Decision Trees

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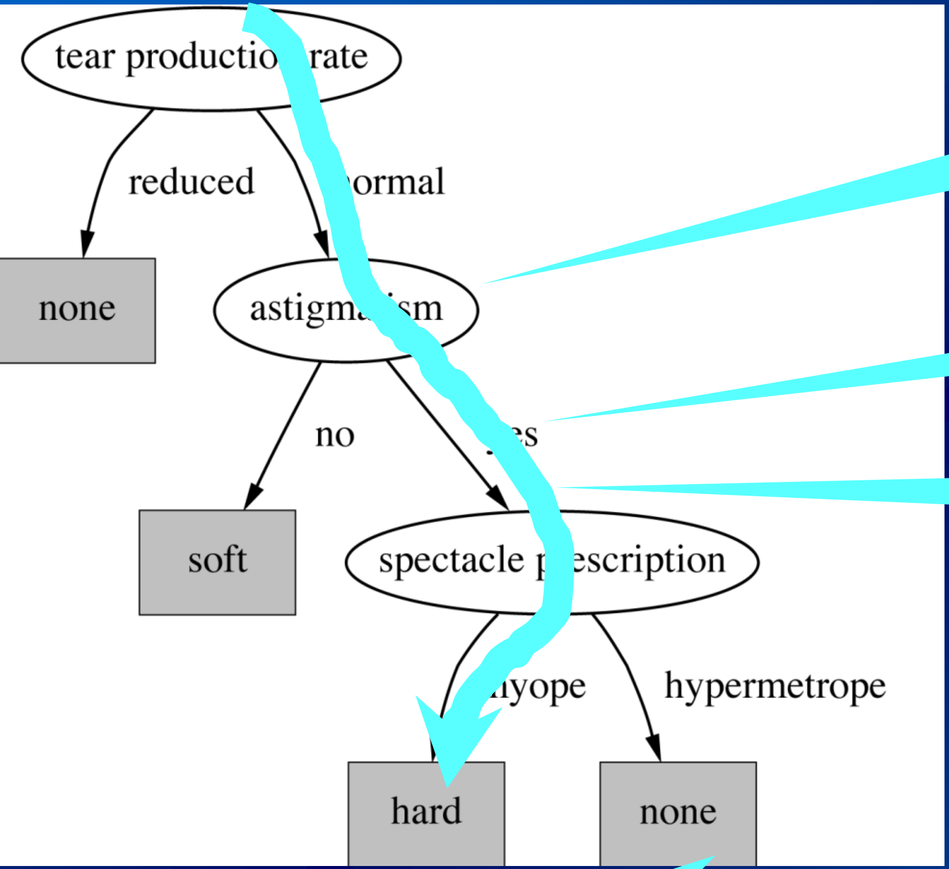
Decision Trees

- **Predict a class variable**
- Visual output self-understandable

Decision trees

Model the process of deciding to which class belongs a new example of the domain



Internal nodes: Variables

Branches: modalities

Paths: Inducted decisions

Leafs: Predicted class

Associated classification rules

If tear prod rate=normal ***and***

astigmatism= yes ***and***

spectacle presciption=myope

then hard lent

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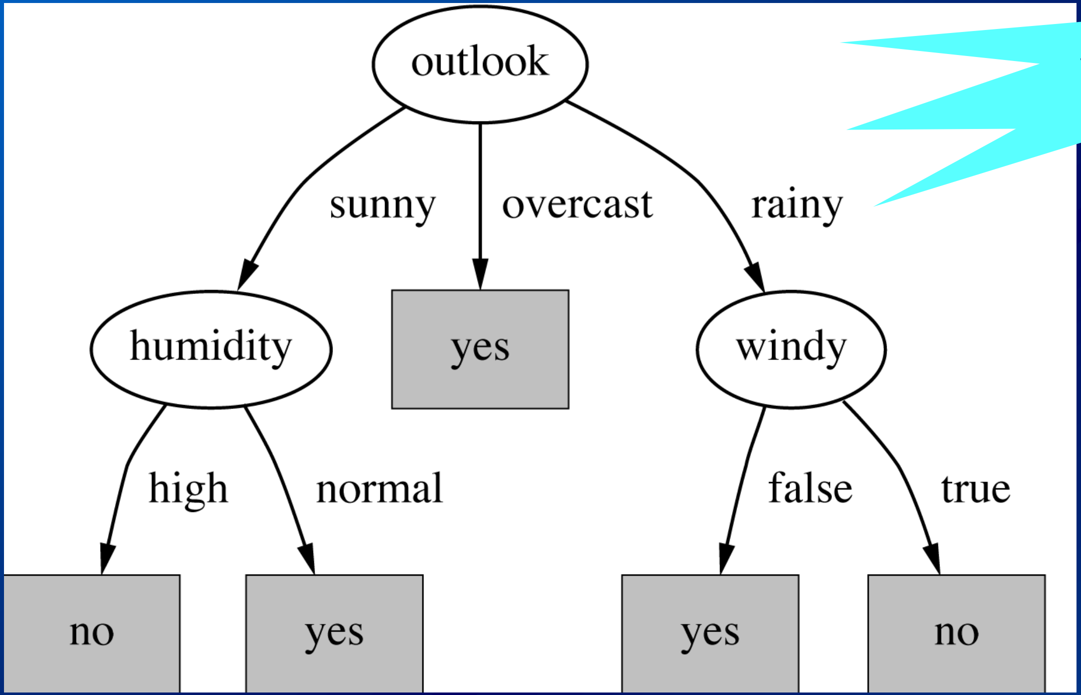
Decision Tree: example 2



Easy to understand

Decision tree for the weather data

Construction:

- Top-down strategy
- Which spliting variable?
- Which branches?
- How to label leafs?

Leafs: Voting

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Decision Trees

- Many models:
  - For numerical/qualitative response variables
  - For binary, nominal, ordinal, numerical explanatory variables
  - Binary tree/multiway-tree

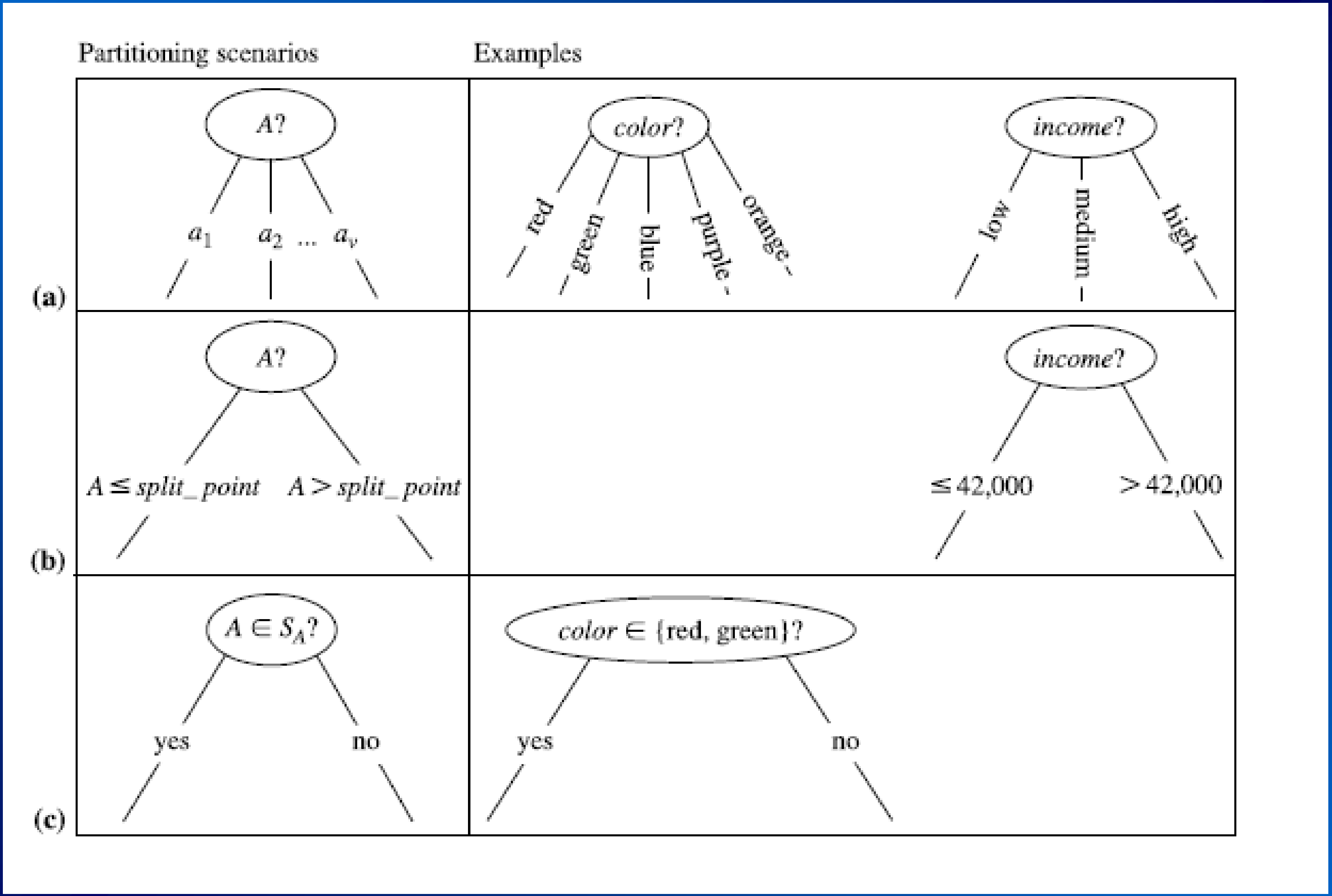
  - Split criterion (information gain, gini index…)
  - Stop criterion (pre-prunning, post-prunning)

