Decision Trees

~Abhishek Kumar

Decision Tree

- Supervised
- Classification algorithm

Predict if John will play tennis

Training examples: **9 yes / 5 no**

Day	Outlook	Humidity	Wind	Play
D1	Sunny	High	Weak	No
D2	Sunny	High	Strong	No
D3	Overcast	High	Weak	Yes
D4	Rain	High	Weak	Yes
D5	Rain	Normal	Weak	Yes
D6	Rain	Normal	Strong	No
D7	Overcast	Normal	Strong	Yes
D8	Sunny	High	Weak	No
D9	Sunny	Normal	Weak	Yes
D10	Rain	Normal	Weak	Yes
D11	Sunny	Normal	Strong	Yes
D12	Overcast	High	Strong	Yes
D13	Overcast	Normal	Weak	Yes
D14	Rain	High	Strong	No

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New data:

Day	Outlook	Humidity	Wind	Play
D15	Rain	High	Weak	?

Predict if John will play tennis

- Hard to guess
- Try to *understand* when John plays

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Predict if John will play tennis

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- Divide & conquer:
  - split into subsets
  - are they pure? (all yes or all no)
  - if yes: stop
  - if not: repeat

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D7	Overcast	Normal	Strong	Yes
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D15	Rain	High	Weak	?

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D7	Overcast	Normal	Strong	Yes
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D11	Sunny	Normal	Strong	Yes
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D13	Overcast	Normal	Weak	Yes
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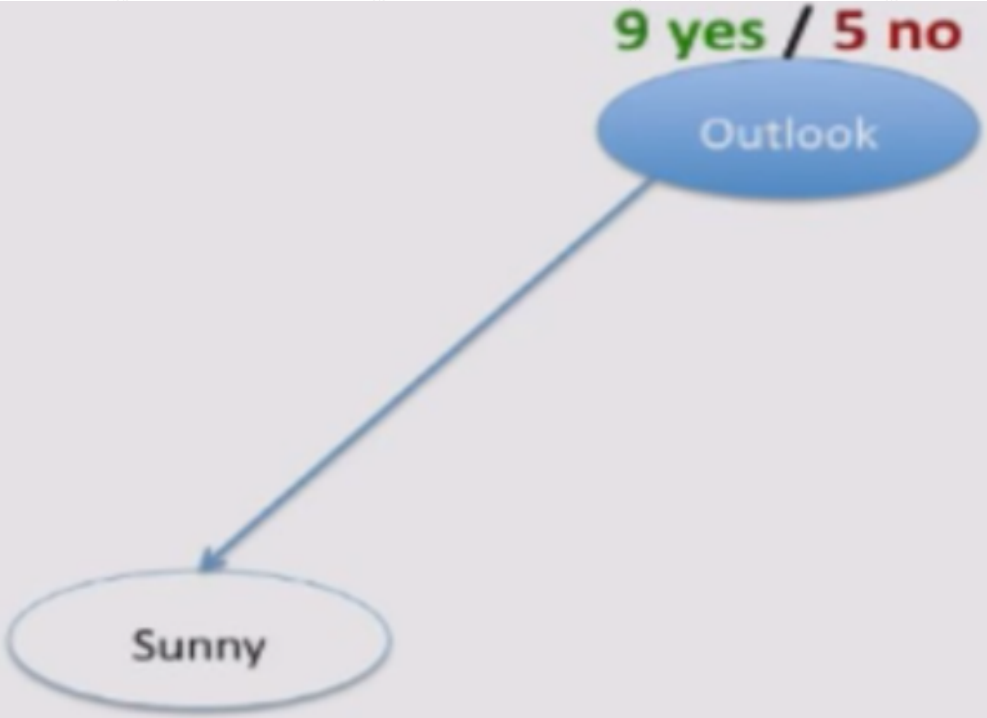
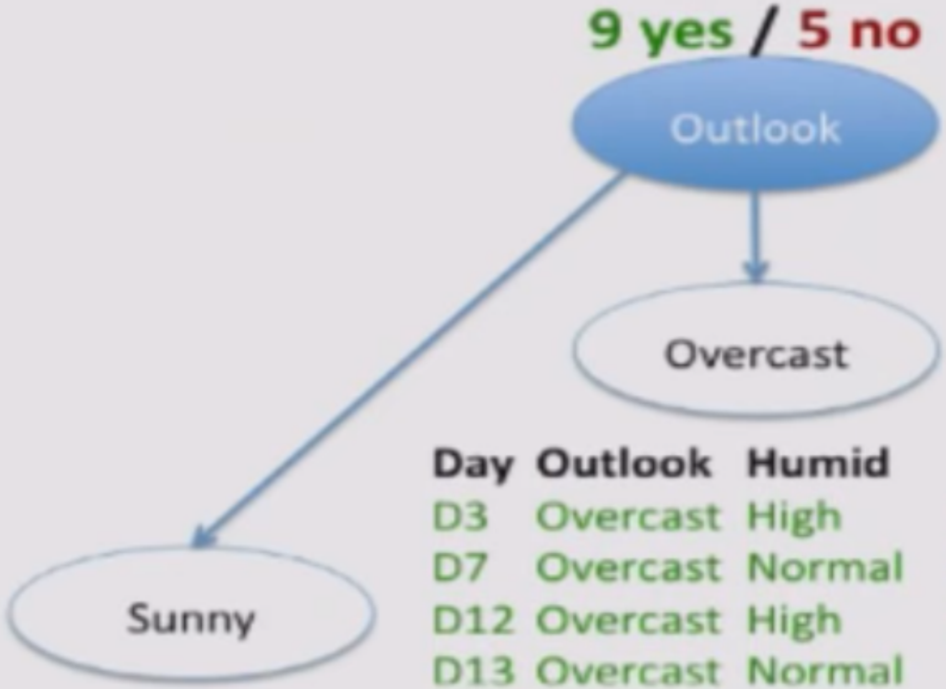
New data:

Day	Outlook	Humidity	Wind	Play
D15	Rain	High	Weak	?

