Statistical Methods in AI (CS7.403)

Lecture-5: Decision Tree Learning

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https://ravika.github.io

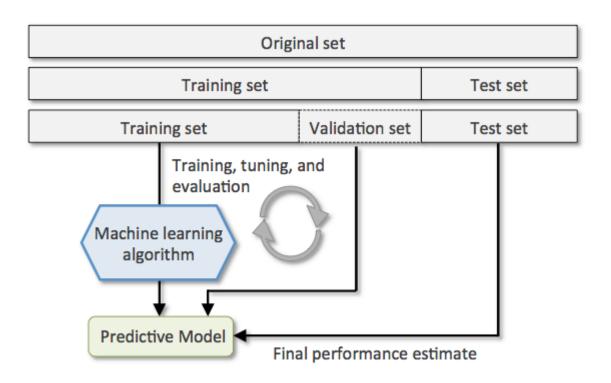




Center for Visual Information Technology (CVIT)

IIIT Hyderabad

The Train-Validation-Test paradigm



Supervised Learning

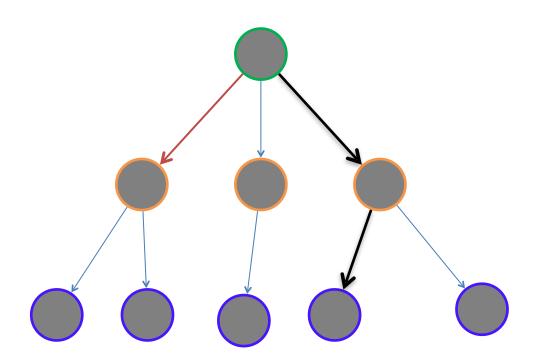
Classification

Regression

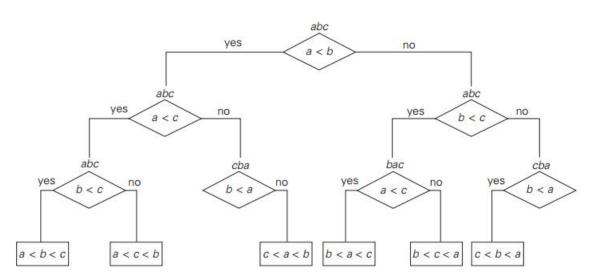
Reinforcement Learning

Trees

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



if/then if/else/then

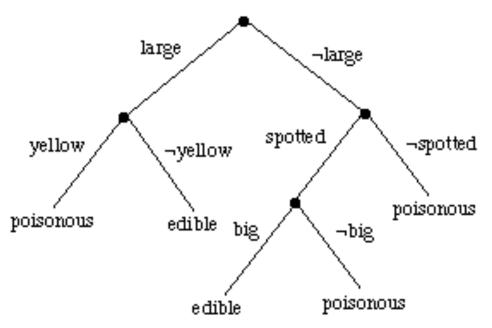




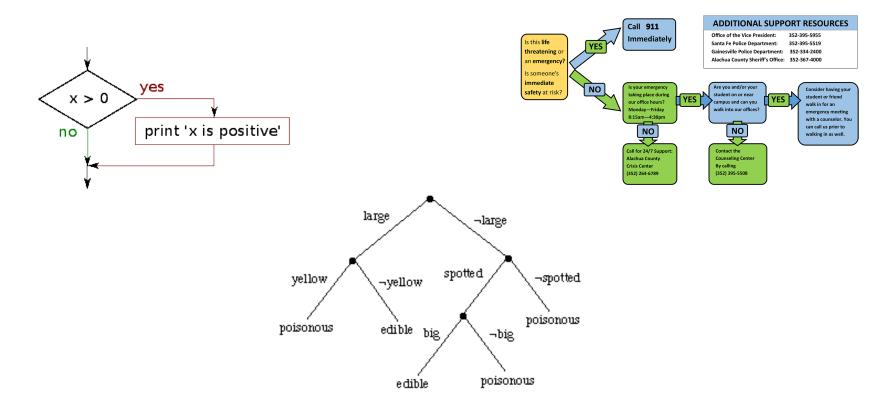
Emergency Response



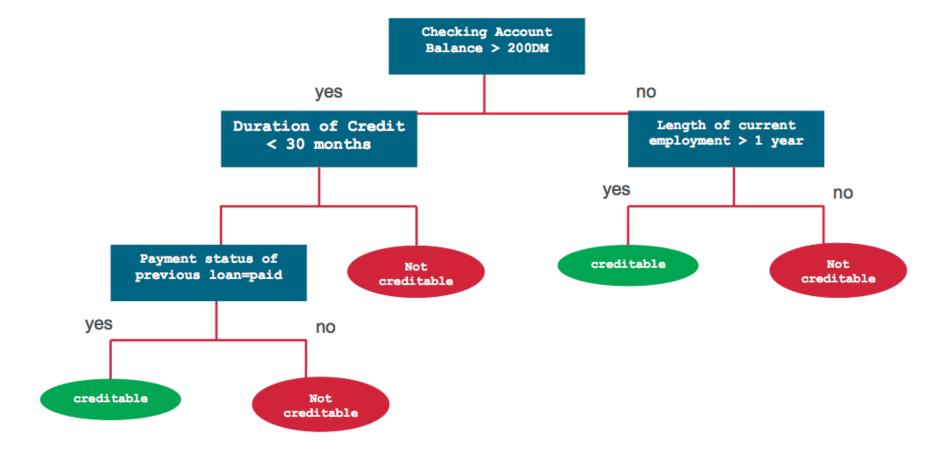
Edible Mushroom



Hand-crafted, fixed trees



Credit Approval



Credit Approval (Raw Data)

