Decision Trees

CSC 461: Machine Learning

Fall 2022

Prof. Marco Alvarez
University of Rhode Island

Introduction

Supervised learning setup

- Data instance
  - ✓ in general, $x \in \mathbb{R}^d$ is a **feature vector** of discrete values, but continuous values can also be handled
  - ✓ $y \in \{1,2,\ldots,k\}$
- Hypothesis
  - ✓ each hypothesis **g** is a **decision tree**

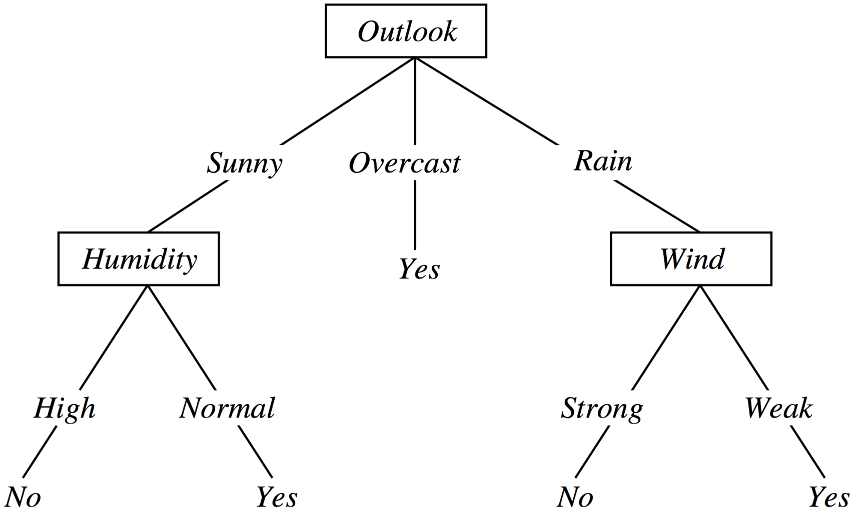
$$g : \mathscr{X} \mapsto \mathscr{Y}, g \in \mathscr{H}$$

Tennis dataset

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

Machine Learning, Tom Mitchell, McGraw Hill, 1997

Example (Decision Tree)



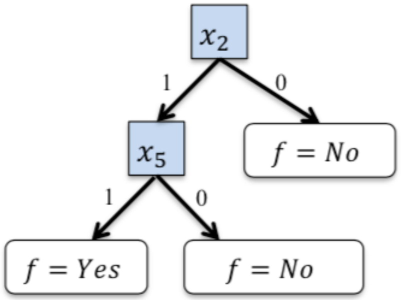
Machine Learning, Tom Mitchell, McGraw Hill, 1997

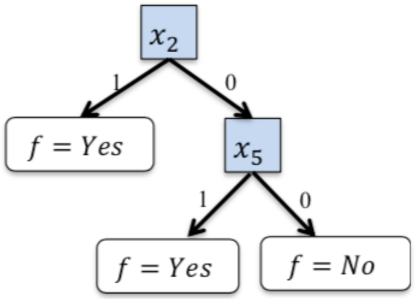
Representation

- Nodes test features/attributes
- Branches represent possible values for a feature
- Leaves represent outputs (classes)
- Assuming boolean inputs/outputs, draw the trees:

$A \wedge B$
$A \vee B$
$(A \wedge B) \vee (C \wedge \neg D \wedge E)$

What functions are represented?

