Statistical Machine Learning

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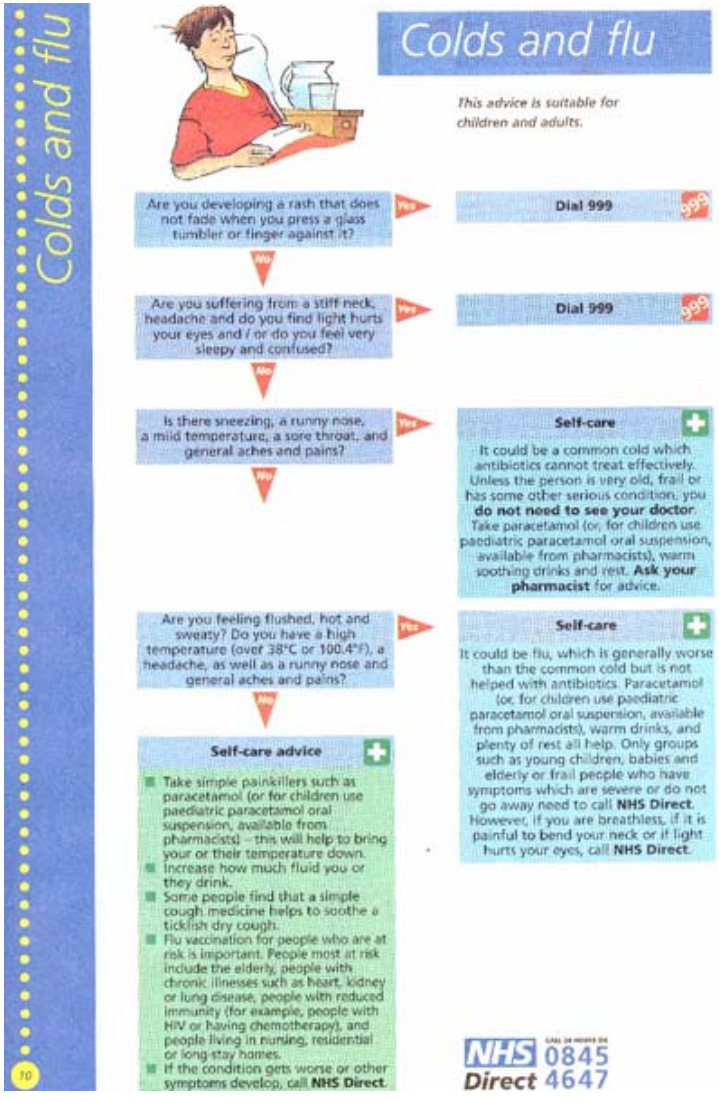
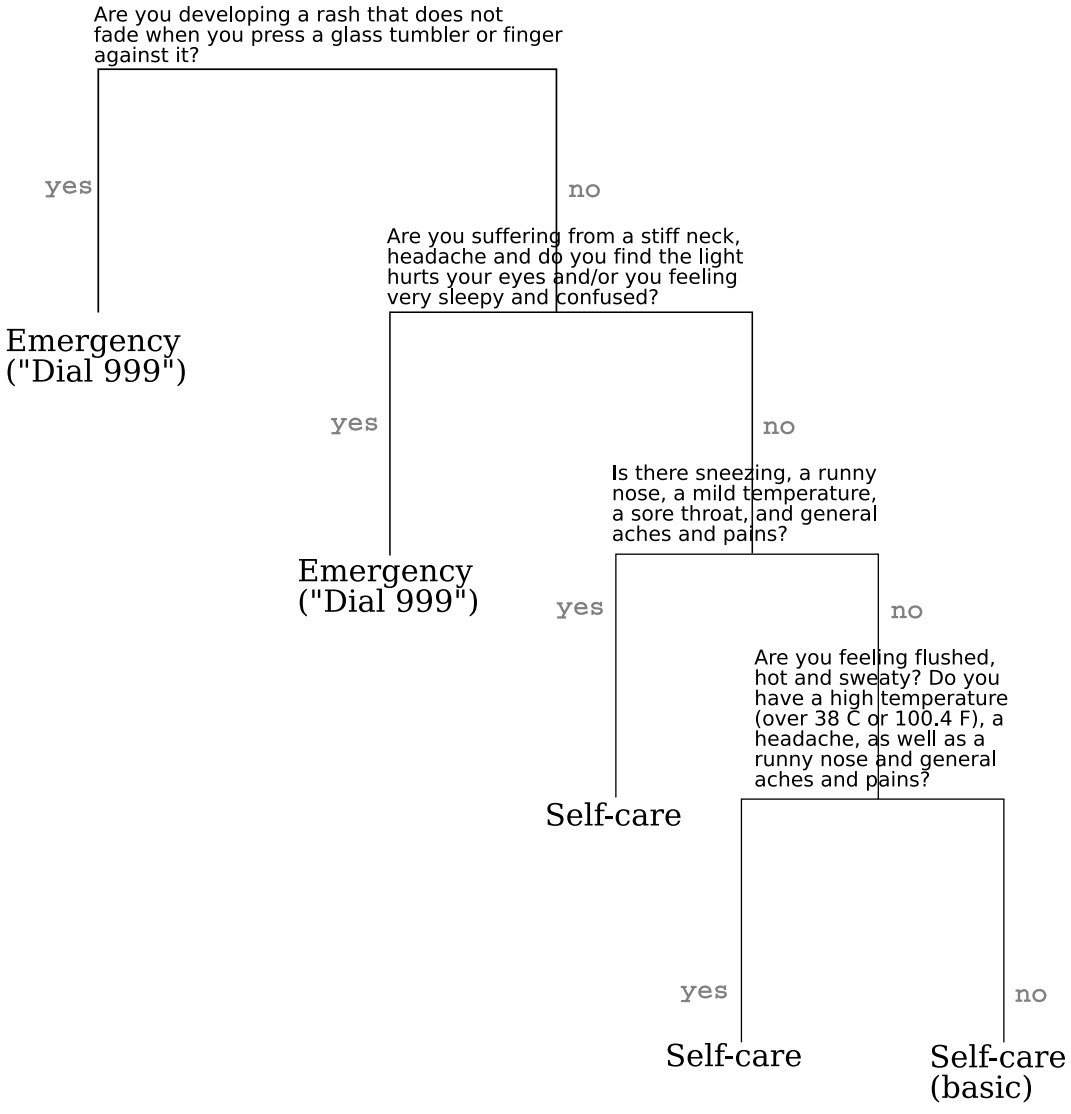
Slide credits and other course material can be found at:
http://www.stats.ox.ac.uk/~palamara/SML20_BDI.html