| | | _ | | _ | _ | _ | _ | | | | | | | | | |
|----|----|-------|--------|----|----|----|----|-------|----|-----|-----|-----|-----|-----|-------|-------|
| 4 | Α | В | С | D | E | F | G | Н | | J | K | L | М | N | 0 | Р |
| 64 | A1 | A2 | A3 | A4 | A5 | A6 | Α7 | 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 | b | 26.67 | 4.25 | u | g | cc | V | 4.29 | t | t | 1 | t | g | 120 | 0 | + |
| 67 | b | 34.17 | 1.54 | u | g | cc | 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 | b | 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 | b | 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 | a | 38.58 | 5 | u | g | CC | 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 | р | 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

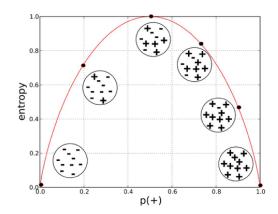
temp

outlook

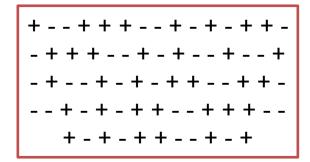
windy

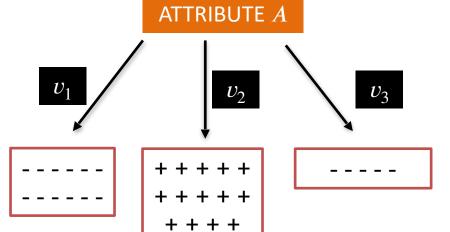
play

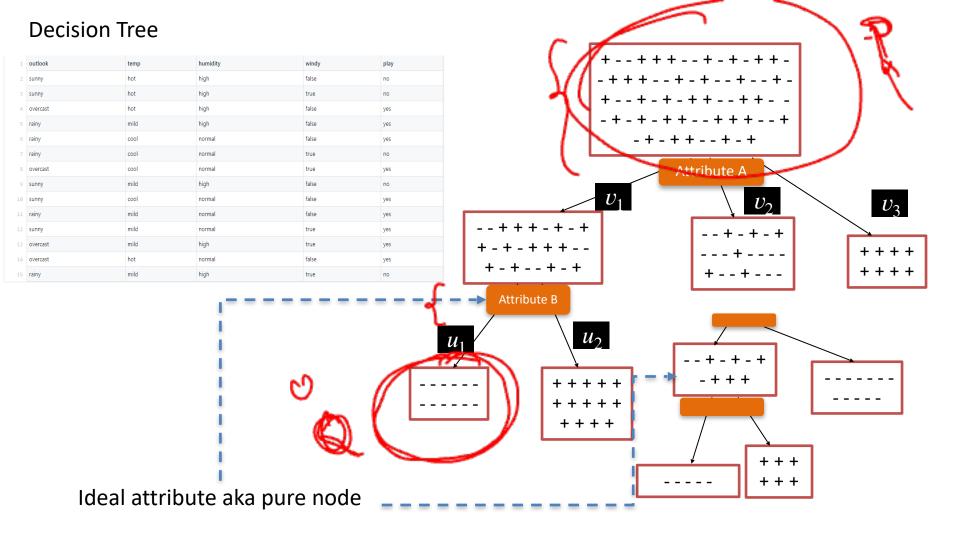
| 1 | outlook | temp | humidity | windy | play |
|----|----------|------|----------|-------|------|
| 2 | sunny | hot | high | false | no |
| 3 | sunny | hot | high | true | no |
| 4 | overcast | hot | high | false | yes |
| 5 | rainy | mild | high | false | yes |
| 6 | rainy | cool | normal | false | 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 |



