

Decision Trees

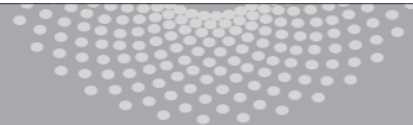
Aarti Singh

Machine Learning 10-315

Nov 2 , 2020



MACHINE LEARNING DEPARTMENT



Carnegie Mellon.
School of Computer Science

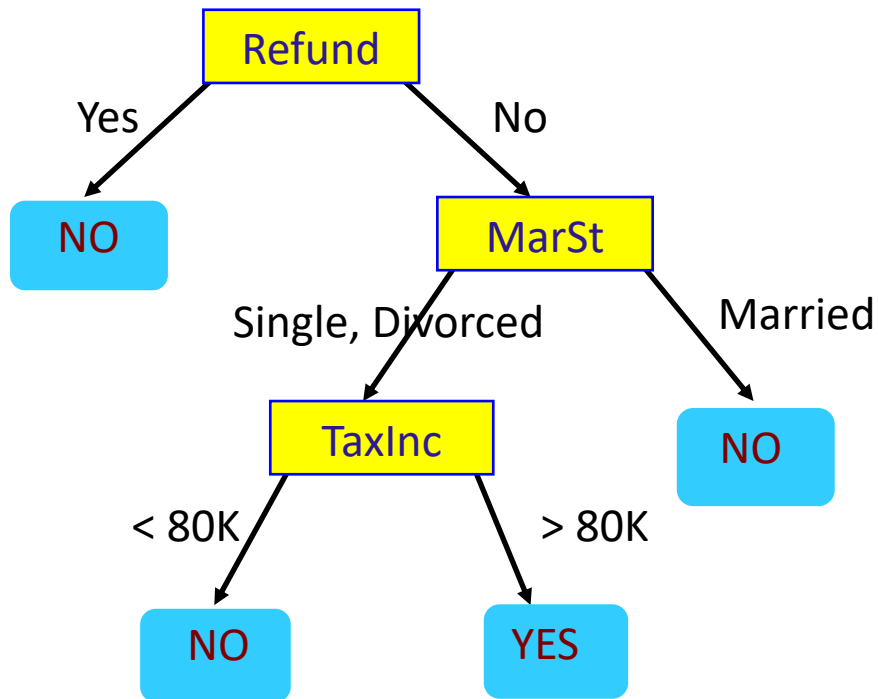
Decision Trees

- Start with discrete features, then discuss continuous

Representation

- What does a decision tree represent

Decision Tree for Tax Fraud Detection



X_1	X_2	X_3	Y
Refund	Marital Status	Taxable Income	Cheat

- Each internal node: test one feature X_i
- Each branch from a node: selects some value for X_i
- Each leaf node: prediction for Y

