## **CMPUT 466** Machine Learning: Day 3 **Professor: Bailey Kacsmar** kacsmar@ualberta.ca Winter 2024

Many of these slides are derived from Alona Fyshe, Alex Thomo. Thanks!

From Last Class: Probability Density Functions (PDFs) Maximum likelihood estimation and MAP

#### MAP and MLE, Basically, Probabilistic Modeling

Given: observations, find a model or function that "shows agreement" and:

#### MAP and MLE, Basically, Probabilistic Modeling

Given: observations, find a model or function that "shows agreement" and:

- The ability to generalize well
- The ability to incorporate prior knowledge and assumptions
- Scalability

### Finding the "best" model?

- Consider learning parameters of a distribution
- Given a set of observations, and some knowledge, the goal is ...

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## Essentially...parameter estimation

### Finding the "best" model?

- Consider learning parameters of a distribution
- Given a set of observations, and some knowledge, the goal is ...

# Essentially...parameter estimation MLE MAP

#### Resume: Maximum Likelihood Estimation (MLE)

### **Rich vs Poor**

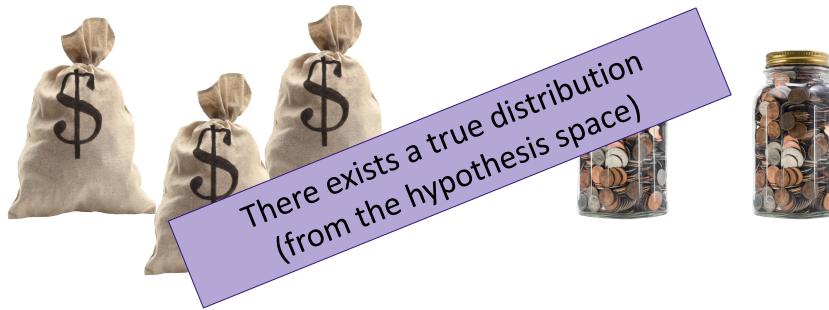
What is the probability of a person being rich, given you know nothing else about that person?







What is the probability of a person being rich, given you know nothing else about that person?



### Let's say 3/5?

We assume that the wealth of the people in our dataset *D* is

independently distributed  $\theta$  = Probability of being rich = P(rich) ? = Probability of being poor = P(poor) $D = \{r, p, r, r, p\}$   $\alpha_r = \# rich$   $\alpha_p = \# poor$ P(D) = P(r and p and r and r and p)=P(rich) \* P(poor) \* P(rich) \*\* A  $\theta^{\alpha F}$ P(rich) \* P(poor) $= \theta * (1 - \theta) * \theta * \theta * (1 - \theta)$  $= (1 - \theta)^{\alpha_p} * \theta^{\alpha_r} \quad \text{argmax } P$ 11

## That's Maximum Likelihood Estimation (MLE)

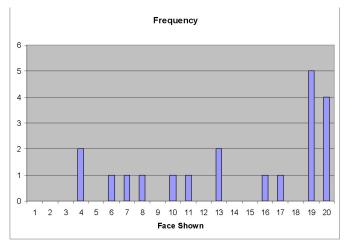
## It's not always the best solution...

## That's Maximum Likelihood Estimation (MLE)

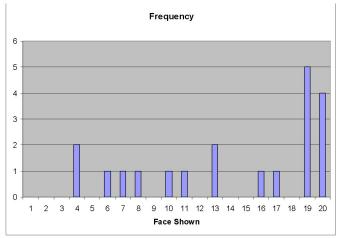
#### It's not always the best solution... Because: The assumption that the function is constant is problematic.

## Consider: Issues with MLE estimate

I bought a loaded 20-faced die (d20) on EBay...but it didn't come with any specs. How can I find out how it behaves?

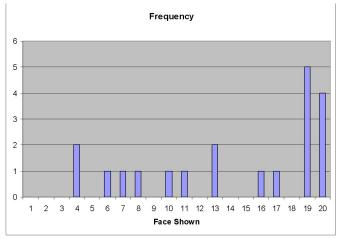


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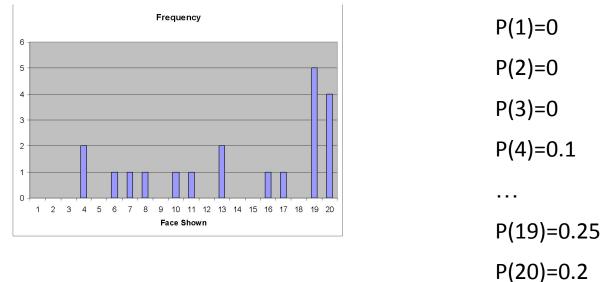
#### 1. Collect some data (20 rolls)

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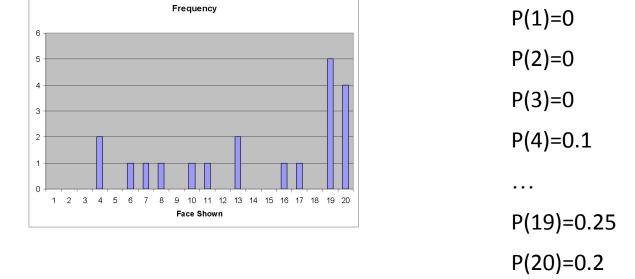


Collect some data (20 rolls)
 Estimate P(i)=CountOf(rolls of i)/CountOf(any roll)

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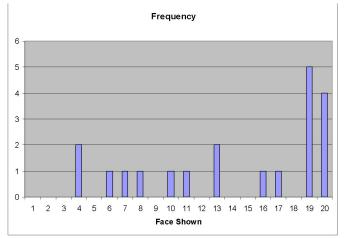
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But: Do I really think it's *impossible* to roll a 1,2 or 3?

## A better solution?

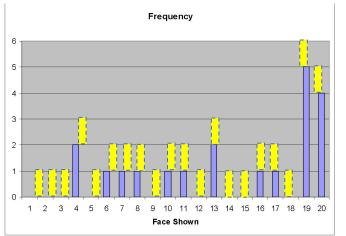
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Collect some data (20 rolls)
 Estimate P(i)

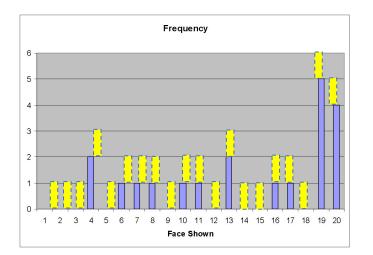
## A better solution

I bought a loaded 20-faced die (d20) on EBay...but it didn't come with any specs. How can I find out how it behaves?



