Statistical Methods in AI (CSE/ECE 471)

Lecture-3: Decision Tree Learning

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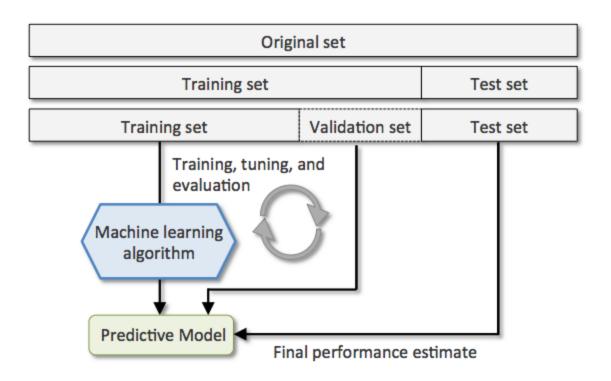
Announcements

- IMPORTANT: All assignments/projects will need to be in Python.
- This week's tutorial: Probability recap, ML datasets, visualization approaches. Bring your laptops.
- Ask questions. Take notes.

Announcements

- Assignments Questions involving equations/ mathematical derivation
 - Write up in latex [overleaf.com] → submit
 - Write neatly on paper → scan as photo/pdf
 [camscanner] → submit
- TA office hours, locations have been announced.

The Train-Validation-Test paradigm



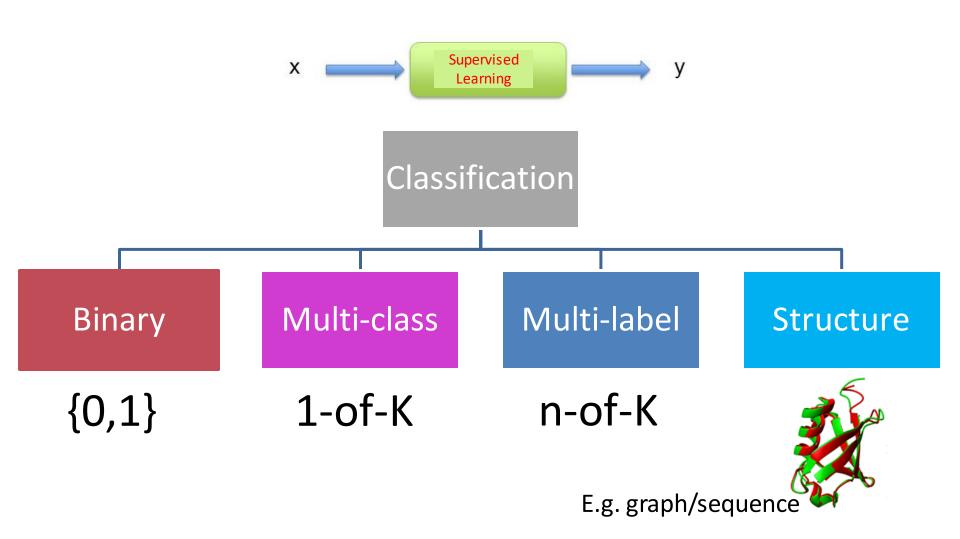


Classification

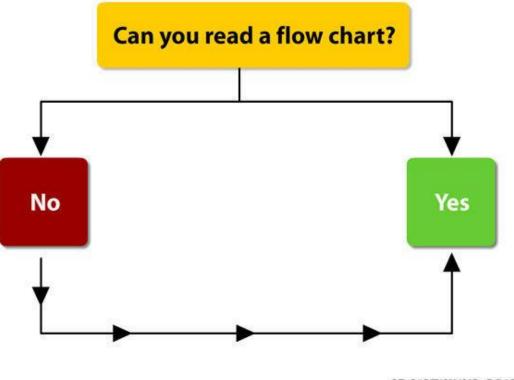
Regression

Reinforcement

Learning



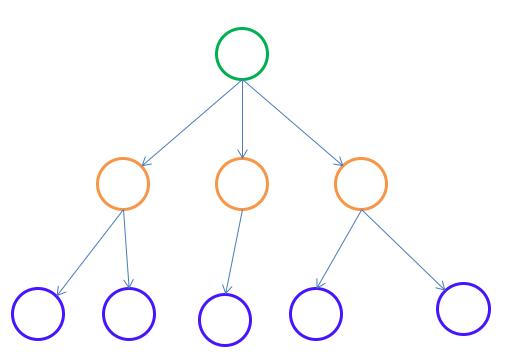
Flowcharts



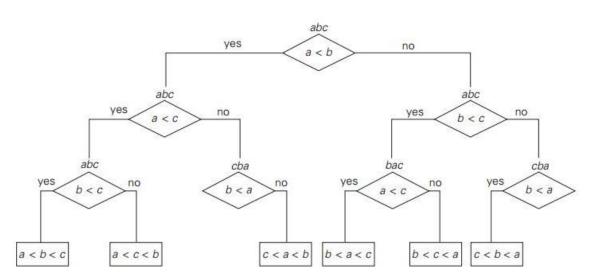
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Trees

