# hiesarclical set of rules Decision Trees <br> Sourav Sen Gupta <br> CDS 2015 | PGDBA | 6 Oct 2015 

## 

## Deciding factors may be

## $\simeq$ heuristic rules

$\longrightarrow$ If there are patrons (people inside) — Yes/No If you are hungry already - Yes / No
$\longrightarrow$ Alternative options in the vicinity - Yes / No
The estimated time for waiting - In minutes
$\longrightarrow$ If you already have a reservation — Yes/No
$\longrightarrow$ If it is a Friday/Saturday night — Yes/No
If there is a Bar area to wait - Yes/No
The range of price at the place - High/Medium/Low
$\longrightarrow I f$ it is raining at the time - Yes/No
The genre of cuisine - French, Italian, Thai, Burger


Ref. - "Artificial Intelligence : A Modern Approach" - Stuart J. Russell and Peter Norvig

ML Pipeline


## Training Data

| Example | $\downarrow$ 侕 $\downarrow$ |  |  | $f$ | Attributes |  | $\forall$ |  | $t$ |  | $\left[\begin{array}{c}\text { Goal } \\ \text { WillWait }\end{array}\right.$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | Alt | Bar | Fri | Hun | Pat | Price | Rain | Res | Type | Est |  |
| $X_{1}$ | Yes | No | No | Yes | Some | \$\$\$ | No | Yes | French | 0-10 | Yes |
| $X_{2}$ | Yes | No | No | Yes | Full | \$ | No | No | Thai | 30-60 | NO |
| ${ }^{1}$ | No | Yes | No | No | Some | \$ | No | No | Burger | 0-10 | Yes |
| ${ }_{4}$ | Yes | No | Yes | Yes | Full | \$ | Yes | No | Thai | 10-30 | Tes |
| $\mathrm{N}_{5}$ | Yes | No | Yes | No | Full | \$\$\$ | No | Yes | French | $>60$ | NO |
| ${ }^{1}$ | No | Yes | No | Yes | Some | \$\$ | Yes | Yes | Italian | 0-10 | Yes |
| $\mathrm{X}_{7}$ | No | Yes | No | No | None | \$ | Yes | No | Burger | 0-10 | NO |
| $\chi_{8}$ | No | No | No | Yes | Some | \$\$ | Yes | Yes | Thai | 0-10 | Yes |
| 0 | No | Yes | Yes | No | Full | \$ | Yes | No | Burger | $>60$ | 150 |
| - | Yes | Yes | Yes | Yes | Full | \$ \$ \$ | No | Yes | Italian | 10-30 | No |
| $\left(X_{11}\right)$ | No | No | No | No | None | \$ | No | No | Thai | 0-10 | (10) |
| $N=28 x_{12}$ | Yes | Yes | Yes | Yes | Full | \$ | No | No | Burger | 30-60 | Yes |
| TEST | Yes | Yes | Yes | No | Full | \$\$\$ | No | No | Thai | 30-60 | ? |



## Entropy \& Information Gain

-Why a logarithm function?

$$
\log \left(p_{1} \times p_{2}\right)=\log \left(p_{1}\right)+\log \left(p_{2}\right)
$$

- Shannon Entropy:

Issue: increasing number of events shrinks the probability.
Solution: use logarithm of probability instead and take the average.

## How do we construct the tree ? i.e., how to pick attribute (nodes)?

Idea: a good attribute splits the examples into subsets that are (ideally) "all positive" or "all negative"

## 000000 <br> 000000

For a training set containing $p$ positive examples and $n$ negatiye examples, we have:

$$
H\left(\frac{p}{p+n} \frac{(n)}{p+n}\right)=-\frac{p}{p+n} \log _{2} \frac{p}{p+n}-\frac{n}{p+n} \log _{2} \frac{n}{p+n}
$$

## Information Gain

Reduction in Eutopy
Informaif = Parent Entropy - E(Child Entropy)