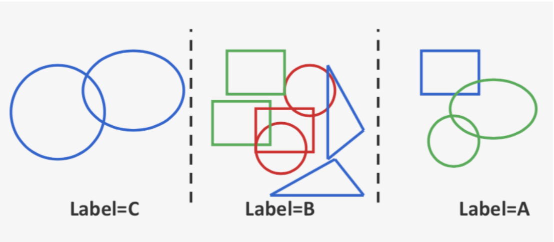




from: 10-315 Machine Learning, Maria-Florina (Nina) Balcan, CMU, Spring 2019

Build/test your own tree

- Assume features: color and shape

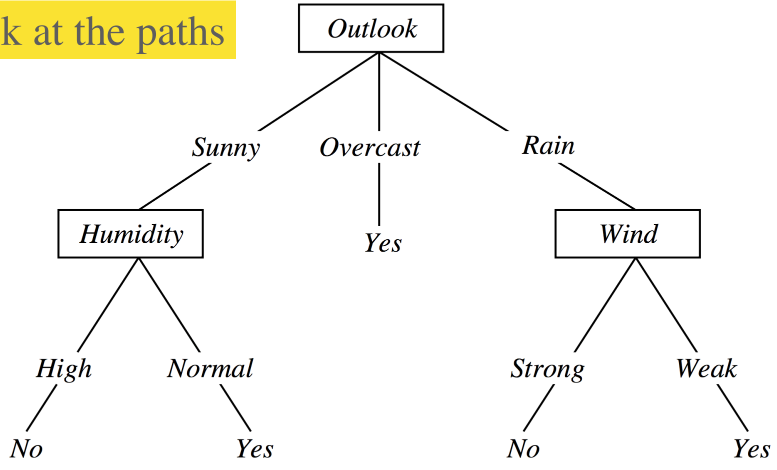


- What are the labels for a red triangle and a green triangle?

from: CS 5350 Machine Learning, Vivek Srikumar, University of Utah, Fall 2019

Extracting rules from the tree

Look at the paths



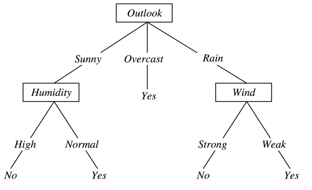
Machine Learning, Tom Mitchell, McGraw Hill, 1997

Disjunction of conjunctions

$$\ldots \lor (\ldots \land \ldots) \lor (\ldots \land \ldots) \lor \ldots$$

If … $(Outlook = Sunny \land Humidity = Normal) \lor$
$(Outlook = Overcast) \lor$
$(Outlook = Rain \land Wind = Weak)$

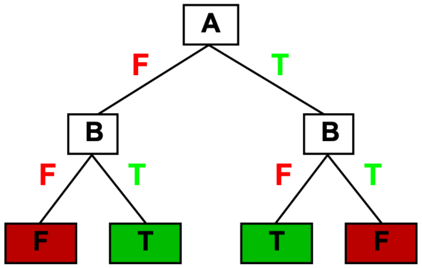
then it belongs to class YES



Expressiveness

- A decision tree can represent any boolean/ discrete function (discrete input/discrete output)

A	B	A xor B
F	F	F
F	T	T
T	F	T
T	T	F



http://aima.eecs.berkeley.edu/slides-pdf/chapter18.pdf

Hypothesis space

How many distinct decision trees can be created with d=5 boolean features?

		x			y
0	0	0	0	0	T/F
0	0	0	0	1	T/F
0	0	0	1	0	T/F
0	0	0	1	1	T/F
0	0	1	0	0	T/F
…					T/F
1	1	1	1	1	T/F

$2^5 = 32$ entries

how many boolean functions with 5 features are there, given that entries can be T/F?

$$2^{2^5}$$

Try d == 10

Hypothesis space

- More expressive hypothesis space …
  - ✓ allows learning complex target functions
  - ✓ increases number of consistent hypotheses
  - ✓ may not **generalize**, due to **overfitting**
- DT learning goal
  - ✓ find a **small tree <u>consistent</u> with the training data**
  - ✓ **NP-complete** (polynomial algorithm may not exist)

Consistent hypotheses

- A hypothesis **g** is consistent with a set of training examples **D** if and only if **g(x) = y** for all pairs **(x, y)** in **D**
  - ✓ **"hope"**: if **g** is consistent with training data, then it would be accurate on new instances