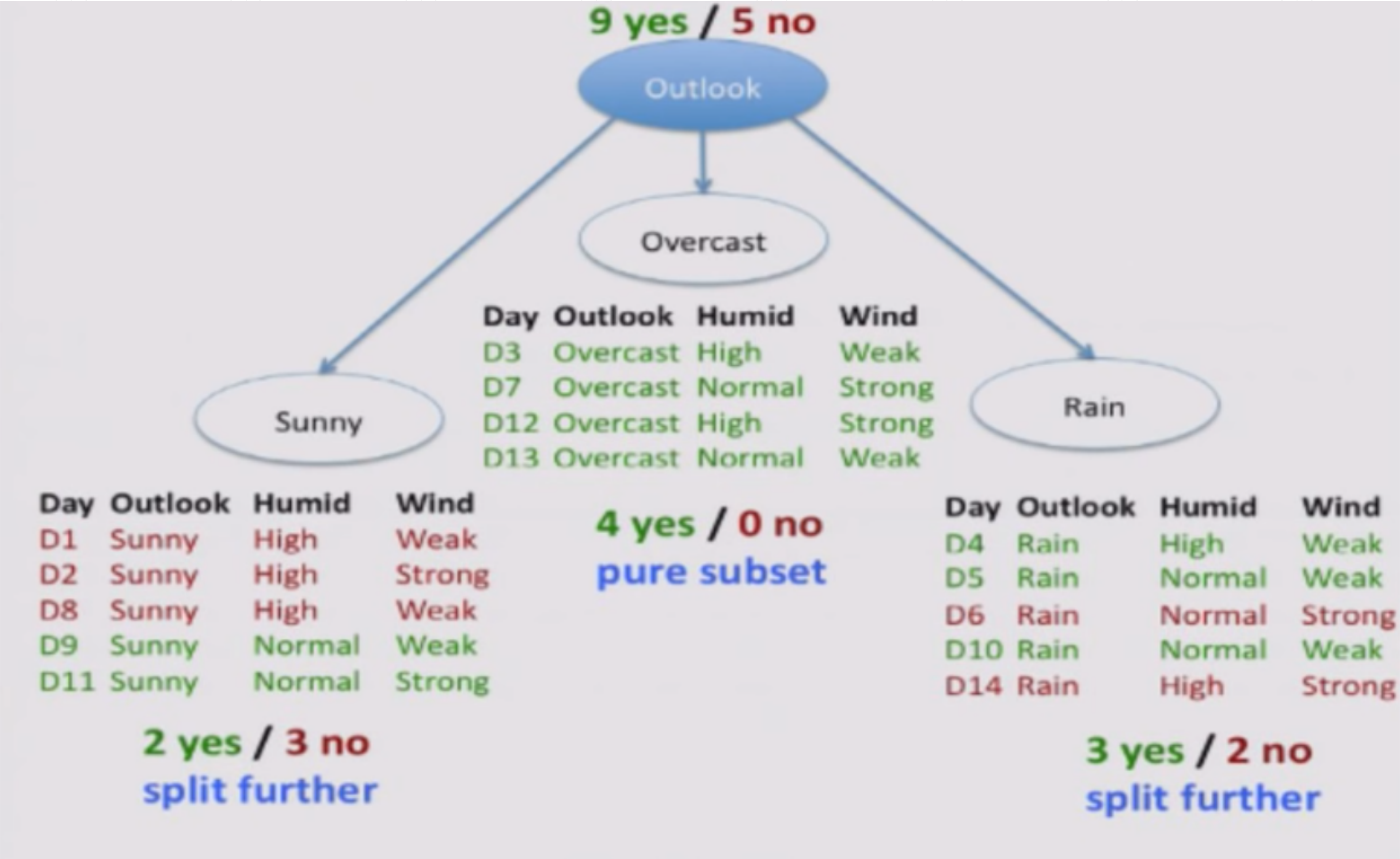


Day	Outlook	Humid	Wind
D1	Sunny	High	Weak
D2	Sunny	High	Strong
D8	Sunny	High	Weak
D9	Sunny	Normal	Weak
D11	Sunny	Normal	Strong



Day	Outlook	Humid	Wind
D3	Overcast	High	Weak
D7	Overcast	Normal	Strong
D12	Overcast	High	Strong
D13	Overcast	Normal	Weak

Day	Outlook	Humid	Wind
D1	Sunny	High	Weak
D2	Sunny	High	Strong
D8	Sunny	High	Weak
D9	Sunny	Normal	Weak
D11	Sunny	Normal	Strong



9 yes / 5 no
Outlook
Overcast
Sunny
Rain

Day	Outlook	Humid	Wind
D3	Overcast	High	Weak
D7	Overcast	Normal	Strong
D12	Overcast	High	Strong
D13	Overcast	Normal	Weak

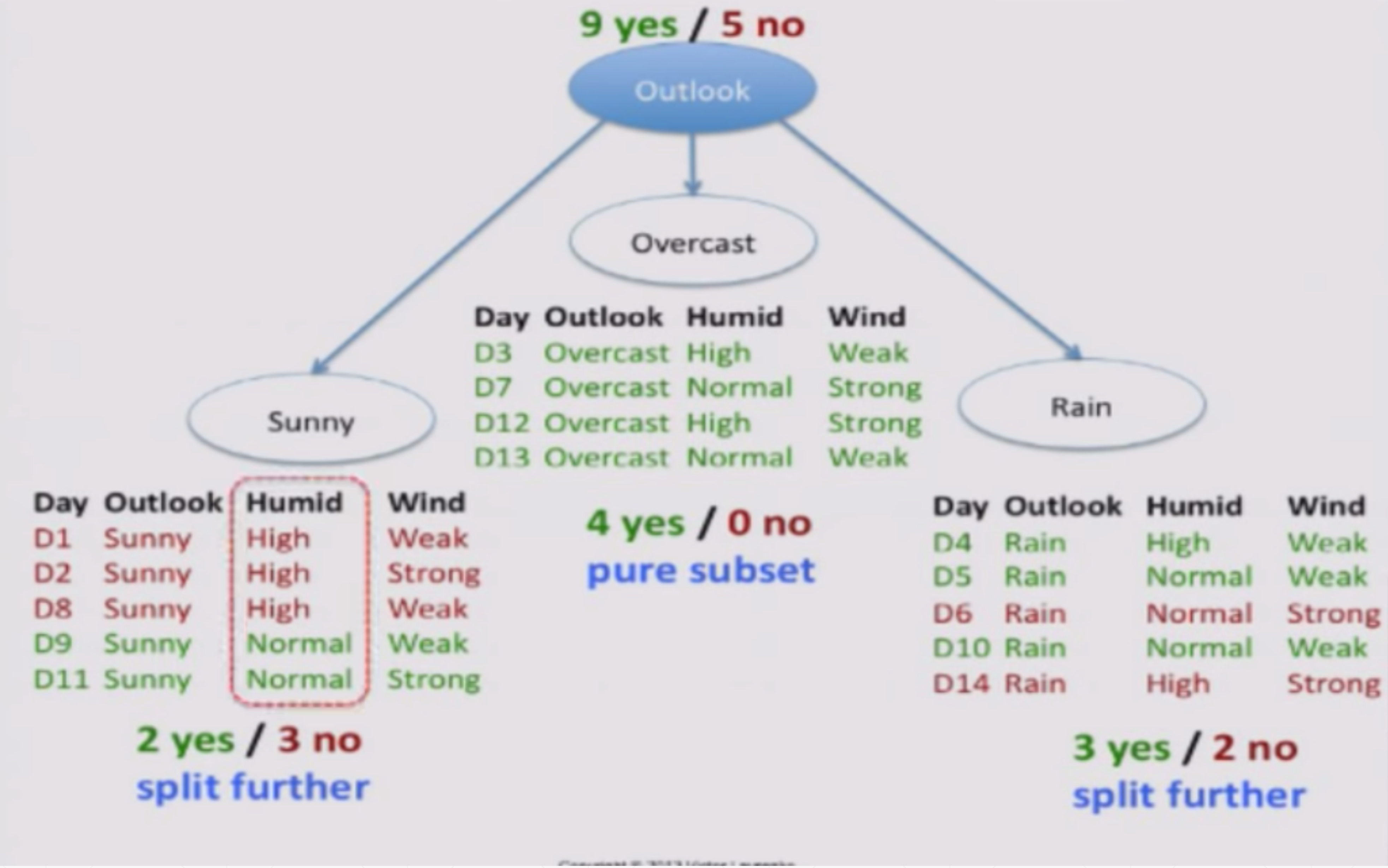
4 yes / 0 no
pure subset

Day	Outlook	Humid	Wind
D1	Sunny	High	Weak
D2	Sunny	High	Strong
D8	Sunny	High	Weak
D9	Sunny	Normal	Weak
D11	Sunny	Normal	Strong

