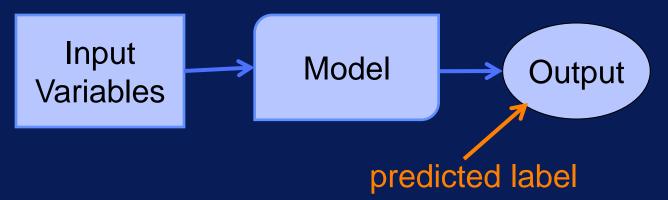
# Generalization & Overfitting

### After this video you will be able to...

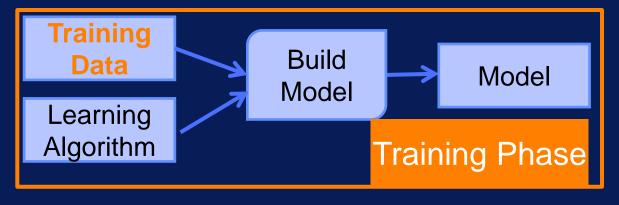
- Define what generalization is
- Describe how overfitting is related to generalization
- Explain why overfitting should be avoided

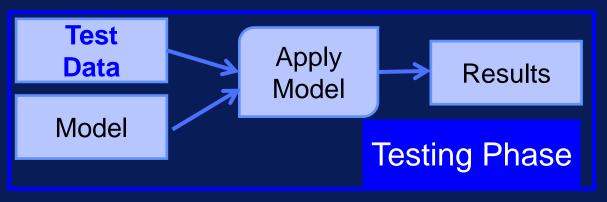
### **Errors in Classification**

- Success: Output = Target true label
- Error: Output != Target
- Error rate = Error = Misclassification Error
  - # errors / # samples = % error



## **Training vs. Testing Phases**





#### **Errors in Classification**

Error on Training Data

Training Error

Error on
Test
Data
Test Error

Test error indicates how well model will perform on new data!

#### Generalization

Performs well on new data



Good Generalization



Test Error = Generalization Error

## Overfitting

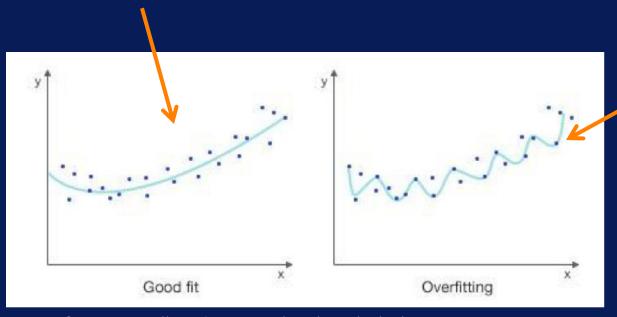


**Test Error** 

## Model is fitting to structure of data

## **Overfitting**

Model is fitting to noise in data

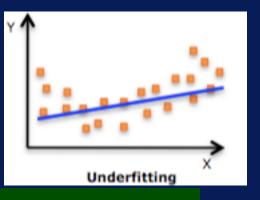


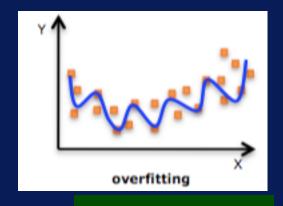
Source: http://blog.fliptop.com/blog/2015/03/02/bias-variance-and-overfitting-machine-learning-overview/

## Overfitting & Generalization

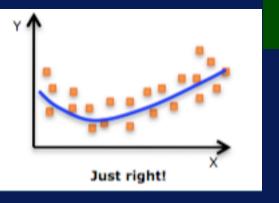


## **Overfitting & Underfitting**





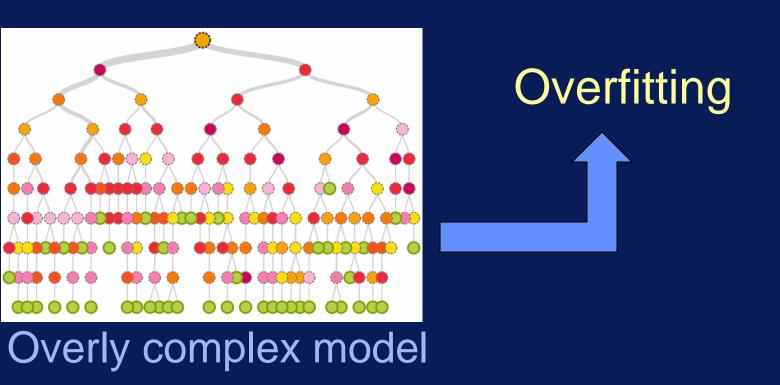
**Underfitting** 



Overfitting

Just Right

## What Causes Overfitting?



## **Generalization & Overfitting**

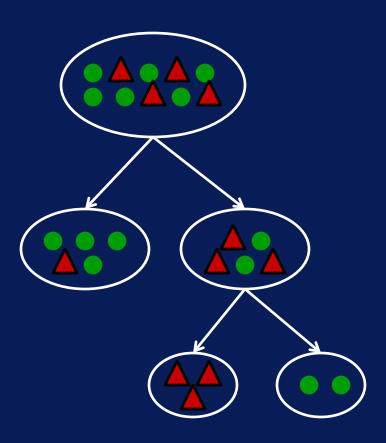


## Overfitting in Decision Trees

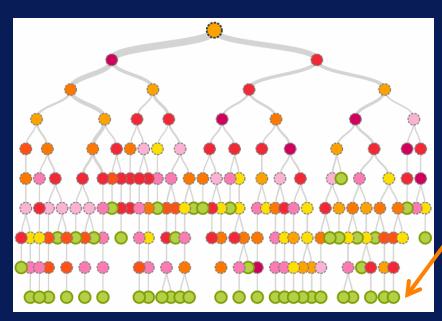
## After this video you will be able to...

