### Nearest Neighbor, Decision Tree

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https://www.ischool.utexas.edu/~dannag/Courses/IntroToMachineLearning/CourseContent.html

#### Review

- Last week:
  - Binary classification applications
  - Evaluating classification models
  - Biological neurons: inspiration
  - Artificial neurons: Perceptron & Adaline
  - Gradient descent
- Assignments (Canvas)
  - Lab assignment 1 due tonight
  - Problem set 3 due next week
- Questions?

### Today's Topics

- Multiclass classification applications and evaluating models
- Motivation for new ML era: need non-linear models
- Nearest neighbor classification
- Decision tree classification
- Parametric versus non-parametric models

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#### Today's Focus: Multiclass Classification

Predict 3+ classes

#### Multiclass Classification: Cancer Diagnosis

Doctor-level performance in recognizing 2,032 diseases



https://www.nature.com/articles/nature21056

https://news.stanford.edu/2017/01/25/artificial-intelligence-used-identify-skin-cancer/

#### Multiclass Classification: Face Recognition



Social media



Visual assistance for people with vision impairments



Security https://www.anyvision.co/

#### Multiclass Classification: Shopping



Camfind (https://venturebeat.com/2014/09/24/camfind-appbrings-accurate-visual-search-to-google-glass-exclusive/)

#### Multiclass Classification: Song Recognition



https://gbksoft.com/blog/how-to-make-a-shazam-like-app/



#### 1. Split data into a "training set" and "test set"



2. Train model on "training set" to try to minimize prediction error on it













#### **Evaluation Methods**

• Confusion matrix; e.g.,

• Accuracy: percentage correct

• Precision:  $\frac{TP}{TP + FP}$ • Recall:  $\frac{TP}{TP + FN}$ 



http://gabrielelanaro.github.io/blog/2016/0 2/03/multiclass-evaluation-measures.html

### Today's Topics

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#### Recall: Historical Context of ML Models



#### Recall: Vision for Perceptron



Frank Rosenblatt (Psychologist) "[The perceptron is] the embryo of an electronic computer that [the Navy] expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence.... [It] is expected to be finished in about a year at a cost of \$100,000."

1958 New York Times article: https://www.nytimes.com/1958/07/08/archives/newnavy-device-learns-by-doing-psychologist-shows-embryo-of.html

https://en.wikipedia.org/wiki/Frank\_Rosenblatt

#### "Perceptrons" Book: Instigator for "AI Winter"



- Input: two binary values x<sub>1</sub> and x<sub>2</sub>
- Output:
  - 1, when exactly one input equals 1
  - 0, otherwise

<b>x</b> <sub>1</sub>	x <sub>2</sub>	$x_1 XOR x_2$
0	0	?
0	1	?
1	0	?
1	1	?

- Input: two binary values x<sub>1</sub> and x<sub>2</sub>
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0	0	0
0	1	1
1	0	?
1	1	?

- Input: two binary values x<sub>1</sub> and x<sub>2</sub>
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<b>x</b> <sub>1</sub>	<b>x</b> <sub>2</sub>	$x_1 XOR x_2$
0	0	0
0	1	1
1	0	1
1	1	?

- Input: two binary values x<sub>1</sub> and x<sub>2</sub>
- Output:
  - 1, when exactly one input equals 1
  - 0, otherwise

<b>x</b> <sub>1</sub>	<b>x</b> <sub>2</sub>	$x_1 XOR x_2$
0	0	0
0	1	1
1	0	1
1	1	0

How to separate 1s from 0s with a perceptron (linear function)?



<b>x</b> <sub>1</sub>	<b>x</b> <sub>2</sub>	x <sub>1</sub> XOR x <sub>2</sub>
0	0	0
0	1	1
1	0	1
1	1	0



Frank Rosenblatt (Psychologist) "[The perceptron is] the embryo of an electronic computer that [the Navy] expects will be able to walk, talk, see, write, reproduce itself and be conscious of its

How can a machine be "conscious" when it can't solve the XOR problem?

navy-device-learns-by-doing-psychologist-shows-embryo-of.html

#### How to Overcome Limitation?

#### Non-linear models: e.g.,

- Linear regression: perform non-linear transformation of input features
- K-nearest neighbors
- Decision trees
- And many more to follow...