0. *Imagine* some data (20 rolls, each i shows up 1x)
1. Collect some data (20 rolls)
2. Estimate P(i)

## A better solution?



$$\hat{P}(i) = \frac{CountOf(i) + 1}{CountOf(ANY) + CountOf(IMAGINED)}$$

P(1)=1/40P(2)=1/40P(3)=1/40P(4)=(2+1)/40. . . P(19)=(5+1)/40 P(20)=(4+1)/40=1/8

0.2 vs. 0.125 – really different! Maybe I should "imagine" less data?

# What if we know that poor people are much more common than rich people?













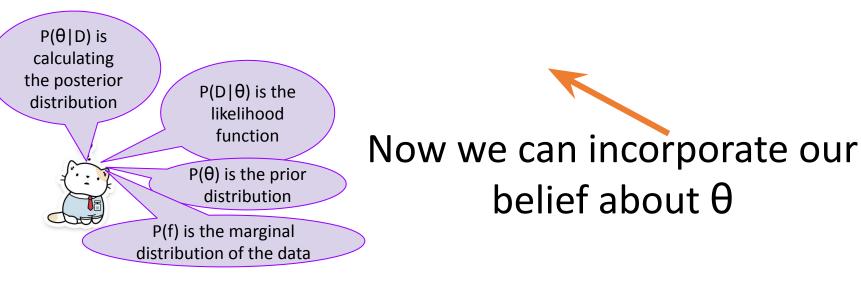








## We have a belief about $\theta$ •P( $\theta$ |D) = P(D| $\theta$ )\*P( $\theta$ )/P(D)



### We have a belief about $\, heta$

## • $P(\theta | D) = P(D | \theta) * P(\theta) / P(D)$

## $\propto$ P(D| $\theta$ )\*P( $\theta$ )

# Now we can incorporate our belief about $\theta$

This is a MAP (Maximum A Posteriori) Estimate 24

## We have a belief about $\, heta$

• $P(\theta | D) = P(D | \theta) * P(\theta) / P(D)$ × P(D|θ)\*P(θ) P(θ) probable model(aka Model(aka) M belief about  $\theta$ This is a Man (Maximum A Posteriori) Estimate

#### **Conjugate Prior**

- Our likelihood so far has been based on a Bernoulli distribution.
- Beta is a conjugate prior to Bernoulli
  - This means their pdfs (probability density functions) play nice together
  - P(D|θ)\*P(θ) will be easy to deal with
  - Called the posterior likelihood

### **Estimating Parameters**

- Maximum Likelihood Estimate (MLE): choose  $\theta$  that maximizes probability of observed data  $\hat{\theta} = \arg \max_{\theta} P(\mathcal{D} \mid \theta)$
- Maximum a Posteriori (MAP) estimate: choose  $\theta$ that is most probable given **prior probability and the data**  $\hat{\theta} = \arg \max_{\theta} P(\theta \mid D)$  $= \arg \max_{\theta} = \frac{P(D \mid \theta)P(\theta)}{P(D)}$

A tutorial:

http://www.cs.ubc.ca/~murphyk/Teaching/CS340-Fall06/reading/bernoulli.pdf

#### Today: Supervised Learning, Classification, Decision Trees

### Recall (again)

(Adapted from Leslie Kaelbling's example in the MIT courseware)

• Imagine I'm trying predict whether my neighbor is going to drive into work, so I can ask for a ride.

- Whether she drives into work seems to depend on the following attributes of the day:
  - temperature
  - expected precipitation
  - day of the week
  - what she's wearing

#### Memory



• Now, we find ourselves on a snowy "-5" degree Monday, and the neighbor is wearing casual clothes.

Temp	Precip	Day	Clothes	
25	None	Sat	Casual	Walk
-5	Snow	Mon	Casual	Drive
15	Snow	Mon	Casual	Walk
-5	Snow	Mon	Casual	

### Averaging

• One strategy would be to predict the majority outcome.

Temp	Precip	Day	Clothes	
25	None	Sat	Casual	Walk
25	None	Sat	Casual	Walk
25	None	Sat	Casual	Drive
25	None	Sat	Casual	Drive
25	None	Sat	Casual	Walk
25	None	Sat	Casual	Walk
25	None	Sat	Casual	Walk
25	None	Sat	Casual	Walk

### Generalization

- Dealing with previously unseen cases
- Will she walk or drive?

Temp	Precip	Day	Clothes	
22	None	Fri	Casual	Walk
3	None	Sun	Casual	Walk
10	Rain	Wed	Casual	Walk
30	None	Mon	Casual	Drive
20	None	Sat	Formal	Drive
25	None	Sat	Casual	Drive
-5	Snow	Mon	Casual	Drive
27	None	Tue	Casual	Drive
24	Rain	Mon	Casual	?

We might plausibly make any of the following arguments:

- She's going to walk because it's raining today and the only other time it rained, she walked.
- She's going to drive because she has always driven on Mondays...<sup>32</sup>

#### Today:

## Today: A different way to not ask our neighbour whether she's driving to work

### **Decision Trees**

• Predict by splitting on attribute values

Тетр	Precip	Day	Clothes	
22	None	Fri	Casual	Walk
3	None	Sun	Casual	Walk
10	Rain	Wed	Casual	Walk
30	None	Mon	Casual	Drive
20	None	Sat	Formal	Drive
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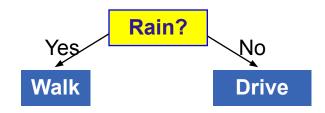


### **Decision Trees**

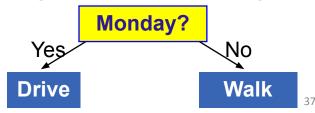
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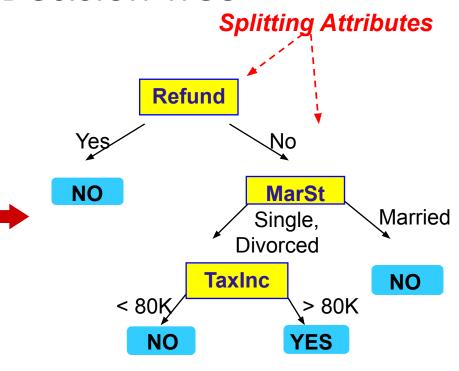


-She's going to drive because she has always driven on Mondays...



