Decision Trees

Classification and Regression Trees, impurity functions, solution properties

Data Analytics and Mining, 2024

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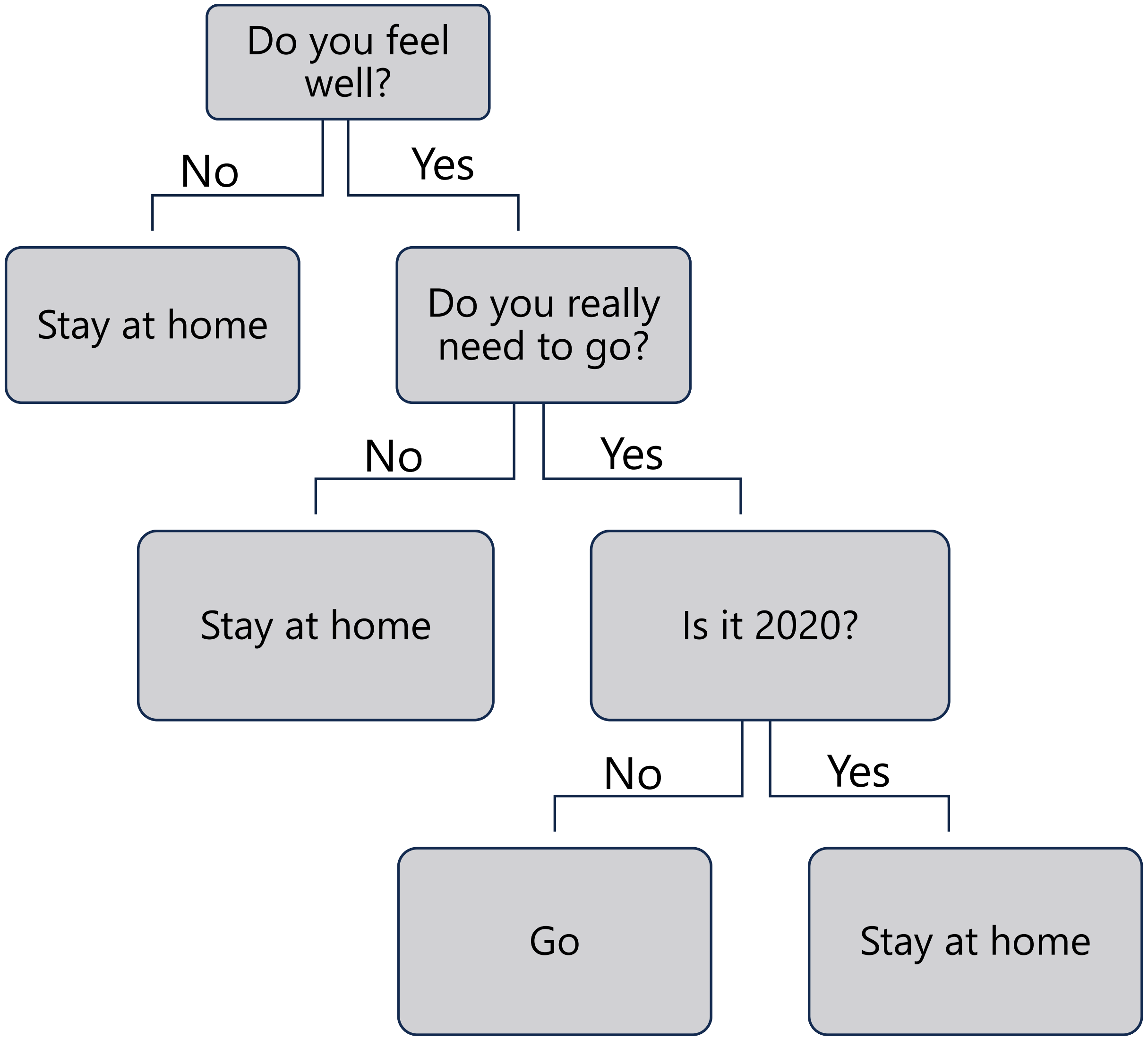
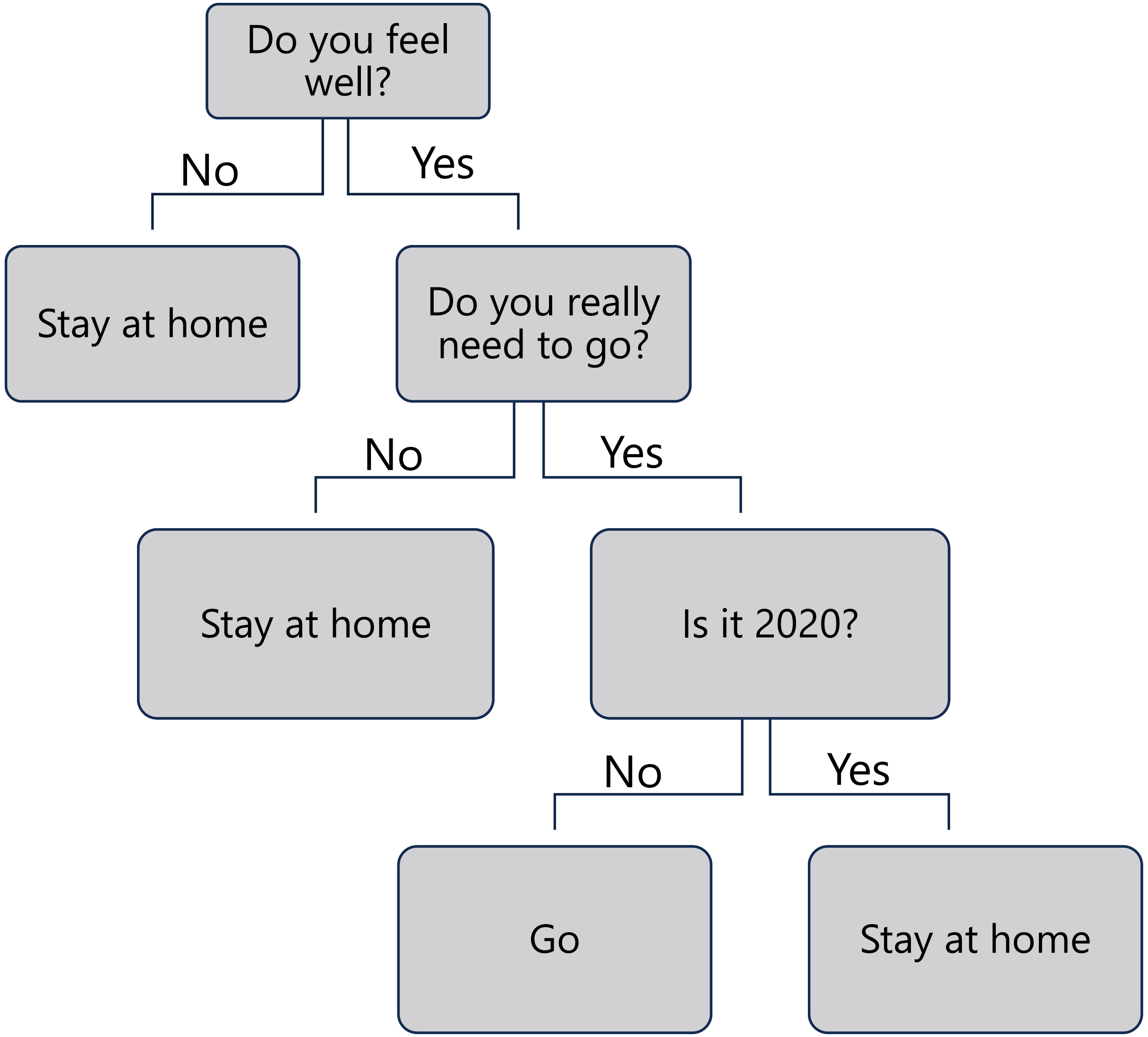
Basics

"Should you go to work?" chart



“Should you go to work?” chart

Directed graph



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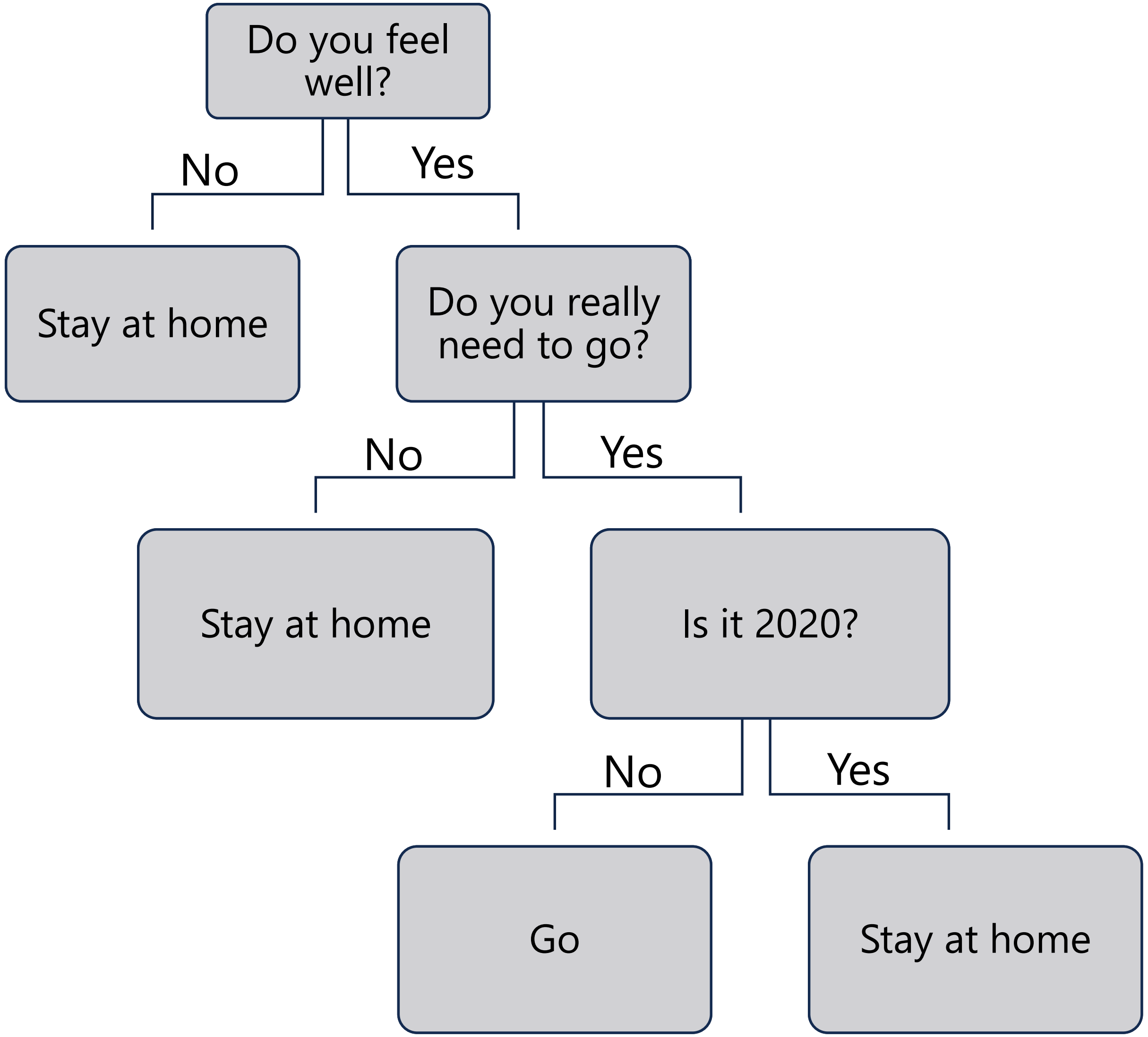
Directed graph