- Discuss overfitting in the context of decision tree models
- Explain how overfitting is addressed in decision tree induction
- Define pre-pruning and post-pruning

### **Decision Tree Induction**



## **Overfitting in Decision Tree**



Source: http://piepdx.org/blog/2013/12/10/which-one-is-is

If nodes are fitting to noise in training data, model will not generalize well

## **Avoiding Overfitting in Decision Tree**

Pre-Pruning

Stop growing tree before fully grown

Post-Pruning

Grow tree to max size, then prune

Control number of nodes to limit complexity of tree

### **Pre-Pruning**

- Restrictive stopping conditions for growing tree:
  - Stop if number of records < some threshold</li>
  - Stop if improvement in impurity measure < some threshold</li>

#### Pre-Pruning

Stop growing tree before fully grown

## **Post-Pruning**

- Pruning
  - Remove nodes from bottom up
  - Replace subtree with leaf node if generalization error improves or does not change

#### Post-Pruning

Grow tree to max size, then prune

## Overfitting in Decision Tree

Pre-Pruning

Stop growing tree before fully grown

Post-Pruning

Grow tree to max size, then prune

- Post-pruning used more often
- But is more computational expensive

## **Tree Pruning to Avoid Overfitting**

Pre-Pruning

Stop growing tree before fully grown

Post-Pruning

Grow tree to max size, then prune

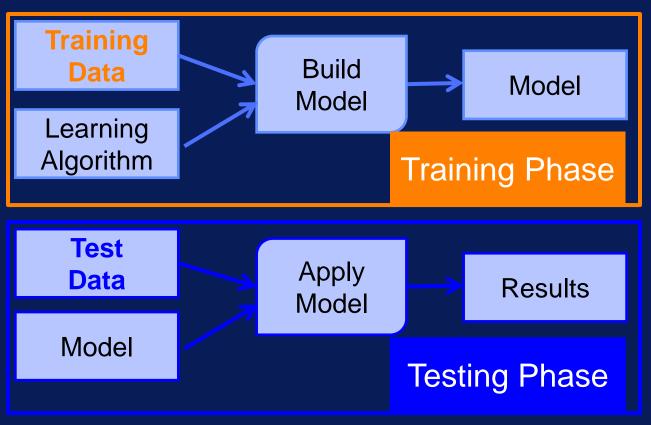
Control number of nodes to limit complexity of tree

# Using a Validation Set

## After this video you will be able to...

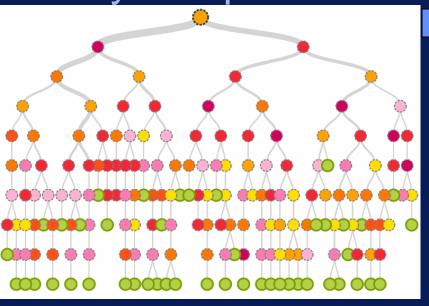
- Describe how a validation set can be used to avoid overfitting
- Articulate how training, validation, and test sets are used
- List three ways that validation can be performed

## **Training vs. Testing Phases**



## **Avoiding Overfitting**

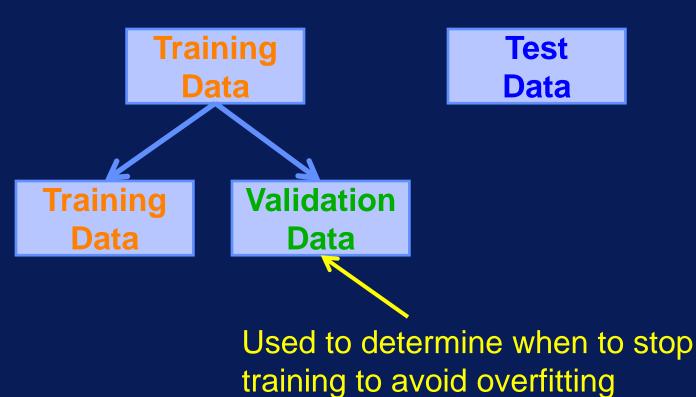
Overly complex model



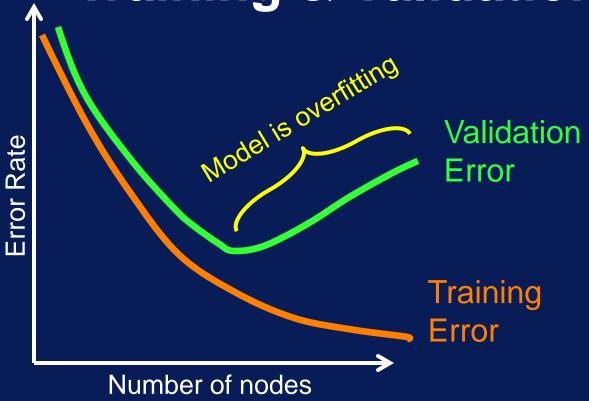
Overfitting

When to stop training before model gets too complex?

