Decision Trees

Week Goals

- Decision Trees: training and application
- Overfitting in Decision Trees
- Working with categorical features

Example: Predicting the Apartment Price

- **Target**: price of an apartment

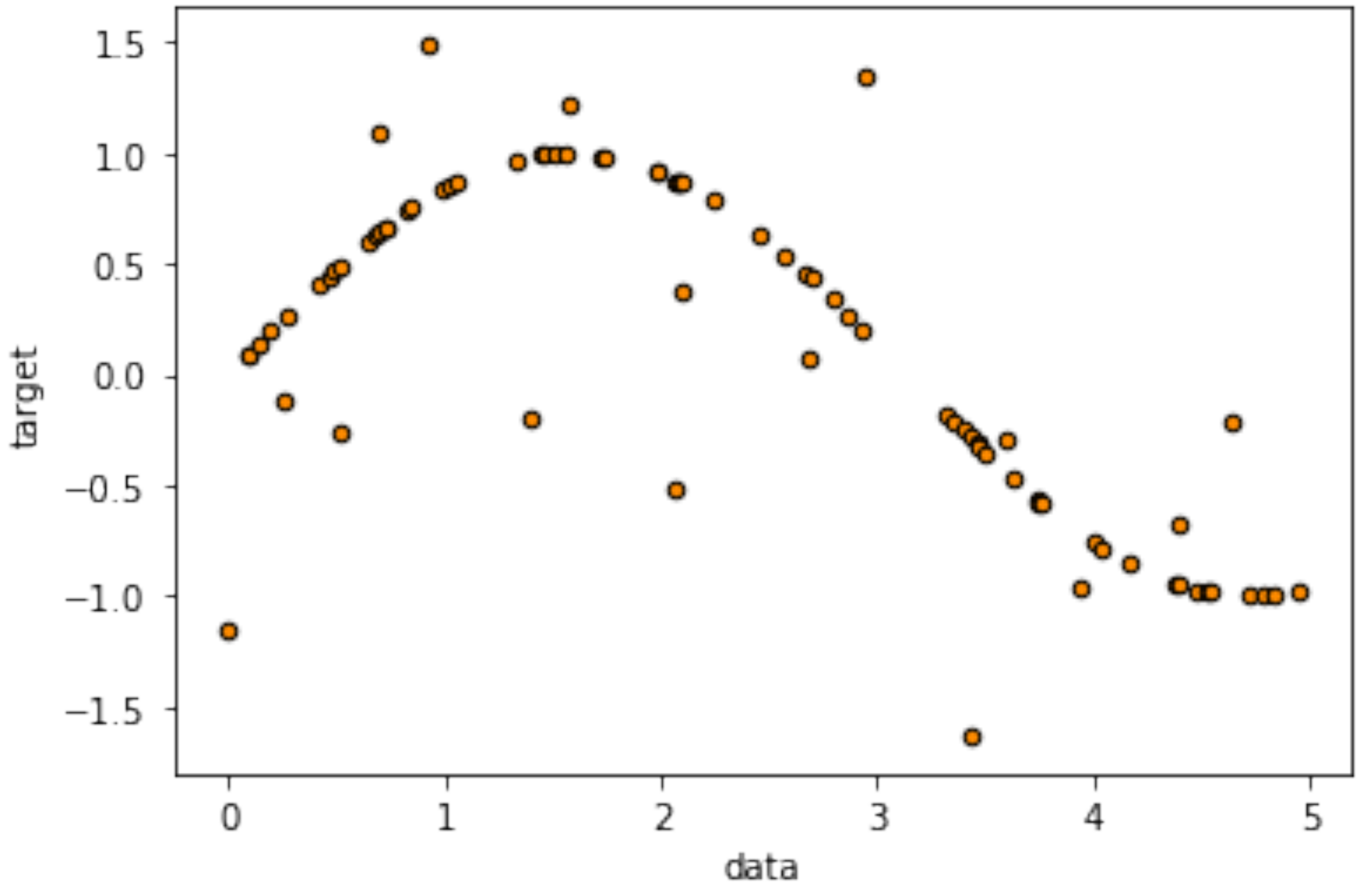
- **Features**: Area, Floor, Distance to nearest metro station, etc.

Example: Predicting the Apartment Price

- Linear Model:

$$a(x) = w_0 + w_1 * (area) + w_2 * \left(floor\right) + w_3 * (dist.\ ) + \ldots$$

- It is likely that the dependency is not linear



Example: Predicting the Apartment Price

- Linear Model:

$$a(x) = w_0 + w_1 * (area) + w_2 * \left(floor\right) + w_3 * (dist.\ ) + \ldots$$

- It is likely that the features are interconnected

Example: Predicting the Apartment Price

- Linear model with polynomial features:

$$a(x) = w_0 + w_1 * (area) + w_2 * \left(floow\right) \; + w_3 * (\,dist\,.)$$

$$+ w_4 * (area)^2 + w_5 * \left(floor\right)^2 + w_6 * (dist\,.)^2$$

$$+ w_7 * (area) * \left(floor\right) + \ldots$$

Example: Predicting the Apartment Price

- Linear model with polynomial features:

$$a(x) = w_0 + w_1 * (area) + w_2 * \left(floow\right) + w_3 * (\ dist\ .)$$

$$+ w_4 * (area)^2 + w_5 * \left(floor\right)^2 + w_6 * (dist\ .)^2$$

$$+ w_7 * (area) * \left(floor\right) + \ldots$$

- It maybe hard to interpret the result

- What does $(dist\ .) * \left(floor\right)^2$ mean?

Example: Predicting the Apartment Price

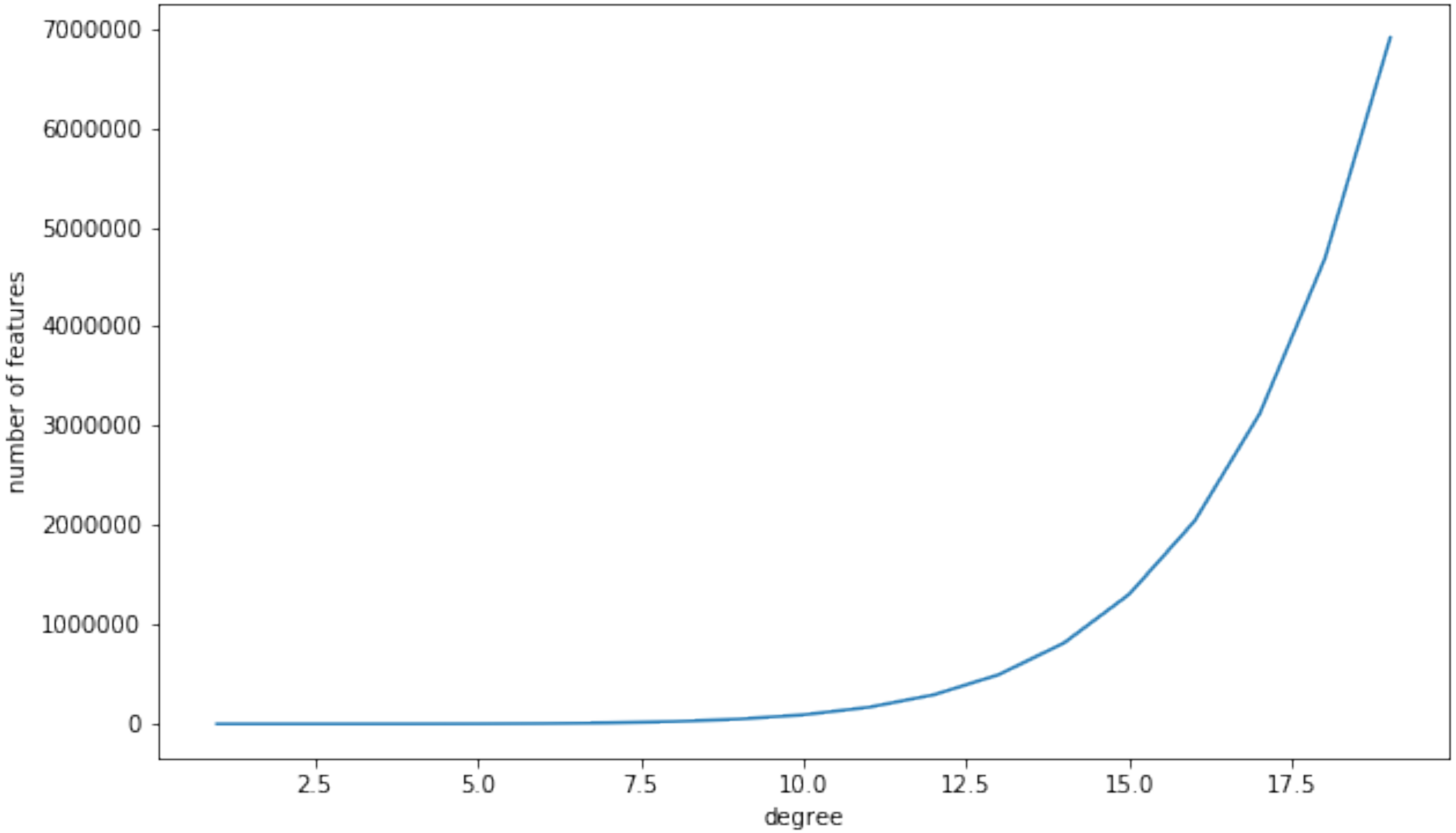
- Linear model with polynomial features:

$$a(x) = w_0 + w_1 * (area) + w_2 * \left(floow\right) + w_3 * (\,dist\,.\,)$$
$$+w_4 * (area)^2 + w_5 * \left(floor\right)^2 + w_6 * (dist\,.\,)^2$$
$$+w_7 * (area) * \left(floor\right) + \ldots$$

- Assume we had 10 features
- Polynomial of power 2 → 55 extra features
- Polynomial of power 3 → 220 extra features

Example: Predicting the Apartment Price

Linear model with polynomial features:



Example: Predicting the Apartment Price

- Add intervals of the features:

$$a(x) = w_0 + w_1 * [30 < area < 50] + w_2 * [50 < area < 80]$$

$$+ w_{20} * [2 < floor < 5] + \dots$$

$$+ w_{100} * [30 < area < 50][2 < floor < 5] + \dots$$

- It is easier to interpret features:

$$[30 < area < 50][2 < floor < 5]$$

- But we will have even more features!

Summary

- We need an efficient algorithm to find non-linear dependency between features and target variables

- Decision trees will allow us to do that

Decision Trees

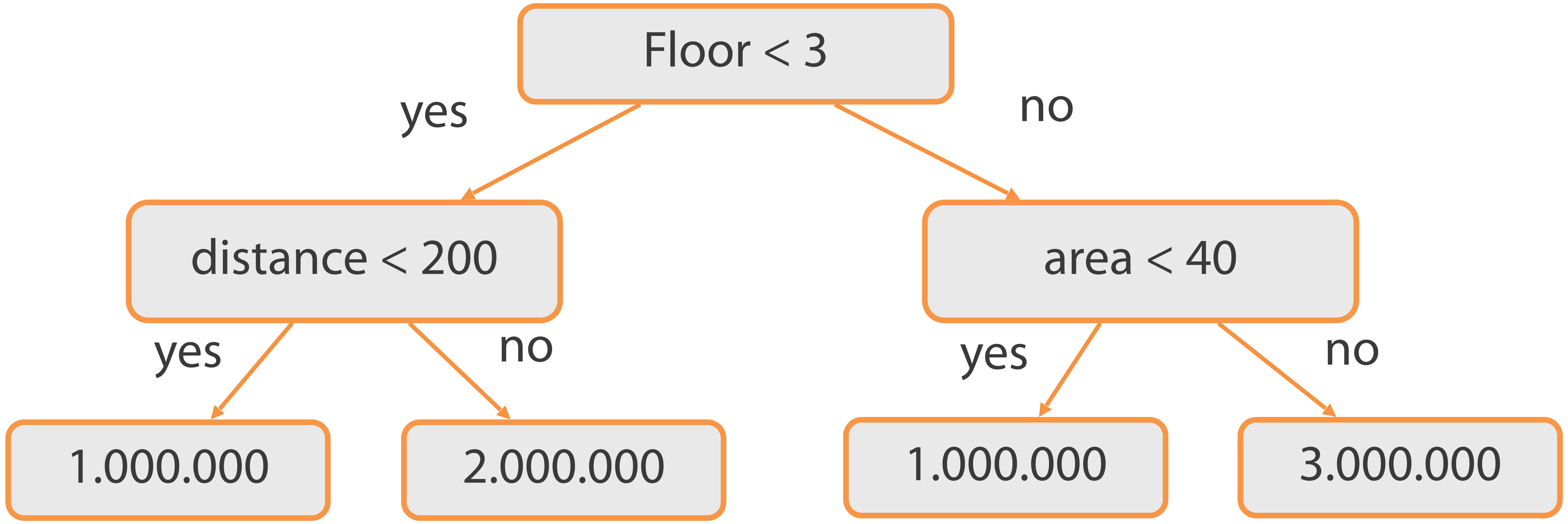
Logical Rule

$$[30 < area < 50]\,[2 < floor < 5]\,[500 < dist. < 1000]$$

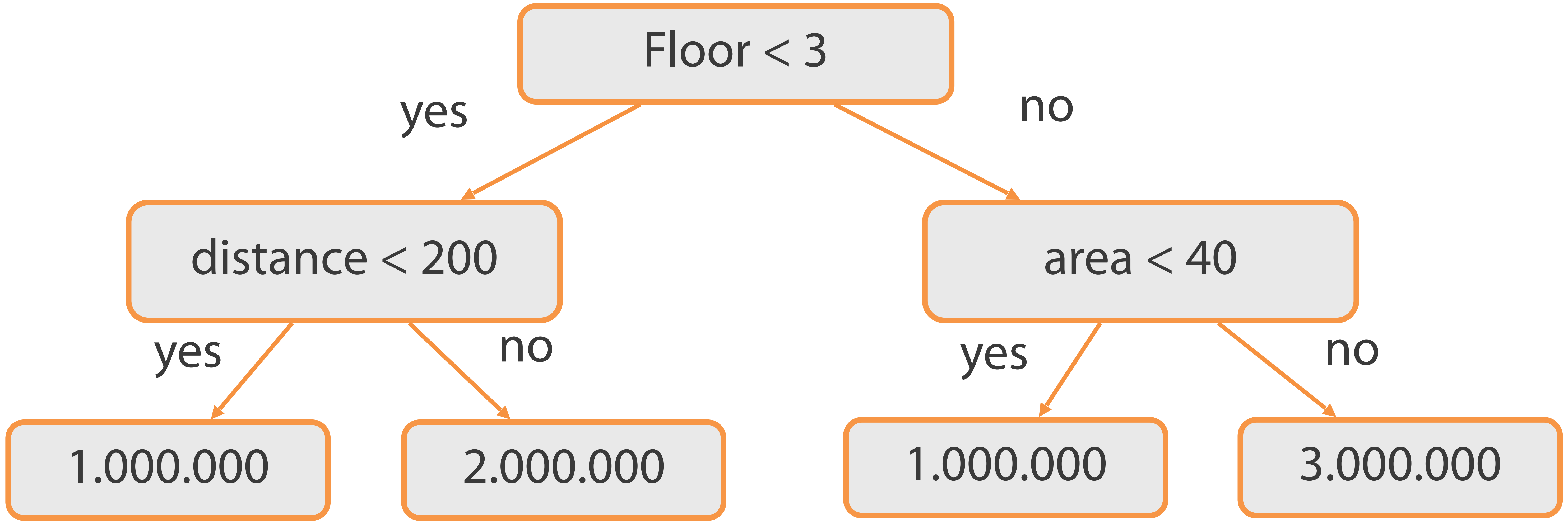
- Easy to explain
- Find non-linear dependencies

- We need to find good logical rules
- We need to build models out of them

Decision Trees

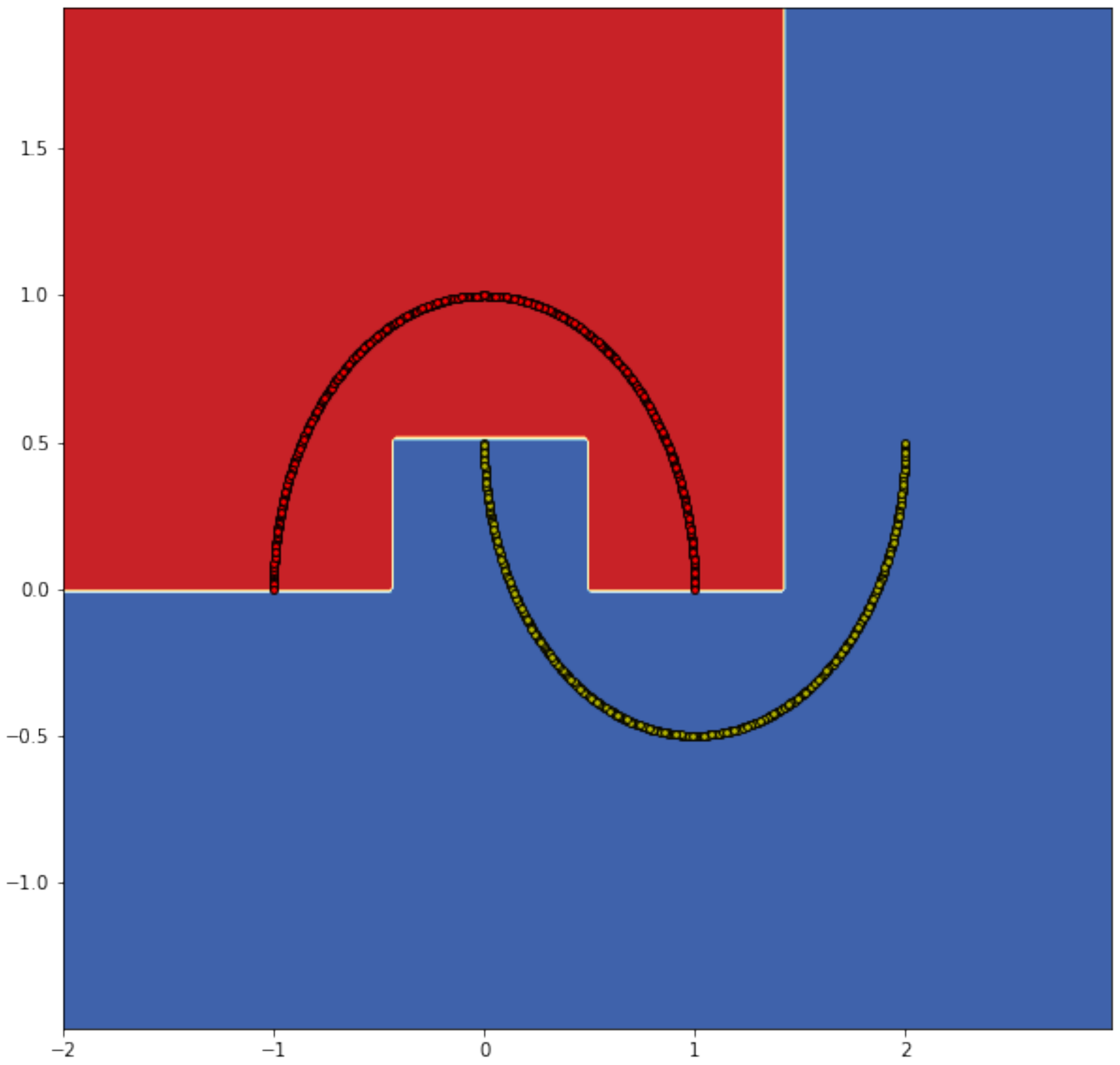


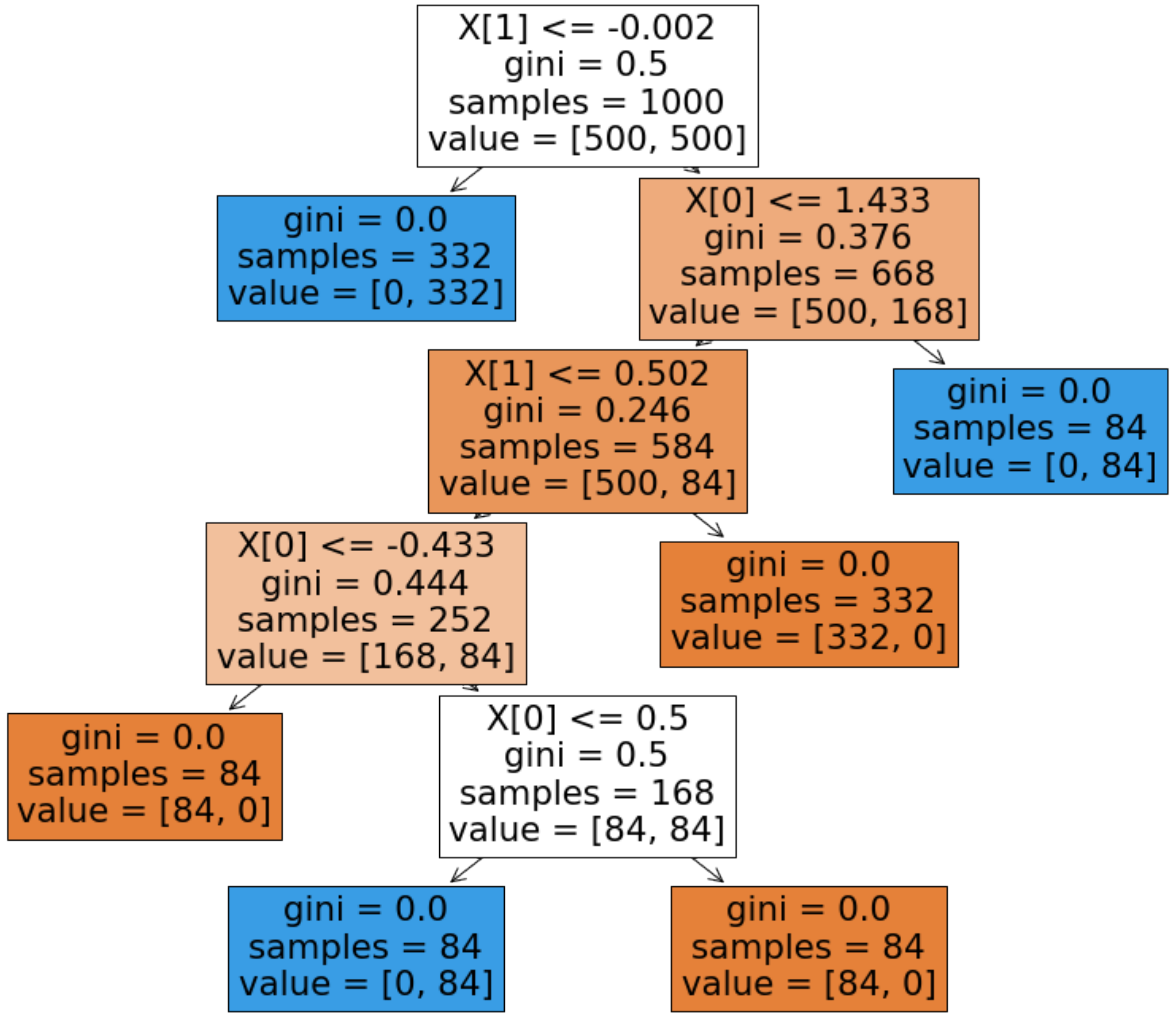
Decision Trees



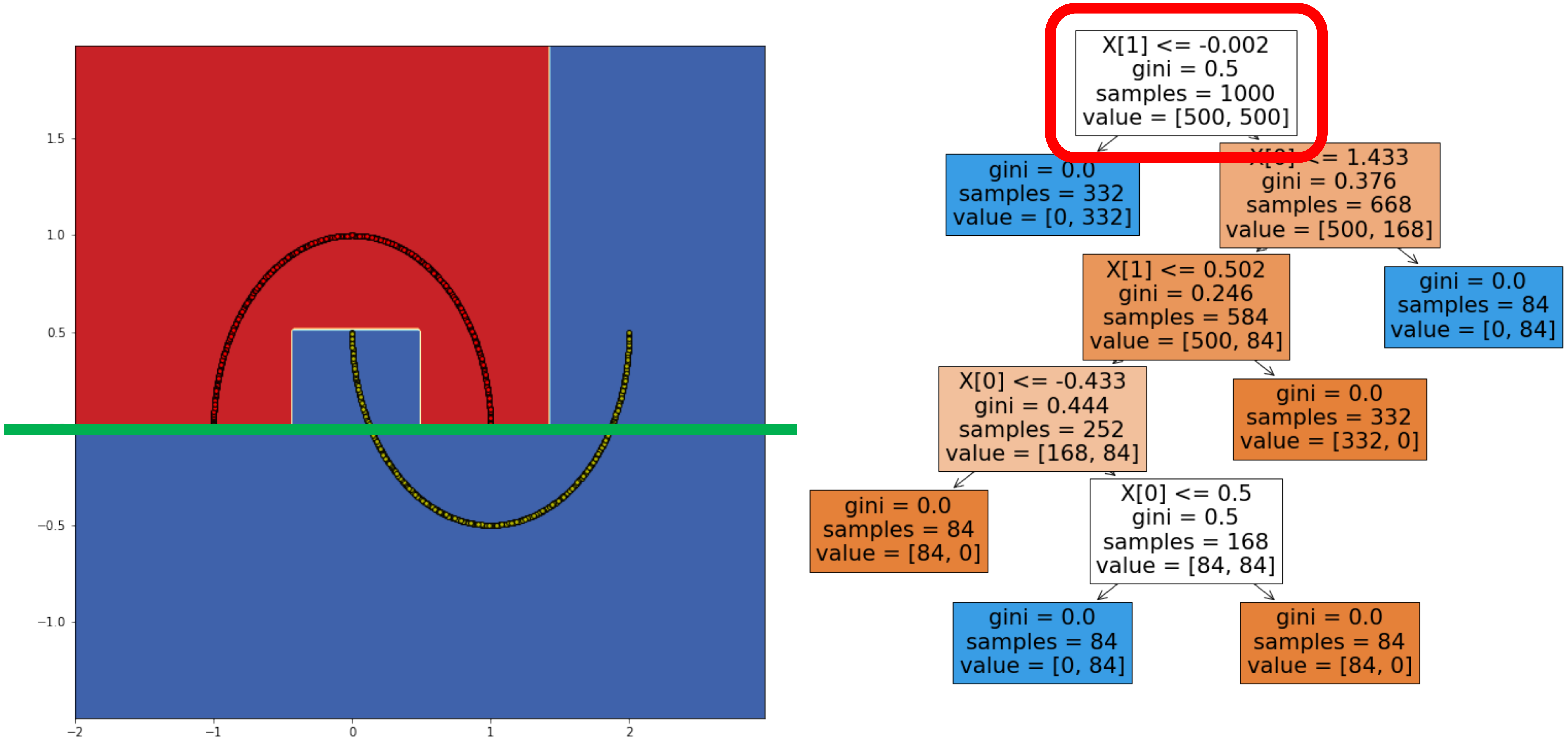
- **Internal Nodes**: splitting criterion $\left[x_j < t\right]$
- **Leaves**: predictions $c \in \mathbb{Y}$