- ■Node
- Root
- **□**Leaf
- □ Edge/Branch
- **□**Path
- **□**Depth



if/then if/else/then

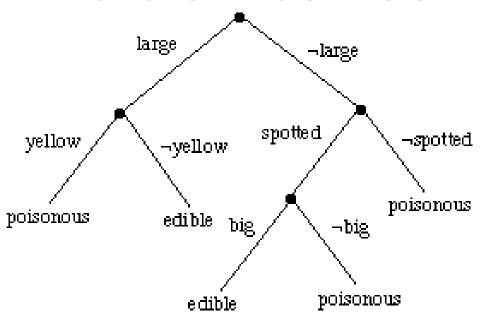




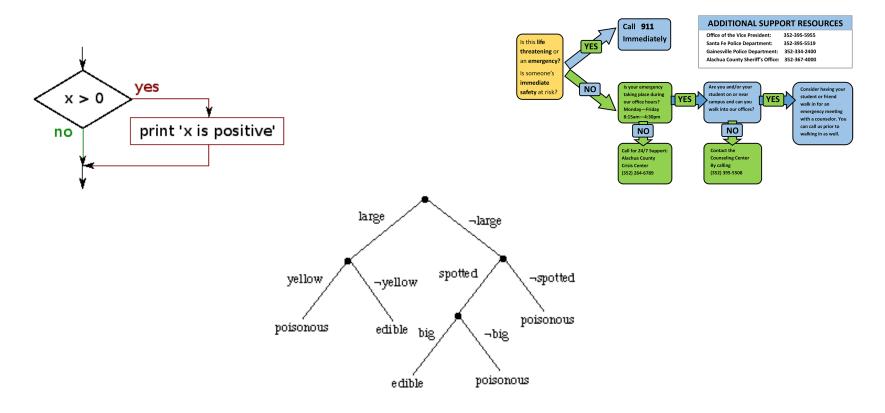
Emergency Response



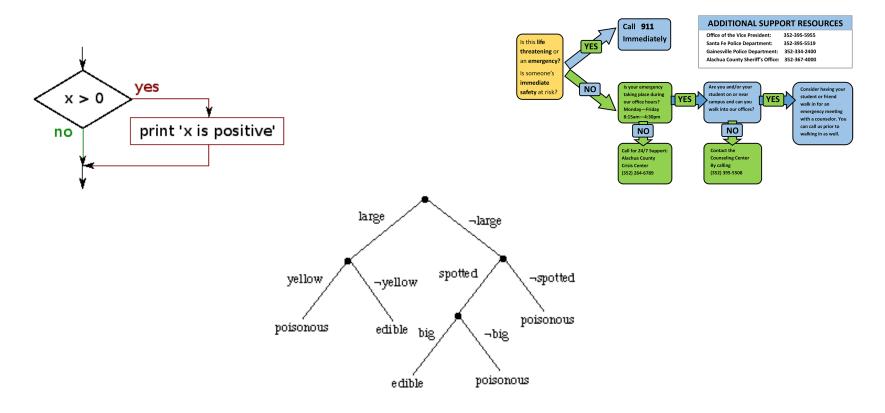
Edible Mushroom



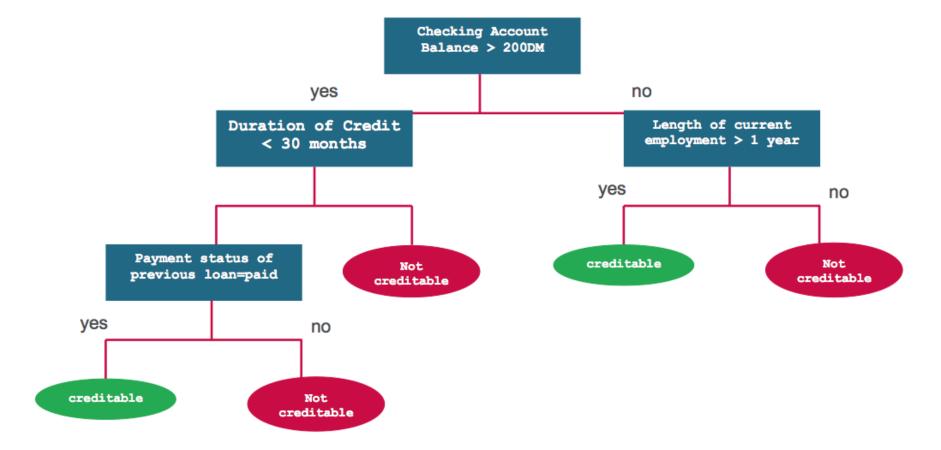
Hand-crafted, fixed trees



Hand-crafted, fixed trees



Credit Approval



Credit Approval (Raw Data)

4	Α	В	С	D	E	F	G	н	1	J	K	L	М	N	0	Р
64	A1	A2	A3	A4	A5	A6	A7	A8	A9	A10	A11	A12	A13	A14	A15	class
65	a	20.42	0.835	u	g	q	v	1.585	t	t	1	f	g	0	0	+
66		26.67	4.25	u	g	СС	v	4.29	t	t	1	t	g	120	0	+
67	b	34.17	1.54	u	g	СС	v	1.54	t	t	1	t	g	520	50000	+
68	a	36	1	u	g	С	v	2	t	t	11	f	g	0	456	+
69	b	25.5	0.375	u	g	m	v	0.25	t	t	3	f	g	260	15108	+
70		19.42	6.5	u	g	w	h	1.46	t	t	7	f	g	80	2954	+
71	b	35.17	25.125	u	g	X	h	1.625	t	t	1	t	g	515	500	+
72		32.33	7.5	u	g	e	bb	1.585	t	f	0	t	S	420	0	-
73	b	34.83	4	u	g	d	bb	12.5	t	f	0	t	g		0	-
74		38.58	5	u	g	СС	v	13.5	t	f	0	t	g	980	0	-
75	b	44.25	0.5	u	g	m	v	10.75	t	f	0	f	S	400	0	-
76	b	44.83	7	у	p	С	v	1.625	f	f	0	f	g	160	2	-
77	b	20.67	5.29	u	g	q	v	0.375	t	t	1	f	g	160	0	-
78	b	34.08	6.5	u	g	aa	v	0.125	t	f	0	t	g	443	0	-

2	sunny	hot	high	false	no
3	sunny	hot	high	true	no
4	overcast	hot	high	false	yes
5	rainy	mild	high	false	yes
6	rainy	cool	normal	false	yes
7	rainy	cool	normal	true	no
8	overcast	cool	normal	true	yes
9	sunny	mild	high	false	no
10	sunny	cool	normal	false	yes
11	rainy	mild	normal	false	yes
12	sunny	mild	normal	true	yes
13	overcast	mild	high	true	yes
14	overcast	hot	normal	false	yes
15	rainy	mild	high	true	no