Many decisions are tree-structured

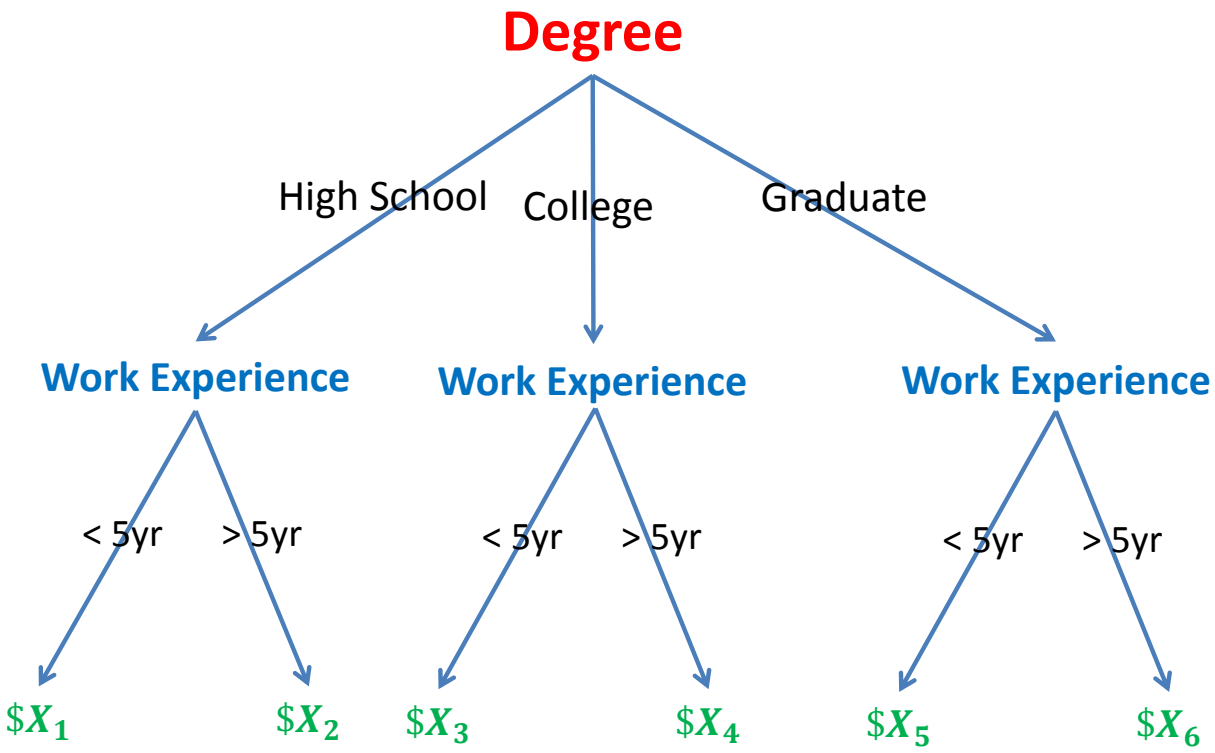


Many decisions are tree-structured



Many decisions are tree-structured

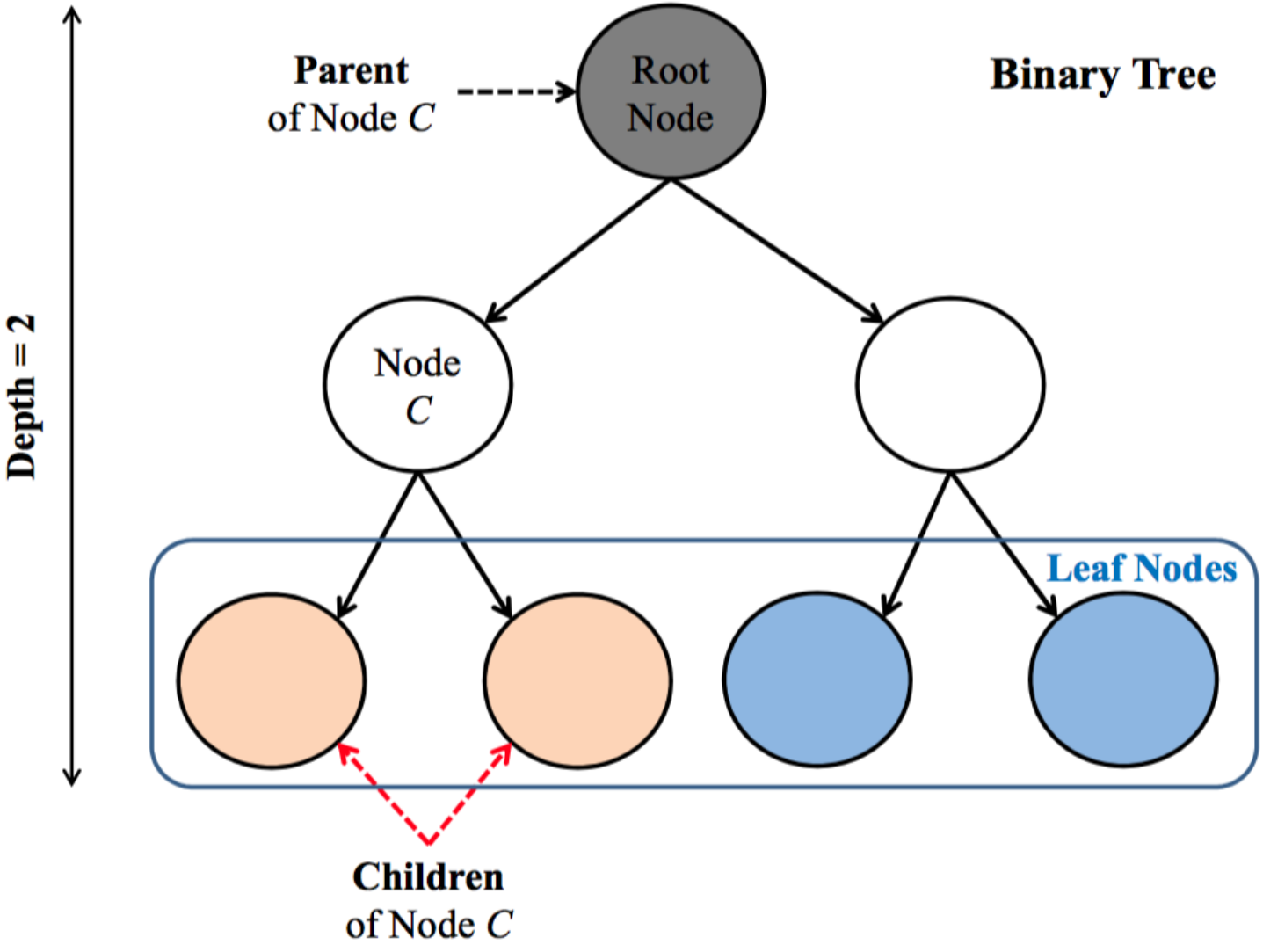
- Employee salary



Terminology

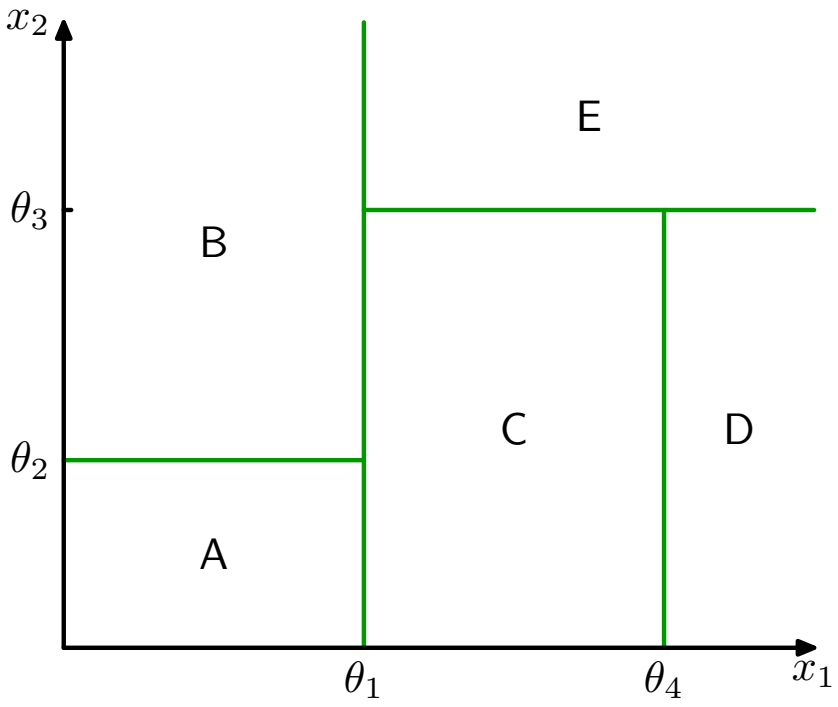
- **Parent** of a node c is the immediate predecessor node.
- **Children** of a node c are the immediate successors of c, equivalently nodes which have c as a parent.
- **Branch** are the edges/arrows connecting the nodes.
- **Root** node is the top node of the tree; the only node without parents.
- **Leaf** nodes are nodes which do not have children.
- **Stumps** are trees with just the root node and two leaf nodes.
- A $K-$**ary** tree is a tree where each node (except for leaf nodes) has K children. Usually working with binary trees $(K = 2)$.
- **Depth** of a tree is the maximal length of a path from the root node to a leaf node.

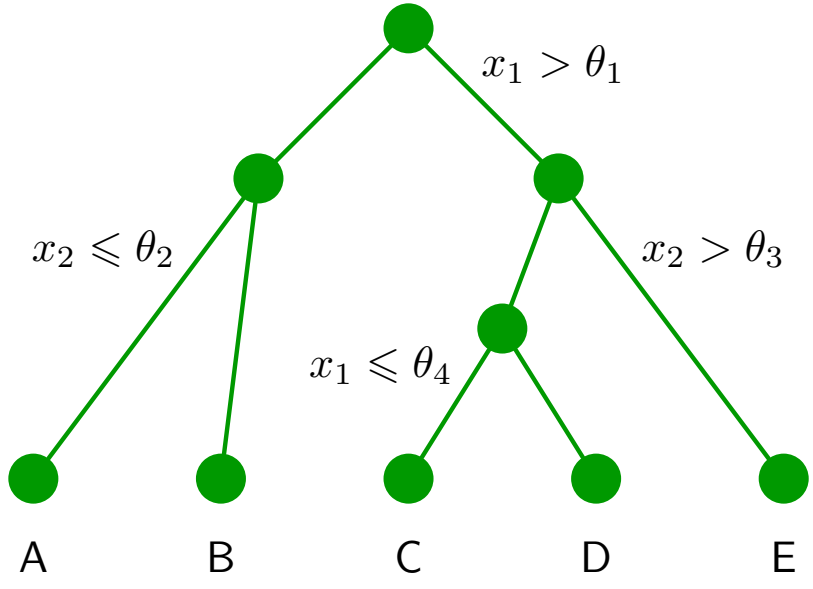
Terminology



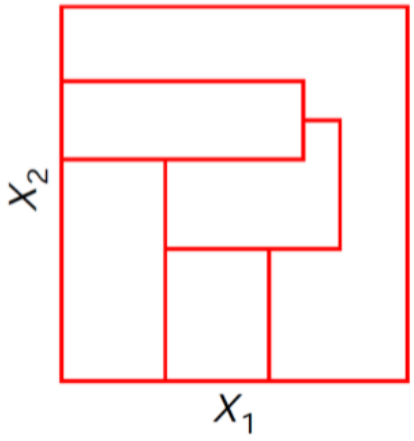
A tree partitions the feature space

- A Decision Tree is a hierarchically organized structure, with each node splitting the data space into pieces based on value of a feature.
  - Equivalent to a partition of $\mathcal{R}_d$ into K disjoint feature regions $\{\mathcal{R}_j, \ldots, \mathcal{R}_j\}$, where each $\mathcal{R}_j \subset \mathbb{R}^p$
  - On each feature region $\mathcal{R}_j$, the same decision/prediction is made for all $x \in \mathcal{R}_j$.

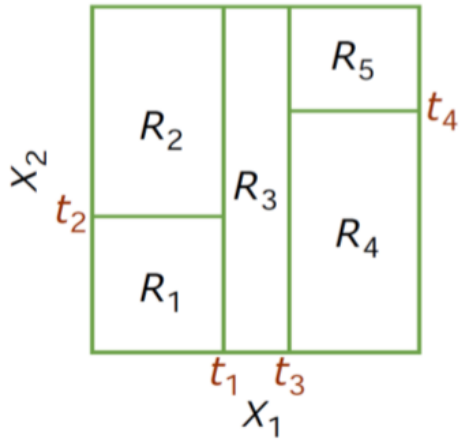




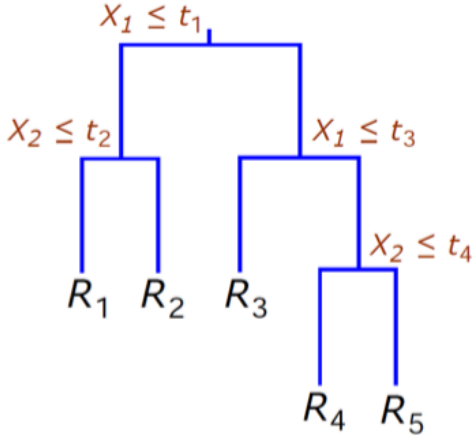
Partitions and regression trees



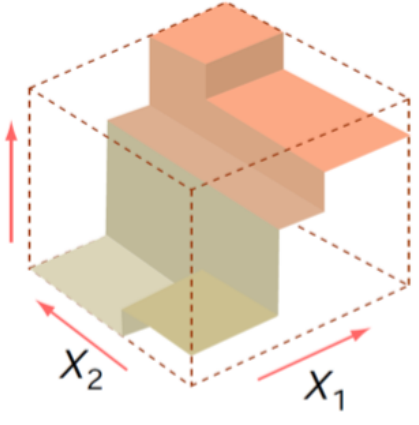
(a) General partition that cannot be obtained from recursive binary splitting.



(b) Partition of a two-dimensional feature space by recursive binary splitting, as used in CART, applied to some fake data.



(c) Tree corresponding to the partition in the top right panel.

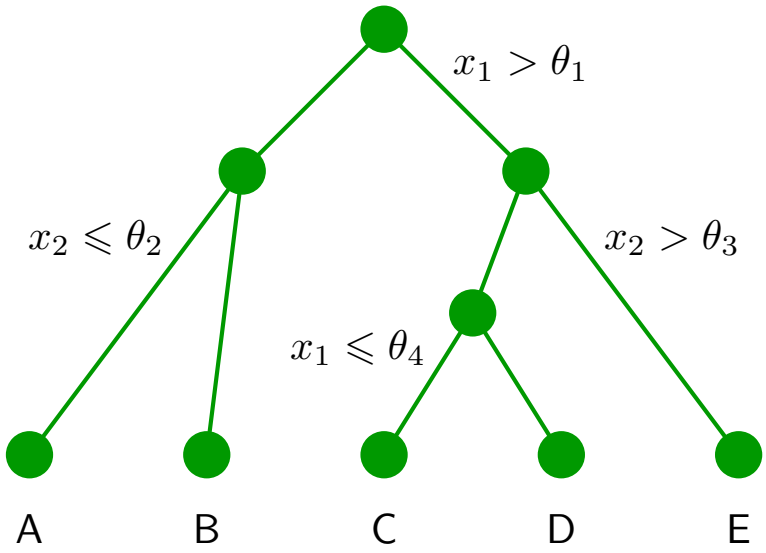


(d) A perspective plot of the prediction surface.

Learning a tree model

Three things to learn:

1. The structure of the tree.
2. The threshold values (θ_i).
3. The values for the leaves ($A, B, \ldots$).



Classification Tree

Classification Tree:

- Given the dataset $D = (x_1, y_1), \ldots, (x_n, y_n)$ where $x_i \in \mathbb{R}, y_i \in Y = \{1, \ldots, m\}$.
- minimize the misclassification error in each leaf
- the estimated probability of each class k in region $\mathcal{R}_j$ is simply:

$$\beta_{jk} = \frac{\sum_i \mathbb{I}(y_i = k) \cdot \mathbb{I}(x_i \in \mathcal{R}_j)}{\sum_i \mathbb{I}(x_i \in \mathcal{R}_j)}$$

- This is the frequency in which label k occurs in the leaf $\mathcal{R}_j$. (These estimates can be regularized.)