ID3, CART (previous AID, CHAID…)

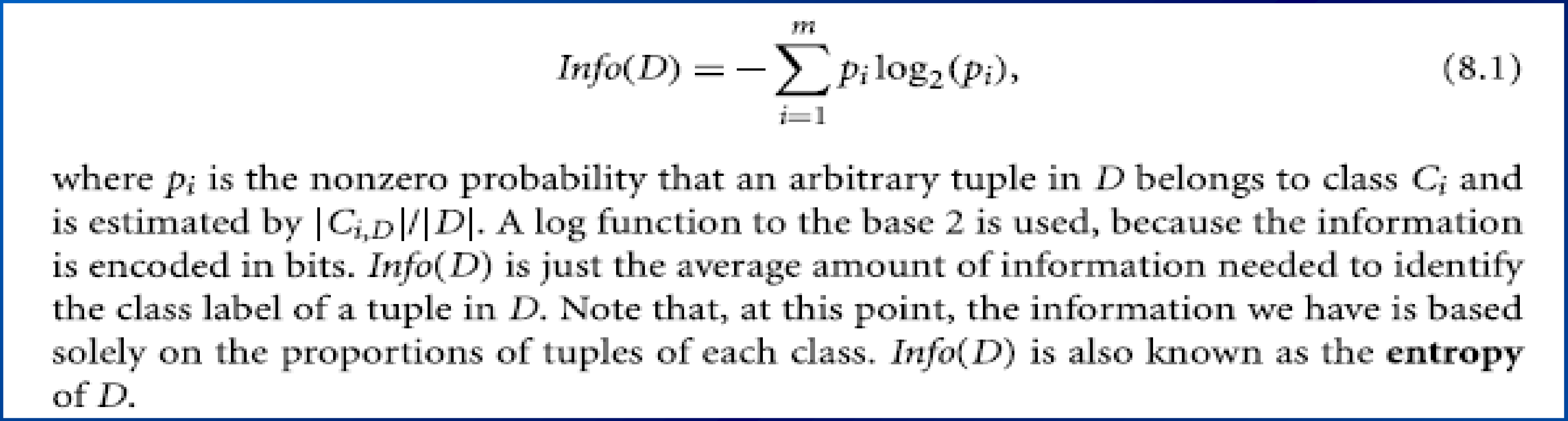
Decision Trees

- General algorithm:
  - Set all individuals at the root node
  - Optimize split in children nodes
  - For every child: decide between
    - Continue splitting (repeating process)
    - Stop

Decision Trees

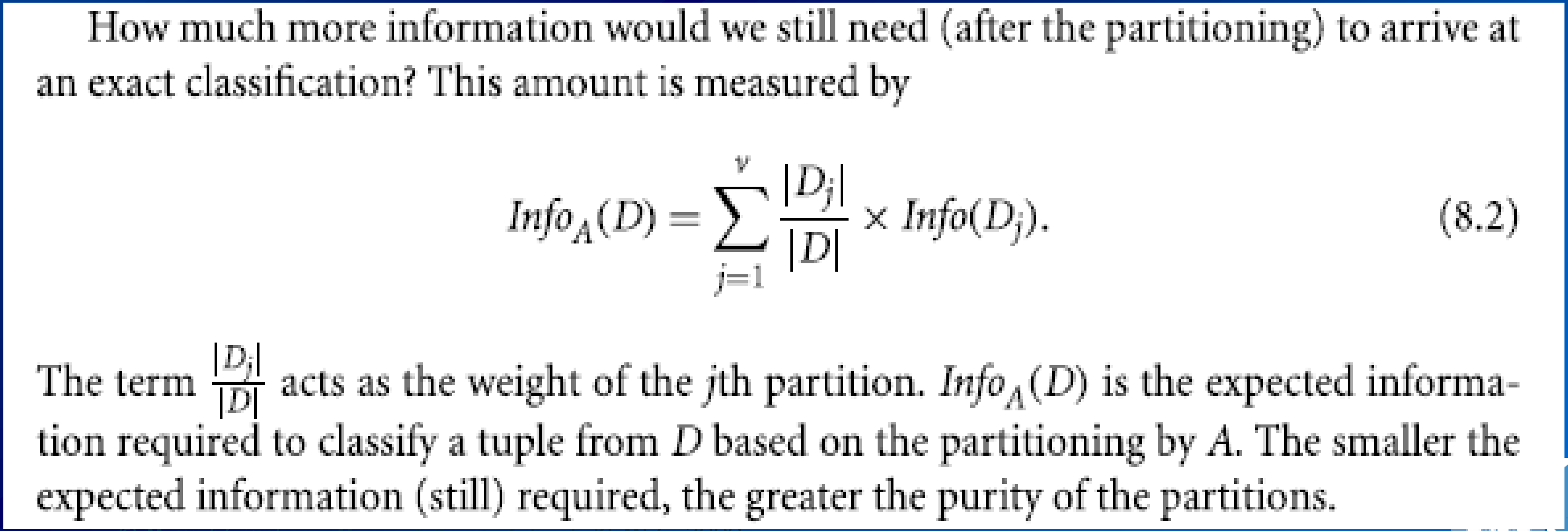


ID3: Entropy & Information Gain



$$Info(D) = -\sum_{i=1}^{m} p_i \log_2(p_i), \tag{8.1}$$

where p_i is the nonzero probability that an arbitrary tuple in D belongs to class C_i and is estimated by $|C_{i,D}|/|D|$. A log function to the base 2 is used, because the information is encoded in bits. $Info(D)$ is just the average amount of information needed to identify the class label of a tuple in D. Note that, at this point, the information we have is based solely on the proportions of tuples of each class. $Info(D)$ is also known as the **entropy** of D.



How much more information would we still need (after the partitioning) to arrive at an exact classification? This amount is measured by

$$Info_A(D) = \sum_{j=1}^{v} \frac{|D_j|}{|D|} \times Info(D_j). \tag{8.2}$$

The term $\frac{|D_j|}{|D|}$ acts as the weight of the jth partition. $Info_A(D)$ is the expected information required to classify a tuple from D based on the partitioning by A. The smaller the expected information (still) required, the greater the purity of the partitions.