#### Example of a (Good?) Decision Tree

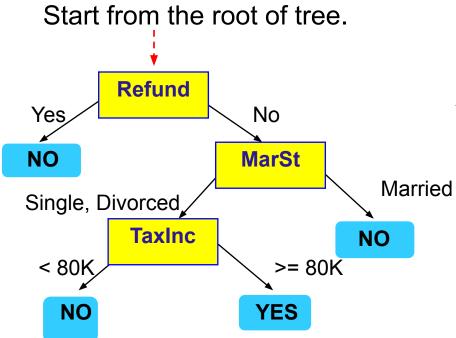
		rical	ical	IOUS
	cate	oprical categ	orical	nuous class
Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes



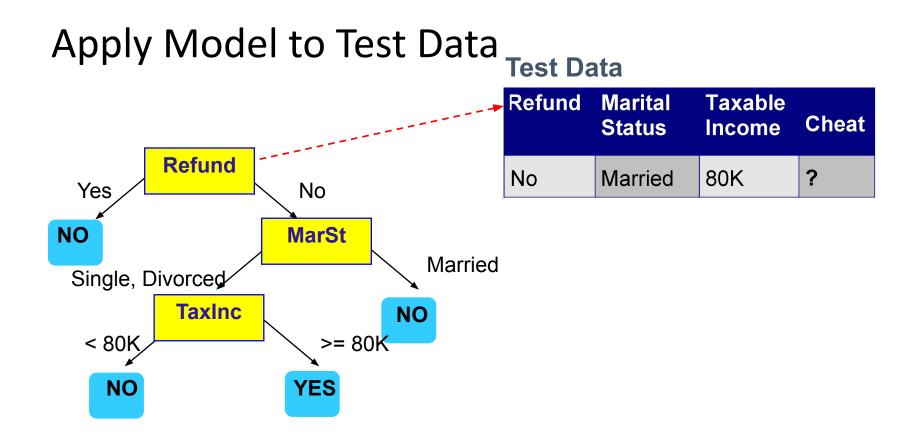
Model: Decision Tree

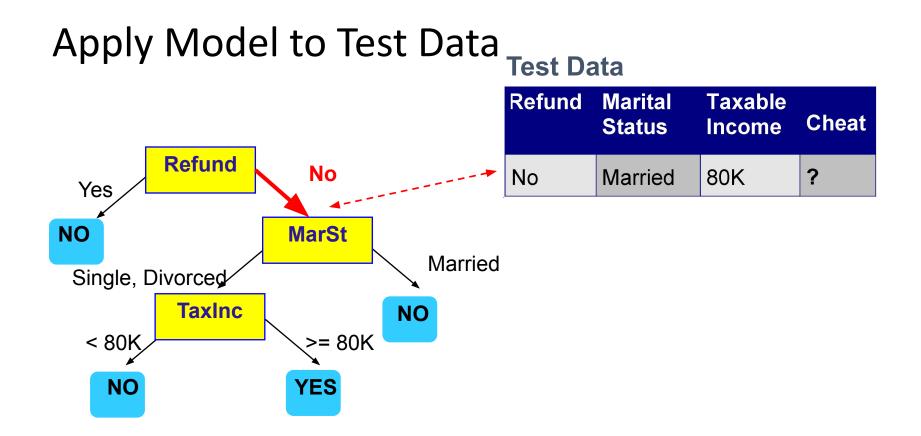
#### **Training Data**

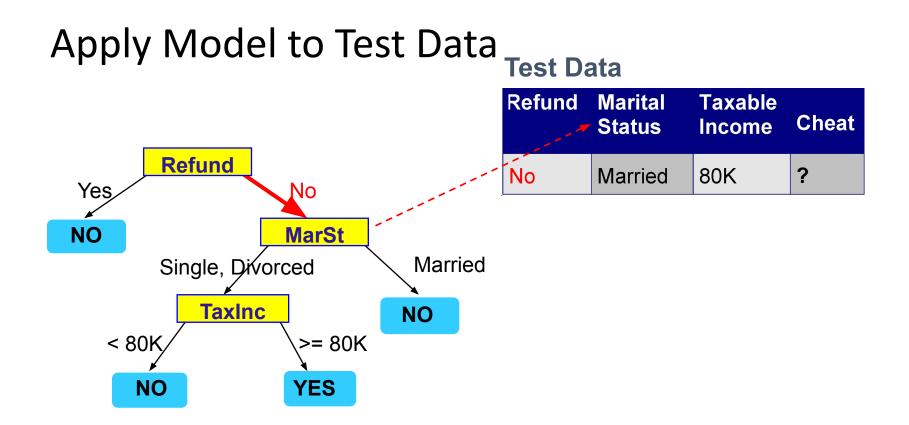
# Apply Model to Test Data Test Data

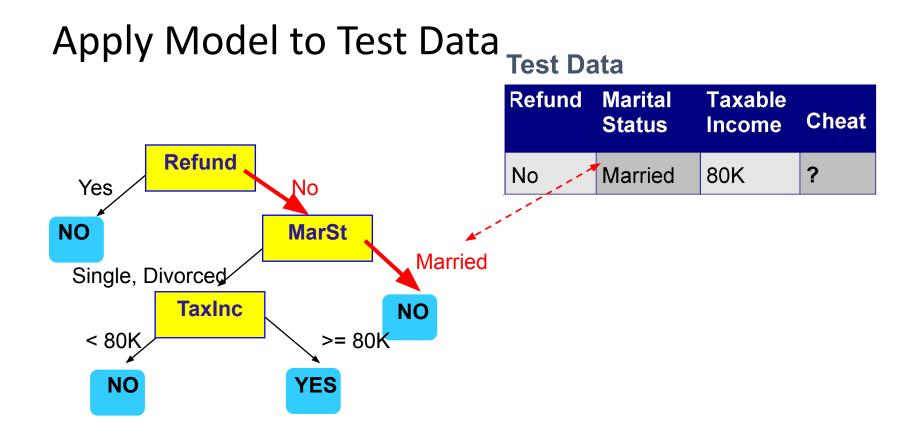


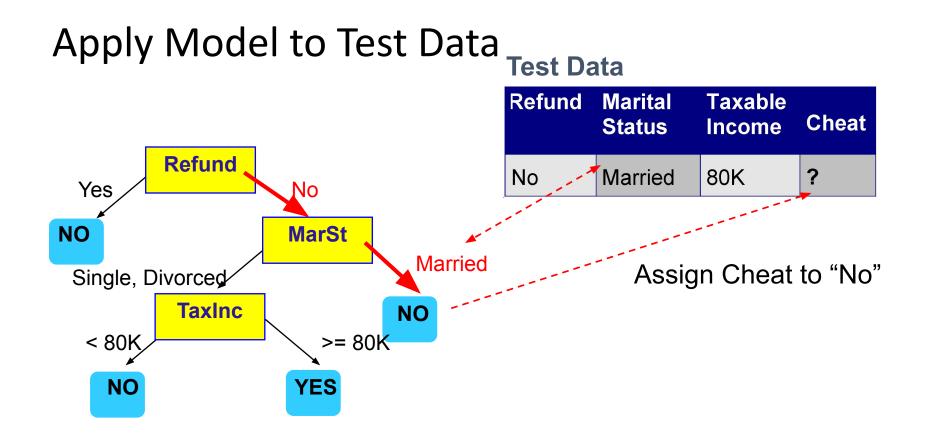
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?











- Top down in a recursive **divide-and-conquer** fashion
  - First:

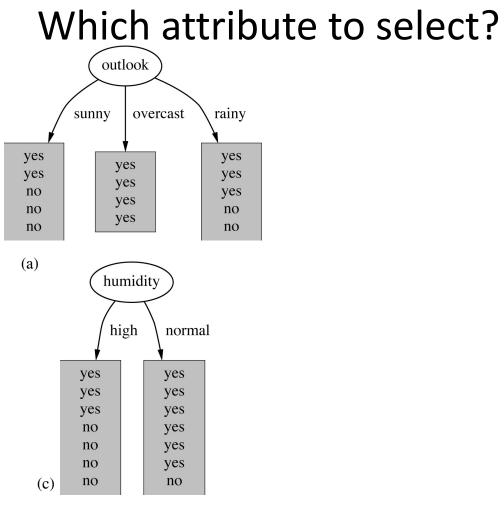
- Top down in a recursive **divide-and-conquer** fashion
  - First: an attribute is selected for the root node and a branch is created for each possible attribute value
  - Then:

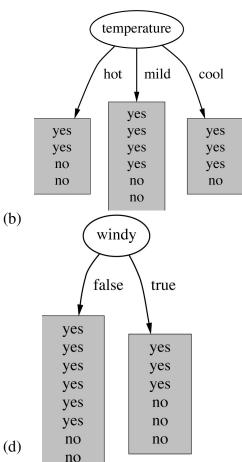
- Top down in a recursive **divide-and-conquer** fashion
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  - Then: the instances are split into subsets (one for each branch extending from the node)
  - Finally:

- Top down in a recursive **divide-and-conquer** fashion
  - First: an attribute is selected for the root node and a branch is created for each possible attribute value
  - Then: the instances are split into subsets (one for each branch extending from the node)