One notion of entropy is that of Shannon Entropy

$$
H(\mathcal{S})=-\sum_{c \in \mathcal{C}} p(c) \log (p(c))
$$

# Come Gan 

7 | 1 | 3 | 4 | 6 | 8 | 12 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| 2 | 5 | 7 | 9 | 10 | 11 |



$$
\begin{array}{cccc}
p=1 / 6 & p=1 / 6 & p=1 / 3 & p=1 / 3 \\
H=1 & H=1 & H=1 & H=1 \\
\hline
\end{array}
$$

## Parent Entropy

$H=-\frac{1}{2} \log _{2} \frac{1}{2}-\frac{1}{2} \log _{2} \frac{1}{2}=1$
E(Child Entropy)

$$
\begin{aligned}
& H=\frac{1}{6} \cdot 1+\frac{1}{6} \cdot 1+\frac{1}{3} \cdot 1+\frac{1}{3} \cdot 1
\end{aligned}
$$

| 1 | 3 | 4 | 6 | 8 | 12 |
| :--- | :--- | :--- | :--- | :--- | :--- |
| 2 | 5 | 7 | 9 | 10 |  | 257910 11



E(Child Entropy)

$$
H=\frac{1}{6} \cdot 0+\frac{1}{3} \cdot 0+\frac{1}{2} \cdot 0.918
$$

## How to pick nodes?

$\square$ A chosen attribute $A$, with $\underline{K}$ distinct values, divides the training set $E$ into subsets $E_{1}, \ldots, E_{K}$.
The Expected Entropy (EH) remaining after trying attribute $A$ (with branches $i=1,2, \ldots, \boldsymbol{K}$ ) is

$$
E H(A)=\sum_{i=1}^{K} \frac{p_{i}+n_{i}}{p+n_{i}} H\left(\frac{p_{i}}{p_{i}+n_{i}}, \frac{n_{i}}{p_{i}+n_{i}}\right)
$$

Information gain (I) or reduction in entropy for this attribute is:

$$
I(A)=H\left(\frac{p}{p+n}, \frac{n}{p+n}\right)-E H(A)^{\wedge}
$$

= Entropy in the parent node - remaining Expected Entropy in the child nodes



Classification Tree


## Classification tree



- How to deal with continuous features?
- Create the splits randomly
- Compute information gain for each split
- Choose the one with maximum gain

A generic data point is denoted by a vector $\mathbf{v}=\left(x_{1}, x_{2}, \cdots, x_{d}\right)$


## Classification tree



A generic data point is denoted by a vector $\mathbf{v}=\left(x_{1}, x_{2}, \cdots, x_{d}\right)$

$$
\mathcal{S}_{j}=\mathcal{S}_{j}^{\mathrm{L}} \cup \mathcal{S}_{j}^{\mathrm{R}}
$$

- Note that the histogram shows the posterior distribution for each class:

$$
p(\text { Class } \mid \text { Data })
$$

## Choosing Split



## Expressiveness of decision trees

The tree on previous slide is a Boolean decision tree:
$\checkmark$ the decision is a binary variable (true, false), and
$\boldsymbol{v}$ the attributes are discrete.
$\boldsymbol{\checkmark}$ It returns ally iff the input attributes satisfy one of the paths leading to an ally leaf:

$$
\text { ally } \Leftrightarrow(\text { neck }=\text { tie } \wedge \text { smile }=\text { yes }) \vee(\text { neck }=\neg \text { tie } \wedge \text { body }=\text { triangle }),
$$

i.e. in general
$\mathbf{x}$ Goal $\Leftrightarrow\left(\right.$ Path $_{1} \vee$ Path $\left._{2} \vee \ldots\right)$, where
$\boldsymbol{x}$ Path is a conjuction of attribute-value tests, i.e.
$\boldsymbol{x}$ the tree is equivalent to a DNF of a function.
Any function in propositional logic can be expressed as a dec. tree.
$\checkmark$ Trees are a suitable representation for some functions and unsuitable for others.
$\checkmark$ What is the cardinality of the set of Boolean functions of $n$ attributes?
$\boldsymbol{x}$ It is equal to the number of truth tables that can be created with $n$ attributes.
$\boldsymbol{x}$ The truth table has $2^{n}$ rows, i.e. there is $2^{2^{n}}$ different functions
$\boldsymbol{x}$ The set of trees is even larger; several trees represent the same function.
$\boldsymbol{\sim}$ We need a clever algorithm to find good hypotheses (trees) in such a large space.