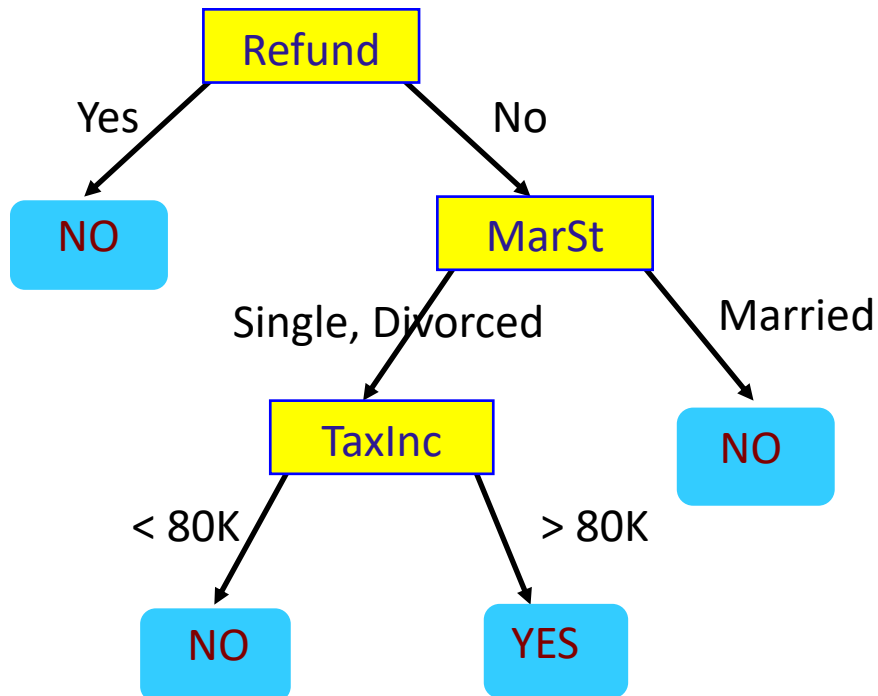
Prediction

- Given a decision tree, how do we assign label to a test point

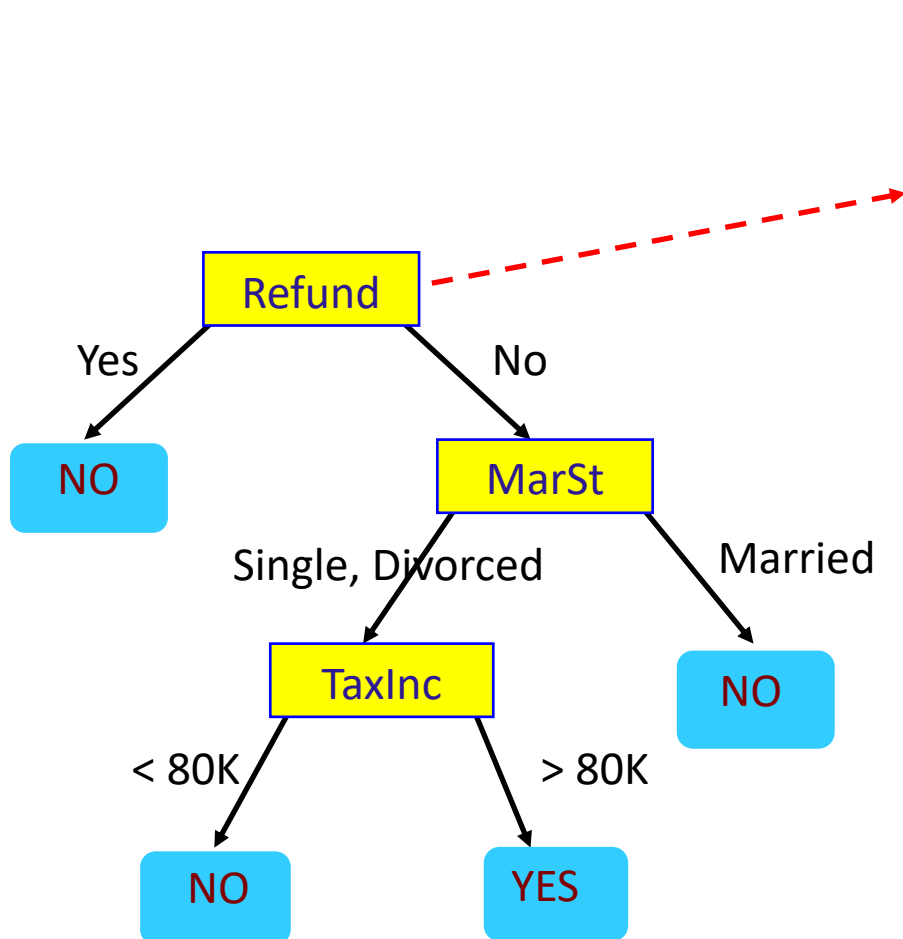
Decision Tree for Tax Fraud Detection

Query Data

X_1	X_2	X_3	Y
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



Decision Tree for Tax Fraud Detection



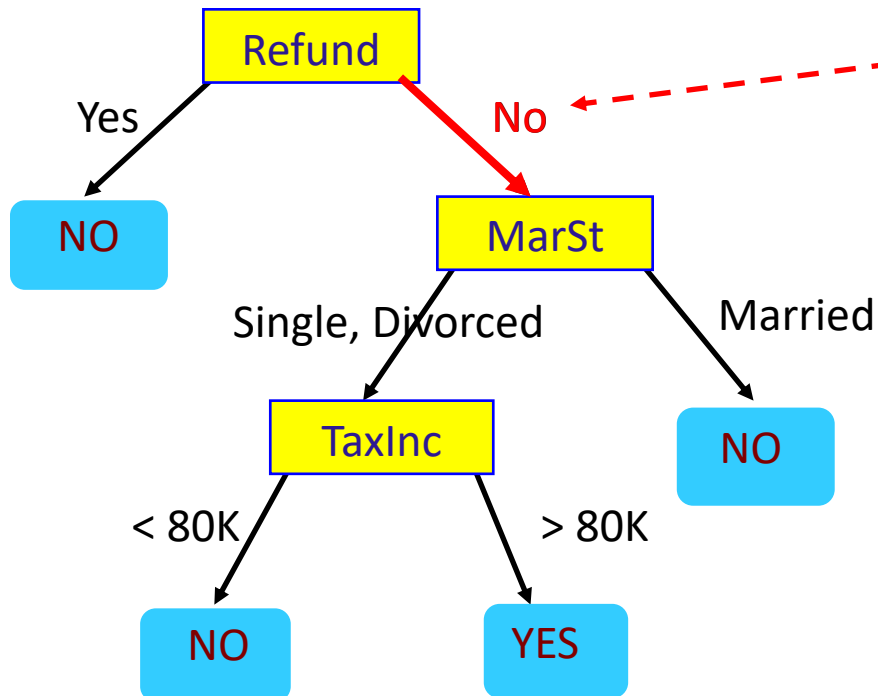
Query Data

X_1	X_2	X_3	Y
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

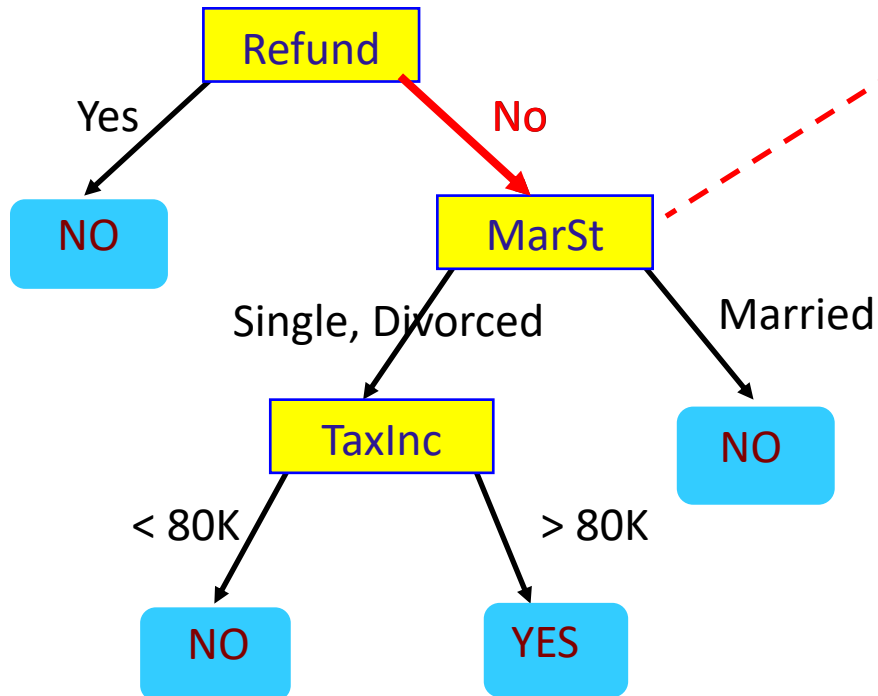
Decision Tree for Tax Fraud Detection

Query Data

X_1	X_2	X_3	Y
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?