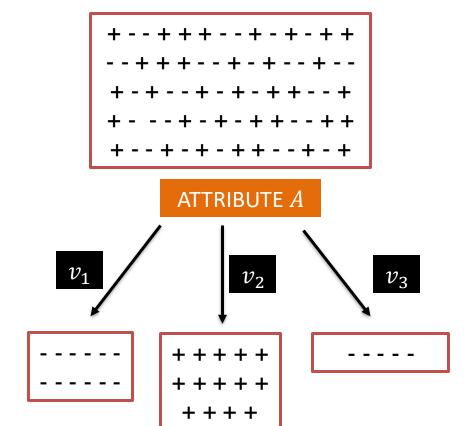
humidity

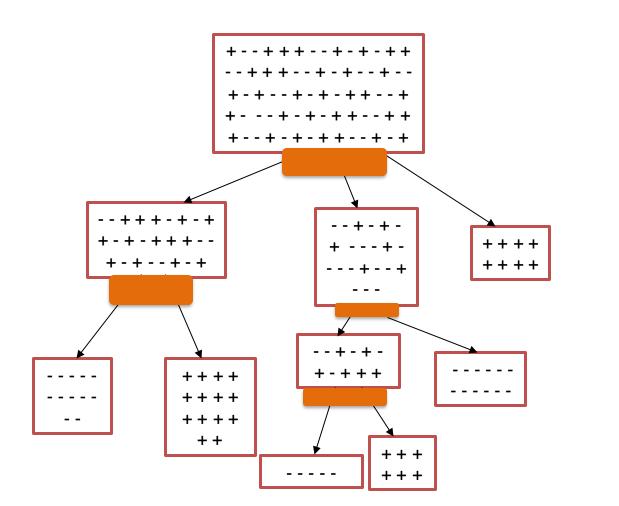
temp

windy

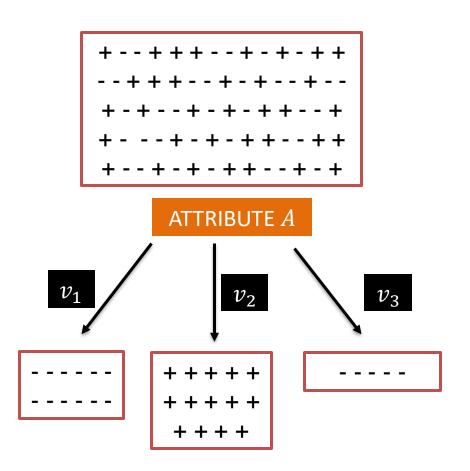
play

outlook

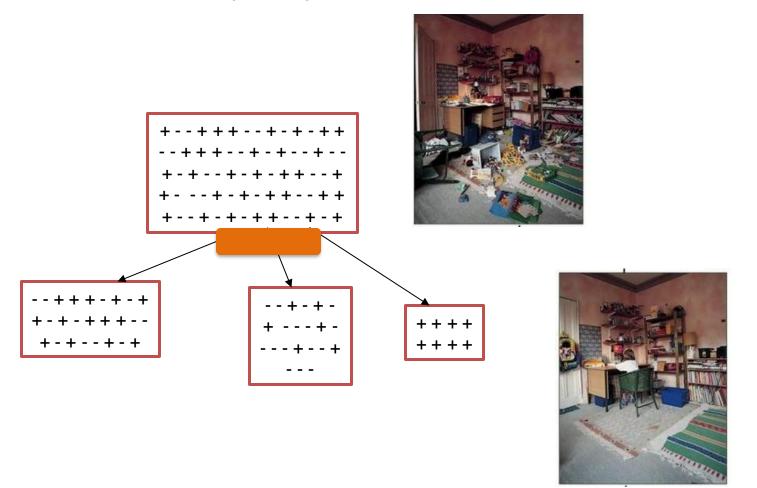


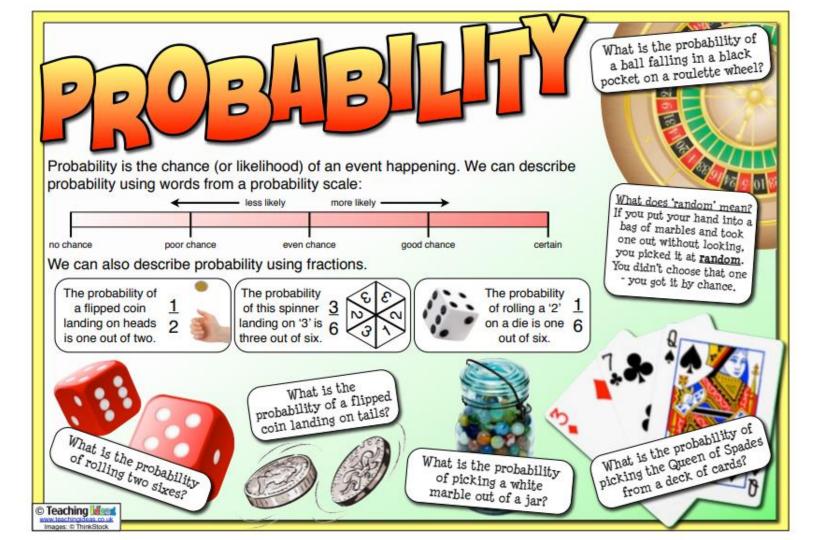


How much 'impurity' does this attribute decrease?



How much 'impurity' does this attribute decrease?





Discrete probability distribution

- Variables that have only a finite number of possible outcomes
- For example ...a six-sided die is thrown

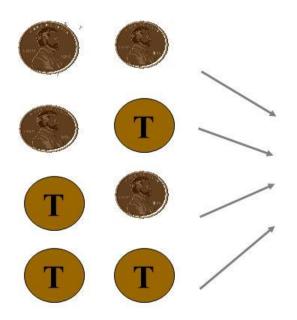
Possibilities
$$r=1$$
 1 2 3 4 5 6
Probability that $Z=r$ 1/6 1/6 1/6 1/6 1/6 1/6

$$0 \le P(X_j) \le 1 \qquad \sum P(X_j) = 1$$

Discrete probability distribution

Event: Toss two coins

Count the number of tails

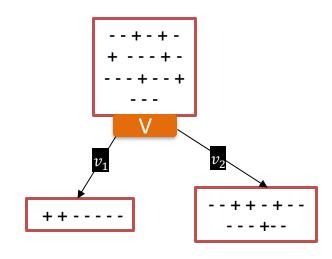


Probability Distribution

<u>Values</u>	Probability
0	1/4 = .25
1	2/4 = .50
2	1/4 = .25

Properties of an impurity measure

- Class labels: Binary {+1,-1}
- C



An *impurity measure* is a function i(V) such that

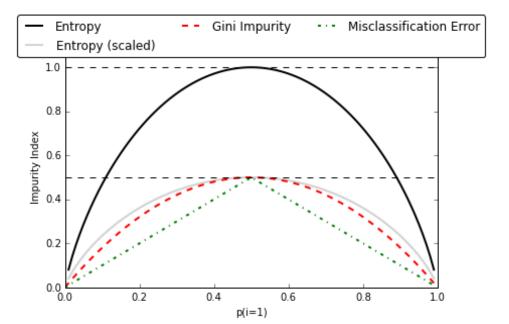
- $i(V) \ge 0$, with i(V) = 0 iff V consists of a single class
- a larger value of i(V) indicates that the distribution defined by (q,(1-q)) is closer to the uniform distribution

Impurity function: candidates

Entropy:
$$i(V) = -(q \log q + (1 - q) \log(1 - q))$$

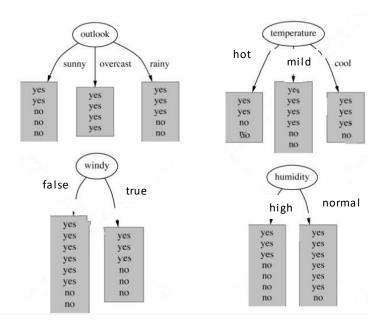
Gini index: i(V) = 2q(1 - q)

Misclassification rate: $i(V) = \min(q, 1-q)$



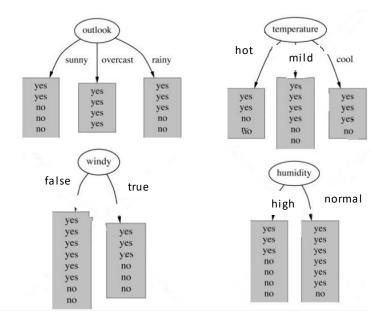
Example

Day	Temperature	Outlook	Humidity	Windy	Play Golf?
07-05	hot	sunny	high	false	no
07-06	hot	sunny	high	true	no
07-07	hot	overcast	high	false	yes
07-09	cool	rain	normal	false	yes
07-10	cool	overcast	normal	true	yes
07-12	mild	sunny	high	false	no
07-14	cool	sunny	normal	false	yes
07-15	mild	rain	normal	false	yes
07-20	mild	sunny	normal	true	yes
07-21	mild	overcast	high	true	yes
07-22	hot	overcast	normal	false	yes
07-23	mild	rain	high	true	no
07-26	cool	rain	normal	true	no
07-30	mild	rain	high	false	yes



