기계학습 (2022년도 2학기)

Decision Trees

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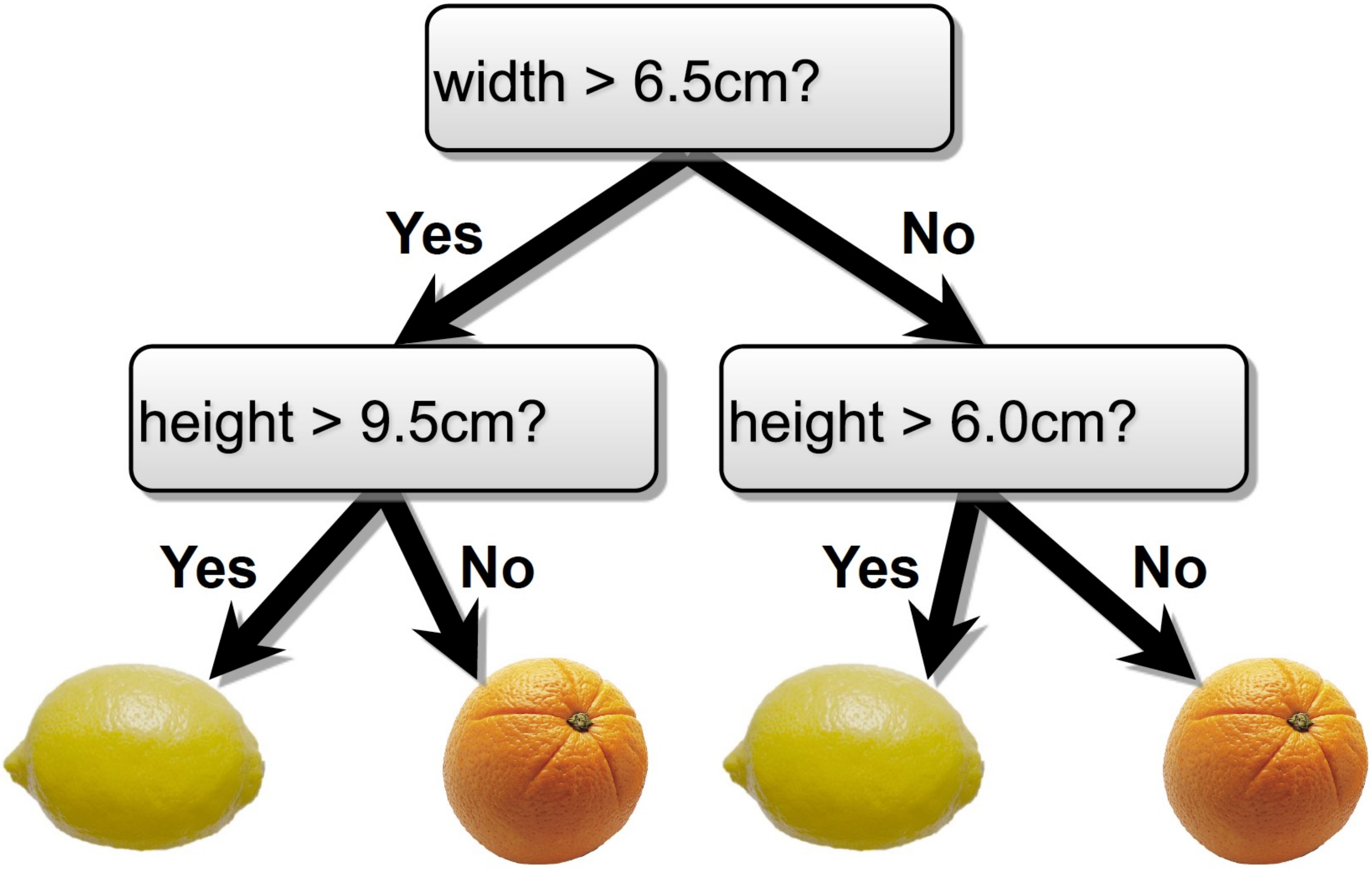
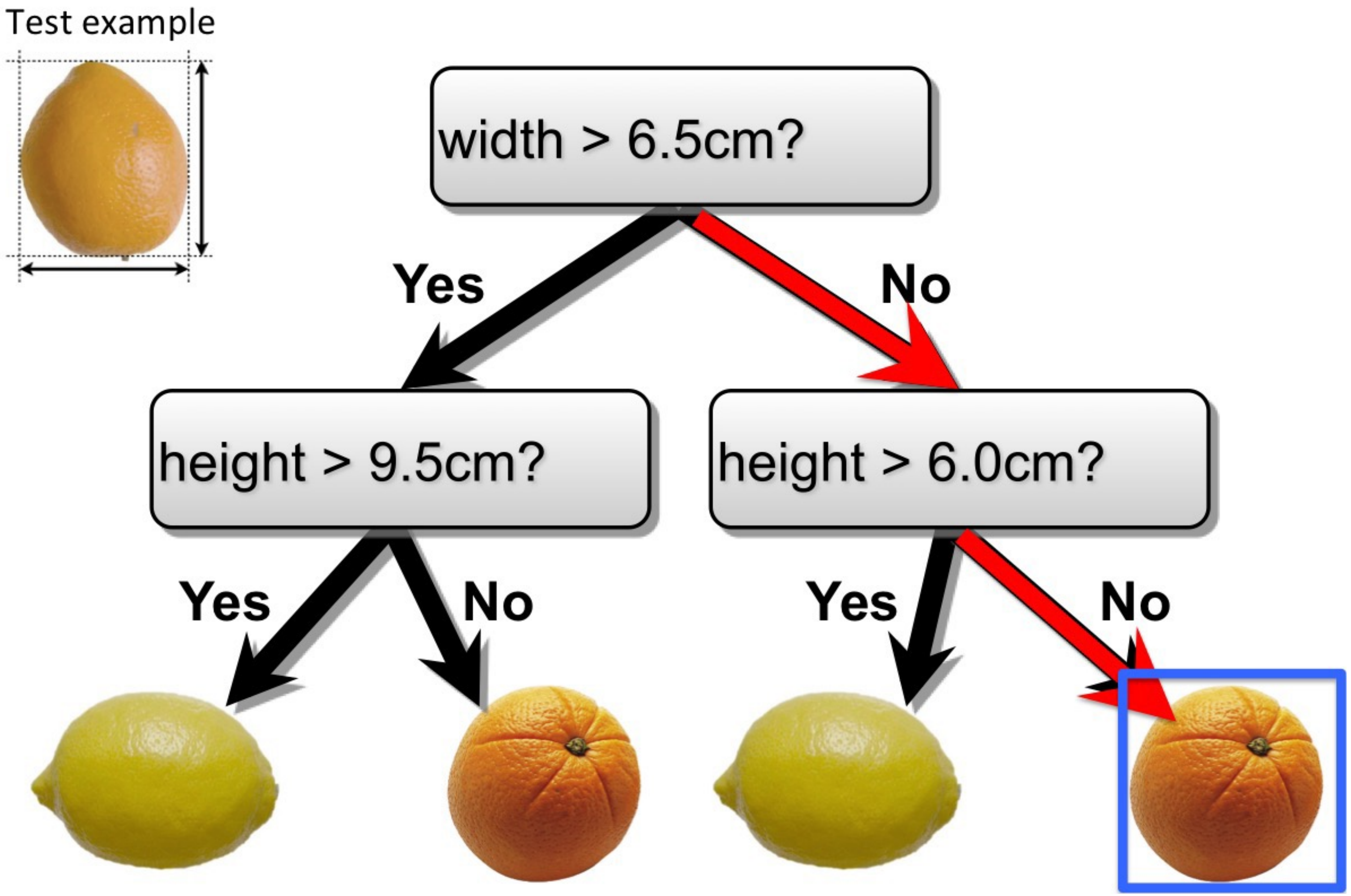
Today

- Decision Trees
  - Simple but powerful learning algorithm
  - One of the most widely used learning algorithms in Kaggle competitions
- Useful information theoretic concepts (entropy, mutual information, etc.)

