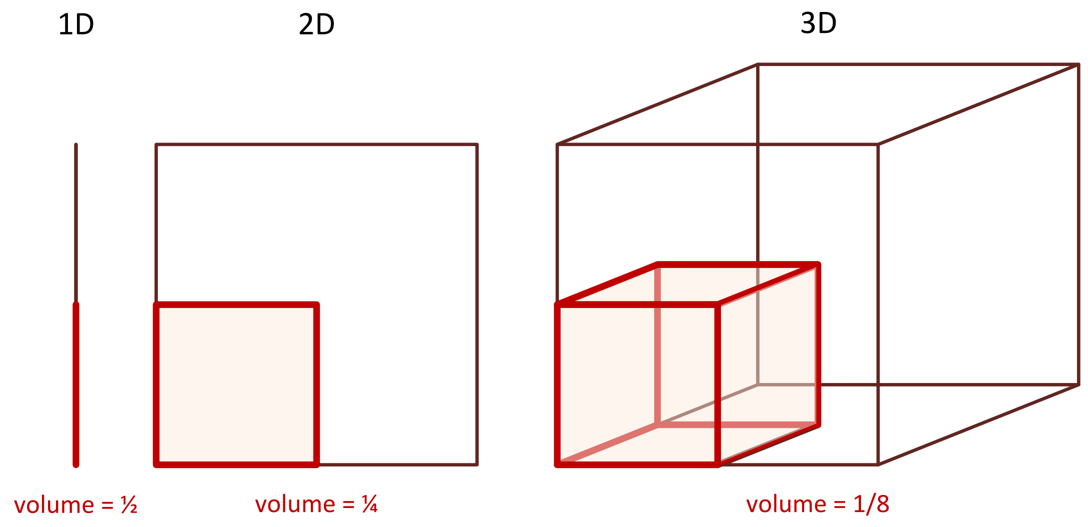
$$d(A,B) = \left|x_1^A - x_1^B\right| \cdot \sqrt{1 + \underbrace{\left(\frac{x_2^A - x_2^B}{x_1^A - x_1^B}\right)^2}_{\ll 1}} \approx \left|x_1^A - x_1^B\right|$$

(i.e., the distance between A and B is independent of the second feature vector x_2)

High Dimensionality

What Happens in High Dimensionality?

- When using (Euclidean) distance, higher dimensionality of data (i.e., more features) requires significantly more samples in order to have the same predictive power

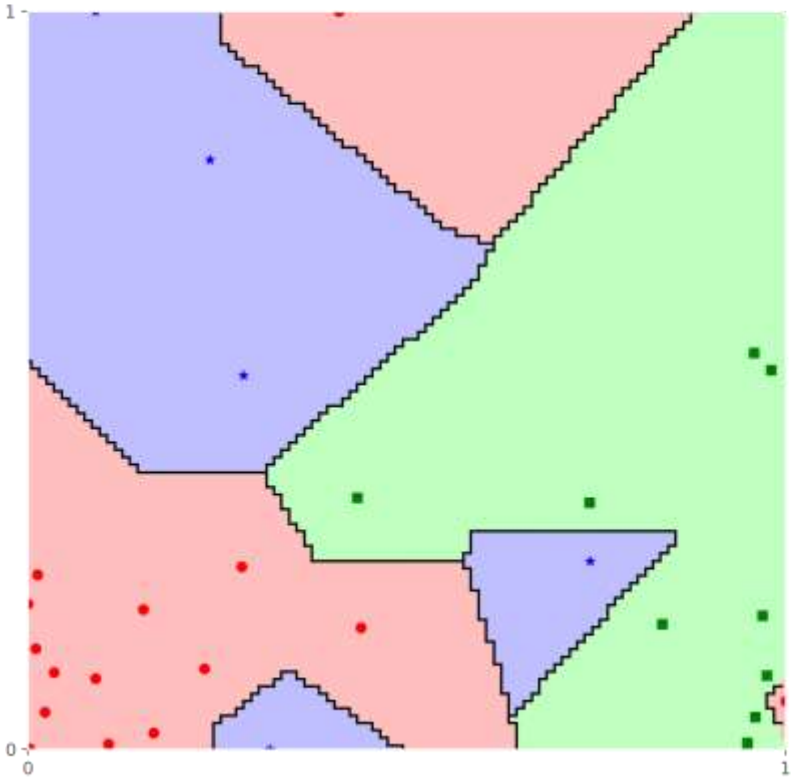


Model Fit

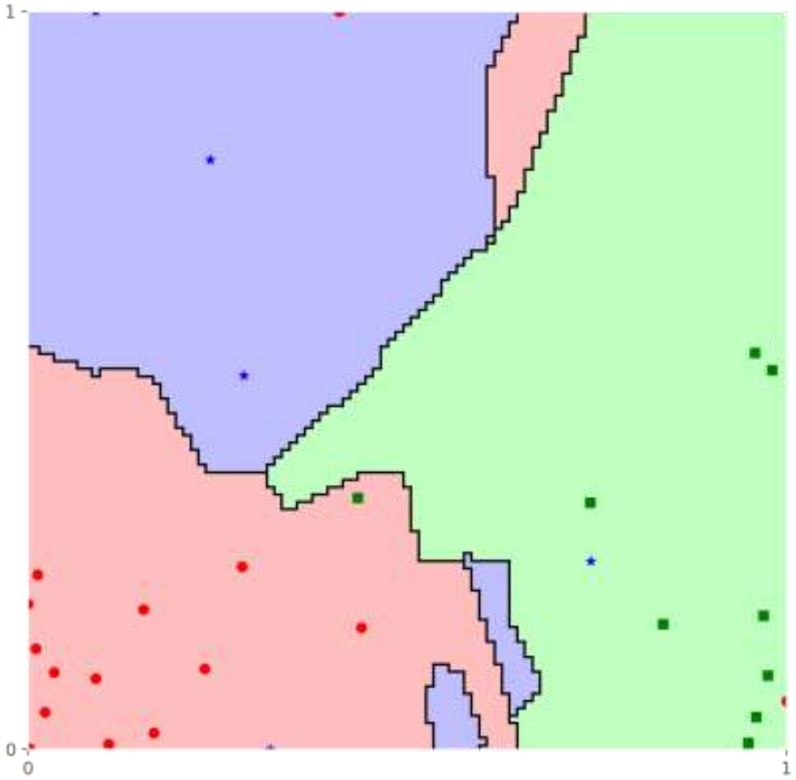
Model Fit | Motivating Example (cont.)