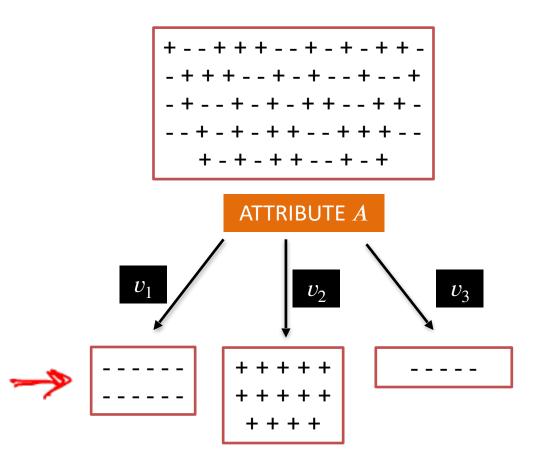
An ideal attribute



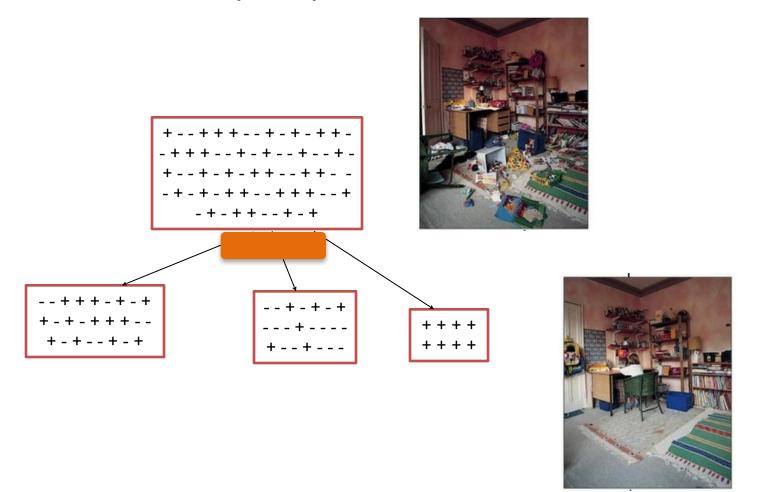


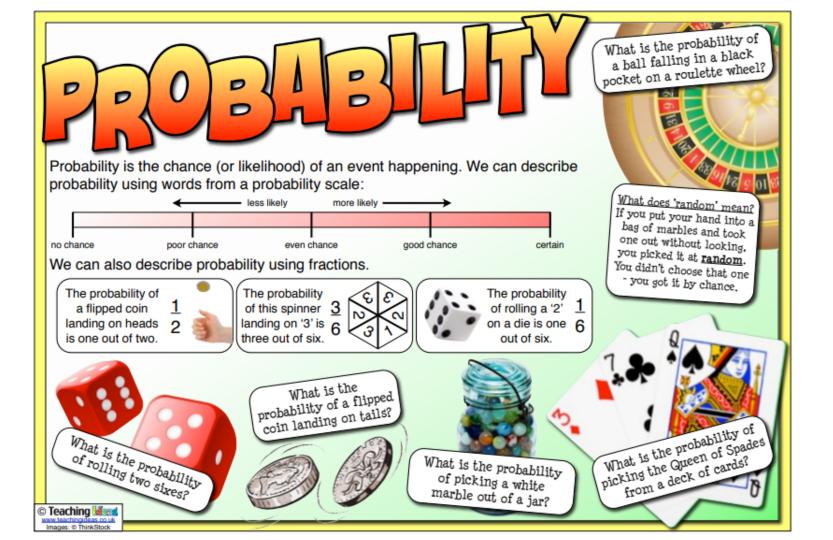


How much 'impurity' does this attribute decrease?



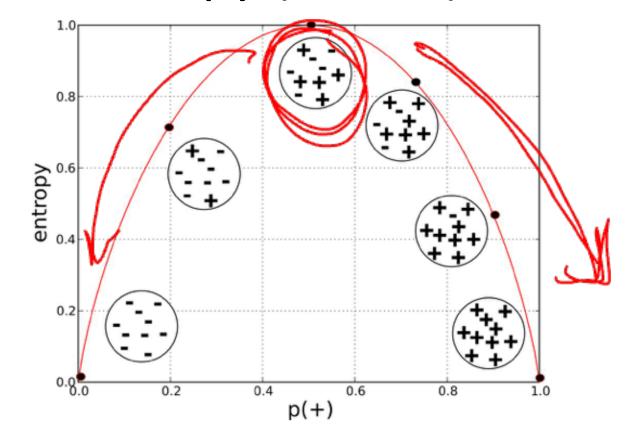
How much 'impurity' does this attribute decrease?





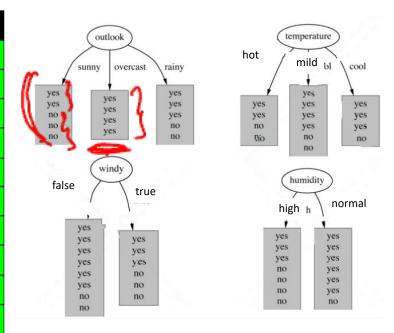
Information and Entropy

Entropy (2 class)



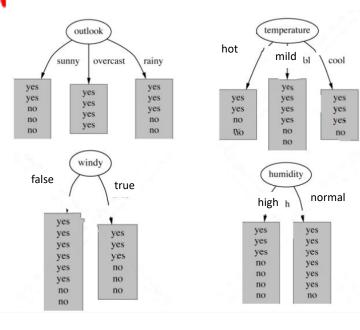
Example

| 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 |
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| 07-15 | mild | rain | normal | false | yes |
| 07-20 | mild | sunny | normal | true | yes |
| 07-21 | mild | overcast | high | 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:
$$i(V) = -(q \log q + (1 - q) \log(1 - q))$$