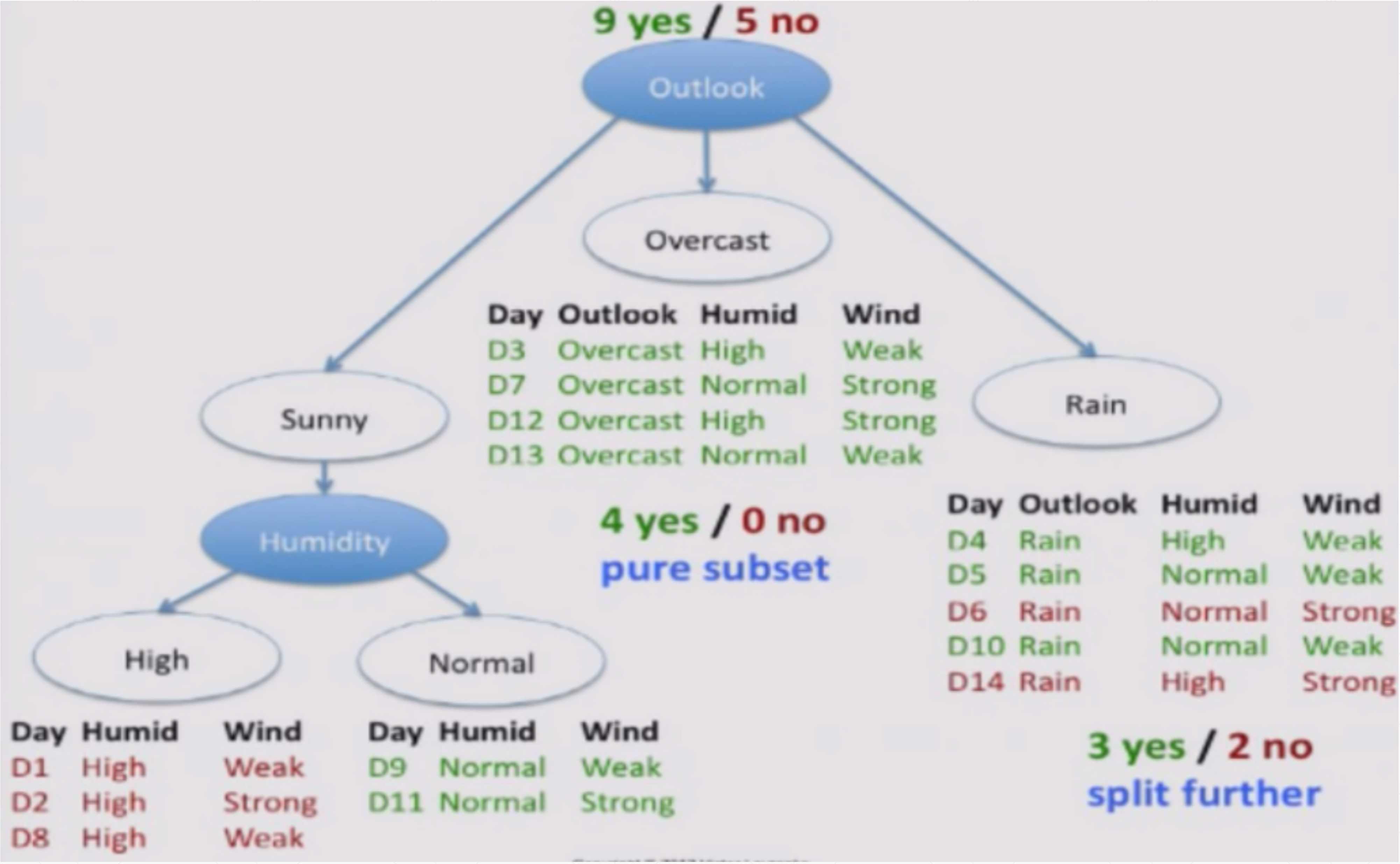
2 yes / 3 no
split further

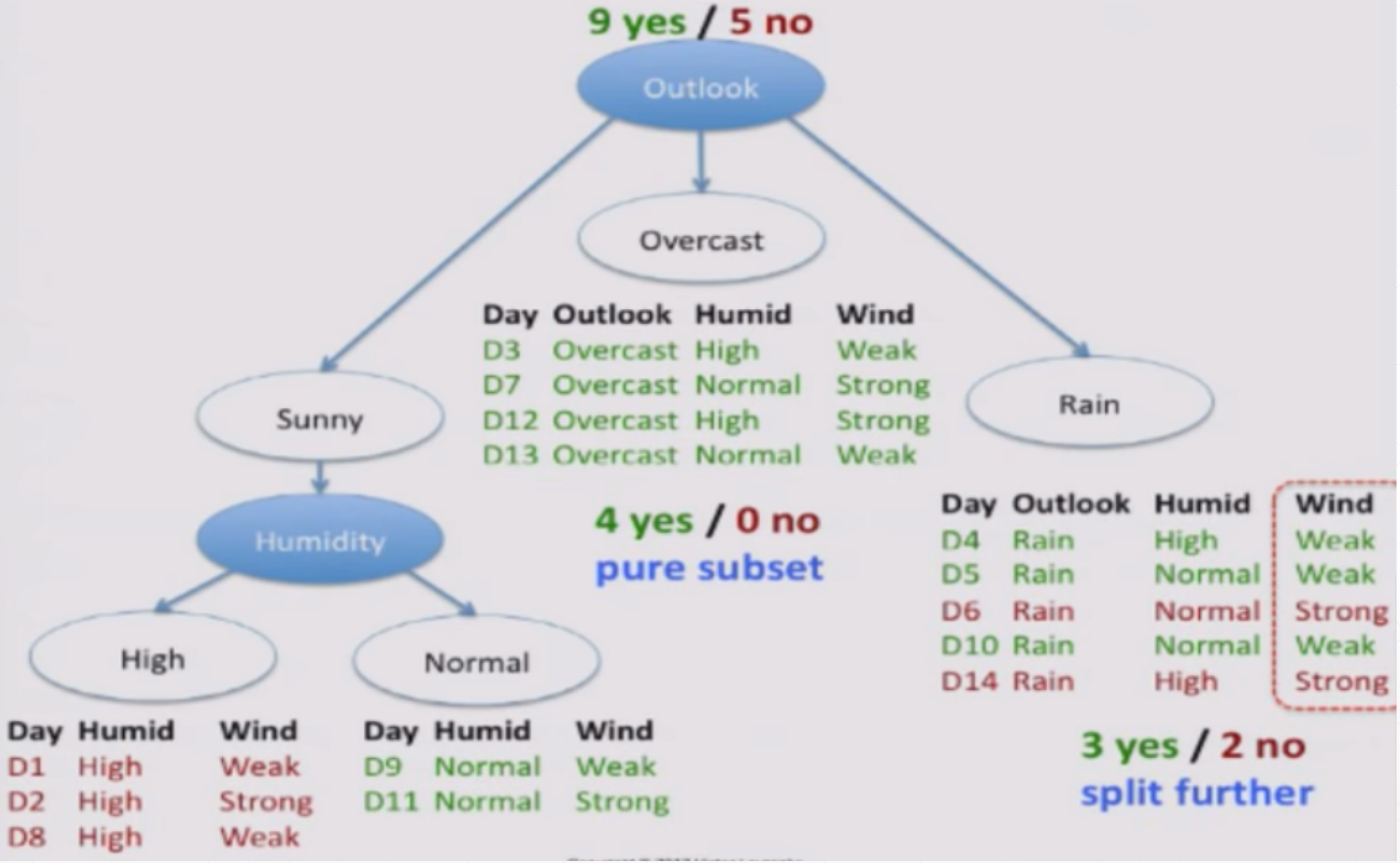
Day	Outlook	Humid	Wind
D4	Rain	High	Weak
D5	Rain	Normal	Weak
D6	Rain	Normal	Strong
D10	Rain	Normal	Weak
D14	Rain	High	Strong

3 yes / 2 no
split further



9 yes / 5 no
Outlook
Overcast
Sunny
Rain
Day Outlook Humid Wind
D3 Overcast High Weak
D7 Overcast Normal Strong
D12 Overcast High Strong
D13 Overcast Normal Weak
4 yes / 0 no
pure subset
Day Outlook Humid Wind
D1 Sunny High Weak
D2 Sunny High Strong
D8 Sunny High Weak
D9 Sunny Normal Weak
D11 Sunny Normal Strong
2 yes / 3 no
split further
Day Outlook Humid Wind
D4 Rain High Weak
D5 Rain Normal Weak
D6 Rain Normal Strong
D10 Rain Normal Weak
D14 Rain High Strong
3 yes / 2 no
split further


9 yes / 5 no
Outlook
Overcast
Day Outlook Humid Wind
D3 Overcast High Weak
D7 Overcast Normal Strong
D12 Overcast High Strong
D13 Overcast Normal Weak
4 yes / 0 no
pure subset
Rain
Day Outlook Humid Wind
D4 Rain High Weak
D5 Rain Normal Weak
D6 Rain Normal Strong
D10 Rain Normal Weak
D14 Rain High Strong
3 yes / 2 no
split further
Sunny
Humidity
High
Day Humid Wind
D1 High Weak
D2 High Strong
D8 High Weak
Normal
Day Humid Wind
D9 Normal Weak
D11 Normal Strong