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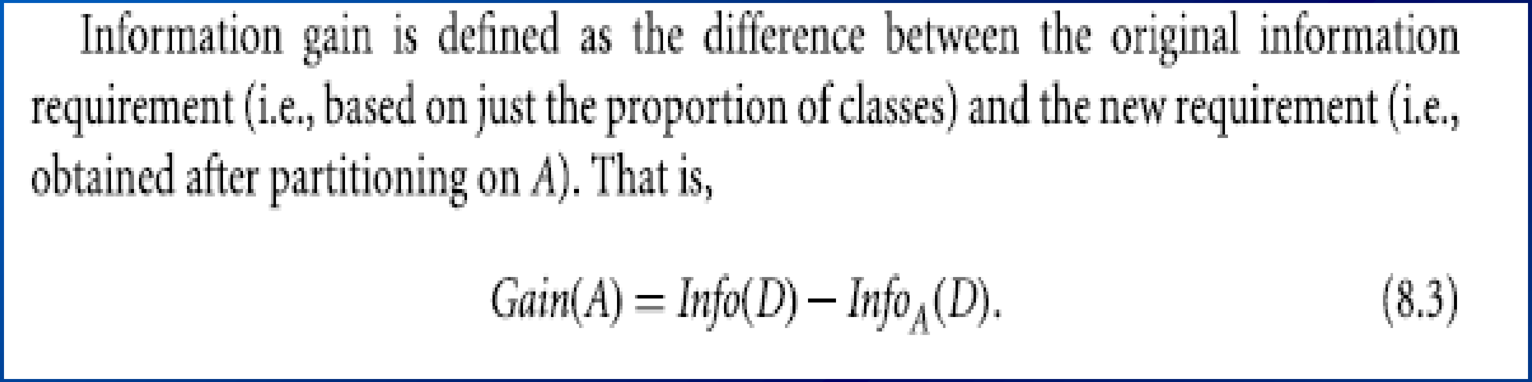
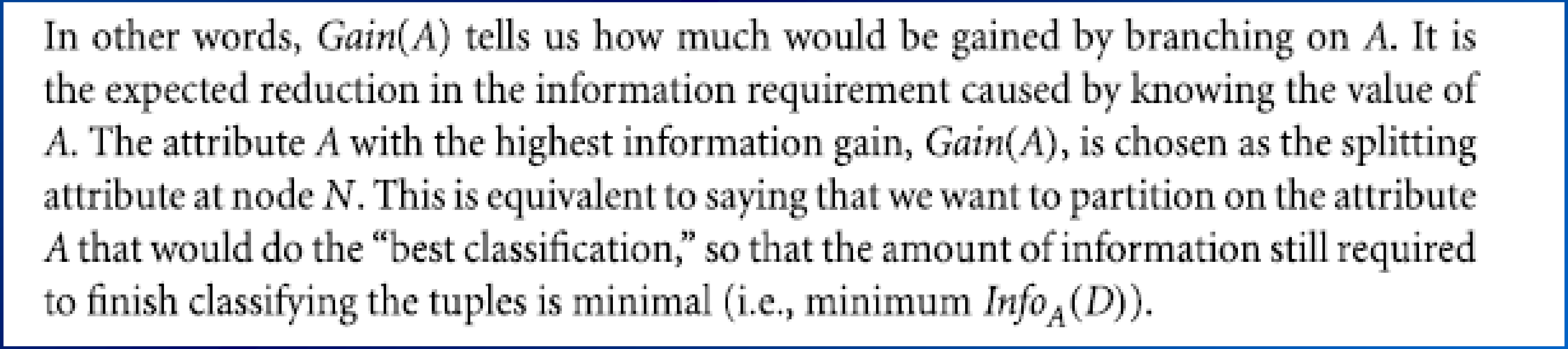
ID3: Entropy & Information Gain



Information gain is defined as the difference between the original information requirement (i.e., based on just the proportion of classes) and the new requirement (i.e., obtained after partitioning on A). That is,

$$Gain(A) = Info(D) - Info_A(D). \quad (8.3)$$



In other words, $Gain(A)$ tells us how much would be gained by branching on A. It is the expected reduction in the information requirement caused by knowing the value of A. The attribute A with the highest information gain, $Gain(A)$, is chosen as the splitting attribute at node N. This is equivalent to saying that we want to partition on the attribute A that would do the "best classification," so that the amount of information still required to finish classifying the tuples is minimal (i.e., minimum $Info_A(D)$).

ID3: Entropy & Information Gain

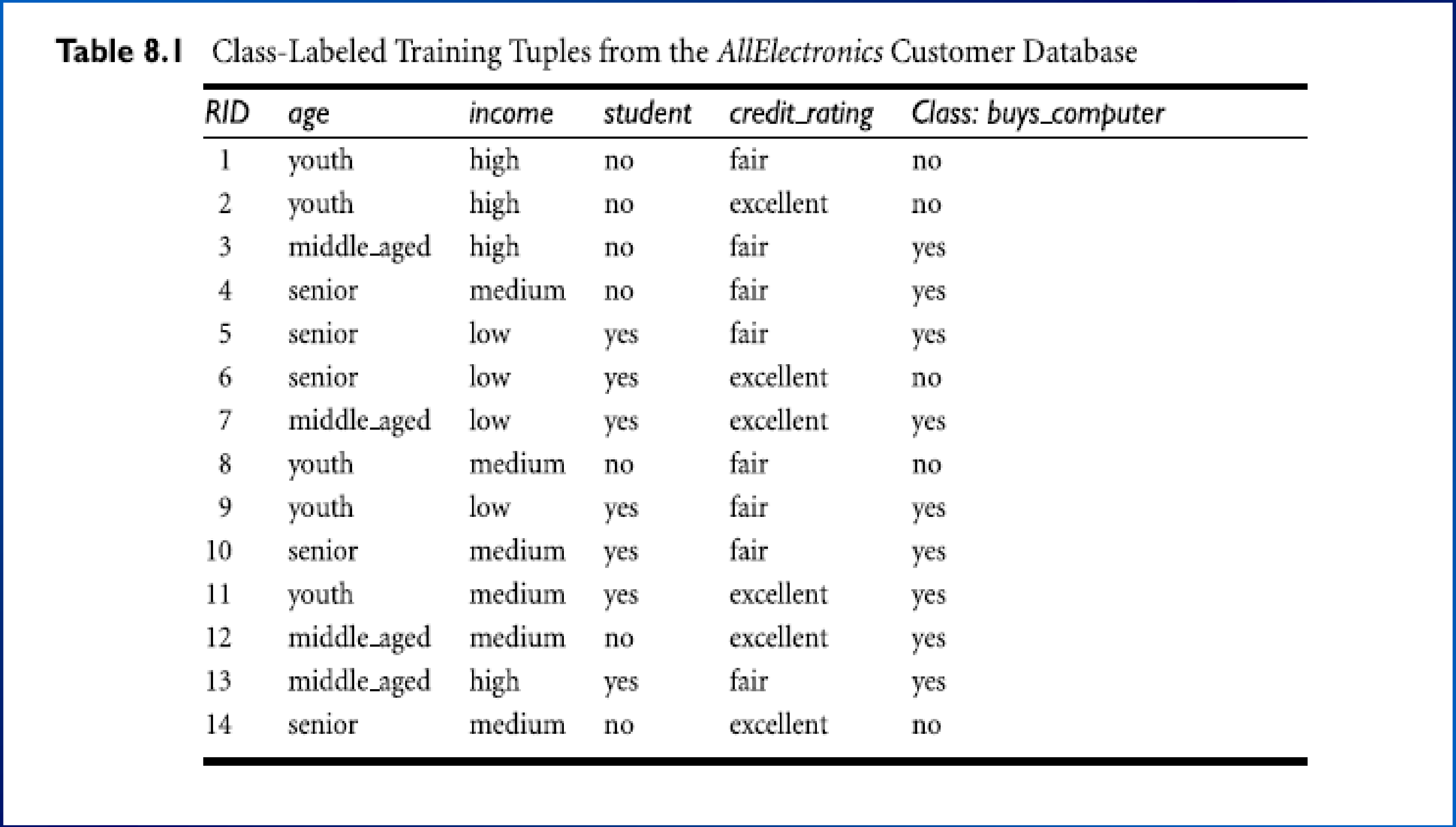


Table 8.1 Class-Labeled Training Tuples from the *AllElectronics* Customer Database