  - Finally: the same procedure is repeated recursively for each branch, using only instances that reach the branch
- Process stops if all instances have the same class

#### New Example: Playing soccer

Outlook	Тетр	Humidity	Windy	Play
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Sunny	Mild	High	False	No
Sunny	Cool	Normal	False	Yes
Rainy	Mild	Normal	False	Yes
Sunny	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Rainy	Mild	High	True	No





#### WE NEED...A criterion for attribute selection

• Which is the best attribute?

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- Which is the best attribute?
- The one which will result in the smallest tree
   Heuristic: choose the attribute that produces the "purest" nodes
- Popular impurity criterion: entropy of nodes
  - Lower the entropy, purer the node.

# EntropyH(X) = E(I(X)) Expected value of the information in X

#### Entropy

- H(X) = E(I(X)) **Expected** value of the **information** in X
- •Expected value:  $E(f(X)) = \sum_{i} P(x_i) * f(x_i)$

• Information: 
$$I(x_i) = -\log_2 P(x_i)$$

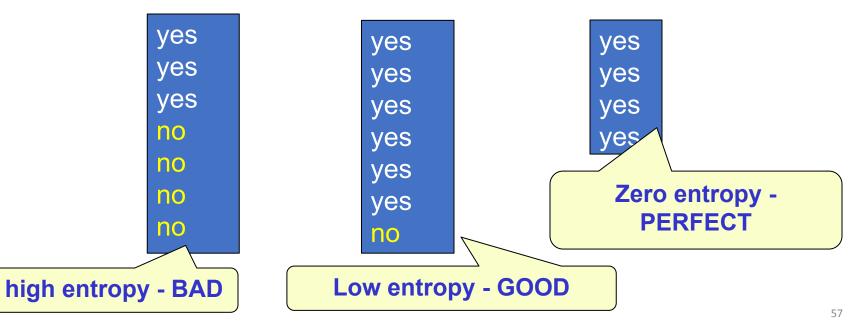
• Entropy: 
$$H(X) = E(I(X)) = \sum_{i} P(x_i)I(x_i) = -\sum_{i} P(x_i)\log_2 P(x_i)$$

• Strategy: choose attribute that results in lowest entropy of the children nodes.