Decision Trees

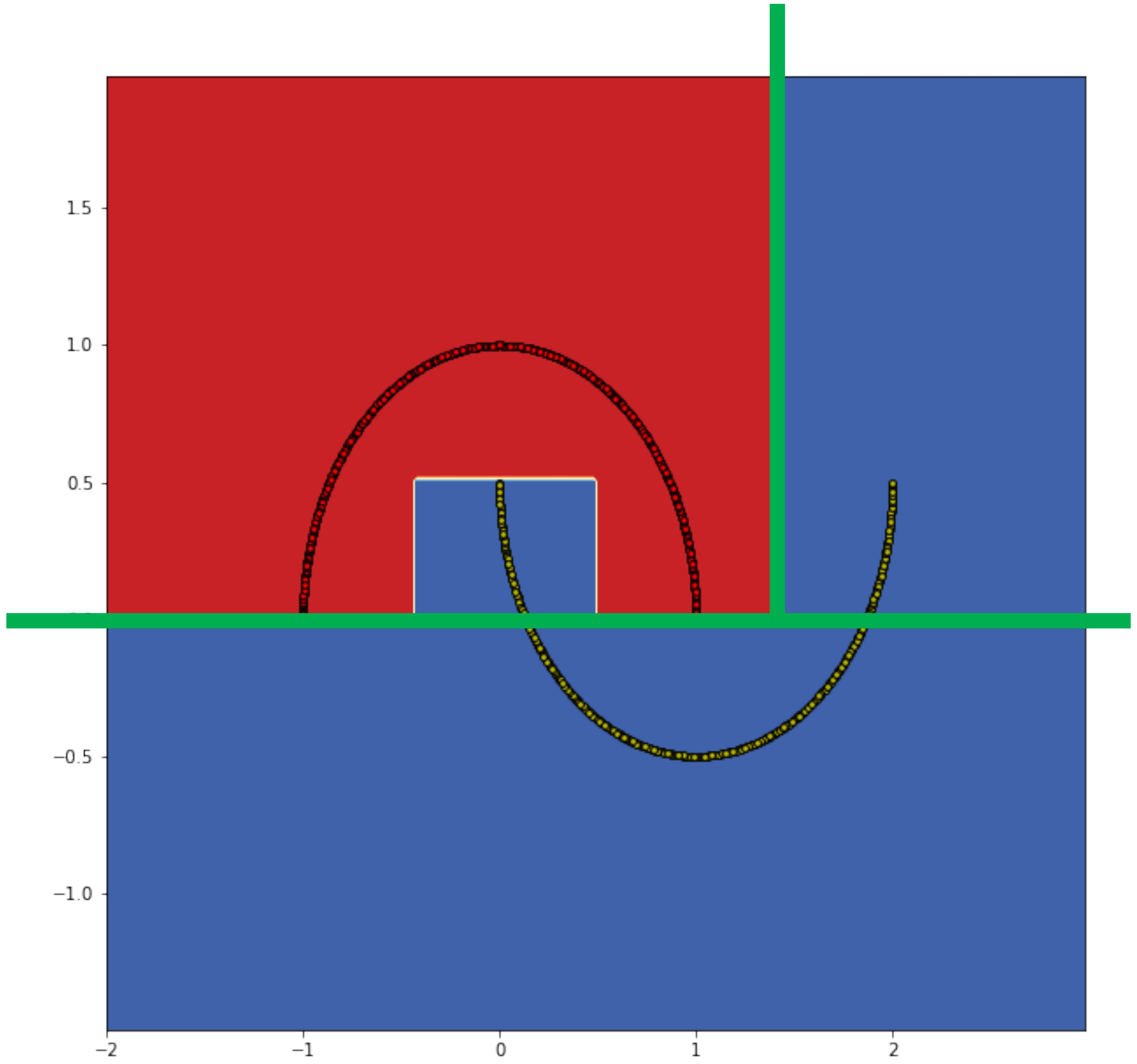


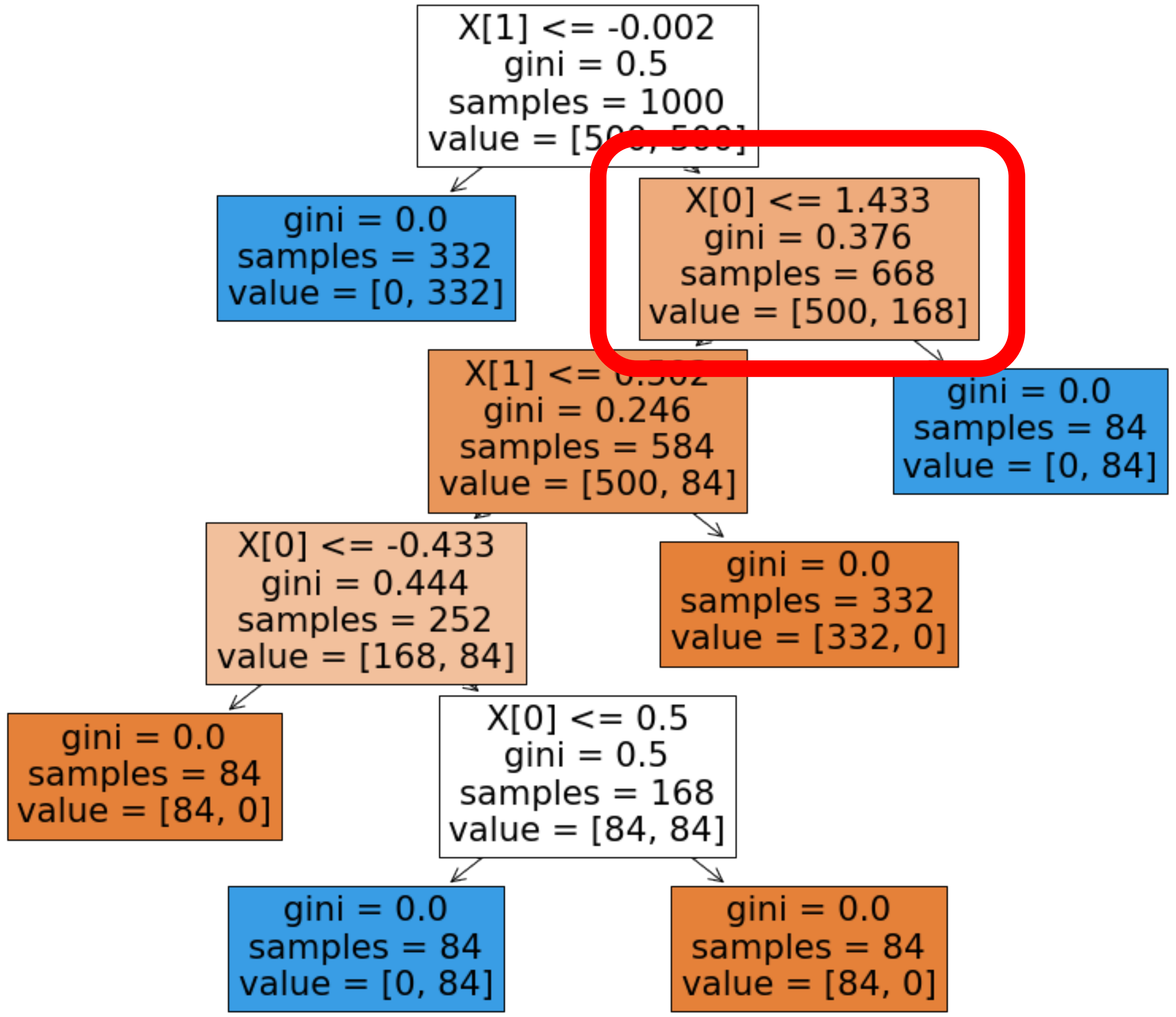


Decision Trees



Decision Trees





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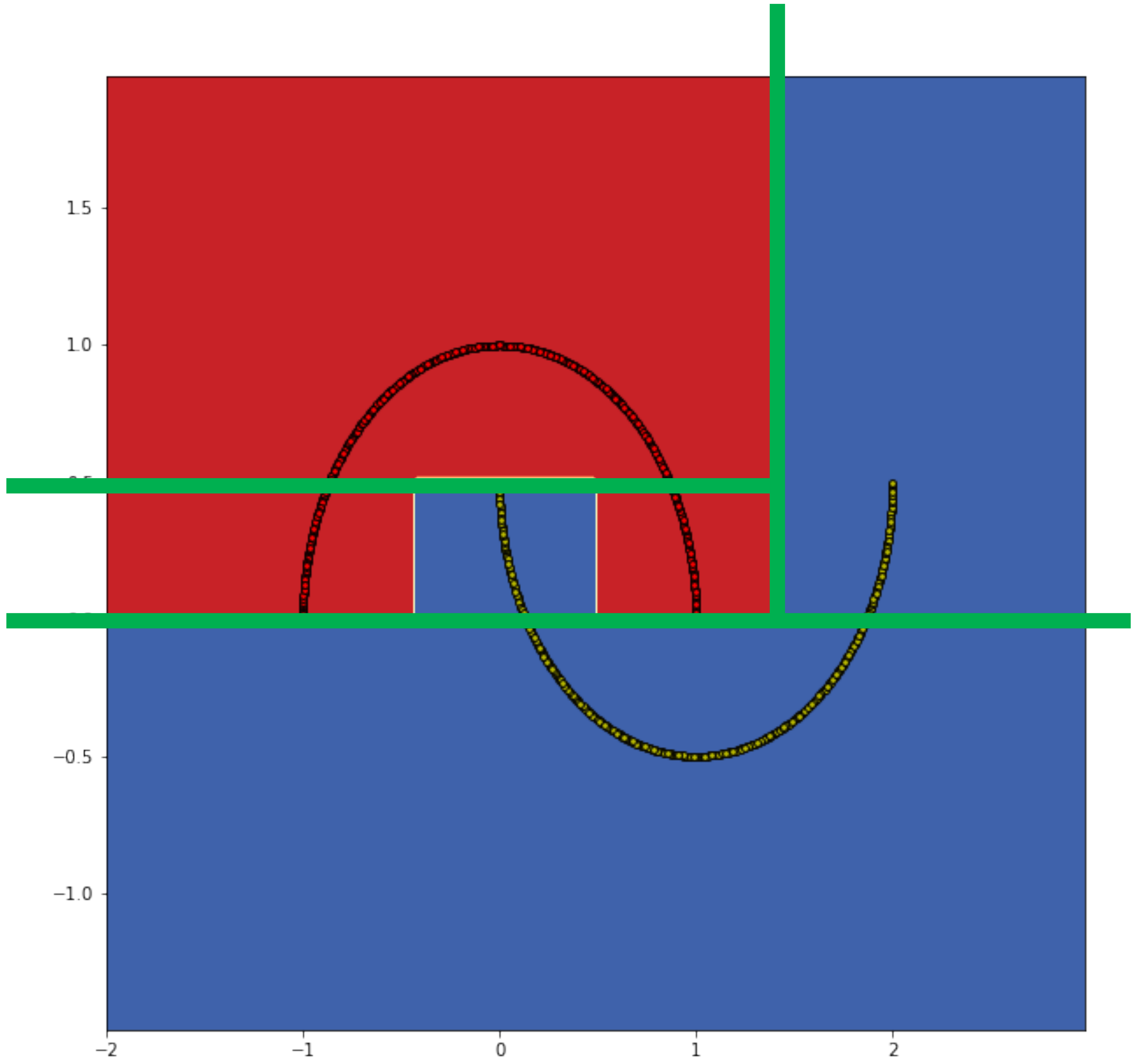
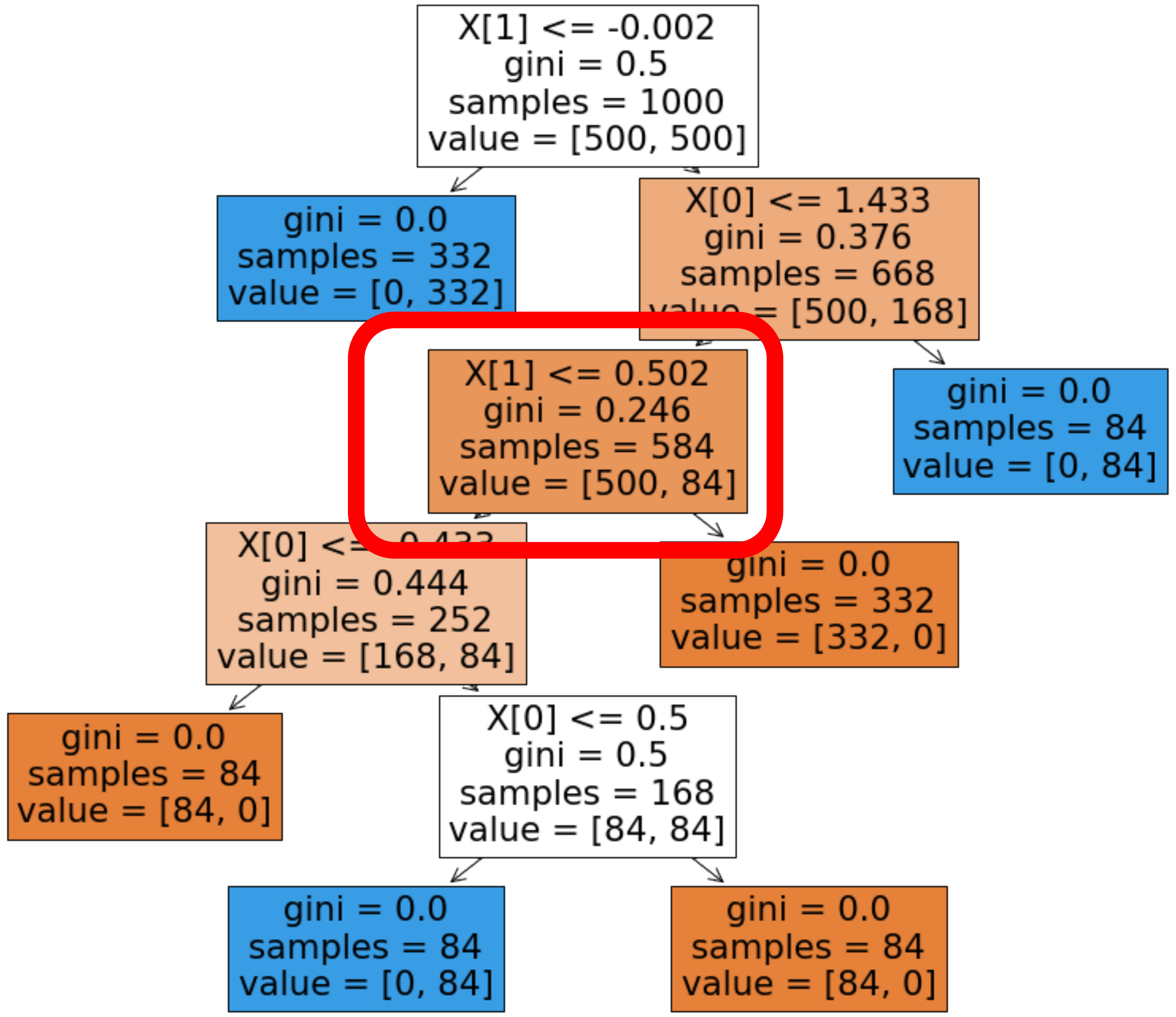
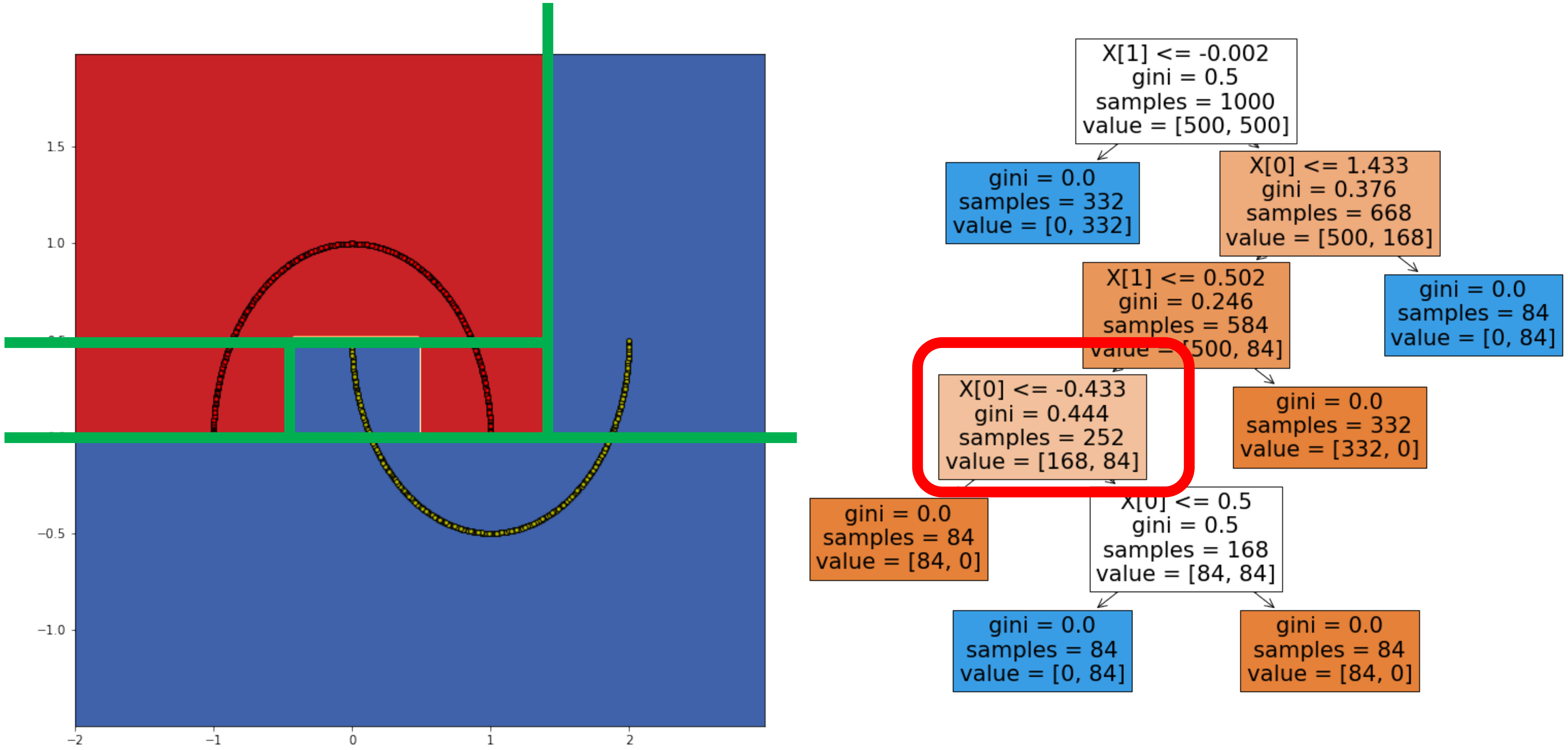
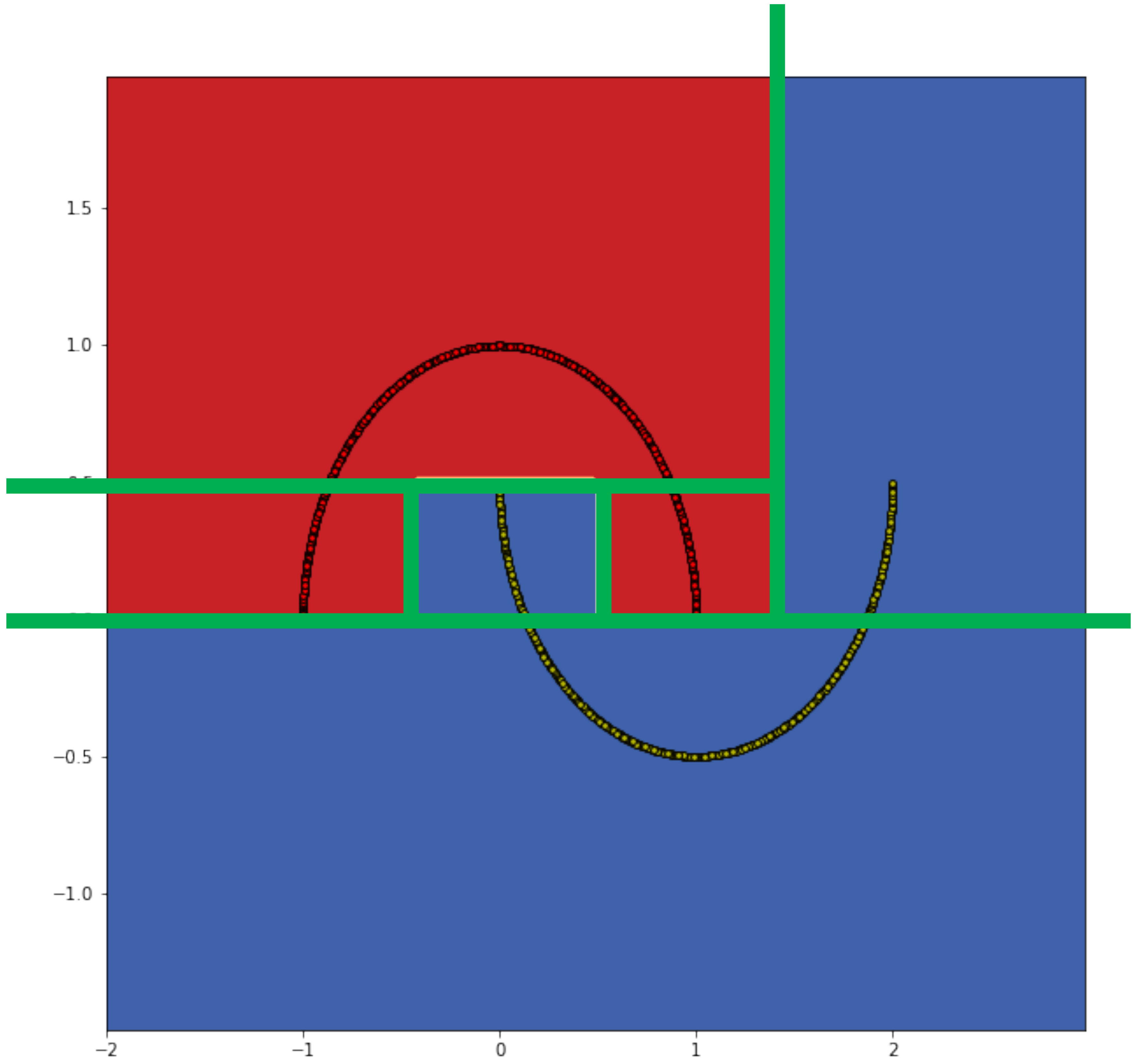


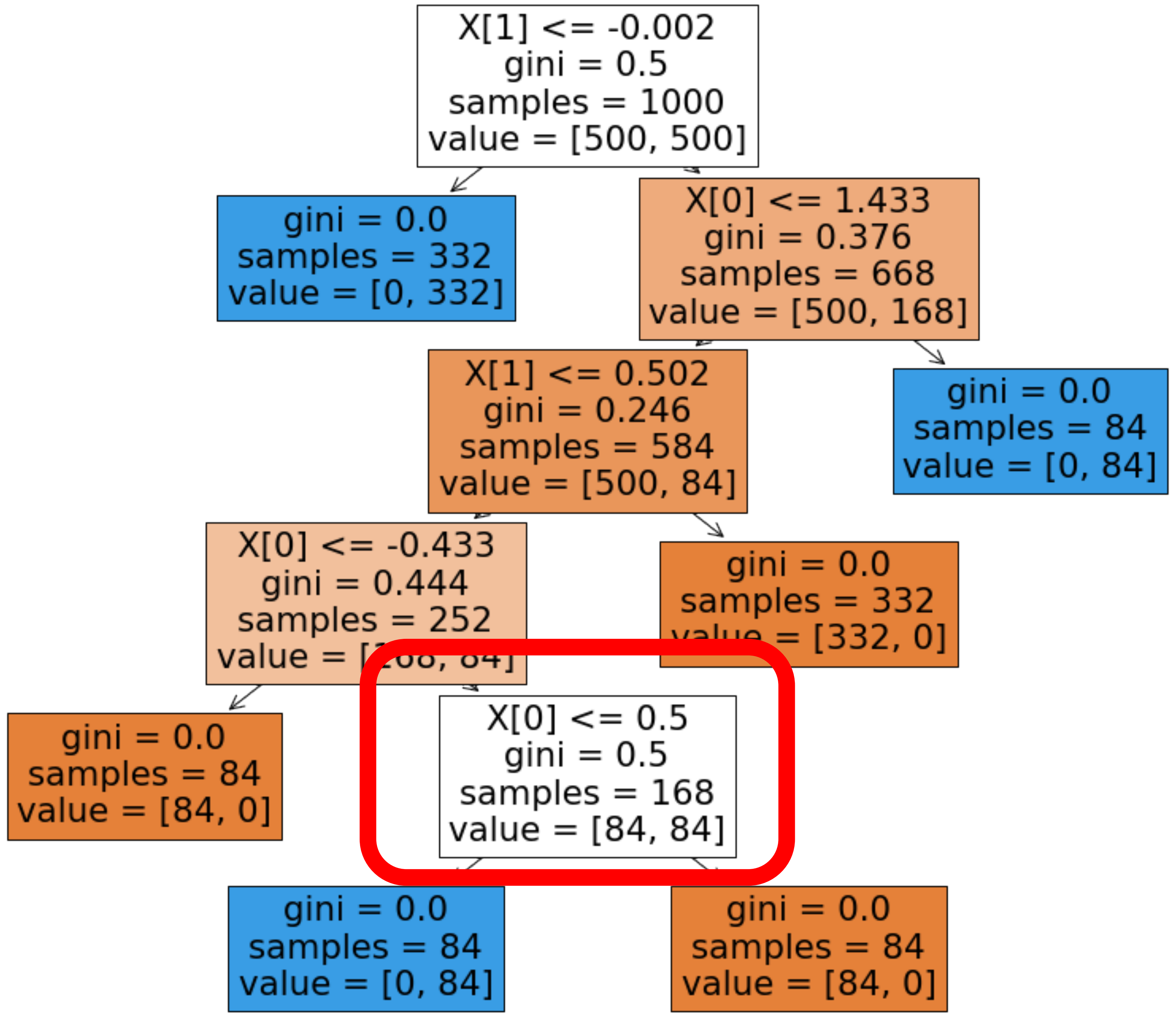


Decision Trees

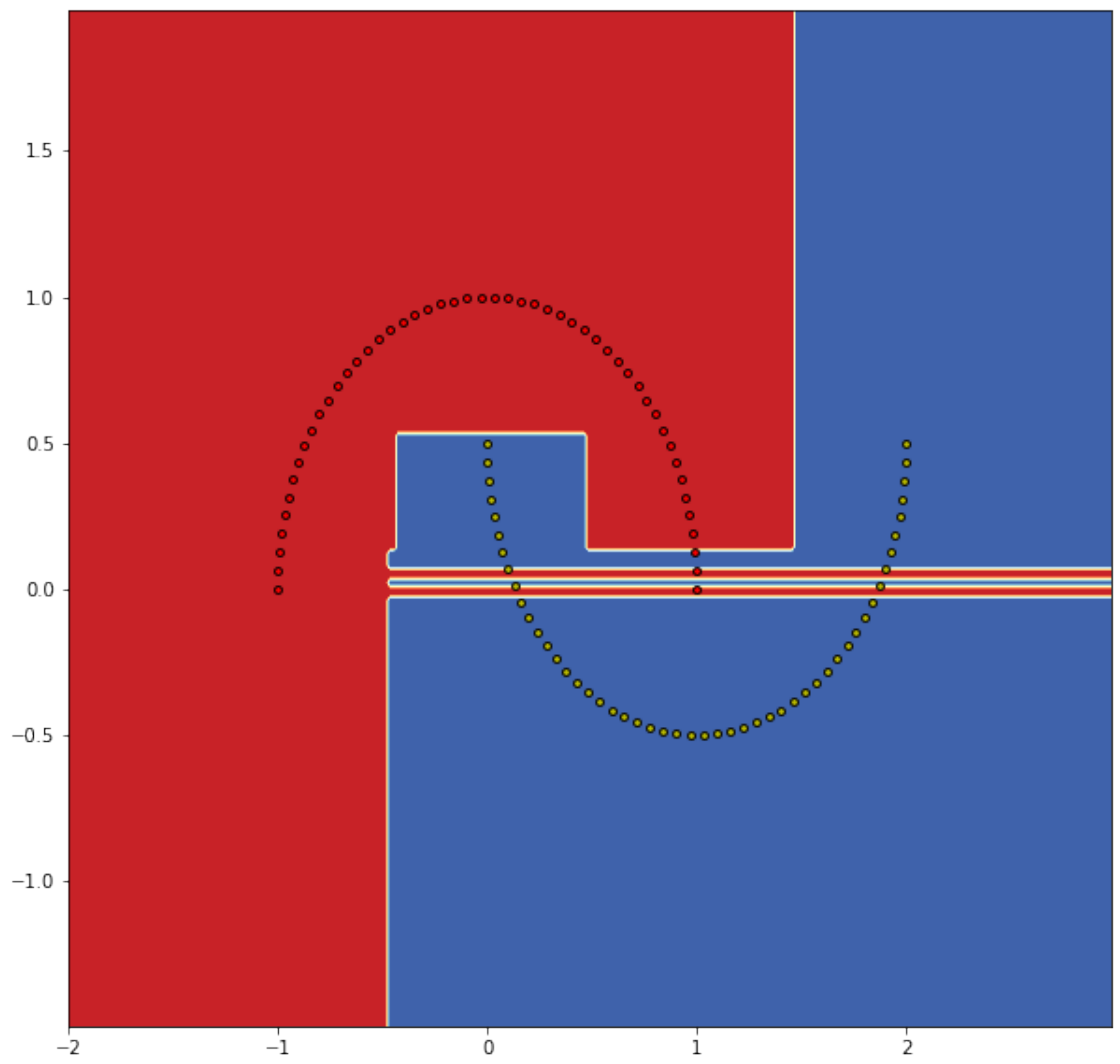


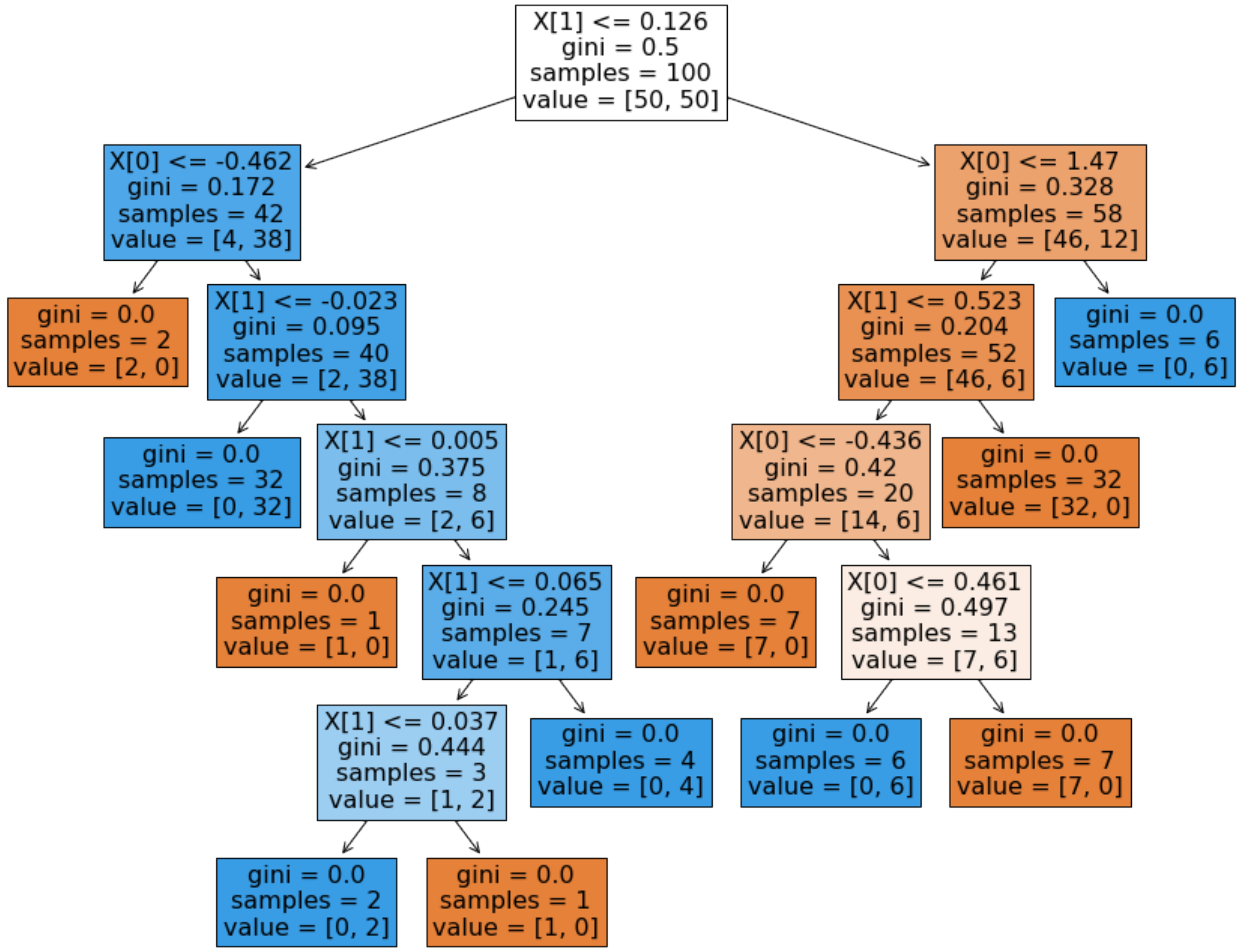
Decision Trees





Decision Trees and Overfitting





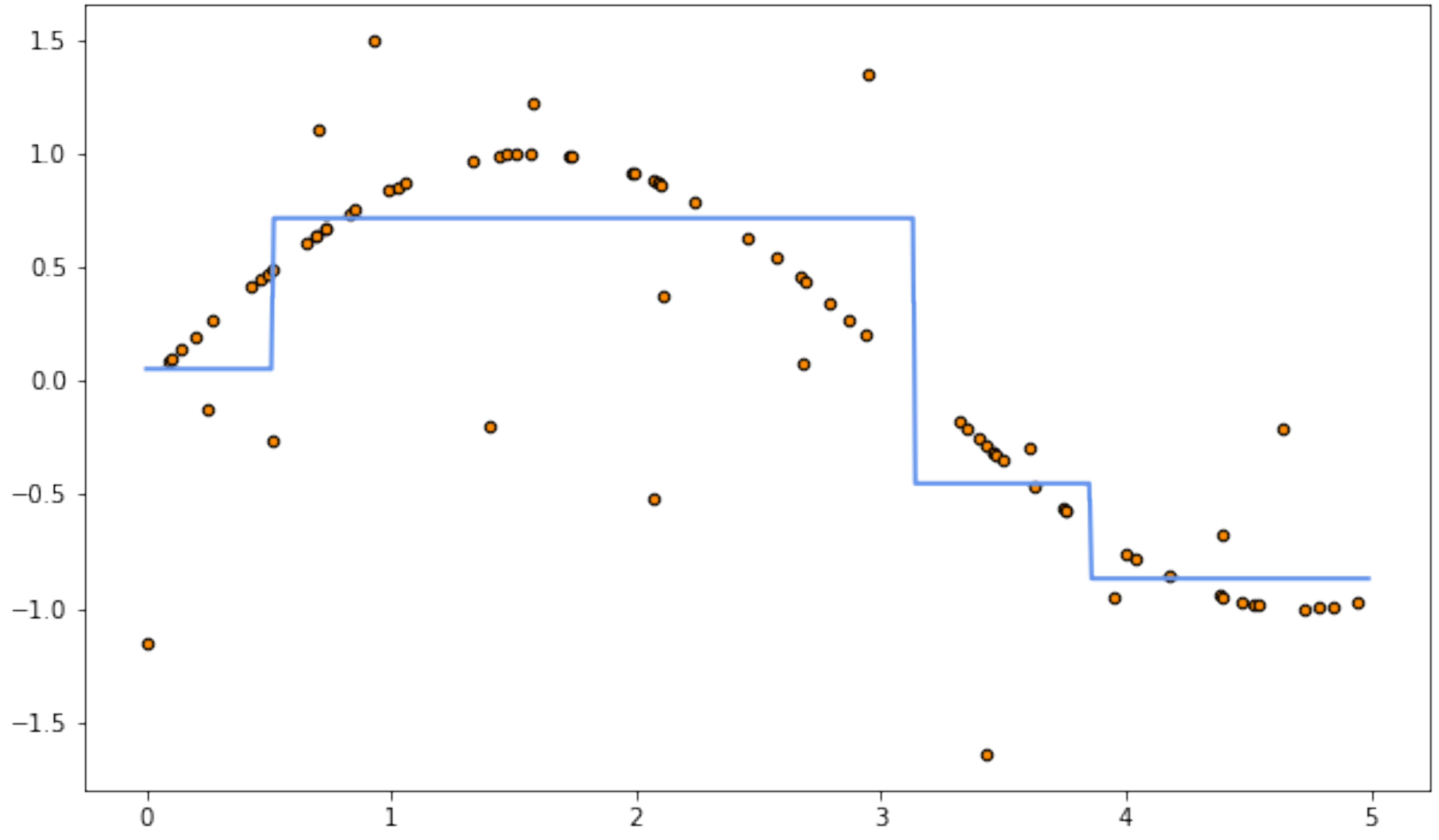
Complexity of Decision Trees

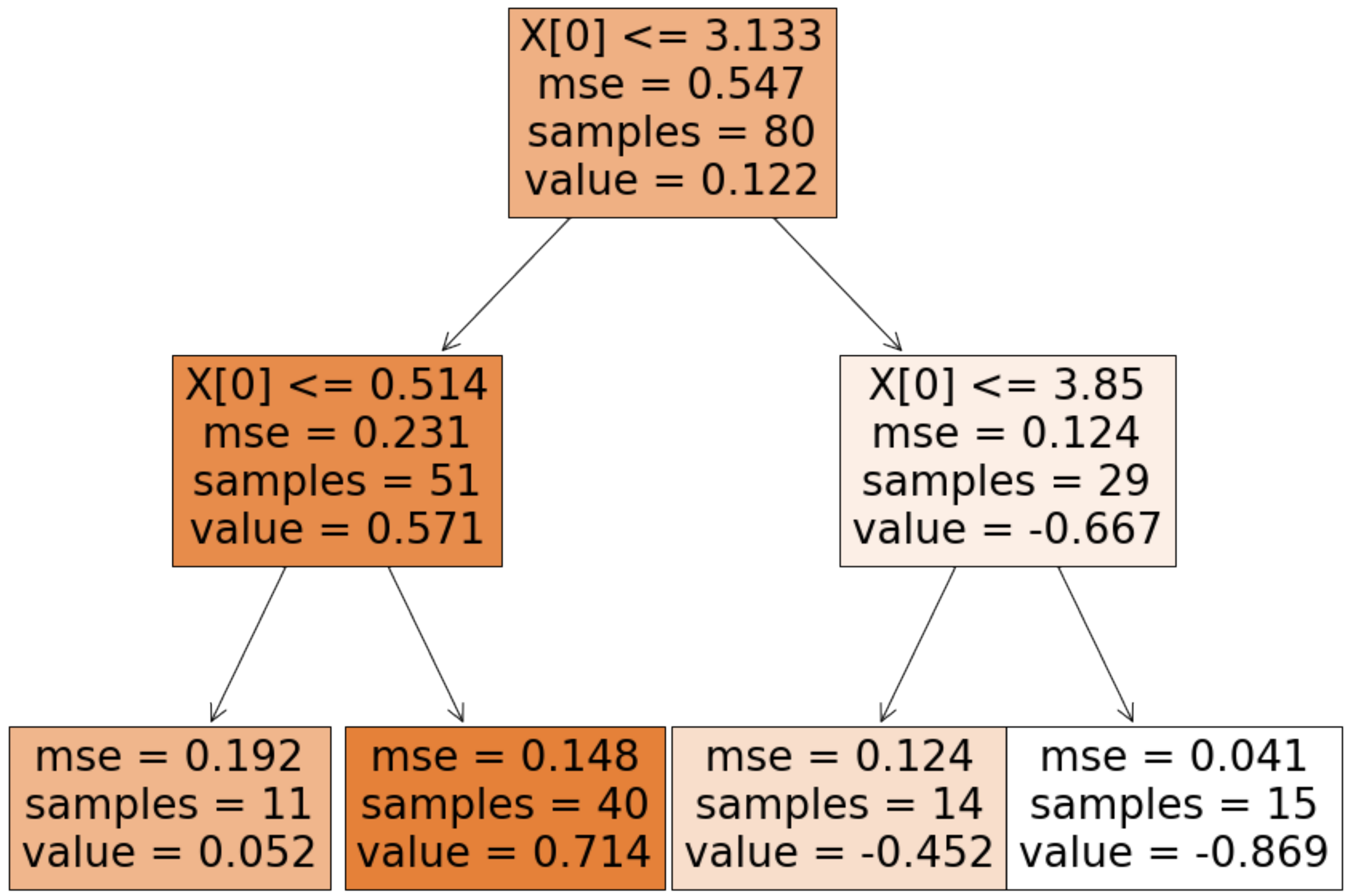
- We can keep splitting until we have only one object in each leaf

