Lecture 06

Decision Trees

STAT 451: Intro to Machine Learning, Fall 2020

Sebastian Raschka

http://stat.wisc.edu/~sraschka/teaching/stat451-fs2020/

Topics

1. **Intro to decision trees**

2. Recursive algorithms & Big-O

3. Types of decision trees

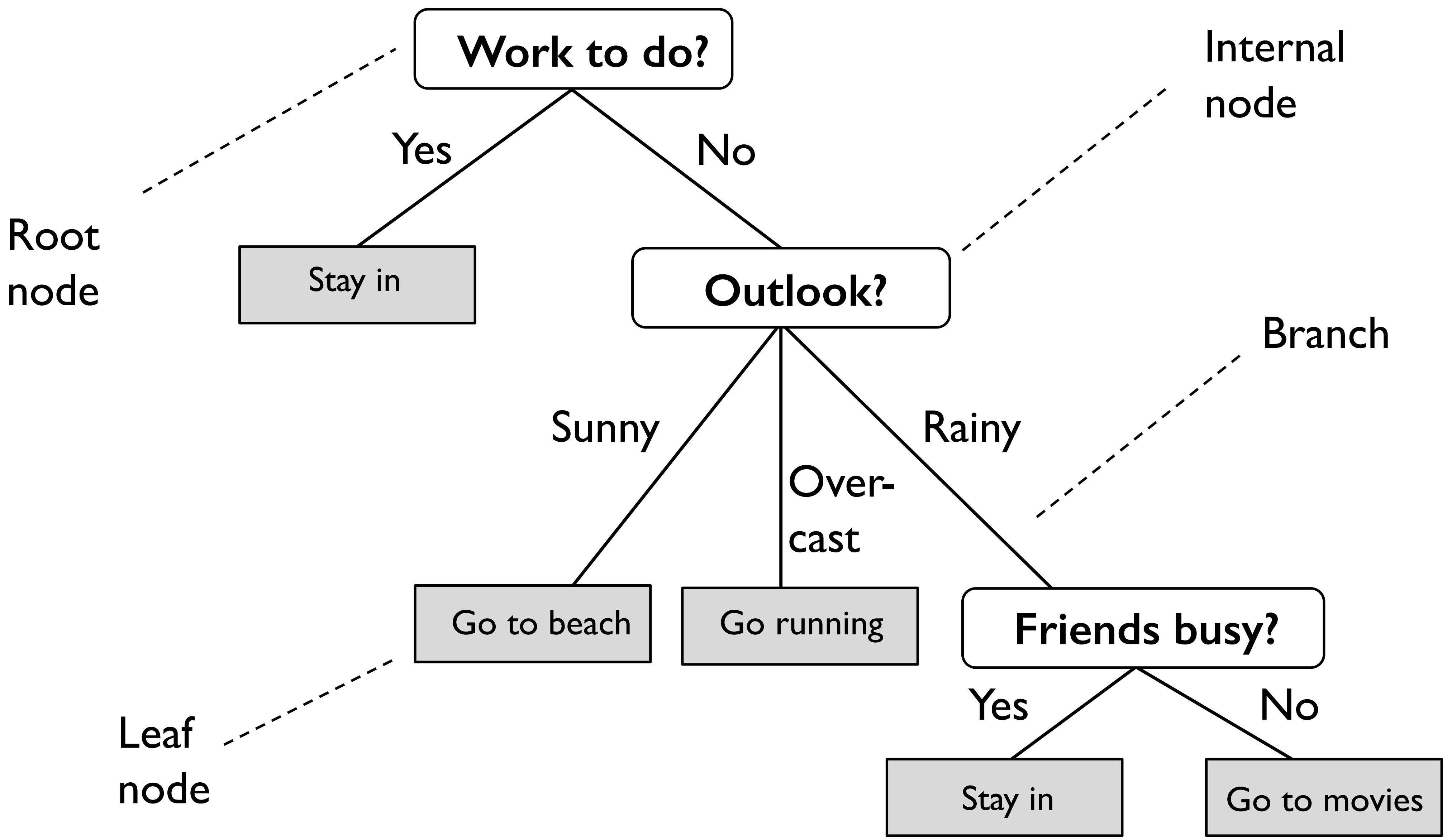
4. Splitting criteria

5. Gini & Entropy vs misclassification error

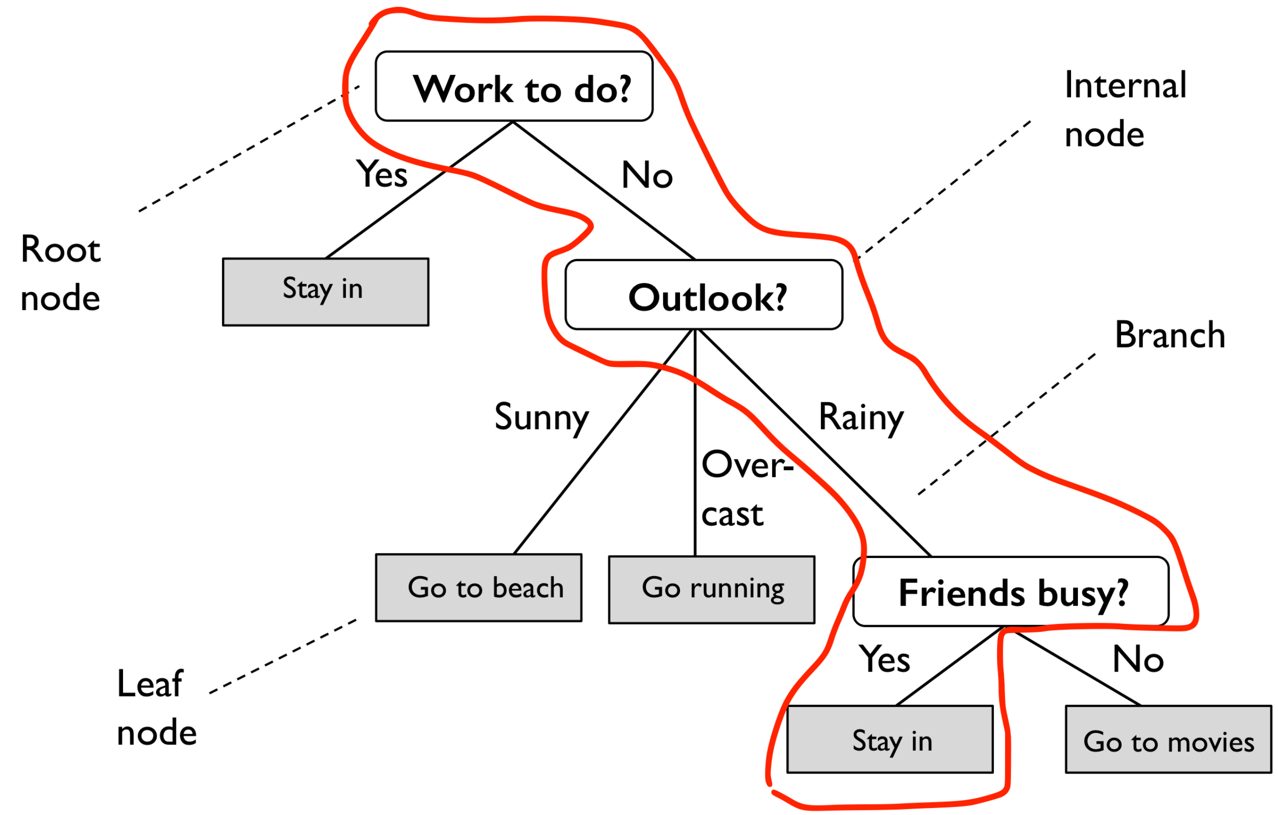
6. Improvements & dealing with overfitting

