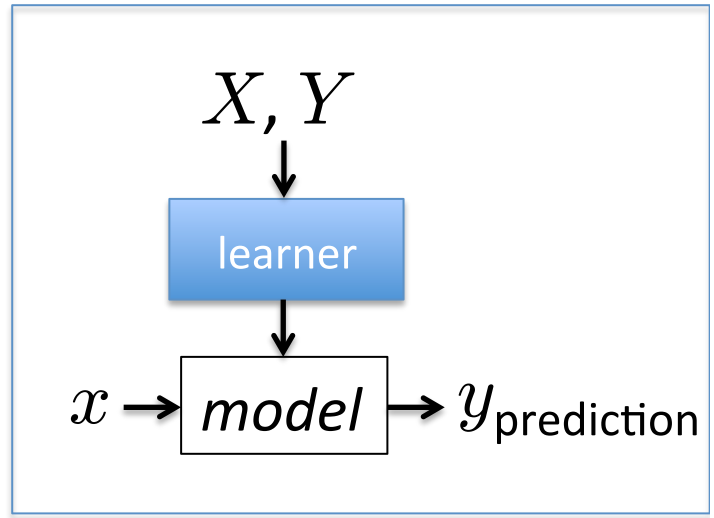
Evaluation

Stages of (Batch) Machine Learning

Given: labeled training data $X, Y = \left\{ \left\langle x^{(i)}, y^{(i)} \right\rangle \right\}_{i=1}^{n}$

- Assumes each $x^{(i)} \sim \mathcal{D}(\mathcal{X})$ with $y^{(i)} = f_{target}\left(x^{(i)}\right)$



Train the model:

model ← *classifier*.train(X, Y)

Apply the model to new data: $x \sim \mathcal{D}(\mathcal{X})$

- Given: new unlabeled instance

$y_{\text{prediction}}$ ← *model*.predict(x)

Classification Metrics

$$\text{accuracy} = \frac{\#\text{ correct predictions}}{\#\text{ test instances}}$$

$$\text{error} = 1 - \text{accuracy} = \frac{\#\text{ incorrect predictions}}{\#\text{ test instances}}$$

Confusion Matrix

- Given a dataset of P positive instances and N negative instances:

		Predicted Class	
		Yes	No
Actual Class	Yes	TP	FN
	No	FP	TN

$$\text{accuracy} = \frac{TP + TN}{P + N}$$

- Imagine using classifier to identify positive cases (i.e., for information retrieval)

$$\text{precision} = \frac{TP}{TP + FP}$$

Probability that a randomly selected result is relevant

$$\text{recall} = \frac{TP}{TP + FN}$$

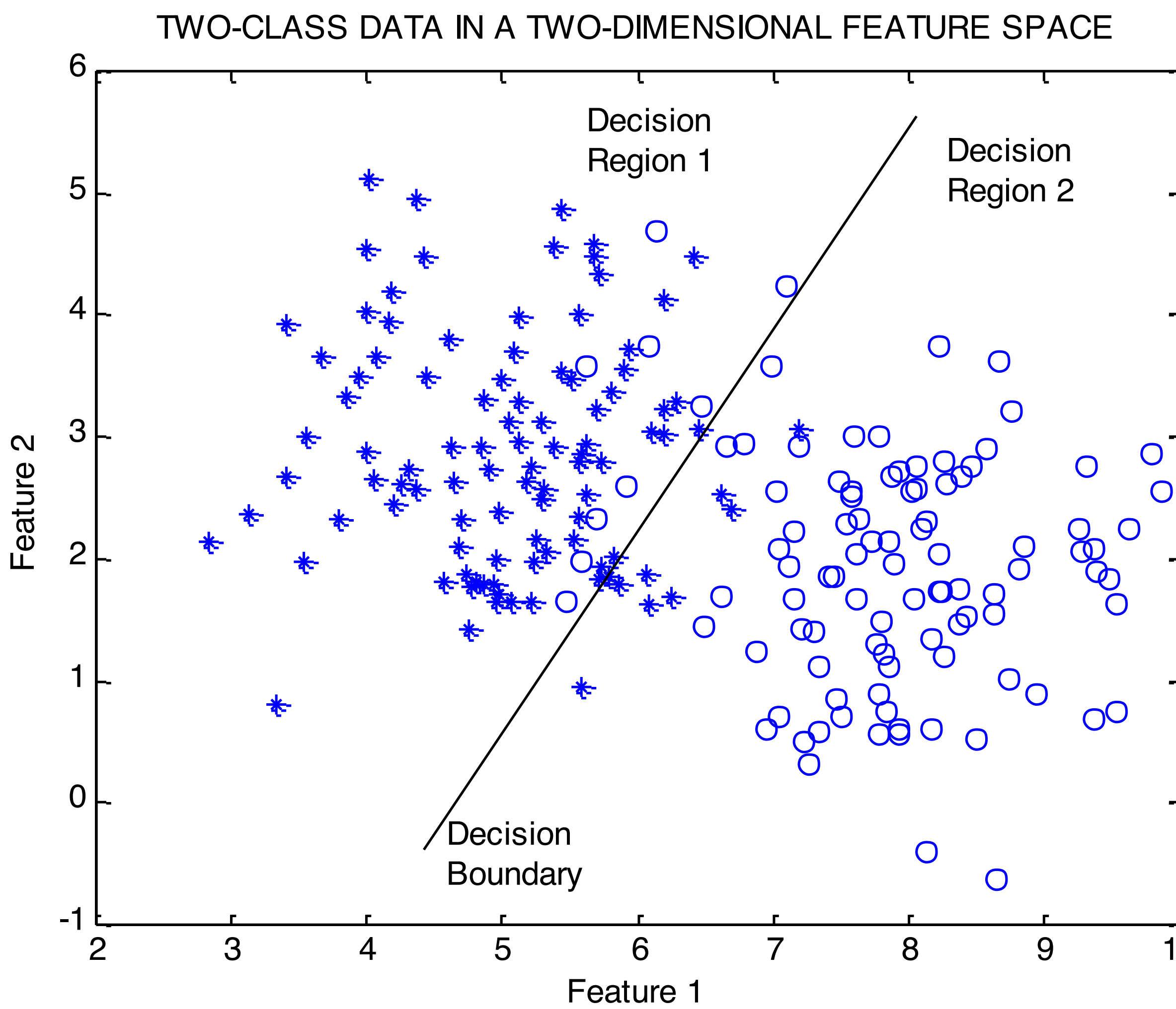
Probability that a randomly selected relevant document is retrieved

Training Data and Test Data

- Training data: data used to build the model
- Test data: new data, not used in the training process

- Training performance is often a poor indicator of generalization performance
  - Generalization is what we really care about in ML
  - Easy to overfit the training data
  - Performance on test data is a good indicator of generalization performance
  - i.e., test accuracy is more important than training accuracy

