

Evaluation

BCSE3066

Instructor: Pratyush Kumar Deka

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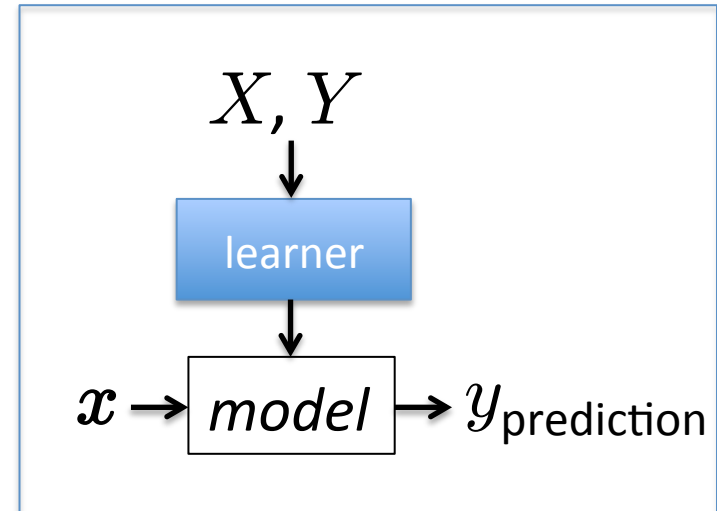
Stages of (Batch) Machine Learning

Given: labeled training data $X, Y = \{\langle \mathbf{x}_i, y_i \rangle\}_{i=1}^n$

- Assumes each $\mathbf{x}_i \sim \mathcal{D}(\mathcal{X})$ with $y_i = f_{target}(\mathbf{x}_i)$

Train the model:

$model \leftarrow classifier.train(X, Y)$



Apply the model to new data:

- Given: new unlabeled instance $x \sim \mathcal{D}(\mathcal{X})$

$y_{prediction} \leftarrow model.predict(x)$

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

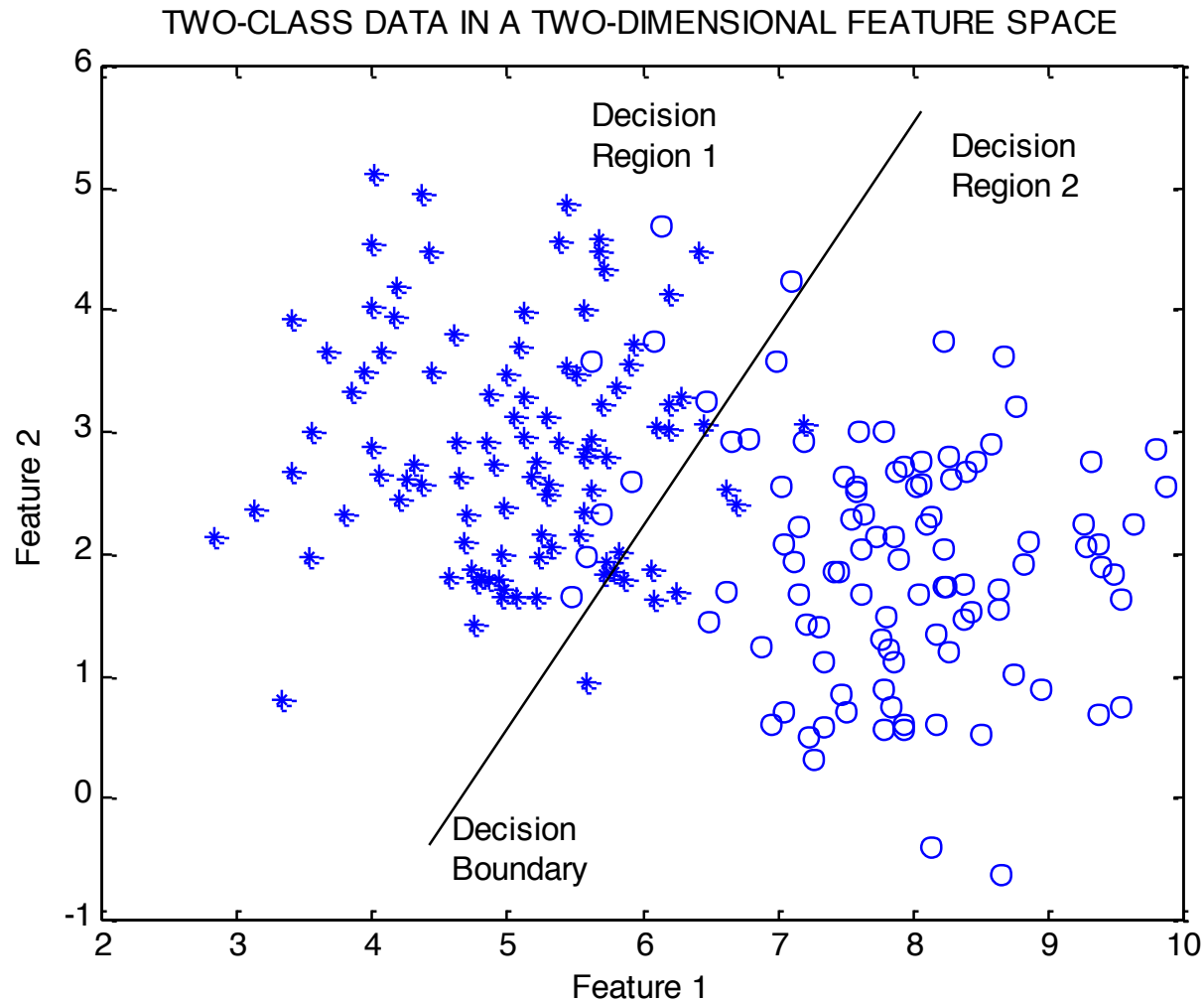
$$\text{recall} = \frac{TP}{TP + FN}$$

Probability that a randomly selected relevant document is retrieved

