Decision Trees

Duke Course Notes

Cynthia Rudin

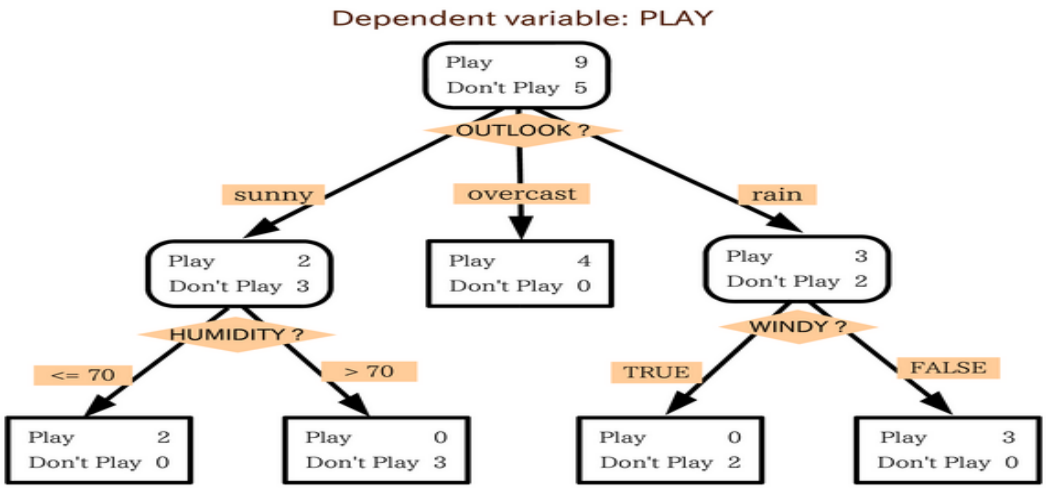
Credit: Russell & Norvig, Mitchell, Kohavi & Quinlan, Carter, Vanden Berghen

Why trees?

- interpretable/intuitive, popular in medical applications because they mimic the way a doctor thinks
- model discrete outcomes nicely
- can be very powerful, can be as complex as you need them
- C4.5 and CART - from "top 10" - decision trees are very popular

Some real examples (from Russell & Norvig, Mitchell)

- BP's GasOIL system for separating gas and oil on offshore platforms - decision trees replaced a hand-designed rules system with 2500 rules. C4.5-based system outperformed human experts and saved BP millions. (1986)
- Learning to fly a Cessna on a flight simulator by watching human experts fly the simulator (1992)
- Can also learn to play tennis, analyze C-section risk, etc.



How to build a decision tree:

- Start at the top of the tree.
- Grow it by "splitting" attributes one by one. To determine which attribute to split, look at "node impurity."
- Assign leaf nodes the majority vote in the leaf.
- When we get to the bottom, prune the tree to prevent overfitting

Why is this a good way to build a tree?

I have to warn you that C4.5 and CART are not elegant by any means that I can define elegant. But the resulting trees can be very elegant. Plus there are 2 of the top 10 algorithms in data mining that are decision tree algorithms! So it's worth it for us to know what's under the hood... even though, well... let's just say it ain't pretty.

Example: Will the customer wait for a table? (from Russell & Norvig)

Here are the attributes:

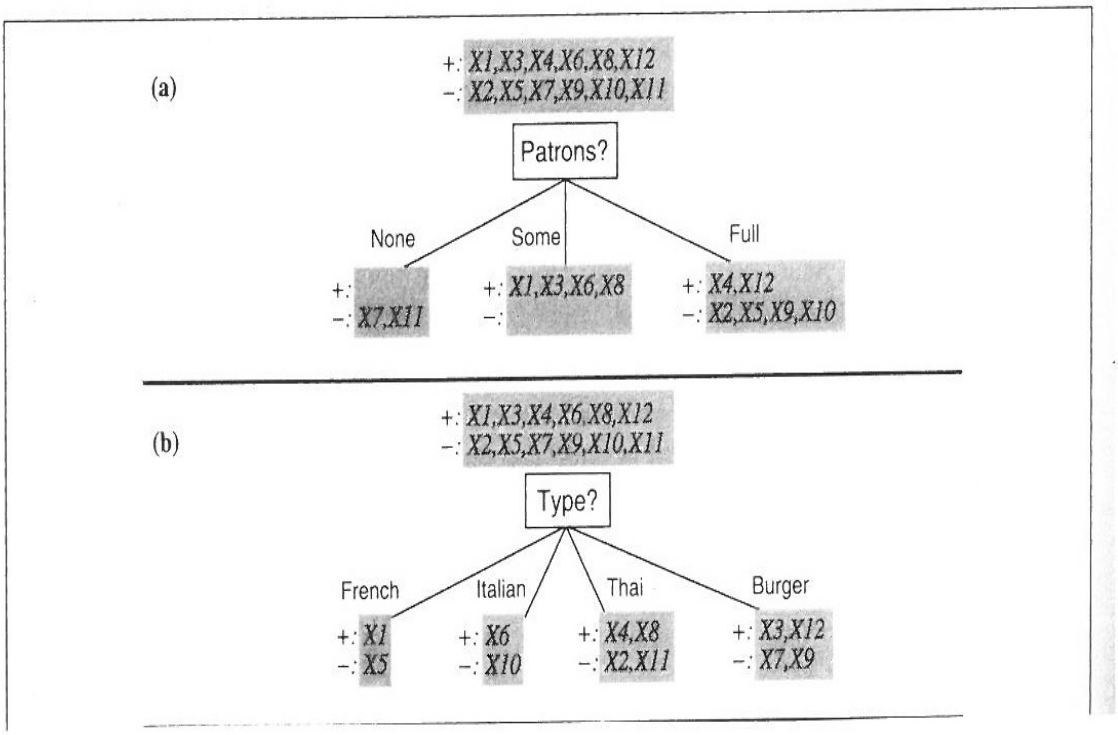
1. *Alternate*: whether there is a suitable alternative restaurant nearby.
2. *Bar*: whether the restaurant has a comfortable bar area to wait in.
3. *Fri/Sat*: true on Fridays and Saturdays.
4. *Hungry*: whether we are hungry.
5. *Patrons*: how many people are in the restaurant (values are *None*, *Some*, 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).