Simple Decision Boundary



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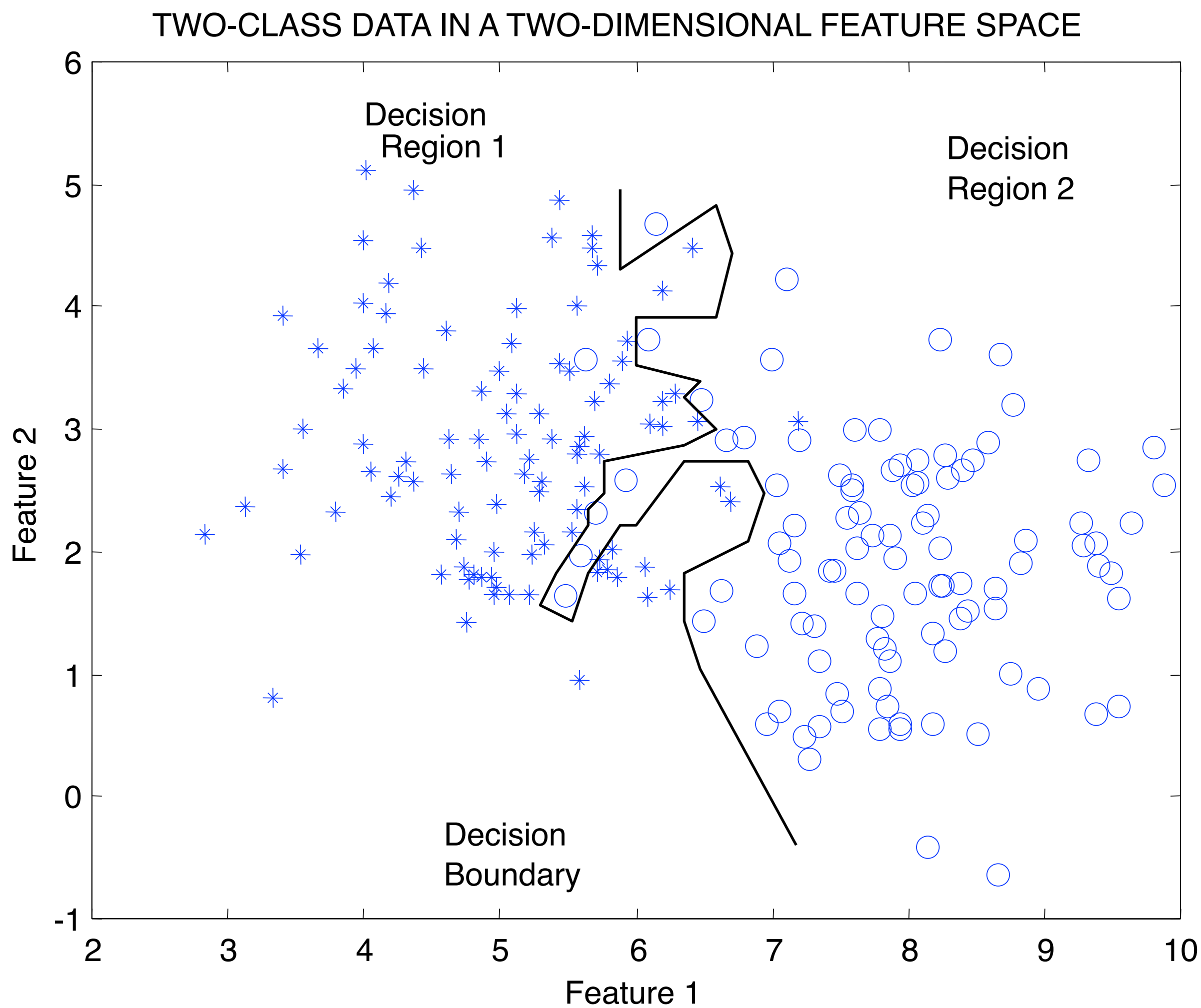
More Complex Decision Boundary



