

CS 360: Machine Learning

Prof. Sara Mathieson

Fall 2020



Haverford
COLLEGE

Admin

- Lab 2 due **Tuesday**
 - Post on Piazza!
- TA hours **Sunday 8:30-10pm** (Fiona)
- Next office hours **Mon 9:45-11am**
- We are working on getting a **peer tutor**

Video on if possible!!

Outline for September 18

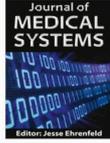
- Recap high level Decision Tree algorithm
- Entropy and information gain
- Continuous features
- Lab 2 implementation suggestions

Outline for September 18

- Recap high level Decision Tree algorithm
- Entropy and information gain
- Continuous features
- Lab 2 implementation suggestions

Real-World Examples

- Medical diagnostics



[Journal of Medical Systems](#)
October 2002, Volume 26, [Issue 5](#), pp 445–463 | [Cite as](#)

Decision Trees: An Overview and Their Use in Medicine

Authors [Authors and affiliations](#)

Vili Podgorelec , Peter Kokol, Bruno Stiglic, Ivan Rozman

- Credit risk analysis



[Computational Economics](#)
April 2000, Volume 15, [Issue 1-2](#), pp 107–143 | [Cite as](#)

Credit Risk Assessment Using Statistical and Machine Learning: Basic Methodology and Risk Modeling Applications

Authors [Authors and affiliations](#)

J. Galindo, P. Tamayo

- Modeling calendar scheduling preferences

Decision Trees in Chemistry reactions

- Example of decision trees in practice
- Use decision trees to interpret another ML algorithm (SVMs)

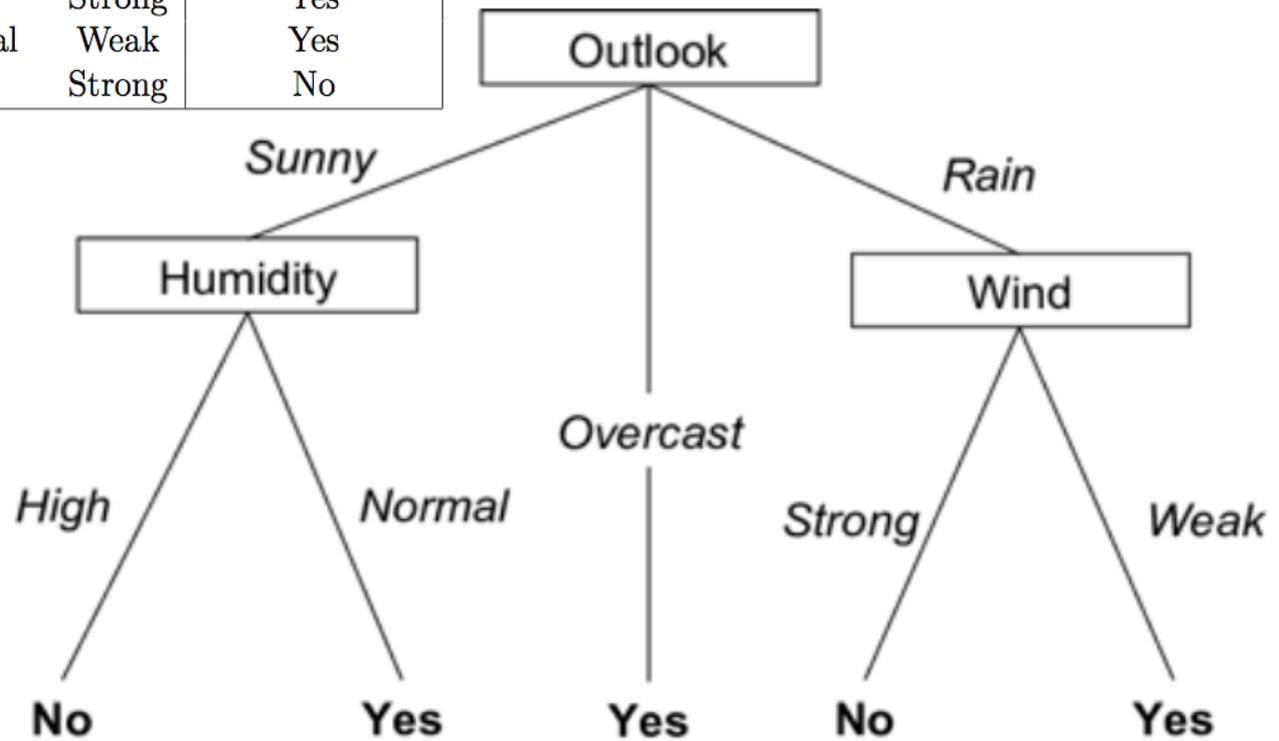
Machine-learning-assisted materials discovery using failed experiments

Paul Raccuglia, Katherine C. Elbert, Philip D. F. Adler, Casey Falk, Malia B. Wenny, Aurelio Mollo, Matthias Zeller, Sorelle A. Friedler , Joshua Schrier  & Alexander J. Norquist 