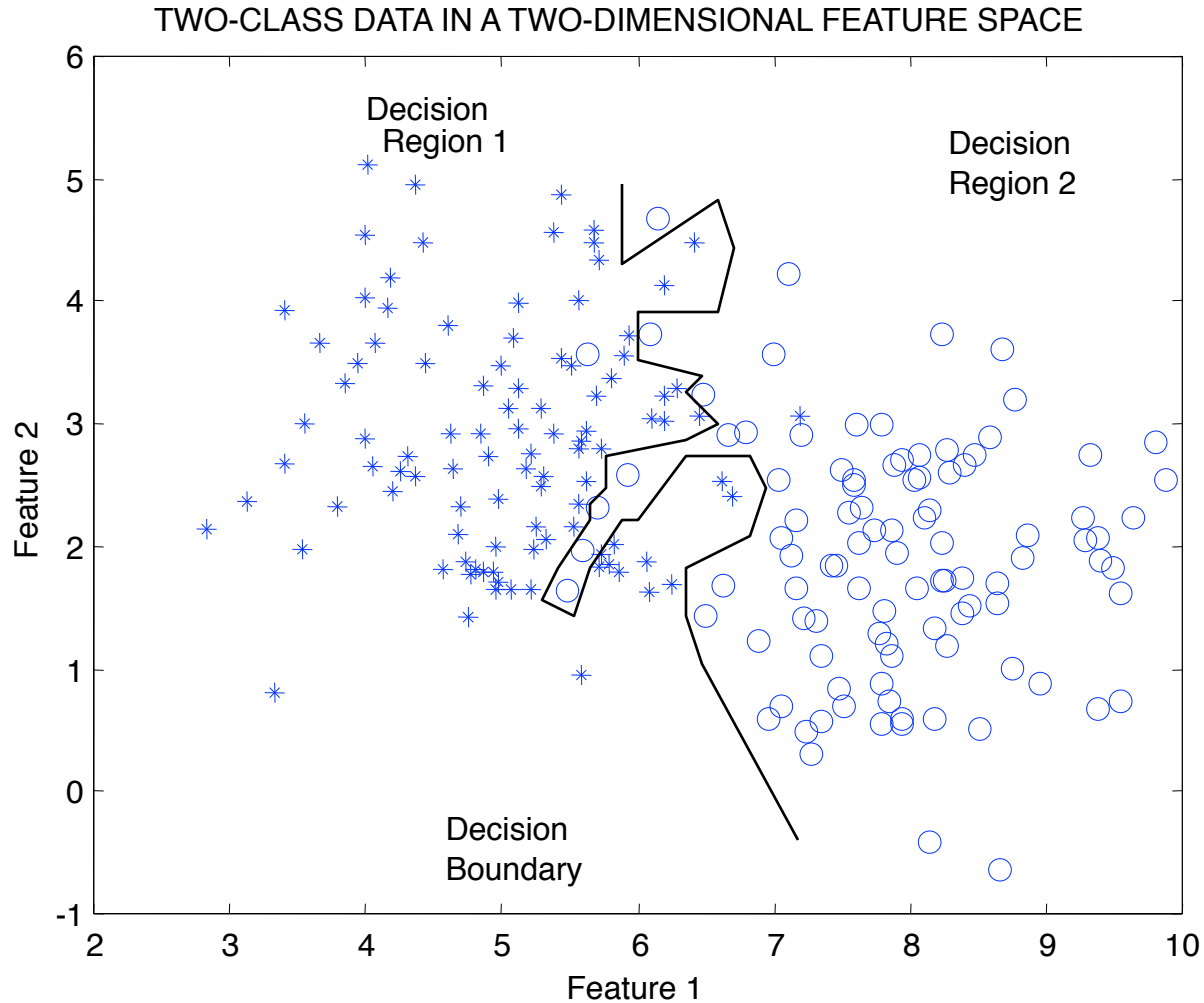
Training Data and Test Data

- 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

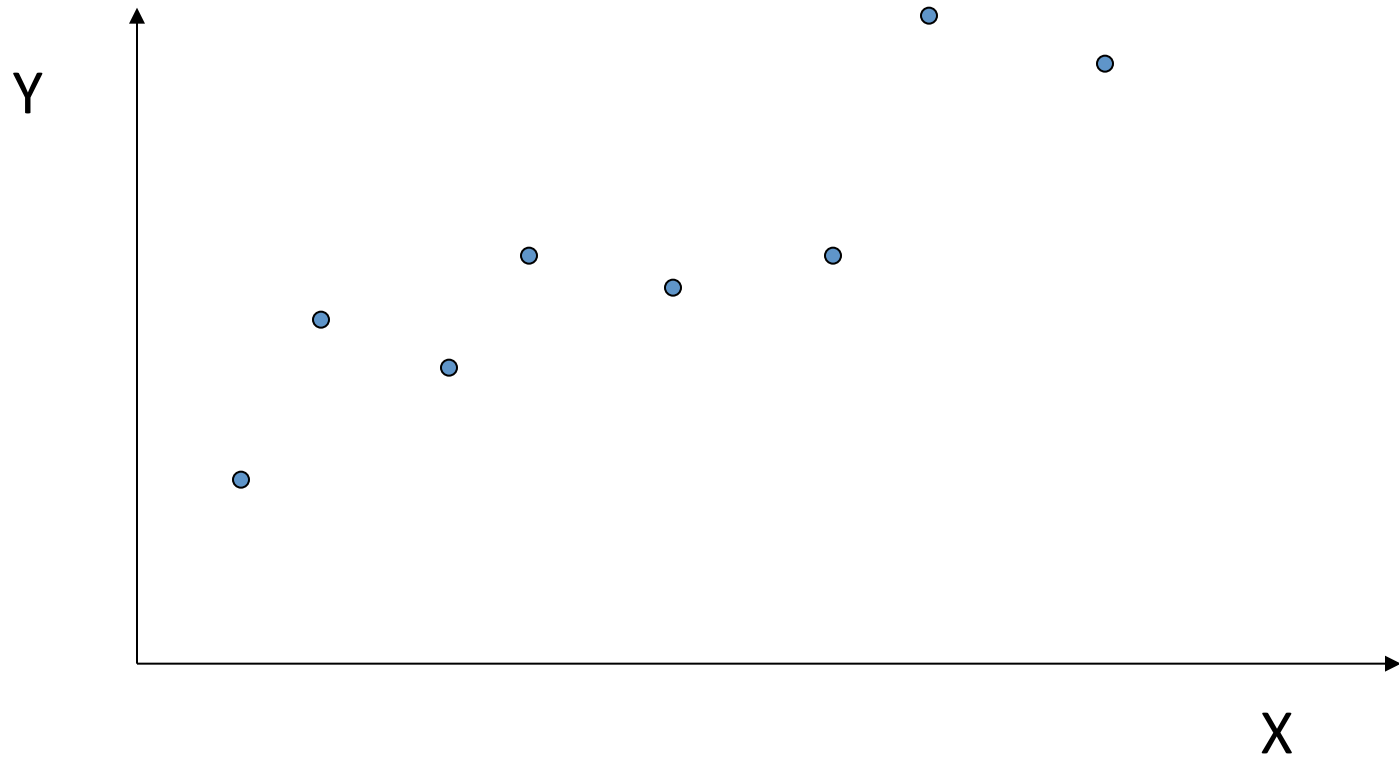
Simple Decision Boundary



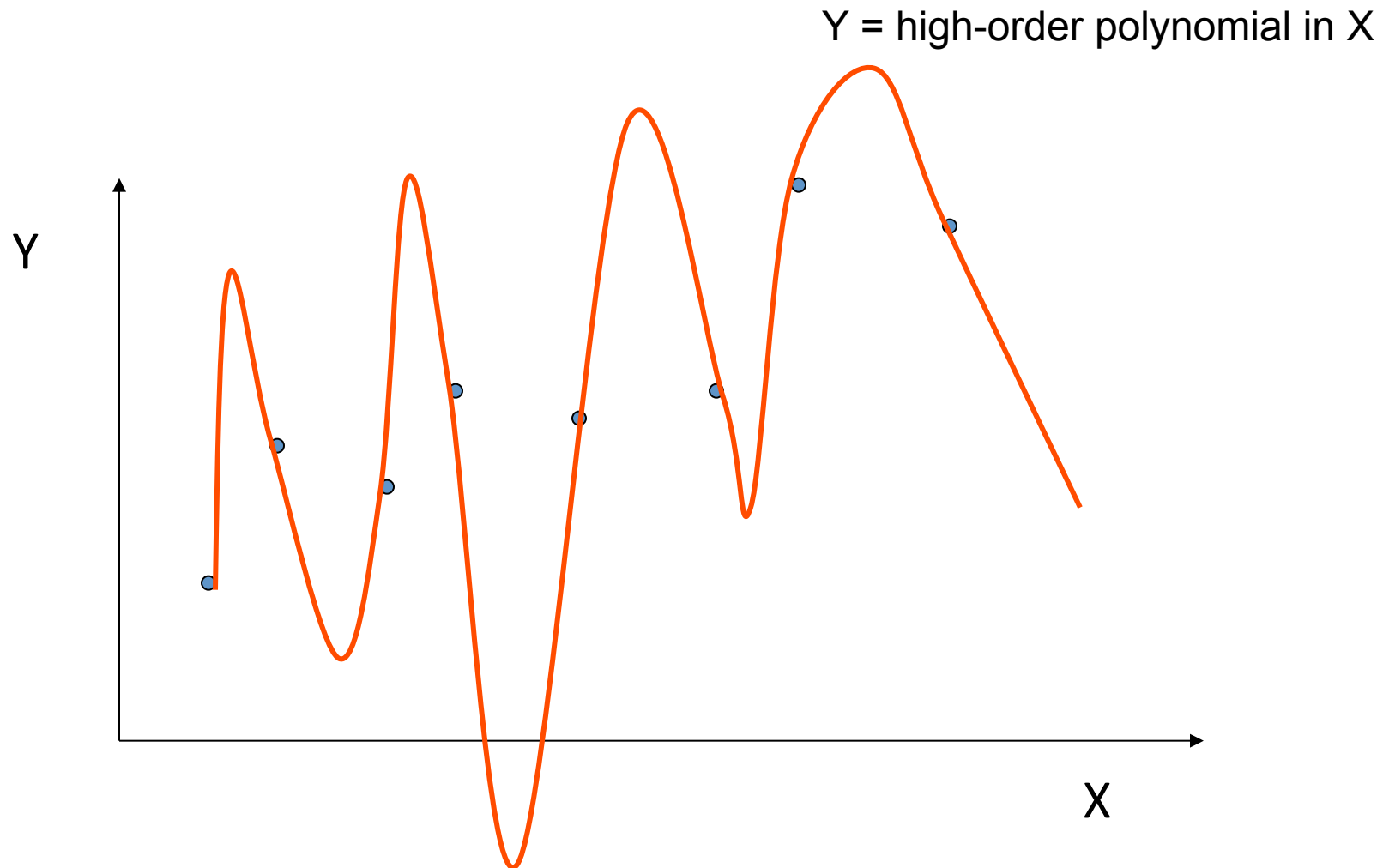
More Complex Decision Boundary