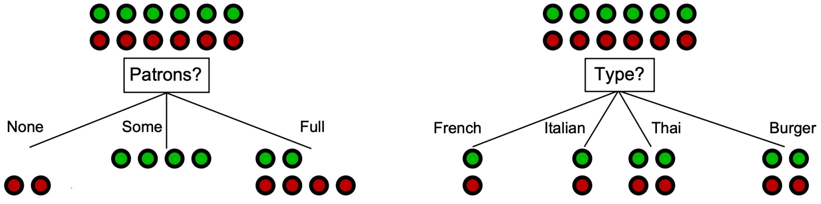
- There is a tree consistent with any training set (just list all paths) — **it may not generalize well**
- Preferably we want more **compact** trees that can **generalize** better

Learning a Decision Tree

Induction of a Decision Tree

- Build the tree using a **top-down** approach
  - ✓ selecting one feature to split at a time
- **Greedy** algorithm
  - ✓ makes the **optimal** choice at each step **(which feature to split)**
  - ✓ the greedy nature of the algorithm cannot guarantee **optimality (smallest tree consistent with the data)**
- **NP-complete** problem
  - ✓ "Although a solution to an NP-complete problem can be verified "quickly", there is no known way to find a solution quickly" [wikipedia]

Which feature is better? Why?

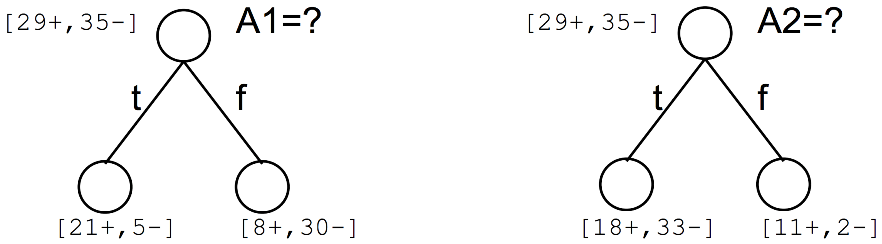


- Which feature is more **informative**?

- Which provides the minimum **0/1 loss** if we use the majority vote for classifying new instances?

http://aima.eecs.berkeley.edu/slides-pdf/chapter18.pdf

Which feature is better?



Machine Learning, Tom Mitchell, McGraw Hill, 1997

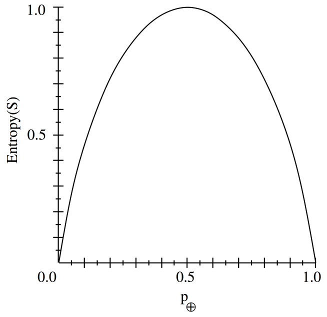
How to choose the splitting feature?

- Information Gain
  - ✓ used in **ID3**
- Gain Ratio
  - ✓ used in C4.5
- Gini Measure
  - ✓ used in CART
- …

ID3 was invented by Ross Quinlan

Entropy

- Assume a set S of positive/negative instances
  - ✓ entropy measures the **impurity** of S



w.r.t. a binary variable

$$E(S) = -p_{\oplus} \log_2 p_{\oplus} - p_{\ominus} \log_2 p_{\ominus}$$

Entropy

- Assuming **k** possible values, each with different probabilities, then:

$$E(S) = -\sum_{i=1}^{k} p_i \log_2 p_i$$

What is the entropy if all instances belong to the same category?

