CS57300
PURDUE UNIVERSITY
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# DATA MINING

# DECISION TREES

# TREE LEARNING

- Top-down recursive divide and conquer algorithm
  - Start with all training examples at root
  - Select **best** attribute/feature: Take a greedy view to decide how "good" an attribute is
  - Partition examples by selected attribute
  - Recurse and repeat
- Other issues:
  - When to stop growing
  - Pruning irrelevant parts of the tree

# CHOOSING AN ATTRIBUTE/FEATURE

- Be greedy: choose an attribute that can immediately minimize the misclassification rate (i.e., as if no further subtree will grow)
- A good feature splits the examples into subsets that distinguish among the class labels as much as possible... ideally into pure sets of "all positive" or "all negative”
- A good attribute leads to **highly certain** prediction for training examples sharing the same value on that attribute!

# MEASURING UNCERTAINTY: ENTROPY

- Used to quantify the amount of randomness of a probability distribution.
- Definition: Suppose a discrete random variable X has a distribution of P(X). The **entropy** H(X) of X is defined by:

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

# ENTROPY OF A RANDOM VARIABLE

A completely random binary variable with P(X)=[0.5,0.5] has entropy:

$H(X) = -(0.5 \log_2 0.5 + 0.5 \log_2 0.5) = -(-0.5 + -0.5) = 1$

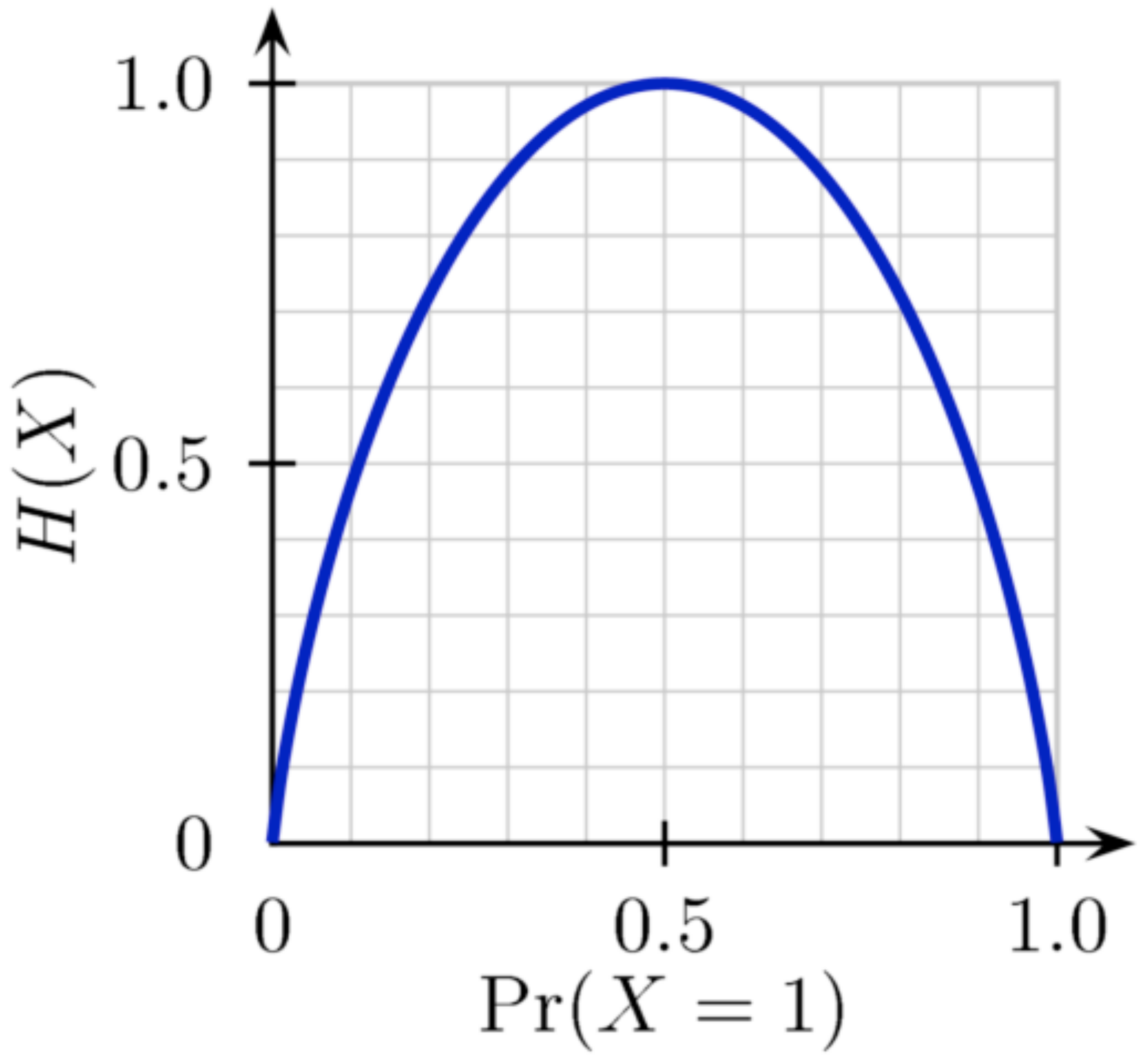
A deterministic variable with P(X)=[1,0] has entropy:

$H(X) = -(1 \log_2 1 + 0 \log_2 0) = -(0+0) = 0$

A biased variable with P(X)=[0.75,0.25] has entropy:

$H(X) = 0.8113$

The entropy of a probability distribution **p** expresses the **amount of uncertainty** that we have about the values of X



# MEASURING CHANGE OF UNCERTAINTY: INFORMATION GAIN

- How much does a feature split decrease the entropy?

$$Gain(S, A) = \underline{Entropy(S)} - \sum_{v \in values(A)} \frac{|S_v|}{|S|} Entropy(S_v)$$

| age | income | student | credit_rating | buys_computer |
|---|---|---|---|---|
| <=30 | high | no | fair | no |
| <=30 | high | no | excellent | no |
| 31…40 | high | no | fair | yes |
| >40 | medium | no | fair | yes |
| >40 | low | yes | fair | yes |
| >40 | low | yes | excellent | no |
| 31…40 | low | yes | excellent | yes |
| <=30 | medium | no | fair | no |
| <=30 | low | yes | fair | yes |
| >40 | medium | yes | fair | yes |
| <=30 | medium | yes | excellent | yes |
| 31…40 | medium | no | excellent | yes |
| 31…40 | high | yes | fair | yes |
| >40 | medium | no | excellent | no |