9 yes / 5 no
Outlook
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D3 Overcast High Weak
D7 Overcast Normal Strong
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Sunny
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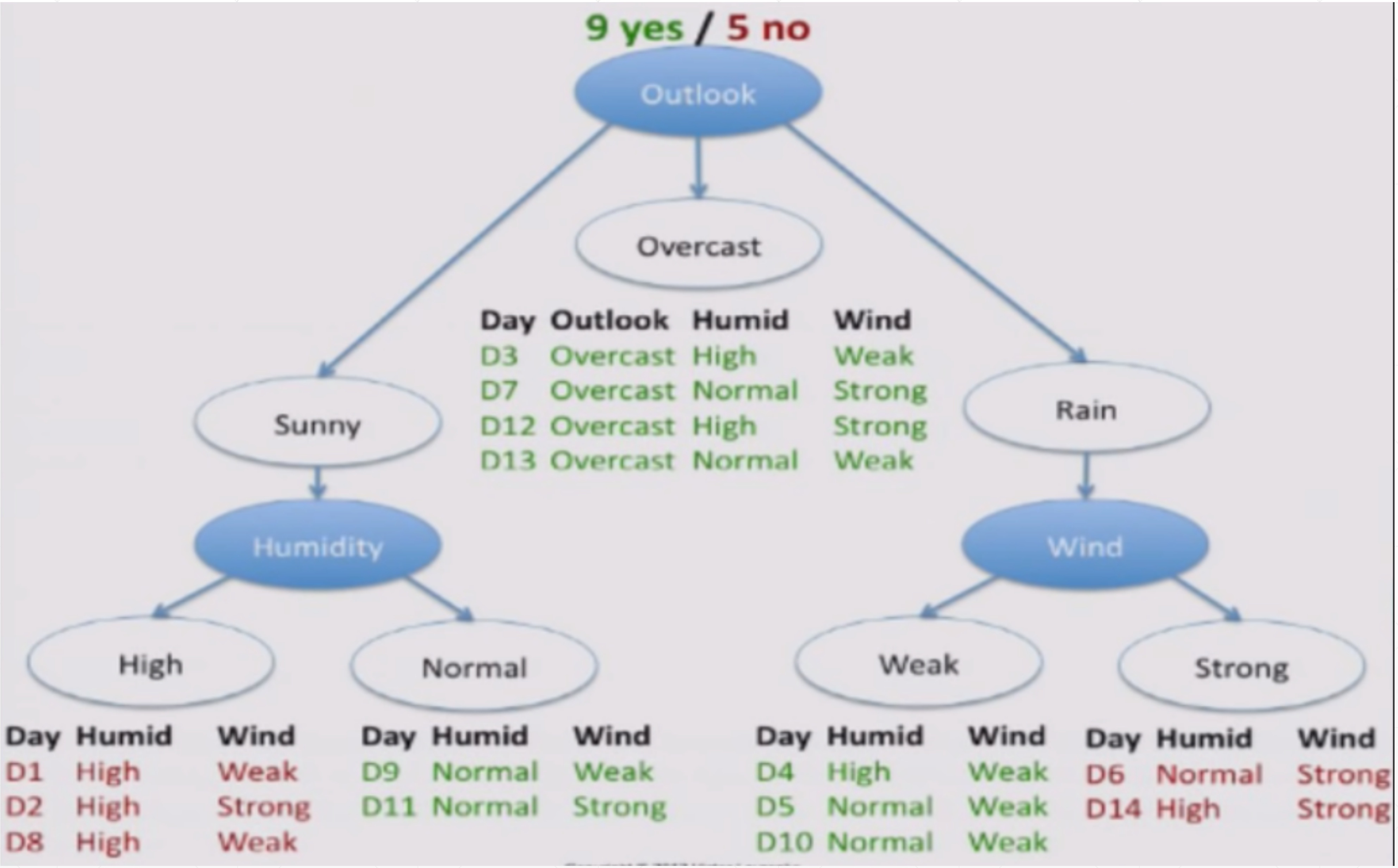
D8 High Weak
Day Humid Wind
D9 Normal Weak
D11 Normal Strong
Rain
Day Outlook Humid Wind
D4 Rain High Weak
D5 Rain Normal Weak
D6 Rain Normal Strong
D10 Rain Normal Weak
D14 Rain High Strong
3 yes / 2 no
split further