7. Code example

Decision Tree Terminology



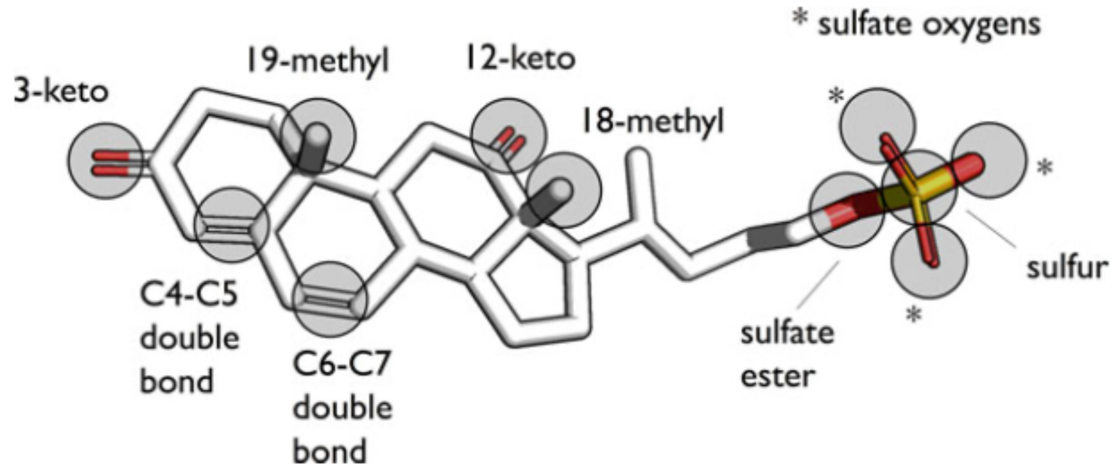
Decision Trees as Rulesets

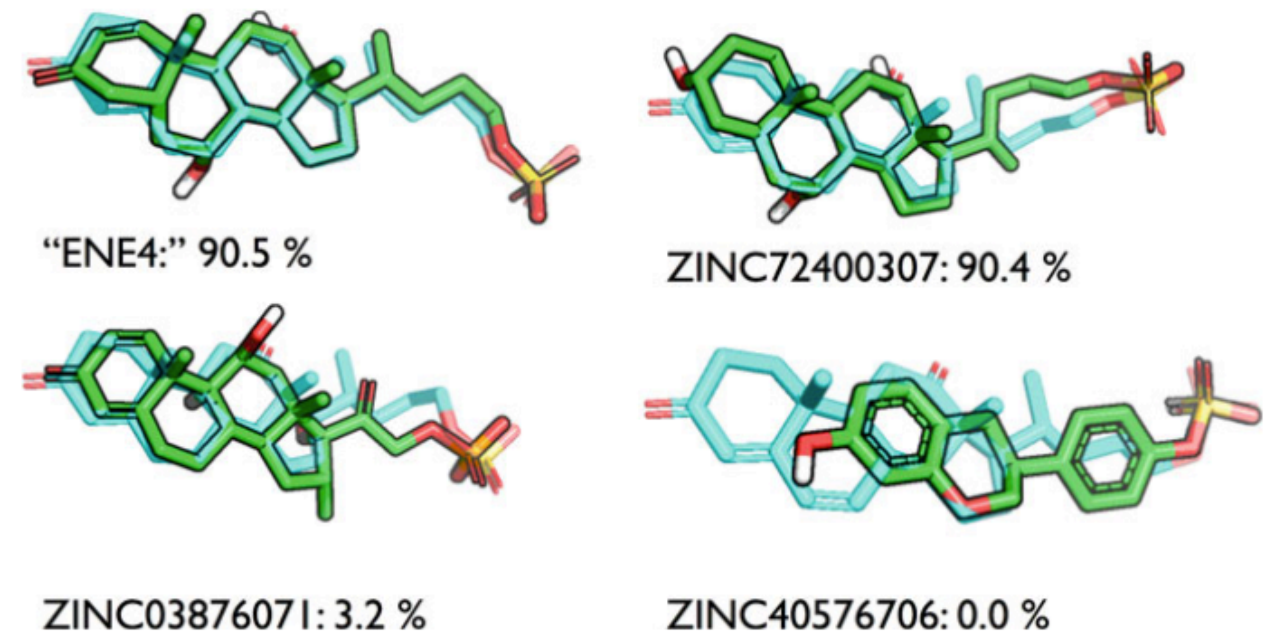


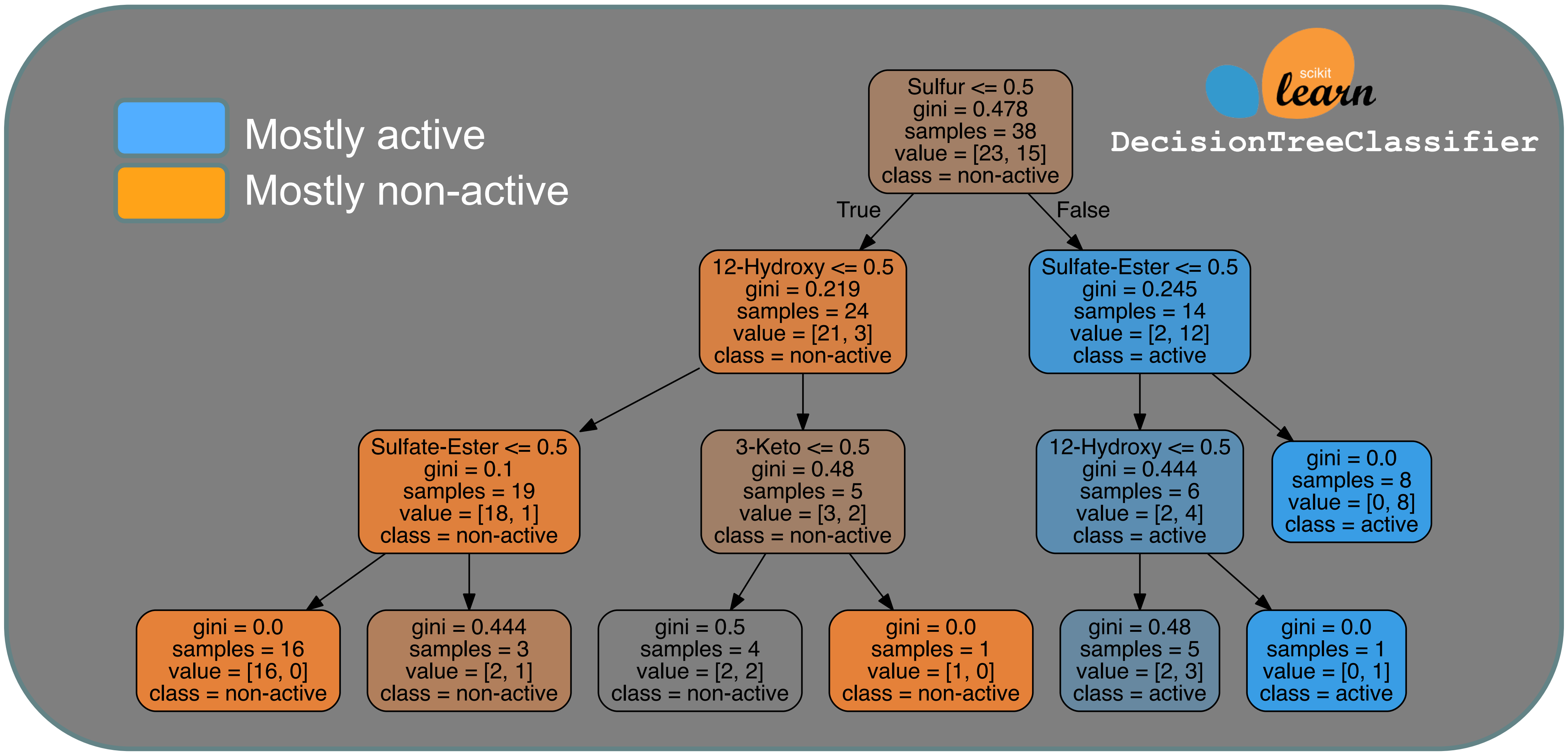
IF ______________________ ___ ______________________

___ ______________________

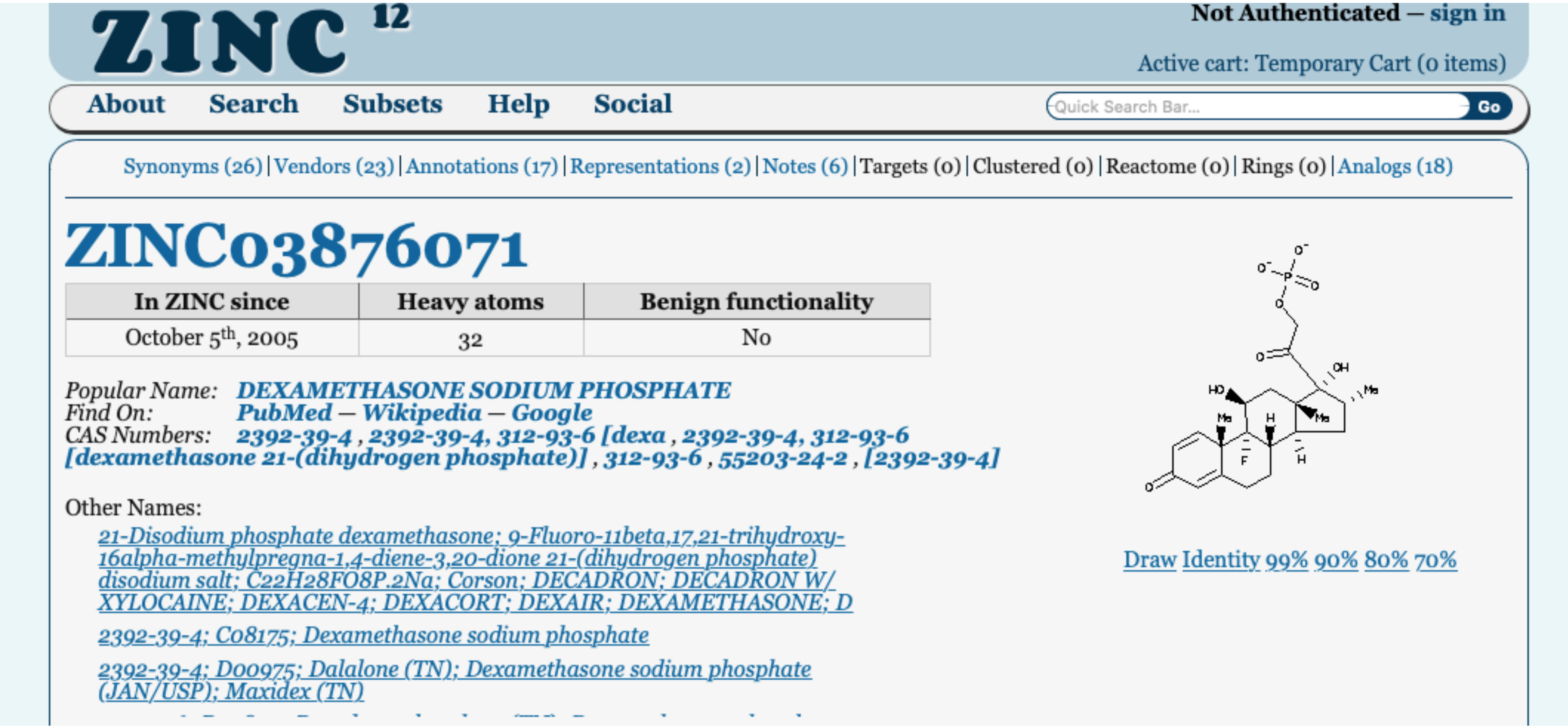
THEN ________ ___ ___________







Sebastian Raschka, Leslie A. Kuhn, Anne M. Scott, and Weiming Li (2018) *Computational Drug Discovery and Design: Automated Inference of Chemical Group Discriminants of Biological Activity from Virtual Screening Data.* Springer. ISBN: 978-1-4939-7755-0



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In ZINC since	Heavy atoms	Benign functionality
October 5th, 2005	32	No

Popular Name: ***DEXAMETHASONE SODIUM PHOSPHATE***
Find On: ***PubMed — Wikipedia — Google***
CAS Numbers: ***2392-39-4 , 2392-39-4, 312-93-6 [dexa , 2392-39-4, 312-93-6 [dexamethasone 21-(dihydrogen phosphate)] , 312-93-6 , 55203-24-2 , [2392-39-4]***

Other Names:

21-Disodium phosphate dexamethasone; 9-Fluoro-11beta,17,21-trihydroxy-16alpha-methylpregna-1,4-diene-3,20-dione 21-(dihydrogen phosphate) disodium salt; C22H28FO8P.2Na; Corson; DECADRON; DECADRON W/ XYLOCAINE; DEXACEN-4; DEXACORT; DEXAIR; DEXAMETHASONE; D

2392-39-4; C08175; Dexamethasone sodium phosphate

2392-39-4; D00975; Dalalone (TN); Dexamethasone sodium phosphate (JAN/USP); Maxidex (TN)

Draw Identity 99% 90% 80% 70%

Random forests, adaptive boosting, gradient boosting

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Recursion / Recursive Algorithms

```
def some_fun(x):
    if x == []:
        return 0
    else:
        return 1 + some_fun(x[1:])
```

What does this function do?