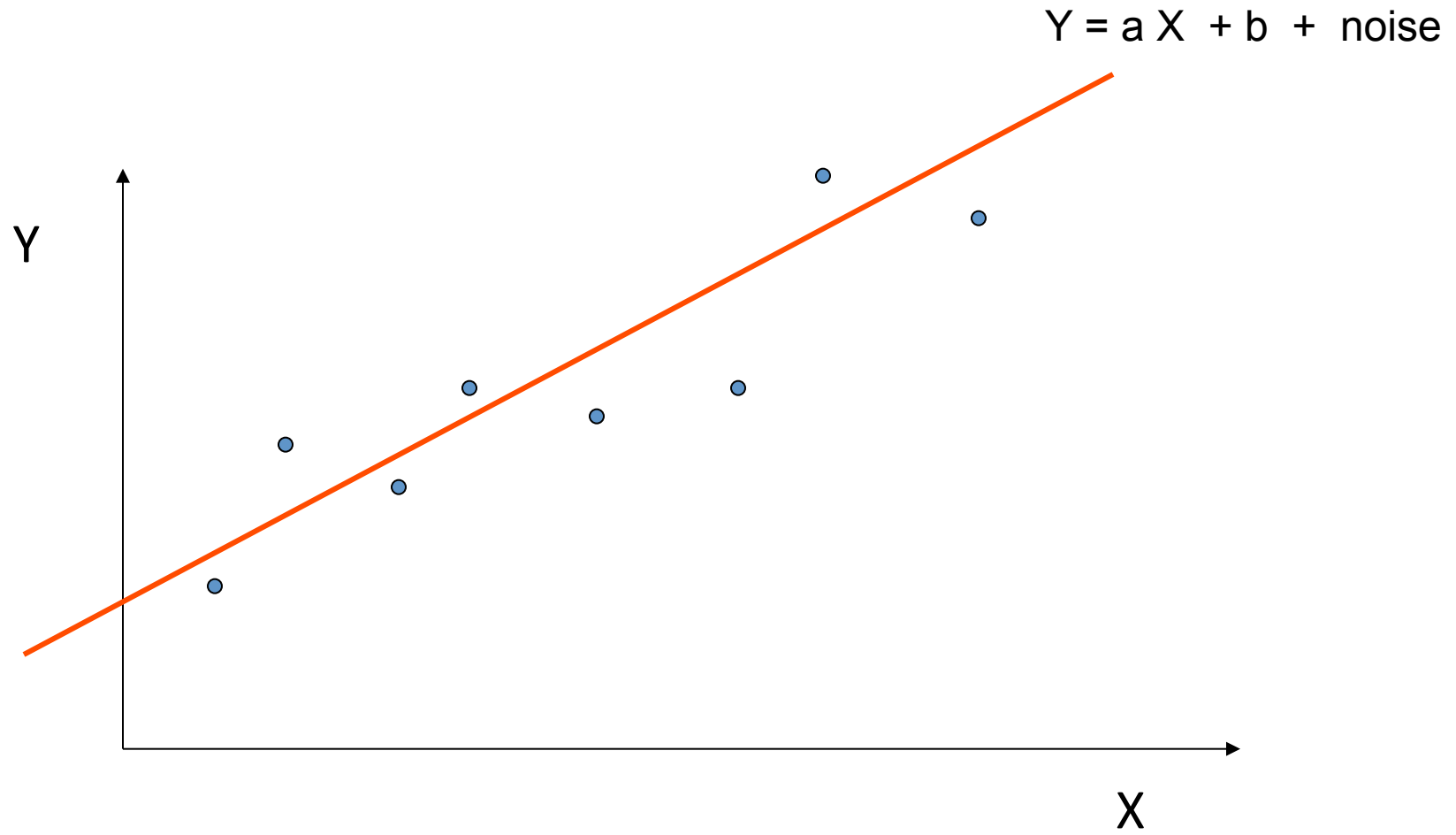
Example: The Overfitting Phenomenon



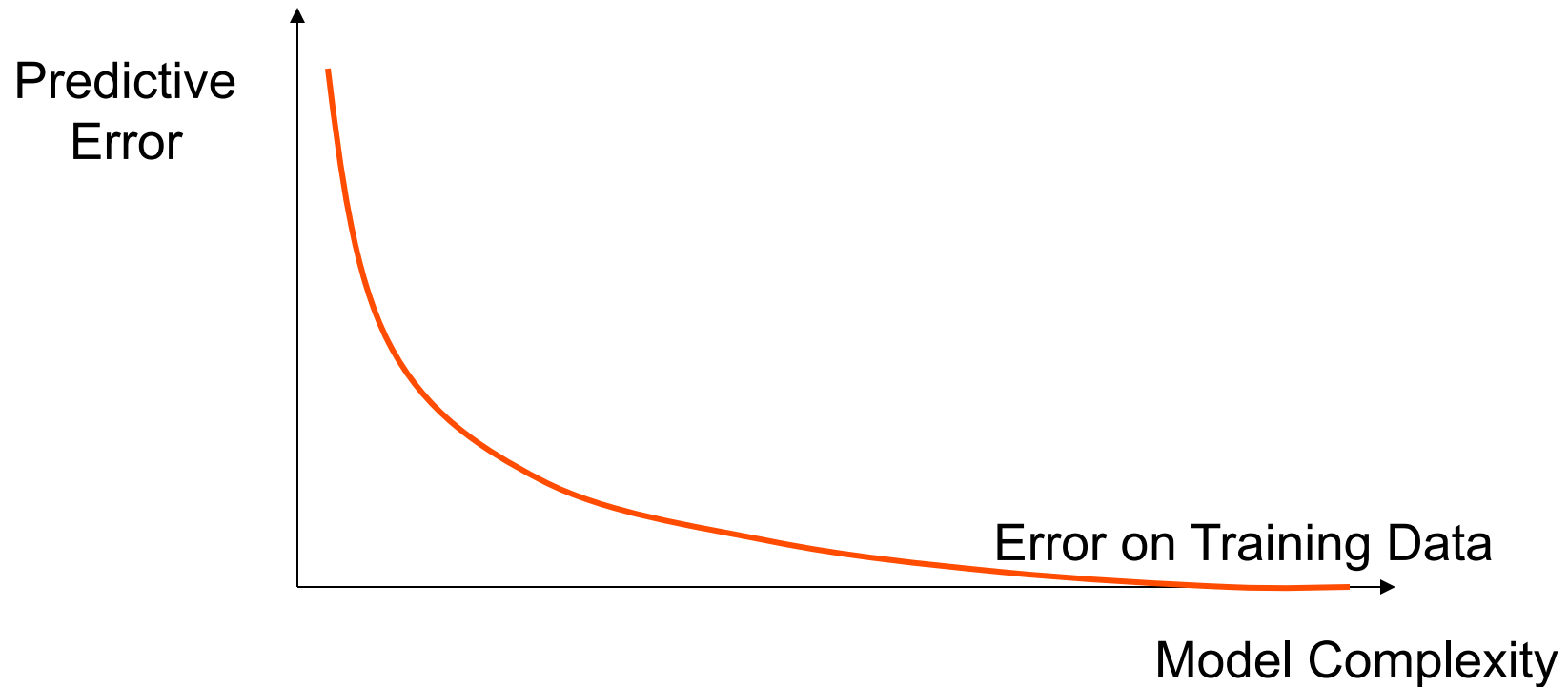
A Complex Model



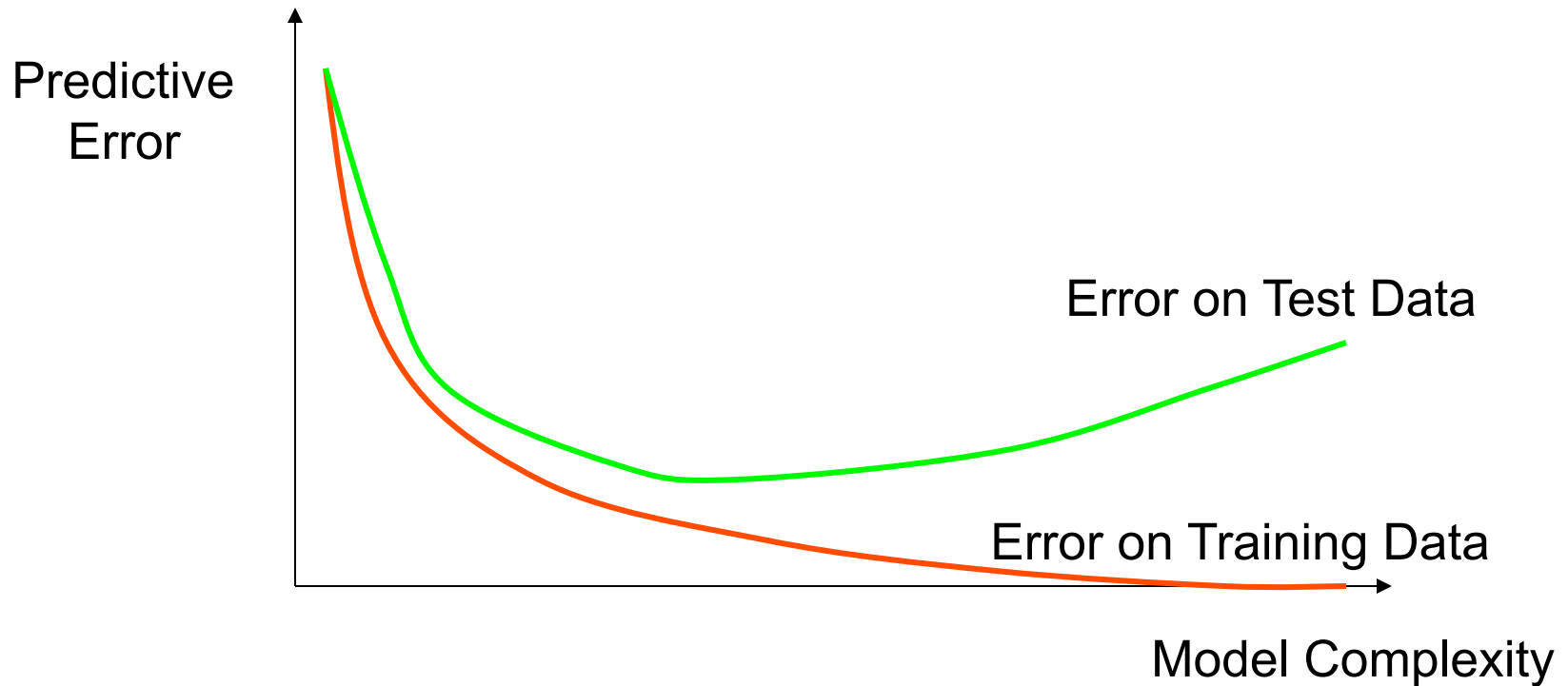
The True (simpler) Model



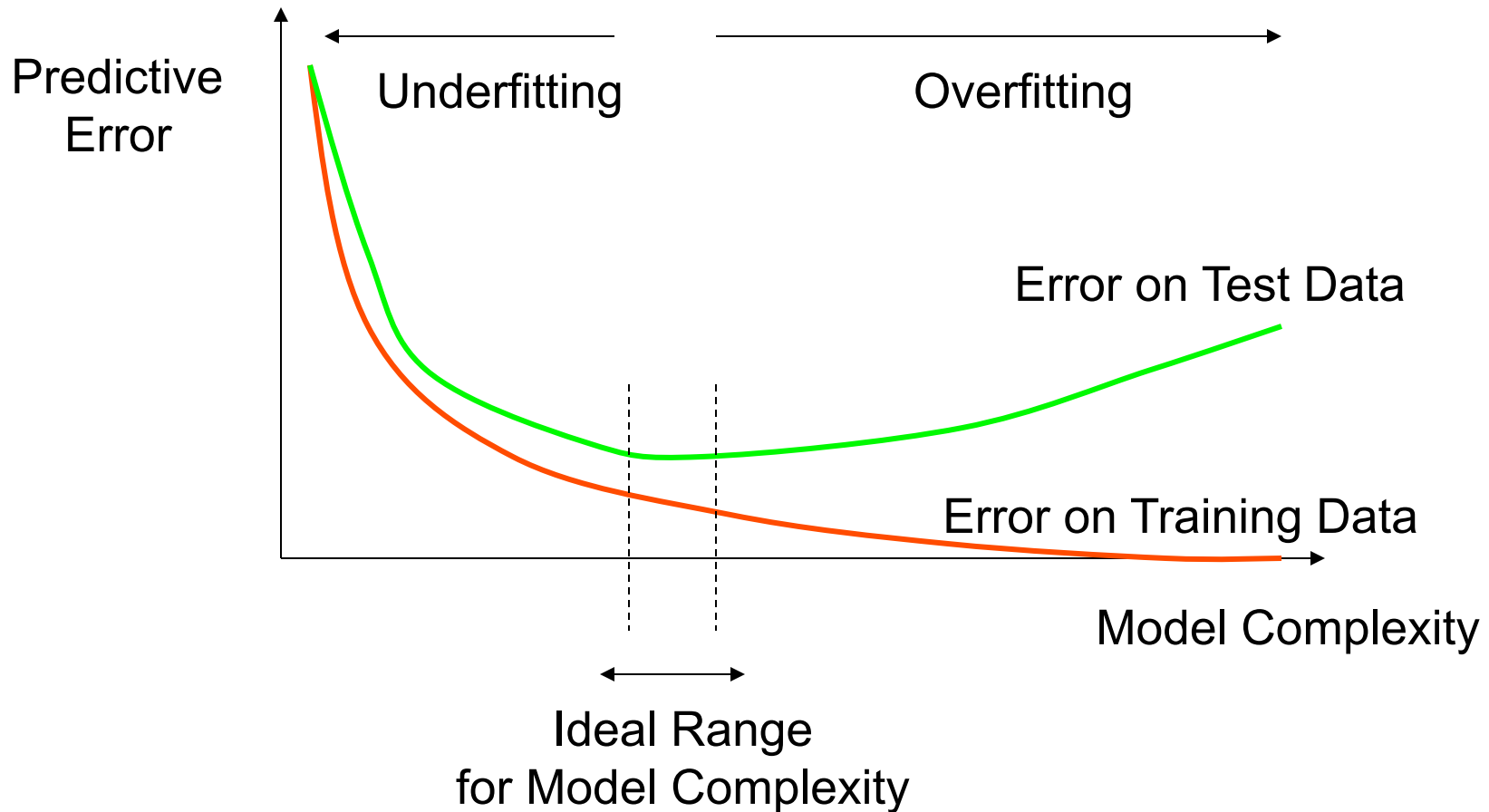
How Overfitting Affects Prediction