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

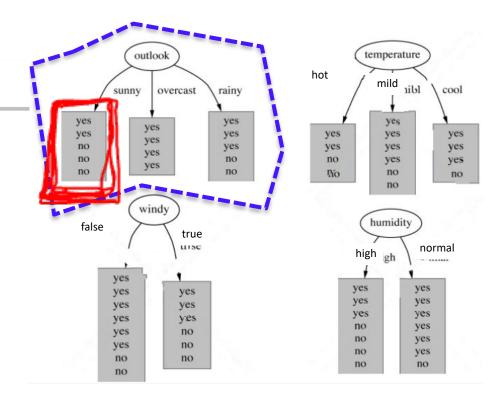
Step-2: Compute impurity score for each unique value of candidate attributes

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

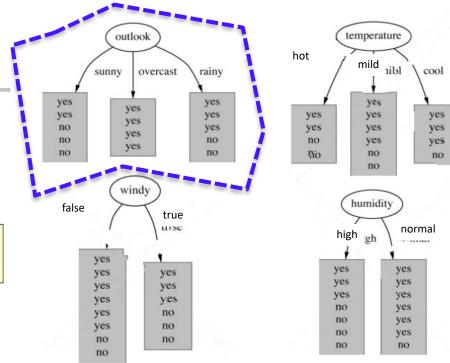
Entropy:
$$i(V) = -(q \log q + (1 - q) \log(1 - q))$$

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

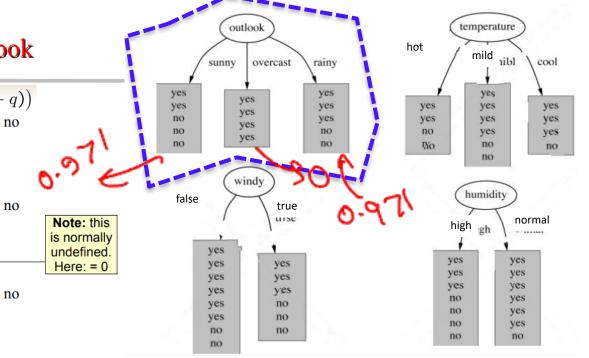
$$E(\text{Outlook} = \text{sunny}) = -\frac{2}{5} \log \left(\frac{2}{5} \right) - \frac{3}{5} \log \left(\frac{3}{5} \right) = 0.971$$

Outlook = overcast: 4 examples yes, 0 examples no

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

Outlook = sunny 2 examples yes, 3 examples no

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



Step-3: Compute impurity score for candidate attribute

Note: this

is normally

undefined.

Here: = 0

Outlook = rainy
 3 examples yes, 2 examples no

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

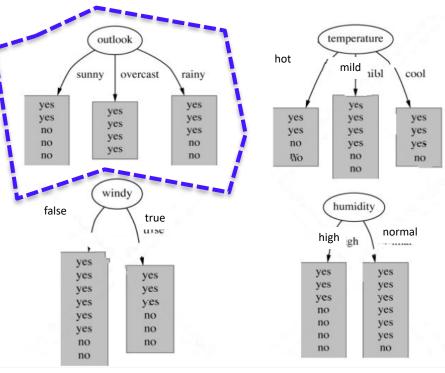
• Outlook = overcast: 4 examples yes, 0 examples no

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

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



Step-3: Compute impurity score for candidate attribute

Note: this

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• 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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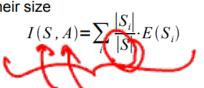
Outlook = sunny 2 examples yes, 3 examples no

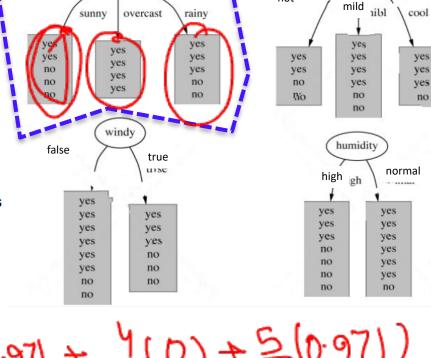
$$E(\text{Outlook} = \text{rainy}) = -\frac{3}{5} \log \left(\frac{3}{5} \right) - \frac{2}{5} \log \left(\frac{2}{5} \right) = 0.971$$

- 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





temperature

hot

outlook

Step-3: Compute impurity score for candidate attribute

Note: this

is normally

undefined.

Here: = 0



3 examples yes, 2 examples no Outlook = rainy

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

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

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

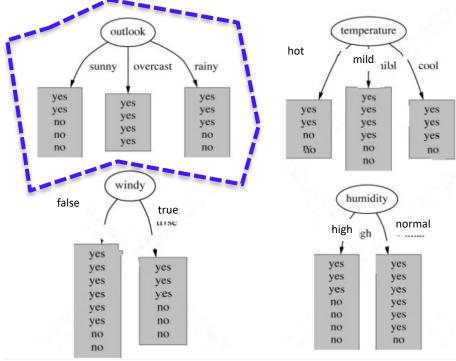
Outlook = sunny 2 examples yes, 3 examples no

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

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

Average entropy for attribute *Outlook*:

e entropy for attribute
$$Outlook$$
:
$$I(Outlook) = \frac{5}{14} \cdot 0.971 + \frac{4}{14} \cdot 0 + \frac{5}{14} \cdot 0.971 = 0.693$$