EXAMPLE

$k = 2$



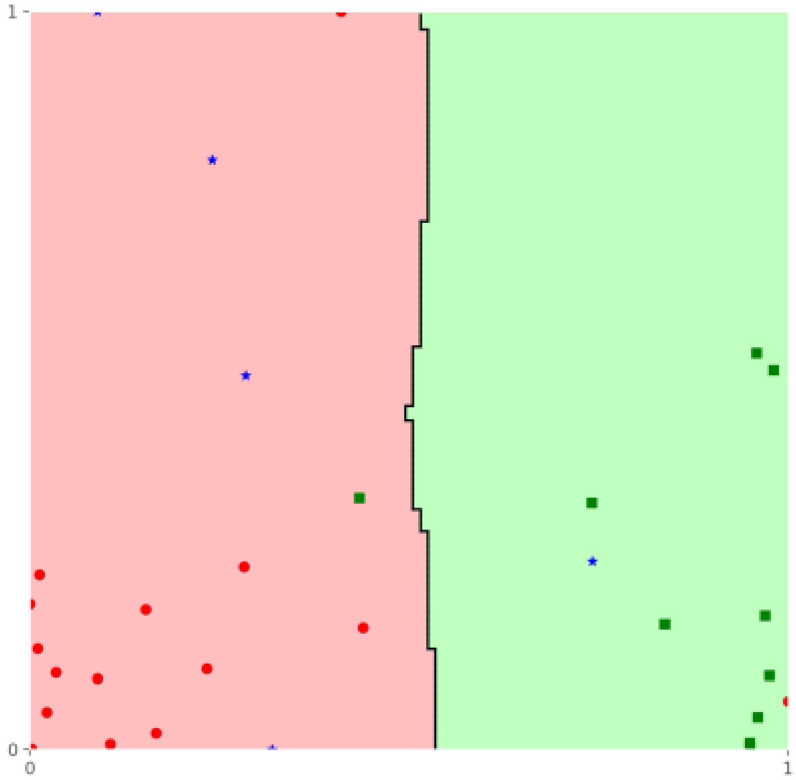
$k = 3$



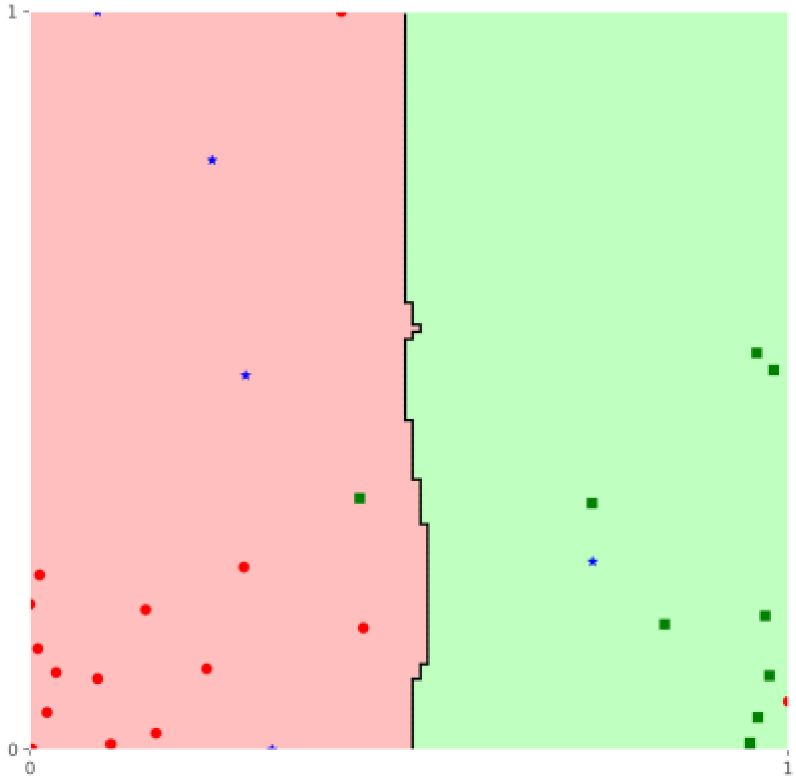
Model Fit | Motivating Example (cont.)

EXAMPLE

$k = 15$



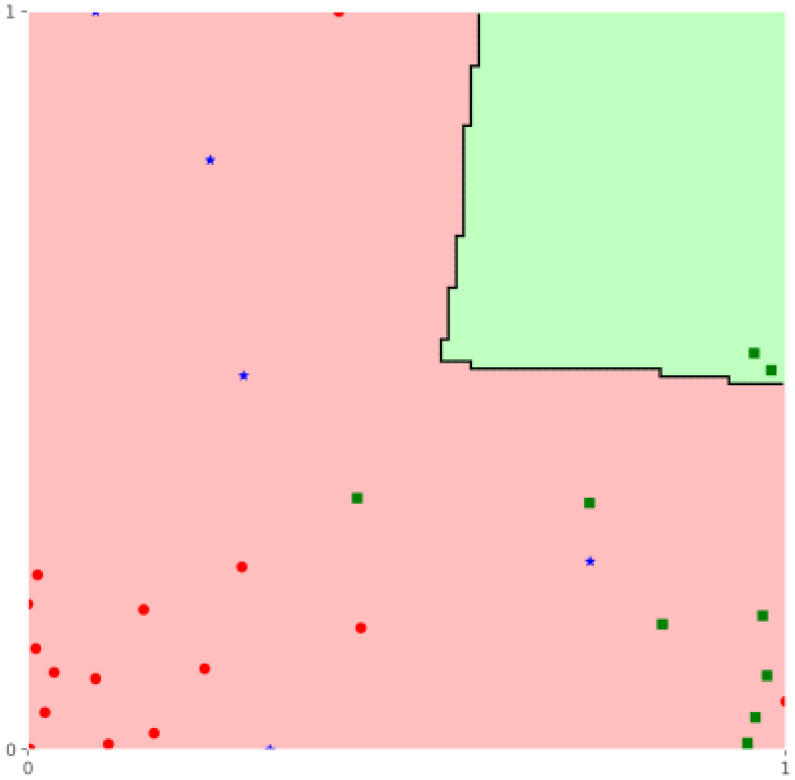
$k = 16$



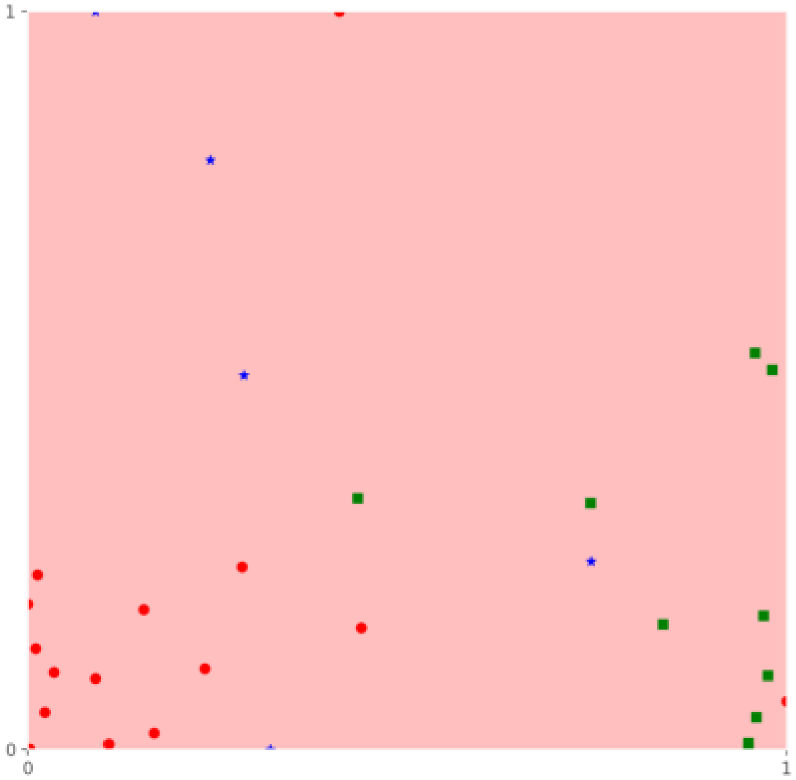
Model Fit | Motivating Example (cont.)