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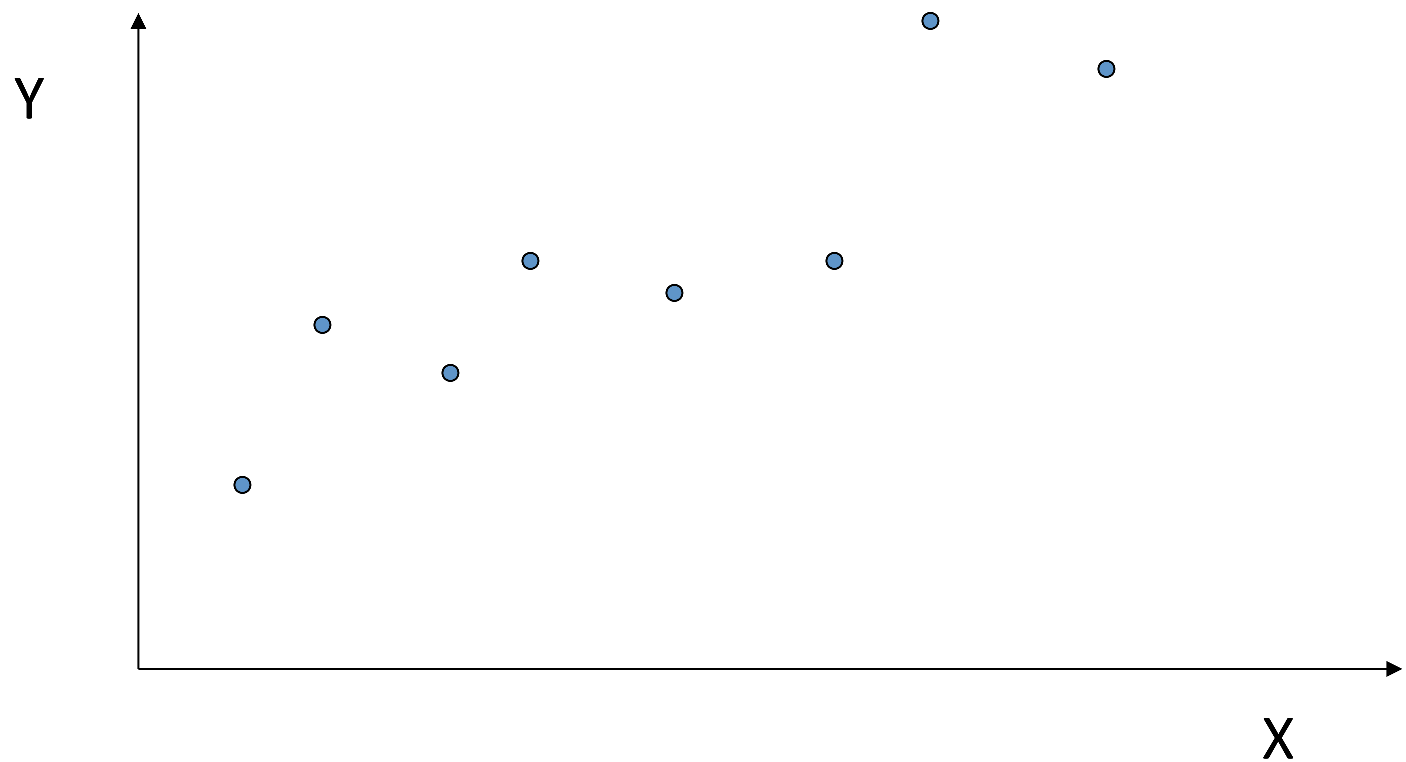
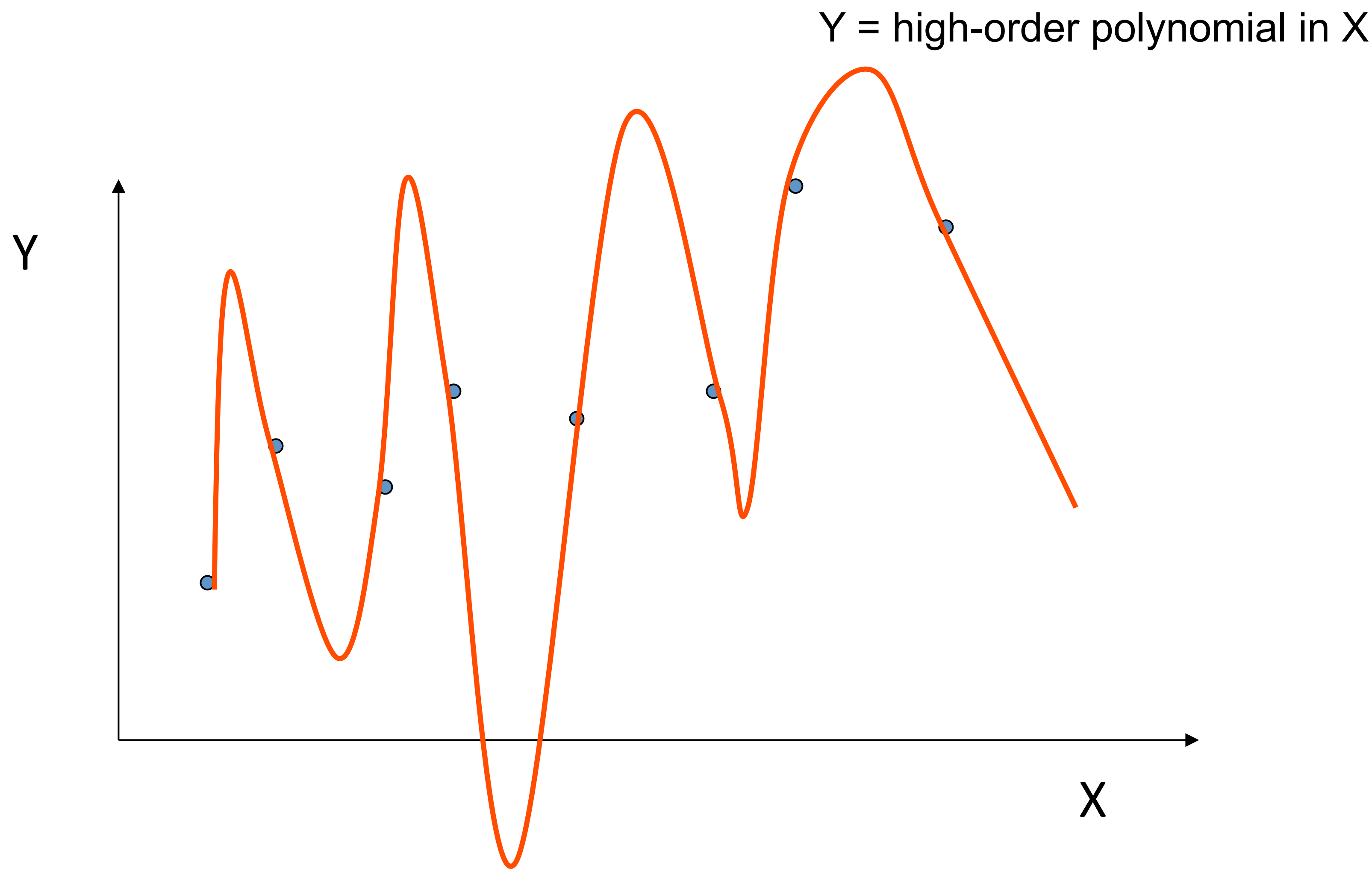
Example: The Overfitting Phenomenon



