

Decision Trees

Classification and Regression Trees, impurity functions, solution properties

Machine Learning and Data Mining, 2024

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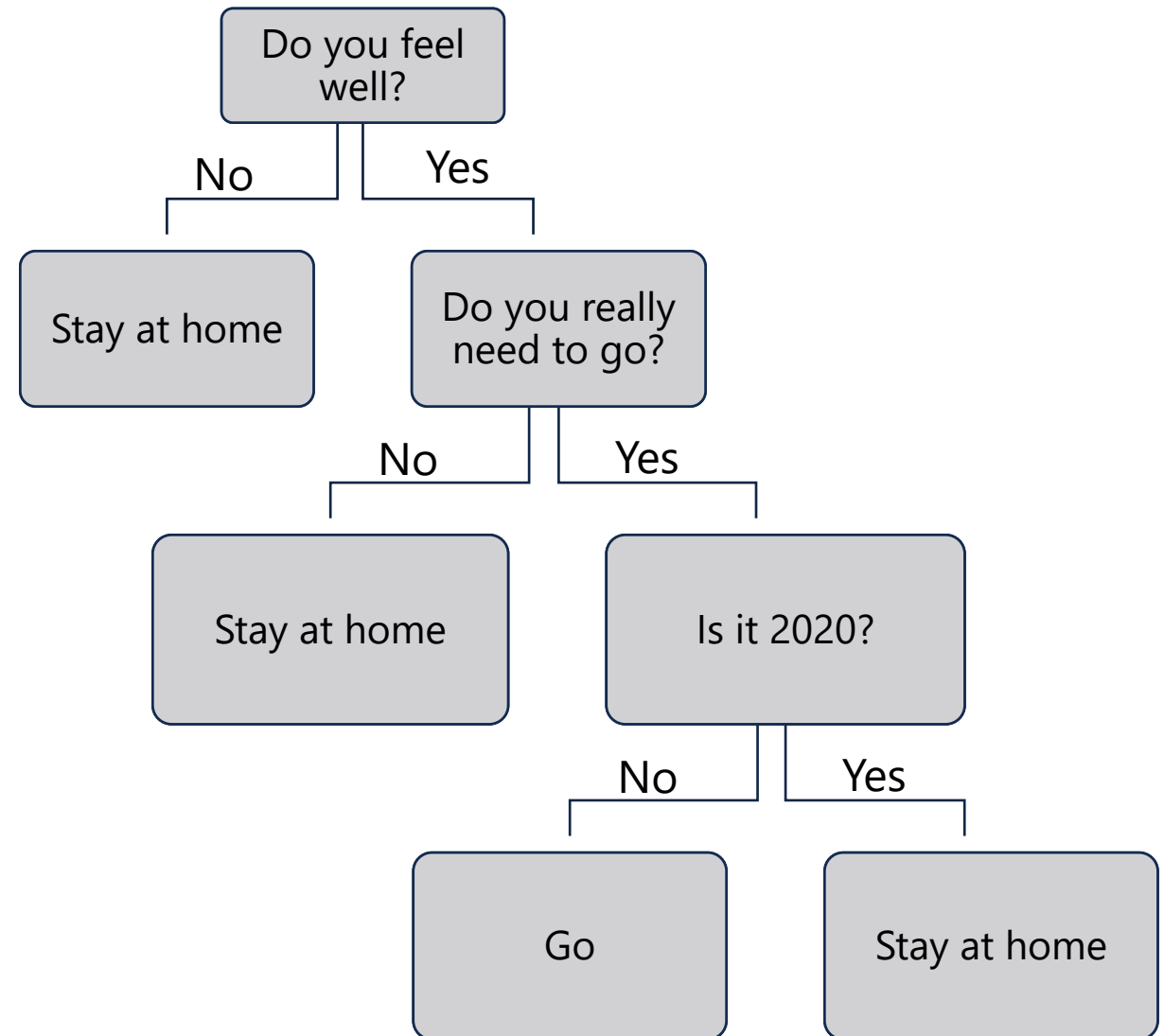
MMCP