Divide & Conquer Algorithms: Quicksort

```
def quicksort(array):
    if len(array) < 2:
        return array
    else:
        pivot = array[0]
        smaller, bigger = [], []
        for ele in array[1:]:
            if ele <= pivot:
                smaller.append(ele)
            else:
                bigger.append(ele)
        return quicksort(smaller) + [pivot] + quicksort(bigger)
```

Divide & Conquer Algorithms: Quicksort

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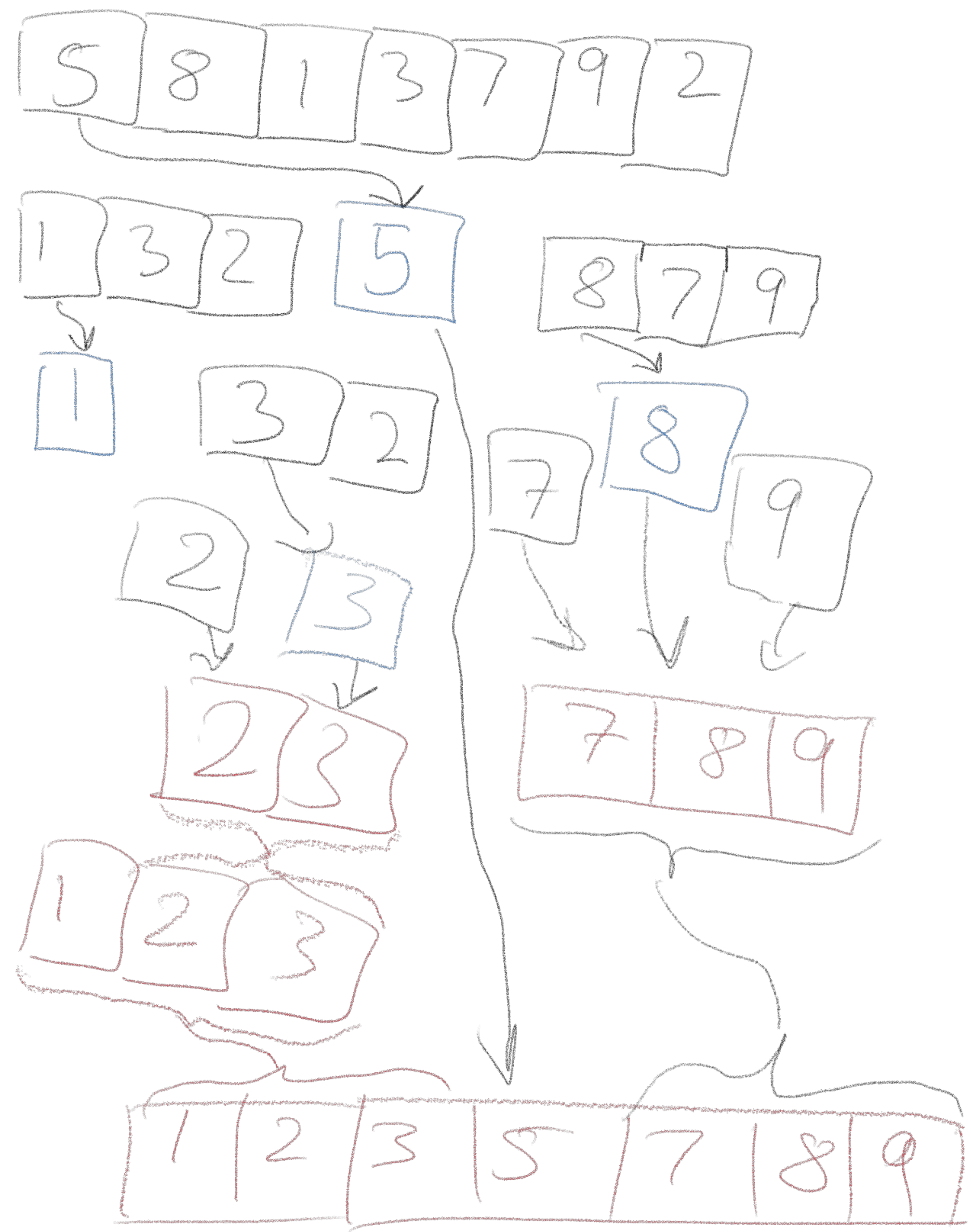

Time complexity of quicksort:

$$\mathcal{O}(\underline{\hspace{6cm}})$$

```
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        return quicksort(smaller) + [pivot] + quicksort(bigger)
```

Array Sorting Algorithms

Algorithm	Time Complexity			Space Complexity
	Best	Average	Worst *	Worst
Quicksort	Ω(n log(n))	Θ(n log(n))	O(n^2)	O(log(n))
Mergesort	Ω(n log(n))	Θ(n log(n))	O(n log(n))	O(n)
Timsort	Ω(n)	Θ(n log(n))	O(n log(n))	O(n)
Heapsort	Ω(n log(n))	Θ(n log(n))	O(n log(n))	O(1)
Bubble Sort	Ω(n)	Θ(n^2)	O(n^2)	O(1)
Insertion Sort	Ω(n)	Θ(n^2)	O(n^2)	O(1)
Selection Sort	Ω(n^2)	Θ(n^2)	O(n^2)	O(1)
Tree Sort	Ω(n log(n))	Θ(n log(n))	O(n^2)	O(n)
Shell Sort	Ω(n log(n))	Θ(n(log(n))^2)	O(n(log(n))^2)	O(1)
Bucket Sort	Ω(n+k)	Θ(n+k)	O(n^2)	O(n)
Radix Sort	Ω(nk)	Θ(nk)	O(nk)	O(n+k)
Counting Sort	Ω(n+k)	Θ(n+k)	O(n+k)	O(k)
Cubesort	Ω(n)	Θ(n log(n))	O(n log(n))	O(n)

http://www.bigocheatsheet.com

* "worst" ~ inversely-sorted array

Decision Tree in Pseudocode

GenerateTree($\mathcal{D}$):

- if $y = 1 \; \forall \; \langle \mathbf{x}, \mathbf{y} \rangle \in \mathcal{D}$ or $y = 0 \; \forall \; \langle \mathbf{x}, y \rangle \in \mathcal{D}$:
    - return Tree
- else:
    - Pick best feature x_j:
        - $\mathcal{D}_0$ at Child$_0$: $x_j = 0 \; \forall \; \langle \mathbf{x}, y \rangle \in \mathcal{D}$
        - $\mathcal{D}_1$ at Child$_1$: $x_j = 1 \; \forall \; \langle \mathbf{x}, y \rangle \in \mathcal{D}$

    return Node(x_j, GenerateTree($\mathcal{D}_0$), GenerateTree($\mathcal{D}_1$))

Time Complexity ("Big-O")

Growing the tree: $\mathcal{O}(\ldots$

Tip: It can be shown that optimal split is on boundary between adjacent examples (similar feature value) with different class labels.

Fayyad, Usama Mohammad. "On the induction of decision trees for multiple concept learning." (1992).

Time Complexity ("Big-O")

Querying the tree: $\mathcal{O}(\ldots$

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Decision Tree in Pseudocode

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Generic Tree Growing Algorithm

1) Pick the feature that, when parent node is split, results in the largest information gain

2) Stop if child nodes are pure or information gain <= 0

3) Go back to step 1 for each of the two child nodes

Generic Tree Growing Algorithm

1) Pick the feature that, when parent node is split, results in the largest information gain

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3) Go back to step 1 for each of the two child nodes

- How make predictions of features in dataset not sufficient to make child nodes pure?

Design choices

- How to split
  - what measurement/criterion as measure of goodness
  - binary vs multi-category split

- When to stop
  - if leaf nodes contain only examples of the same class
  - feature values are all the same for all examples
  - statistical significance test

ID3 -- Iterative Dichotomizer 3

- one of the earlier/earliest decision tree algorithms
- Quinlan, J. R. 1986. Induction of Decision Trees. Mach. Learn. 1, 1 (Mar. 1986), 81-106.
- cannot handle numeric features
- no pruning, prone to overfitting
- short and wide trees (compared to CART)
- maximizing information gain/minimizing entropy
- discrete features, binary and multi-category features

C4.5

- continuous and discrete features
- Ross Quinlan 1993, Quinlan, J. R. (1993). C4. 5: Programming for machine learning. *Morgan Kauffmann*, *38*, 48.
- continuous is very expensive, because must consider all possible ranges
- handles missing attributes (ignores them in gain compute)
- post-pruning (bottom-up pruning)
- Gain Ratio

CART

- Breiman, L. (1984). *Classification and regression trees*. Belmont, Calif: Wadsworth International Group.
- continuous and discrete features
- strictly binary splits (taller trees than ID3, C4.5)
- binary splits can generate better trees than C4.5, but tend to be larger and harder to interpret; k-attributes has a ways to create a binary partitioning
- variance reduction in regression trees
- Gini impurity, twoing criteria in classification trees
- cost complexity pruning

Others

- CHAID (CHi-squared Automatic Interaction Detector); Kass, G. V. (1980). "An exploratory technique for investigating large quantities of categorical data". *Applied Statistics*. 29 (2): 119–127.
- MARS (Multivariate adaptive regression splines); Friedman, J. H. (1991). "Multivariate Adaptive Regression Splines". *The Annals of Statistics*. 19: 1
- C5.0 (patented)
- ...