## Learning a Decision Tree



## A computer game

## Example 2:

Some robots changed their attitudes:


No obvious simple rule.
How to build a decision tree discriminating the 2 robot classes?

## Alternative hypotheses

Example 2: Attribute description:



## How to choose the best tree?

We want a tree that is
$\checkmark$ consistent with the data,
$\checkmark$ is as small as possible, and
$\checkmark$ which also works for new data.
Consistent with data?
$\checkmark$ All 3 trees are consistent.
Small?

$\checkmark$ The right-hand side one is the simplest one: |  | left | middle | right |
| :--- | :---: | :---: | :---: |
|  | depth | 2 | 2 |
| leaves | 4 | 4 | 3 |
|  | conditions | 3 | 2 |

Will it work for new data?
$\checkmark$ We have no idea!
$\checkmark$ We need a set of new testing data (different data from the same source).

## Learning a Decision Tree

It is an intractable problem to find the smallest consistent tree among $>2^{2^{n}}$ trees.
We can find approximate solution: a small (but not the smallest) consistent tree.
Top-Down Induction of Decision Trees (TDIDT):
$\checkmark$ A greedy divide-and-conquer strategy.
$\boldsymbol{v}$ Progress:

1. Test the most important attribute.
2. Divide the data set using the attribute values.
3. For each subset, build an independent tree (recursion).
$\boldsymbol{\checkmark}$ "Most important attribute": attribute that makes the most difference to the classification.
$\checkmark$ All paths in the tree will be short, the tree will be shallow

## Attribute importance

| head |  | body |  | smile |  | neck |  | holds |  | class |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| triangle |  | circle |  | yes |  | tie |  | nothing |  | ally |
| triangle |  | triangle |  | no |  | nothing |  | ball |  | ally |
| circle |  | triangle |  | yes |  | nothing |  | flower |  | ally |
| circle |  | circle |  | yes |  | tie |  | nothing |  | ally |
| triangle |  | square |  | no |  | tie |  | ball |  | enemy |
| circle |  | square |  | no |  | tie |  | sword |  | enemy |
| square |  | square |  | yes |  | bow |  | nothing |  | enemy |
| circle |  | circle |  | no |  | bow |  | sword |  | enemy |
| triangle: | 2:1 | triangle: | 2:0 | yes: | 3:1 | tie: | 2:2 | ball: | 1:1 |  |
| circle: | 2:2 | circle: | 2:1 | no: | 1:3 | bow: | 0:2 | sword: | 0:2 |  |
| square: | 0:1 | square: | 0:3 |  |  | nothing: | 2:0 | flower: | 1:0 |  |
|  |  |  |  |  |  |  |  | nothing: | 2:1 |  |

A perfect attribute divides the examples into sets each of which contain only a single class. (Do you remember the simply created perfect attribute from Example 1?)
A useless attribute divides the examples into sets each of which contains the same distribution of classes as the set before splitting.
None of the above attributes is perfect or useless. Some are more useful than others.

## Choosing the test attribute

Information gain:
$\boldsymbol{\nu}$ Formalization of the terms "useless", "perfect", "more useful".
$\boldsymbol{\checkmark}$ Based on entropy, a measure of the uncertainty of a random variable $V$ with possible values $v_{i}$ :

$$
H(V)=-\sum_{i} p\left(v_{i}\right) \log _{2} p\left(v_{i}\right)
$$

$\checkmark$ Entropy of the target class $C$ measured on a data set $S$ (a finite-sample estimate of the true entropy):

$$
H(C, S)=-\sum_{i} p\left(c_{i}\right) \log _{2} p\left(c_{i}\right)
$$

where $p\left(c_{i}\right)=\frac{N_{S}\left(c_{i}\right)}{|S|}$, and $N_{S}\left(c_{i}\right)$ is the number of examples in $S$ that belong to class $c_{i}$.
$\checkmark$ The entropy of the target class $C$ remaining in the data set $S$ after splitting into subsets $S_{k}$ using values of attribute $A$ (weighted average of the entropies in individual subsets):

$$
H(C, S, A)=\sum_{k} p\left(S_{k}\right) H\left(C, S_{k}\right), \quad \text { where } p\left(S_{k}\right)=\frac{\left|S_{k}\right|}{|S|}
$$