No loops

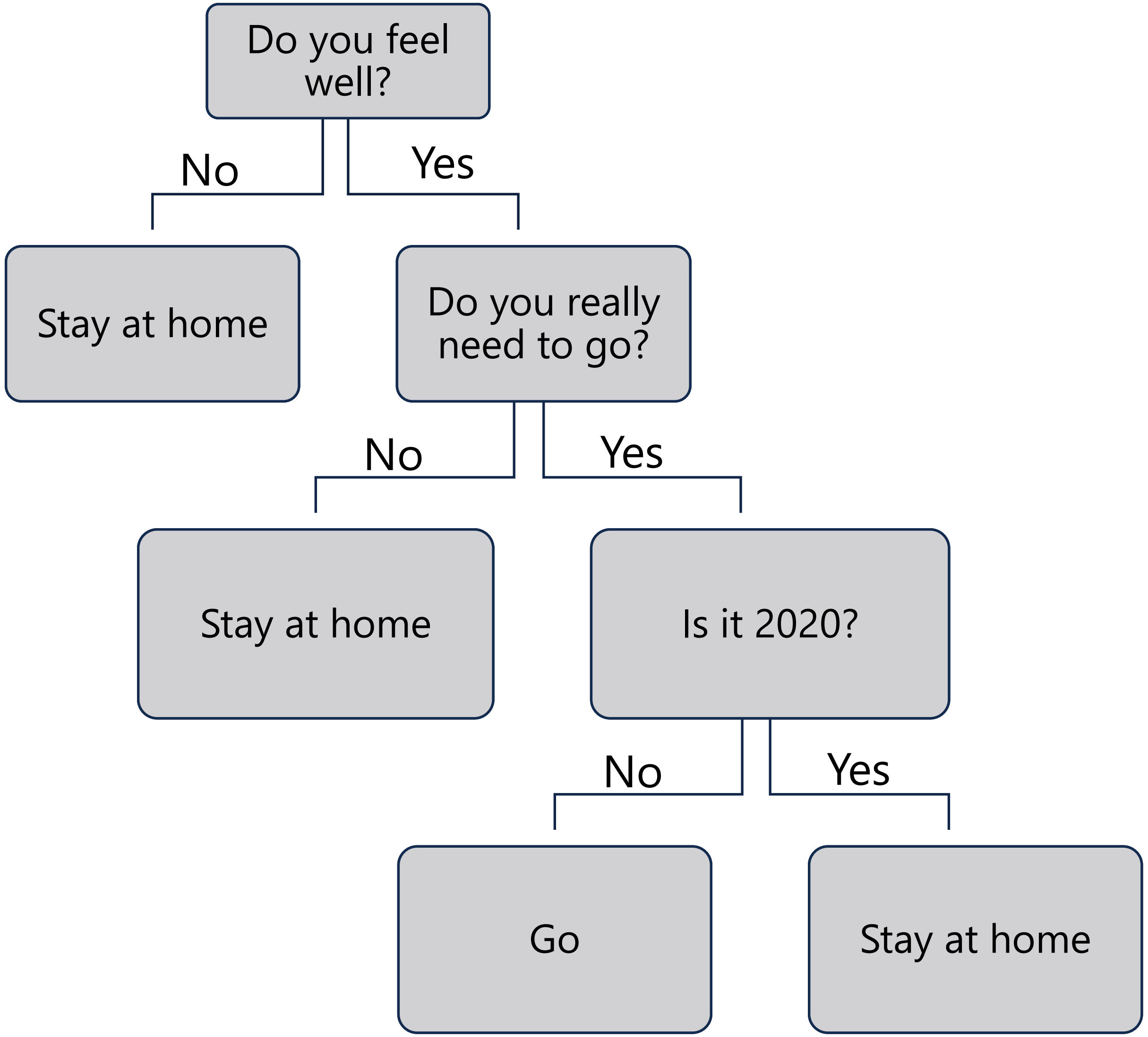


“Should you go to work?” chart

Directed graph

No loops

Single root node



“Should you go to work?” chart

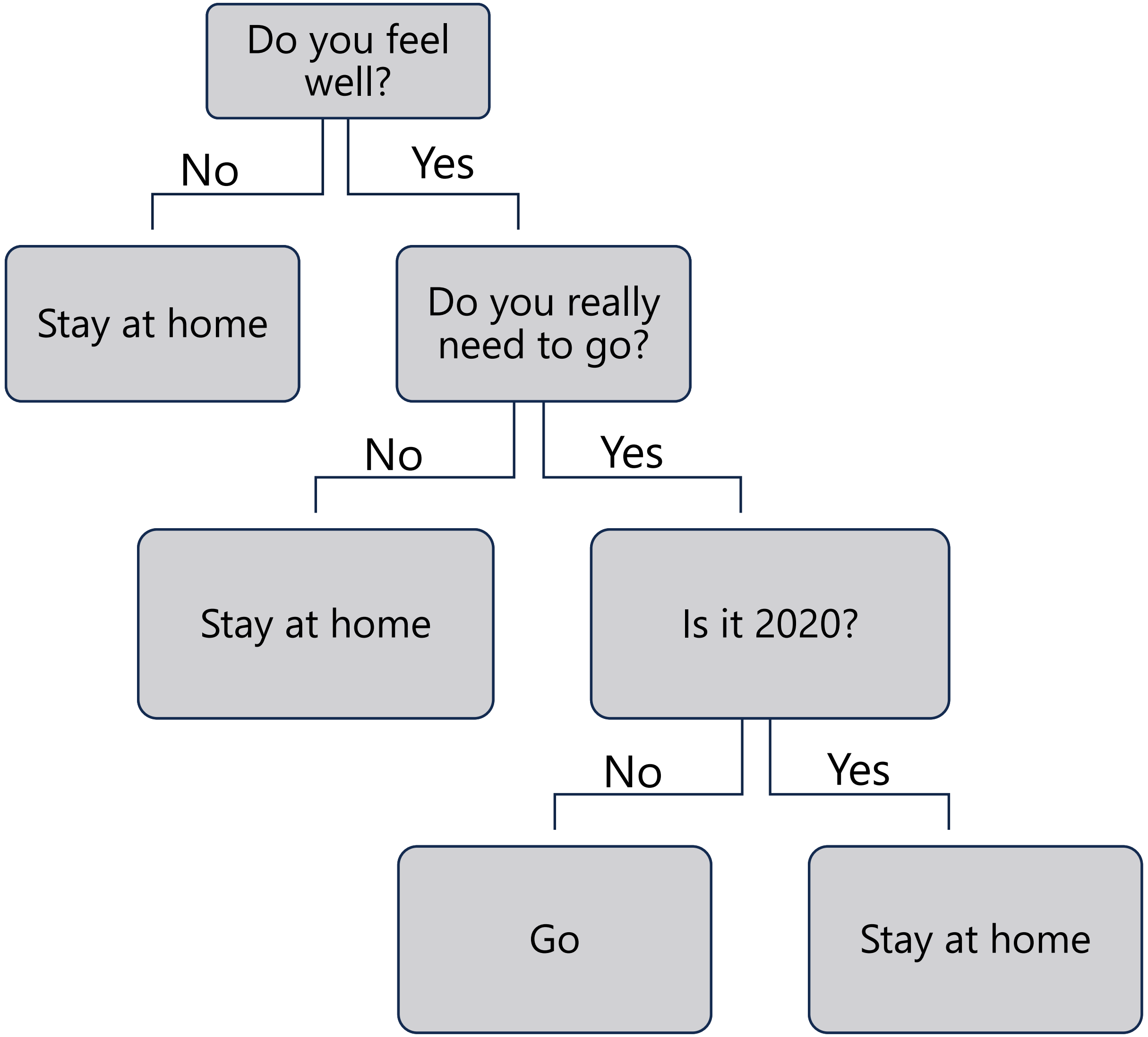
Directed graph

No loops

Single root node

Each node has:

– either 0 child nodes (**terminal node**, “leaf”)