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#### Historical Context of ML Models



E. Fix and J.L. Hodges. Discriminatory Analysis, Nonparametric Discrimination: Consistency Properties. Technical Report 4, USAF School of Aviation Medicine, Randolph Field, 1951

#### **Recall: Instance-Based Learning**



#### Memorizes examples and uses a similarity measure to those examples to make predictions

Figure Source: Hands-on Machine Learning with Scikit-Learn & TensorFlow, Aurelien Geron

#### e.g., Predict What Scene The Image Shows



#### e.g., Predict What Scene The Image Shows

#### 1. Create Large Database


2. Organize Database so Visually Similar Examples Neighbor Each Other



3. Predict Class Using Label of Most Similar Example(s) in the Database





Label: ?

3. Predict Class Using Label of Most Similar Example(s) in the Database





3. Predict Class Using Label of Most Similar Example(s) in the Database





#### Label: ?

3. Predict Class Using Label of Most Similar Example(s) in the Database





## K-Nearest Neighbor Classification



Novel Examples:

• Given:

## K-Nearest Neighbor Classification



Novel Examples:

• Given:

- Predict:
  - When k = 1:
    - Class 1
  - When k = **6**:
    - How to avoid ties?
      - Set "k" to odd value for binary problems
      - Prefer "closer" neighbors

How to measure distance between a novel example and test example?

• Commonly use, Minkowski distance:

$$D\left(X,Y
ight) = \left(\sum_{i=1}^n |x_i-y_i|^p
ight)^{1/p}$$

• When p = 2, Euclidean distance:

$$=\sqrt{\sum_{i=1}^n (x_i-y_i)^2}$$

• When p = 1, Manhattan distance:

$$=\sum_{i=1}^n |x_i-y_i||$$





#### **Euclidean Distance**

• Given:

$$x=1: = \sqrt{\sum_{i=1}^n (x_i-y_i)^2}$$

$$\begin{aligned} dist &= \sqrt{(10.5 - 10.1)^2 + (3 - 2.3)^2} \\ dist &= \sqrt{0.4^2 + 0.7^2} \\ dist &= \sqrt{0.16 + 0.49} \\ dist &= \sqrt{0.65} \\ dist &= 0.81 \end{aligned}$$



**Euclidean Distance** 

• Given:

=1:
$$=\sqrt{\sum_{i=1}^n (x_i-y_i)^2}$$

 $dist = \sqrt{(10.5 - 10.1)^2 + (3 - 2.3)^2}$ Note: May7want to  $dist = \sqrt{0.16 + 0.49}$ scale the data to the dist = 0.81same range first



**Manhattan Distance** 

Given:

•

$$= \sum_{i=1}^n |x_i - y_i|$$

dist = |10.5 - 10.1| + |3 - 2.3|dist = 0.4 + 0.7dist = 1.1



**Manhattan Distance** 

$$=\sum_{i=1}^n |x_i-y_i|$$

How to measure distance for novel categorical test data?

- e.g., Train = blue
- e.g., Test = blue; identical values so assign distance 0
- e.g., Test = white; different values so assign distance 1







#### What happens to the decision boundary as "k" grows?



#### What happens when "k" equals the training data size?





At what value for "k" is model **overfitting** the most?

k = 1



## K-Nearest Neighbor: How to Use to Predict More than Two Classes?

• Tally number of examples belonging to each class and again choose the majority vote winners

# What are Strengths of KNN?

- Adapts as new data is added
- Training is relatively fast
- Easy to understand

#### What are Weaknesses of KNN?

- For large datasets, requires large storage space
- For large datasets, this approach can be very slow or infeasible
  - Note: can improve speed with efficient data structures such as KD-trees
- Vulnerable to noisy/irrelevant examples
- Sensitive to imbalanced datasets where more frequent class will dominate majority voting

