Decision Trees

6/10/2023

Supervised Classification: Problem Setting

Procediamo con una classificazione che include >2 categorie:
ad esempio le mail: spam|lavoro|newsletter| etc...

Input : Training labeled examples $\{(x^{(i)}, y^{(i)})\}$ of unknown target function f such as $y = f(x)$

- Examples $x^{(i)}$ described by their values on some set of features or attributes
- Unknown target function $f : X \rightarrow Y$
  - X Set of possible instances
  - Y label space

per ogni label Y(i) viene associata una istanza X(i).
Y(1)=Vento <- Forte=X(1).
Y(2)=Tempo <- Sole=X(2)
queste tuple formano una ISTANZA ETICHETTATA.

Output: Hypothesis $h \in H$ that (best) approximates target function f

- Set of function hypotheses $H = \{h | h : X \rightarrow Y\}$
  - hypothesis h are decision trees

quindi, date delle istanze X e delle label Y, cerchiamo una funzione che approssima al meglio delle possibilità queste istanze nelle label.
NB: una singola label Y può assumere uno tra i valori delle possibili istanze X, che cambia da label a label.

Sample Dataset

- Columns denote features of X
- Rows denote labeled instances $(x^{(i)}, y^{(i)})$
- Class label (whether a tennis game was played)

$\langle x^{(i)}, y^{(i)} \rangle$

Predictors				Response
Outlook	**Temperature**	**Humidity**	**Wind**	**Class**
Sunny	Hot	High	Weak	No
Sunny	Hot	High	Strong	No
Overcast	Hot	High	Weak	Yes
Rain	Mild	High	Weak	Yes
Rain	Cool	Normal	Weak	Yes
Rain	Cool	Normal	Strong	No
Overcast	Cool	Normal	Strong	Yes
Sunny	Mild	High	Weak	No
Sunny	Cool	Normal	Weak	Yes
Rain	Mild	Normal	Weak	Yes
Sunny	Mild	Normal	Strong	Yes
Overcast	Mild	High	Strong	Yes
Overcast	Hot	Normal	Weak	Yes
Rain	Mild	High	Strong	No

- What about

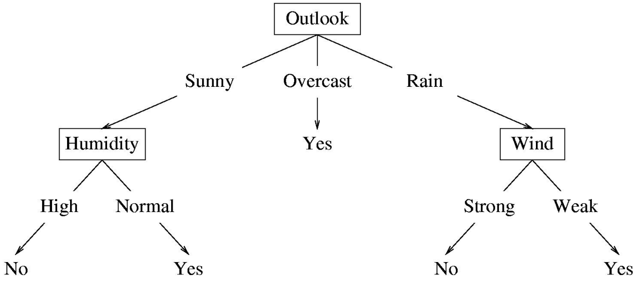
$$x = (Overcast, Mild, Normal, Weak)$$

Decision Trees

queste "Ipotesi H" sono alberi decisionali!

- Make predictions by splitting on features according to a tree structure.

Questa struttura permette una facile comprensione anche senza avere basi matematiche, ma dipende dai dati che ho. Se avessi tutti gli eventi possibili, l'albero sarebbe affidabilissimo, ma anche banale perché non predice nulla.

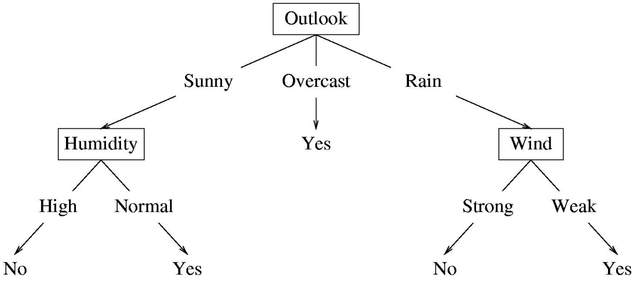


- Each internal node tests one attribute
- Each branch from a node selects one value of that attribute
- Each leaf nodes predicts Y

Decision Trees

- Make predictions by splitting on features according to a tree structure.

L'ideale sarebbe avere qualche caso, lavorare bene su quello e poi avere buoni riferimenti per dati non osservati!
Se non li osservo, come faccio a giudicarli? uso validation set.