Example: A tree model for deciding where to eat

Decide whether to wait for a table at a restaurant, based on the following attributes (Example from Russell and Norvig, AIMA)

- Alternate: is there an alternative restaurant nearby?
- Bar: is there a comfortable bar area to wait in?
- Fri/Sat: is today Friday or Saturday?
- Hungry: are we hungry?
- Patrons: number of people in the restaurant (None, Some, Full)
- Price: price range ($, $$, $$$)
- Raining: is it raining outside?
- Reservation: have we made a reservation?
- Type: kind of restaurant (French, Italian, Thai, Burger)
- Wait Estimate: estimated waiting time (0-10, 10-30, 30-60, >60)

Example: A tree model for deciding where to eat

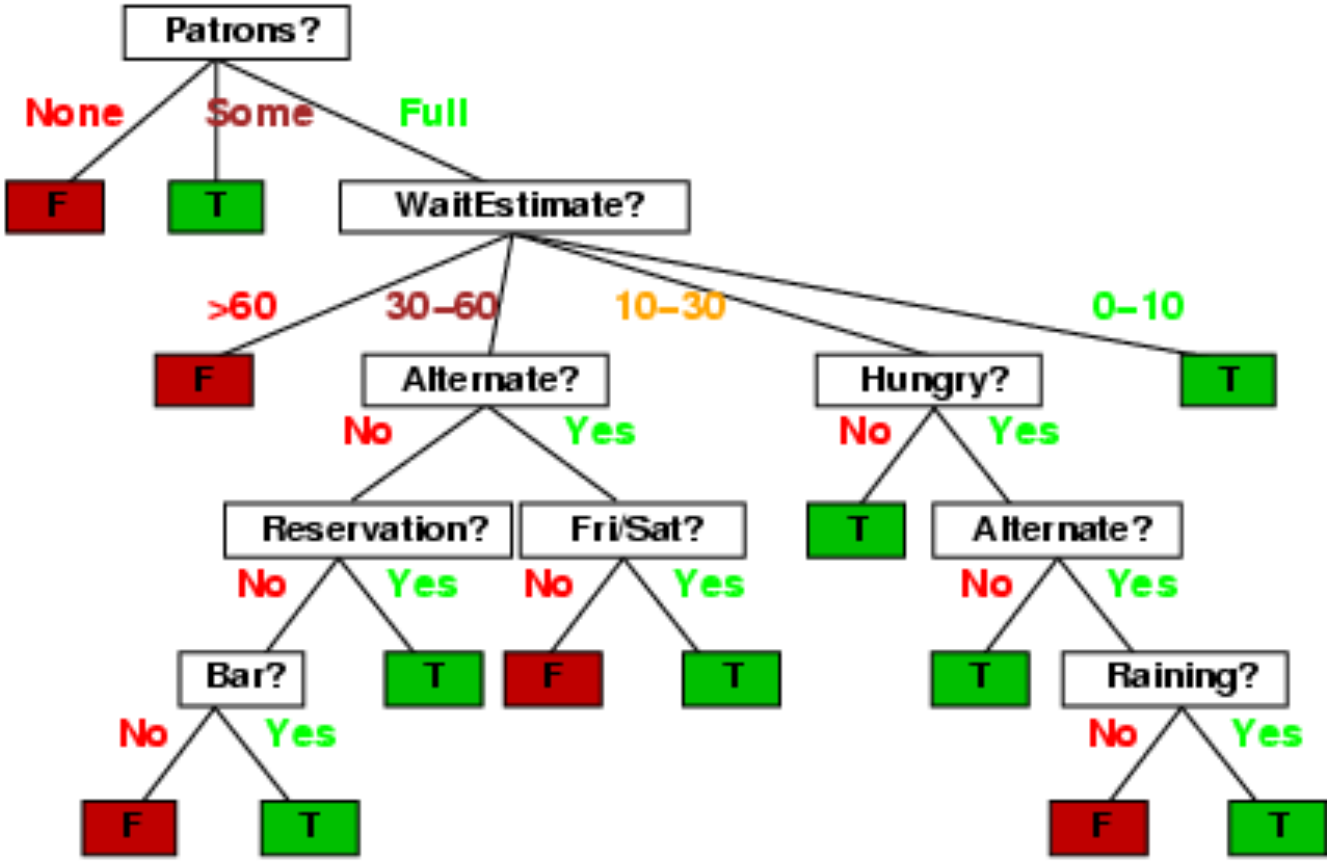
Choosing a restaurant

(Example from Russell & Norvig, AIMA)

Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
X_1	*T*	*F*	*F*	*T*	*Some*	*$$$*	*F*	*T*	*French*	*0–10*	*T*
X_2	*T*	*F*	*F*	*T*	*Full*	*$*	*F*	*F*	*Thai*	*30–60*	*F*
X_3	*F*	*T*	*F*	*F*	*Some*	*$*	*F*	*F*	*Burger*	*0–10*	*T*
X_4	*T*	*F*	*T*	*T*	*Full*	*$*	*F*	*F*	*Thai*	*10–30*	*T*
X_5	*T*	*F*	*T*	*F*	*Full*	*$$$*	*F*	*T*	*French*	*>60*	*F*
X_6	*F*	*T*	*F*	*T*	*Some*	*$$*	*T*	*T*	*Italian*	*0–10*	*T*
X_7	*F*	*T*	*F*	*F*	*None*	*$*	*T*	*F*	*Burger*	*0–10*	*F*
X_8	*F*	*F*	*F*	*T*	*Some*	*$$*	*T*	*T*	*Thai*	*0–10*	*T*
X_9	*F*	*T*	*T*	*F*	*Full*	*$*	*T*	*F*	*Burger*	*>60*	*F*
X_{10}	*T*	*T*	*T*	*T*	*Full*	*$$$*	*F*	*T*	*Italian*	*10–30*	*F*
X_{11}	*F*	*F*	*F*	*F*	*None*	*$*	*F*	*F*	*Thai*	*0–10*	*F*
X_{12}	*T*	*T*	*T*	*T*	*Full*	*$*	*F*	*F*	*Burger*	*30–60*	*T*

Classification of examples is positive (T) or negative (F)

A possible decision tree



Is this the best decision tree?

Decision tree training/learning

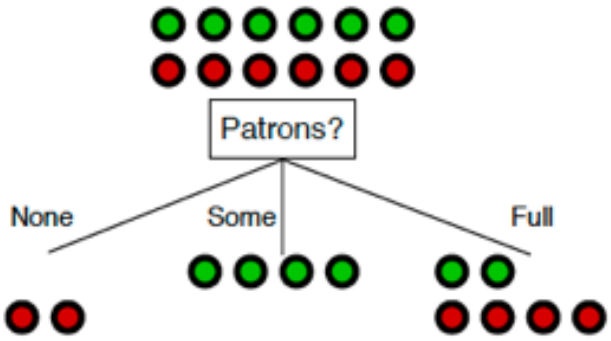
For simplicity assume both features and outcome are binary (take YES/NO values).

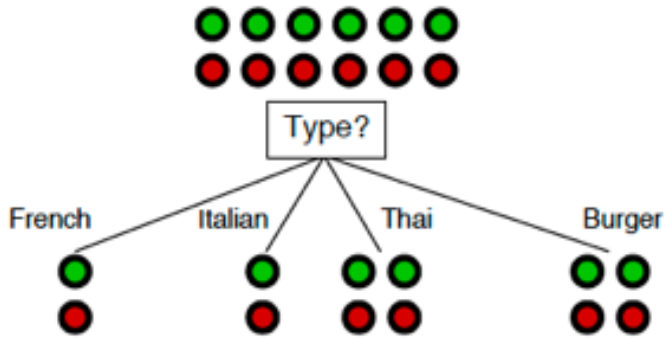
Algorithm 1 DecisionTreeTrain ($data, features$)

$guess \leftarrow$ the most frequent label in $data$
if all labels in $data$ are the same **then**
  return LEAF ($guess$)
else
  $f \leftarrow$ the "best" feature $\in features$
  $NO \leftarrow$ the subset of $data$ on which $f = NO$
  $YES \leftarrow$ the subset of $data$ on which $f = YES$
  $left \leftarrow$ DecisionTreeTrain (NO, $features - \{f\}$)
  $right \leftarrow$ DecisionTreeTrain (YES, $features - \{f\}$)
  return NODE($f, left, right$)
end if

First decision: at the root of the tree

Which attribute to split?





Patrons? is a better choice—gives **information** about the classification

Idea: use information gain to choose which attribute to split

Information gain

- Basic idea: **Gaining information** reduces uncertainty
- Given a random variable X with K different values, $(a_1, \ldots, a_K)$, we can use different measures of "purity" of a node:
  - **Entropy** (measured in bits, max$= 1$):

$$H[X] = -\sum_{k=1}^{K} P(X = a_k) \times \log_2 P(X = a_k)$$

  - **Misclassification error** (max$= 0.5$): if c is the most common class label

$$1 - P(X = c)$$

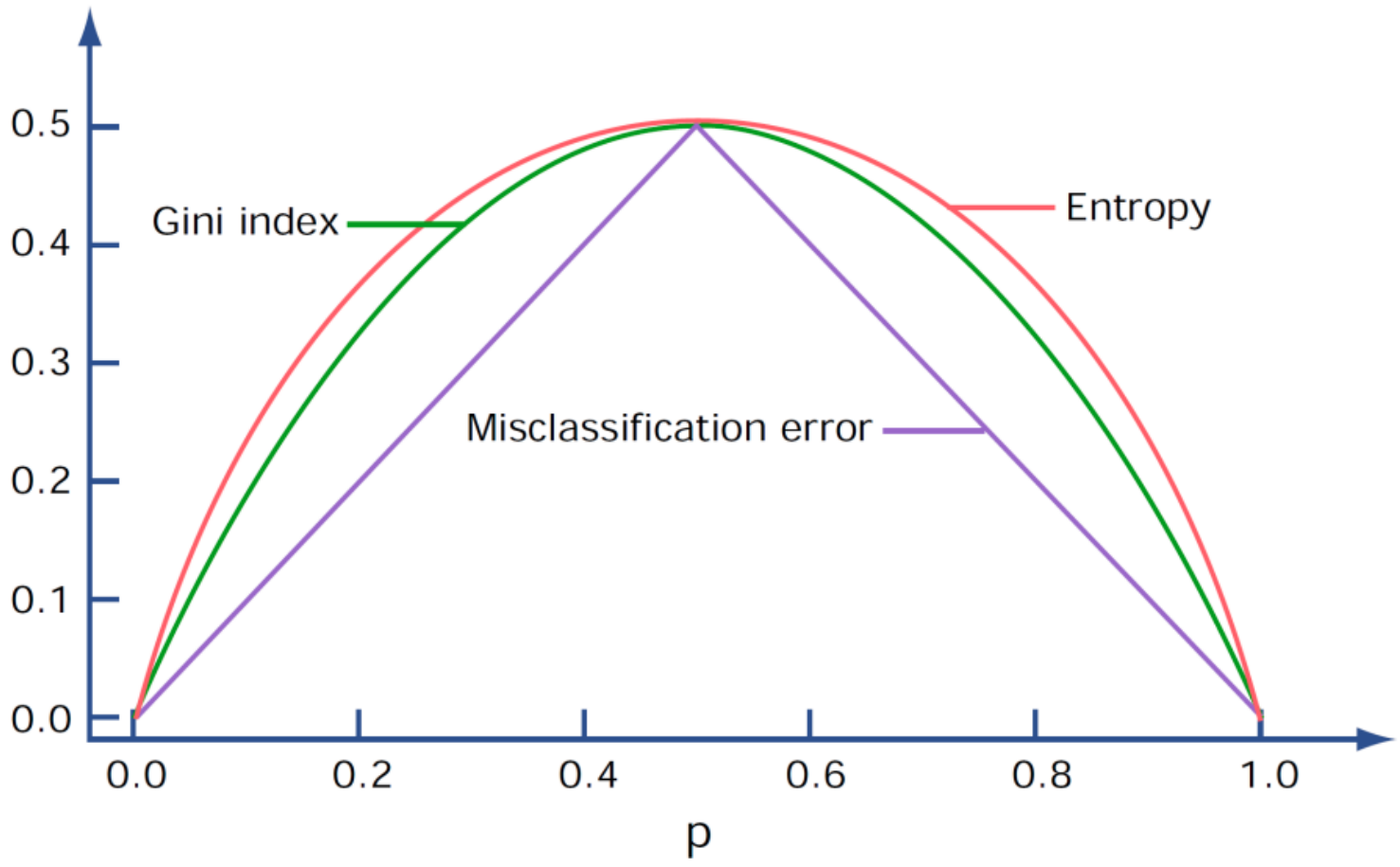
  - **GINI Index** (max$= 0.5$):

$$\sum_{k=1}^{K} P(X = a_k)(1 - P(X = a_k))$$

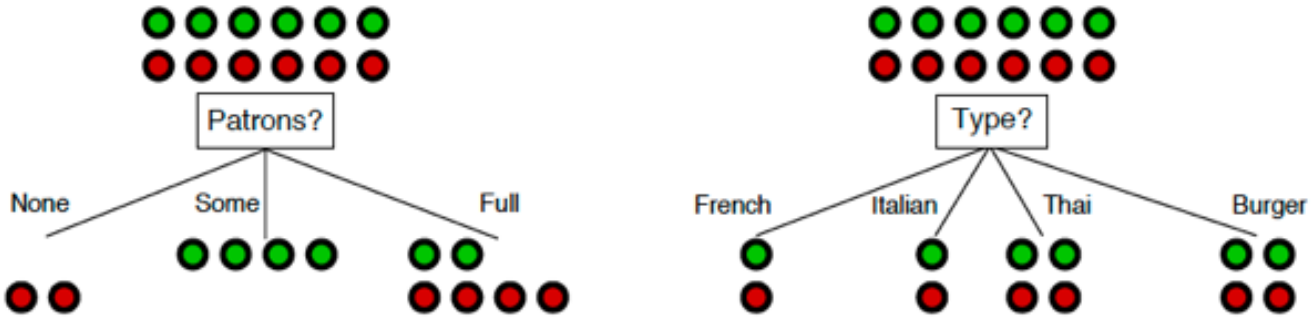
  - E.g. compare splits $[(300, 100), (100, 300)]$ and $[(200, 400), (200, 0)]$, taking average of scores for nodes produced (but note different max values). which node will each measure prefer, and would you agree?