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

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

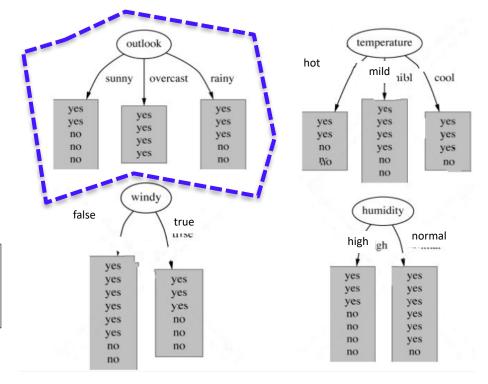
Average entropy for attribute *Outlook*:

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

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

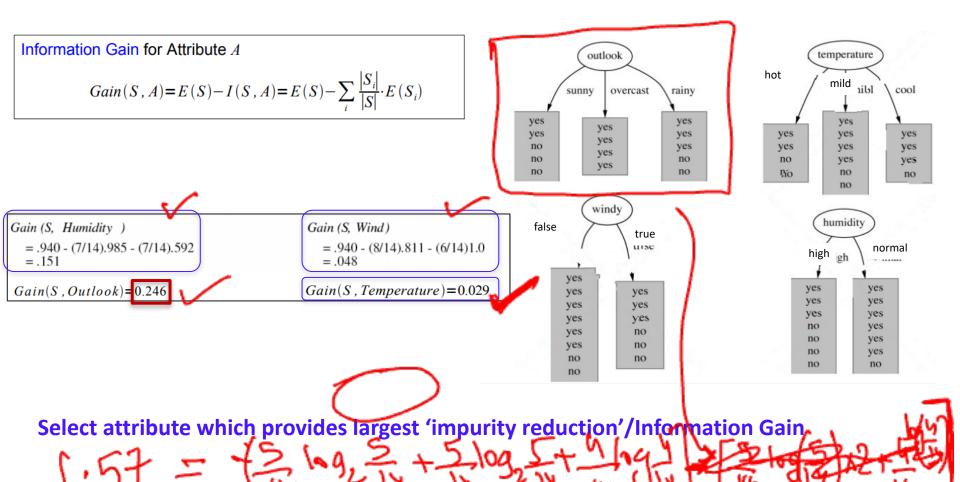
Information Gain for Attribute A

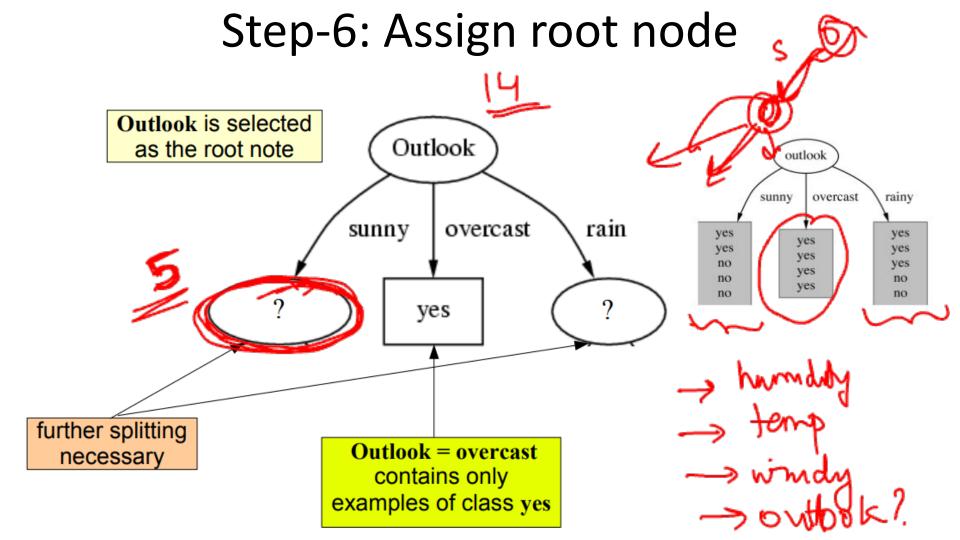
$$Gain(S, A) = E(S) - I(S, A) = E(S) - \sum_{i} \frac{|S_{i}|}{|S|} \cdot E(S_{i})$$