Here are the examples:

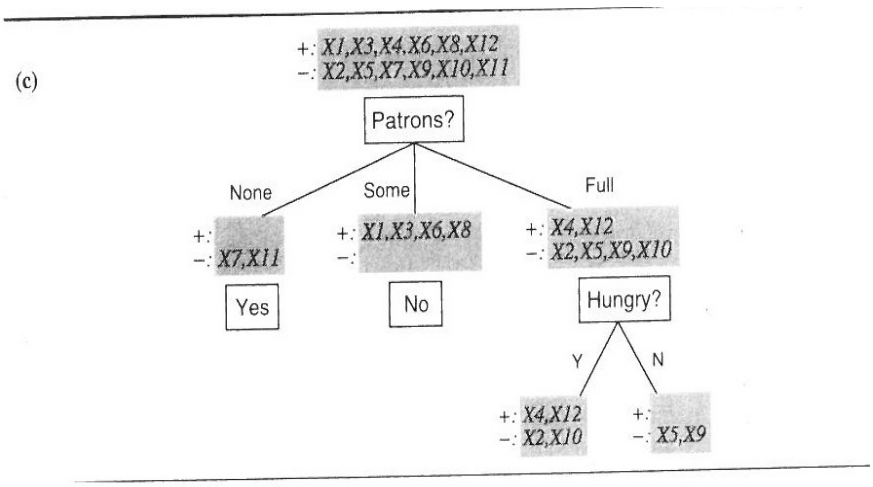
Example	Attributes										Goal
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
X_1	*Yes*	*No*	*No*	*Yes*	*Some*	*$$$*	*No*	*Yes*	*French*	*0–10*	*Yes*
X_2	*Yes*	*No*	*No*	*Yes*	*Full*	*$*	*No*	*No*	*Thai*	*30–60*	*No*
X_3	*No*	*Yes*	*No*	*No*	*Some*	*$*	*No*	*No*	*Burger*	*0–10*	*Yes*
X_4	*Yes*	*No*	*Yes*	*Yes*	*Full*	*$*	*No*	*No*	*Thai*	*10–30*	*Yes*
X_5	*Yes*	*No*	*Yes*	*No*	*Full*	*$$$*	*No*	*Yes*	*French*	*>60*	*No*
X_6	*No*	*Yes*	*No*	*Yes*	*Some*	*$$*	*Yes*	*Yes*	*Italian*	*0–10*	*Yes*
X_7	*No*	*Yes*	*No*	*No*	*None*	*$*	*Yes*	*No*	*Burger*	*0–10*	*No*
X_8	*No*	*No*	*No*	*Yes*	*Some*	*$$*	*Yes*	*Yes*	*Thai*	*0–10*	*Yes*
X_9	*No*	*Yes*	*Yes*	*No*	*Full*	*$*	*Yes*	*No*	*Burger*	*>60*	*No*
X_{10}	*Yes*	*Yes*	*Yes*	*Yes*	*Full*	*$$$*	*No*	*Yes*	*Italian*	*10–30*	*No*
X_{11}	*No*	*No*	*No*	*No*	*None*	*$*	*No*	*No*	*Thai*	*0–10*	*No*
X_{12}	*Yes*	*Yes*	*Yes*	*Yes*	*Full*	*$*	*No*	*No*	*Burger*	*30–60*	*Yes*

Figure 18.5 Examples for the restaurant domain.

Here are two options for the first feature to split at the top of the tree. Which one should we choose? Which one gives me the most information?



What we need is a formula to compute "information." Before we do that, here's another example. Let's say we pick one of them (Patrons). Maybe then we'll pick Hungry next, because it has a lot of "information":



We'll build up to the derivation of **C4.5**. Origins: Hunt 1962, ID3 of Quinlan 1979 (600 lines of Pascal), C4 (Quinlan 1987). C4.5 is 9000 lines of C (Quinlan 1993). We start with some basic information theory.

Information Theory (from slides of Tom Carter, June 2011)

"Information" from observing the occurrence of an event
:= #bits needed to encode the probability of the event $p = -\log_2 p$.

E.g., a coin flip from a fair coin contains 1 bit of information. If the event has probability 1, we get no information from the occurrence of the event.