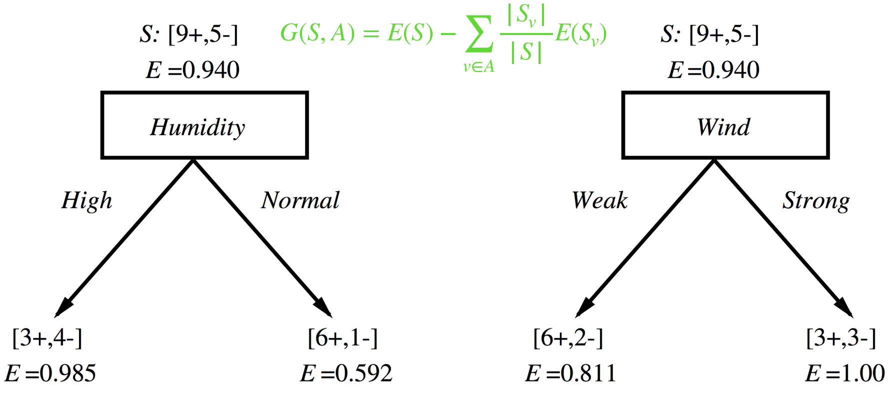
Information Gain

- Expected reduction in **Entropy** after splitting

$$G(S,A) = E(S) - \sum_{v \in A} \frac{|S_v|}{|S|} E(S_v)$$

- **Information gain** increases for low entropy values

Calculate the Information Gain



$$G(S,A) = E(S) - \sum_{v \in A} \frac{|S_v|}{|S|} E(S_v)$$

Machine Learning, Tom Mitchell, McGraw Hill, 1997

Induction of a Decision Tree

```
Algorithm GrowTree($D, F$)
Input   : data $D$; set of features $F$.
Output  : feature tree $T$ with labelled leaves.
if Homogeneous($D$) then return Label($D$) ;    // Homogeneous, Label: see text
$S$ ←BestSplit($D, F$) ;                        // e.g., BestSplit-Class (Algorithm 5.2)
split $D$ into subsets $D_i$ according to the literals in $S$;
for each $i$ do
    if $D_i \neq \emptyset$ then $T_i$ ←GrowTree($D_i, F$) else $T_i$ is a leaf labelled with
    Label($D$);
end
return a tree whose root is labelled with $S$ and whose children are $T_i$
```

Machine Learning: The Art and Science of Algorithms that Make Sense of Data, Peter Flach, Cambridge University Press, 2012

Induction of a Decision Tree

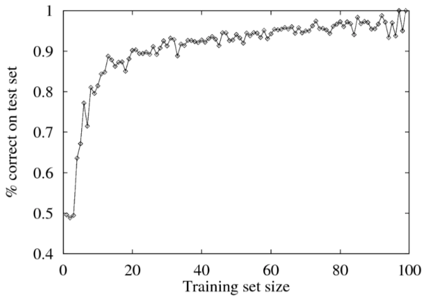
Algorithm BestSplit-Class(D, F) – find the best split for a decision tree.

```
Input  : data $D$; set of features $F$.
Output : feature $f$ to split on.
$I_{min} \leftarrow 1$;
for each $f \in F$ do
    split $D$ into subsets $D_1, \ldots, D_l$ according to the values $v_j$ of $f$;
    if $Imp(\{D_1, \ldots, D_l\}) < I_{min}$ then
        $I_{min} \leftarrow Imp(\{D_1, \ldots, D_l\})$;
        $f_{best} \leftarrow f$;
    end
end
return $f_{best}$
```

Machine Learning: The Art and Science of Algorithms that Make Sense of Data, Peter Flach, Cambridge University Press, 2012

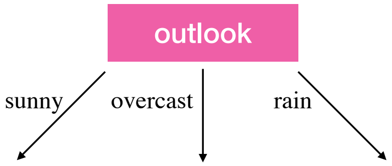
Resulting tree

- Tree is expected to be small and consistent with training examples
- Tree does not necessarily agree with the correct function (bigger training datasets help)