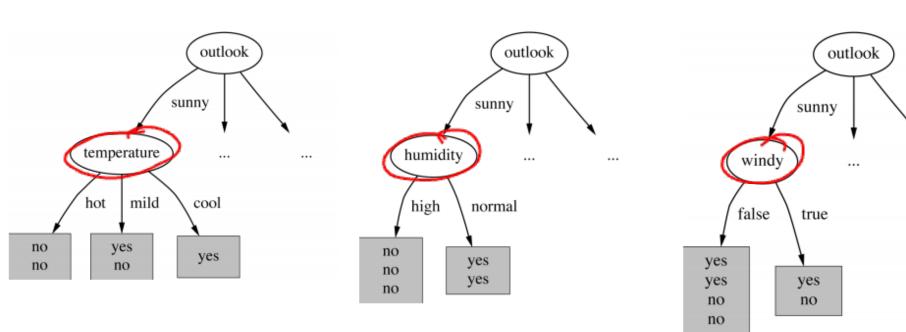
Gain(S, Outlook) = 0.246

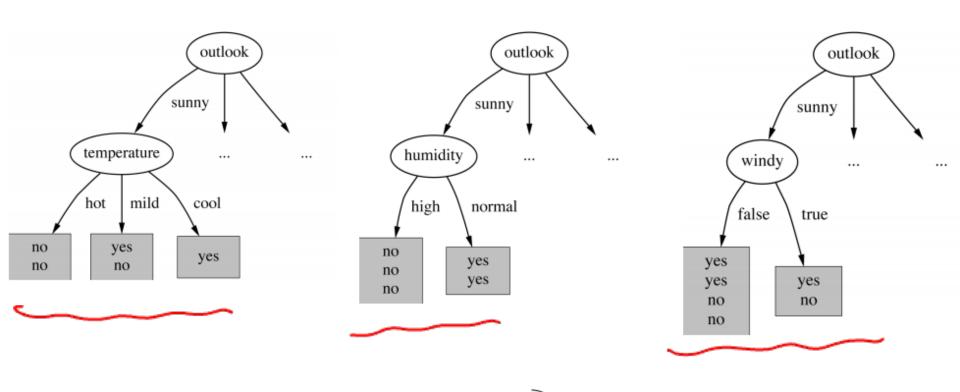
Step-5: Compare Information Gain provided by all candidates





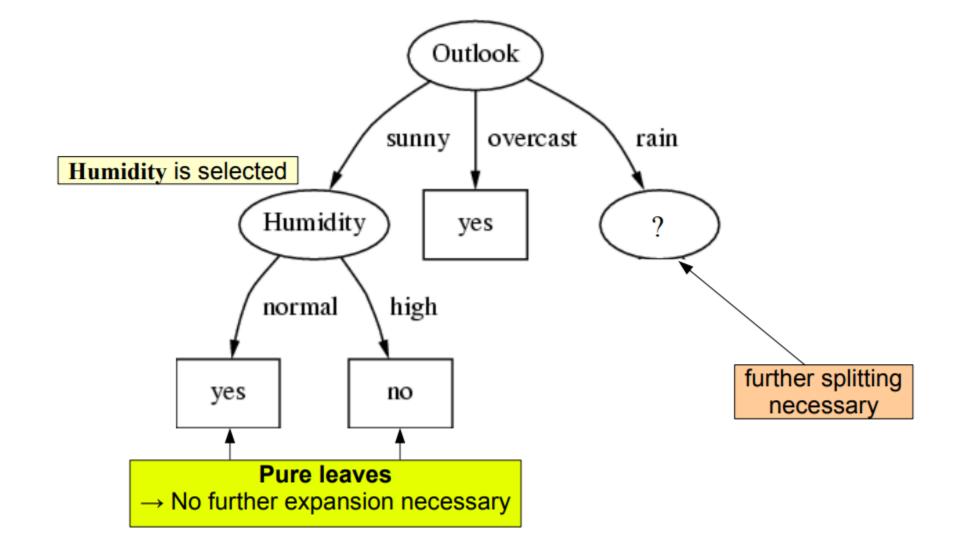
Recurse and repeat Steps 1-6





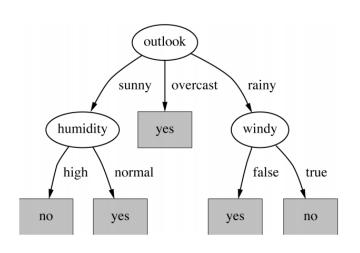
Gain(Temperature) = 0.571 bits Gain(Humidity) = 0.971 bits Gain(Windy) = 0.020 bits

Humidity is selected



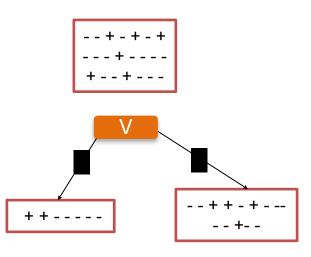
Final Decision Tree

| 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 |



Properties of an impurity measure

- Class labels: Binary {\frac{1}{7},-1}
- C



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

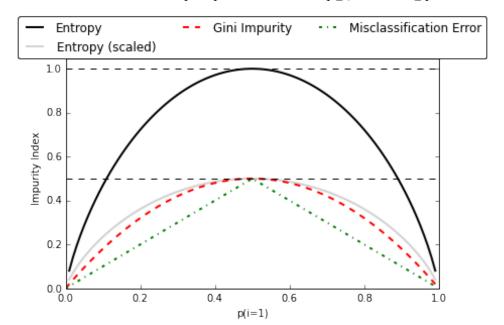
- $f(V) \geq 0$ with i(V) = 0 iff V consists of a single class
- a larger value of i(V) indicates that the distribution defined by (q,(1-q)) is closer to the uniform distribution