Where did this definition of information come from? Turns out it's pretty cool. We want to define I so that it obeys all these things:

- $I(p) \geq 0, I(1) = 0$; the information of any event is non-negative, no information from events with prob 1
- $I(p_1 \cdot p_2) = I(p_1) + I(p_2)$; the information from two independent events should be the sum of their informations
- $I(p)$ is continuous, slight changes in probability correspond to slight changes in information

Together these lead to:

$$I(p^2) = 2I(p) \text{ or generally } I(p^n) = nI(p),$$

this means that

$$I(p) = I\left((p^{1/m})^m\right) = mI\left(p^{1/m}\right) \text{ so } \frac{1}{m}I(p) = I\left(p^{1/m}\right)$$

and more generally,

$$I\left(p^{n/m}\right) = \frac{n}{m}I(p).$$

This is true for any fraction n/m, which includes rationals, so just define it for all positive reals:

$$I(p^a) = aI(p).$$

The functions that do this are $I(p) = -\log_b(p)$ for some b. Choose $b = 2$ for "bits."

Flipping a fair coin gives $-\log_2(1/2) = 1$ bit of information if it comes up either heads or tails.

A biased coin landing on heads with $p = .99$ gives $-\log_2(.99) = .0145$ bits of information.

A biased coin landing on heads with $p = .01$ gives $-\log_2(.01) = 6.643$ bits of information.

Entropy. Say one of many of possible events could occur. What's the mean information of those events? Assume the events $v_1, ..., v_J$ occur with probabilities $p_1, ..., p_J$, where $[p_1, ..., p_J]$ is a discrete probability distribution.

$$\mathbf{E}_{p\sim[p_1,...,p_J]} I(p) = \sum_{j=1}^{J} p_j I(p_j) = -\sum_j p_j \log_2 p_j =: H(\mathbf{p})$$

where $\mathbf{p}$ is the vector $[p_1, ..., p_J]$. $H(\mathbf{p})$ is called the **entropy** of discrete distribution $\mathbf{p}$.

So if there are only 2 events (binary), with probabilities $\mathbf{p} = [p, 1-p]$,

$$H(\mathbf{p}) = -p\log_2(p) - (1-p)\log_2(1-p).$$

If the probabilities were $[1/2, 1/2]$,

$$H(\mathbf{p}) = -2\frac{1}{2}\log_2\frac{1}{2} = 1 \quad \text{(Yes, we knew that.)}$$

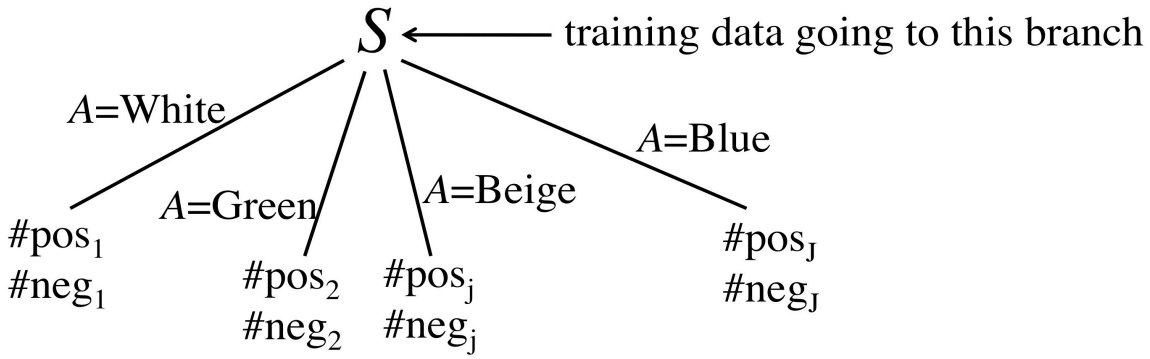
Or if the probabilities were $[0.99, 0.01]$,

$$H(\mathbf{p}) = 0.08 \text{ bits.}$$

As one of the probabilities in the vector $\mathbf{p}$ goes to 1, $H(\mathbf{p}) \to 0$, which is what we want.

Back to C4.5, which uses Information Gain as the splitting criteria.

Back to C4.5 (source material: Russell & Norvig, Mitchell, Quinlan)
We consider a "test" split on attribute A at a branch.



In S we have #pos positives and #neg negatives. For each branch j, we have $\#\text{pos}_j$ positives and $\#\text{neg}_j$ negatives.