Nature **533**, 73–76 (05 May 2016) | [Download Citation](#) 

Handout 2

| Day | Outlook | Temperature | Humidity | Wind | PlayTennis (y) |
|----------|----------|-------------|----------|--------|--------------------|
| x_1 | Sunny | Hot | High | Weak | No |
| x_2 | Sunny | Hot | High | Strong | No |
| x_3 | Overcast | Hot | High | Weak | Yes |
| x_4 | Rain | Mild | High | Weak | Yes |
| x_5 | Rain | Cool | Normal | Weak | Yes |
| x_6 | Rain | Cool | Normal | Strong | No |
| x_7 | Overcast | Cool | Normal | Strong | Yes |
| x_8 | Sunny | Mild | High | Weak | No |
| x_9 | Sunny | Cool | Normal | Weak | Yes |
| x_{10} | Rain | Mild | Normal | Weak | Yes |
| x_{11} | Sunny | Mild | Normal | Strong | Yes |
| x_{12} | Overcast | Mild | High | Strong | Yes |
| x_{13} | Overcast | Hot | Normal | Weak | Yes |
| x_{14} | Rain | Mild | High | Strong | No |



Handout 2

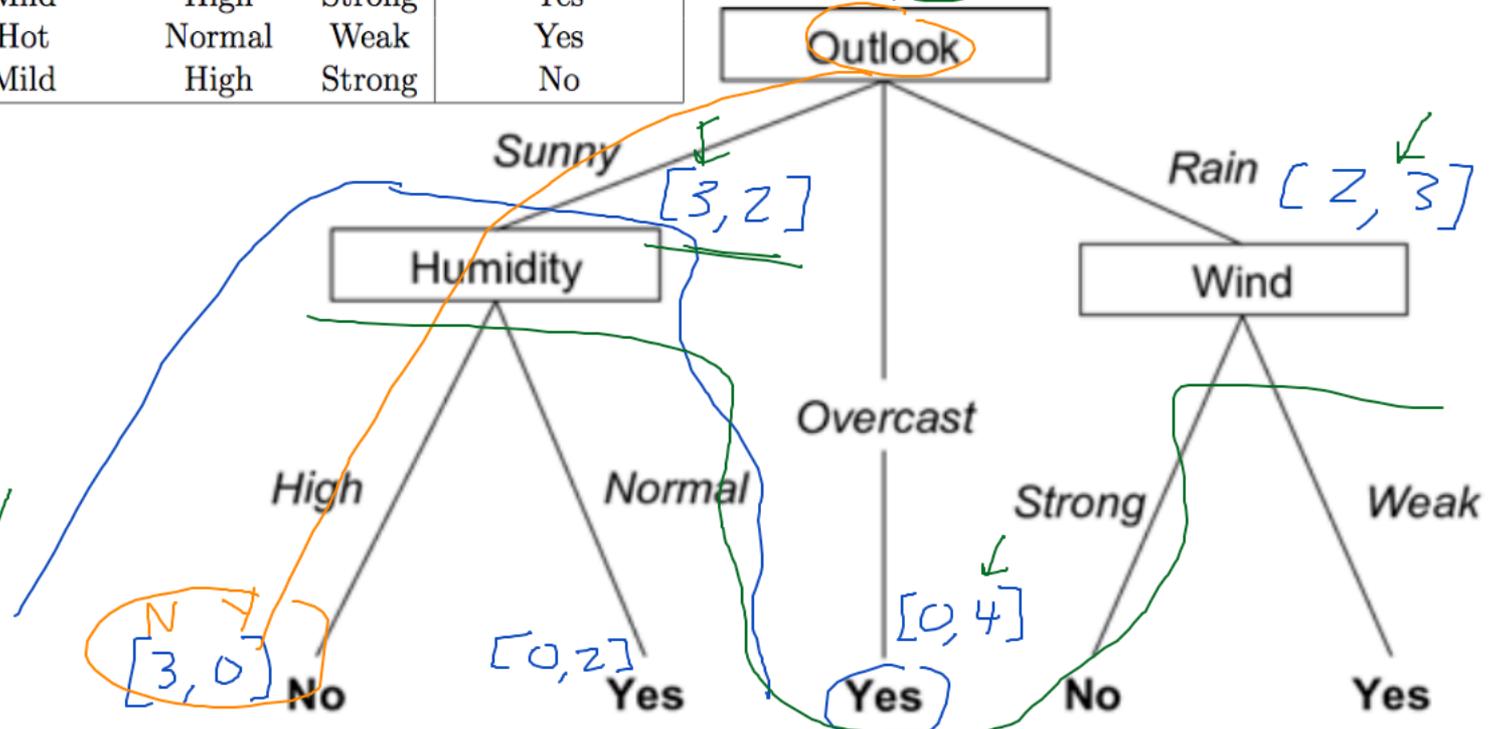
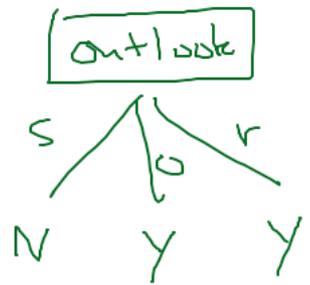
| Day | Outlook | Temperature | Humidity | Wind | PlayTennis (y) |
|----------|----------|-------------|----------|--------|----------------|
| x_1 | Sunny | Hot | High | Weak | No |
| x_2 | Sunny | Hot | High | Strong | No |
| x_3 | Overcast | Hot | High | Weak | Yes |
| x_4 | Rain | Mild | High | Weak | Yes |
| x_5 | Rain | Cool | Normal | Weak | Yes |
| x_6 | Rain | Cool | Normal | Strong | No |
| x_7 | Overcast | Cool | Normal | Strong | Yes |
| x_8 | Sunny | Mild | High | Weak | No |
| x_9 | Sunny | Cool | Normal | Weak | Yes |
| x_{10} | Rain | Mild | Normal | Weak | Yes |
| x_{11} | Sunny | Mild | Normal | Strong | Yes |
| x_{12} | Overcast | Mild | High | Strong | Yes |
| x_{13} | Overcast | Hot | Normal | Weak | Yes |
| x_{14} | Rain | Mild | High | Strong | No |