“Should you go to work?” chart

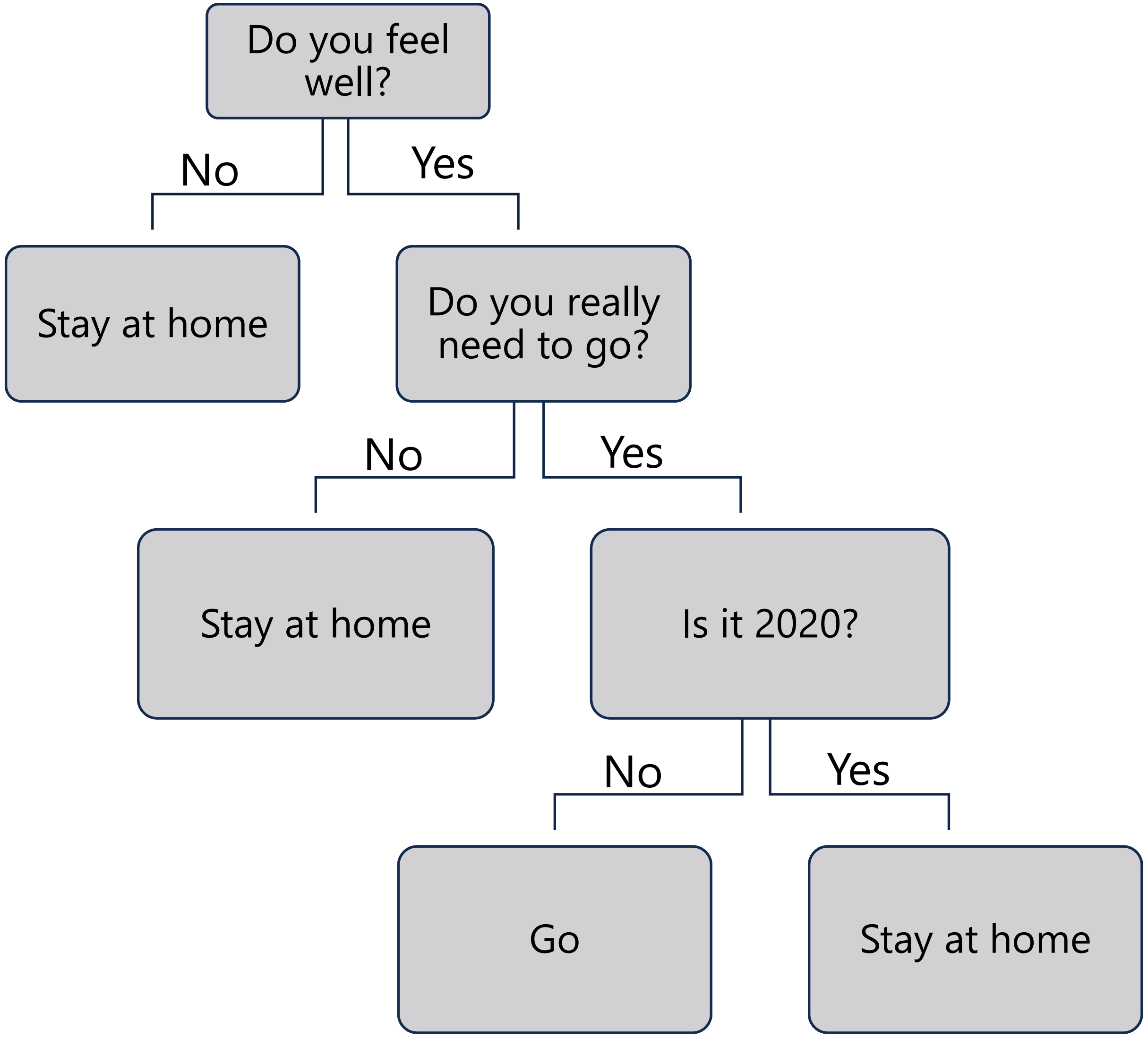
Directed graph

No loops

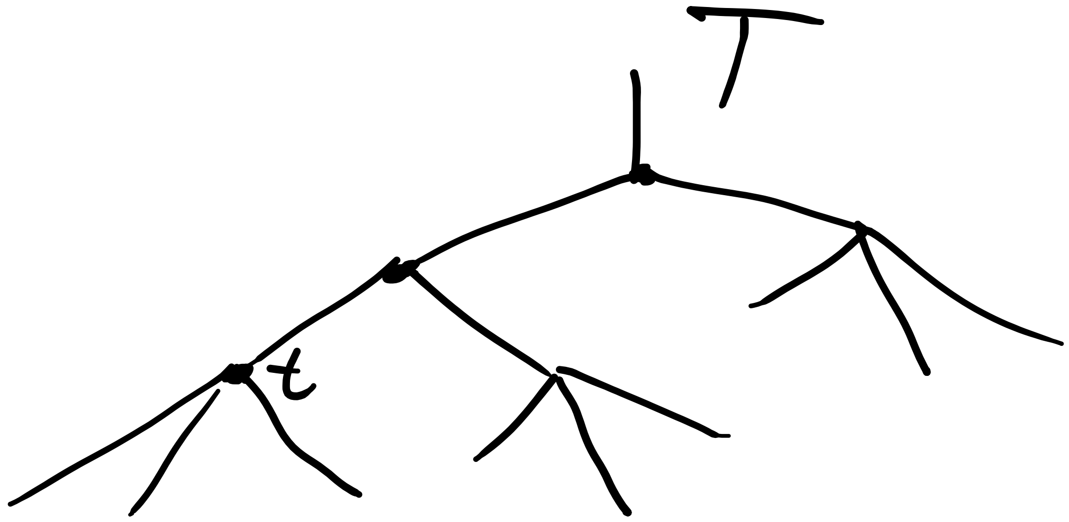
Single root node

Each node has:

- either 0 child nodes (**terminal node**, “leaf”)
- or ≥2 child nodes (**internal node**)
  - 2 nodes for binary trees



Defining a tree (general approach)



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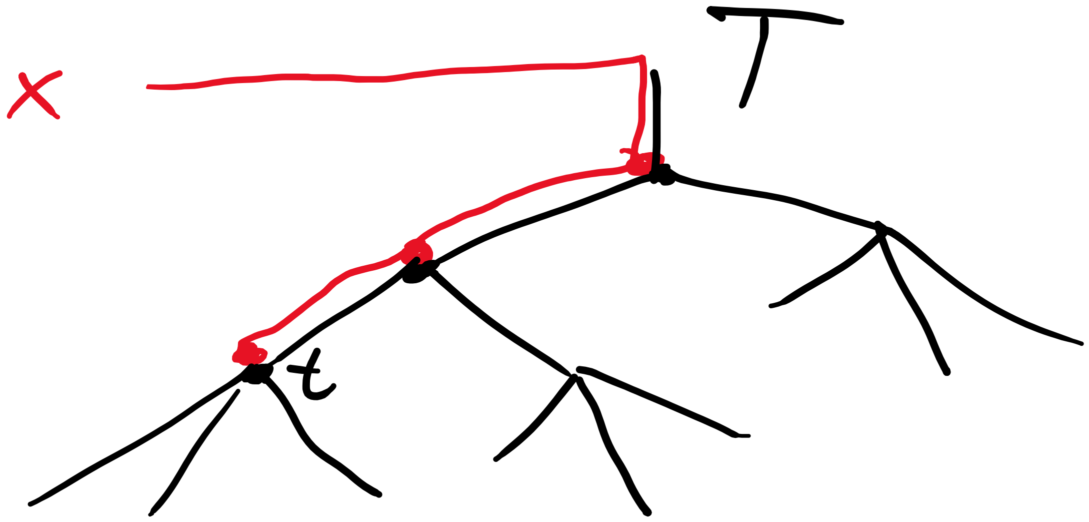

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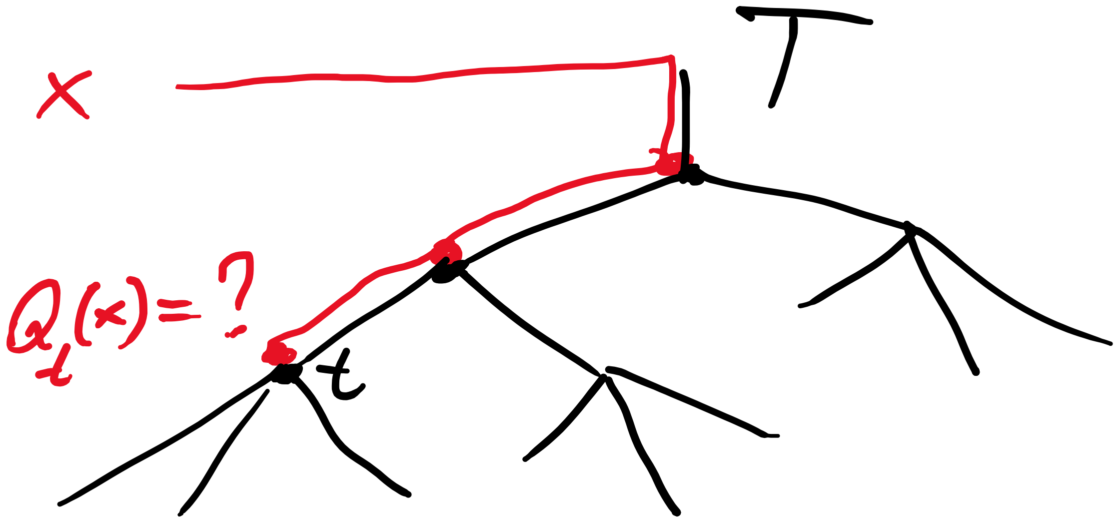