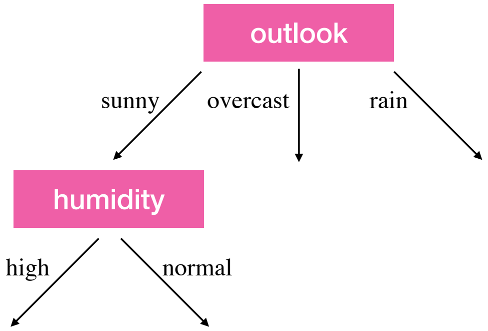
Example

Day	Outlook	Temperature	Humidity	Wind	Play
D1	sunny	hot	high	weak	no
D2	sunny	hot	high	strong	no
D3	overcast	hot	high	weak	yes
D4	rain	mild	high	weak	yes
D5	rain	cool	normal	weak	yes
D6	rain	cool	normal	strong	no
D7	overcast	cool	normal	strong	yes
D8	sunny	mild	high	weak	no
D9	sunny	cool	normal	weak	yes
D10	rain	mild	normal	weak	yes
D11	sunny	mild	normal	strong	yes
D12	overcast	mild	high	strong	yes
D13	overcast	hot	normal	weak	yes
D14	rain	mild	high	strong	no



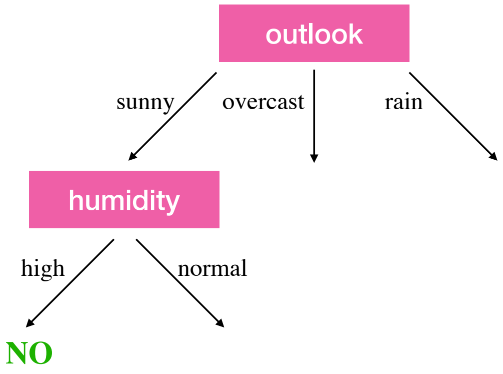
Day	Outlook	Temperature	Humidity	Wind	Play
D1	sunny	hot	high	weak	no
D2	sunny	hot	high	strong	no
D3	overcast	hot	high	weak	yes
D4	rain	mild	high	weak	yes
D5	rain	cool	normal	weak	yes
D6	rain	cool	normal	strong	no
D7	overcast	cool	normal	strong	yes
D8	sunny	mild	high	weak	no
D9	sunny	cool	normal	weak	yes
D10	rain	mild	normal	weak	yes
D11	sunny	mild	normal	strong	yes
D12	overcast	mild	high	strong	yes
D13	overcast	hot	normal	weak	yes
D14	rain	mild	high	strong	no

calculate IG and select highest



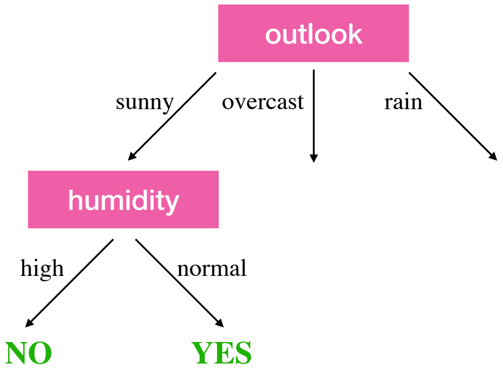
Day	Temperature	Humidity	Wind	Play
D1	hot	high	weak	no
D2	hot	high	strong	no
D8	mild	high	weak	no
D9	cool	normal	weak	yes
D11	mild	normal	strong	yes

calculate IG and select highest



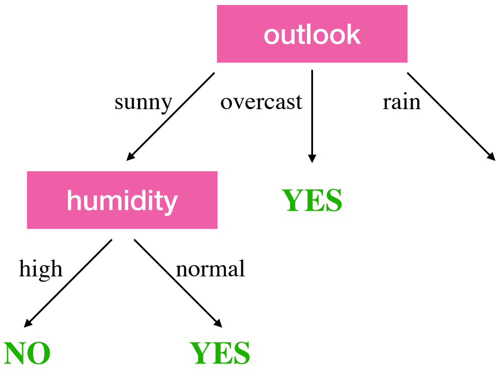
Day	Temperature	Wind	Play
D1	hot	weak	no
D2	hot	strong	no
D8	mild	weak	no