November 22, 2024

Basics

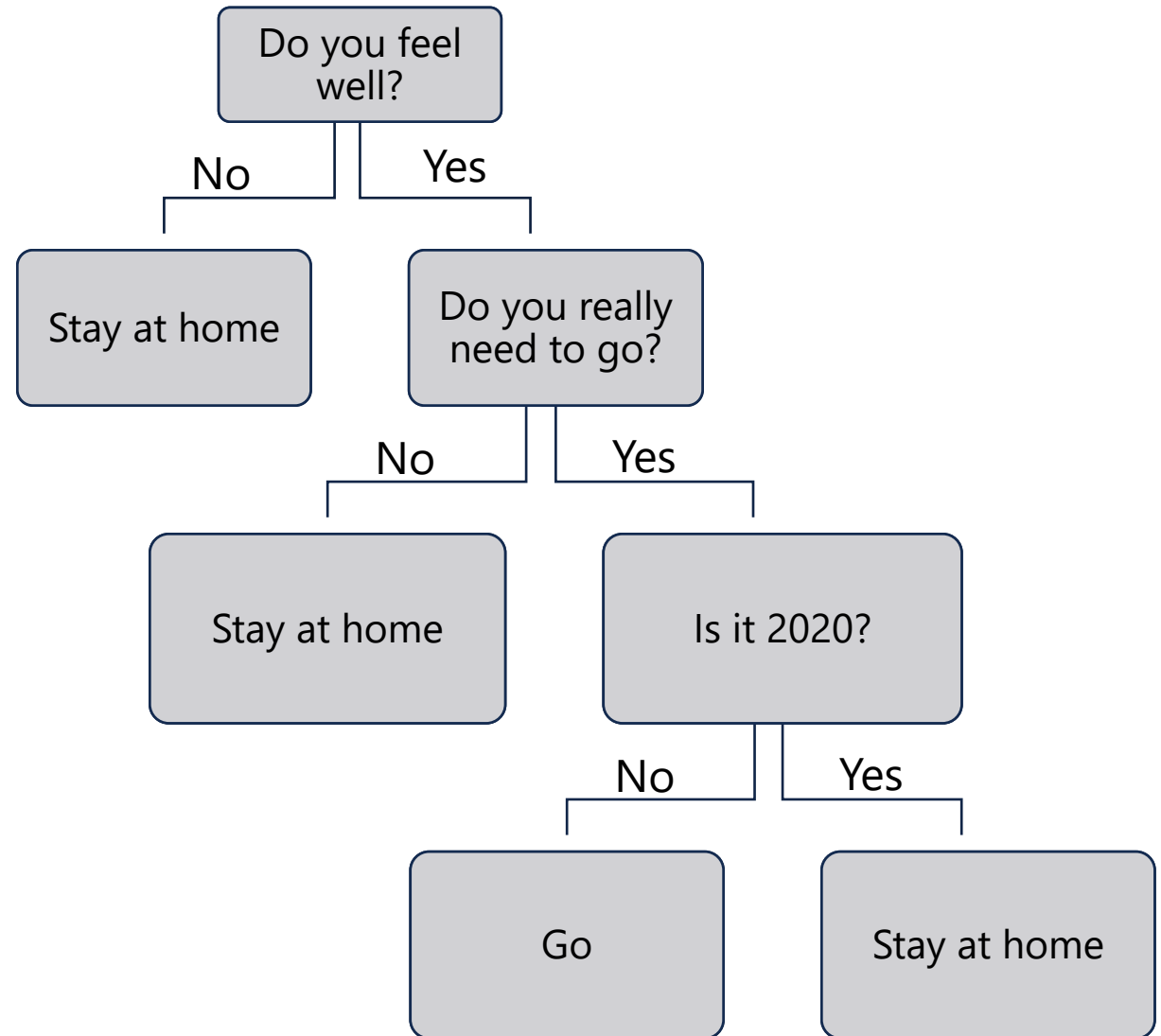


"Should you go to work?" chart



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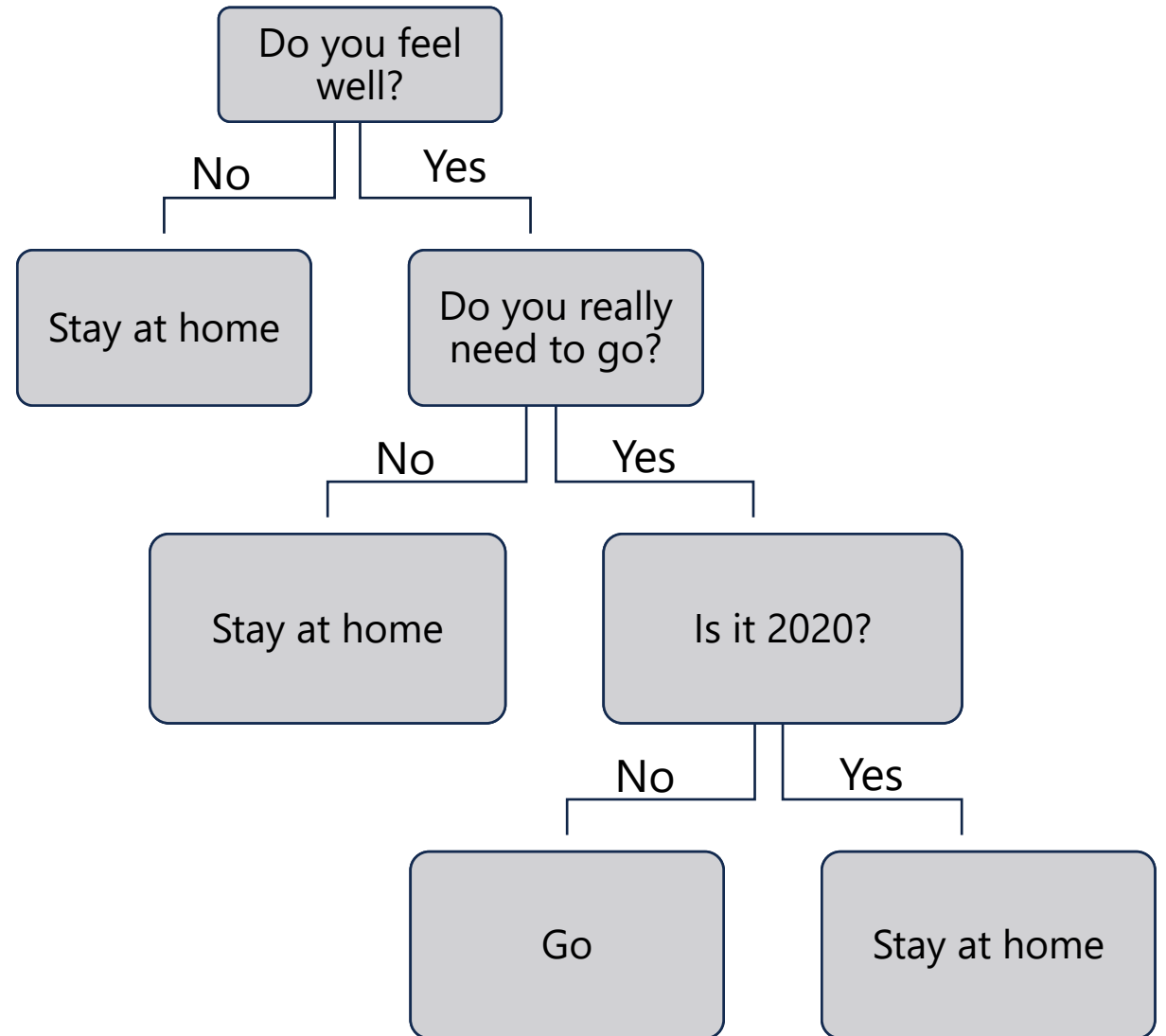
Directed graph



"Should you go to work?" chart

Directed graph

No loops

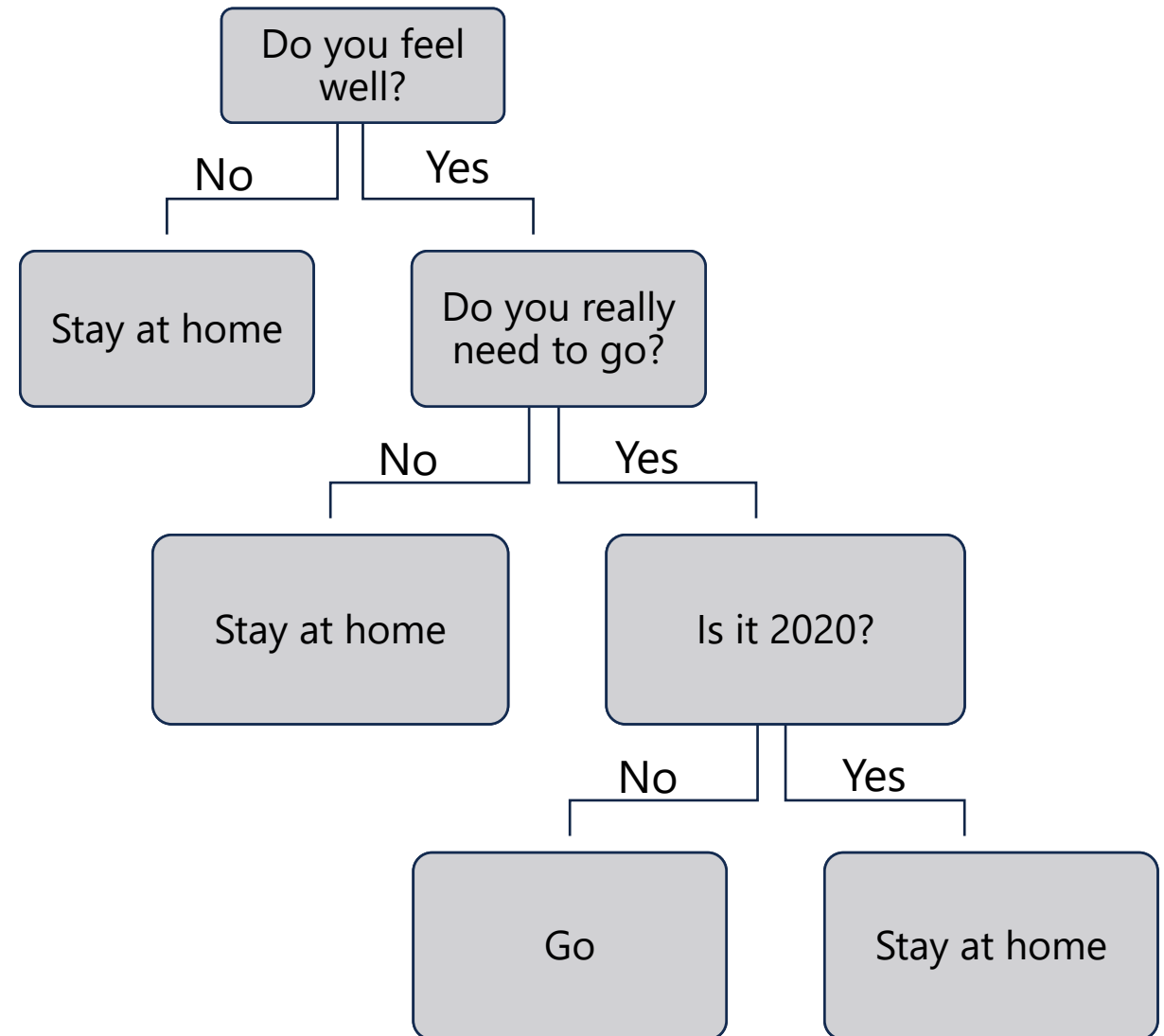


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Directed graph

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Single root node



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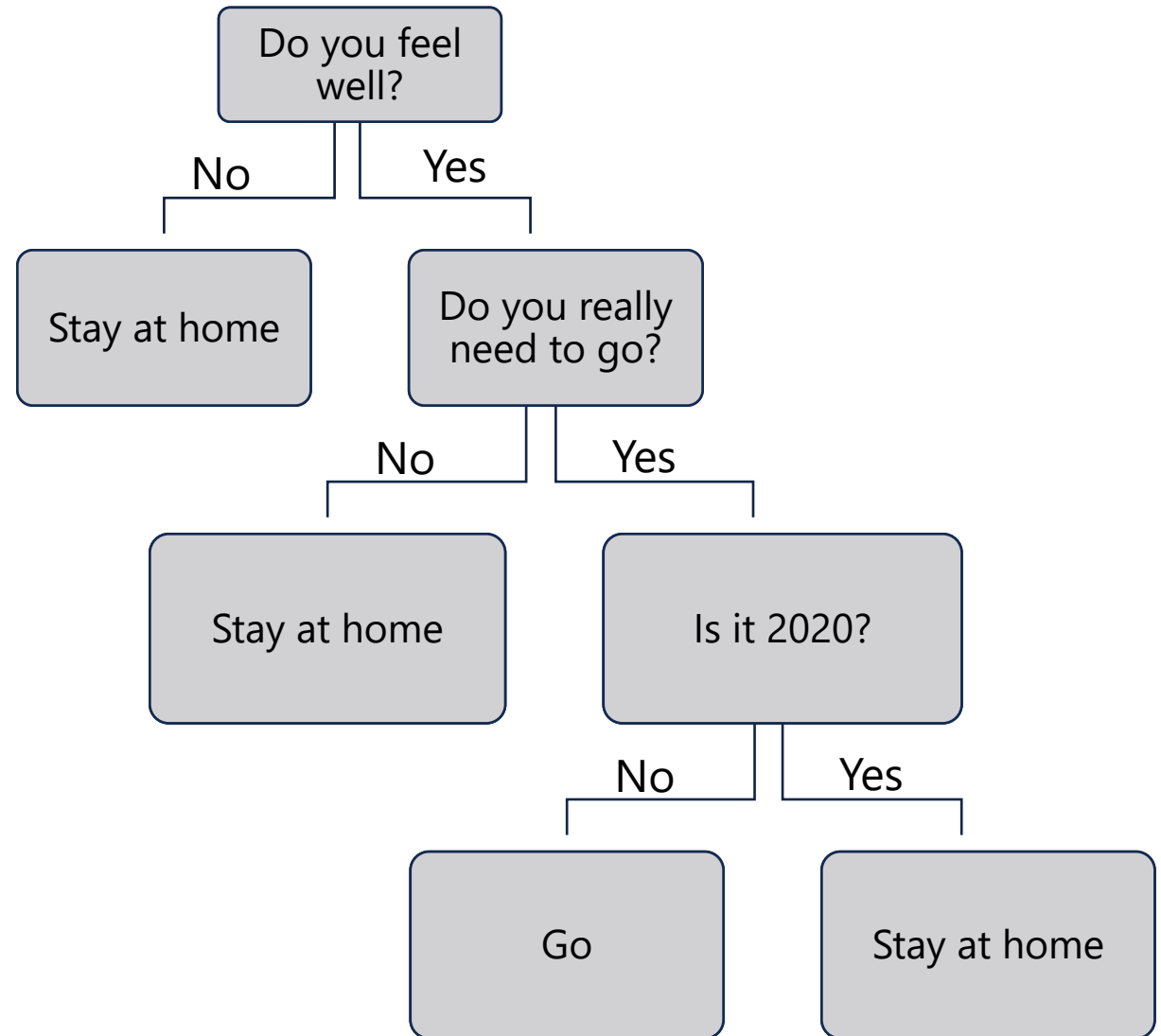
Directed graph