For each node $t \in T$ define a check function $Q_t(x)$

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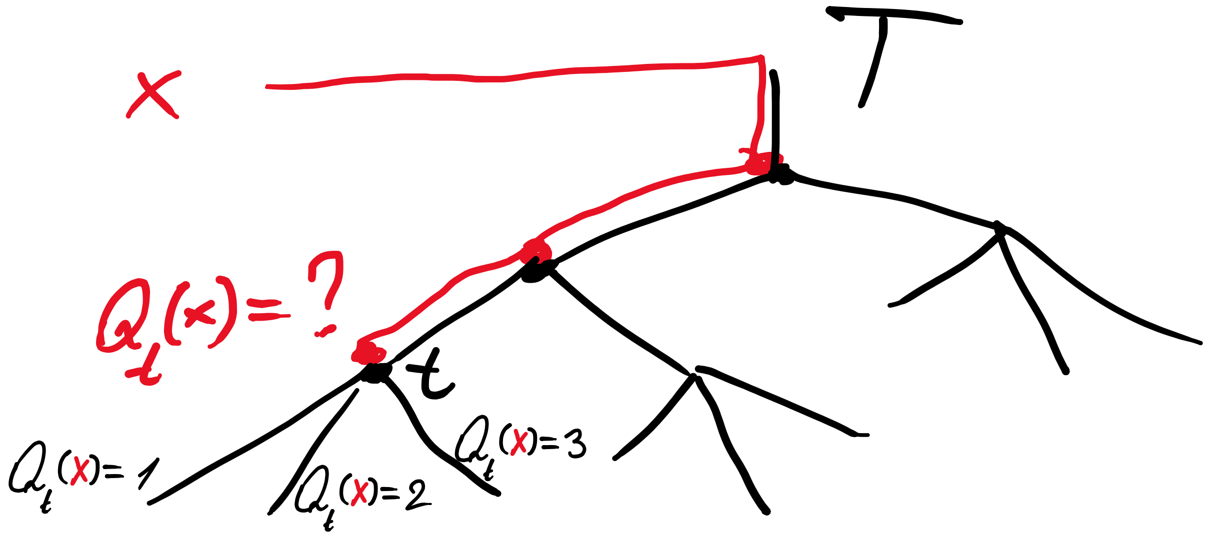

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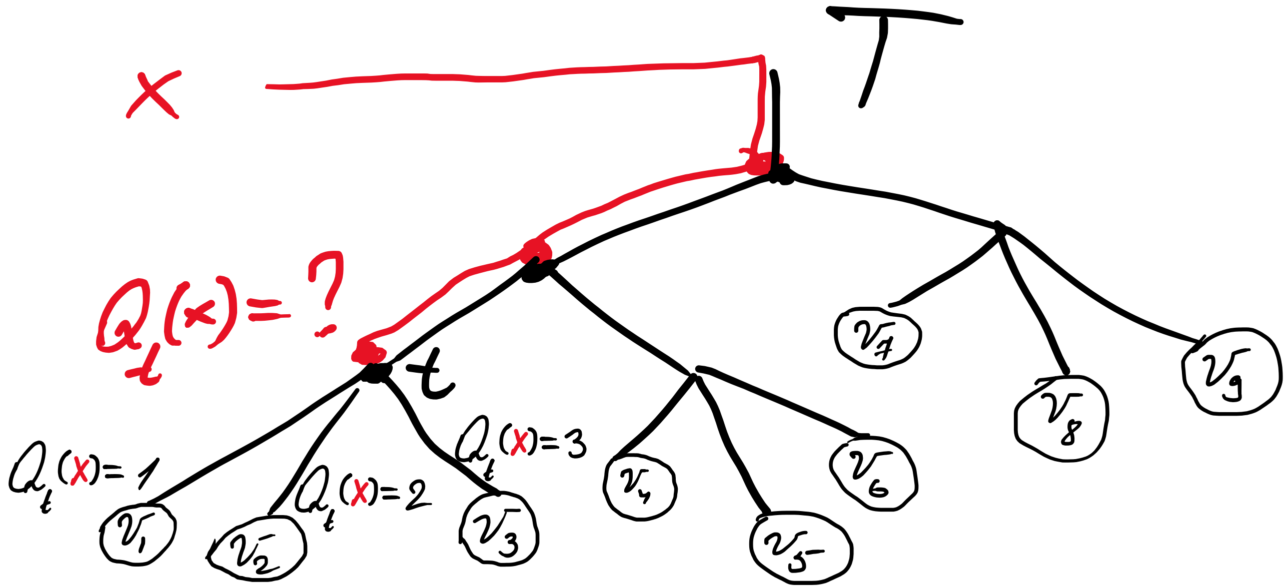
For each child node of t assign a set of unique values of $Q_t(x)$

Defining a tree (general approach)



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

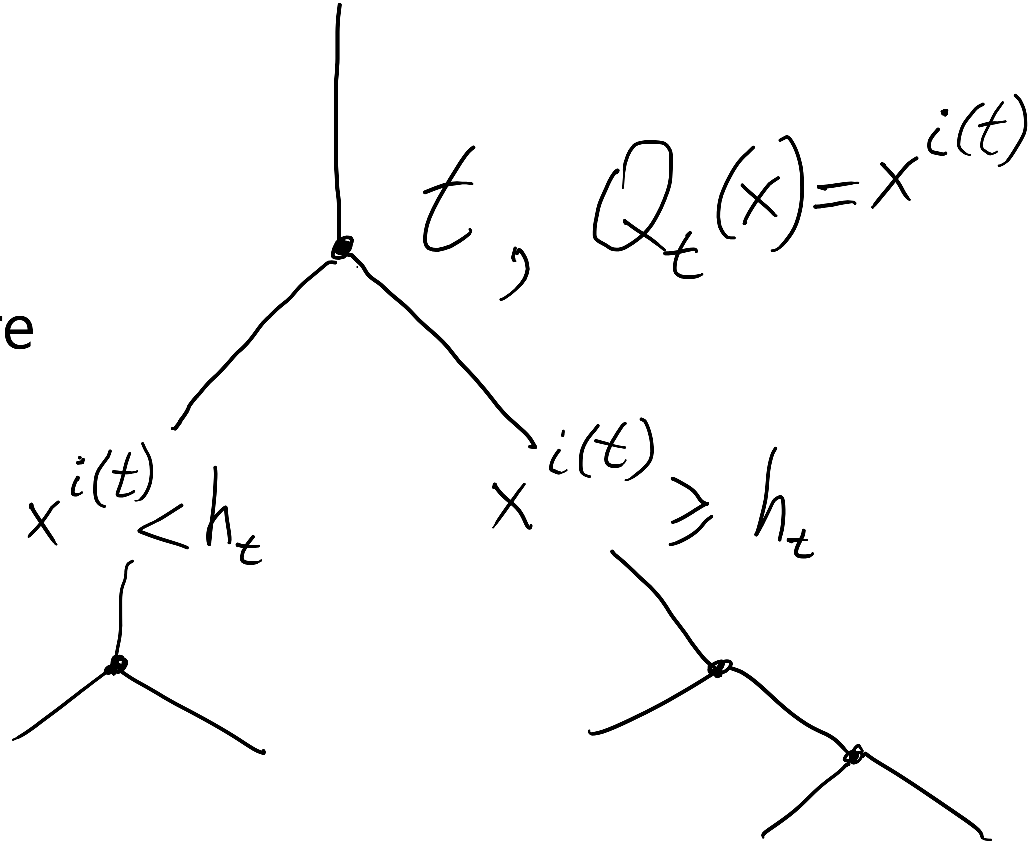
Check function:

$Q_t(x) = x^{i(t)}$ — 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

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

the decrease of impurity:

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

is maximized (over k and i).

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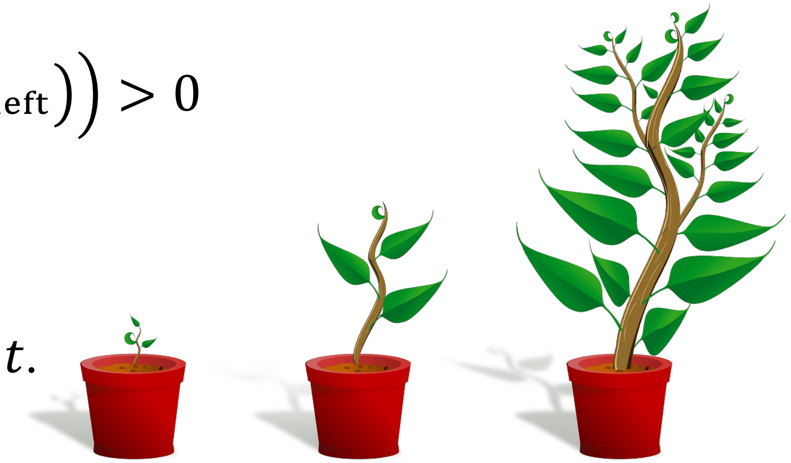
is maximized (over k and i).

Set the check function $Q_t(x) = x^i$, and threshold $h_t = x_k^i$,
attach the two new corresponding child nodes t^{left} and t^{right} to t.