How Overfitting Affects Prediction



How Overfitting Affects Prediction



Comparing Classifiers

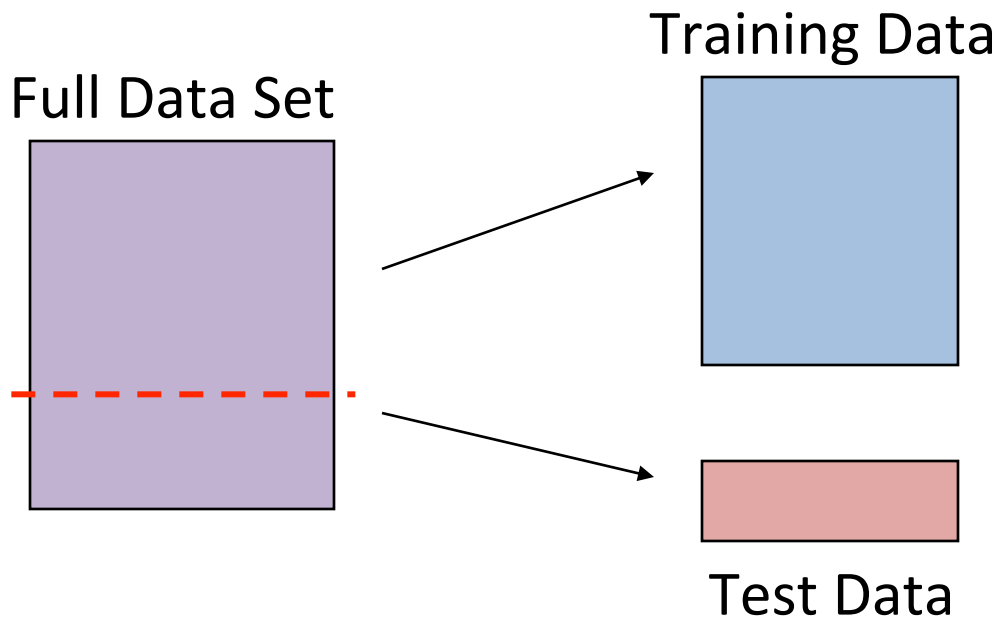
Say we have two classifiers, $C1$ and $C2$, and want to choose the best one to use for future predictions

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...