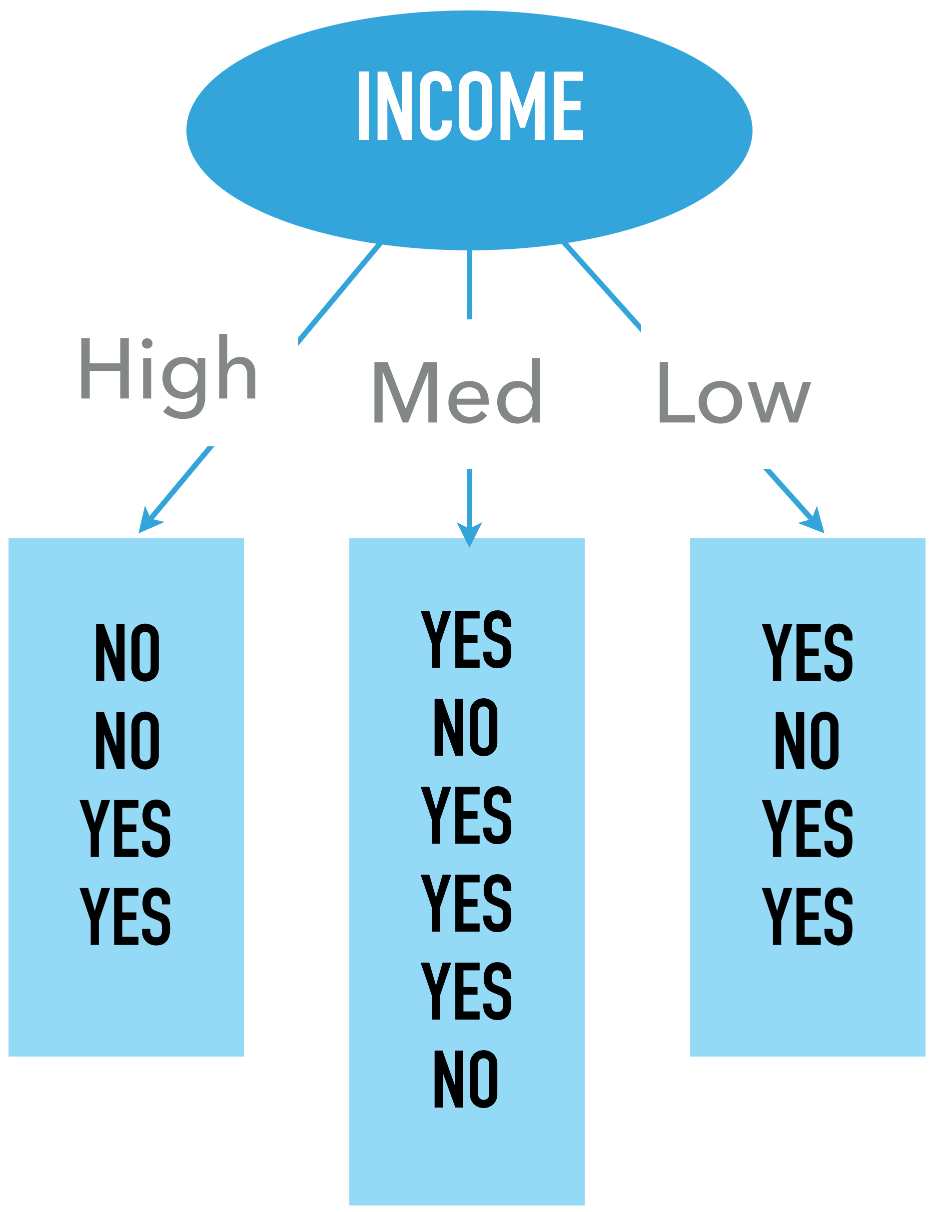
Entropy(S)

= -9/14 Log 9/14 -5/14 Log 5/14

= 0.9400

# INFORMATION GAIN

$$Gain(S, A) = Entropy(S) - \sum_{v \in values(A)} \frac{|S_v|}{|S|} Entropy(S_v)$$




Entropy(Income=High)
= -2/4 Log 2/4 -2/4 Log 2/4 = 1

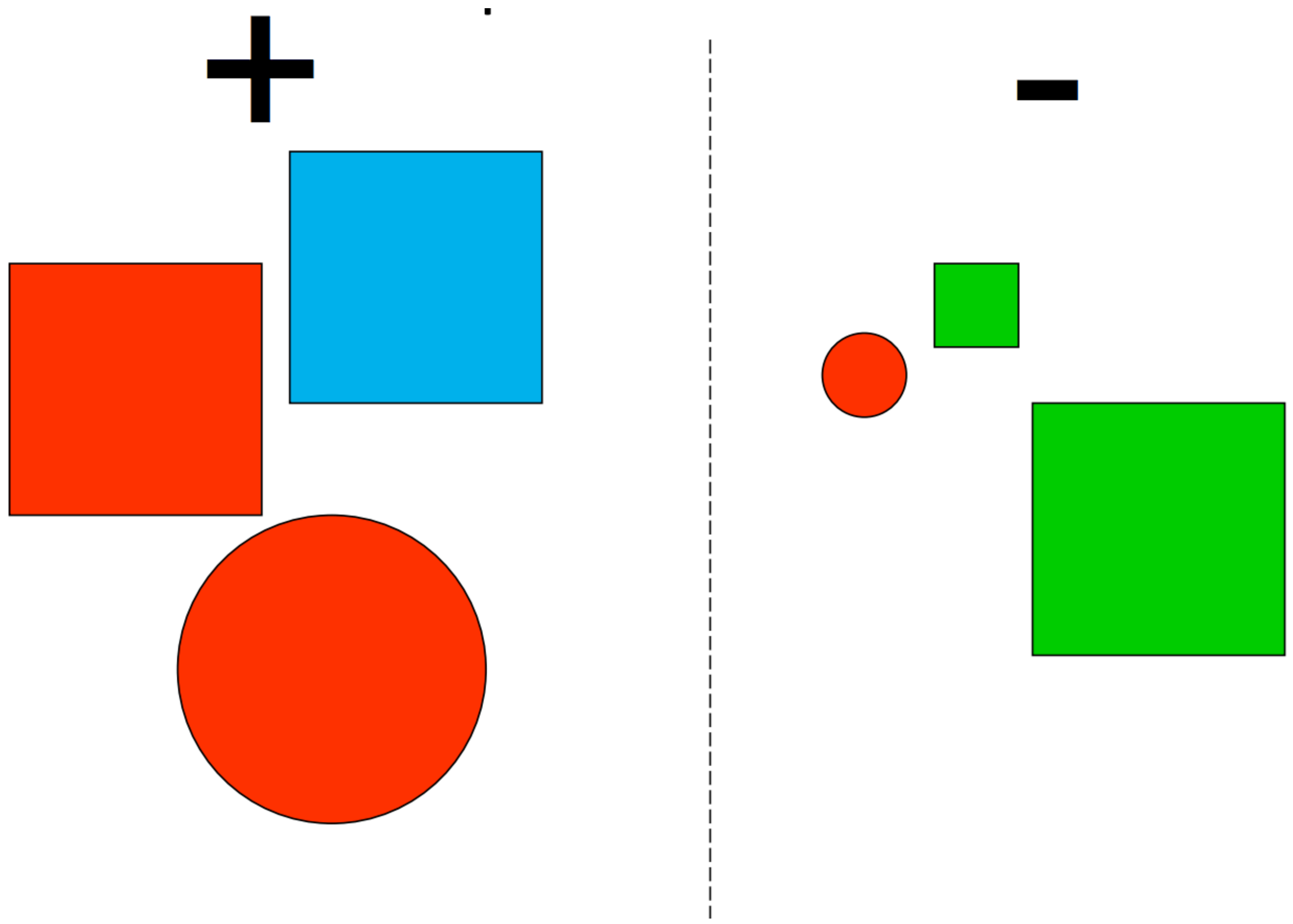
Entropy(Income=Med)
= -4/6 Log 4/6 -2/6 Log 2/6 = 0.9183