9 yes / 5 no
Outlook
Overcast
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D3 Overcast High Weak
D7 Overcast Normal Strong
D12 Overcast High Strong
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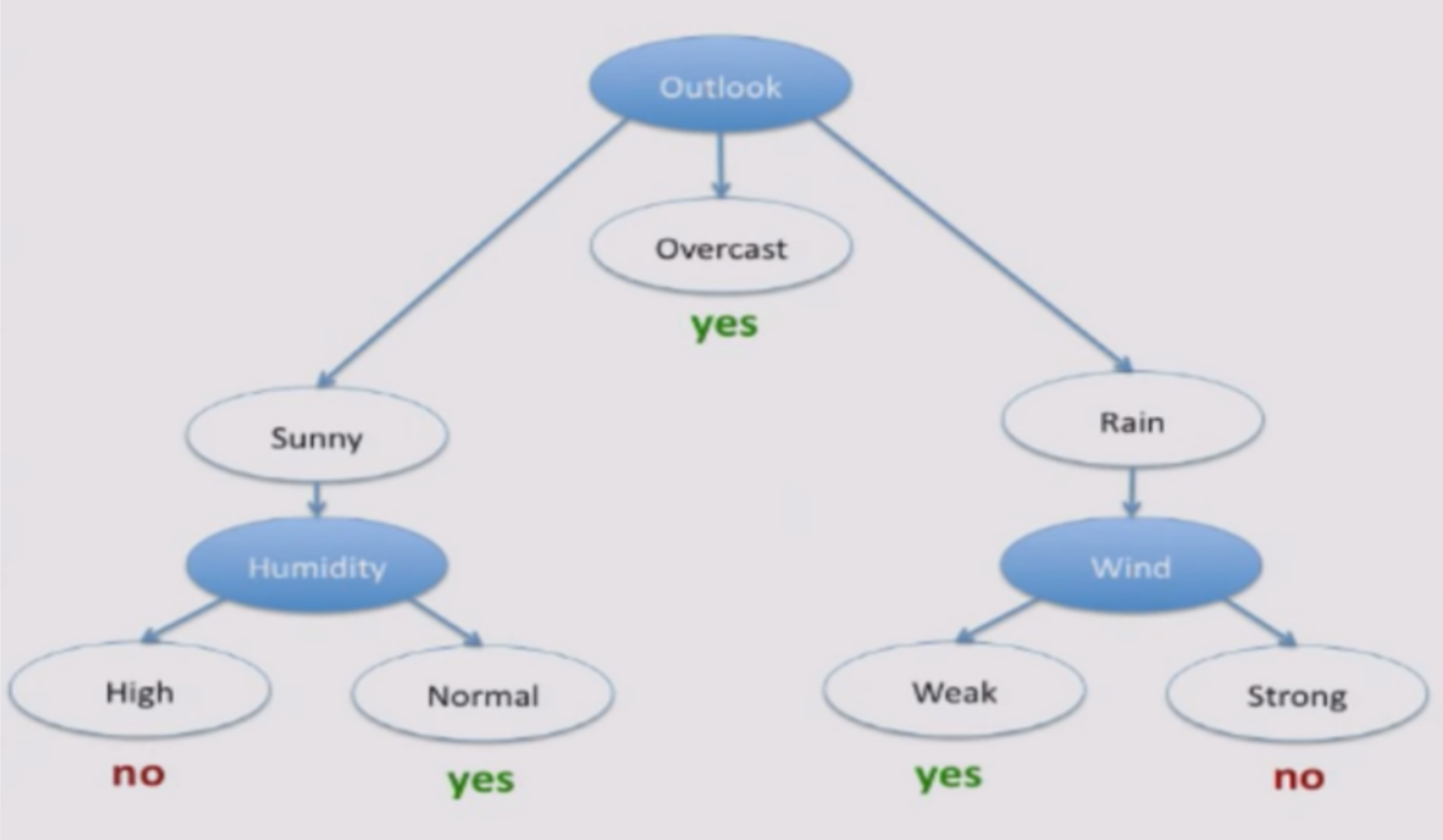
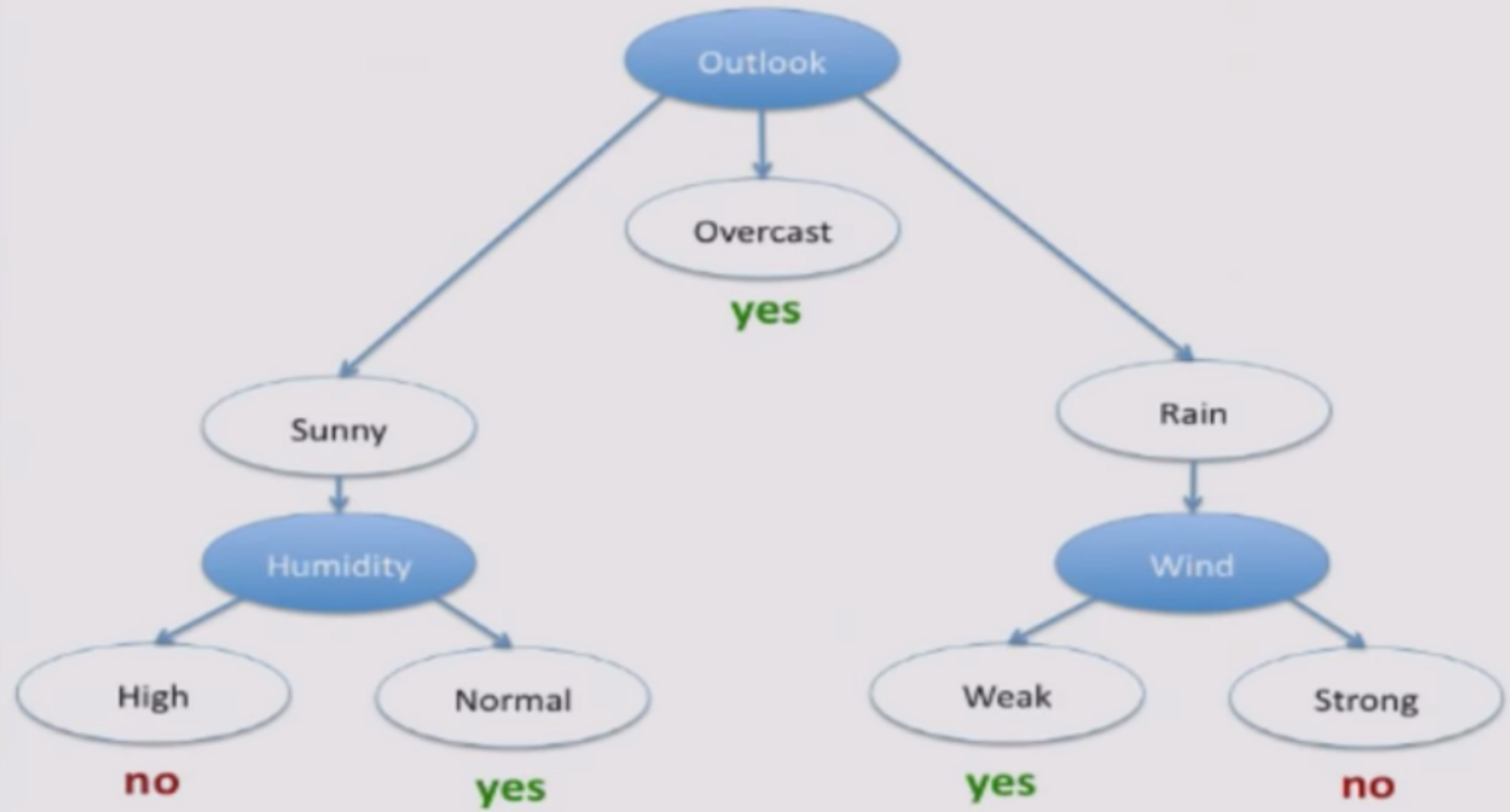
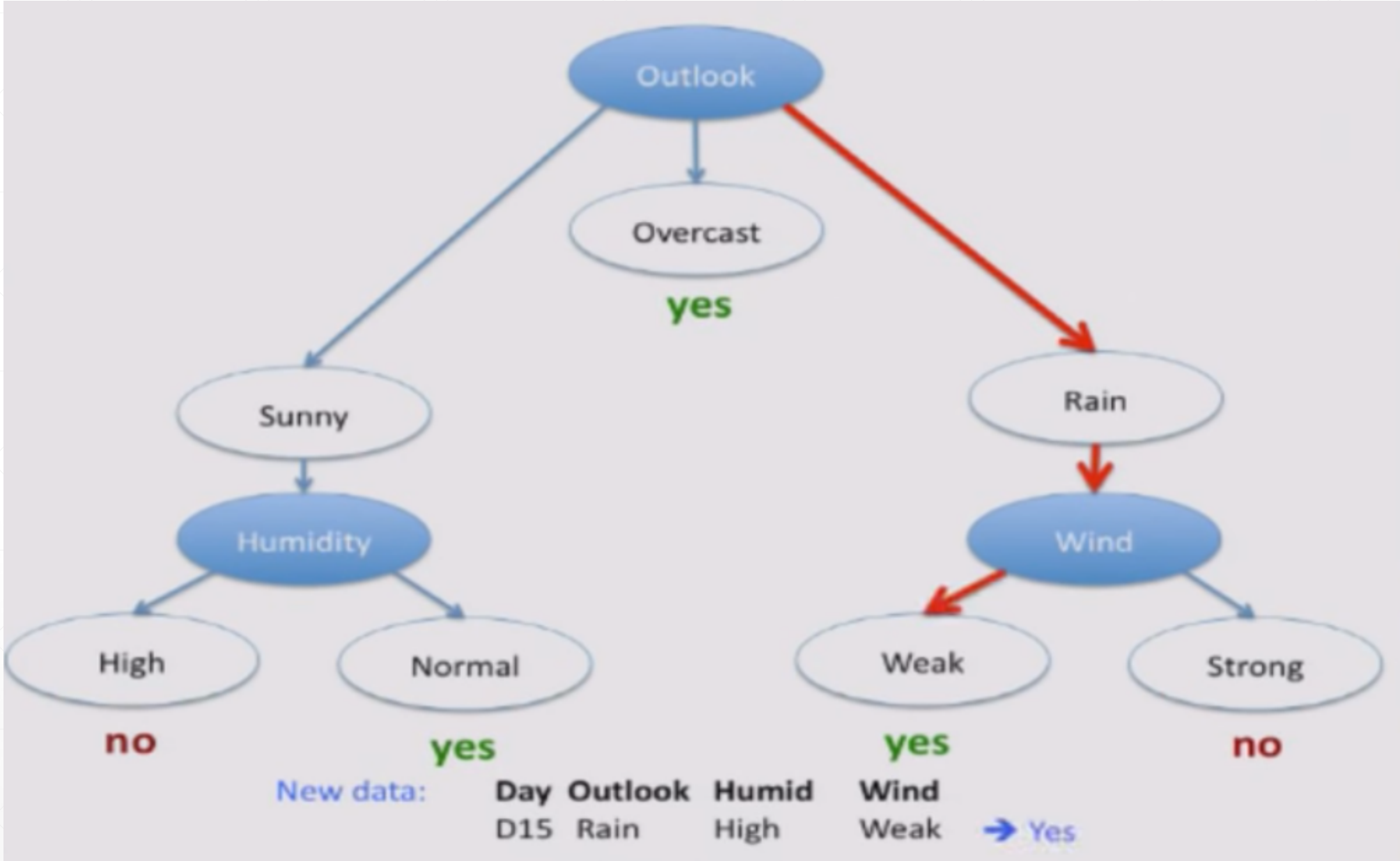
Sunny
Rain
Humidity
Wind
High
Normal
Weak
Strong
Day Humid Wind
D1 High Weak
D2 High Strong
D8 High Weak
Day Humid Wind
D9 Normal Weak
D11 Normal Strong
Day Humid Wind
D4 High Weak
D5 Normal Weak
D10 Normal Weak
Day Humid Wind
D6 Normal Strong
D14 High Strong