Decision Trees

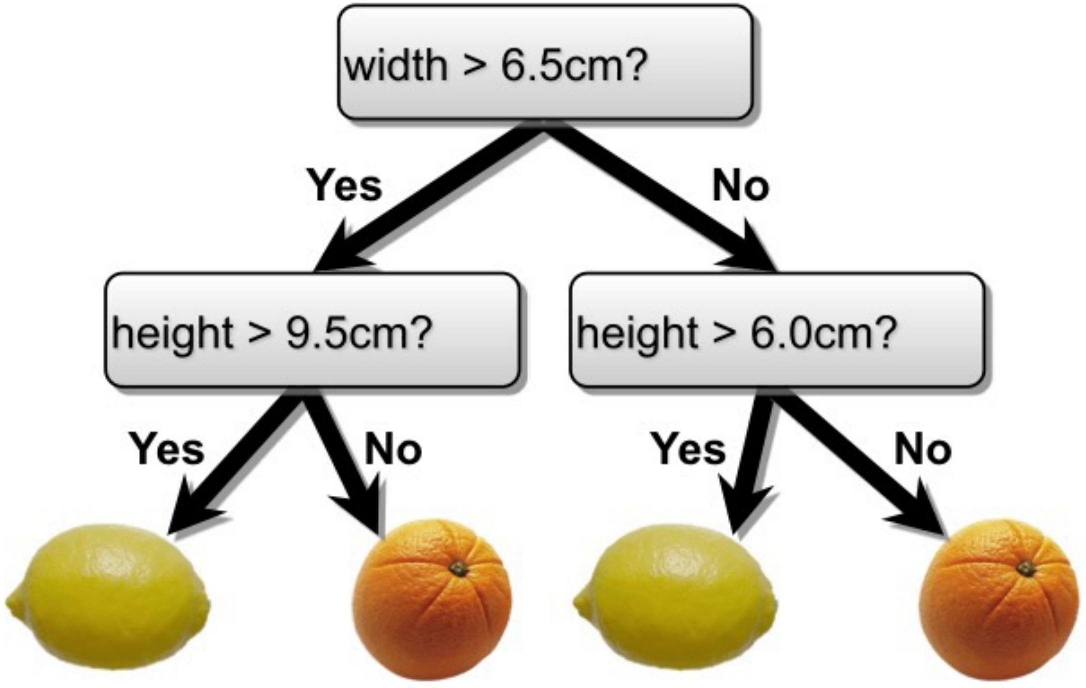


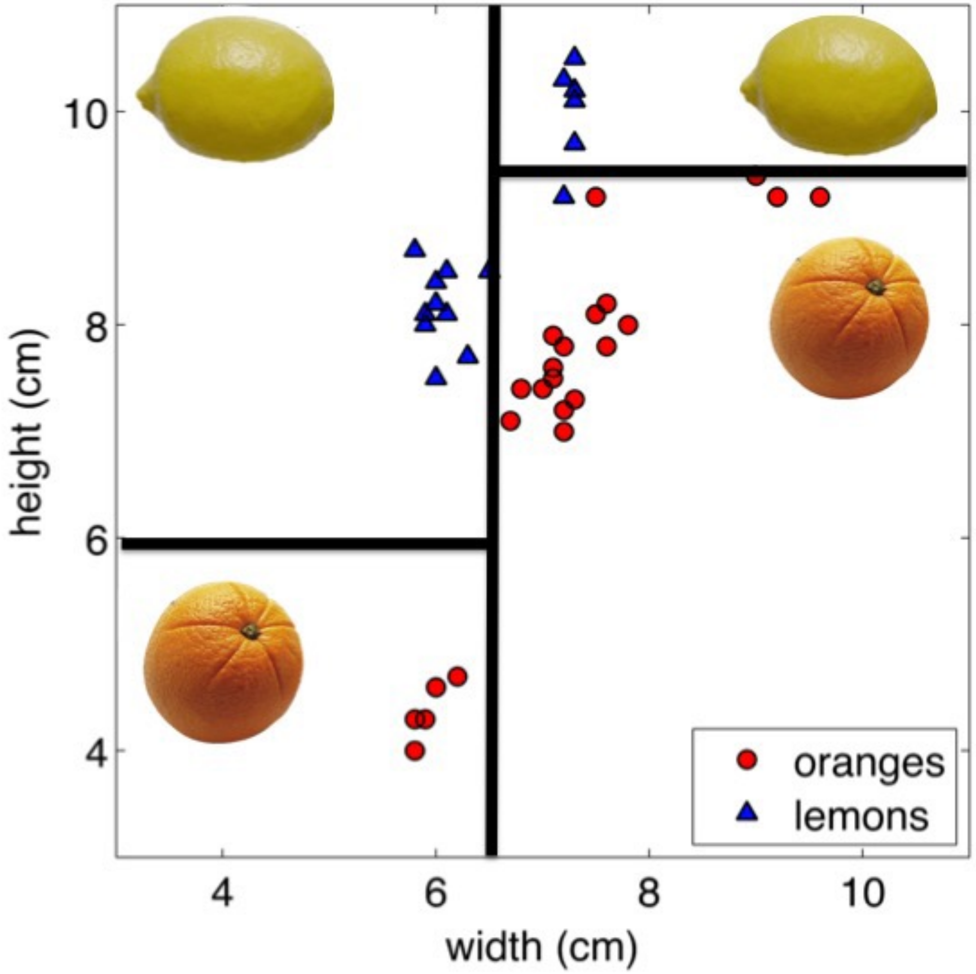
Decision Trees



Decision Trees

- Decision trees make predictions by recursively splitting on different attributes according to a tree structure.





When to Consider Decision Trees

- Instances describable by attribute-value pairs
- Target function is discrete valued
- Disjunctive hypothesis may be required
- Possibly noisy training data

Examples:

- Equipment or medical diagnosis
- Credit risk analysis
- Modeling calendar scheduling preferences

Example with Discrete Inputs

- What if the attributes are discrete?

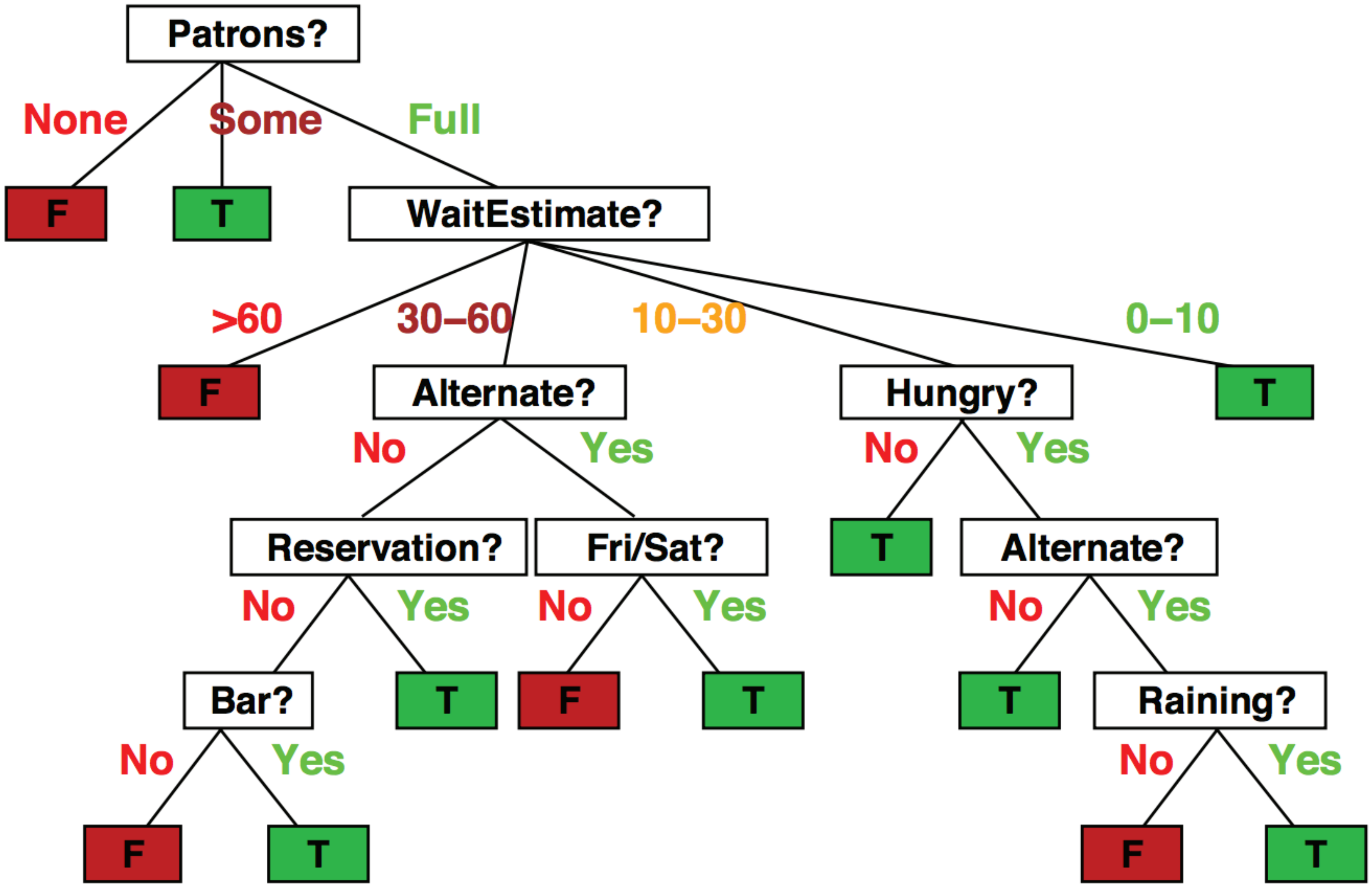
Example	Input Attributes										Goal
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
$\mathbf{x}_1$	Yes	No	No	Yes	Some	$$$	No	Yes	French	0–10	$y_1 =$ Yes
$\mathbf{x}_2$	Yes	No	No	Yes	Full	$	No	No	Thai	30–60	$y_2 =$ No
$\mathbf{x}_3$	No	Yes	No	No	Some	$	No	No	Burger	0–10	$y_3 =$ Yes
$\mathbf{x}_4$	Yes	No	Yes	Yes	Full	$	Yes	No	Thai	10–30	$y_4 =$ Yes
$\mathbf{x}_5$	Yes	No	Yes	No	Full	$$$	No	Yes	French	>60	$y_5 =$ No
$\mathbf{x}_6$	No	Yes	No	Yes	Some	$$	Yes	Yes	Italian	0–10	$y_6 =$ Yes
$\mathbf{x}_7$	No	Yes	No	No	None	$	Yes	No	Burger	0–10	$y_7 =$ No
$\mathbf{x}_8$	No	No	No	Yes	Some	$$	Yes	Yes	Thai	0–10	$y_8 =$ Yes
$\mathbf{x}_9$	No	Yes	Yes	No	Full	$	Yes	No	Burger	>60	$y_9 =$ No
$\mathbf{x}_{10}$	Yes	Yes	Yes	Yes	Full	$$$	No	Yes	Italian	10–30	$y_{10} =$ No
$\mathbf{x}_{11}$	No	No	No	No	None	$	No	No	Thai	0–10	$y_{11} =$ No
$\mathbf{x}_{12}$	Yes	Yes	Yes	Yes	Full	$	No	No	Burger	30–60	$y_{12} =$ Yes

Attributes:

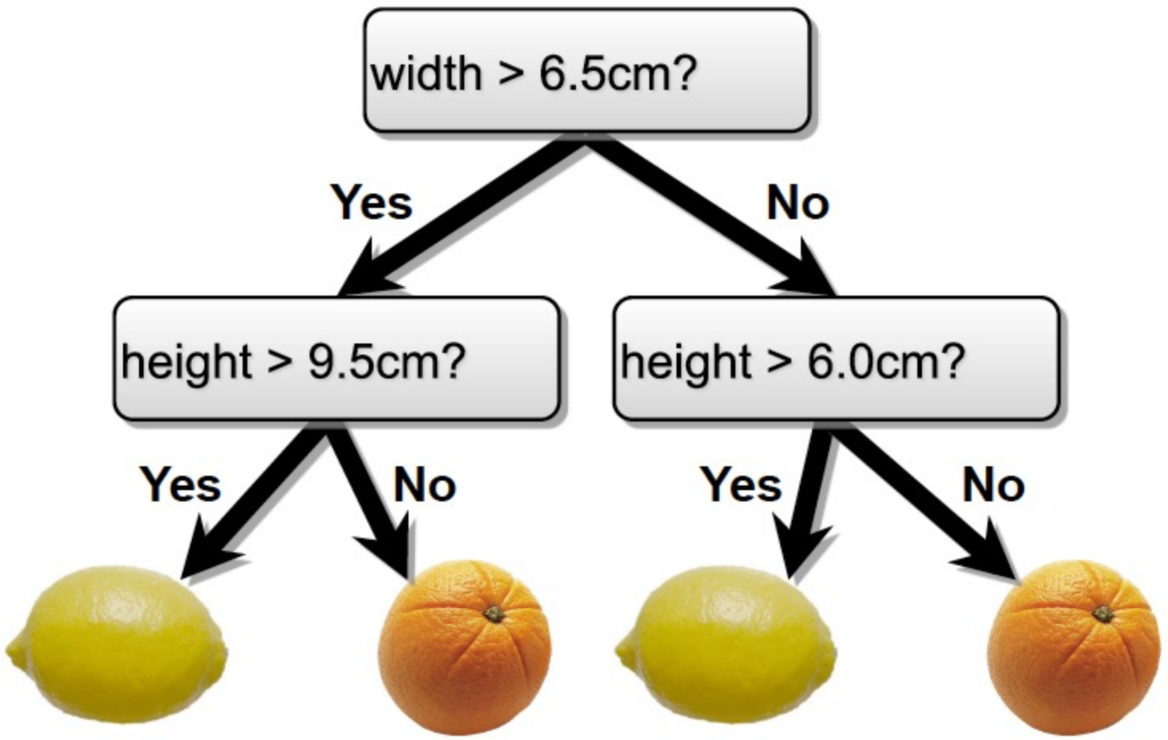
1.	Alternate: whether there is a suitable alternative restaurant nearby.
2.	Bar: whether the restaurant has a comfortable bar area to wait in.
3.	Fri/Sat: true on Fridays and Saturdays.
4.	Hungry: whether we are hungry.
5.	Patrons: how many people are in the restaurant (values are None, Some, and Full).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

Decision Tree: Example with Discrete Inputs

- The tree to decide whether to wait (T) or not (F)

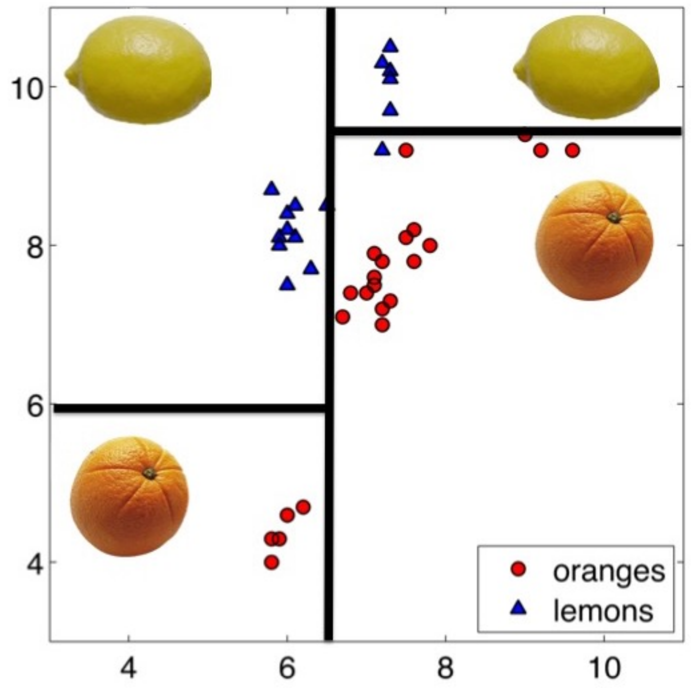


Decision Trees



- Internal nodes test attributes
- Branching is determined by attribute value
- Leaf nodes are outputs (predictions)

Decision Tree: Classification and Regression



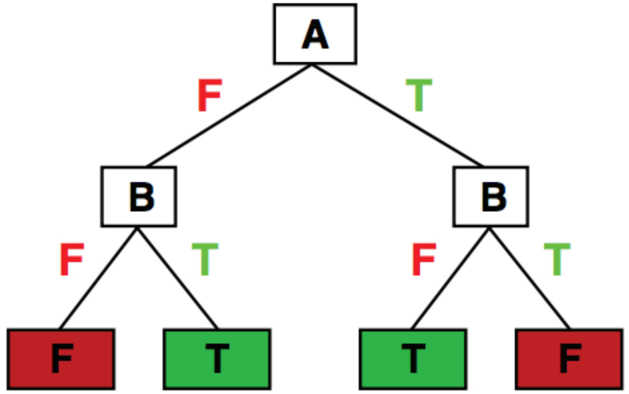
- Each path from root to a leaf defines a region R_m of input space
- Let $\left\{\left(x^{(m_1)}, t^{(m_1)}\right), \dots, \left(x^{(m_k)}, t^{(m_k)}\right)\right\}$ be the training examples that fall into R_m
- **Classification tree:**
  - discrete output
  - leaf value y_m typically set to the most common value in $\left\{t^{(m_1)}, \dots, t^{(m_k)}\right\}$
- **Regression tree:**
  - continuous output
  - leaf value y_m typically set to the mean value in $\left\{t^{(m_1)}, \dots, t^{(m_k)}\right\}$

Note: We will focus on classification

Expressiveness

- Discrete-input, discrete-output case:
  - Decision trees can express any function of the input attributes
  - E.g., for Boolean functions, truth table row→path to leaf:

A	B	A xor B
F	F	F
F	T	T
T	F	T
T	T	F



- Continuous-input, continuous-output case:
  - Can approximate any function arbitrarily closely
- Trivially, there is a consistent decision tree for any training set with one path to leaf for each example (unless *f* nondeterministic in *x*) but it probably won't generalize to new examples
  (모든 training data sample들이 별도의 leaf node를 가지도록 decision tree를 만들 수 있으나 general하지 않음)

How do we Learn a Decision Tree?

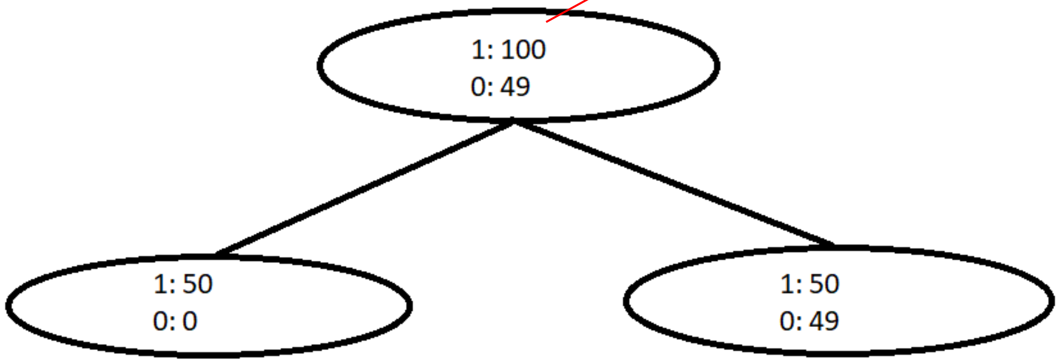
- How do we construct a useful decision tree?

- Learning the simplest (smallest) decision tree is an NP complete problem [if you are interested, check: Hya l & Rivest'76]
  - Resort to a **greedy heuristic**:
    - Start from an empty decision tree
    - Split on the “best" attribute
    - Recurse
  - Which attribute is the “best"?
    - Choose based on accuracy?

Choosing a Good Split

- Why isn't accuracy a good measure?

(class 1과 class 0에 속하는 sample의 갯수가 각각 100개, 49개)



- Is this split good? Zero accuracy gain.
  (윗쪽 node만 이용한 분류와 아래쪽 node 2개를 사용한 분류 결과는 모두 1로 동일)

- Instead, we will use techniques from **information theory**

Idea: Use counts at leaves to define probability distributions, so we can measure uncertainty

Choosing a Good Split

- Which attribute is better to split on, X_1 or X_2?
  - Deterministic: good (all are true or false; just one class in the leaf)
  - Uniform distribution: bad (all classes in leaf equally probable)
  - What about distributons in between?