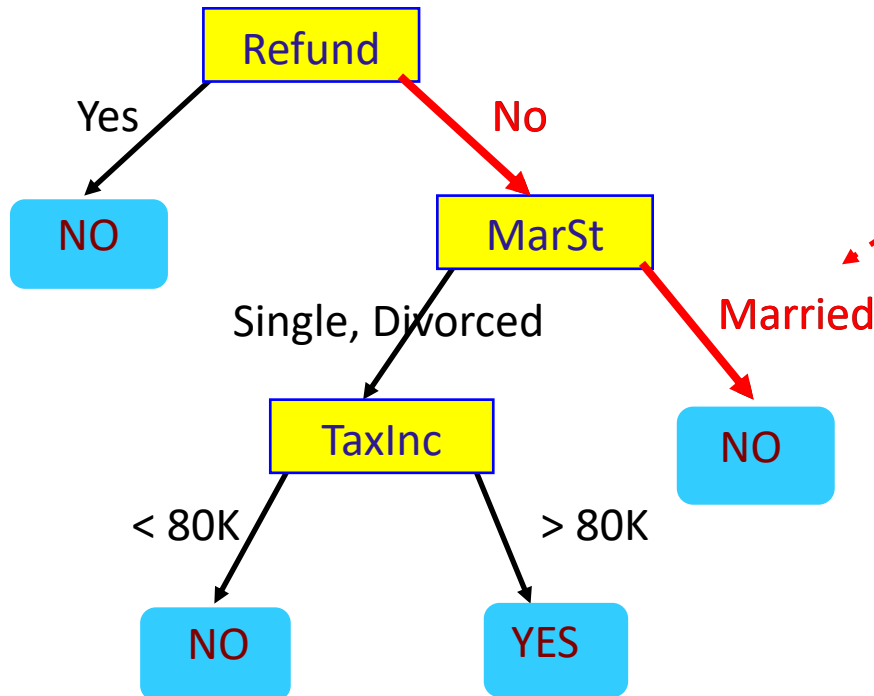
Decision Tree for Tax Fraud Detection



Query Data

X_1	X_2	X_3	Y
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

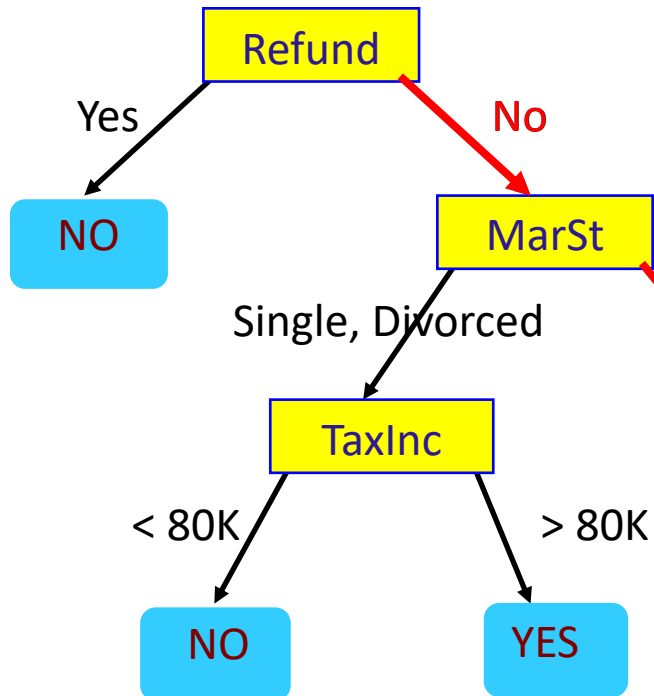
Decision Tree for Tax Fraud Detection



Query Data

X_1	X_2	X_3	Y
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Decision Tree for Tax Fraud Detection



Query Data

X_1	X_2	X_3	Y
Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

Assign Cheat to "No"

So far...

- What does a decision tree represent
- Given a decision tree, how do we assign label to a test point

Discriminative or Generative?

Now ...

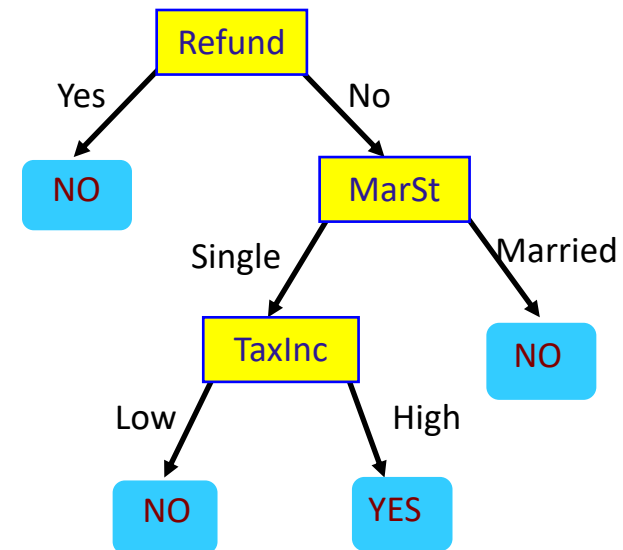
- How do we learn a decision tree from training data

How to learn a decision tree

- Top-down induction [ID3]

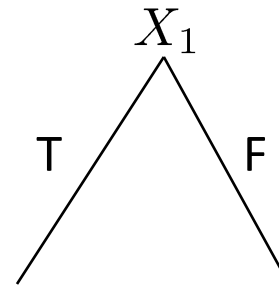
Main loop:

1. $X \leftarrow$ the “best” decision feature for next *node*
2. Assign X as decision feature for *node*
3. For each value of X , create new descendant of *node* (Discrete features)
4. Sort training examples to leaf nodes
5. If training examples perfectly classified, Then STOP, Else iterate over new leaf nodes (steps 1-5) after removing current feature
6. When all features exhausted, assign majority label to the leaf node



Which feature is best?

X_1	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

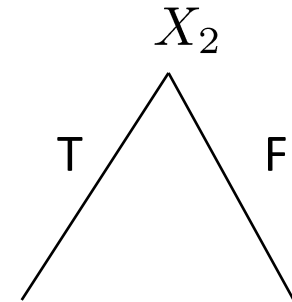


Y: 4 Ts
0 Fs

Y: 1 Ts
3 Fs

Absolutely
sure

Kind of
sure



Y: 3 Ts
1 F

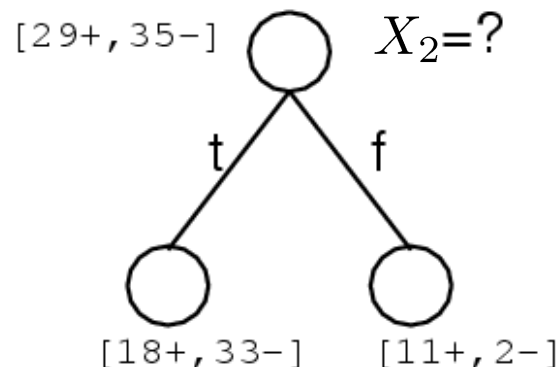
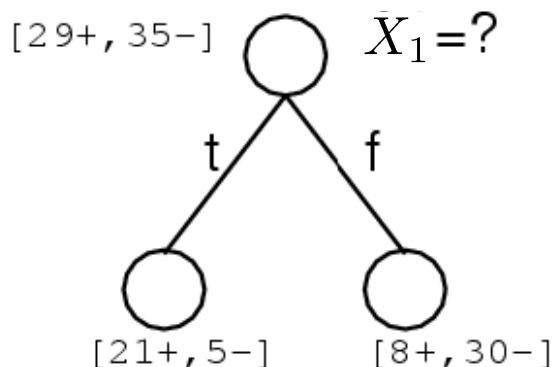
Y: 2 Ts
2 Fs

Kind of
sure

Absolutely
unsure

Good split if we are more certain
about classification after split –
Uniform distribution of labels is bad

Which feature is best?