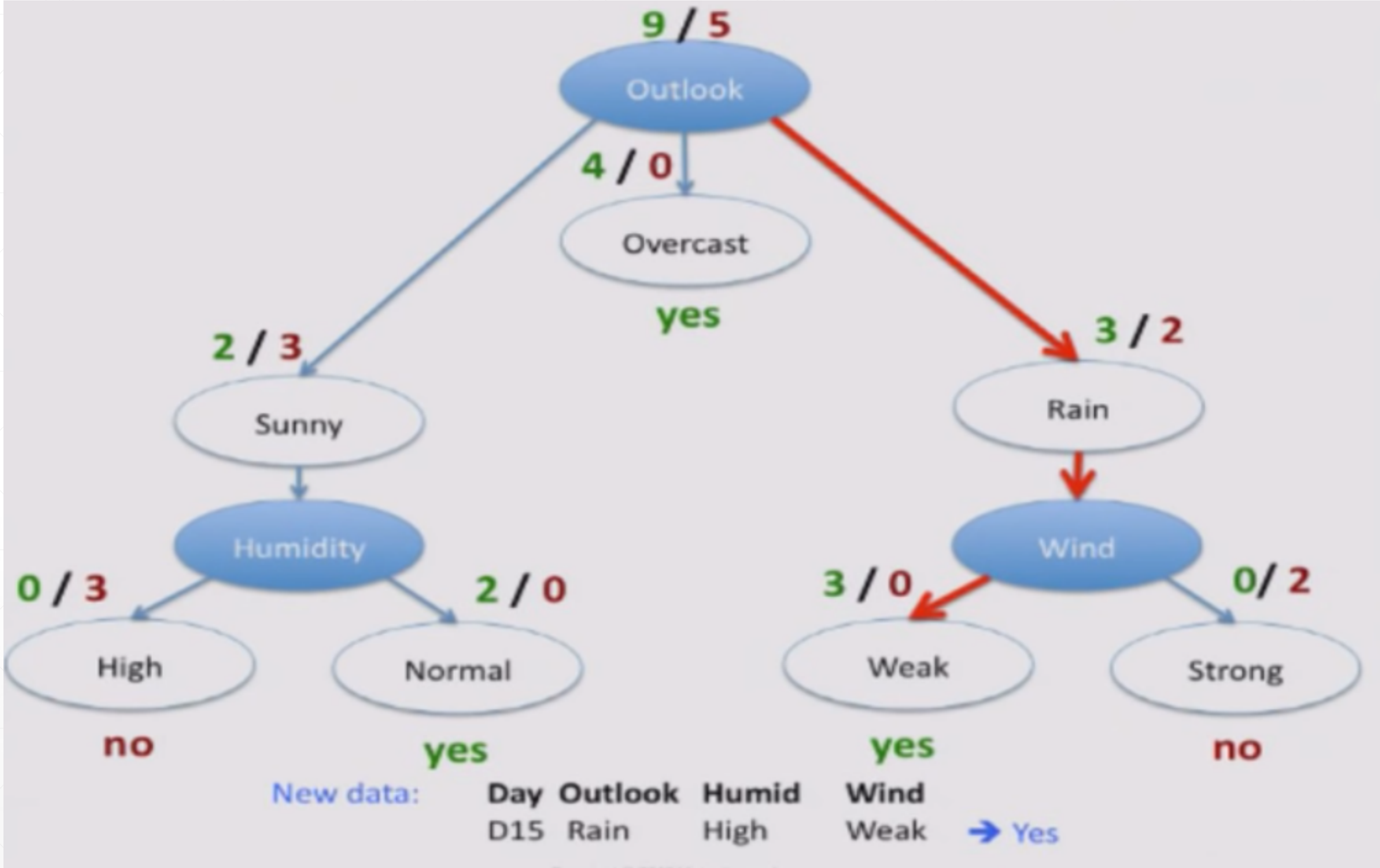

Outlook
Overcast
yes
Sunny
Rain
Humidity
Wind
High
Normal
Weak
Strong
no
yes
yes
no



New data:

Day	Outlook	Humid	Wind
D15	Rain	High	Weak


Outlook
Overcast
yes
Sunny
Rain
Humidity
Wind
High
Normal
Weak
Strong
no
yes
yes
no
New data:
Day Outlook Humid Wind
D15 Rain High Weak
Yes


9 / 5
Outlook
4 / 0
Overcast
yes
2 / 3
Sunny
3 / 2
Rain
Humidity
Wind
0 / 3
2 / 0
3 / 0
0/ 2
High
Normal
Weak
Strong
no
yes
yes
no
New data:
Day Outlook Humid Wind
D15 Rain High Weak → Yes

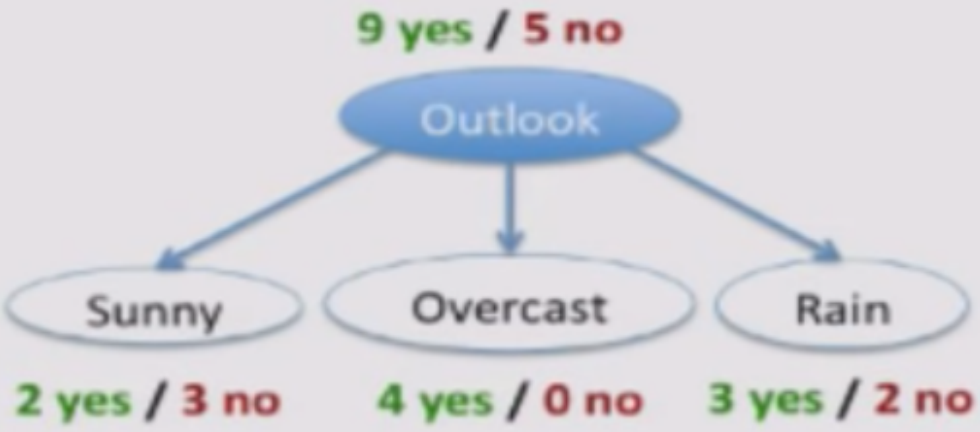
ID3 algorithm

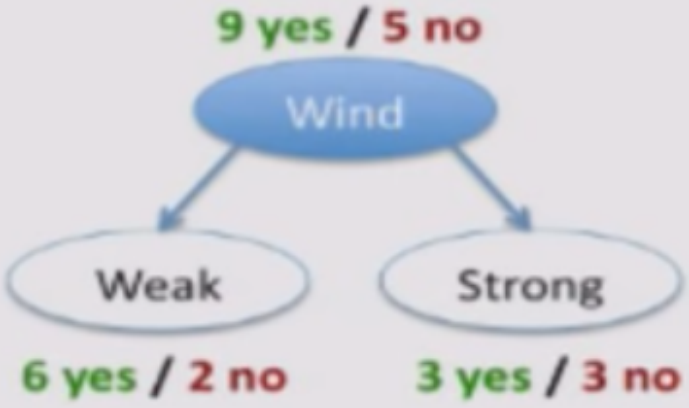
- Split (node, {examples}):
  1. A ← the best attribute for splitting the {examples}
  2. Decision attribute for this node ← A
  3. For each value of A, create new child node
  4. Split training {examples} to child nodes
  5. For each child node / subset:

     if subset is pure: STOP

     else: Split (child_node, {subset})
- Ross Quinlan (ID3: 1986), (C4.5: 1993)
- Breimanetal (CaRT: 1984) from statistics

Which attribute to split on?





Which attribute to split on?

- Want to measure "purity" of the split
  - more certain about Yes/No after the split
    - pure set (4 yes / 0 no) => completely certain (100%)
    - impure (3 yes / 3 no) => completely uncertain (50%)
  - can't use P("yes" | set):
    - must be symmetric: 4 yes / 0 no as pure as 0 yes / 4 no

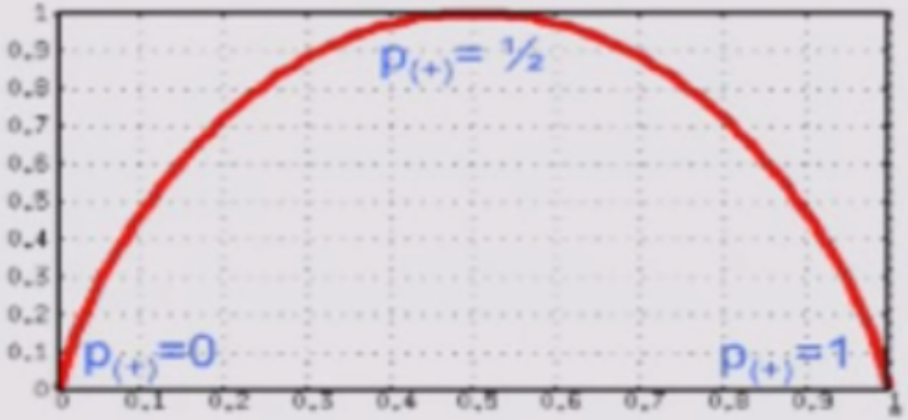
Entropy

- Entropy: $H(S) = - p_{(+)} \log_2 p_{(+)} - p_{(-)} \log_2 p_{(-)}$ bits
  - S … subset of training examples
  - $p_{(+)}$ / $p_{(-)}$ … % of positive / negative examples in S
- Interpretation: assume item X belongs to S
  - how many bits need to tell if X positive or negative
- impure (3 yes / 3 no):

$$H(S) = -\frac{3}{6}\log_2\frac{3}{6} - \frac{3}{6}\log_2\frac{3}{6} = 1 \text{ bits}$$

- pure set (4 yes / 0 no):

$$H(S) = -\frac{4}{4}\log_2\frac{4}{4} - \frac{0}{4}\log_2\frac{0}{4} = 0 \text{ bits}$$



Information Gain

- Want many items in pure sets
- Expected drop in entropy after split:

$$Gain(S,A) = H(S) - \sum_{V \in Values(A)} \frac{|S_V|}{|S|} H(S_V)$$

V ... possible values of A
S ... set of examples {X}
S_v ... subset where $X_A = V$