The training probabilities in branch j are:

$$\left[\frac{\#\text{pos}_j}{\#\text{pos}_j + \#\text{neg}_j}, \frac{\#\text{neg}_j}{\#\text{pos}_j + \#\text{neg}_j}\right].$$

The Information Gain is calculated like this:

$$\begin{aligned}
\text{Gain}(S, A) &= \text{expected reduction in entropy due to branching on attribute } A \\
&= \text{original entropy} - \text{entropy after branching} \\
&= H\left(\left[\frac{\#\text{pos}}{\#\text{pos} + \#\text{neg}}, \frac{\#\text{neg}}{\#\text{pos} + \#\text{neg}}\right]\right) \\
&\quad - \sum_{j=1}^{J} \frac{\#\text{pos}_j + \#\text{neg}_j}{\#\text{pos} + \#\text{neg}} H\left[\frac{\#\text{pos}_j}{\#\text{pos}_j + \#\text{neg}_j}, \frac{\#\text{neg}_j}{\#\text{pos}_j + \#\text{neg}_j}\right].
\end{aligned}$$

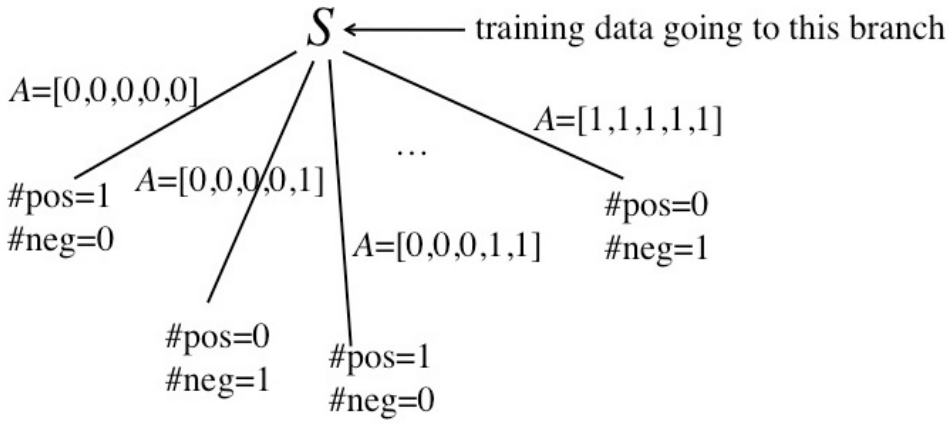
Back to the example with the restaurants.

$$\begin{aligned}
\text{Gain}(S, \text{Patrons}) &= H\left(\left[\frac{1}{2}, \frac{1}{2}\right]\right) - \left[\frac{2}{12}H([0,1]) + \frac{4}{12}H([1,0]) + \frac{6}{12}H\left(\left[\frac{2}{6}, \frac{4}{6}\right]\right)\right] \\
&\approx 0.541 \text{ bits.}
\end{aligned}$$

$$\begin{aligned}
\text{Gain}(S, \text{Type}) &= 1 - \left[\frac{2}{12}H\left(\left[\frac{1}{2}, \frac{1}{2}\right]\right) + \frac{2}{12}H\left(\left[\frac{1}{2}, \frac{1}{2}\right]\right)\right. \\
&\quad \left. + \frac{4}{12}H\left(\left[\frac{2}{4}, \frac{2}{4}\right]\right) + \frac{4}{12}H\left(\left[\frac{2}{4}, \frac{2}{4}\right]\right)\right] \approx 0 \text{ bits.}
\end{aligned}$$

Actually Patrons has the highest gain among the attributes, and is chosen to be the root of the tree. In general, we want to choose the feature A that maximizes $\text{Gain}(S, A)$.

One problem with Gain is that it likes to partition too much, and favors numerous splits: e.g., if each branch contains 1 example:



Then,

$$H\left[\frac{\#\text{pos}_j}{\#\text{pos}_j + \#\text{neg}_j}, \frac{\#\text{neg}_j}{\#\text{pos}_j + \#\text{neg}_j}\right] = 0 \text{ for all } j,$$

so all the terms for the entropy after branching would be zero and we'd choose that attribute over all the others.

An alternative to Gain is the *Gain Ratio*. We want to have a large Gain, but also we want a small number of partitions. We'll choose our attribute according to:

$$\begin{array}{rl} \dfrac{\text{Gain}(S, A)}{\text{SplitInfo}(S, A)} & \begin{array}{l} \leftarrow \text{ want large} \\ \leftarrow \text{ want small} \end{array} \end{array}$$

where $\text{SplitInfo}(S, A)$ comes from the partition:

$$\text{SplitInfo}(S, A) = -\sum_{j=1}^{J} \frac{|S_j|}{|S|} \log\left(\frac{|S_j|}{|S|}\right)$$

where $|S_j|$ is the number of examples in branch j. We want each term in the sum to be large. That means we want $\frac{|S_j|}{|S|}$ to be large, which means we want $|S_j|$ to be large, meaning that we want lots of examples in each branch.

Keep splitting until:

- no more examples left (no point trying to split)
- all examples have the same class
- no more attributes to split

For the restaurant example, we get this:

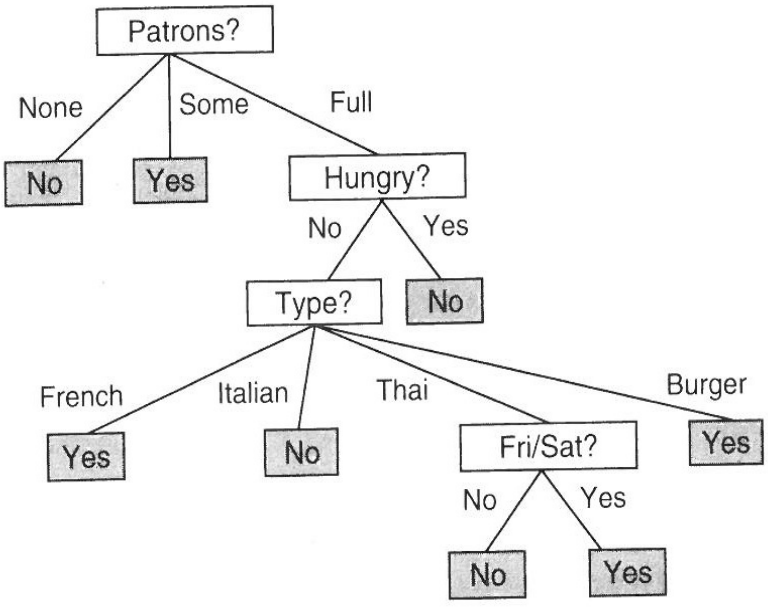


Figure 18.8 The decision tree induced from the 12-example training set.

A wrinkle: actually, it turns out that the class labels for the data were themselves generated from a tree. So to get the label for an example, they fed it into a tree, and got the label from the leaf. That tree is here:

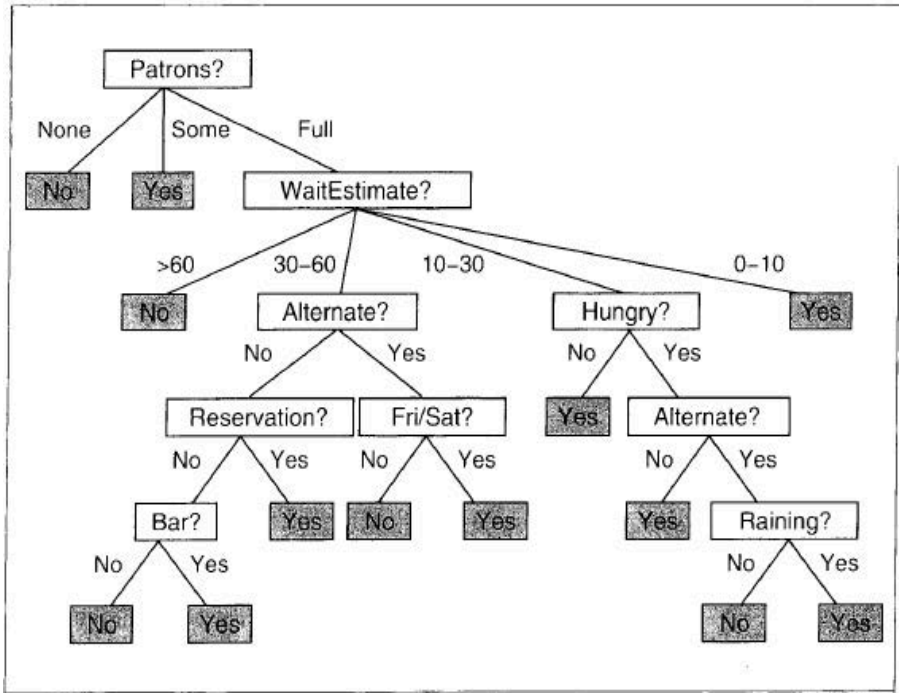


Figure 18.4 A decision tree for deciding whether to wait for a table.

But the one we found is simpler!

Does that mean our algorithm isn't doing a good job?

There are possibilities to replace $H([p, 1-p])$.

- Gini index $2p(1-p)$ used by CART.
- Misclassification error $1-\max(p, 1-p)$. (Say an event has prob p of success. Using majority vote, we classify the event to happen when $p > 1/2$ and classify the event not to happen when $p \leq 1/2$. This value is thus the proportion of time we guess incorrectly.)

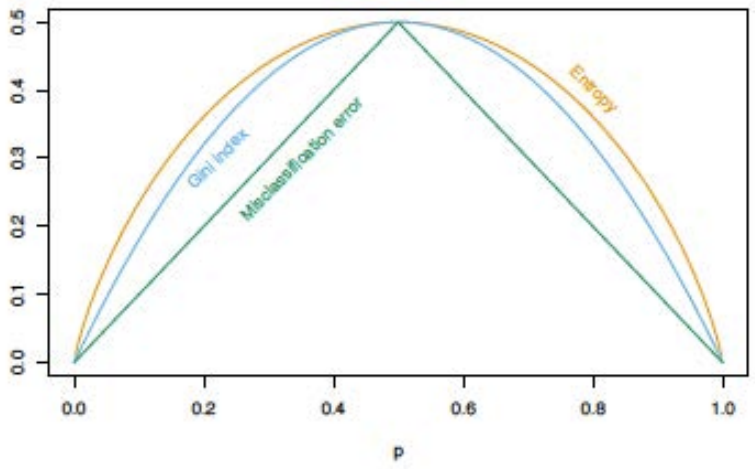


FIGURE 9.3. *Node impurity measures for two-class classification, as a function of the proportion p in class 2. Cross-entropy has been scaled to pass through* $(0.5, 0.5)$.

Pruning

Let's start with C4.5's pruning. C4.5 recursively makes choices as to whether to prune on an attribute:

- Option 1: leaving the tree as is
- Option 2: collapse that part of the tree into a leaf. The leaf has the most frequent label in the data S going to that part of the tree.
- Option 3: replace that part of the tree with one of its subtrees, corresponding to the most common branch in the split

To figure out which decision to make, C4.5 computes upper bounds on the probability of error for each option. I'll show you how to do that shortly.