Pick the attribute/feature which yields maximum information gain:

$$\arg \max_i I(Y, X_i) = \arg \max_i [H(Y) - H(Y|X_i)]$$

$H(Y)$ – entropy of Y $H(Y|X_i)$ – conditional entropy of Y

Andrew Moore's Entropy in a Nutshell



Low Entropy

..the values (locations of soup) sampled entirely from within the soup bowl



High Entropy

..the values (locations of soup) unpredictable... almost uniformly sampled throughout our dining room

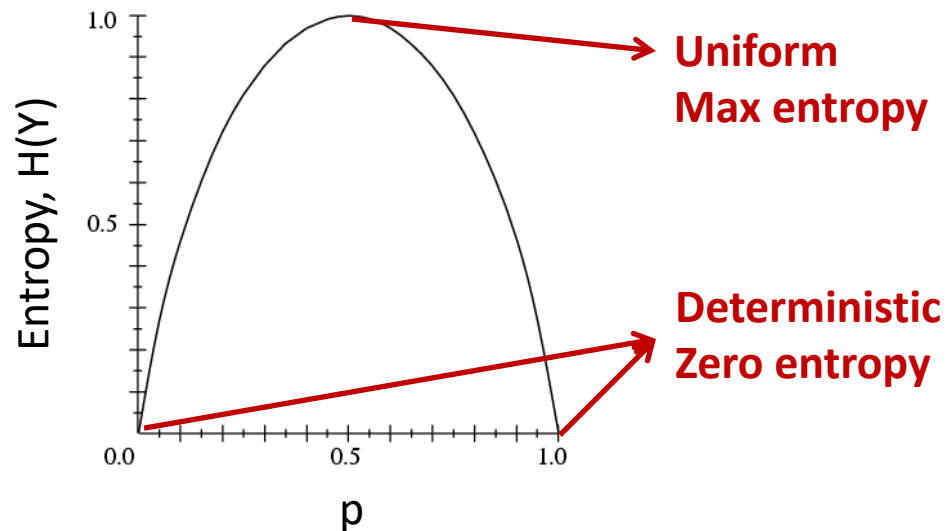
Entropy

- Entropy of a random variable Y

$$H(Y) = - \sum_y P(Y = y) \log_2 P(Y = y)$$

***More uncertainty,
more entropy!***

$Y \sim \text{Bernoulli}(p)$



Information Theory interpretation: $H(Y)$ is the expected number of bits needed to encode a randomly drawn value of Y (under most efficient code)

Information Gain

- Advantage of attribute = decrease in uncertainty

- Entropy of Y before split

$$H(Y) = - \sum_y P(Y = y) \log_2 P(Y = y)$$

- Entropy of Y after splitting based on X_i

- Weight by probability of following each branch

$$\begin{aligned} H(Y | X_i) &= \sum_x P(X_i = x) H(Y | X_i = x) \\ &= - \sum_x P(X_i = x) \sum_y P(Y = y | X_i = x) \log_2 P(Y = y | X_i = x) \end{aligned}$$

- Information gain is difference

$$I(Y, X_i) = H(Y) - H(Y | X_i)$$

Max Information gain = min conditional entropy

Which feature is best to split?

Pick the attribute/feature which yields maximum information gain:

$$\begin{aligned}\arg \max_i I(Y, X_i) &= \arg \max_i [H(Y) - H(Y|X_i)] \\ &= \arg \min_i H(Y|X_i)\end{aligned}$$

Entropy of Y

$$H(Y) = - \sum_y P(Y = y) \log_2 P(Y = y)$$

Conditional entropy of Y

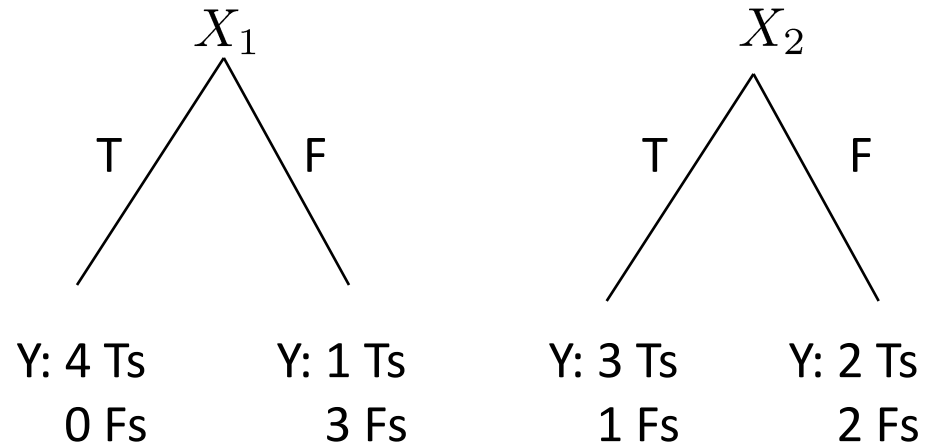
$$H(Y | X_i) = \sum_x P(X_i = x) H(Y | X_i = x)$$

Feature which yields maximum reduction in entropy (uncertainty) provides maximum information about Y

Information Gain

$$H(Y | X_i) = - \sum_x P(X_i = x) \sum_y P(Y = y | X_i = x) \log_2 P(Y = y | X_i = x)$$

X_1	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



$$\hat{H}(Y|X_1) = -\frac{1}{2}[1 \log_2 1 + 0 \log_2 0] - \frac{1}{2}\left[\frac{1}{4} \log_2 \frac{1}{4} + \frac{3}{4} \log_2 \frac{3}{4}\right]$$

$$\hat{H}(Y|X_2) = -\frac{1}{2}\left[\frac{3}{4} \log_2 \frac{3}{4} + \frac{1}{4} \log_2 \frac{1}{4}\right] - \frac{1}{2}\left[\frac{1}{2} \log_2 \frac{1}{2} + \frac{1}{2} \log_2 \frac{1}{2}\right]$$