Step-1: Compute impurity score of training label distribution

Day	Temperature	Outlook	Humidity	Windy	Play Golf?
07-05	hot	sunny	high	false	no
07-06	hot	sunny	high	true	no
07-07	hot	overcast	high	false	yes
07-09	cool	rain	normal	false	yes
07-10	cool	overcast	normal	true	yes
07-12	mild	sunny	high	false	no
07-14	cool	sunny	normal	false	yes
07-15	mild	rain	normal	false	yes
07-20	mild	sunny	normal	true	yes
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07-23	mild	rain	high	true	no
07-26	cool	rain	normal	true	no
07-30	mild	rain	high	false	yes



Entropy:
$$i(V) = -(q \log q + (1-q) \log(1-q))$$

$$E(S) = -\left(\frac{9}{14}log(\frac{9}{14}) + \frac{5}{14}log(\frac{5}{14})\right) = 0.94$$

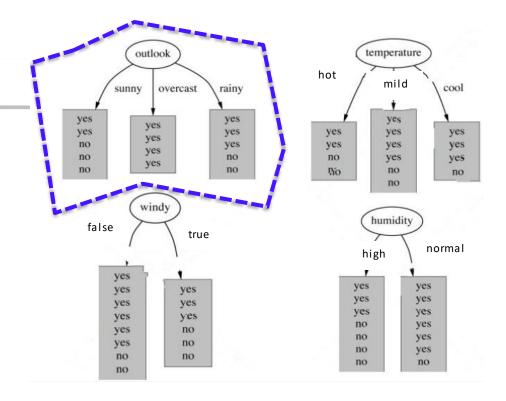
Step-2: Compute impurity score for each unique value of candidate attributes

Example: Attribute Outlook

Entropy:
$$i(V) = -(q \log q + (1 - q) \log(1 - q))$$

Outlook = rainy
 3 examples yes, 2 examples no

$$E(\text{Outlook} = \text{sunny}) = -\frac{2}{5} \log \left(\frac{2}{5} \right) - \frac{3}{5} \log \left(\frac{3}{5} \right) = 0.971$$



Step-2: Compute impurity score for each unique value of candidate attributes

Example: Attribute Outlook

Entropy:
$$i(V) = -(q \log q + (1 - q) \log(1 - q))$$

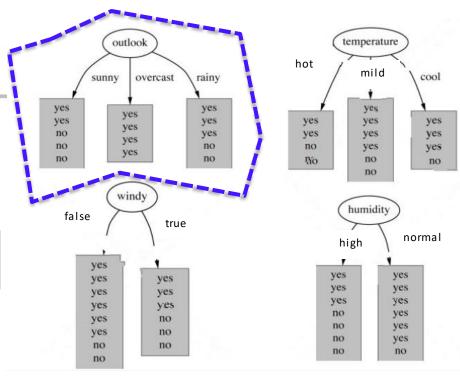
Outlook = rainy
 3 examples yes, 2 examples no

$$E(\text{Outlook} = \text{sunny}) = -\frac{2}{5} \log \left(\frac{2}{5} \right) - \frac{3}{5} \log \left(\frac{3}{5} \right) = 0.971$$

• Outlook = overcast: 4 examples yes, 0 examples no

$$E(\text{Outlook} = \text{overcast}) = -1 \log(1) - 0 \log(0) = 0$$

Note: this is normally undefined. Here: = 0



Step-2: Compute impurity score for each unique value of candidate attributes

Example: Attribute Outlook

Entropy:
$$i(V) = -(q \log q + (1 - q) \log(1 - q))$$

• Outlook = rainy 3 examples yes, 2 examples no

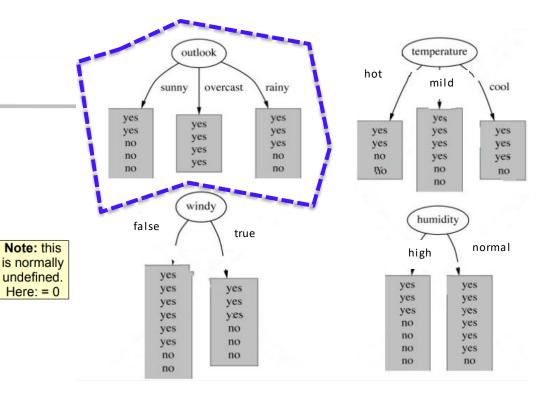
$$E(\text{Outlook} = \text{sunny}) = -\frac{2}{5} \log \left(\frac{2}{5} \right) - \frac{3}{5} \log \left(\frac{3}{5} \right) = 0.971$$

Outlook = overcast: 4 examples yes, 0 examples no

$$E(\text{Outlook} = \text{overcast}) = -1 \log(1) - 0 \log(0) = 0$$

Outlook = sunny2 examples yes, 3 examples no

$$E(\text{Outlook} = \text{rainy}) = -\frac{3}{5} \log \left(\frac{3}{5} \right) - \frac{2}{5} \log \left(\frac{2}{5} \right) = 0.971$$



Step-3: Compute impurity score for candidate attribute

Note: this

is normally

undefined.

Here: = 0

• Outlook = rainy 3 examples yes, 2 examples no

$$E(\text{Outlook} = \text{sunny}) = -\frac{2}{5} \log \left(\frac{2}{5} \right) - \frac{3}{5} \log \left(\frac{3}{5} \right) = 0.971$$

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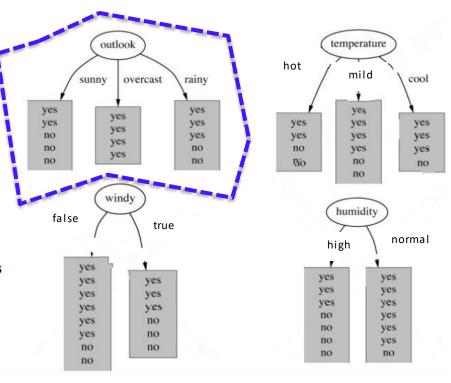
2 examples yes, 3 examples no

$$E(\text{Outlook} = \text{rainy}) = -\frac{3}{5} \log \left(\frac{3}{5} \right) - \frac{2}{5} \log \left(\frac{2}{5} \right) = 0.971$$

- Entropy only computes the quality of a single (sub-)set of examples
 - · corresponds to a single value

Outlook = sunny

- How can we compute the quality of the entire split?
 - corresponds to an entire attribute



Step-3: Compute impurity score for candidate attribute

• Outlook = rainy 3 examples yes, 2 examples no

$$E(\text{Outlook} = \text{sunny}) = -\frac{2}{5} \log \left(\frac{2}{5} \right) - \frac{3}{5} \log \left(\frac{3}{5} \right) = 0.971$$

• Outlook = overcast: 4 examples yes, 0 examples no

$$E(\text{Outlook} = \text{overcast}) = -1 \log(1) - 0 \log(0) = 0$$

Note: this is normally undefined. Here: = 0

Outlook = sunny
 2 examples yes, 3 examples no

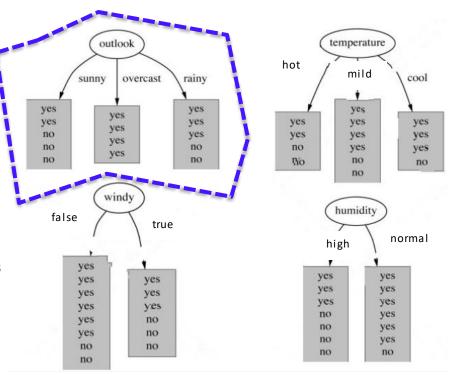
$$E(\text{Outlook} = \text{rainy}) = -\frac{3}{5}\log\left(\frac{3}{5}\right) - \frac{2}{5}\log\left(\frac{2}{5}\right) = 0.971$$

- Entropy only computes the quality of a single (sub-)set of examples
 - · corresponds to a single value
- How can we compute the quality of the entire split?
 - · corresponds to an entire attribute

Solution:

- Compute the weighted average over all sets resulting from the split
 - weighted by their size

$$I(S, A) = \sum_{i} \frac{|S_{i}|}{|S|} \cdot E(S_{i})$$



Step-3: Compute impurity score for candidate attribute

Note: this

is normally

undefined.