A Complex Model



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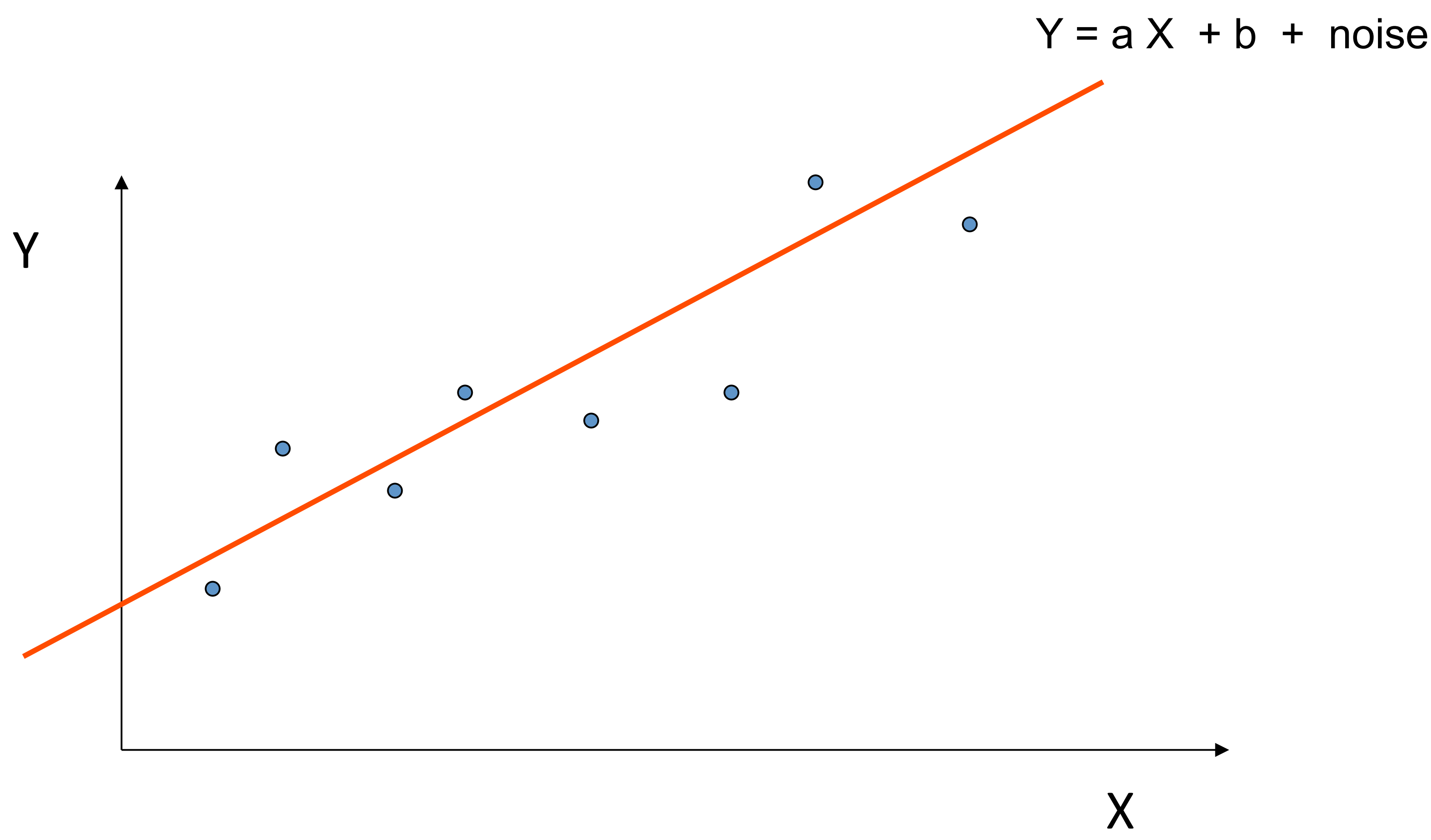
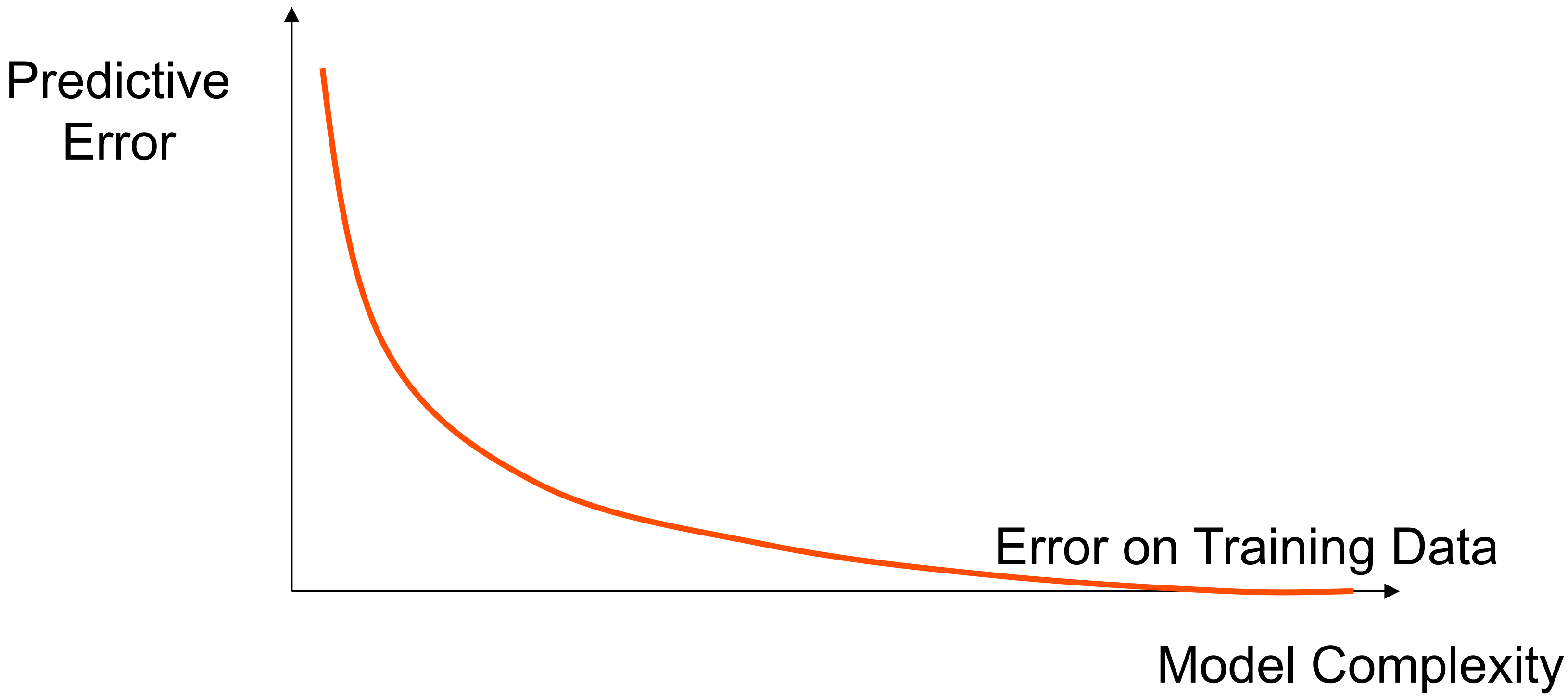
The True (simpler) Model



How Overfitting Affects Prediction



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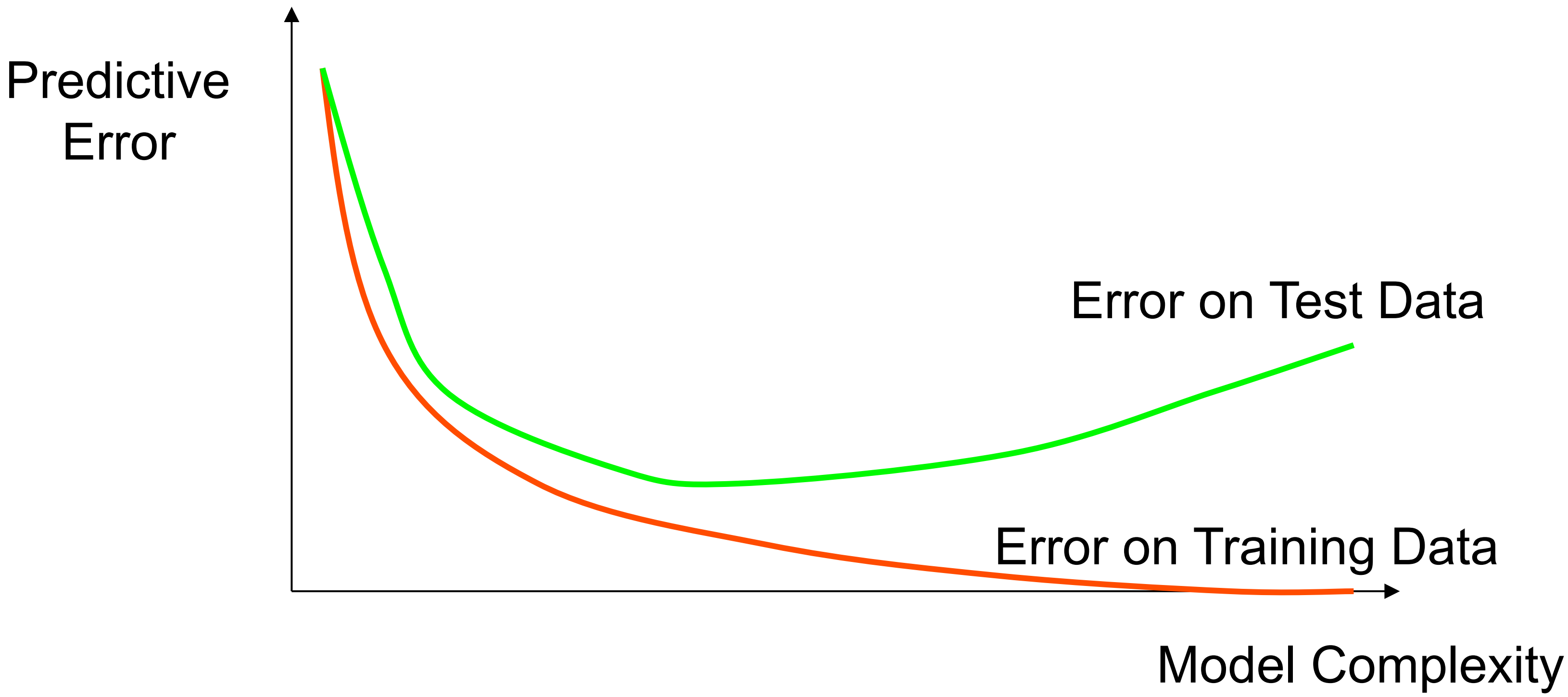
How Overfitting Affects Prediction