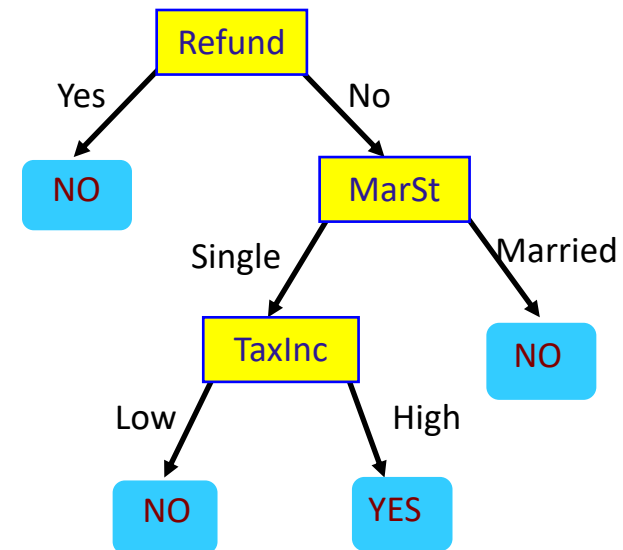
$$\hat{H}(Y|X_1) < \hat{H}(Y|X_2) > 0$$

How to learn a decision tree

- Top-down induction [ID3]

Main loop:

1. $X \leftarrow$ the “best” decision feature for next *node*
2. Assign X as decision feature for *node*
3. For each value of X , create new descendant of *node* (Discrete features)
4. Sort training examples to leaf nodes
5. If training examples perfectly classified, Then STOP, Else iterate over new leaf nodes (steps 1-5) after removing current feature
6. When all features exhausted, assign majority label to the leaf node

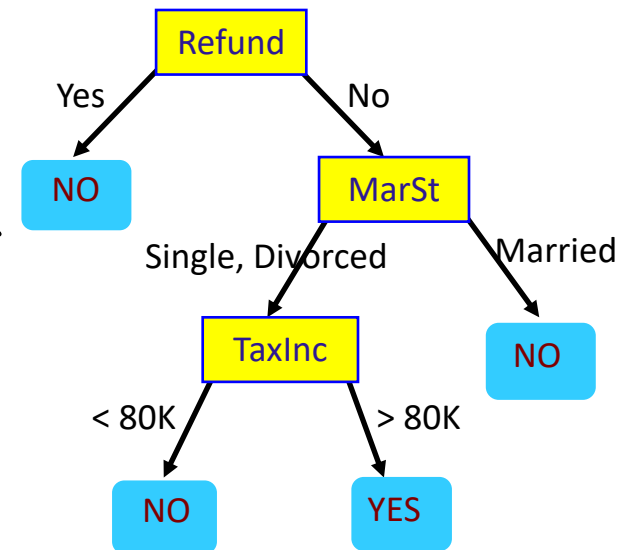


How to learn a decision tree

- Top-down induction [ID3, C4.5, C5, ...]

Main loop: C4.5

1. $X \leftarrow$ the “best” decision feature for next *node*
2. Assign X as decision feature for *node*
3. For “best” split of X , create new descendants of *node*
4. Sort training examples to leaf nodes
5. If training examples perfectly classified, Then STOP, Else iterate over new leaf nodes
6. Prune back tree to reduce overfitting
7. Assign majority label to the leaf node



Handling continuous features (C4.5)

Convert continuous features into discrete by setting a threshold.

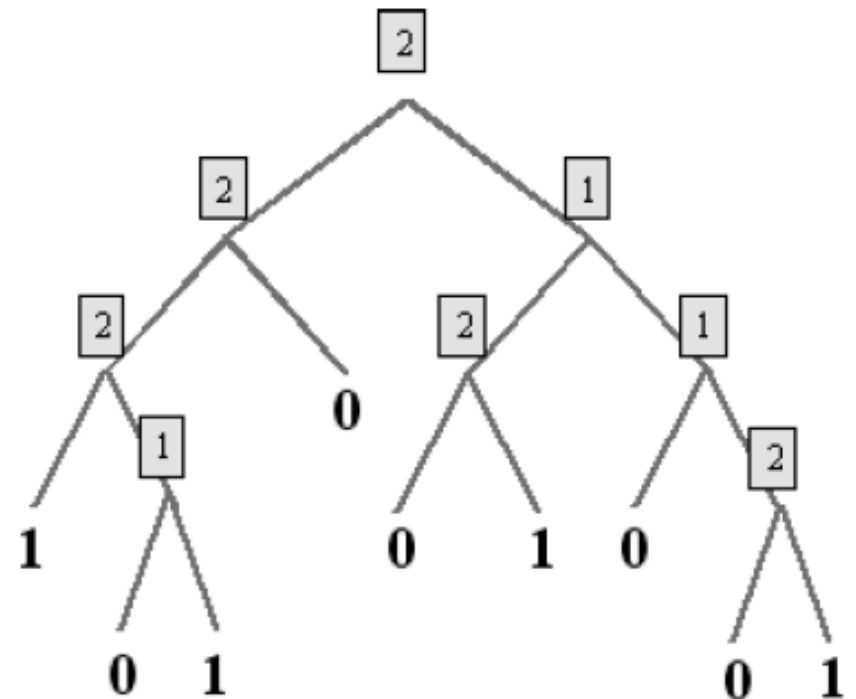
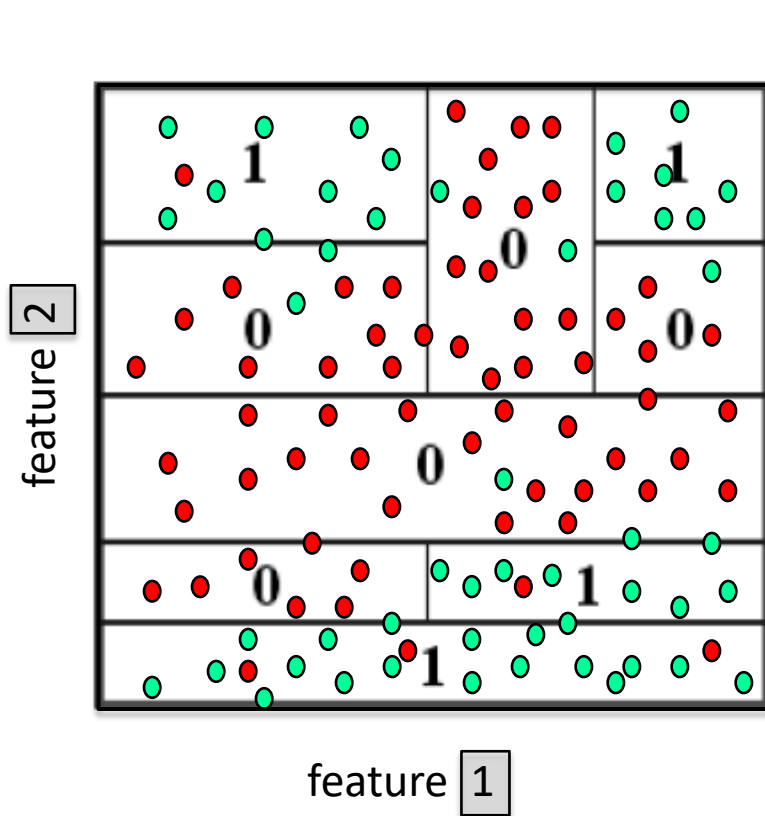
What threshold to pick?