EXAMPLE

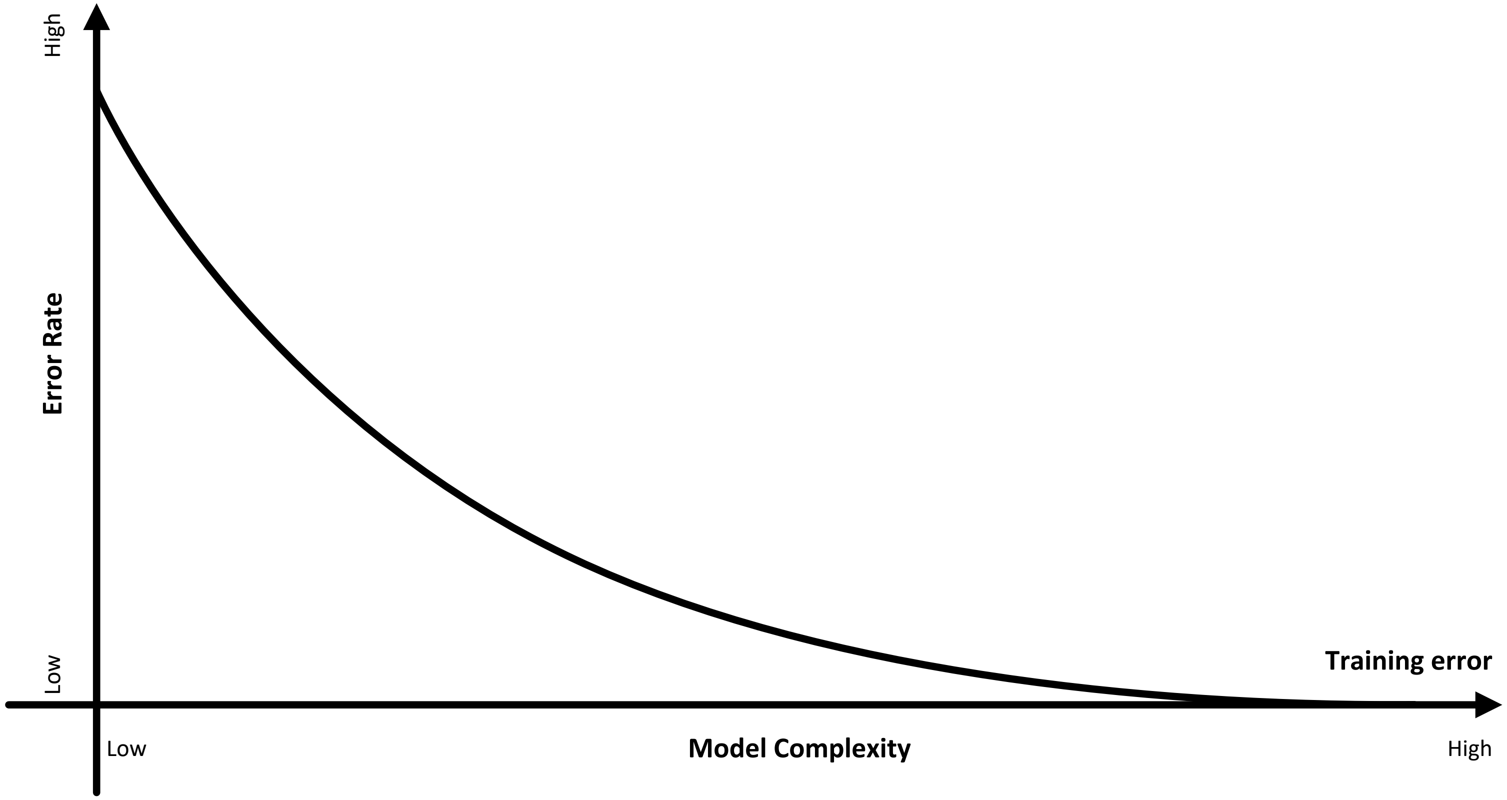
$k = 25$



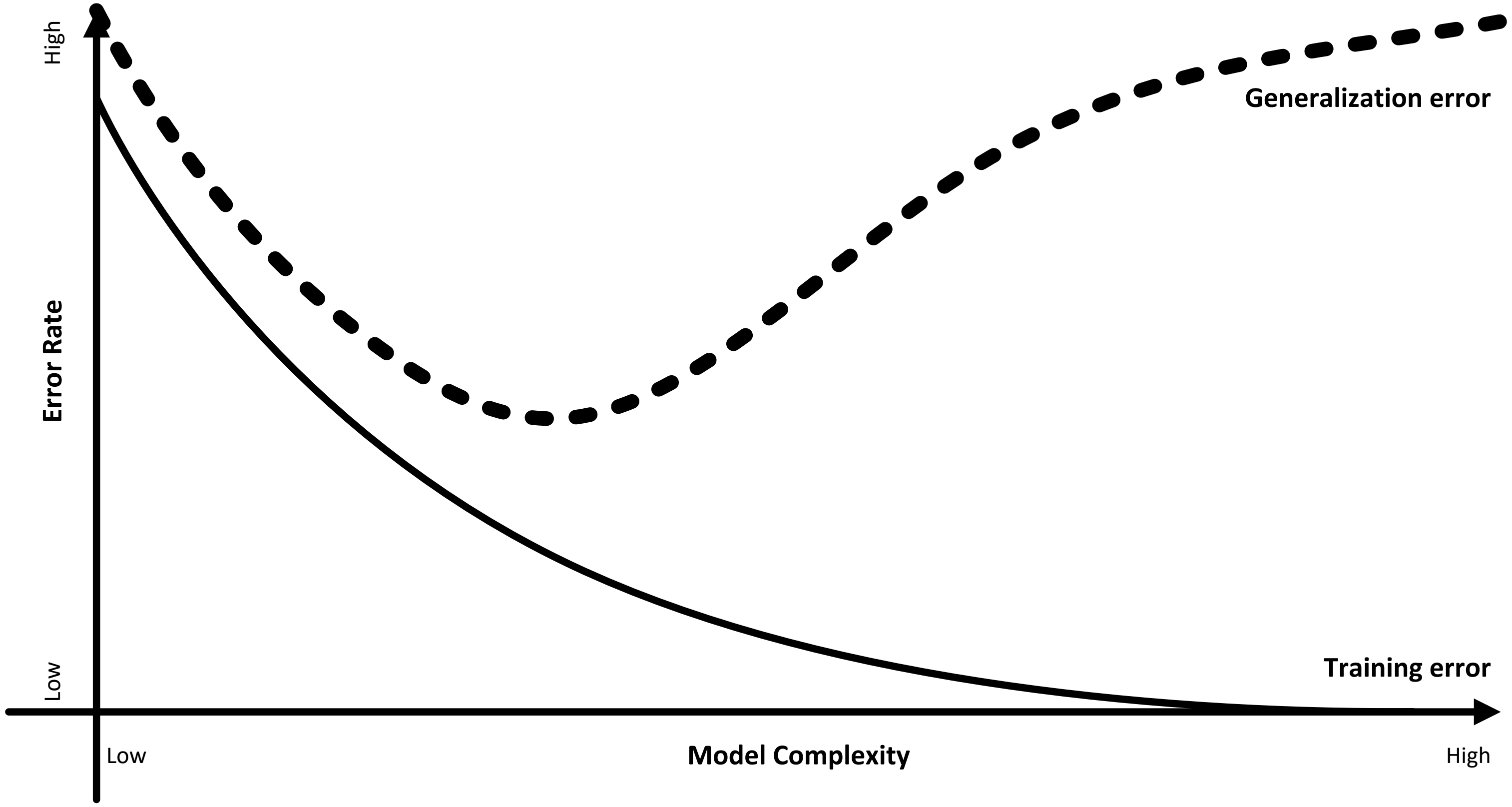
$k = 26$



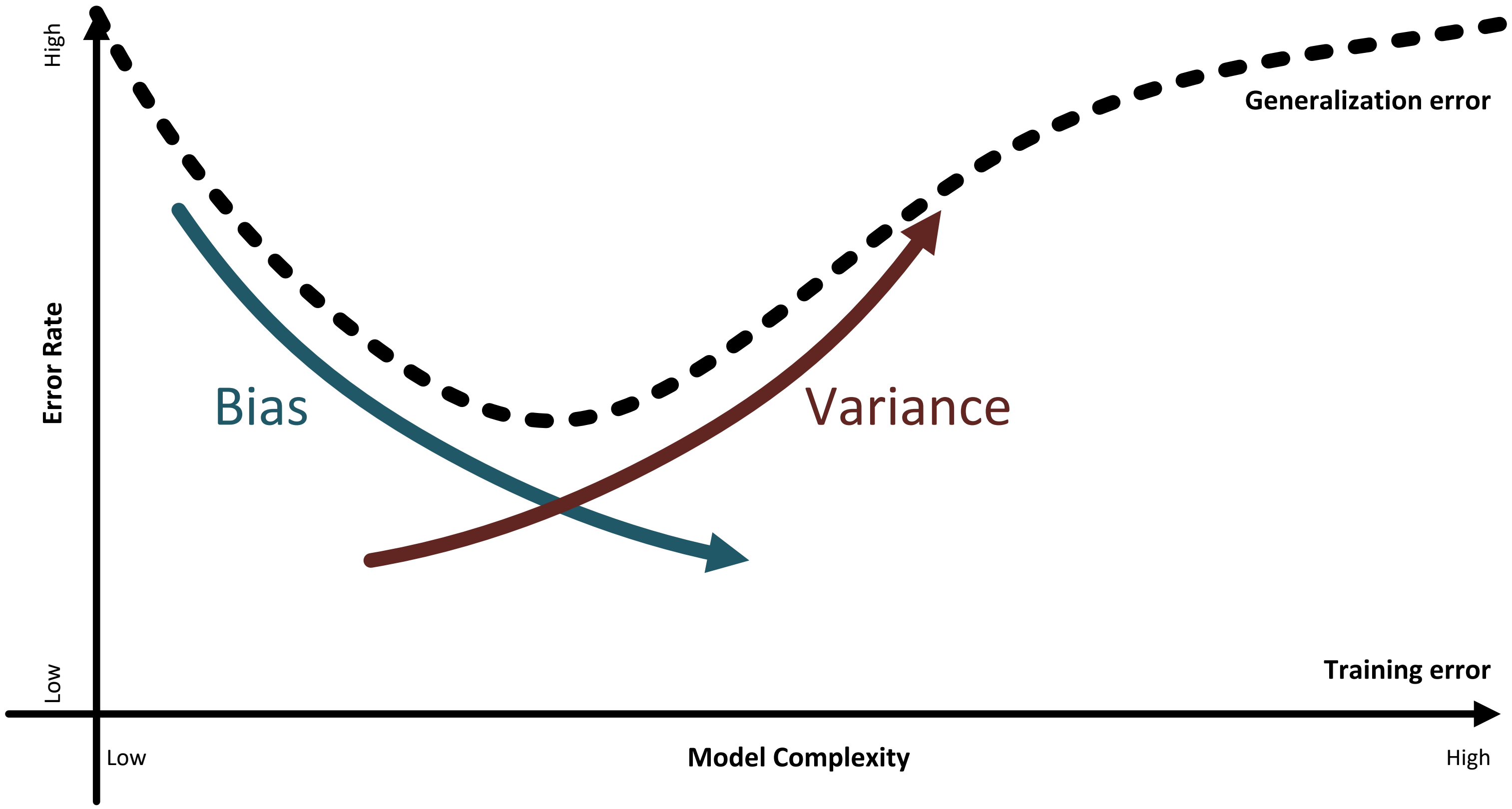
The Training Error can go down to zero (effectively