Note: Let's take a slight detour and remember concepts from information theory

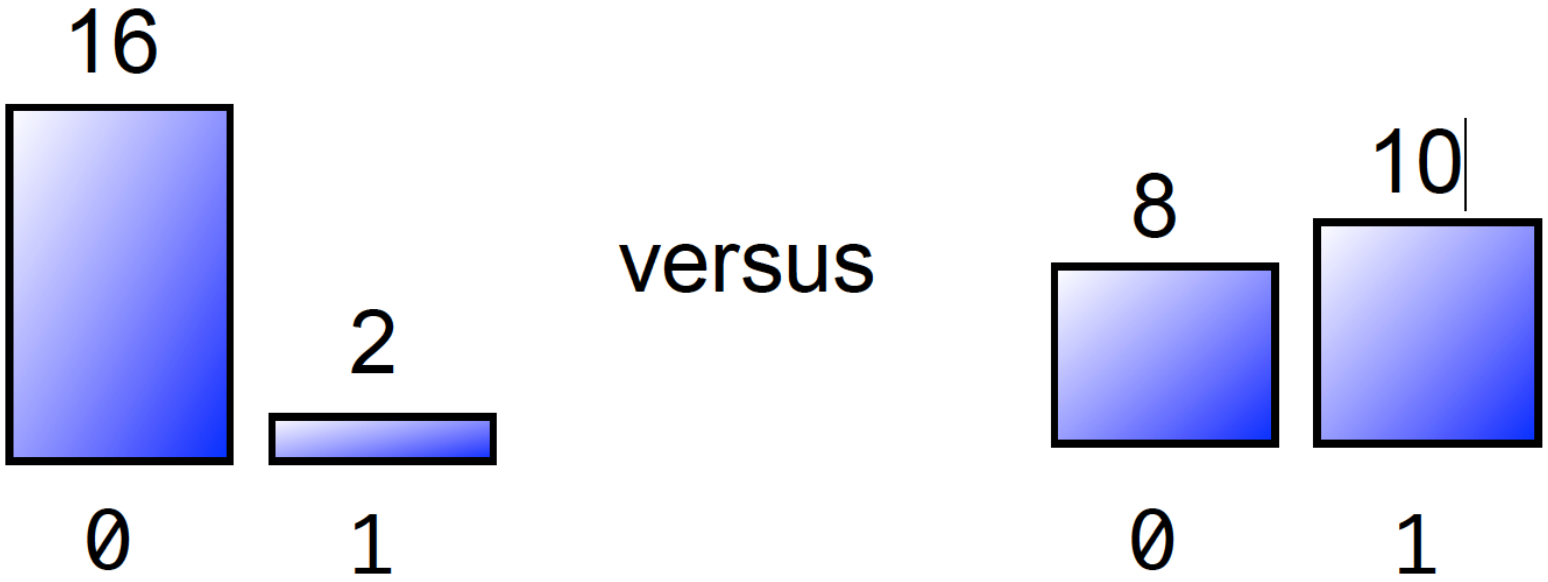
We Flip Two Different Coins

- *Sequence 1:*

0 0 0 1 0 0 0 0 0 0 0 0 0 0 0 0 1 0 0 ... ?

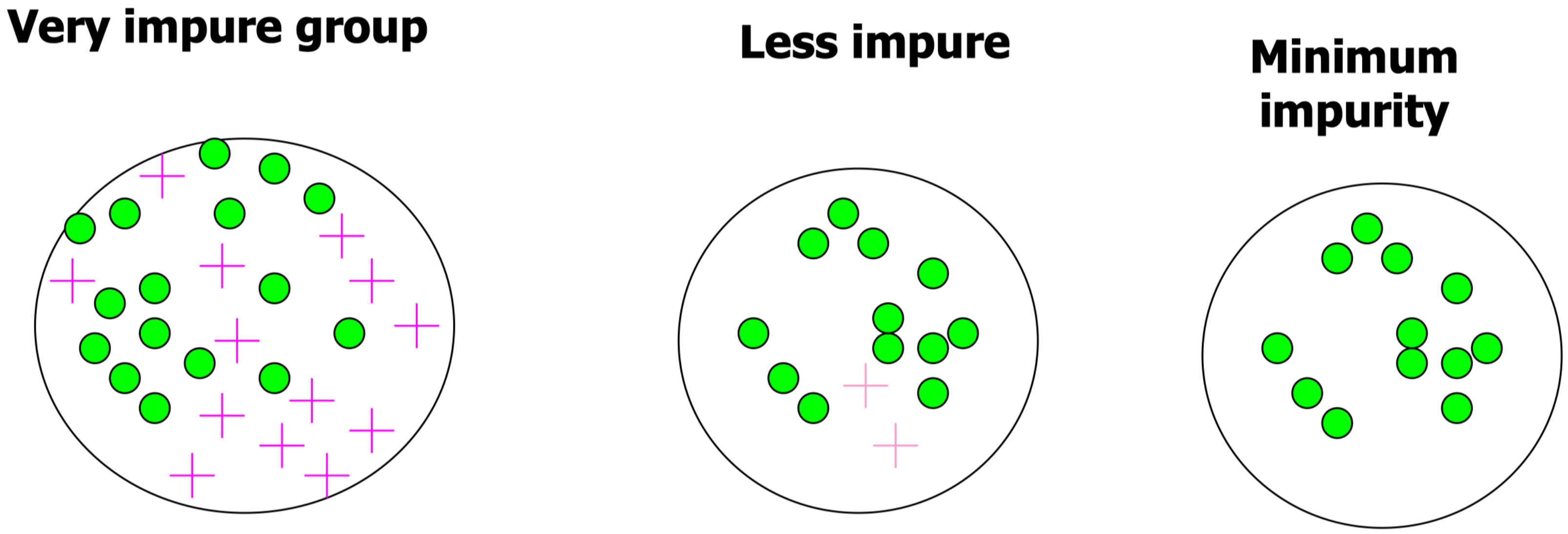
- *Sequence 2:*

0 1 0 1 0 1 1 1 0 1 0 0 1 1 0 1 0 1 ... ?



Impurity/Entropy (informal)

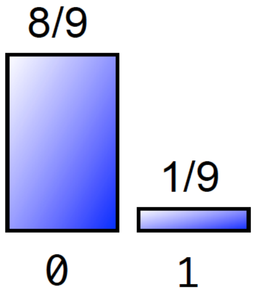
- Measures the level of impurity in a group of examples

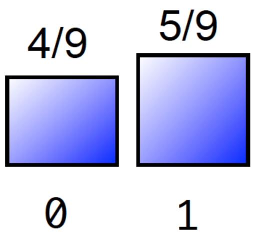


Quantifying Uncertainty

- **Entropy** is a measure of expected “surprise":
  (정보이론(Information theory)에서 나옴. Entropy가 클수록 또는 불확실성이 큰 이벤트 일수록 많은 정보를 가지고 있음)

$$H(X) = -\sum_{x \in X} p(x) \log_2 p(x)$$





$$-\frac{8}{9}\log_2\frac{8}{9} - \frac{1}{9}\log_2\frac{1}{9} \approx \frac{1}{2}$$

$$-\frac{4}{9}\log_2\frac{4}{9} - \frac{5}{9}\log_2\frac{5}{9} \approx 0.99$$

- Measures the information content of each observation
- Unit = **bits**
- A fair coin flip has 1 bit of entropy

Quantifying Uncertainty

- **Entropy** is a measure of expected “surprise":
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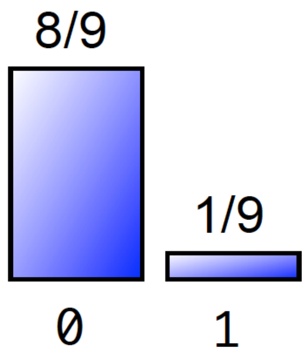

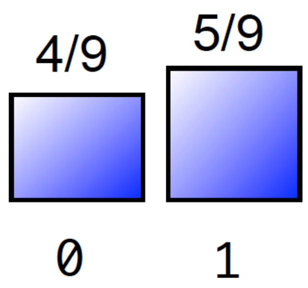

$$-\frac{8}{9}\log_2\frac{8}{9} - \frac{1}{9}\log_2\frac{1}{9} \approx \frac{1}{2}$$

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- Measures the information content of each observation
- Unit = **bits**
- A fair coin flip has 1 bit of entropy (앞뒤 확률이 동일함: 가장 불확실성이 큼)

What does Entropy mean for learning from examples?

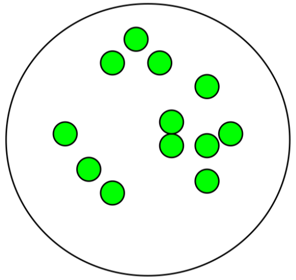
2-Class Cases

$$\text{Entropy} \quad H(x) = -\sum_{i=1}^{n} P(x=i)\log_2 P(x=i)$$

- What is the entropy of a group in which all examples belong to the same class?
  - entropy = $-(1\times\log_2 1 + 0\times\log_2 0) = 0$

  not a good training set for learning

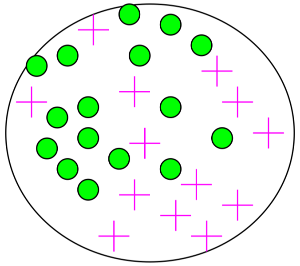
Minimum impurity



- What is the entropy of a group with 50% in either class?
  - entropy = $-(0.5\times\log_2 0.5 + 0.5\log_2 0.5) = 1$