Search for best one as per information gain. Infinitely many??

Don't need to search over more than $\sim n$ (number of training data), e.g. say X_1 takes values $x_1^{(1)}, x_1^{(2)}, \dots, x_1^{(n)}$ in the training set. Then possible thresholds are

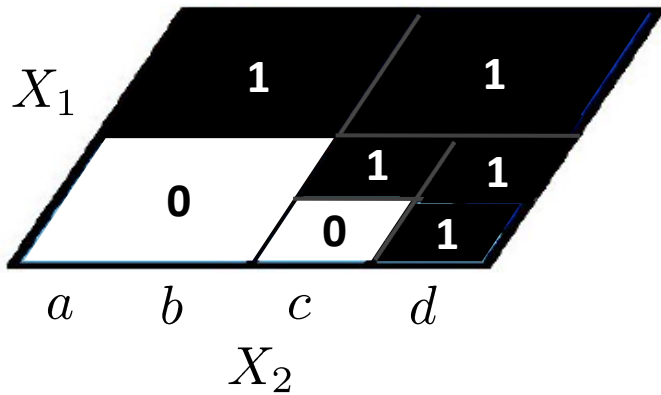
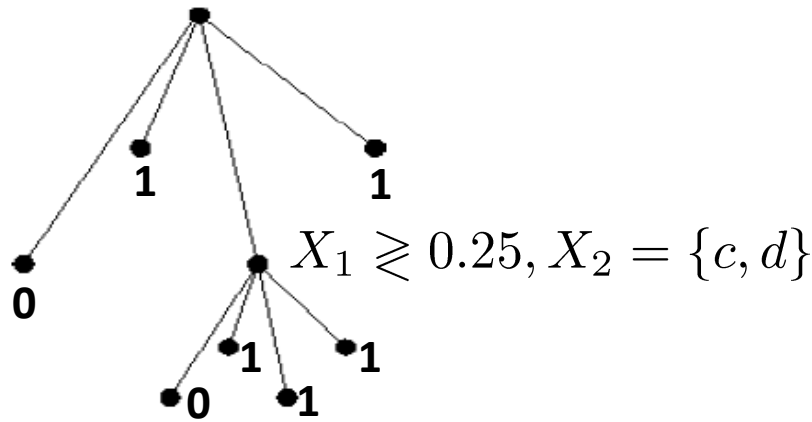
$$[x_1^{(1)} + x_1^{(2)}]/2, [x_1^{(2)} + x_1^{(3)}]/2, \dots, [x_1^{(n-1)} + x_1^{(n)}]/2$$

Dyadic decision trees (split on mid-points of features)



Decision Tree more generally...

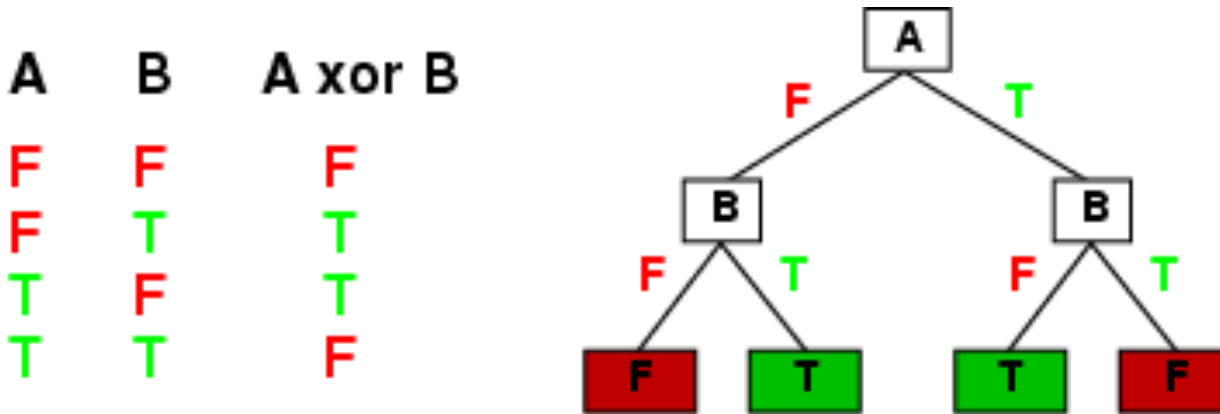
$$X_1 \geq 0.5, X_2 = \{a, b\} \text{ or } \{c, d\}$$



- Features can be discrete, continuous or categorical
- Each internal node: test some set of features $\{X_i\}$
- Each branch from a node: selects a set of value for $\{X_i\}$
- Each leaf node: prediction for Y

Expressiveness of Decision Trees

- Decision trees in general (without pruning) can express any function of the input features.
- E.g., for Boolean functions, truth table row \rightarrow path to leaf:



- There is a decision tree which perfectly classifies a training set with one path to leaf for each example - **overfitting**
- But it won't generalize well to new examples - prefer to find more **compact** decision trees

When to Stop?

- Many strategies for picking simpler trees:

- Pre-pruning

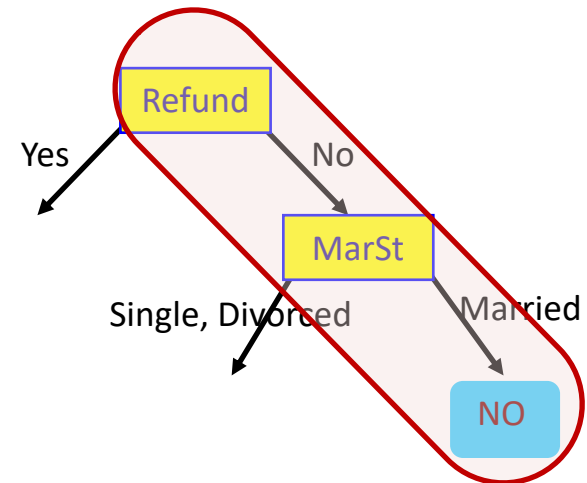
- Fixed depth (e.g. ID3)
- Fixed number of leaves

- Post-pruning

- Chi-square test

- Convert decision tree to a set of rules
- Eliminate variable values in rules which are independent of label (using chi-square test for independence)
- Simplify rule set by eliminating unnecessary rules

- Information Criteria: MDL (Minimum Description Length)