### Why low entropy?

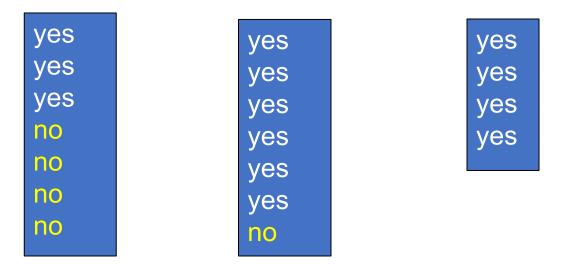
# Measuring Purity with Entropy

- Entropy is a measure of **disorder.** Aka **amount of information**.
  - The higher the entropy, the messier the bag
  - The lower the entropy, the purer the bag

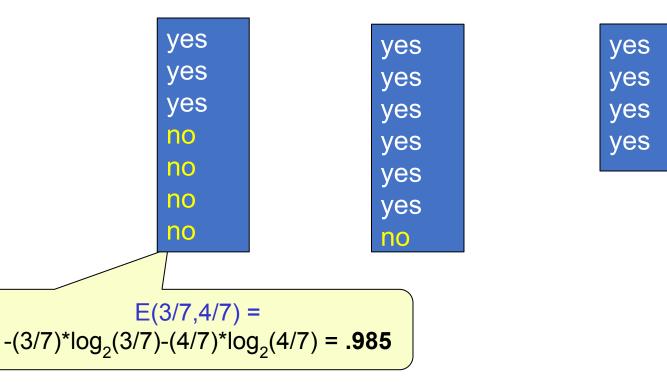


 $E(a/d, b/d) = -(a/d)*\log_2(a/d) - (b/d)*\log_2(b/d)$  where:

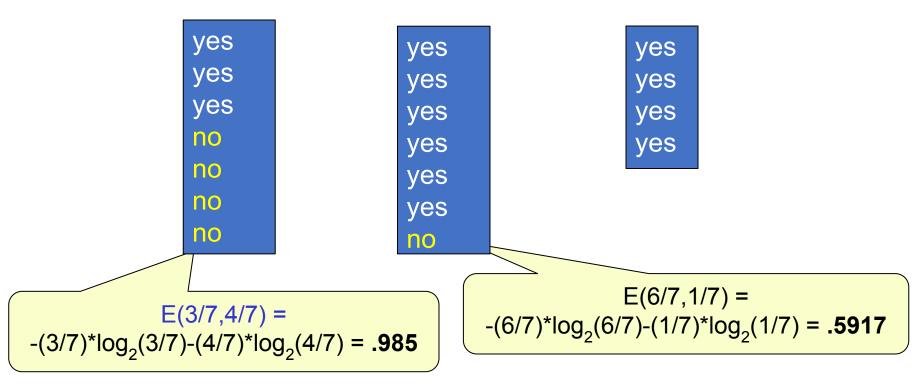
**d**=total # of rows, **a** = # yes, **b** = # no



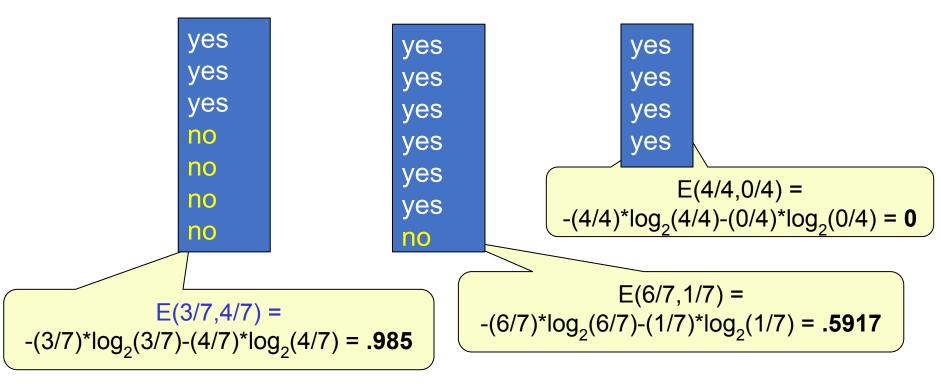
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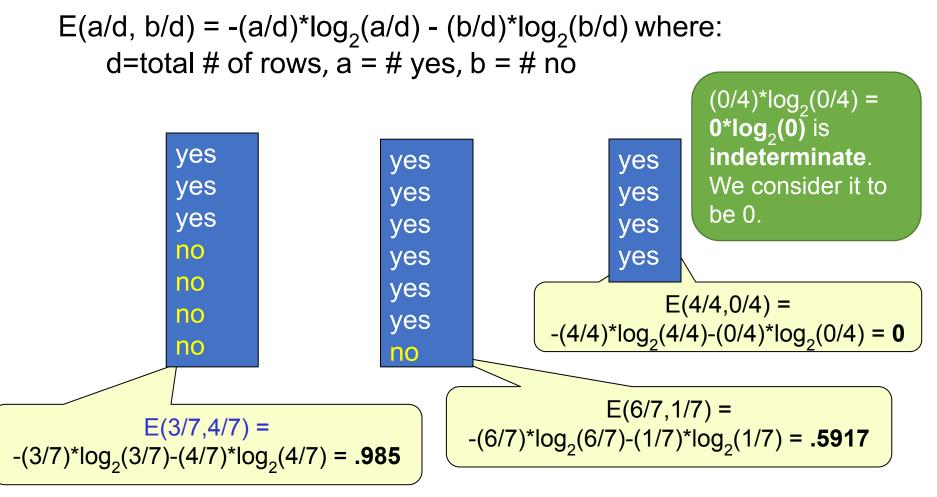


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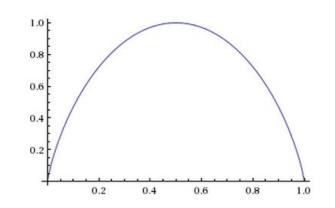
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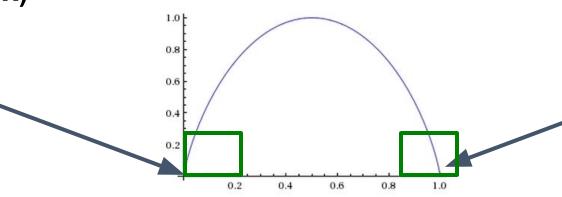


- In the entropy formula: a/d + b/d = 1
- Denote
  - a/d with x b/d with 1-x.

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- $E(a/d, b/d) = -(a/d)*\log_2(a/d) (b/d)*\log_2(b/d) =$
- -x\*log<sub>2</sub>(x) (1-x)\*log<sub>2</sub>(1-x)



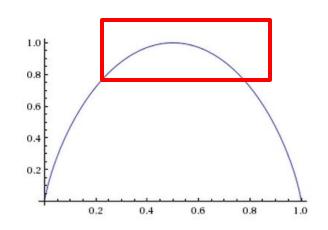
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- -x\*log<sub>2</sub>(x) (1-x)\*log<sub>2</sub>(1-x)

Question to think about: Can entropy be larger than 1?





