

# Decision Trees

Classification and Regression Trees, impurity functions, solution properties

Machine Learning and Data Mining, 2023

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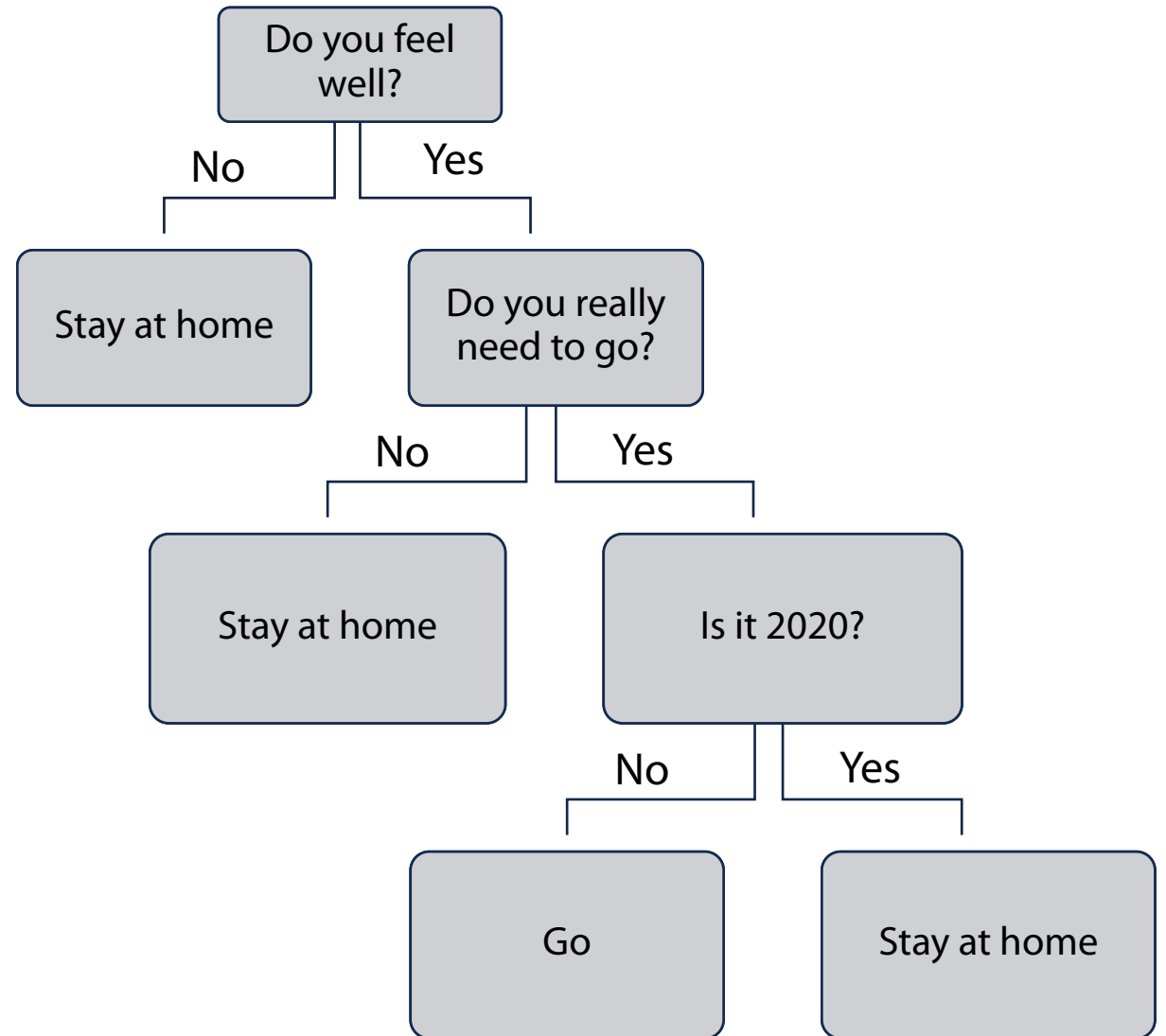
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# Basics

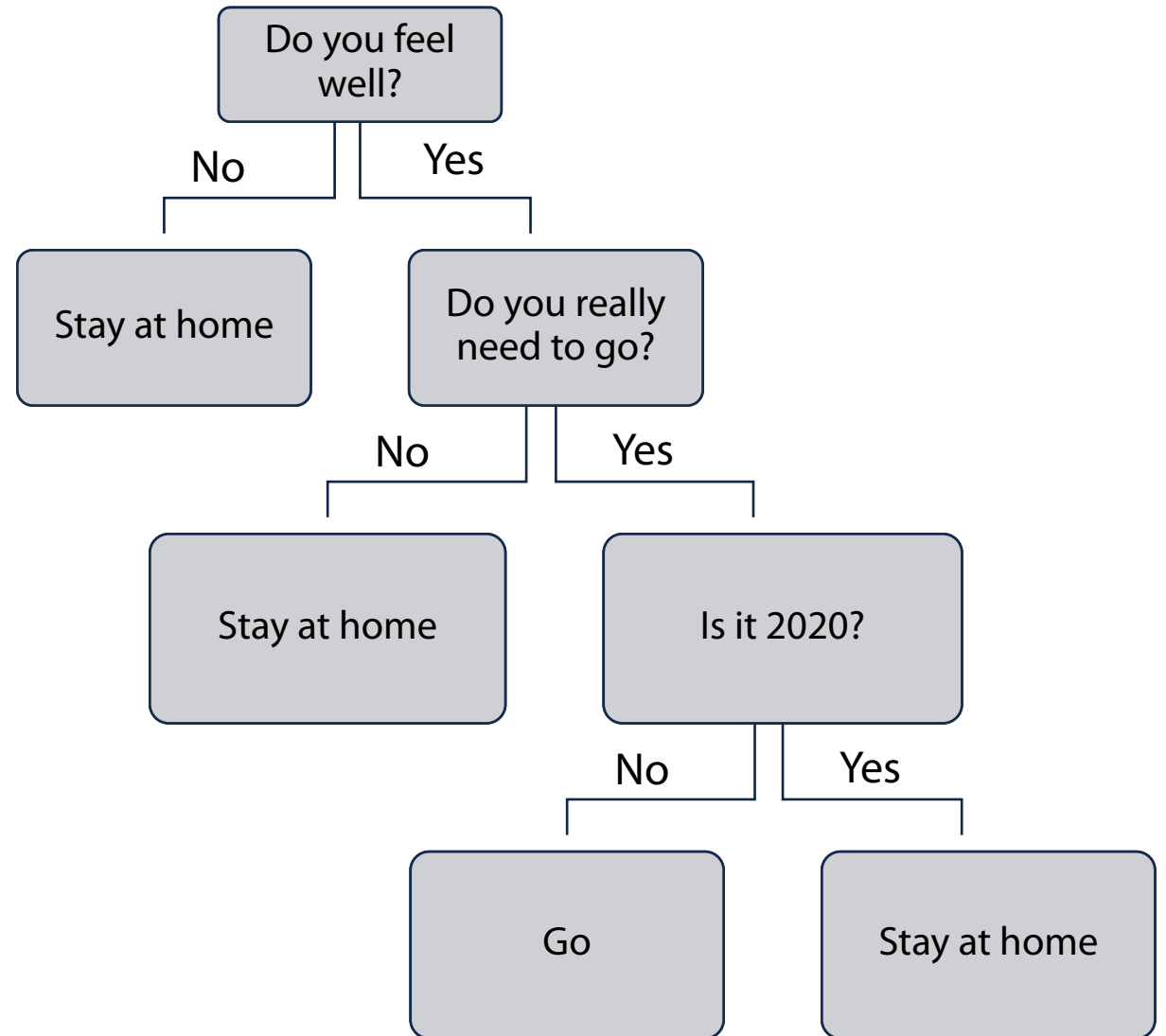


# “Should you go to work?” chart



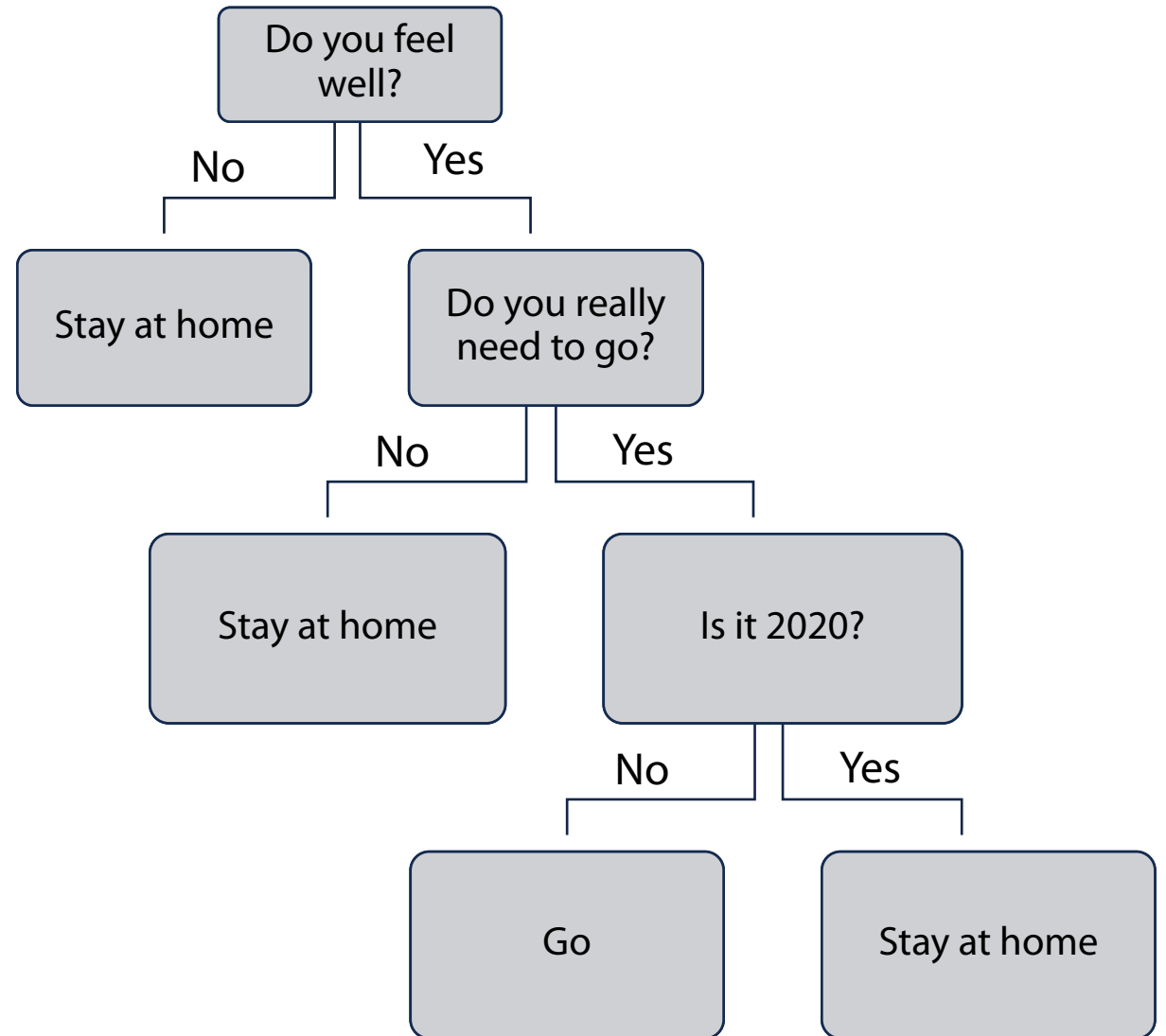
# “Should you go to work?” chart

► Directed graph



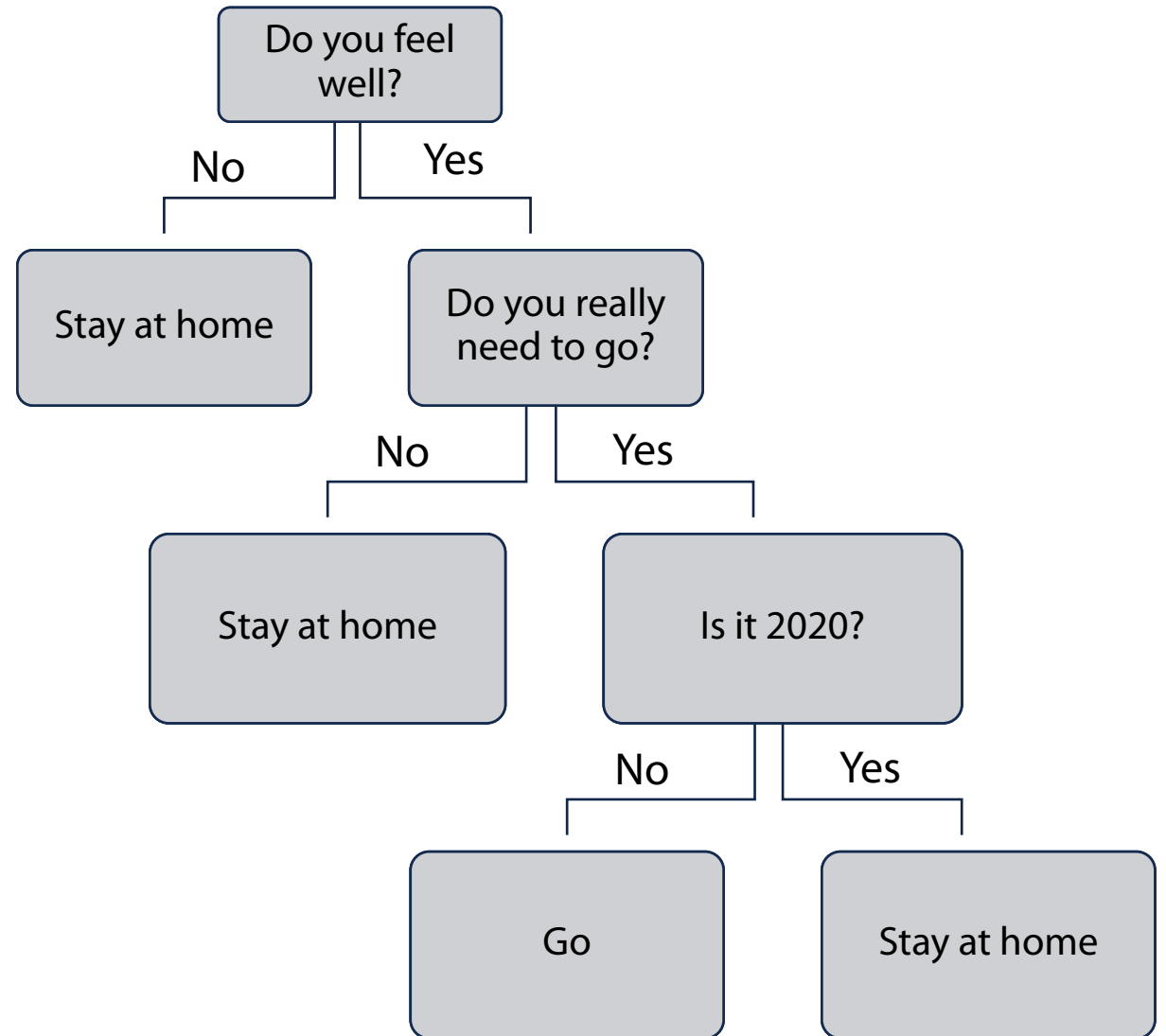
# “Should you go to work?” chart

- ▶ Directed graph
- ▶ No loops



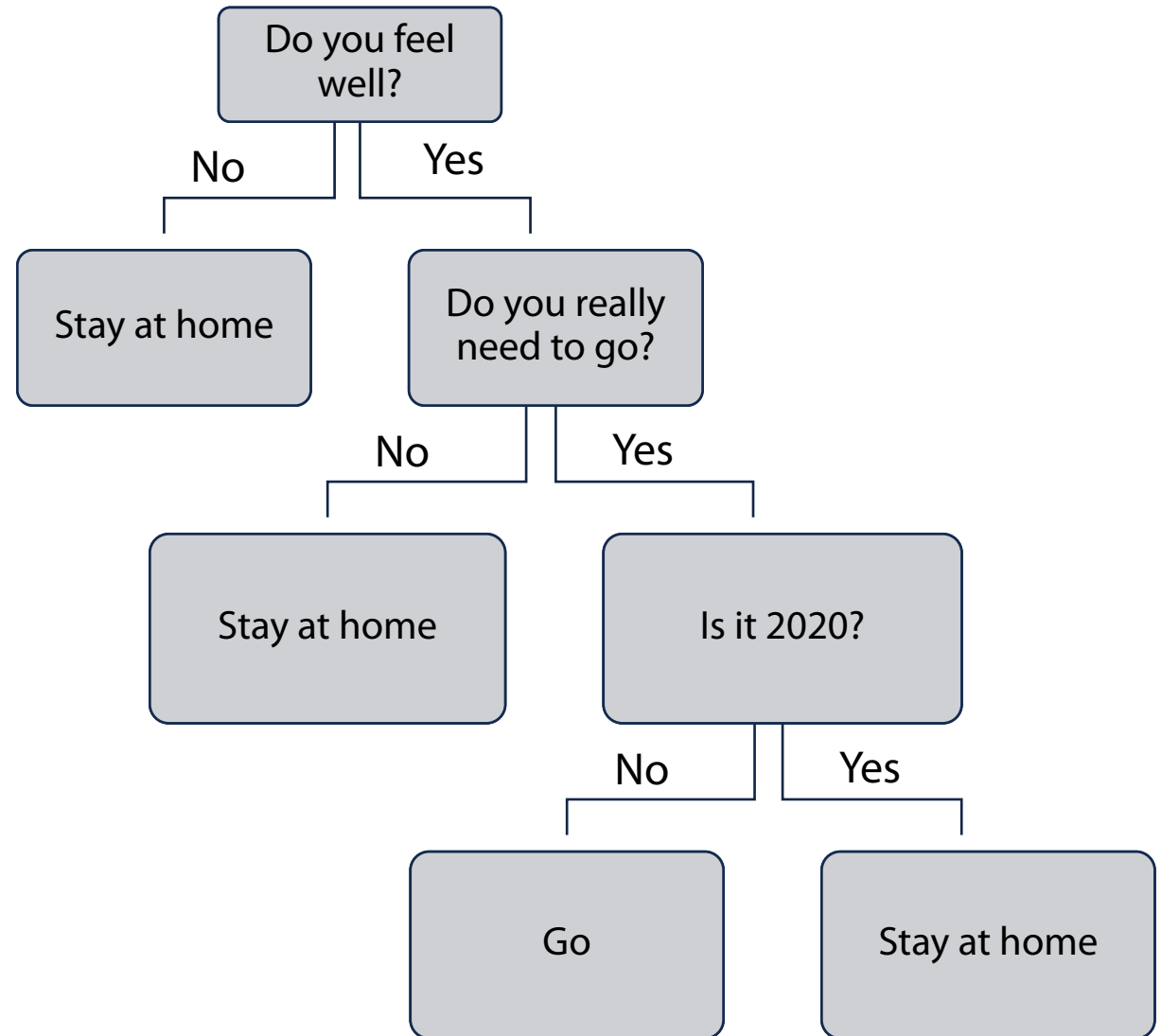
# “Should you go to work?” chart

- ▶ Directed graph
- ▶ No loops
- ▶ Single root node



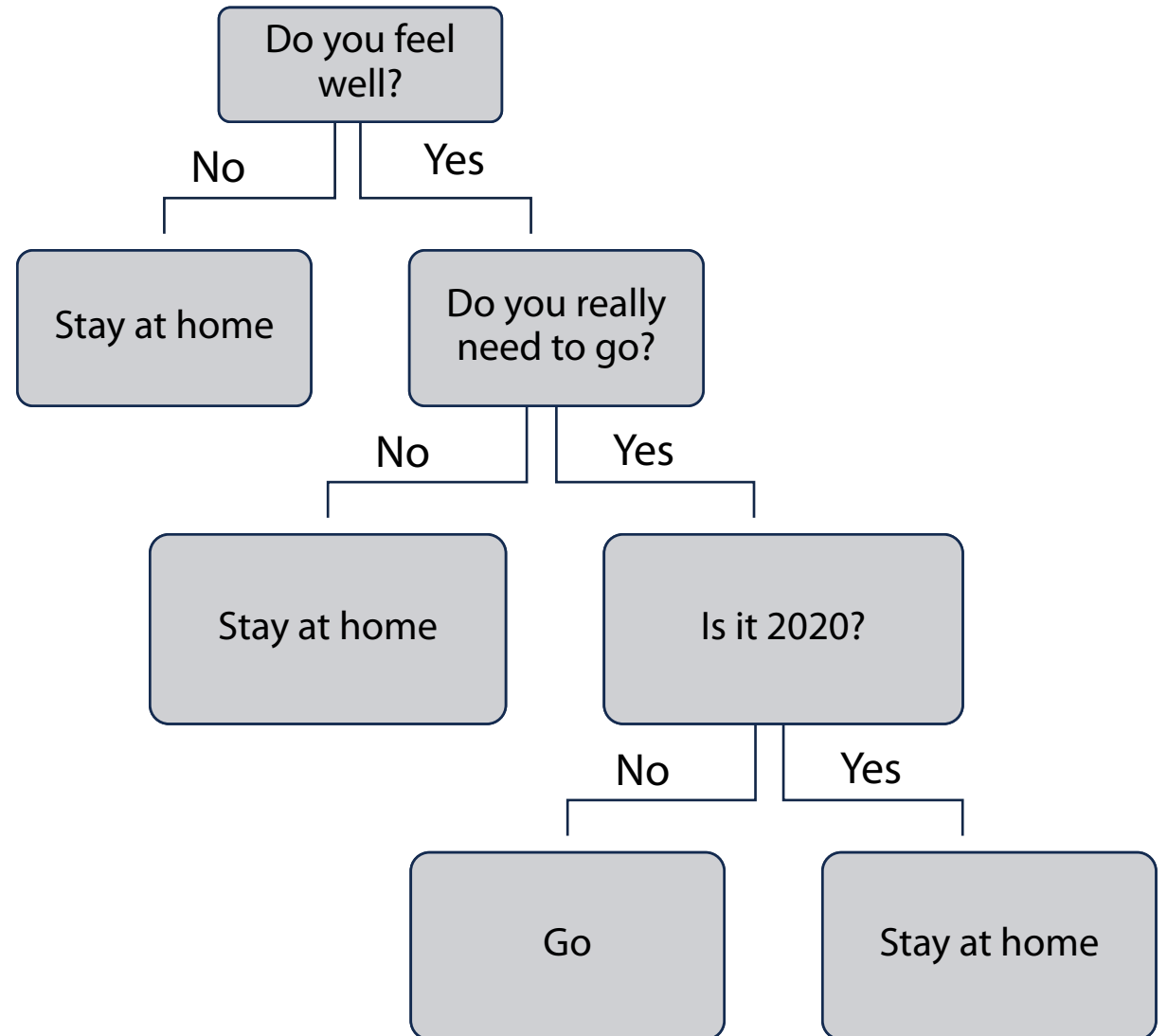
# “Should you go to work?” chart

- ▶ Directed graph
- ▶ No loops
- ▶ Single root node
- ▶ Each node has:
  - either 0 child nodes (**terminal node**, “leaf”)



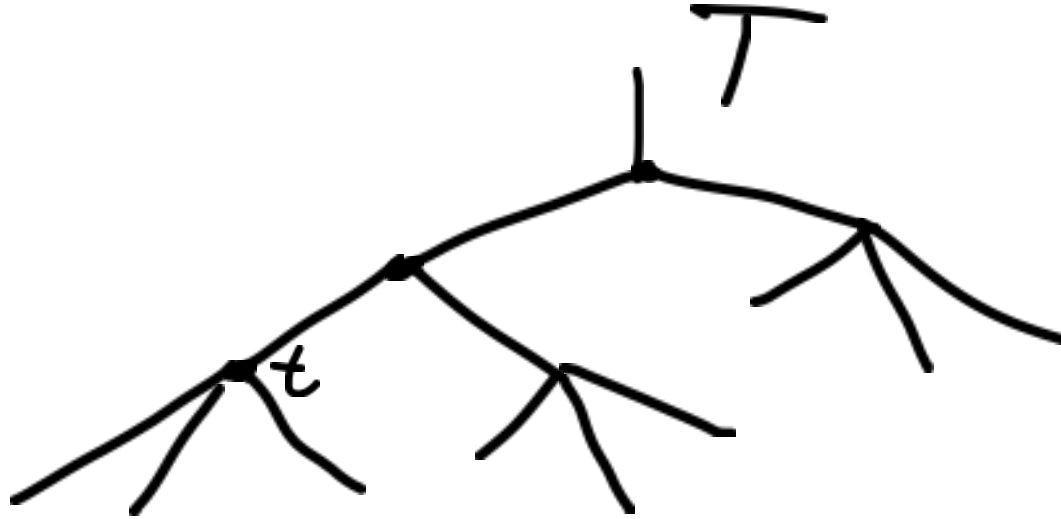
# “Should you go to work?” chart

- ▶ Directed graph
- ▶ No loops
- ▶ Single root node
- ▶ Each node has:
  - either 0 child nodes (**terminal node**, “leaf”)
  - or  $\geq 2$  child nodes (**internal node**)
  - 2 nodes for binary trees

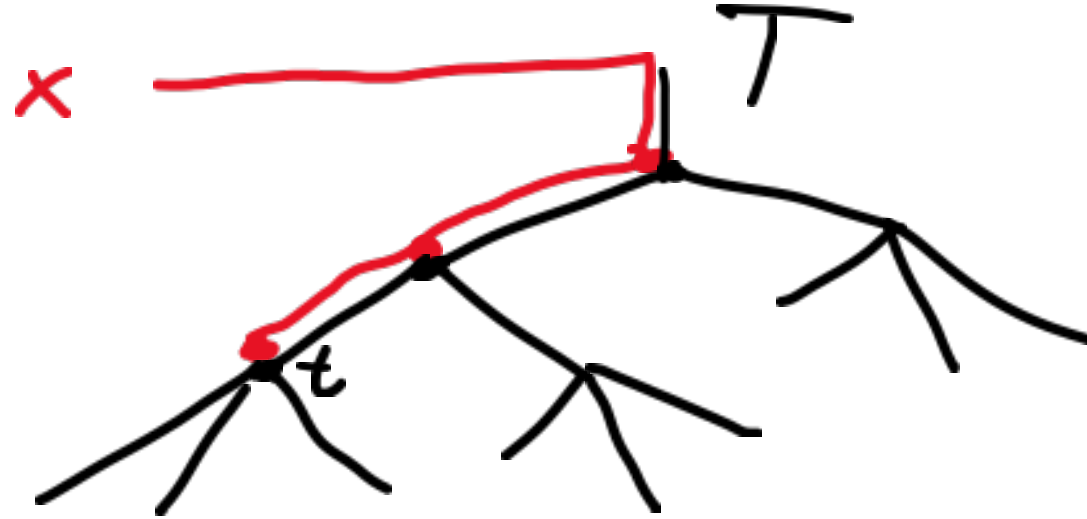




# Defining a tree (general approach)



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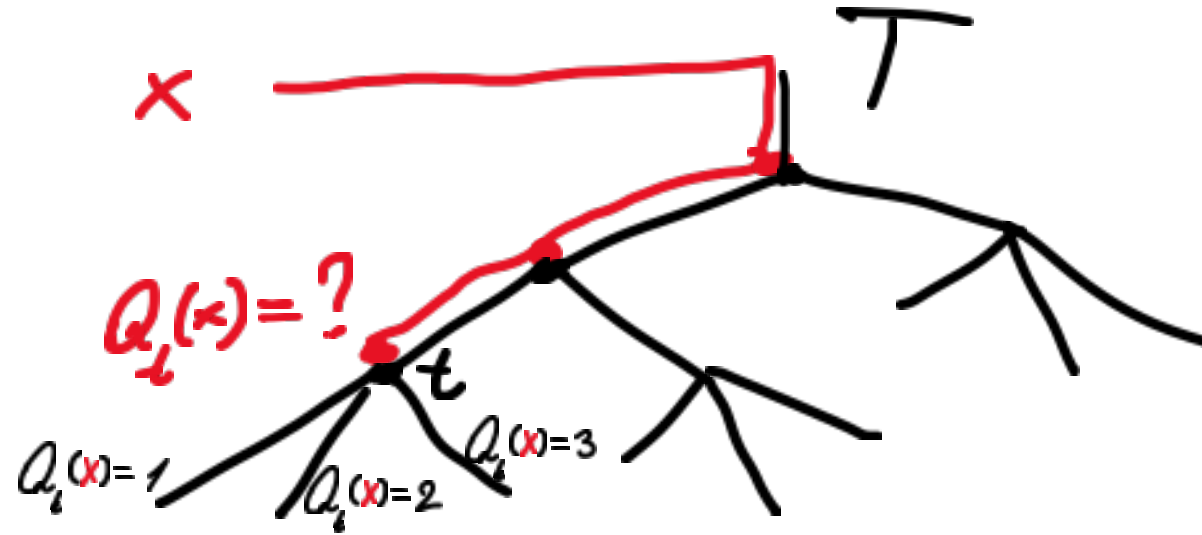


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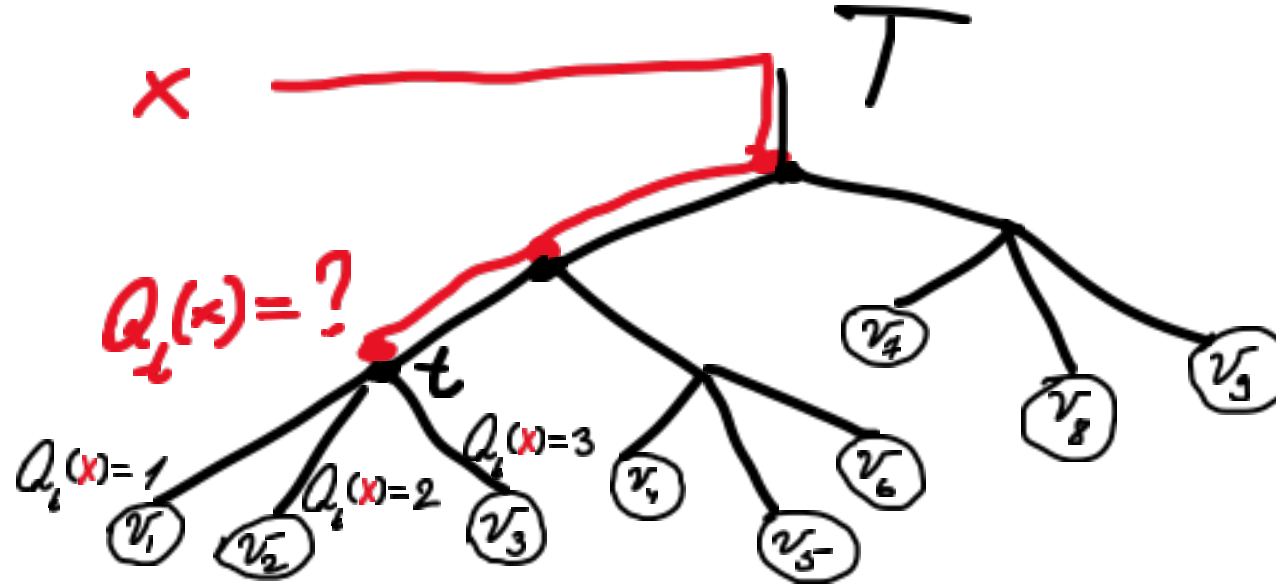
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- ▶ For each node  $t \in T$  define a check function  $Q_t(x)$
- ▶ For each child node of  $t$  assign a set of unique values of  $Q_t(x)$
- ▶ Assign each terminal node  $i$  a prediction value  $v_i$

# Classification and Regression Trees (CART)



# CART

Binary trees

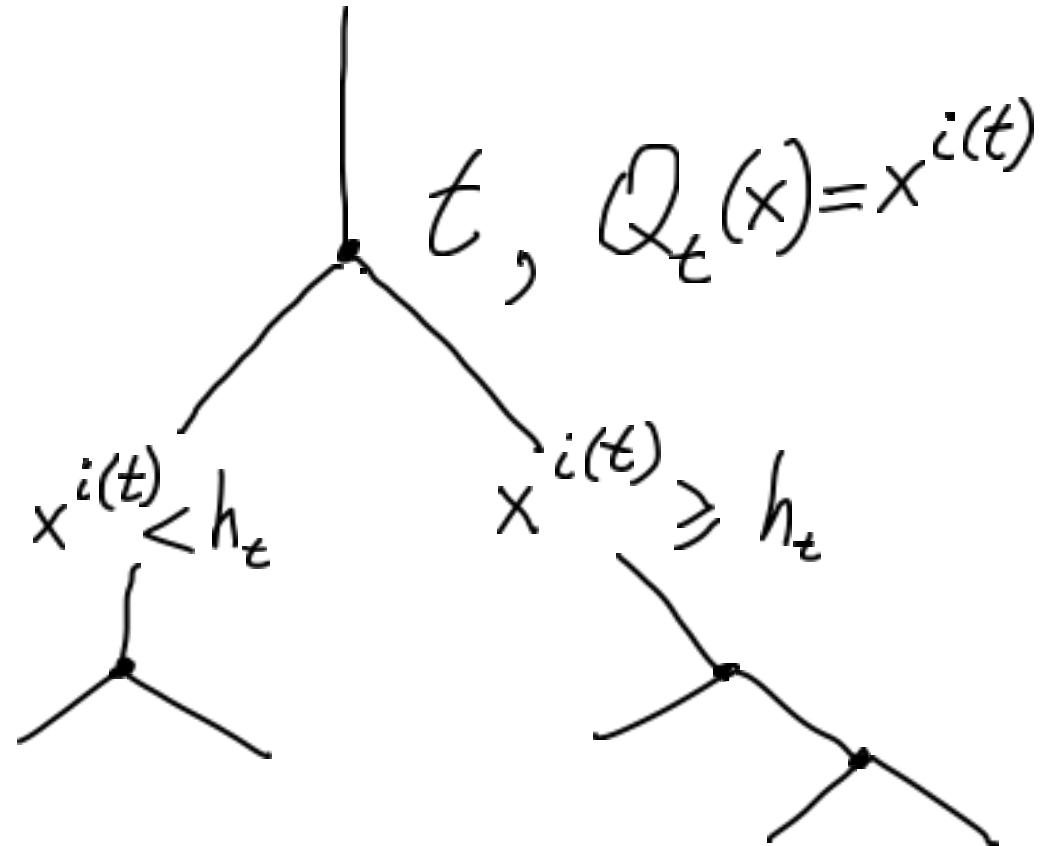
Check function:

$Q_t(x) = x^{i(t)}$  — pick a single ( $i$ -th) feature

Child nodes:

Left or right depending on whether

$$Q_t(x) \geq h_t$$



Finding the best tree is not trivial. In practice a **greedy algorithm** is used.

# Growing a tree

Given a dataset  $D = \{(x_1, y_1), \dots, (x_N, y_N)\}$ , and **impurity function**  $I(D)$

Start from a single root node  $t_0$ , all data residing in it:  $D_{t_0} = D$





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While stop condition not met, repeat for each leaf node  $t$ :

Find feature  $i$  and element  $(x_k, y_k) \in D_t$ , such that for the two subsets

$$D_{t^{\text{left}}} = \{(x, y) \mid (x, y) \in D_t, x^i < x_k^i\},$$

$$D_{t^{\text{right}}} = \{(x, y) \mid (x, y) \in D_t, x^i \geq x_k^i\}$$

the decrease of impurity:

$$|D_t| \cdot \Delta I_t = |D_t| \cdot I(D_t) - \left( |D_{t^{\text{right}}}| \cdot I(D_{t^{\text{right}}}) + |D_{t^{\text{left}}}| \cdot I(D_{t^{\text{left}}}) \right) > 0$$

is maximized (over  $k$  and  $i$ ).



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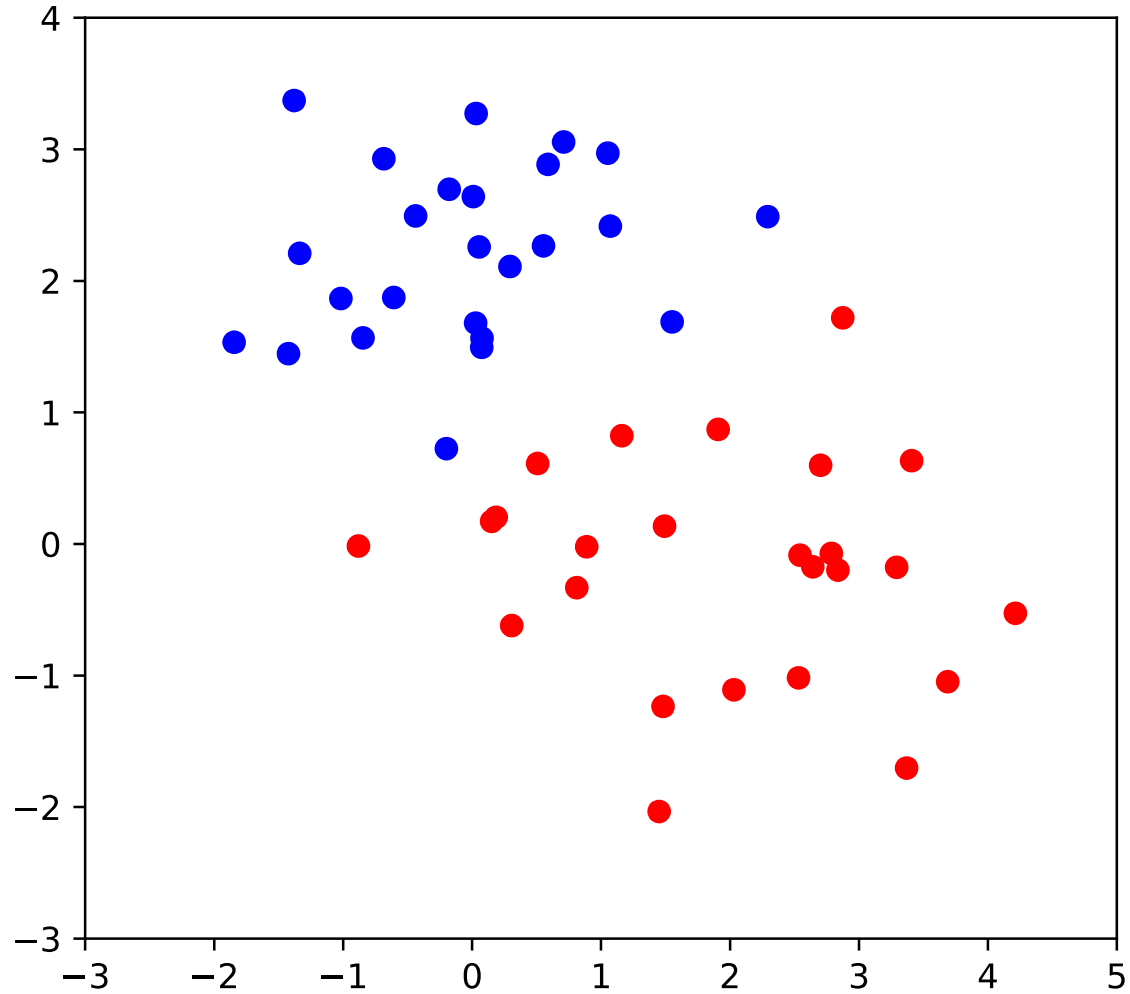
is maximized (over  $k$  and  $i$ ).

Set the check function  $Q_t(x) = x^i$ , and threshold  $h_t = x_k^i$ ,

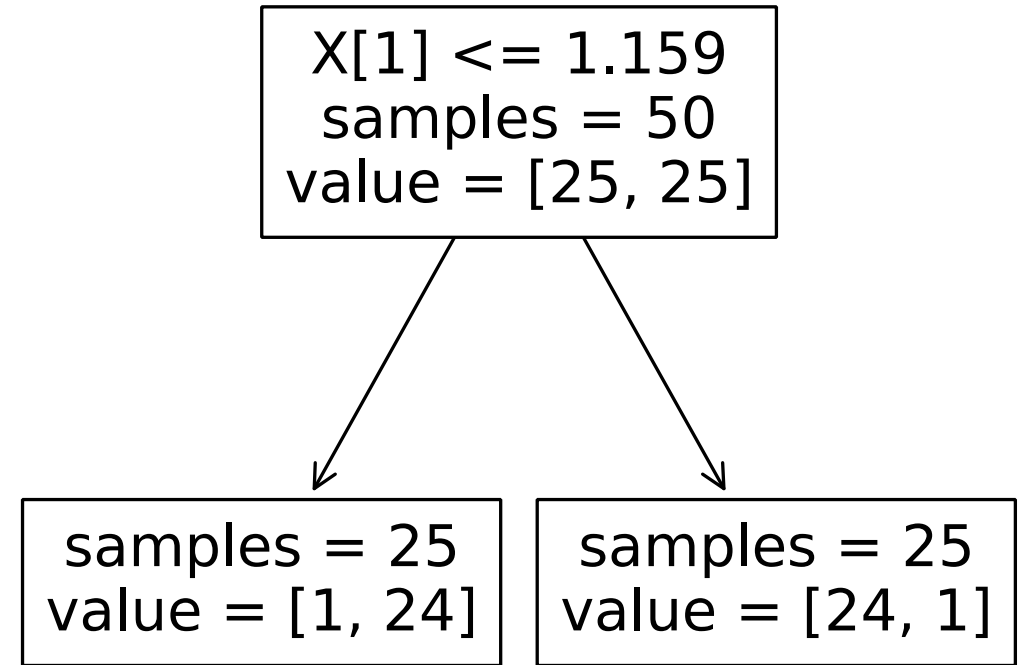
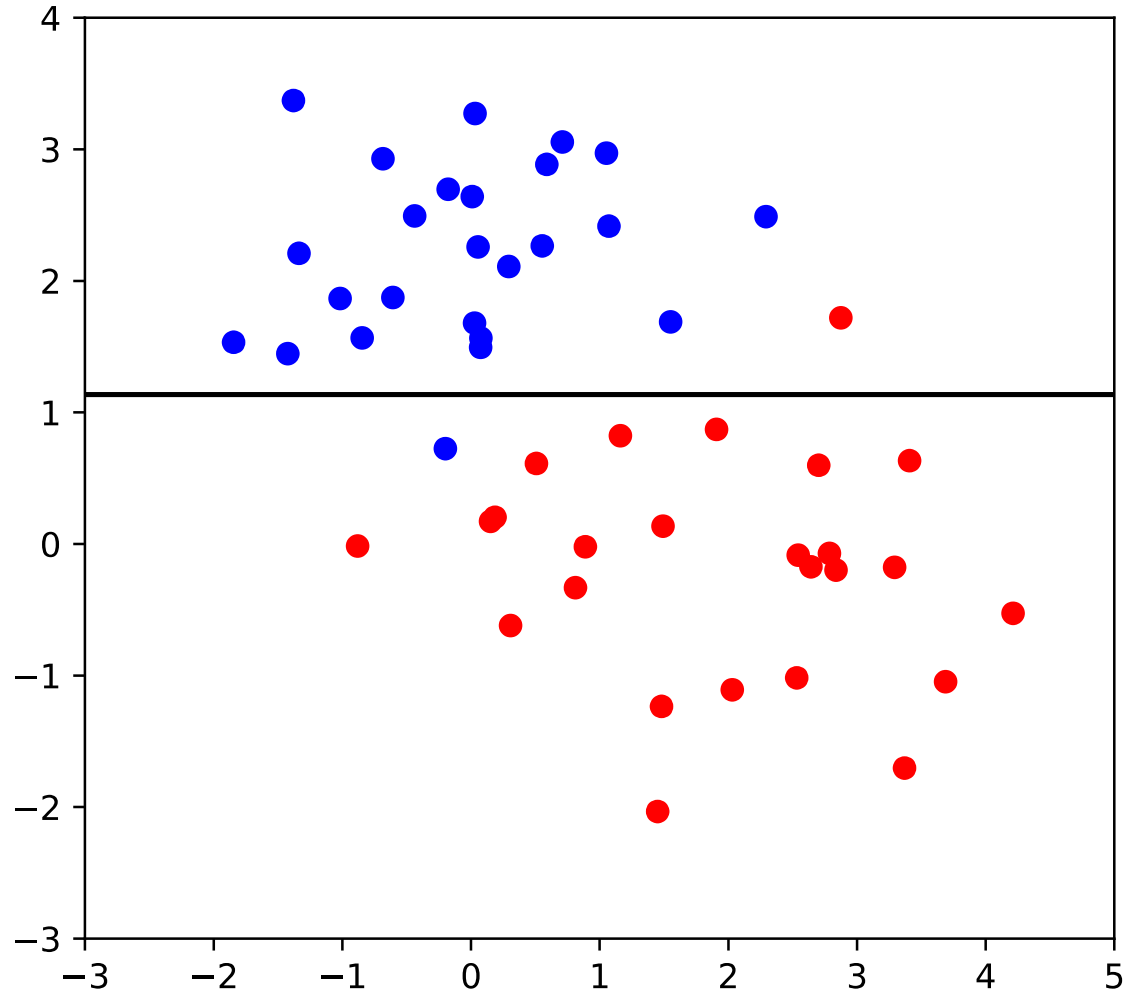
attach the two new corresponding child nodes  $t^{\text{left}}$  and  $t^{\text{right}}$  to  $t$ .



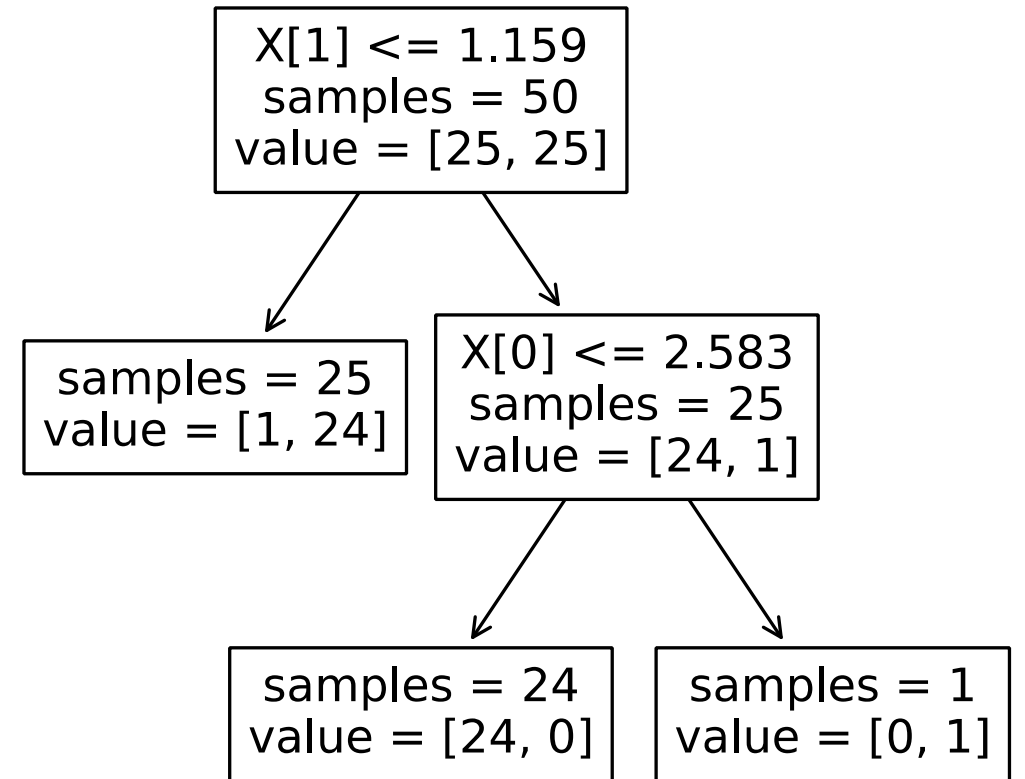
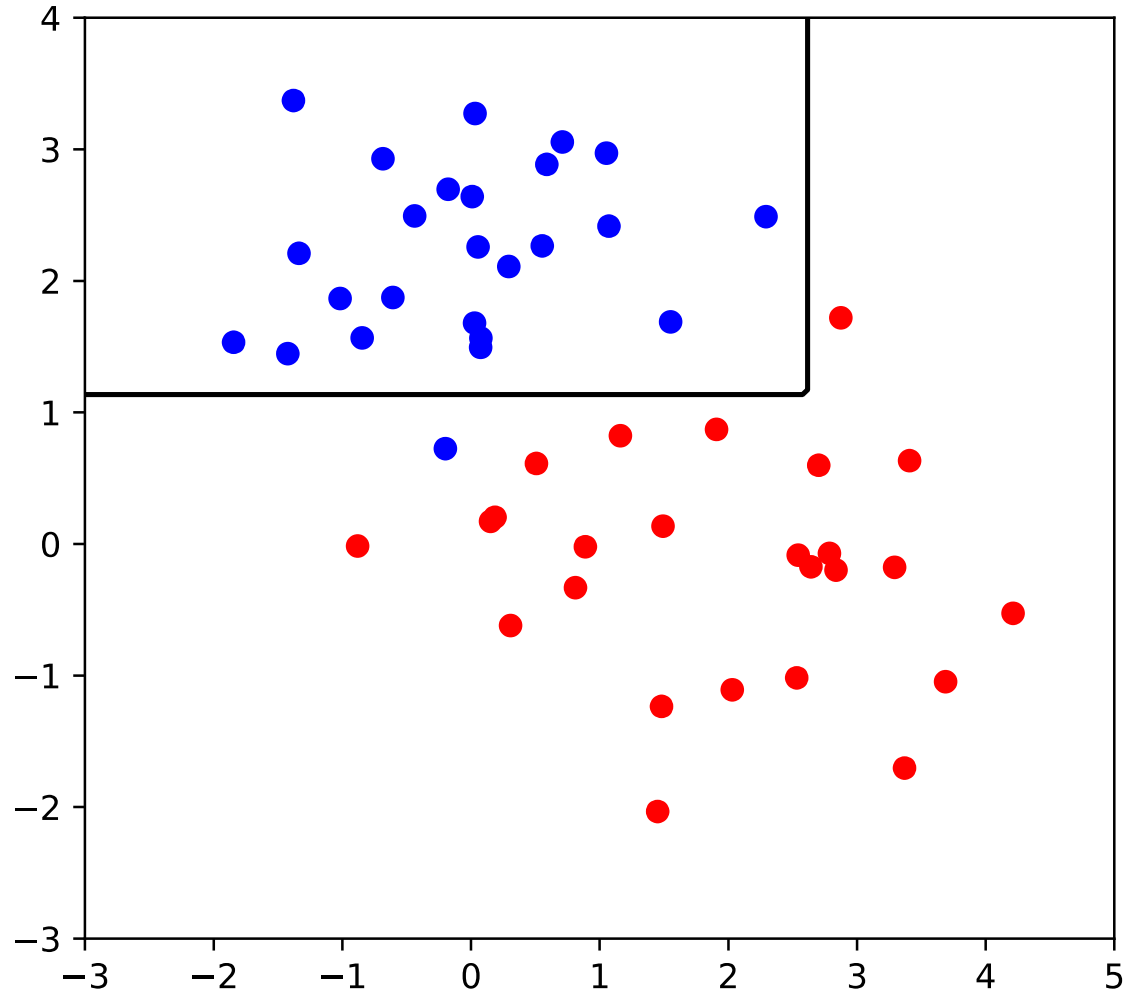
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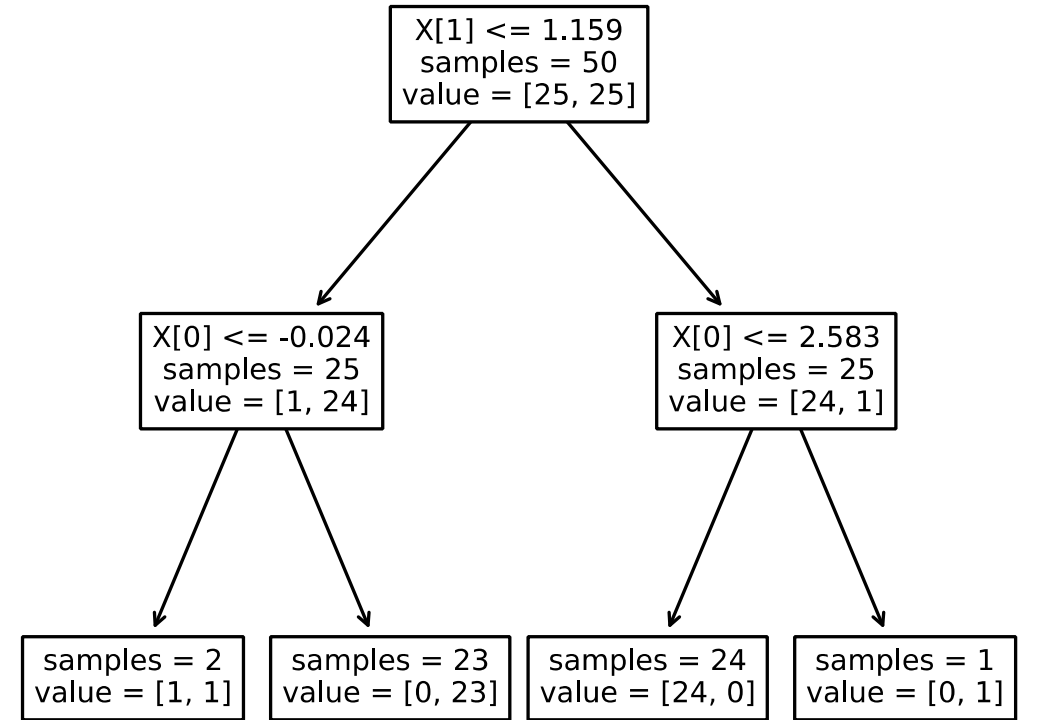
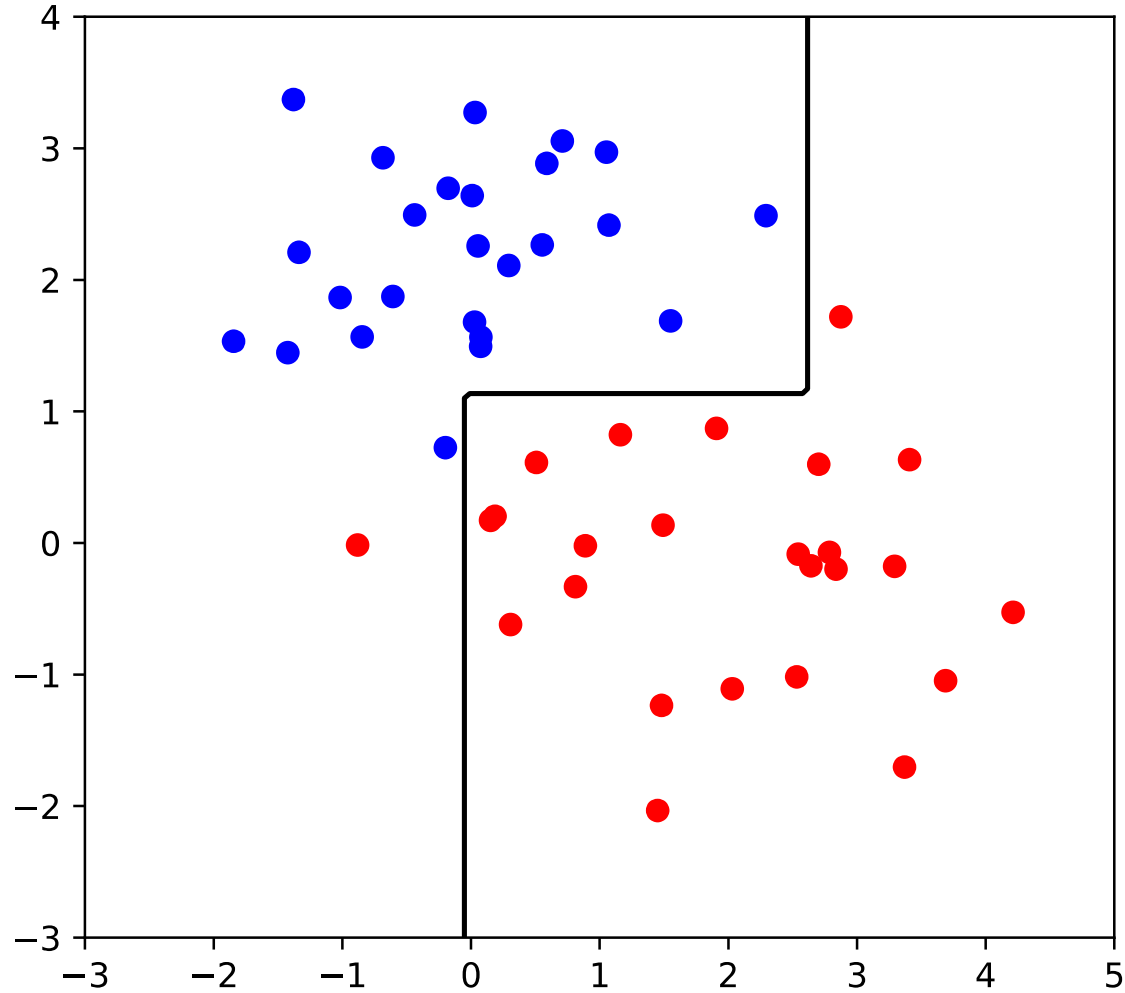
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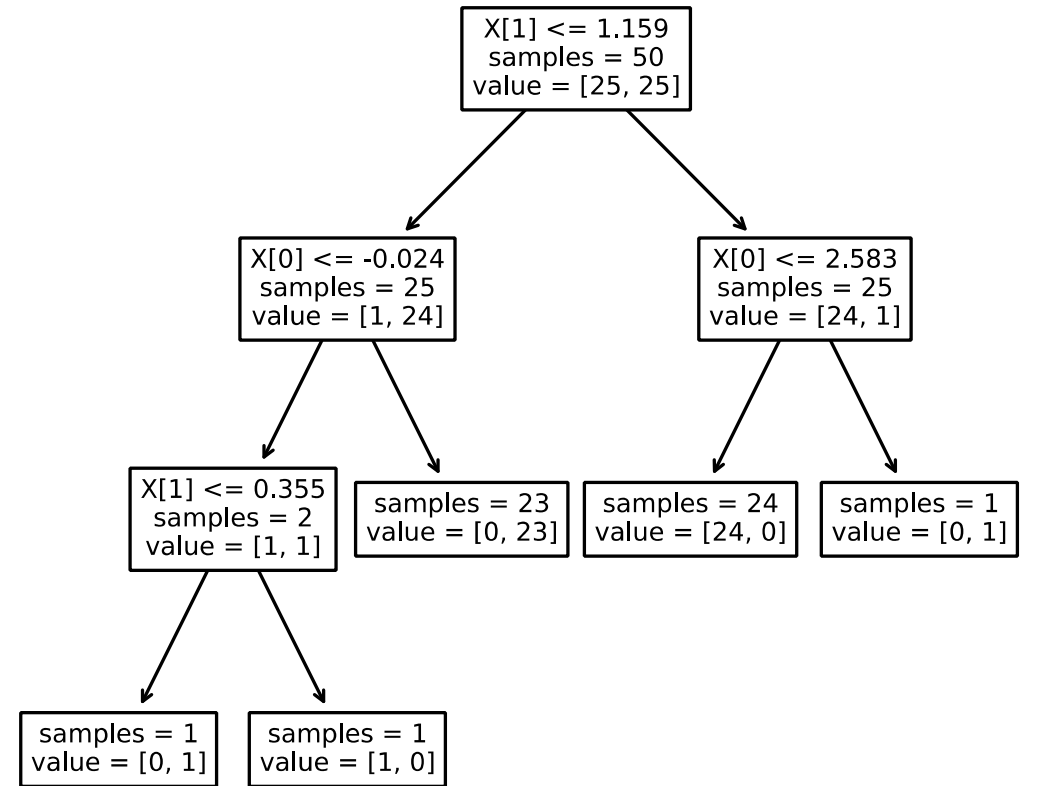
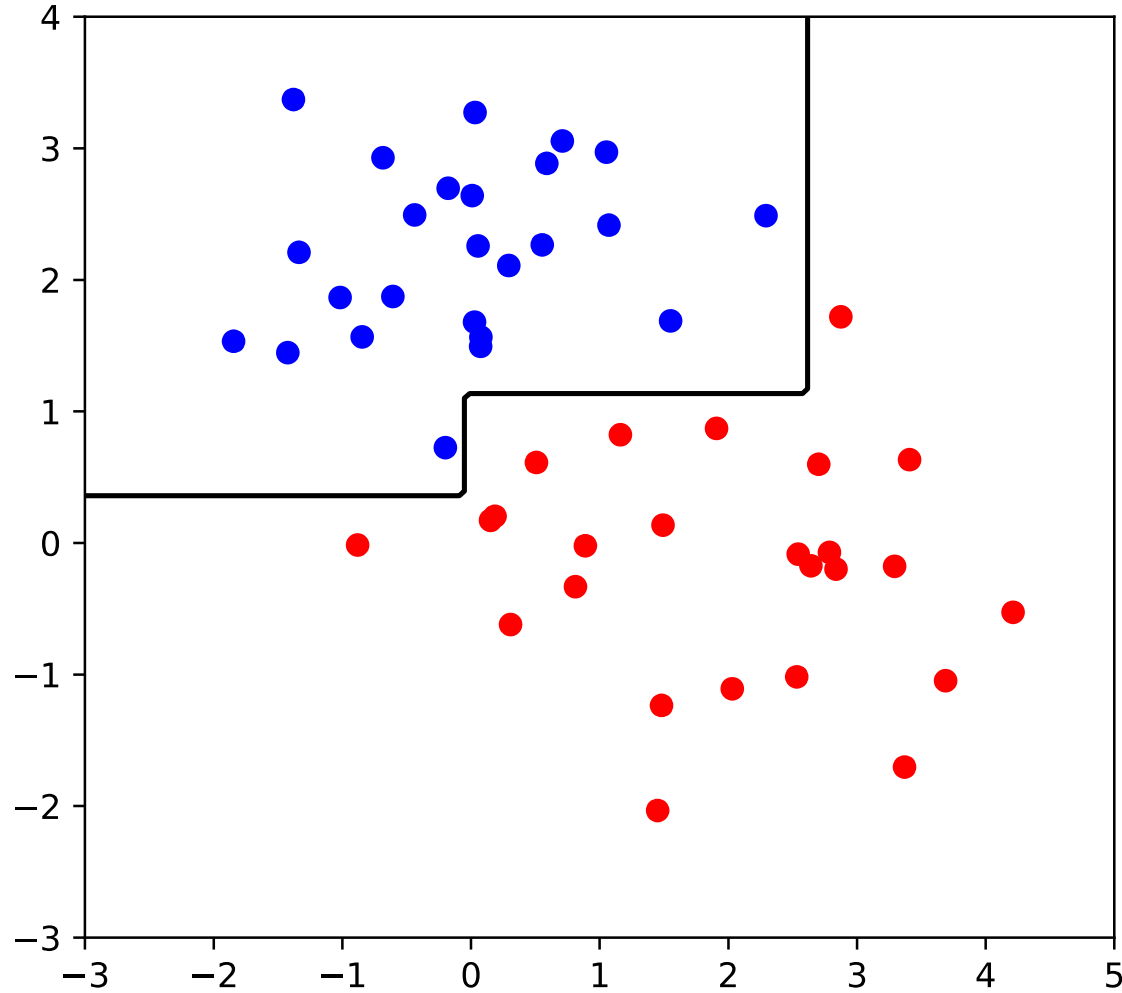
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# Impurity measures

## Regression

MSE:

$$I(D_t) = \frac{1}{|D_t|} \sum_{(x,y) \in D_t} \left( y - \mu_{D_t} \right)^2$$

mean target



MAE:

$$I(D_t) = \frac{1}{|D_t|} \sum_{(x,y) \in D_t} \left| y - m_{D_t} \right|$$

median target



# Impurity measures

What about classification?

Define class probabilities:

$$p_j = \frac{1}{|D_t|} \sum_{(x,y) \in D_t} \mathbb{I}[y = j]$$

Then, impurity function  $\phi(D_t) = \phi(p_1, \dots, p_C)$  should satisfy:

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- $\phi$  is defined for  $p_j \geq 0$  and  $\sum_j p_j = 1$
- $\phi$  is maximized when all  $p_j = 1/C$
- $\phi$  is minimized when a single  $p_j = 1$ , while others  $p_i = 0, i \neq j$
- $\phi$  is symmetric wrt its arguments

# Impurity measures

## Classification

Gini criterion:

$$I(D_t) = \sum_{i=1}^C p_i(1 - p_i) = 1 - \sum_{i=1}^C p_i^2$$

Probability of an error  
when predicting randomly  
with prior class  
probabilities  $p_i$

Entropy:

$$I(D_t) = - \sum_{i=1}^C p_i \log p_i$$

Shortest possible expected  
message length for the  
alphabet distributed under  $p_i$

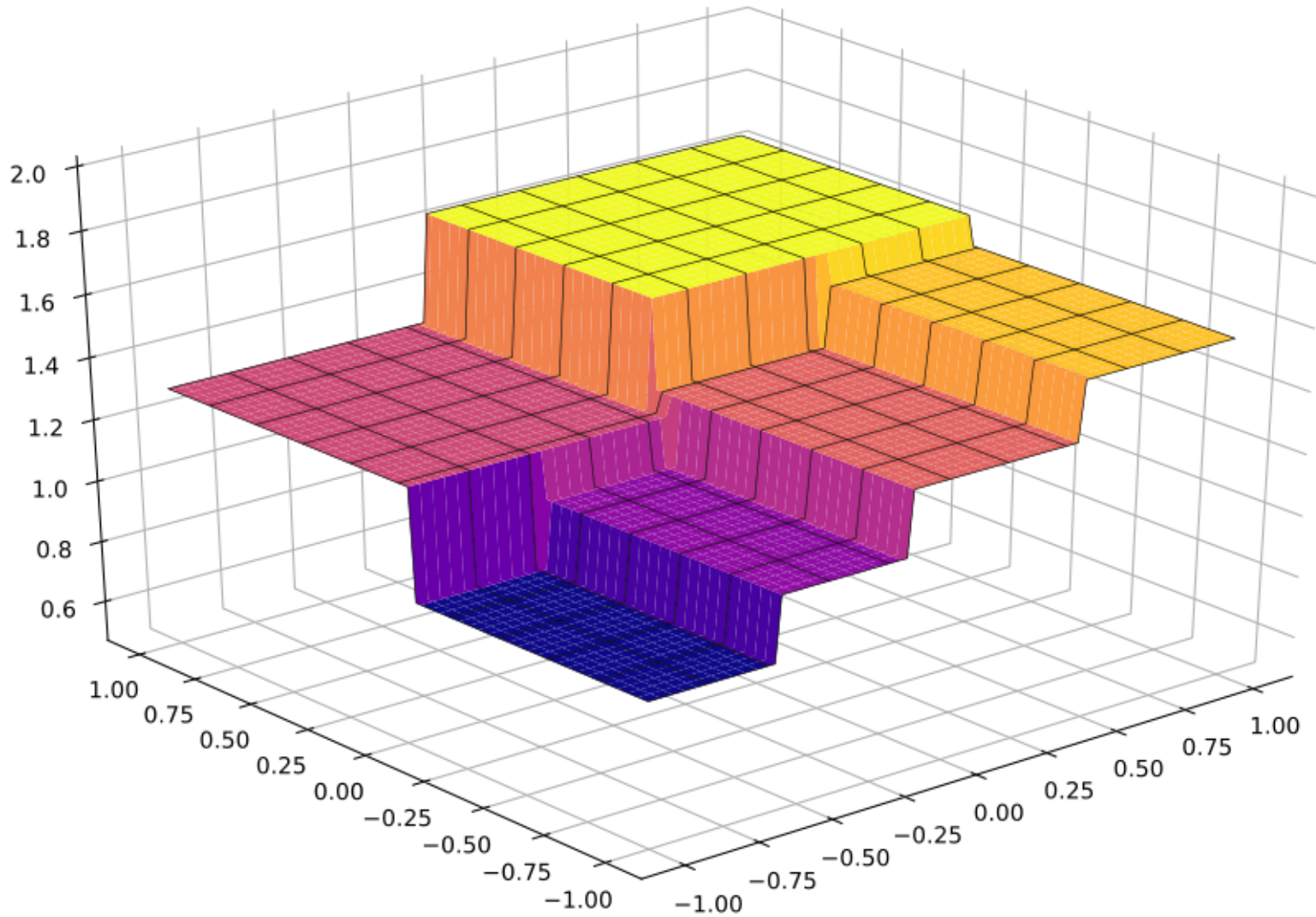
# Stopping criteria

- ▶ Maximum tree depth
- ▶ Maximum number of leaves
- ▶ Minimum number of samples in node to make a split
- ▶ Minimum number of samples in a leaf
- ▶ Minimum impurity gain
- ▶ You name it...

# Solution properties

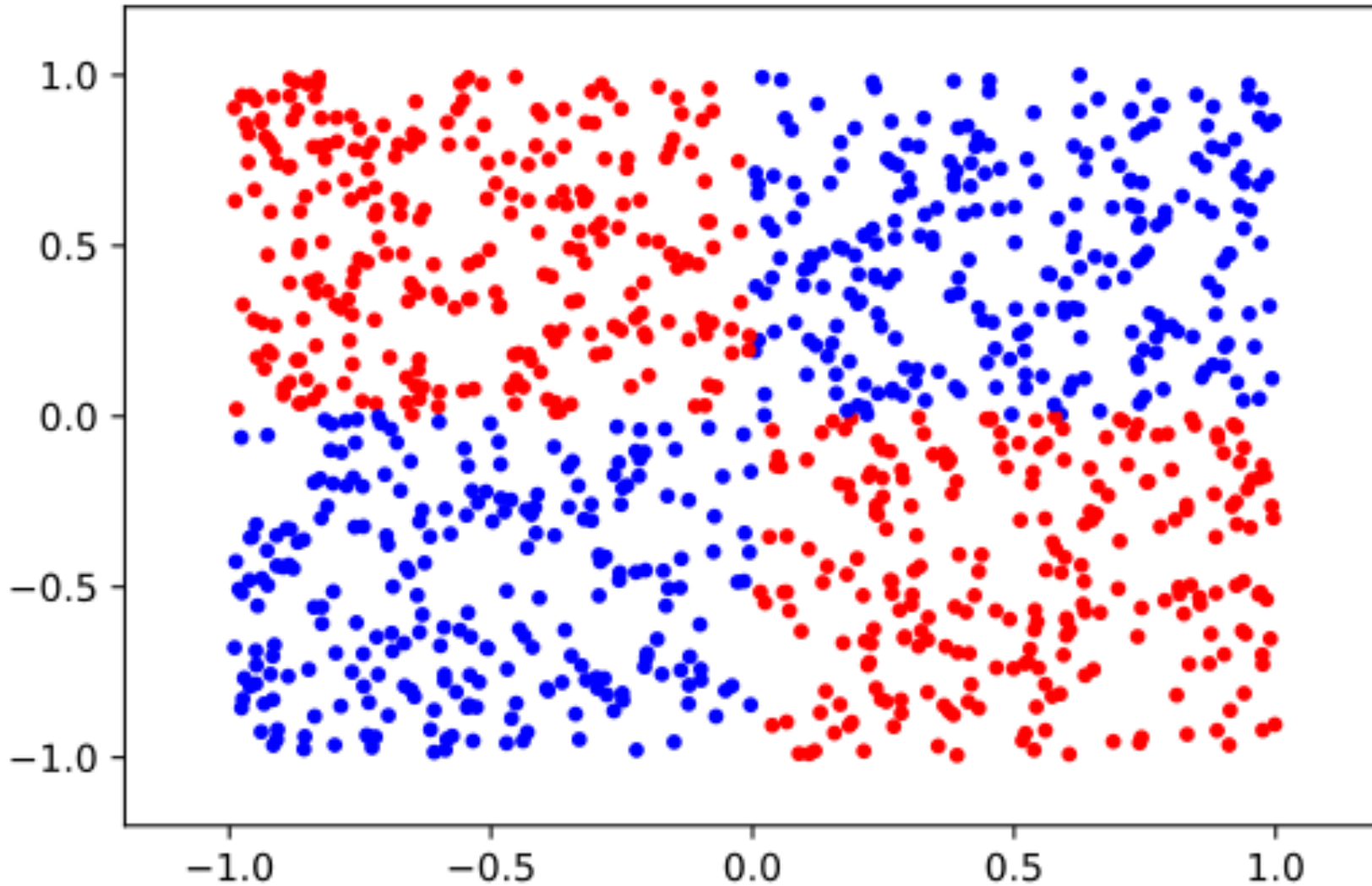


# Prediction function



- ▶ Decision boundaries always **orthogonal to feature axes**
- ▶ Resulting function is a **piecewise constant**

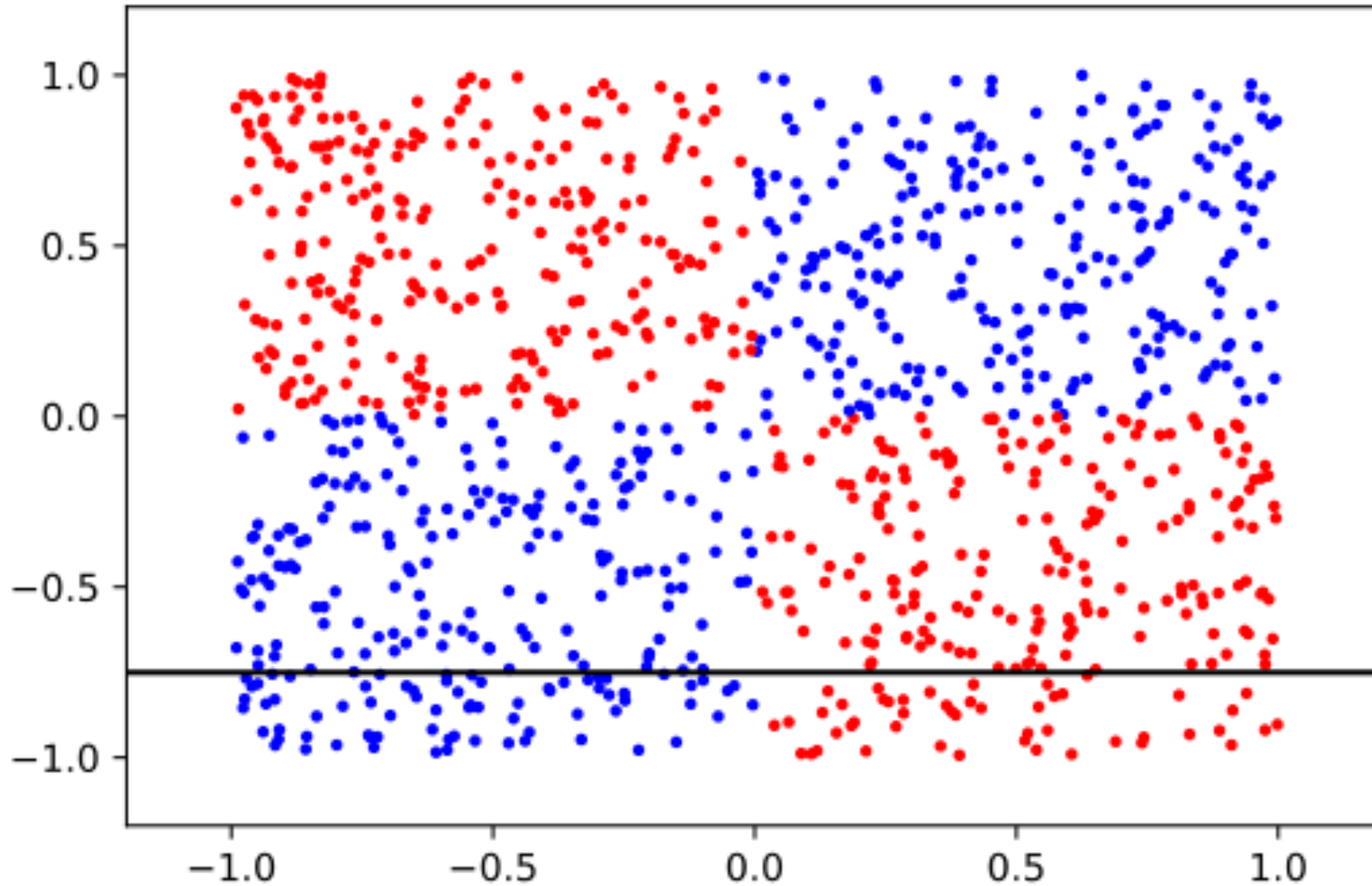
# XOR example



The greedy algorithm does not necessarily lead to the optimal solution!



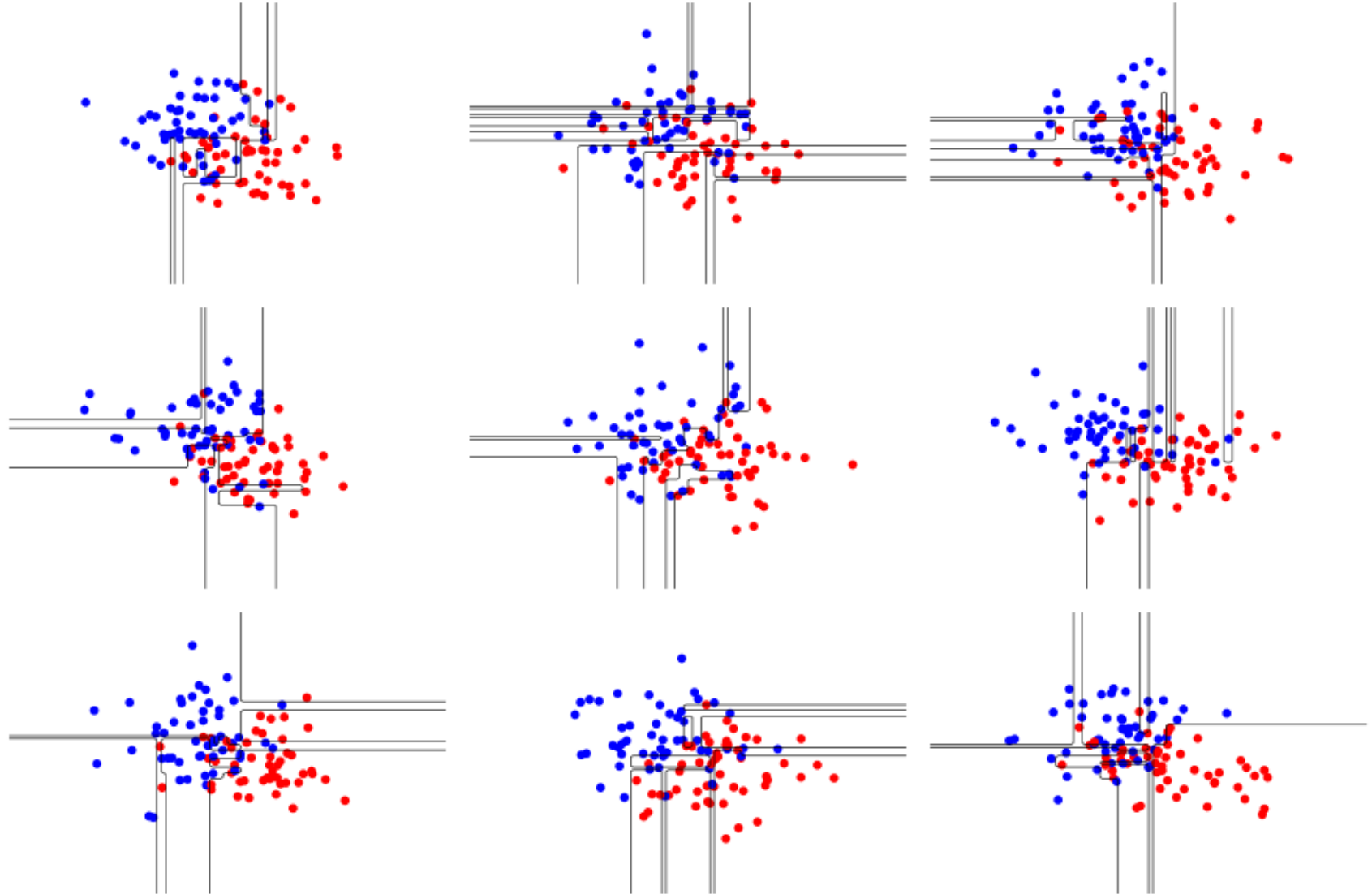
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# High Variance

- ▶ Without a stopping criterion the tree will grow until every object is classified correctly
- ▶ Can be regularized by a stopping criterion or with **pruning**



# Cost-Complexity Pruning

Original algorithm optimizes the sample-weighted impurity in the terminal nodes of the tree  $T$ :

$$R(T) = \sum_{t \in \text{leaves}(T)} |D_t| \cdot I(D_t)$$

Can modify this objective by adding a regularizer proportional to the **number of terminal nodes**  $|T|$ :

$$R_\alpha(T) = R(T) + \alpha |T|$$

Idea: build a full tree under  $R(T)$ , then remove some of the nodes to optimize  $R_\alpha(T)$ .

# Cost-Complexity Pruning

Let  $T_t$  be the subtree tree whose root node is  $t \in T$

$T_t$  will be pruned out if:

$$R(T_t) + \alpha |T_t| > R(t) + \alpha$$

or in other words if:

$$\alpha > \alpha_{\text{eff}}(t) = \frac{R(t) - R(T_t)}{|T_t| - 1}$$

# Categorical features

- ▶ Ordinal → label encoding (preserving the order!)
- ▶ Nominal → order the categories with:
  - positive class probability (binary classification)
  - target mean/median (regression)
  - (make sure the categories are **well populated** to avoid overfitting!)

# Thank you!



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