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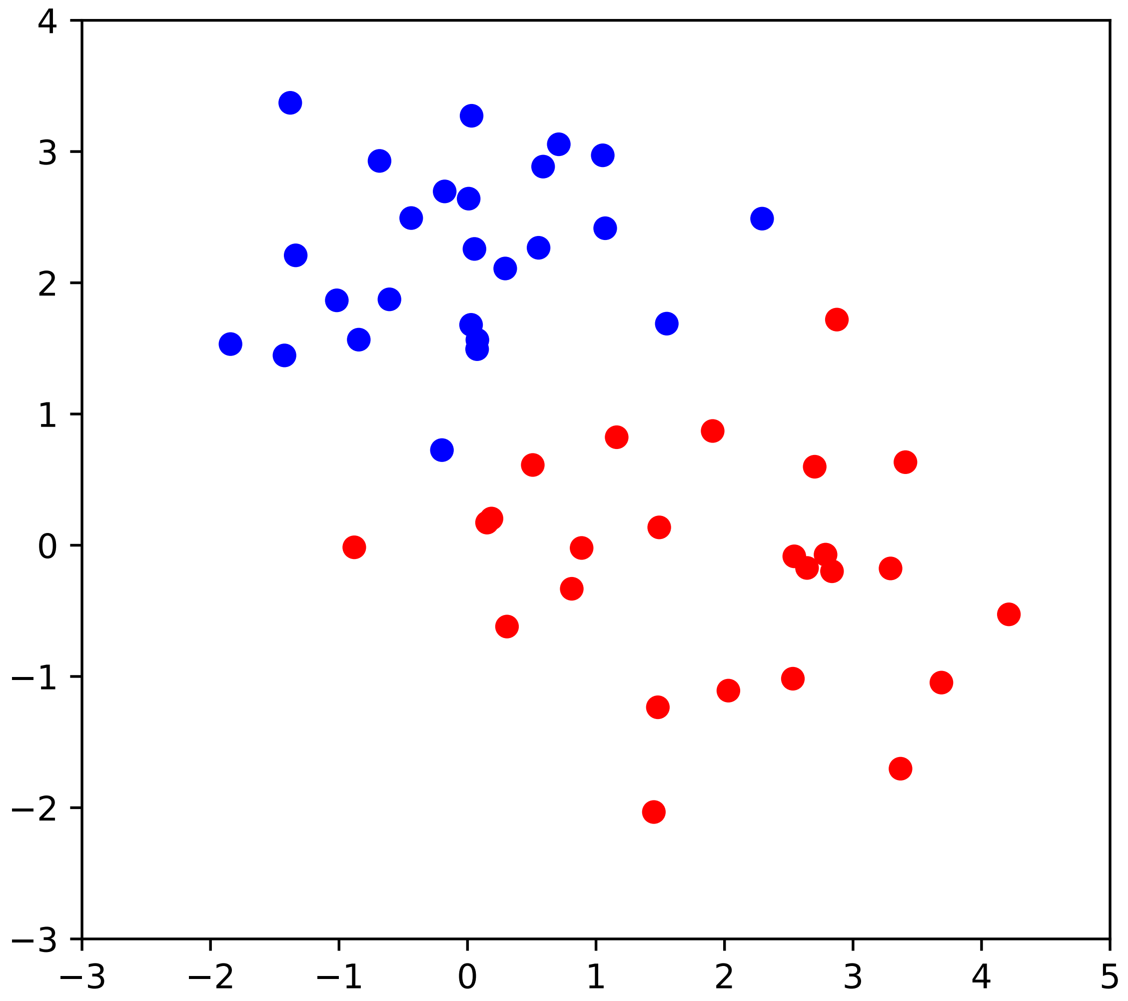

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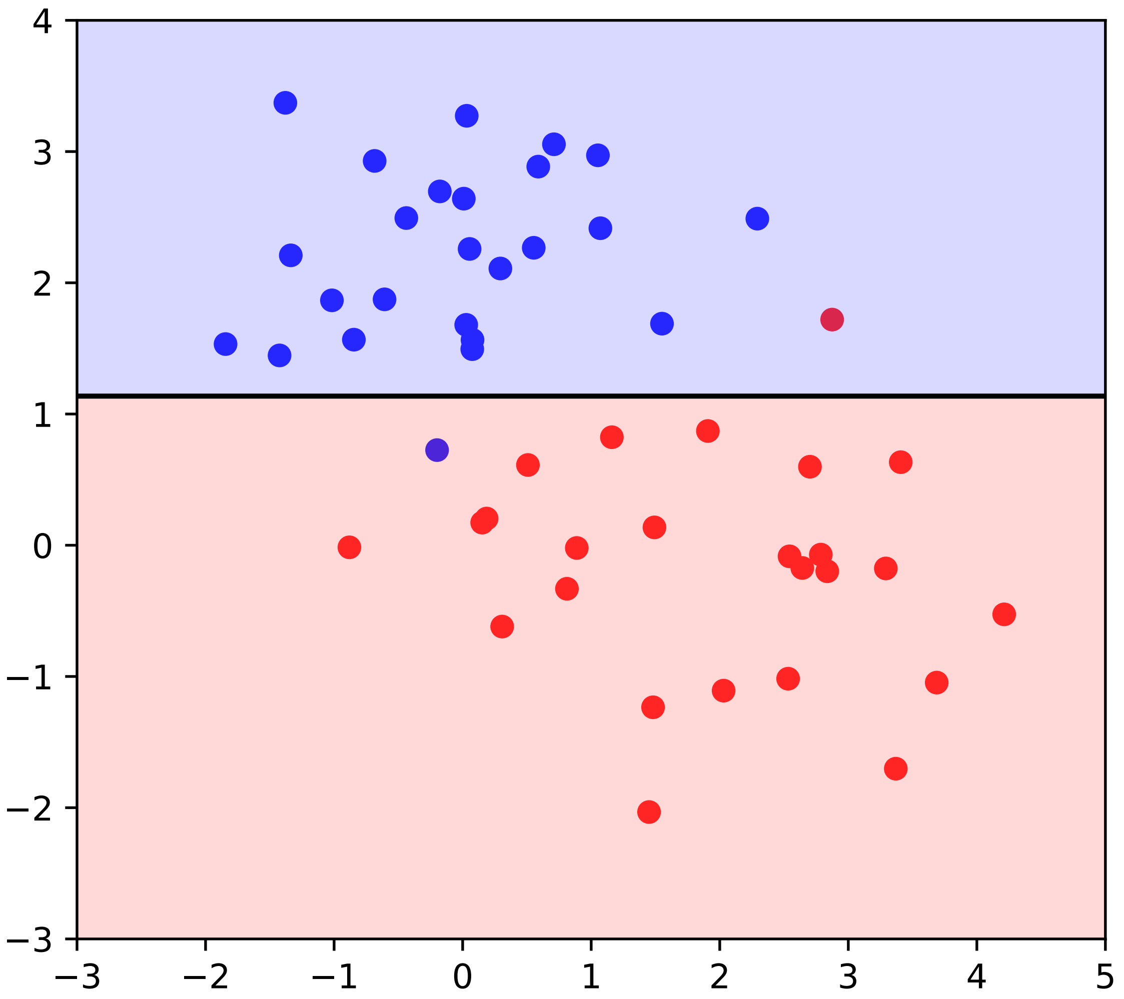