Entropy(Income=Low)
= -3/4 Log 3/4 -1/4 Log 1/4 = 0.8113

Gain(S,Income)
= 0.9400 - (4/14 [1] + 6/14 [0.9183] + 4/14 [0.8113])
= 0.029

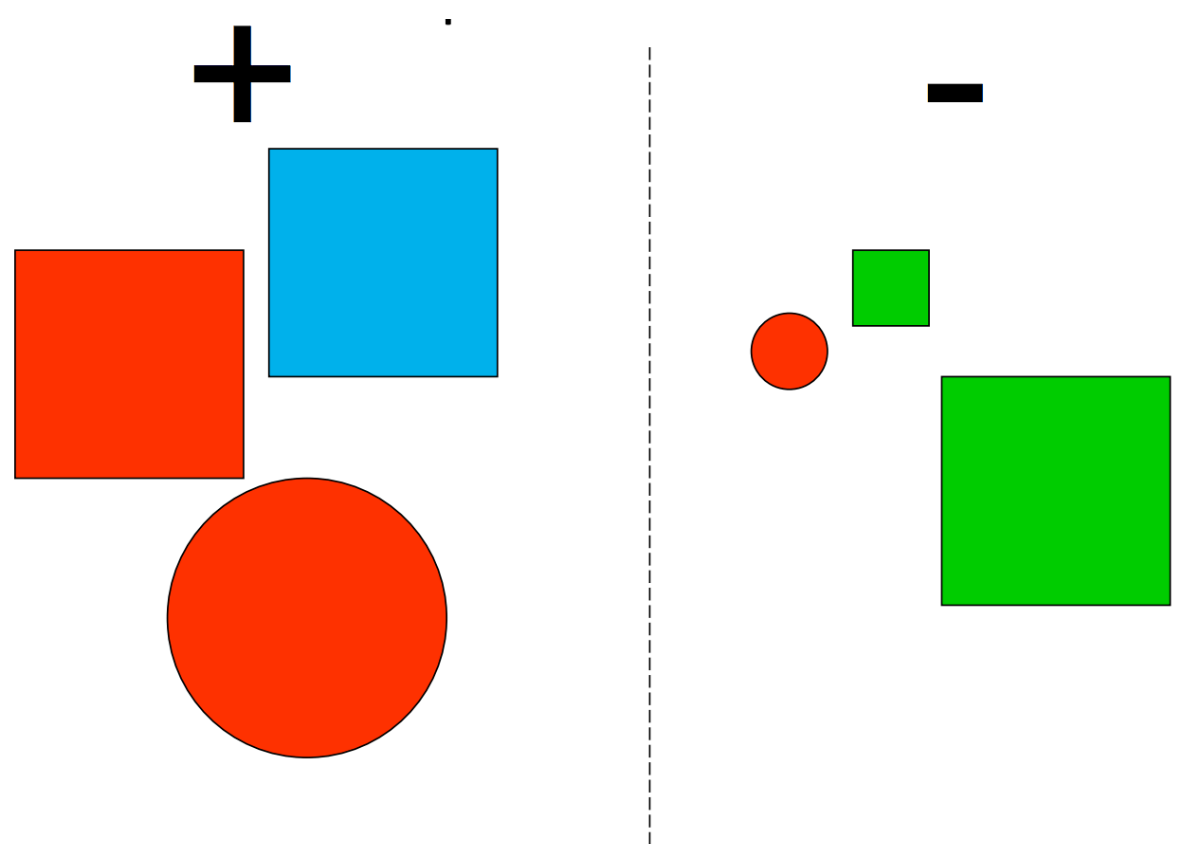
# EXAMPLE: CHOOSE THE ATTRIBUTE WITH LARGEST INFORMATION GAIN

- Features: color, shape, size
- What's the best feature to use at root?



# EXAMPLE: CHOOSE THE ATTRIBUTE WITH LARGEST INFORMATION GAIN

| Example | Color | Shape | Size | Class |
|---|---|---|---|---|
| 1 | Red | Square | Big | + |
| 2 | Blue | Square | Big | + |
| 3 | Red | Circle | Big | + |
| 4 | Red | Circle | Small | - |
| 5 | Green | Square | Small | - |
| 6 | Green | Square | Big | - |




- H(S) = -(0.5*log0.5+0.5*log0.5)=1
- Gain(S, Color) =1-0.5*(-0.67*log0.67-0.33*log0.33)-0.17*(-1*log1-0*log0)-0.33*(-1*log1-0*log0) = 0.54
- Gain(S, Shape) = 1- 0.67*(-0.5*log0.5-0.5*log0.5)-0.33*(-0.5*log0.5-0.5*log0.5)=0
- Gain(S, Size) = 1-0.67*(-0.75*log0.75-0.25*log0.25)-0.33*(-1*log1-0*log0)=0.46

# BUILDING TREE RECURSIVELY

**Buildtree**(examples, attributes)

/*examples: a list of training examples at the current node
attributes: a set of candidate attributes to place question on*/

**If** examples={} **then** return

**If** examples have the same label *y* **then** return a leaf node with label *y*

**If** attributes={} **then** return a leaf node with the majority label in examples

*A* = Best_attribute(examples, attributes) /*Suppose attribute *A* has *n* possible values*/

Create an internal node, *node(A)*, with *n* children

**For** attribute *A*'s *i*-th possible value *A(i)*:

The i-th child of node(A) = **Buildtree**({examples with its value on *A* being *A(i)*}, attributes-{*A*})

# DEALING WITH CONTINUOUS ATTRIBUTES

- Discretize the value of a continuous attribute into several intervals
  - Two bins for the continuous variable x: $x<=t$, $x>t$
  - $Gain(S, x, t)=Entropy(S)-|S_{x<=t}|*Entropy(S_{x<=t})/|S|-|S_{x>t}|*Entropy(S_{x>t})/|S|$
  - $Gain(S, x)=max_t\ Gain(S, x, t)$