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Single root node

Each node has:

- either 0 child nodes (**terminal node**, "leaf")



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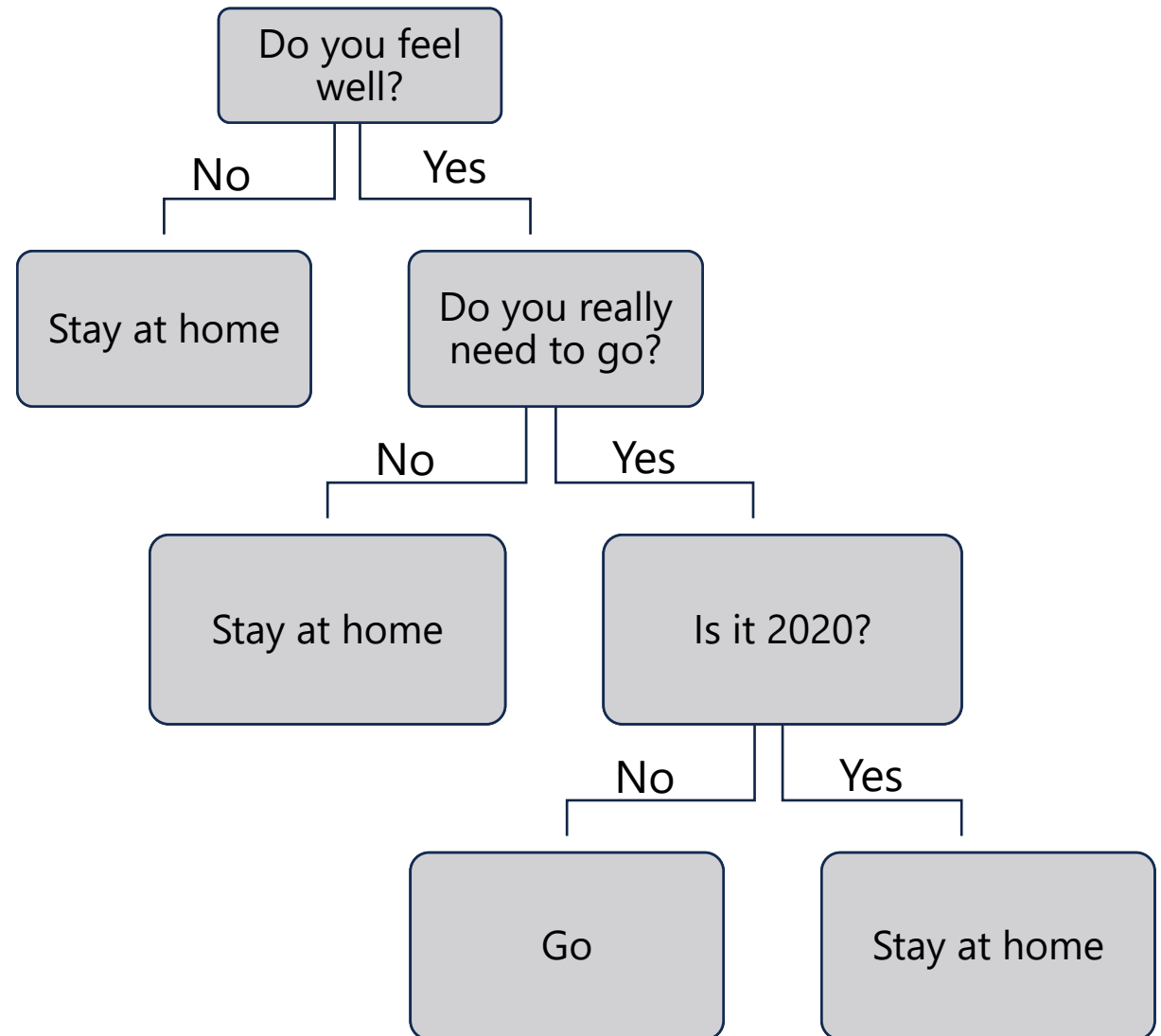
Directed graph

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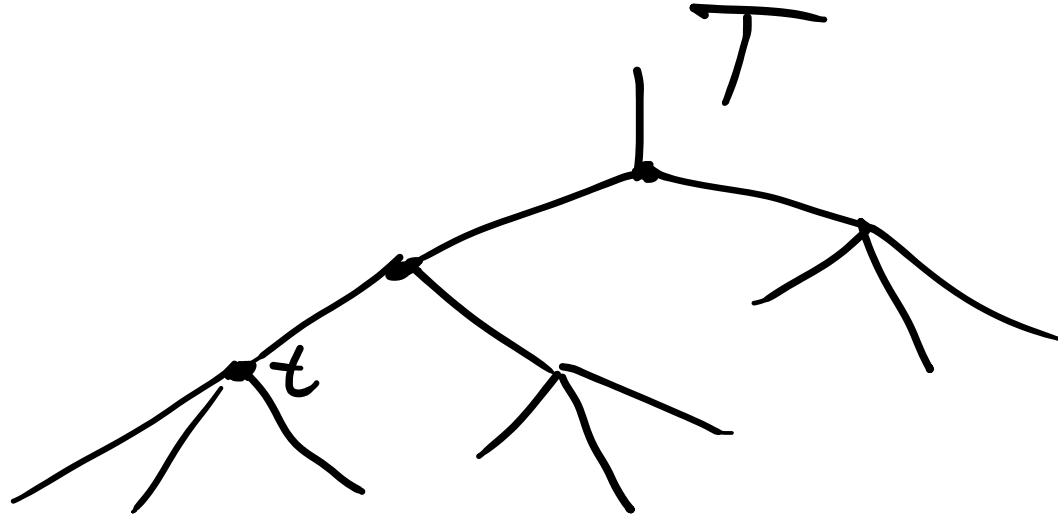
Single root node

Each node has:

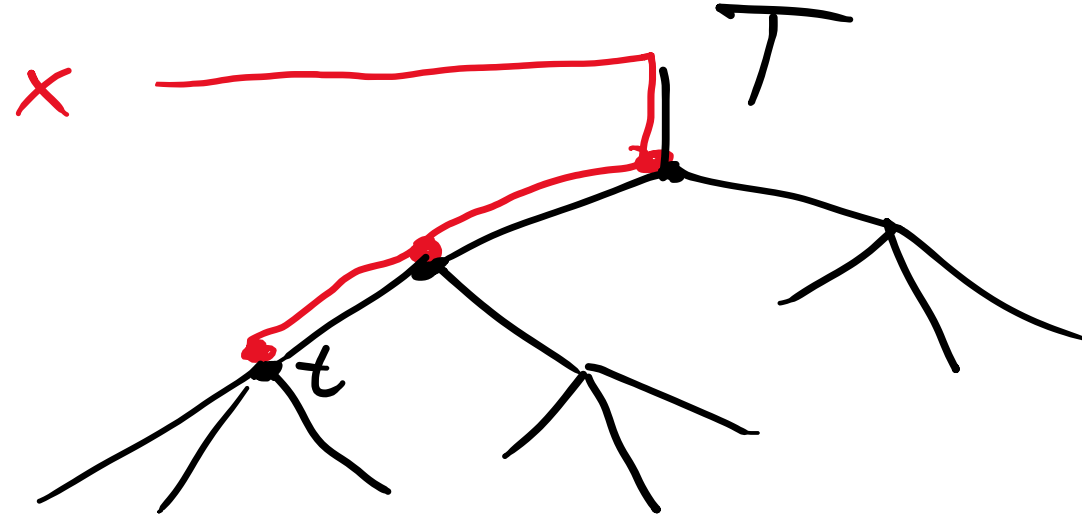
- either 0 child nodes (**terminal node**, "leaf")
- or ≥ 2 child nodes (**internal node**)
 - 2 nodes for binary trees