memorizing the entire dataset)



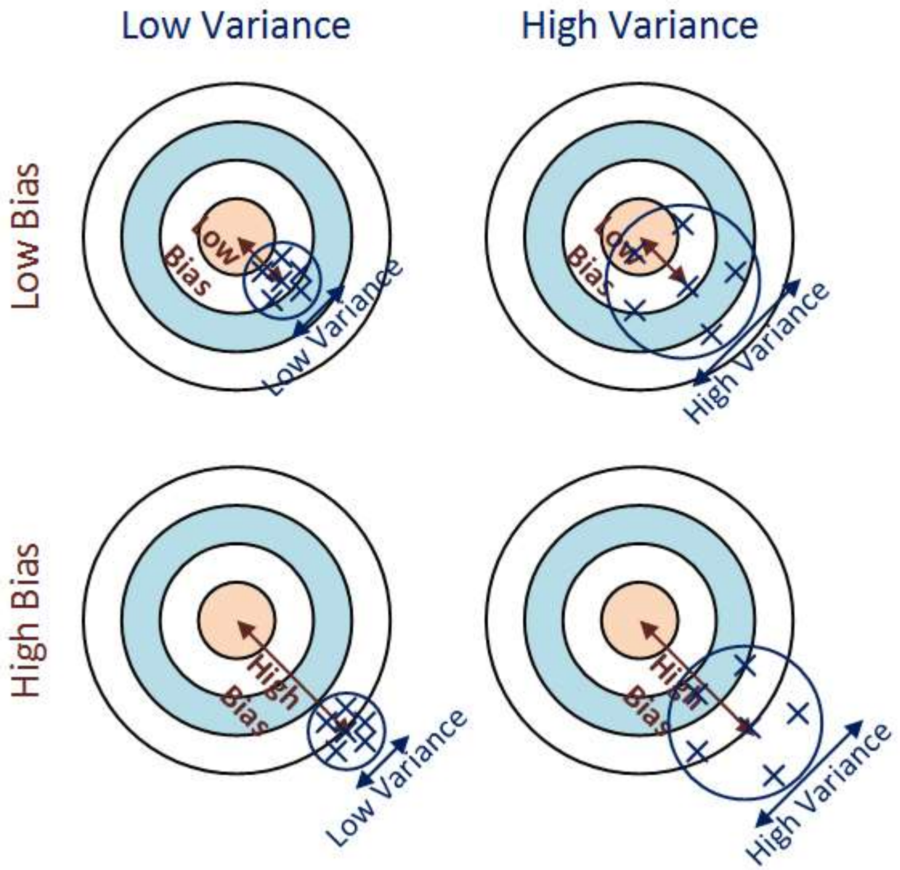
As the model gets more complex, the Generalization Error initially goes down; however, after reaching a minimum, it goes back up



