CSDS 440: Machine Learning

Soumya Ray (he/him, sray@case.edu)
Olin 516

Office hours T, Th 11:15-11:45 or by appointment

Zoom recording here

Announcements

- Written 1 due this week
- Quiz 1 next Thursday, in class, 30-45 minutes, closed book/notes
 - Topics: everything up to and including decision trees
 - Remember to review probability and statistics

Recap

- What is the geometry of the tree's decision boundary?
- Tree learners don't need a m____ s___ representation, can represent
 c____ concepts, are human i____ and easy to e____.
- But they have trouble with features that have lots of v_____, features that i_____, and o_____ easily.
- What is goal of learning algorithm performance evaluation?
- Given a finite dataset, we want the training set to an algorithm to be as I____ as possible. We also want the test sets to be i____.
- In this procedure, we p____ the data into f___. Each iteration we use ___ as the train set and ____ as the test set.
- What is leave one out cross validation?
- What is stratified CV?
- What is internal CV?

Today

Metrics

Contingency Table

Class according to Target Concept / Oracle (Correct Answer)

ifier		Positive	Negative	
s according to Learned Classifier (Predicted Answer)	Positive	True Positives (TP)	False Positives (FP) (Type I error)	
	Negative	False Negatives (FN) (Type II error)	True Negatives (TN)	

Accuracy

 Most commonly used measure for comparing classification algorithms

$$Accuracy = \frac{TP + TN}{TP + TN + FP + FN}$$

Error Rate

Inverse of Accuracy

$$ErrorRate = \frac{FP + FN}{TP + TN + FP + FN}$$

Weaknesses of Accuracy

- Does not account for:
 - Skewed class distributions
 - Differential misclassification costs
 - Confidence estimates from learning algorithms

Weighted/Balanced Accuracy

Corrects for skewed class distributions

$$WAcc = \frac{1}{2} \left(\frac{TP}{Allpos} + \frac{TN}{Allneg} \right)$$

$$= \frac{1}{2} \left(\frac{TP}{TP + FN} + \frac{TN}{TN + FP} \right)$$
True Positive Rate True Negative Rate

Measuring one class

- Often, just a single class is "interesting"
 - Call this the "positive" class

	Positive	Negative	
Positive	True Positives (TP)	False Positives (FP) (Type I error)	
Negative	False Negatives (FN) (Type II error)	True atives	

Precision

 Of the examples the learner predicted positive, how many were actually positive?

$$Precision = \frac{TP}{TP + FP}$$

Recall/TP rate/Sensitivity

 Of the examples that were actually positive, how many did the learner predict correctly?

$$Recall = \frac{TP}{TP + FN} = \frac{TP}{Allpos}$$

Specificity/TN rate

Counterpart of recall for the negative class

$$Specificity = \frac{TN}{TN + FP} = \frac{TN}{Allneg}$$

• So:

$$WAcc = \frac{1}{2} \left(Sensitivity + Specificity \right)$$

F₁ score

 Combines precision and recall into a single measure, giving each equal weight

$$\frac{1}{F_1} = \frac{1}{2} \left(\frac{1}{Precision} + \frac{1}{Recall} \right)$$

$$F_{1} = \frac{2}{\frac{1}{Precision} + \frac{1}{Recall}}$$

Beyond point estimates

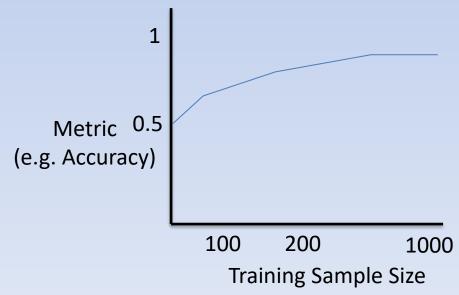
Everything above is a "point estimate"

 Because they will be computed on the basis of a sample, we can also compute variance estimates for each quantity

 Important to show "stability" of solutions, and when comparing across algorithms (later)

Learning Curves

- Often useful to plot each metric as a function of training sample size
- Provides insight into how many examples the algorithm needs to become effective



Metrics with Confidence Measures

 Many learning algorithms can produce models that can provide estimates of how confident they are about a prediction

• Example: Pruned Decision Trees

Metrics with Confidence Measures

	True Class	Confidence On +
Example 1	+	0.9
Example 2	-	0.8
Example 3	+	0.4
Example 4	-	0.3

 We can create multiple classifiers by thresholding the confidence

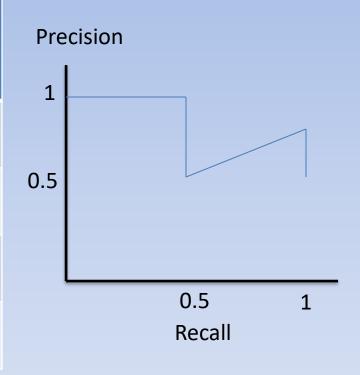
 In this case, we can plot Precision-Recall (PR) and Receiver Operating Characteristic (ROC) graphs tracking all of the classifiers

Precision-Recall graphs

	True Class	Confidence On +	Recall (x axis)	Precision (y axis)
Example 1	+	0.9		
Example 2	-	0.8		
Example 3	+	0.4		
Example 4	-	0.3		

Precision-Recall graphs

	True Class	Confidence On +	Recall (x axis)	Precision (y axis)
Example 1	+	0.9	0.5	1
Example 2	-	0.8	0.5	0.5
Example 3	+	0.4	1	0.67
Example 4	-	0.3	1	0.5

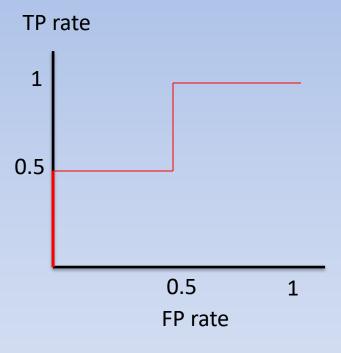


ROC graphs

	True Class	Confidence On +	FP Rate (1-Spec.) (x axis)	Sens./Recall (y axis)
Example 1	+	0.9		
Example 2	-	0.8		
Example 3	+	0.4		
Example 4	-	0.3		

ROC graphs

	True Class	Confidence On +	FP Rate (x axis)	Sens./Recall (y axis)
Example 1	+	0.9	0	0.5
Example 2	-	0.8	0.5	0.5
Example 3	+	0.4	0.5	1
Example 4	-	0.3	1	1



Properties of ROC graphs

- Random guessing is a diagonal line
 - Also majority class classifier
 - If your classifier is any good its ROC must lie above the diagonal
- Monotonically increasing
- Often use "AUC" / "AROC" as comparison statistic (later)
- Can be misleading if class distribution is too skewed (use PR graphs instead)