- **C4.5** Tree algorithm: Classification uses entropy to measure uncertainty.
- **CART** (class. and regression tree) algorithm: Classification uses Gini.

Different measures of uncertainty



Which attribute to split?



Patrons? is a better choice—gives information about the classification

Patron vs. Type?

By choosing Patron, we end up with a partition (3 branches) with smaller entropy, ie, smaller uncertainty (0.45 bit)

By choosing Type, we end up with uncertainty of 1 bit.

Thus, we choose Patron over Type.

Uncertainty if we go with "Patron"

For "None" branch

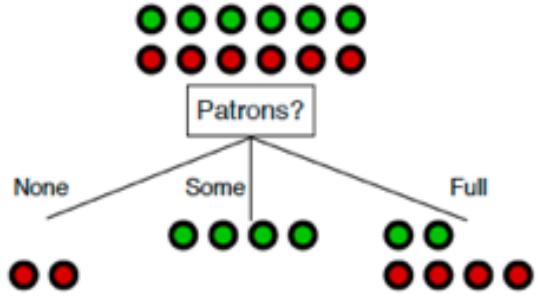
$$-\left(\frac{0}{0+2}\log\frac{0}{0+2}+\frac{2}{0+2}\log\frac{2}{0+2}\right)=0$$

For "Some" branch

$$-\left(\frac{4}{4+0}\log\frac{4}{4+0}+\frac{4}{4+0}\log\frac{4}{4+0}\right)=0$$

For "Full" branch

$$-\left(\frac{2}{2+4}\log\frac{2}{2+4}+\frac{4}{2+4}\log\frac{4}{2+4}\right)\approx 0.9$$



For choosing "Patrons"

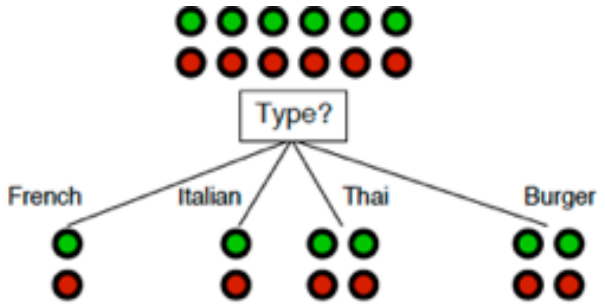
weighted average of each branch: this quantity is called conditional entropy

$$\frac{2}{12}*0+\frac{4}{12}*0+\frac{6}{12}*0.9=0.45$$

Conditional entropy for Type

For "French" branch

$$-\left(\frac{1}{1+1}\log\frac{1}{1+1}+\frac{1}{1+1}\log\frac{1}{1+1}\right)=1$$



For "Italian" branch

$$-\left(\frac{1}{1+1}\log\frac{1}{1+1}+\frac{1}{1+1}\log\frac{1}{1+1}\right)=1$$

For "Thai" and "Burger" branches

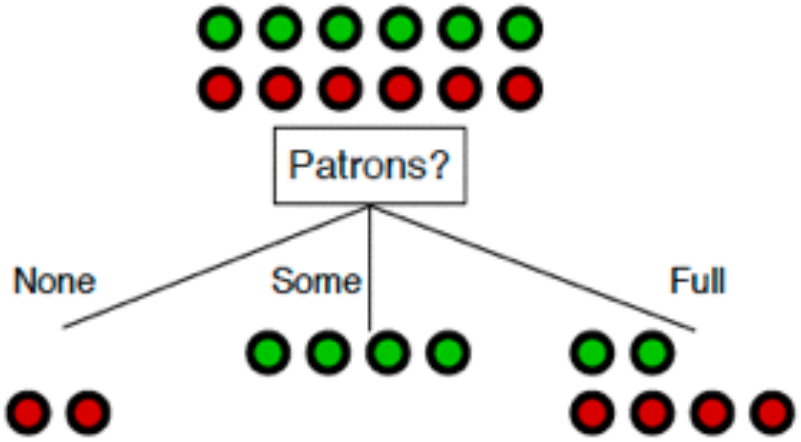
$$-\left(\frac{2}{2+2}\log\frac{2}{2+2}+\frac{2}{2+2}\log\frac{2}{2+2}\right)=1$$

For choosing "Type"

weighted average of each branch:

$$\frac{2}{12}*1+\frac{2}{12}*1+\frac{4}{12}*1+\frac{4}{12}*1=1$$

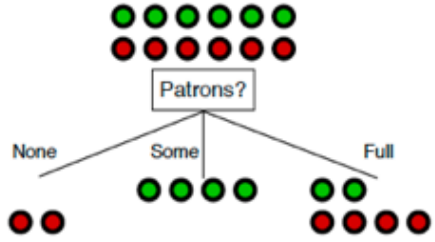
Do we split on “Non” or “Some”?



No, we do not

The decision is deterministic, as seen from the training data

next split?

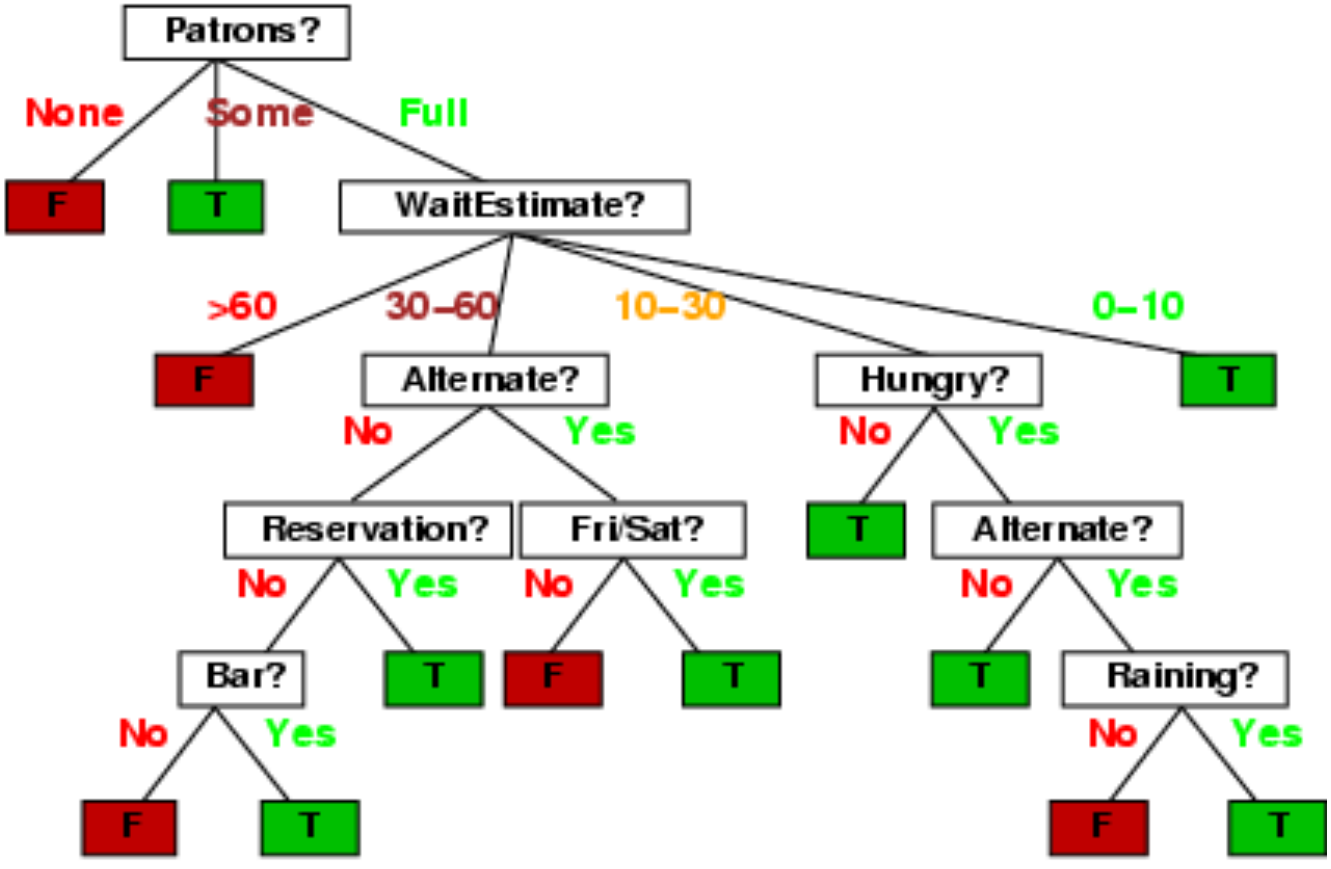


We will look only at the 6 instances with Patrons == Full

Example	Attributes										Target
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
X_1	T	F	F	T	Some	$$$	F	T	French	0–10	T
X_2	T	F	F	T	Full	$	F	F	Thai	30–60	F
X_3	F	T	F	F	Some	$	F	F	Burger	0–10	T
X_4	T	F	T	T	Full	$	F	F	Thai	10–30	T
X_5	T	F	T	F	Full	$$$	F	T	French	>60	F
X_6	F	T	F	T	Some	$$	T	T	Italian	0–10	T
X_7	F	T	F	F	None	$	T	F	Burger	0–10	F
X_8	F	F	F	T	Some	$$	T	T	Thai	0–10	T
X_9	F	T	T	F	Full	$	T	F	Burger	>60	F
X_{10}	T	T	T	T	Full	$$$	F	T	Italian	10–30	F
X_{11}	F	F	F	F	None	$	F	F	Thai	0–10	F
X_{12}	T	T	T	T	Full	$	F	F	Burger	30–60	T

Classification of examples is positive (T) or negative (F)

Greedily, we build



An Algorithm for Classification Trees

Assume binary classification for simplicity ($y_i \in \{0, 1\}$), and numerical features (see Section 9.2.4 in ESL for categorical features and binary trees).

1. Start with $\mathcal{R}_1 = \mathcal{X} = \mathbb{R}^p$.
2. For each feature $j = 1, \ldots, p$, for each value $v \in \mathbb{R}$ that we can split on:
   1. Split data set:
   $$I_< = \{i : x_i^{(j)} < v\} \qquad I_> = \{i : x_i^{(j)} \geq v\}$$
   2. Estimate parameters:
   $$\beta_< = \frac{\sum_{i \in I_<} y_i}{|I_<|} \qquad \beta_> = \frac{\sum_{i \in I_>} y_i}{|I_>|}$$
   3. Compute the **quality of split**, e.g., using entropy (note: we take $0 \log 0 = 0$)
   $$\frac{|I_<|}{|I_<| + |I_>|} \mathrm{B}(\beta_<) + \frac{|I_>|}{|I_<| + |I_>|} \mathrm{B}(\beta_>)$$
   where
   $$\mathrm{B}(q) = -[q \log_2(q) + (1 - q) \log_2(1 - q)]$$
3. Choose split, i.e., feature j and value v, with maximum quality.
4. Recurse on both children, with datasets $(x_i, y_i)_{i \in I_<}$ and $(x_i, y_i)_{i \in I_>}$.

Comparing the features with conditional entropy

- Given two random variables X and Y, conditional entropy is

$$H[Y|X] = \sum_k P(X = a_k) \times H[Y|X = a_k]$$

- In the algorithm,
  - X: the attribute to be split (e.g. patrons)
  - Y: the labels (e.g. wait or not)
  - Estimated $P(X = a_k)$ is the weight in the quality calculation
- Relation to **information gain**

$$\text{Gain}[Y, X] = H[Y] - H[Y|X]$$

  - When $H[Y]$ is fixed, we need only to compare conditional entropy.
  - Minimizing conditional entropy is equivalent to maximizing information gain.