# ADDITIONAL ATTRIBUTE SELECTION CRITERIA: GINI GAIN

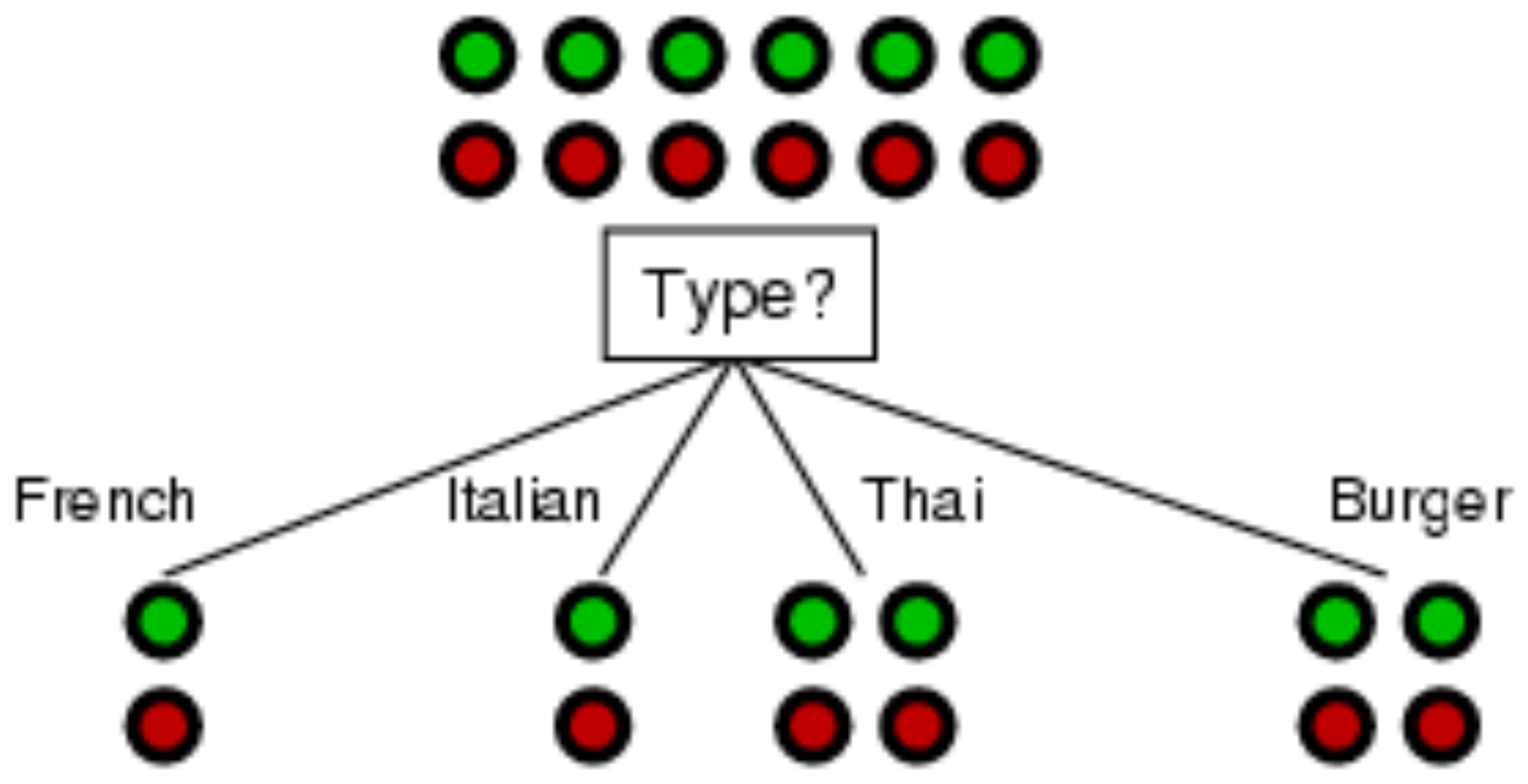
- Similar to information gain
- Uses gini index instead of entropy

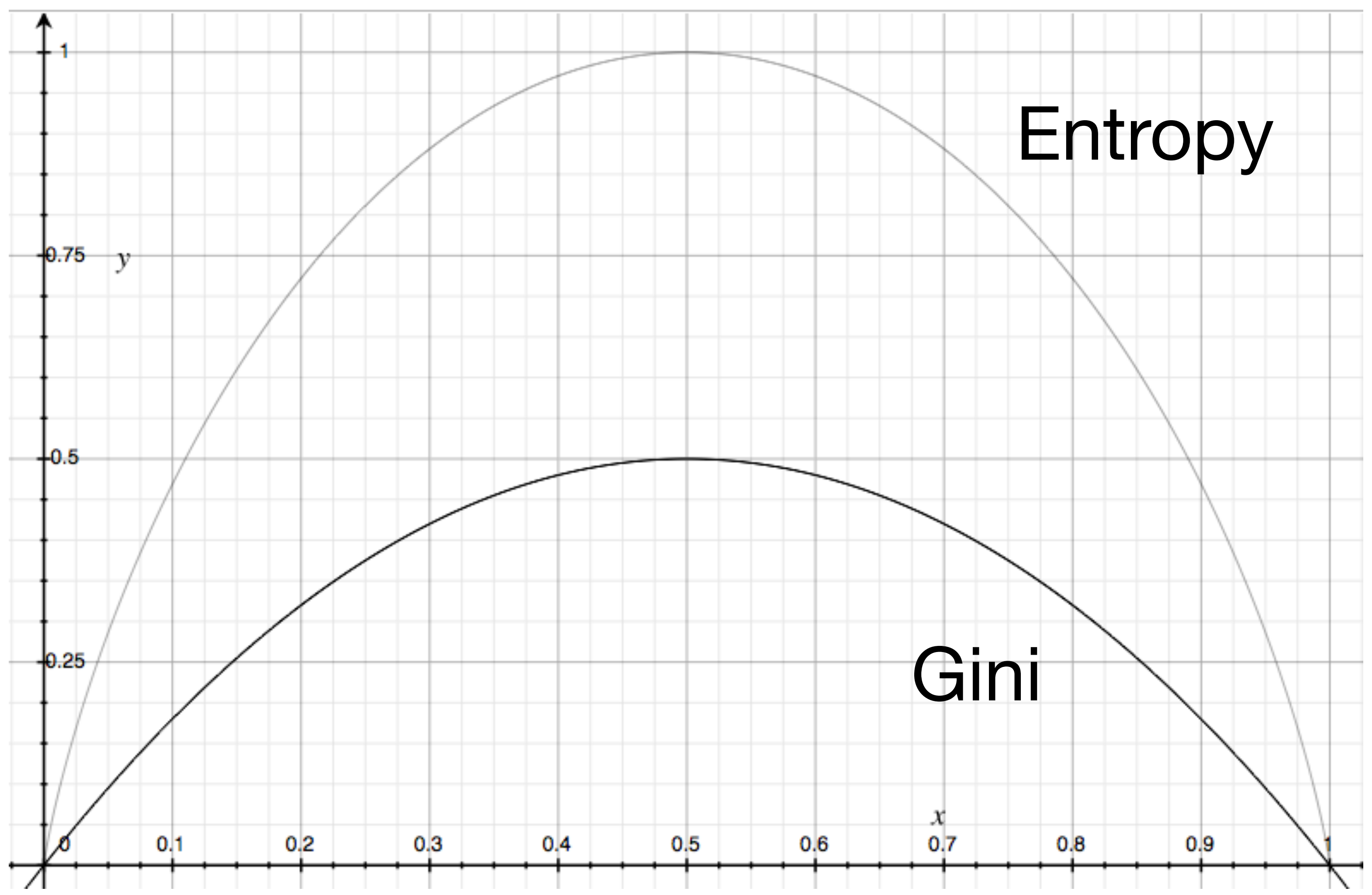
$$Gini(X) = 1 - \sum_{x} p(x)^2$$

- Measures decrease in gini index after split:

$$Gain(S, A) = Gini(S) - \sum_{v \in values(A)} \frac{|S_A|}{|S|} Gini(S_A)$$

# COMPARING INFORMATION GAIN TO GINI GAIN

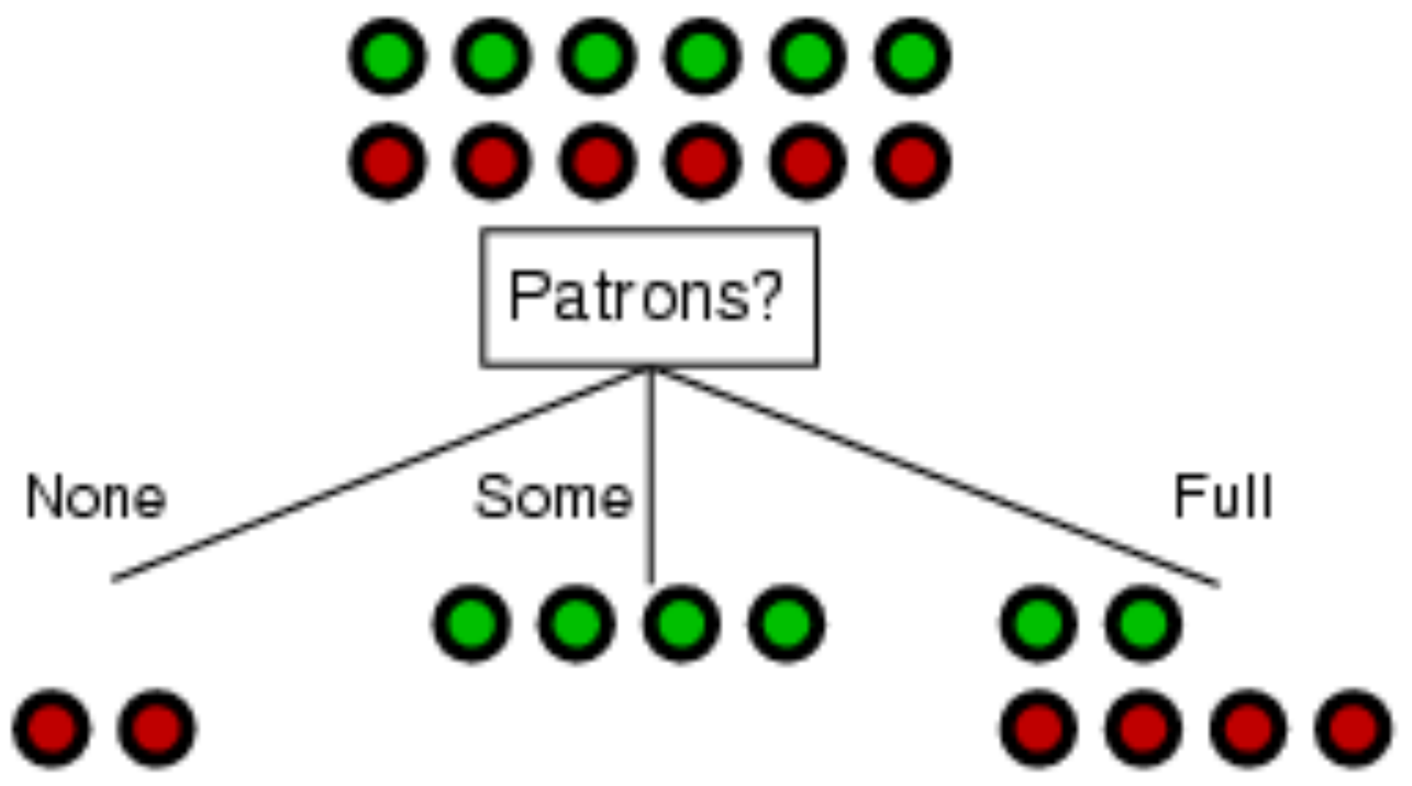


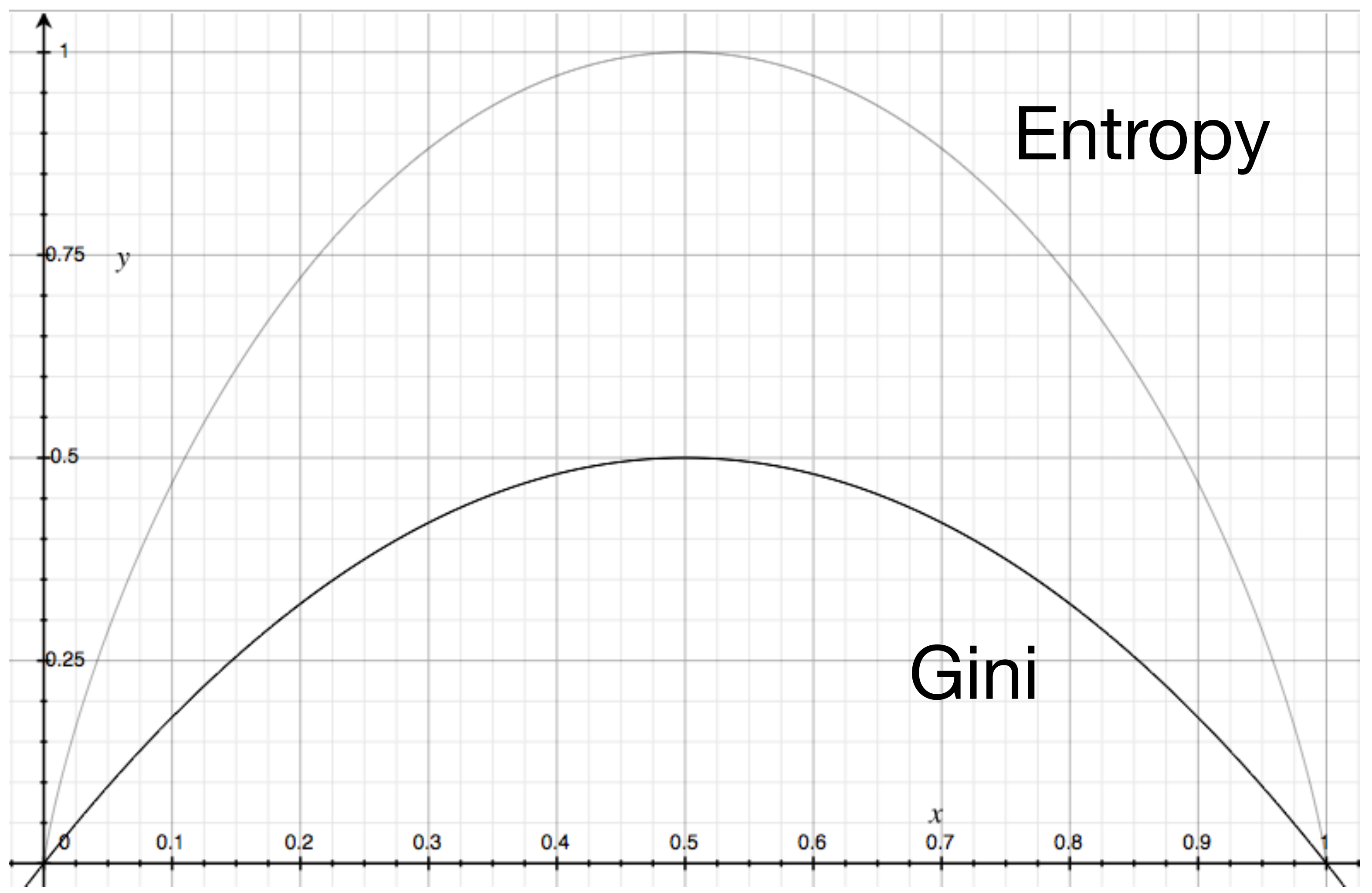




$$IG = 0$$

$$GG = 0$$

# COMPARING INFORMATION GAIN TO GINI GAIN




$$IG = 1.0 - \left[\frac{2}{12}\,0\right] - \left[\frac{4}{12}\,0\right] - \left[\frac{6}{12}\,0.919\right] = 0.541$$

$$GG = 0.5 - \left[\frac{2}{12}\,0\right] - \left[\frac{4}{12}\,0\right] - \left[\frac{6}{12}\,0.444\right] = 0.278$$

# ADDITIONAL ATTRIBUTE SELECTION CRITERIA: CHI-SQUARE SCORE

- Widely used to test independence between two categorical attributes (e.g., feature and class label)
- Considers counts in a contingency table and calculates the normalized squared deviation of observed (actual) values from expected (predicted) values

$$\chi^2 = \sum_{i=1}^{k} \frac{(o_i - e_i)^2}{e_i}$$

- Sampling distribution is known to be chi-square distributed, given that cell counts are above minimum thresholds

# CALCULATING EXPECTED VALUES FOR A CELL

$$\chi^2 = \sum_{i=1}^{k} \frac{(o_i - e_i)^2}{e_i}$$

Class

| Attribute | | + | - |
|---|---|---|---|
| | 0 | a | b |
| | 1 | c | d |

**N**

$$o_{(0,+)} = a$$

$$\begin{aligned} e_{(0,+)} &= p(A=0, C=+) \cdot N \\ &= p(A=0)p(C=+|A=0) \cdot N \\ &= p(A=0)p(C=+) \cdot N \qquad \text{(assuming independence)} \\ &= \left[\frac{a+b}{N}\right] \cdot \left[\frac{a+c}{N}\right] \cdot N \end{aligned}$$

# EXAMPLE CALCULATION

**Observed**

| | Buy | No buy |
|---|---|---|
| High | 2 | 2 |
| Med | 4 | 2 |
| Low | 3 | 1 |

**Expected**

| | Buy | No buy |
|---|---|---|
| High | 2.57 | 1.43 |
| Med | 3.86 | 2.14 |
| Low | 2.57 | 1.43 |

$$\chi^2 = \sum_{i=1}^{k} \frac{(o_i - e_i)^2}{e_i} = \left(\frac{(2-2.57)^2}{2.57}\right) + \left(\frac{(4-3.86)^2}{3.86}\right) + \left(\frac{(3-2.57)^2}{2.57}\right)$$

$$+ \left(\frac{(2-1.43)^2}{1.43}\right) + \left(\frac{(2-2.14)^2}{2.14}\right) + \left(\frac{(1-1.43)^2}{1.43}\right)$$

$$= 0.57$$

# WHEN TO STOP GROWING

- Full growth methods
  - There are no examples left
  - All examples at a node belong to the same class
  - There are no attributes left for further splits
- What impact does this have on the quality of the learned trees?
  - Trees **overfit** the training data and accuracy on testing data suffers

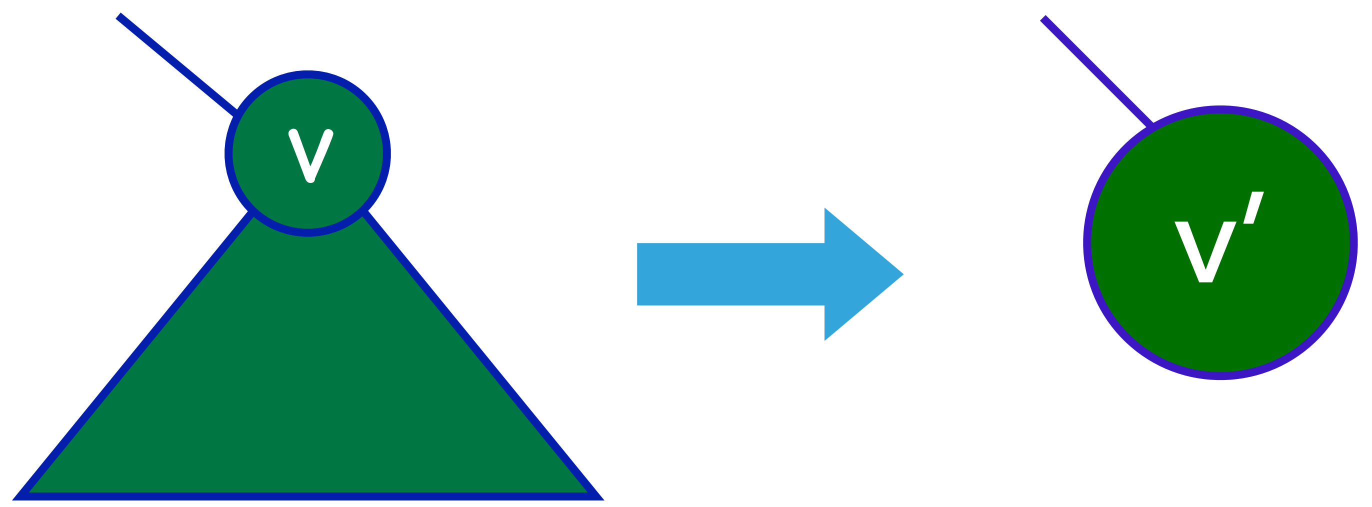
# OVERFITTING

- Consider a distribution $D$ of data representing a population and a sample $D_S$ drawn from $D$, which is used as training data
- Given a model space $M$, a score function $S$, and a learning algorithm that returns a model $m \in M$, the algorithm **overfits** the training data $D_S$ if:
  $\exists m' \in M$ such that $S(m, D_S) > S(m', D_S)$ but $S(m, D) < S(m', D)$
  - In other words, there is another model (m′) that is better on the entire distribution and if we had learned from the full data we would have selected it instead

# HOW TO AVOID OVERFITTING IN DECISION TREES

- Post-pruning
  - Separate the training data into a training set and a validation set (i.e., a pruning set).
  - Fully grow a tree
  - Use the pruning set to evaluate the utility of pruning (i.e. deleting) nodes from the tree
- Pre-pruning
  - Apply a statistical test to decide whether to expand a node
  - Add penalty terms in scoring functions to prefer trees with smaller sizes

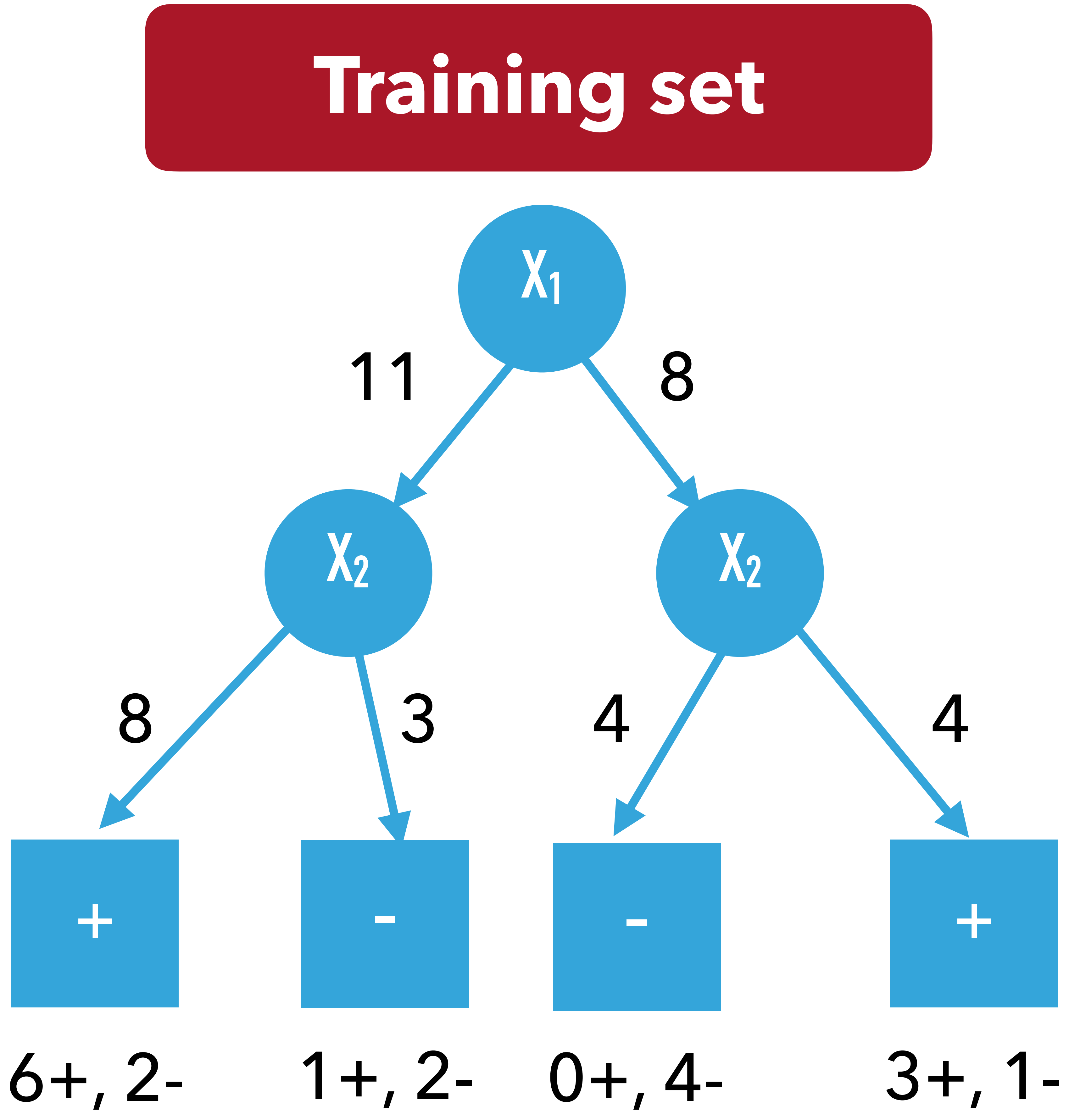
# POST-PRUNING METHOD: REDUCED ERROR PRUNING




- Grow a full tree *T* using the **training set**
- Let *v* be an internal node of the current tree *T*
- If we prune at *v* to create a new tree *T′*, in *T′*, the subtree rooted at *v* will be replaced by a leaf node *v′*, whose label is the majority label for all **training examples** fall under *v*
- Define the gain of pruning at *v* as, in the **pruning set**, # of misclassified examples under *v* (in *T*) - # of misclassified examples that in *v′* (in *T′*)
- Repeat: Prune at node with largest gain until only negative gain nodes remain

Source: www.ailab.si/blaz/predavanja/uisp/slides/uisp05-PostPruning.ppt

# REDUCED ERROR PRUNING EXAMPLE

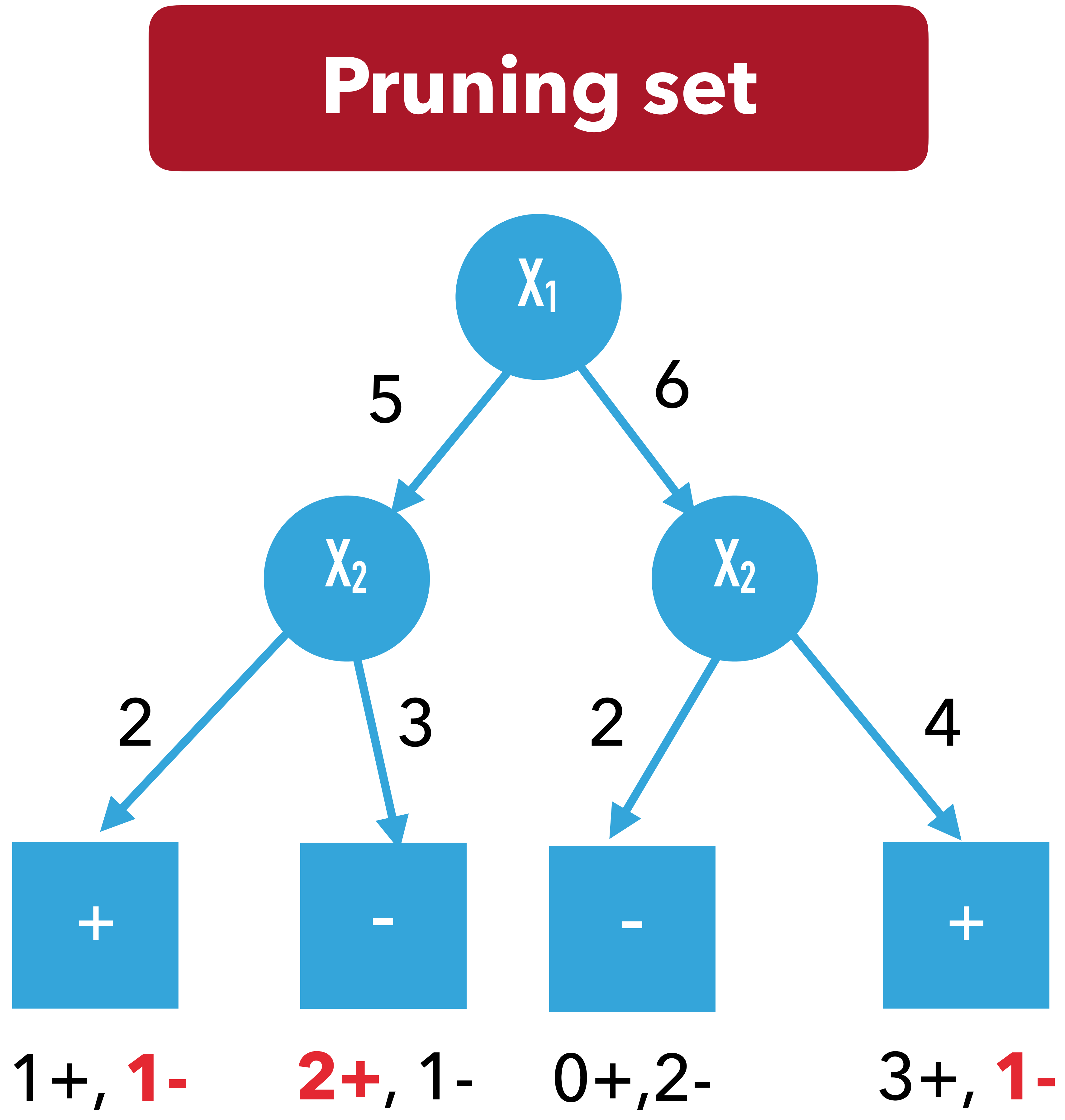



Gain at node $X_2$ (left): 3-2=1

Gain at node $X_2$ (right): 1-3=-2

Gain at node $X_1$: 4-5=-1

Prune at node $X_2$ (left)!



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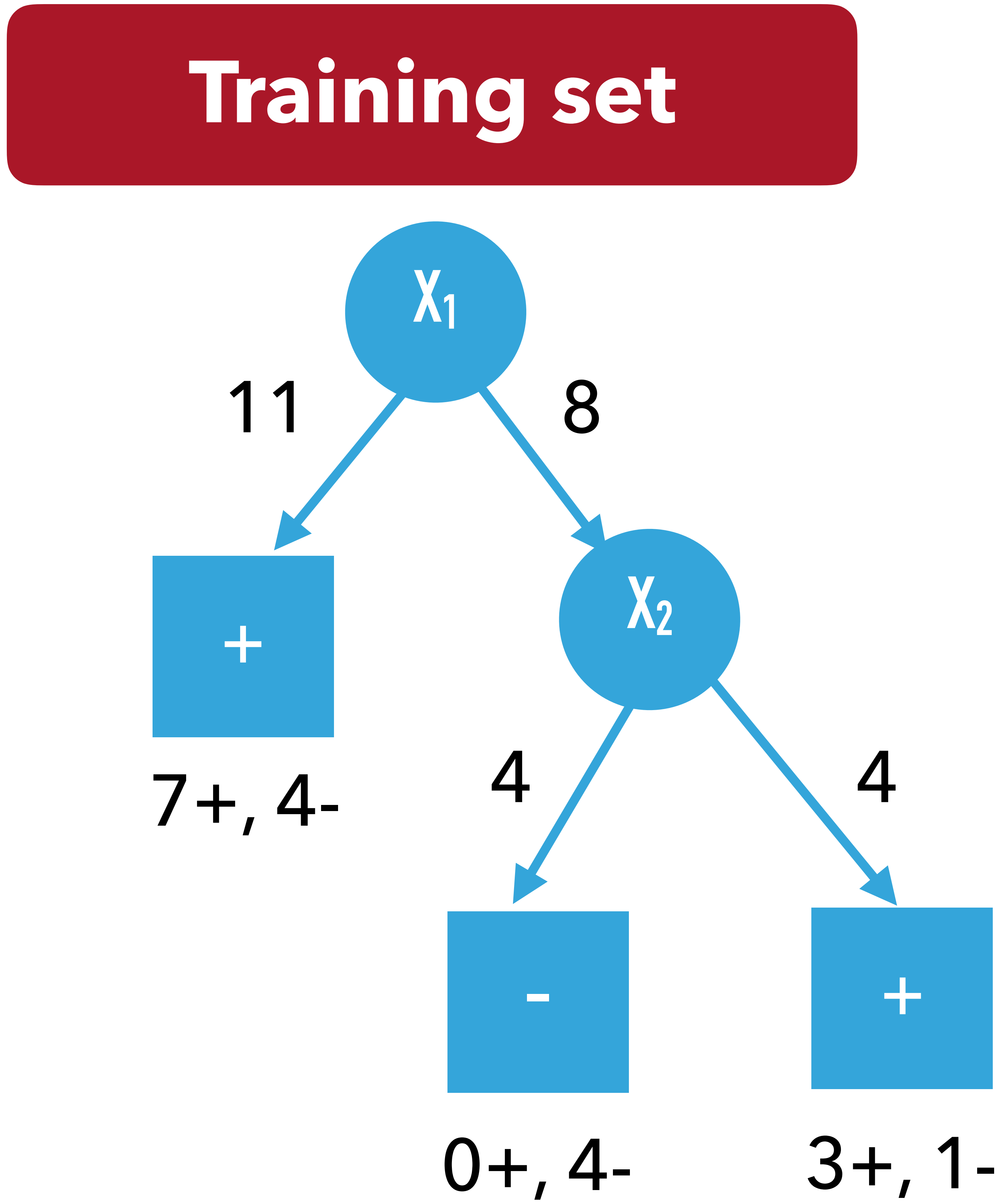


Gain at node $X_2$: 1-3=-2

Gain at node $X_1$: 3-5=-2

Done!