Information Criteria

- Penalize complex models by introducing cost

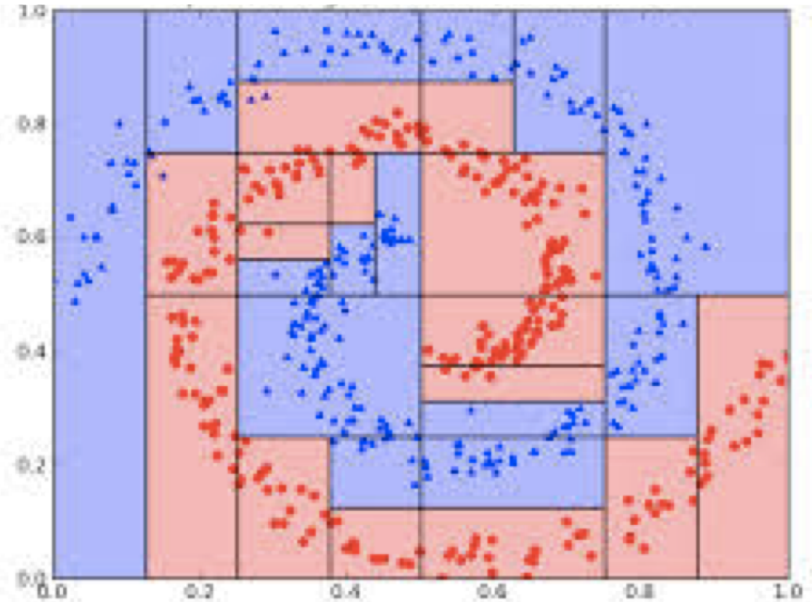
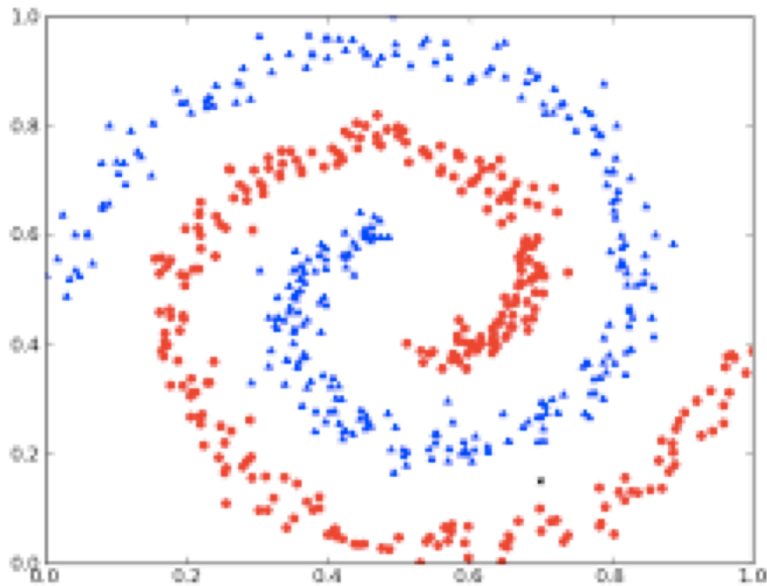
$$\hat{f} = \arg \min_T \left\{ \underbrace{\frac{1}{n} \sum_{i=1}^n \text{loss}(\hat{f}_T(X_i), Y_i)}_{\text{log likelihood}} + \underbrace{\text{pen}(T)}_{\text{cost}} \right\}$$

$$\begin{aligned} \text{loss}(\hat{f}_T(X_i), Y_i) &= (\hat{f}_T(X_i) - Y_i)^2 && \text{regression} \\ &= \mathbf{1}_{\hat{f}_T(X_i) \neq Y_i} && \text{classification} \end{aligned}$$

$\text{pen}(T) \propto |T|$ penalize trees with more leaves

CART – optimization can be solved by dynamic programming

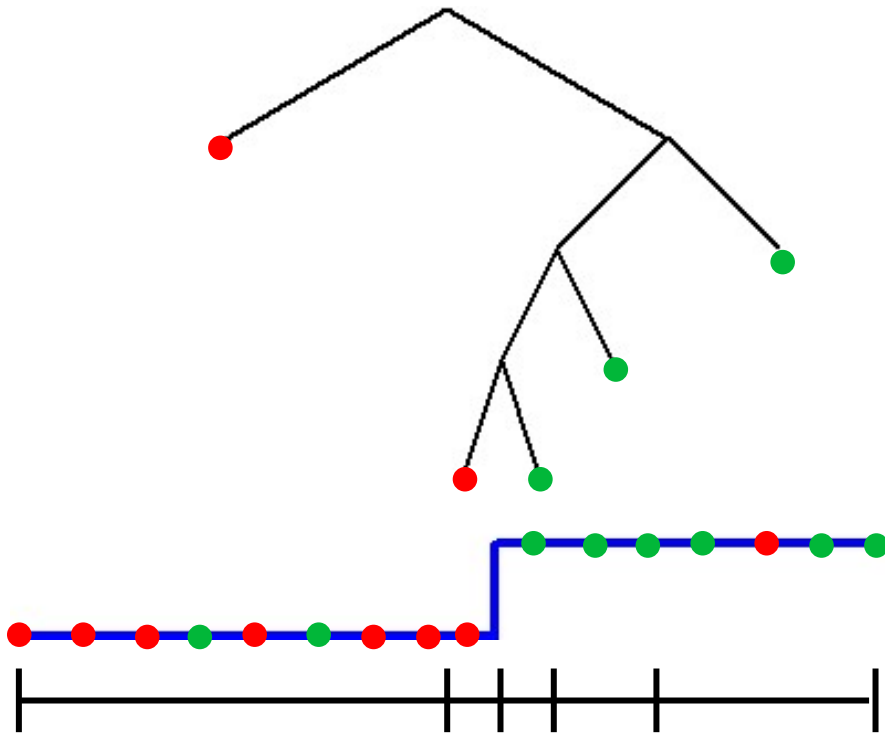
Example of 2-feature decision tree classifier