Defining a tree (general approach)



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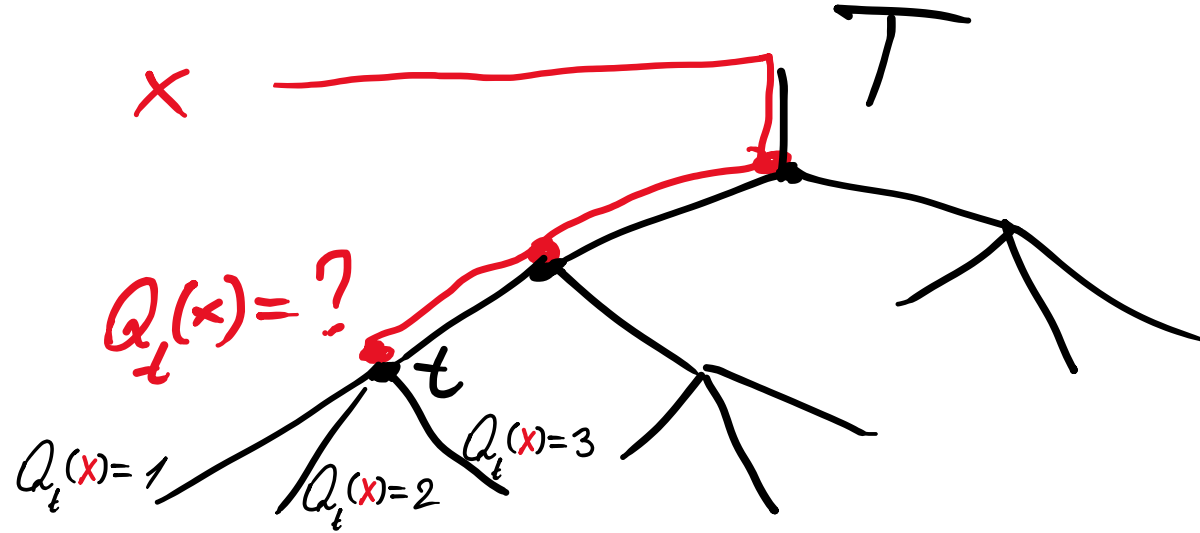


Defining a tree (general approach)



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

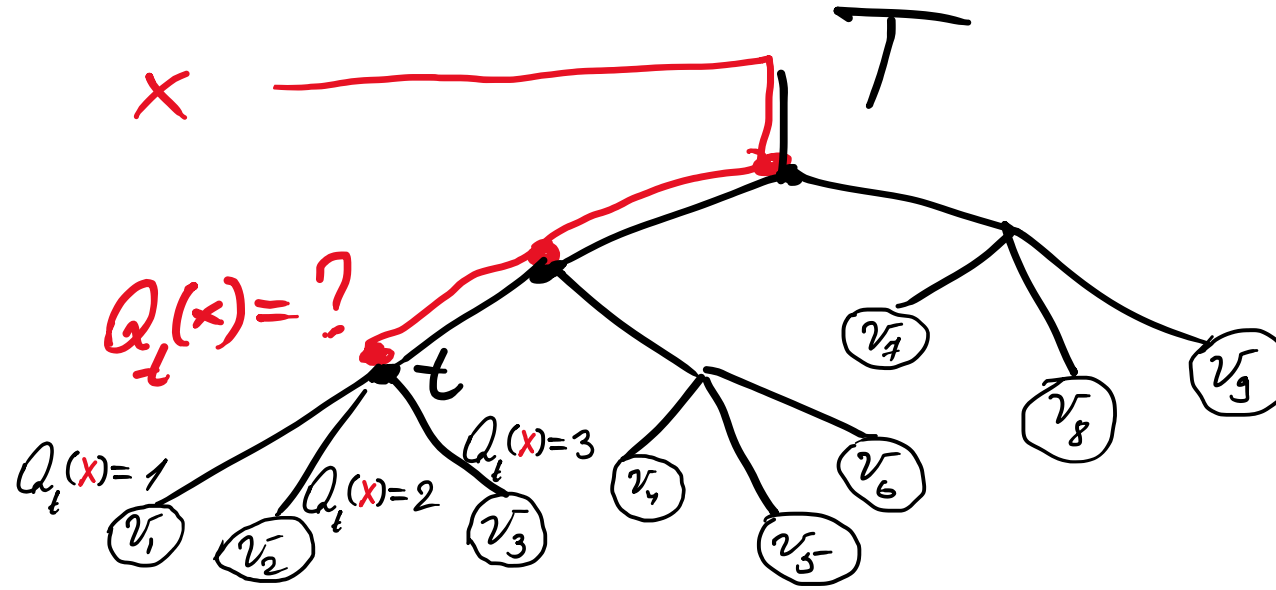
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Assign each terminal node i a prediction value v_i

Classification and Regression Trees (CART)