Here: = 0

3 examples yes, 2 examples no Outlook = rainv

$$E(\text{Outlook} = \text{sunny}) = -\frac{2}{5} \log \left(\frac{2}{5} \right) - \frac{3}{5} \log \left(\frac{3}{5} \right) = 0.971$$

• Outlook = overcast: 4 examples yes, 0 examples no

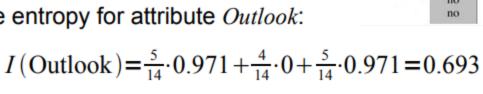
$$E(\text{Outlook} = \text{overcast}) = -1 \log(1) - 0 \log(0) = 0$$

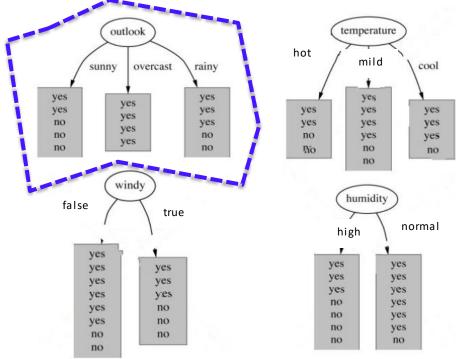
2 examples yes, 3 examples no Outlook = sunnv

$$E(\text{Outlook} = \text{rainy}) = -\frac{3}{5} \log \left(\frac{3}{5} \right) - \frac{2}{5} \log \left(\frac{2}{5} \right) = 0.971$$

$$I(S, A) = \sum_{i} \frac{|S_i|}{|S|} \cdot E(S_i)$$

Average entropy for attribute *Outlook*:





Step-4: Compute Information Gain (reduction in impurity score) provided by candidate attribute

$$I(S, A) = \sum_{i} \frac{|S_{i}|}{|S|} \cdot E(S_{i})$$

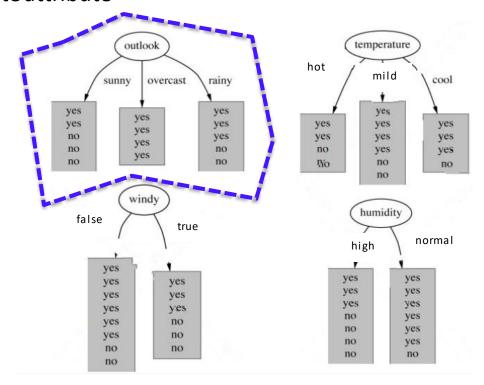
Average entropy for attribute *Outlook*:

$$I(\text{Outlook}) = \frac{5}{14} \cdot 0.971 + \frac{4}{14} \cdot 0 + \frac{5}{14} \cdot 0.971 = 0.693$$

$$E(S) = -\left(\frac{9}{14}log\left(\frac{9}{14}\right) + \frac{5}{14}log\left(\frac{5}{14}\right)\right) = 0.94$$

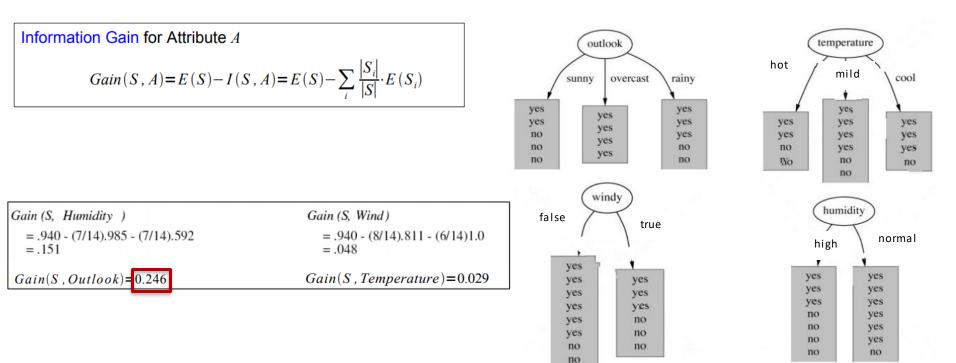
Information Gain for Attribute A

$$Gain(S, A) = E(S) - I(S, A) = E(S) - \sum_{i} \frac{|S_{i}|}{|S|} \cdot E(S_{i})$$