$d=2$ + rain acc = $\frac{100}{140}$

$d=1$ + rain acc = $\frac{10}{14}$

No Yes
[5, 9] ← depth = 0

depth = 1



Recursive algorithm: Partition data structure

| Day | Outlook | Temperature | Humidity | Wind | PlayTennis (y) |
|----------|----------|-------------|----------|--------|--------------------|
| x_1 | Sunny | Hot | High | Weak | No |
| x_2 | Sunny | Hot | High | Strong | No |
| x_3 | Overcast | Hot | High | Weak | Yes |
| x_4 | Rain | Mild | High | Weak | Yes |
| x_5 | Rain | Cool | Normal | Weak | Yes |
| x_6 | Rain | Cool | Normal | Strong | No |
| x_7 | Overcast | Cool | Normal | Strong | Yes |
| x_8 | Sunny | Mild | High | Weak | No |
| x_9 | Sunny | Cool | Normal | Weak | Yes |
| x_{10} | Rain | Mild | Normal | Weak | Yes |
| x_{11} | Sunny | Mild | Normal | Strong | Yes |
| x_{12} | Overcast | Mild | High | Strong | Yes |
| x_{13} | Overcast | Hot | Normal | Weak | Yes |
| x_{14} | Rain | Mild | High | Strong | No |

Recursive algorithm: Partition data structure

| Day | Outlook | Temperature | Humidity | Wind | PlayTennis (y) |
|----------|----------|-------------|----------|--------|--------------------|
| x_1 | Sunny | Hot | High | Weak | No |
| x_2 | Sunny | Hot | High | Strong | No |
| x_3 | Overcast | Hot | High | Weak | Yes |
| x_4 | Rain | Mild | High | Weak | Yes |
| x_5 | Rain | Cool | Normal | Weak | Yes |
| x_6 | Rain | Cool | Normal | Strong | No |
| x_7 | Overcast | Cool | Normal | Strong | Yes |
| x_8 | Sunny | Mild | High | Weak | No |
| x_9 | Sunny | Cool | Normal | Weak | Yes |
| x_{10} | Rain | Mild | Normal | Weak | Yes |
| x_{11} | Sunny | Mild | Normal | Strong | Yes |
| x_{12} | Overcast | Mild | High | Strong | Yes |
| x_{13} | Overcast | Hot | Normal | Weak | Yes |
| x_{14} | Rain | Mild | High | Strong | No |

| | | | | | |
|----------|-------|------|--------|--------|-----|
| x_1 | Sunny | Hot | High | Weak | No |
| x_2 | Sunny | Hot | High | Strong | No |
| x_8 | Sunny | Mild | High | Weak | No |
| x_9 | Sunny | Cool | Normal | Weak | Yes |
| x_{11} | Sunny | Mild | Normal | Strong | Yes |