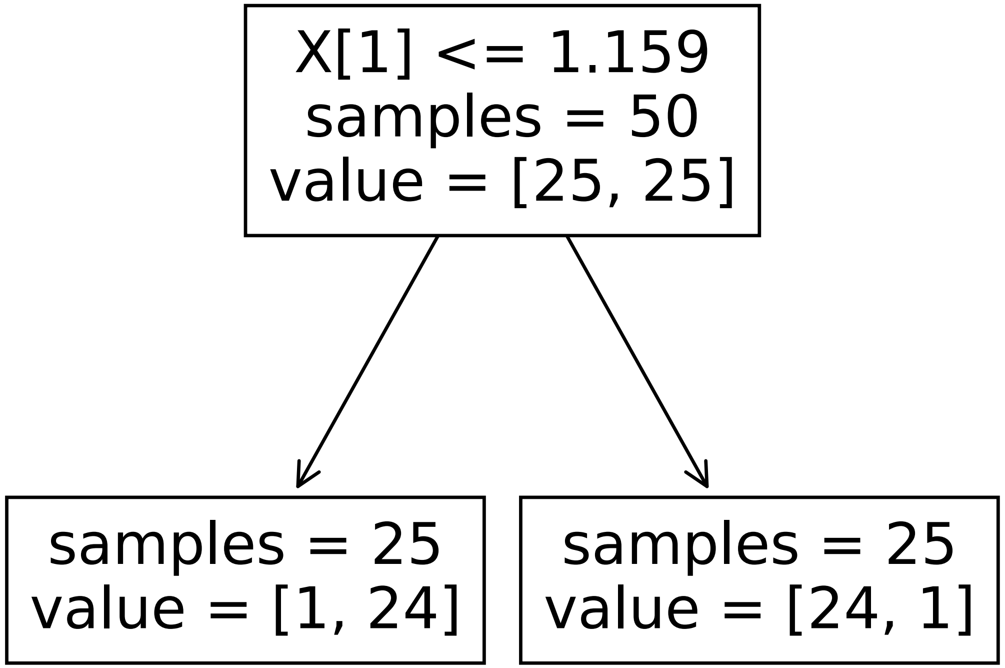

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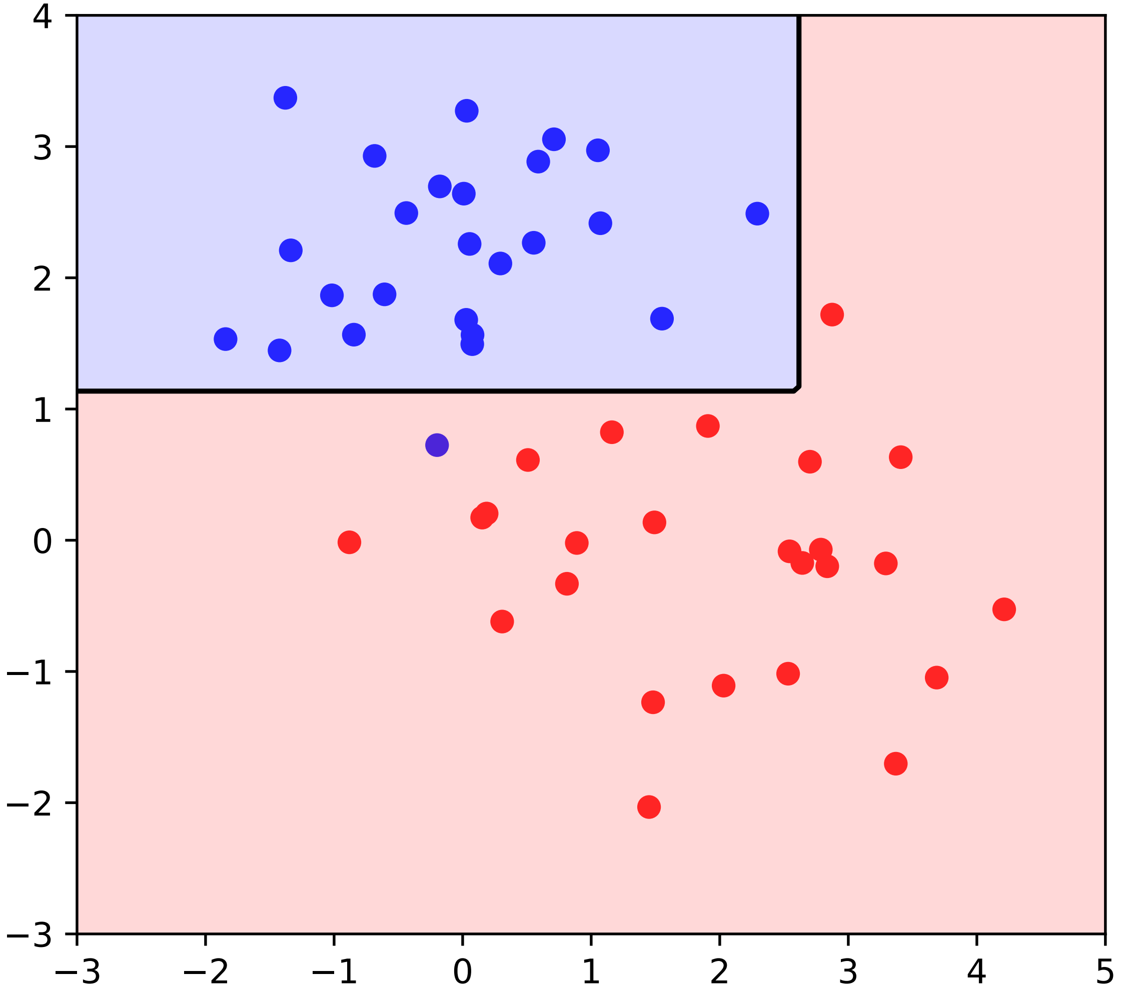

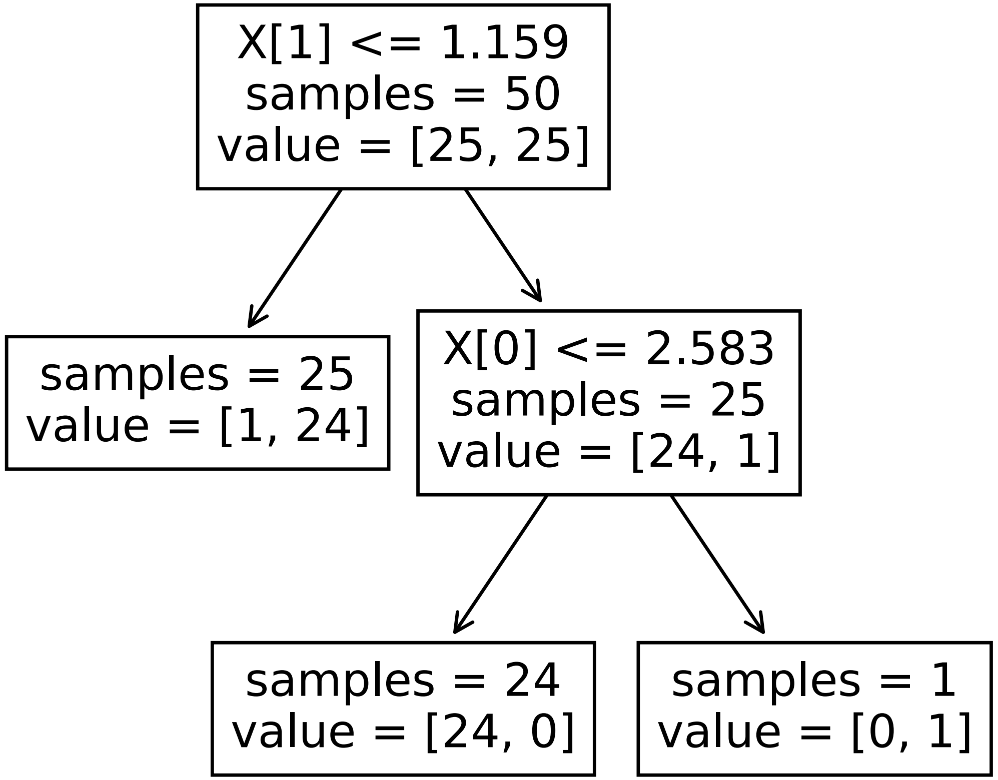

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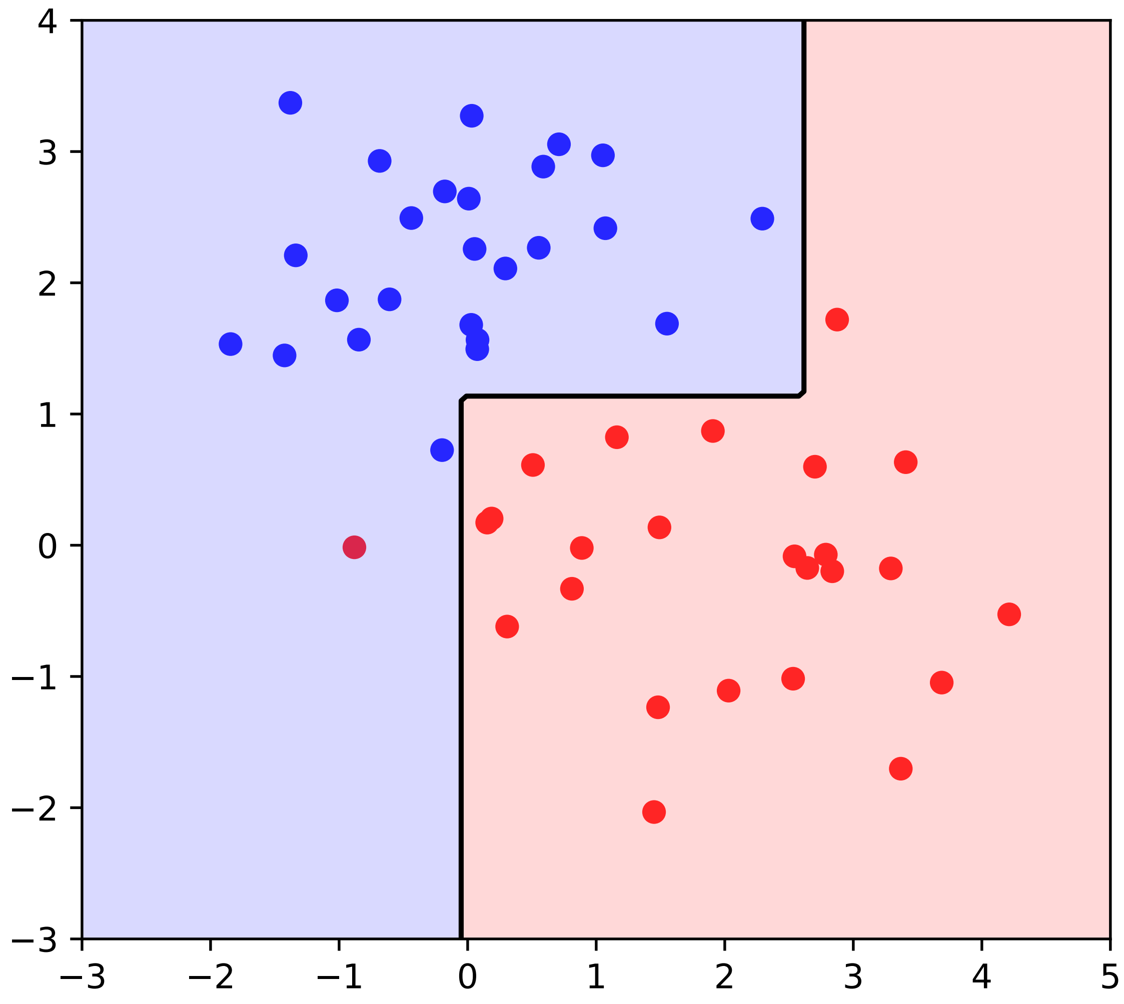