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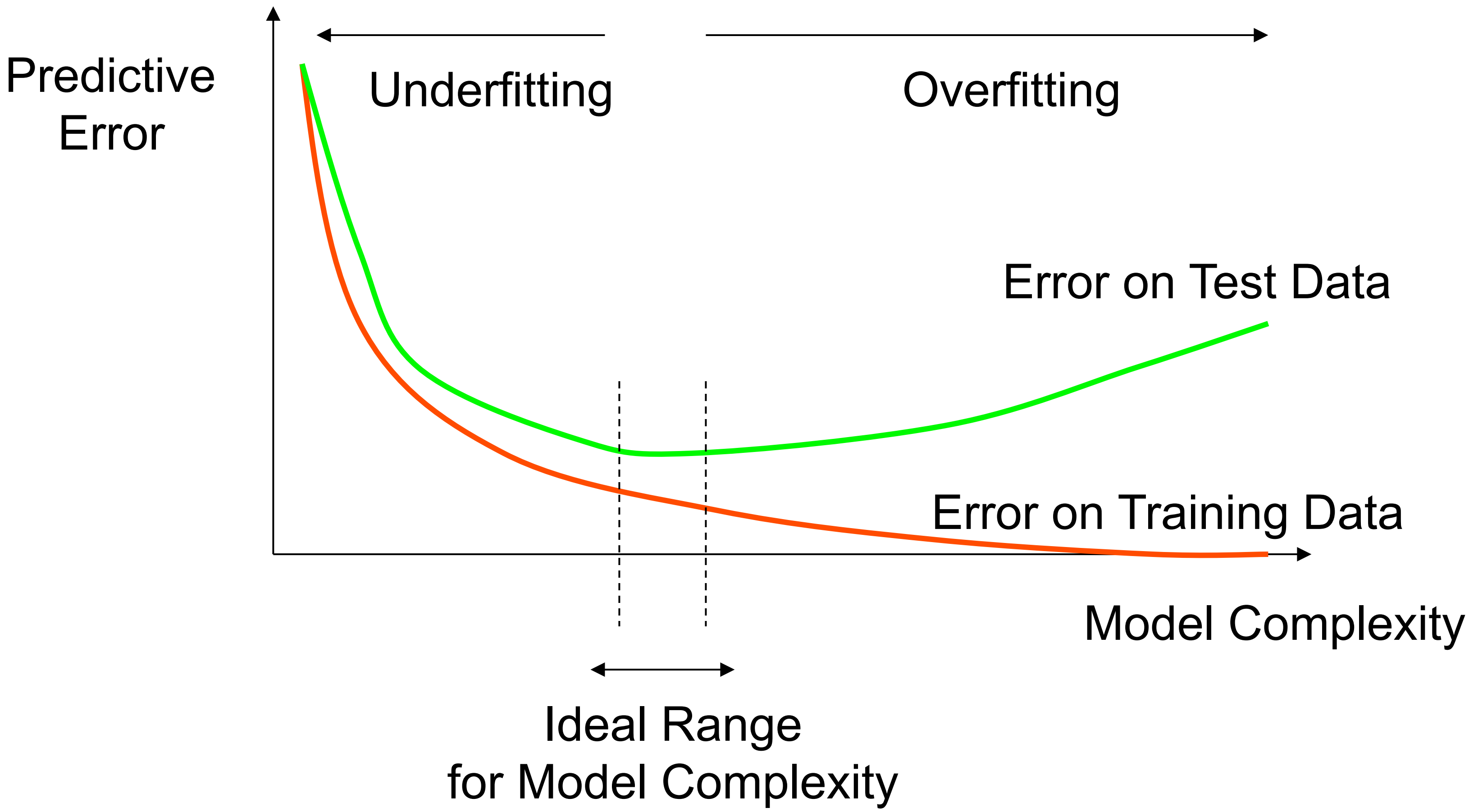
How Overfitting Affects Prediction



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Comparing Classifiers

Say we have two classifiers, *C1* and *C2*, and want to choose the best one to use for future predictions

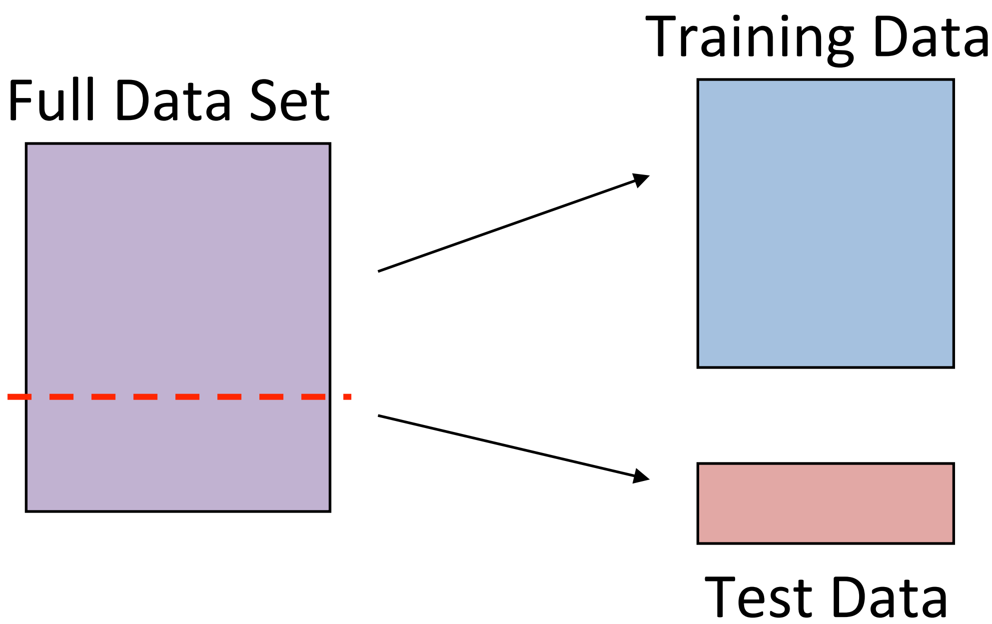
Can we use training accuracy to choose between them?

- No!
  - e.g., C1 = pruned decision tree, C2 = 1-NN
    training_accuracy(1-NN) = 100%, but may not be best

Instead, choose based on test accuracy...

Based on Slide by Padhraic Smyth, UCIrvine

Training and Test Data



Idea:
Train each model on the "training data"...