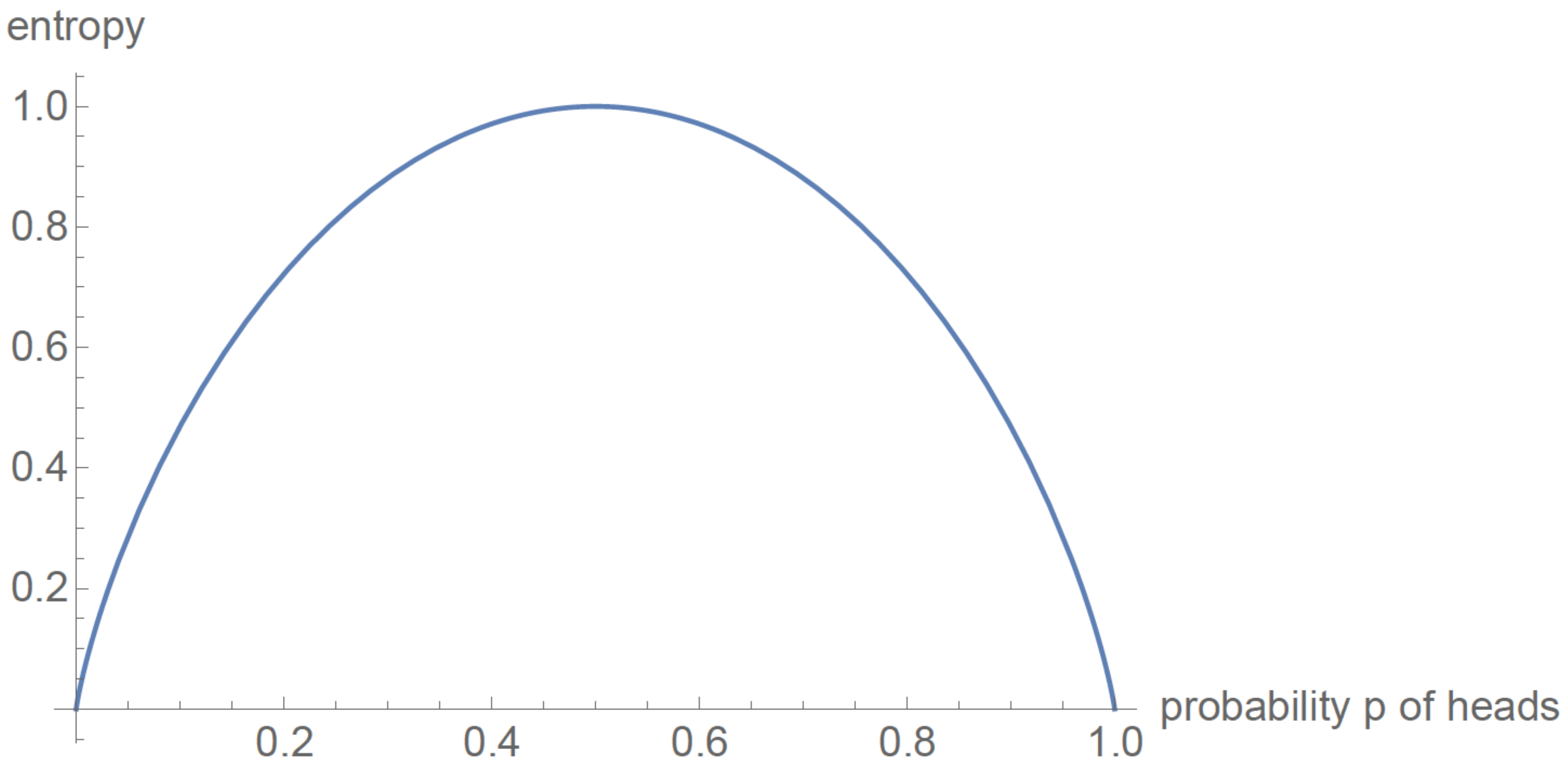
  good training set for learning

Very impure group



Quantifying Uncertainty

$$H(X) = -\sum_{x \in X} p(x) \log_2 p(x)$$



Entropy

- “High Entropy":
  - Variable has a uniform like distribution
  - Flat histogram
  - Values sampled from it are less predictable
- “Low Entropy"
  - Distribution of variable has many peaks and valleys
  - Histogram has many lows and highs
  - Values sampled from it are more predictable

Entropy of a Joint Distribution

- Example: X = {Raining, Not raining}, Y = {Cloudy, Not cloudy}

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

$$
\begin{aligned}
H(X,Y) &= -\sum_{x\in X}\sum_{y\in Y} p(x,y)\log_2 p(x,y) \\
&= -\frac{24}{100}\log_2\frac{24}{100} - \frac{1}{100}\log_2\frac{1}{100} - \frac{25}{100}\log_2\frac{25}{100} - \frac{50}{100}\log_2\frac{50}{100} \\
&\approx 1.56\text{bits}
\end{aligned}
$$

Specific Conditional Entropy

- Example: X = {Raining, Not raining}, Y = {Cloudy, Not cloudy}

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

- What is the entropy of cloudiness Y , given that it is raining?

$$\begin{aligned} H(Y|X=x) &= -\sum_{y \in Y} p(y|x) \log_2 p(y|x) \\ &= -\frac{24}{25}\log_2\frac{24}{25} - \frac{1}{25}\log_2\frac{1}{25} \\ &\approx 0.24\text{bits} \end{aligned}$$

- We used: $p(y|x) = \frac{p(x,y)}{p(x)}$, and $p(x) = \sum_y p(x,y)$ (sum in a row)

Conditional Entropy

- Example: X = {Raining, Not raining}, Y = {Cloudy, Not cloudy}

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

- The expected conditional entropy:

$$
\begin{aligned}
H(Y|X) &= \sum_{x \in X} p(x) H(Y|X = x) \\
&= -\sum_{x \in X} \sum_{y \in Y} p(x, y) \log_2 p(y|x)
\end{aligned}
$$

Conditional Entropy

- Example: X = {Raining, Not raining}, Y = {Cloudy, Not cloudy}

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

- What is the entropy of cloudiness, given the knowledge of whether or not it is raining?

$$
\begin{aligned}
H(Y|X) &= \sum_{x \in X} p(x) H(Y|X=x) \\
&= \boxed{\frac{1}{4} H(\text{cloudy}|\text{is raining})} + \boxed{\frac{3}{4} H(\text{cloudy}|\text{not raining})} \\
&\approx 0.75 \text{ bits}
\end{aligned}
$$

Some useful properties of Conditional Entropy

- H is always non-negative

- Chain rule:

$$H(X,Y) = H(X|Y) + H(Y) = H(Y|X) + H(X)$$

- If X and Y independent, then X doesn't tell us anything about Y:

$$H(Y|X) = H(Y)$$

- But X tells us everything about Y

$$H(Y|X) = 0$$

- By knowing X, we can only decrease uncertainty about Y

$$H(Y|X) \leq H(Y)$$

Information Gain

- Example: X = {Raining, Not raining}, Y = {Cloudy, Not cloudy}

	Cloudy	Not Cloudy
Raining	24/100	1/100
Not Raining	25/100	50/100

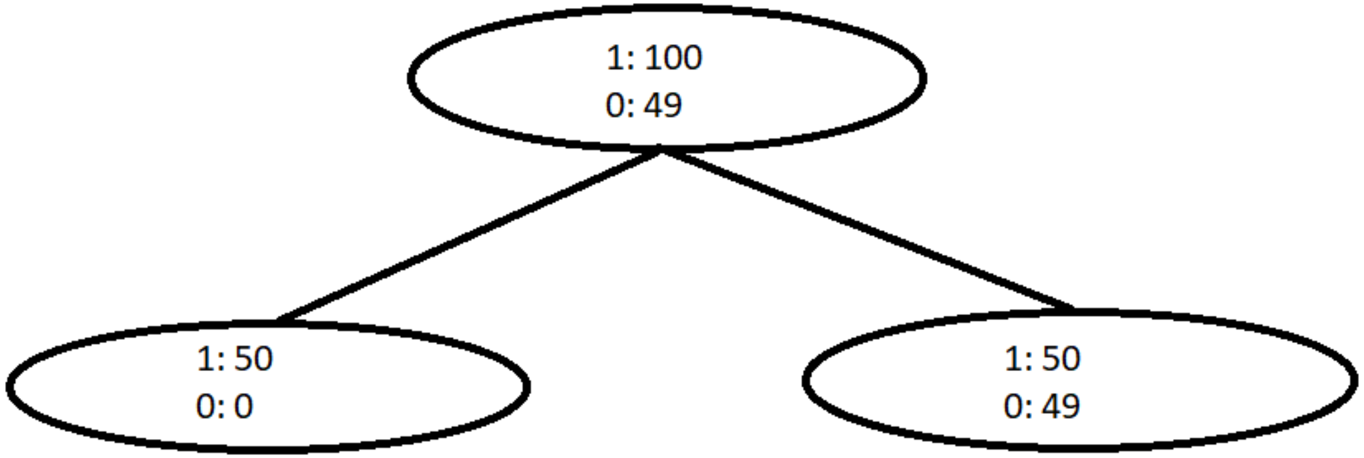
- How much information about cloudiness do we get by discovering whether it is raining?

$$\begin{aligned} IG(Y|X) &= H(Y) - H(Y|X) \\ &\approx 0.25 \text{ bits} \end{aligned}$$

- This is called the **information gain** in Y due to X, or the **mutual information** of Y and X
- If X is completely uninformative about Y: $IG(Y|X) = 0$
- If X is completely informative about Y: $IG(Y|X) = H(Y)$

Revisiting Our Original Example

- **Information Gain** = entropy(parent) – [average entropy(children)]
- Information gain measures the informativeness of a variable, which is exactly what we desire in a decision tree attribute!
- What is the information gain of this split?