Training and Test Data



Idea:

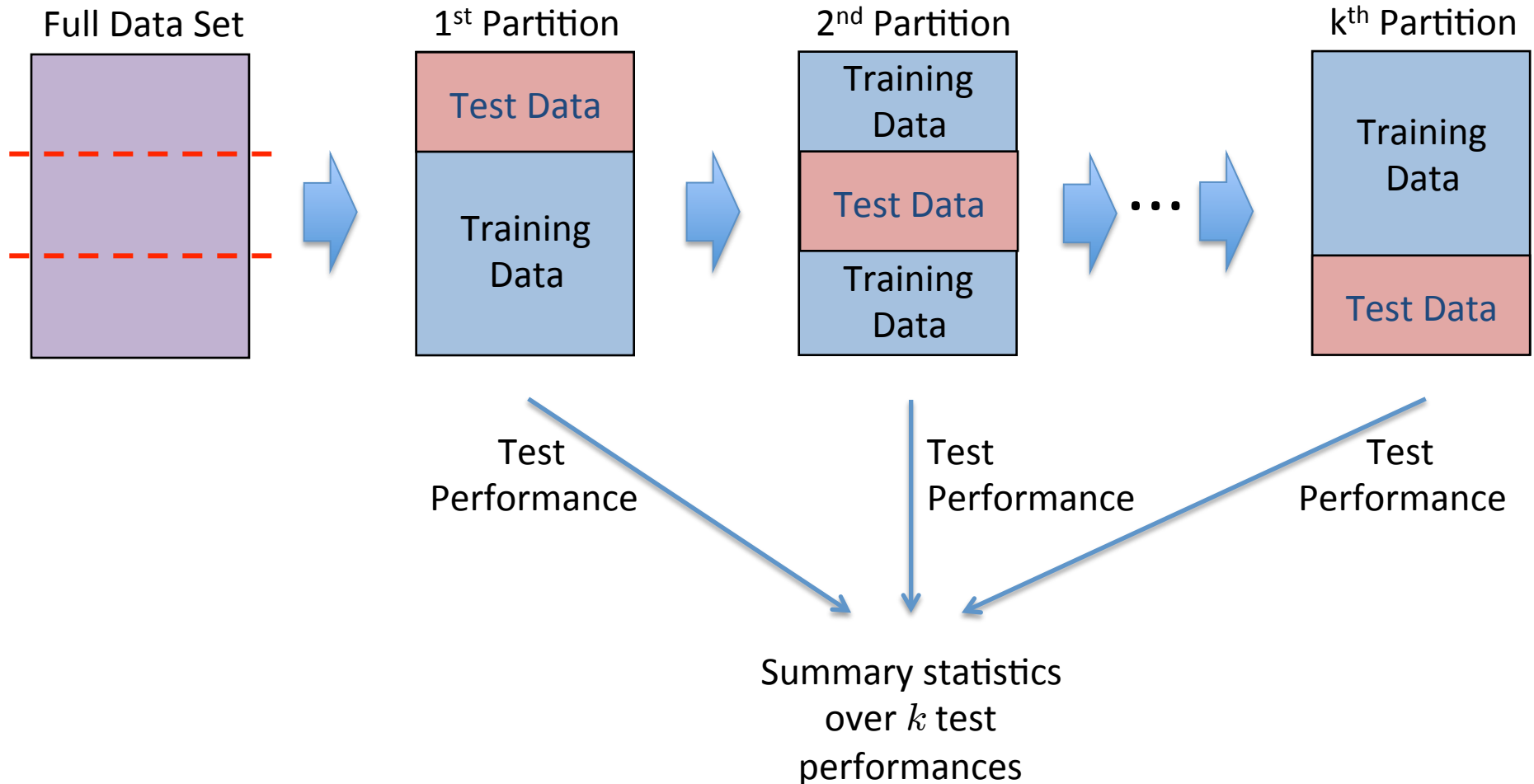
Train each model on the “training data”...

...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 $k = n$

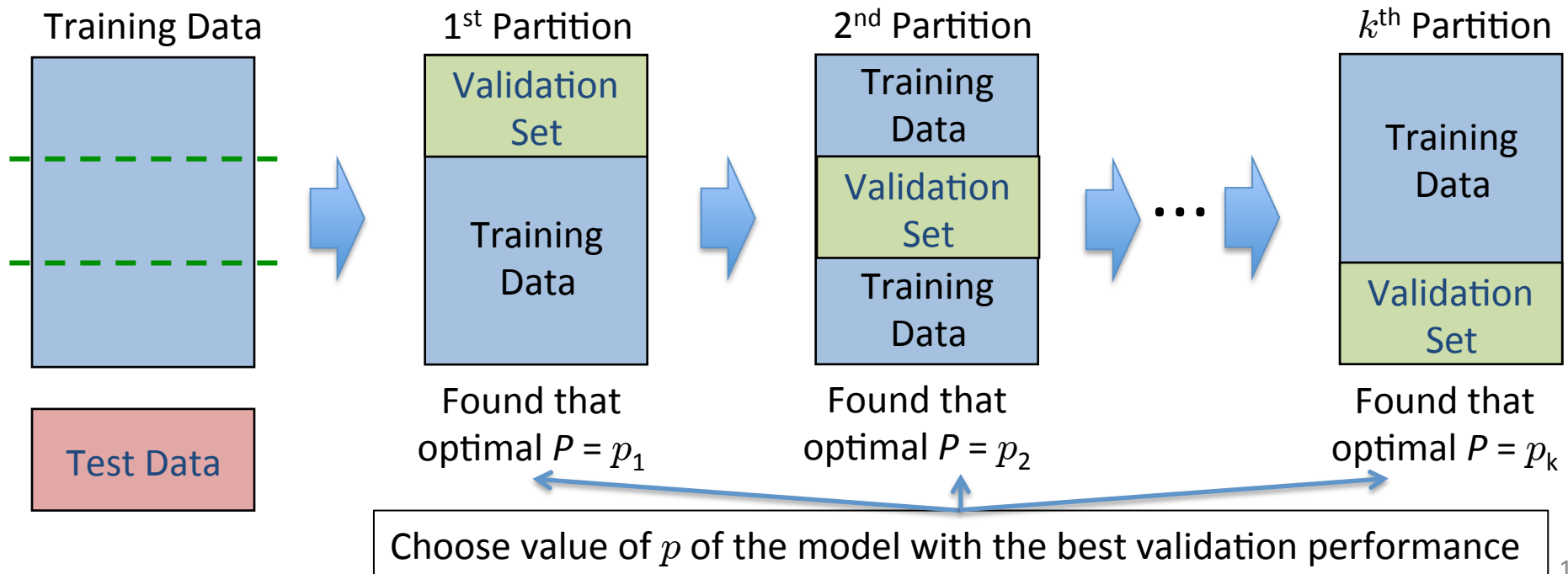
Example 3-Fold CV



Optimizing Model Parameters

Can also use CV to choose value of model parameter P

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



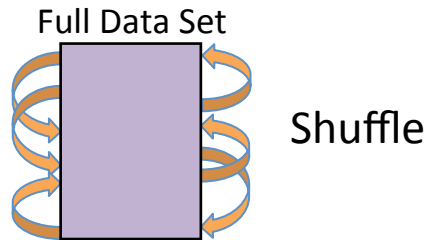
More on Cross-Validation

- 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!