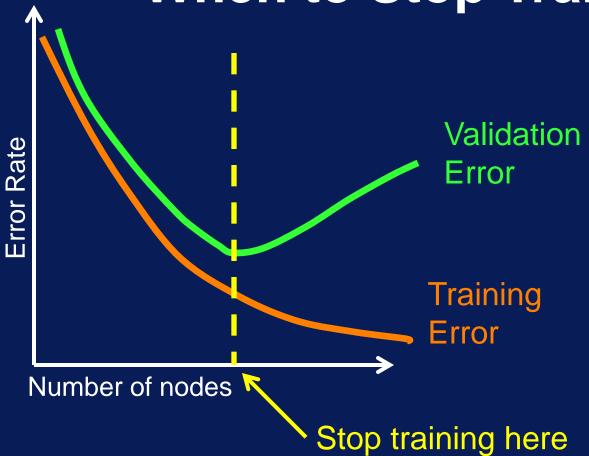
#### Validation Set



## **Training & Validation Errors**



## When to Stop Training



## Ways to Create & Use Validation Set

- Holdout method
- Random subsampling
- K-fold cross-validation
- Leave-one-out cross-validation

#### **Holdout Method**

determine when training

should stop

All data available for building model Used for Holdout set used to

training model

**Training Data** 

Validation Data

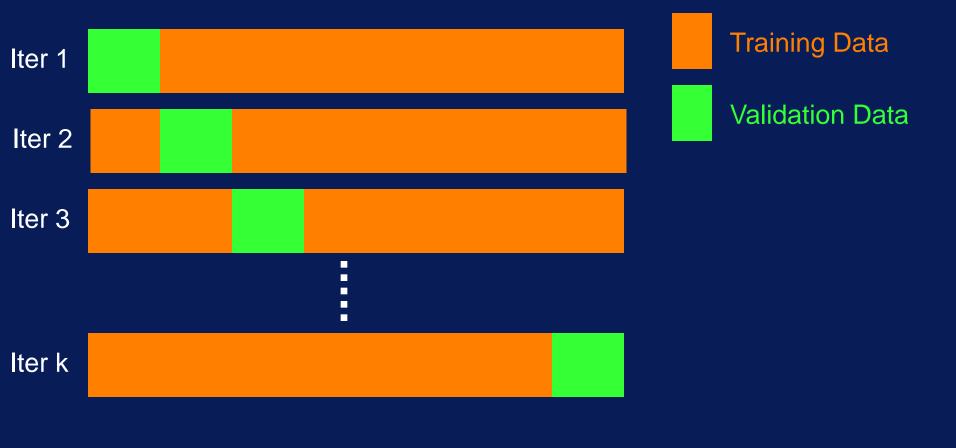
## Repeated Holdout

**Training Data** 

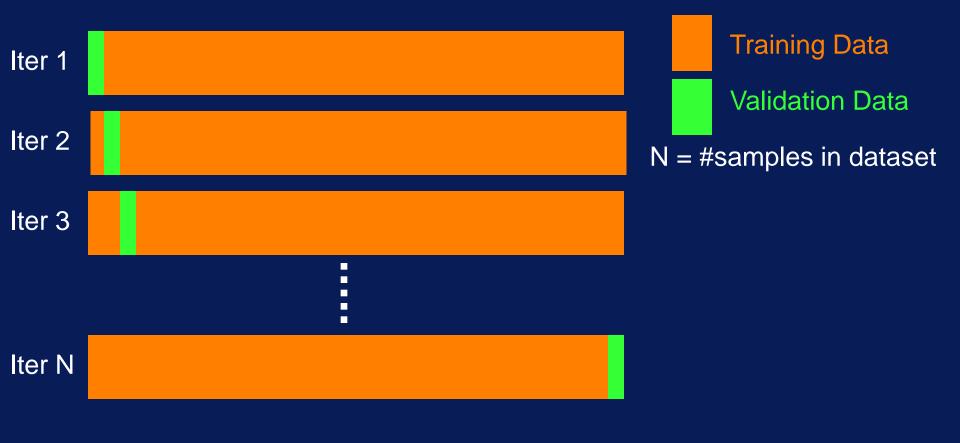
Validation Data

- Repeating holdout method several times
- Randomly select different hold out set each iteration
- Average validation errors over all repetitions

#### **K-Fold Cross-Validation**



#### Leave-One-Out Cross-Validation



#### **Uses of Validation Set**

Validation Data

- Uses:
  - Address overfitting
  - Estimate generalization performance

#### **Datasets**

Training Data

Adjust model parameters

Validation Data

Determine when to stop training (avoid overfitting)

Estimate generalization performance

**Test Data** 

Evaluate performance on new data

Cannot be used in any way in model creation!

## Validation Set Summary

Training Data

Validation Data

> Test Data

- Datasets: training, validation, test
- Validation set: avoid overfitting, estimate generalization
- Using validation: holdout, repeated holdout, crossvalidation (k-fold, leave-one-out)

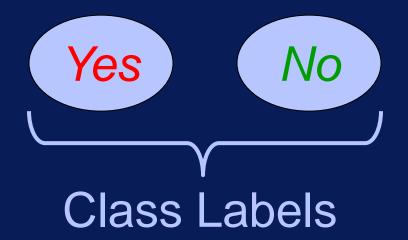
### Metrics to Evaluate Model Performance

### After this video you will be able to...

- Discuss how performance metrics can be used to evaluate models
- Name three model evaluation metrics
- Explain why accuracy may be misleading

#### Classification

Is this animal a mammal?