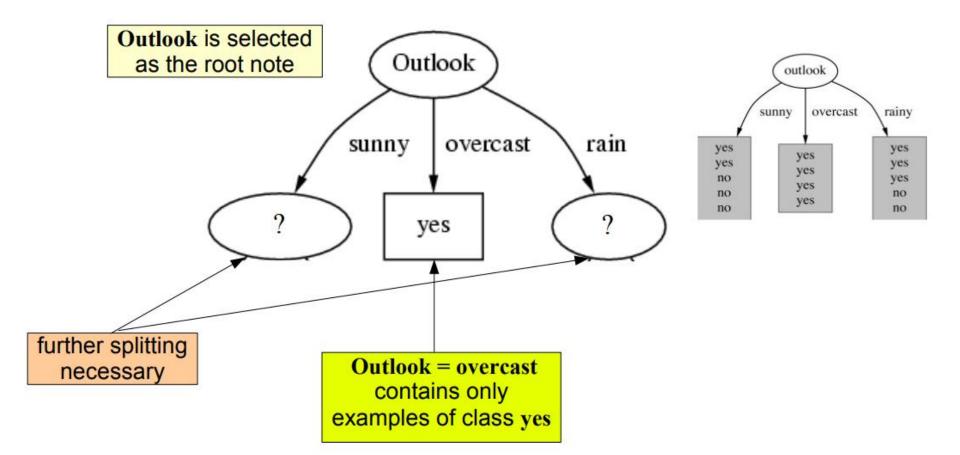
Gain(S, Outlook) = 0.246

Step-5: Compare Information Gain provided by all candidates

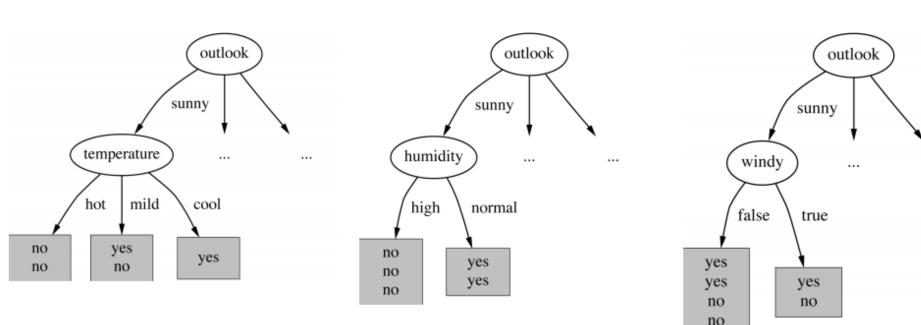


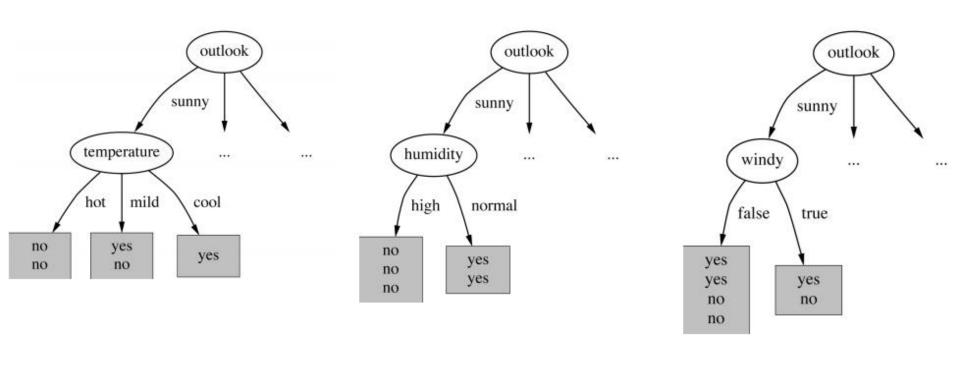
Select attribute which provides largest 'impurity reduction'/Information Gain

Step-6: Assign root node



Recurse and repeat Steps 1-6

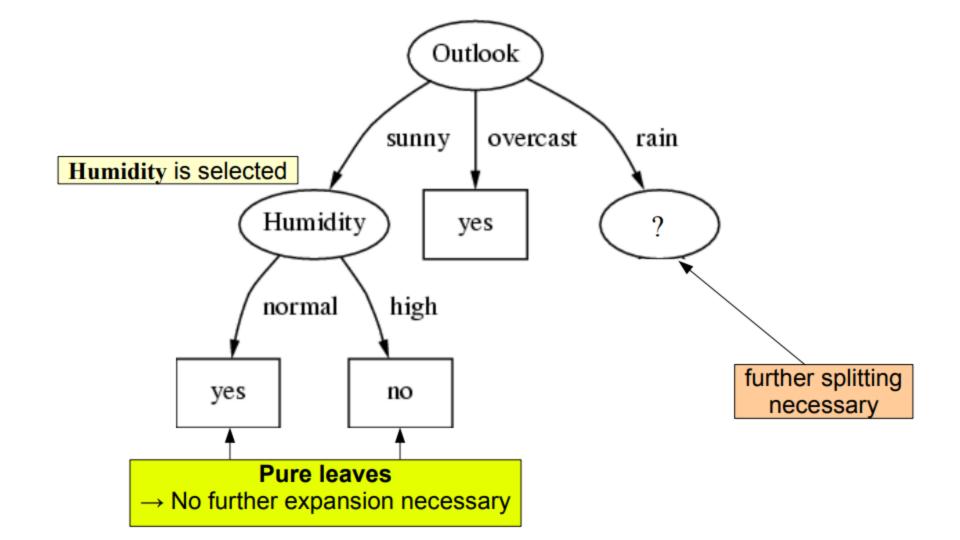




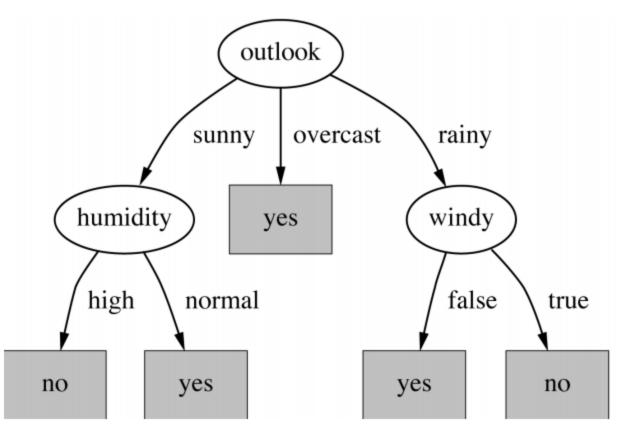
$$Gain(Temperature) = 0.571 \text{ bits}$$

 $Gain(Humidity) = 0.971 \text{ bits}$
 $Gain(Windy) = 0.020 \text{ bits}$

Humidity is selected

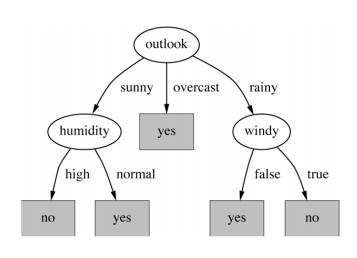


Final Decision Tree



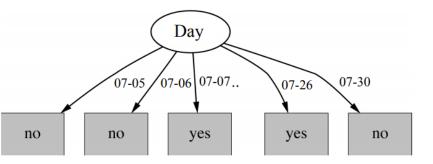
Final Decision Tree

Day	Temperature	Outlook	Humidity	Windy	Play Golf?
07-05	hot	sunny	high	false	no
07-06	hot	sunny	high	true	no
07-07	hot	overcast	high	false	yes
07-09	cool	rain	normal	false	yes
07-10	cool	overcast	normal	true	yes
07-12	mild	sunny	high	false	no
07-14	cool	sunny	normal	false	yes
07-15	mild	rain	normal	false	yes
07-20	mild	sunny	normal	true	yes
07-21	mild	overcast	high	true	yes
07-22	hot	overcast	normal	false	yes
07-23	mild	rain	high	true	no
07-26	cool	rain	normal	true	no
07-30	mild	rain	high	false	yes



- Problematic: attributes with a large number of values
 - extreme case: each example has its own value
 - e.g. example ID; Day attribute in weather data

- Problematic: attributes with a large number of values
 - extreme case: each example has its own value
 - e.g. example ID; Day attribute in weather data
- Subsets are more likely to be pure if there is a large number of different attribute values
 - Information gain is biased towards choosing attributes with a large number of values



Entropy of split:

$$I(\text{Day}) = \frac{1}{14} (E([0,1]) + E([0,1]) + ... + E([0,1])) = 0$$

Information gain is maximal for Day (0.940 bits)

$$Gain(S, Temperature) = 0.029$$

Gain(S, Outlook) = 0.246

Attributes with large # of values

- This may cause several problems:
 - Overfitting
 - selection of an attribute that is non-optimal for prediction
 - Fragmentation
 - data are fragmented into (too) many small sets