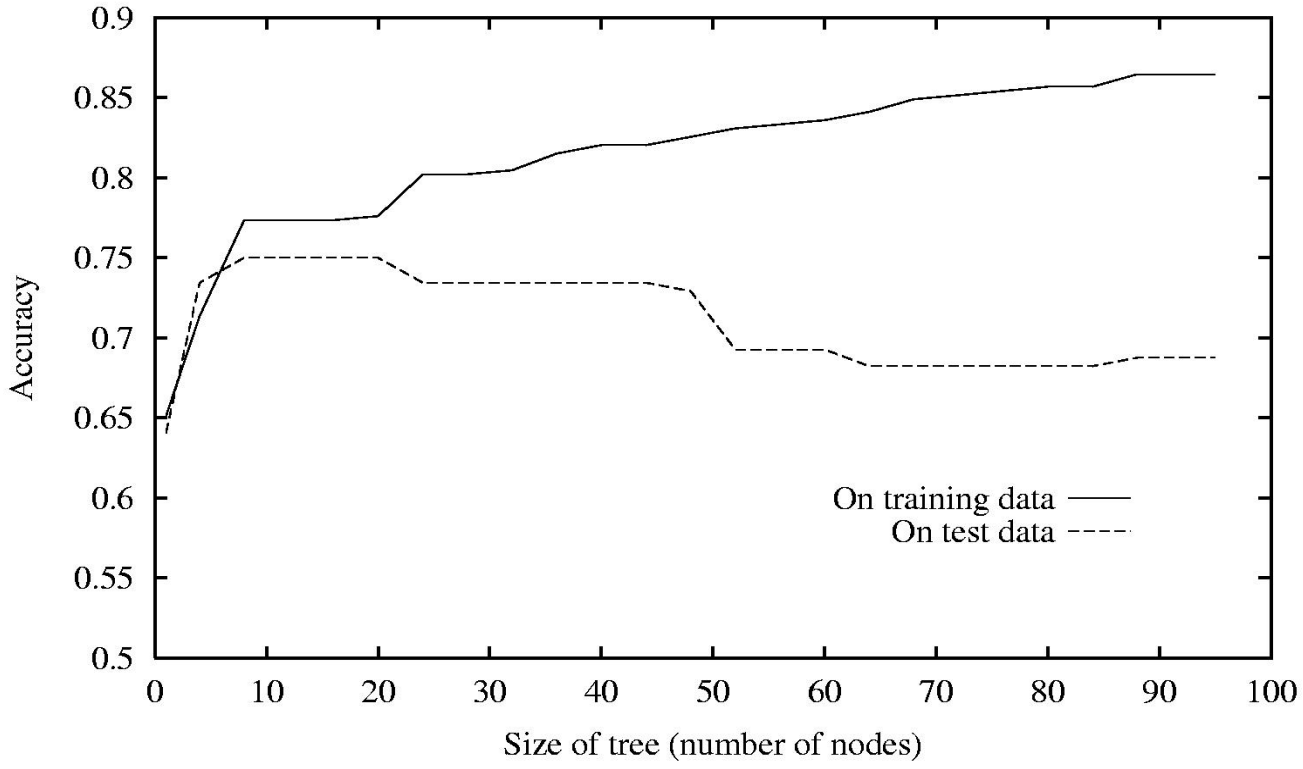
Patrons vs Type

$$\text{Gain}[Y, \text{Patrons}] = H[Y] - H[Y|\text{Patrons}] = 1 - 0.45 = 0.55$$

$$\text{Gain}[Y, \text{Type}] = H[Y] - H[Y|\text{Type}] \quad = 1 - 1 \quad = 0$$

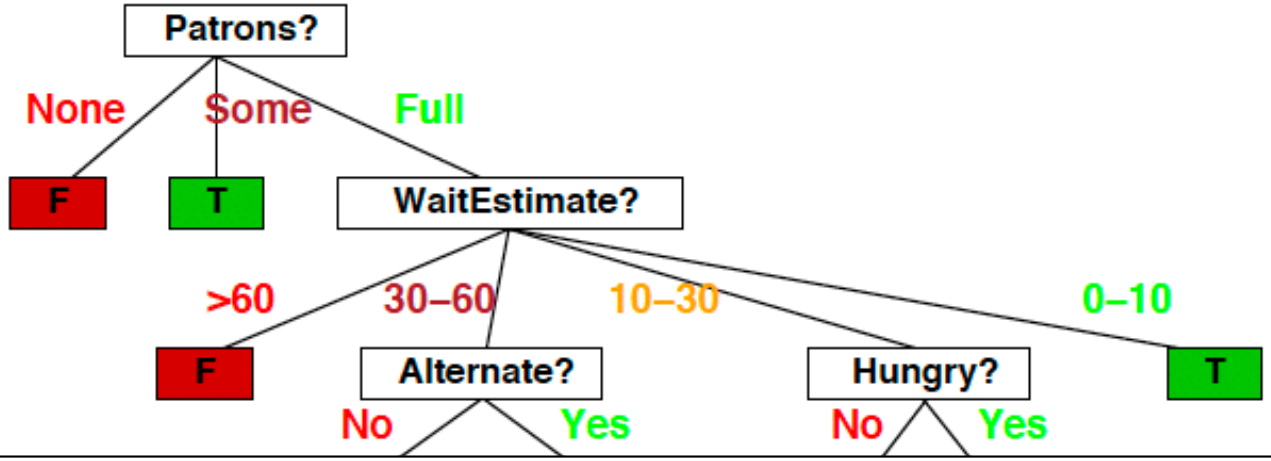
What is the optimal Tree Depth?

- We need to be careful to pick an appropriate tree depth.
- If the tree is too deep, we can overfit.
- If the tree is too shallow, we underfit
- Max depth is a hyper-parameter that should be tuned by the data.
- Alternative strategy is to create a very deep tree, and then to prune it.



Control the size of the tree

We would prune to have a smaller one



If we stop here, not all training sample would be classified correctly.

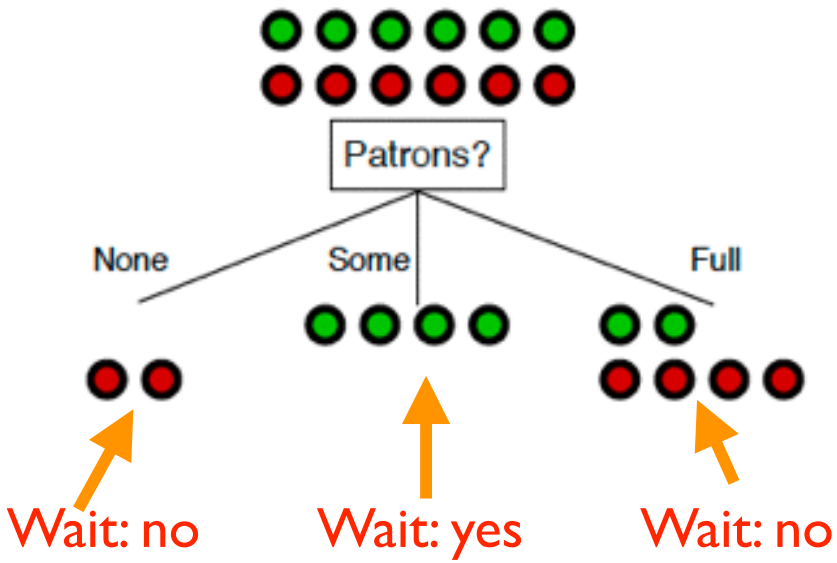
More importantly, how do we classify a new instance?

We label the leaves of this smaller tree with the majority of training samples' labels

Example

Example

We stop after the root (first node)



Computational Considerations

Numerical Features

- We could split on any feature, with any threshold
- However, for a given feature, the only split points we need to consider are the the n values in the training data for this feature.
- If we sort each feature by these n values, we can quickly compute our impurity metric of interest (cross entropy or others), skipping values where labels are unchanged.
  - This takes $O(d\, n \log n)$ time (sorting n elements takes $O(n \log n)$ steps).

Categorical Features

- Assuming q distinct categories, there are $2^{q-1} - 1$ possible binary partitions we can consider.
- However, things simplify in the case of binary classification (or regression, see Section 9.2.4 in ESL for details).

Summary of learning classification trees

Advantages

- Easily interpretable by human (as long as the tree is not too big)
- Computationally efficient
- Handles both numerical and categorical data
- It is parametric thus compact: unlike Nearest Neighborhood Classification, we do not have to carry our training instances around
- Building block for various ensemble methods (more on this later)

Disadvantages

- Heuristic training techniques
- Finding partition of space that minimizes empirical error is NP-hard.
- We resort to greedy approaches with limited theoretical underpinning.
- Unstable: small changes in input data lead to different trees. Mitigated by ensable methods (e.g. random forests, coming up).

Regression Tree

Regression Tree:

- Given the dataset $D = (x_1, y_1), \ldots, (x_n, y_n)$ where $x_i \in \mathbb{R}, y_i \in Y = \{1, \ldots, m\}$.
- minimize the squared loss (may use others!) in each leaf
- the parameterized function is:

$$\hat{f}(x) = \sum_{j=1}^{K} \beta_j \cdot \mathbb{I}(x \in \mathcal{R}_j)$$

- Using squared loss, optimal parameters are:

$$\hat{\beta}_j = \frac{\sum_{i=1}^{n} y_i \cdot \mathbb{I}(x_i \in \mathcal{R}_j)}{\sum_{i=1}^{n} \mathbb{I}(x_i \in \mathcal{R}_j)}$$

  i.e. the sample mean.

An Algorithm for Regression Trees

Assume numerical features (see Section 9.2.4 in ESL for categorical).

1. Start with $\mathcal{R}_1 = \mathcal{X} = \mathbb{R}^p$.
2. For each feature $j = 1, \ldots, p$, for each value $v \in \mathbb{R}$ that we can split on:
   1. Split data set:

$$I_< = \{i : x_i^{(j)} < v\} \qquad I_> = \{i : x_i^{(j)} \geq v\}$$

   2. Estimate parameters:

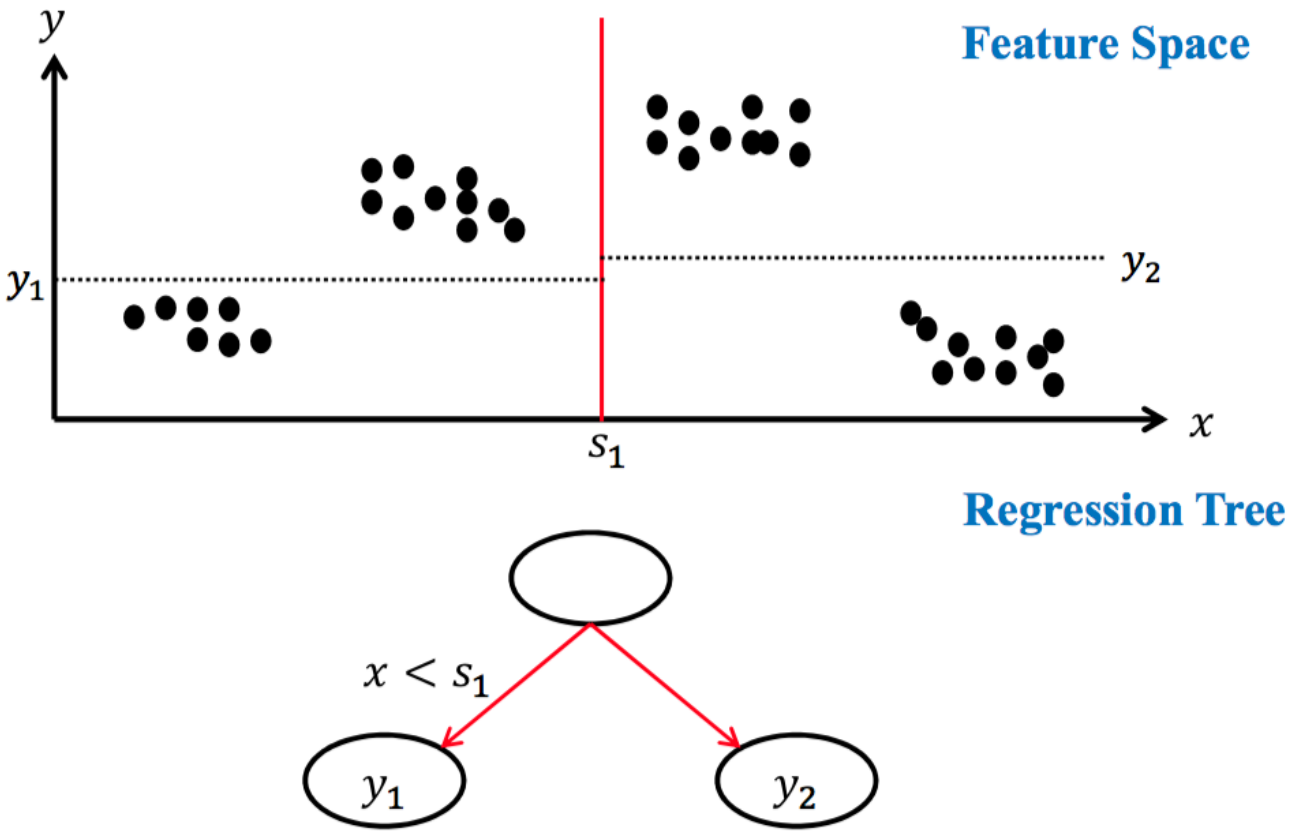
$$\beta_< = \frac{\sum_{i \in I_<} y_i}{|I_<|} \qquad \beta_> = \frac{\sum_{i \in I_>} y_i}{|I_>|}$$