### Types of

Is this animal a mammal?



Yes No

Class Labels

True Predicted Label Label

Error Type

Yes



True Positive (TP)

No



True Negative (TN)

No



False Positive (FP)

Yes

False Negative (FN)

### Accuracy Rate

Accuracy = 
$$\begin{array}{r}
\text{# correct predictions} \\
\text{Rate} \\
&= \frac{\text{# total predictions}}{\text{TP + TN}} \\
&= \frac{\text{TP + FN}}{\text{TP + FN}}
\end{array}$$

# Error Rate

Error =  $\frac{\text{# incorrect predictions}}{\text{# total predictions}}$   $= \frac{\text{FN+ TP}}{\text{TP + TN + FP + FN}}$  = 1 - Accurate Rate

Predicted Label
No
No
No
Yes
Yes
No
No
Yes
No
Yes

True

Yes

No

No

Yes

Yes

No

Yes

Yes

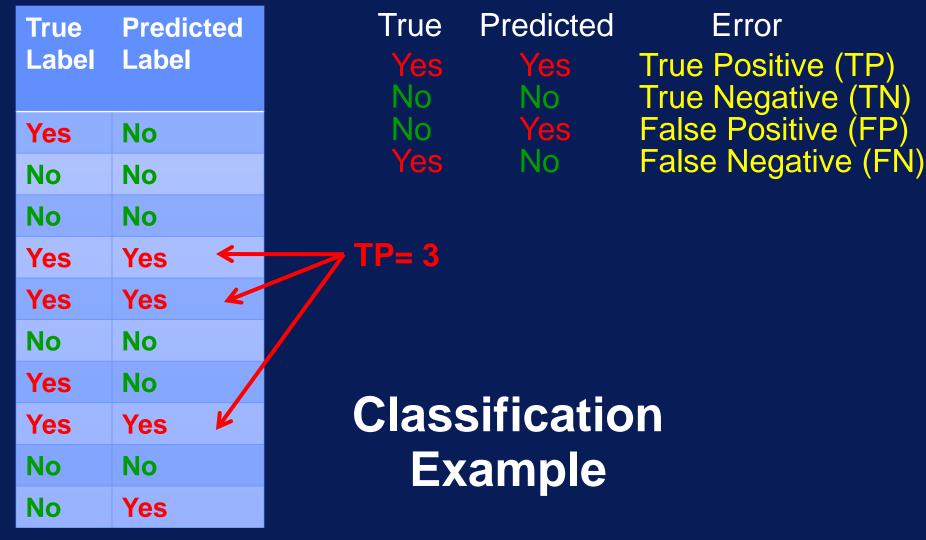
No

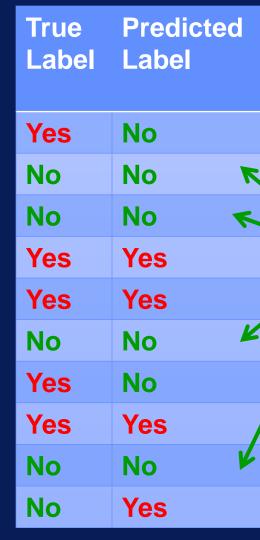
No

Label

True **Predicted** Error Yes Yes True Positive (TP) No No True Negative (TN) False Positive (FP) Yes No False Negative (FN) Yes No

### Classification Example







TN = 4

### Classification Example

### Accuracy Rate

Accuracy = 
$$\frac{\text{# correct predictions}}{\text{# total predictions}}$$

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

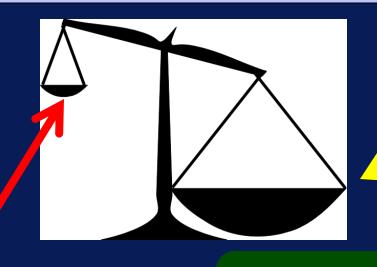
$$= (3 + 4) / 10 = 7 / 10 = 0.7$$

### Error Rate

$$= 1 - 0.7 = 0.3$$

### **Limitation with Accuracy**

Is this tumor cancerous?



most are negative examples

very few positive examples

Class Imbalance Problem

# Limitation with Accuracy

Is this tumor cancerous?



- Say 3% of samples are cancer
- If model <u>always</u> predicts noncancer
  - Accuracy = 97%
  - But no cancer cases detected!

# Precision & Recall

True Predicted Error

Yes Yes True Positive (TP)

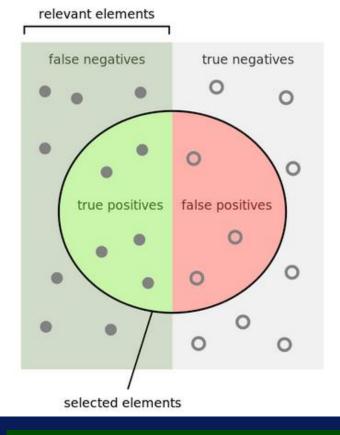
No No True Negative (TN)

No Yes False Positive (FP)

Yes No False Negative (FN)

Precision = 
$$\frac{TP}{TP + FP} \leftarrow \frac{All \text{ samples with Predicted = Yes}}{Predicted = Yes}$$

Recall =  $\frac{TP}{TP + FN} \leftarrow \frac{All \text{ samples with True = Yes}}{True = Yes}$ 



How many selected items are relevant?