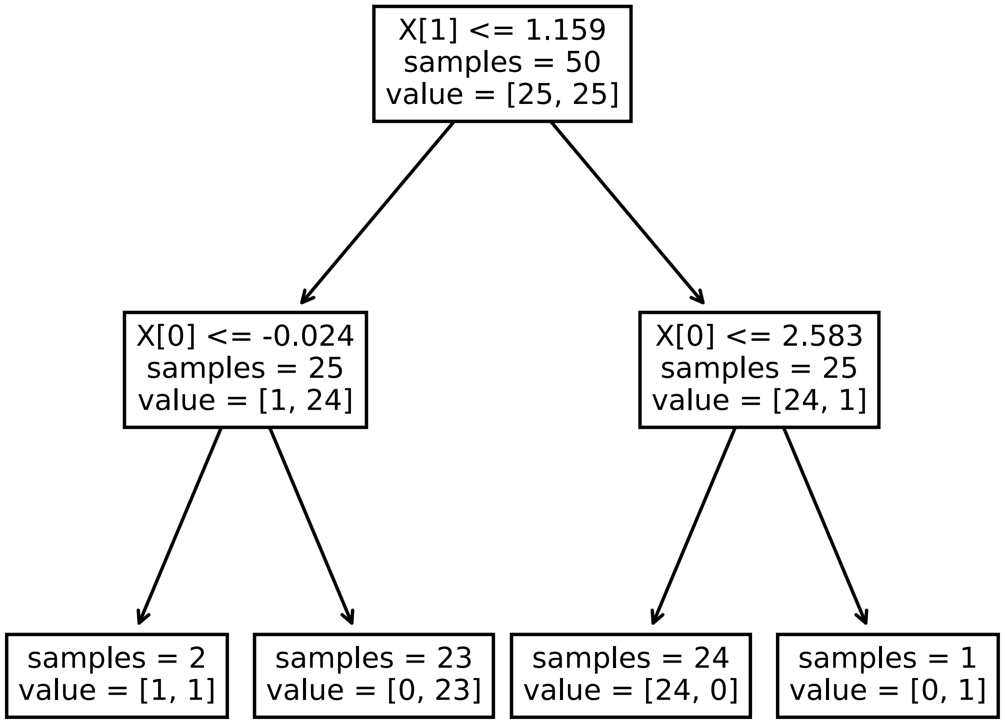

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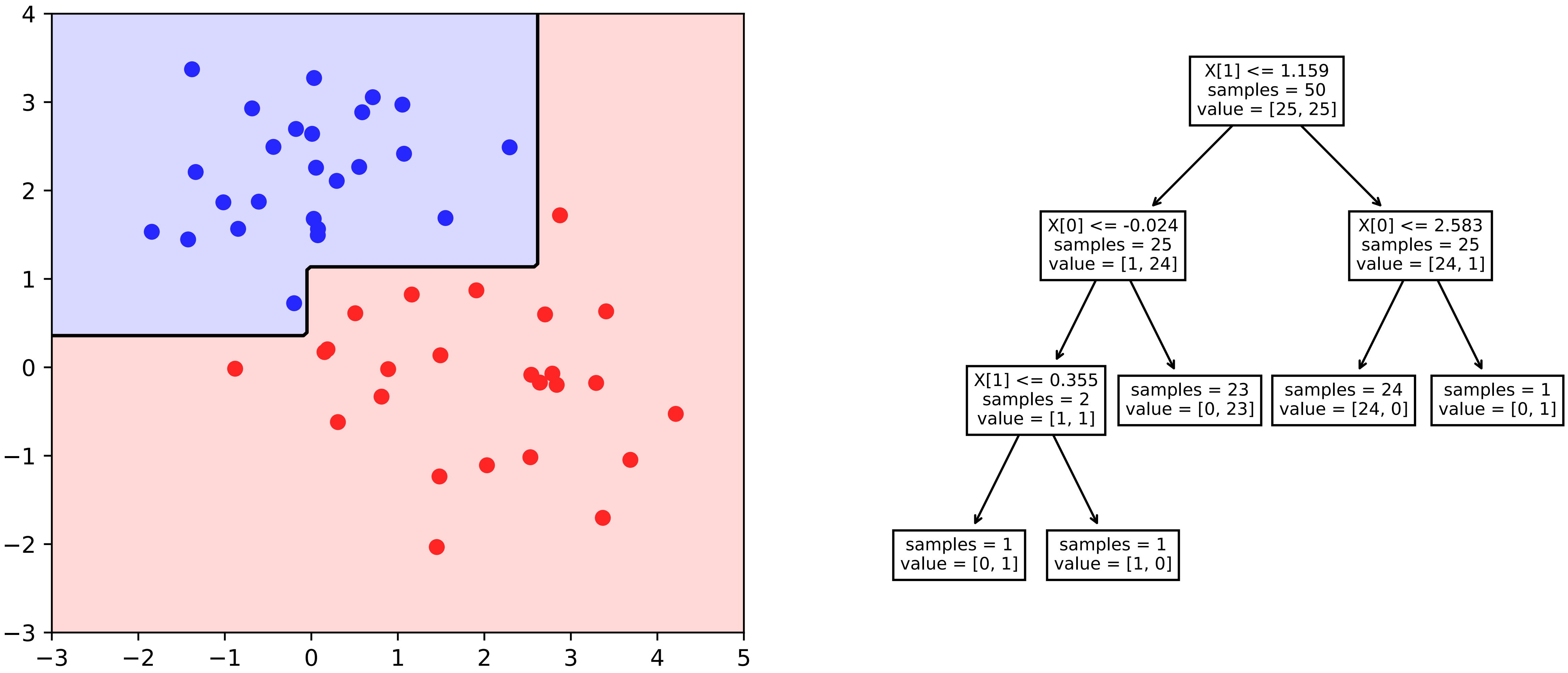

Impurity measures

Regression

mean target

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

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:

Impurity measures

What about classification?