   3. **Quality of split**: highest quality is achieved for minimum squared loss, which is defined as

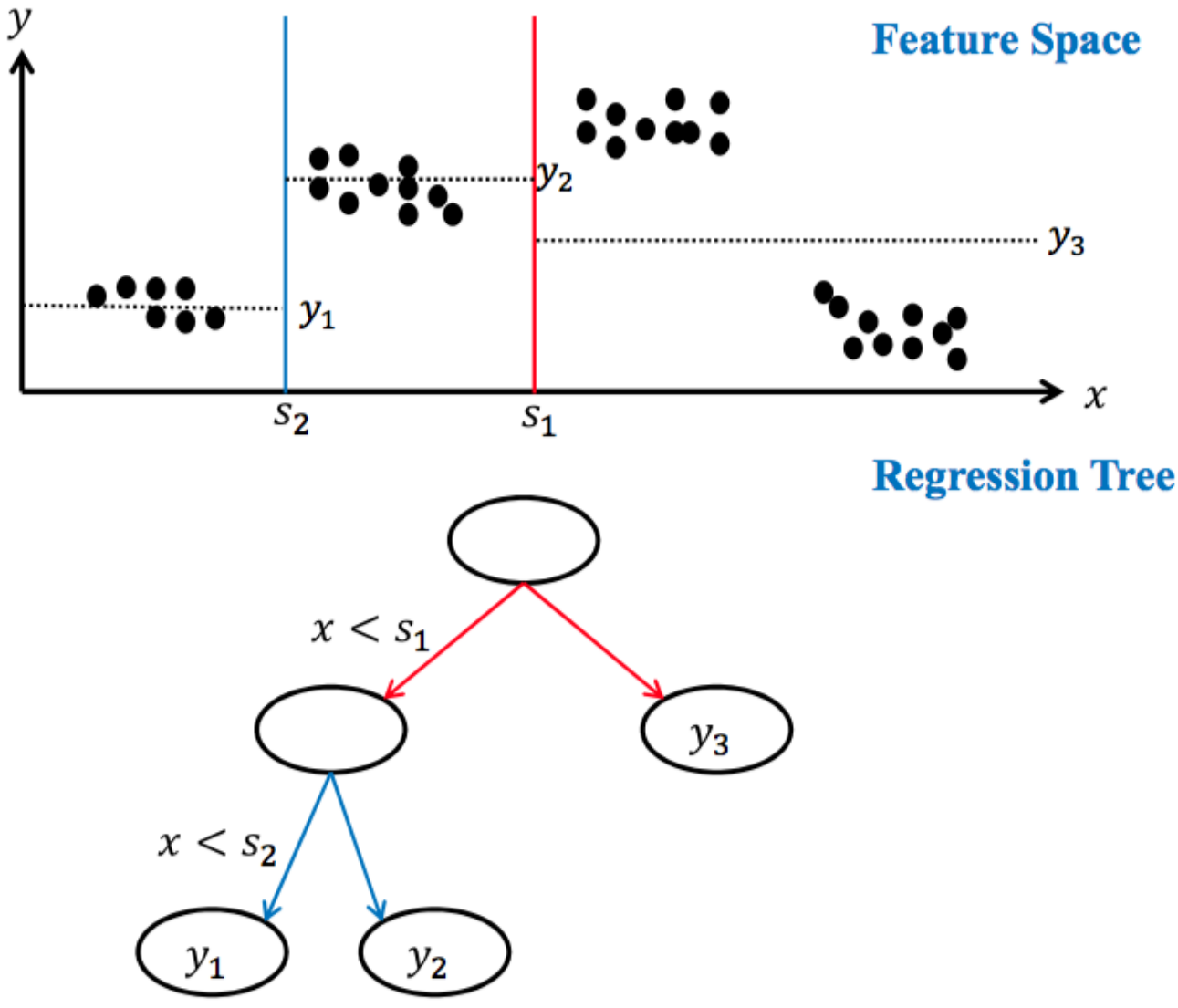
$$\sum_{i \in I_<} (y_i - \beta_<)^2 + \sum_{i \in I_>} (y_i - \beta_>)^2$$

3. Choose split, i.e., feature j and value v, with maximum quality.
4. Recurse on both children, with datasets $(x_i, y_i)_{i \in I_<}$ and $(x_i, y_i)_{i \in I_>}$.

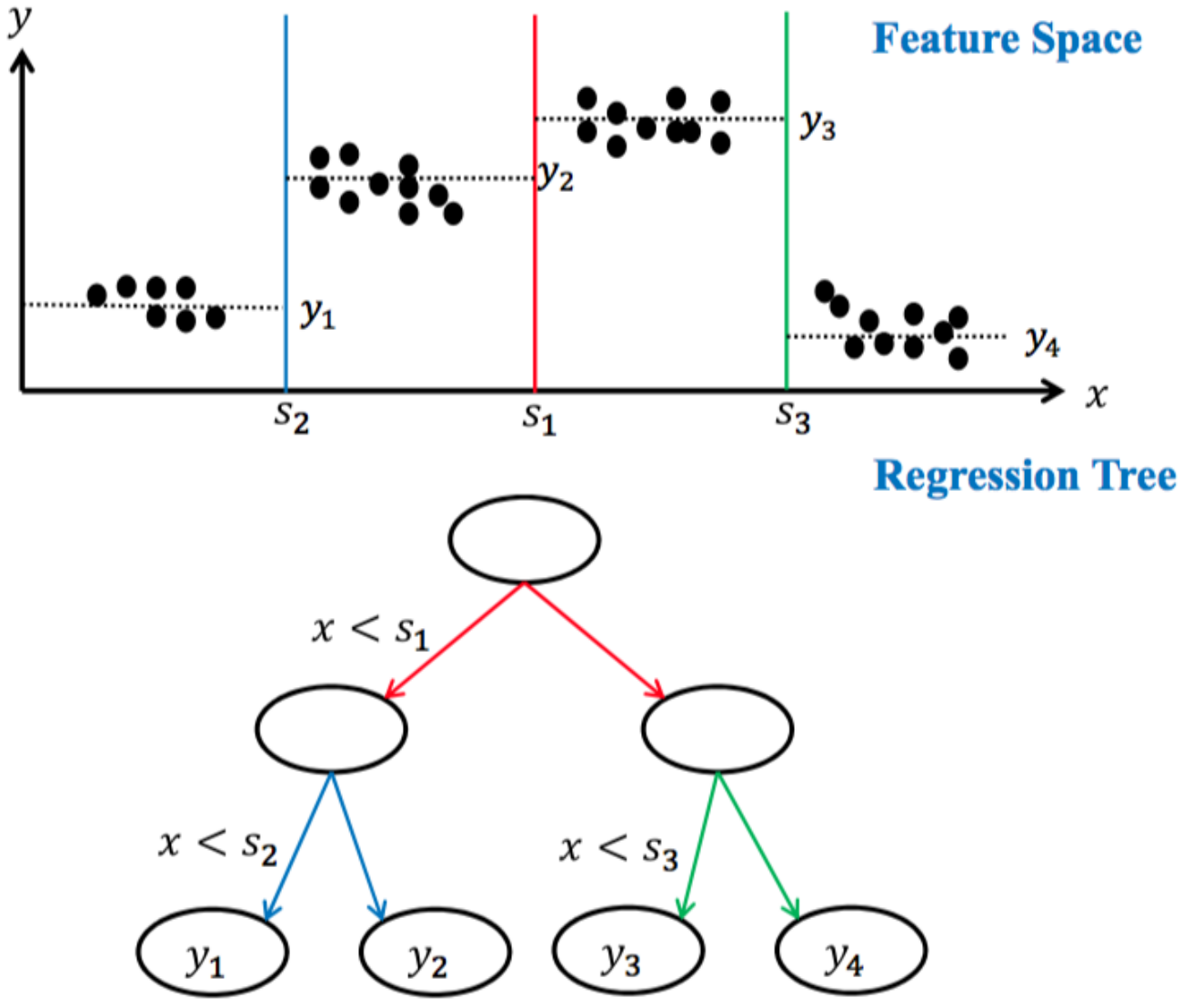
Example of Regression Trees



Example of Regression Trees



Example of Regression Trees



Model Complexity

- When should a regression tree growing be stopped?
- As for classification, can use pruning (early stopping or post-pruning)
- In general, can also use a regularized objective

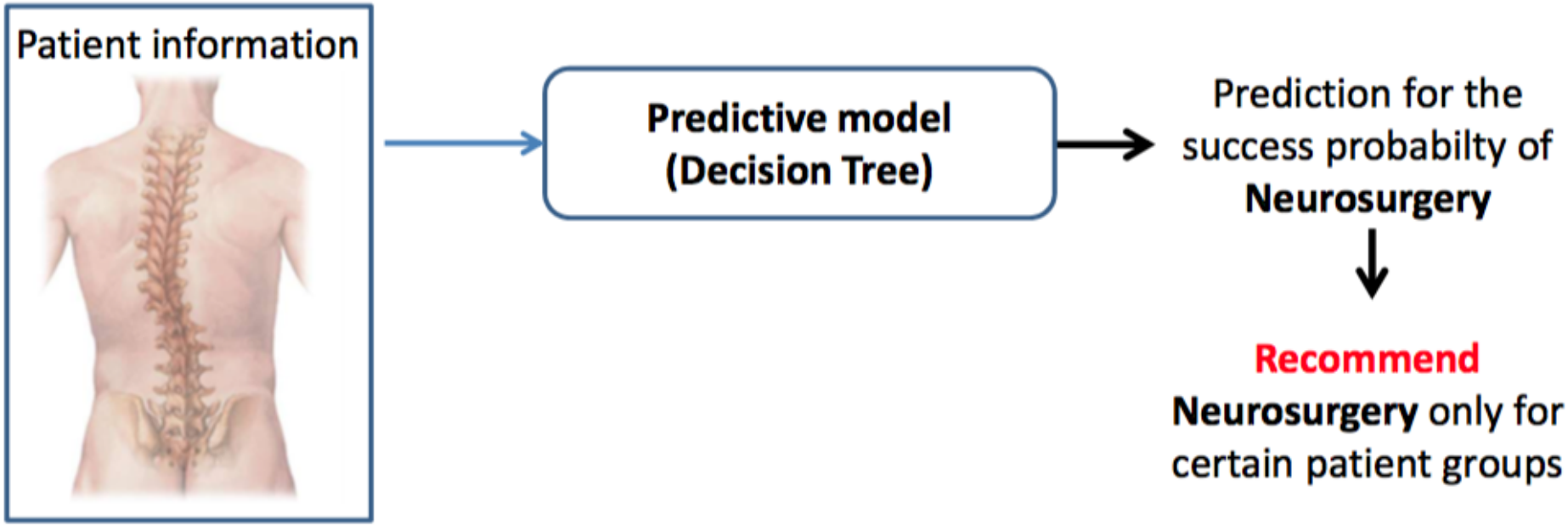
$$R^{\text{emp}}(T) + C \times \text{size}(T)$$

  - Early stopping: row the tree from scratch and stop once the criterion objective starts to increase.
  - Pruning: first grow the full tree and prune nodes (starting at leaves), until the objective starts to increase.
  - Pruning is preferred as the choice of tree is less sensitive to “wrong” choices of split points and variables to split on in the first stages of tree fitting.
  - Use cross-validation to determine optimal C.