CART

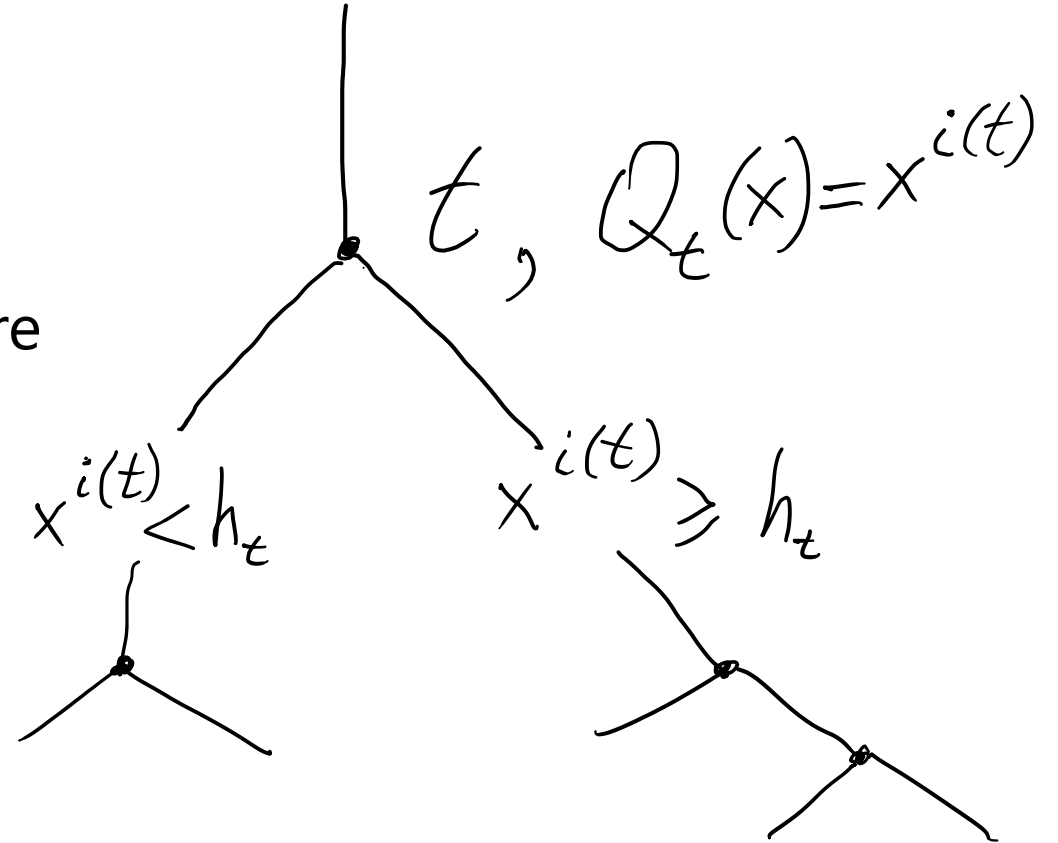
Binary trees

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: $D_{t_0} = D$



<https://pixabay.com/users/openclipart-vectors-30363/>

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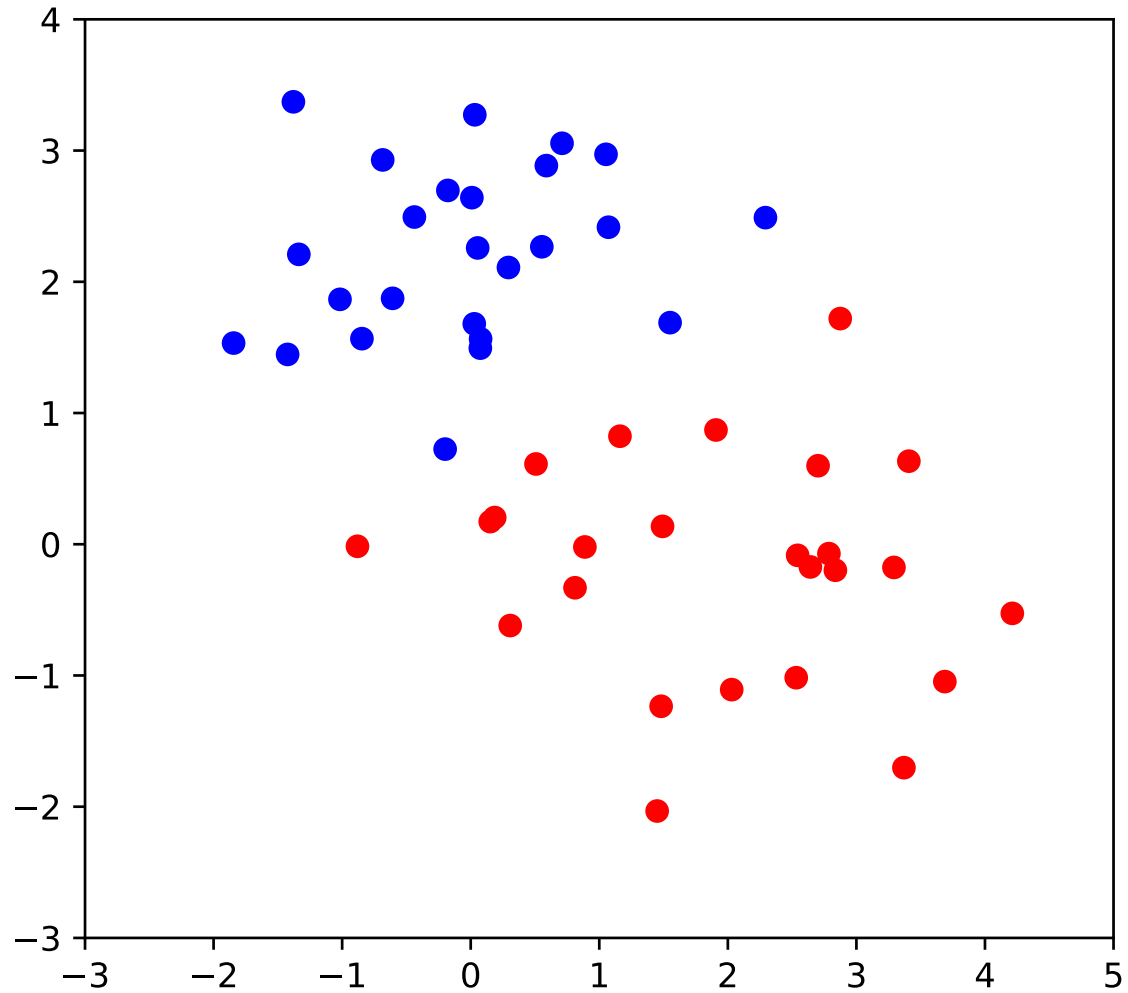
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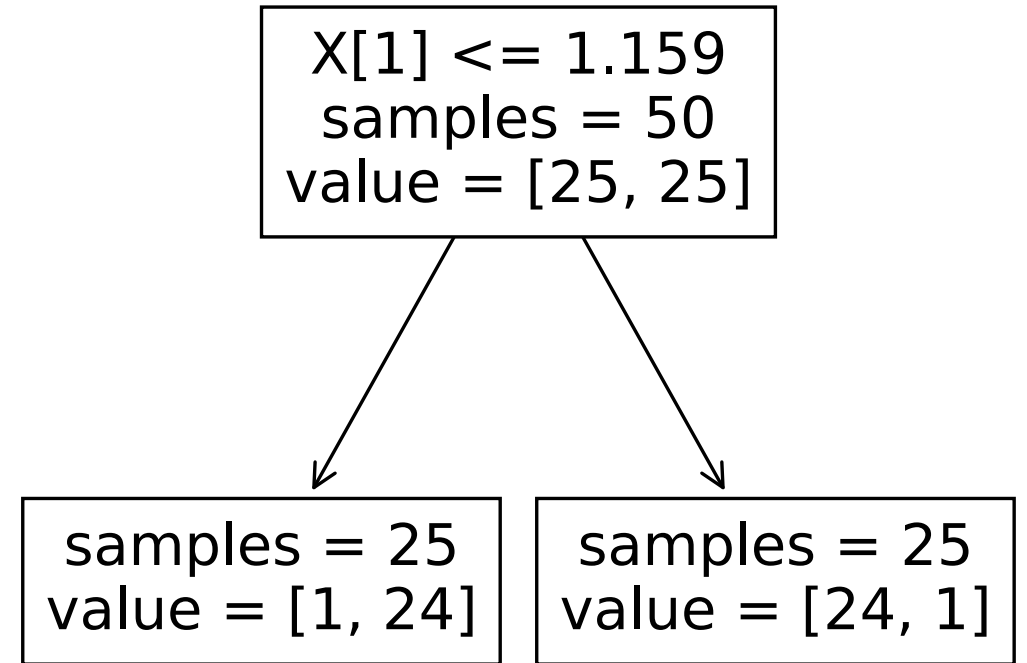
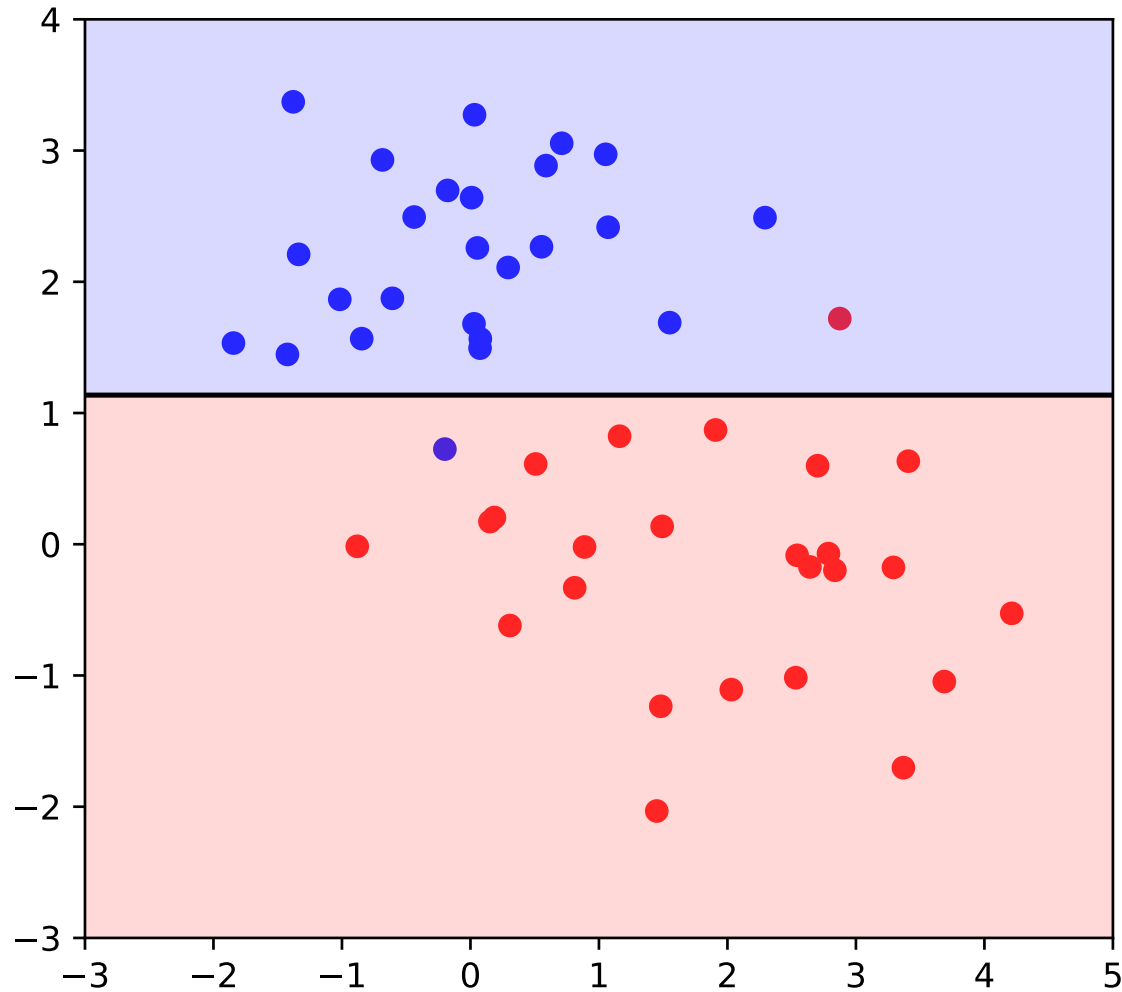
Set the check function $Q_t(x) = x^i$, and threshold $h_t = x_k^i$,
attach the two new corresponding child nodes t^{left} and t^{right} to t .