$\checkmark$ The information gain of attribute $A$ for a data set $S$ is

$$
\operatorname{Gain}(A, S)=H(C, S)-H(C, S, A) .
$$

Choose the attribute with the highest information gain, i.e. the attribute with the lowest $H(C, S, A)$.

## Choosing the test attribute (special case: binary classification)

$\checkmark$ For a Boolean random variable $V$ which is true with probability $q$, we can define:

$$
H_{B}(q)=-q \log _{2} q-(1-q) \log _{2}(1-q)
$$

$\checkmark$ Entropy of the target class $C$ measured on a data set $S$ with $N_{p}$ positive and $N_{n}$ negative examples:

$$
H(C, S)=H_{B}\left(\frac{N_{p}}{N_{p}+N_{n}}\right)=H_{B}\left(\frac{N_{p}}{|S|}\right)
$$

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## Choosing the test attribute (example)

| head |  | body |  | smile |  | neck |  | holds |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
| triangle: | $2: 1$ | triangle: | $2: 0$ | yes: | $3: 1$ | tie: | $2: 2$ | ball: |
| circle: | $2: 2$ | circle: | $2: 1$ | no: | $1: 3$ | bow: | $0: 2$ | sword: |
| square: | $0: 1$ | square: | $0: 3$ |  |  | nothing: | $2: 0$ | flower: |
|  |  |  |  |  |  |  |  | nothing: |
|  |  |  |  |  |  |  |  |  |

## head:

$p\left(S_{\text {head=tri }}\right)=\frac{3}{8} ; H\left(C, S_{\text {head=tri }}\right)=H_{B}\left(\frac{2}{2+1}\right)=0.92$
$p\left(S_{\text {head=cir }}\right)=\frac{4}{8} ; H\left(C, S_{\text {head=cir }}\right)=H_{B}\left(\frac{2}{2+2}\right)=1$
$p\left(S_{\text {head=sq }}\right)=\frac{1}{8} ; H\left(C, S_{\text {head }=\text { sq }}\right)=H_{B}\left(\frac{0}{0+1}\right)=0$
$H(C, S$, head $)=\frac{3}{8} \cdot 0.92+\frac{4}{8} \cdot 1+\frac{1}{8} \cdot 0=0.84$
Gain $($ head, $S)=1-0.84=0.16$
body:
$p\left(S_{\text {body=tri }}\right)=\frac{2}{8} ; H\left(C, S_{\text {body }}\right.$ tri $)=H_{B}\left(\frac{2}{2+0}\right)=0$
$p\left(S_{\text {body=cir }}\right)=\frac{3}{8} ; H\left(C, S_{\text {body=cir }}\right)=H_{B}\left(\frac{2}{2+1}\right)=0.92$
$p\left(S_{\text {body=sq }}\right)=\frac{3}{8} ; H\left(C, S_{\text {body }=\text { sq }}\right)=H_{B}\left(\frac{0}{0+3}\right)=0$
$H(C, S$, bod $y)=\frac{2}{8} \cdot 0+\frac{3}{8} \cdot 0.92+\frac{3}{8} \cdot 0=0.35$
$\operatorname{Gain}($ body,$S)=1-0.35=0.65$
smile:
$p\left(S_{\text {smile }=\text { yes }}\right)=\frac{4}{8} ; H\left(C, S_{\text {yes }}\right)=H_{B}\left(\frac{3}{3+1}\right)=0.81$
$p\left(S_{\text {smile=no }}\right)=\frac{4}{8} ; H\left(C, S_{\mathrm{no}}\right)=H_{B}\left(\frac{1}{1+3}\right)=0.81$
$H(C, S$, smile $)=\frac{4}{8} \cdot 0.81+\frac{4}{8} \cdot 0.81+\frac{3}{8} \cdot 0=0.81$
$\operatorname{Gain}($ smile,S $)=1-0.81=0.19$
neck:
$p\left(S_{\text {neck=tie }}\right)=\frac{4}{8} ; H\left(C, S_{\text {neck=tie }}\right)=H_{B}\left(\frac{2}{2+2}\right)=1$
$p\left(S_{\text {neck=bow }}\right)=\frac{2}{8} ; H\left(C, S_{\text {neck=bow }}\right)=H_{B}\left(\frac{0}{0+2}\right)=0$
$p\left(S_{\text {neck=no }}\right)=\frac{2}{8} ; H\left(C, S_{\text {neck=no }}\right)=H_{B}\left(\frac{2}{2+0}\right)=0$
$H(C, S$, neck $)=\frac{4}{8} \cdot 1+\frac{2}{8} \cdot 0+\frac{2}{8} \cdot 0=0.5$
$\operatorname{Gain}($ neck,$S)=1-0.5=0.5$