- We can ideally fit **any** training data

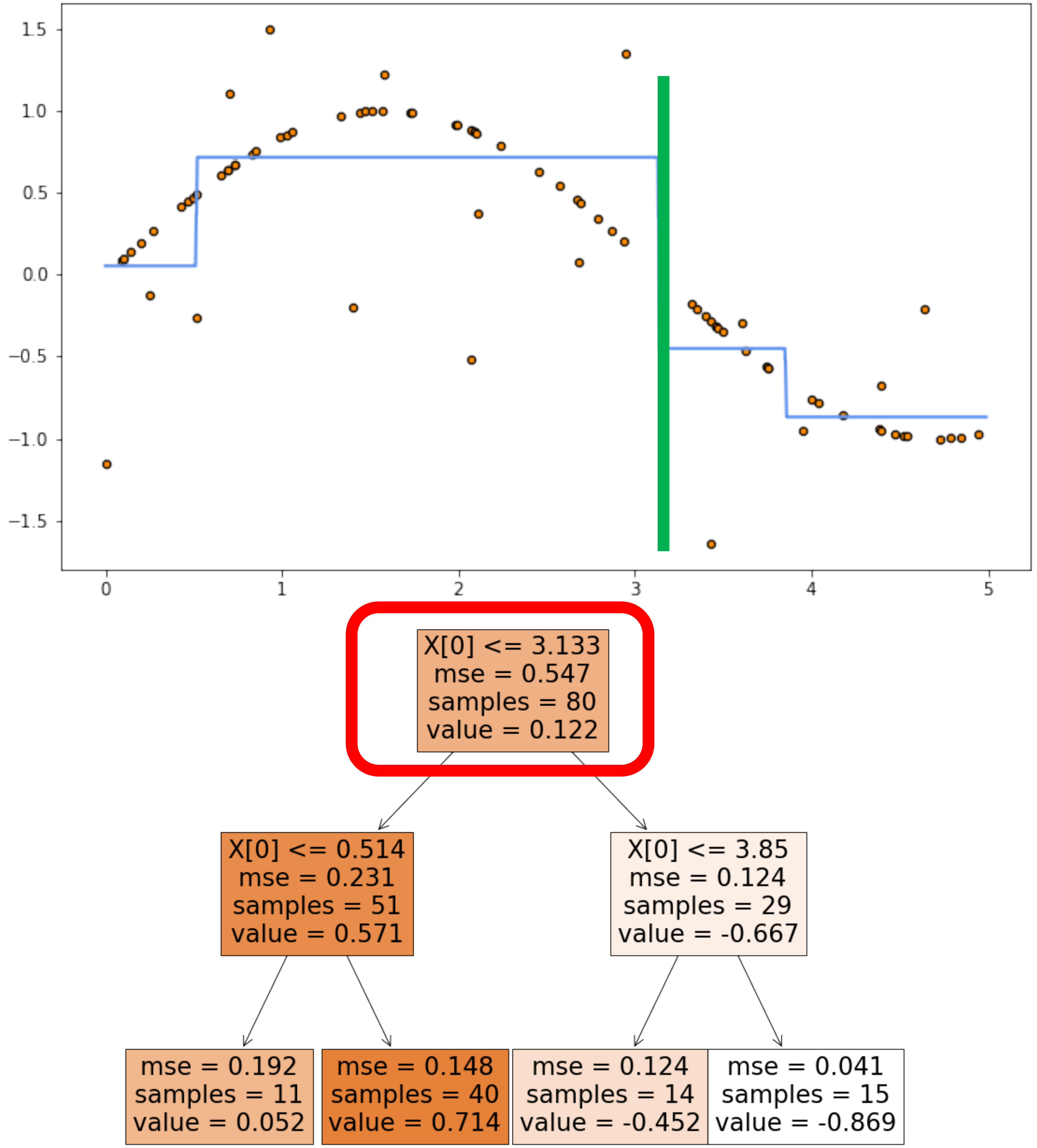
- Unless there are several objects with the same features and different target values

Decision Trees for Regression Task





Decision Trees for Regression Task



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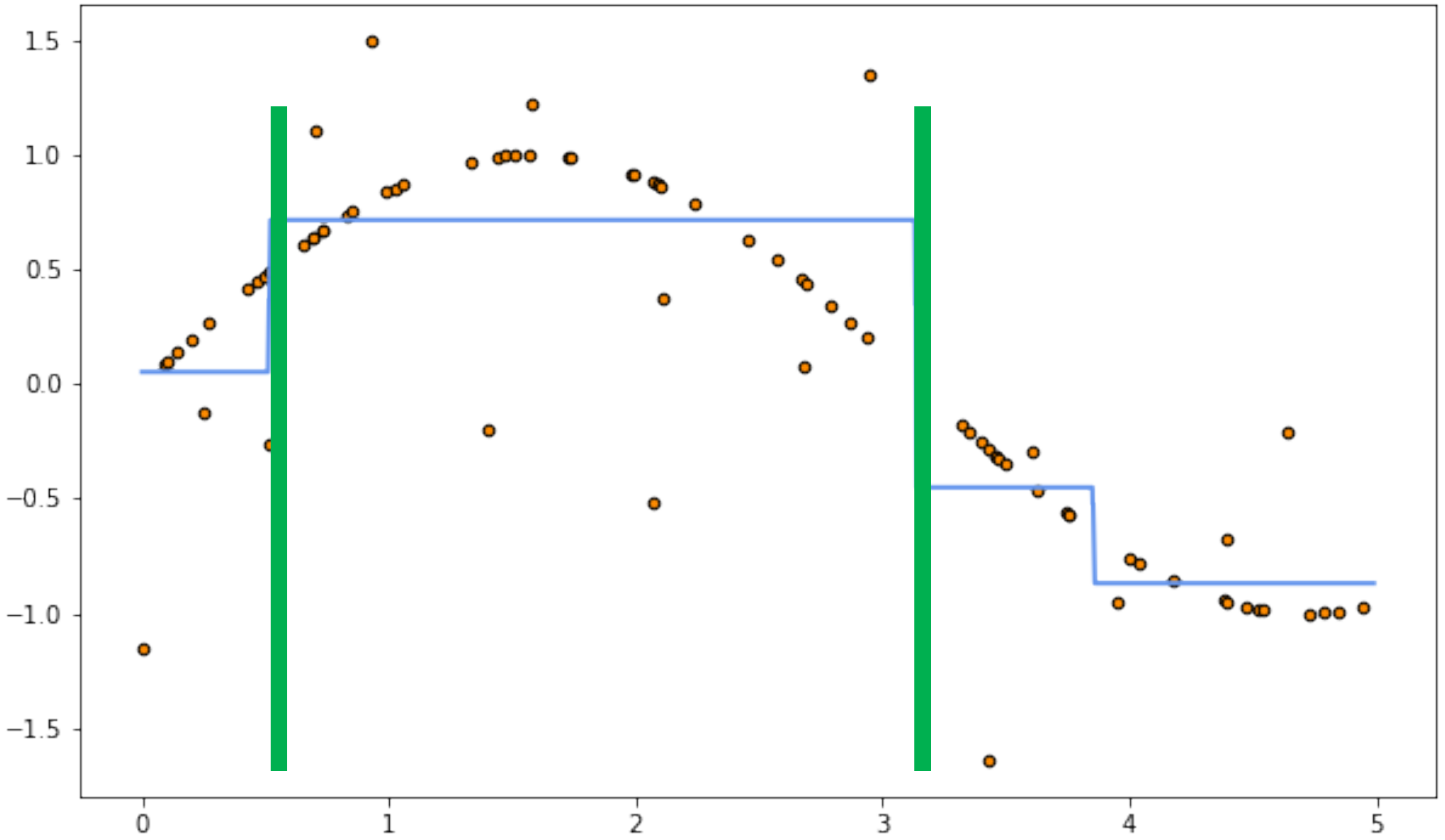
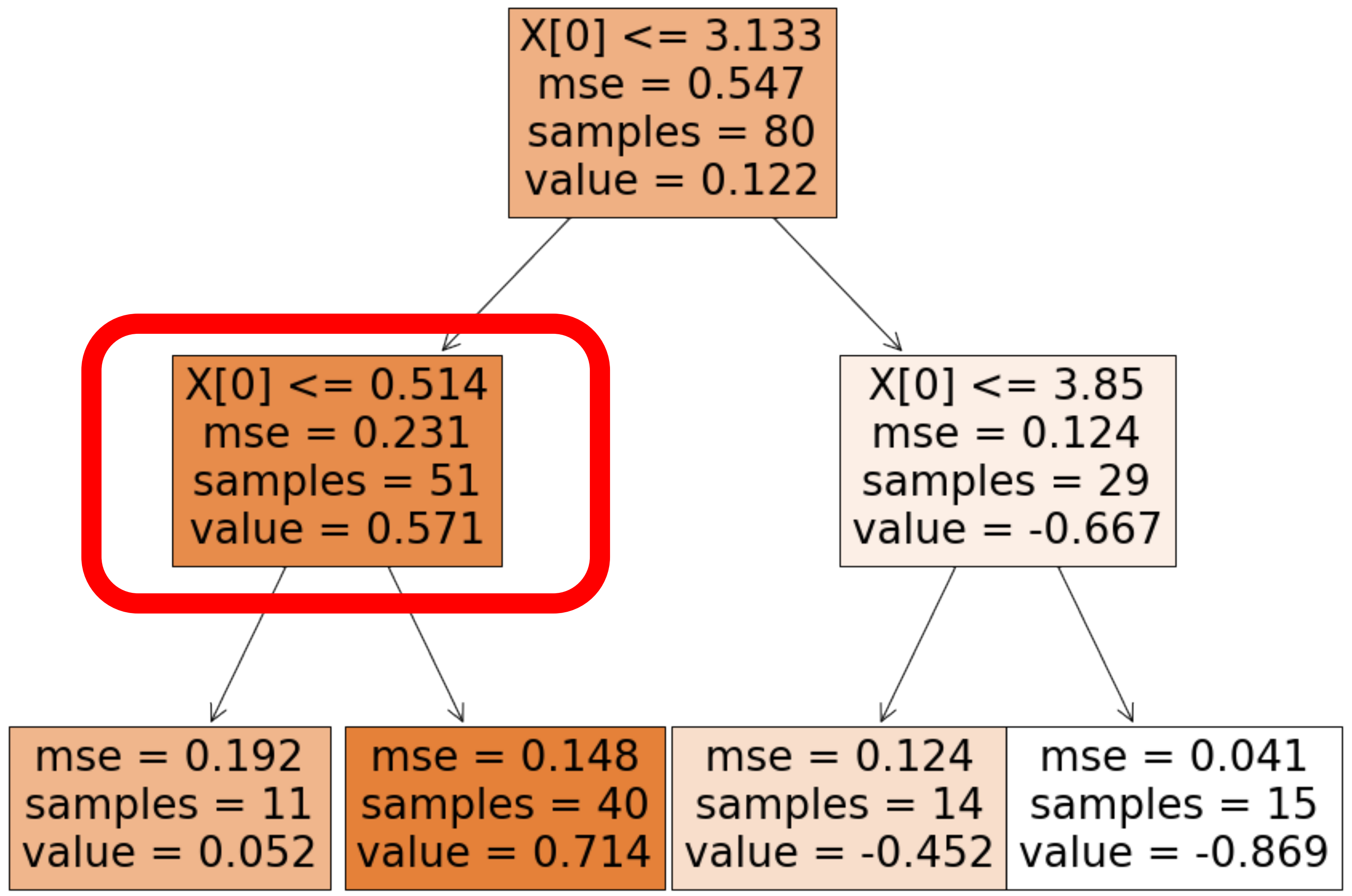
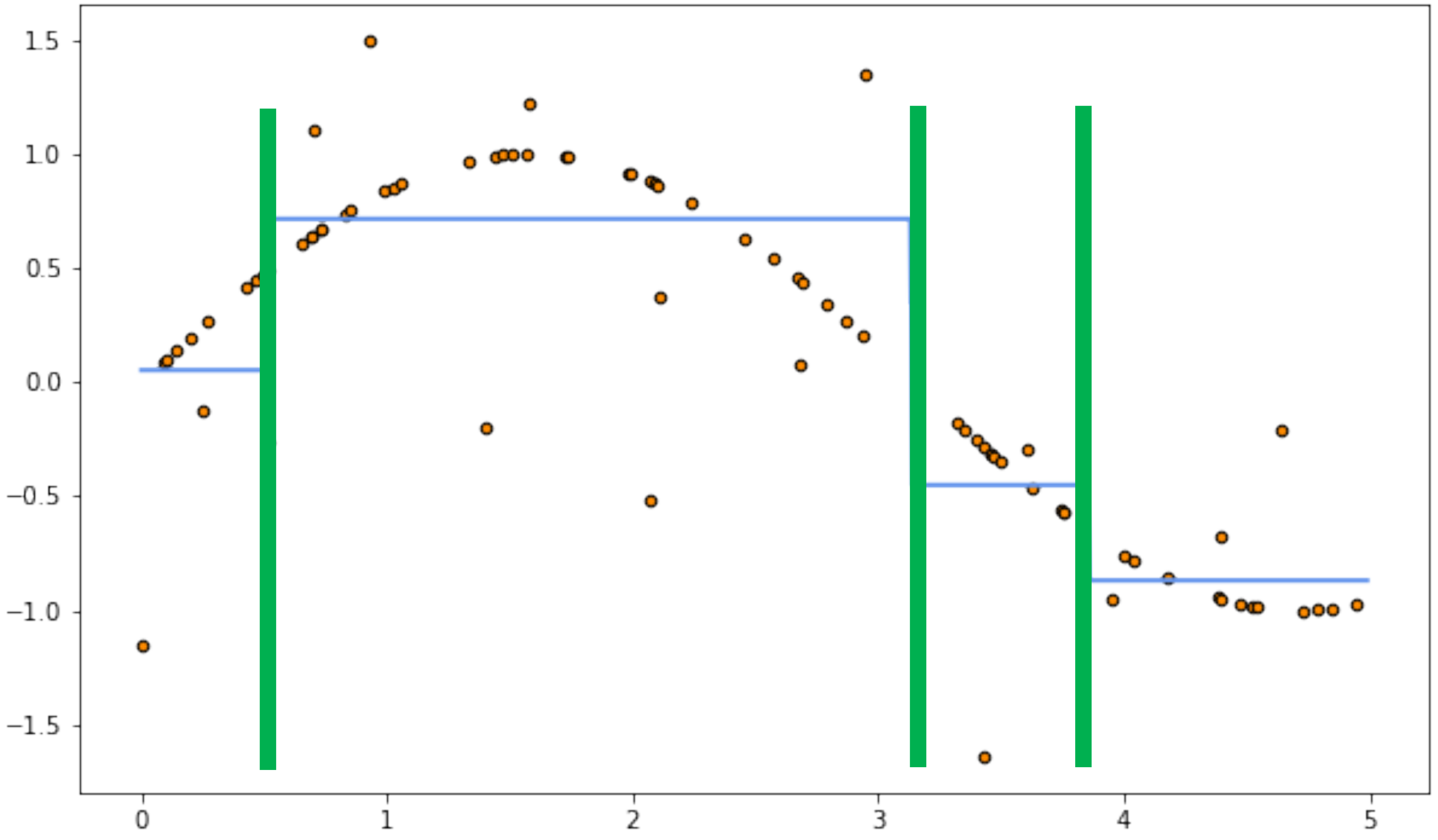
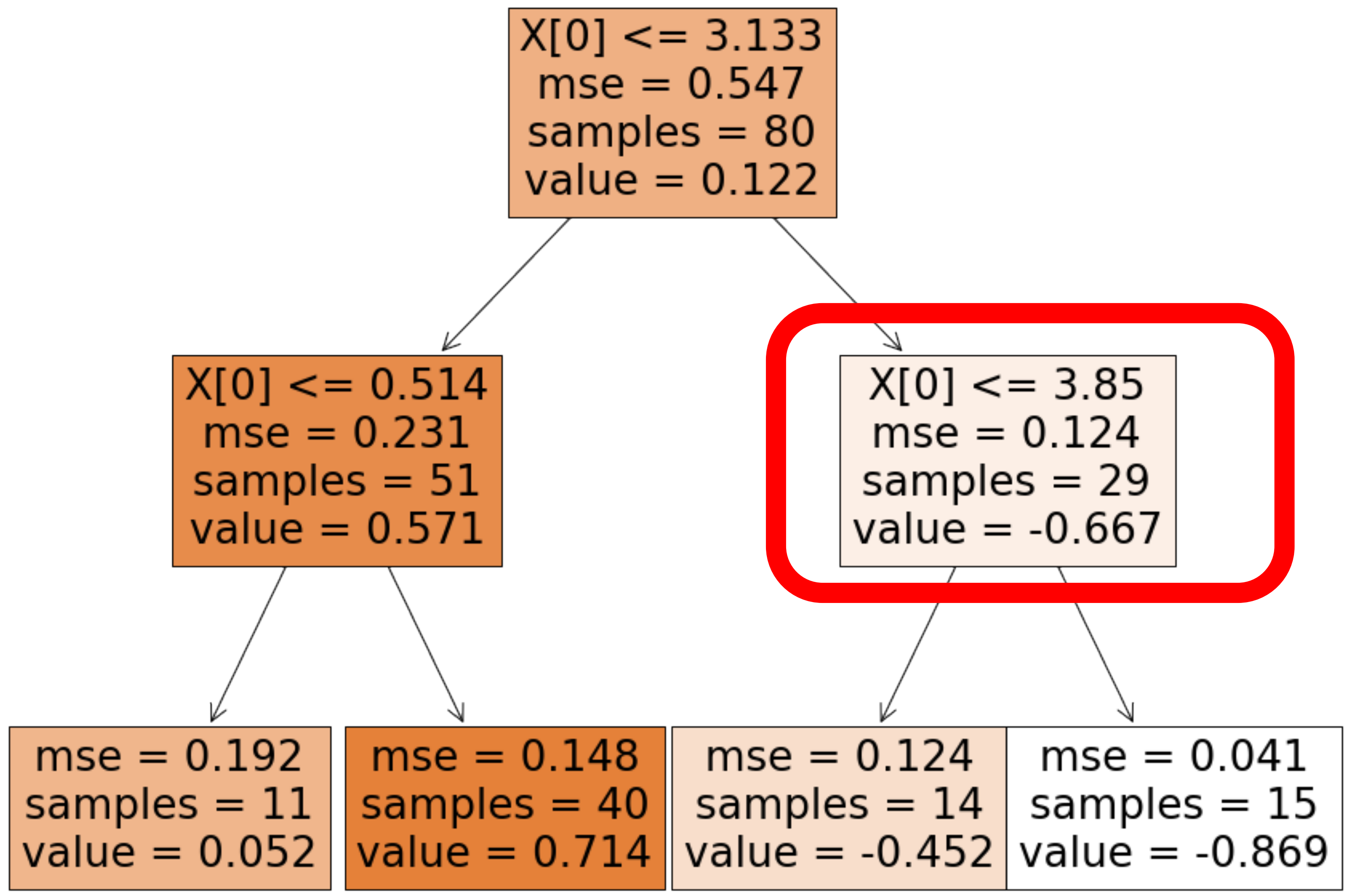


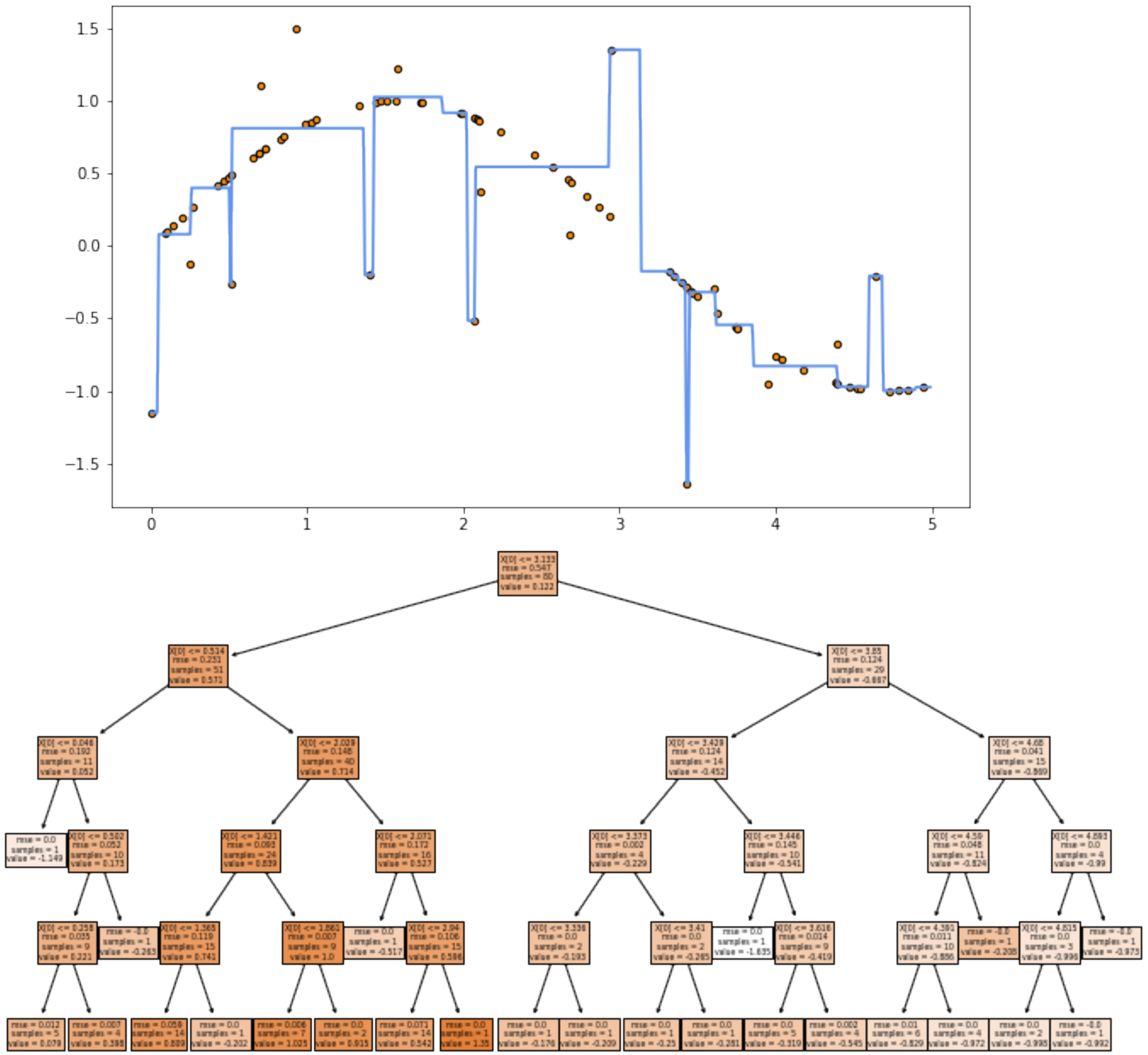


Decision Trees for Regression Task





Decision Trees for Regression and Overfitting

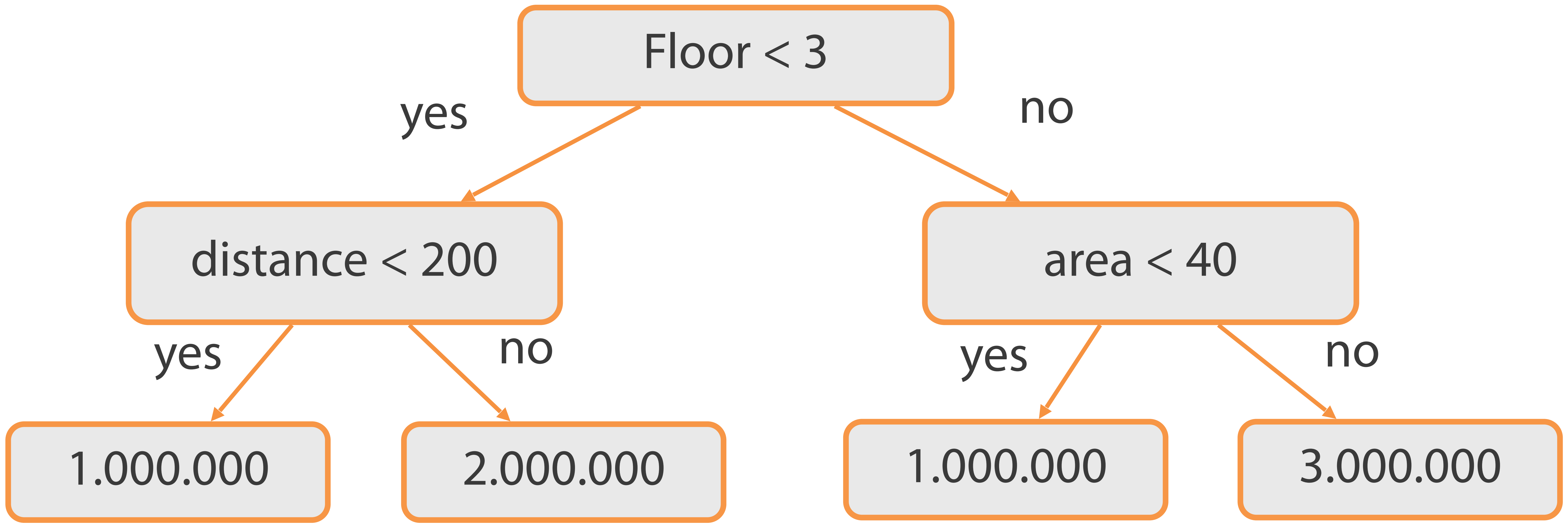


Summary

- Decision trees — combination of simple logic rules
- Decision Trees split feature space into several areas with constant prediction in each of them
- It is quite easy to overfit, when you use decision trees

Structure of Decision Trees

Decision Trees



- **Internal Nodes**: splitting criterion
- **Leaves**: predictions $c \in \mathbb{Y}$

Splitting Criterion

- Step function: $\left[x_j < t\right]$ — not the only option
- Use a linear model: $[\langle w, \ x \rangle < t]$
- A specific metric: $\left[\rho\left(x, \ x_0\right) < t\right]$
- …

- But we can build arbitrary complex models even with the most simple predicates

Predictions in Leaves: Regression

- We will use constant predictions $c_v \in \mathbb{Y}$
- Average value:

$$c_v = \frac{1}{|R_v|} \sum_{(x_i, y_i) \in R_v} y_i$$

Predictions in Leaves: Classification

- We will use constant predictions $c_v \in \mathbb{Y}$
- The most common class:

$$c_v = \underset{k \in \mathbb{Y}}{\operatorname{argmax}} \sum_{(x_i, y_i) \in R_v} [y_i = k]$$

Predictions in Leaves: Classification

- We will use constant predictions $c_v \in \mathbb{Y}$
- The most common class:

$$c_v = \underset{k \in \mathbb{Y}}{\operatorname{argmax}} \sum_{(x_i, y_i) \in R_v} [y_i = k]$$

- Class probabilities

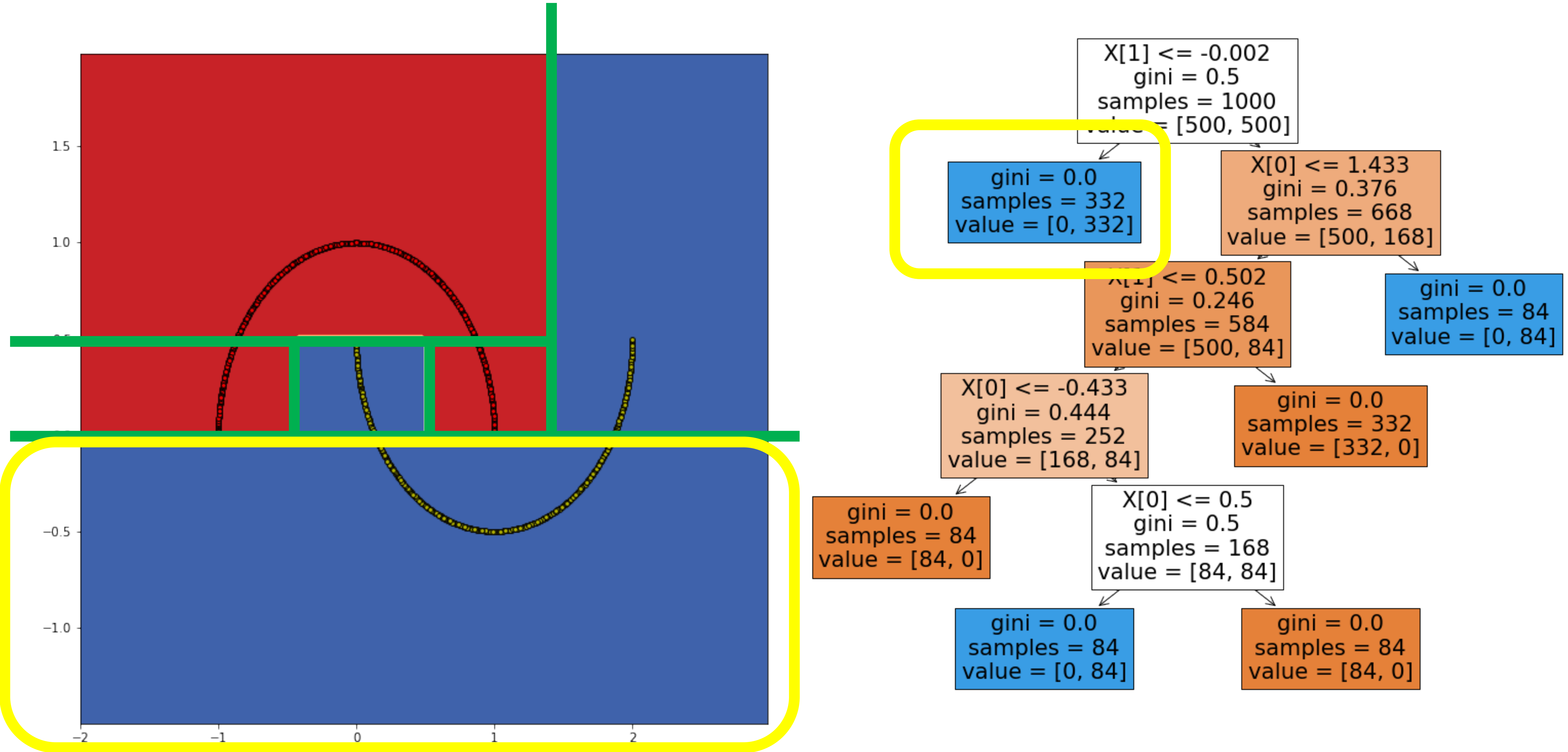
$$c_{vk} = \frac{1}{|R_v|} \sum_{(x_i, y_i) \in R_v} [y_i = k]$$

Predictions in Leaves

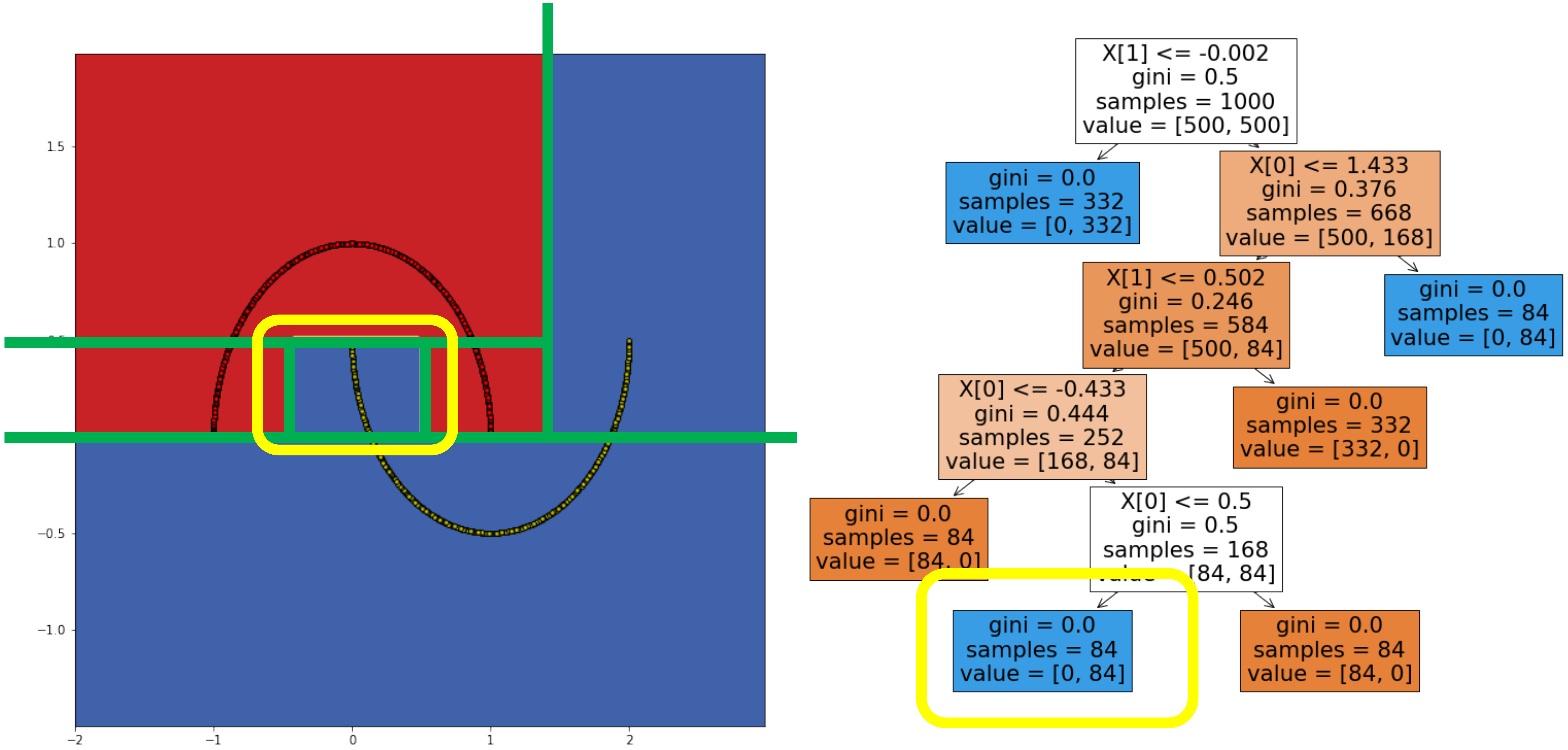
- We could use more complex prediction functions in leaves
- E.g. linear regression:

$$c_v(x) = \langle w_v, \; x \rangle$$

Decision Tree



Decision Tree



Decision Tree: Interpretation

- Tree splits feature space on disjoint sub-spaces $R_1, \ldots, R_J$
- Each sub-space R_j corresponds to the leaf
- At each sub-space R_j prediction c_j is constant

$$a(x) = \sum_{j=1}^{J} c_j \left[x \in R_j\right]$$

Decision Tree: Interpretation

$$a(x) = \sum_{j=1}^{J} c_j \left[x \in R_j \right]$$

- Decision tree constructs new powerful features
- The predictions then are linear combination of new features

Summary

- One could use different approaches in splitting and making predictions in leaves. Usually the simplest one is good enough.

- One could think about decision tree as linear model over new features

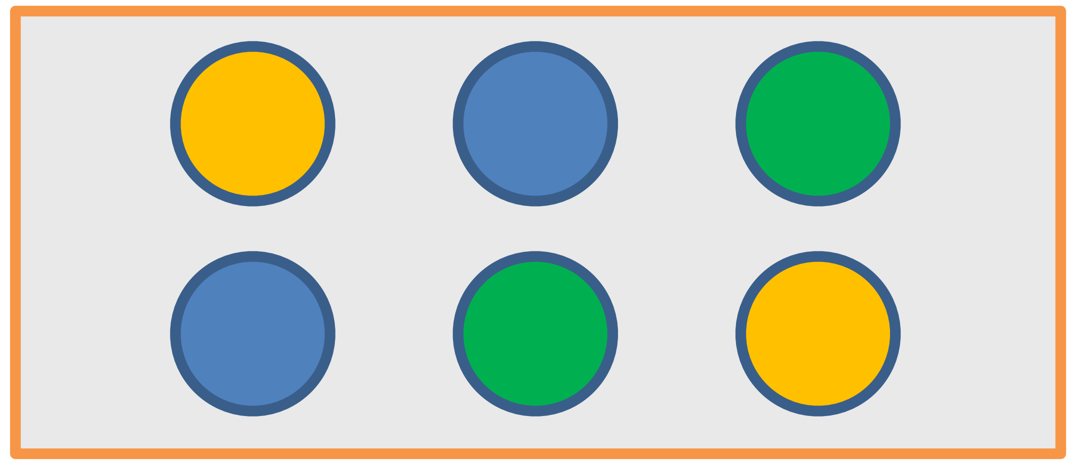
How to Train Decision Trees?

Greedy Tree Construction

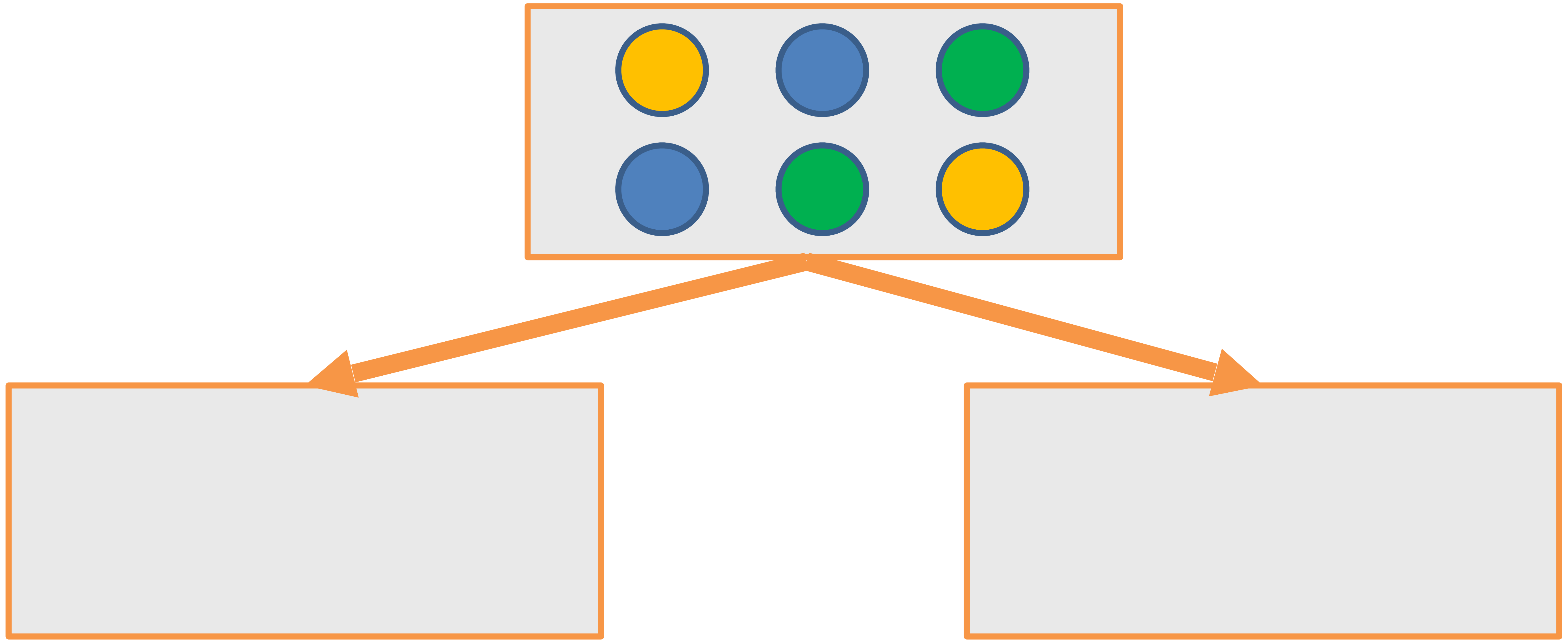
- Let’s develop the algorithm on the example

- We start from the classification task

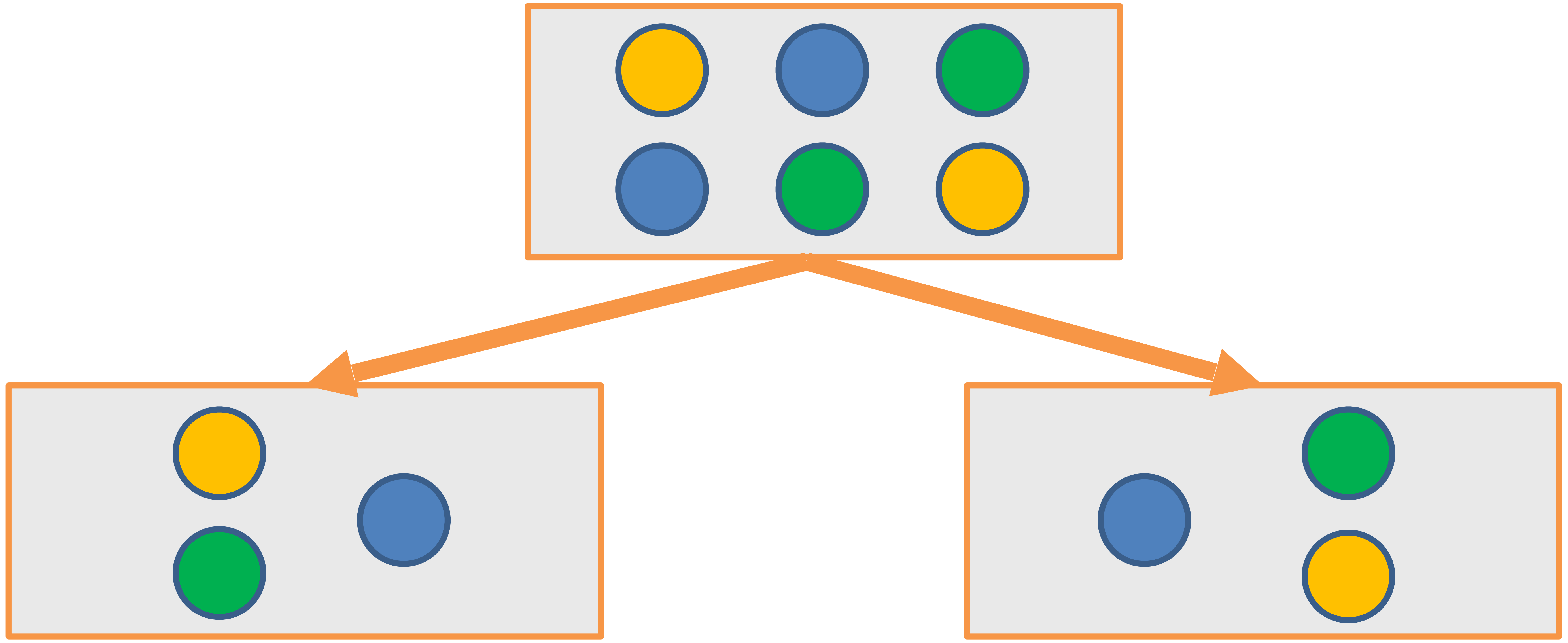
Greedy Tree Construction



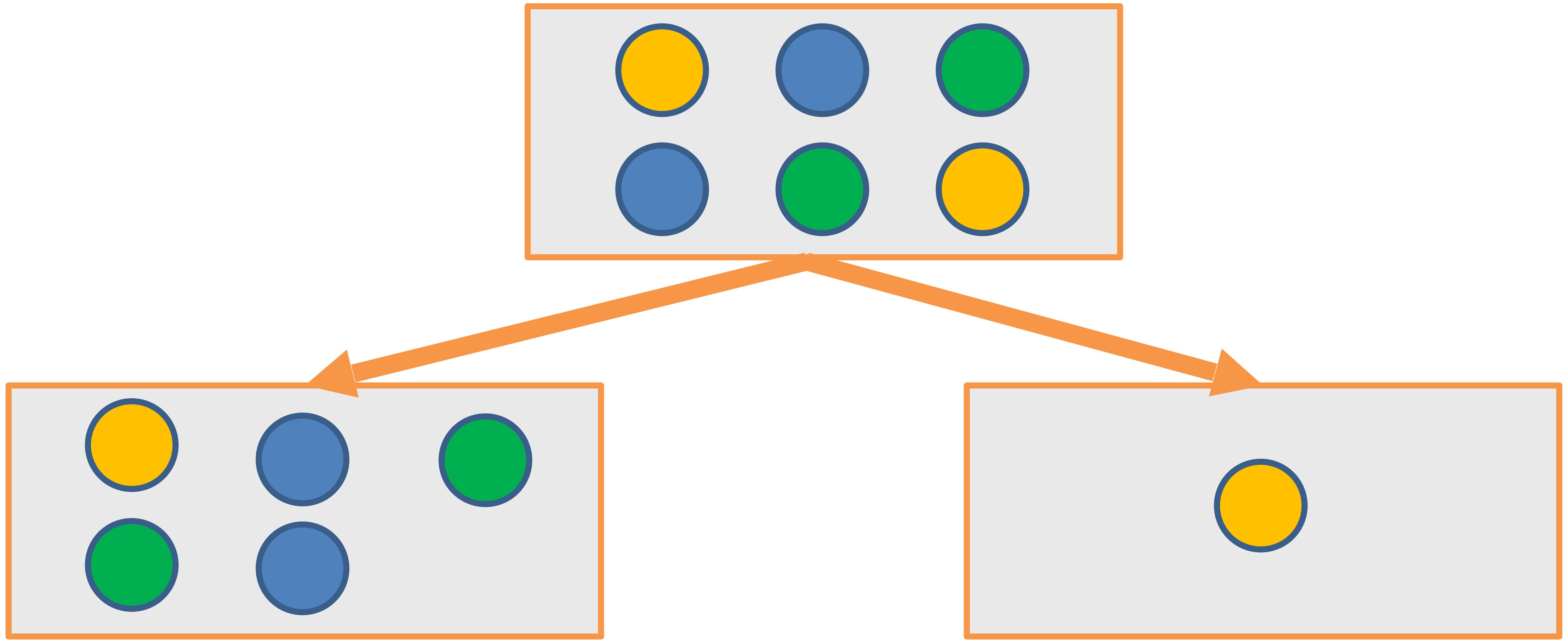
Greedy Tree Construction



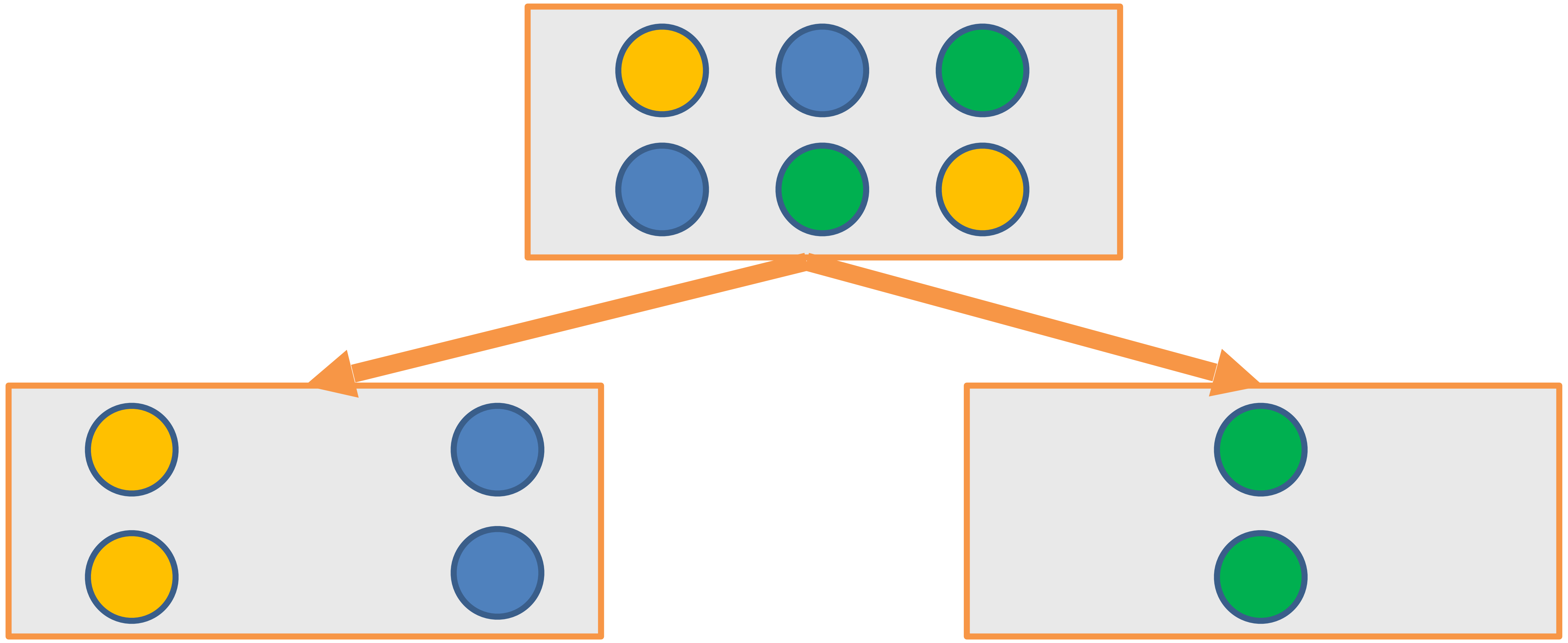
Greedy Tree Construction



Greedy Tree Construction



Greedy Tree Construction



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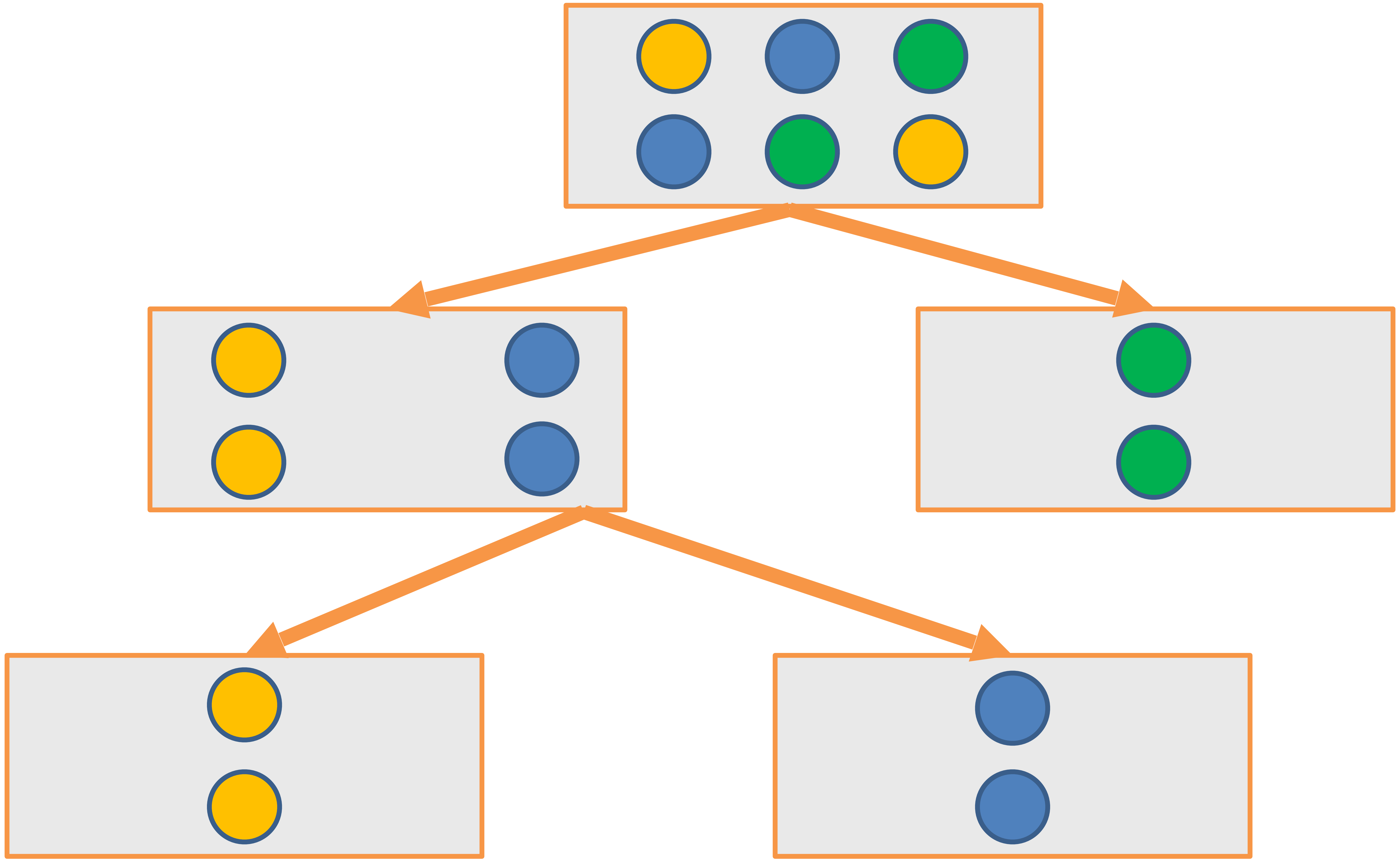
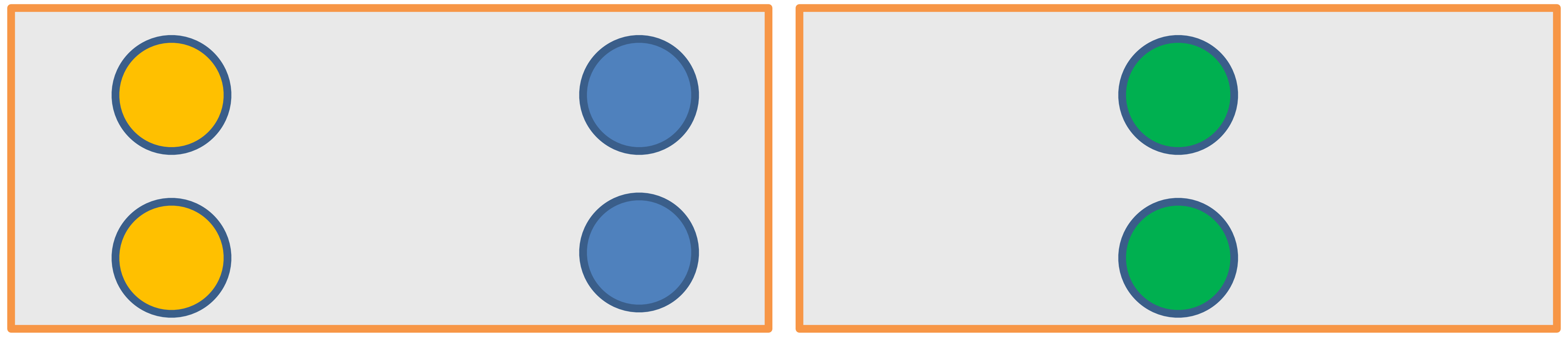


How to Choose Between Two Splits ?



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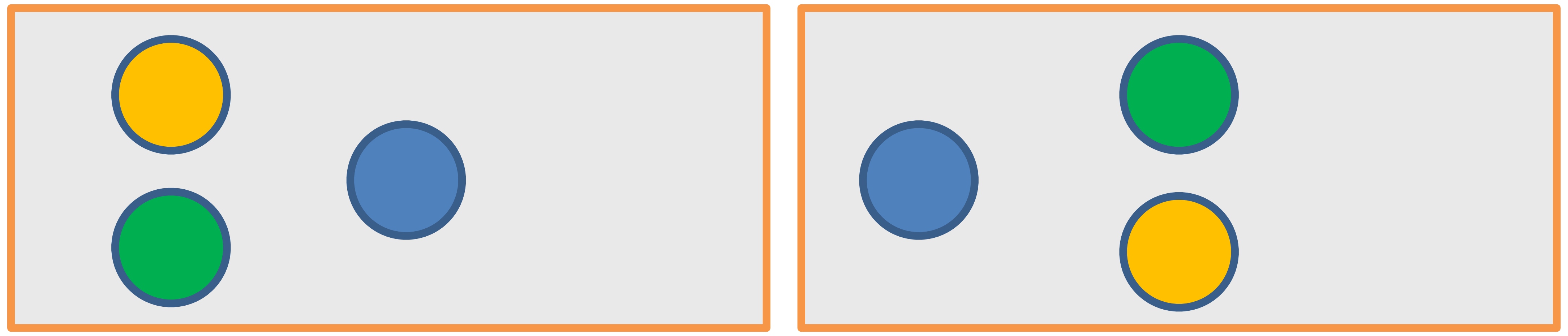
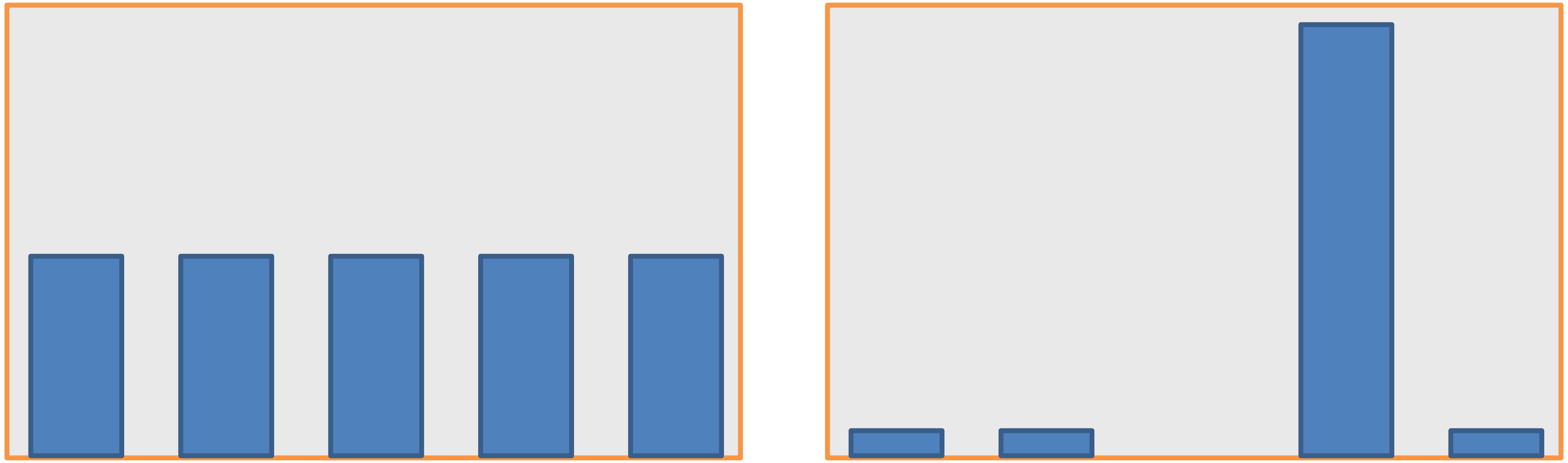


Entropy

We consider entropy as a way to measure the uncertainty of an experiment's outcome



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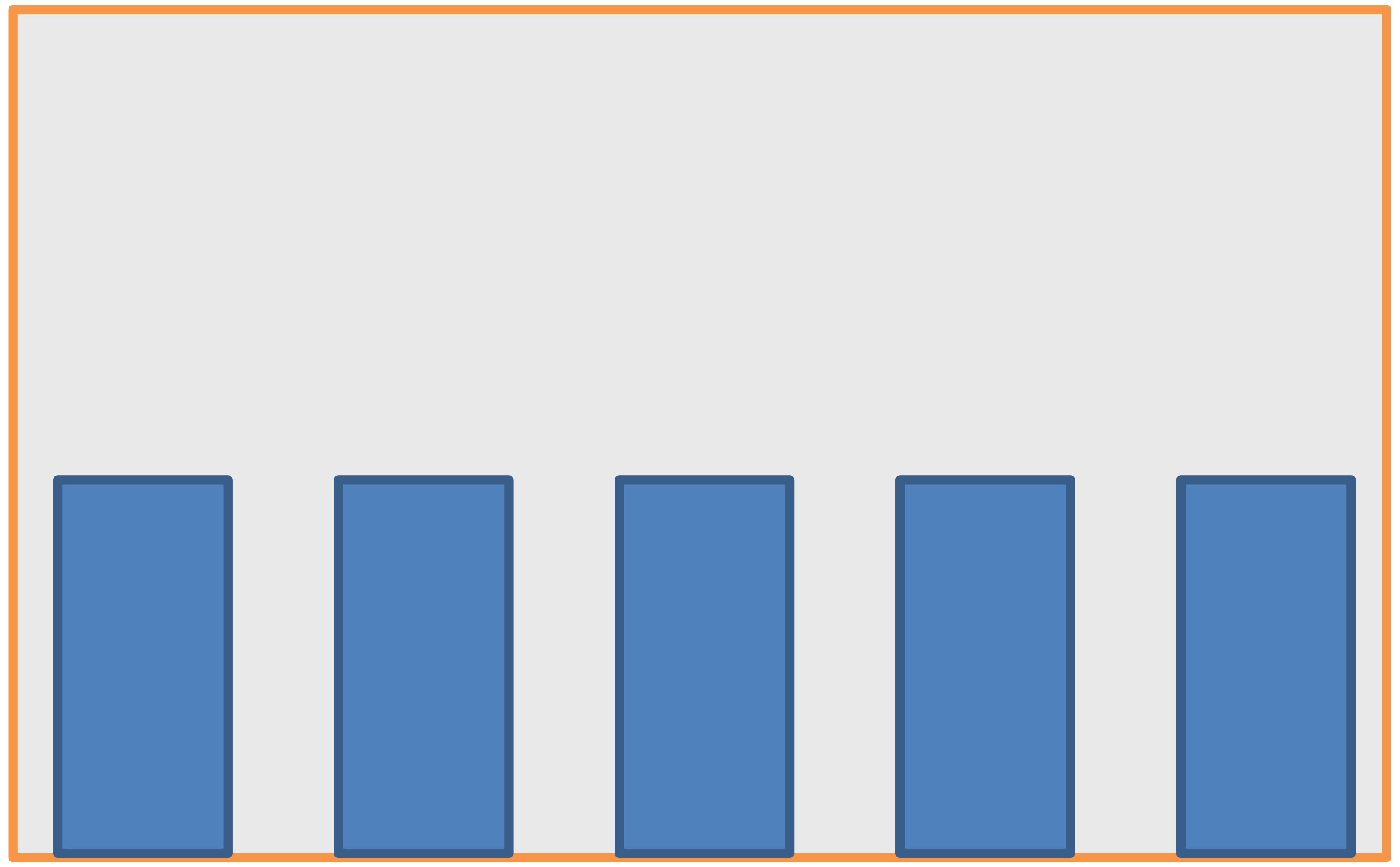
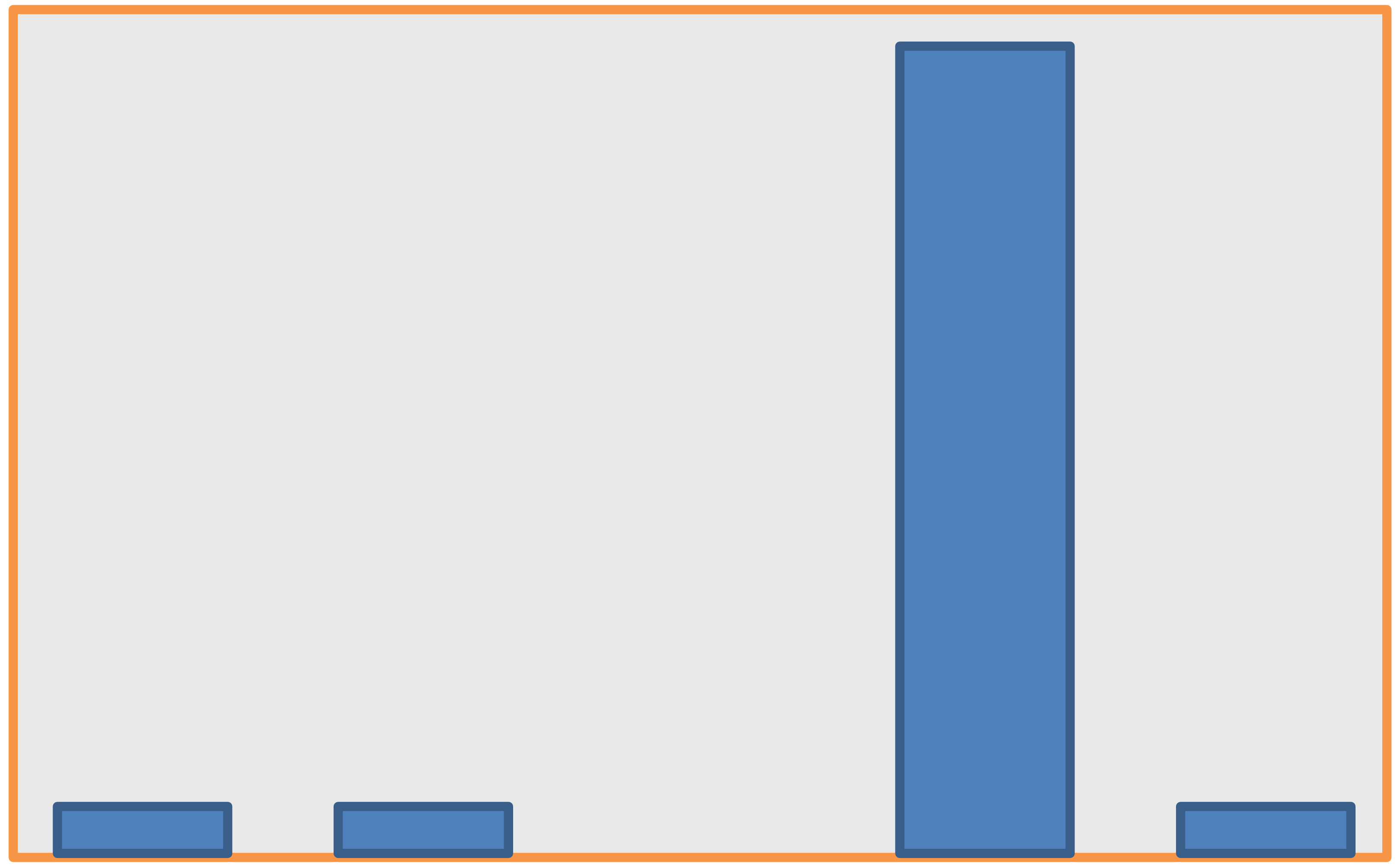


High entropy



Low entropy

Entropy

- Assume we are given discrete distribution with n possible outcomes
- Probability of outcomes: $p_1, p_2, \ldots, p_n$
- Entropy of distribution:

$$H(p_1, \ldots, p_n) = -\sum_{i=1}^{n} p_i \log_2 p_i$$

Entropy

$$H\left(p_1, \ldots, p_n\right) = -\sum_{i=1}^{n} p_i \log_2 p_i$$

- $p = (0.2,\ 0.2,\ 0.2,\ 0.2,\ 0.2)$
  - $H = 2.3219$

Entropy

$$H(p_1, \ldots, p_n) = -\sum_{i=1}^{n} p_i \log_2 p_i$$

- $p = (0.2,\ 0.2,\ 0.2,\ 0.2,\ 0.2)$
  - $H = 2.3219$

- $p = (0.9,\ 0.05,\ 0.05,\ 0,\ 0)$
  - $H = 0.5689$

Entropy

$$H\left(p_1, \ldots, p_n\right) = -\sum_{i=1}^{n} p_i \log_2 p_i$$

- $p = (0.2,\ 0.2,\ 0.2,\ 0.2,\ 0.2)$
  - $H = 2.3219$
- $p = (0.9,\ 0.05,\ 0.05,\ 0,\ 0)$
  - $H = 0.5689$
- $p = (0,\ 0,\ 0,\ 1,\ 0)$
  - $H = 0$

Entropy

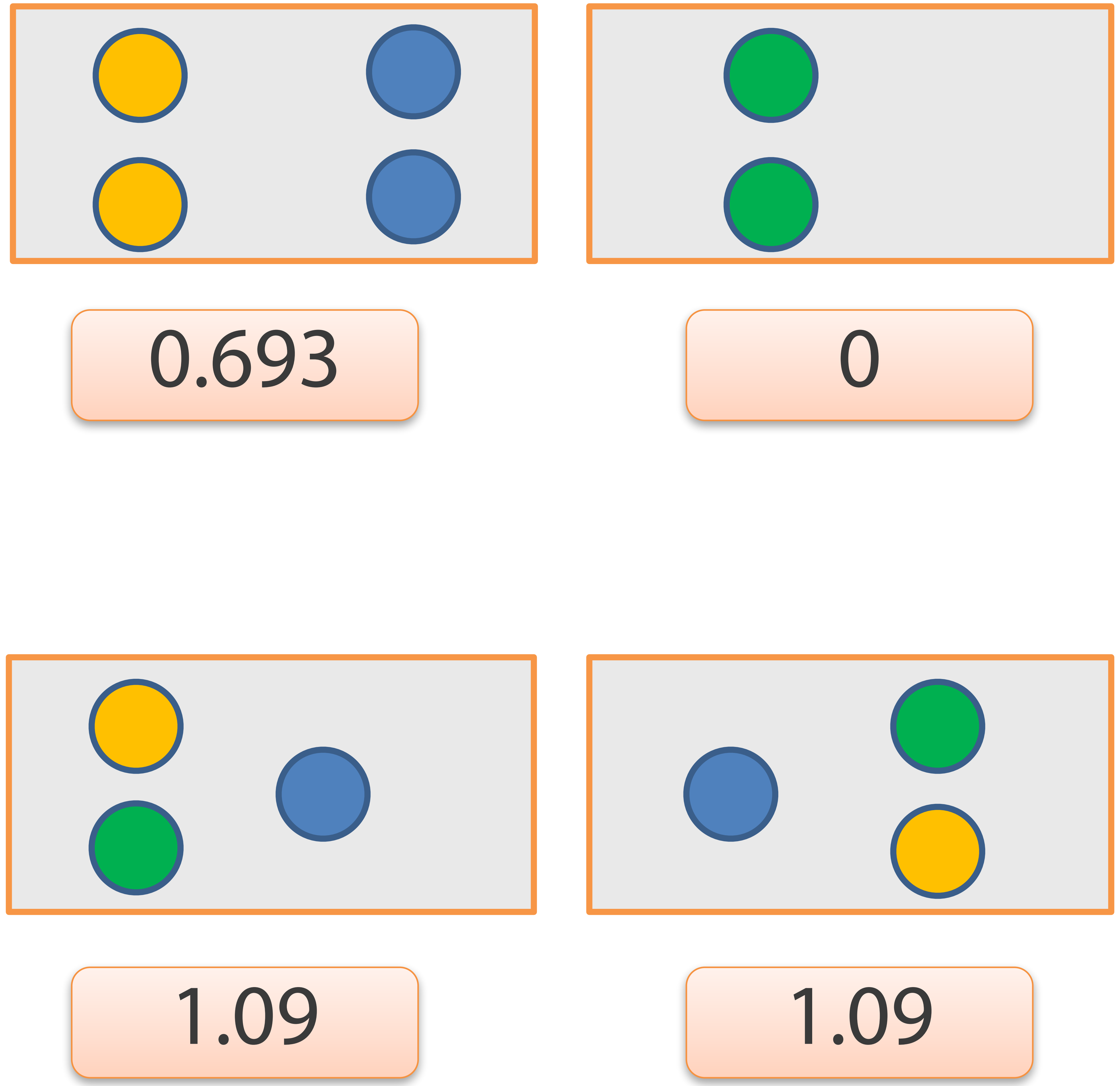
- In classification tasks the number of possible outcomes is the number of classes K

- Probability to be at the class k — fraction of objects of class k

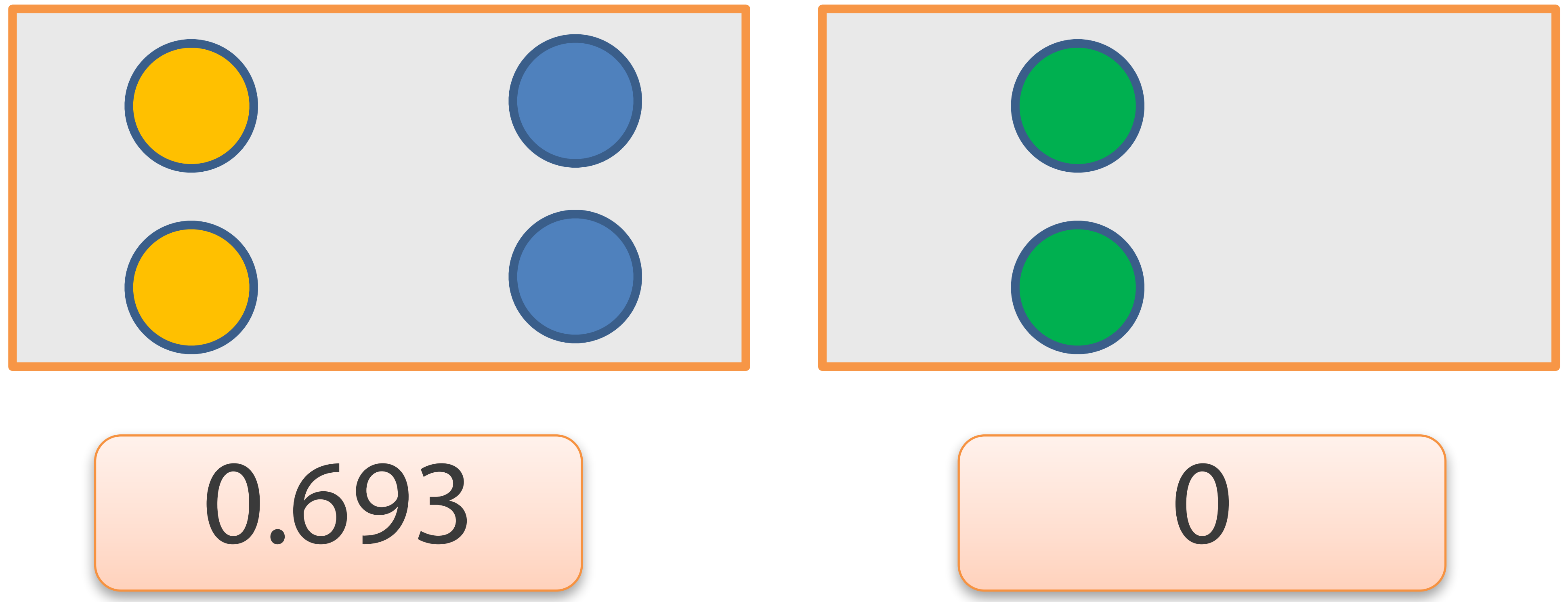
$$p_k = \frac{1}{|R|} \sum_{(x_i, y_i) \in R} [y_i = k]$$

- Zero Entropy — there are **only** objects form **one class** at the leaf
- Max. Entropy — there are **equal proportion** of objects from **each class**

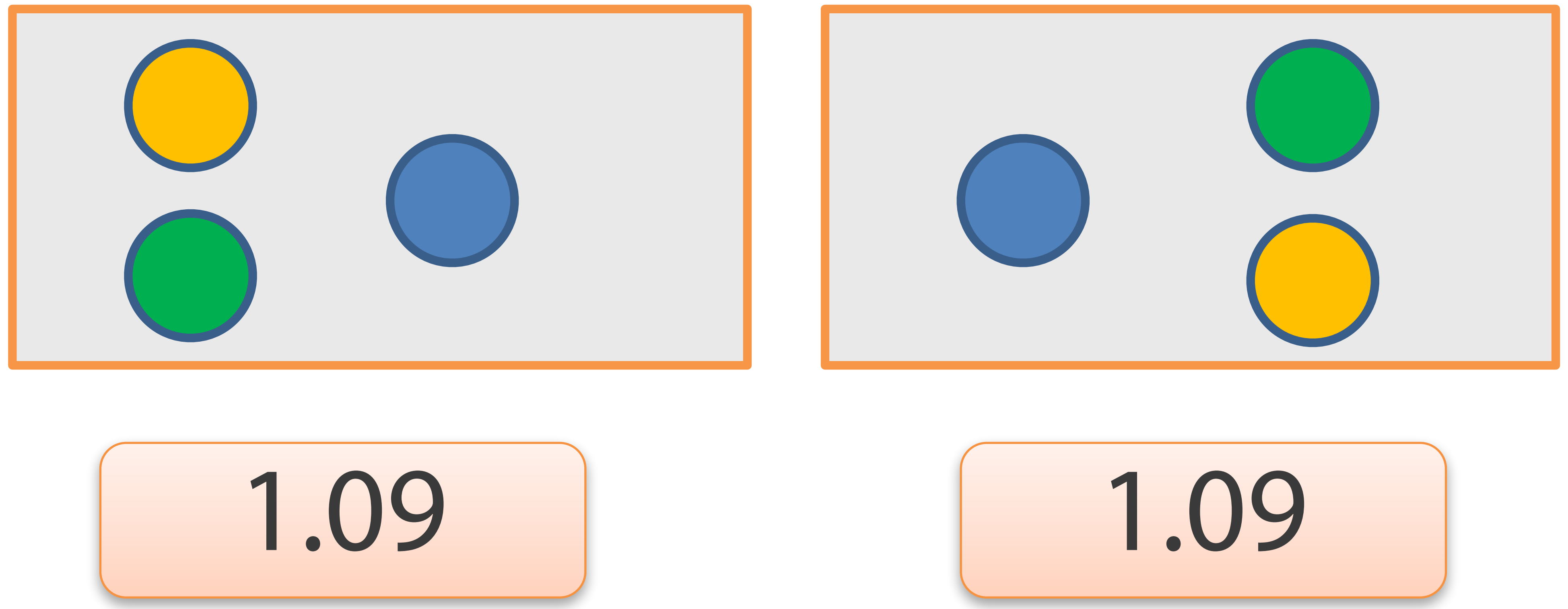
How to Select Between Two Splits?



How to Select Between Two Splits?



- $(0.5,\ 0.5,\ 0)$ and $(0,\ 0,\ 1)$
- $0.693 + 0 = 0.693$



- $(0.33,\ 0.33,\ 0.33)$ and $(0.33,\ 0.33,\ 0.33)$
- $1.09 + 1.09 = 2.18$

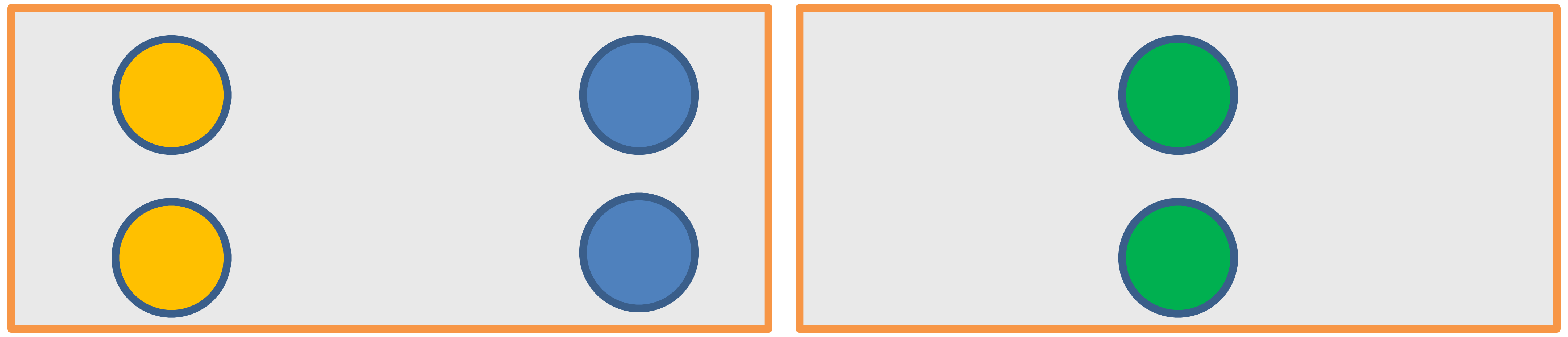
Summary

- Decision tree could be constructed in a greedy manner from the root node to the leaves

- For classification task we could choose a split, so that it minimizes class diversity at resulting groups

Measures of Impurity

How to Choose Between Two Splits ?



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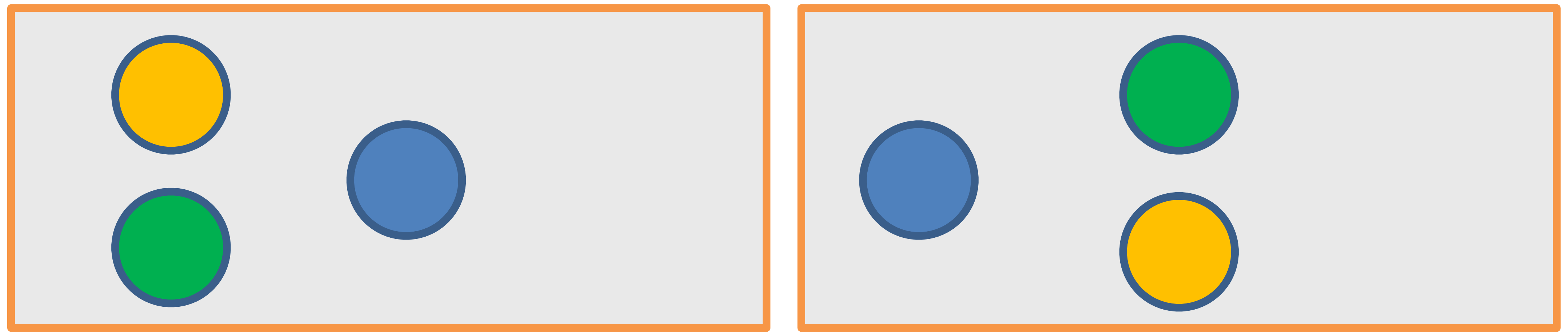


Entropy

$$H(p_1, \ldots, p_K) = -\sum_{i=1}^{K} p_i \log_2 p_i$$

- Measure of diversity at the node

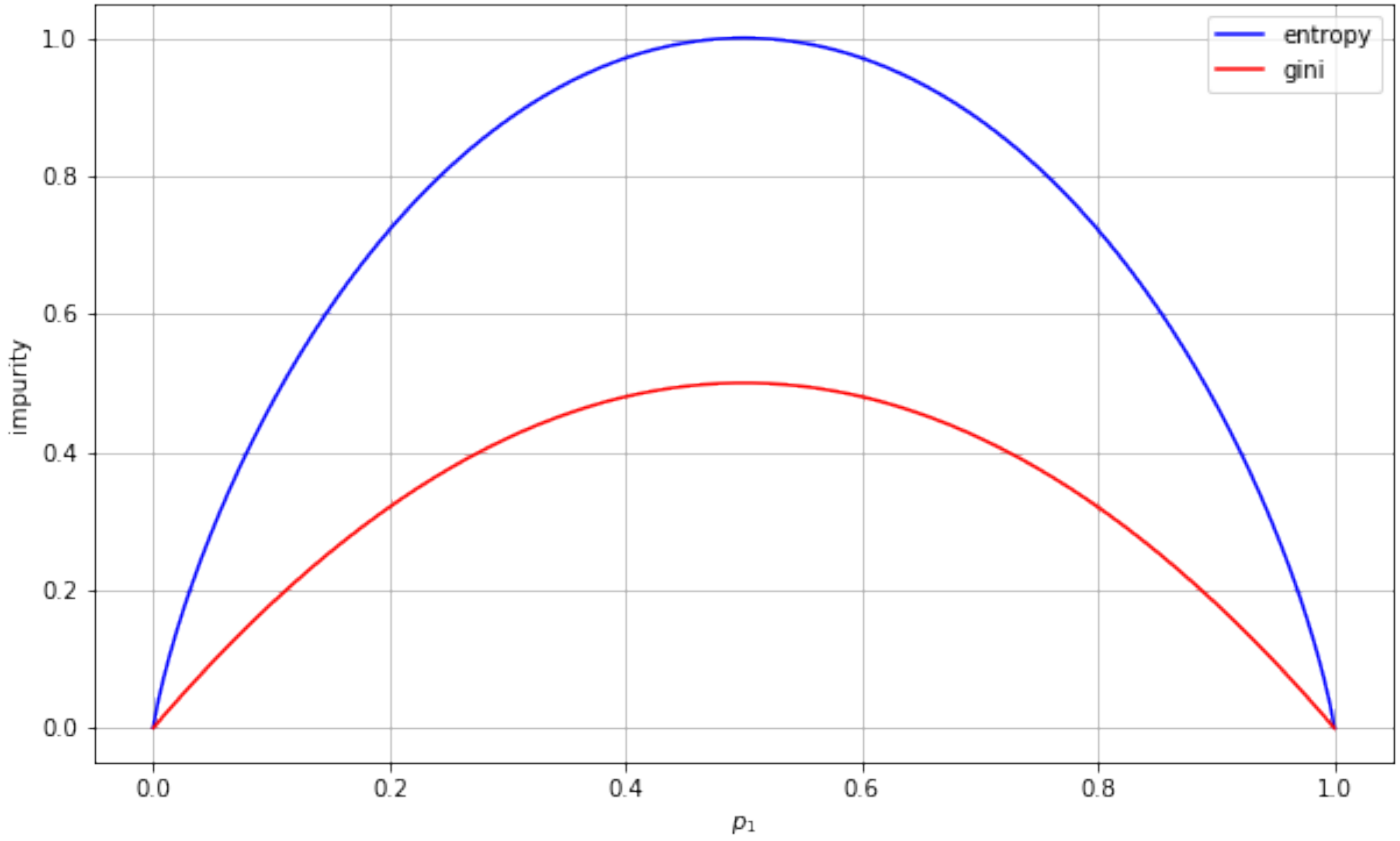
Gini Index

$$H(p_1, \ldots, p_K) = \sum_{i=1}^{K} p_i \left(1 - p_i\right)$$

- Consider a classifier, which outputs class k with probability p_k

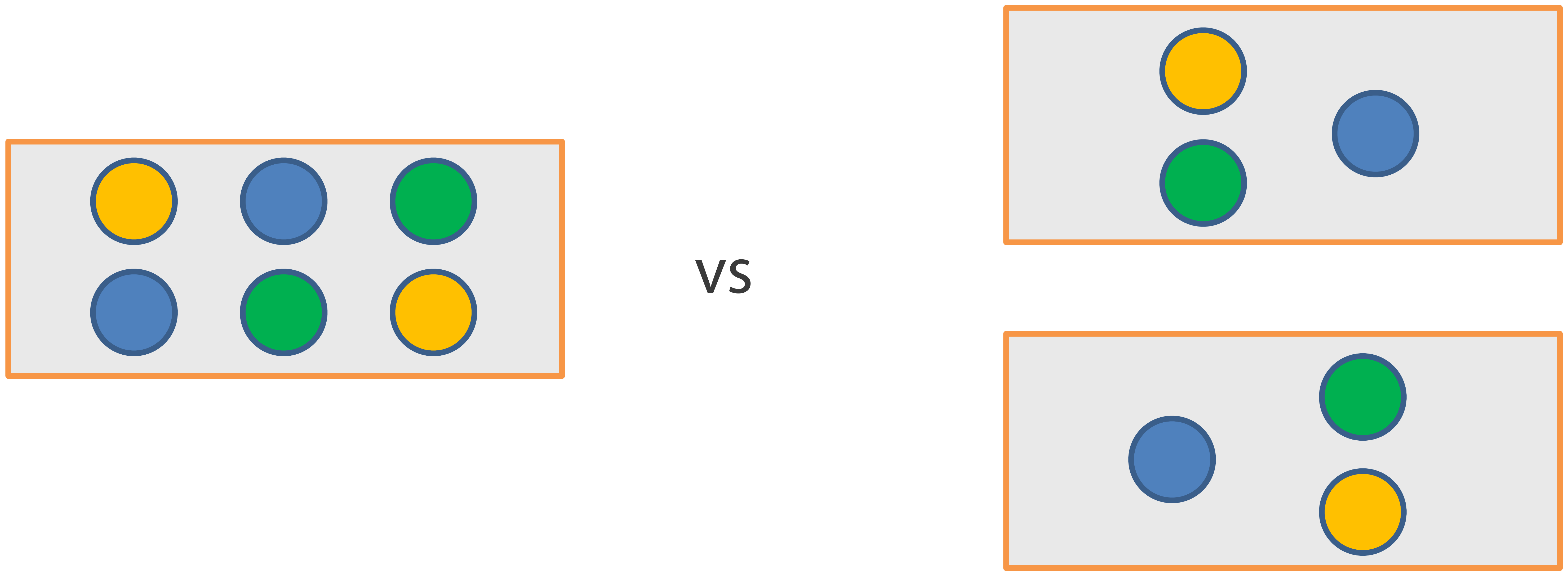
- Gini index is a probability that the object will be classified incorrectly if the class is assigned with probabilities $p_1, \ldots, p_k$

Gini Index vs Entropy



Impurity Criterions

- How to decide which split is better?
- Compare the impurity before the split (in the initial node R) and in the two nodes after the split (R_ℓ and R_r)



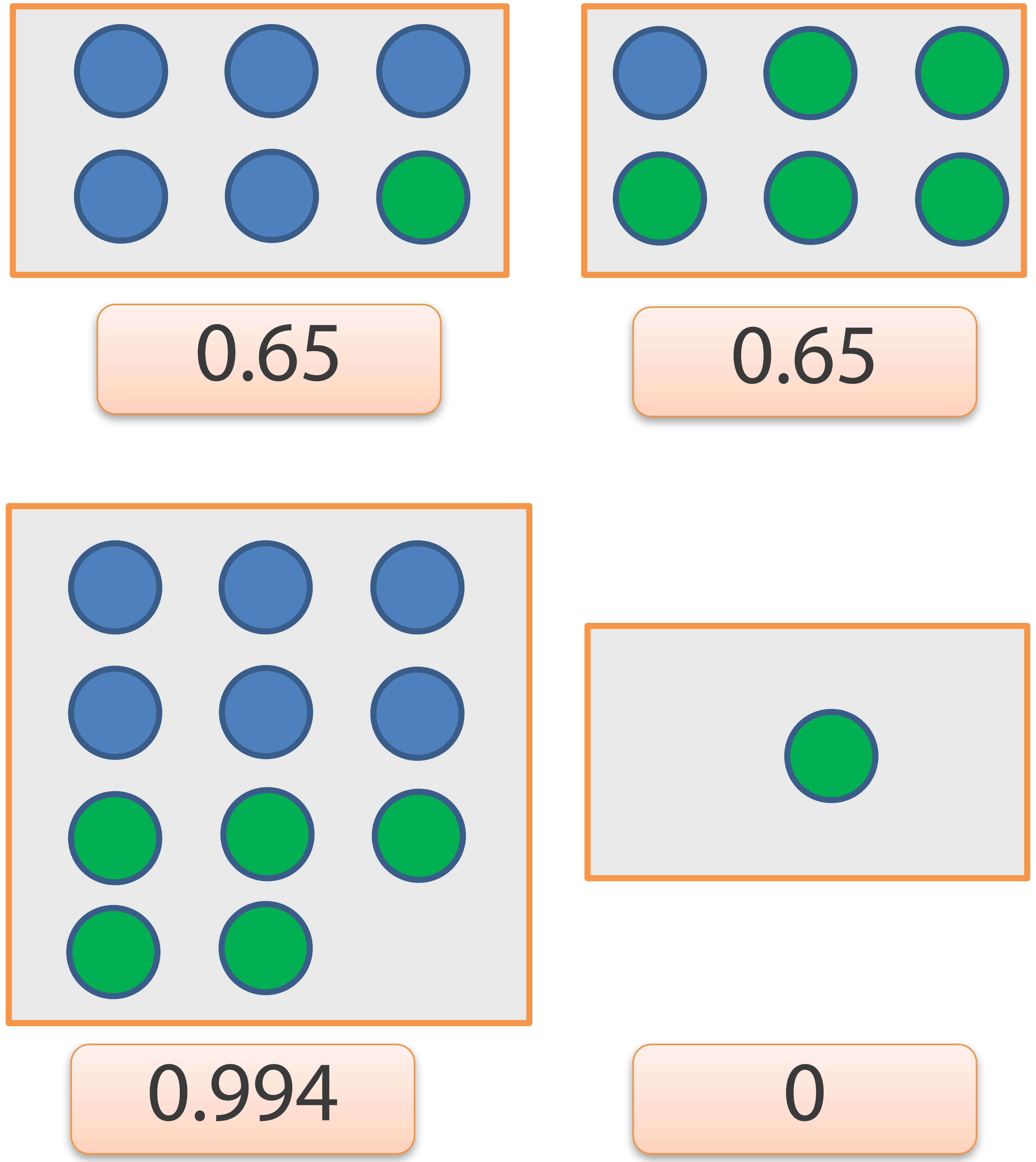
Impurity Criterions

- How to decide which split is better?
- Compare the impurity before the split (in the initial node R) and in the two nodes after the split (R_ℓ and R_r)

$$Q(R, j, t) = H(R) - \frac{|R_\ell|}{|R|} H(R_\ell) - \frac{|R_r|}{|R|} H(R_r) \to \max_{j,\ t}$$

How to Compare Two Splits?

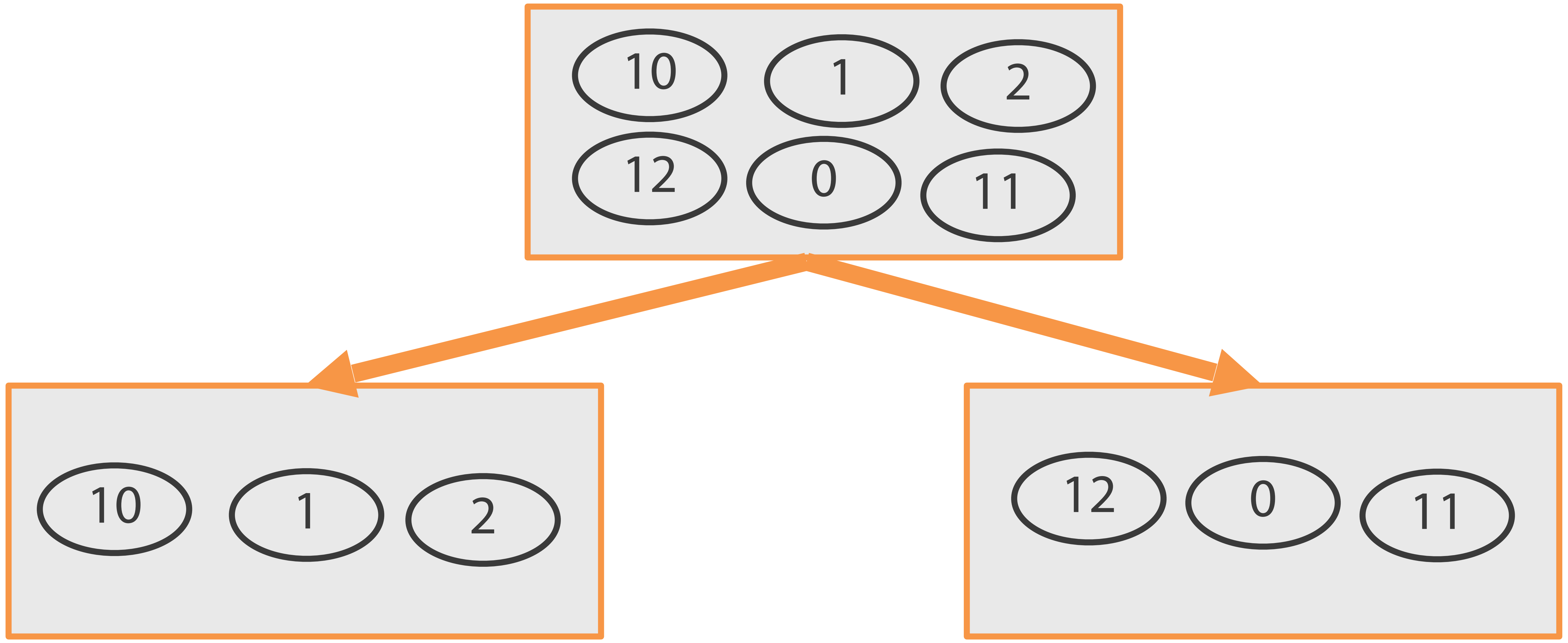
$$H(R) = 1$$



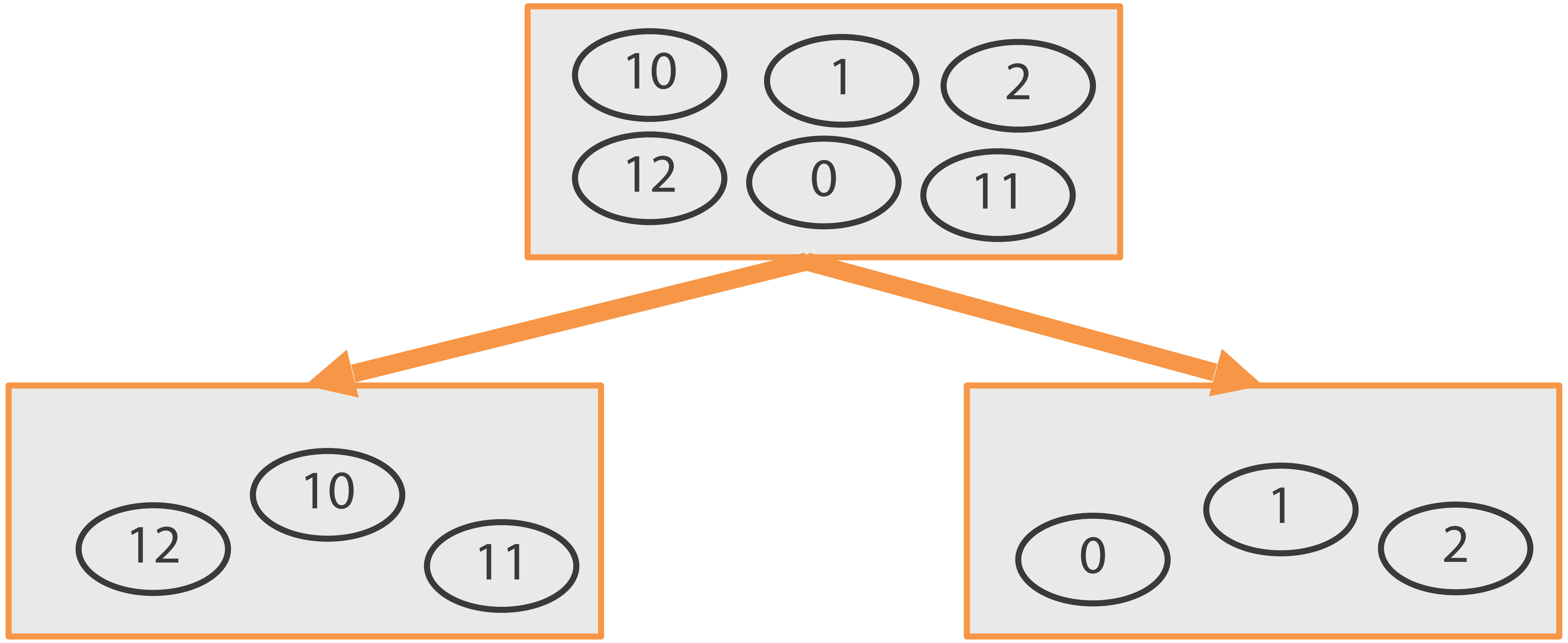
- $Q(R) = 1 - \frac{1}{2}0.65 - \frac{1}{2}0.65$
- $Q(R) = 0.35$

- $Q(R) = 1 - \frac{11}{12}0.994 - \frac{1}{12}0$
- $Q(R) = 0.088$

Greedy Construction: Regression



Greedy Construction: Regression



Regression Task

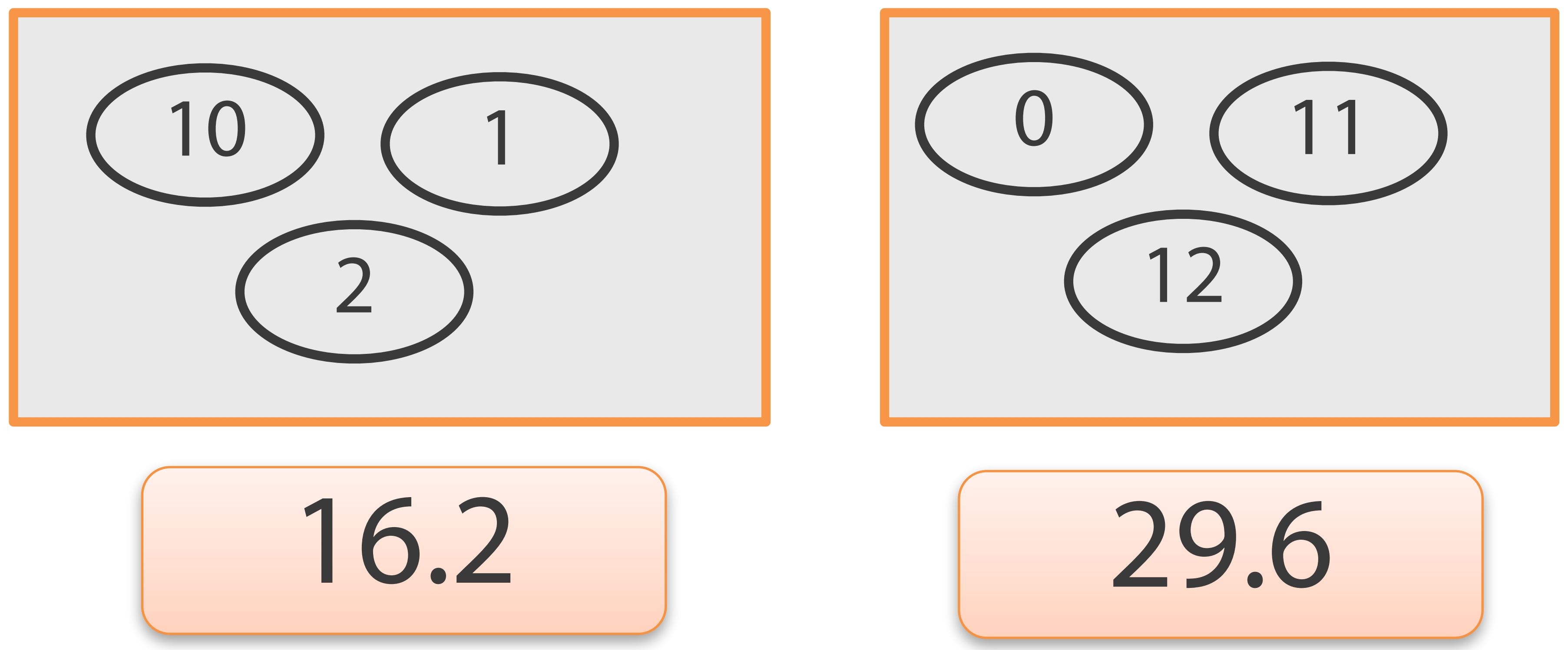
$$H(R) = \frac{1}{|R|} \sum_{(x_i,\, y_i) \in R} \left(y_i - y_R\right)^2$$

$$y_R = \frac{1}{|R|} \sum_{(x_i,\, y_i) \in R} y_i$$

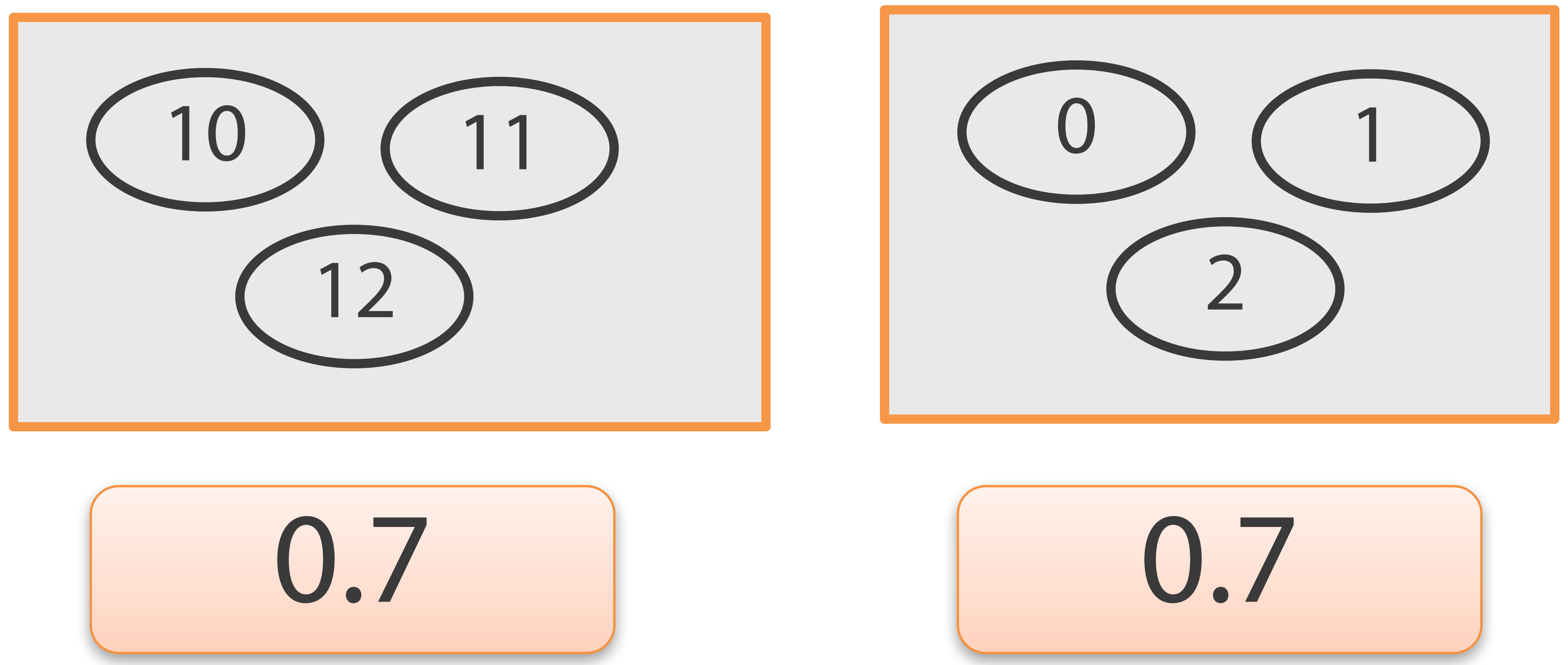
- So we can measure the variance of answers in the node

How to Compare Two Splits?

$$H(R) = 25.6$$



- $Q(R) = 25.6 - \frac{1}{2}16.2 - \frac{1}{2}29.6$
- $Q(R) = 2.7$



- $Q(R) = 25.6 - \frac{1}{2}0.7 - \frac{1}{2}0.7$
- $Q(R) = 24.9$

Summary

- We can choose the split, so that it reduces the diversity of answers in the resulting nodes

- We use impurity criterion to measure the quality of the split

- There are different criterions that might be used.
  The most popular are:
  - Entropy and Gini for classification
  - Variance for regression

Greedy Tree Construction

How to Construct a Tree?

- Optimal option:
  - Try all possible trees and select the smallest one

- That is too computationally expensive

How to Construct a Tree?

- We know how to choose the best split for a given node

- Let’s use greedy algorithm

- We start from the root node and will be splitting until some stopping criterion is satisfied

Stopping Criterions

- Restrict the maximal depth
- Restrict the number of leaves
- Fix the minimal number of objects in the node
- Set the minimal decrease in the diversity when splitting
- etc.

Greedy Algorithm

1. Put the whole dataset into the root: $R_1 = X$

2. Start the tree construction: $\text{SplitNode}(1, R_1)$

Greedy Algorithm

$\mathrm{SplitNode}\left(m,\ R_m\right)$

1. If stopping criterion is satisfied, then quit

2. Find the best split (feature and threshold):

$$j,\ t = \underset{\mathrm{j,t}}{\mathrm{argmax}} Q(R_m,\ j,\ t)$$

3. Split the objects:

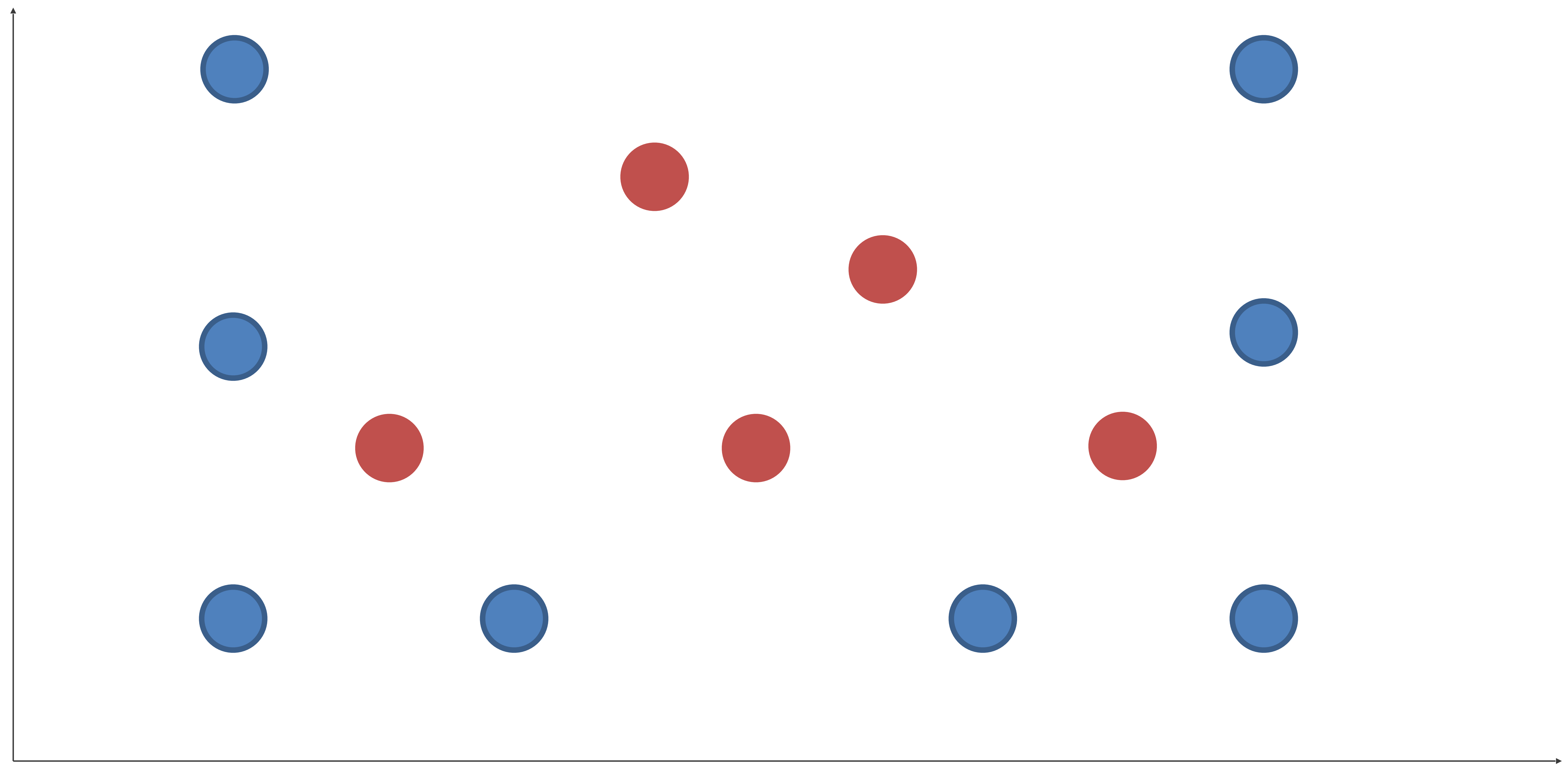
$$R_\ell = \left\{\left\{(x,\ y) \in R_m \middle| \left[x_j < t\right]\right\}\right.,$$

$$R_r = \left\{\left\{(x,\ y) \in R_m \middle| \left[x_j \geq t\right]\right\}\right.$$

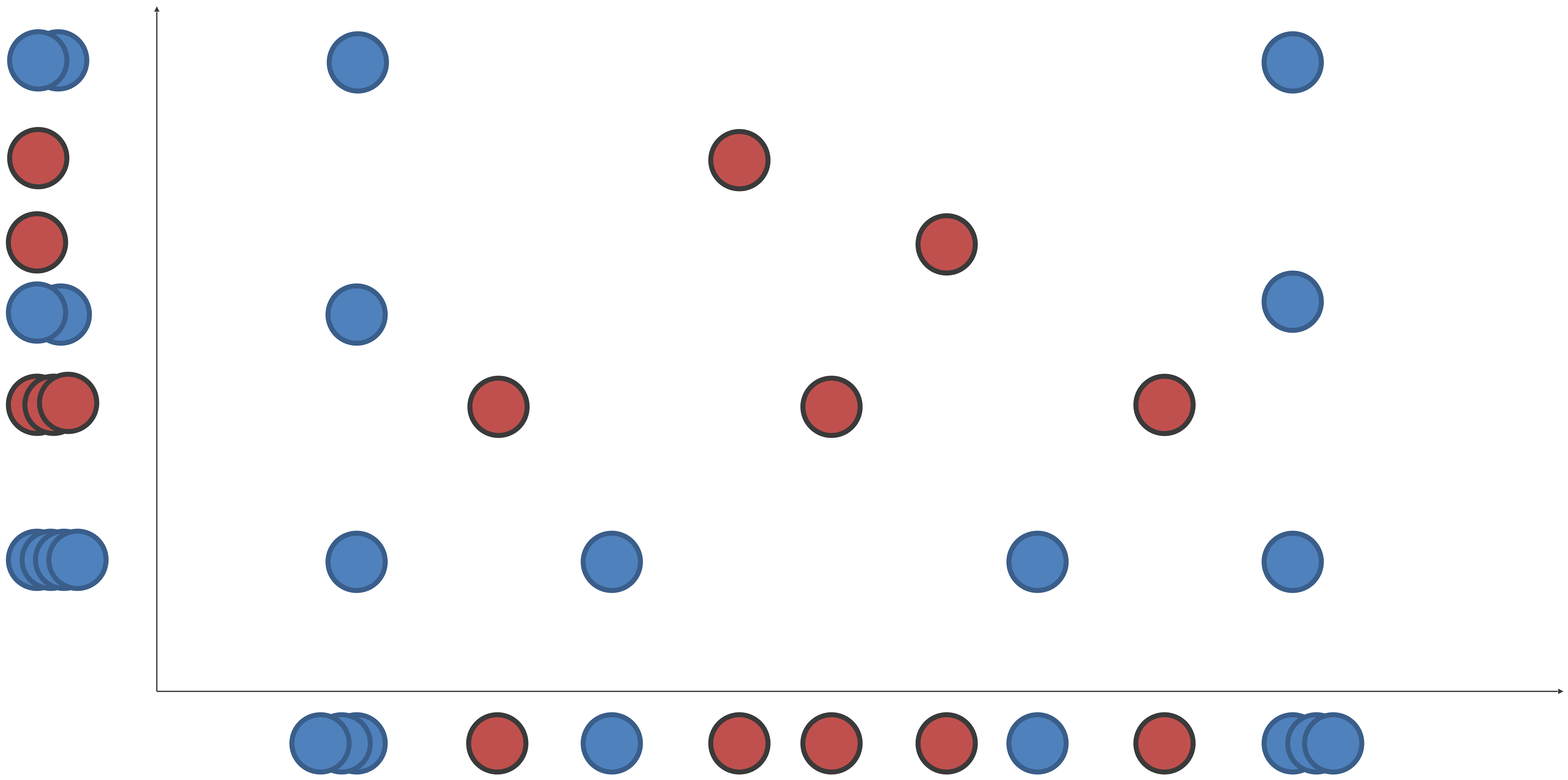
4. Repeat for the child nodes:

$\mathrm{SplitNode}\left(\ell,\ R_\ell\right)$ and $\mathrm{SplitNode}\left(r,\ R_r\right)$

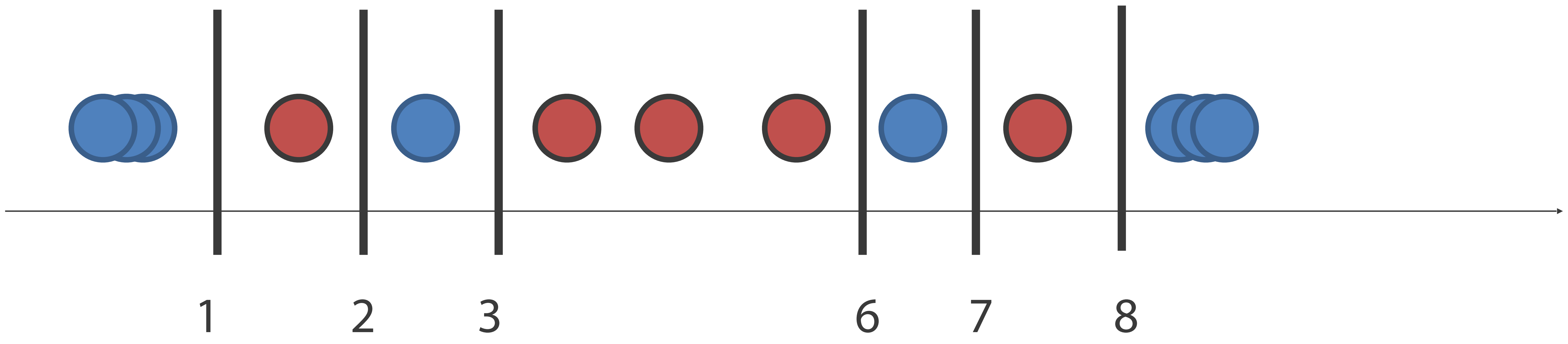
Greedy Algorithm



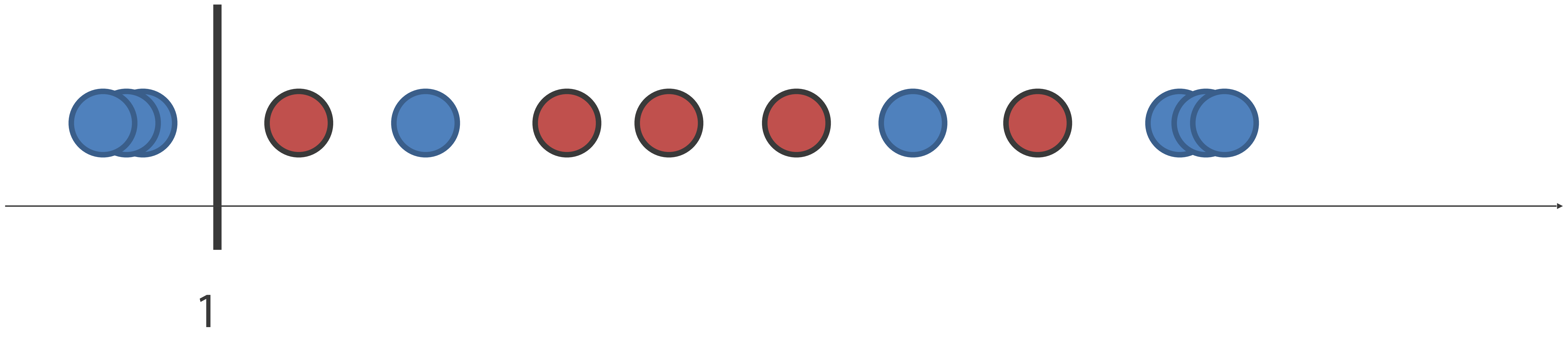
Greedy Algorithm



Splitting on the first feature



Splitting on the first feature

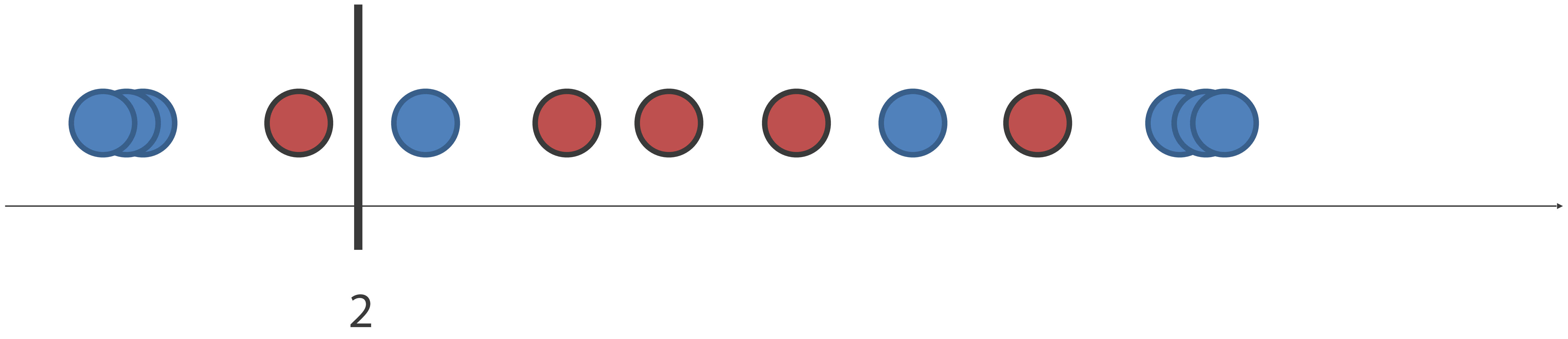


(1, 0)
H(p) = 0

(1/2, 1/2)
H(p) = 1

$$\frac{3}{13}H\left(p_l\right)+\frac{10}{13}H\left(p_r\right)=0.76$$

Splitting on the first feature

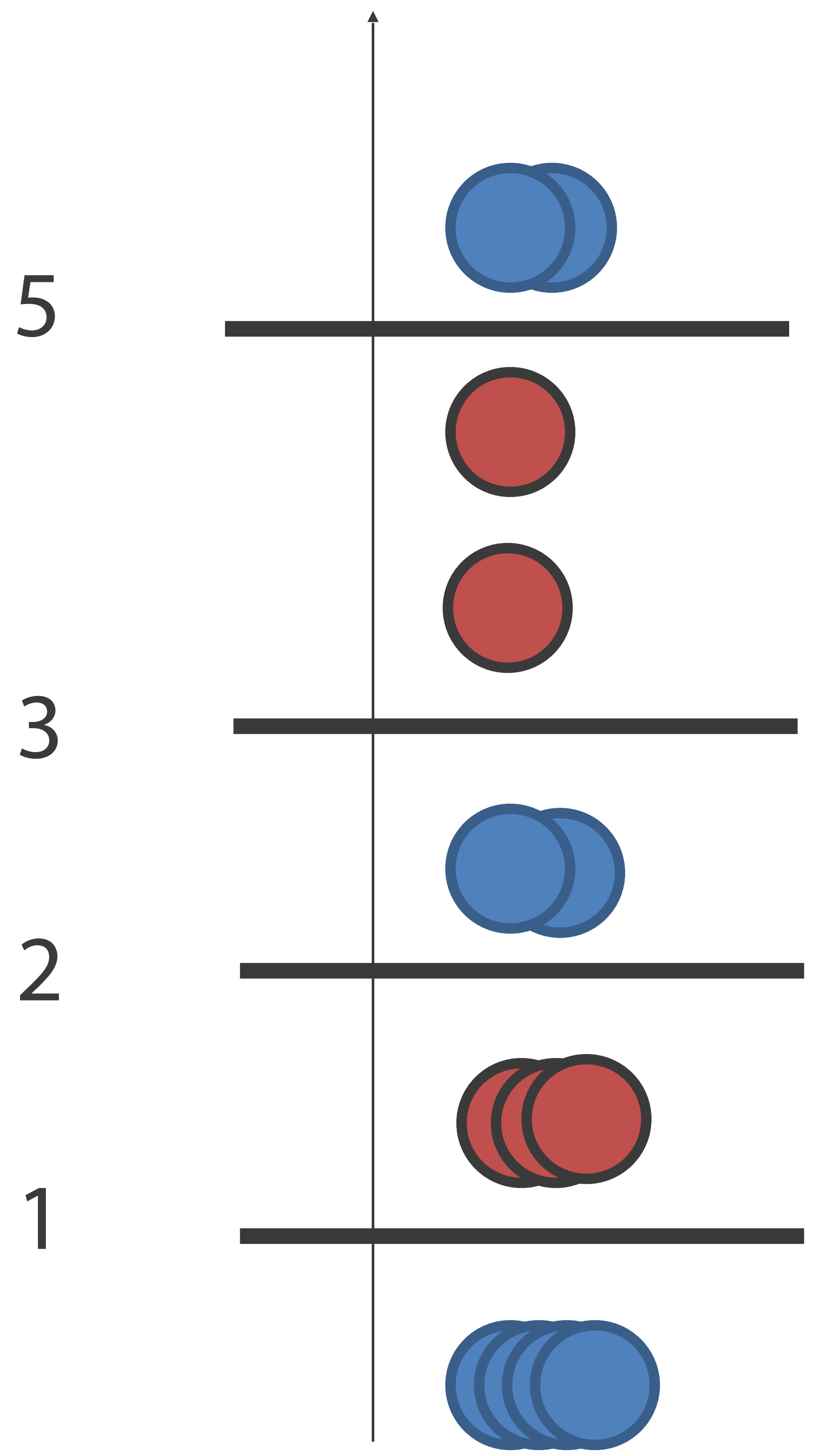


(3/4, 1/4)
H(p) = 0.81

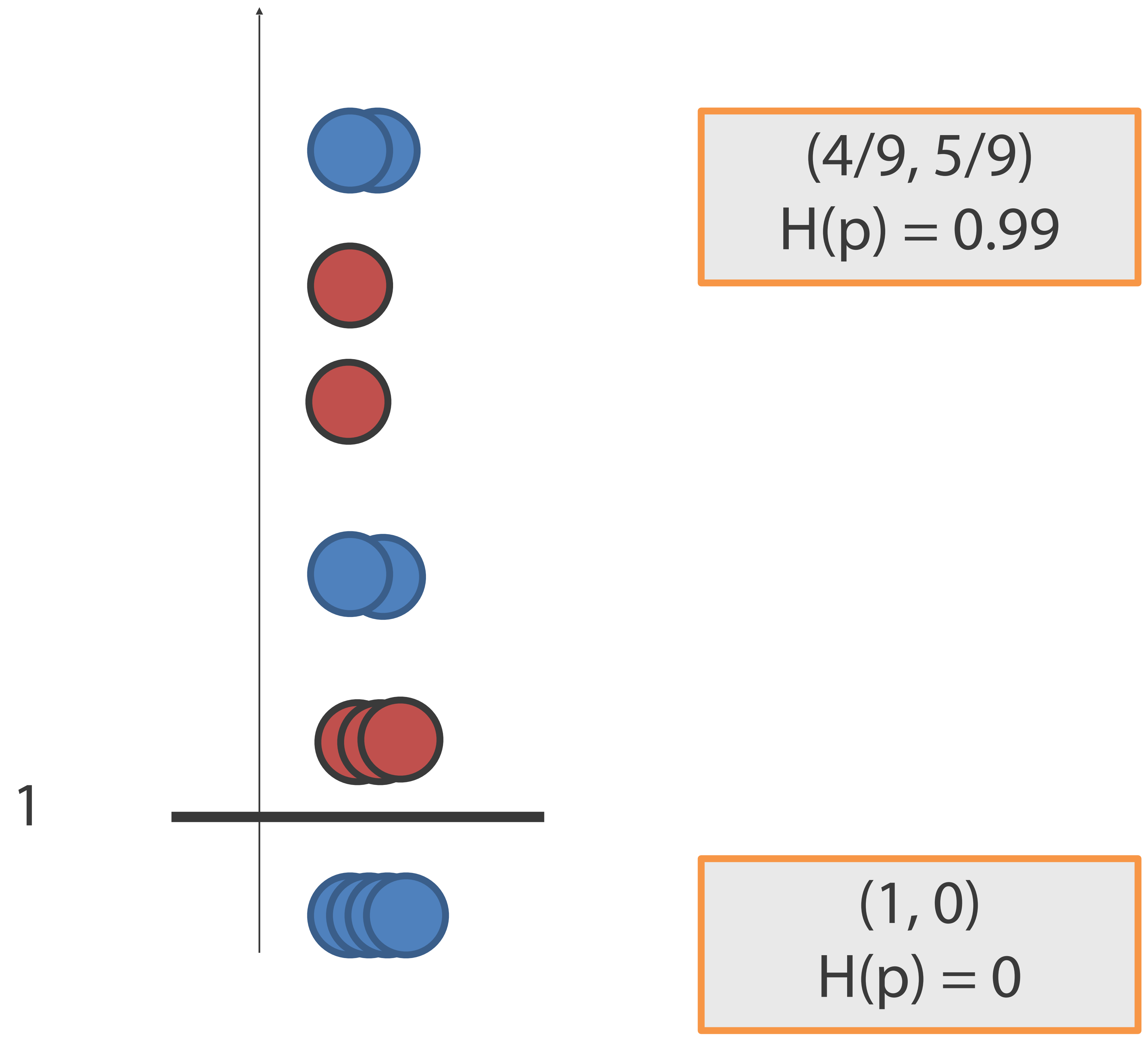
(5/9, 4/9)
H(p) = 0.99

$$\frac{4}{13}H\left(p_l\right) + \frac{9}{13}H\left(p_r\right) = 0.93$$

Splitting on the Second Feature

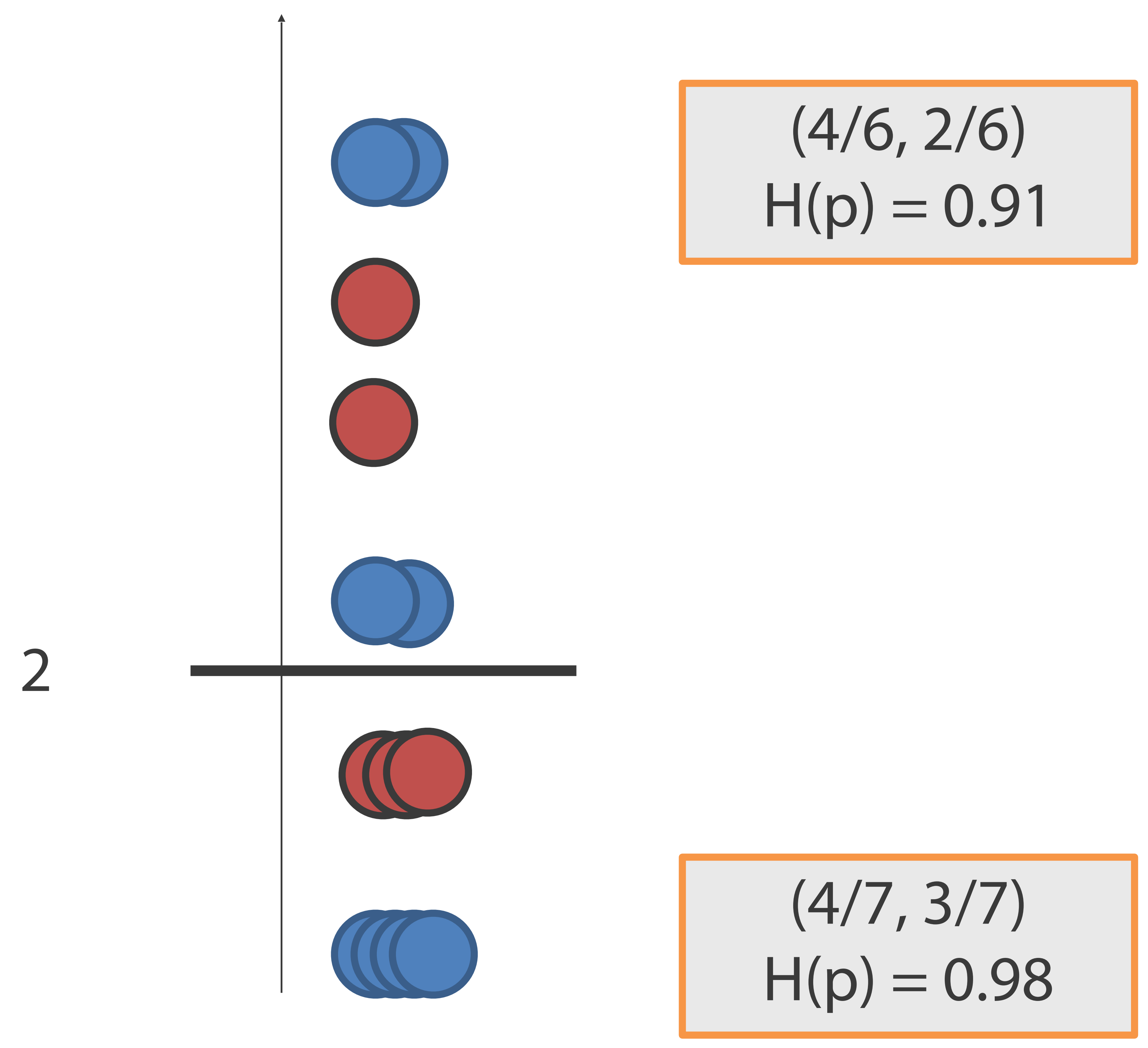


Splitting on the Second Feature



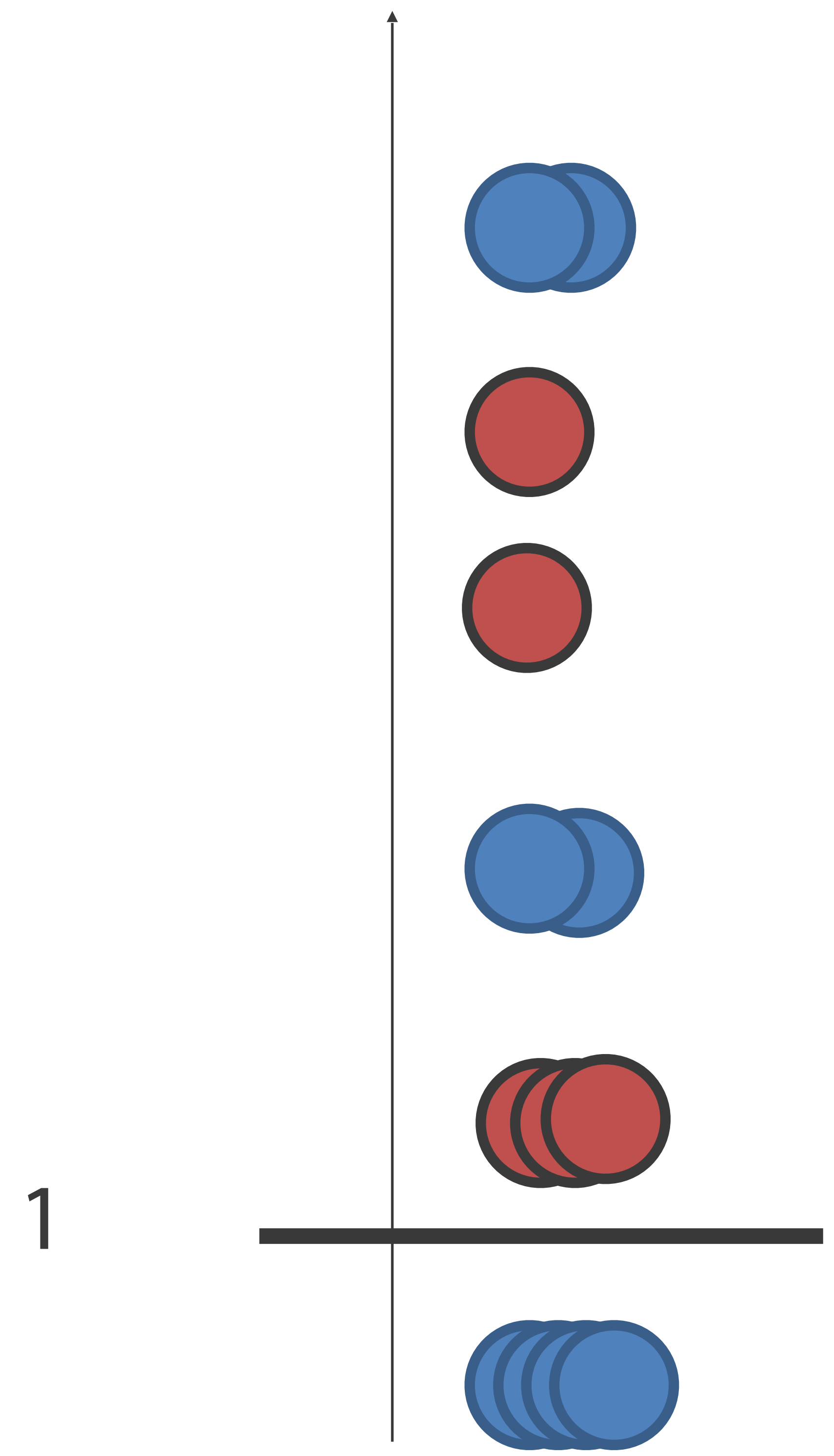
$$\frac{4}{13}H\left(p_l\right) + \frac{9}{13}H\left(p_r\right) = 0.68$$

Splitting on the Second Feature



$$\frac{7}{13}H\left(p_l\right) + \frac{6}{13}H\left(p_r\right) = 0.94$$

Splitting on the Second Feature



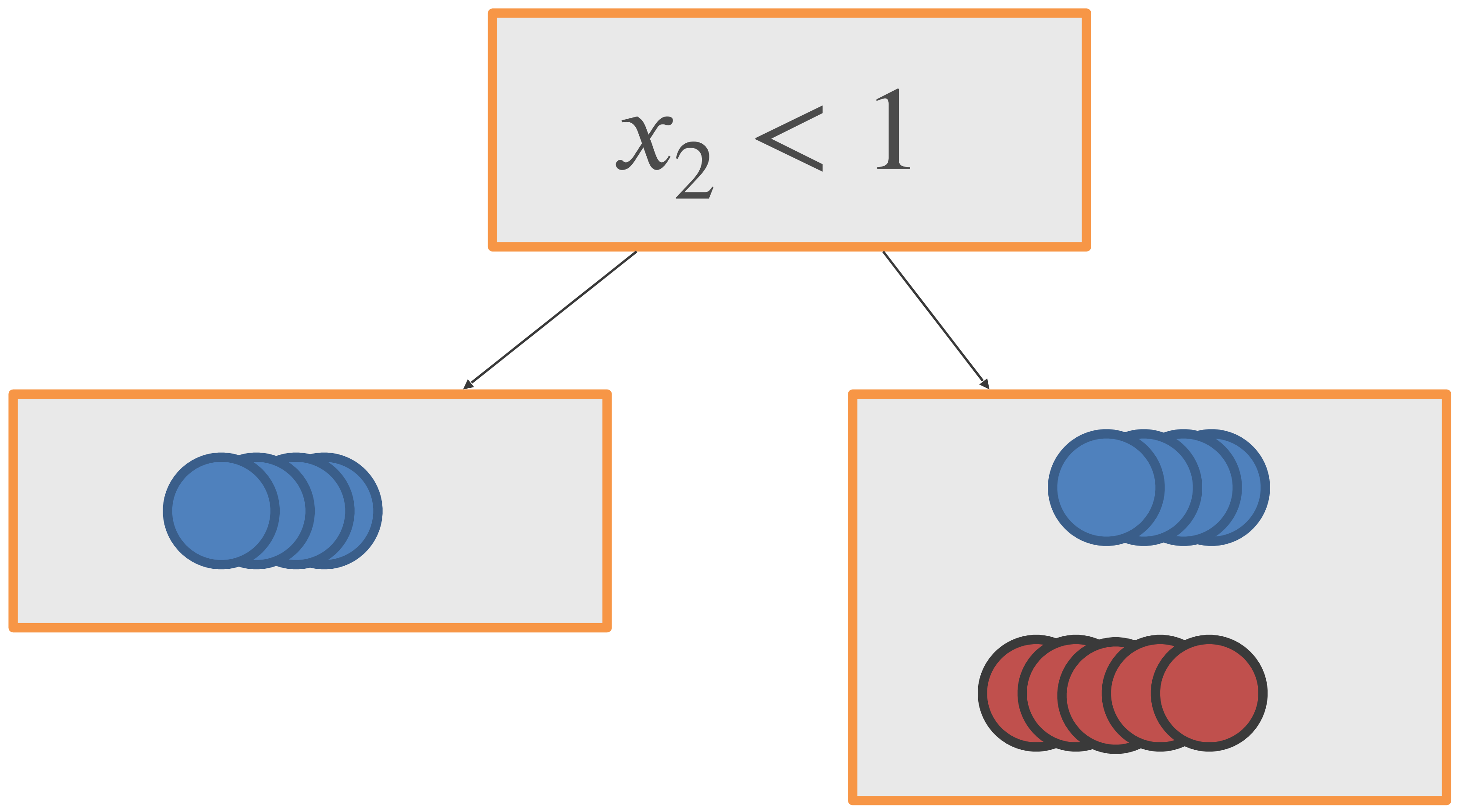
(4/9, 5/9)
H(p) = 0.99

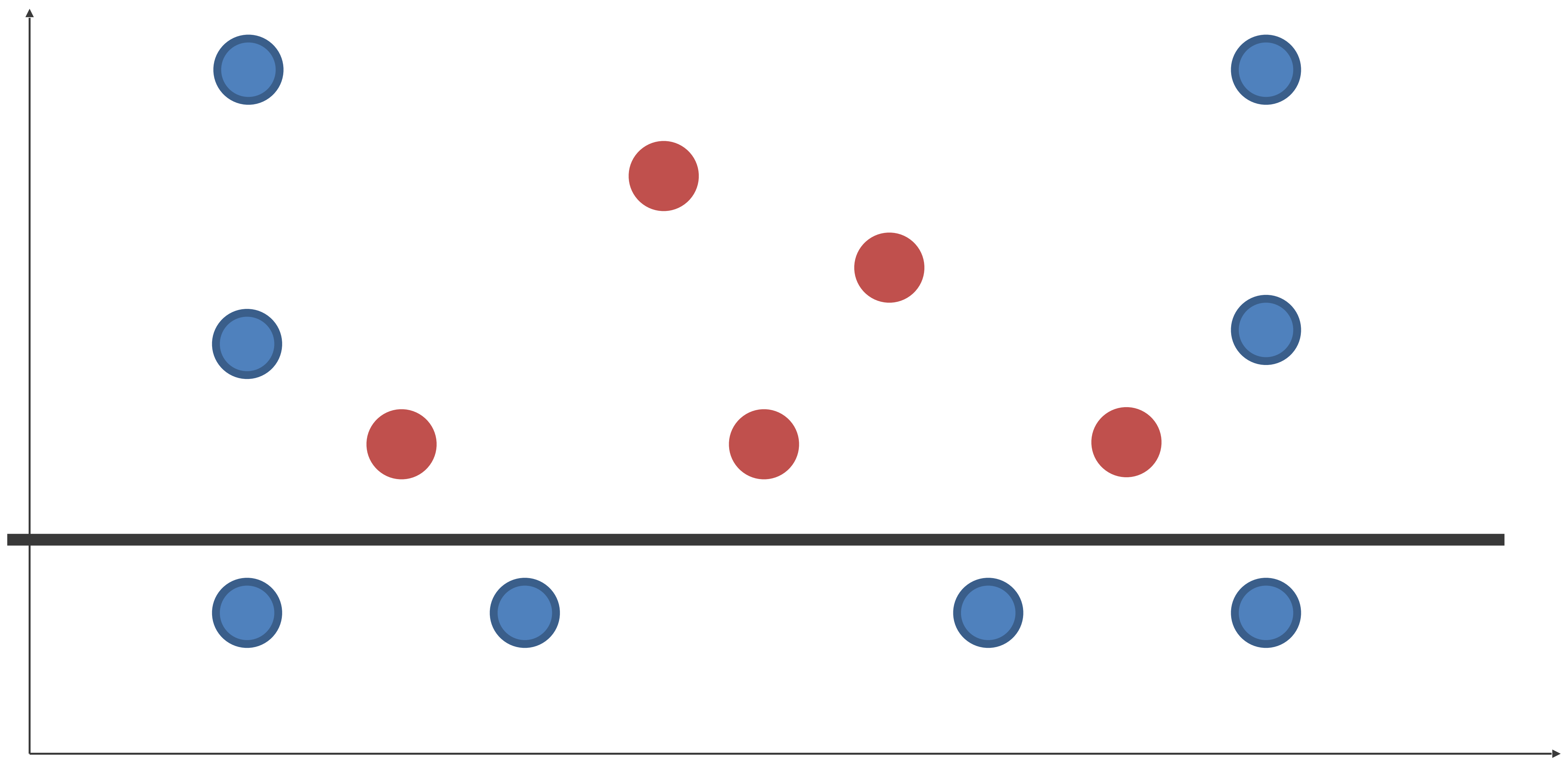
(1, 0)
H(p) = 0

$$\frac{4}{13}H\left(p_l\right) + \frac{9}{13}H\left(p_r\right) = 0.68$$

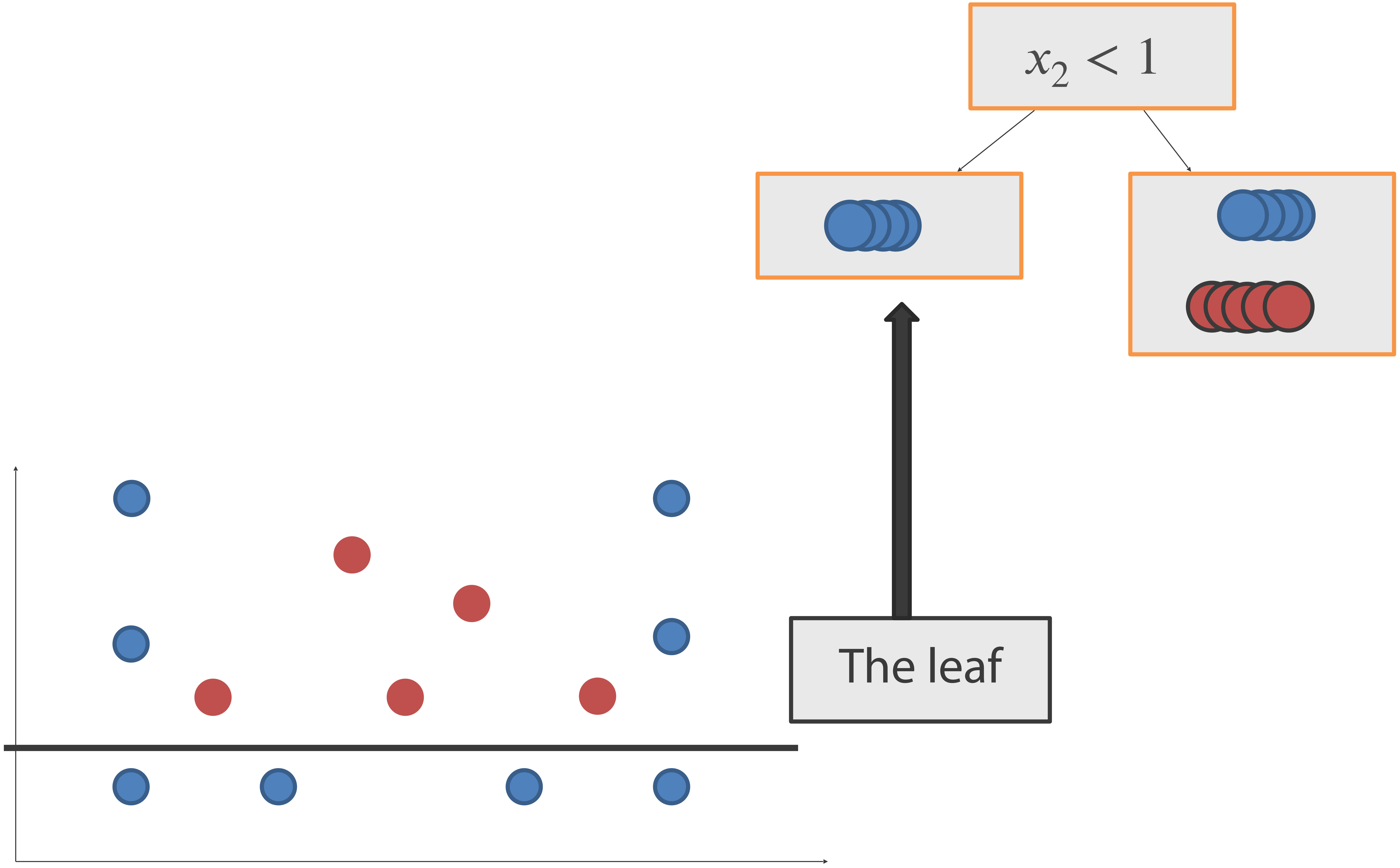
The Best Split

Greedy Algorithm

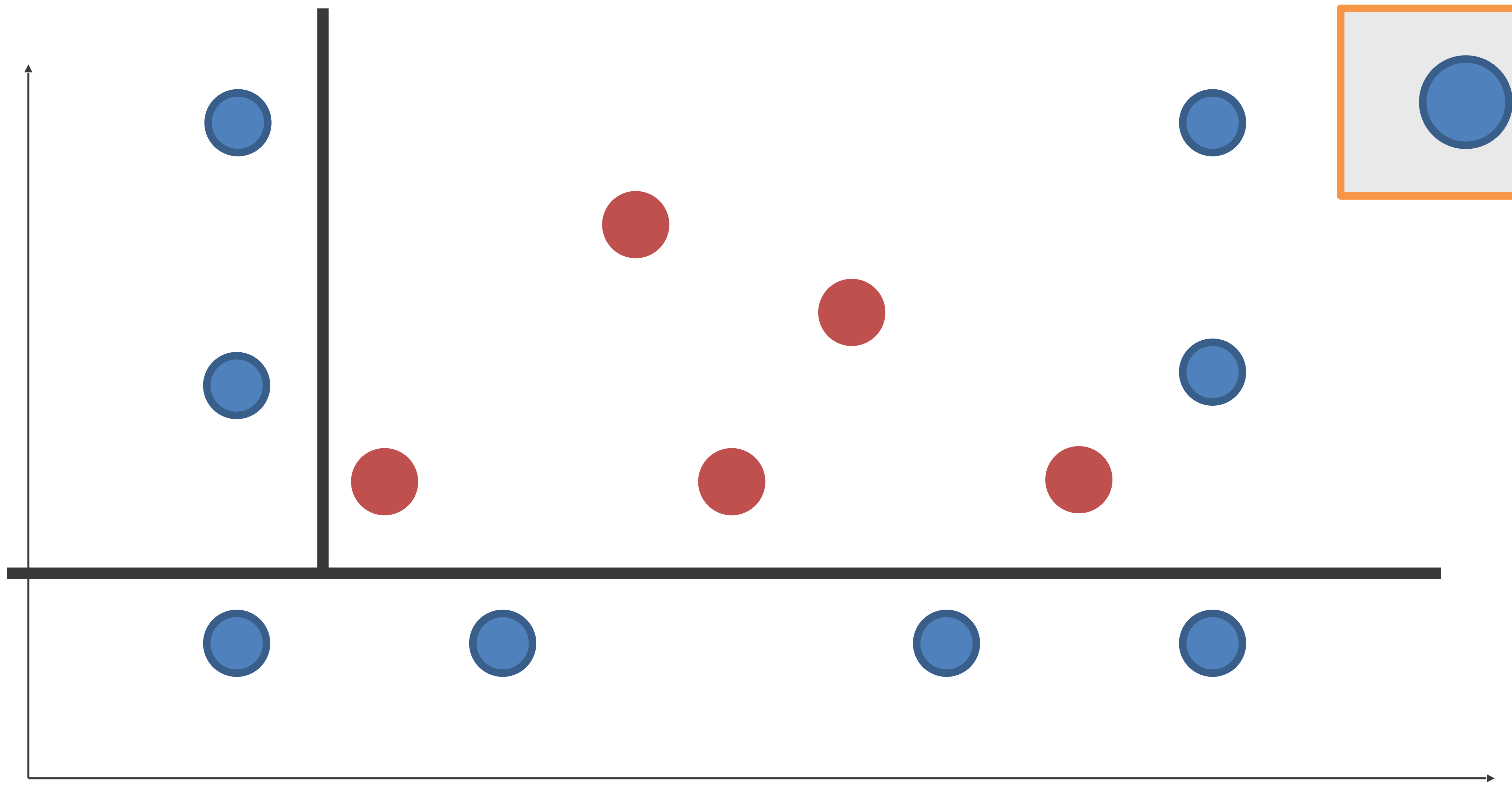


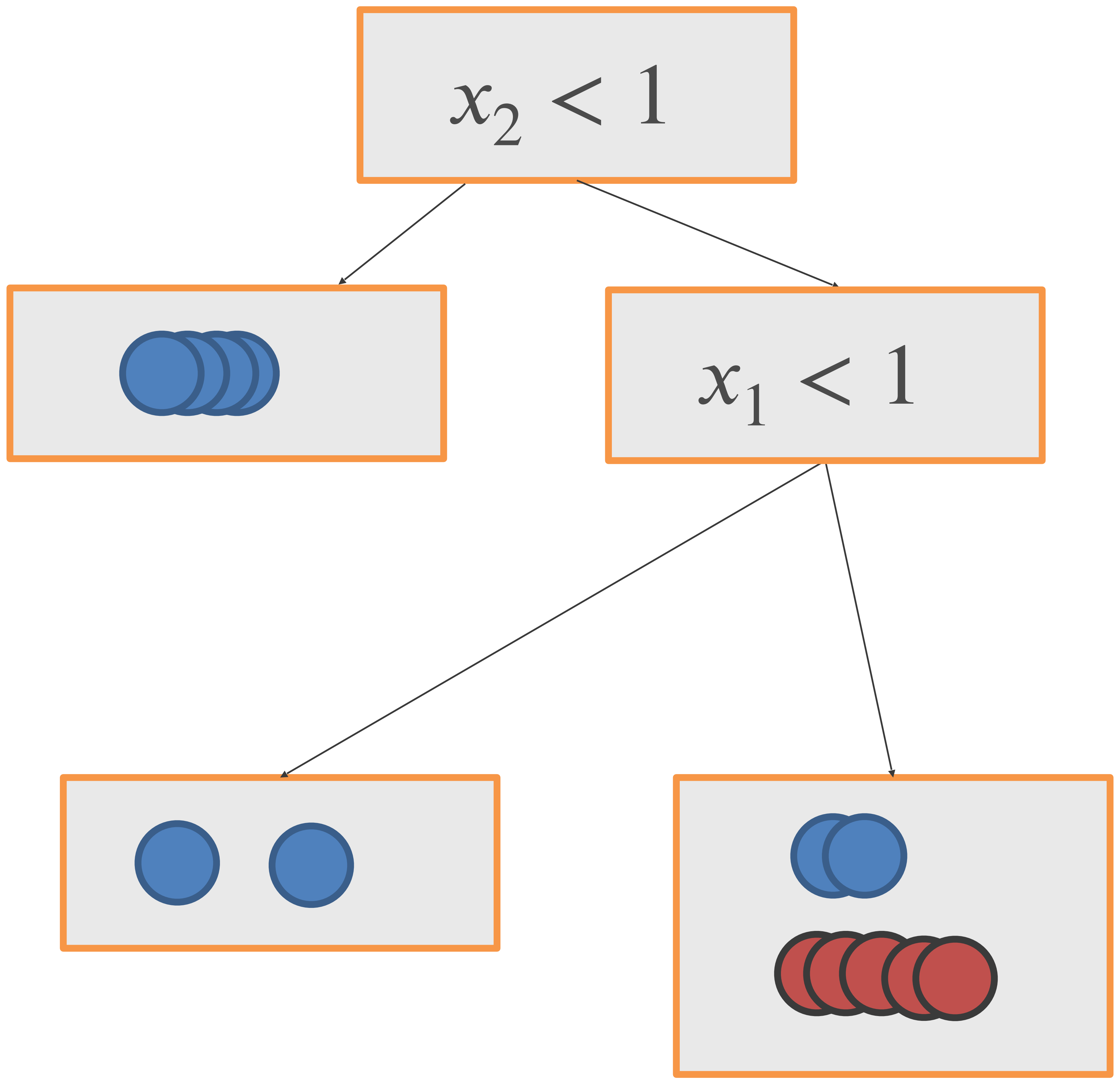


Greedy Algorithm

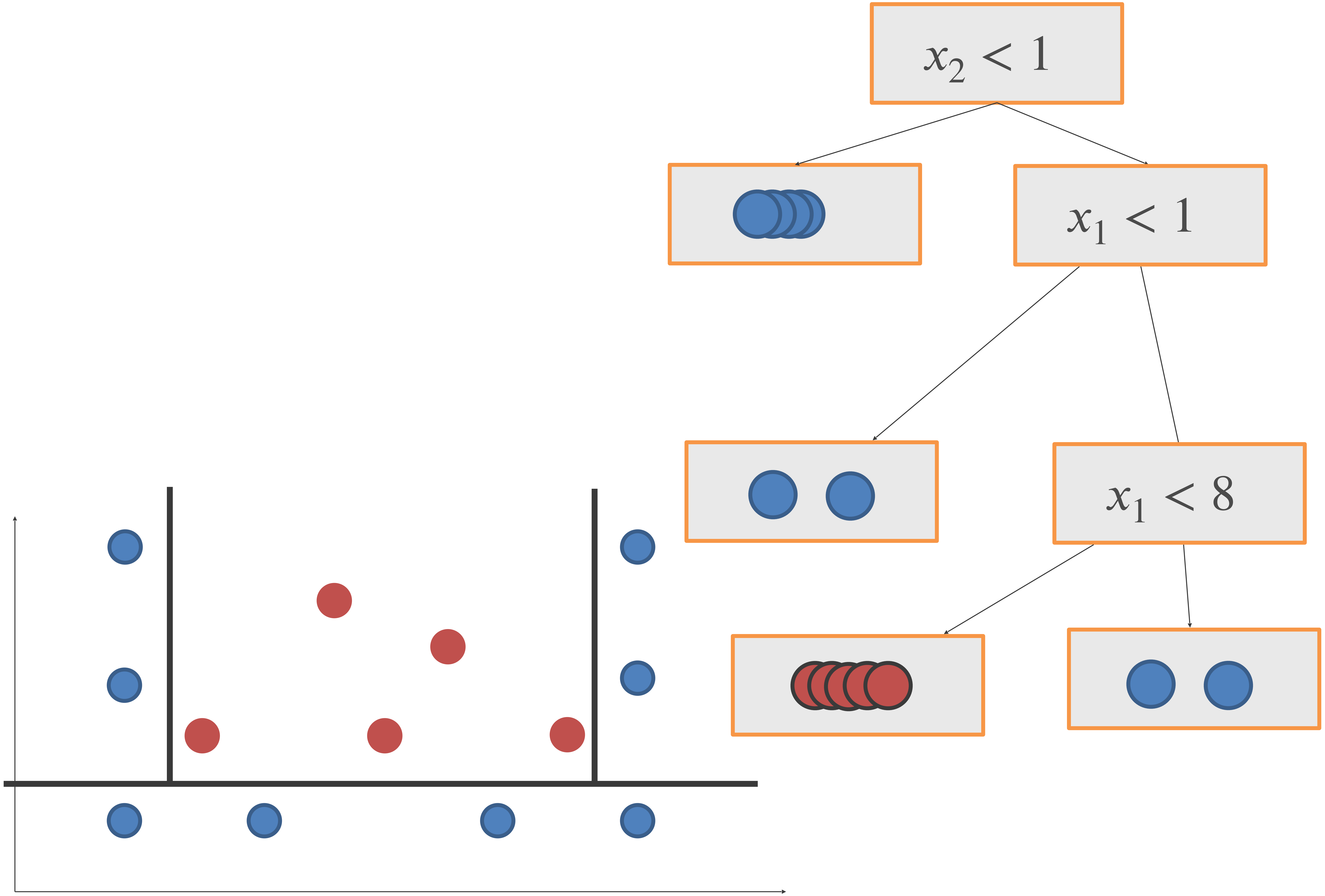


Greedy Algorithm





Greedy Algorithm

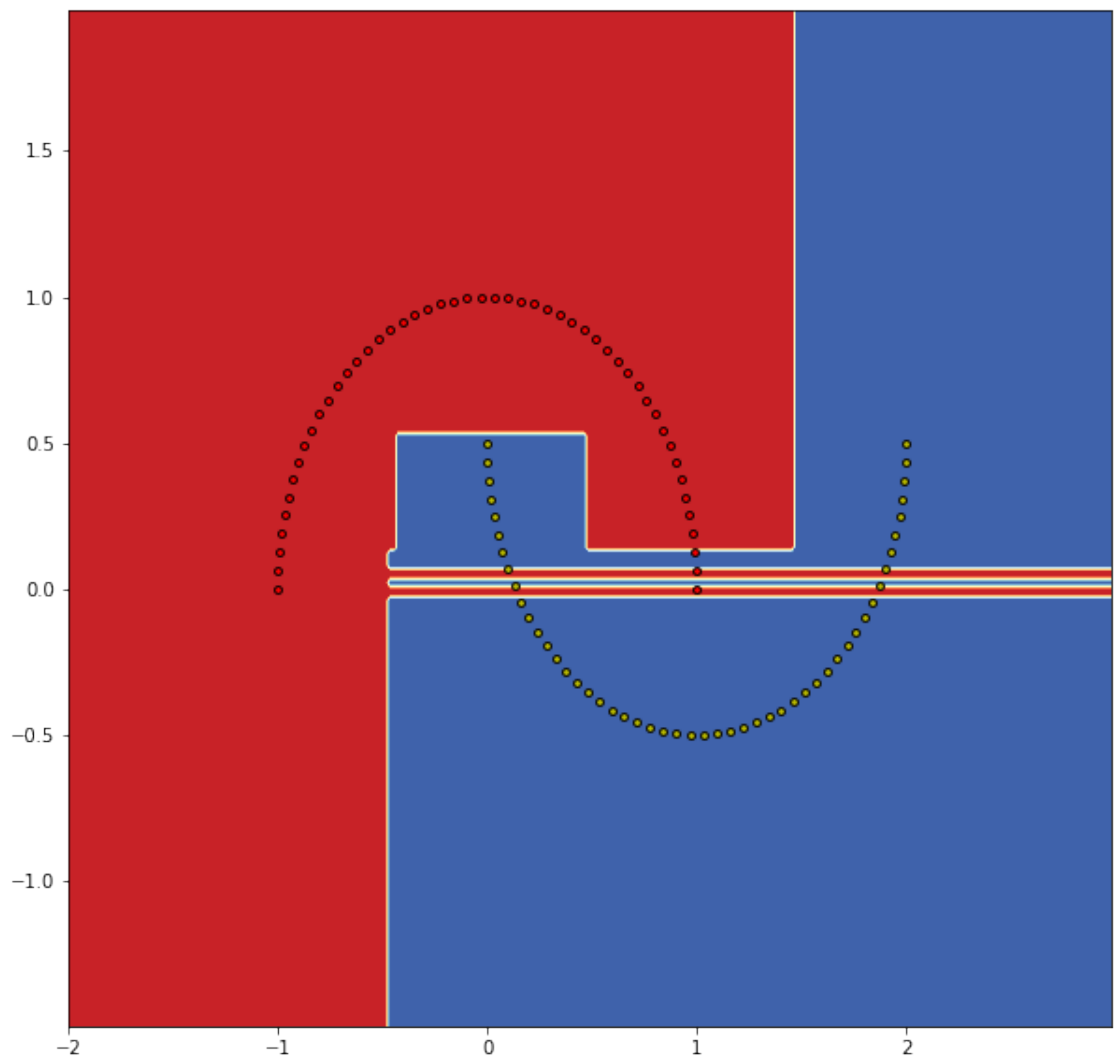


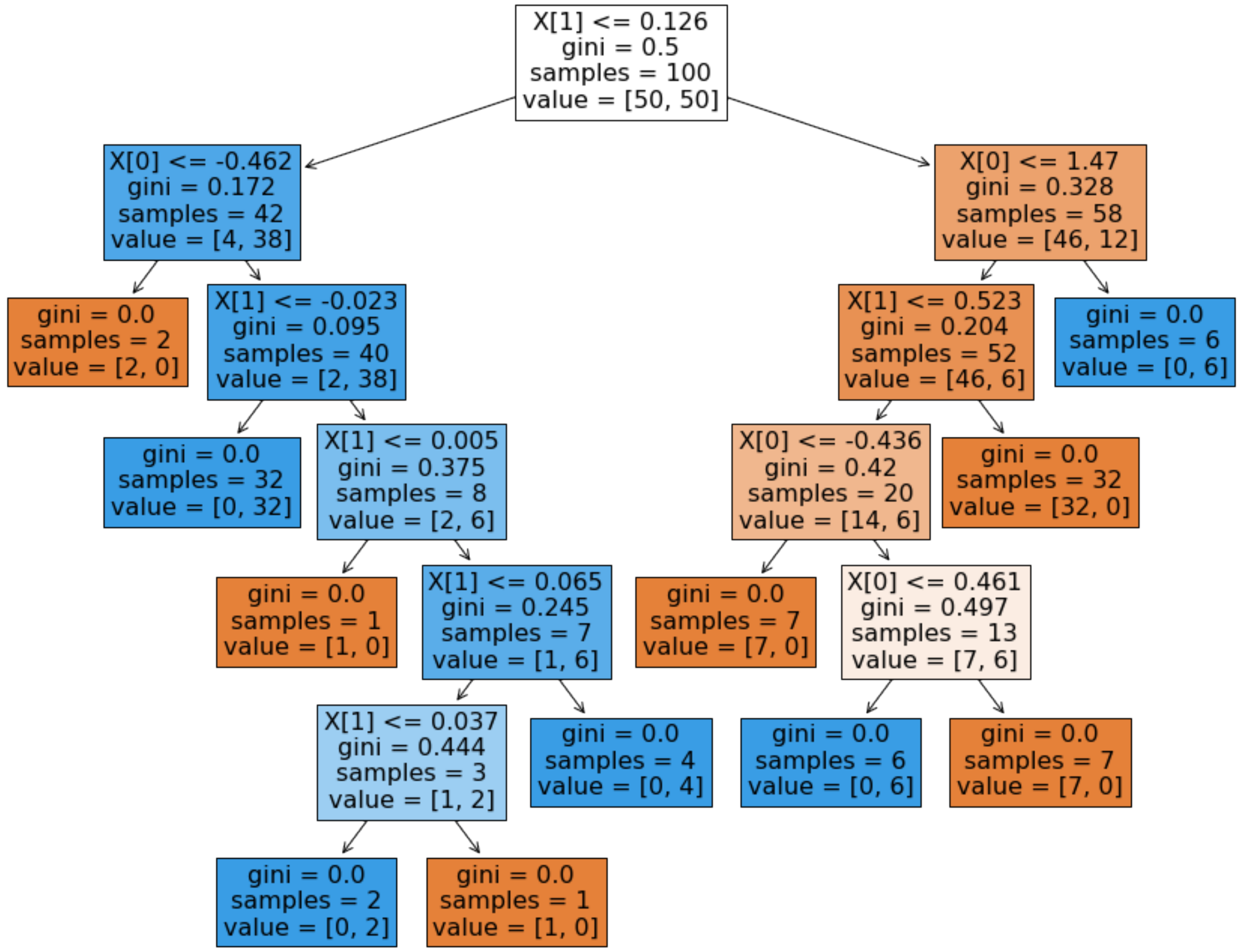
Summary

- We use greedy algorithm to construct a tree
- At each step we select the best split
- The algorithm is quite complex and requires brute force of all the splits at each step

High Variance of Decision Trees

Decision Trees and Overfitting

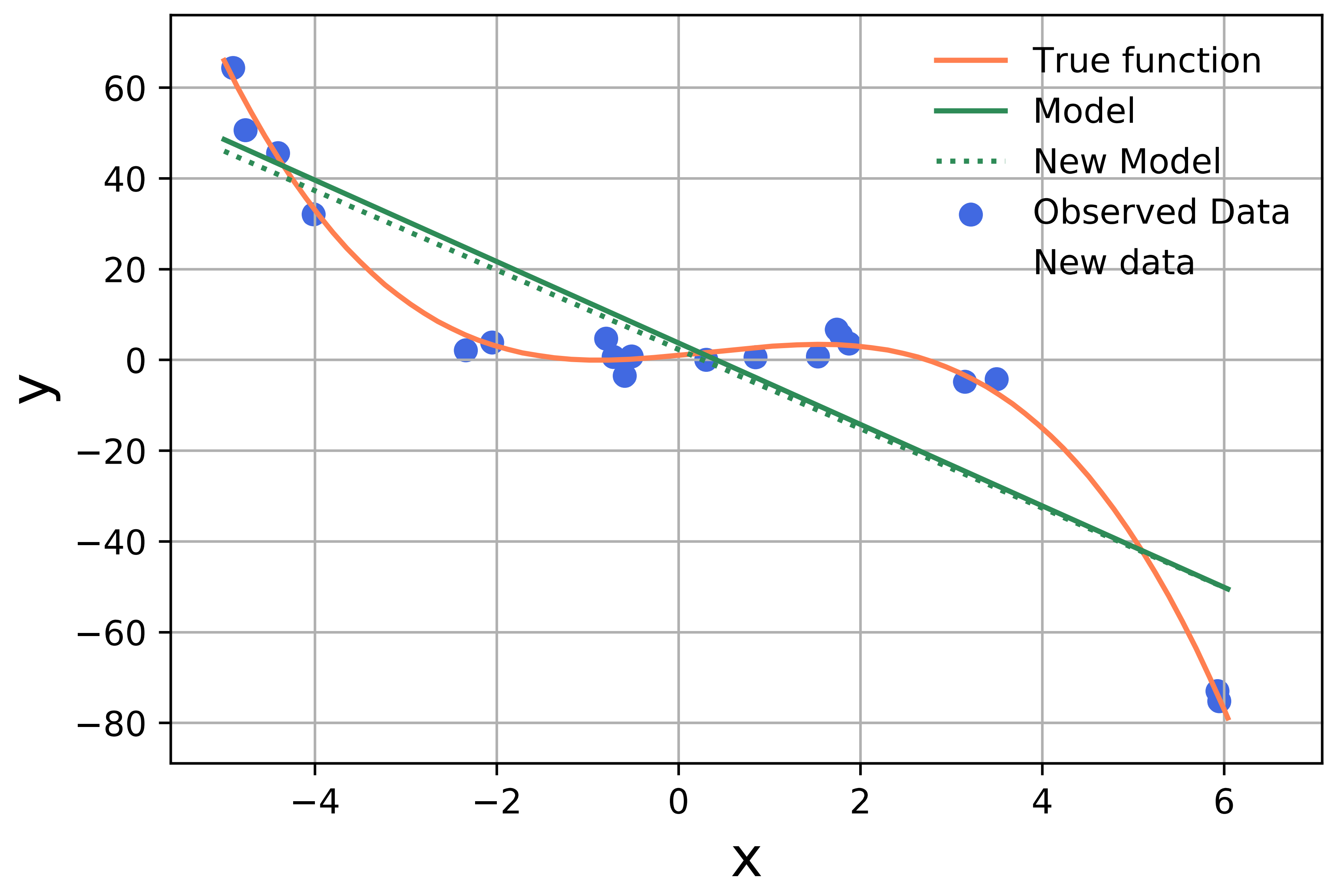




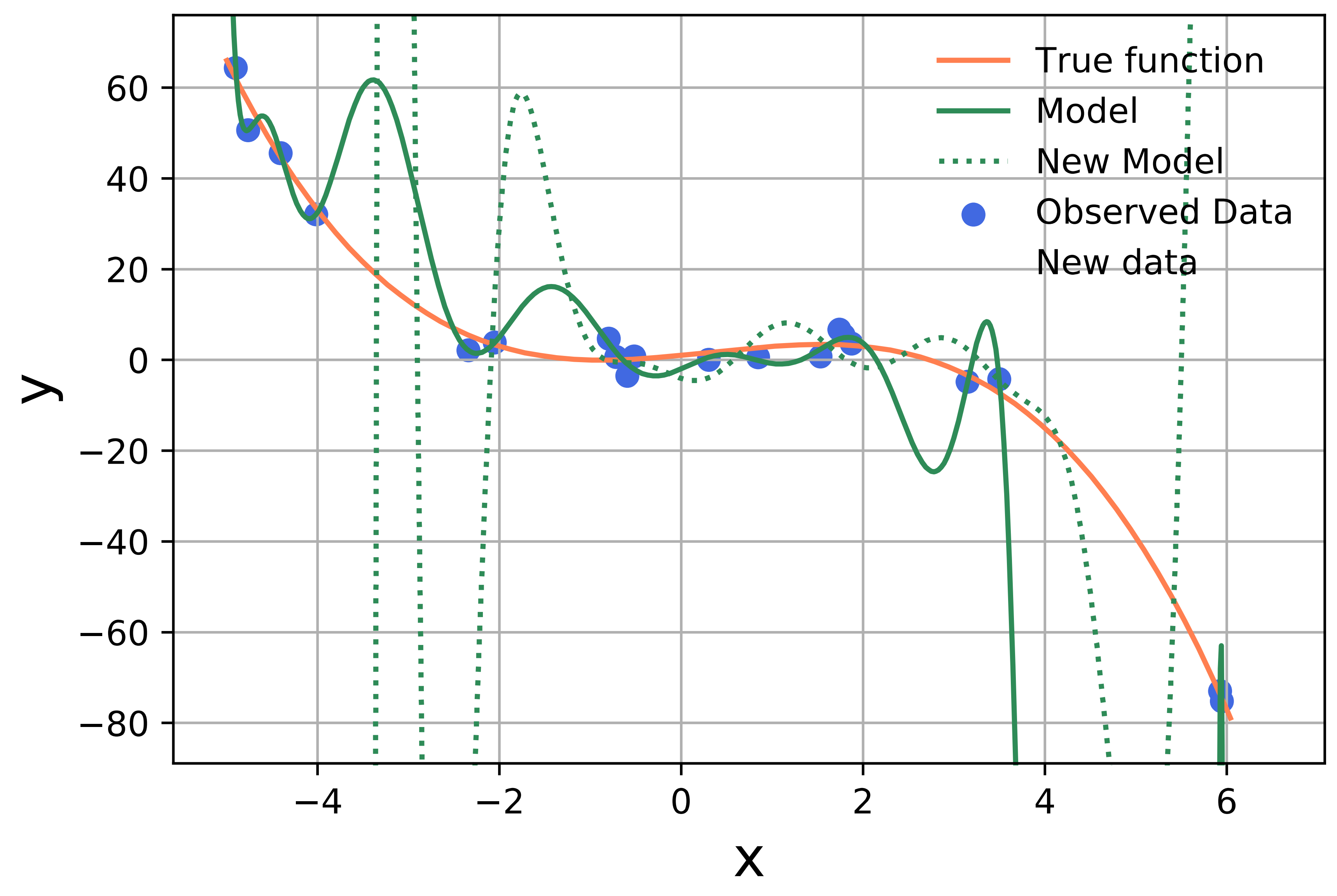
Variance

Variance – sensitivity of the model to the fluctuations in the data

Low Variance



High Variance

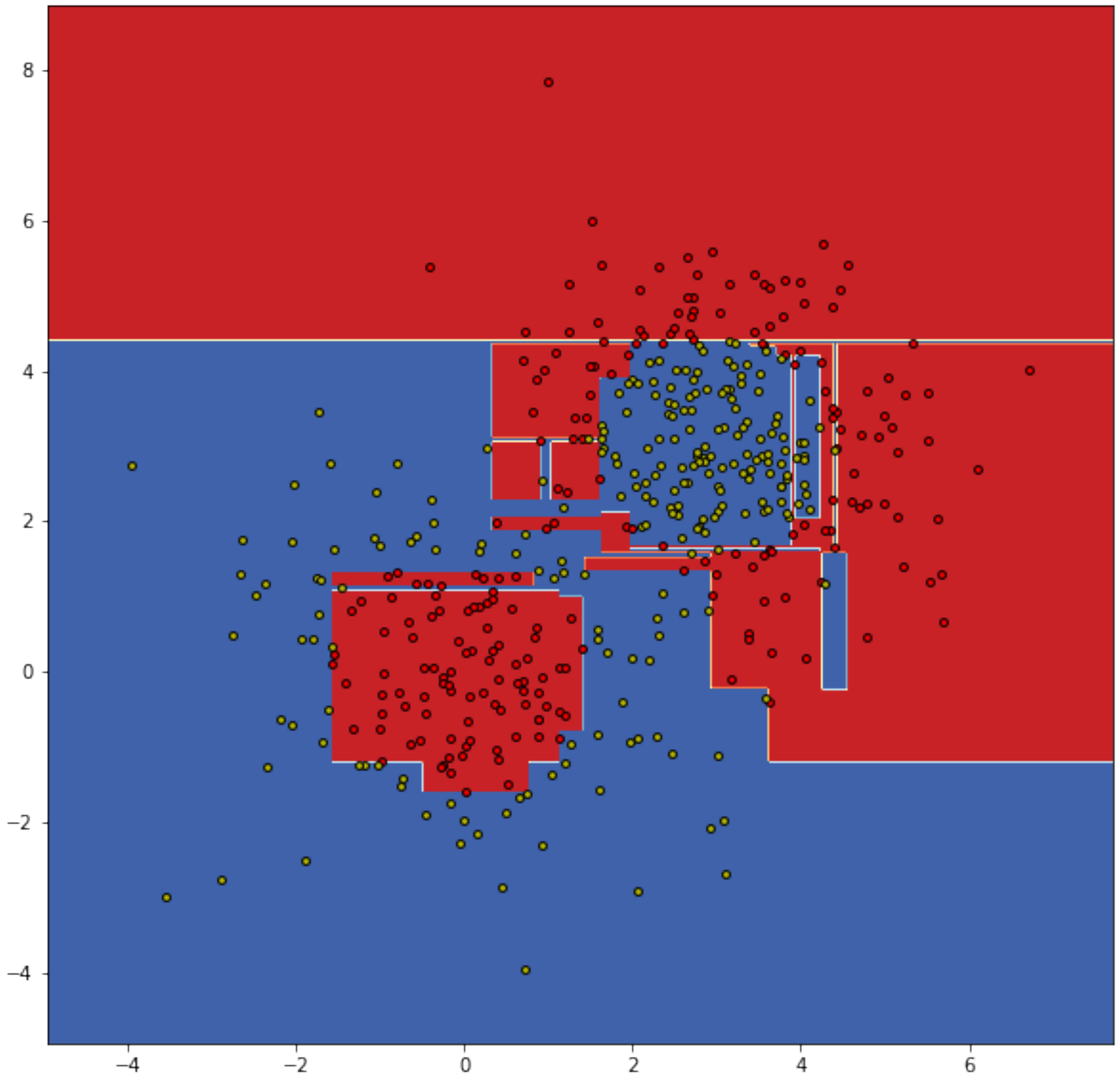


Stability of a Model

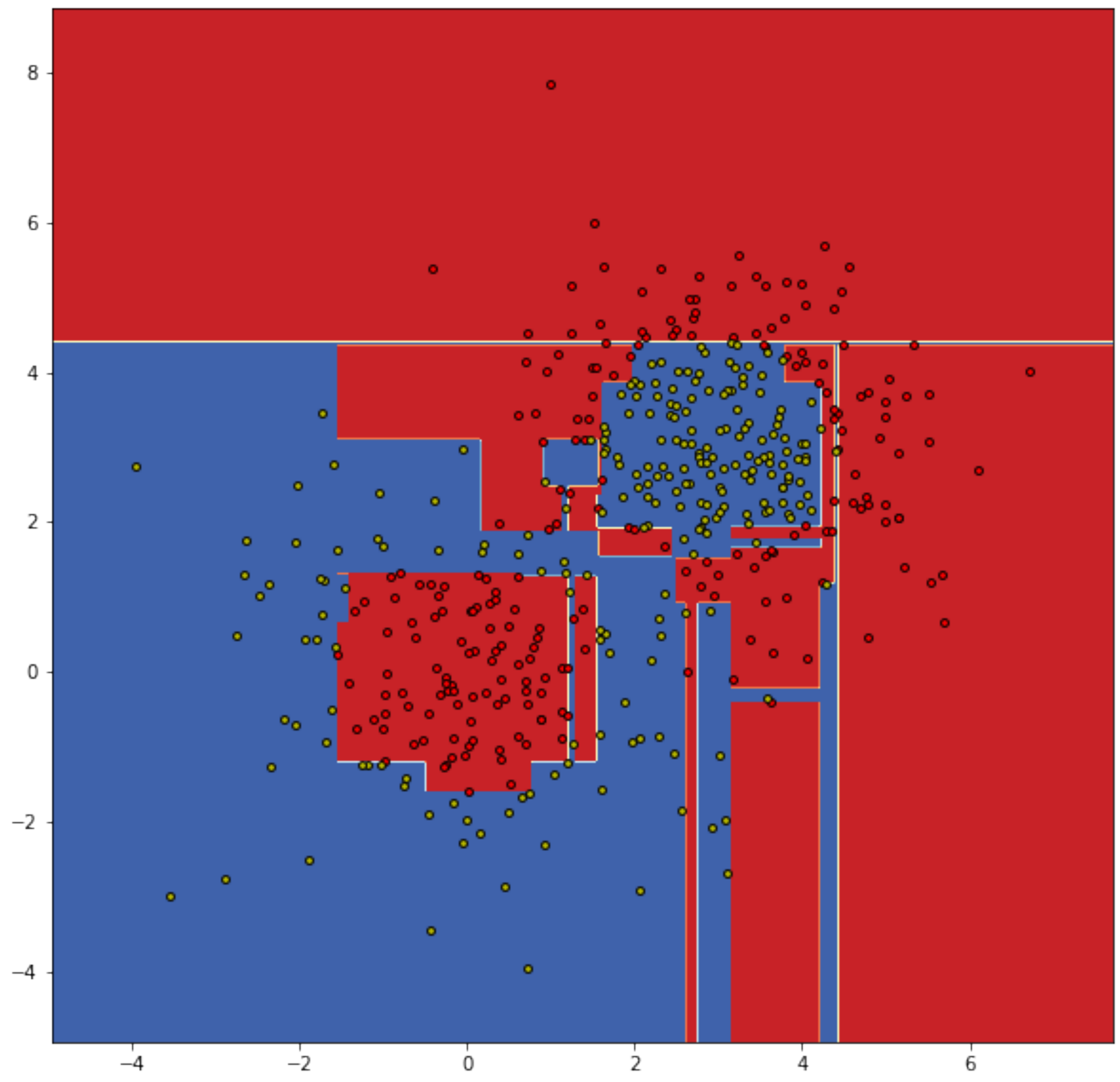
- $X = (x_i, y_i)_{i=1}^{\ell}$ — training dataset
- If the model has low variance, we expect is to look similar if we use different subset of the initial training dataset

- $\widetilde{X}$ — random subsample, approx. 90% from the initial
- Let us train decision trees on different $\widetilde{X}$

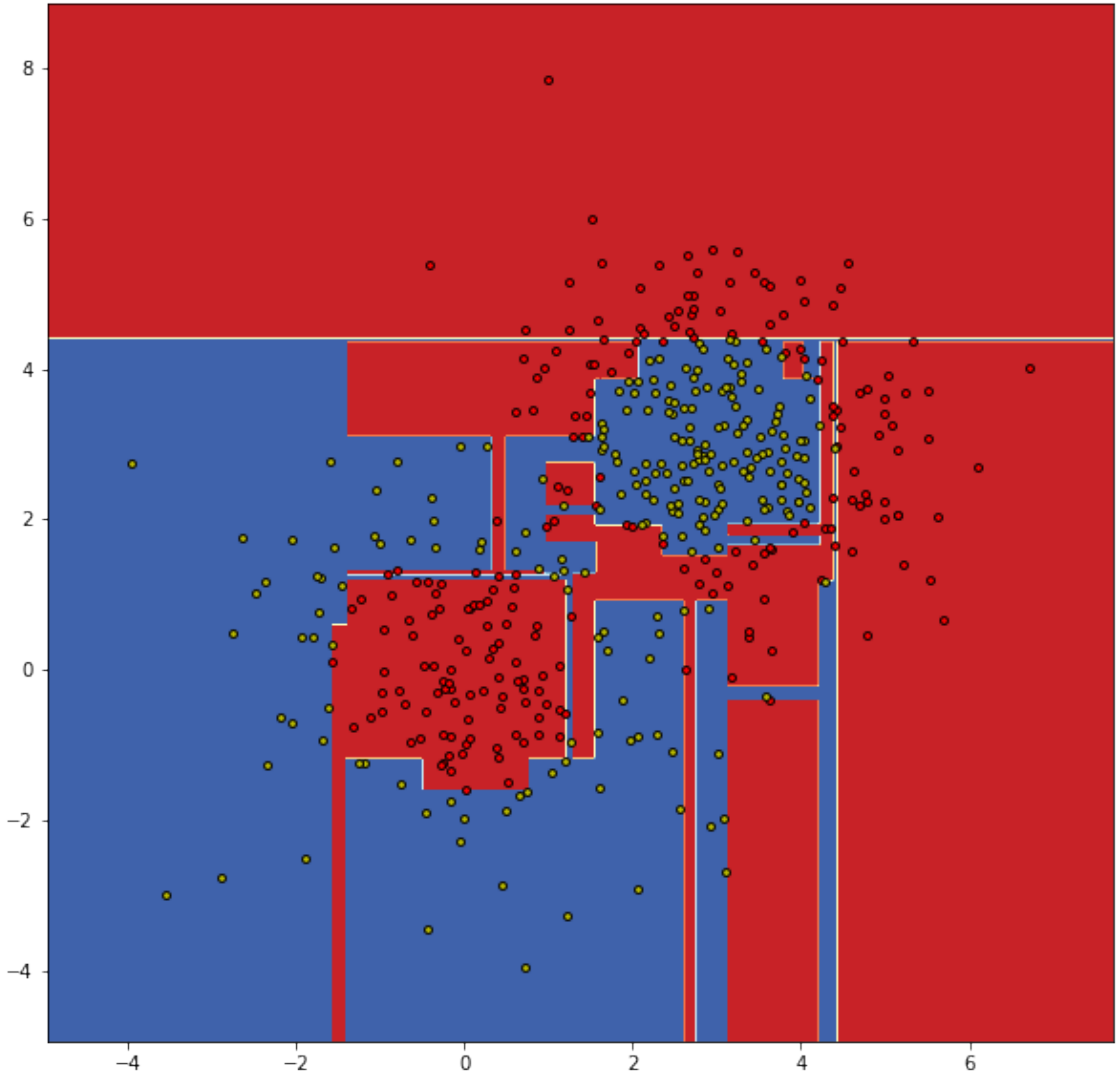
Training Decision Tree on Subsamples



Training Decision Tree on Subsamples

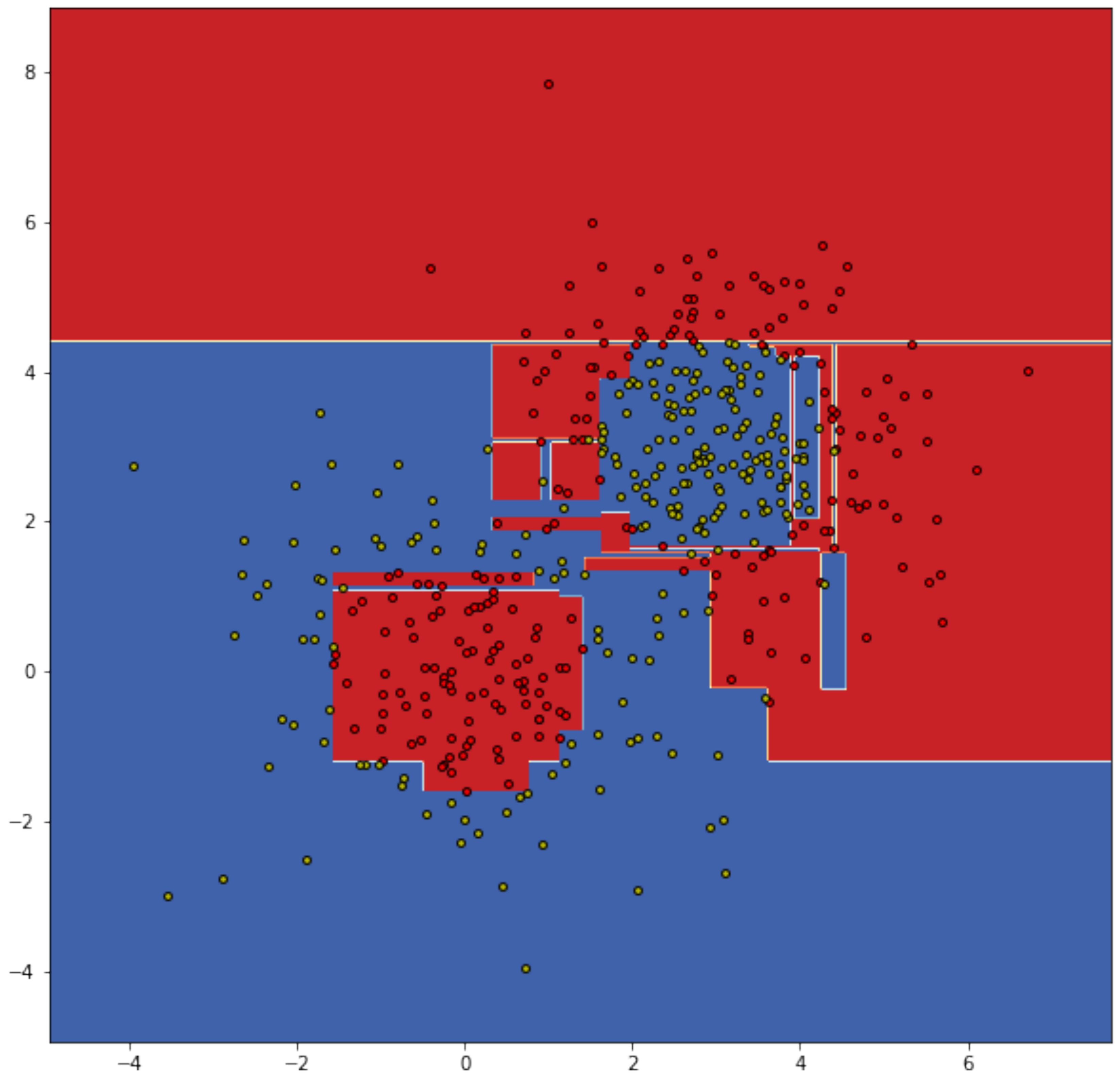


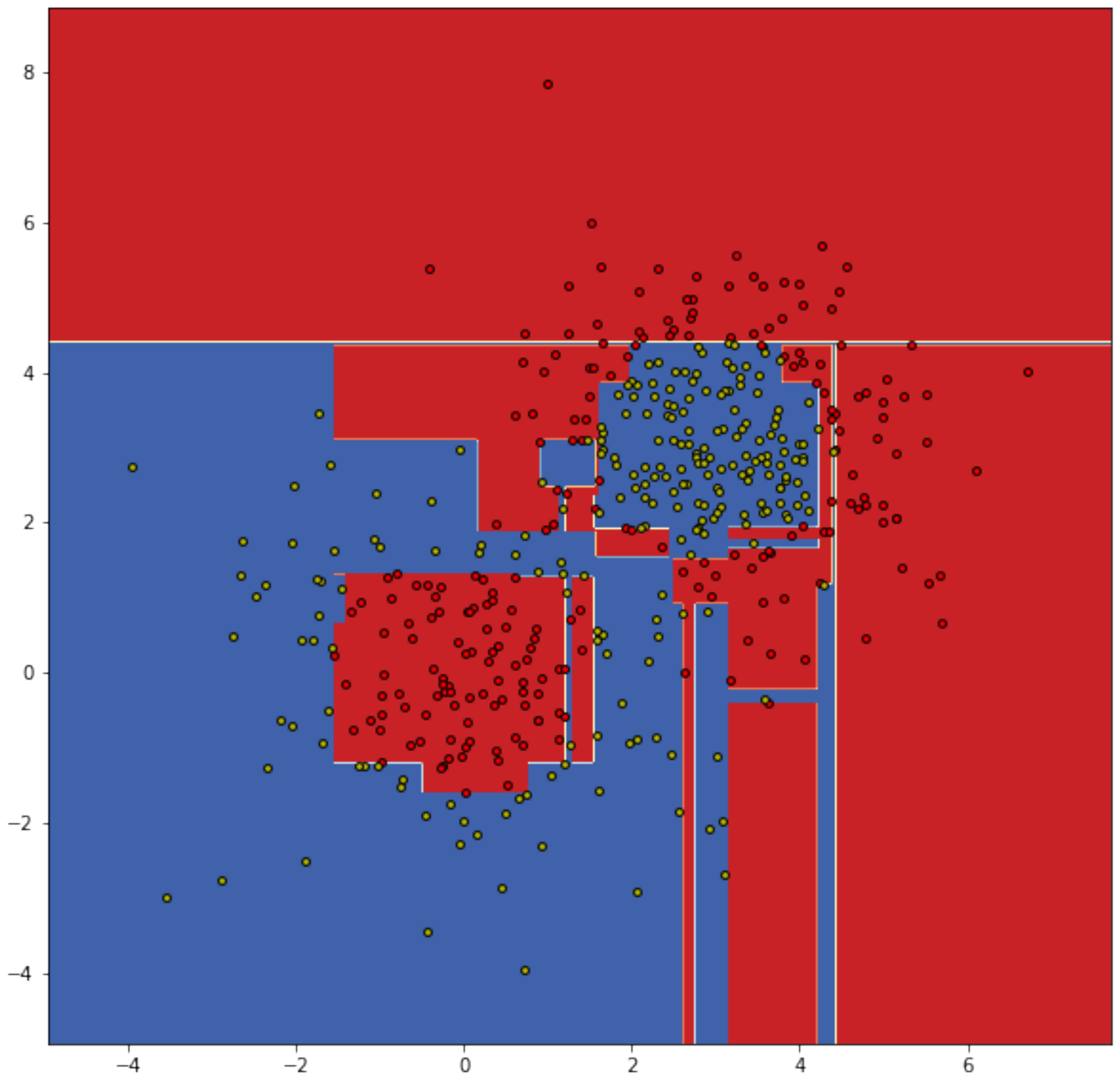
Training Decision Tree on Subsamples



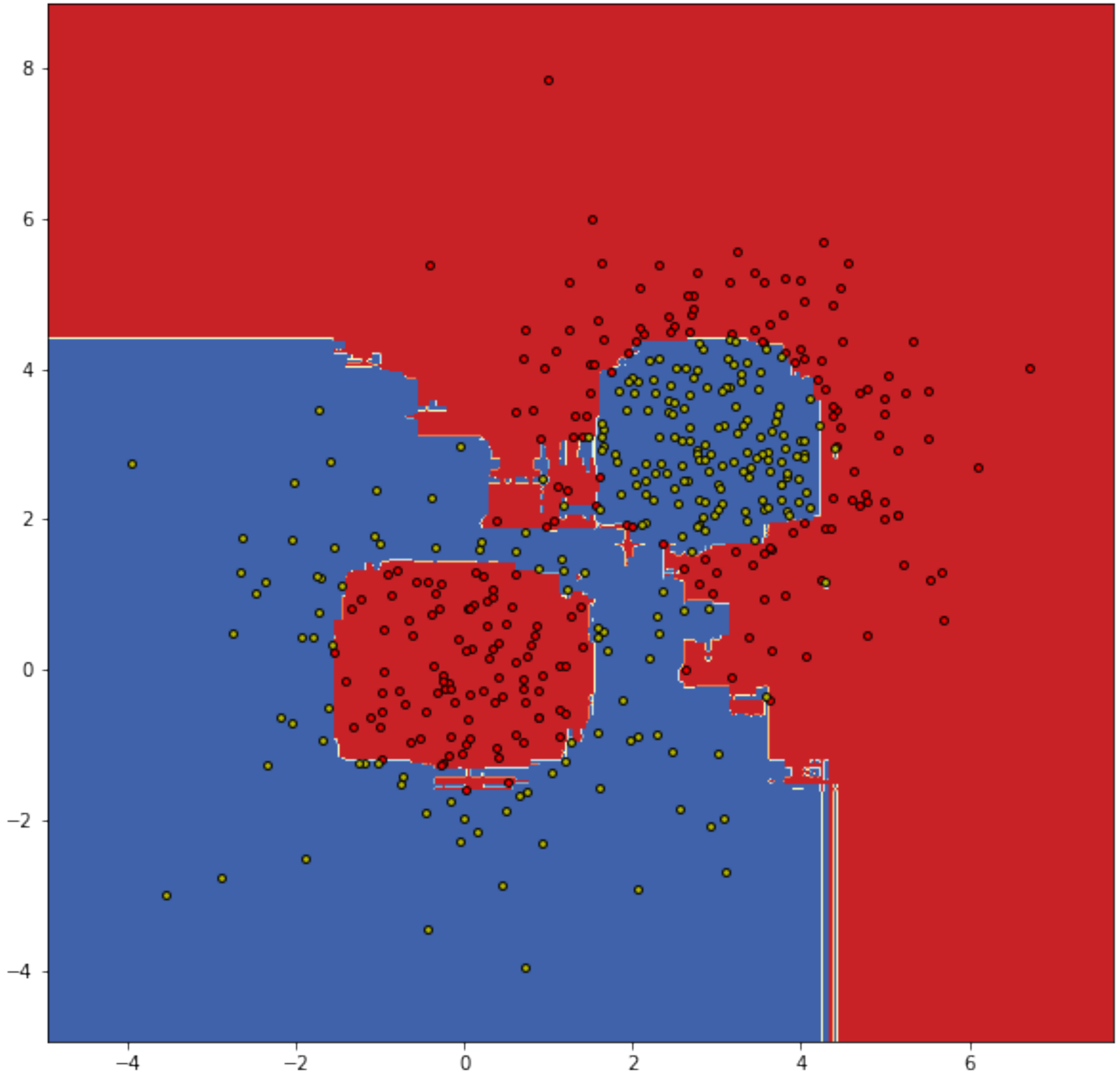
Decision Trees

- High variance
- Lack of smoothness





Composition of Models



Summary

- Decision trees are very sensitive to the changes in the dataset
- Prediction surface of decision trees in very non-smooth
- In practice composition of decision trees is used