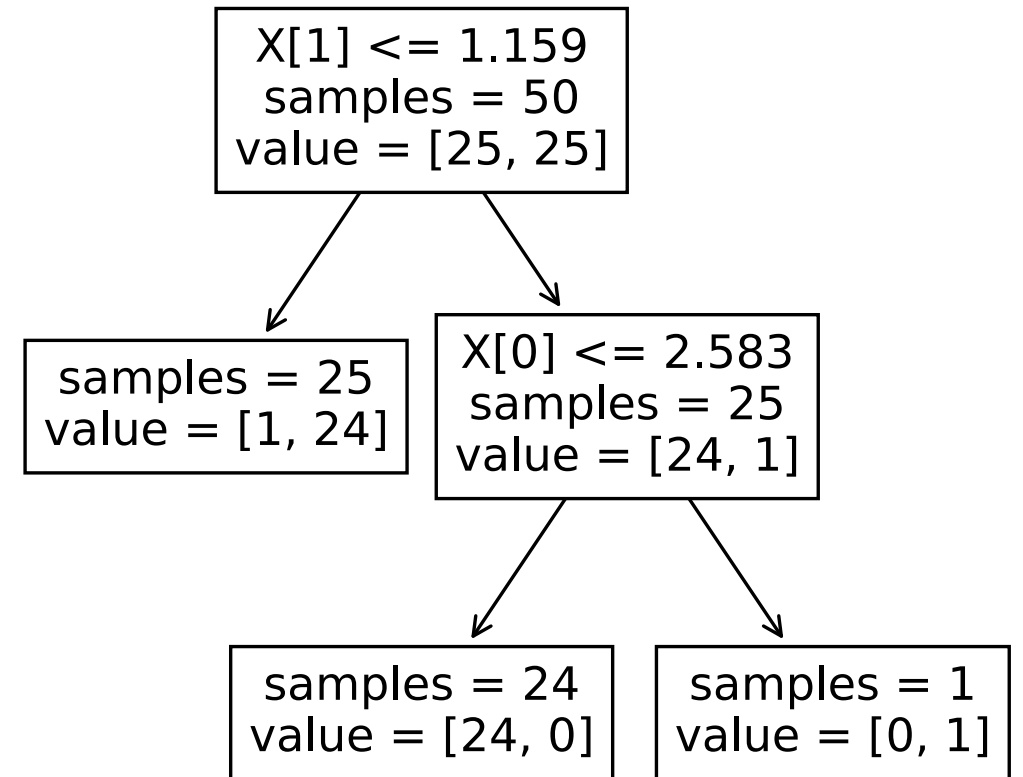
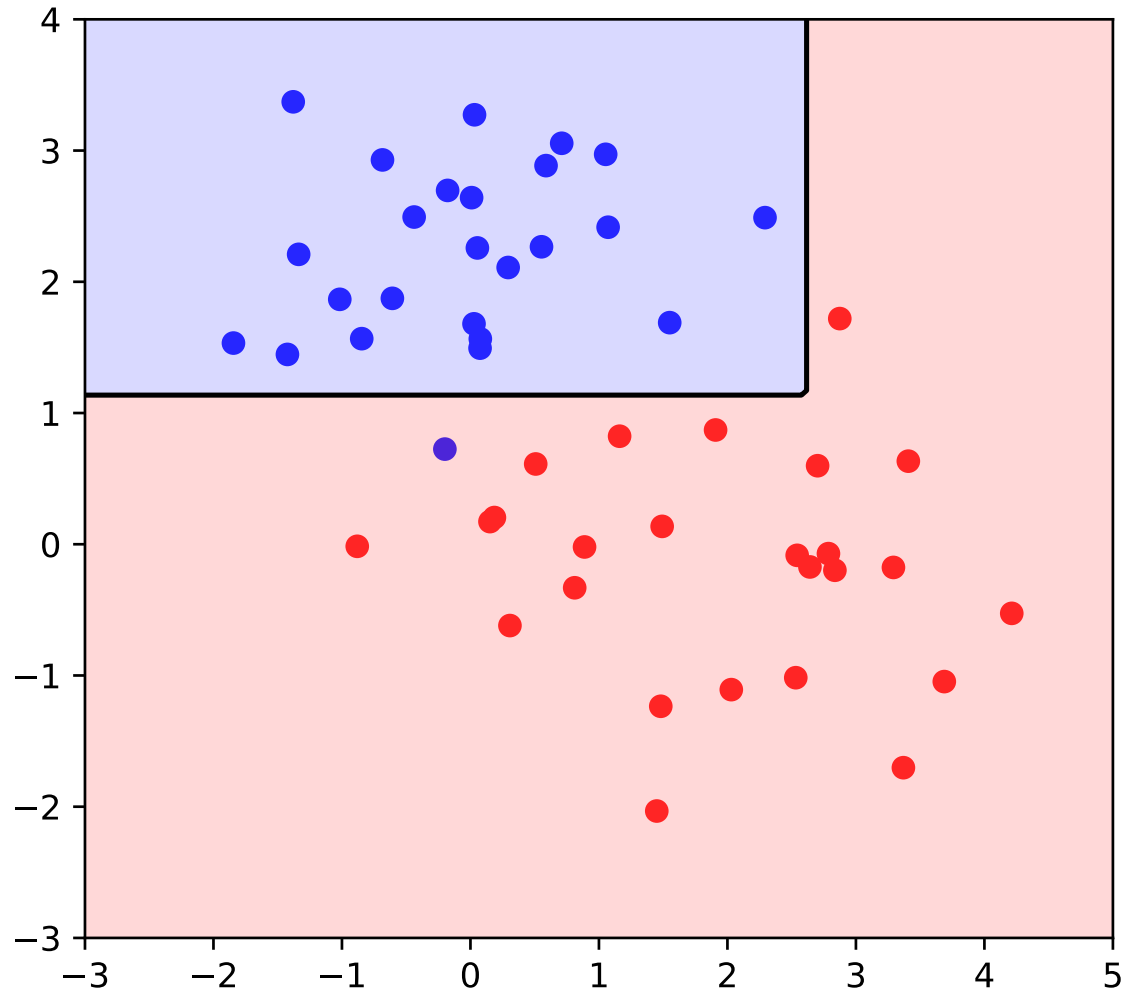
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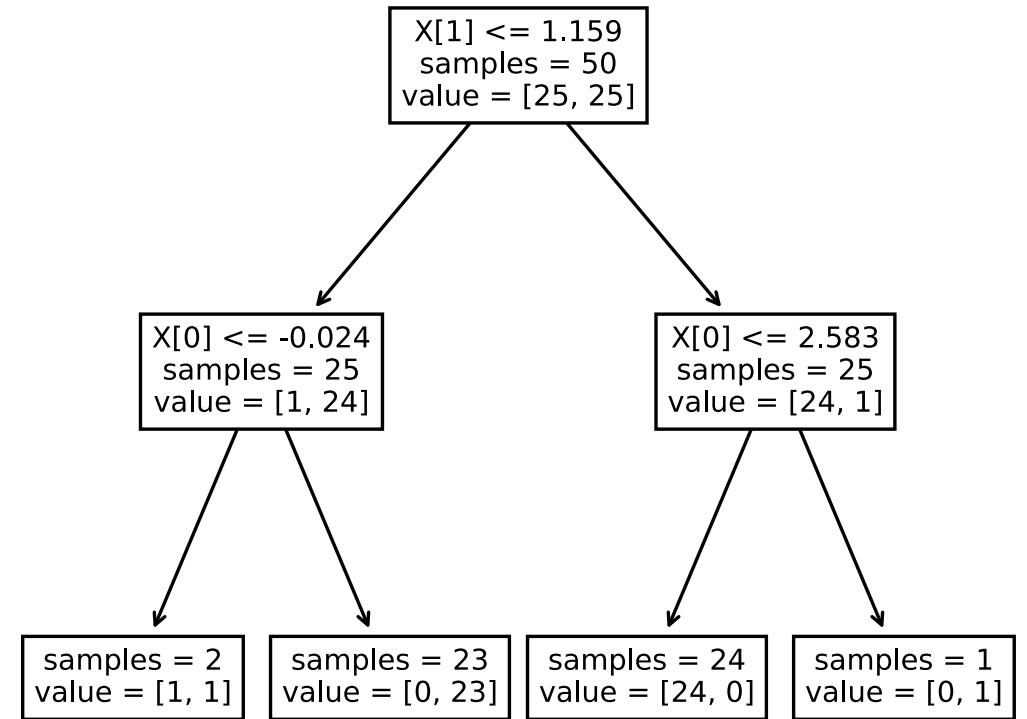