# Today's Topics

- Multiclass classification applications and evaluating models
- Motivation for new ML era: need non-linear models
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- Parametric versus non-parametric models

# Historical Context of ML Models

Quinlan, J. R. (1986). Induction of decision trees. *Machine learning*, 1(1), 81-106. Hunt, E.B. (1962). Concept learning: An information processing problem. New York: Wiley. Quinlan, J.R. (1979). Discovering rules by induction from large collections of examples. In D. Michie (Ed.), Expert systems in the micro electronic age. Edinburgh University Press.



## Example: Decision Tree



#### Test Example

#### Example: Decision Tree decision nodes salary at least \$50,000 yes decline commute more yes than 1 hour no offers free decline yes coffee offer no **Decision Tree:**

accept

offer

decline

offer

Should I accept a new

job offer?

Salary: \$44,869 Commute: 35 min Free Coffee: Yes

offer

leaf nodes

## Test Example Salary: \$62,200



Example: Decision Tree

## Example: Decision Tree



Machine must learn to create a decision tree

## Decision Tree: Generic Structure

- Goal: predict class label (aka: class, ground truth)
- Representation: Tree
  - Internal (non-leaf) nodes = tests an attribute
  - Branches = attribute value
  - Leaf = classification label

### Decision Tree: Generic Structure

- Goal: predict class label (aka: class, ground truth)
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## Decision Tree: Generic Structure

- Goal: predict class label
- Representation: Tree
  - Internal (non-leaf) nodes = tests an attribute
  - Branches = attribute value
  - How can a machine learn a decision tree?

## Decision Tree: Generic Learning Algorithm

 Greedy approach (NP complete problem) Function BuildTree(n,A) // n: samples (rows), A: attributes aka – "data" aka – "feature names"

# Decision Tree: Generic Learning Algorithm

• Greedy approach (NP complete problem)

Function BuildTree(n,A) // n: samples (rows), A: attributes

If empty(A) or all n(L) are the same

status = leaf

class = most common class in n(L)



# Decision Tree: Generic Learning Algorithm

• Greedy approach (NP complete problem)

Function BuildTree(n,A) // n: samples (rows), A: attributes If empty(A) or all n(L) are the same

```
status = leaf
```

```
class = most common class in n(L)
```

```
else
```

```
status = internala \leftarrow bestAttribute(n,A)Key DecisionLeftNode = BuildTree(n(a=1), A \ {a})RightNode = BuildTree(n(a=0), A \ {a})end
```



## Next "Best" Attribute: Use Entropy



Fraction of examples belonging to class *i* 

In a binary setting,

- Entropy is 0 when fraction of examples belonging to a class is 0 or 1
- Entropy is 1 when fraction of examples belonging to each class is 0.5



https://www.logcalculator.net/log-2
$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i$$

e.g., Will you like a movie?

Movie	Type	Length	IMDb Rating	Liked?
m1	Comedy	Short	7.2	Yes
m2	Drama	Medium	9.3	Yes
m3	Comedy	Medium	5.1	No
m4	Drama	Long	6.9	No
m5	Drama	Medium	8.3	Yes
m6	Drama	Short	4.5	No
m7	Comedy	Short	8.0	Yes
m8	Drama	Medium	7.5	Yes

$$Entropy = -\left[\frac{5}{8}\log_2\frac{5}{8}\right] +$$

$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i$$

e.g., Will you like a movie?

Movie	Type	Length	IMDb Rating	Liked?
m1	Comedy	Short	7.2	Yes
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m4	Drama	Long	6.9	No
m5	Drama	Medium	8.3	Yes
m6	Drama	Short	4.5	No
m7	Comedy	Short	8.0	Yes
m8	Drama	Medium	7.5	Yes

$$Entropy = -(\frac{5}{8}\log_2\frac{5}{8} + \frac{3}{8}\log_2\frac{3}{8})$$

$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i$$

e.g., Will you like a movie?