Possible decision tree pruning rules

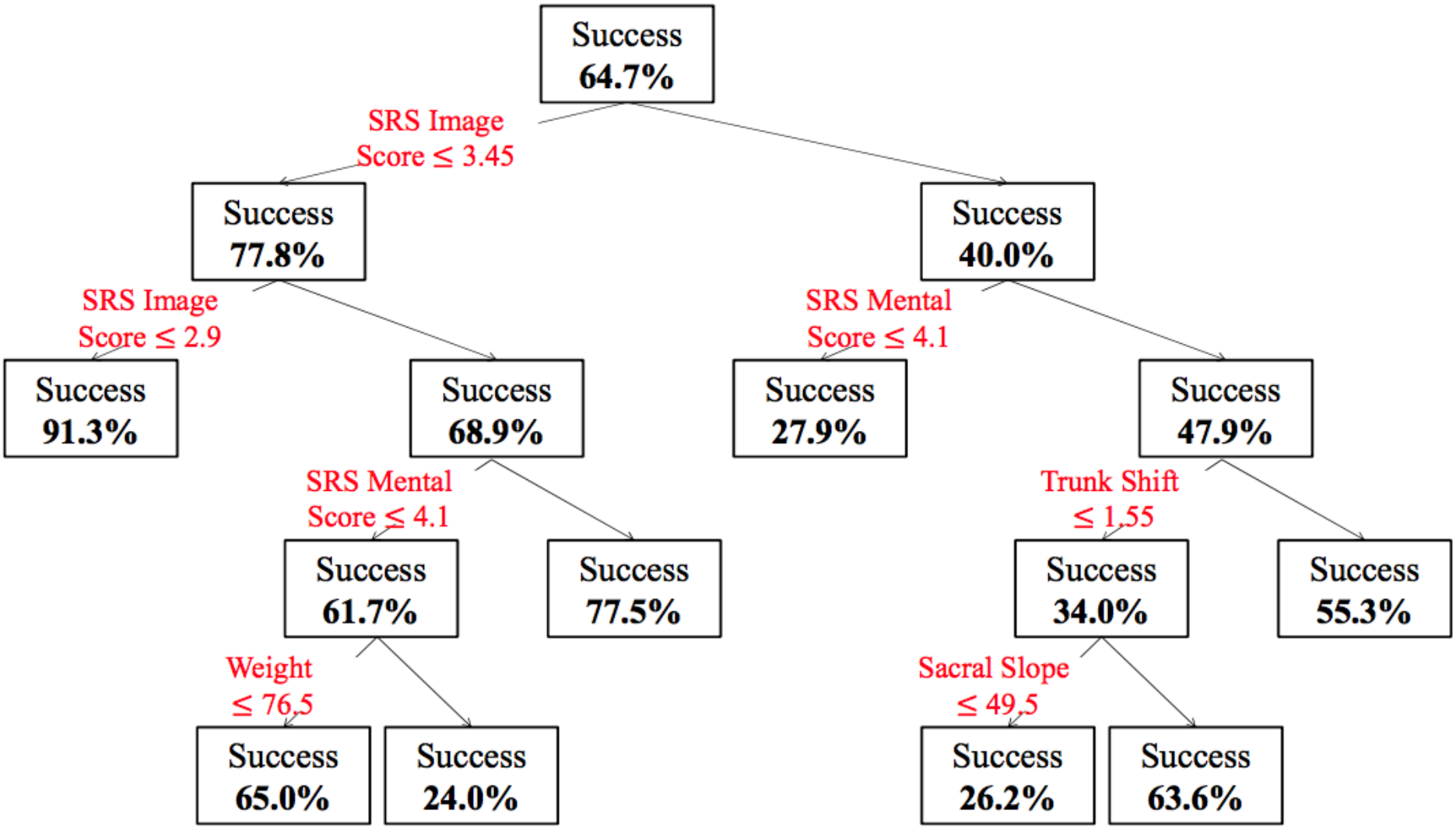
- Stop when the number of leaves is more than a threshold
- Stop when the leaf's error is less than a threshold
- Stop when the number of instances in each leaf is less than a threshold
- Stop when the p-value between two divided leafs is smaller than a certain threshold (e.g. 0.05 or 0.01) based on chosen statistical tests.

Example: Neurosurgery

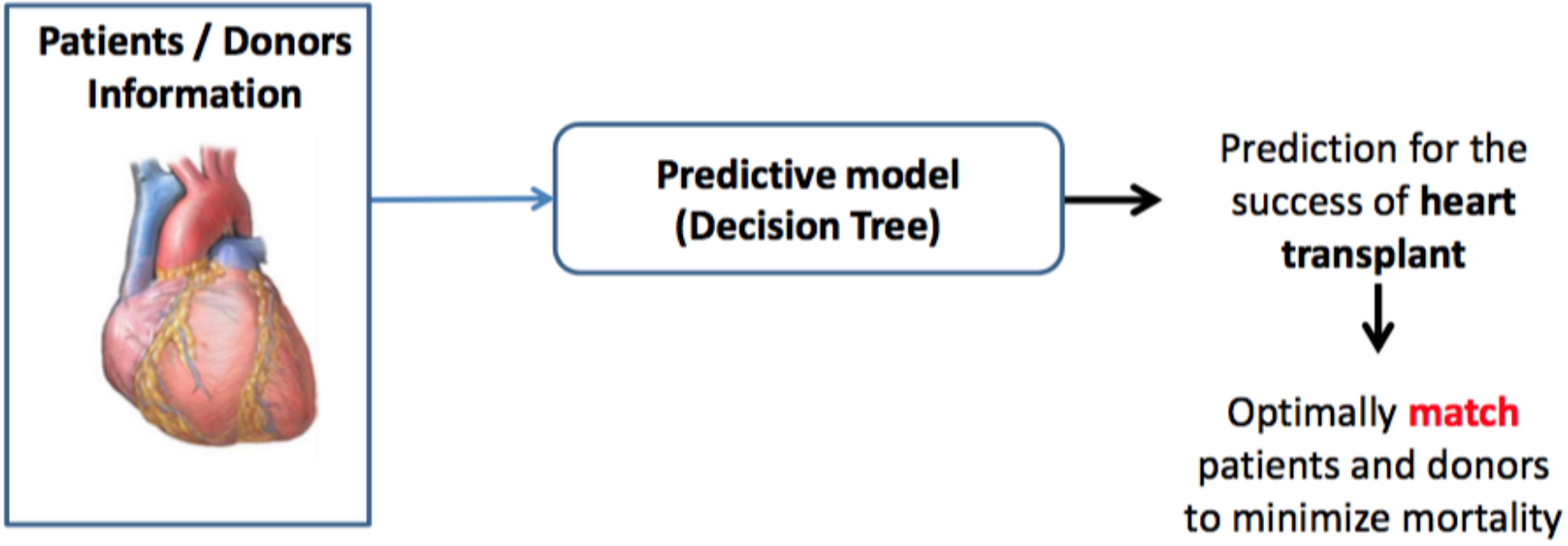


Type	Explanation	Note
Patient	1,449 patients with neurosurgery	2 year follow-up
Feature	91 Features (61 Continuous / 30 Binary)	
Label	MCID 1: 938 Patients (64.7%) MCID 0: 511 Patients (35.3%)	

Example: Neurosurgery

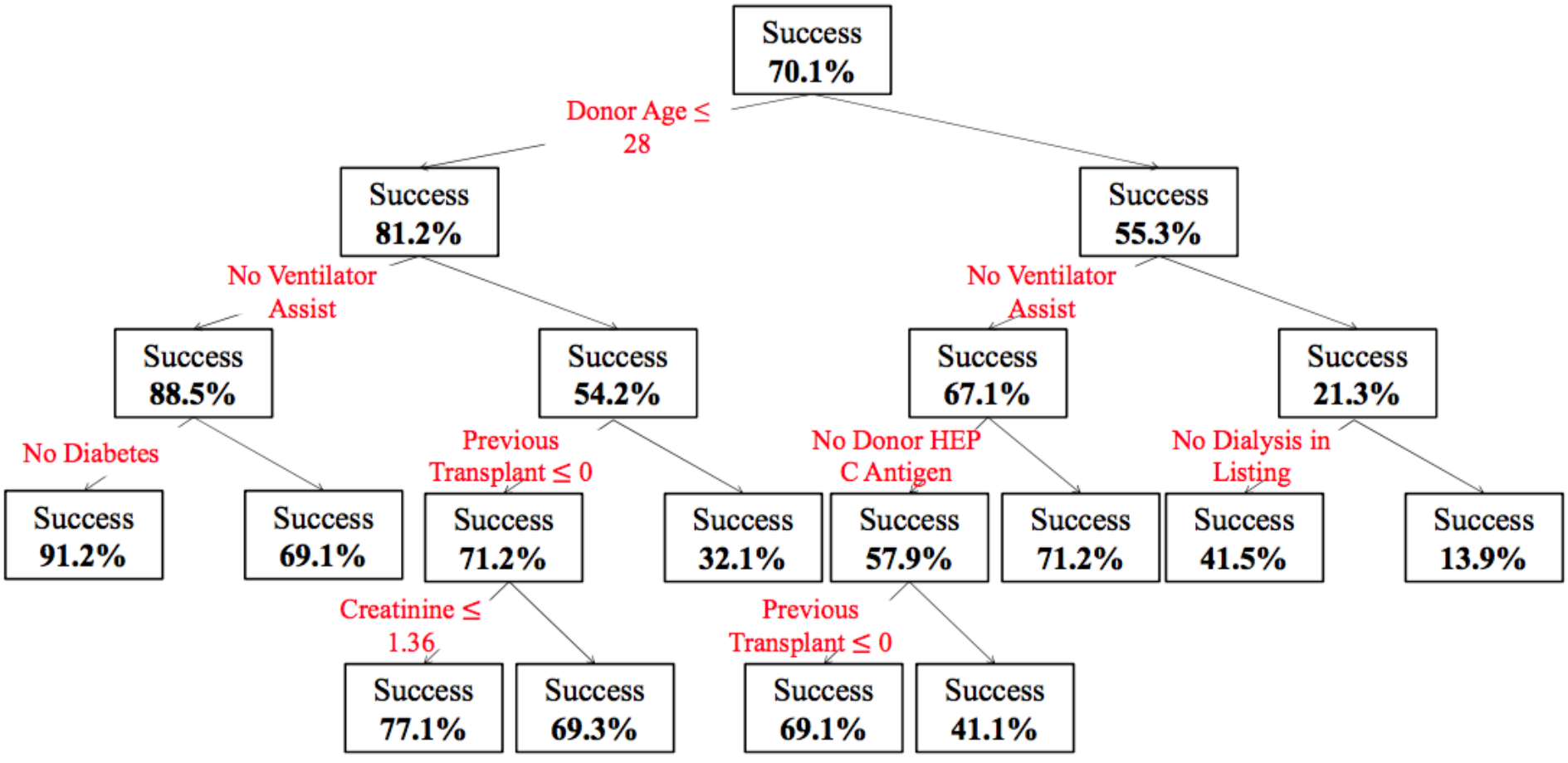


Example: Heart Transplant



Type	Explanation	Note
Patient	56,716 patients (heart transplant patients)	follow-up until they died
Feature	141 Features (84 Continuous / 57 Binary)	From 1986 to 2015
Label	Dead: 16,986 Patients (29.95%) Alive: 39,730 Patients (70.05%)	