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

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

Impurity measures

Classification

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

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

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

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

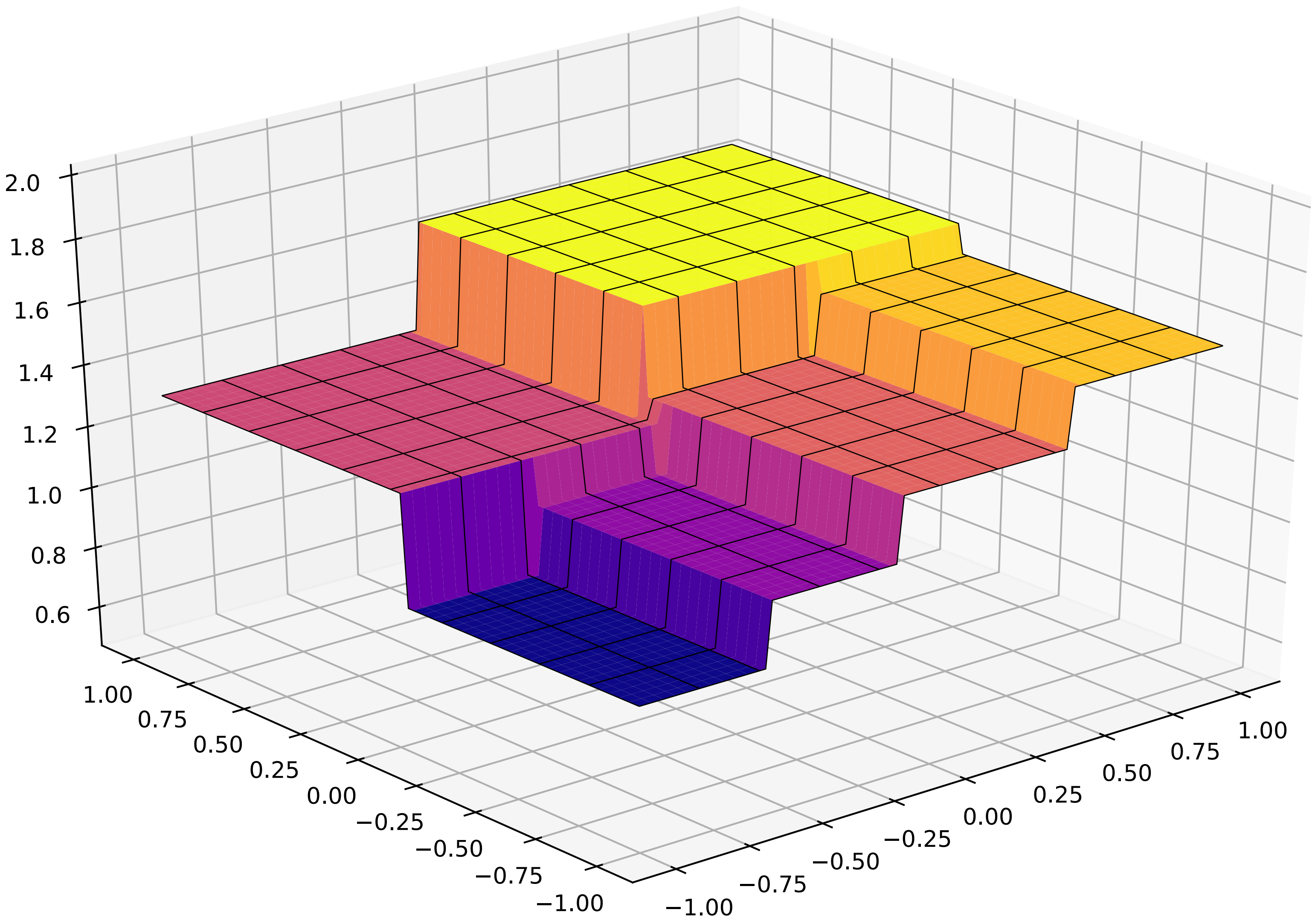
Minimum number of samples in a leaf

Minimum impurity gain

You name it…

Solution properties

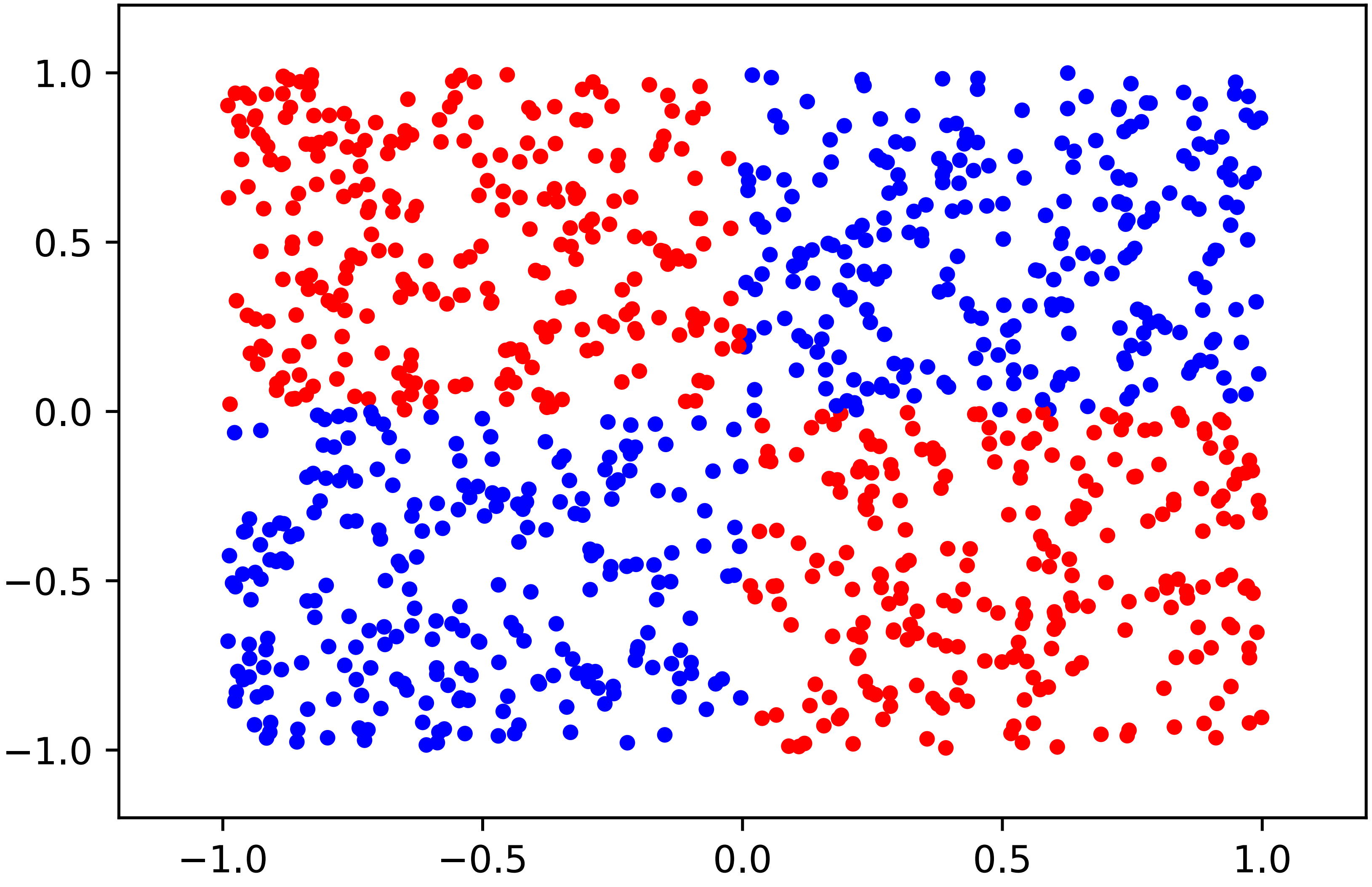
Prediction function



Decision boundaries always **orthogonal to feature axes**

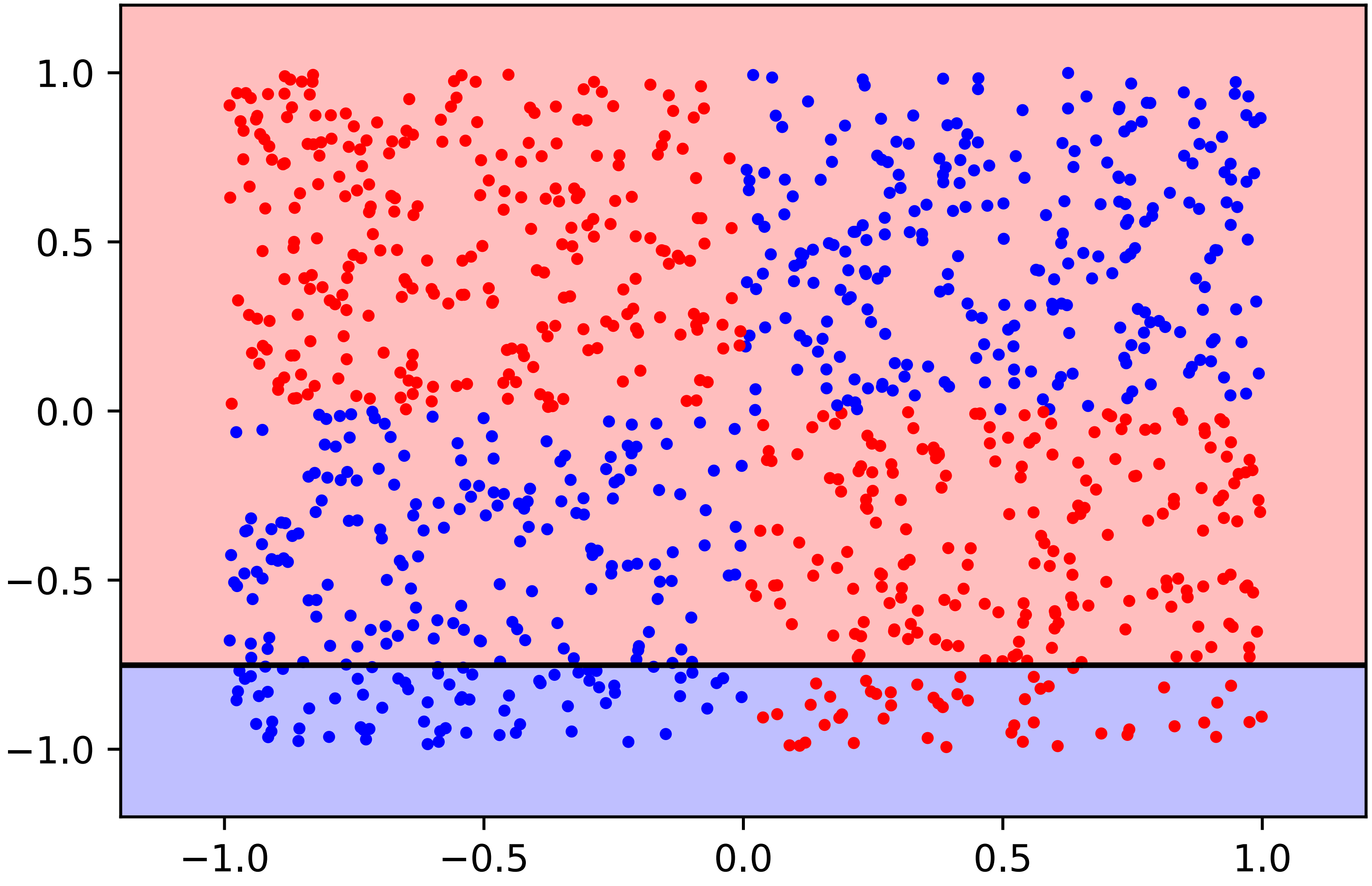
Resulting function is a **piecewise constant**

XOR example



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

XOR example



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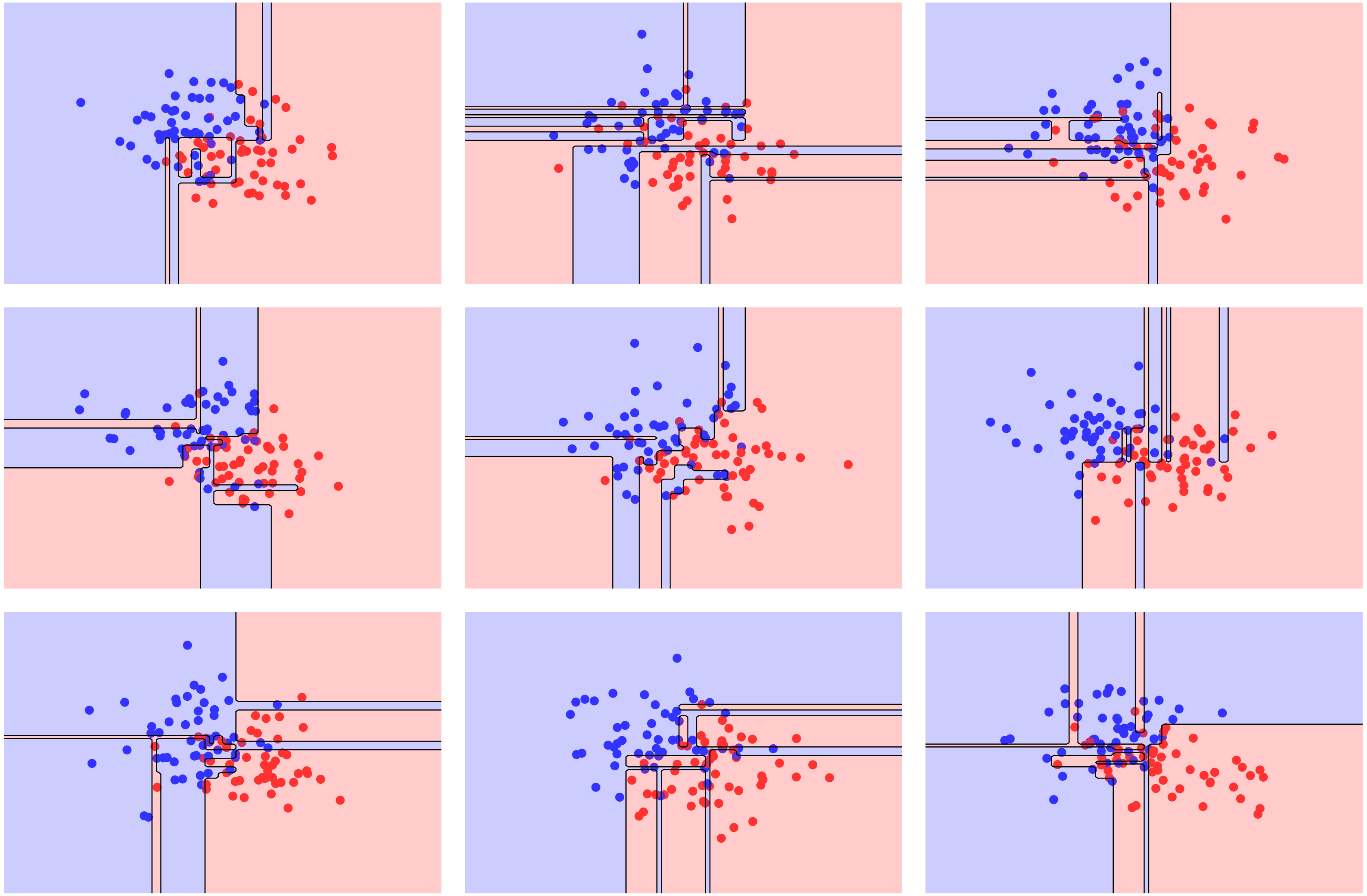
High Variance

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 ∈ 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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