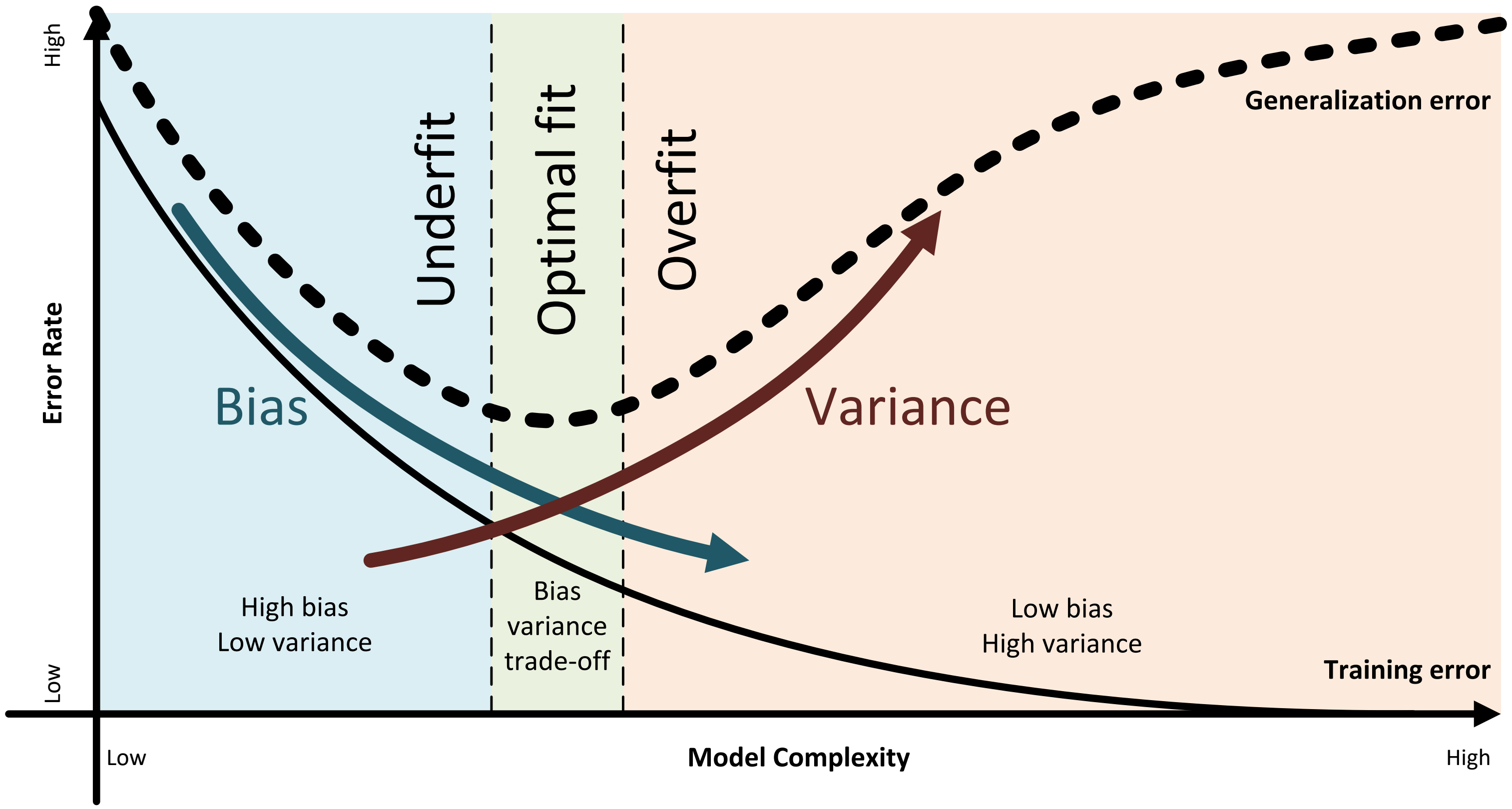
The Generalization Error is made of two components: Bias and Variance



The Bias is a systematic, non-random error; the Variance is an idiosyncratic, random error



Errors, Complexity, Fit, Bias, and Variance

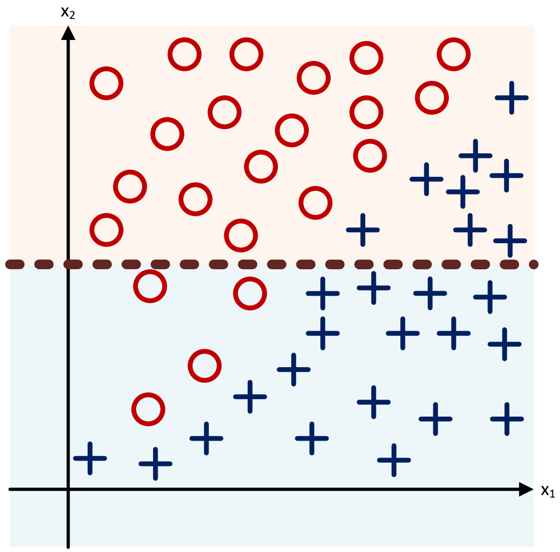


Errors, Complexity, Fit, Bias, and Variance (cont.)