calculate IG and select highest



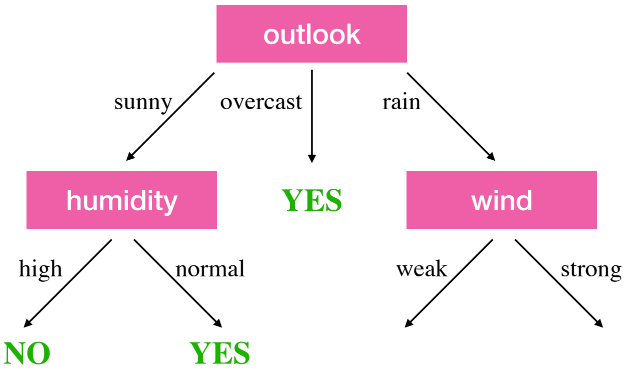
Day	Temperature	Wind	Play
D9	cool	weak	yes
D11	mild	strong	yes

calculate IG and select highest



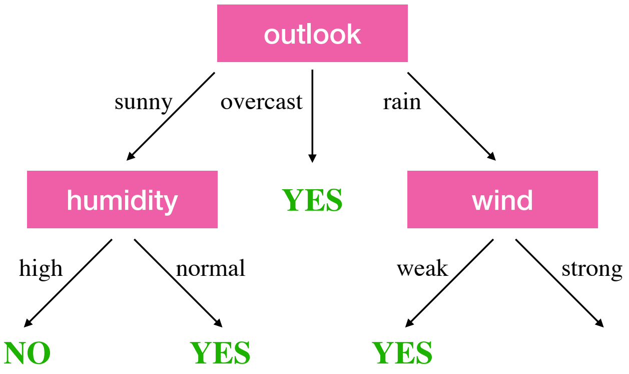
Day	Temperature	Humidity	Wind	Play
D3	hot	high	weak	yes
D7	cool	normal	strong	yes
D12	mild	high	strong	yes
D13	hot	normal	weak	yes

calculate IG and select highest



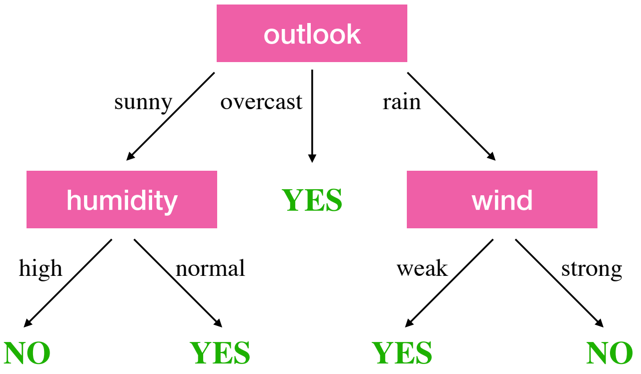
Day	Temperature	Humidity	Wind	Play
D4	mild	high	weak	yes
D5	cool	normal	weak	yes
D6	cool	normal	strong	no
D10	mild	normal	weak	yes
D14	mild	high	strong	no

calculate IG and select highest



Day	Temperature	Humidity	Play
D4	mild	high	yes
D5	cool	normal	yes
D10	mild	normal	yes

calculate IG and select highest



Day	Temperature	Humidity	Play
D6	cool	normal	no
D14	mild	high	no

calculate IG and select highest

Final Remarks

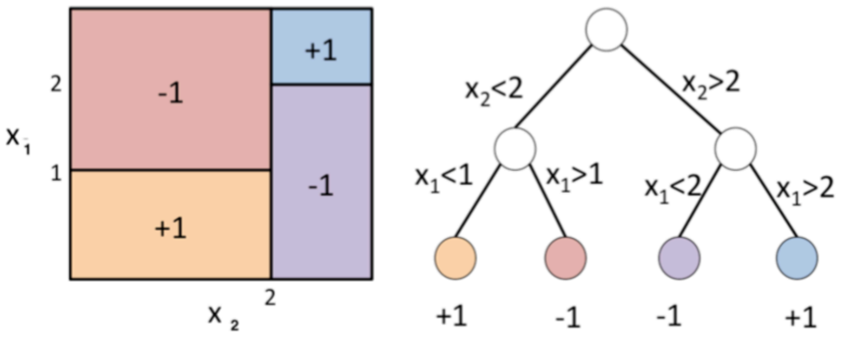
Continuous features

- Transform continuous into discrete features
  - ✓ use thresholds defined by domain experts or automatically calculated from training data
- For example:
  - ✓ sort values (training set)
  - ✓ find split points where class changes