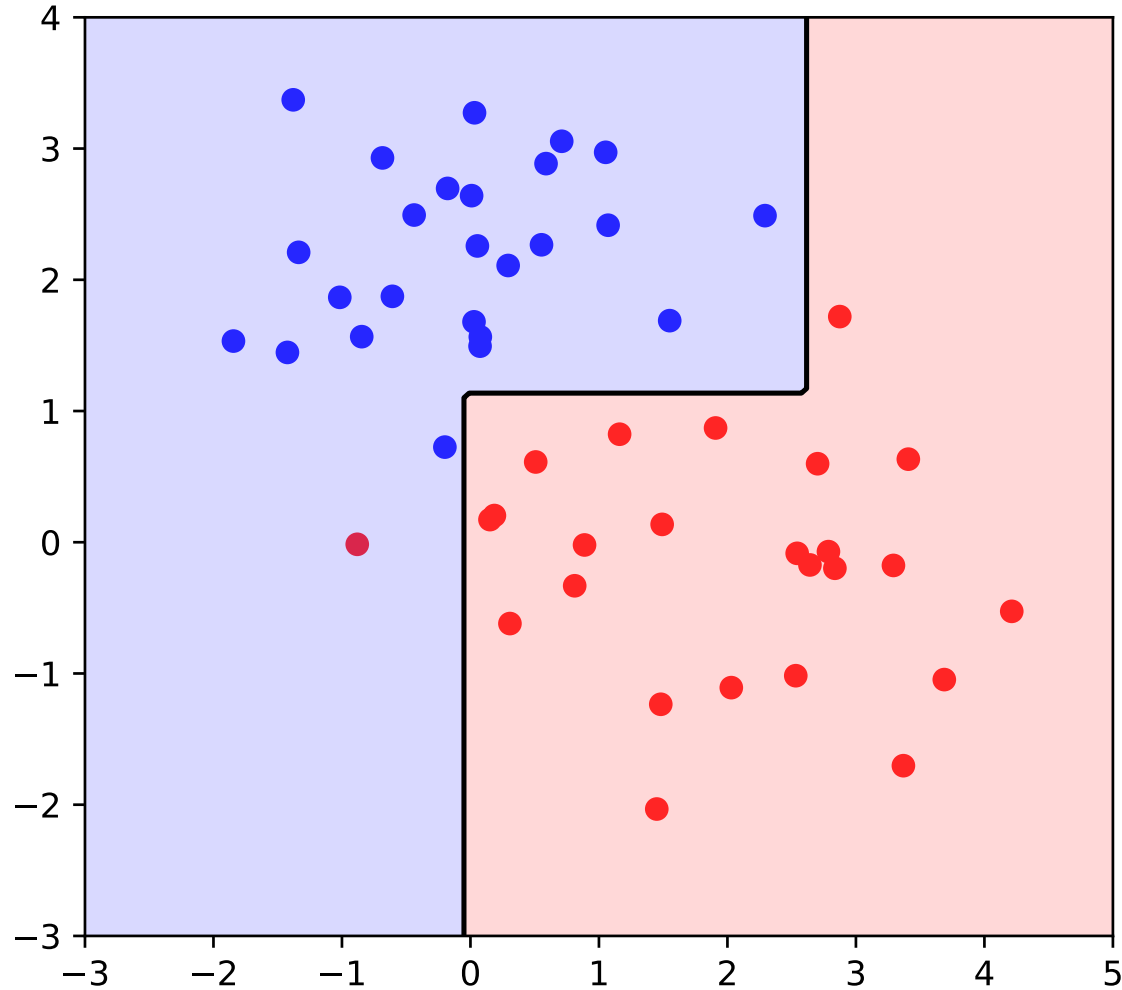
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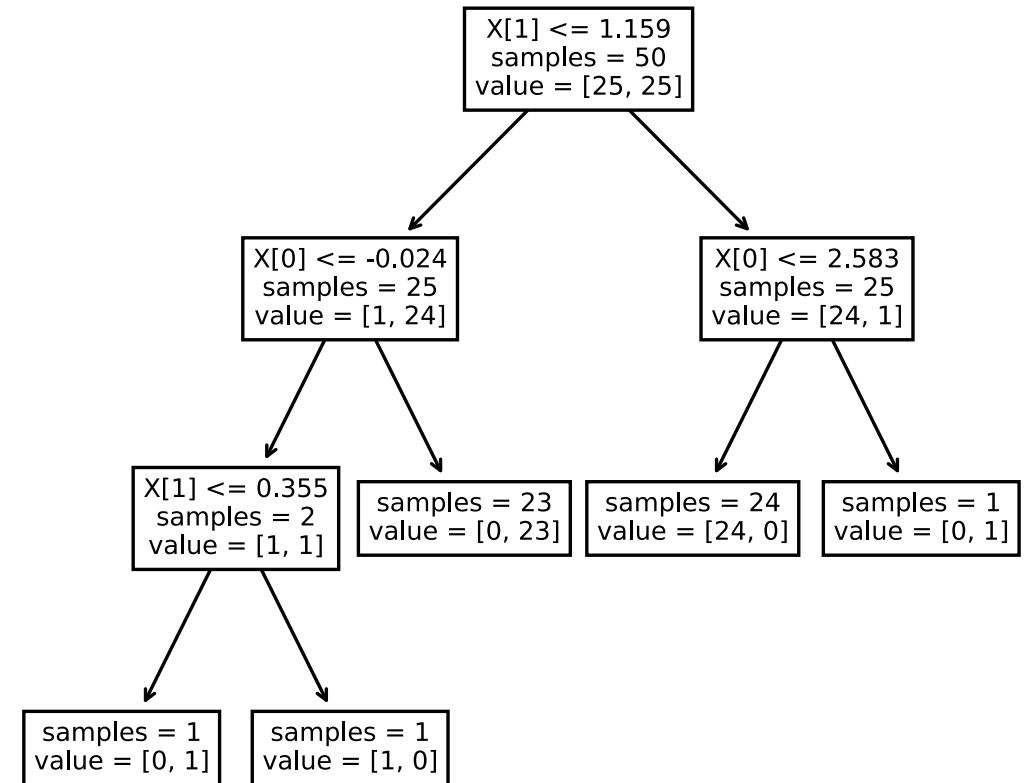
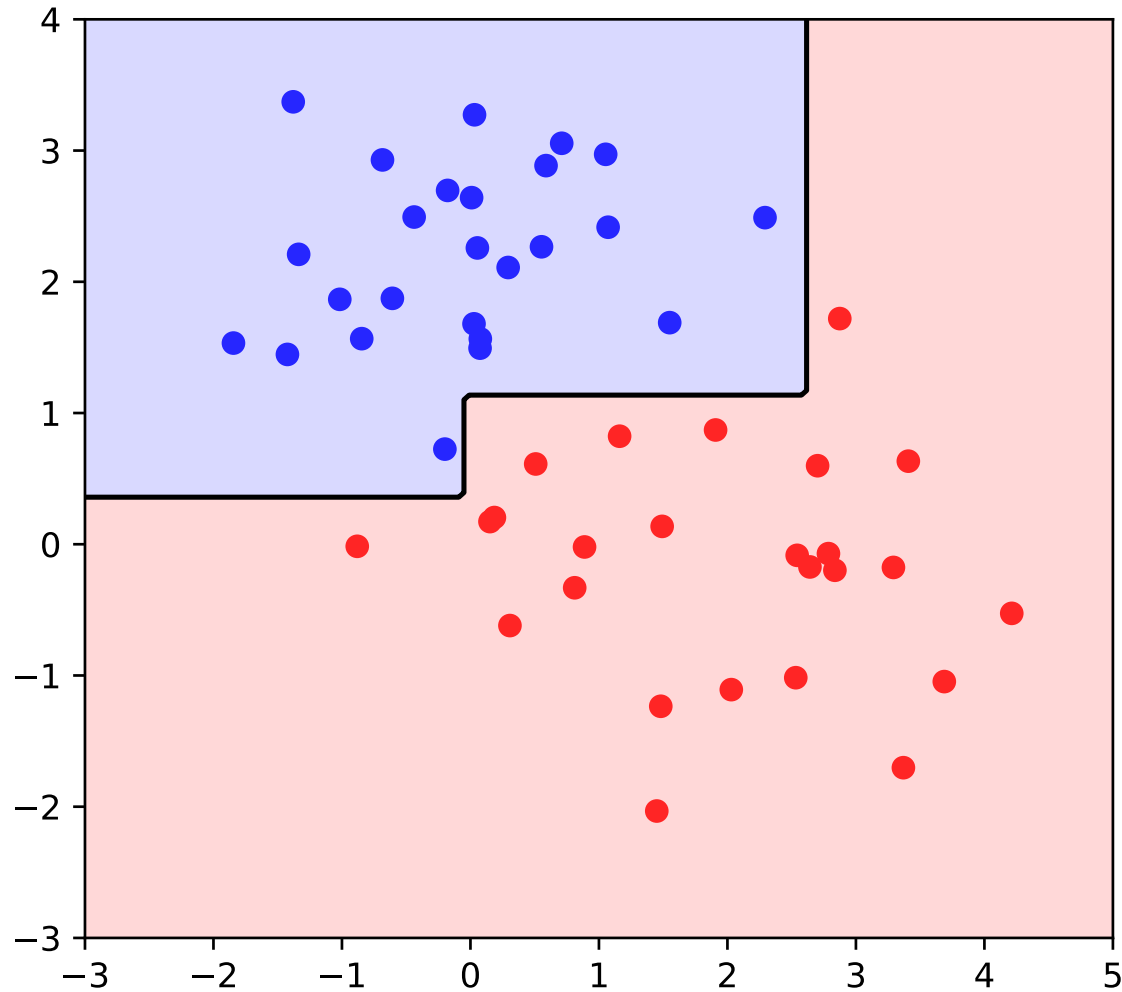
Growing a tree