EXAMPLE

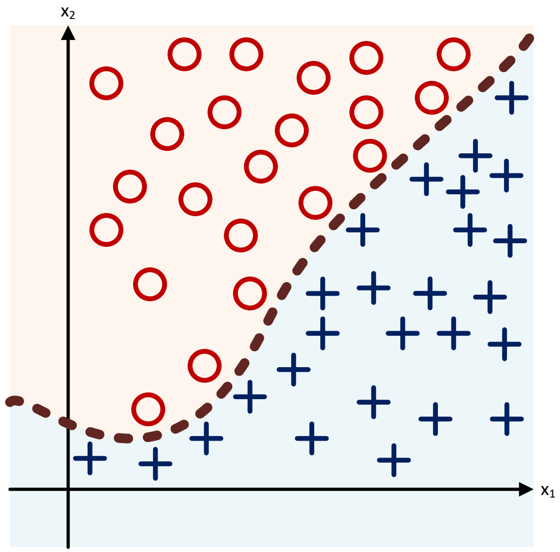
Underfit

high bias/low variance



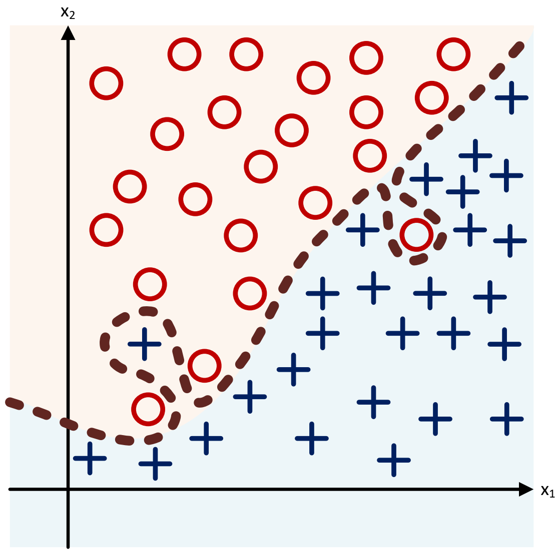
Optimal Fit

bias-variance trade-off

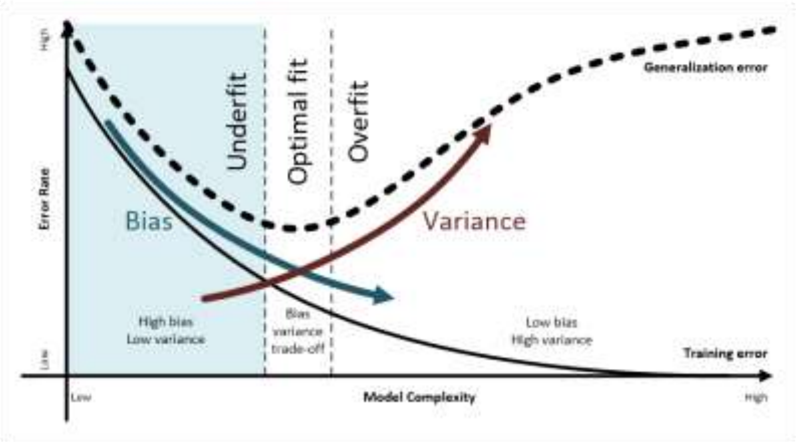


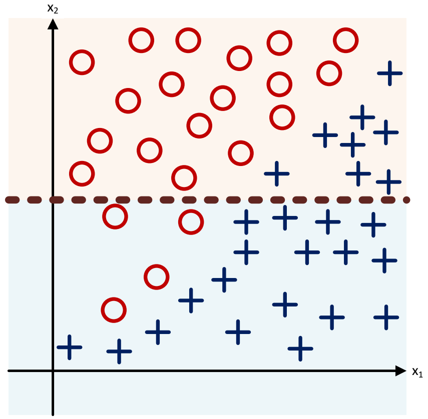
Overfit

low bias/high variance



Underfit

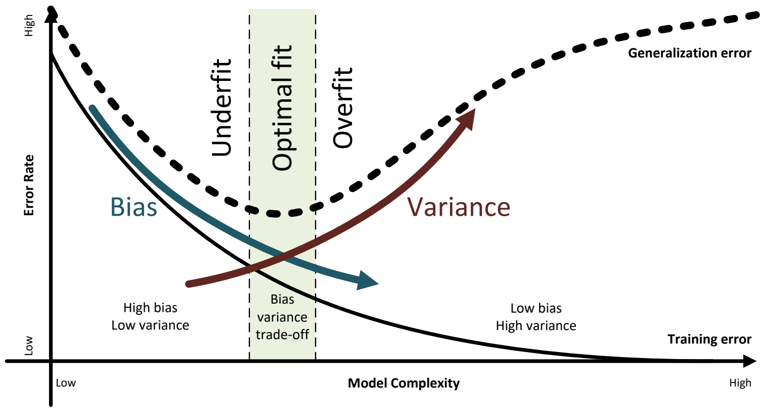


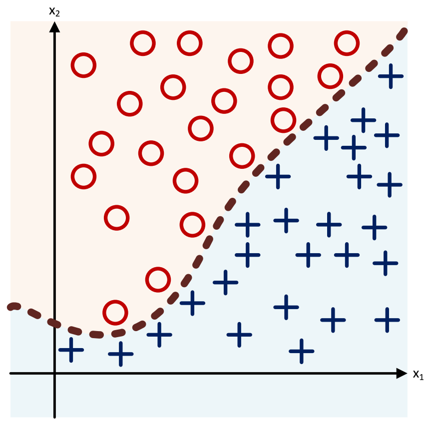


- Underfit
  - Model too simple
  - It cannot represent the desired behavior very well; both its training and generalization error are poor
  - High bias; low variance

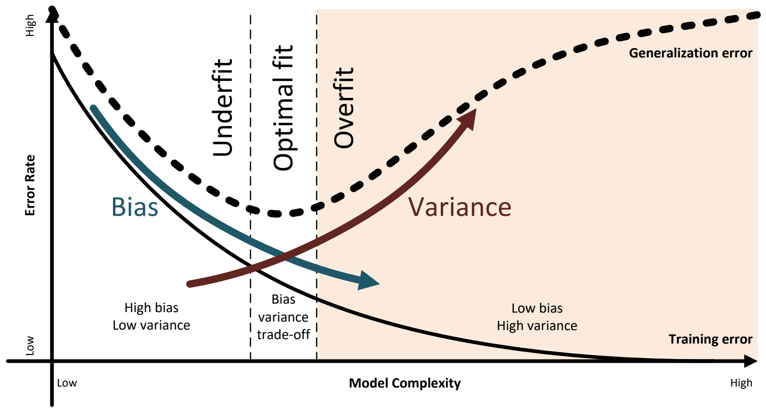
Optimal Fit

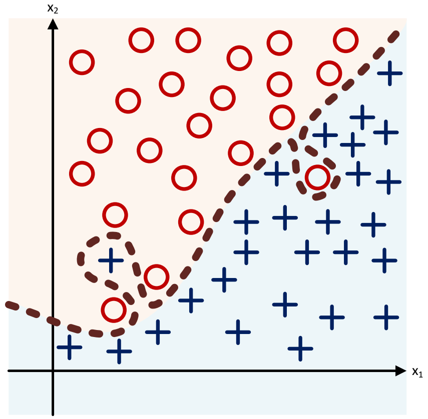
- Optimal Fit
  - Model has the right level of complexity
  - It performs well on the training set (low training error) and generalize well to unknown data points (low generalization error)