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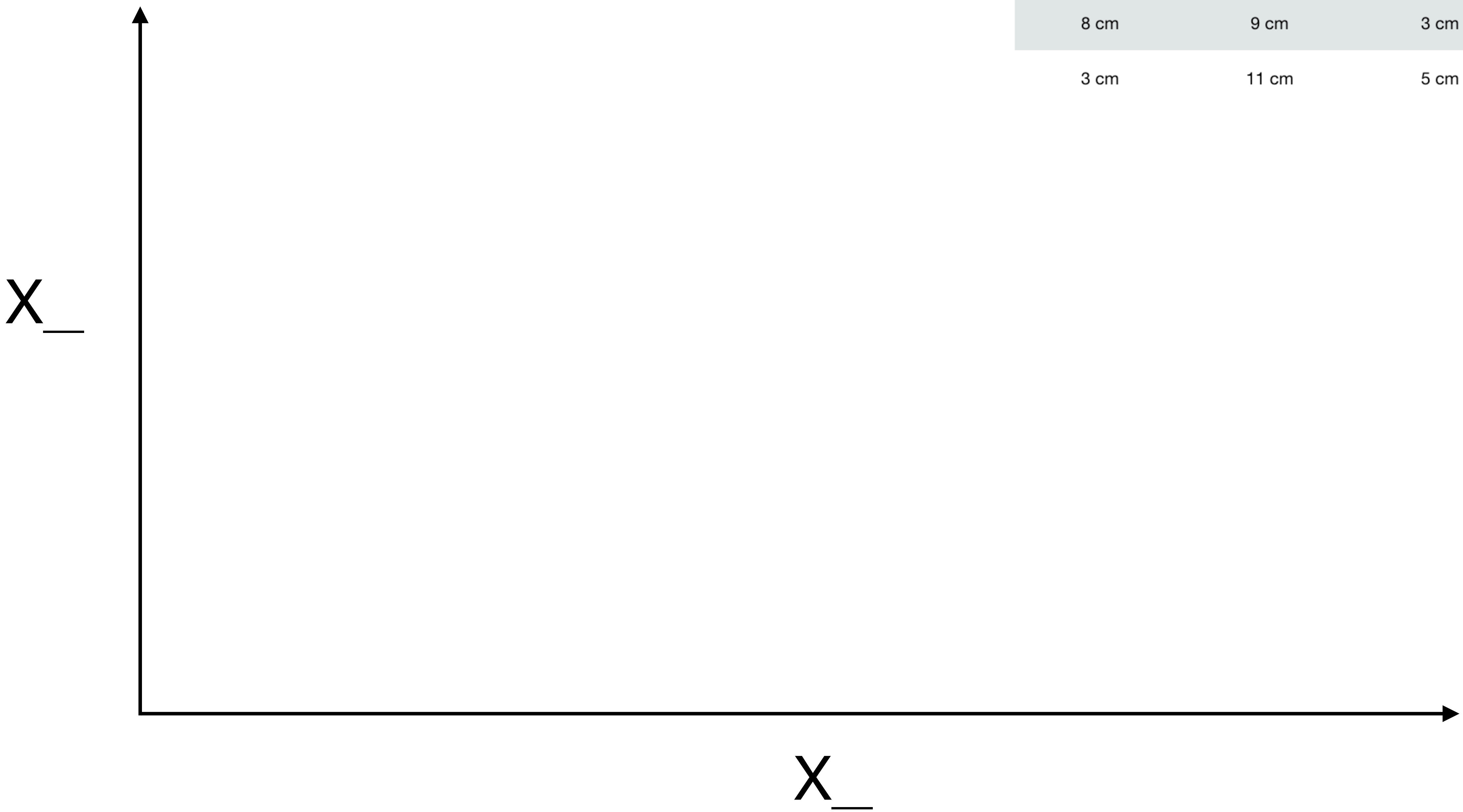
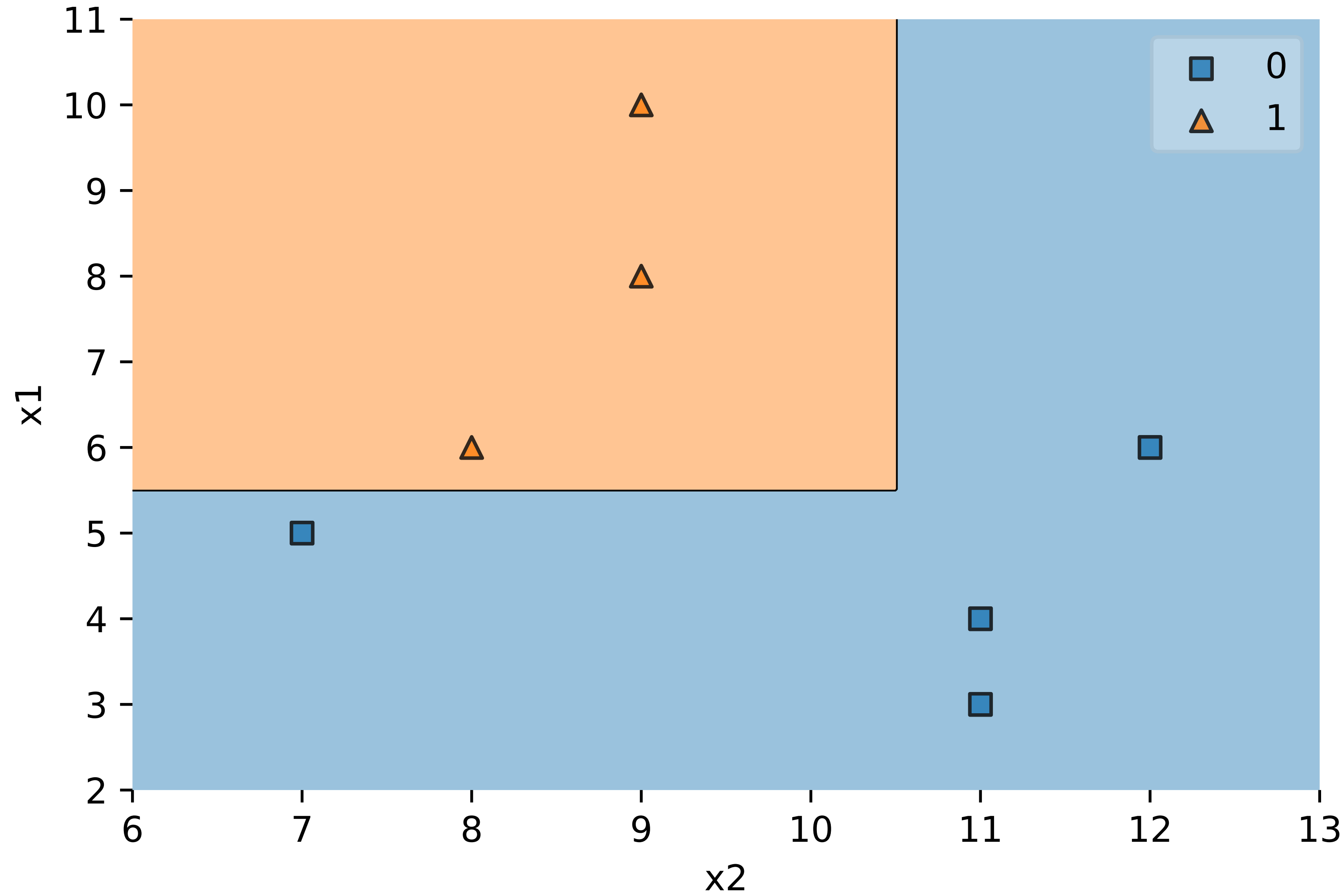
Finding a Decision Rule

x_1	x_2	x_3	y
6 cm	8 cm	9 cm	1
4 cm	11 cm	2 cm	0
6 cm	12 cm	4 cm	0
10 cm	9 cm	3 cm	1
5 cm	7 cm	8 cm	0
8 cm	9 cm	3 cm	1
3 cm	11 cm	5 cm	0