How to assign label to each leaf

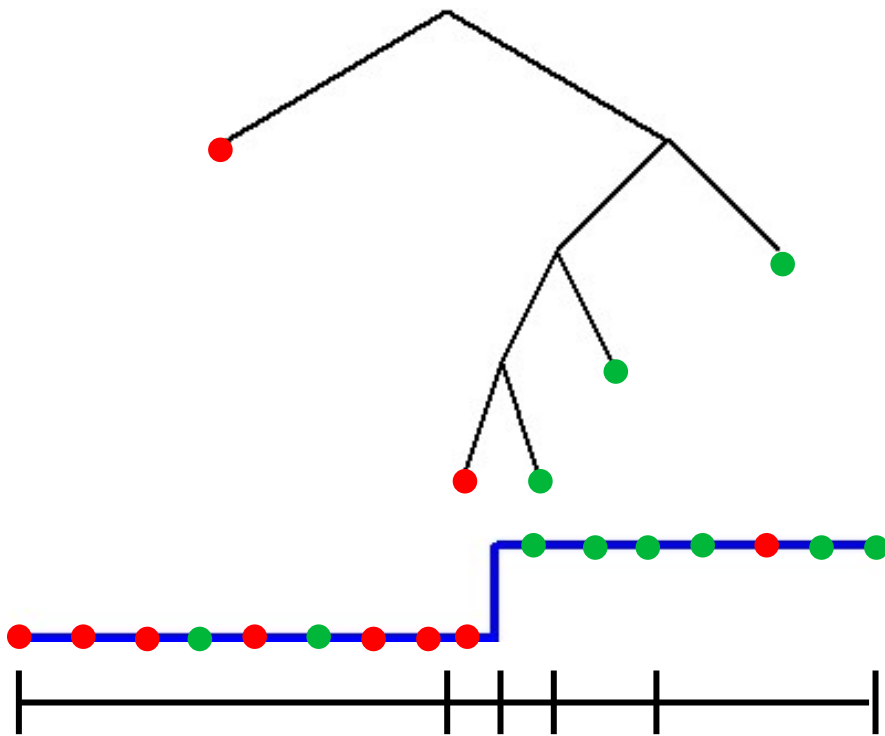
Classification – Majority vote

Regression – ?

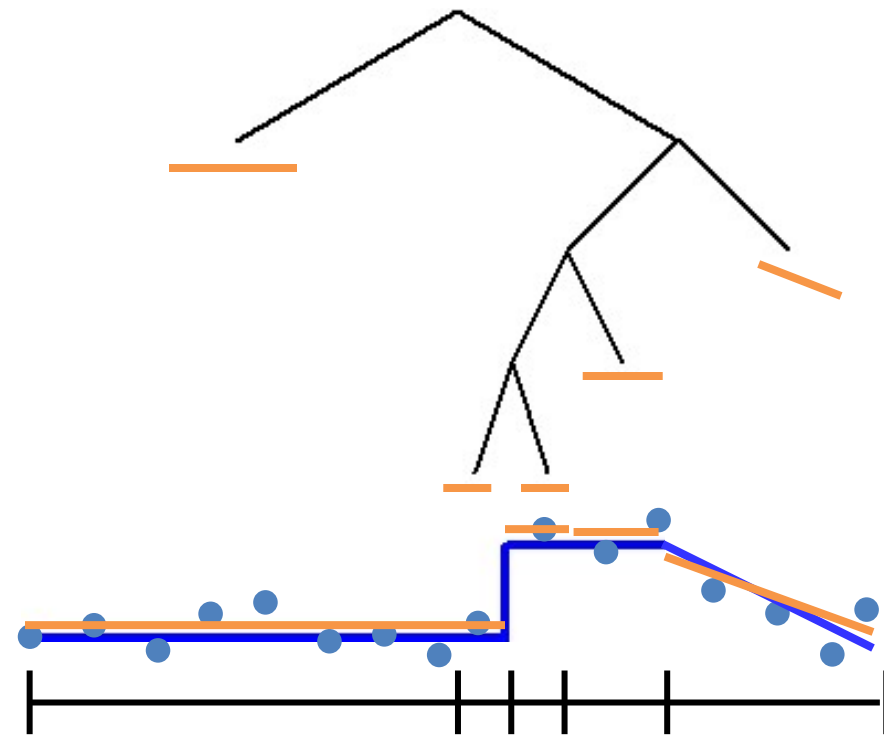


How to assign label to each leaf

Classification – Majority vote



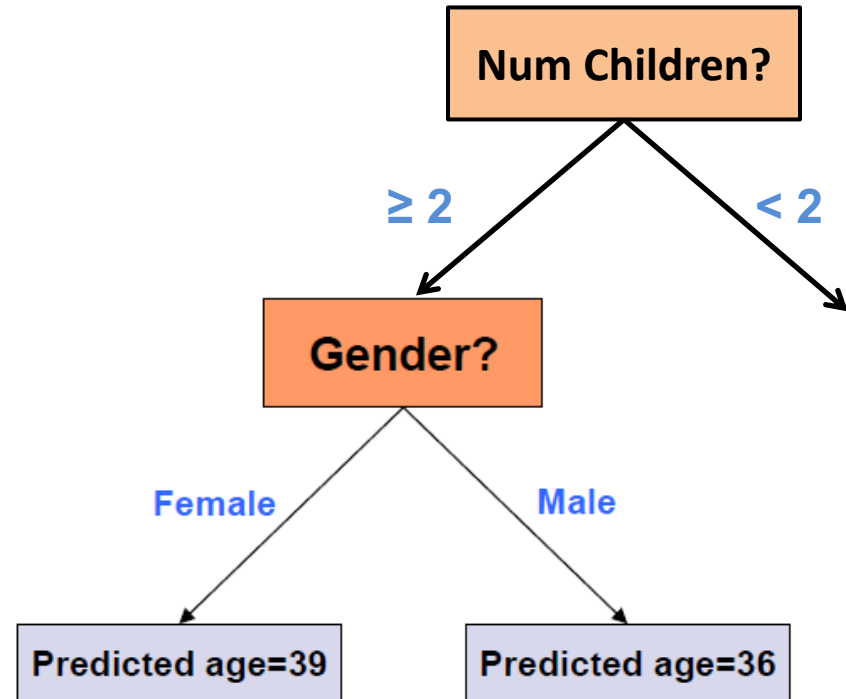
Regression – Constant/
Linear/Poly fit



Regression trees

$X^{(1)}$ $X^{(p)}$ Y

Gender	Rich?	Num. Children	# travel per yr.	Age
F	No	2	5	38
M	No	0	2	25
M	Yes	1	0	72
:	:	:	:	:



Average (fit a constant) using training data at the leaves

What you should know

- Decision trees are one of the most popular data mining tools
 - Simplicity of design
 - Interpretability
 - Ease of implementation
 - Good performance in practice (for small dimensions)
- Information gain to select attributes (ID3, C4.5,...)
- Decision trees will overfit!!!
 - Must use tricks to find “simple trees”, e.g.,
 - Pre-Pruning: Fixed depth/Fixed number of leaves
 - Post-Pruning: Chi-square test of independence
 - Complexity Penalized/MDL model selection
- Can be used for classification, regression and density estimation too