# Entropy for more than two class values

For three class values:

 $\mathsf{E}(a/d, b/d, c/d) = -(a/d)^* \log_2(a/d) - (b/d)^* \log_2(b/d) - (c/d)^* \log_2(c/d)$ 

a/d + b/d + c/d = 1

#### Entropy for more than two class values

For three class values:

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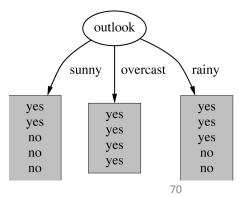
a/d + b/d + c/d = 1

For more class values:  $E(a_1/d,..., a_n/d) = -(a_1/d)*\log_2(a_1/d) - ... - (a_n/d)*\log_2(a_n/d)$  $a_1/d + ... + a_n/d = 1$ 

Outlook	Тетр	Humidity	Windy	Play
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Overcast	Hot	High	False	Yes
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Overcast	Cool	Normal	True	Yes
Sunny	Mild	High	False	No
Sunny	Cool	Normal	False	Yes
Rainy	Mild	Normal	False	Yes
Sunny	Mild	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes
Rainy	Mild	High	True	No



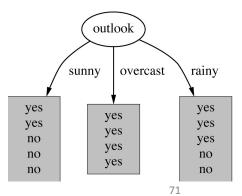
#### Attribute "Outlook"



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outlook=sunny

entropy(2/5,3/5) = -2/5\*log2(2/5) -3/5\*log2(3/5) = .971



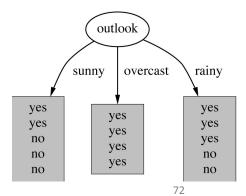
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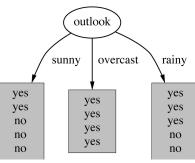
outlook=overcast

entropy(4/4,0/4) = -1\*log2(1) - 0\*log2(0) = 0



#### Attribute "Outlook"

outlook=sunny entropy(2/5,3/5) = -2/5\*log2(2/5) -3/5\*log2(3/5) = .971 outlook=overcast entropy(4/4,0/4) = -1\*log2(1) -0\*log2(0) = 0 outlook=rainy entropy(3/5,2/5) = -3/5\*log2(3/5)-2/5\*log2(2/5) = .971



#### Attribute "Outlook"

outlook=sunny

entropy(2/5,3/5) = -2/5\*log2(2/5) -3/5\*log2(3/5) = .971

outlook=overcast

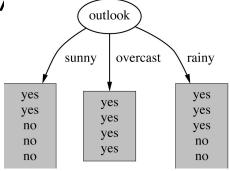
entropy(4/4,0/4) = -1\*log2(1) - 0\*log2(0) = 0

outlook=rainy

entropy(3/5,2/5) = -3/5\*log2(3/5)-2/5\*log2(2/5) = .971

**Expected info**:

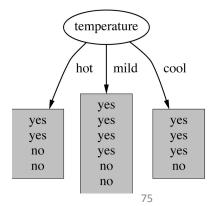
AE = .971\*(5/14) + 0\*(4/14) + .971\*(5/14) = .693



74

temperature=hot

entropy(2/4,2/4) = -2/4\*log2(2/4) - 2/4\*log2(2/4) = 1

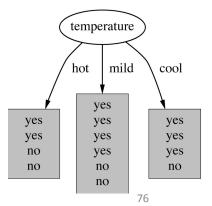


temperature=hot

entropy(2/4,2/4) = -2/4\*log2(2/4) - 2/4\*log2(2/4) = 1

temperature=mild

 $entropy(4/6,2/6) = -4/6*\log 2(4/6) - 2/6*\log 2(2/6) = .918$ 



temperature=hot

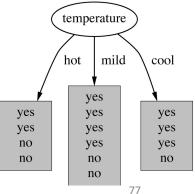
 $entropy(2/4,2/4) = -2/4*\log(2/4) - 2/4*\log(2/4) = 1$ 

temperature=mild

entropy(4/6,2/6) = -4/6\*log2(4/6) - 2/6\*log2(2/6) = .918

temperature=cool

 $entropy(3/4,1/4) = -3/4*\log^2(3/4)-1/4*\log^2(1/4) = .811$ 



temperature=hot

entropy(2/4,2/4) = -2/4\*log2(2/4) - 2/4\*log2(2/4) = 1

temperature=mild

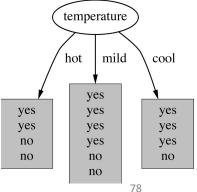
 $entropy(4/6,2/6) = -4/6*\log 2(4/6) - 2/6*\log 2(2/6) = .918$ 

temperature=cool

 $entropy(3/4,1/4) = -3/4*\log^2(3/4)-1/4*\log^2(1/4) = .811$ 

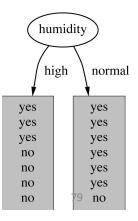
**Expected info**:

 $AE = 1^{*}(4/14) + .918^{*}(6/14) + .811^{*}(4/14) = 0.911$ 



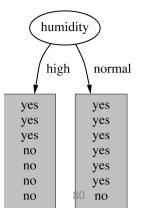
#### Attribute "Humidity"

humidity=high entropy $(3/7,4/7) = -3/7*\log^2(3/7) - 4/7*\log^2(4/7) = .985$ 



#### Attribute "Humidity"

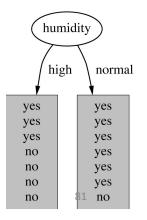
humidity=high entropy $(3/7,4/7) = -3/7*\log 2(3/7) - 4/7*\log 2(4/7) = .985$ humidity=normal entropy $(6/7,1/7) = -6/7*\log 2(6/7) - 1/7*\log 2(1/7) = .592$ 



#### Attribute "Humidity"

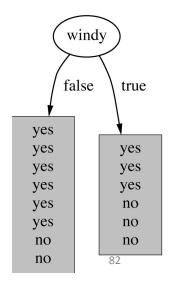
humidity=high entropy $(3/7,4/7) = -3/7*\log 2(3/7) - 4/7*\log 2(4/7) = .985$ humidity=normal entropy $(6/7,1/7) = -6/7*\log 2(6/7) - 1/7*\log 2(1/7) = .592$ Expected info:

AE = .985\*(7/14) + .592\*(7/14) = **.789** 



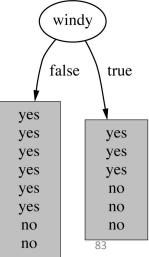
#### Attribute "Windy"

# windy=false entropy(6/8,2/8) = -6/8\*log2(6/8) -2/8\*log2(2/8) = .811



#### Attribute "Windy"

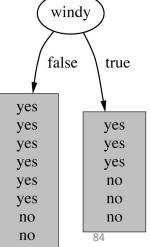
windy=false entropy(6/8,2/8) =  $-6/8*\log 2(6/8) - 2/8*\log 2(2/8) = .811$ windy=true entropy(3/6,3/6) =  $-3/6*\log 2(3/6) - 3/6*\log 2(3/6) = 1$ 



#### Attribute "Windy"

windy=false entropy(6/8,2/8) = -6/8\*log2(6/8) -2/8\*log2(2/8) = .811 windy=true entropy(3/6,3/6) = -3/6\*log2(3/6) -3/6\*log2(3/6) = 1 Expected info:

 $AE = .811^{*}(8/14) + 1^{*}(6/14) = .892$ 



#### And the winner is...

#### And the winner is...

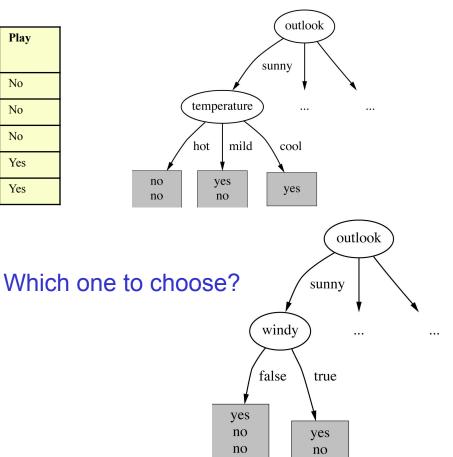
"Outlook"

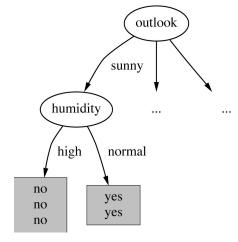
...So, the root will be "Outlook"



#### Continuing to split (for Outlook="Sunny")

Outlook	Тетр	Humidity	Windy	Play
Sunny	Hot	High	False	No
Sunny	Hot	High	True	No
Sunny	Mild	High	False	No
Sunny	Cool	Normal	False	Yes
Sunny	Mild	Normal	True	Yes



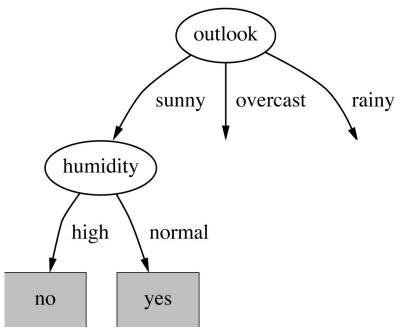


# Continuing to split (for Outlook="Sunny")

temperature=hot: entropy(2/2,0/2) = 0temperature=mild: entropy(1/2, 1/2) = 1temperature=cool: entropy(1/1,0/1) = 0, AE = 0\*(2/5) + 1\*(2/5) + 0\*(1/5) = .4humidity=high: entropy(3/3,0/3) = 0**humidity**=normal: info(2/2,0/2) = 0, AE = 0windy=false: entropy $(1/3, 2/3) = -1/3*\log_2(1/3) - 2/3*\log_2(2/3) = .918$ windy=true: entropy(1/2, 1/2) = 1AE = .918\*(3/5) + 1\*(2/5) = .951

#### Winner is "humidity"

#### Tree so far



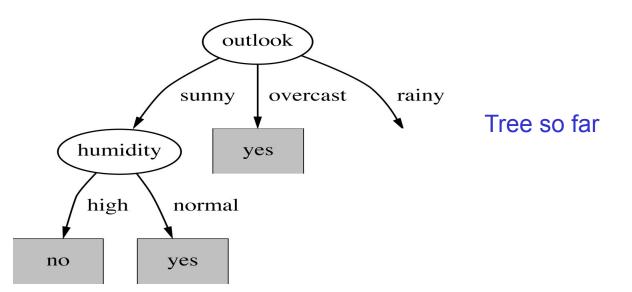
#### Continuing to split (for Outlook="Overcast")

Outlook	Тетр	Humidity	Windy	Play
Overcast	Hot	High	False	Yes
Overcast	Cool	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes

#### Continuing to split (for Outlook="Overcast")

Outlook	Тетр	Humidity	Windy	Play
Overcast	Hot	High	False	Yes
Overcast	Cool	Normal	True	Yes
Overcast	Mild	High	True	Yes
Overcast	Hot	Normal	False	Yes

• Nothing to split here, "play" is always "yes".



#### Continuing to split (for Outlook="Rainy")

Outlook	Тетр	Humidity	Windy	Play
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Rainy	Mild	Normal	False	Yes
Rainy	Mild	High	True	No

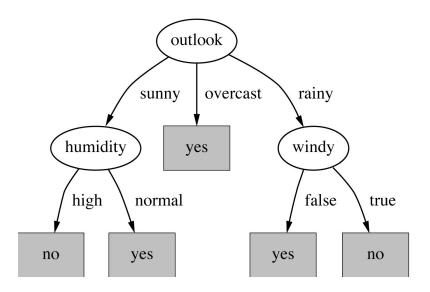
# Continuing to split (for Outlook="Rainy")

Outlook	Тетр	Humidity	Windy	Play
Rainy	Mild	High	False	Yes
Rainy	Cool	Normal	False	Yes
Rainy	Cool	Normal	True	No
Rainy	Mild	Normal	False	Yes
Rainy	Mild	High	True	No

• We can easily see that "Windy" is the one to choose. (Why?)