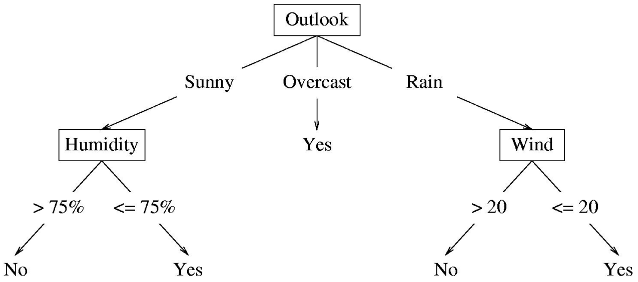


- What prediction would we make for

$$x = (Overcast, Mild, Normal, Weak)$$

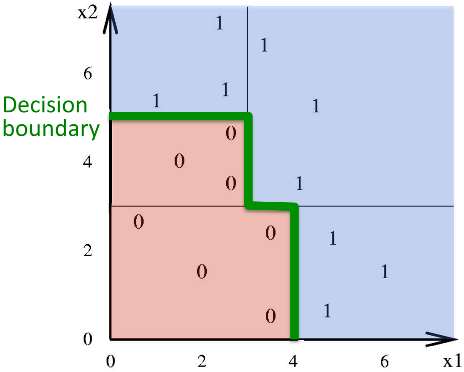
Decision Trees

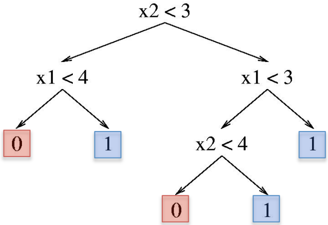
- If features are continuous, internal nodes can test the value of a feature against a threshold



Decision Trees - Decision Boundary

- Decision trees divide the feature space into axis-parallel (hyper-)rectangles
- Each rectangular region is labeled with one label





Another Example (Russel & Norivg)

Model a patron's decision whether to wait for a table

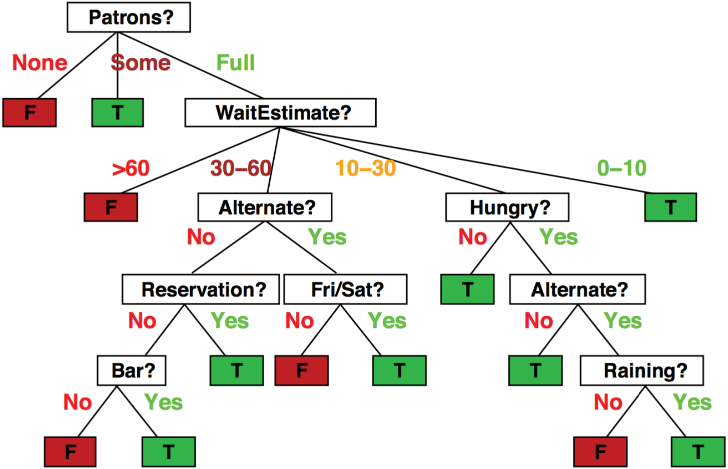
Example	Input Attributes										Goal
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
$\mathbf{x}_1$	*Yes*	*No*	*No*	*Yes*	*Some*	*$$$*	*No*	*Yes*	*French*	*0–10*	$y_1 =$ *Yes*
$\mathbf{x}_2$	*Yes*	*No*	*No*	*Yes*	*Full*	*$*	*No*	*No*	*Thai*	*30–60*	$y_2 =$ *No*
$\mathbf{x}_3$	*No*	*Yes*	*No*	*No*	*Some*	*$*	*No*	*No*	*Burger*	*0–10*	$y_3 =$ *Yes*
$\mathbf{x}_4$	*Yes*	*No*	*Yes*	*Yes*	*Full*	*$*	*Yes*	*No*	*Thai*	*10–30*	$y_4 =$ *Yes*
$\mathbf{x}_5$	*Yes*	*No*	*Yes*	*No*	*Full*	*$$$*	*No*	*Yes*	*French*	*>60*	$y_5 =$ *No*
$\mathbf{x}_6$	*No*	*Yes*	*No*	*Yes*	*Some*	*$$*	*Yes*	*Yes*	*Italian*	*0–10*	$y_6 =$ *Yes*
$\mathbf{x}_7$	*No*	*Yes*	*No*	*No*	*None*	*$*	*Yes*	*No*	*Burger*	*0–10*	$y_7 =$ *No*
$\mathbf{x}_8$	*No*	*No*	*No*	*Yes*	*Some*	*$$*	*Yes*	*Yes*	*Thai*	*0–10*	$y_8 =$ *Yes*
$\mathbf{x}_9$	*No*	*Yes*	*Yes*	*No*	*Full*	*$*	*Yes*	*No*	*Burger*	*>60*	$y_9 =$ *No*
$\mathbf{x}_{10}$	*Yes*	*Yes*	*Yes*	*Yes*	*Full*	*$$$*	*No*	*Yes*	*Italian*	*10–30*	$y_{10} =$ *No*
$\mathbf{x}_{11}$	*No*	*No*	*No*	*No*	*None*	*$*	*No*	*No*	*Thai*	*0–10*	$y_{11} =$ *No*
$\mathbf{x}_{12}$	*Yes*	*Yes*	*Yes*	*Yes*	*Full*	*$*	*No*	*No*	*Burger*	*30–60*	$y_{12} =$ *Yes*