Impurity function: candidates

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

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

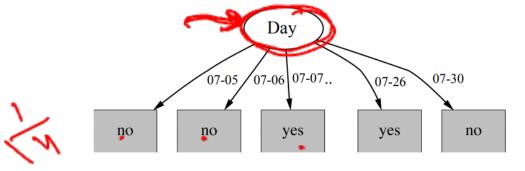
Misclassification rate: $i(V) = \min(q, 1 - q)$



- 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



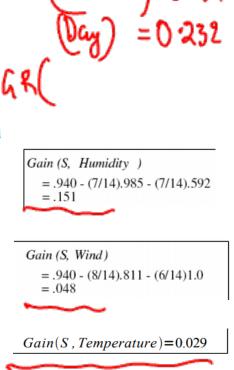
- Problematic: attributes with a large number of values
 - extreme case: each example has its own value
 - e.g. example ID; Day attribute in weather data
 - Subsets are more likely to be pure if there is a large number of ζ
 - Information gain is biased towards choosing attributes with a large number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

Intrinsic information of Day attribute:

$$\frac{3}{2} \log \frac{1}{2} + \frac{4}{3} \log \frac{10}{10} = 14 \times \left(-\frac{1}{14} \cdot \log\left(\frac{1}{14}\right)\right) = 3.807$$

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

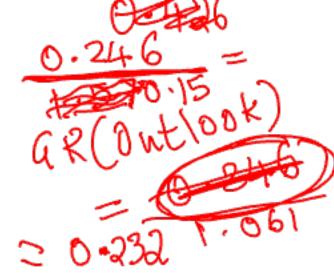
Gain Ratio

- 0.246 = 0.157
- 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 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

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

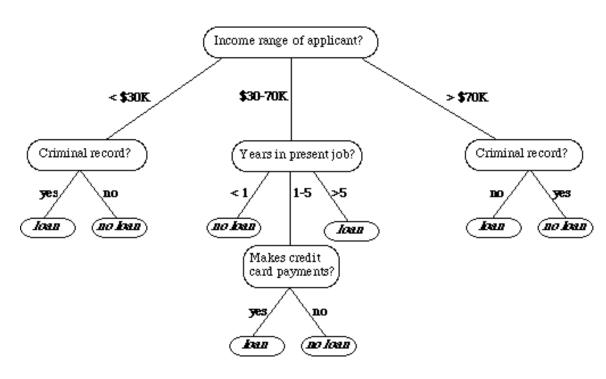
Split points can be placed between values or directly at values

Handling numerical attributes

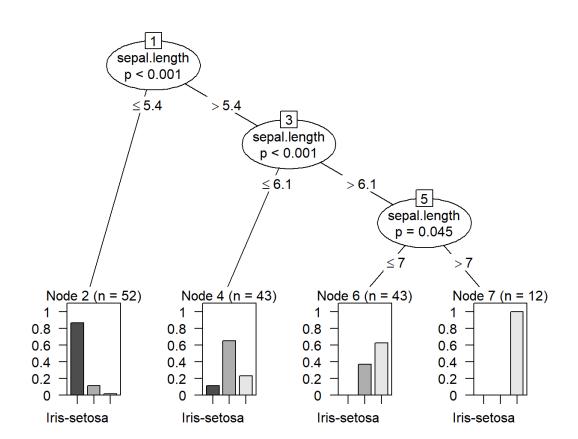
- Splitting (multi-way) on a nominal attribute exhausts all information in that attribute
 - Nominal attribute is tested (at most) once on any path in the tree
- Not so for binary splits on numerical attributes (why?)
- Attribute may be tested multiple times in the tree
- Tree may become hard to read

Handling numerical attributes

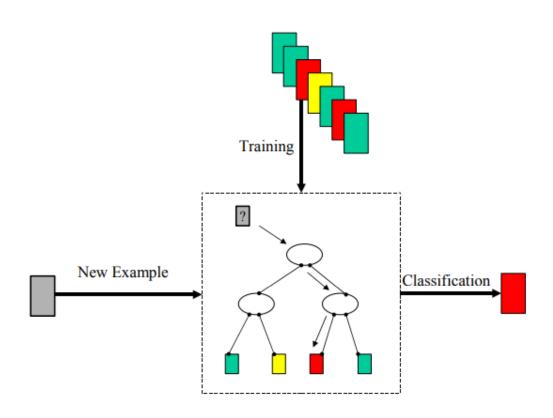
Discretization / Clustering



Decision Tree with numerical attribute



Deployment



Learning Algorithm for Decision Trees

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

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

$$x_j, y \in \{0, 1\}$$

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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_i

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

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

DT algs differ on this choice!