- Mutual Information
  - between attribute A and class labels of S

$-\frac{9}{14}\log_2\frac{9}{14} - \frac{5}{14}\log_2\frac{5}{14}$ 9 yes / 5 no

$H(S) = 0.94$

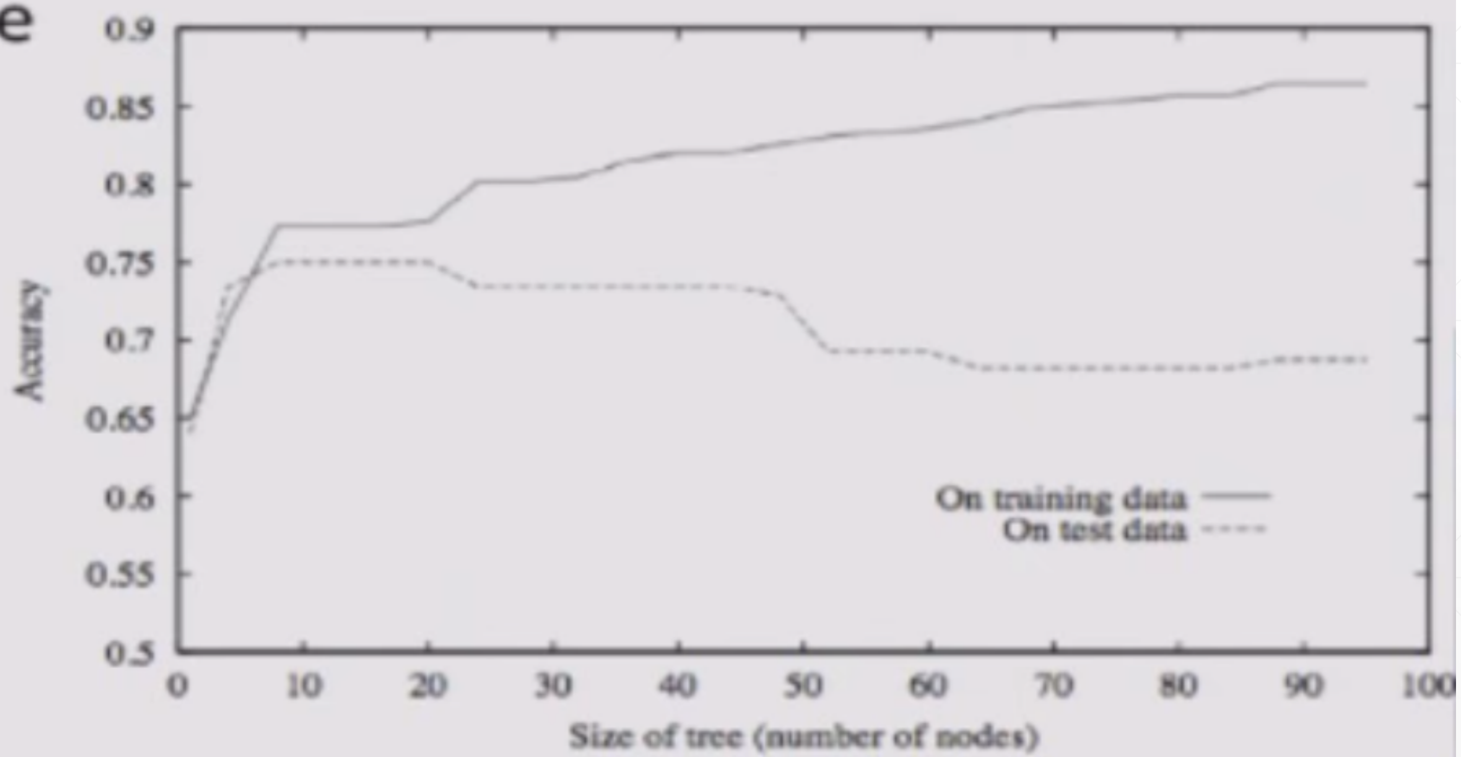
6 yes / 2 no
$-\frac{6}{8}\log_2\frac{6}{8} - \frac{2}{8}\log_2\frac{2}{8}$
$H(S_{weak}) = 0.81$

3 yes / 3 no
$-\frac{3}{6}\log_2\frac{3}{6} - \frac{3}{6}\log_2\frac{3}{6}$
$H(S_{strong}) = 1.0$

Gain (S, Wind)
$= H(S) - {}^{8}/_{14}\, H(S_{weak}) - {}^{6}/_{14}\, H(S_{weak})$
$= 0.94 - {}^{8}/_{14} * 0.81 - {}^{6}/_{14} * 1.0$
$= 0.049$

Overfitting in Decision Trees

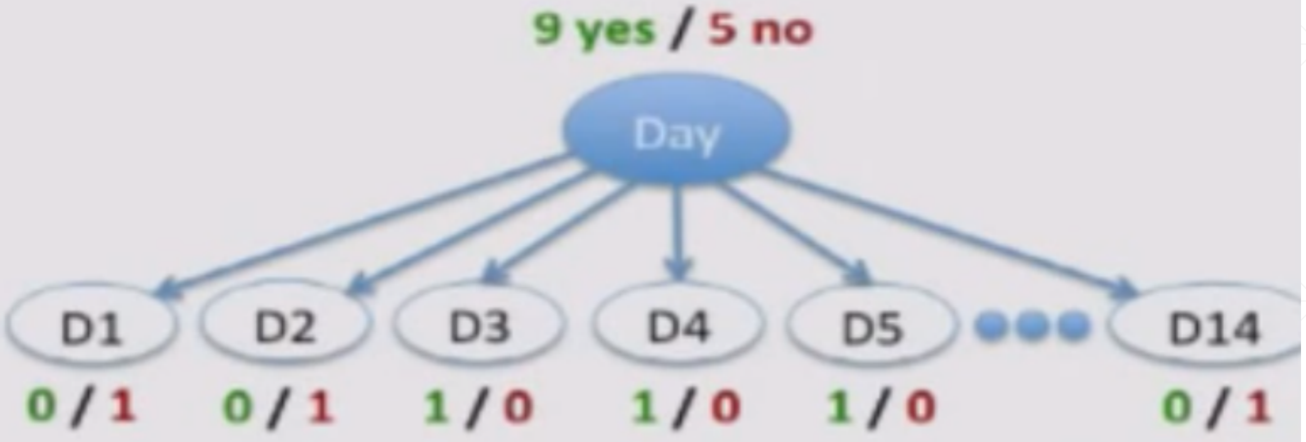
- Can always classify training examples perfectly
  - keep splitting until each node contains 1 example
  - singleton = pure
- Doesn't work on new data



Avoid overfitting

- Stop splitting when not statistically significant
- Grow, then post-prune
  - based on validation set
- Sub-tree replacement pruning (WF 6.1)
  - for each node:
    - pretend remove node + all children from the tree
    - measure performance on validation set
  - remove node that results in greatest improvement
  - repeat until further pruning is harmful

Problems with Information Gain



all subsets perfectly pure => optimal split

- Biased towards attributes with many values
- Won't work for new data: D15 Rain High Weak
- Use GainRatio:

$$SplitEntropy(S,A) = -\sum_{V \in Values(A)} \frac{|S_V|}{|S|} \log \frac{|S_V|}{|S|}$$

A ... candidate attribute
V ... possible values of A
S ... set of examples {X}
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$$SplitEntropy(S,A) = -\sum_{V \in Values(A)} \frac{|S_V|}{|S|} \log \frac{|S_V|}{|S|}$$