#### The final decision tree



- Note: not all leaves need to be pure; sometimes identical instances have different classes
- $\Rightarrow$  Splitting stops when data can't be split any further

#### Algorithms

 Algorithm described so far is called "ID3" - Iterative Dichotomiser developed by Ross Quinlan at University of Sydney Australia

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 Algorithm described so far is called "ID3" - Iterative Dichotomiser developed by Ross Quinlan at University of Sydney Australia

- Led to development of C4.5 (and its commercial version, C5.0, J48 in Java) which deals with
  - noisy data
  - missing values
  - numeric attributes
  - pruning the tree

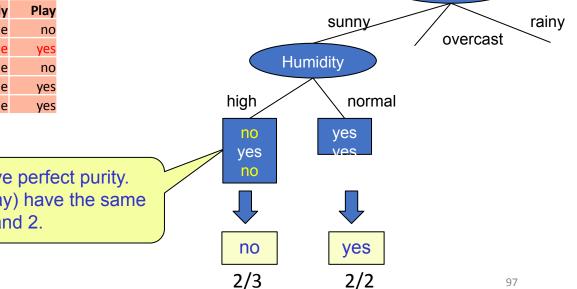
# Noisy data



Outlook

- Not all leaves need to be pure; sometimes identical tuples have different class values
  - Splitting stops when data can't be split any further

ID	Outlook	Temp	Humidity	Windy	Play
1	sunny	hot	high	false	no
2	sunny	hot	high	false	yes
8	sunny	mild	high	false	no
9	sunny	cool	normal	false	yes
11	sunny	mild	normal	true	yes



No chance to split and achieve perfect purity. All attributes (except ID and Play) have the same values for tuple 1 and 2.

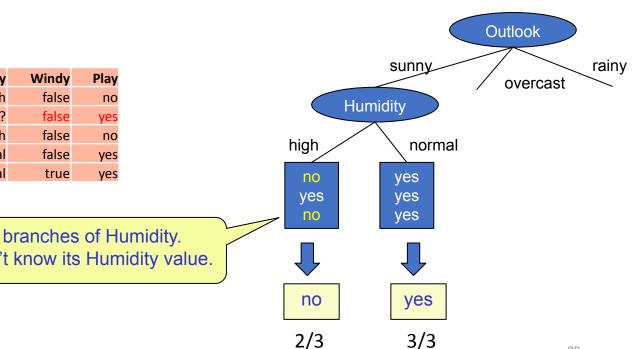
# Missing data



Sometimes, some attributes of some tuples have missing values

ID	Outlook	Temp	Humidity	Windy	Play
1	sunny	hot	high	false	no
2	sunny	hot	?	false	yes
8	sunny	mild	high	false	no
9	sunny	cool	normal	false	yes
11	sunny	mild	normal	true	yes

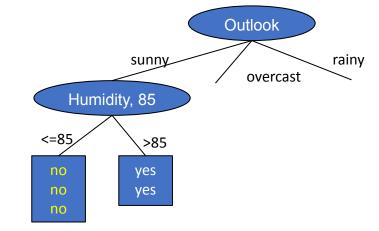
Tuple 2 is sent both branches of Humidity. This is because we don't know its Humidity value.



### Continuous-valued attributes

- Some attributes can be numeric (continuous).
- No problem, we can have binary splits (≥v, <v), still use Entropy

ID	Outlook	Temp	Humidity	Windy	Play
1	sunny	85	85	false	no
2	sunny	80	90	true	no
3	overcast	83	86	false	yes
4	rainy	70	96	false	yes
5	rainy	68	80	false	yes
6	rainy	65	70	true	no
7	overcast	64	65	true	yes
8	sunny	72	95	false	no
9	sunny	69	70	false	yes
10	rainy	75	80	false	yes
11	sunny	75	70	true	yes
12	overcast	72	90	true	yes
13	overcast	81	75	false	yes
14	rainy	71	91	true	no



ID	Outlook	Temp	Humidity	Windy	Play
1	sunny	69	70	false	no
2	sunny	75	70	true	no
8	sunny	85	85	false	no
9	sunny	80	90	false	yes
11	sunny	72	95	true	99 yes



#### Pruning the tree

- Not always a good idea to grow the tree exhaustively
  - Saying goes:
    - "tree will over fit the training data"
    - "tree will not abstract well to classify new data"

#### Pruning the tree

- Not always a good idea to grow the tree exhaustively
  - Saying goes:
    - "tree will over fit the training data"
    - "tree will not abstract well to classify new data"
- Solutions
  - Pre-pruning
    - Stop when error on new data doesn't go down much
  - Post-pruning
    - Chi-squared test for generalizability. See: http://www.saedsayad.com/decision\_tree\_overfitting.htm

#### **Decision Trees**

• Pros:

•

- Easy to visualize/interpret
- Efficient to use
- Handles discrete and continuous values

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#### **Decision Trees**

- Pros:
  - Easy to visualize/interpret
  - Efficient to use
  - Handles discrete and continuous values
- Cons:
  - Can create overly-complex trees (pruning helps)
  - Unstable (small changes in data can give very different trees)
  - Finding optimal tree exhaustively is a combinatorial problem (and is thus very expensive to compute and verify)

#### Applications

- CNNs (convolutional neural nets) are often hard to interpret
  - I.e. it's unclear why the model makes a particular classification decision
- Proposed that decision trees can help us to interpret CNNs
  - <u>https://openaccess.thecvf.com/content\_CVPR\_2019/papers/Z</u> <u>hang\_Interpreting\_CNNs\_via\_Decision\_Trees\_CVPR\_2019\_pap</u> <u>er.pdf</u>

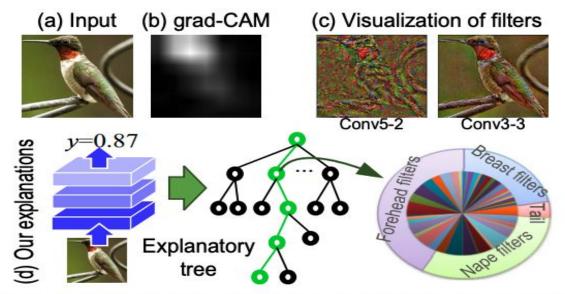


Figure 1. Different types of explanations for CNNs. We compare (d) our task of quantitatively and semantically explaining CNN predictions with previous studies of interpreting CNNs, such as (b) the grad-CAM [26] and (c) CNN visualization [23]. Given an input image (a), we infer a parse tree (green lines) within the decision tree to project neural activations onto clear concepts of object parts. Our method quantitatively explains which filters/parts (in the small/big round) are used for the prediction and how much they contribute to the prediction. We visualize numerical contributions from randomly selected 10% filters for clarity.

#### Forestsssssssssssssssss...



#### Are cool.