Features:

1.	Alternate: whether there is a suitable alternative restaurant nearby.
2.	Bar: whether the restaurant has a comfortable bar area to wait in.
3.	Fri/Sat: true on Fridays and Saturdays.
4.	Hungry: whether we are hungry.
5.	Patrons: how many people are in the restaurant (values are None, Some, and Full).
6.	Price: the restaurant's price range ($, $$, $$$).
7.	Raining: whether it is raining outside.
8.	Reservation: whether we made a reservation.
9.	Type: the kind of restaurant (French, Italian, Thai or Burger).
10.	WaitEstimate: the wait estimated by the host (0-10 minutes, 10-30, 30-60, >60).

A possible Decision Tree

- Will I eat at this restaurant?



Core Aspects in Decision Tree & Supervised Learning

- How to automatically find a good hypothesis for training data?
  - This is an algorithmic question, the main topic of computer science
- When do we generalize and do well on unseen data?
  - Learning theory quantifies ability to generalize as a function of the amount of training data and the hypothesis space
  - Occam's razor: use the simplest hypothesis consistent with data!
- Decision trees: find a small decision tree that explains data well
  - NP-hard problem
  - Very nice practical heuristics; top down algorithms, e.g , ID3

Ockham's Razor

- Principle stated by William of Ockham (1285-1347)
- "Entia non sunt multiplicanda praeter necessitatem"
- entities are not to be multiplied beyond necessity

- **Idea**: The simplest consistent explanation is the best
  - Therefore, the smallest decision tree that correctly classifies all of the training examples is best
    - Finding the provably smallest decision tree is NP-hard
    - So instead of constructing the absolute smallest tree consistent with the training examples, construct one that is pretty small

Decision Trees: ID3 algorithm

ID3: Iterative Dichotomiser 3 (Ross Quinlan)

- greedy approach to build a decision tree top down from the root

Algorithm:

- Start with the whole training set and an empty decision tree.
- Pick the “best” feature/attribute
- Split on that feature and recurse on subpartitions.

Decision Trees: ID3 algorithm

ID3 algorithm

node $\leftarrow$ root
repeat
  $A \leftarrow$ the “best” decision attribute for next level nodes
  forall *value a of A* **do**
    add a new descendent node corresponding to attribute a
  end
  Assign training examples to leaf nodes
until *all training examples are perfectly classified*;

Key Question: Which attribute is the best?

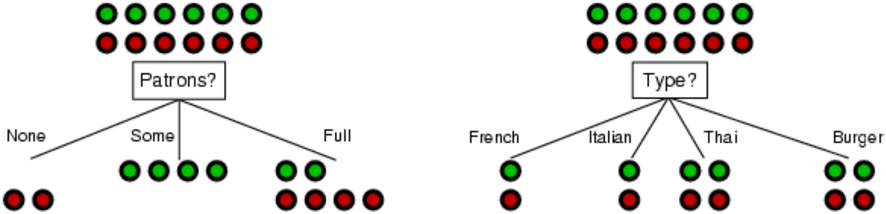
Choosing the Best Attribute

Key Problem : choosing which attribute to split a given set of examples

- Some possibilities are:
  - **Random** Select any attribute at random
  - **Least-Values** Choose the attribute with the smallest number of possible values
  - **Most-Values** Choose the attribute with the largest number of possible values
  - **Max-Gain** Choose the attribute that has the largest expected *information gain*
    - i.e., attribute that results in smallest expected size of subtrees rooted at its children
- The ID3 algorithm uses the Max-Gain method of selecting the best attribute

Choosing an Attribute

- **Idea** a good attribute splits the examples into subsets that are (ideally) “all positive” or “all negative”



- which split is more informative?