Recursive algorithm: Partition data structure

| Day | Outlook | Temperature | Humidity | Wind | PlayTennis (y) |
|----------|----------|-------------|----------|--------|--------------------|
| x_1 | Sunny | Hot | High | Weak | No |
| x_2 | Sunny | Hot | High | Strong | No |
| x_3 | Overcast | Hot | High | Weak | Yes |
| x_4 | Rain | Mild | High | Weak | Yes |
| x_5 | Rain | Cool | Normal | Weak | Yes |
| x_6 | Rain | Cool | Normal | Strong | No |
| x_7 | Overcast | Cool | Normal | Strong | Yes |
| x_8 | Sunny | Mild | High | Weak | No |
| x_9 | Sunny | Cool | Normal | Weak | Yes |
| x_{10} | Rain | Mild | Normal | Weak | Yes |
| x_{11} | Sunny | Mild | Normal | Strong | Yes |
| x_{12} | Overcast | Mild | High | Strong | Yes |
| x_{13} | Overcast | Hot | Normal | Weak | Yes |
| x_{14} | Rain | Mild | High | Strong | No |

| | | | | | |
|----------|-------|------|--------|--------|-----|
| x_1 | Sunny | Hot | High | Weak | No |
| x_2 | Sunny | Hot | High | Strong | No |
| x_8 | Sunny | Mild | High | Weak | No |
| x_9 | Sunny | Cool | Normal | Weak | Yes |
| x_{11} | Sunny | Mild | Normal | Strong | Yes |

| | | | | | |
|----------|----------|------|--------|--------|-----|
| x_3 | Overcast | Hot | High | Weak | Yes |
| x_7 | Overcast | Cool | Normal | Strong | Yes |
| x_{12} | Overcast | Mild | High | Strong | Yes |
| x_{13} | Overcast | Hot | Normal | Weak | Yes |

Recursive algorithm: Partition data structure

| Day | Outlook | Temperature | Humidity | Wind | PlayTennis (y) |
|----------|----------|-------------|----------|--------|--------------------|
| x_1 | Sunny | Hot | High | Weak | No |
| x_2 | Sunny | Hot | High | Strong | No |
| x_3 | Overcast | Hot | High | Weak | Yes |
| x_4 | Rain | Mild | High | Weak | Yes |
| x_5 | Rain | Cool | Normal | Weak | Yes |
| x_6 | Rain | Cool | Normal | Strong | No |
| x_7 | Overcast | Cool | Normal | Strong | Yes |
| x_8 | Sunny | Mild | High | Weak | No |
| x_9 | Sunny | Cool | Normal | Weak | Yes |
| x_{10} | Rain | Mild | Normal | Weak | Yes |
| x_{11} | Sunny | Mild | Normal | Strong | Yes |
| x_{12} | Overcast | Mild | High | Strong | Yes |
| x_{13} | Overcast | Hot | Normal | Weak | Yes |
| x_{14} | Rain | Mild | High | Strong | No |

| | | | | | |
|----------|-------|------|--------|--------|-----|
| x_1 | Sunny | Hot | High | Weak | No |
| x_2 | Sunny | Hot | High | Strong | No |
| x_8 | Sunny | Mild | High | Weak | No |
| x_9 | Sunny | Cool | Normal | Weak | Yes |
| x_{11} | Sunny | Mild | Normal | Strong | Yes |

| | | | | | |
|----------|----------|------|--------|--------|-----|
| x_3 | Overcast | Hot | High | Weak | Yes |
| x_7 | Overcast | Cool | Normal | Strong | Yes |
| x_{12} | Overcast | Mild | High | Strong | Yes |
| x_{13} | Overcast | Hot | Normal | Weak | Yes |

| | | | | | |
|----------|------|------|--------|--------|-----|
| x_4 | Rain | Mild | High | Weak | Yes |
| x_5 | Rain | Cool | Normal | Weak | Yes |
| x_6 | Rain | Cool | Normal | Strong | No |
| x_{10} | Rain | Mild | Normal | Weak | Yes |
| x_{14} | Rain | Mild | High | Strong | No |

Recursive algorithm: Partition data structure

| Day | Outlook | Temperature | Humidity | Wind | PlayTennis (y) |
|----------|----------|-------------|----------|--------|--------------------|
| x_1 | Sunny | Hot | High | Weak | No |
| x_2 | Sunny | Hot | High | Strong | No |
| x_3 | Overcast | Hot | High | Weak | Yes |
| x_4 | Rain | Mild | High | Weak | Yes |
| x_5 | Rain | Cool | Normal | Weak | Yes |
| x_6 | Rain | Cool | Normal | Strong | No |
| x_7 | Overcast | Cool | Normal | Strong | Yes |
| x_8 | Sunny | Mild | High | Weak | No |
| x_9 | Sunny | Cool | Normal | Weak | Yes |
| x_{10} | Rain | Mild | Normal | Weak | Yes |
| x_{11} | Sunny | Mild | Normal | Strong | Yes |
| x_{12} | Overcast | Mild | High | Strong | Yes |
| x_{13} | Overcast | Hot | Normal | Weak | Yes |
| x_{14} | Rain | Mild | High | Strong | No |

temp →

| | | | | | |
|-----------------------------|------------------|----------------|-----------------|-------------------|---------------|
| x_1 | Sunny | Hot | High | Weak | No |
| x_2 | Sunny | Hot | High | Strong | No |
| x_8 | Sunny | Mild | High | Weak | No |
| x_9 | Sunny | Cool | Normal | Weak | Yes |
| x_{11} | Sunny | Mild | Normal | Strong | Yes |