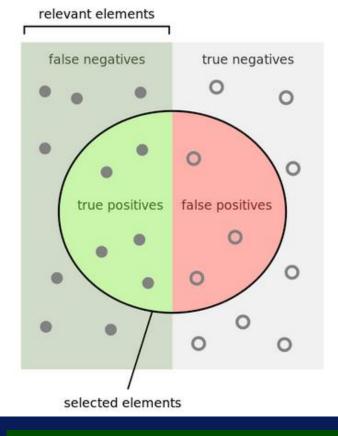
How many relevant items are selected?

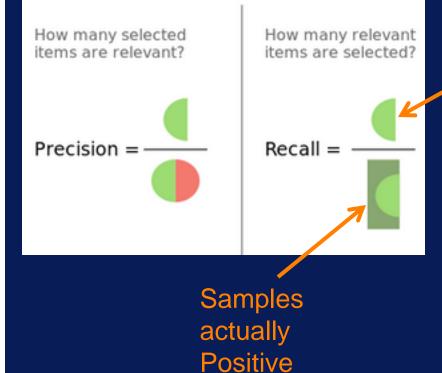
Recall =

Samples correctly predicted as Positive

#### Recall

Source: https://en.wikipedia.org/wiki/Precision\_and\_recall

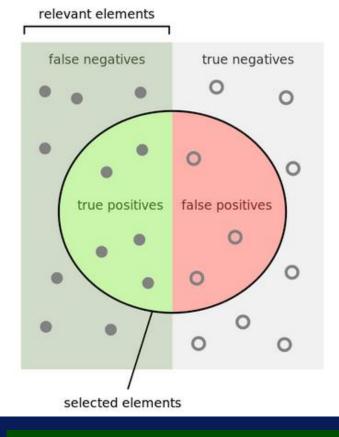


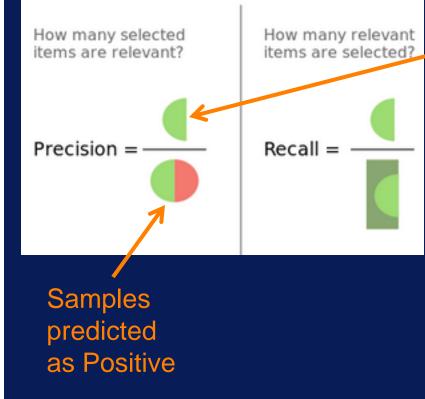


Samples correctly predicted as Positive

#### Recall

Source: https://en.wikipedia.org/wiki/Precision\_and\_recall





Samples correctly predicted as Positive

#### Recall

Source: https://en.wikipedia.org/wiki/Precision\_and\_recall

# Precision & Recall

Precision = 
$$\frac{TP}{TP + FP}$$
 =  $\frac{Positive samples correctly predicted}{All samples predicted as Positive}$ 

$$Recall = \frac{TP}{TP + FN} = \frac{Positive samples correctly predicted}{All samples with true label Positive}$$

Measure of completeness

exactness

#### **Precision & Recall**

Precision



Recall

- Use together
- Goal: Maximize both

#### F-Measure

**Precision** 



Recall

- F<sub>1</sub>: evenly weighted
- F<sub>2</sub>: weights Recall more
- F<sub>0.5</sub>: weights Precision more

# **Evaluation Metrics**

True Predicted
Yes Yes
No No
No Yes
Yes
No

Error
True Positive (TP)
True Negative (TN)
False Positive (FP)
False Negative (FN)

Accuracy Rate

Error Rate

Precision & Recall

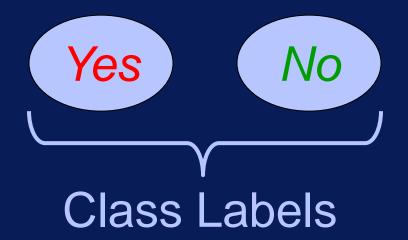
F₁-Measure

### After this video you will be able to...

- Describe how a confusion matrix can be used to evaluate a classifier
- Interpret the confusion matrix of a model
- Relate accuracy to values in a confusion matrix

#### Classification

Is this animal a mammal?



### Types of Classification Errors

Is this animal a mammal?



True Predicted Label

Error Type

Yes



True Positive (TP)





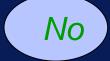
True Negative (TN)





False Positive (FP)





False Negative (FN)

Is this animal a mammal?