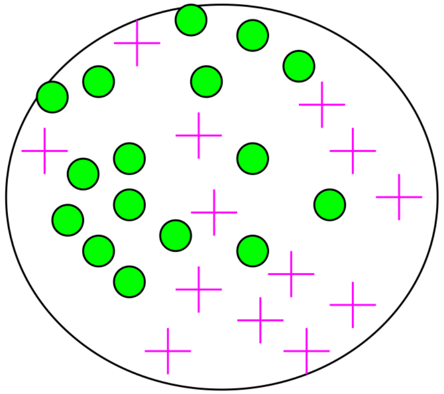


- Root entropy: $H(Y) = -\frac{49}{149}\log_2(\frac{49}{149}) - \frac{100}{149}\log_2(\frac{100}{149}) \approx 0.91$
- Leafs entropy: $H(Y|left) = 0,\ H(Y|right) \approx 1$
- $IG(split) \approx 0.91 - (\frac{1}{3}\cdot 0 + \frac{2}{3}\cdot 1) \approx 0.24 > 0$

More Example for Calculating Information Gain

- **Information Gain** = entropy(parent) – [average entropy(children)]

Entire population (30 instances)

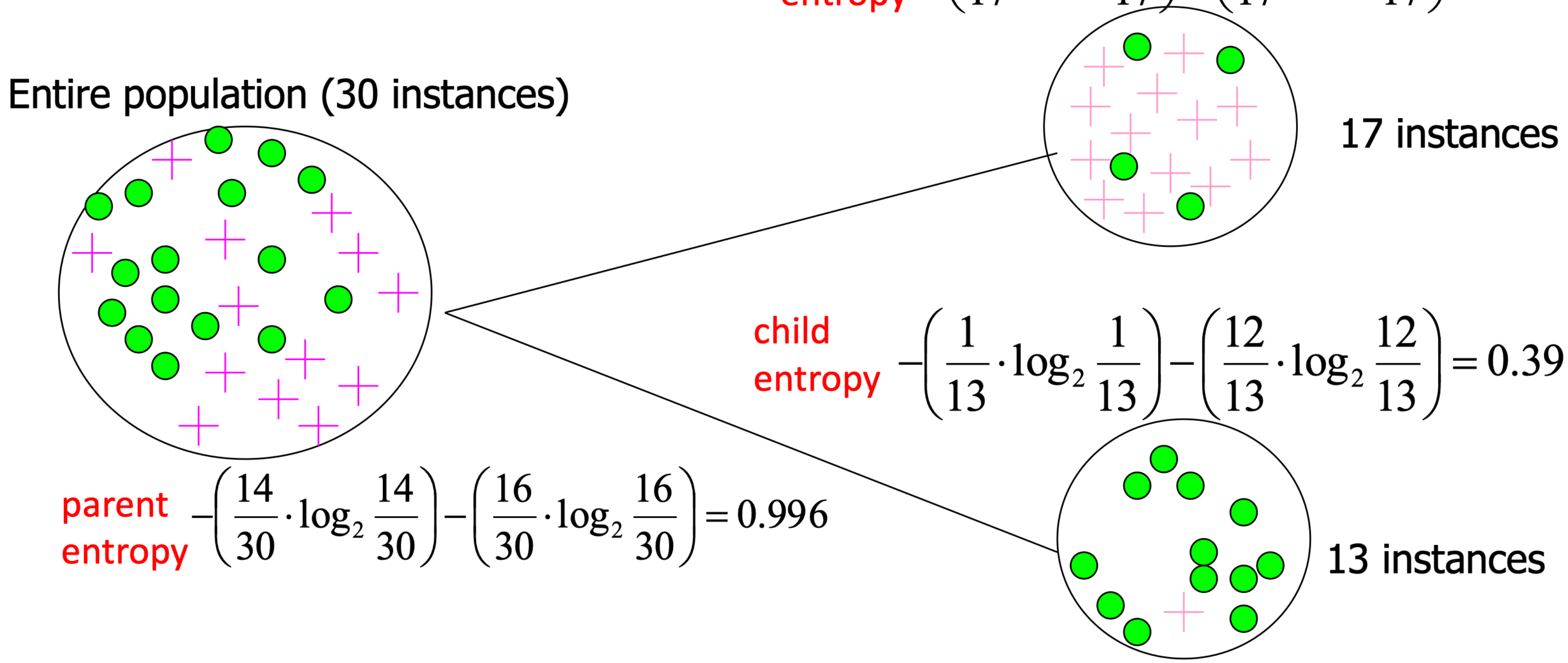


parent entropy $-\left(\frac{14}{30}\cdot\log_2\frac{14}{30}\right)-\left(\frac{16}{30}\cdot\log_2\frac{16}{30}\right)=0.996$

More Example for Calculating Information Gain

- **Information Gain** = entropy(parent) – [average entropy(children)]

child entropy $-\left(\frac{13}{17}\cdot\log_2\frac{13}{17}\right)-\left(\frac{4}{17}\cdot\log_2\frac{4}{17}\right)=0.787$



child entropy $-\left(\frac{1}{13}\cdot\log_2\frac{1}{13}\right)-\left(\frac{12}{13}\cdot\log_2\frac{12}{13}\right)=0.391$

parent entropy $-\left(\frac{14}{30}\cdot\log_2\frac{14}{30}\right)-\left(\frac{16}{30}\cdot\log_2\frac{16}{30}\right)=0.996$

More Example for Calculating Information Gain

- **Information Gain** = entropy(parent) – [average entropy(children)]

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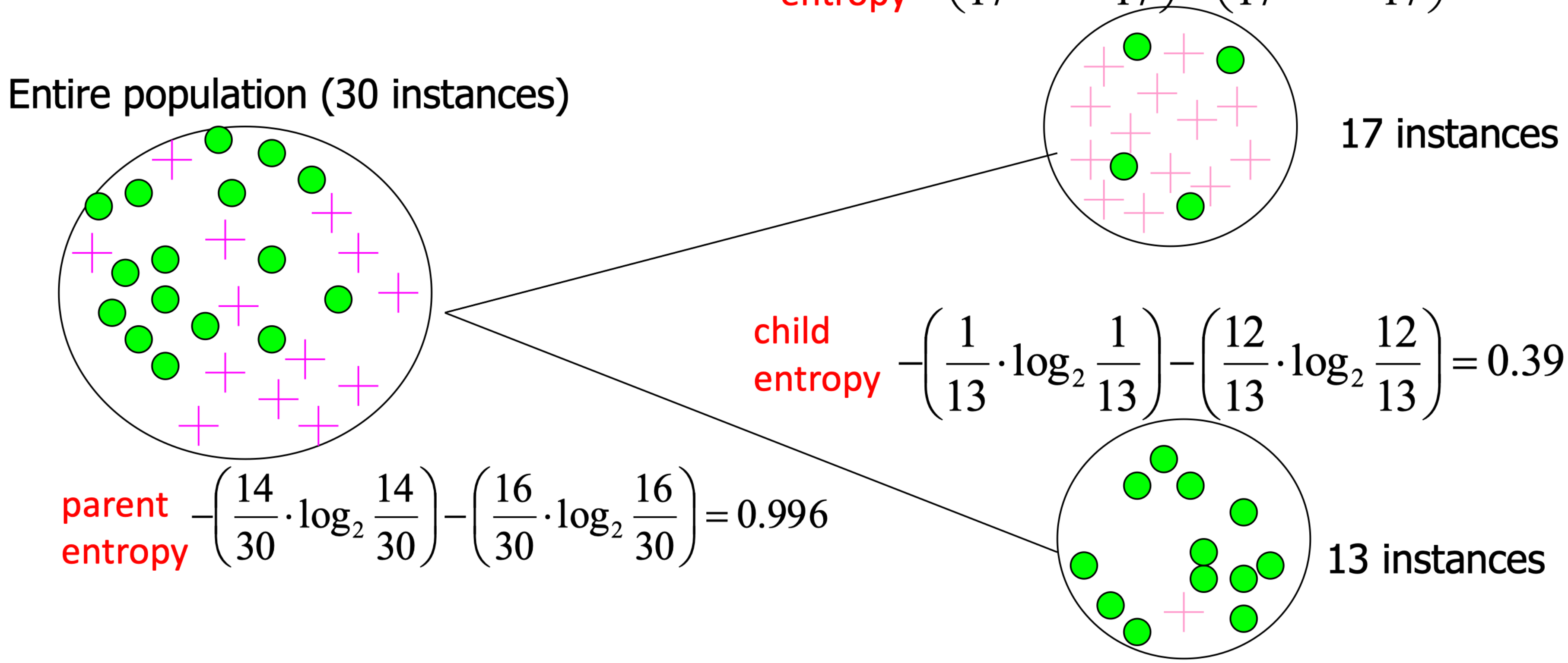