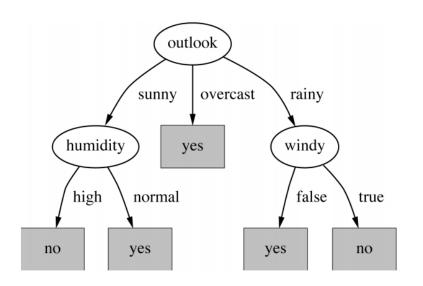
- ID3
 - **CAT4.5**
 - **CART**

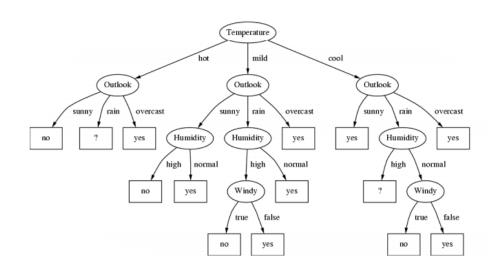
return new node(x_i , GROWTREE(S_0), GROWTREE(S_1))

Other issues to address

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

Small is often better





The Smallest Decision Tree

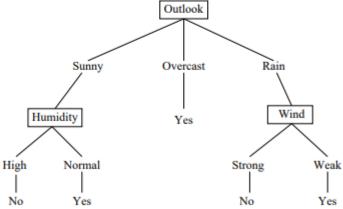
- Learning the smallest DT is NP-hard (Hyafil & Rivest '76)
- Greedy Heuristic
 - Start from empty decision tree
 - Split on next best attribute (feature)
 - Recurse

Overfitting in Decision Trees

Consider adding noisy training example #15:

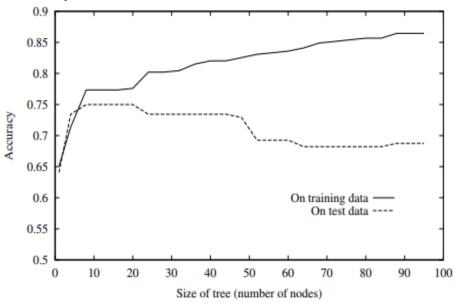
Sunny, Hot, Normal, Strong, PlayTennis = No

What effect on earlier tree?



Overfitting in Decision Trees

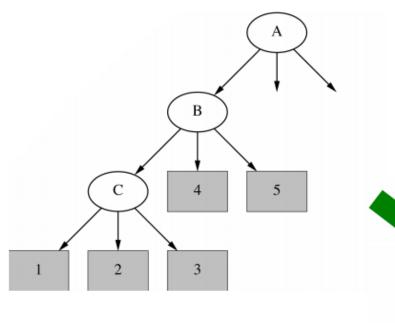
 Overfitting can occur with noisy training examples, and also when small numbers of examples are associated with leaf nodes (→ coincidental or accidental regularities)



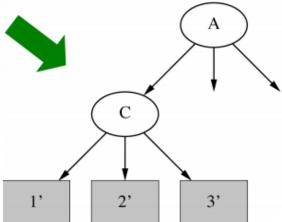
Avoiding overfitting

- 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

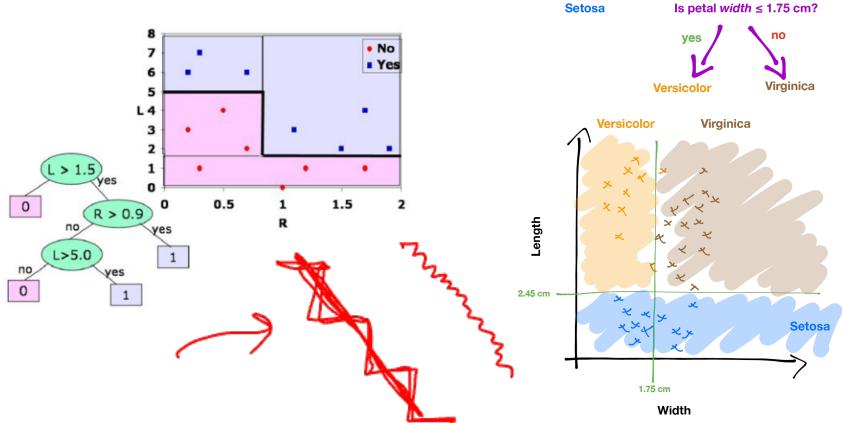


Decision Trees -> Code

| 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"
```

Decision Boundaries



Is petal length ≤ 2.45 cm?

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.

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

Advantages of DT

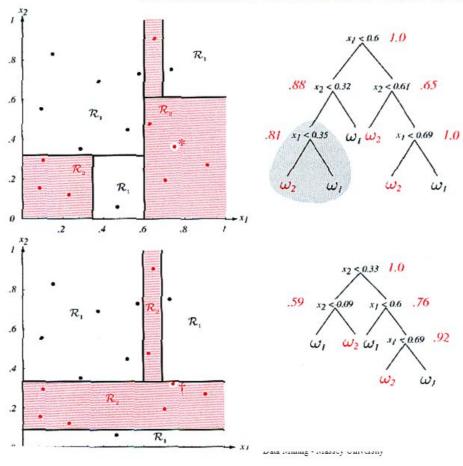
- Easy to use, understand
- Produce rules that are easy to interpret & implement
- Variable selection & reduction is automatic
- Do not require the assumptions of statistical models
- Can work without extensive handling of missing data

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/
- Entropy: https://towardsdatascience.com/entropy-how-decision-trees-make-decisions-2946b9c18c8
- Entropy: https://plus.maths.org/content/information-surprise

- 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