Attributes with large # of values – measure

- Intrinsic information of a split
 - entropy of distribution of instances into branches
 - i.e. how much information do we need to tell which branch an instance belongs to

$$IntI(S, A) = -\sum_{i} \frac{|S_{i}|}{|S|} \log \left| \frac{|S_{i}|}{|S|} \right|$$

- Example:
 - Intrinsic information of Day attribute:

$$IntI(Day) = 14 \times \left(-\frac{1}{14} \cdot \log\left(\frac{1}{14}\right)\right) = 3.807$$

- Observation:
 - Attributes with higher intrinsic information are less useful

Gain Ratio

- modification of the information gain that reduces its bias towards multi-valued attributes
- takes number and size of branches into account when choosing an attribute
 - corrects the information gain by taking the intrinsic information of a split into account
- Definition of Gain Ratio:

$$GR(S, A) = \frac{Gain(S, A)}{IntI(S, A)}$$

- Example:
 - Gain Ratio of Day attribute

$$GR(\text{Day}) = \frac{0.940}{3.807} = 0.246$$

Handling numerical attributes

- Standard method: binary splits
 - E.g. Temperature < 78</p>
- Multiple split points possible
- Computationally more demanding

Handling numerical attributes – some optimizations

- Assume a numerical attribute for Temperature
- First step:
 - Sort all examples according to the value of this attribute
 - Could look like this:

```
64 65 68 69 70 71 72 72 75 75 80 81 83 85
Yes No Yes Yes Yes No No Yes Yes No Yes Yes No
```

Handling numerical attributes – some optimizations

- Assume a numerical attribute for Temperature
- First step:
 - Sort all examples according to the value of this attribute
 - Could look like this:

- One split between each pair of values
 - E.g. Temperature < 71.5: yes/4, no/2 Temperature ≥ 71.5 : yes/5, no/3

$$I(\text{Temperature} @ 71.5) = \frac{6}{14} \cdot E(\text{Temperature} < 71.5) + \frac{8}{14} E(\text{Temperature} \ge 71.5) = 0.939$$

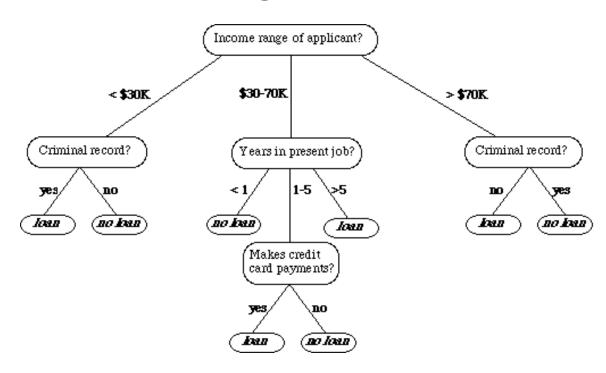
Split points can be placed between values or directly at values

Handling numerical attributes

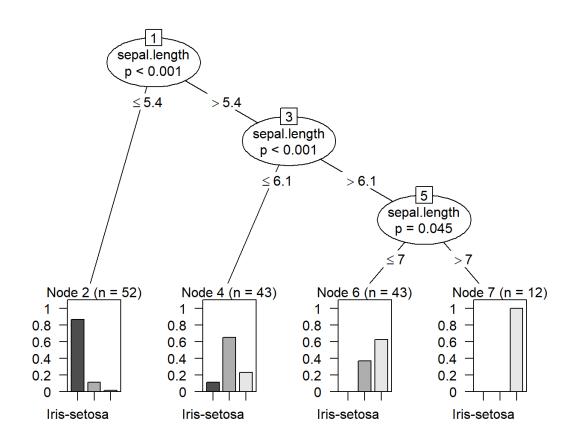
- Splitting (multi-way) on a nominal attribute exhausts all information in that attribute
 - Nominal attribute is tested (at most) once on any path in the tree
- Not so for binary splits on numerical attributes (why?)
- Attribute may be tested multiple times in the tree
- Tree may become hard to read

Handling numerical attributes

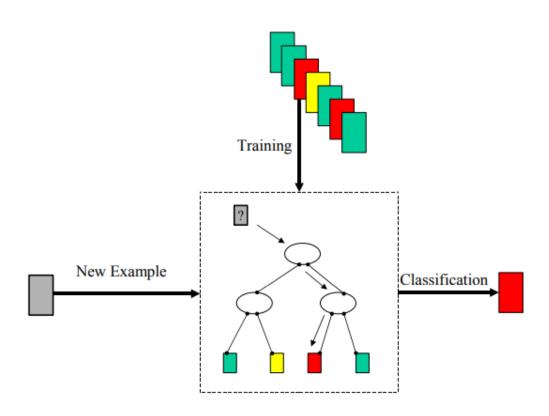
Discretization / Clustering



Decision Tree with numerical attribute



Deployment



Learning Algorithm for Decision Trees

$$S = \{ (\mathbf{x}_1, y_1), ..., (\mathbf{x}_N, y_N) \}$$

$$\mathbf{x} = (x_1, ..., x_d)$$

$$x_j, y \in \{0, 1\}$$
 GrowTree(S)

if $(y = 0 \text{ for all } \langle \mathbf{x}, y \rangle \in S)$ return new leaf(0)

else if $(y = 1 \text{ for all } \langle \mathbf{x}, y \rangle \in S)$ return new leaf(1)

else

choose best attribute x_j

 $S_0 = \text{all } \langle \mathbf{x}, y \rangle \in S \text{ with } x_j = 0;$

 $S_1 = \text{all } \langle \mathbf{x}, y \rangle \in S \text{ with } x_i = 1;$

1 (C = ====

DT algs differ on this choice!

- ID3
 - **CAT4.5**
 - CART

return new node(x_j , GROWTREE(S_0), GROWTREE(S_1))

Other issues to address

- Missing attributes
- Attribute values not seen during tree induction (construction)
- Attribute missing in 'test phase'
 - Divide into pieces etc.

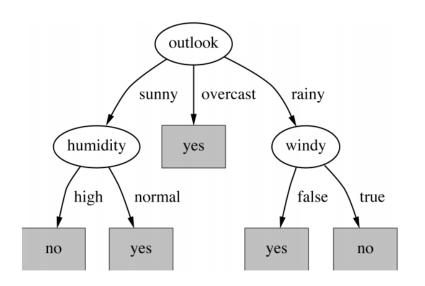
I, Donald J. Trump, am currently inclined to use a position of power to modify the location that is above the country of Mexico and below the country of Canada to be held up to the standards it cemented to be of excellent status, at an earlier point in the country's lifetime.