	Predicted Class Label			
True		Yes	No	
Class Label  Yes  No	True Positive (TP)	False Negative (FN)		
	No	False Positive (FP)	True Negative (TN)	

Class Labels

True Label	Predicted Label
Yes	No
No	No
No	No
Yes	Yes
Yes	Yes
No	No
Yes	No
Yes	Yes
No	No
No	Yes

	Predicted Class Label		
True Class Label		Yes	No
	Yes	TP	FN
	No	FP	TN

True Label	Predicted Label
Yes	No
No	No
No	No
Yes	Yes
Yes	Yes
No	No
Yes	No
Yes	Yes
No	No
No	Yes

	Predicted Class Label		
True Class		Yes	No
Label	Yes	<b>TP = 3</b>	
	No		

True Label	Predicted Label
Yes	No
No	No K
No	No K
Yes	Yes
Yes	Yes
No	No Z
Yes	No
Yes	Yes
No	No V
No	Yes

	Predicted Class Label		
True Class		Yes	No
Label	Yes	TP = 3	
	No		TN = 4

True Label	Predicted Label
Yes	No
No	No
No	No
Yes	Yes
Yes	Yes
No	No
Yes	No 📕
Yes	Yes
No	No
No	Yes

	Predicted Class Label		
True Class		Yes	No
Label	Yes	TP = 3	FN = 2
	No		TN = 4

FN

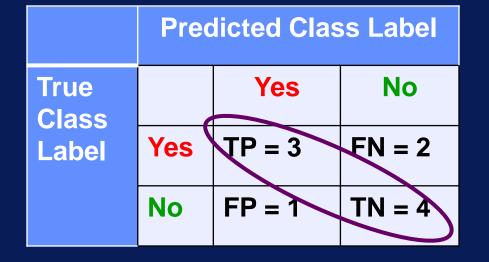
True Label	Predicted Label
Yes	No
No	No
No	No
Yes	Yes
Yes	Yes
No	No
Yes	No
Yes	Yes
No	No
No	Yes 😕

	Predicted Class Label		
True Class		Yes	No
Label	Yes	TP = 3	FN = 2
	No	FP = 1	TN = 4

True Label	Predicted Label
Yes	No
No	No
No	No
Yes	Yes
Yes	Yes
No	No
Yes	No
Yes	Yes
No	No
No	Yes

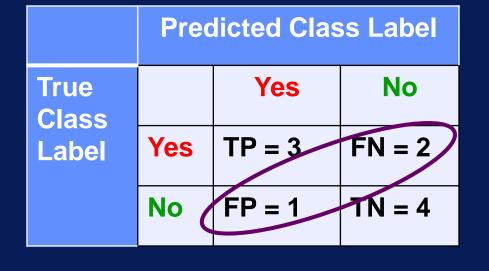
	Predicted Class Label		
True Class Label		Yes	No
	Yes	TP = 3	FN = 2
	No	FP = 1	TN = 4

True Label	Predicted Label
Yes	No
No	No
No	No
Yes	Yes
Yes	Yes
No	No
Yes	No
Yes	Yes
No	No
No	Yes



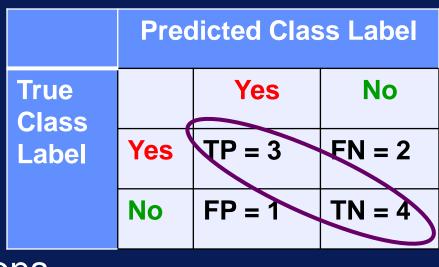
Correct Predictions: 7 out of 10 = 0.7

	Predicted
abel	Label
es	No
lo	No
lo	No
es	Yes
es	Yes
lo	No
es	No
es	Yes
lo	No
lo	Yes



Incorrect Predictions: 3 out of 10 = 0.3

# **Confusion Matrix** & Accuracy Rate

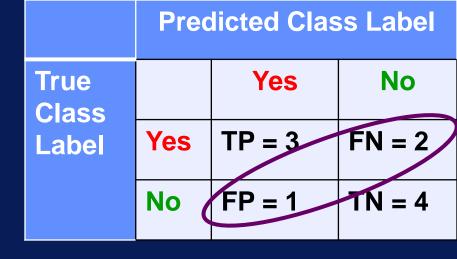


Accuracy = 
$$\frac{\text{# correct predictions}}{\text{# total predictions}}$$

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

$$= (3 + 4) / 10 = 7 / 10 = 0.7$$

## Confusion Matrix & Error Rate



$$= 1 - 0.7 = 0.3$$

## **Misclassifications in Confusion Matrix**

	Predicted Class Label					
True Class		Yes	No			
Label	Yes	TP = 3	FN = 2			
	No	FP = 1	TN = 4			

High value means classifying Positive class is problematic

High value means classifying Negative class is problematic

# **Confusion Matrix**

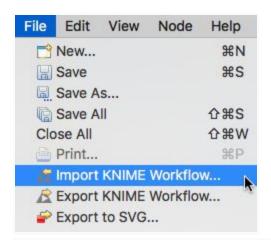
	Predicted Class Label						
True Class		Yes	No				
Label	Yes	TP	FN				
	No	FP	TN				

### Completed KNIME Workflows

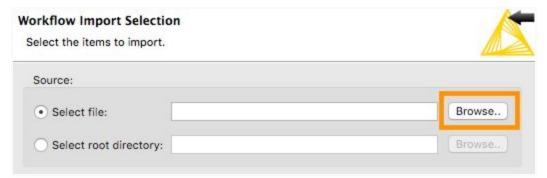
The completed KNIME workflows for this course are available here:

KNIME-workflows.zip

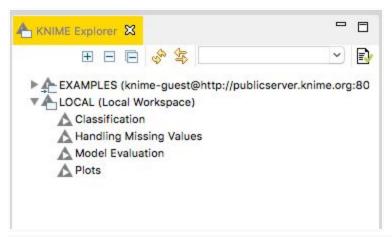
To load these in KNIME, select File -> Import KNIME Workflow:



Next, click on the *Browse* button and select the workflow to import:



Finally, click on *Finish*. The workflow will be added to your *LOCAL* Workspace, and you can load it by double-clicking on the name:



Finally, double-click on the *File Reader* Node and change the *valid URL* parameter to the location of *daily\_weather.csv* on your computer:



### Comparing Classification Results for KNIME and Spark

You may have noticed that the classification results from KNIME and Spark MLlib decision trees are not exactly the same. This document describes the differences in the setup that can lead to this disparity.