| | | | | | |
|--------------------------------|---------------------|-----------------|-------------------|-------------------|----------------|
| x_3 | Overcast | Hot | High | Weak | Yes |
| x_7 | Overcast | Cool | Normal | Strong | Yes |
| x_{12} | Overcast | Mild | High | Strong | Yes |
| x_{13} | Overcast | Hot | Normal | Weak | Yes |

temp

| | | | | | |
|--------------------------------|-----------------|-----------------|-------------------|-------------------|----------------|
| x_4 | Rain | Mild | High | Weak | Yes |
| x_5 | Rain | Cool | Normal | Weak | Yes |
| x_6 | Rain | Cool | Normal | Strong | No |
| x_{10} | Rain | Mild | Normal | Weak | Yes |
| x_{14} | Rain | Mild | High | Strong | No |

Partition class

```
class Example:
```

```
    def __init__(self, features, label):  
        """Helper class (like a struct) that stores info about each example."""  
        # dictionary. key=feature name: value=feature value for this example  
        self.features = features  
        self.label = label # in {-1, 1}
```

```
class Partition:
```

```
    def __init__(self, data, F):  
        """Store information about a dataset"""  
        self.data = data # list of examples  
        # dictionary. key=feature name: value=set of possible values  
        self.F = F  
        self.n = len(self.data)
```

Partition class

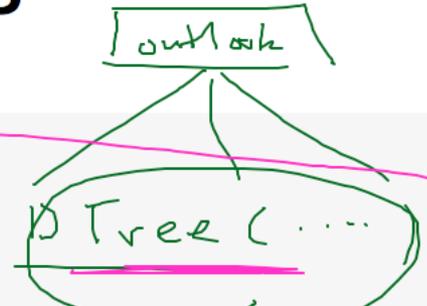
DTree
class

class Example:

```
def __init__(self, features, label):
```

```
    """Helper class (like a struct) that stores info about each example."""  
    # dictionary. key=feature name: value=feature value for this example  
    self.features = features  
    self.label = label # in {-1, 1}
```

```
self.children = {}  
self.children["sun"] = DTree(...)
```



class Partition:

```
def __init__(self, data, F):
```

```
    """Store information about a dataset"""  
    self.data = data # list of examples  
    # dictionary. key=feature name: value=set of possible values  
    self.F = F  
    self.n = len(self.data)
```