RID	*age*	*income*	*student*	*credit_rating*	*Class: buys_computer*
1	youth	high	no	fair	no
2	youth	high	no	excellent	no
3	middle_aged	high	no	fair	yes
4	senior	medium	no	fair	yes
5	senior	low	yes	fair	yes
6	senior	low	yes	excellent	no
7	middle_aged	low	yes	excellent	yes
8	youth	medium	no	fair	no
9	youth	low	yes	fair	yes
10	senior	medium	yes	fair	yes
11	youth	medium	yes	excellent	yes
12	middle_aged	medium	no	excellent	yes
13	middle_aged	high	yes	fair	yes
14	senior	medium	no	excellent	no

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ID3: Entropy & Information Gain

$$Info(D) = -\frac{9}{14}\log_2\left(\frac{9}{14}\right) - \frac{5}{14}\log_2\left(\frac{5}{14}\right) = 0.940 \text{ bits.}$$

$$Gain(age) = Info(D) - Info_{age}(D) = 0.940 - 0.694 = 0.246 \text{ bits.}$$

$$Gain(income) = 0.029 \text{ bits}, \; Gain(student) = 0.151 \text{ bits},$$

$$Gain(credit\_rating) = 0.048 \text{ bits.}$$

Ross Quinlan
American

ID3 algorithm

- **ID3** ≡ Induction Decision Tree [Quinlan, 1979]
- Machine Learning Technique
- Decision Tree Induction
- Top-Down strategy
- Qualitative variables
- Multi-way trees
- Don't repeat variables
- From a set of **examples (instances** + belonging class) build up the *best* decision tree which explains the instances

$$\begin{tikzcd}
 & \textbf{Compactness} \rightarrow \text{the more compact the better} \\
\textbf{Criteria} \arrow[ur] \arrow[dr] & \\
 & \textbf{Goodness} \rightarrow \text{predictive/discriminant ability}
\end{tikzcd}$$

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Ross Quinlan
American

C4.5 algorithm

- C4.5: Refines ID3 [Quinlan, 1986]
- Machine Learning Technique
- Decision Tree Induction
- Top-Down strategy
- Qualitative variables
- Multi-way trees
- Uses impurity ratio
- Heuristics for prunning
- From a set of **examples (instances** + belonging class) build up the *best* decision tree which explains the instances

$$\begin{tikzcd}
 & \textbf{Compactness} \rightarrow \text{the more compact the better} \\
\textbf{Criteria} \arrow[ur] \arrow[dr] & \\
 & \textbf{Goodness} \rightarrow \text{predictive/discriminant ability}
\end{tikzcd}$$

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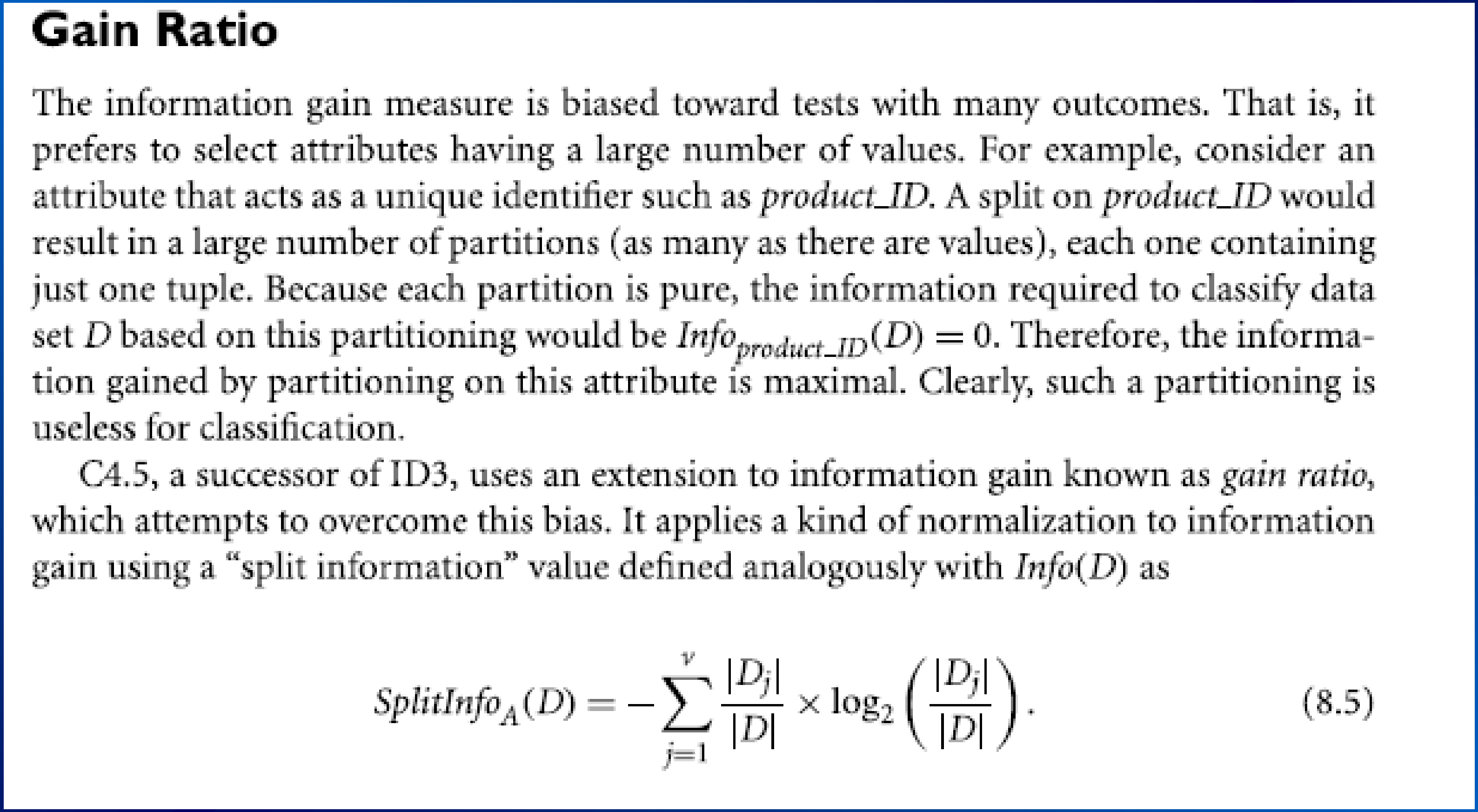
C4.5: Gain Ratio



Gain Ratio

The information gain measure is biased toward tests with many outcomes. That is, it prefers to select attributes having a large number of values. For example, consider an attribute that acts as a unique identifier such as *product_ID*. A split on *product_ID* would result in a large number of partitions (as many as there are values), each one containing just one tuple. Because each partition is pure, the information required to classify data set D based on this partitioning would be $Info_{product\_ID}(D) = 0$. Therefore, the information gained by partitioning on this attribute is maximal. Clearly, such a partitioning is useless for classification.