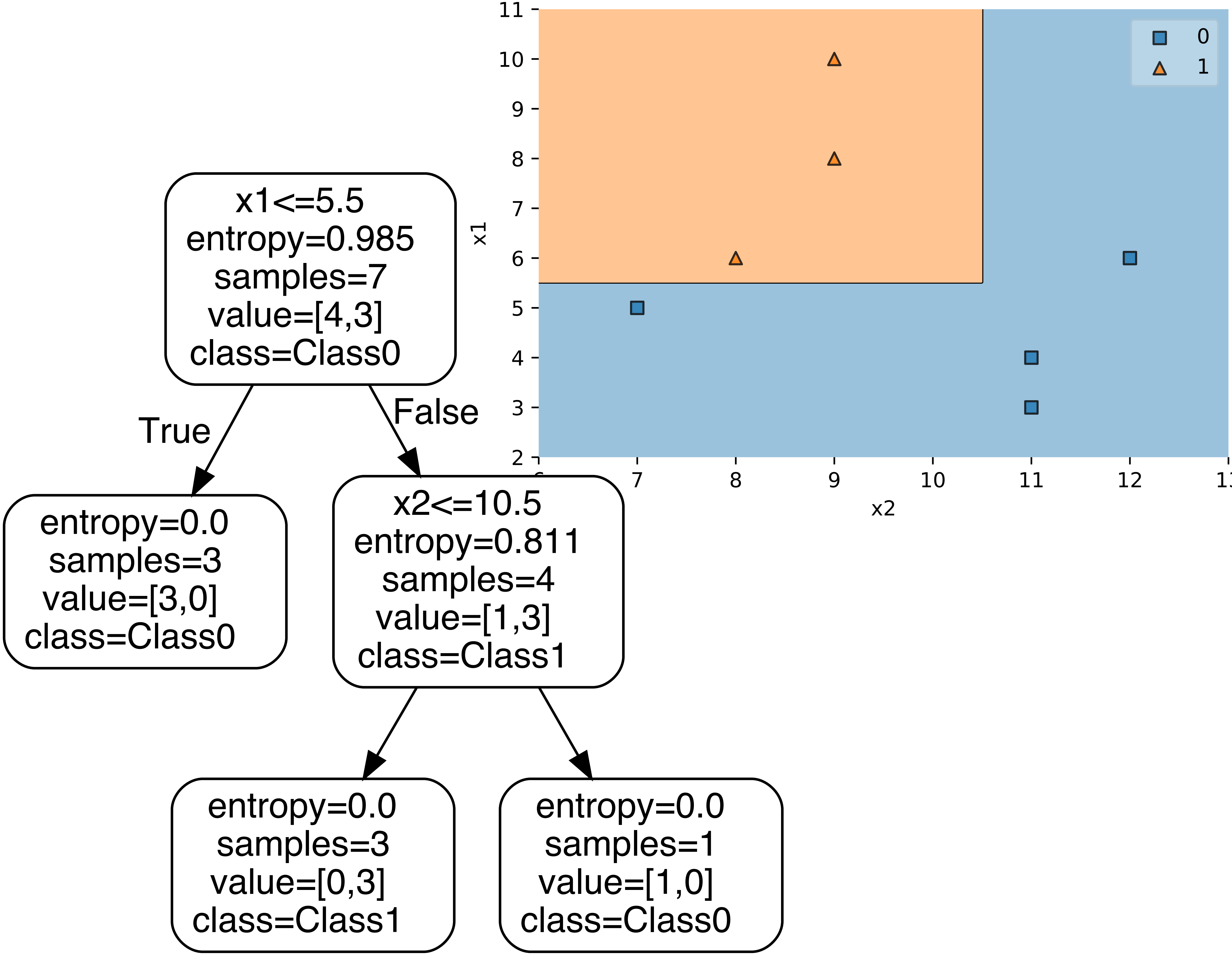
Drawing a Decision Boundary

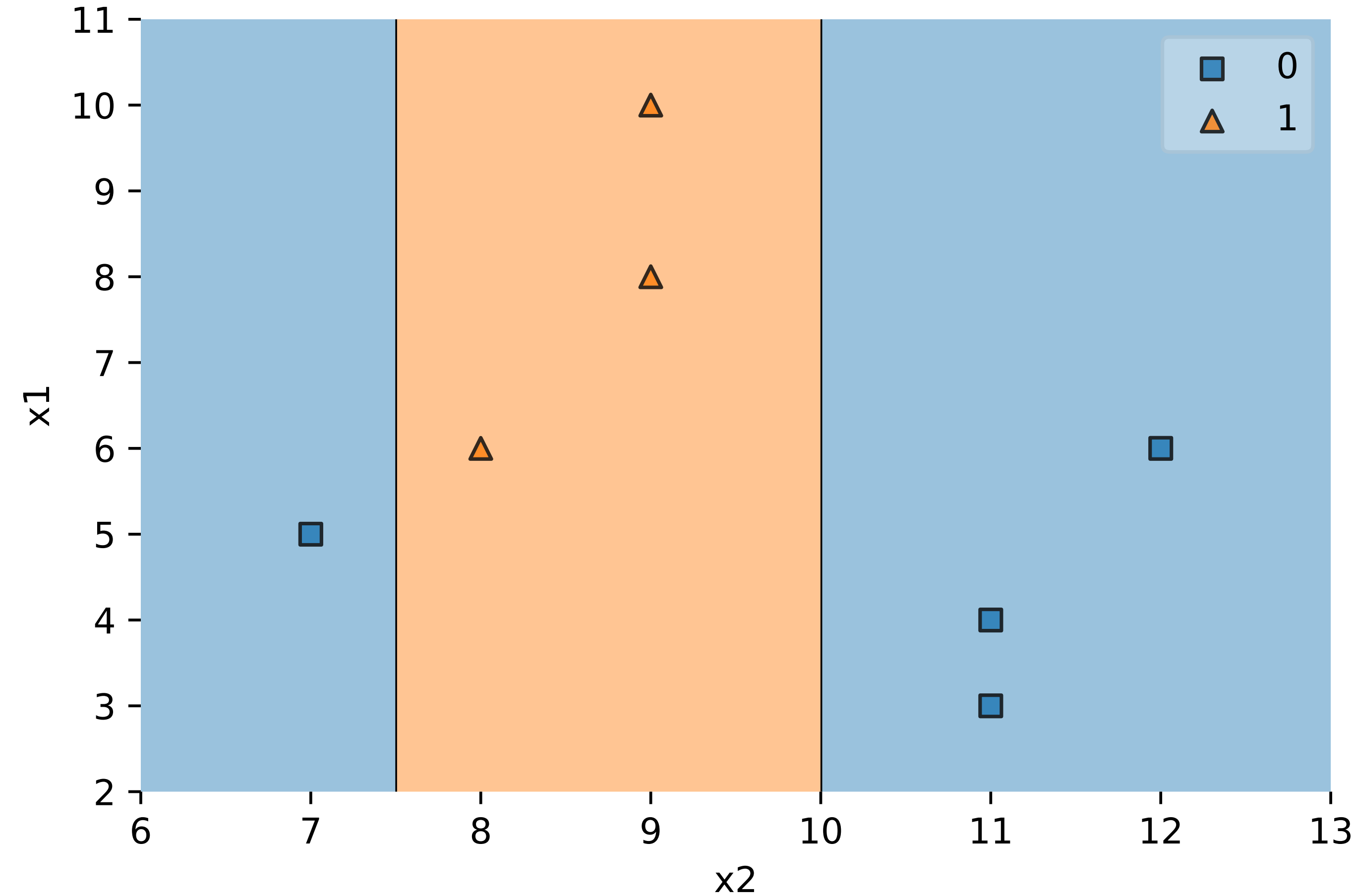
x_1	x_2	x_3	y
6 cm	8 cm	9 cm	1
4 cm	11 cm	2 cm	0
6 cm	12 cm	4 cm	0
10 cm	9 cm	3 cm	1
5 cm	7 cm	8 cm	0
8 cm	9 cm	3 cm	1
3 cm	11 cm	5 cm	0



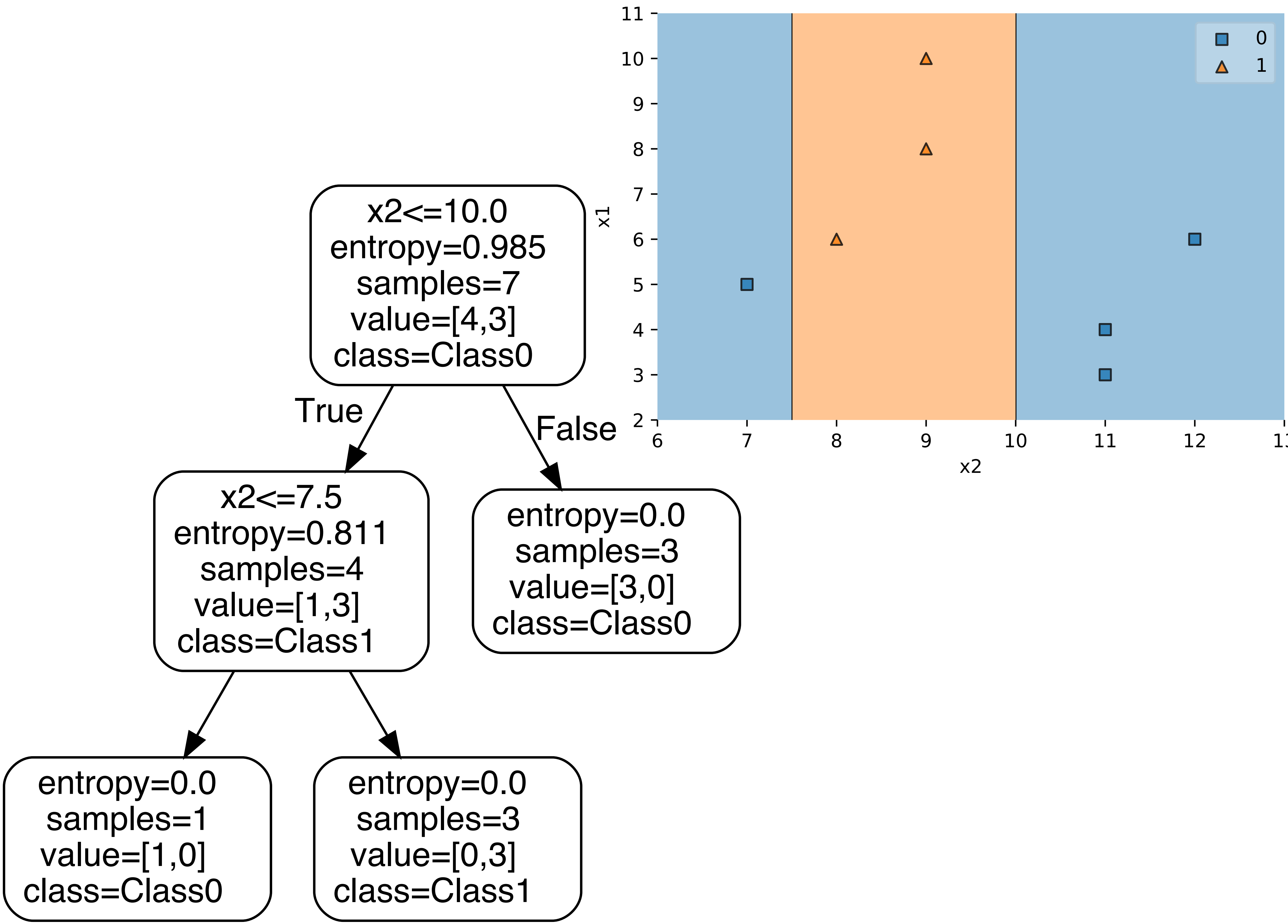


0
1
x1
x2


x1<=5.5
entropy=0.985
samples=7
value=[4,3]
class=Class0
True
False
entropy=0.0
samples=3
value=[3,0]
class=Class0
x2<=10.5
entropy=0.811
samples=4
value=[1,3]
class=Class1
entropy=0.0
samples=3
value=[0,3]
class=Class1
entropy=0.0
samples=1
value=[1,0]
class=Class0
0
1
x1
x2
2
3
4
5
6
7
8
9
10
11
12
13



0
1
x1
x2
11
10
9
8
7
6
5
4
3
2
6
7
8
9
10
11
12
13


x2<=10.0
entropy=0.985
samples=7
value=[4,3]
class=Class0
True
False
x2<=7.5
entropy=0.811
samples=4
value=[1,3]
class=Class1
entropy=0.0
samples=3
value=[3,0]
class=Class0
entropy=0.0
samples=1
value=[1,0]
class=Class0
entropy=0.0
samples=3
value=[0,3]
class=Class1
0
1
x1
x2

The Splitting Criterion

Information Gain

$$GAIN(\mathscr{D}, x_j) = H(\mathscr{D}) - \sum_{v \in Values(x_j)} \frac{|\mathscr{D}_v|}{|\mathscr{D}|} H(\mathscr{D}_v)$$