$F = \{ \text{outlook} : (\text{sun}, \text{rain}, \text{overcast}), \}$

↑
key

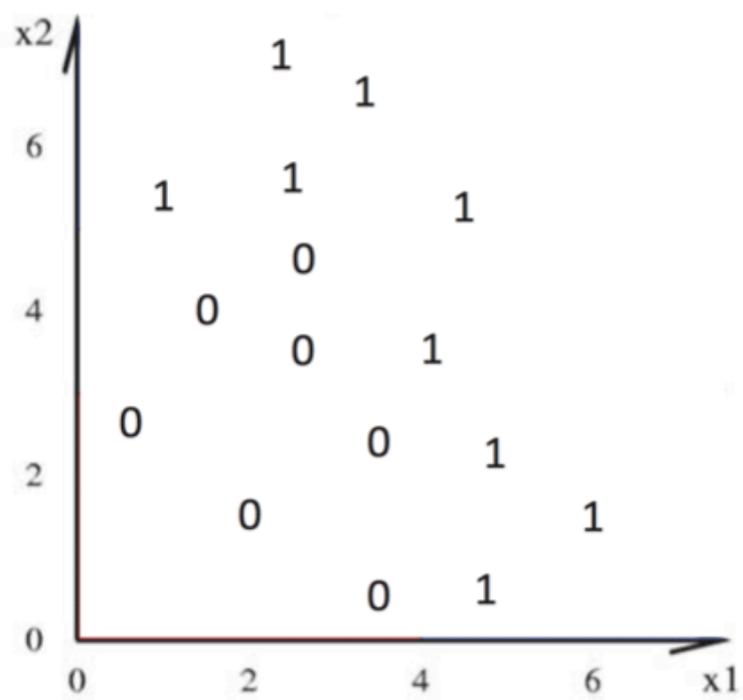
↑
value

Tree

```
self.left = Tree(...)  
self.right = Tree(...)
```

Handout 2: continuous features

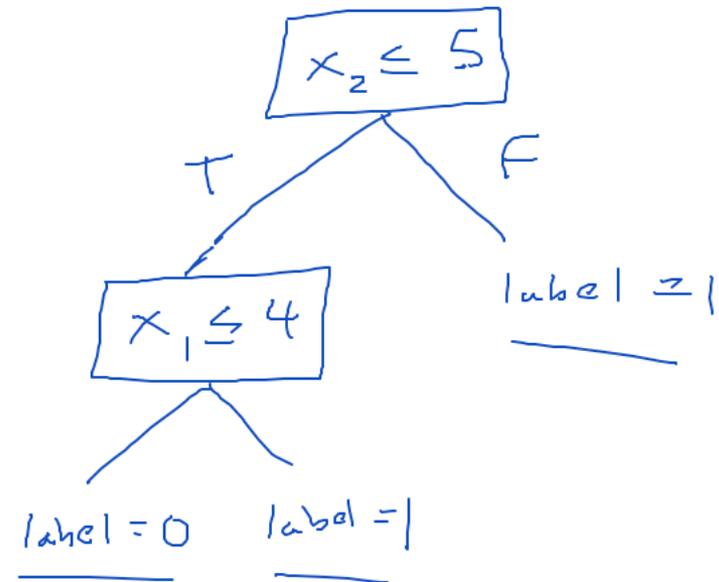
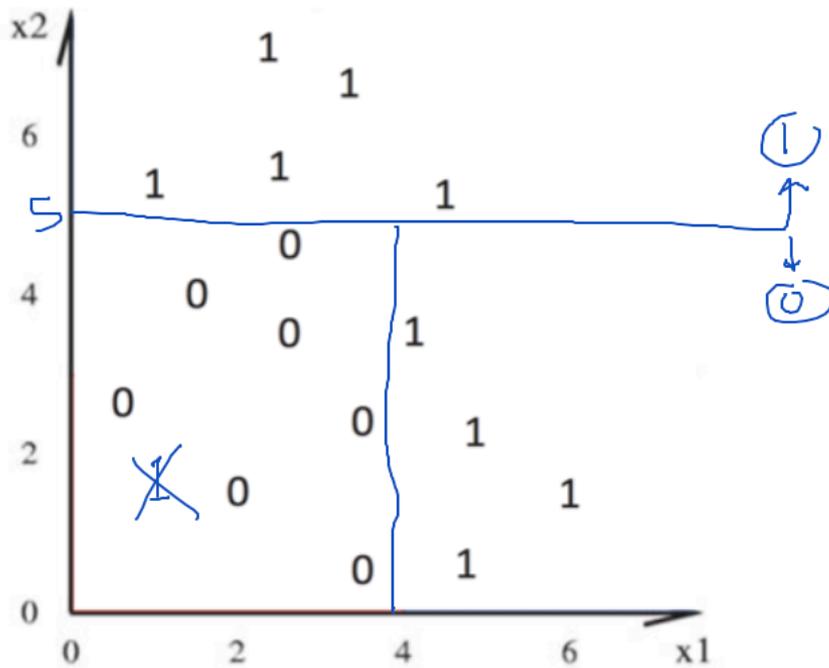
4. For the dataset below, the label $y \in \{0, 1\}$. What is n ? What is p ? Devise a decision tree for this data that perfectly classifies the given examples. Internal node labels should be of the form " $x_j \leq a$ ", where a is some constant.



5. Repeat Question (2) for this decision tree (i.e. label each node with the "0" and "1" counts.)

Handout 2: continuous features

4. For the dataset below, the label $y \in \{0, 1\}$. What is n ? What is p ? Devise a decision tree for this data that perfectly classifies the given examples. Internal node labels should be of the form " $x_j \leq a$ ", where a is some constant.



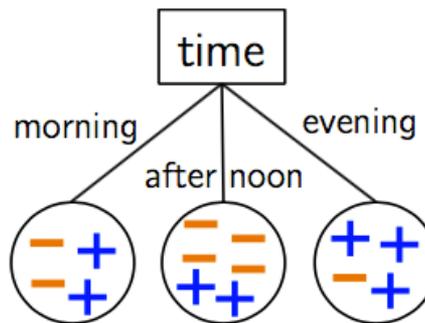
5. Repeat Question (2) for this decision tree (i.e. label each node with the "0" and "1" counts.)

Reading check-in: work individually for a few minutes

1. Match the decision tree component on the left with its corresponding data component on the right.

- | | |
|------------------|----------------|
| • internal nodes | class labels |
| • branches | feature names |
| • leaves | feature values |

2. Say I am trying to predict if a student will like a course (+) or dislike it (-). One of the features is the time of day the course is offered. If I just choose this one feature and build a decision tree, here is how the training examples cluster at the leaves:



(a) How would you classify a new example with value **evening** for the feature **time**?

(b) What is the overall *training error* if I use the majority class label at each leaf?

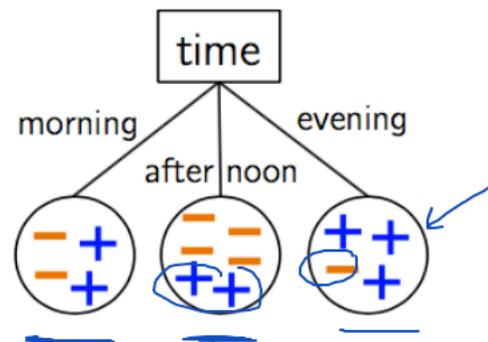
3. If a decision tree is overfitting, is the *depth* more likely to be low or high?