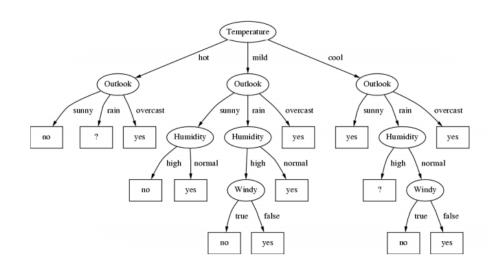






Small is often better





The Smallest Decision Tree

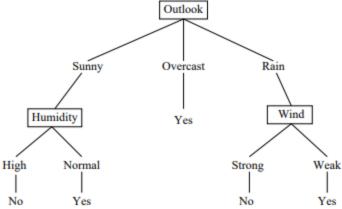
- Learning the smallest DT is NP-hard (Hyafil & Rivest '76)
- Greedy Heuristic
 - Start from empty decision tree
 - Split on next best attribute (feature)
 - Recurse

Overfitting in Decision Trees

Consider adding noisy training example #15:

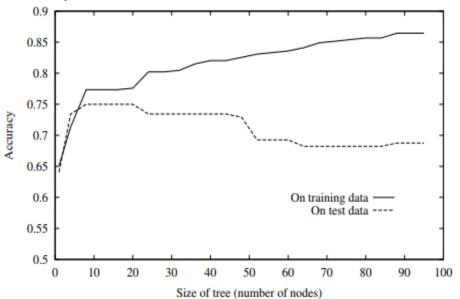
Sunny, Hot, Normal, Strong, PlayTennis = No

What effect on earlier tree?



Overfitting in Decision Trees

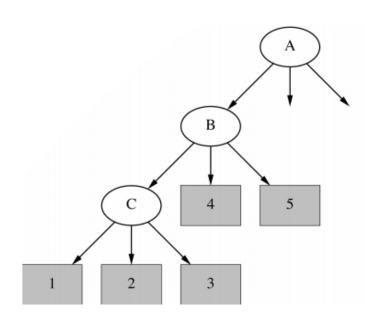
 Overfitting can occur with noisy training examples, and also when small numbers of examples are associated with leaf nodes (→ coincidental or accidental regularities)



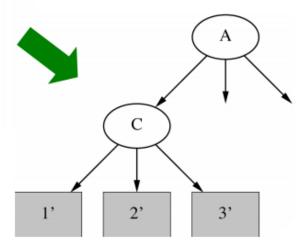
Avoiding overfitting

- Pre-pruning: stop growing tree based on statistical tests of significance
- Post-pruning: Grow full tree, then prune

Post-pruning by subtree raising



- Delete node B
- Redistribute instances of leaves 4 and 5 into C



Decision Trees -> Code

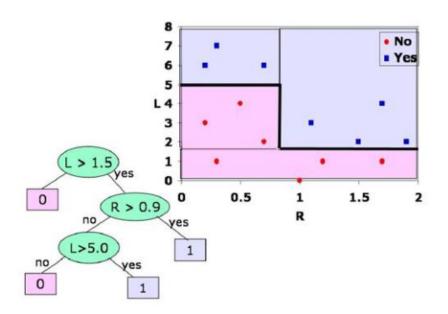
rec	Age	Income	Student	Credit_rating	Buys_computer(CLASS)
r1	<=30	High	No	Fair	No
r2	<=30	High	No	Excellent	No
r3	3140	High	No	Fair	Yes
r4	>40	Medium	No	Fair	Yes
r5	>40	Low	Yes	Fair	Yes
r6	>40	Low	Yes	Excellent	No
r7	3140	Low	Yes	Excellent	Yes
r8	<=30	Medium	No	Fair	No
r9	<=30	Low	Yes	Fair	Yes
r10	>40	Medium	Yes	Fair	Yes
r11	<=30	Medium	Yes	Excellent	Yes
r12	3140	Medium	No	Excellent	Yes
r13	3140	High	Yes	Fair	Yes
r14	>40	Medium	No	Excellent	No

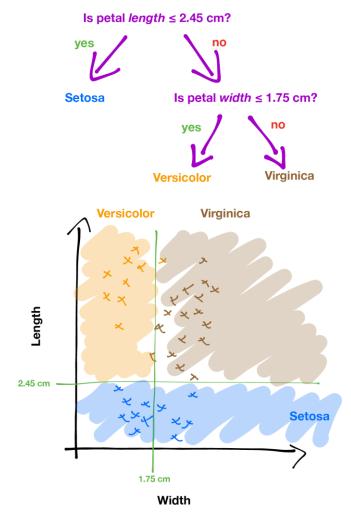
```
IF age = "<=30" AND student = "no" THEN
 buys computer = "no"
IF age = "<=30" AND student = "yes" THEN
 buys computer = "yes"
IF age = "31...40"
                                    THEN
  buys computer = "yes"
IF age = ">40" AND credit rating = "excellent"
 buys computer = "no"
IF age = ">40" AND credit_rating = "fair" THEN
  buys computer = "yes"
```

Attributes with Differing Costs

- Measuring attribute costs something
 - prefer cheap ones if possible
 - use costly ones only if good gain
- Introduce cost term in selection measure
 - no guarantee in finding optimum, but give bias towards cheapest
- Example applications
 - robot & sonar: time required to position
 - medical diagnosis: cost of a laboratory test

Decision Boundaries





Decision trees for classification

Some real examples (from Russell & Norvig, Mitchell)

- BP's GasOIL system for separating gas and oil on offshore platforms - decision trees replaced a hand-designed rules system with 2500 rules. C4.5-based system outperformed human experts and saved BP millions. (1986)
- learning to fly a Cessna on a flight simulator by watching human experts fly the simulator (1992)
- can also learn to play tennis, analyze C-section risk, etc.

Advantages of DT

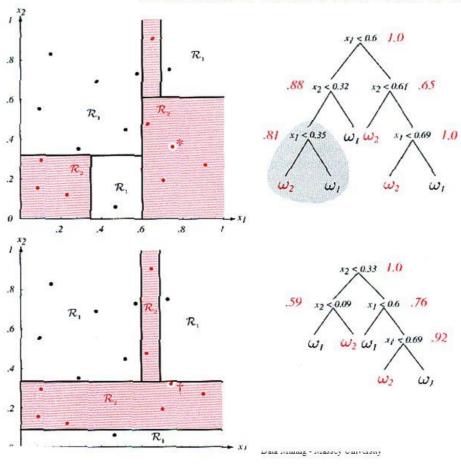
- Easy to use, understand
- Produce rules that are easy to interpret & implement
- Variable selection & reduction is automatic
- Do not require the assumptions of statistical models
- Can work without extensive handling of missing data

Disadvantages

 May not perform well where there is structure in the data that is not well captured by horizontal or vertical splits

 Since the process deals with one variable at a time, no way to capture interactions between variables

Decision Trees are not stable



Moving just one example slightly may lead to quite different trees and space partition!

Lack of stability against small perturbation of data.

Figure from Duda, Hart & Stork, Chap. 8

References and Reading

- https://en.wikipedia.org/wiki/Decision tree learning
- Cool demo: http://www.r2d3.us/visual-intro-to-machine-learning-part-1/
- Entropy in decision trees: https://bricaud.github.io/personal-blog/entropy-in-decision-trees/

- Textbook References
 - [TM] Machine Learning by Tom Mitchell (3.1 3.5, 3.7 3.8)
 - [PRML] Pattern Recognition and Machine Learning by Chris Bishop (1.2 (intro), 1.6)
 - [DHS] Duda and Hart (8.1 8.4)
- Code
 - https://scikit-learn.org/stable/modules/tree.html
 - https://scikit-learn.org/stable/auto_examples/tree/plot_unveil_tree_structure.html