Choosing a Good Split

- How can we quantify uncertainty in prediction for a given leaf node?
  - If all examples in leaf have same class: good, low uncertainty
  - If each class has same amount of examples in leaf: bad, high uncertainty
- **Idea**: Use counts at leaves to define probability distributions; use a probabilistic notion of uncertainty to decide splits.
- A brief detour through information theory...

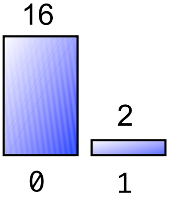
Quantifying Uncertainty

- The entropy of a discrete random variable is a number that quantifies the uncertainty inherent in its possible outcomes.
- The mathematical definition of entropy that we give in a few slides may seem arbitrary, but it can be motivated axiomatically.
- To explain entropy, consider flipping two different coins...

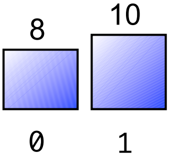
We Flip Two Different Coins

Sequence 1:
0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 1 0 0 ... ?

Sequence 2:
0 1 0 1 0 1 1 1 0 1 0 0 1 1 0 1 0 1 ... ?

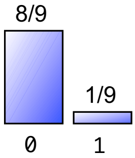


versus

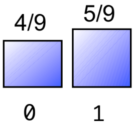


Quantifying Uncertainty

- The entropy of a loaded coin with probability p of heads is given by
$$-plog_2(p) - (1-p)log_2(1-p)$$



$$-\frac{8}{9}\log_2\frac{8}{9} - \frac{1}{9}\log_2\frac{1}{9} \approx \frac{1}{2}$$

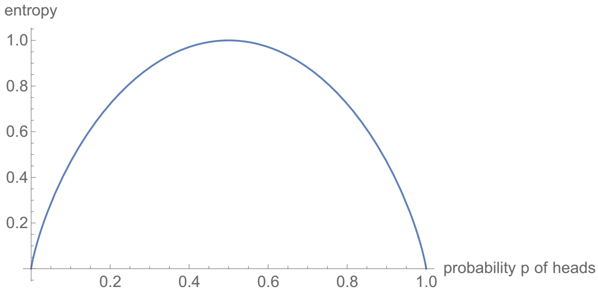


$$-\frac{4}{9}\log_2\frac{4}{9} - \frac{5}{9}\log_2\frac{5}{9} \approx 0.99$$

- Notice: the coin whose outcomes are more certain has a lower entropy.
- In the extreme case $p = 0$ or $p = 1$, we were certain of the outcome before observing. So, we gained no certainty by observing it, i.e., entropy is 0.

Quantifying Uncertainty

- Can also think of entropy as the expected information content of a random draw from a probability distribution.



- Claude Shannon showed: you cannot store the outcome of a random draw using fewer expected bits than the entropy without losing information.
- Interpretation from information theory: expected number of bits needed to encode label of a randomly drawn example in S.
- So units of entropy are bits; a fair coin flip has 1 bit of entropy.

Entropy

- More generally, the entropy of a discrete random variable Y is given by
$$H(Y) = -\sum_{y \in Y} P(y) \log_2 P(y)$$
- “High Entropy”
  - Variable has a uniform like distribution over many outcomes
  - Flat histogram
  - Values sampled from it are less predictable
- “Low Entropy"
  - Distribution is concentrated on only a few outcomes
  - Histogram is concentrated in a few areas
  - Values sampled from it are more predictable

Entropy

- Suppose we observe partial information X about a random variable Y
  - For example, X = sign(Y).
- We want to work towards a definition of the expected amount of information that will be conveyed about Y by observing X.
  - Or equivalently, the expected reduction in our uncertainty about Y after observing X.