Shannon Entropy

Refer to lecture notes

Entropy

$$H = -\sum_{i} p(i \mid x_j) \log_2(p(i \mid x_j))$$

Gini Impurity

$$Gini = 1 - \sum_{i} \left(p(i \,|\, x_j)^2 \right)$$

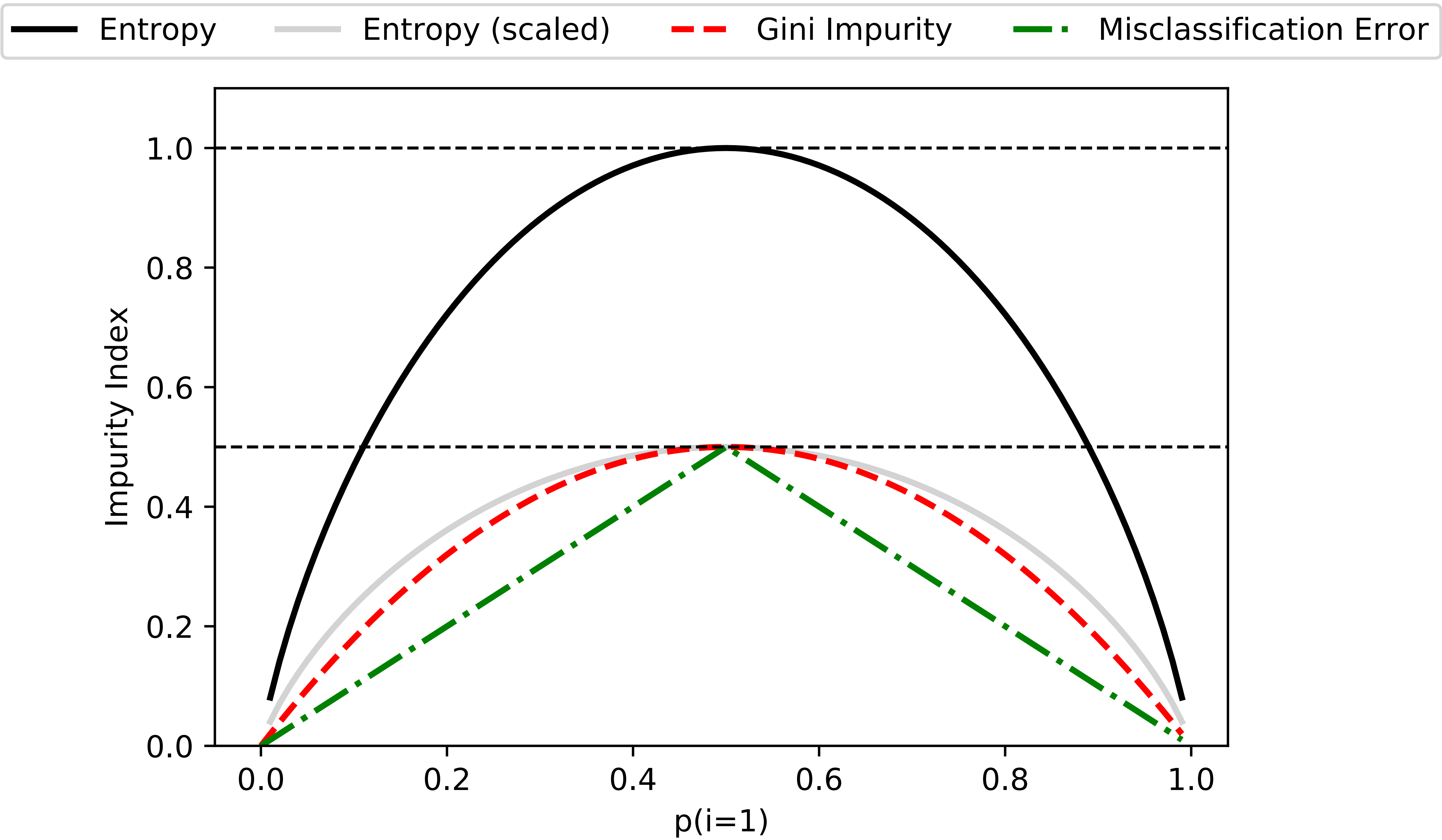
Misclassification Error

$$ERR = \frac{1}{n} \sum_{i=1}^{n} L(\hat{y}^{[i]}, y^{[i]}),$$

$$L(\hat{y}, y) = \begin{cases} 0 \textbf{ if } \hat{y} = y, \\ 1 \textbf{ otherwise.} \end{cases}$$

Misclassification Error

$$ERR = 1 - \max_i (p(i \mid x_j))$$



Entropy
Entropy (scaled)
Gini Impurity
Misclassification Error
Impurity Index
p(i=1)
0.0
0.2
0.4
0.6
0.8
1.0

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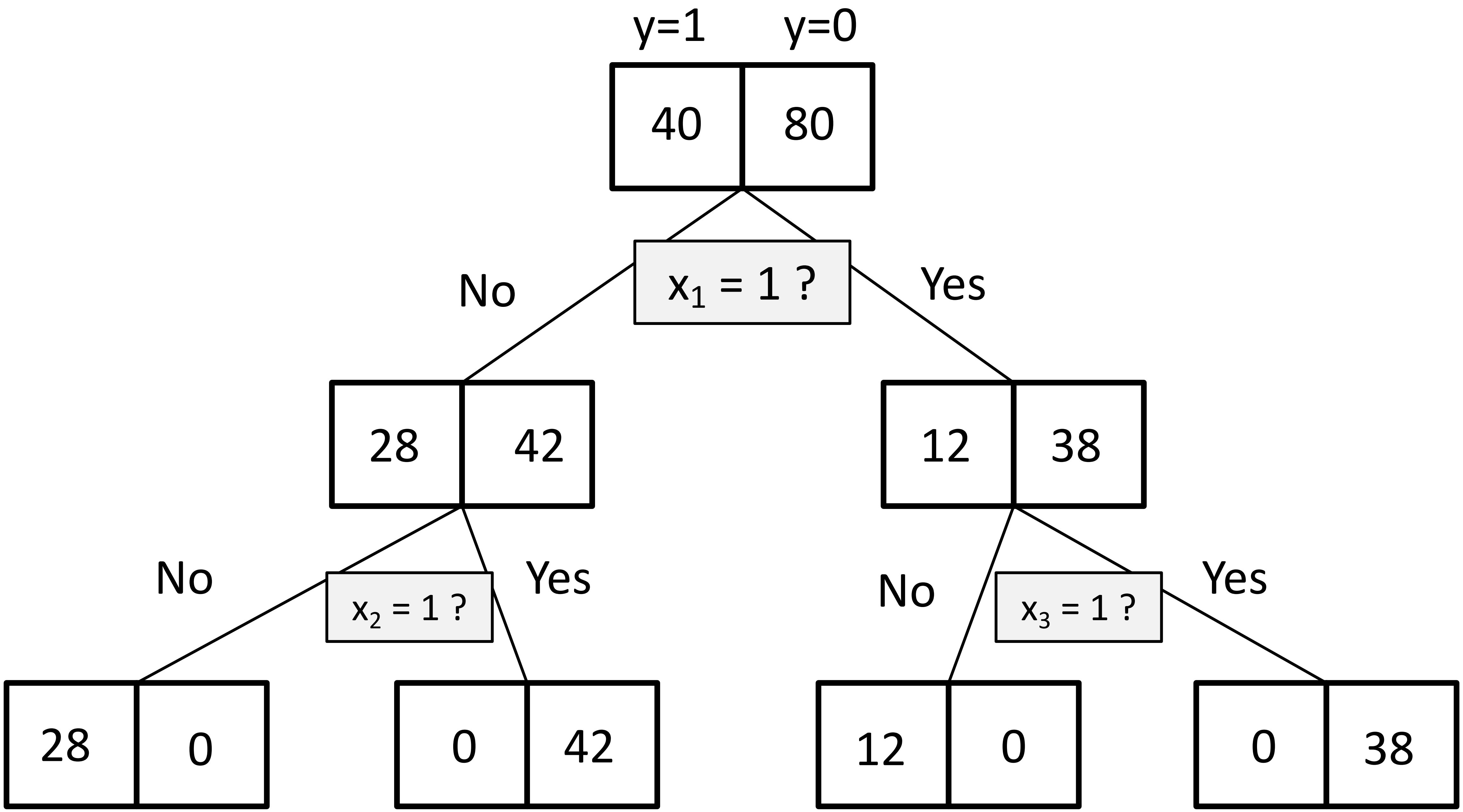
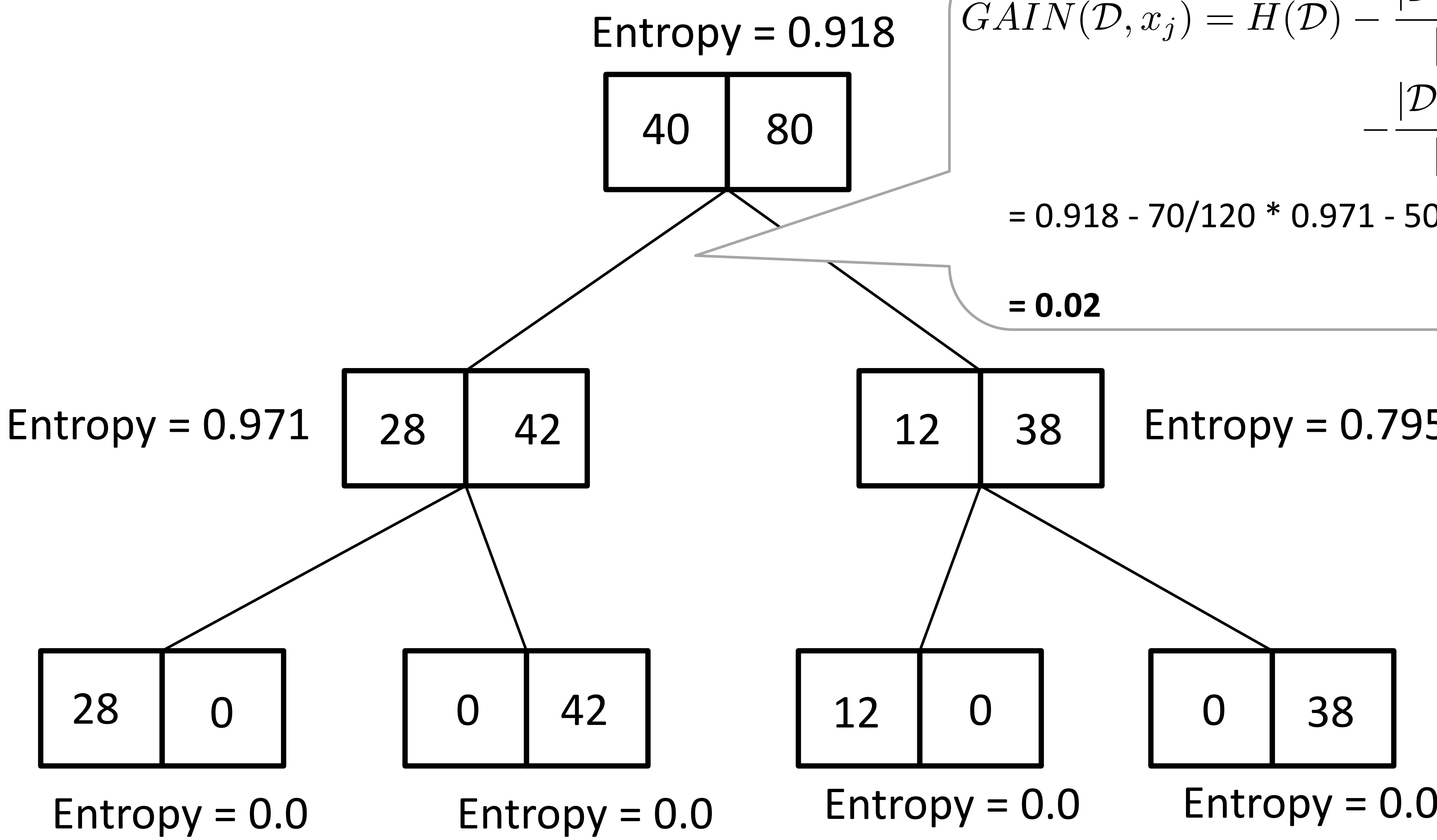
Why Growing Decision Trees via Entropy instead of Misclassification Error?