Example: Heart Transplant

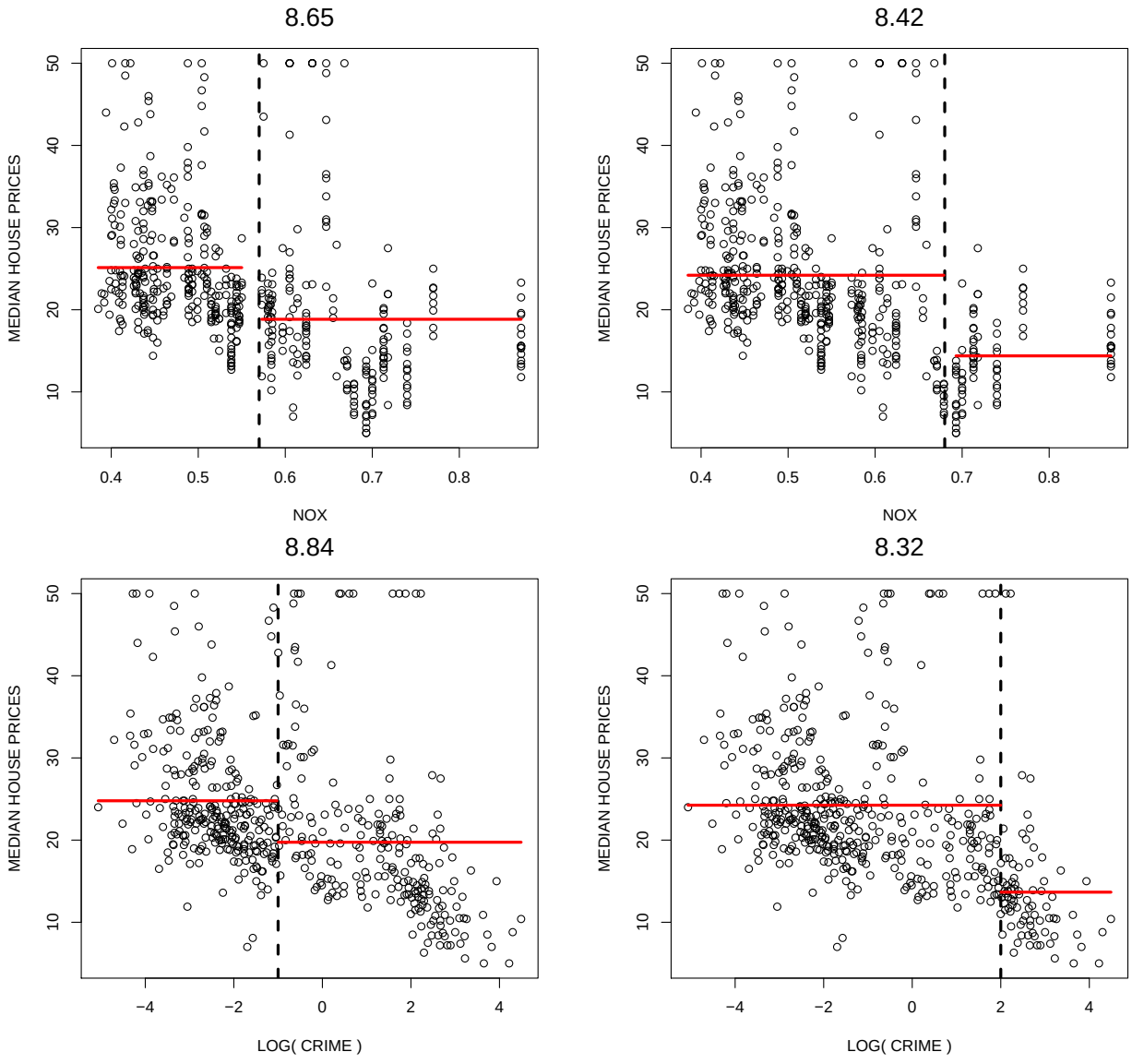


Example: Boston Housing Data

```
crim    per capita crime rate by town
nox     nitric oxides concentration (parts per 10 million)
rm      average number of rooms per dwelling
dis     weighted distances to five Boston employment centres
lstat   percentage of lower status of the population
... (6 more features)
```

- Predict median house value.

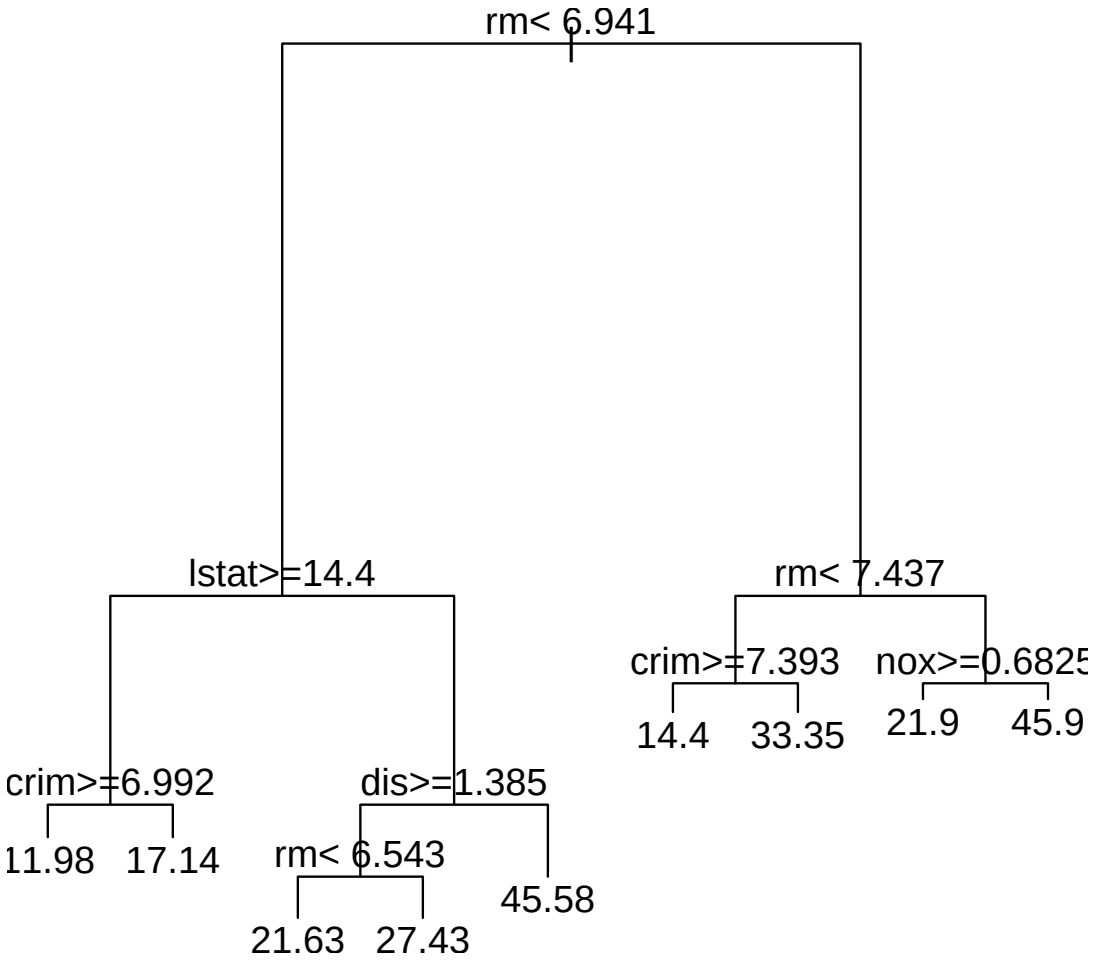
Example: Boston Housing Data



Different possible splits (features and thresholds) result in different quality measures.

Example: Boston Housing Data

- Overall, the best first split is on variable `rm`, average number of rooms per dwelling.
- Final tree contains predictions in leaf nodes.



Example: Pima Indians Diabetes Dataset

Goal: predict whether or not a patient has diabetes.

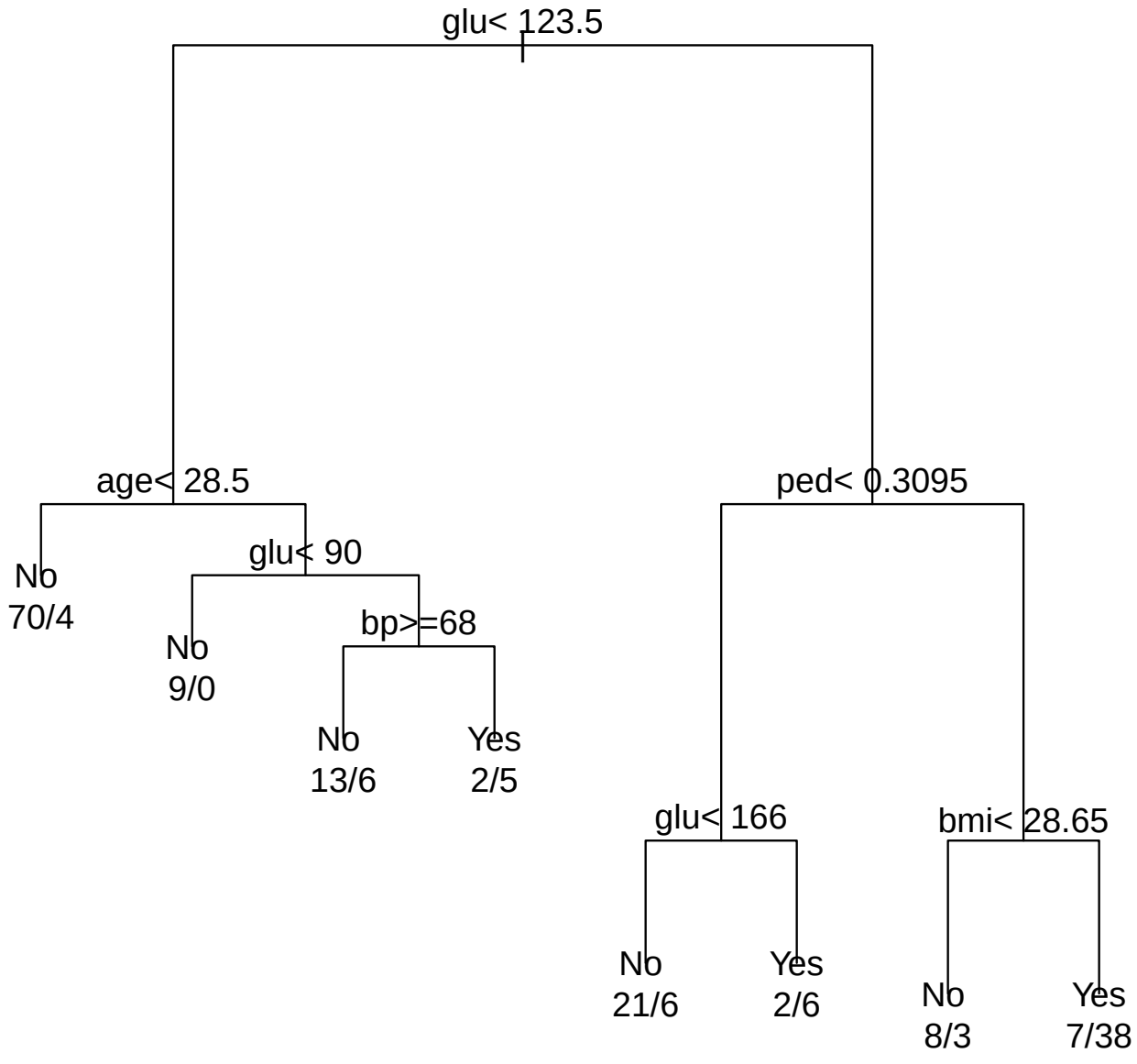
```
> library(rpart)
> library(MASS)
> data(Pima.tr)
> rp <- rpart(Pima.tr[,8] ~ ., data=Pima.tr[,-8])
> rp
n= 200

node), split, n, loss, yval, (yprob)
      * denotes terminal node

 1) root 200 68 No (0.66000000 0.34000000)
   2) glu< 123.5 109 15 No (0.86238532 0.13761468)
     4) age< 28.5 74  4 No (0.94594595 0.05405405) *
     5) age>=28.5 35 11 No (0.68571429 0.31428571)
      10) glu< 90 9  0 No (1.00000000 0.00000000) *
      11) glu>=90 26 11 No (0.57692308 0.42307692)
        22) bp>=68 19  6 No (0.68421053 0.31578947) *
        23) bp< 68 7  2 Yes (0.28571429 0.71428571) *
   3) glu>=123.5 91 38 Yes (0.41758242 0.58241758)
     6) ped< 0.3095 35 12 No (0.65714286 0.34285714)
      12) glu< 166 27  6 No (0.77777778 0.22222222) *
      13) glu>=166 8  2 Yes (0.25000000 0.75000000) *
     7) ped>=0.3095 56 15 Yes (0.26785714 0.73214286)
      14) bmi< 28.65 11  3 No (0.72727273 0.27272727) *
      15) bmi>=28.65 45  7 Yes (0.15555556 0.84444444) *
```

Example: Pima Indians Diabetes Dataset

```
> plot(rp,margin=0.1); text(rp,use.n=T)
```



Two possible trees.

```
> rp1 <- rpart(Pima.tr[,8] ~ ., data=Pima.tr[,-8])
> plot(rp1);text(rp1)
```

```
> rp2 <- rpart(Pima.tr[,8] ~ ., data=Pima.tr[,-8],
                        control=rpart.control(cp=0.05))
> plot(rp2);text(rp2)
```