Entropy of a Joint Distribution

- Example: X = {Raining, Not raining}, Y = {Cloudy, Not cloudy}

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

$$
\begin{aligned}
H(X,Y) &= -\sum_{x \in X} \sum_{y \in Y} P(x,y) log_2 P(x,y) \\
&= -\frac{24}{100} log_2 \frac{24}{100} - \frac{1}{100} log_2 \frac{1}{100} - \frac{25}{100} log_2 \frac{25}{100} - \frac{50}{100} log_2 \frac{50}{100} \\
&\approx 1.56 bits
\end{aligned}
$$

Specific Conditional Entropy

- Example: X = {Raining, Not raining}, Y = {Cloudy, Not cloudy}

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

- What is the entropy of cloudiness Y, given that it is raining?

$$
\begin{aligned}
H(Y|X=x) &= -\sum_{y \in Y} P(y|x) log_2 P(y|x) \\
&= -\frac{24}{25} log_2 \frac{24}{25} - \frac{1}{25} log_2 \frac{1}{25} \\
&\approx 0.24 bits
\end{aligned}
$$

Conditional Entropy

- Example: X = {Raining, Not raining}, Y = {Cloudy, Not cloudy}

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

- The expected conditional entropy:

$$H(Y|X) = \sum_{x \in X} P(x) H(Y|X = x)$$
$$= -\sum_{x \in X} \sum_{y \in Y} P(x, y) \log_2 p(y|x)$$

Conditional Entropy

- Example: X = {Raining, Not raining}, Y = {Cloudy, Not cloudy}

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

- What is the entropy of cloudiness Y, given the knowledge of whether or not it is raining?

$$\begin{aligned} H(Y|X) &= \sum_{x \in X} P(x) H(Y|X = x) \\ &= \frac{1}{4} H(\text{cloud}|\text{raining}) + \frac{3}{4} H(\text{cloudy}|\text{not raining}) \\ &\approx 0.75 bits \end{aligned}$$

Conditional Entropy

Some useful properties

- H is always non-negative
- Chain rule: $H(X, Y) = H(X|Y) + H(Y) = H(Y|X) + H(X)$
- If X and Y are independent, then X does not affect our uncertainty about Y : $H(Y|X) = H(Y)$
- But knowing Y makes our knowledge of Y certain: $H(Y|Y) = 0$
- By knowing X, we can only decrease uncertainty about Y : $H(Y|X) \leq H(Y)$

Select the next attribute

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

- How much more certain am I about whether it's cloudy if I'm told whether it is raining? My uncertainty in Y minus my expected uncertainty that would remain in Y after seeing X.
- This is called the information gain $IG(Y|X)$ in Y due to X, or the mutual information of Y and X

$$IG(Y|X) = H(Y) - H(Y|X)$$

- If X is completely uninformative about Y : $IG(Y|X) = 0$
- If X is completely informative about Y : $IG(Y|X) = H(Y)$

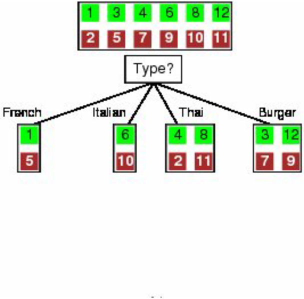
Back to Our Example

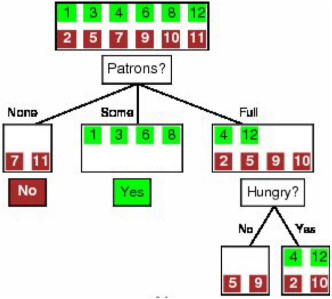
Example	Input Attributes										Goal
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
$\mathbf{x}_1$	Yes	No	No	Yes	Some	$$$	No	Yes	French	0–10	$y_1 =$ Yes
$\mathbf{x}_2$	Yes	No	No	Yes	Full	$	No	No	Thai	30–60	$y_2 =$ No
$\mathbf{x}_3$	No	Yes	No	No	Some	$	No	No	Burger	0–10	$y_3 =$ Yes
$\mathbf{x}_4$	Yes	No	Yes	Yes	Full	$	Yes	No	Thai	10–30	$y_4 =$ Yes
$\mathbf{x}_5$	Yes	No	Yes	No	Full	$$$	No	Yes	French	>60	$y_5 =$ No
$\mathbf{x}_6$	No	Yes	No	Yes	Some	$$	Yes	Yes	Italian	0–10	$y_6 =$ Yes
$\mathbf{x}_7$	No	Yes	No	No	None	$	Yes	No	Burger	0–10	$y_7 =$ No
$\mathbf{x}_8$	No	No	No	Yes	Some	$$	Yes	Yes	Thai	0–10	$y_8 =$ Yes
$\mathbf{x}_9$	No	Yes	Yes	No	Full	$	Yes	No	Burger	>60	$y_9 =$ No
$\mathbf{x}_{10}$	Yes	Yes	Yes	Yes	Full	$$$	No	Yes	Italian	10–30	$y_{10} =$ No
$\mathbf{x}_{11}$	No	No	No	No	None	$	No	No	Thai	0–10	$y_{11} =$ No
$\mathbf{x}_{12}$	Yes	Yes	Yes	Yes	Full	$	No	No	Burger	30–60	$y_{12} =$ Yes