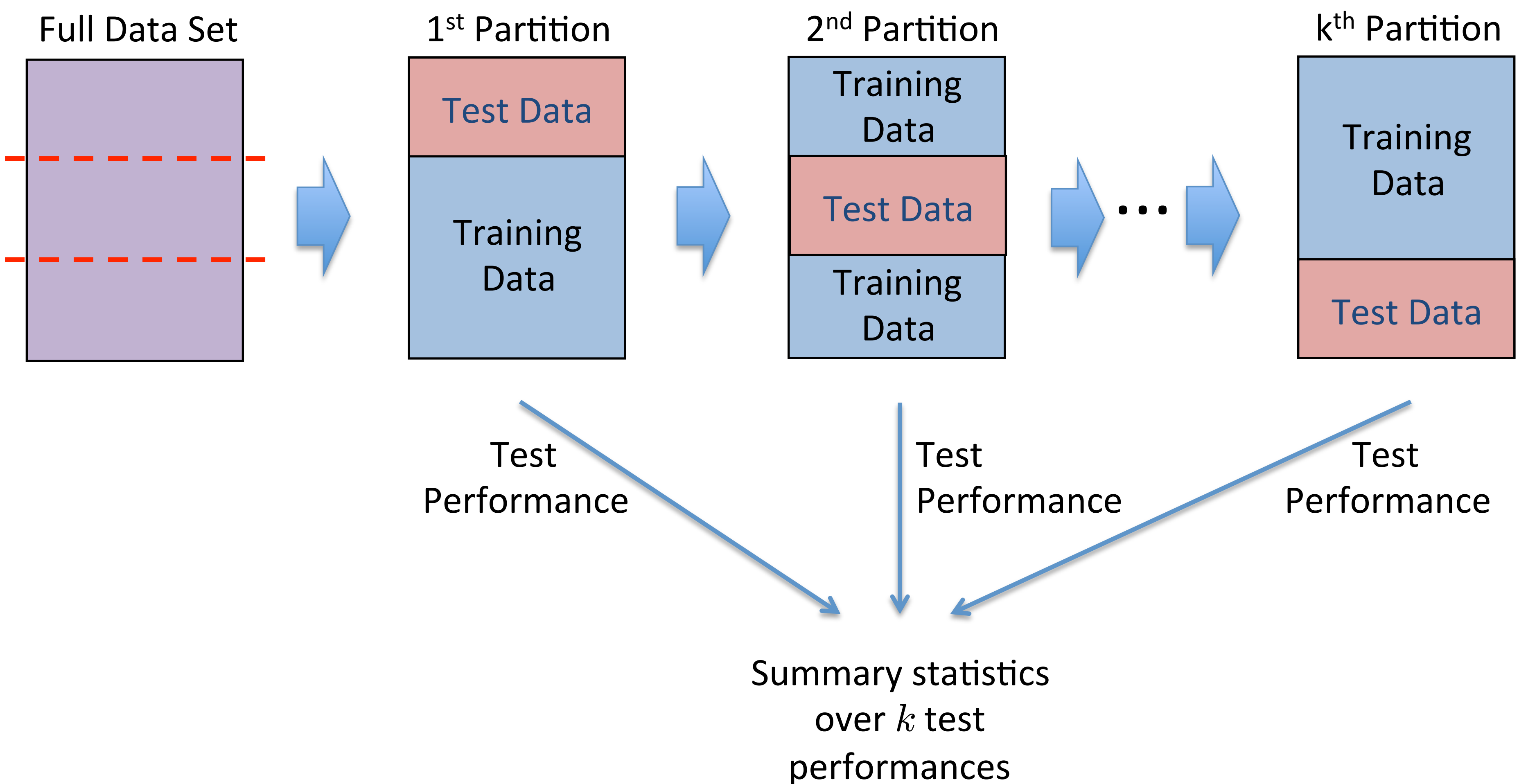
...and then test each model's accuracy on the test data

k-Fold Cross-Validation

- Why just choose one particular "split" of the data?
  - In principle, we should do this multiple times since performance may be different for each split

- k-Fold Cross-Validation (e.g., k=10)
  - randomly partition full data set of n instances into k disjoint subsets (each roughly of size n/k)
  - Choose each fold in turn as the test set; train model on the other folds and evaluate
  - Compute statistics over k test performances, or choose best of the k models
  - Can also do "leave-one-out CV" where $k = n$

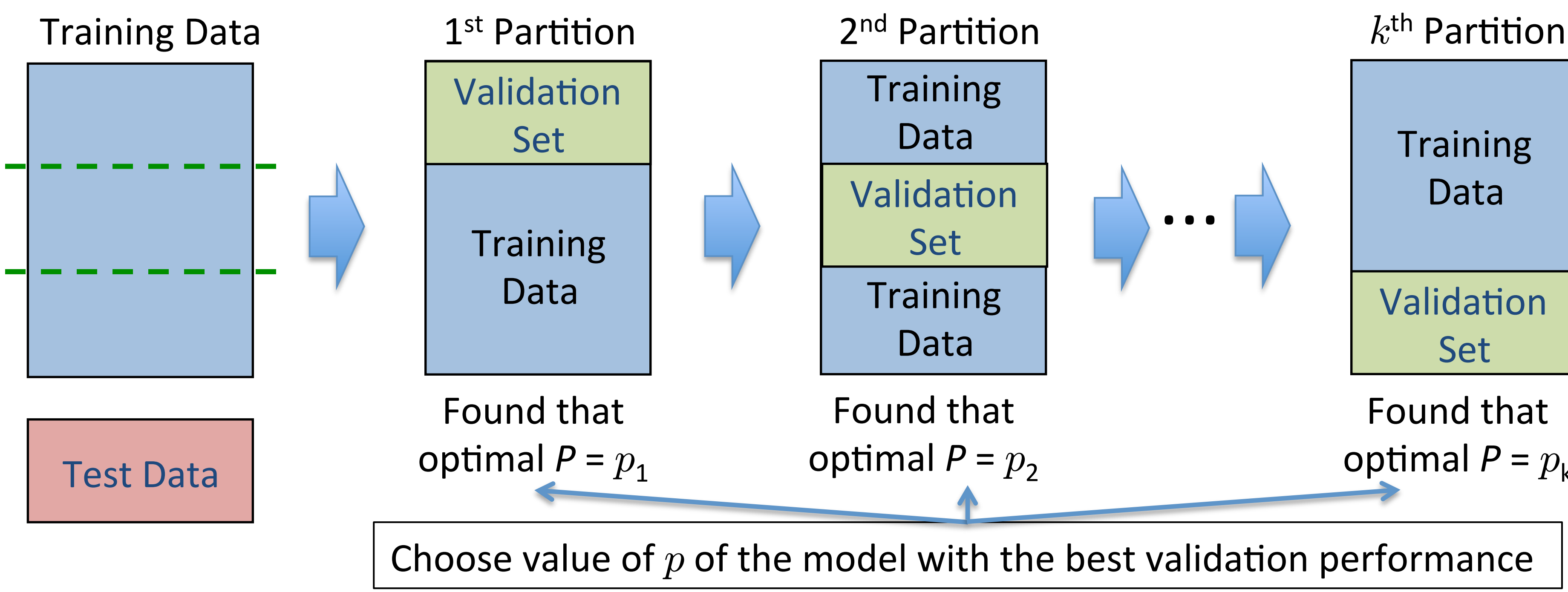
Example 3-Fold CV



Optimizing Model Parameters

Can also use CV to choose value of model parameter P

- Search over space of parameter values $p \in values(P)$
  - Evaluate model with $P = p$ on validation set
- Choose value p' with highest validation performance
- Learn model on full training set with $P = p'$



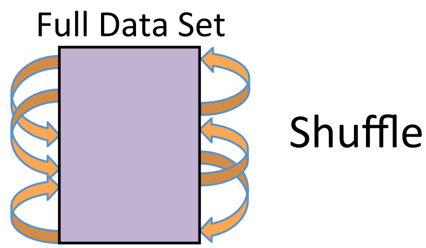
More on Cross-Validation

- Cross-validation generates an approximate estimate of how well the classifier will do on "unseen" data
  - As $k \rightarrow n$, the model becomes more accurate (more training data)
  - ...but, CV becomes more computationally expensive
  - Choosing $k < n$ is a compromise
- Averaging over different partitions is more robust than just a single train/validate partition of the data
- It is an even better idea to do CV repeatedly!