Overfit

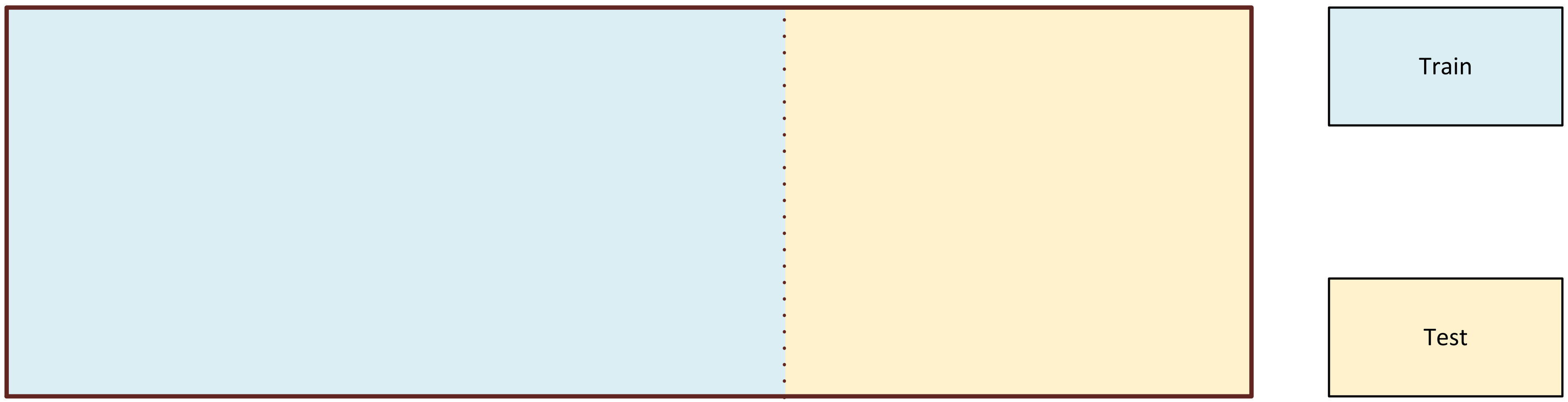




- Overfit
  - Model too complex
  - It performs very well on the training set (low training error) but does not generalize well to unseen data points (high generalization error)
  - Low bias; high variance

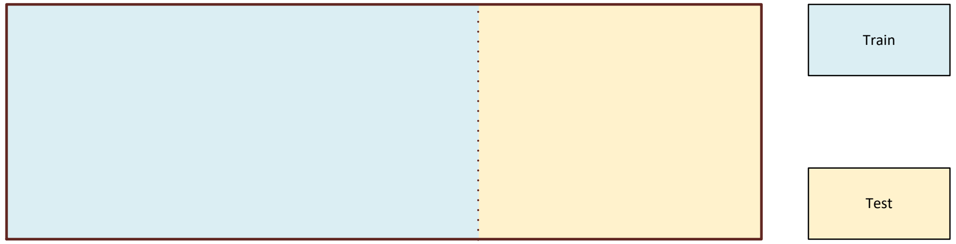
So far, we used the entire dataset to train the models.
Question: How can we estimate the Generalization Error?

Answer: Divide (randomly) the dataset into a Train Set and a Test Set

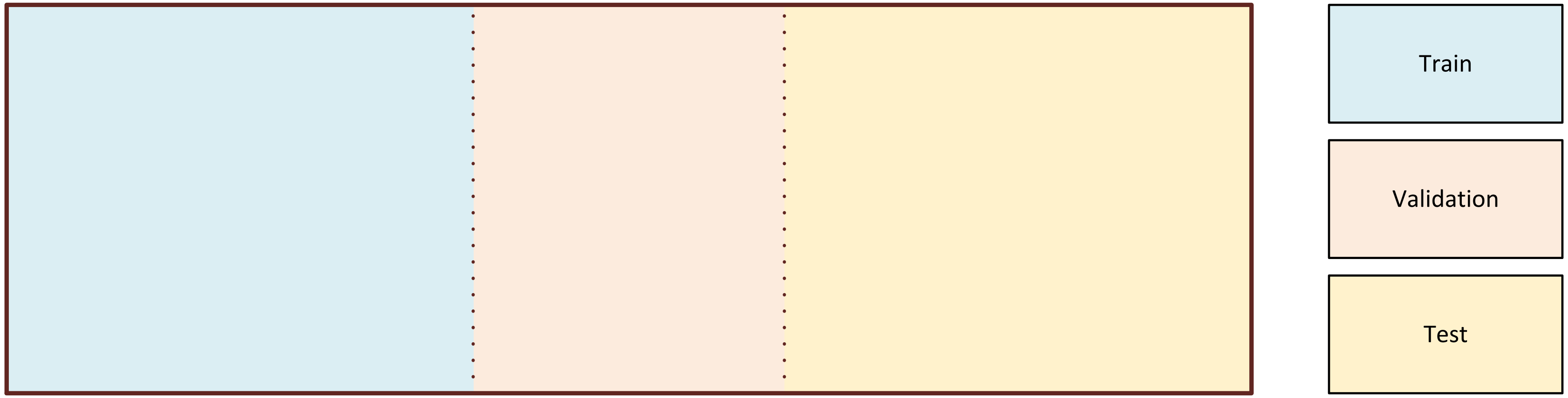


Train and Test Sets

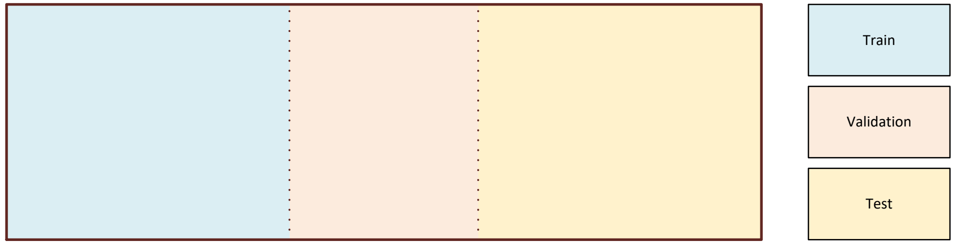
- Set aside the test set; don't look at it until the very end
- Train your model with the train set
  - Remodel as needed until you are satisfied with your model performance on the train set (low training error)
- Evaluate your model on the test set to compute the generalization error
  - Only then do you now know whether your model underfits, overfits, or seems ok
- If you need to go back and remodel you need a new test: as you incorporate knowledge from the test set back into your remodel, the test set's previously unseen data points are not longer unseen
  - Question: How can we really keep our test set aside until the very end



Answer: Divide (randomly) again your Train Set into a (new) Train Set and a Validation Set