Features:

1.	Alternate: whether there is a suitable alternative restaurant nearby.
2.	Bar: whether the restaurant has a comfortable bar area to wait in.
3.	Fri/Sat: true on Fridays and Saturdays.
4.	Hungry: whether we are hungry.
5.	Patrons: how many people are in the restaurant (values are None, Some, and Full).
6.	Price: the restaurant's price range ($, $$, $$$).
7.	Raining: whether it is raining outside.
8.	Reservation: whether we made a reservation.
9.	Type: the kind of restaurant (French, Italian, Thai or Burger).
10.	WaitEstimate: the wait estimated by the host (0-10 minutes, 10-30, 30-60, >60).

Back to Our Example



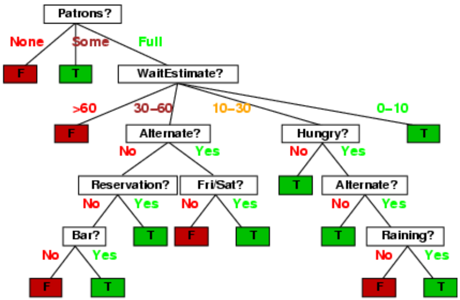


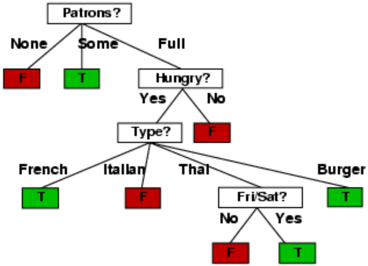
$$IG(Y|X) = H(Y) - H(Y|X)$$

$$IG(Y|type) = 1 - \left[\frac{2}{12}H(Y|Fr.) + \frac{2}{12}H(Y|It.) + \frac{4}{12}H(Y|Thai) + \frac{4}{12}H(Y|Bur.)\right] = 0$$

$$IG(T|Patrons) = 1 - \left[\frac{2}{12}H(Y|None) + \frac{4}{12}H(Y|Some) + \frac{6}{12}H(Y|Full)\right] \approx 0,541$$

Which Tree is Better?





Decision Trees: ID3 algorithm

ID3 algorithm

node $\leftarrow$ root
repeat
    forall *attributes* A **do**
        Calculate $IG(Y|A) = H(Y) - \sum_{a \in A} P(a)(Y|a)$
    end
    $A^* \leftarrow \arg\max_A IG(Y|A)$
    forall *value* a *of* A^* **do**
        add a new descendent node corresponding to each $a \in A^*$
    end
    Assign training examples to new nodes according to the value of attribute A^*
until *all training examples are perfectly classified*;

Decision Tress Miscellany

- Problems
  - Exponentially less data at lower levels
  - Big trees can overfit data
  - Greedy algorithms don't (necessarily) yield the global optmimum
- Handling continuous attributes
  - Split based on a threshold, chosen to maximize information gain
- Decision trees can also be used for regression on real-valued outputs. Choose splits to minimize squared error, rather than maximize information gain

Temporary page!

LaTeX was unable to guess the total number of pages correctly
was some unprocessed data that should have been added to
page this extra page has been added to receive it.
If you rerun the document (without altering it) this surplus pa
away, because LaTeX now knows how many pages to expect fo
document.