Movie	Type	Length	IMDb Rating	Liked?
m1	Comedy	Short	7.2	Yes
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m3	Comedy	Medium	5.1	No
m4	Drama	Long	6.9	No
m5	Drama	Medium	8.3	Yes
m6	Drama	Short	4.5	No
m7	Comedy	Short	8.0	Yes
m8	Drama	Medium	7.5	Yes



- Let C1 = "Yes" and C2 = "No"
- Current entropy?

$$Entropy = -(\frac{5}{8}\log_2 \frac{5}{8} + \frac{3}{8}\log_2 \frac{3}{8})$$

$$Entropy = -(-0.42 - 0.53) = 0.95$$

$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i$$

e.g., Will you like a movie?

Movie	Type	Liked?
m1	Comedy	Yes
m2	Drama	Yes
m3	Comedy	No
m4	Drama	No
m5	Drama	Yes
m6	Drama	No
m7	Comedy	Yes
m8	Drama	Yes

- Let C1 = "Yes" and C2 = "No"
- Entropy if we split on "Type"?
  - Left tree: "Comedy" = ?

$$Entropy = -(\frac{2}{3}\log_2\frac{2}{3} + \frac{1}{3}\log_2\frac{1}{3})$$

$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i$$

e.g., Will you like a movie?

Movie	Type	Liked?
m1	Comedy	Yes
$m^2$	Drama	Yes
m3	Comedy	No
m4	Drama	No
m5	Drama	Yes
m6	Drama	No
m7	Comedy	Yes
m8	Drama	Yes

- Let C1 = "Yes" and C2 = "No"
- Entropy if we split on "Type"?
  - Left tree: "Comedy" = ?

$$Entropy = -(\frac{2}{3}\log_2\frac{2}{3} + \frac{1}{3}\log_2\frac{1}{3})$$

Entropy = -(-0.53 - 0.39) = 0.92

$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i$$

e.g., Will you like a movie?

Movie	Type	Liked?
m1	Comedy	Yes
m2	Drama	Yes
m3	Comedy	No
m4	Drama	No
m5	Drama	Yes
m6	Drama	No
m7	Comedy	Yes
m8	Drama	Yes

- Let C1 = "Yes" and C2 = "No"
  - Entropy if we split on "Type"?
    - Left tree: "Comedy" = 0.92
    - Right tree: "Drama" = ?

$$Entropy = -(\frac{3}{5}\log_2\frac{3}{5} + \frac{2}{5}\log_2\frac{2}{5})$$

$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i$$

e.g., Will you like a movie?

Movie	Type	Liked?
m1	Comedy	Yes
m2	Drama	Yes
m3	Comedy	No
m4	Drama	No
m5	Drama	Yes
m6	Drama	No
m7	Comedy	Yes
m8	Drama	Yes

Let C1 = "Yes" and C2 = "No"

- Left tree: "Comedy" = 0.92
- Right tree: "Drama" = ?

$$Entropy = -(\frac{3}{5}\log_2\frac{3}{5} + \frac{2}{5}\log_2\frac{2}{5})$$

Entropy = -(-0.44 - 0.53) = 0.97

$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i$$

e.g., Will you like a movie?

Movie	Type	Liked?
m1	Comedy	Yes
m2	Drama	Yes
m3	Comedy	No
m4	Drama	No
m5	Drama	Yes
m6	Drama	No
m7	Comedy	Yes
m8	Drama	Yes

- Let C1 = "Yes" and C2 = "No"
- Entropy if we split on "Type"?
  - Left tree: "Comedy" = 0.92
  - Right tree: "Drama" = 0.97
- Information gain by split on "Type"?

$$IG = 0.95 - \left(\frac{3}{8} * 0.92 + \frac{5}{8} * 0.97\right)$$
  
$$IG = 0$$

$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i$$

e.g., Will you like a movie?