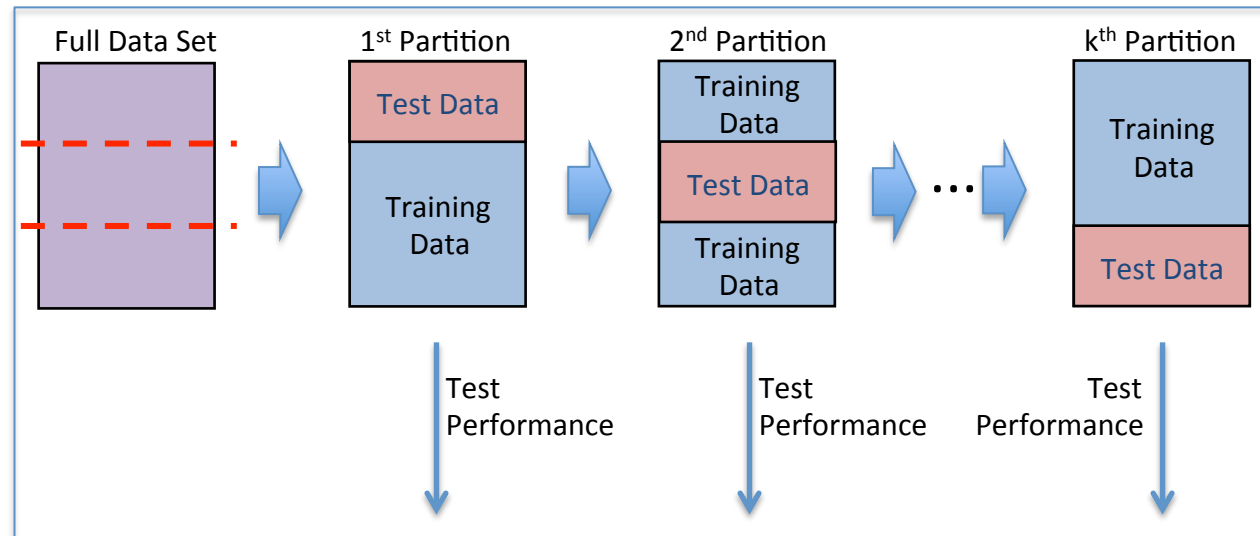
Multiple Trials of k -Fold CV

1.) Loop for t trials:

a.) Randomize
Data Set



b.) Perform
 k -fold CV

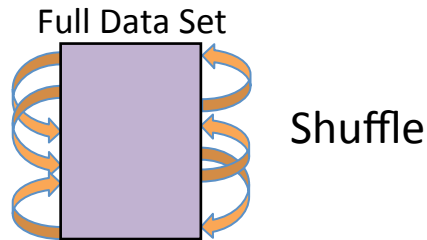


2.) Compute statistics over
 $t \times k$ test performances

Comparing Multiple Classifiers

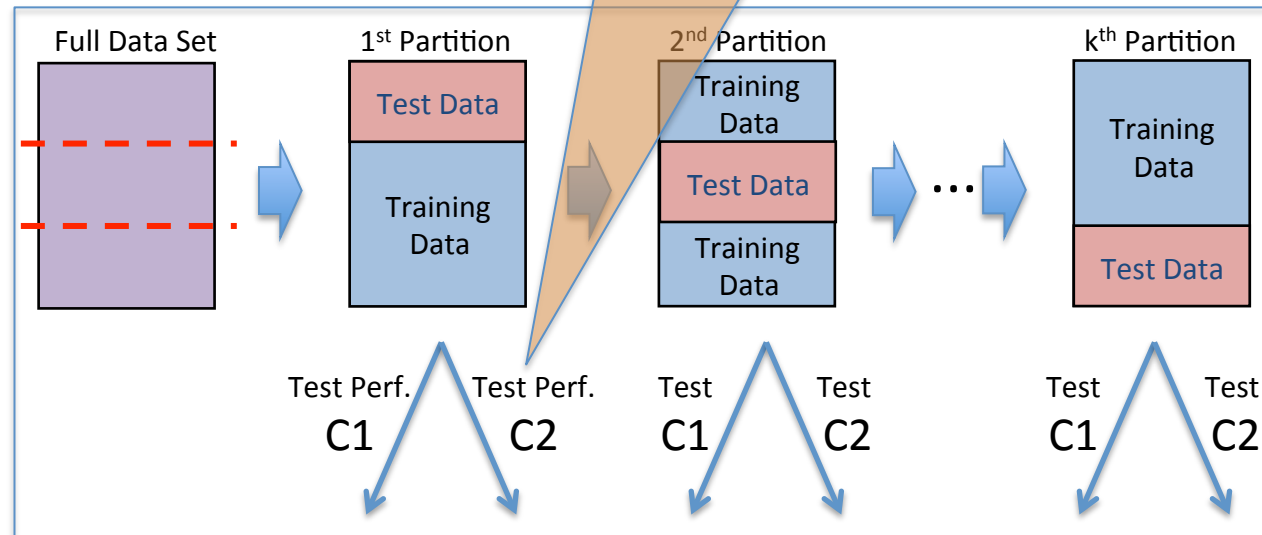
1.) Loop for t trials:

a.) Randomize Data Set



Test each candidate learner on same training/testing splits

b.) Perform k -fold CV

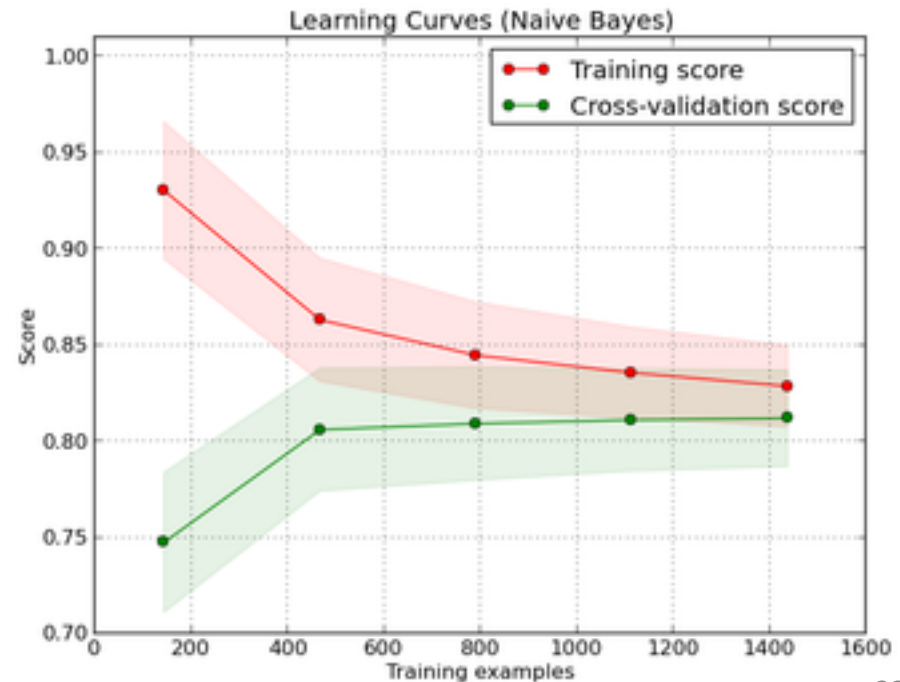
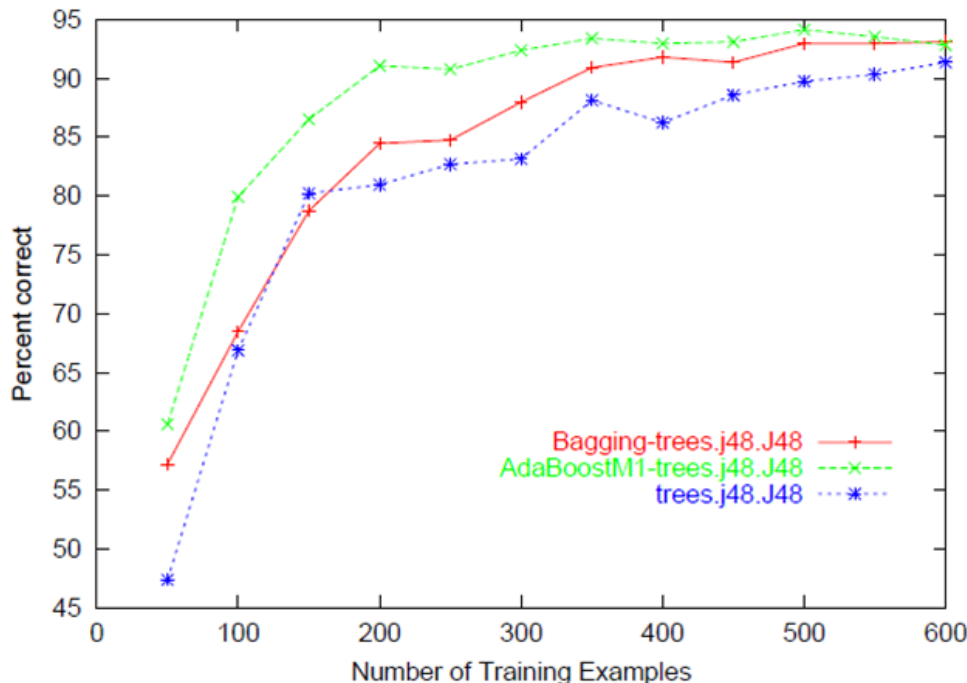


2.) Compute statistics over $t \times k$ test performances

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

Learning Curve

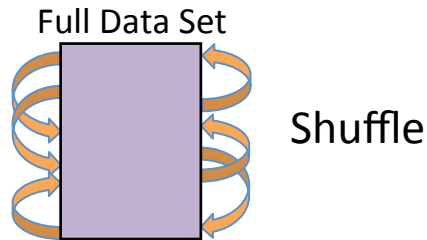
- Shows performance versus the # training examples
 - Compute over a single training/testing split
 - Then, average across multiple trials of CV



Building Learning Curves

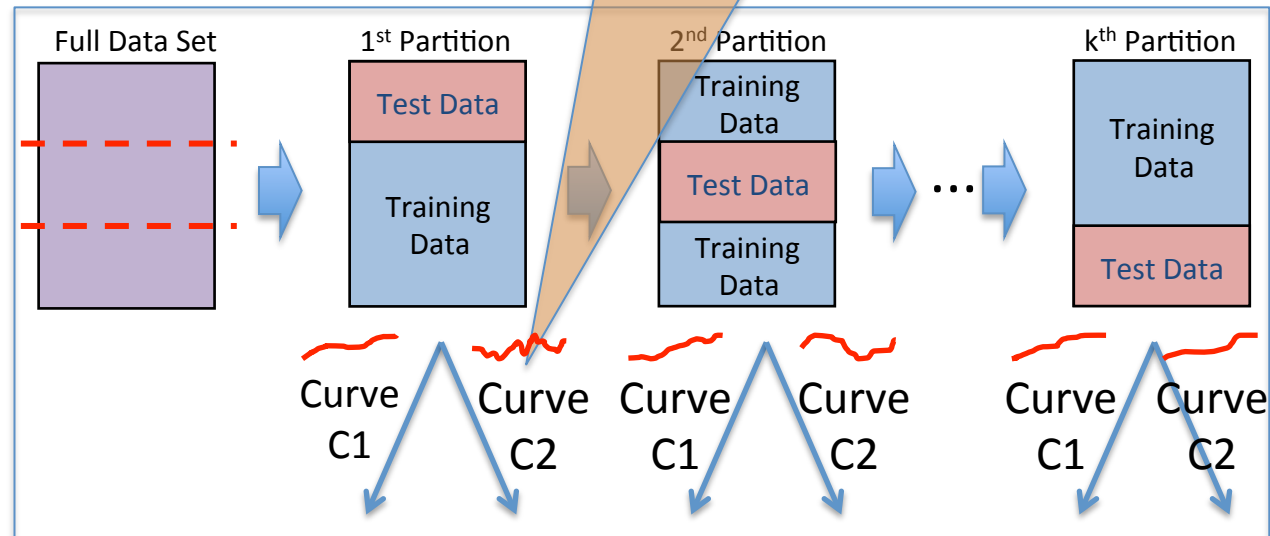
1.) Loop for t trials:

a.) Randomize Data Set



Compute learning curve over each training/testing split

b.) Perform k -fold CV



2.) Compute statistics over $t \times k$ learning curves