Temperature:	40	48	60	72	80	90
PlayTennis:	No	No	Yes	Yes	Yes	No

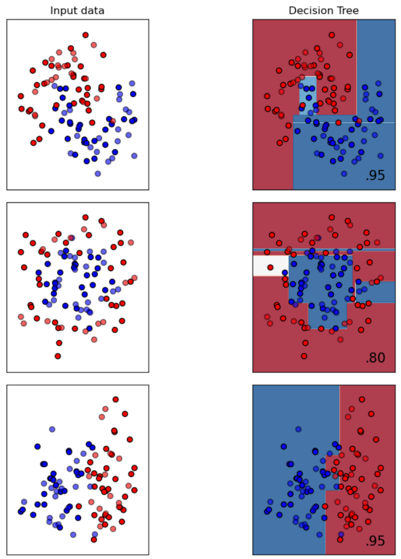
54 85

Nonlinear Decision Boundary



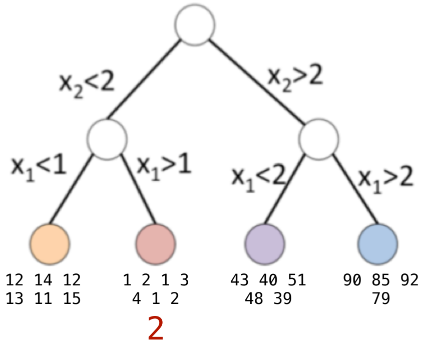
from: CS260 Machine Learning Algorithms, Cho-Jui Hsieh, UCLA, 2019

Nonlinear Decision Boundary



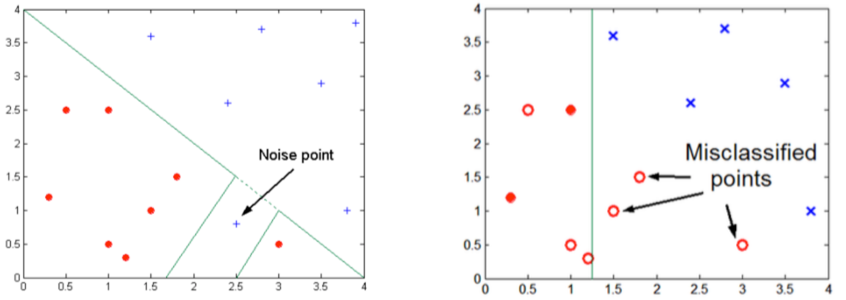
Continuous outputs

- Regression trees
  - ✓ can assign a continuous value to a leaf
  - ✓ e.g. the **average** of all **y** values that fall into the leaf



Model overfitting

A hypothesis **h1** is said to **overfit** the training data if there exists some alternative hypothesis **h2** such that **h1** has smaller error than **h2** over the training examples, but **h2** has a smaller error than **h1** over the entire distribution of instances



due to noise

due to lack of representative instances

from: Data Mining I, Eirini Ntoutsi, Leibniz University, Summer 2019

Preventing overfitting (DTs)

- Remove irrelevant features
- Add more data
- **Stop growing branches** during training
  - ✓ hard thresholds or statistical measures
- Prune the tree post-training

Additional thoughts on DTs

- **Nonlinear** classifiers, which can also provide **interpretability**
- Training may be **slow** but inference is **fast**
  - ✓ what is the big-O of inference?
- Although trees can be small, certain functions will require an exponentially large decision tree
  - ✓ e.g. **majority** (1 if n inputs are positive), **parity** (1 if even number of inputs is positive)