Movie	Length	Liked?
m1	Short	Yes
m2	Medium	Yes
m3	Medium	No
m4	Long	No
m5	Medium	Yes
m6	Short	No
m7	Short	Yes
m8	Medium	Yes

- Let C1 = "Yes" and C2 = "No"
- Entropy if we split on "Length"?
  Left tree: "Short" = ?

$$Entropy = -(\frac{2}{3}\log_2\frac{2}{3} + \frac{1}{3}\log_2\frac{1}{3})$$

Entropy = -(-0.53 - 0.39) = 0.92

$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i$$

e.g., Will you like a movie?

Movie	Length	Liked?
m1	Short	Yes
m2	Medium	Yes
m3	Medium	No
m4	Long	No
m5	Medium	Yes
m6	Short	No
m7	Short	Yes
m8	Medium	Yes

- Let C1 = "Yes" and C2 = "No"
- Entropy if we split on "Length"?
  - Left tree: "Short" = 0.92
  - Middle tree: "Medium" = ?

$$Entropy = -(\frac{3}{4}\log_2\frac{3}{4} + \frac{1}{4}\log_2\frac{1}{4})$$

Entropy = -(-0.32 - 0.5) = 0.82

$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i$$

e.g., Will you like a movie?

Movie	Length	Liked?
m1	Short	Yes
m2	Medium	Yes
m3	Medium	No
m4	Long	No
m5	Medium	Yes
m6	Short	No
m7	Short	Yes
m8	Medium	Yes

- Let C1 = "Yes" and C2 = "No"
- Entropy if we split on "Length"?
  - Left tree: "Short" = 0.92
  - Middle tree: "Medium" = 0.82
  - Right tree: "Long" = ?

$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i$$

e.g., Will you like a movie?

Movie	Length	Liked?
m1	Short	Yes
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m4	Long	No
m5	Medium	Yes
m6	Short	No
m7	Short	Yes
m8	Medium	Yes

- Let C1 = "Yes" and C2 = "No"
- Entropy if we split on "Length"?
  - Left tree: "Short" = 0.92
  - Middle tree: "Medium" = 0.82
  - Right tree: "Long" = 0
- Information gain by split on "Length"?

 $IG = 0.95 - \left(\frac{3}{8} * 0.92 + \frac{4}{8} * 0.82 + \frac{1}{8} * 0\right)$ IG = 0.19

$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i$$

e.g., Will you like a movie?

Movie	IMDb Rating	Liked?
m1	7.2	Yes
m2	9.3	Yes
m3	5.1	No
m4	6.9	No
m5	8.3	Yes
m6	4.5	No
m7	8.0	Yes
m8	7.5	Yes

- Let C1 = "Yes" and C2 = "No"
- Entropy if we split on "IMDb Rating"?
  - Order attribute values:

{4.5, 5.1, 6.9, 7.2, 7.5, 8.0, 8.3, 9.3}

$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i$$

e.g., Will you like a movie?

Movie	IMDb Rating	Liked?
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m8	7.5	Yes

- Let C1 = "Yes" and C2 = "No"
- Entropy if we split on "IMDb Rating"?
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{4.5, 5.1, 6.9, 7.2, 7.5, 8.0, 8.3, 9.3}

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m8	7.5	Yes

- Let C1 = "Yes" and C2 = "No"
- Entropy if we split on "IMDb Rating"?
  - Order attribute values:

{4.5, 5.1, 6.9, 7.2, 7.5, 8.0, 8.3, 9.3}

$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i$$

e.g., Will you like a movie?

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7.2	Yes
9.3	Yes
5.1	No
6.9	No
8.3	Yes
4.5	No
8.0	Yes
7.5	Yes
	8.0 7.5

- Let C1 = "Yes" and C2 = "No"
- Entropy if we split on "IMDb Rating"?
  - Order attribute values:

 $\{4.5, 5.1, 6.9, 7.2, 7.5, 8.0, 8.3, 9.3\}$ 

Split at midpoint and measure entropy

 $IG = 0.95 - \left(\frac{5}{8} * \left(\frac{5}{5}\log_2\frac{5}{5}\right) + \frac{3}{8} * \left(\frac{3}{3}\log_2\frac{3}{3}\right)\right)$ IG = 0.95

$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i$$

e.g., Will you like a movie?