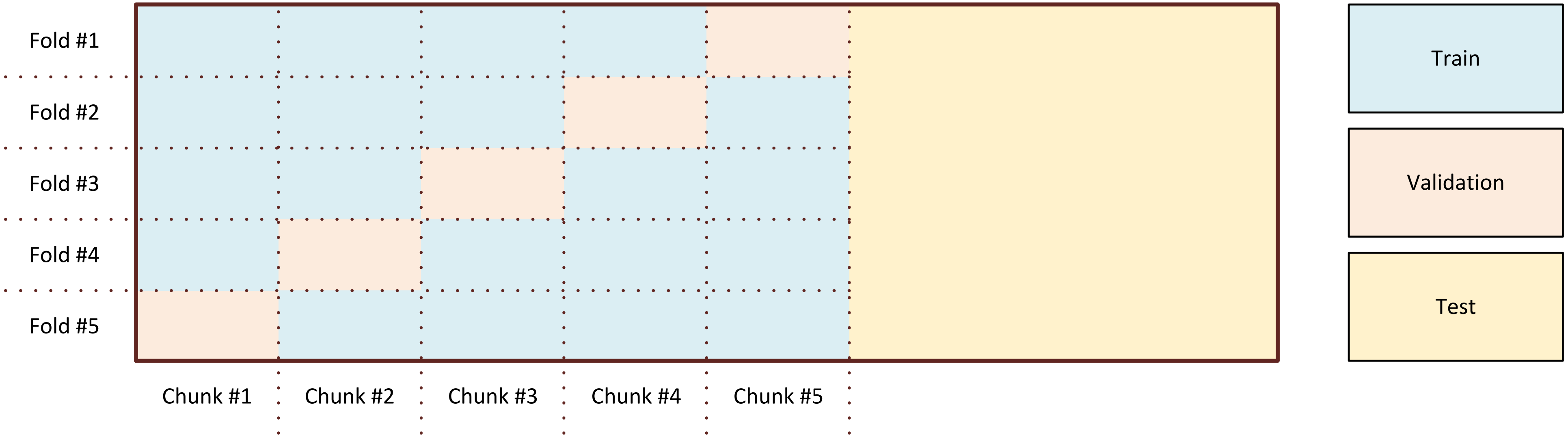


Train, Validation, and Test Sets



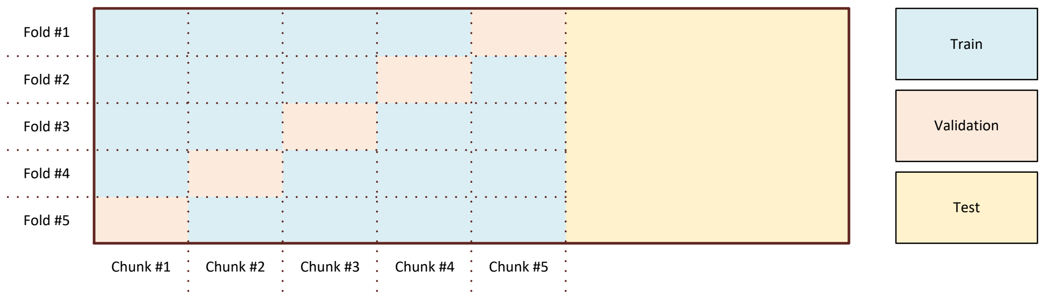
- You still train the model with the train set (model building) but now you use the cross-validation set, not the test set, to estimate the generalization error (model checking)
- After using the cross-validation set and before a new phase of remodeling, you should then reshuffle data between your train set and your cross-validation set
- Question: Reshuffling the train/cross-validation sets seems heavy work. Can we do better?

Answer: Yes, we can. Using k-Fold Cross-Validation

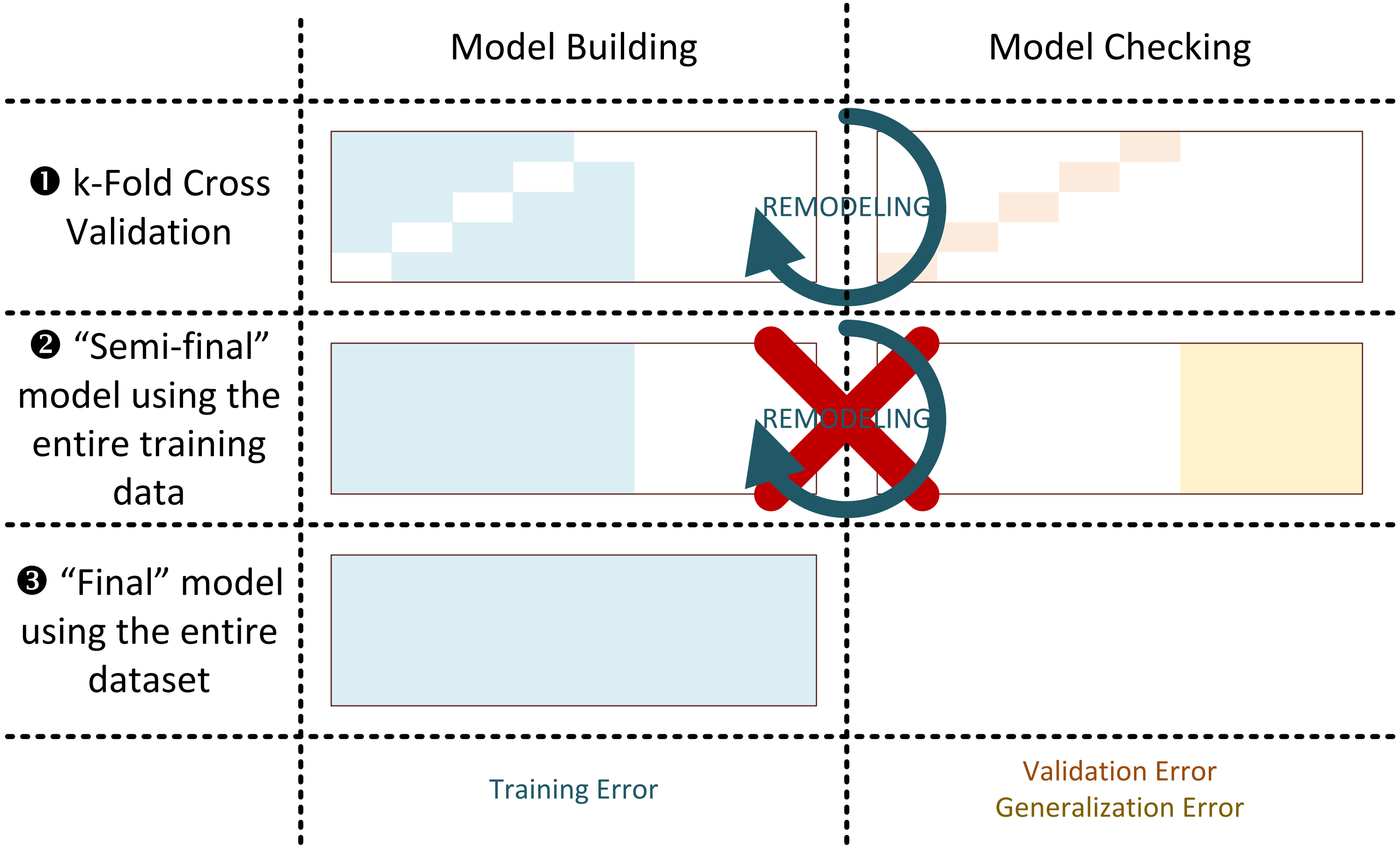


k-Fold Cross-Validation

- Typically, $k = 5$ or 10 with each sample being used both for training ($k - 1$ times) and validation (1 time)
- The training/validation errors are the average training/validation errors across all folds
- After selecting the model that minimize the validation error, you then build a final model that uses all the training data



Model Building and Model Checking with k-Fold Cross-Validation



k-Nearest Neighbors

Pros and Cons

k-Nearest Neighbors | Pros and Cons

- Pros
  - Intuitive and simple to explain
  - Training phase is fast
  - Non-parametric (does not presume a “form” of the decision boundary)
  - The decision boundary easily captures non-linearity

- Cons
  - Not interpretable
  - Prediction phase can be slow when n (number of observations) is large
  - Very sensitive to feature scaling; need to standardize the data
  - Sensitive to irrelevant features
  - Cannot be used if you have sparse data and feature space with dimension $p \geq 4$