## holds:

$p\left(S_{\text {holds }=\text { ball }}\right)=\frac{2}{8} ; H\left(C, S_{\text {holds=ball }}\right)=H_{B}\left(\frac{1}{1+1}\right)=1$
$p\left(S_{\text {holds=swo }}\right)=\frac{2}{8} ; H\left(C, S_{\text {holds=swo }}\right)=H_{B}\left(\frac{0}{0+2}\right)=0$
$p\left(S_{\text {holds }}=\right.$ flo $)=\frac{1}{8} ; H\left(C, S_{\text {holds=flo }}\right)=H_{B}\left(\frac{1}{1+0}\right)=0$
$p\left(S_{\text {holds=no }}\right)=\frac{3}{8} ; H\left(C, S_{\text {holds=no }}\right)=H_{B}\left(\frac{2}{2+1}\right)=0.92$
$H(C, S$, holds $)=\frac{2}{8} \cdot 1+\frac{2}{8} \cdot 0+\frac{1}{8} \cdot 0+\frac{3}{8} \cdot 0.92=0.6$
Gain $($ holds,$S)=1-0.6^{8}=0.4$
The body attribute
$\checkmark$ brings us the largest information gain, thus
$\checkmark$ it shall be chosen for the first test in the tree!

## Entropy gain toy example

At each split we are going to choose the feature that gives the highest information gain.

| $\mathbf{x}^{1}$ | $\mathbf{x}^{2}$ | Y |
| :---: | :---: | :---: |
| T | T | T |
| T | F | T |
| T | T | T |
| T | F | T |
| F | T | T |
| F | F | F |
| F | T | F |
| F | F | F |

Figure 6: 2 possible features to split by

$$
\begin{aligned}
H\left(Y \mid X^{1}\right)=\frac{1}{2} H\left(Y \mid X^{1}=T\right)+\frac{1}{2} H\left(Y \mid X^{1}\right. & =F)=0+\frac{1}{2}\left(\frac{1}{4} \log _{2} \frac{1}{4}+\frac{3}{4} \log _{2} \frac{3}{4}\right) \approx .405 \\
I G\left(X^{1}\right) & =H(Y)-H\left(Y \mid X^{1}\right)=.954-.405=.549
\end{aligned}
$$

$$
\begin{array}{r}
H\left(Y \mid X^{2}\right)=\frac{1}{2} H\left(Y \mid X^{2}=T\right)+\frac{1}{2} H\left(Y \mid X^{2}=F\right)=\frac{1}{2}\left(\frac{1}{4} \log _{2} \frac{1}{4}+\frac{3}{4} \log _{2} \frac{3}{4}\right)+\frac{1}{2}\left(\frac{1}{2} \log _{2} \frac{1}{2}+\frac{1}{2} \log _{2} \frac{1}{2}\right) \approx .905 \\
I G\left(X^{2}\right)=H(Y)-H\left(Y \mid X^{2}\right)=.954-.905=.049
\end{array}
$$