C4.5, a successor of ID3, uses an extension to information gain known as *gain ratio*, which attempts to overcome this bias. It applies a kind of normalization to information gain using a "split information" value defined analogously with $Info(D)$ as

$$SplitInfo_A(D) = -\sum_{j=1}^{v} \frac{|D_j|}{|D|} \times \log_2\left(\frac{|D_j|}{|D|}\right). \qquad (8.5)$$

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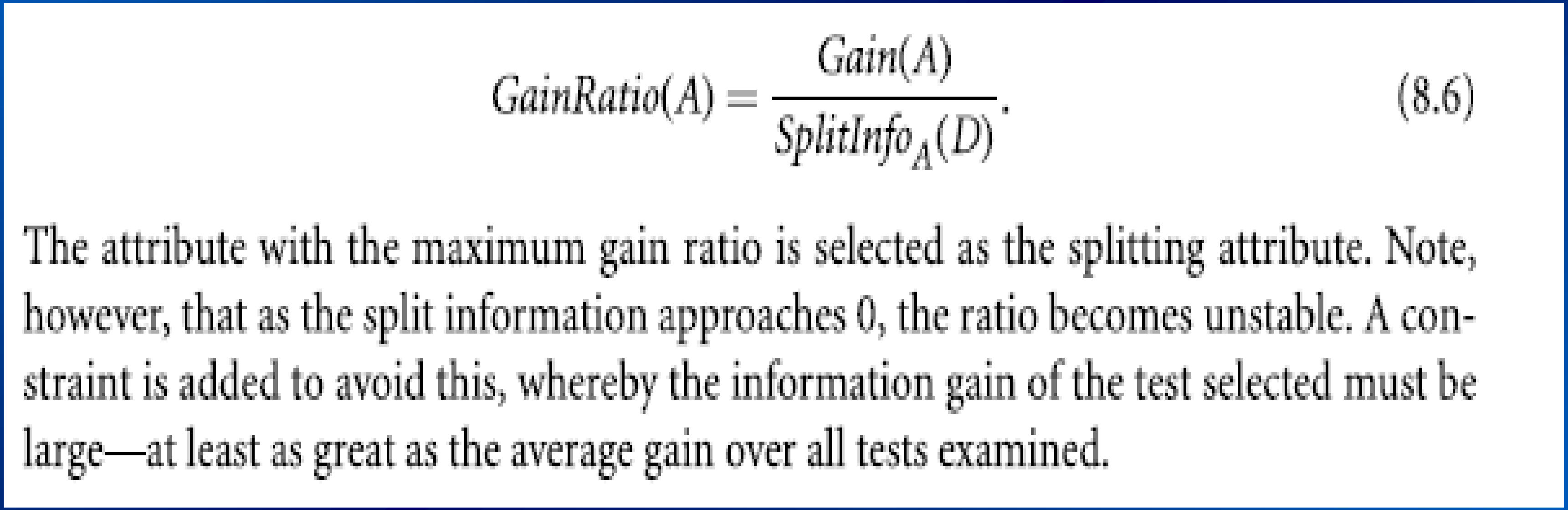
C4.5: Gain Ratio



$$GainRatio(A) = \frac{Gain(A)}{SplitInfo_A(D)}. \quad (8.6)$$

The attribute with the maximum gain ratio is selected as the splitting attribute. Note, however, that as the split information approaches 0, the ratio becomes unstable. A constraint is added to avoid this, whereby the information gain of the test selected must be large—at least as great as the average gain over all tests examined.

ID3

Which variable in decision node?

It is a *greedy* *(voraz)* algorithm

the *best* attribute at each step

is the most discriminant one (potentially more useful)

Maximize a certain G(I,X)

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ID3: Notation

- I ≡ set of examples ≡ $i=\{i_{1..}\ i_n\}$
- X ≡ variable with values $\{x_{1..}\ x_{nx}\}$
- P ≡ set of classes ≡ $\{c_{1.....}\ c_p\}$
- # ≡ Cardinality

$X^{-1}(x_i)$ ≡ set of elements in I with X=xi

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ID3: splitting criteria

- Select variable X which *maximizes* the information gain

$$G(I, X) = H(I) - H(I,X)$$

Divide by H(I)
Avoid effect of n_x

where P response variable (class)

Information of parent node

$$\mathbf{H(I)} = -\sum_{c \in P} p(c|I) * \log_2 p(c|I)$$

Empirical probability of being in class C

$$\mathbf{p(c|I)} = \#c / \#I$$

Entropy of splitting by X

$$\mathbf{H(I, X)} = \sum_{i=1:n_x} p_X(x_i) * H(X^{-1}(x_i))$$

Probability that one example has the value x_i for the variabe X

$$\mathbf{p_X (x_i)} = \#X^{-1}(x_i) / \#I$$

Termination criteria

- All instances in a node belong to same class
- A maximum depth of the tree is achieved

  (maxdepth control parameter in R)
- Splits do not open a minimum number of branches

  (only for n-ary trees)
- Next split produces too small leafs

  (minsplit control parameter in R)
- Improvement of termination function is not enough

  (cp control parameter in R, termination fumction = splitting criterion)

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Post-prunning criteria

- Avoids overfitting and redundancy
- Evaluate the tree with/without the branch
  - If performance is maintained, prune
  - Performance can be measured in different ways
    - Different error functions
    - Statistical tests

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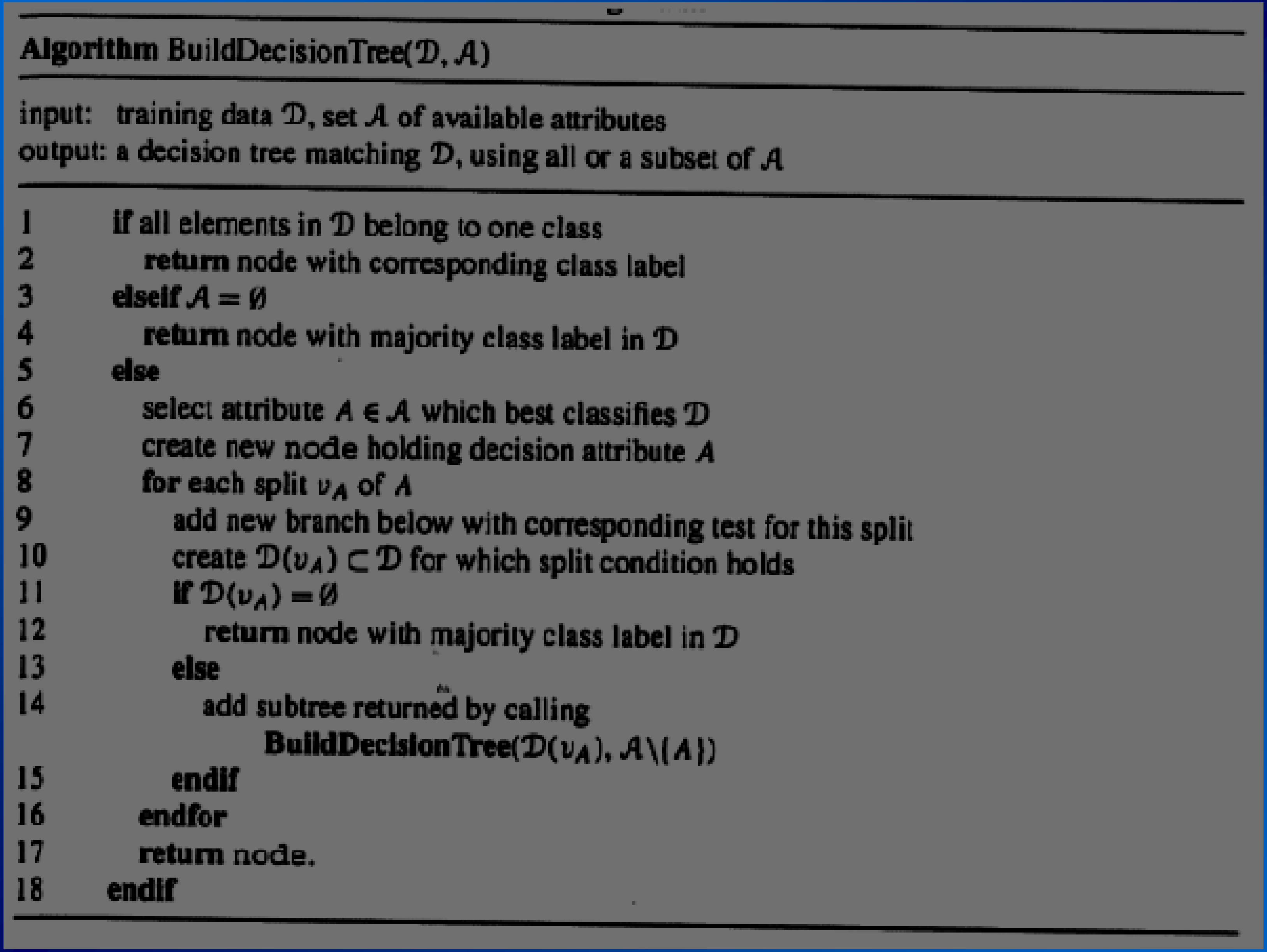