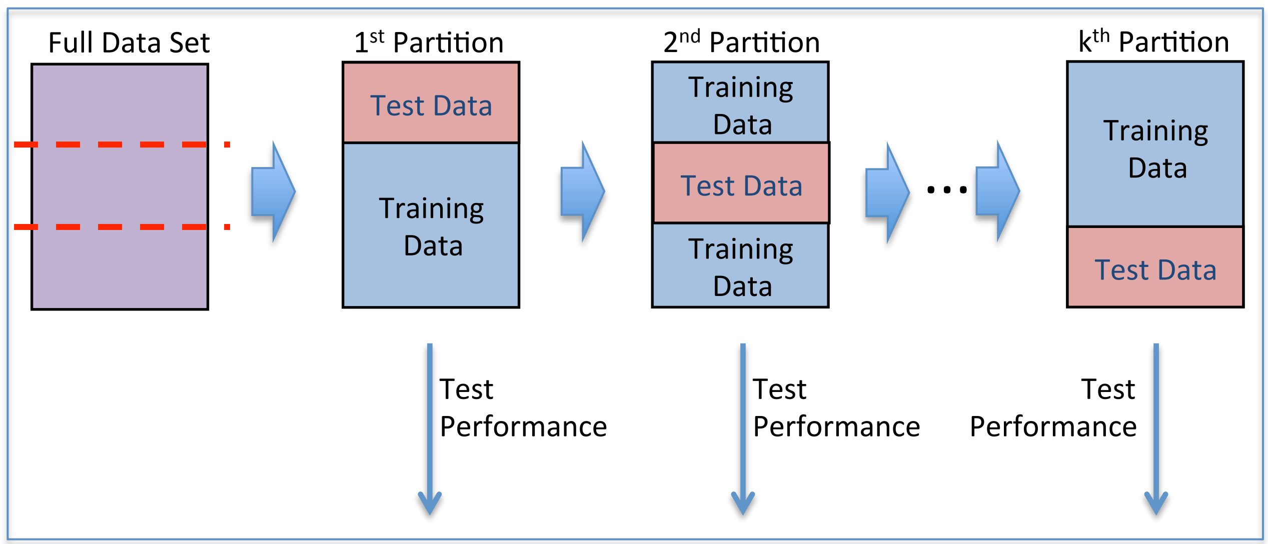
Multiple Trials of k-Fold CV

1.) Loop for t trials:

a.) Randomize Data Set



b.) Perform k-fold CV

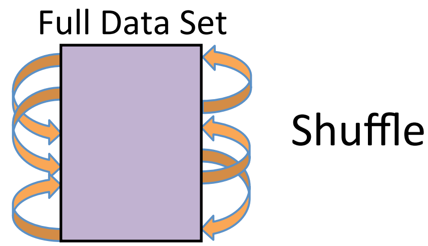


2.) Compute statistics over t x k test performances

Comparing Multiple Classifiers

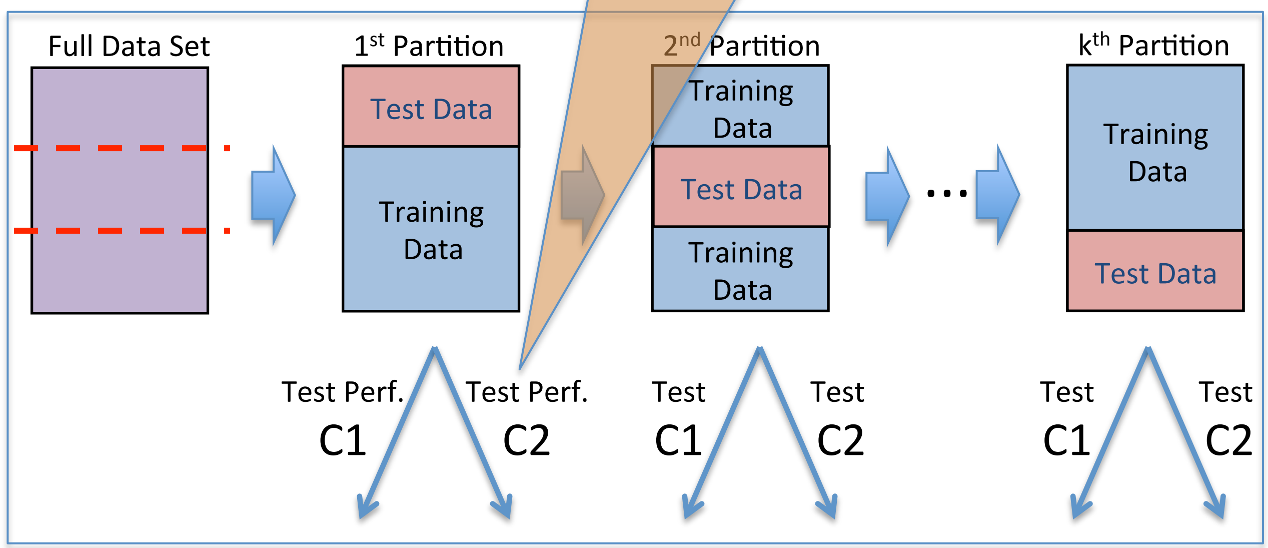
1.) Loop for t trials:

a.) Randomize Data Set



Test each candidate learner on same training/testing splits

b.) Perform k-fold CV

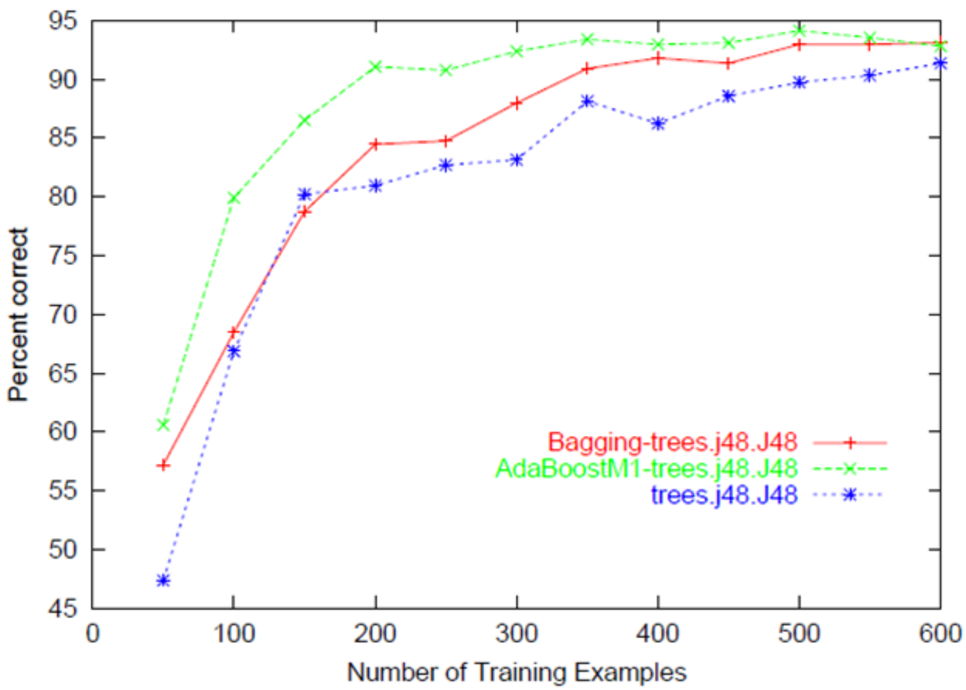


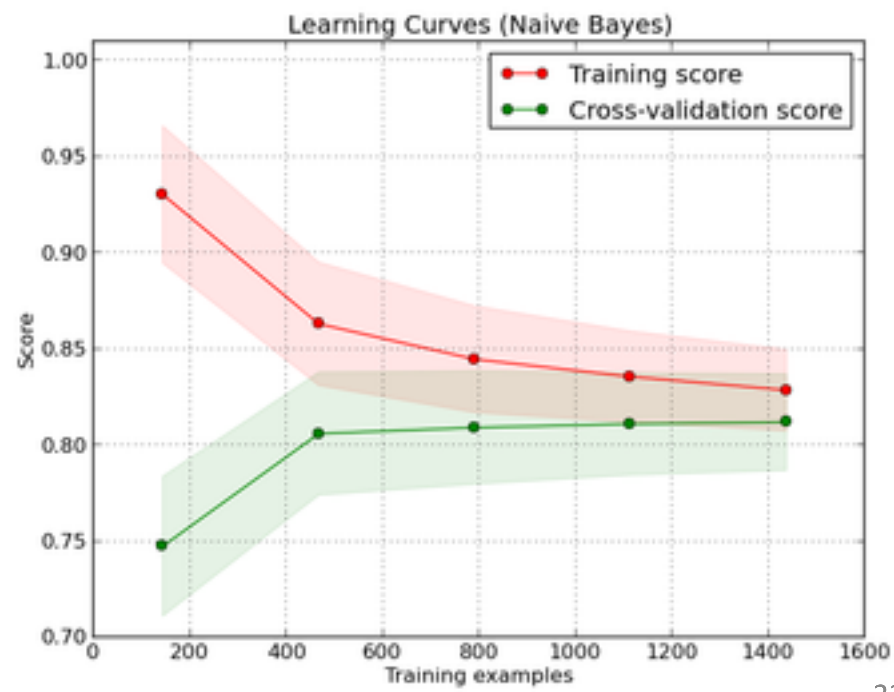
2.) Compute statistics over t x k test performances

Allows us to do paired summary statistics (e.g., paired t-test)

Learning Curve

- Shows performance versus the # training examples
  – Compute over a single training/testing split
  – Then, average across multiple trials of CV

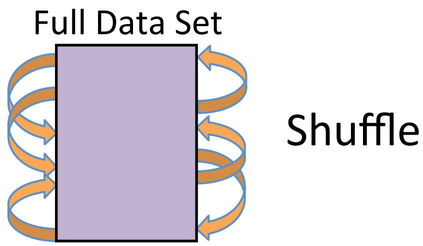




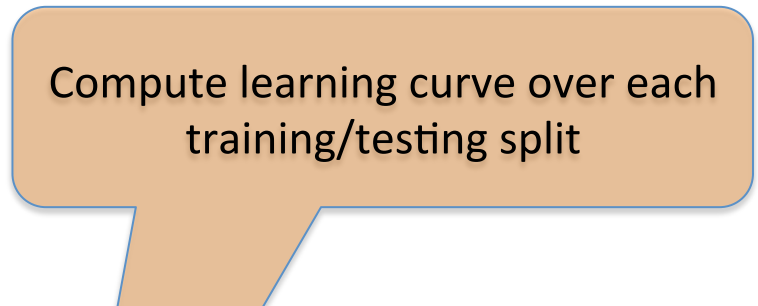
Building Learning Curves

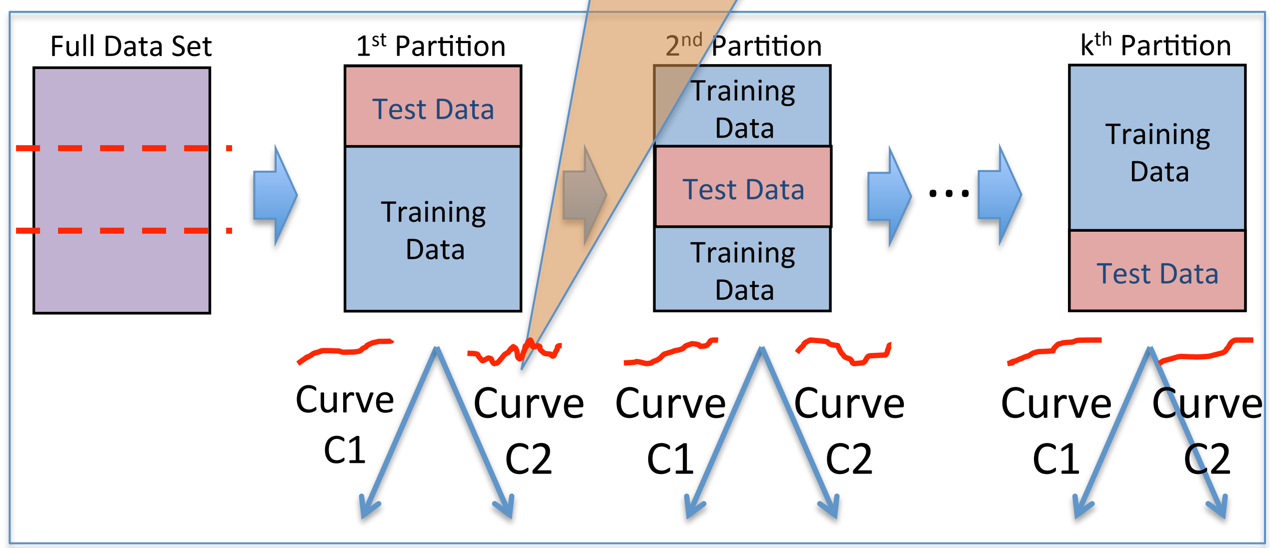
1.) Loop for t trials:

a.) Randomize Data Set



b.) Perform k-fold CV





2.) Compute statistics over t x k learning curves