## Data Partition Rules


$x_{1}=$ word count

- $x_{1}, x_{2}=$ data features
- Each path in the tree corresponds to a region
- Deeper paths correspond to smaller regions


## Data Partition Rules



## Data Partition Rules





## Walkthrough Decision Tree Example

| mpg | cylinders | displacement | horsepower | weight | acceleration | modelyear | maker |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| good | 4 | low | low | low | high | 75to78 | asia |
| bad | 6 | medium | medium | medium | medium | 70to74 | america |
| bad | 4 | medium | medium | medium | low | 75to78 | europe |
| bad | 8 | high | high | high | low | 70to74 | america |
| bad | 6 | medium | medium | medium | medium | 70to74 | america |
| bad | 4 | low | medium | low | medium | 70to74 | asia |
| bad | 4 | low | medium | low | low | 70to74 | asia |
| bad | 8 | high | high | high | low | 75to78 | america |
| : | : | : | : | : | : | : | : |
| : | : | : | : | : | : | : | : |
| : | : | : | : | : | : | : | : |
| bad |  | high | high | high | low | 70to74 | america |
| good | 8 | high | medium | high | high | 79to83 | america |
| bad | 8 | high | high | high | low | 75to78 | america |
| good | 4 | low | low | low | low | 79to83 | america |
| bad | 6 | medium | medium | medium | high | 75 to 78 | america |
| good | 4 | medium | low | low | low | 79to83 | america |
| good | 4 | low | low | medium | high | 79t083 | america |
| bad |  | high | high | high | low | 70to74 | america |
| good | 4 | low | medium | low | medium | 75to78 | europe |
| bad |  | medium | medium | medium | medium | 75to78 | europe |

## 40 Records

- Data (matrix) example : automobiles
- Target : mpg $\in\{$ good, bad\} - 2 class /binary problem


## Decision Tree Split



- Split by feature "cylinders", using feature values for branches


## Decision Tree Splits



- each terminal leaf is labeled by majority (at that leaf). This leaf-label is used for prediction.


## Decision Tree Splits



## Prediction with a tree

## - testpoint:

- cylinder=4
- maker=asia
- horsepower=low
- weight=low
- displacement=medium
- modelyear=75to78


## Regression Tree

Variauce/squark ensor instead of Information

- same tree structure, split criteria Gain
- assume numerical labels
- for each terminal node compute the node label (predicted value) and the mean square error

Estimate a predicted value per tree node

$$
g_{m}=\frac{\sum_{t \in \chi_{m}} y_{t}}{\left|\chi_{m}\right|}
$$

Calculate mean square error

$$
E_{m}=\frac{\sum_{t \in \chi_{m}}\left(y_{t}-g_{m}\right)^{2}}{\left|\chi_{m}\right|}
$$

- choose a split criteria to minimize the weighted error at children nodes


## Regression Tree


labels: 1, 2, 2, 3
labels: 10, 12, 14, 15

$$
\begin{array}{r}
g=\frac{10+12+14+15}{4}=12.75 \\
\text { Error }=\sum_{i}\left(\text { label }_{i}-g\right)^{2}=14.75
\end{array}
$$

- choose a split criteria to minimize the weighted or total error at children nodes
- in the example total error after the split is $14.75+$ $2=16.75$


## Prediction with a tree

- for each test datapoint $x=\left(x^{1}, x^{2}, \ldots, x^{d}\right)$ follow the corresponding path to reach a terminal node $n$
- predict the value/label associated with node $n$


## Overfitting

- decision trees can overfit quite badly
- in fact they are designed to do so due to high complexity of the produced model
- if a decision tree training error doesn't approach zero, it means that data is inconsistent
- 
- some ideas to prevent overfitting:
- create more than one tree, each using a different subset of features; average/vote predictions
- do not split nodes in the tree that have very few datapoints (for example less than 10)
- only split if the improvement is massive


## Pruning

- done also to prevent overfitting
- construct a full decision tree
- then walk back from the leaves and decide to "merge" overfitting nodes
- when split complexity overwhelms the gain obtained by the spit