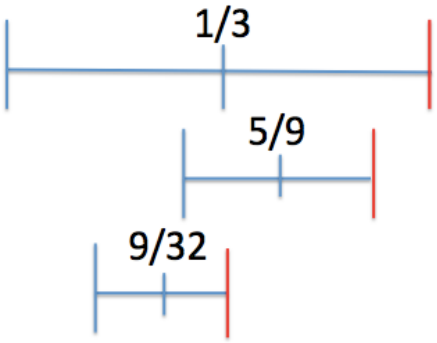
- Prob of error for Option 1 $\leq$ UpperBound$_1$
- Prob of error for Option 2 $\leq$ UpperBound$_2$
- Prob of error for Option 3 $\leq$ UpperBound$_3$

C4.5 chooses the option that has the lowest of these three upper bounds. This ensures that (w.h.p.) the error rate is fairly low.

E.g., which has the smallest upper bound:

- 1 incorrect out of 3
- 5 incorrect out of 9, or
- 9 incorrect out of 32?

Which of these could be the safest choice to reduce the misclassification rate?

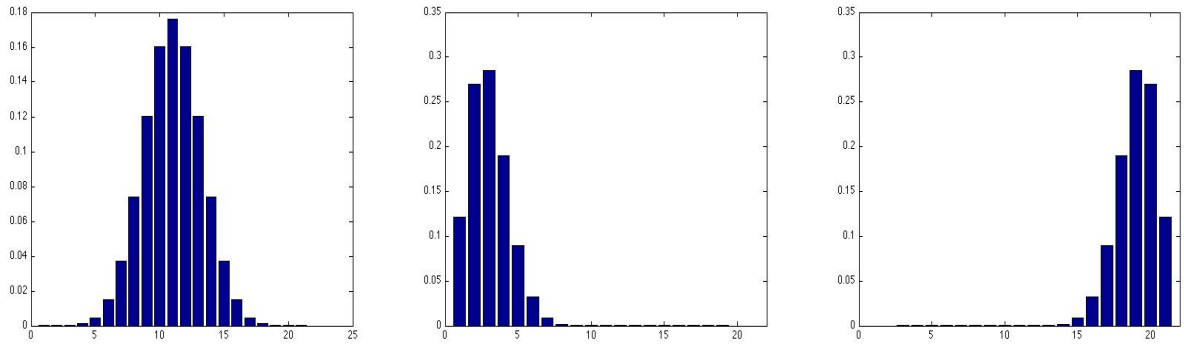


To calculate the upper bounds, calculate confidence intervals on proportions.

The abstract problem is: say you flip a coin N times, with M heads. (Here N is the number of examples in the leaf, M is the number incorrectly classified.) What is an upper bound for the probability p of heads for the coin?

Think visually about the binomial distribution, where we have N coin flips, and how it changes as p changes:

p=0.5 p=0.1 p=0.9

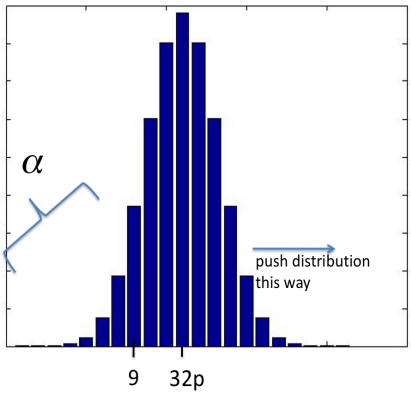


Is 9/32 reasonable for any of these coins? Hint: $9/32 \approx .28$.

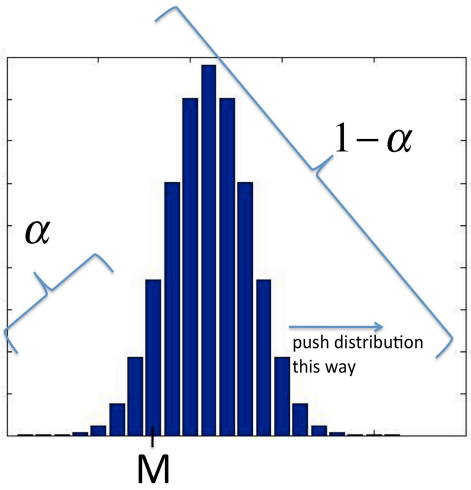
We need 9 to be a reasonable value, which means there should be a decently high probability to get 9 heads (or something more extreme).

We're trying to find an upper bound, meaning the largest reasonable value for the probability of success p of the coin. If p is too large and we flip it 32 times, then having only 9 heads is unlikely.

How large can p be and still have 9 heads be reasonable?



More generally, let's write this in terms of M heads out of N coin flips.