Movie	IMDb Rating	Liked?
m1	7.2	Yes
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m3	5.1	No
m4	6.9	No
m5	8.3	Yes
m6	4.5	No
m7	8.0	Yes
m8	7.5	Yes

- Let C1 = "Yes" and C2 = "No"
- Entropy if we split on "IMDb Rating"?
  - Order attribute values:

{4.5, 5.1, 6.9, 7.2, 7.5, 8.0, 8.3, 9.3}

$$Entropy = -\sum_{i=1}^{n} p_i \log_2 p_i$$

e.g., Will you like a movie?

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m5	8.3	Yes
m6	4.5	No
m7	8.0	Yes
m8	7.5	Yes

- Let C1 = "Yes" and C2 = "No"
- Entropy if we split on "IMDb Rating"?
  - Order attribute values:

 $\{4.5, 5.1, 6.9, 7.2, 7.5, 8.0, 8.3, 9.3\}$ 

# Decision Tree: What is Our First Split?

• Greedy approach (NP complete problem)

Function BuildTree(n,A) // n: samples (rows), A: attributes

If empty(A) or all n(L) are the same

status = leaf class = most common class in n4	1 \	IG = 0	IG = 0.19	IG = 0.95	
else	Movie	Type	Length	IMDb Rating	Liked?
status = internal	m1	Comedy	Short	7.2	Yes
a ← boetAttributo(n Λ)	m2	Drama	Medium	9.3	Yes
	m3	Comedy	Medium	5.1	No
LeftNode = BuildTree(n(a=1), A	m4	Drama	Long	6.9	No
RightNode = BuildTree(n(a=0).	m5	Drama	Medium	8.3	Yes
	m6	Drama	Short	4.5	No
ena	m7	Comedy	Short	8.0	Yes
end	m8	Drama	Medium	7.5	Yes

# Decision Tree: What Tree Results?



# Decision Tree: What Tree Results?



#### Recurse on this tree?

# Decision Tree: What Tree Results?



# Decision Tree: Generic Learning Algorithm

• Greedy approach (NP complete problem)

Function BuildTree(n,A) // n: samples (rows), A: attributes

```
If empty(A) or all n(L) are the same
```

```
status = leaf
```

```
class = most common class in n(L)
```

```
else
```

```
status = internal

a \leftarrow bestAttribute(n,A) Key Decision

LeftNode = BuildTree(n(a=1), A \ {a})

RightNode = BuildTree(n(a=0), A \ {a})

end
```

- Entropy (maximize information gain)
- Gini Index (used in CART algorithm)
- Gain ratio (used in C4.5 algorithm)
- Mean squared error
  - ...

```
end
```

# Overfitting

• At what tree size, does overfitting begin?



http://www.alanfielding.co.uk/multivar/crt/dt\_example\_04.htm

# Regularization to Avoid Overfitting

#### • Pruning

- Pre-pruning: stop tree growth earlier
- Post-pruning: prune tree afterwards



https://www.clariba.com/blog/tech-20140811-decision-trees-with-sap-predictive-analytics-and-sap-hana-emilio-nieto

# Today's Topics

- Multiclass classification applications and evaluating models
- Motivation for new ML era: need non-linear models
- Nearest neighbor classification
- Decision tree classification
- Parametric versus non-parametric models

# Machine Learning Goal

• Learn function that maps input features (X) to an output prediction (Y)

# Y = f(x)

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- Parametric model: has a fixed number of parameters
- Non-parametric model: does not specify the number of parameters

# **Class Discussion**

- For each model, is it parametric or non-parametric?
  - Linear regression
  - K-nearest neighbors
- What are advantages and disadvantages of parametric models?
- What are advantages and disadvantages of non-parametric models?

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# References Used for Today's Material

- Chapter 3 of Deep Learning book by Goodfellow et al.
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