Why Growing Decision Trees via Entropy instead of Misclassification Error?

$$GAIN(\mathscr{D}, x_j) = I(\mathscr{D}) - \sum_{v \in Values(x_j)} \frac{|\mathscr{D}_v|}{|\mathscr{D}|} I(\mathscr{D}_v)$$



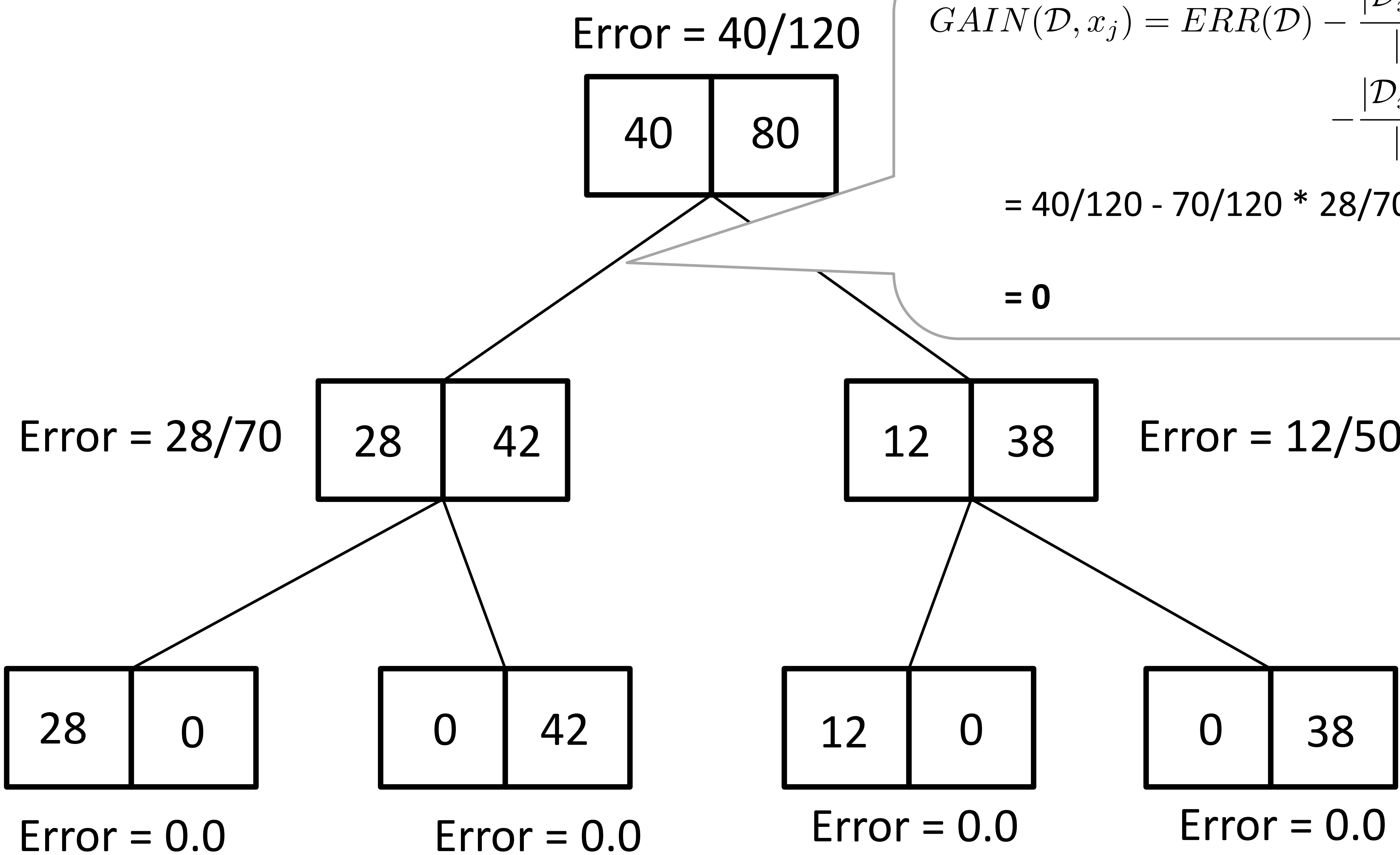
y=1
y=0
40
80
x_1 = 1 ?
No
Yes
28
42
12
38
No
x_2 = 1 ?
Yes
No
x_3 = 1 ?
Yes
28
0
0
42
12
0
0
38



$$GAIN(\mathcal{D}, x_j) = H(\mathcal{D}) - \frac{|\mathcal{D}_{x_j=1}|}{|\mathcal{D}|} H(\mathcal{D}_{x_j=1}) - \frac{|\mathcal{D}_{x_j=0}|}{|\mathcal{D}|} H(\mathcal{D}_{x_j=0})$$

= 0.918 - 70/120 * 0.971 - 50/120 * 0.795

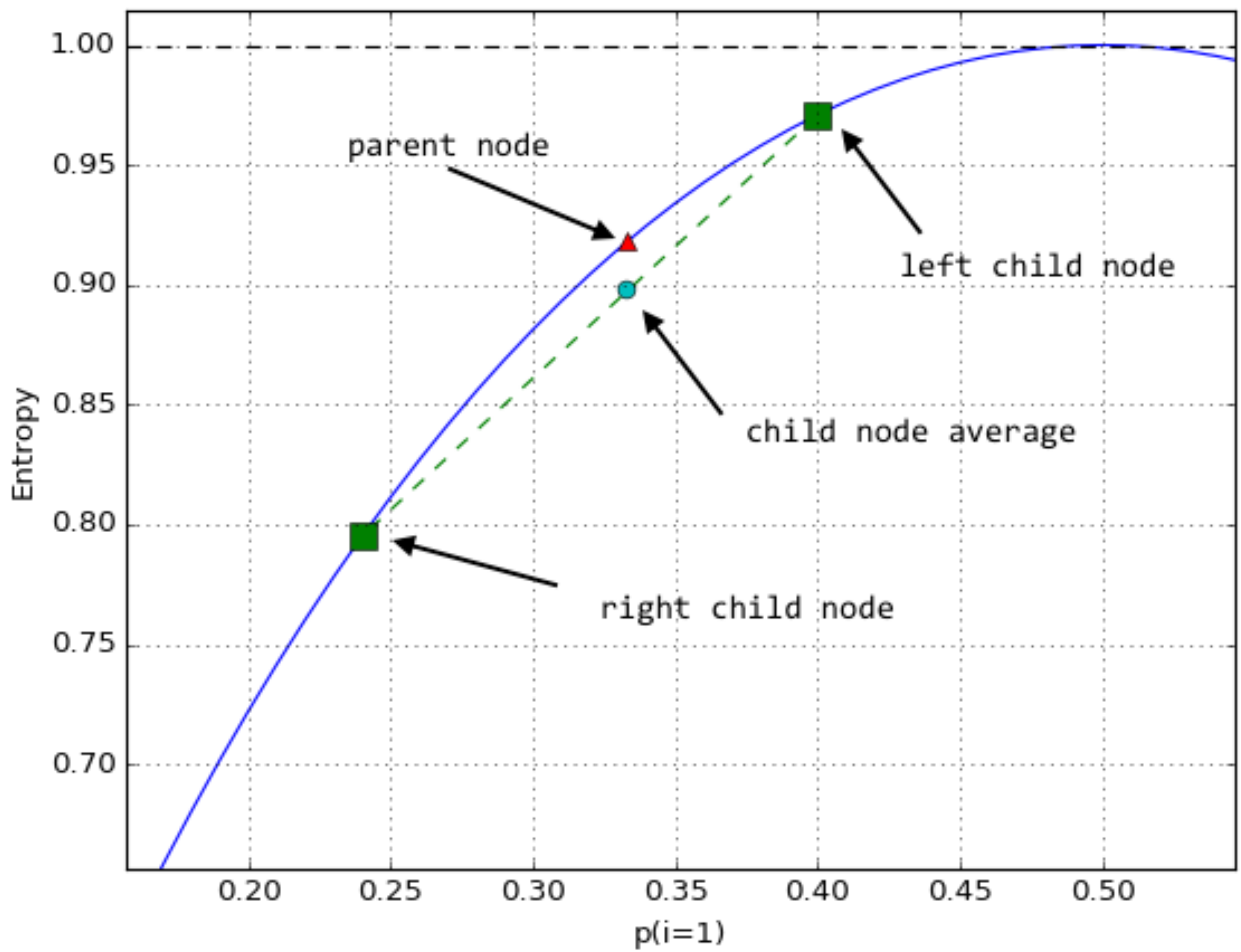
= 0.02



$$
\begin{aligned}
GAIN(\mathcal{D}, x_j) = ERR(\mathcal{D}) &- \frac{|\mathcal{D}_{x_j=1}|}{|\mathcal{D}|} ERR(\mathcal{D}_{x_j=1}) \\
&- \frac{|\mathcal{D}_{x_j=0}|}{|\mathcal{D}|} ERR(\mathcal{D}_{x_j=0})
\end{aligned}
$$

= 40/120 - 70/120 * 28/70 - 50/120 * 12/50

= 0


parent node
left child node
child node average
right child node
Entropy
p(i=1)
1.00
0.95
0.90
0.85
0.80
0.75
0.70
0.20
0.25
0.30
0.35
0.40
0.45
0.50

Topics

Gain Ratio

$$GainRatio(\mathscr{D}, x_j) = \frac{Gain(\mathscr{D}, x_j)}{SplitInfo(\mathscr{D}, x_j)}$$

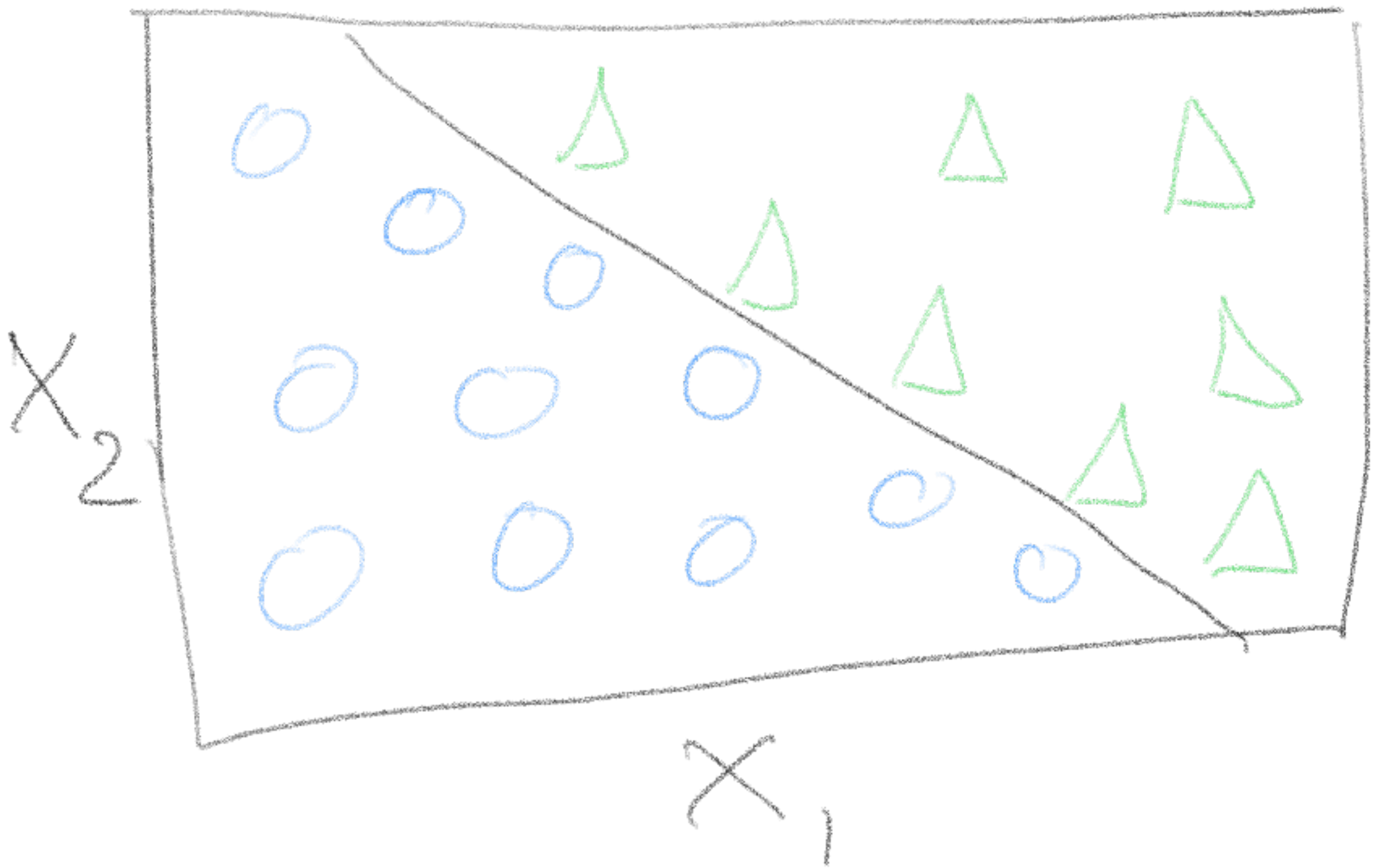
Quinlan 1986

where the split information measures the entropy of the feature:

$$SplitInfo(\mathscr{D}, x_j) = -\sum_{v \in x_j} \frac{|\mathscr{D}_v|}{|\mathscr{D}|} \log_2 \frac{|\mathscr{D}_v|}{|\mathscr{D}|}$$

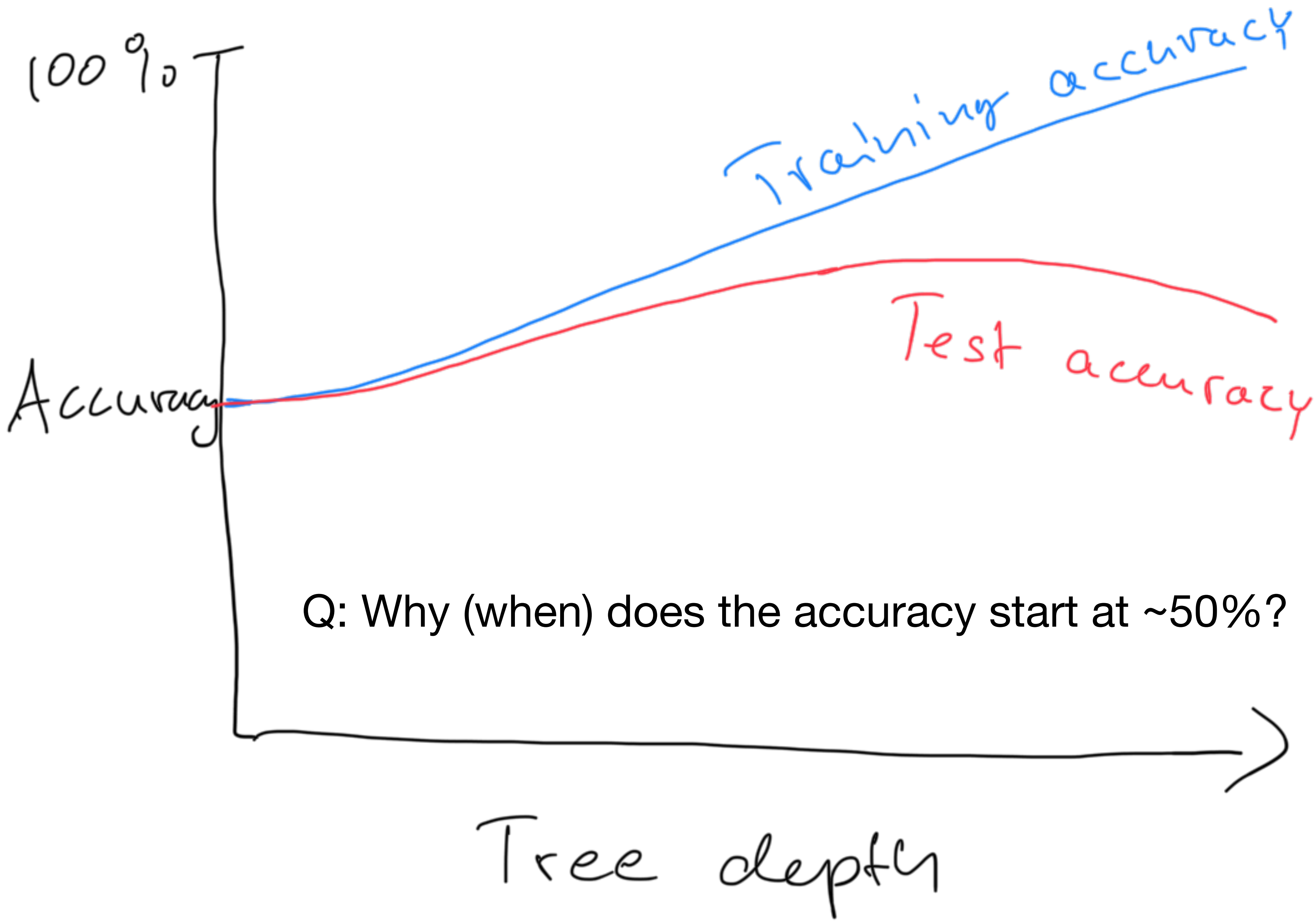
Penalizes splitting categorical attributes with many values (e.g., think date column, or really bad: row ID) via the split information

Shortcomings



How would the decision tree split look like?

Overfitting



Q: Why (when) does the accuracy start at ~50%?

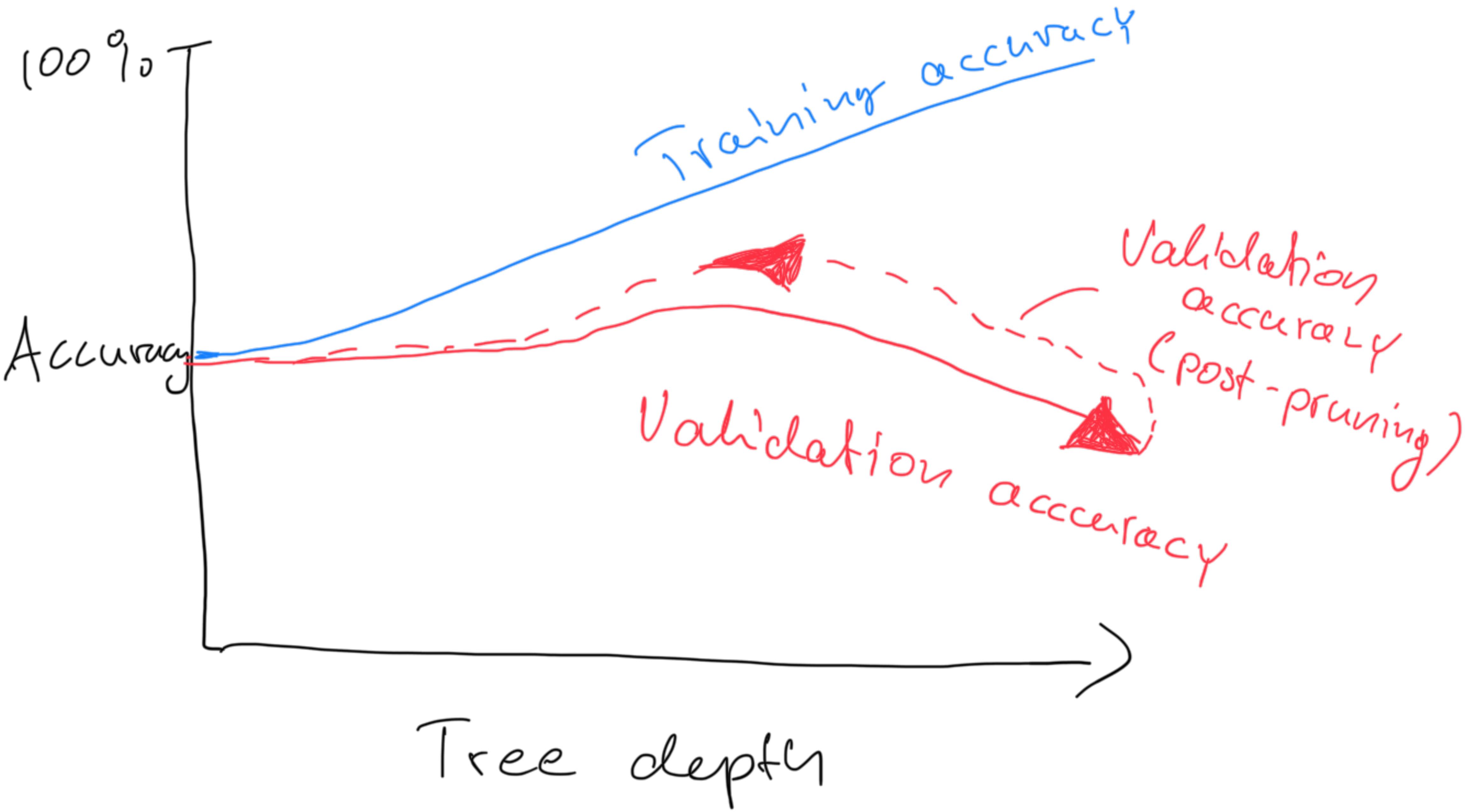
Pre-Pruning

- Set a depth cut-off (maximum tree depth) *a priori*
- Cost-complexity pruning: , where is an impurity measure, is a tuning parameter, and is the total number of nodes.
- Stop growing if split is not statistically significant (e.g., χ^2 test)
- Set a minimum number of data points for each node

Post-Pruning

- Grow full tree first, then remove nodes, in C4.5
- Reduced-error pruning, remove nodes via validation set eval. (problematic for limited data)
- Can also convert trees to rules first and then prune the rules

Post-Pruning



Regression Trees

Decision Tree Summary: Pros and Cons

- (+) Easy to interpret and communicate
- (+) Can represent "complete" hypothesis space
- (-) Easy to overfit
- (-) Elaborate pruning required
- (-) Expensive to just fit a "diagonal line"
- (-) Output range is bounded (dep. on training examples) in regression trees

Decision Trees and ML Categories

- Supervised vs. unsupervised learning algorithm
- Classification vs. regression
- Optimization method: ______
- Eager vs. lazy learning algorithm
- Batch vs. online learning algorithm
- Parametric vs. nonparametric model
- Deterministic vs. stochastic

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Demo

06-trees_demo.ipynb