We define that for M to be reasonable, there must be α probability to achieve that value or something more extreme. Then we can solve for p in terms of α and M:

$$P_{M\sim \mathrm{Bin}(N,p)}(M \text{ or fewer errors}) \approx \alpha.$$

Let's call the solution p_α. I can write out the binomial coefficient terms:

$$\begin{aligned} P_{M\sim\text{Bin}(N,p_\alpha)}(M \text{ or fewer errors}) &\approx \alpha \\ \sum_{z=0}^{M} \text{Bin}(z, N, p_\alpha) &\approx \alpha \\ \sum_{z=0}^{M} \binom{N}{z} p_\alpha^z (1-p_\alpha)^{N-z} &\approx \alpha \text{ for } M > 0. \end{aligned}$$

(Note: for $M = 0$ it's $(1-p_\alpha)^N \approx \alpha$).

We can calculate this numerically without a problem. So now if you give me α M and N, I can give you p_α. C4.5 uses $\alpha = .25$ by default.

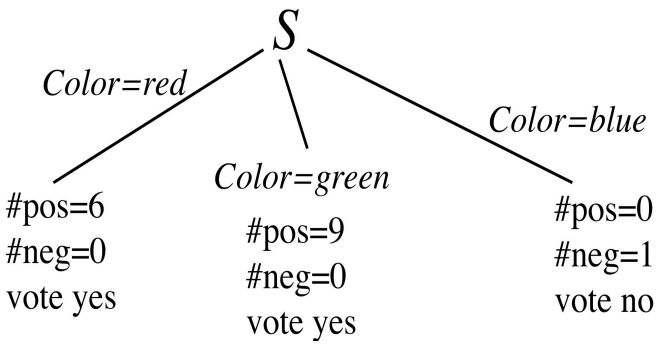
(M for a given branch is how many misclassified examples are in the branch. N for a given branch is just the number of examples in the branch, $|S_j|$.)

So we can calculate the upper bound on a branch, but it's still not clear how to calculate the upper bound on a tree. Actually, we calculate an upper confidence bound on each branch on the tree and average it over the relative frequencies of landing in each branch of the tree. It's best explained by example:

Let's consider a dataset of 16 examples describing toys (from the Kranf Site). We want to know if the toy is fun or not.

Color	Max number of players	Fun?
red	2	yes
red	3	yes
green	2	yes
red	2	yes
green	2	yes
green	4	yes
green	2	yes
green	1	yes
red	2	yes
green	2	yes
red	1	yes
blue	2	no
green	2	yes
green	1	yes
red	3	yes
green	1	yes

Think of a split on color.



Calculate the upper bound on the tree for Option 1: calculate $p_{.25}$ for each branch, which are respectively .206, .143, and .75. Then the average is:

$$\text{Ave of the upper bounds for tree} = \frac{1}{16}\left(6 \cdot .206 + 9 \cdot .143 + 1 \cdot .75\right) = .204.$$

Calculate the upper bound on the tree for Option 2: where we'd collapse the tree to a leaf with 6+9+1 = 16 examples in it, where 15 are positive, and 1 is negative. Calculate p_α that solves $\alpha = \sum_{z=0}^{1} \text{Bin}(z, 16, p_\alpha)$, which is .157. The average is:

$$\text{Ave of the upper bounds for leaf} = \frac{1}{16} 16 \cdot .157 = .157.$$

Option 3 is the same as Option 2. (If the green leaf had a subtree below it then Option 3 would have us keep that subtree, but it's just a leaf here.)

The upper bound on the error for Option 2 is lower, so we'll prune the tree to a leaf. Look at the data – does it make sense to do this?

CART - Classification and Regression Trees (Breiman, Friedman, Olshen, Stone, 1984)

Does only binary splits, not multiway splits (less interpretable, but simplifies splitting criteria).

For splitting, CART uses the Gini index. The Gini index is

$$p(1-p) = \frac{\text{variance of Bin}(n,p)}{n} = \text{variance of Bernoulli}(p).$$

For pruning, CART uses "minimal cost complexity."

Each subtree is assigned a cost.

$$\text{cost(subtree)} = \sum_{\text{leaves } j} \sum_{x_i \in \text{leaf } j} \mathbf{1}_{[y_i \neq \text{leaf's class}]} + C\left[\#\text{leaves in subtree}\right].$$

It eliminates the subtree if it doesn't reduce the error rate enough relative to the number of leaves. We could create a sequence of nested subtrees by gradually increasing C. We can use a validation set or full-blown nested cross-validation to choose C.

This cost function is actually what decision trees should be optimizing all along. However, computers in the 1980's weren't so good, and even now it is challenging to optimize over the set of decision trees. However, we can optimize this function over the set of decision *lists* for categorical data. This what the CORELS algorithm does (Angelino et al. 2017, 2018).