### Random Seed for Partitioning

In the step to partition data into training and test sets, random sampling is used in both KNIME and Spark MLlib. However, note that different random seed values are used. A value of 12345 is used for KNIME, and 13234 is used for Spark. Different seed values will generate different random number sequences. Since the selection of which samples go into the training vs. the test partition is based on these random number sequences, the contents of the training and test datasets will be different with different seed values. Consequently, different training and test sets will change the performance results of the classifier. Cross validation is a common approach to address this variability in performance with a single partitioning of the data.

### Partitioning into Training and Test Sets

You also may have noticed that the sizes of the training and test sets are different between KNIME and Spark. This is due to the different sampling methods that they use to partition data.

Spark uses a sampling method that does not generate a fixed sample size. So if we specify that the test size should be 20% of the available data, the resulting test size is only approximately 20%, not necessarily exactly.

KNIME uses a different way to randomly select samples to be placed in either training and test set. Due to the different sampling techniques, the contents of the training and test sets are different for KNIME and Spark MLlib.

#### **Decision Tree**

KNIME and Spark MLlib use different methods to constrain the complexity of the decision tree model. In both, the minimum number of samples in a node can be specified as a stopping criterion for growing the tree. If the number of samples reaches this threshold, the node is not split.

In Spark, you can also specify the maximum depth of the tree as another stopping criterion (the maxDepth parameter). KNIME does not have this option in its Decision Tree Learner node.

KNIME does have an option for pruning the tree, however. The default setting in the Decision Tree Learner node uses 'Reduced error pruning'. This prunes the tree by replacing a node with the class of the majority of the samples in that node, if doing so does not decrease the accuracy of the classifier. Spark's DecisionTreeClassifier method does not have an option to prune the tree.

#### Performance Results

As we can see, there are several differences in the setup for a decision tree classifier in KNIME and Spark MLlib. These differences result in different trained models, and consequently, different classification performance numbers.

### **Evaluation of Decision Tree in KNIME**

### **Learning Objectives**

At the end of this activity, you will be able to perform the following operations in KNIME:

- 1. Create and interpret a confusion matrix for a decision tree
- 2. Determine the accuracy rate of a decision tree model
- 3. Use highlighting to analyze classification errors

### **Problem Description**

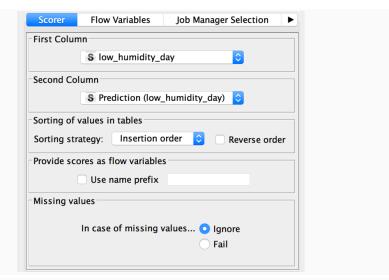
With the decision tree classifier built, we now need to evaluate its performance.

### Steps

### Generate a Confusion Matrix and Determine Accuracy Rate

A confusion matrix shows the type of errors and correct classifications that a classifier makes. It can be generated using a **Scorer** node.

- Open the Decision Tree Workflow that you created from the Classification Hands-On reading.
- 2. Connect a **Scorer** node to the existing **Decision Tree Predictor**.
- 3. The Scorer Configure Dialog should look like this by default. Click OK.



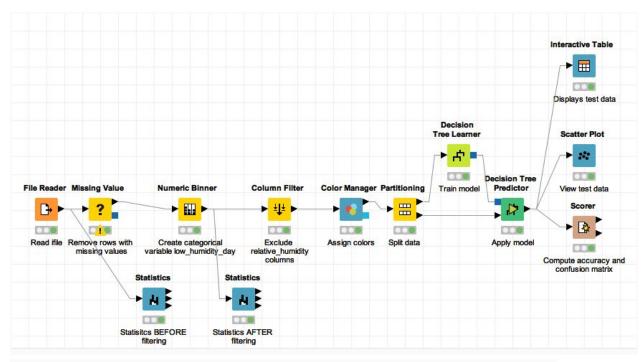
Execute and view the **Scorer** node. It shows the confusion matrix, along with the accuracy of the prediction. Here you should see an accuracy rate of 80.282% if you followed all the hands-on instructions.

low_humidity_day \ Prediction (low_humidity_day) humidity_low humidity_not_low	humidity_low 76 18	humidity_not_low 24 95
Correct classified: 171	Wrong class	ified: 42
Accuracy: 80.282 %	Error: 19.718 %	
Cohen's kappa (к) 0.603		

From the confusion matrix, we see the following:

- There are 213 samples in the test data set (the sum of all the values in the confusion matrix)
- 76 humidity\_low samples with were correctly classified
- 95 humidity not low samples were correctly classified
- The accuracy rate is (76 + 95) / 213 = 171 / 213 = 80.282%
- 24 humidity\_low samples were incorrectly classified as humidity\_not\_low
- 18 humidity\_not\_low samples were incorrectly classified as humidity\_low
- The error rate is (24 + 18) / 213 = 42 / 213 = 19.718%

### Use Highlighting and Scatter Plot to Analyze Classification Errors



A good way to enhance analysis of incorrect predictions is to visualize them. This can be accomplished using a feature called **hiliting**, and viewing the data in a **Scatter Plot** node.