Algorithm BuildDecisionTree($\mathcal{D}$, $\mathcal{A}$)

input: training data $\mathcal{D}$, set $\mathcal{A}$ of available attributes
output: a decision tree matching $\mathcal{D}$, using all or a subset of $\mathcal{A}$

```
if all elements in $\mathcal{D}$ belong to one class
   return node with corresponding class label
elseif $\mathcal{A} = \emptyset$
   return node with majority class label in $\mathcal{D}$
else
   select attribute $A \in \mathcal{A}$ which best classifies $\mathcal{D}$
   create new node holding decision attribute $A$
   for each split $v_A$ of $A$
      add new branch below with corresponding test for this split
      create $\mathcal{D}(v_A) \subset \mathcal{D}$ for which split condition holds
      if $\mathcal{D}(v_A) = \emptyset$
         return node with majority class label in $\mathcal{D}$
      else
         add subtree returned by calling
               BuildDecisionTree($\mathcal{D}(v_A)$, $\mathcal{A} \setminus \{A\}$)
      endif
   endfor
   return node.
endif
```

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ID3: EXAMPLE (9)

	Eye Colour	Hair Colour	Height	Class
E1	Blue	Blonde	Tall	C+
E2	Blue	Brown	Medium	C+
E3	Brown	Brown	Medium	C-
E4	Green	Brown	Medium	C-
E5	Green	Brown	Tall	C+
E6	Brown	Brown	Low	C-
E7	Green	Blonde	Low	C-
E8	Blue	Brown	Medium	C+

ID3: example (10)

I={E1,….E8} C+={E1, E2, E5, E8) C-={E3,,E4,E5,E7}

G(I, Eye-Color) = H(I) - H(I,Eye-Color)

$$\mathbf{H(I)} = -\sum_{C_i \in C} p(c_i|I) * \log_2 p(c_i|I) = \mathbf{-p(c+|I)*} \log_2 p(c+|I) \mathbf{-p(c-|I)*} \log_2 p(c-|I)$$

p(C+|I) = p (C-|I)= 1/2

H(I) = $\mathbf{-1/2 \log_2 1/2 -1/2 \log_2 1/2 = 1}$

$$\mathbf{H(I, Eye\text{-}Color)} = \sum_{x_i} p_X(x_i) * H(X^{-1}(x_i)) = \sum_{x_i} p_{Eye\text{-}Color}(x_i) * H(Eye\text{-}Color^{-1}(x_i))$$

$P_X(x_1) = P_{Eye\text{-}Color}(Blue) = 3/8$

$H(Eye\text{-}Colour^{-1}(Blue)) = - p(C+|Blue) * \log_2 p(C+|Blue) -- p(C-|Blue) * \log_2 p(C-|Blue)$

$= - 1 \log_2 1 - 0 \log_2 0$

$H(I, Eye\text{-}colour) = \mathbf{3/8} (-1 \log_2 1 - 0 \log_2 0) + \mathbf{2/8} (-0 \log_2 0 - 1 \log_2 1) +$

$\mathbf{3/8} (-1/3 \log_2 1/3 - 2/3 \log_2 2/3) = 0.344$

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ID3: example (10)

$$\mathbf{H(I) = -1/2 \log_2 1/2 - 1/2 \log_2 1/2 = 1}$$

$$H(I, \text{Eye-colour}) = \mathbf{3/8}\,(-1 \log_2 1 - 0 \log_2 0) + \mathbf{2/8}\,(-0 \log_2 0 - 1 \log_2 1) + \mathbf{3/8}\,(-1/3 \log_2 1/3 - 2/3 \log_2 2/3) = 0.344$$

$$H(I, \text{Hair-colour}) = \mathbf{2/8}\,(-1/2 \log_2 1/2 - 1/2 \log_2 1/2) + \mathbf{6/8}\,(-3/6 \log_2 3/6 - 3/6 \log_2 3/6) = 1$$

$$H(I, \text{Height}) = 2/8\,(-1 \log_2 1 - 0 \log_2 0) + 4/8\,(-1/2 \log_2 1/2 - 1/2 \log_2 1/2) + 2/8\,(-0 \log_2 0 - 1 \log_2 1) = 0.5$$

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ID3: example (11)

G(I, Eye-colour) = 1 - 0.366 = **0.656**

G(I, Hair-colour) = 1 - 1 = 0

G(I, Height) = 1- 0.5 = 0.5

$$\begin{tikzcd}
 & \text{Eye-colour} \arrow[dl, "\text{Blue}"'] \arrow[d, "\text{Brown}"] \arrow[dr, "\text{Green}"] & \\
\text{E1,E2,E8} & \text{E3,E6} & \text{E4,E7, E5} \\
+ & - & - \quad - \quad +
\end{tikzcd}$$

	Hair-colour	**Height**	**Class**
E4	Brown	Medium	C-
E5	Brown	Tall	C+
E7	Blonde	Low	C-

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ID3: example (12)

H(Green) = $-1/3 \log_2 1/3 - 2/3 \log_2 2/3 = 0{,}918$

(E_5) (E_4,E_7)