A ... candidate attribute
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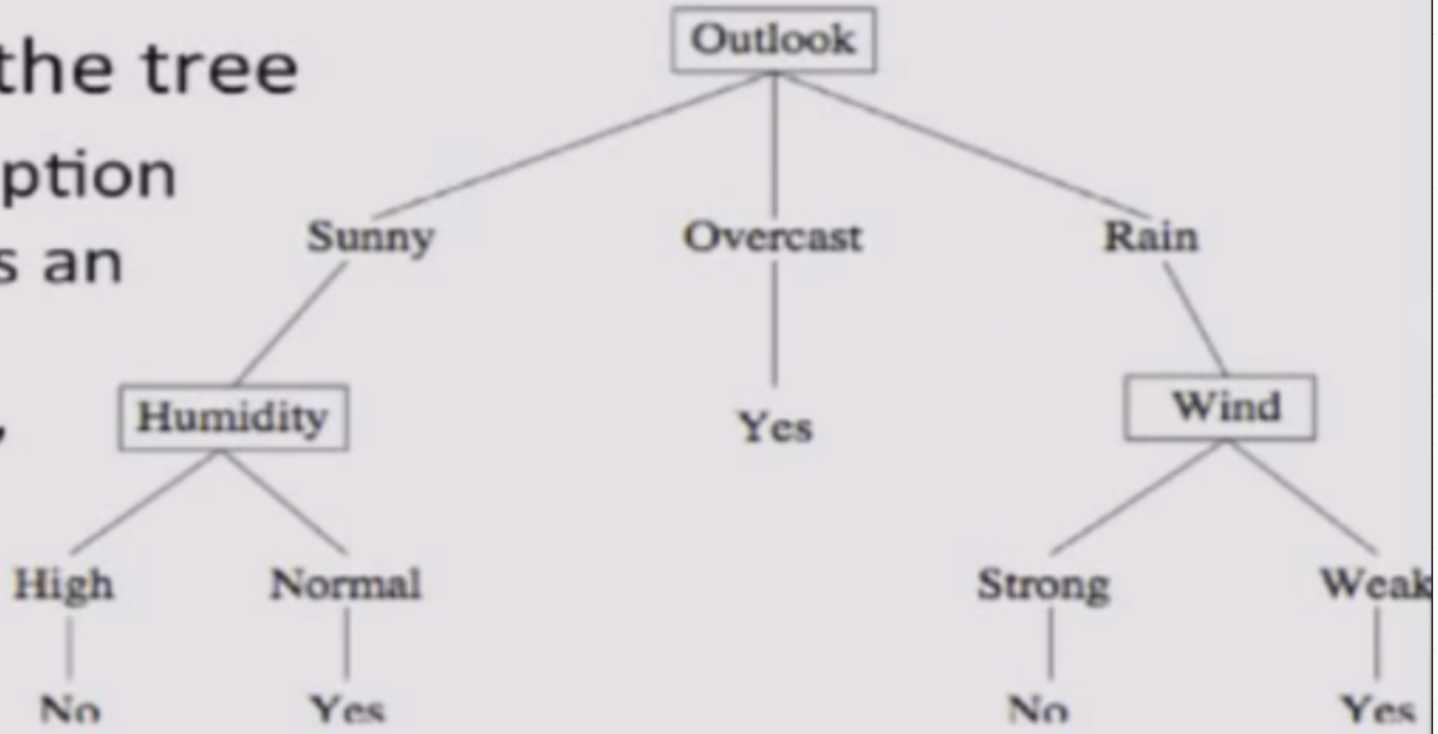
S_v ... subset where $X_A = V$

$$GainRatio(S,A) = \frac{Gain(S,A)}{SplitEntropy(S,A)}$$

penalizes attributes with many values

Trees are interpretable

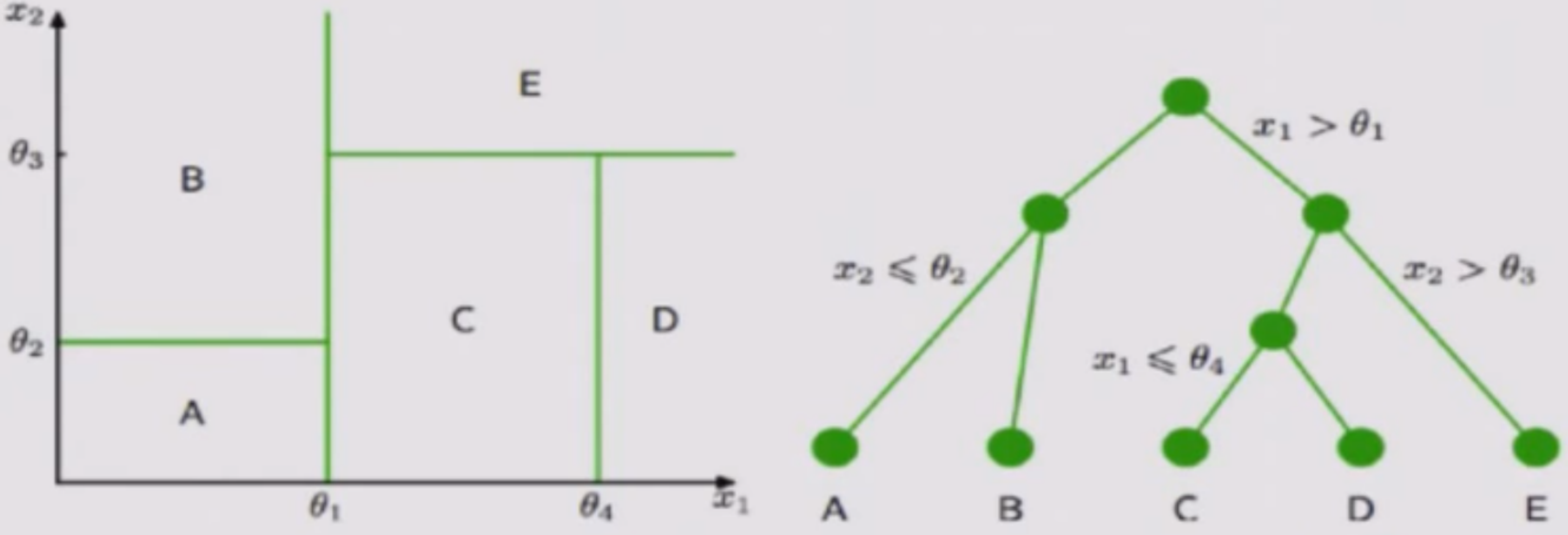
- Read rules off the tree
  - concise description of what makes an item positive
- No “black box”
  - important for users



Rule: (Outlook = Overcast) $\vee$
(Outlook = Rain $\wedge$ Wind = Weak) $\vee$
(Outlook = Sunny $\wedge$ Humidity = Normal)

Continuous Attributes

- Dealing with continuous-valued attributes:
  - create a split: (Temperature > 72.3) = True,False
- Threshold can be optimized (WF 6.1)

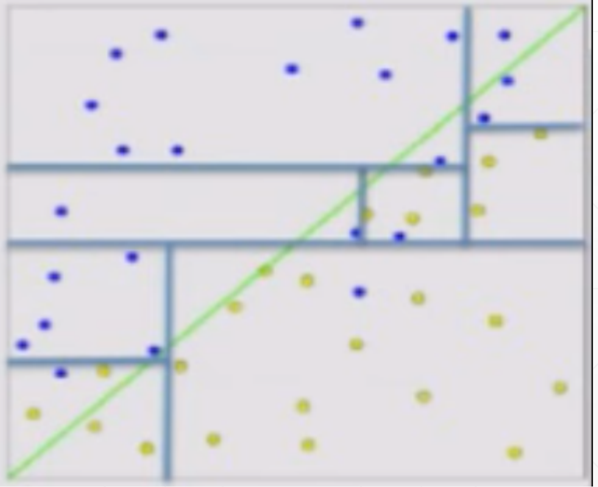


Multi-class and Regression

- Multi-class classification:
  - predict most frequent class in the subset
  - entropy: $H(S) = -\Sigma_c p_{(c)} \log_2 p_{(c)}$
  - $p_{(c)}$ ... % of examples of class c in S
- Regression:
  - predicted output = average of the training examples in the subset
  - requires a different definition of entropy
  - can use linear regression at the leaves (WF 6.5)

Pros and Cons

- Pros:
  - interpretable: humans can understand decisions
  - easily handles irrelevant attributes (Gain = 0)
  - can handle missing data (WF 6.1)
  - very compact: #nodes << D after pruning
  - very fast at testing time: O(depth)
- Cons:
  - only axis-aligned splits of data
  - greedy (may not find best tree)
    - exponentially many possible trees



Random Decision Forest

- Grow K different decision trees:
  - pick a random subset S_r of training examples
  - grow a full ID3 tree T_r (no prunning):
    - when splitting: pick from $d << D$ random attributes
    - compute gain based on S_r instead of full set
  - repeat for $r = 1 \ldots K$
- Given a new data point X:
  - classify X using each of the trees $T_1 \ldots T_K$
  - use majority vote: class predicted most often

Summary

- ID3: grows decision tree from the root down
  - greedily selects next best attribute (using Gain)
  - entropy: how uncertain we are of Yes/No in a set
  - Gain: reduction in uncertainty following a split
- Searches a complete hypothesis space
  - prefers smaller trees, high gain at the root
- Overfitting addressed by post-pruning
  - prune nodes, while accuracy ⇧ on validation set
- Fast, compact, interpretable

Discussion

Thank you!