CART's Regression Trees

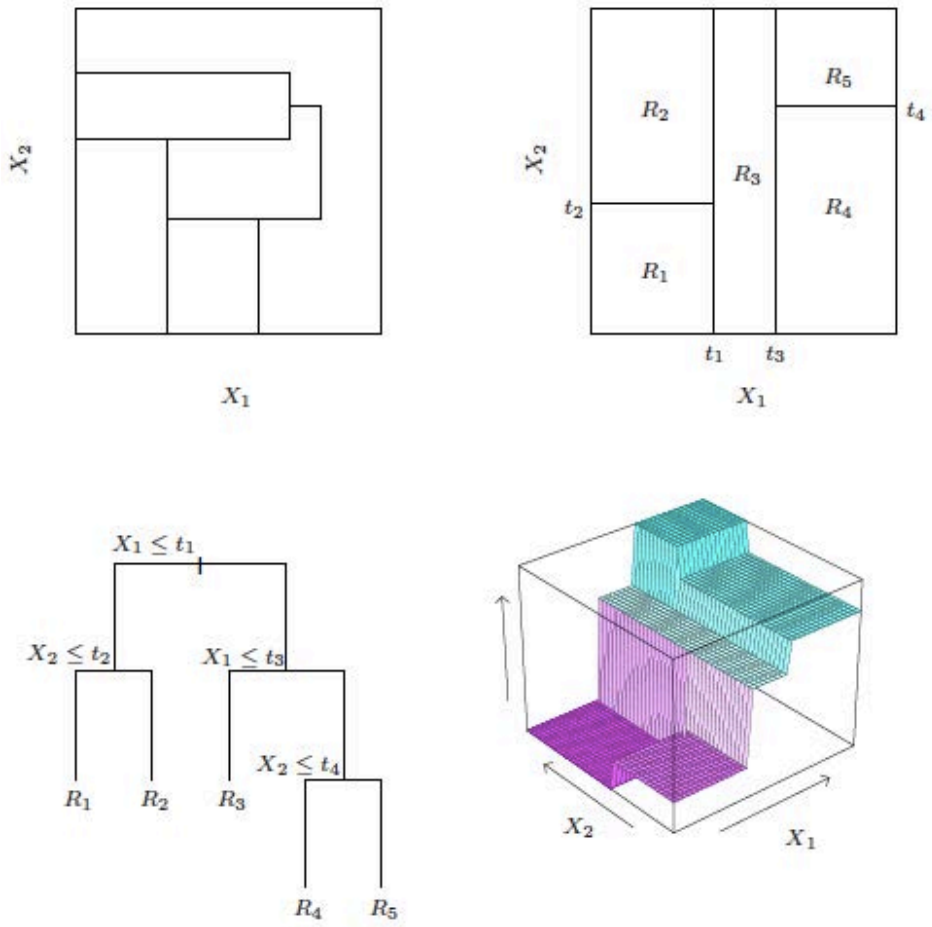


FIGURE 9.2. *Partitions and CART. Top right panel shows a partition of a two-dimensional feature space by recursive binary splitting, as used in CART, applied to some fake data. Top left panel shows a general partition that cannot be obtained from recursive binary splitting. Bottom left panel shows the tree corresponding to the partition in the top right panel, and a perspective plot of the prediction surface appears in the bottom right panel.*

CART decides which attributes to split and where to split them.
In each leaf, we're going to assign $f(x)$ to be a constant.

Can you guess what value to assign?

Consider the empirical error, using the least squares loss:

$$R^{\text{train}}(f) = \sum_i (y_i - f(x_i))^2$$

Break it up by leaves. Call the value of $f(x)$ in leaf j by f_j since it's a constant.

$$\begin{aligned} R^{\text{train}}(f) &= \sum_{\text{leaves } j} \sum_{i \in \text{leaf } j} (y_i - f(x_i))^2 \\ &= \sum_{\text{leaves } j} \sum_{i \in \text{leaf } j} (y_i - f_j)^2 =: \sum_{\text{leaves } j} R_j^{\text{train}}(f_j). \end{aligned}$$

To choose the value of the f_j's so that they minimize R_j^{train}, take the derivative, set it to 0. Let $|S_j|$ be the number of examples in leaf j.

$$\begin{aligned} 0 &= \frac{d}{d\tilde{f}} \sum_{i \in \text{leaf } j} (y_i - \tilde{f})^2 \Big|_{\tilde{f}=f_j} \\ &= -2 \sum_i (y_i - \tilde{f}) \Big|_{\tilde{f}=f_j} = -2 \left(\left(\sum_i y_i \right) - |S_j| \tilde{f} \right) \Big|_{\tilde{f}=f_j} \\ f_j &= \frac{1}{|S_j|} \sum_{i \in \text{leaf } j} y_i = \bar{y}_{S_j}, \end{aligned}$$

where $\bar{y}_{S_j}$ is the sample average of the labels for leaf j's examples.

So now we know what value to assign for f in each leaf. How to split? Greedily want feature j and split point s solving the following.

$$\min_{\substack{j,\, s \\ \text{for each feature } j \text{ do} \\ \text{a linesearch over } s}} \left[\min_{C_1} \sum_{x_i \in \{\text{leaf} | x^{(j)} \le s\}} (y_i - C_1)^2 + \min_{C_2} \sum_{x_i \in \{\text{leaf} | x^{(j)} > s\}} (y_i - C_2)^2 \right].$$

The first term means that we'll choose the optimal $C_1 = \bar{y}_{\{\text{leaf} | x^{(j)} \le s\}}$. The second term means we'll choose $C_2 = \bar{y}_{\{\text{leaf} | x^{(j)} > s\}}$.

For pruning, again CART does minimal cost complexity pruning:

$$\text{cost} = \sum_{\text{leaves } j} \sum_{x_i \in S_j} (y_i - \bar{y}_{S_j})^2 + C[\#\text{ leaves in tree}]$$