Blonde

H(Green, Hair-colour) = $\mathbf{1/3}\ (-\log_2 \ \ -1 \log_2 1) +$

$\mathbf{2/3}\ (-1/2 \log_2 1/2 - 1/2 \log_2 1/2) = 2/3$

H(Green, Height) = $1/3\ (-0 \log_2 0 - 1 \log_2 1) +$

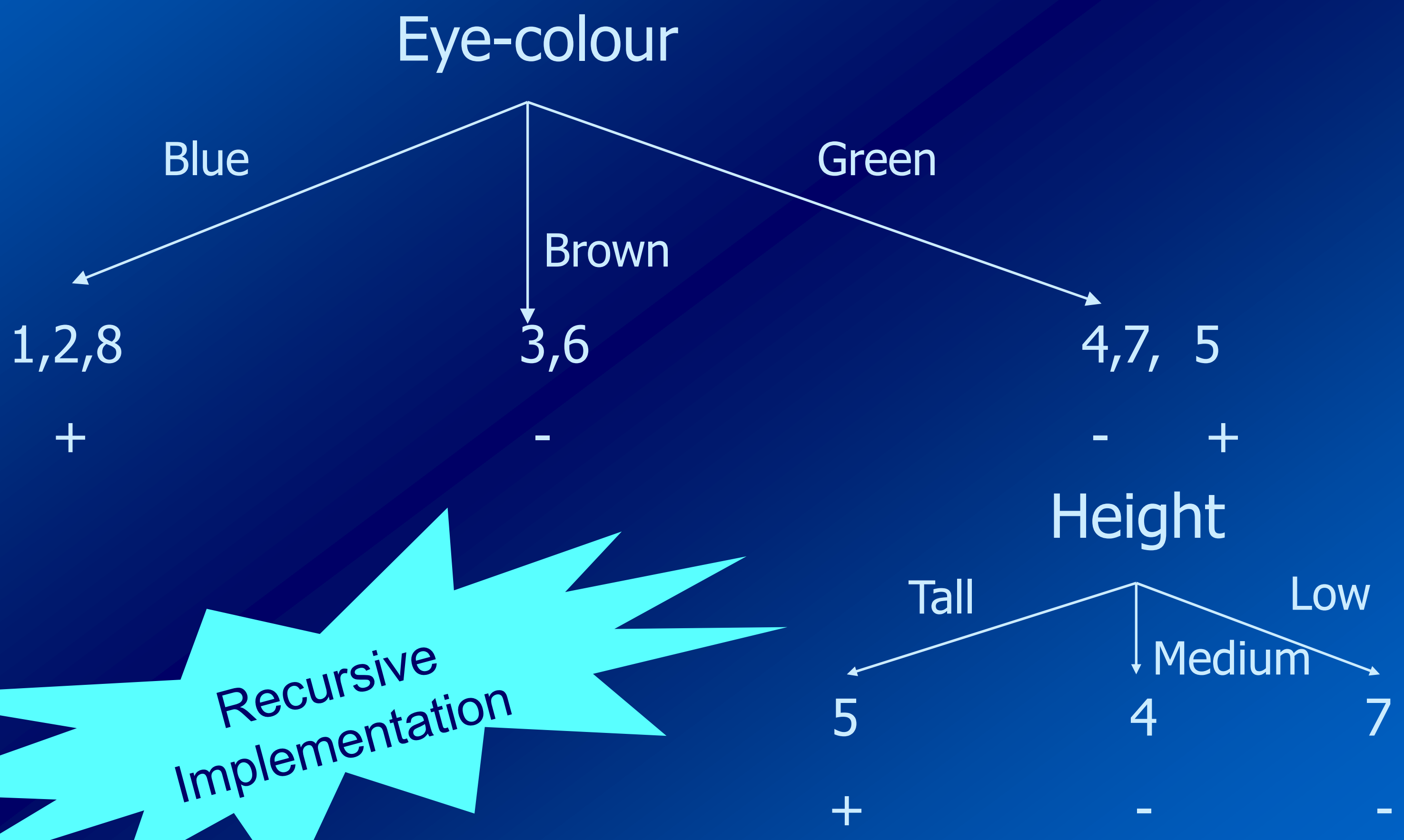
$1/3\ (-1 \log_2 1 - 0 \log_2 0) +$

$1/3\ (-0 \log_2 0 - 1 \log_2 1) = 0$

G(Green, Hair-colour) = 0,918 - 0,666 = 0,252

G(Green, Height) = 0,918 - 0 = **0,918**

ID3: example



Recursive Implementation

ID3: example (14)

Eye-colour = Blue → C+

Eye-colour = Brown → C-

Eye-colour = Green ∧ Height = Tall → C+

Eye-colour = Green ∧ Height = Medium → C-

Eye-colour = Green ∧ Height = Low → C-

Transcription in a set of rules

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ID3: example (15)

Optimizing the set of rules

(Eye-colour = Blue) or (Eye-colour = Green $\wedge$ Height <> Tall) $\rightarrow$ C+

(Eye-colour = Brown) or (Eye-colour = Green $\wedge$ Height = Tall) $\rightarrow$ C-

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Leo Breiman,
American, 1928-2005

The CART solution

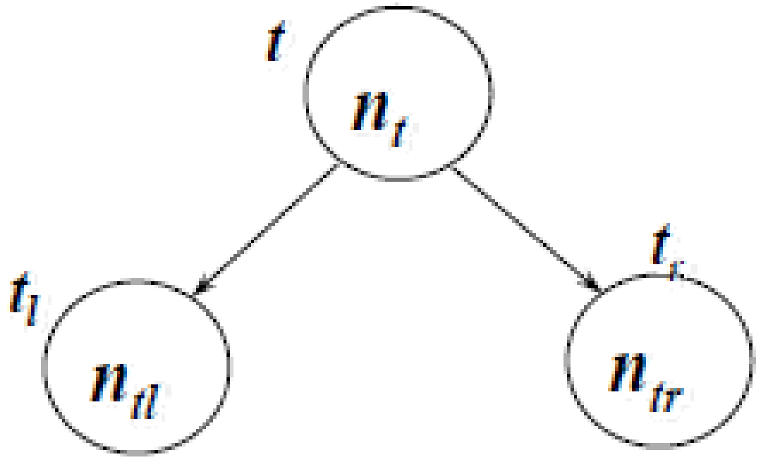
Jerome Friedman,
American

Developed 1974-1984 by 4 statistics professors: Leo Breiman (Berkeley), Jerry Friedman (Stanford), Charles Stone (Berkeley), Richard Olshen (Stanford). Distributed by Salford Systems http://salford-systems.com/

- Just perform Binary trees
- Unifies the categorical and continuous responseunder the same framework.
  - Classification tree
  - Regression tree
- Any kind of explanatory variable
- Split criterion: Impurity of the node
- Post pruning (without stop criterion)
- Delivers honest estimates of the quality of a tree

Selection of the optimal partition

Maximize the decrement of impurity between the parent and its children



$$\Delta i(t) = i(t) - \frac{n_{tl}}{n_t} i(t_l) - \frac{n_{tr}}{n_t} i(t_r)$$

Impurity of a node

For categorical responses:

- Gini

$$i(t) = \sum_{i \neq j} p(j/t)p(i/t) = 1 - \sum_j^q p_j^2$$

- Information (Entropy)

$$i(t) = -\sum_j p(j/t) \log_2 p(j/t)$$

For continuous responses:

- Variance

$$i(t) = \frac{\sum_{i \in t} (y_i - \bar{y}_t)^2}{n_t}$$

Missclassification tax

Gini(Node labelled as C) = p(c|I) * (1-p(c|I)) two classes

Gini(Node labelled as C) = $1-\sum_{c' \in P,\ c\ [illegible]\ c} p(c'|I)^2$, more than 2 classes

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Selection of the optimal tree (from the maximum tree)

We need to define how good (or bad) is a tree:

Obvious criterion = *Probability of misclassification (= cost of the tree)*

How can we compute the Cost of the tree:

We assign every leave to the response class with maximum *p(j/t)*

$$p(j/t) = \frac{p(j,t)}{p(t)} = \frac{\pi_j \, {}^{n_{tj}}\!/_{n_j}}{{}^{n_t}\!/_{n}}$$

If classes *j* autorepresentatives $\quad if\ \pi_j = \frac{n_j}{n} \quad p(j/t) = \frac{n_{tj}}{n_t}$

Cost of the tree

of a node: $r(t) = 1 - \max_j p(j/t)$

If there are missclassification costs

$$r(t) = \min_i \sum_j c(i/j) p(j/t)$$

Cost of the tree: $R(T) = \frac{\sum_{t \in \tilde{T}} p(t) r(t)}{r(root)} \times 100$

(decreasing with size)

Criterion to optimize: $Min\ R(T)$

Cost of a regression tree

- In a regression tree, every individuals is assigned with the mean value of the leave.
- Cost of the tree = residual variance

$$r(t) = \frac{1}{n_t}\sum_{i=1}^{n_t}(y_{it} - \bar{y}_t)^2$$

Penalization for complexity

Criterion to optimize: $Min\left(R(T)+\alpha\left|T\right|\right)$

Where α is the *complexity parameter*, expresses the penalization for building large trees

Run with increasing complexity and

Get a sequence of optimal trees of increasing size….

Evaluate and select the best

Unbalanced Data

- Unequal class frequencies
  - 99% don’t buy, 1% buy
  - 90% healthy, 10% disease
- Getting a majority class of 97% accuracy is useless
- Decision Trees assume balanced classes

  (minority class hardly become a majority in a node)
- Work with balanced traninig datasets

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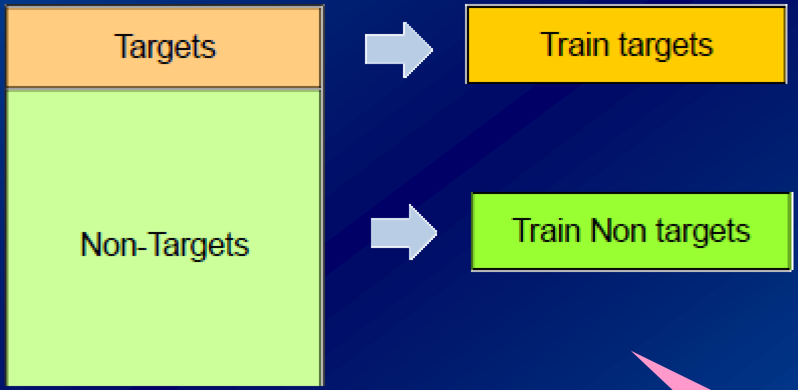
Unbalanced training Data

Bad performance



Otherwise, weight non targets:

$$\sum_{targets} weights = \sum_{non\ targets} weights$$

Keep Proportions

After Learning: Using

- Use the inducted DT to assign the class of a new object:

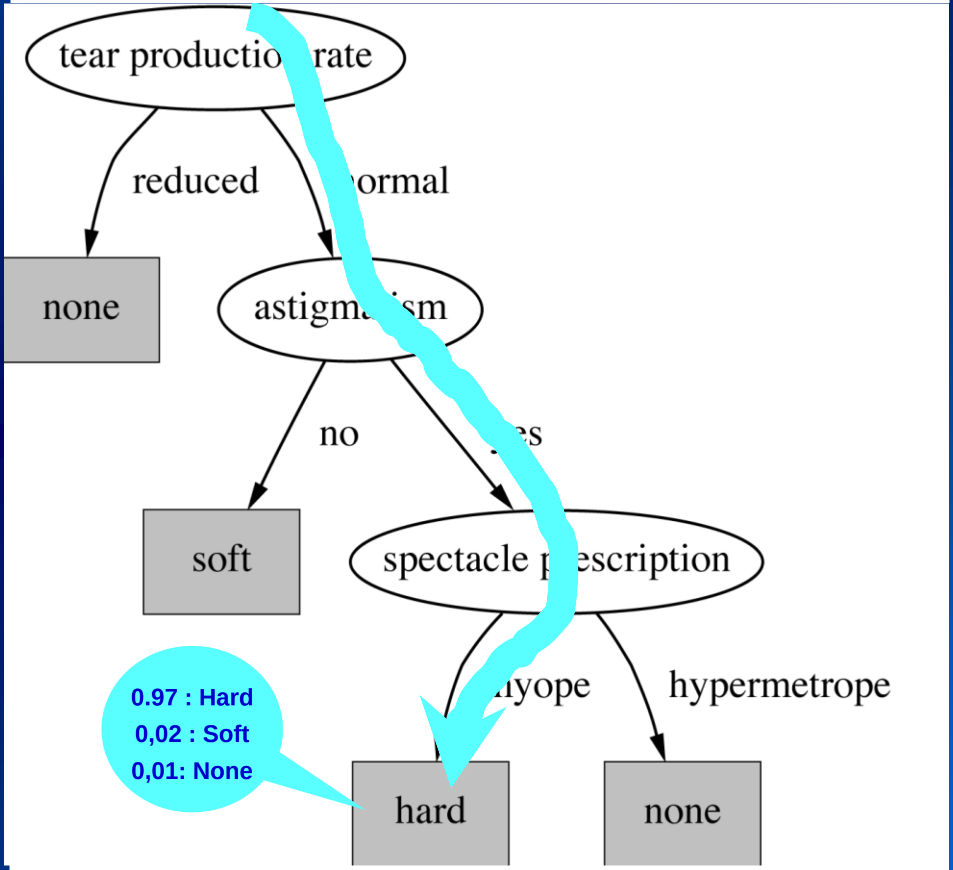
  PREDICTION

- Evaluate node-queries over the object and descend to a leaf

- Assign the label of the leaf as the class of the object

Evenctually, consider the purity of the leaf as the probability of the assignment

John: (normal tear, Astigmatism, myope)



OUTPUT: John requires hard lents

With a probability of 0.97

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Validation in Decision Trees

Missclassification rate

Confusion matrix

Cross-validation

ROC curves: (DT provides single points for ROC space)

use probability of assignment to run ROC

or move some parameter (cp, minleaf….)

Confusion matrix and error rate

	Predicted class YES	Predicted class NO
Real class YES	n_{TP}	n_{FN}
Real class NO	n_{FP}	n_{TN}

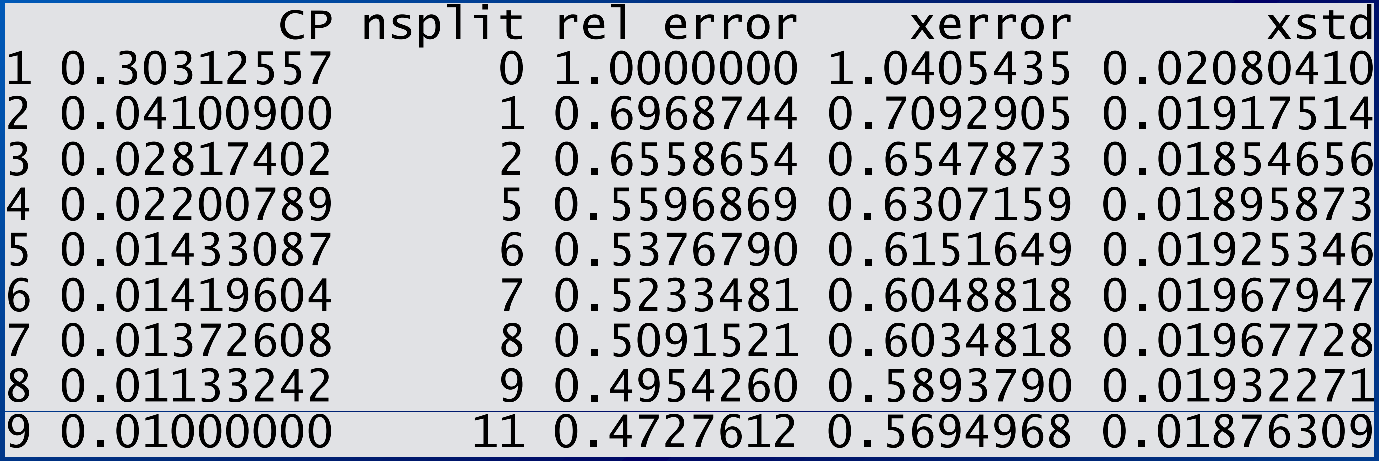
Type-I error

Type-II error

$$Error\ rate = \frac{n_{FN} + n_{FP}}{n}$$

Missclassification rate depends on DT parameters

cpTable



```
          CP nsplit rel error    xerror       xstd
1 0.30312557      0 1.0000000 1.0405435 0.02080410
2 0.04100900      1 0.6968744 0.7092905 0.01917514
3 0.02817402      2 0.6558654 0.6547873 0.01854656
4 0.02200789      5 0.5596869 0.6307159 0.01895873
5 0.01433087      6 0.5376790 0.6151649 0.01925346
6 0.01419604      7 0.5233481 0.6048818 0.01967947
7 0.01372608      8 0.5091521 0.6034818 0.01967728
8 0.01133242      9 0.4954260 0.5893790 0.01932271
9 0.01000000     11 0.4727612 0.5694968 0.01876309
```

Cp: complexity parameter

Rel error: relative missclassification rate of the tree at each cp

Xerror: Crossvalidated missclassification error

Xstd: standard deviation of crossvalidated missclassification error

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Pros and cons of DT

- Easy to interpret
- Branches provide assignment rules (Results operationalized)
- Branches provide good support to decision making
- Automatic detection of complex interactions among variables
- Computationaly efficient ……
- But…. Rough approach to the response (approached by leaps (discontinuities)
- But… worse performance than other classifiers

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rpart   package:rpart
Recursive Partitioning and Regression Trees

rpart(formula, data, weights na.action = na.rpart, method, parms, control, cost, ...)

formula: a formula, as in the 'lm' function.
data: an optional data frame in which to interpret the variables named in the formula
weights: optional case weights.
na.action: The default action deletes all observations for which 'y' is missing, but keeps those in which one or more predictors are missing.
method: one of '"anova"', '"poisson"', '"class"' or '"exp"'. If 'method' is missing then the routine tries to make an intellegent guess.
parms=list(prior=c(.85,.15), split='information')
control=rpart.control(minsplit=20, minbucket=round(minsplit/3), cp=0.01,maxcompete=4, maxsurrogate=5, usesurrogate=2, xval=10, maxdepth=30, ...)

minsplit: the minimum number of observations that must exist in a node, in order for a split to be attempted.
minbucket: the minimum number of observations in any terminal '<leaf>' node.
cp: complexity parameter.
maxcompete: the number of competitor splits retained in the output.
maxsurrogate: the number of surrogate splits retained in the output.
usesurrogate: 1= use surrogates, in order, to split subjects missing the primary variable; if all surrogates are missing the observation is not split. 2= if all surrogates are missing, then send the observation in the majority direction.
xval: number of cross-validations
maxdepth: Set the maximum depth of any node of the final tree, with the root node counted as depth 0