- 1. Connect an Interactive Table node to the Decision Tree Predictor.
- 2. Execute and view this Interactive Table to see the input values for each sample (row), along with the ACTUAL/TRUE low\_humidity\_day value and the PREDICTED low\_humidity\_day value. The red and blue squares next to the Row ID color-codes the actual/true label (low or not). You can use this table to analyze samples whose true value differs from the predicted value (incorrect prediction).
- 3. Connect a **Scatter Plot** node to the **Decision Tree Predictor**.
- 4. Execute and view the **Scatter Plot** node, and place the window side-by-side with the **Interactive Table** window.
- 5. Go through the table looking for rows with predictions that are different from the true value.
- 6. When you find such a row, click anywhere on that row. At the top of the window click Hilite > Hilite Selected. This will make that row yellow in the table and in the Scatter Plot. It may be easiest to use the up and down arrow keys to navigate the rows of the table. In this example, we are just going to highlight the first 5 misclassifications.
- 7. Do this for any row with a misclassification. This allows you to pinpoint the misclassified samples and analyze them further. Analyzing the misclassified samples can bring insight into how to improve model performance. For example, if many samples with

avg\_temperature\_9am between 60 and 70 degrees are misclassified, this suggests that more samples with these values for avg\_temperature\_9am are needed to train the model.

91.65   77.036   70.6   3.825   85.5   4.765   0   0	Row ID	D air_pr	. D air_te	. <b>D</b> avg_w	D avg_w	D max	<b>D</b> max	D rain_a	D rain_d	S low_humidi	S Prediction
15	10	_			Access to the second second			0	-		humidity low
11	15		70.865					0	0		
131	17										
33 918,37 63,914 53,7 14,451 72,1 17,045 0 0 0 municity, low humidity, not last set of the set of t	31										
88 914.66 \$0.36 177.6 8.523 186.3 10.021 0 20 humidity, not, low humidity, not and the property of the propert	33										
914.9   64.688   174.6   5.659   184.5   6.867   0   0   humidity, not, low humidity, and, low humidity, and, low humid	38										
18.5	43										
17. 916.05 87.188 210 1.566 109.3 2.595 0 0 0 humidity.low humidity.low lumidity.low lumidity.lo	46										
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### Save Your Workflow

or File>Save As.		

Save your workflow using <control>-s on Windows or <command>-s on Mac, or selecting File>Save

### **Evaluation of Decision Tree in Spark**

By the end of this activity, you will be able to perform the following in Spark:

- 1. Determine the accuracy of a classifier model
- 2. Display the confusion matrix for a classifier model

In this activity, you will be programming in a Jupyter Python Notebook. If you have not already started the Jupyter Notebook server, see the instructions in the Reading *Instructions for Starting Jupyter*.

Step 1. **Open Jupyter Python Notebook.** Open a web browser by clicking on the web browser icon at the top of the toolbar:



Navigate to localhost:8889/tree/Downloads/big-data-4:

localhost:8889/tree/Downloads/big-data-4

Open the model evaluation notebook by clicking on *model-evaluation.ipynb*:



Step 2. Load predictions. Execute the first cell to load the classes used in this activity:

```
In [1]: from pyspark.sql import SQLContext
    from pyspark.ml.evaluation import MulticlassClassificationEvaluator
    from pyspark.mllib.evaluation import MulticlassMetrics
```

Execute the next cell to load the predictions CSV file that we created at the end of the Week 3 Hands-On *Classification in Spark* into a DataFrame:

Step 3. **Compute accuracy.** Let's create an instance of *MulticlassClassificationEvaluator* to determine the accuracy of the predictions:

The first two arguments specify the names of the label and prediction columns, and the third argument specifies that we want the overall precision.

We can compute the accuracy by calling evaluate():

```
In [4]: accuracy = evaluator.evaluate(predictions)
print("Accuracy = %g " % (accuracy))

Accuracy = 0.809524
```

Step 4. **Display confusion matrix.** The *MulticlassMetrics* class can be used to generate a confusion matrix of our classifier model. However, unlike *MulticlassClassificationEvaluator*, *MulticlassMetrics* works with RDDs of numbers and not DataFrames, so we need to convert our *predictions* DataFrame into an RDD.

If we use the *rdd* attribute of *predictions*, we see this is an *RDD* of *Rows*:

```
In [5]: predictions.rdd.take(2)
Out[5]: [Row(prediction=1.0, label=1.0), Row(prediction=1.0, label=1.0)]
```

Instead, we can map the RDD to *tuple* to get an RDD of numbers:

```
In [6]: predictions.rdd.map(tuple).take(2)
Out[6]: [(1.0, 1.0), (1.0, 1.0)]
```

Let's create an instance of *MulticlassMetrics* with this RDD:

```
In [7]: metrics = MulticlassMetrics(predictions.rdd.map(tuple))
```

**NOTE**: the above command can take longer to execute than most Spark commands when first run in the notebook.

The *confusionMatrix()* function returns a Spark *Matrix*, which we can convert to a Python Numpy array, and transpose to view: