Decision Tree

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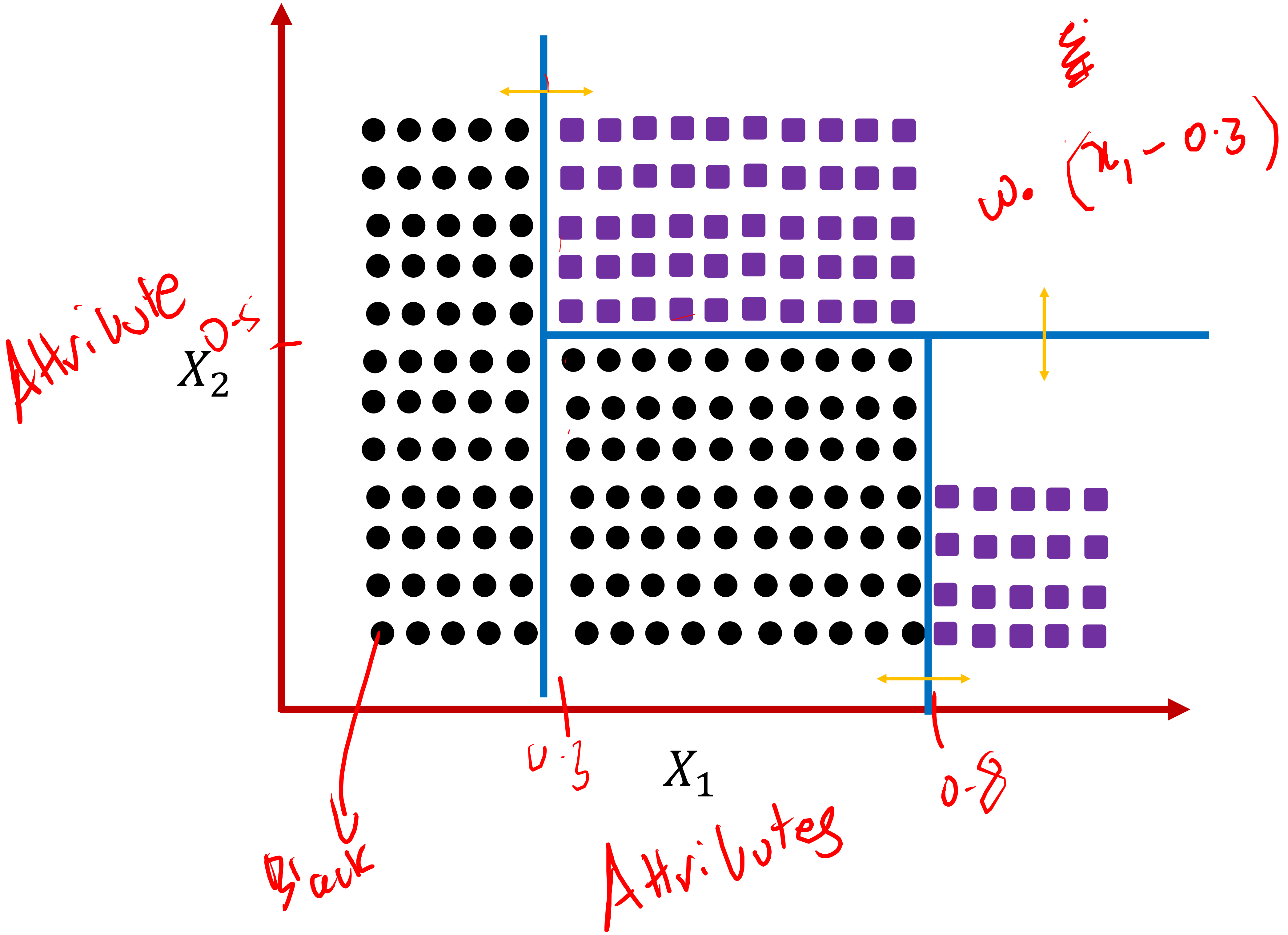
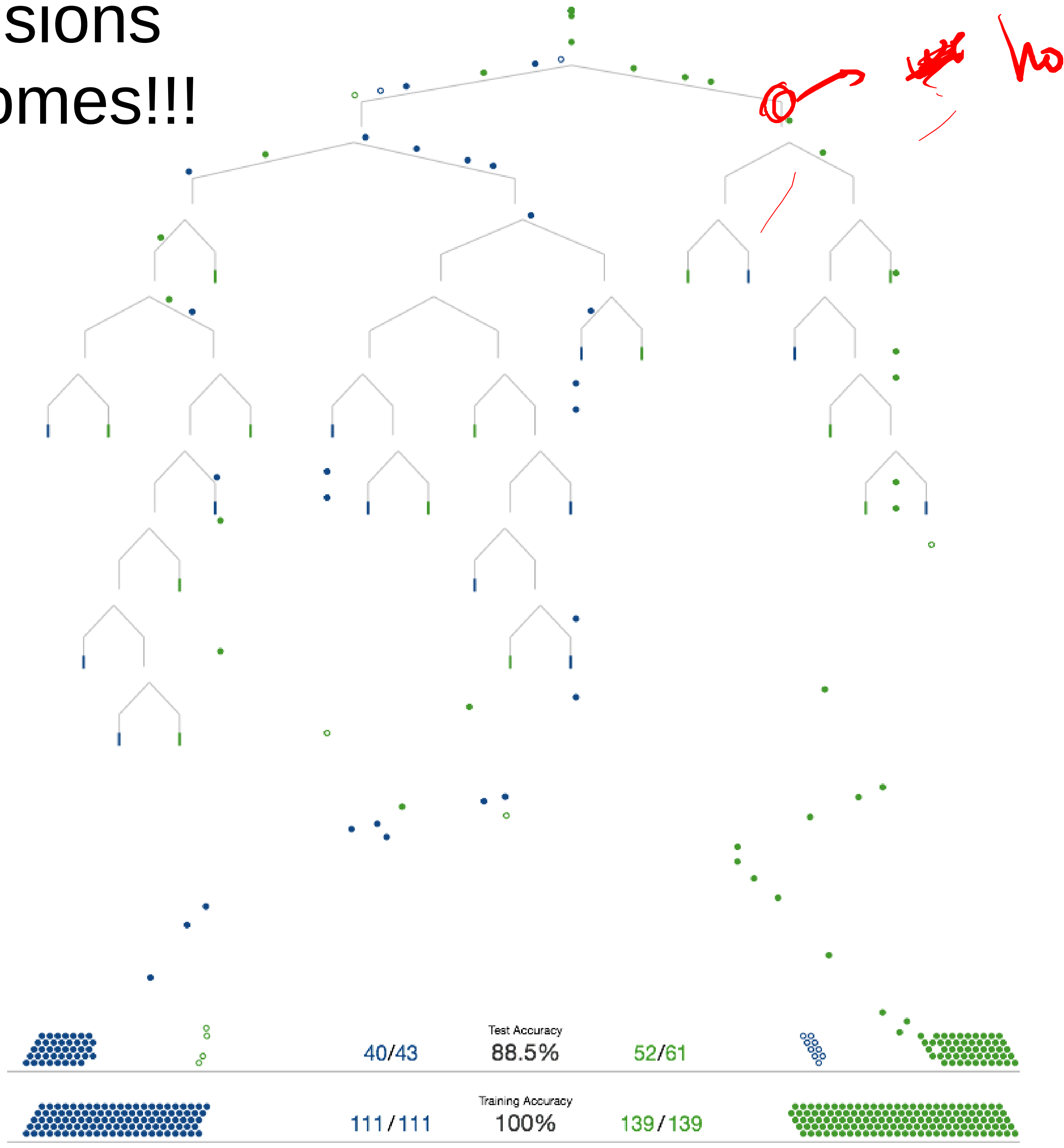
These slides are adopted from Polo, Vivek Srikumar, Mahdi Roozbahani and Chao Zhang.

Data



Visual Introduction to Decision Tree

Interpretable decisions for verifiable outcomes!!!



how many floors in NY?

[Building a tree to distinguish homes in New York from homes in San Francisco]

Decision Tree: Example (2)

	O	T	H	W	Play?
1	S	H	H	W	-
2	S	H	H	S	-
3	O	H	H	W	+
4	R	M	H	W	+
5	R	C	N	W	+
6	R	C	N	S	-
7	O	C	N	S	+
8	S	M	H	W	-
9	S	C	N	W	+
10	R	M	N	W	+
11	S	M	N	S	+
12	O	M	H	S	+
13	O	H	N	W	+
14	R	M	H	S	-

Outlook: Sunny, Overcast, Rainy

Temperature: Hot, Medium, Cool

Humidity: High, Normal, Low

Wind: Strong, Weak

Will I play tennis today?

Decision trees (DT)

play vs ~~not~~ ! play

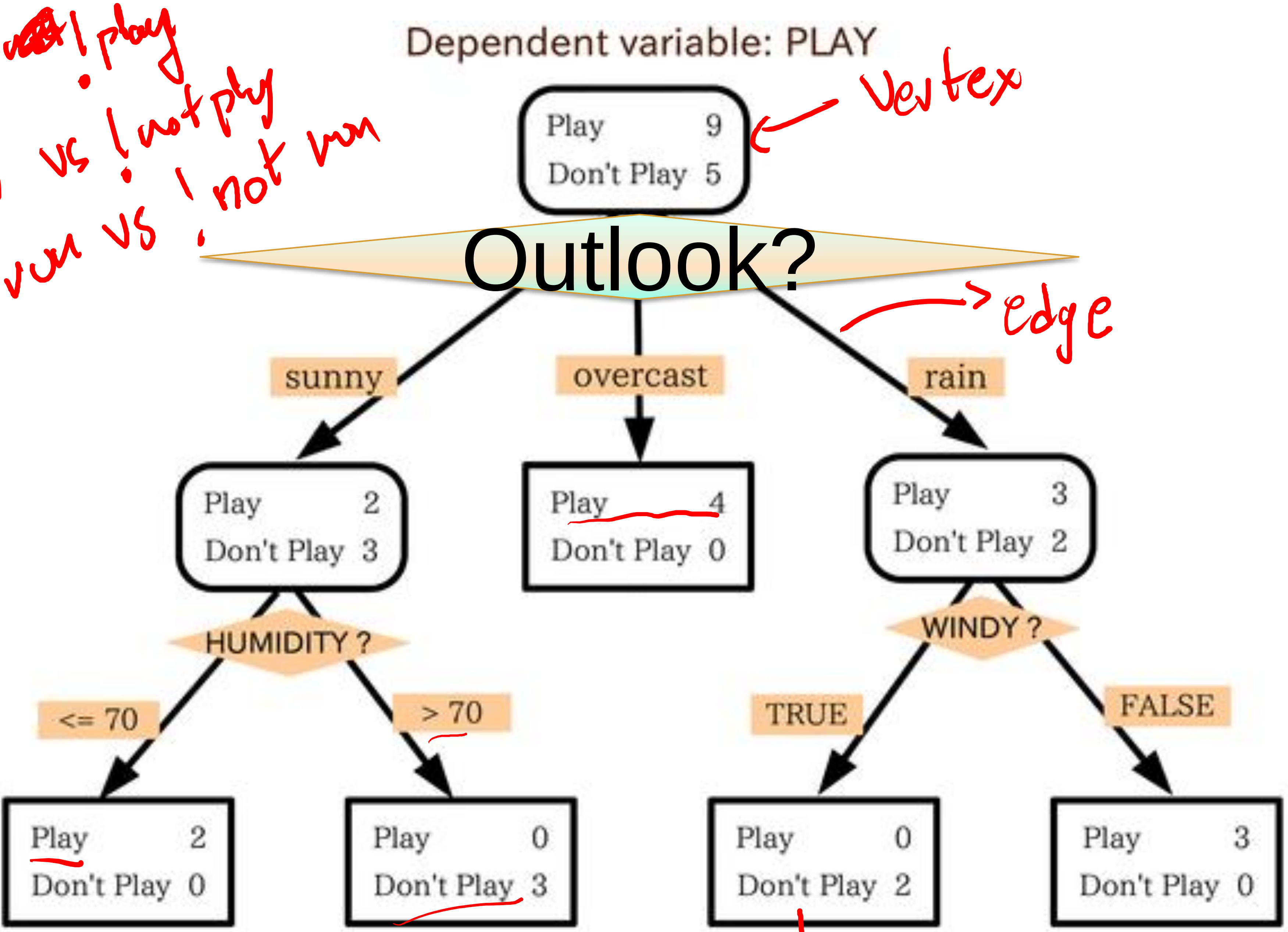
not play vs ! not play

go for run vs ! not run

play

not play

go for a run



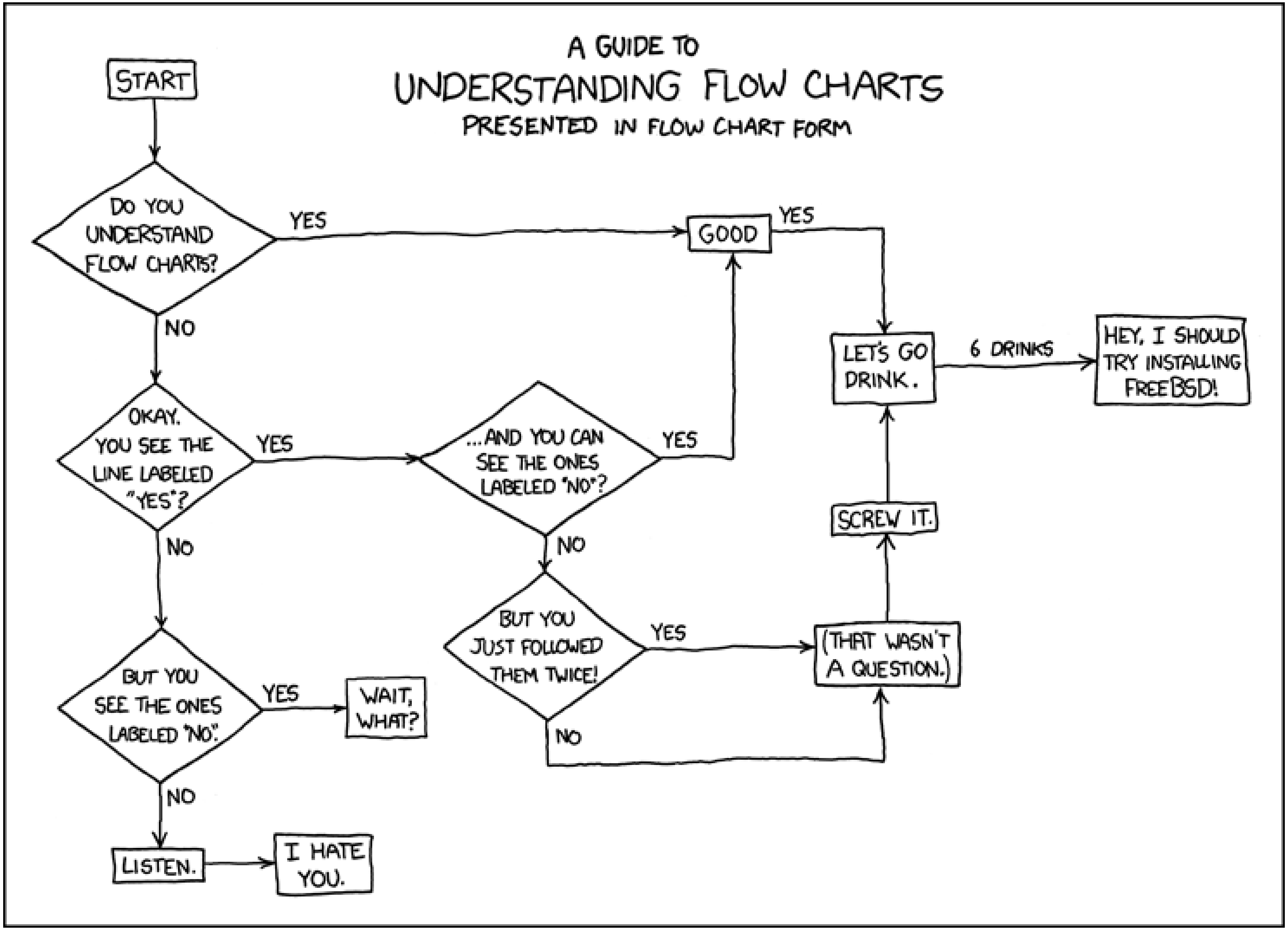
leaf node

The classifier:

$f_T(x)$: majority class in the leaf in the tree T containing x

Model parameters: The tree structure and size

Flow charts - xkcd



Decision trees

Pieces:

1. Find the best attribute to split on
2. Find the best split on the chosen attribute
3. Decide on when to stop splitting

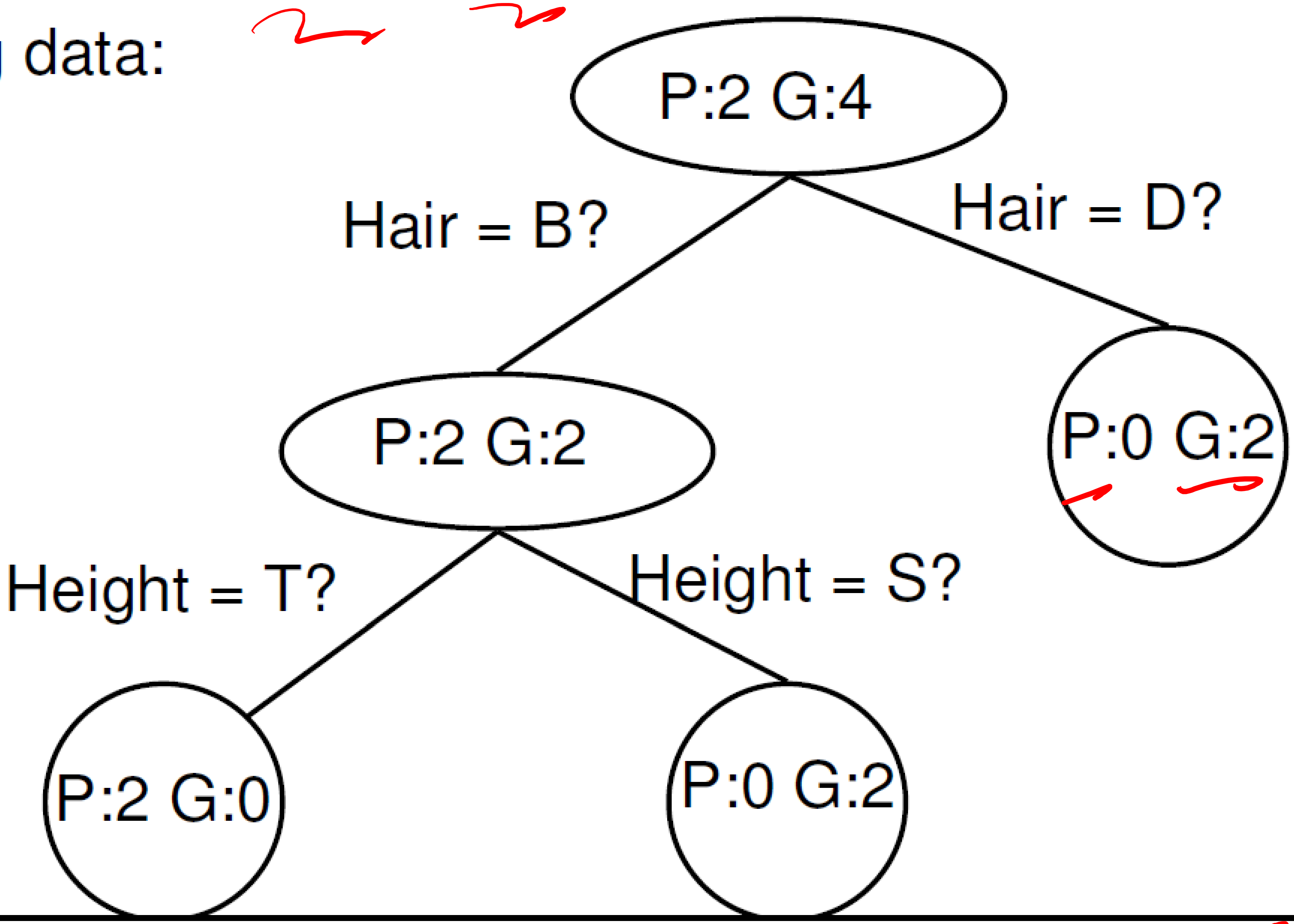
Categorical or Discrete attributes

- Three variables:
  - Hair = {blond, dark} → not an ordered set
  - Height = {tall,short}
  - Country = {Gromland, Polvia}

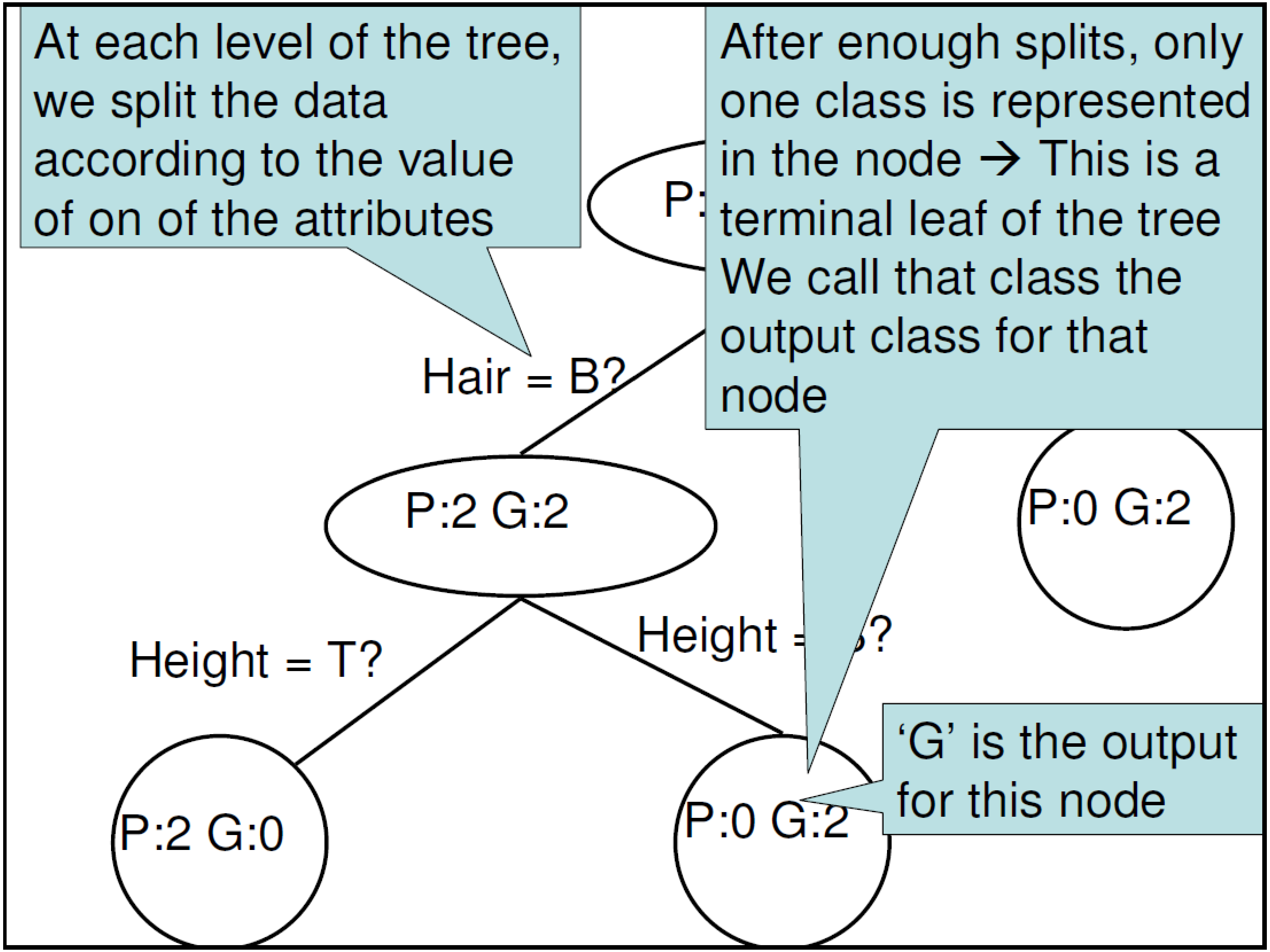
Label

Training data:

(B,T,P)
(B,T,P)
(B,S,G)
(D,S,G)
(D,T,G)
(B,S,G)



ordered set → [0:10] (5<6?)

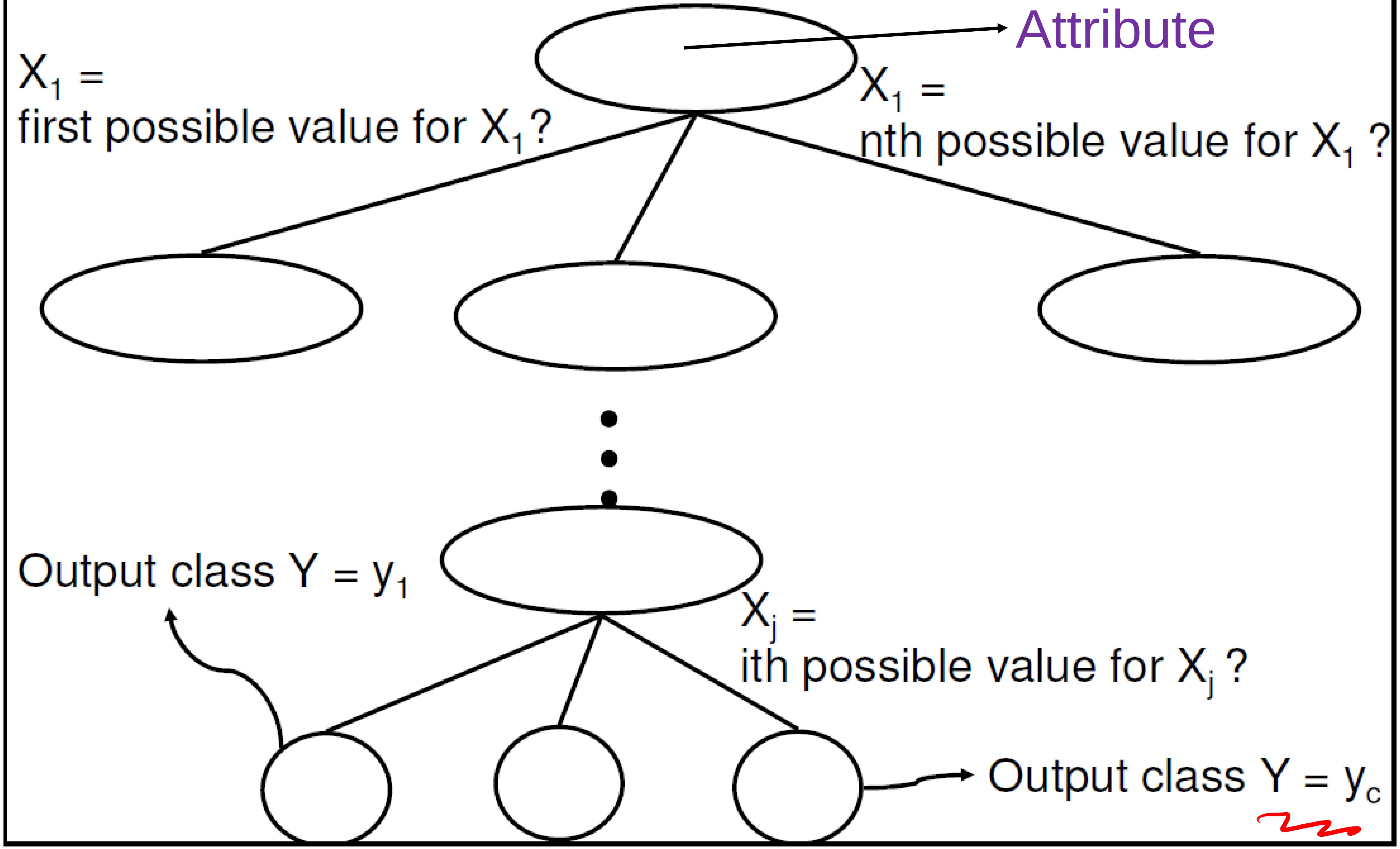


At each level of the tree, we split the data according to the value of on of the attributes

After enough splits, only one class is represented in the node → This is a terminal leaf of the tree We call that class the output class for that node

'G' is the output for this node

General Decision Tree (Discrete Attributes)



Attribute

X_1 = first possible value for X_1?

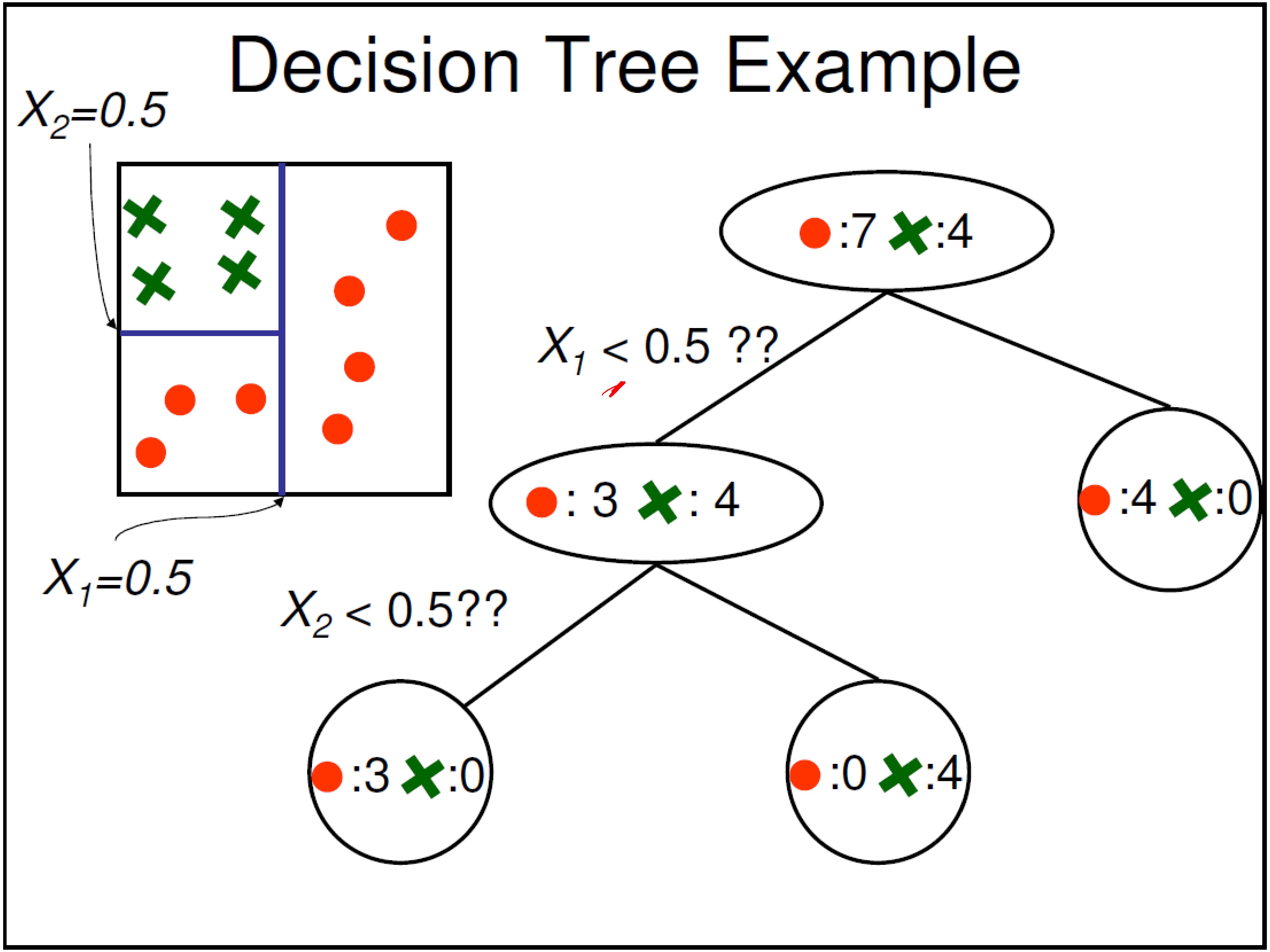
X_1 = nth possible value for X_1 ?

X_j = ith possible value for X_j ?

Output class $Y = y_1$

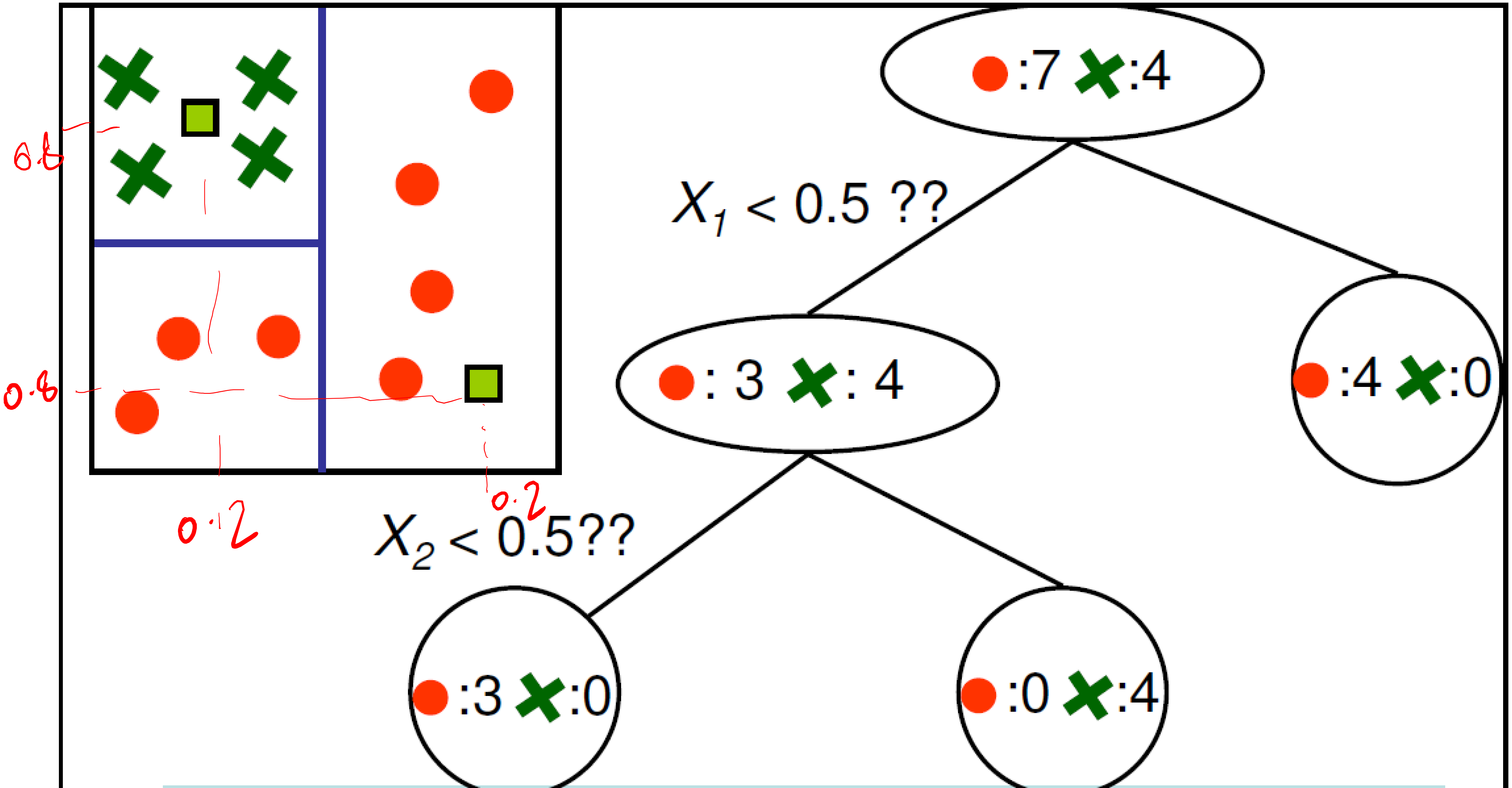
Output class $Y = y_c$

Continuous attributes or ordered attributes



Decision Tree Example

Test data

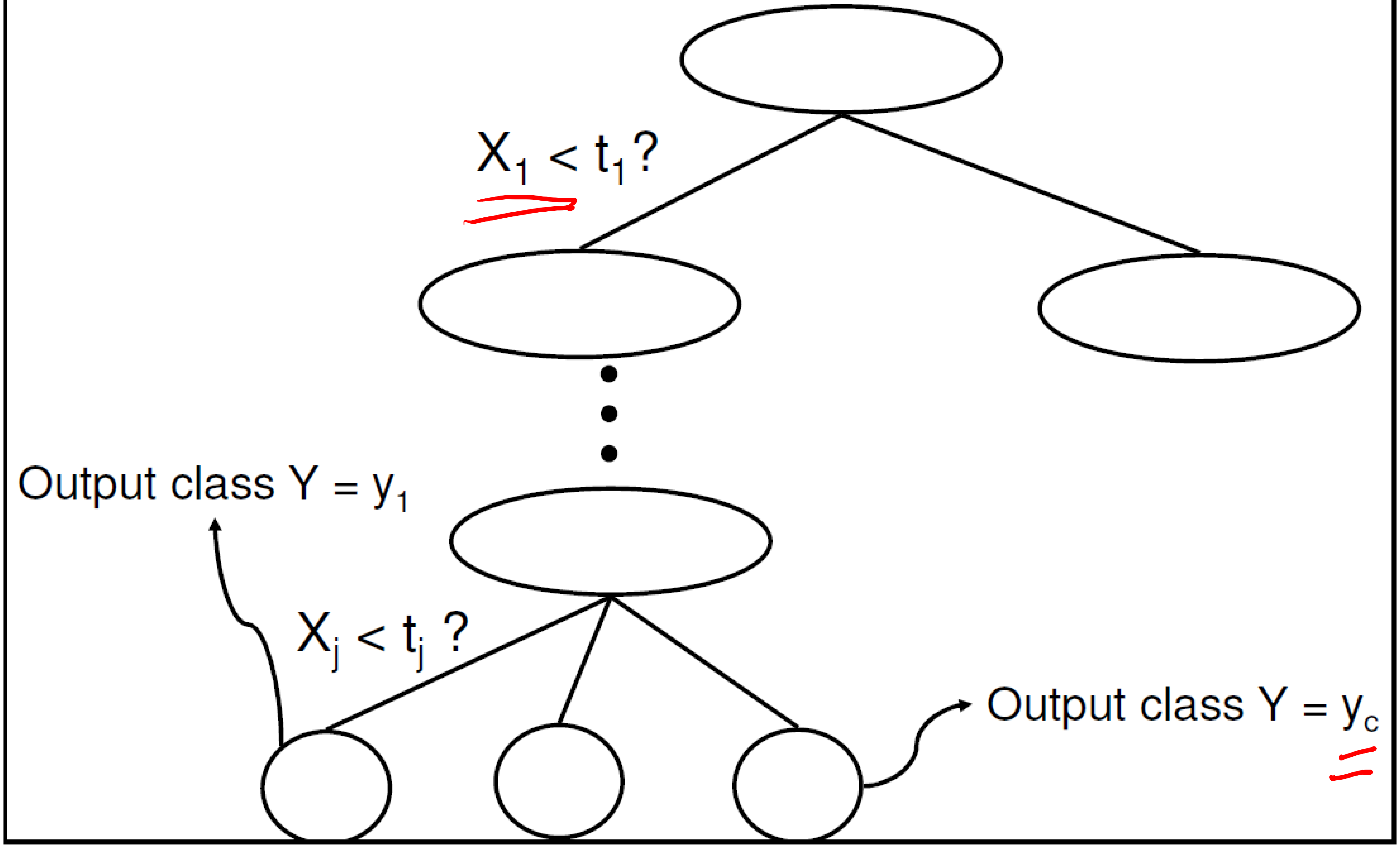


The class of a new input can be classified by following the tree all the way down to a leaf and by reporting the output of the leaf. For example:

(0.2,0.8) is classified as ✖

(0.8,0.2) is classified as ●

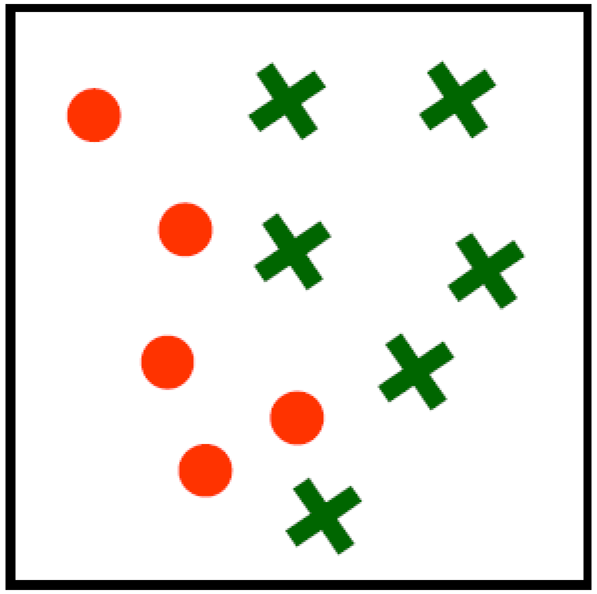
General Decision Tree (Continuous Attributes)



Basic Questions

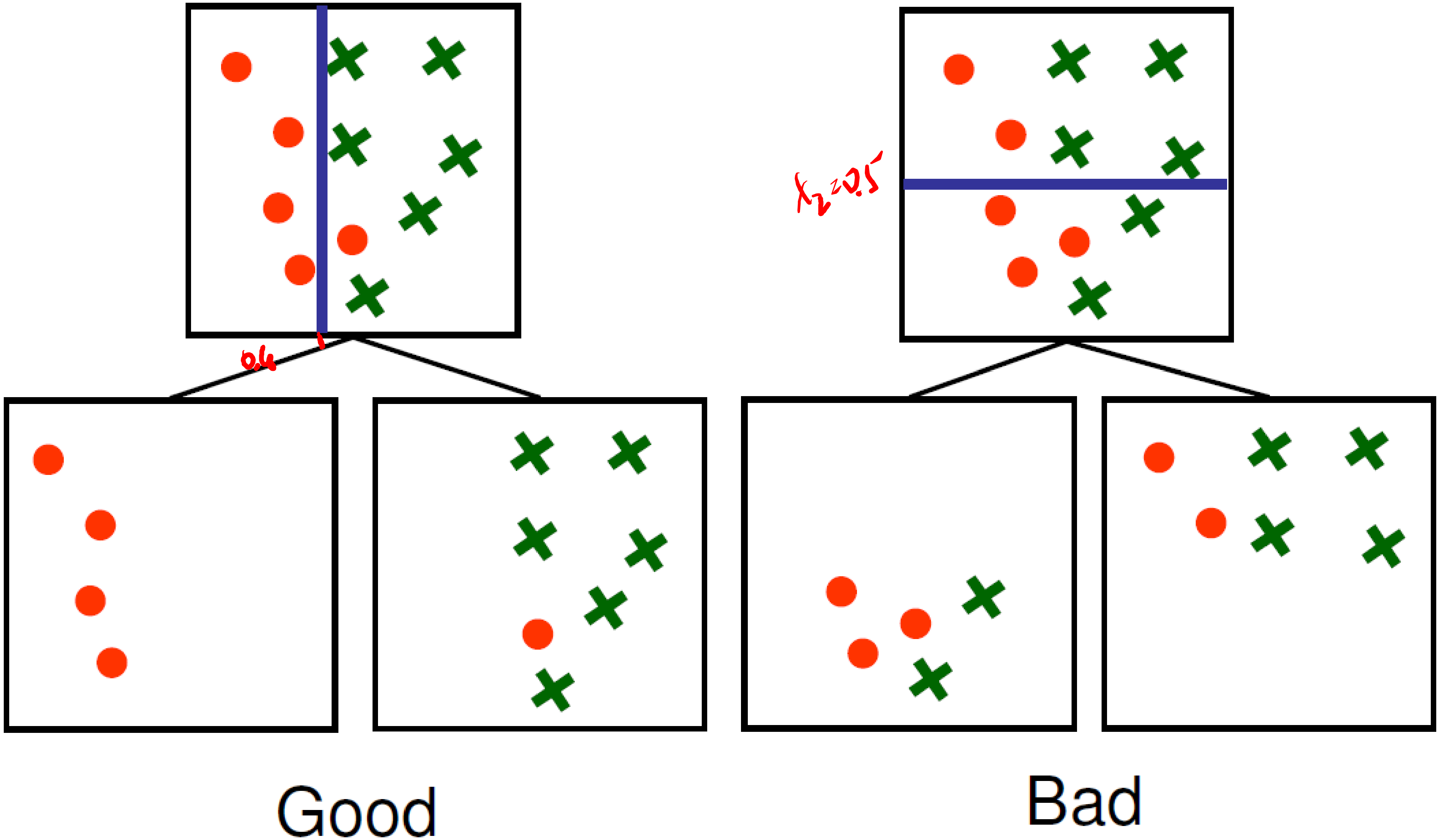
- How to choose the attribute/value to split on at each level of the tree?
- When to stop splitting? When should a node be declared a leaf?
- If a leaf node is impure, how should the class label be assigned?
- If the tree is too large, how can it be pruned?

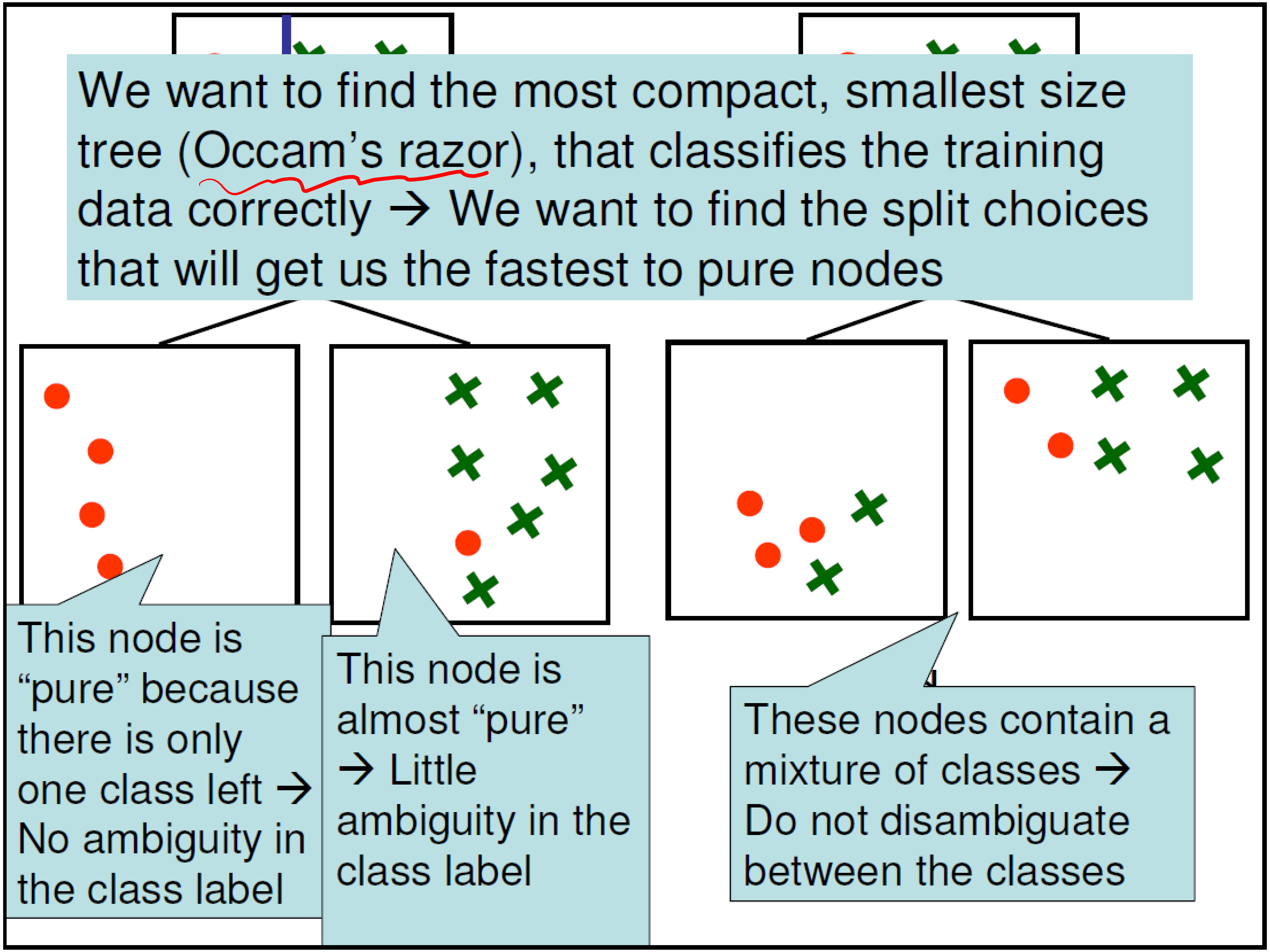
How to choose the attribute/value to split on at each level of the tree?



- Two classes (red circles/green crosses)
- Two attributes: X_1 and X_2
- 11 points in training data
- Idea → Construct a decision tree such that the leaf nodes predict correctly the class for all the training examples

How to choose the attribute/value to split on at each level of the tree?





We want to find the most compact, smallest size tree (Occam's razor), that classifies the training data correctly → We want to find the split choices that will get us the fastest to pure nodes

This node is "pure" because there is only one class left → No ambiguity in the class label

This node is almost "pure" → Little ambiguity in the class label

These nodes contain a mixture of classes → Do not disambiguate between the classes

Information Content

Coin flip

C_{1H}	0
C_{1T}	6

P(C_{1H}) = 0/6 = 0

P(C_{1T}) = 6/6 = 1

C_{2H}	1
C_{2T}	5

P(C_{2H}) = 1/6

P(C_{2T}) = 5/6

C_{3H}	2
C_{3T}	4

P(C_{3H}) = 2/6

P(C_{3T}) = 4/6

Which coin will give us the purest information?

Entropy ~ Uncertainty

Lower uncertainty, higher information gain

$$H(X) = -\sum_{i=1}^{N} P(x=i)\log_2 P(x=i) \rightarrow \sum_{i=1}^{N} p(x_i)\log_2\left(\frac{1}{p(x_i)}\right)$$

Entropy$_1$ = $-\overset{\to 0}{\cancel{0}}$ log 0 – 1 $\overset{\to 0}{\cancel{\log}}$ 1 = – 0 – 0 = 0

Entropy$_2$ = – (1/6) $\log_2$ (1/6) – (5/6) $\log_2$ (5/6) = 0.65

Entropy$_3$ = – (2/6) $\log_2$ (2/6) – (4/6) $\log_2$ (4/6) = 0.92

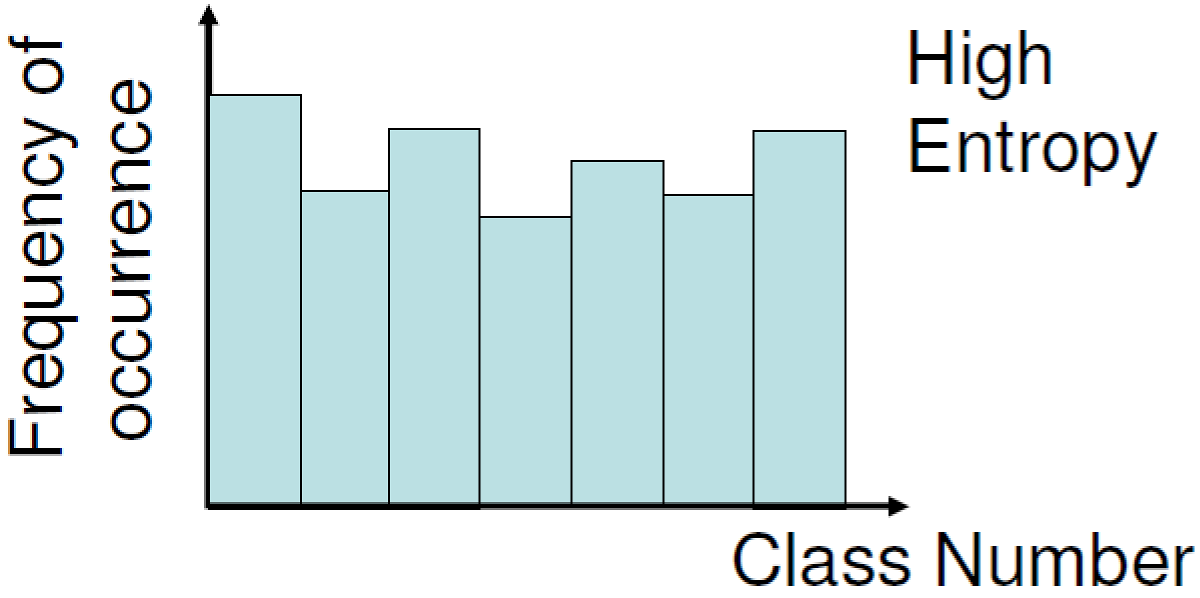
Entropy

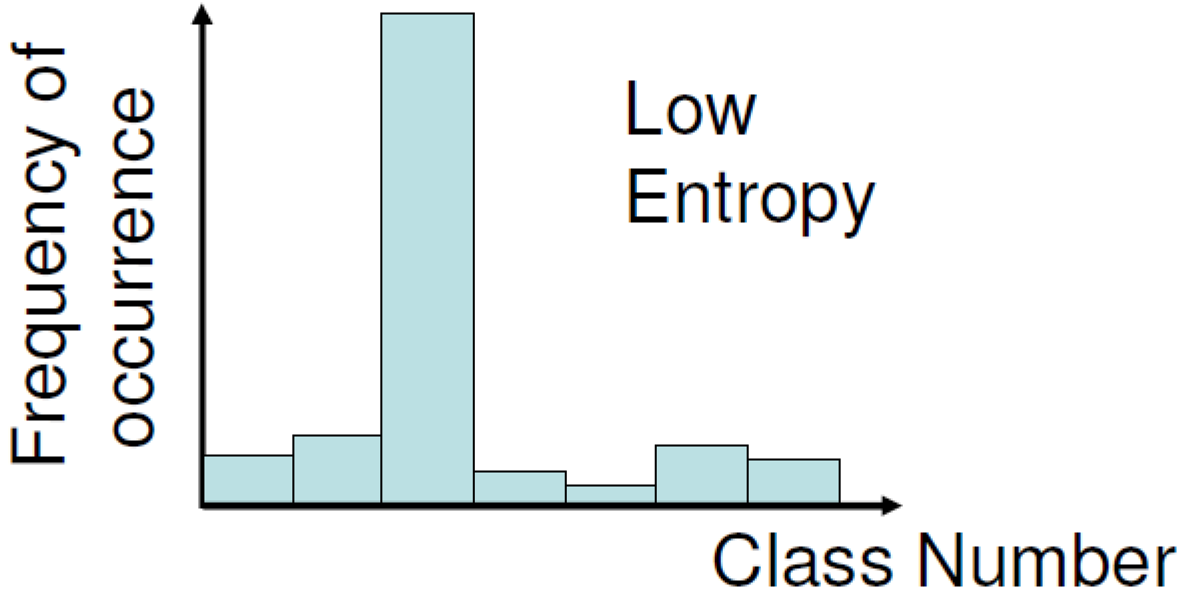
- In general, the average number of bits necessary to encode *n* values is the entropy:

$$\boxed{H = -\sum_{i=1}^{n} P_i \log_2 P_i}$$

- P_i = probability of occurrence of value *i*
  - High entropy → All the classes are (nearly) equally likely
  - Low entropy → A few classes are likely; most of the classes are rarely observed

Entropy

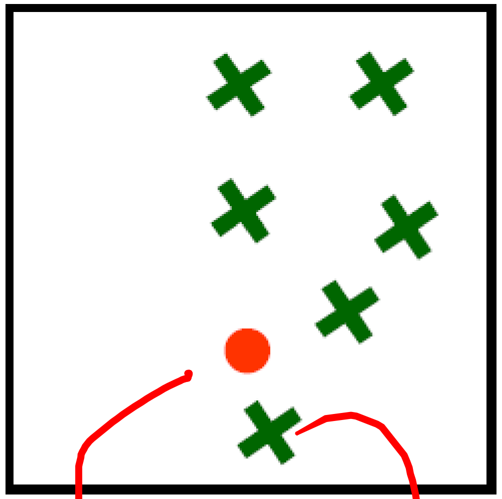




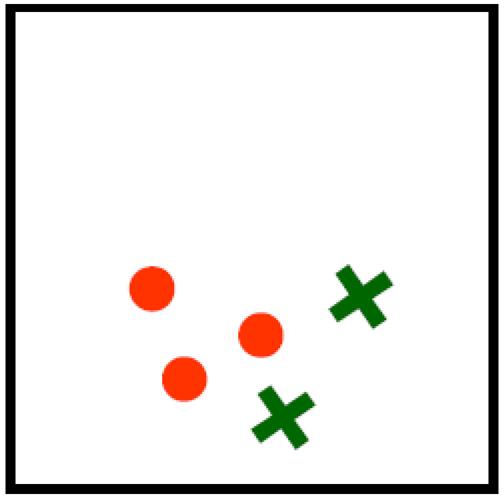
The entropy captures the degree of “purity” of the distribution

Example Entropy Calculation

①



②



red circle → $N_A = 1$

$N_B = 6$ ← green cross

$N_A = 3$

$N_B = 2$

$p_A = N_A/(N_A+N_B) = 1/7$

$p_B = N_B/(N_A+N_B) = 6/7$

$p_A = N_A/(N_A+N_B) = 3/5$

$p_B = N_B/(N_A+N_B) = 2/5$

$H_1 = -p_A \log_2 p_A - p_B \log_2 p_B$

$= 0.59$

$H_2 = -p_A \log_2 p_A - p_B \log_2 p_B$

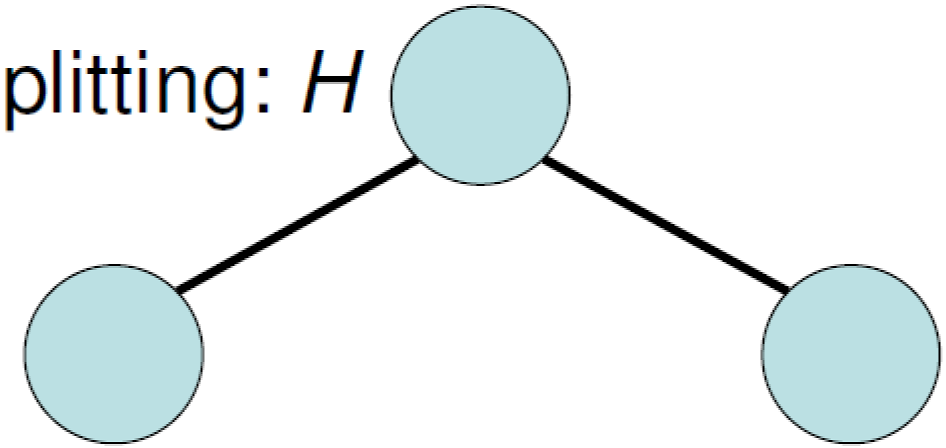
$= 0.97$

$H_1 < H_2$ => (2) less pure than (1)

low entropy is important
↓
Occam's razor

Conditional Entropy

Entropy before splitting: H



After splitting, a fraction P_L of the data goes to the left node, which has entropy H_L

After splitting, a fraction P_R of the data goes to the left node, which has entropy H_R

The average entropy after splitting is:

$$\boxed{H_L \text{x } P_L + H_R \text{x } P_R}$$

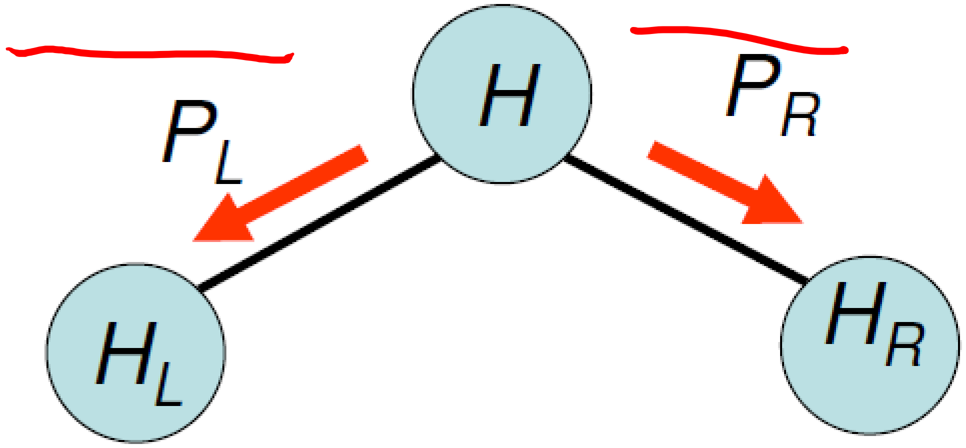
$\sum P_i H_i$

Entropy of left node

"Conditional Entropy"

Probability that a random input is directed to the left node

Information Gain



We want nodes as pure as possible

→We want to reduce the entropy as much as possible

→ We want to maximize the difference between the entropy of the parent node and the expected entropy of the children

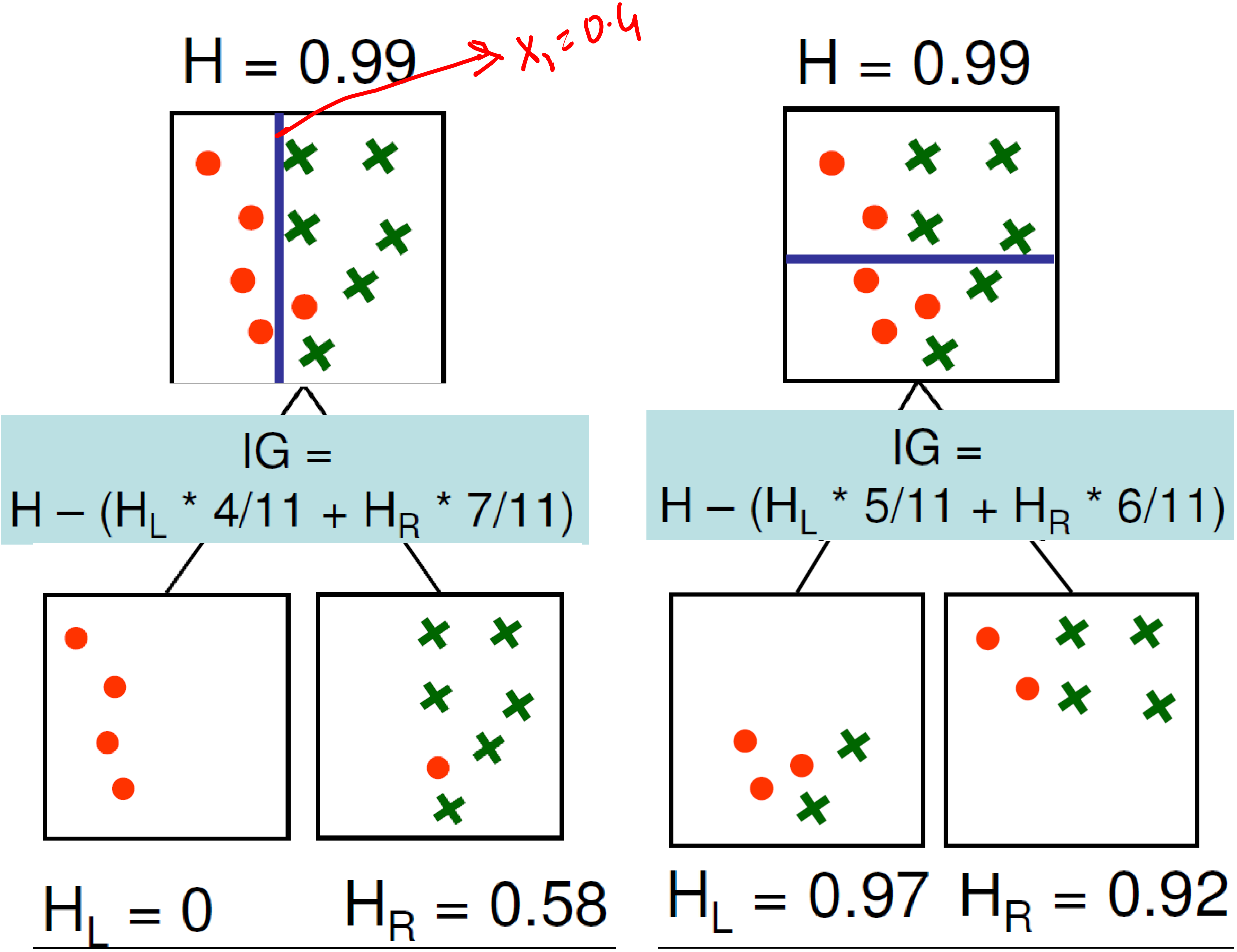
Information Gain (IG) = Amount by which the ambiguity is decreased by splitting the node

Maximize:

$$\boxed{IG = H - (H_L \text{x } P_L + H_R \text{x } P_R)}$$

Notations

- Entropy: $H(Y)$ = Entropy of the distribution of classes at a node
- Conditional Entropy:
  - *Discrete*: $H(Y|X_j)$ = Entropy after splitting with respect to variable *j*
  - *Continuous*: $H(Y|X_j,t)$ = Entropy after splitting with respect to variable *j* with threshold *t*
- Information gain:
  - *Discrete*: $IG(Y|X_j) = H(Y) - H(Y|X_j)$ = Entropy after splitting with respect to variable *j*
  - *Continuous*: $IG(Y|X_j,t) = H(Y) - H(Y|X_j,t)$ = Entropy after splitting with respect to variable *j* with threshold *t*



$H = 0.99$

$\rightarrow x_1 = 0.4$

IG =

$H - (H_L * 4/11 + H_R * 7/11)$

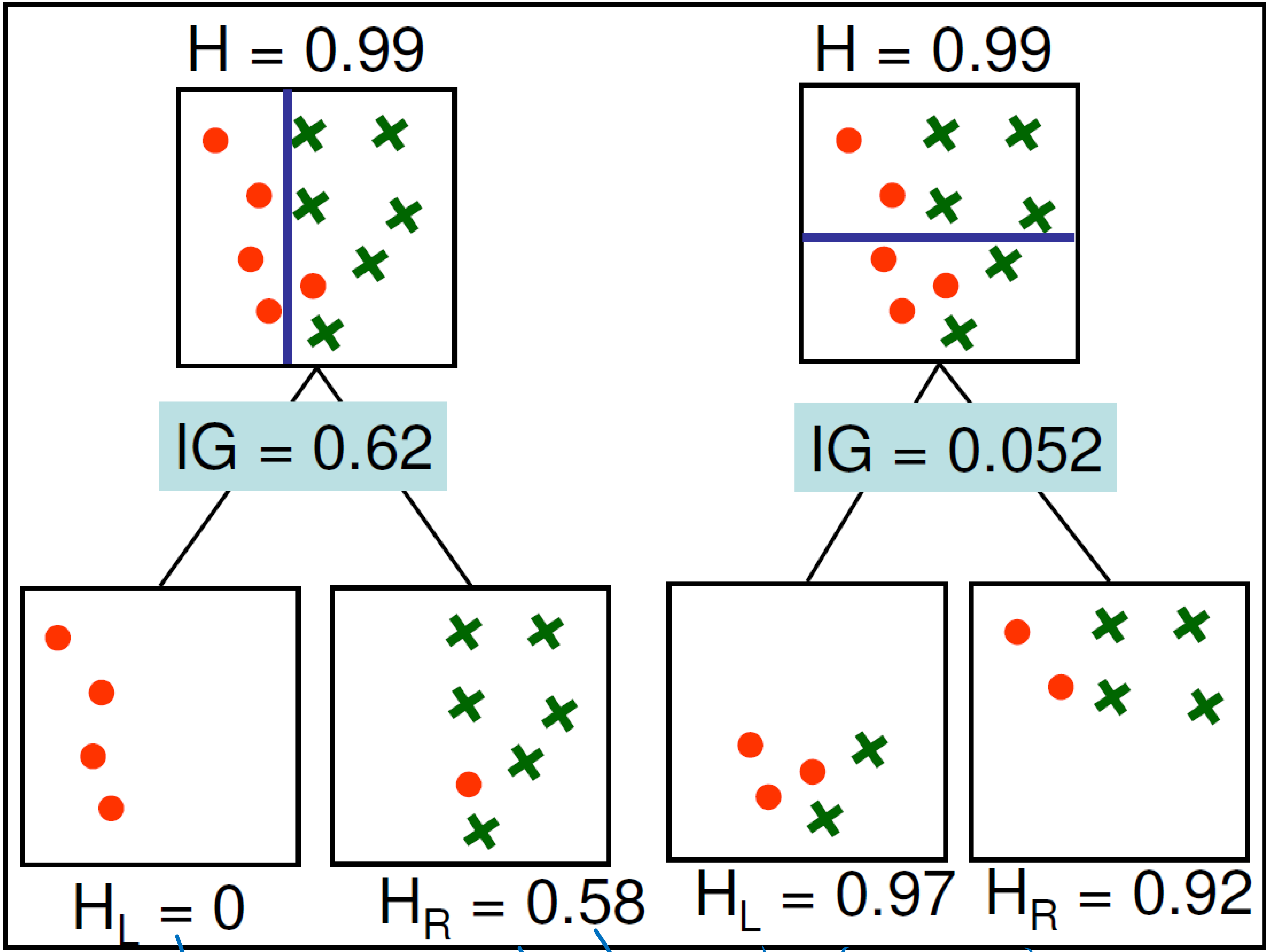
$H_L = 0$ $H_R = 0.58$

$H = 0.99$

IG =

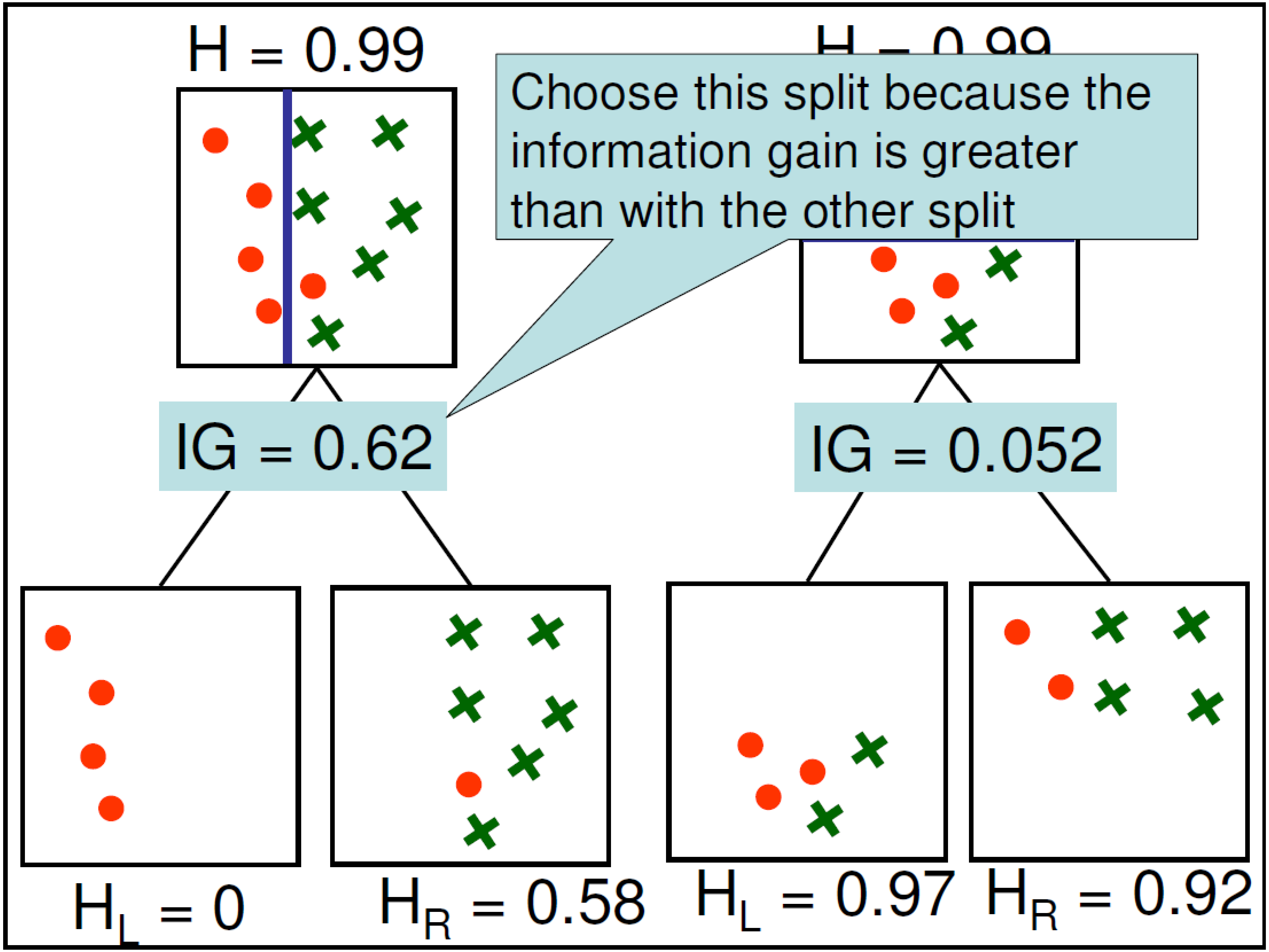
$H - (H_L * 5/11 + H_R * 6/11)$

$H_L = 0.97$ $H_R = 0.92$



$\sum_i P(x_i) \log_2(1/P(x_i))$

$1/7 \cdot \log_2(7/1) + 6/7 \log_2(7/6)$



H = 0.99

H = 0.99

Choose this split because the information gain is greater than with the other split

IG = 0.62

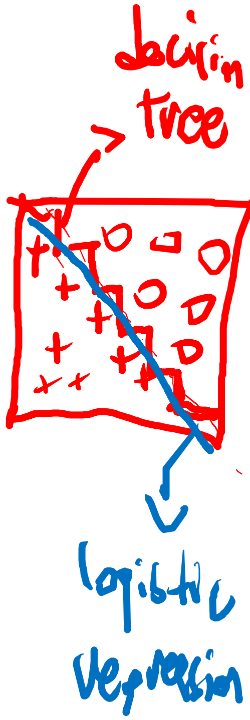
IG = 0.052

H_L = 0

H_R = 0.58

H_L = 0.97

H_R = 0.92



Announcements

- Touchpoint deliverables due today. Video + PPT
- Touchpoint next class. Individual BlueJeans calls with mentors.
- Please make sure to attend your touchpoints for feedback!!!
- Physical touchpoint survey needed back today
- Questions??

Decision Tree:

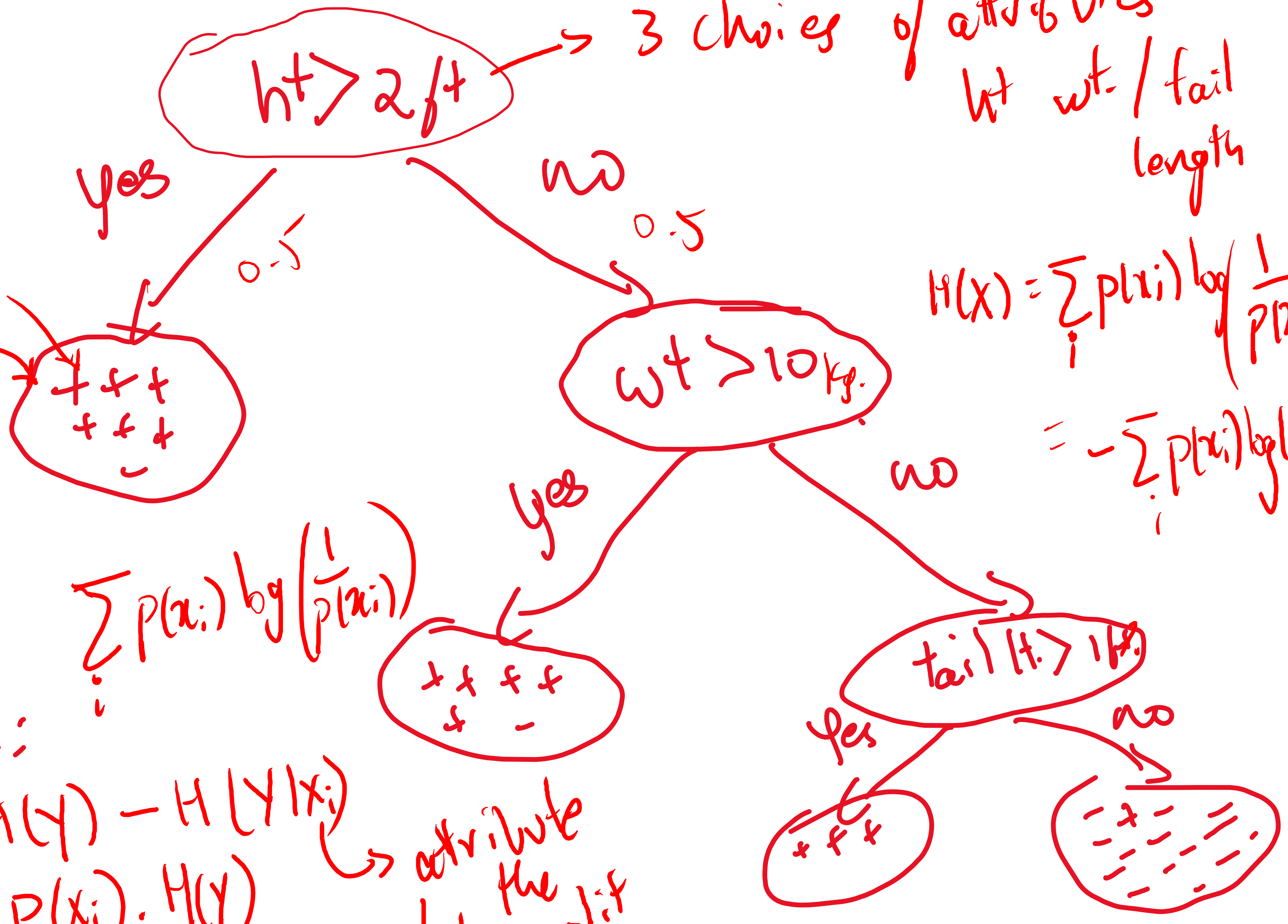
Cat vs Dog

→ 3 choices of attributes

ht wt / tail length

$$H(X) = \sum_i p(x_i)\log\left(\frac{1}{p(x_i)}\right)$$

$$= -\sum_i p(x_i)\log(p(x_i))$$



if node pure entropy ↓ low

Entropy:

$$H(X) = \sum_i p(x_i)\log\left(\frac{1}{p(x_i)}\right)$$

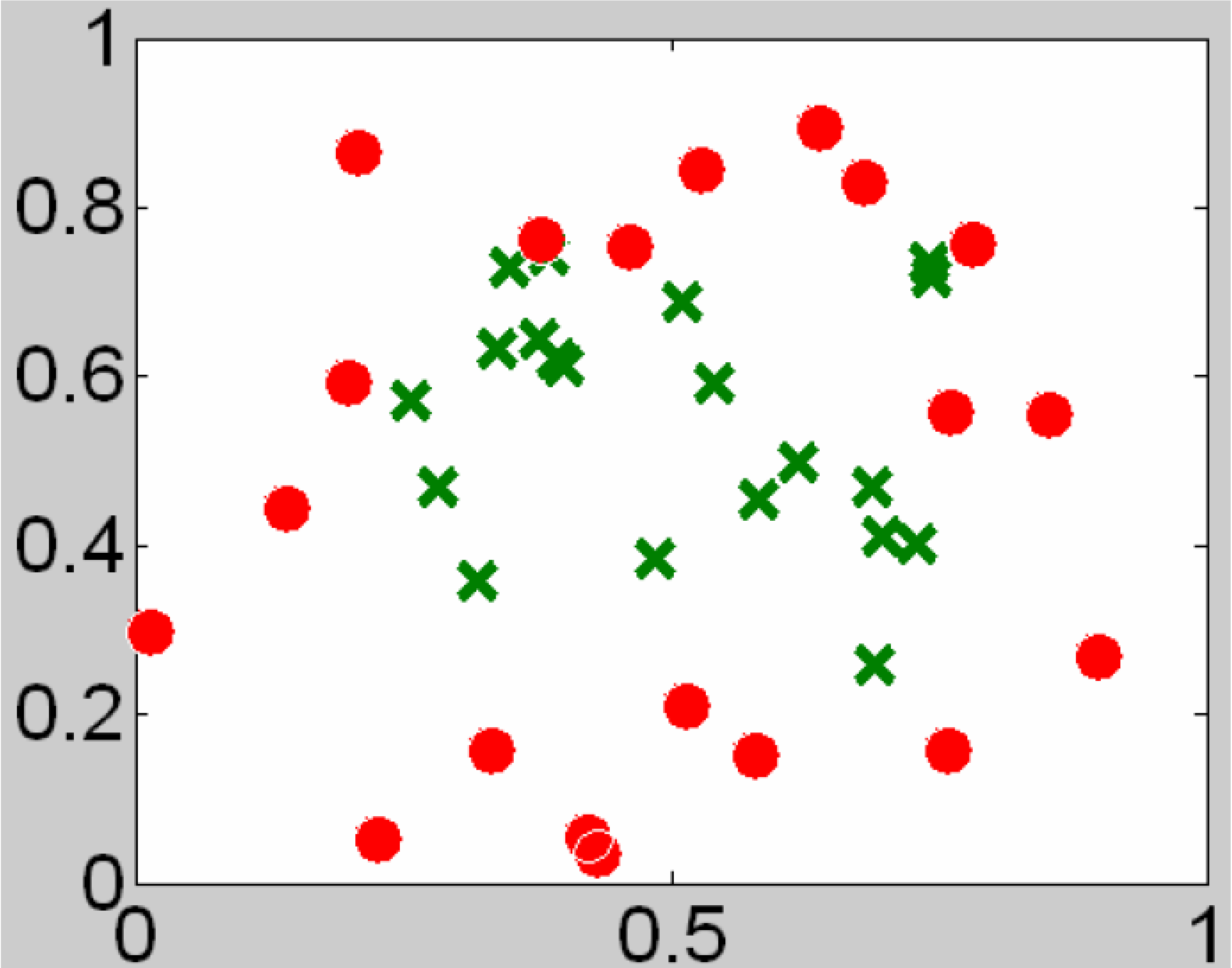
info. gain:

$$I.G. = H(Y) - H(Y|X_i)$$

→ attribute for the split

$$H(Y|X_i) = \sum_i P(X_i) \cdot H(Y)$$

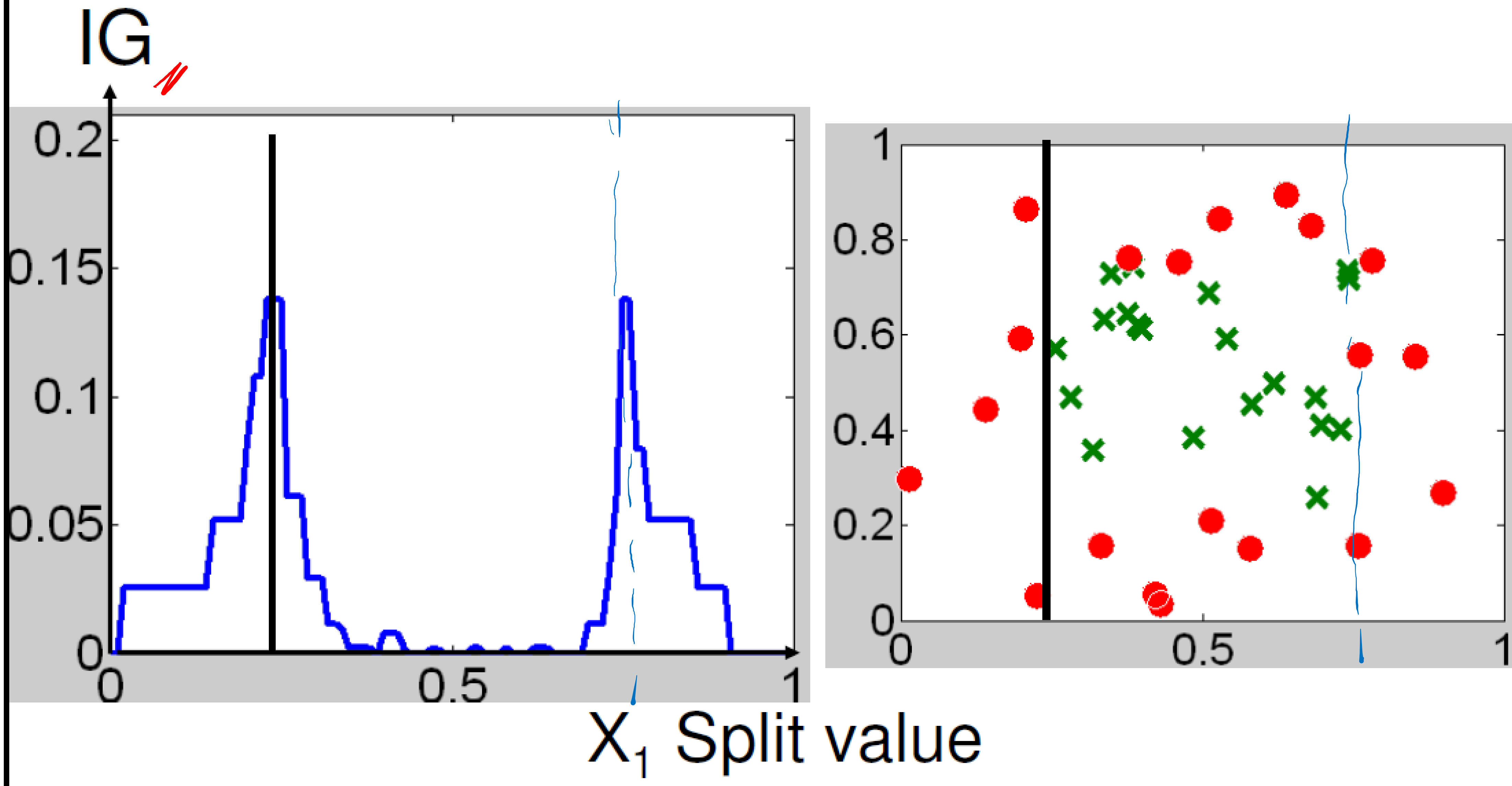
More Complete Example



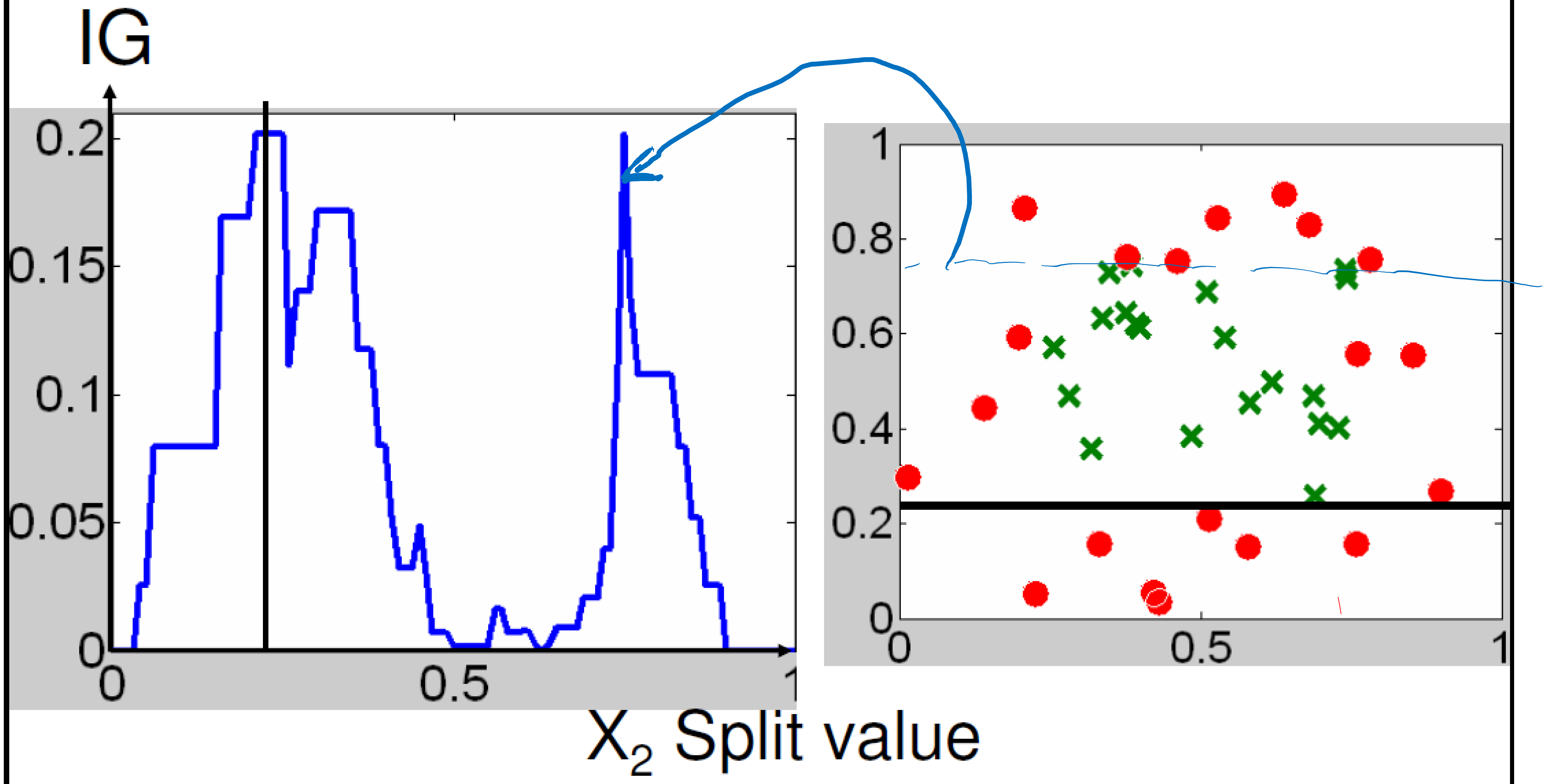
● = 20 training examples from class A

✖ = 20 training examples from class B

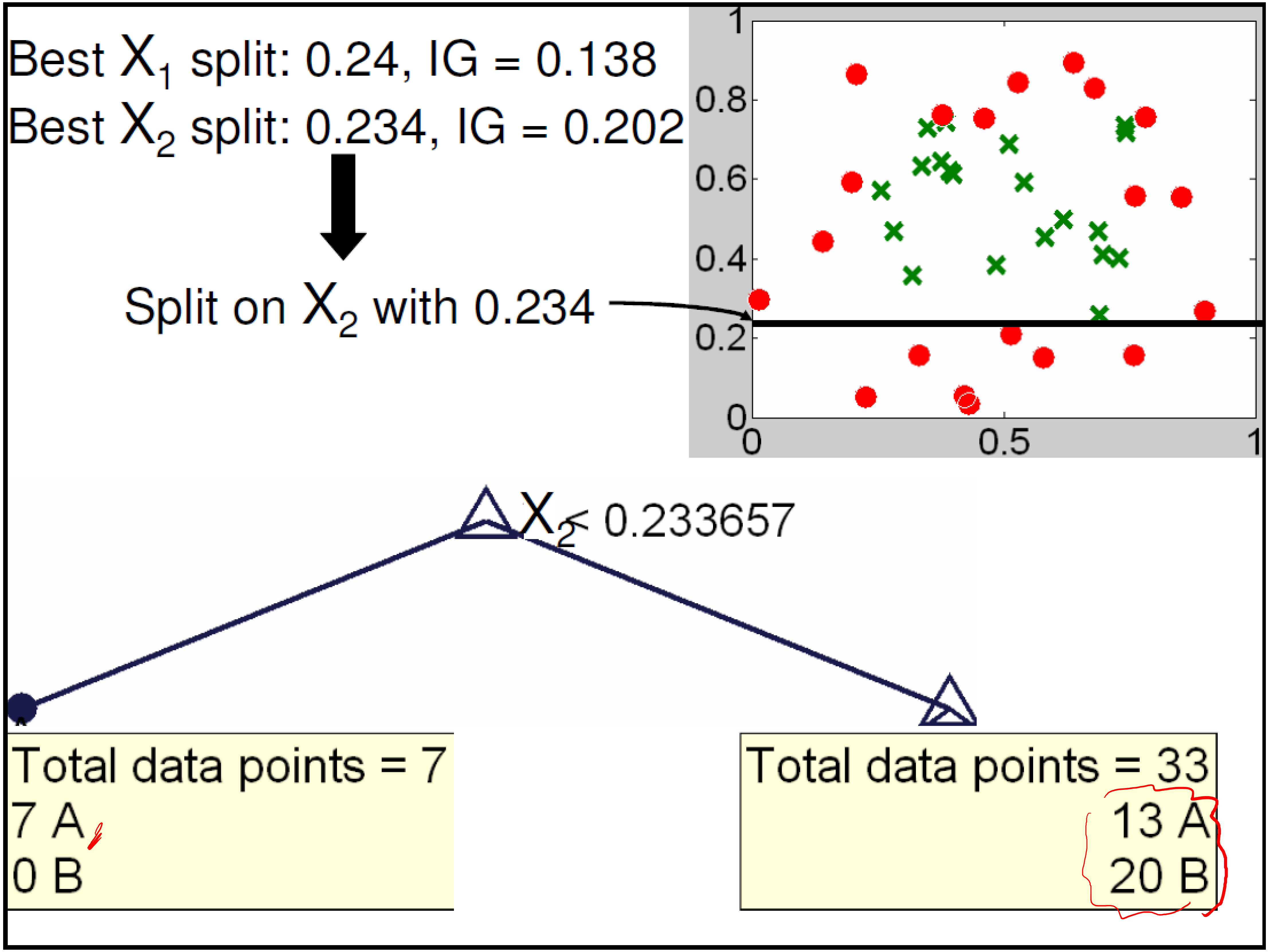
Attributes = X_1 and X_2 coordinates



Best split value (max Information Gain) for X_1 attribute: 0.24 with IG = 0.138



Best split value (max Information Gain) for X_2 attribute: 0.234 with IG = 0.202



Best X_1 split: 0.24, IG = 0.138

Best X_2 split: 0.234, IG = 0.202

Split on X_2 with 0.234

$X_2 < 0.233657$

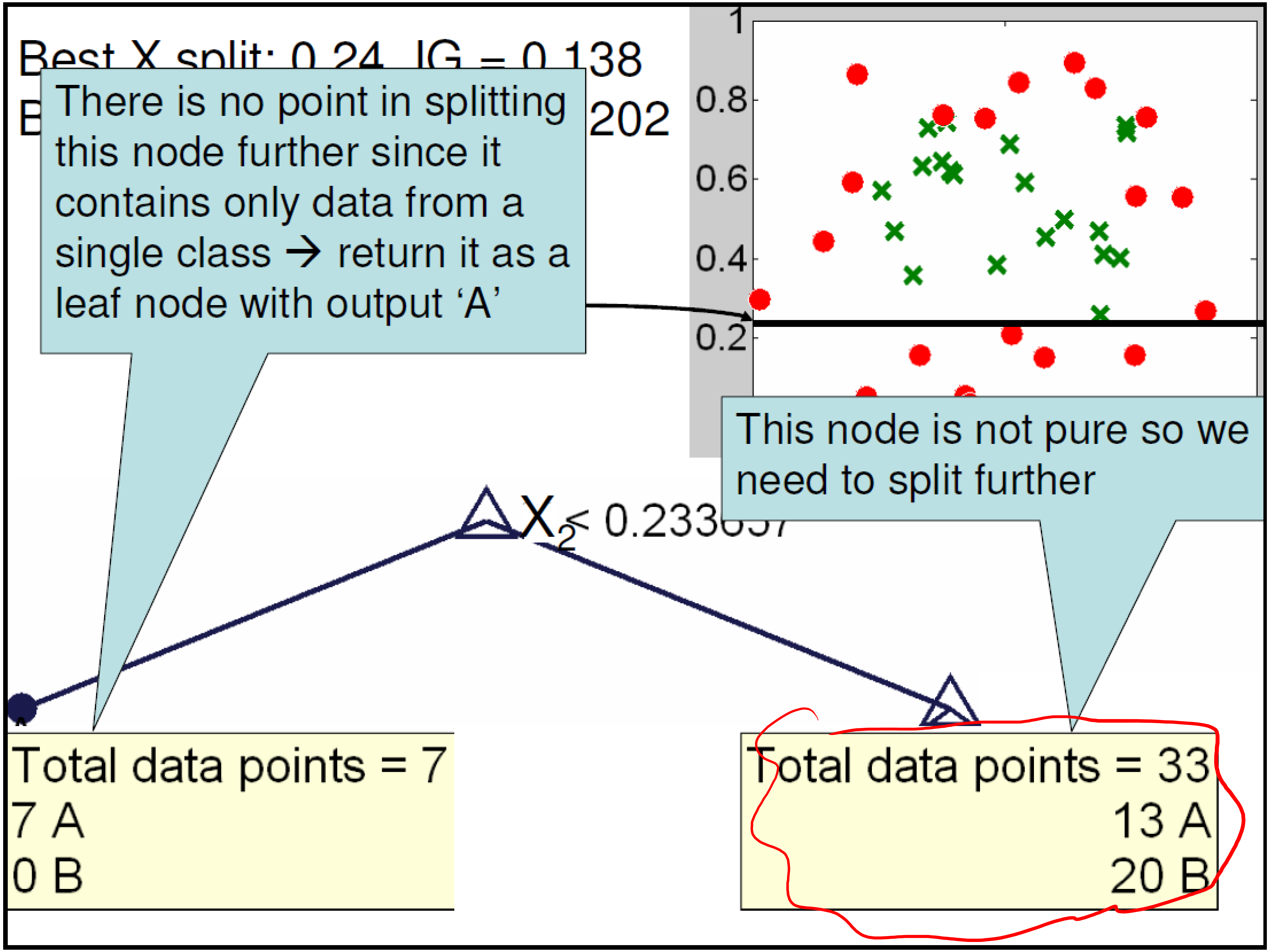
Total data points = 7
7 A
0 B

Total data points = 33
13 A
20 B

Left direction for **smaller** value, **right** direction for **bigger** value

Best X split: 0.24, IG = 0.138

B 202

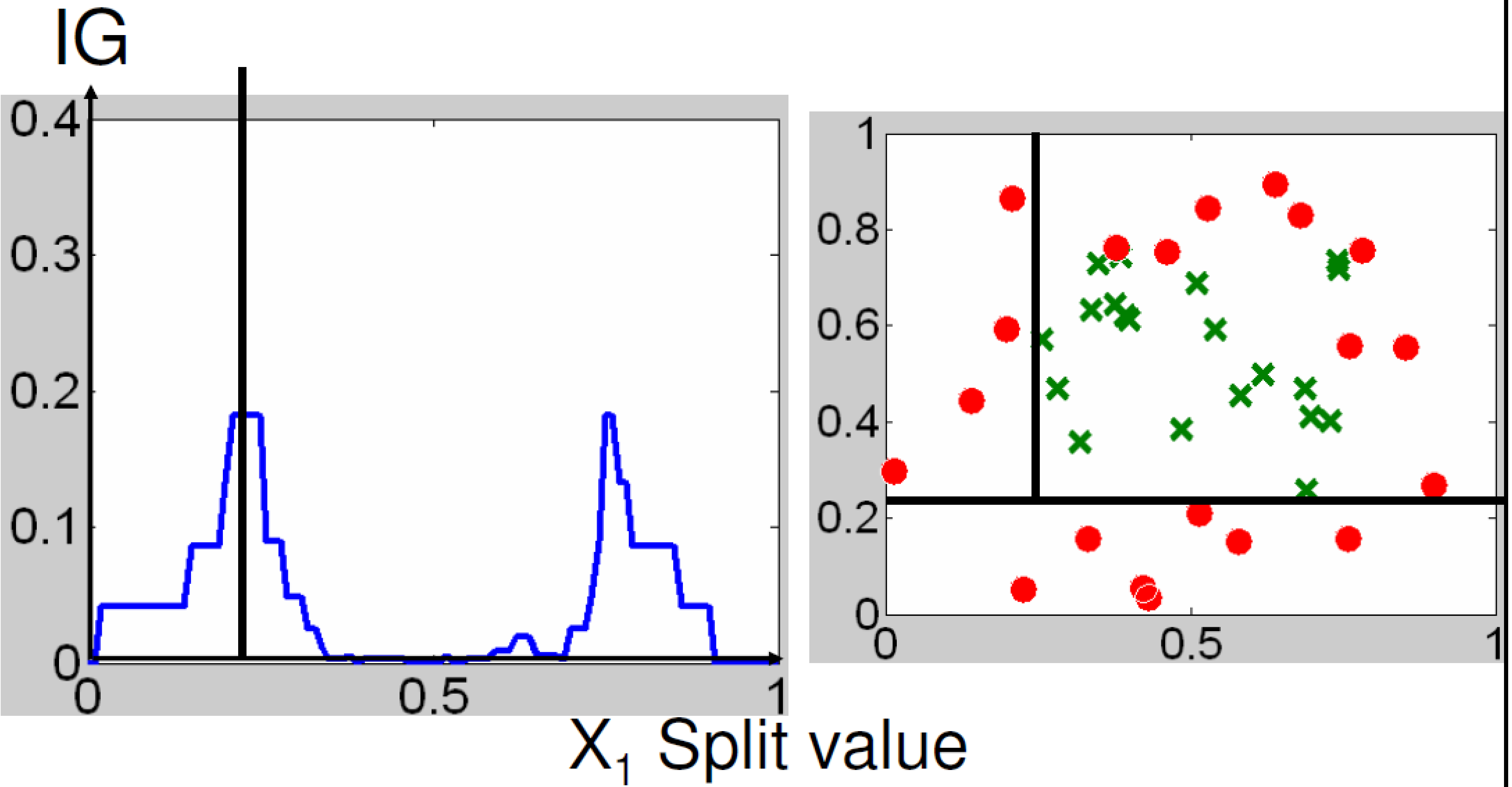


There is no point in splitting this node further since it contains only data from a single class → return it as a leaf node with output ‘A’

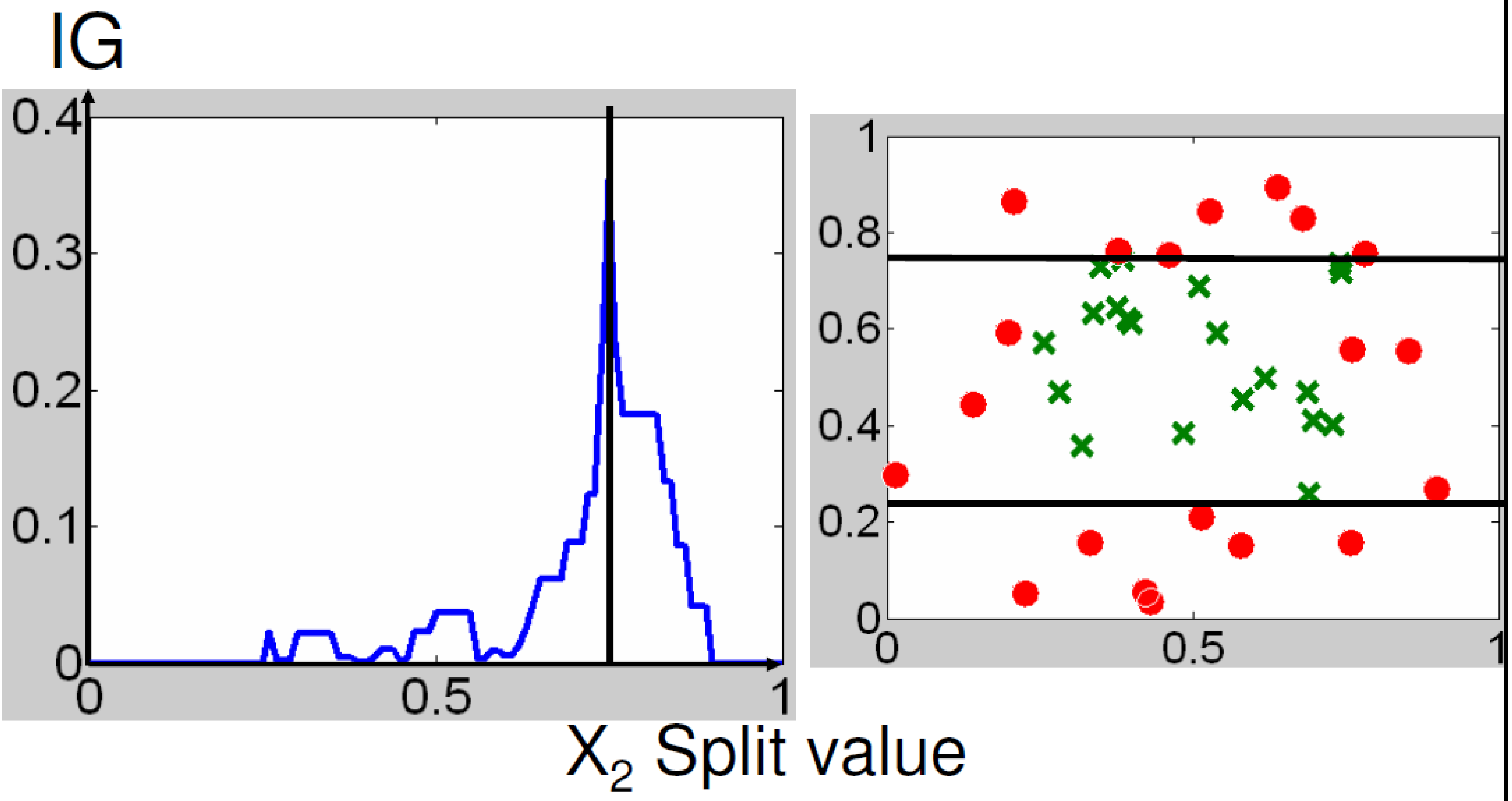
This node is not pure so we need to split further

Total data points = 7
7 A
0 B

Total data points = 33
13 A
20 B



Best split value (max Information Gain) for X_1 attribute: 0.22 with IG ~ 0.182

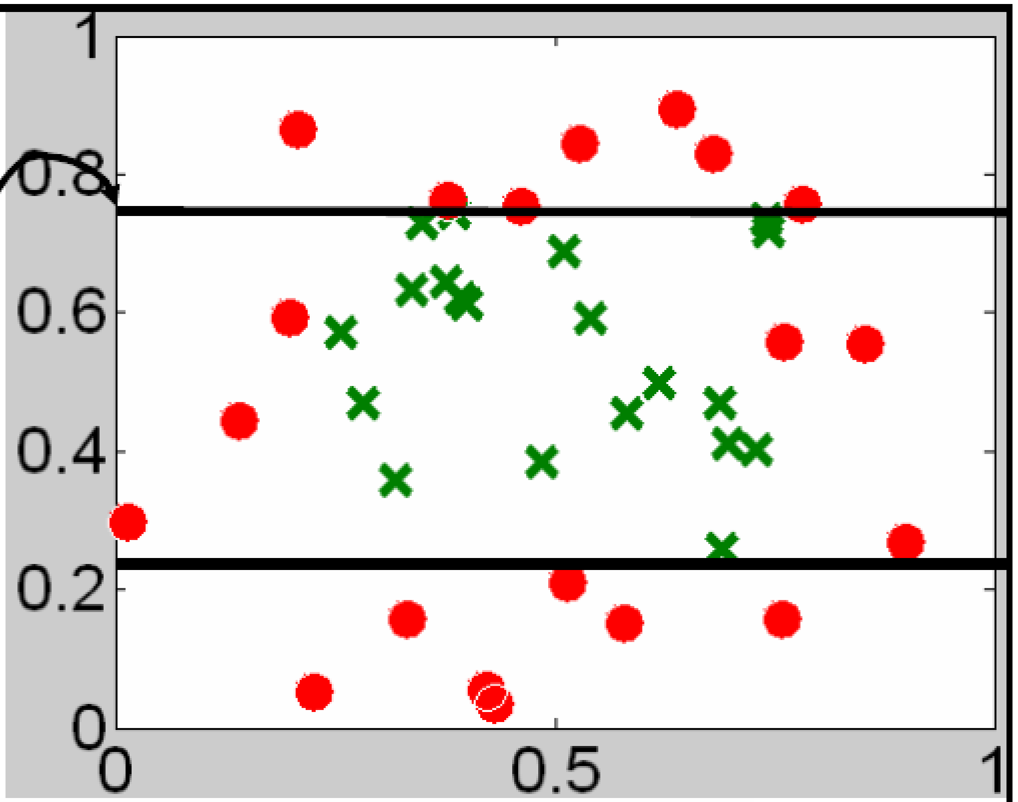


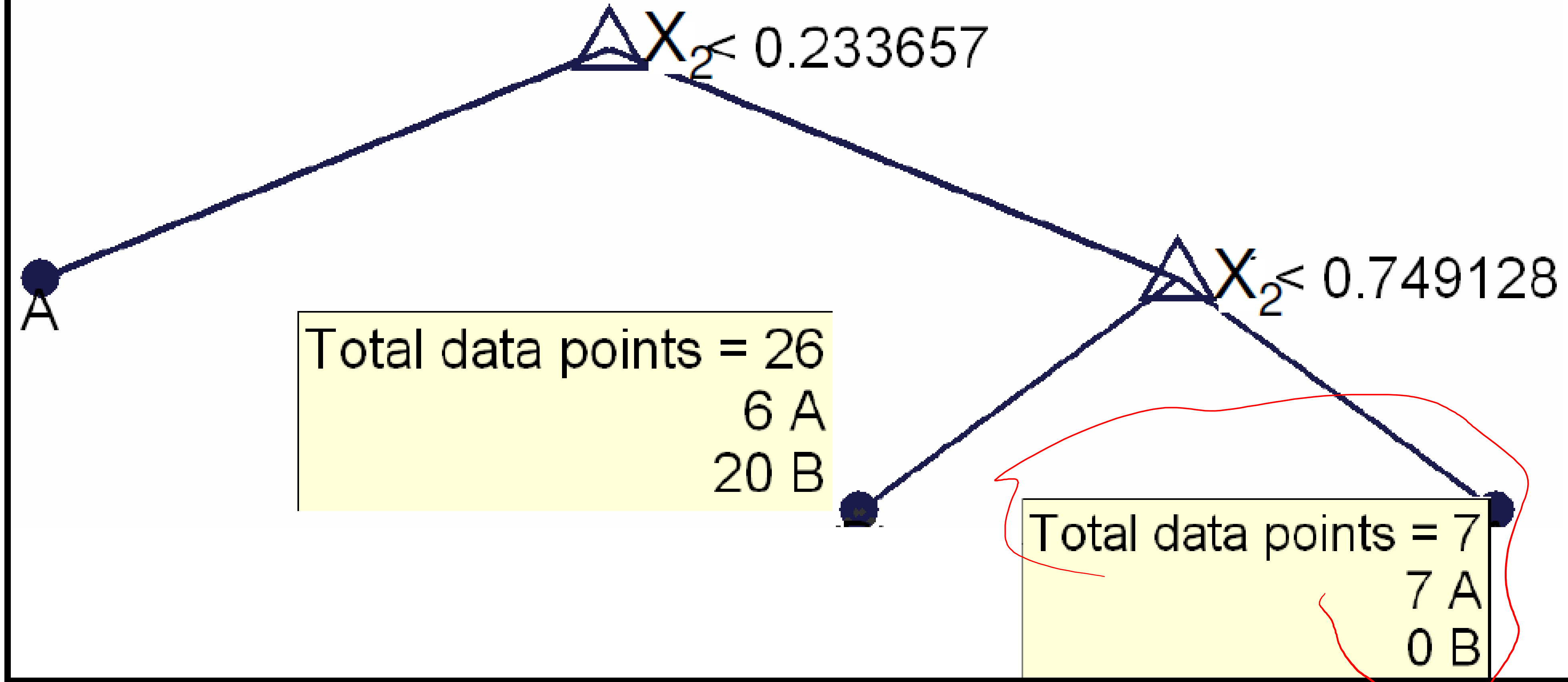
Best split value (max Information Gain) for X_2 attribute: 0.75 with IG ~ 0.353

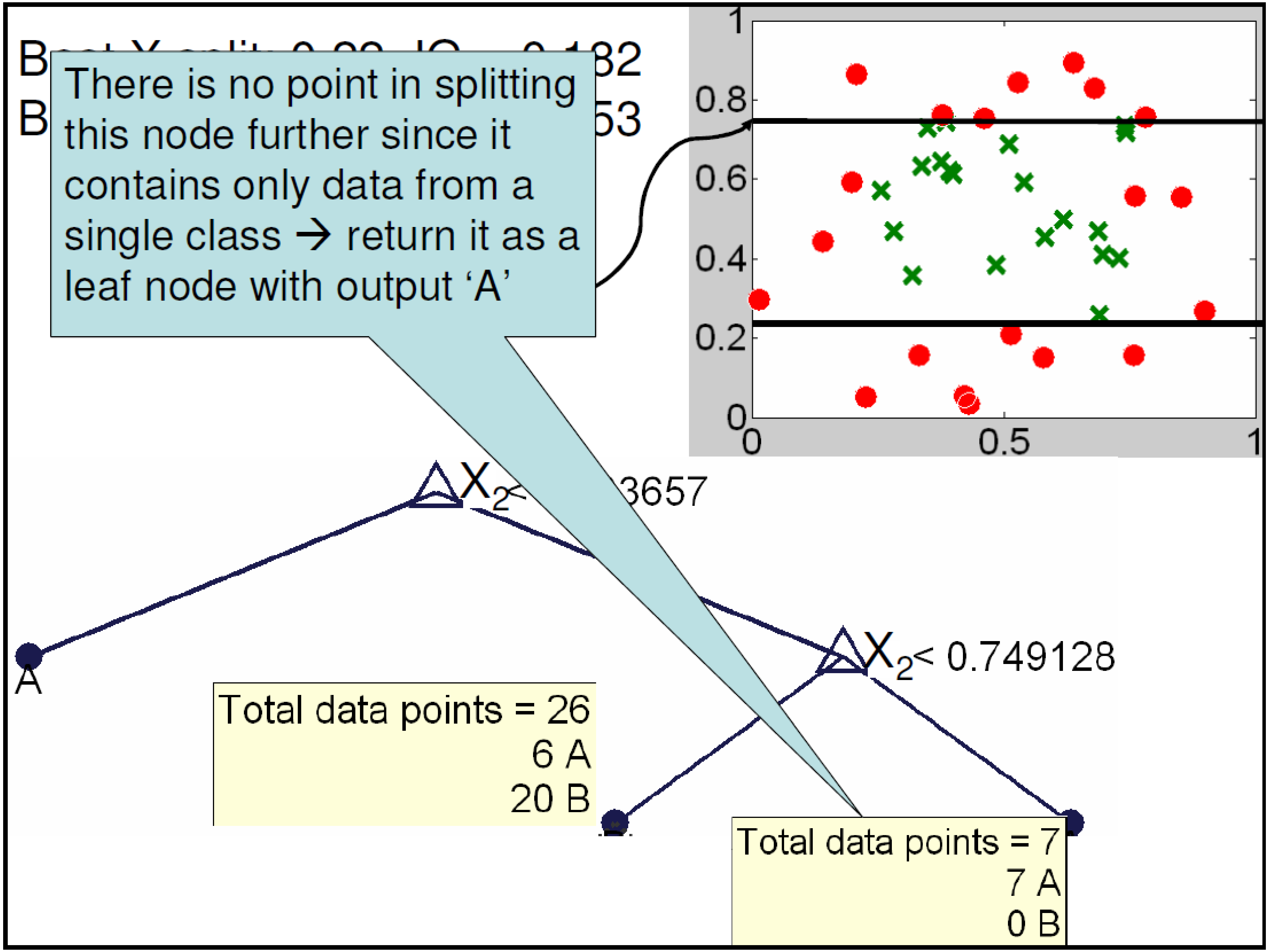
Best X_1 split: 0.22, IG = 0.182

Best X_2 split: 0.75, IG = 0.353

Split on X_2 with 0.75





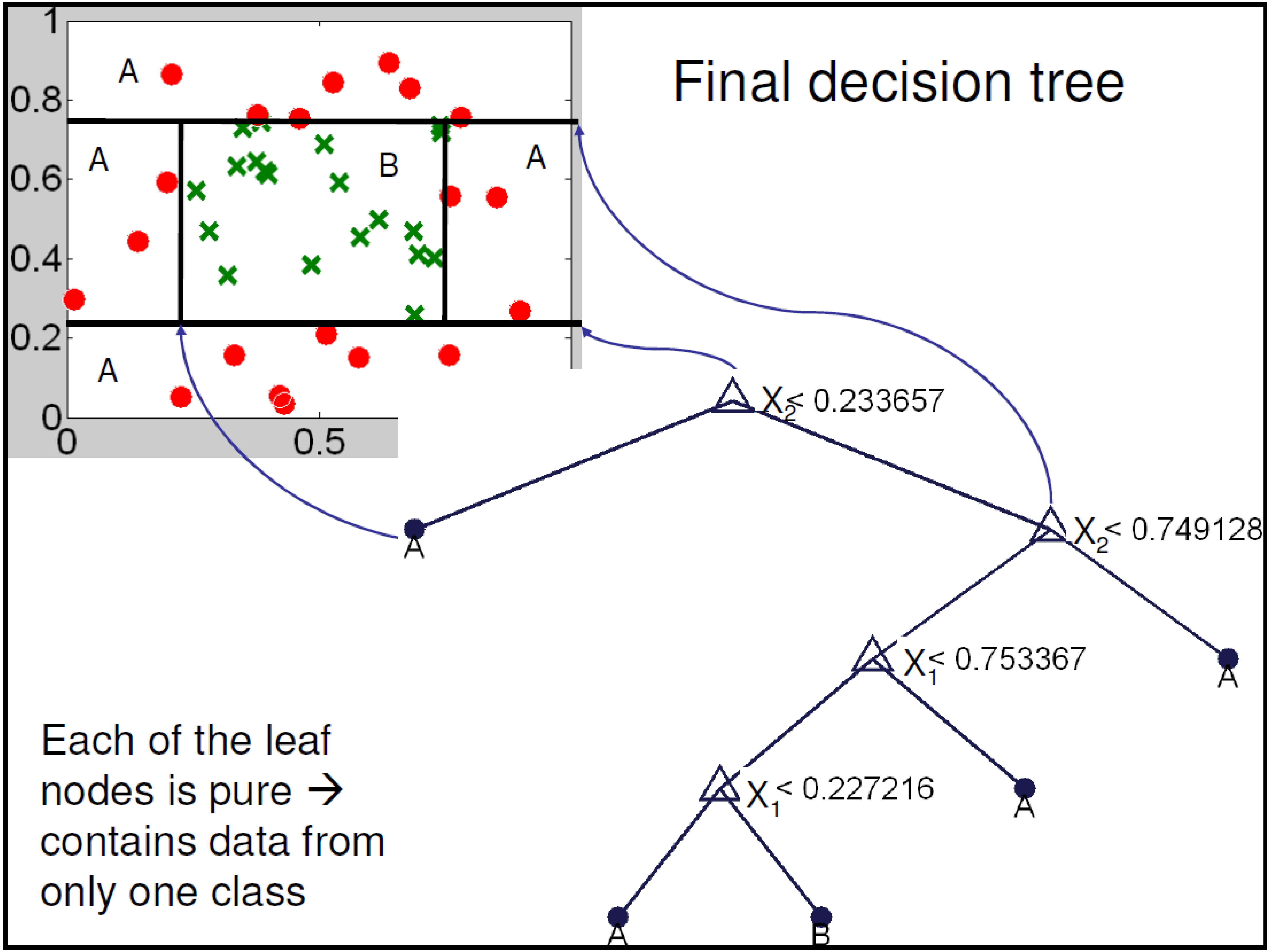


There is no point in splitting this node further since it contains only data from a single class → return it as a leaf node with output 'A'

Total data points = 26
6 A
20 B

Total data points = 7
7 A
0 B

Final decision tree



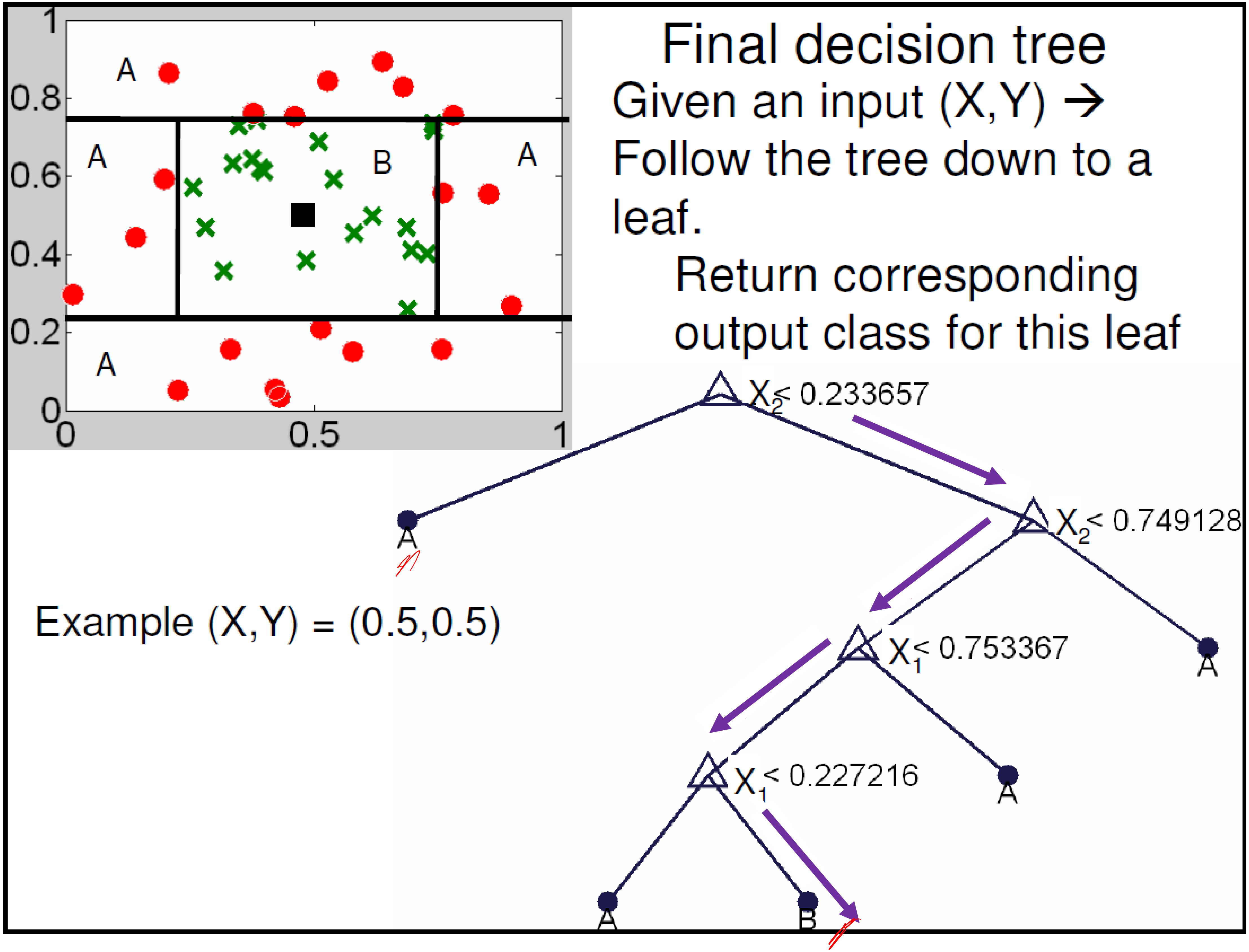
Each of the leaf nodes is pure → contains data from only one class

Final decision tree

Given an input (X,Y) → Follow the tree down to a leaf.

Return corresponding output class for this leaf

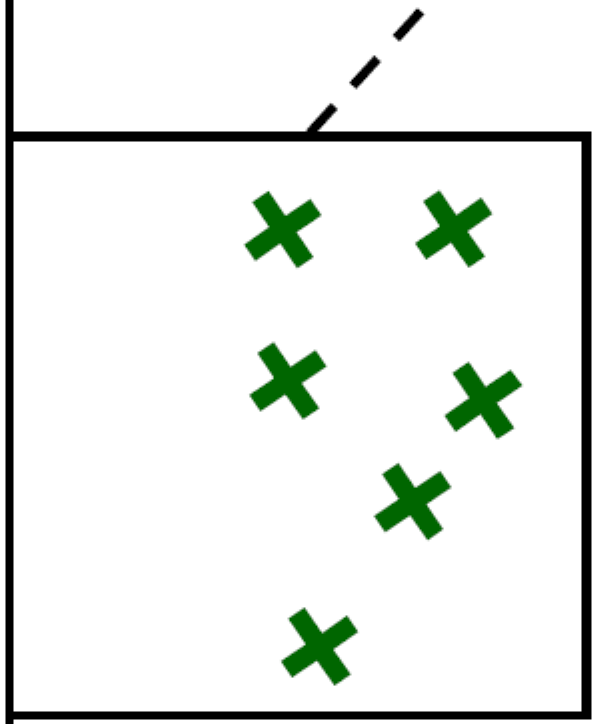
Example (X,Y) = (0.5,0.5)



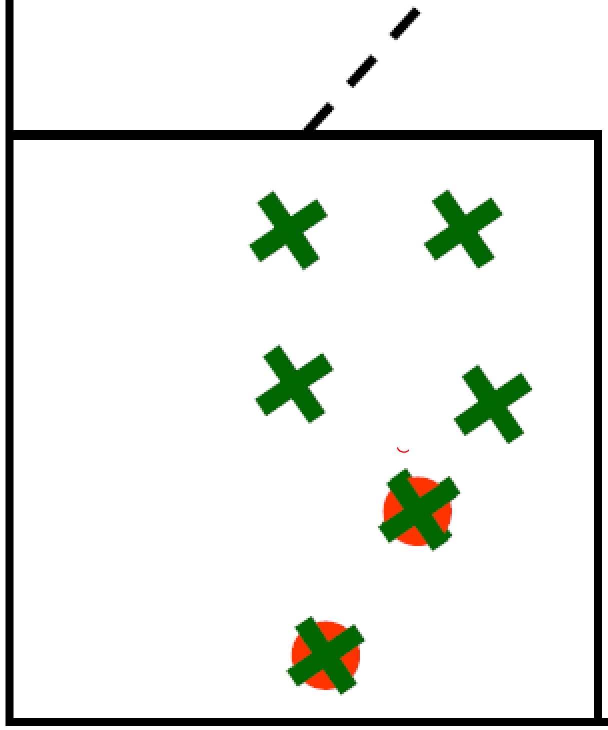
Basic Questions

- How to choose the attribute/value to split on at each level of the tree?
- When to stop splitting? When should a node be declared a leaf?
- If a leaf node is impure, how should the class label be assigned?
- If the tree is too large, how can it be pruned?

Pure and Impure Leaves and When to Stop Splitting



All the data in the node comes from a single class → We declare the node to be a leaf and stop splitting. This leaf will output the class of the data it contains



Several data points have exactly the same attributes even though they are from different class → We cannot split any further → We still declare the node to be a leaf, but it will output the class that is the majority of the classes in the node (in this example, ‘B’)

Decision Tree Algorithm (Continuous Attributes)

- LearnTree(X, Y)
  - Input: → no. of training points → M dim.
    - Set X of R training vectors, each containing the values $(x_1,..,x_M)$ of data M attributes $(X_1,..,X_M)$
    - A vector Y of R elements, where y_j = class of the jth datapoint
  - If all the datapoints in X have the same class value y
    - Return a leaf node that predicts y as output
  - If all the datapoints in X have the same attribute value $(x_1,...,x_M)$
    - Return a leaf node that predicts the majority of the class values in Y as output
  - Try all the possible attributes X_j and threshold t and choose the one, j^*, for which IG($Y|X_j,t$) is maximum
  - X_L, Y_L = set of datapoints for which $x_{j^*} < t$ and corresponding classes
  - X_H, Y_H = set of datapoints for which $x_{j^*} >= t$ and corresponding classes
  - Left Child ← LearnTree(X_L, Y_L)
  - Right Child ← LearnTree(X_H, Y_H)

Stopping condition

Decision Tree Algorithm (Discrete Attributes)

- LearnTree(X, Y)
  - Input:
    - Set X of R training vectors, each containing the values (x_1,..,x_M) of M attributes (X_1,..,X_M)
    - A vector Y of R elements, where y_j = class of the jth datapoint
  - If all the datapoints in X have the same class value y
    - Return a leaf node that predicts y as output
  - If all the datapoints in X have the same attribute value (x_1,..,x_M)
    - Return a leaf node that predicts the majority of the class values in Y as output
  - Try all the possible attributes X_j and choose the one, j^*, for which IG(Y|X_j) is maximum
  - For every possible value v of X_{j^*}:
    - X_v, Y_v= set of datapoints for which $x_{j^*} = v$ and corresponding classes
    - Child$_v$ ← LearnTree(X_v, Y_v)

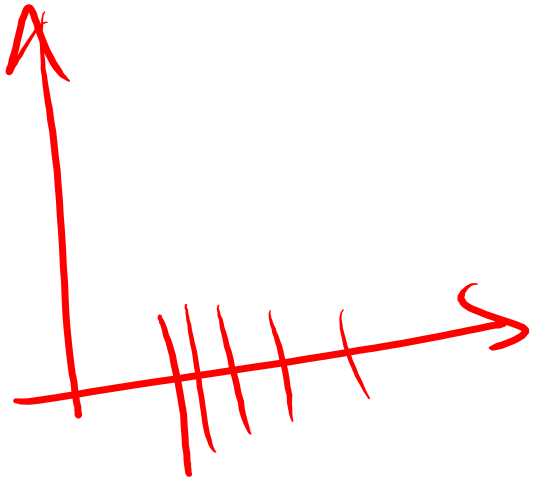
Decision Trees So Far

- Given N observations from training data, each with D attributes X and a class attribute Y, construct a sequence of tests (decision tree) to predict the class attribute Y from the attributes X
- Basic strategy for defining the tests ("when to split") → maximize the information gain on the training data set at each node of the tree
- Problems (next):
  - Computational issues → How expensive is it to compute the IG
  - The tree will end up being much too big → *pruning*
  - Evaluating the tree on training data is dangerous → *overfitting*

Basic Questions

- How to choose the attribute/value to split on at each level of the tree?
- When to stop splitting? When should a node be declared a leaf?
- If a leaf node is impure, how should the class label be assigned?
- If the tree is too large, how can it be pruned?

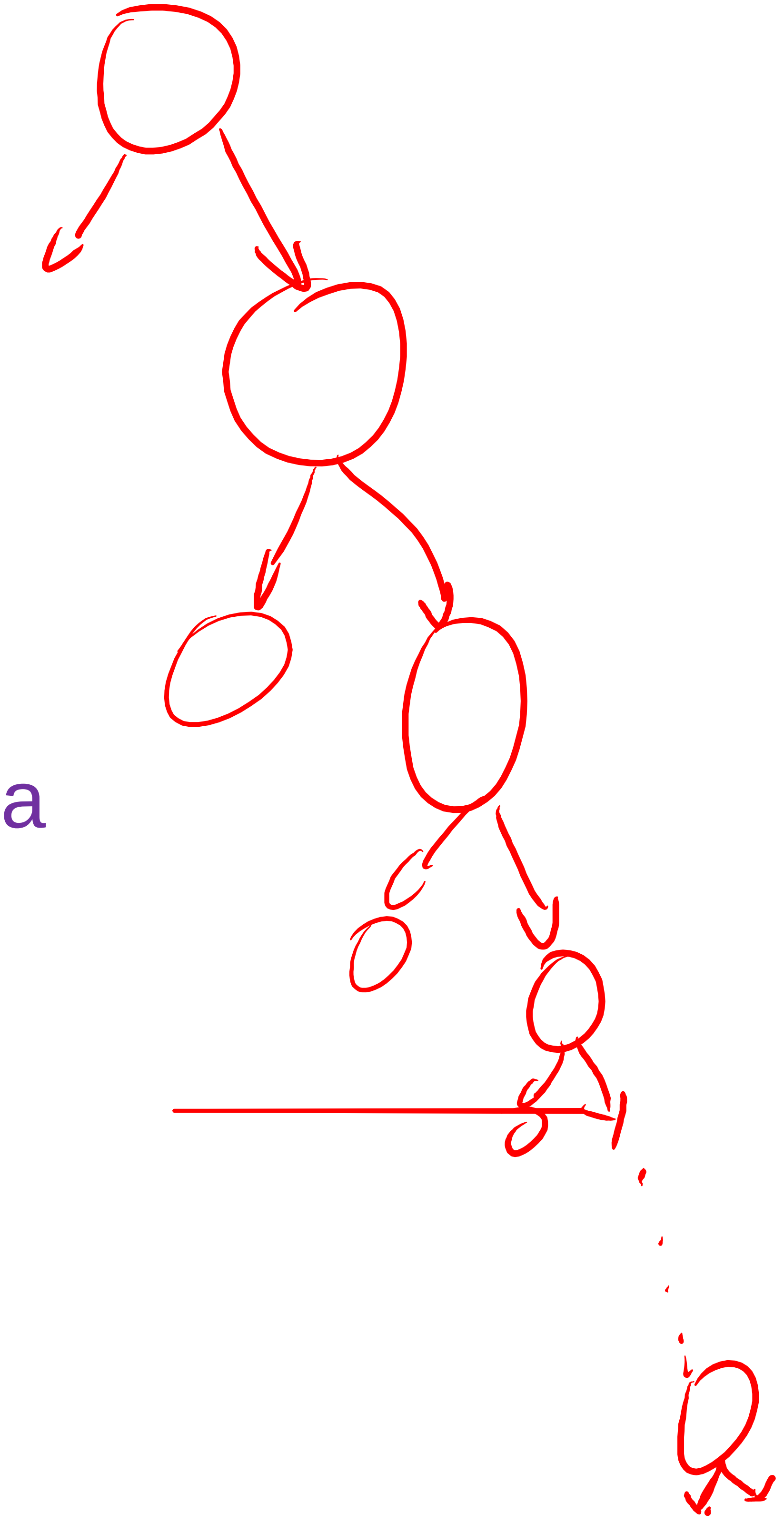
What will happen if a tree is too large?



Overfitting

High variance

Instability in predicting test data



How to avoid overfitting?

- Acquire more training data
- Remove irrelevant attributes (manual process – not always possible)
- Grow full tree, then post-prune
- Ensemble learning

Reduced-Error Pruning

Split data into training and validation sets

Grow tree based on training set

Do until further pruning is harmful:

1. Evaluate impact on validation set of pruning each possible node (plus those below it)

2. Greedily remove the node that most improves validation set accuracy

How to decide to remove it a node using pruning

- Pruning of the decision tree is done by replacing a whole subtree by a leaf node.
- The replacement takes place if a decision rule establishes that the expected error rate in the subtree is greater than in the single leaf.

If we had simply predicted the **majority class** (negative), we make 2 errors instead of 4

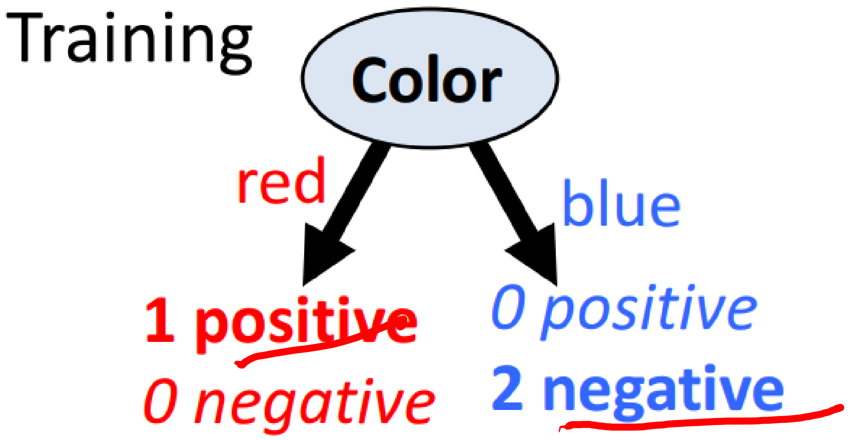
negative

Pruned!

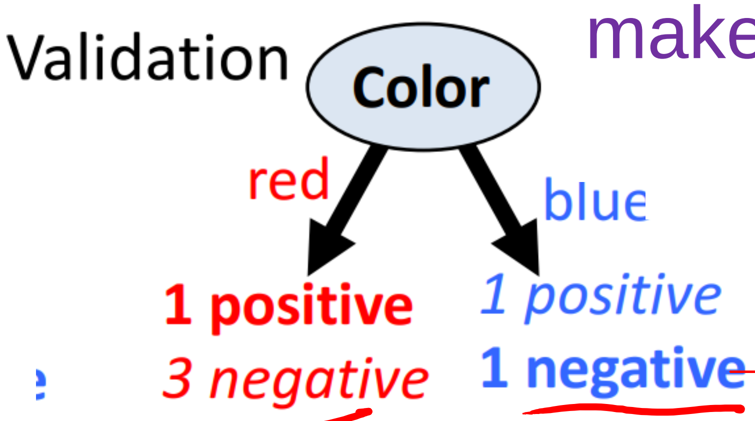
val. accuracy

$\frac{4}{6} = \frac{2}{3}$

$1/3$



3 training data points
Actual Label: 1 positive class and 2 negative class
Predicted Label: 1 positive class and 2 negative class
3 correct and **0** incorrect



6 validation data points
Actual label:2 positive and 4 negative
Predicted Label: 4 positive and 2 negative
2 correct and **4** incorrect