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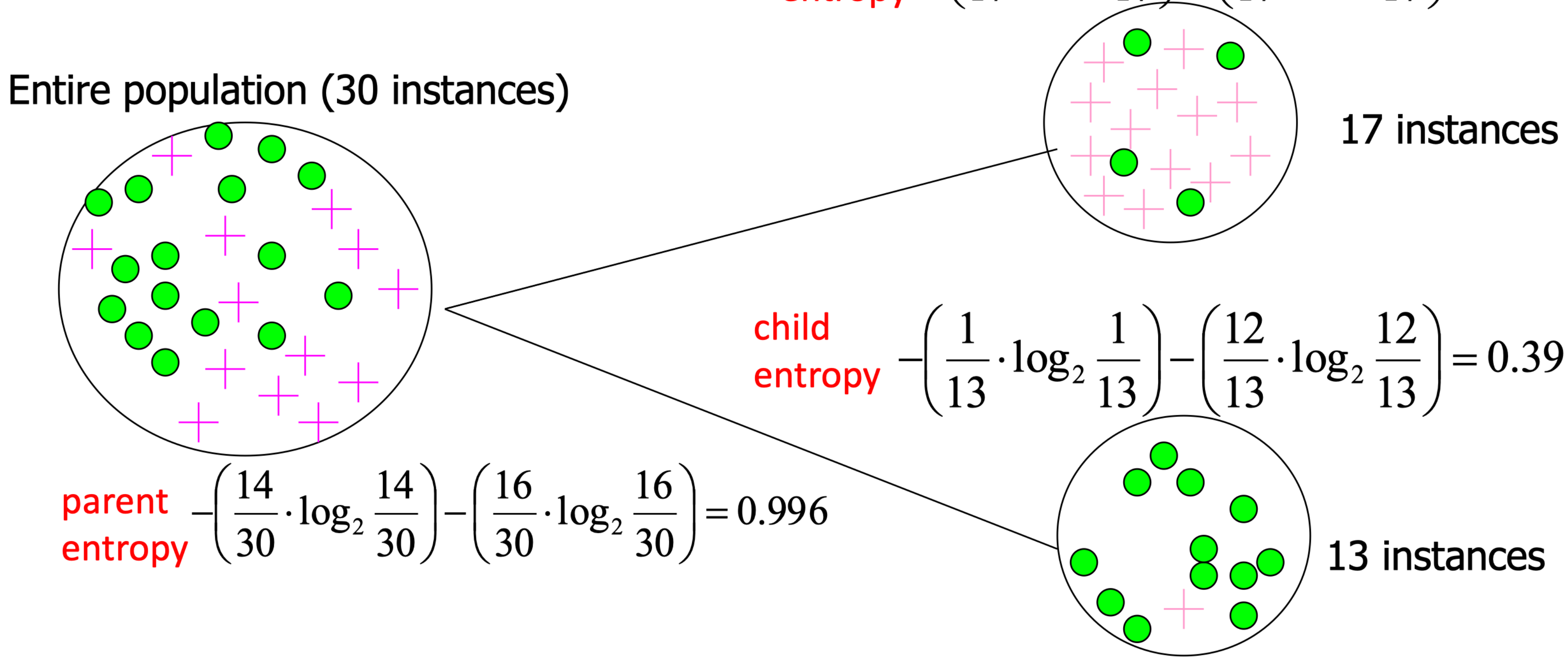
parent entropy $-\left(\frac{14}{30}\cdot\log_2\frac{14}{30}\right)-\left(\frac{16}{30}\cdot\log_2\frac{16}{30}\right)=0.996$

- (Weighted) Average Entropy of Children = $\left(\frac{17}{30}\times 0.787\right)+\left(\frac{13}{30}\times 0.391\right)=0.615$

More Example for Calculating Information Gain

- **Information Gain** = entropy(parent) – [average entropy(children)]



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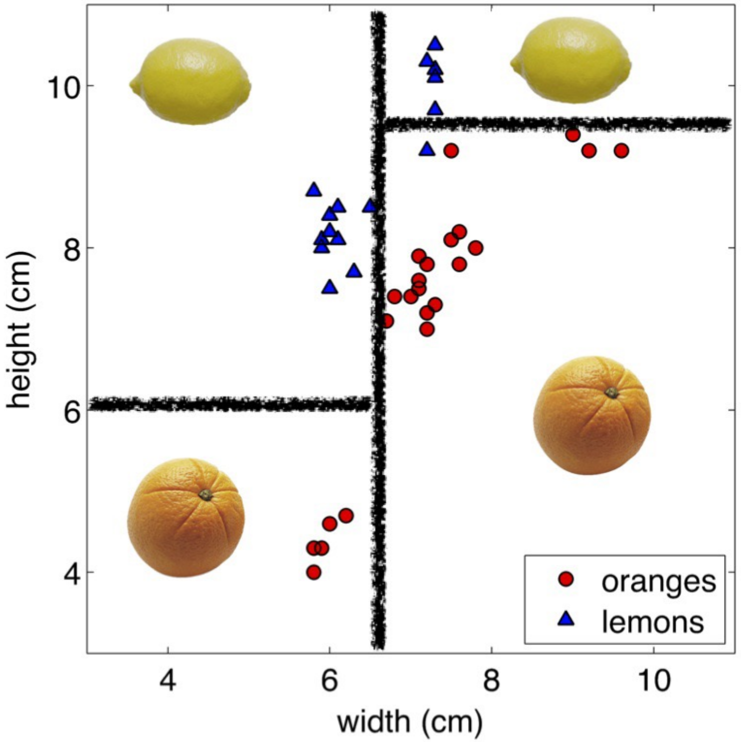
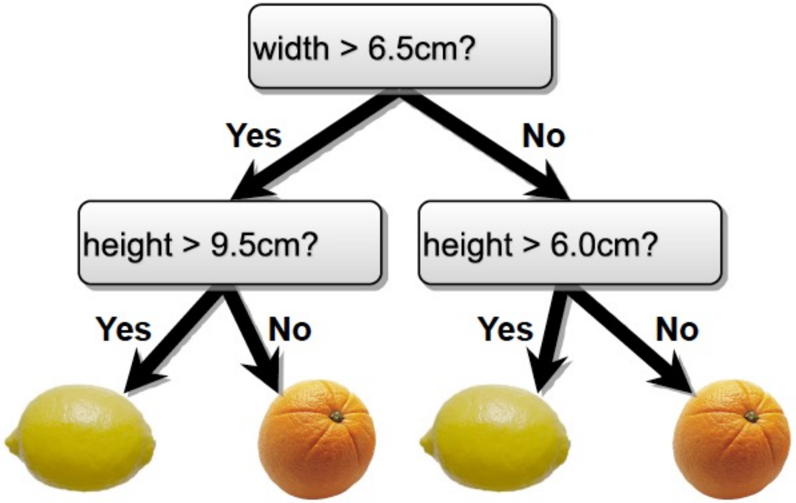
- (Weighted) Average Entropy of Children $=\left(\frac{17}{30}\times 0.787\right)+\left(\frac{13}{30}\times 0.391\right)=0.615$
- Information gain $= 0.996 - 0.615 = 0.38$

Constructing Decision Trees





- At each level, one must choose:
  1. Which variable to split.
  2. Possibly where to split it.
- Choose them based on how much information we would gain from the decision! (choose attribute that gives the best gain)

Decision Tree Construction Algorithm

- Simple, greedy, recursive approach, builds up tree node-by-node

1. pick an attribute to split at a non-terminal node
2. split examples into groups based on attribute value
3. for each group:
    - if no examples - return majority from parent
    - else if all examples in same class - return class
    - else loop to step 1

Back to Our Example

Example	Input Attributes										Goal
	Alt	*Bar*	*Fri*	*Hun*	*Pat*	*Price*	*Rain*	*Res*	*Type*	*Est*	*WillWait*
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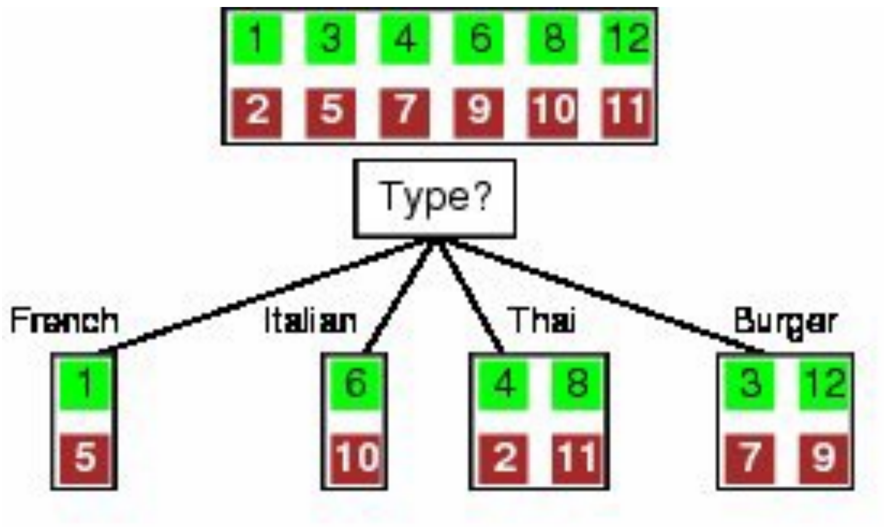
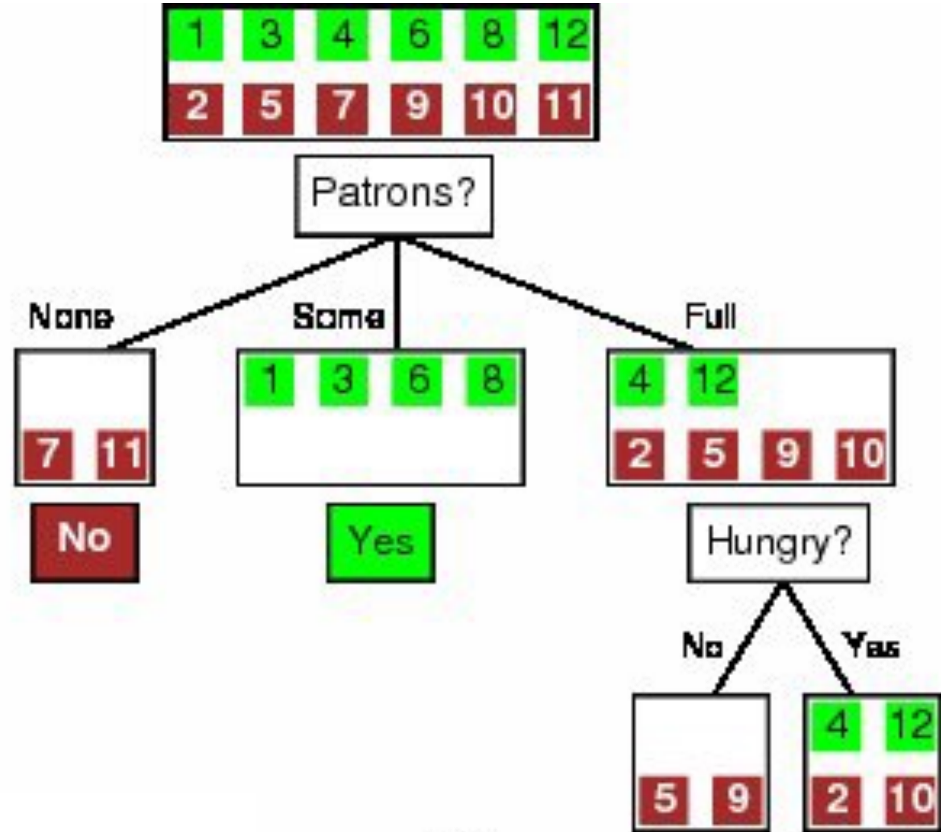
$\mathbf{x}_{10}$	Yes	Yes	Yes	Yes	Full	$$$	No	Yes	Italian	10–30	$y_{10} =$ No
$\mathbf{x}_{11}$	No	No	No	No	None	$	No	No	Thai	0–10	$y_{11} =$ No
$\mathbf{x}_{12}$	Yes	Yes	Yes	Yes	Full	$	No	No	Burger	30–60	$y_{12} =$ Yes

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).