Reading check-in: work individually for a few minutes

1. Match the decision tree component on the left with its corresponding data component on the right.

- internal nodes class labels
- branches feature names
- leaves feature values

2. Say I am trying to predict if a student will like a course (+) or dislike it (-). One of the features is the time of day the course is offered. If I just choose this one feature and build a decision tree, here is how the training examples cluster at the leaves:



(a) How would you classify a new example with value **evening** for the feature **time**?

+ (like)

(b) What is the overall training error if I use the majority class label at each leaf?

$$\text{error} = \frac{2 + 2 + 1}{14} = \frac{5}{14}$$

acc: $\frac{9}{14}$

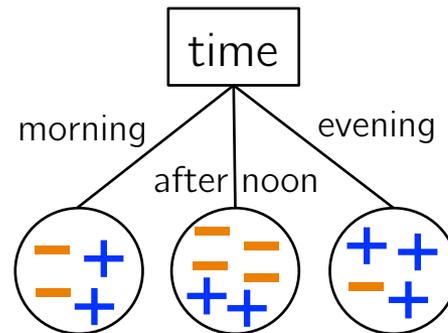
3. If a decision tree is overfitting, is the *depth* more likely to be low or high?

high

Reading Check-in

- 1)
- internal nodes
 - branches
 - leaves
- class labels
feature names
feature values

- 2) (a) +
(b) 5/14



- 3) high

Outline for September 18

- Recap high level Decision Tree algorithm
- Entropy and information gain
- Continuous features
- Lab 2 implementation suggestions

Entropy

Idea: avg # bits needed to transmit info

| Year | prob (p) | Idea | Cumulative prob | Binary | | |
|------------|----------|------|-----------------|--------|--|--|
| Senior | 0.5 | | | | | |
| Junior | 0.25 | | | | | |
| Sophomore | 0.125 | | | | | |
| First year | 0.125 | | | | | |

Entropy

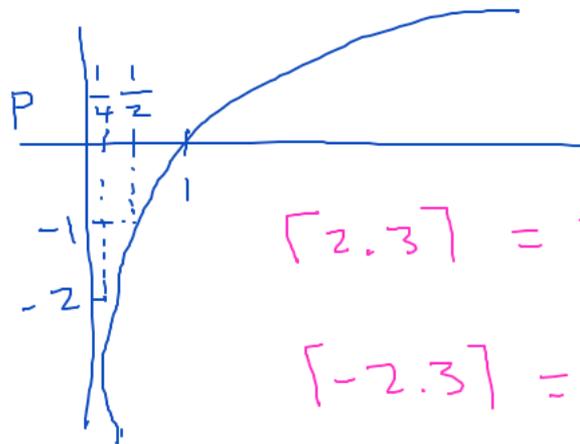
Idea: avg # bits needed to transmit info

| Year | prob (p) | Idea | Cumulative prob | Binary | $-\lceil \log_2(p) \rceil$ | code |
|------------|----------|------|-----------------|----------|----------------------------|------|
| Senior | 0.5 | 0 | 0 | 0.000... | 1 | 0 |
| Junior | 0.25 | 1 | 0.5 | 0.100... | 2 | 10 |
| Sophomore | 0.125 | 01 | 0.75 | 0.110... | 3 | 110 |
| First year | 0.125 | 10 | 0.875 | 0.111... | 3 | 111 |

11011010001110

binary =>

decimal



$$\lceil 2.3 \rceil = 3$$

$$\lceil -2.3 \rceil = -3$$

$$\dots + 0 \cdot 2^2 + 1 \cdot 2^1 + 1 \cdot 2^0 + 1 \cdot 2^{-1} + 1 \cdot 2^{-2}$$

$$5 = 1 \cdot 2^2 + 0 \cdot 2^1 + 1 \cdot 2^0$$

$$\Rightarrow 101$$

$$5.5 \Rightarrow 101.1$$

↑
1/2
↑
1/4

Entropy

$$H(Y) = - \sum_{c \in \text{vals}(Y)} p(Y=c) \log_2 p(Y=c)$$

bits

$$H(\text{year}) = \frac{1}{2} \cdot 1 + \frac{1}{4} \cdot 2 + \left(\frac{1}{8} \cdot 3\right) 2$$
$$= \underline{1.75} \text{ bits}$$

~~$$= \frac{1 + 2 + 3 + 3}{4} = 2.25$$~~

Conditional Entropy

one feature name

value

$$H(Y | X=v) = - \sum_{c \in \text{vals}(Y)} p(Y=c | X=v) \log_2 p(Y=c | X=v)$$

A B

$$p(\text{Yes} | \text{outlook} = \text{sun}) = \frac{p(\text{Yes AND sun})}{p(\text{sun})}$$

label $\in \{\text{yes}, \text{no}\}$

sun
rain
over
cast

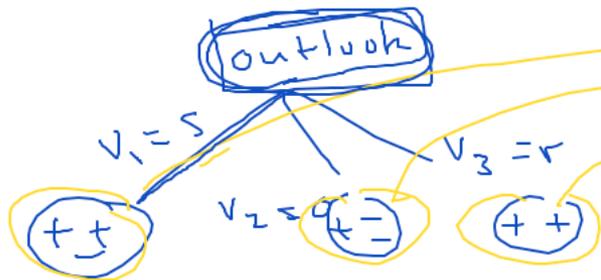
$v = \text{sun}$
 $\frac{5}{14}$

low

$$H(Y | X) = \sum_{v \in \text{vals}(X)} p(X=v) H(Y | X=v)$$

$v \in \text{vals}(X)$

entropy of label



Info Gain : $H(Y) - H(Y|X)$

high

Handout 4: work with your group!
(second question only)

Handout 4

Try first and then
check your answers!

| Movie | Type | Length | Director | Famous actors | Liked? |
|-------|----------|--------|----------|---------------|--------|
| m1 | Comedy | Short | Adamson | No | Yes |
| m2 | Animated | Short | Lasseter | No | No |
| m3 | Drama | Medium | Adamson | No | Yes |
| m4 | Animated | Long | Lasseter | Yes | No |
| m5 | Comedy | Long | Lasseter | Yes | No |
| m6 | Drama | Medium | Singer | Yes | Yes |
| m7 | Animated | Short | Singer | No | Yes |
| m8 | Comedy | Long | Adamson | Yes | Yes |
| m9 | Drama | Medium | Lasseter | No | Yes |

$$P(Li = \text{yes}) = 2/3$$

$$H(Li) = 0.92$$

$$H(Li | T) = 0.61$$

$$H(Li | Le) = 0.61$$

$$H(Li | D) = 0.36 \quad \text{MIN ENTROPY}$$

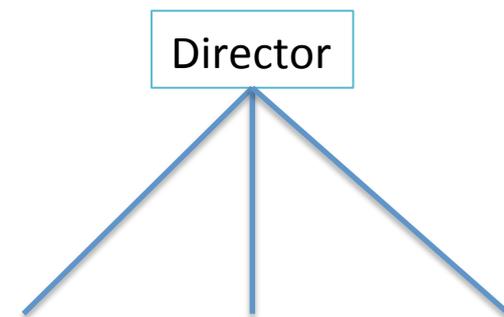
$$H(Li | F) = 0.85$$

$$\text{Gain}(Li, T) = 0.92 - 0.61 = 0.31$$

$$\text{Gain}(Li, Le) = 0.92 - 0.61 = 0.31$$

$$\text{Gain}(Li, D) = 0.92 - 0.36 = 0.56 \quad \text{MAX INFO GAIN}$$

$$\text{Gain}(Li, F) = 0.92 - 0.85 = 0.07$$



Start of the tree

Outline for September 18

- Recap high level Decision Tree algorithm
- Entropy and information gain
- **Continuous features**
- Lab 2 implementation suggestions

Continuous Features

(do this for the TRAIN only!)

| X | Y |
|----|---|
| 10 | Y |
| 7 | Y |
| 8 | N |
| 3 | Y |
| 7 | N |
| 12 | Y |
| 2 | Y |

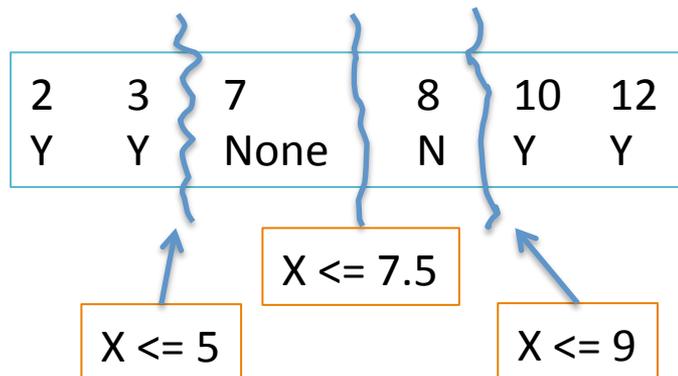
- 1) Sort examples based on given feature

| | | | | | | |
|---|---|---|---|---|----|----|
| 2 | 3 | 7 | 7 | 8 | 10 | 12 |
| Y | Y | Y | N | N | Y | Y |

- 2) Different label with same feature value, collapse to "None"

| | | | | | |
|---|---|------|---|----|----|
| 2 | 3 | 7 | 8 | 10 | 12 |
| Y | Y | None | N | Y | Y |

- 3) Whenever label changes, make a feature (use avg)



Outline for September 18

- Recap high level Decision Tree algorithm
- Entropy and information gain
- Continuous features
- Lab 2 implementation suggestions

Implementation Suggestions

- Start slow with **entropy**! Build up function by function
- Think back to **trees in data structures**
- Distinguish between **data** (X,y) and **options for data** (values for each feature, classes for y)