Attribute Selection



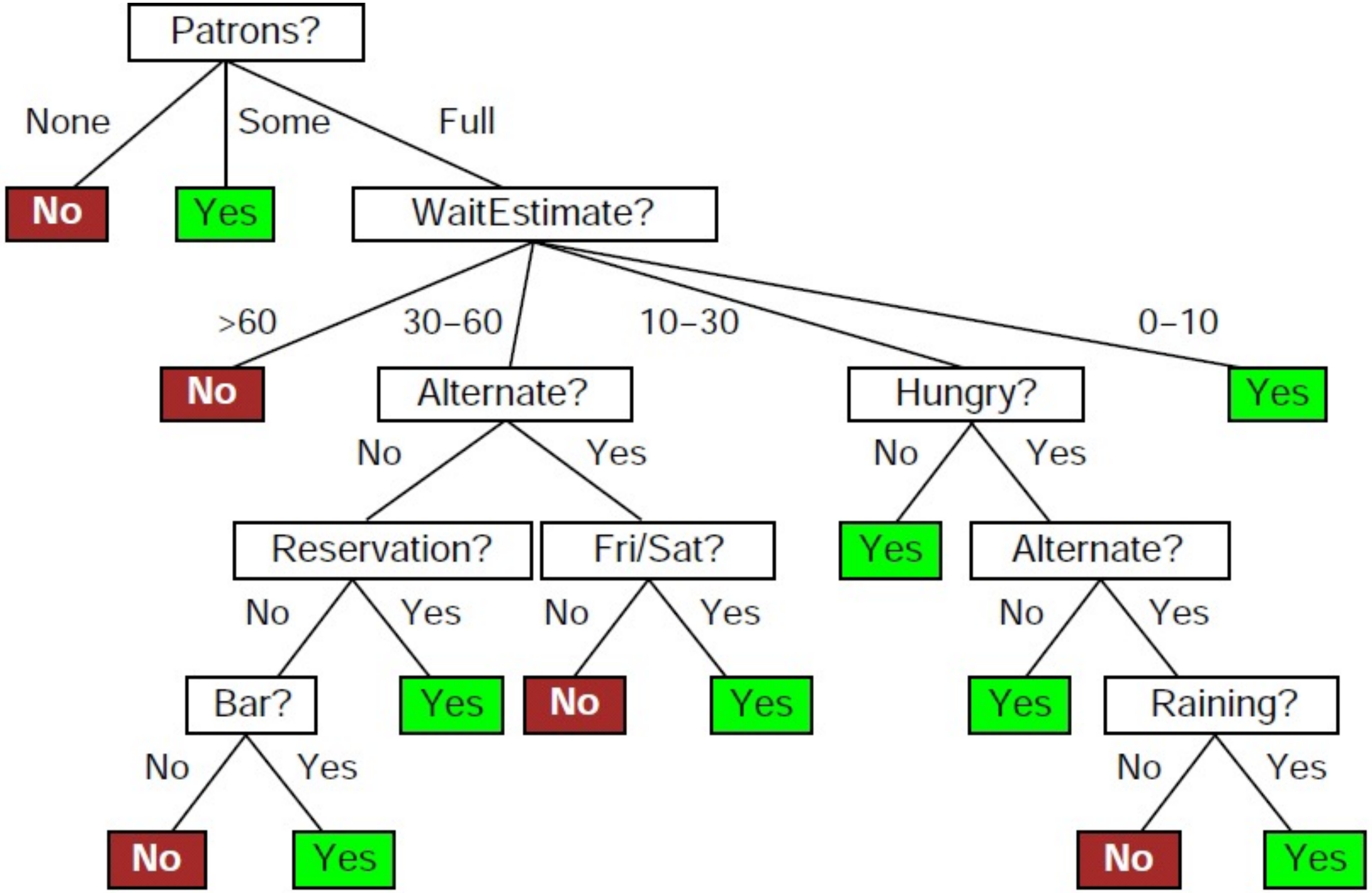


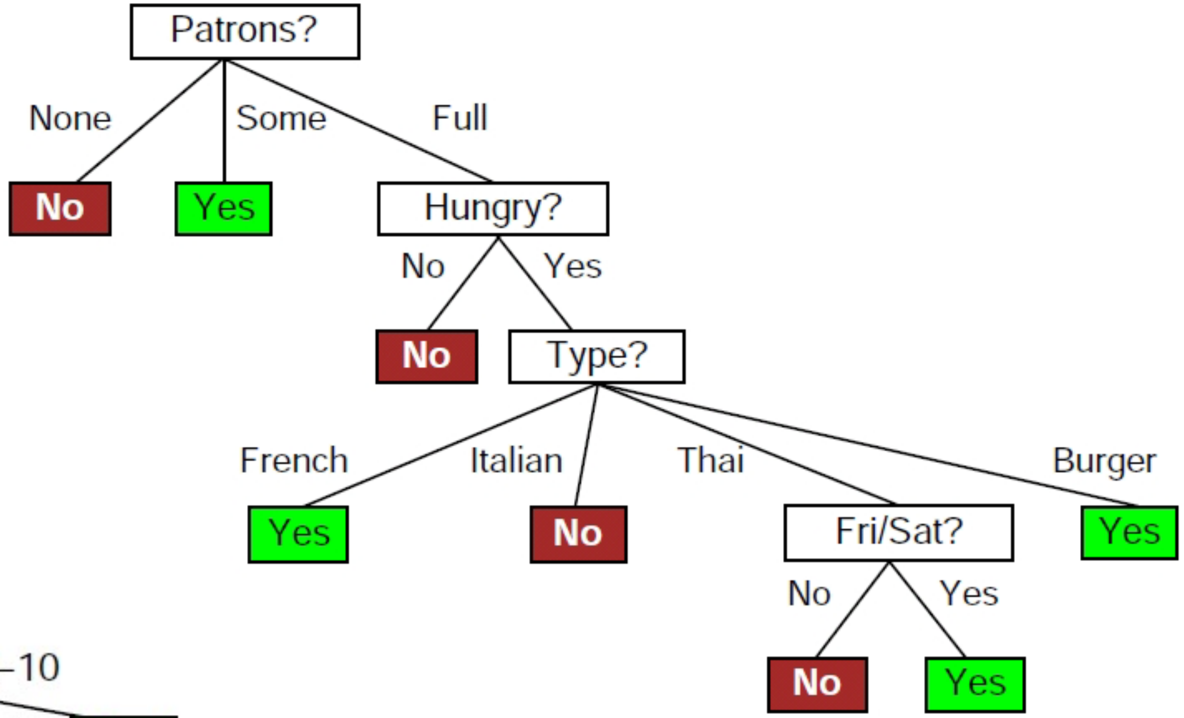
$$IG(Y) = H(Y) - H(Y|X)$$

$$IG(type) = 1 - \left[\frac{2}{12}H(Y|\text{Fr.}) + \frac{2}{12}H(Y|\text{It.}) + \frac{4}{12}H(Y|\text{Thai}) + \frac{4}{12}H(Y|\text{Bur.})\right] = 0$$

$$IG(Patrons) = 1 - \left[\frac{2}{12}H(0,1) + \frac{4}{12}H(1,0) + \frac{6}{12}H(\frac{2}{6},\frac{4}{6})\right] \approx 0.541$$

Which Tree is Better?





What Makes a Good Tree?

- Not too small: need to handle important but possibly subtle distinctions in data
- Not too big:
  - Computational efficiency (avoid redundant, spurious attributes)
  - Avoid over-fitting training examples
  - Human interpretability
- **“Occam's Razor"**: find the simplest hypothesis that fits the observations
  - Useful principle, but hard to formalize (how to define simplicity?)
  - See Domingos, 1999, “The role of Occam's razor in knowledge discovery"
- We desire small trees with informative nodes near the root

Decision Tree Miscellany

- Problems:
  - You have exponentially less data at lower levels
  - Too big of a tree can overfit the data
  - Greedy algorithms don't necessarily yield the global optimum
- Handling continuous attributes
  - Split based on a threshold, chosen to maximize information gain
- Decision trees can also be used for regression on real-valued outputs. Choose splits to minimize squared error, rather than maximize information gain.

Comparison to k-NN

- Advantages of decision trees over k-NN
  - Good with discrete attributes
  - Easily deals with missing values (just treat as another value)
    (예: nominal feature, 즉 categorical feature인 경우 새로운 class로 취급)
  - Robust to scale of inputs
  - Fast at test time
  - More interpretable
- Advantages of k-NN over decision trees
  - Able to handle attributes/features that interact in complex ways (e.g. pixels)
  - Can incorporate interesting distance measures (e.g. shape contexts)
  - Typically make better predictions in practice
    - As we'll see next lecture, ensembles of decision trees are much stronger. But they lose many of the advantages listed above.