Growing a tree



Growing a tree



Impurity measures

Regression

MSE:

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

mean target



MAE:

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

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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- ϕ is defined for $p_j \geq 0$ and $\sum_j p_j = 1$
- ϕ is maximized when all $p_j = 1/C$
- 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

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

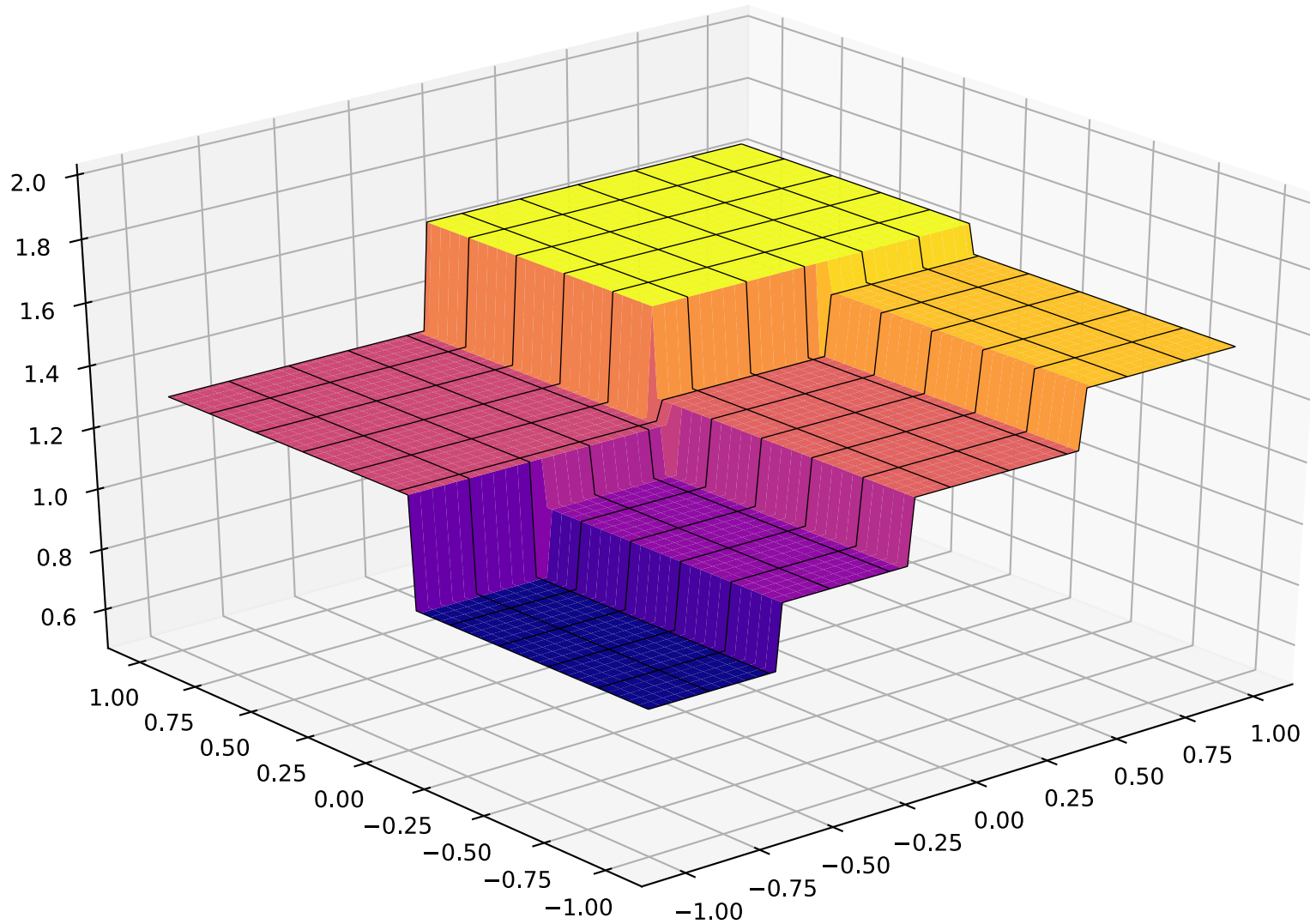
Minimum impurity gain

You name it...

Solution properties



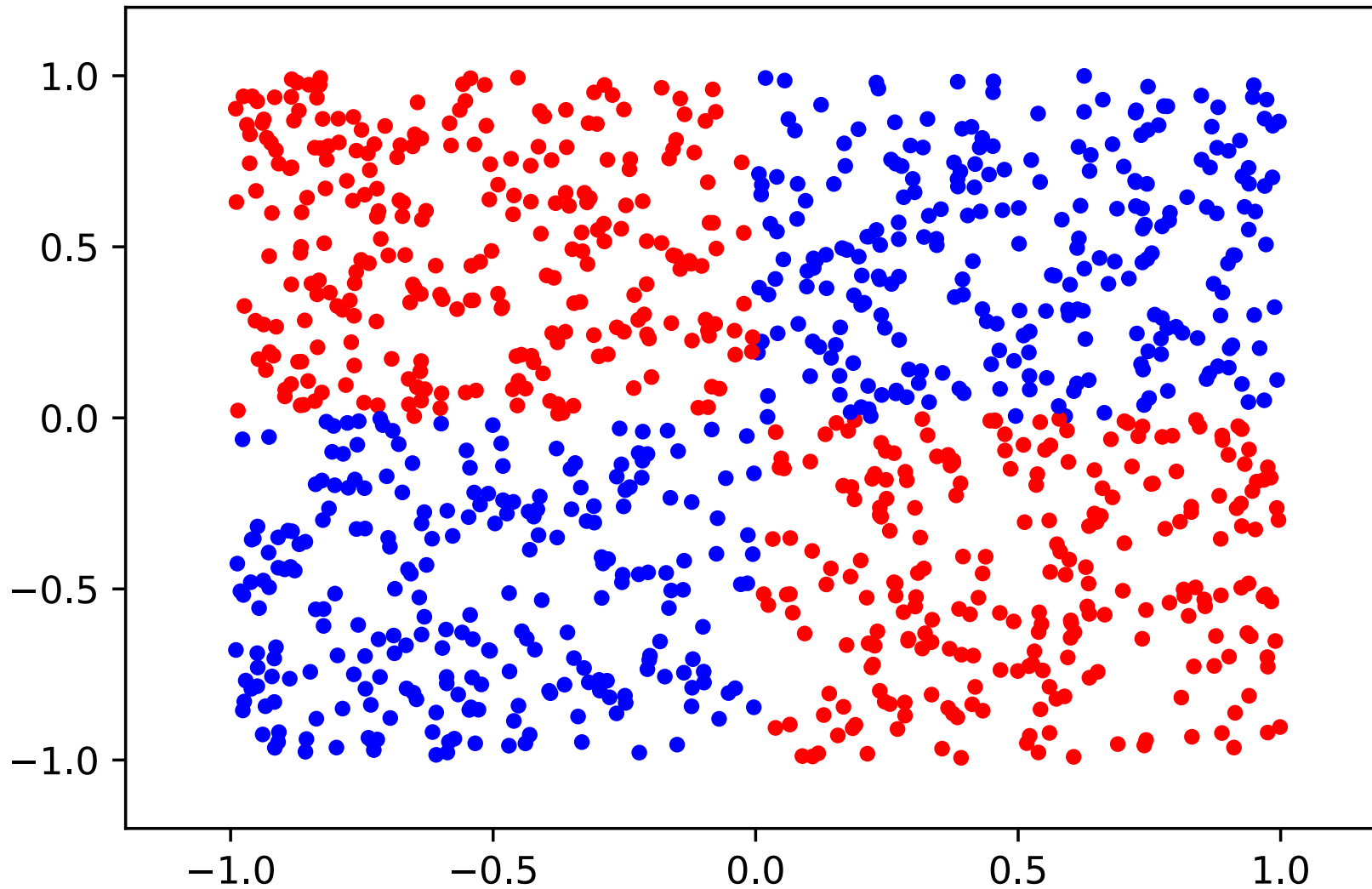
Prediction function



Decision boundaries
always **orthogonal to
feature axes**

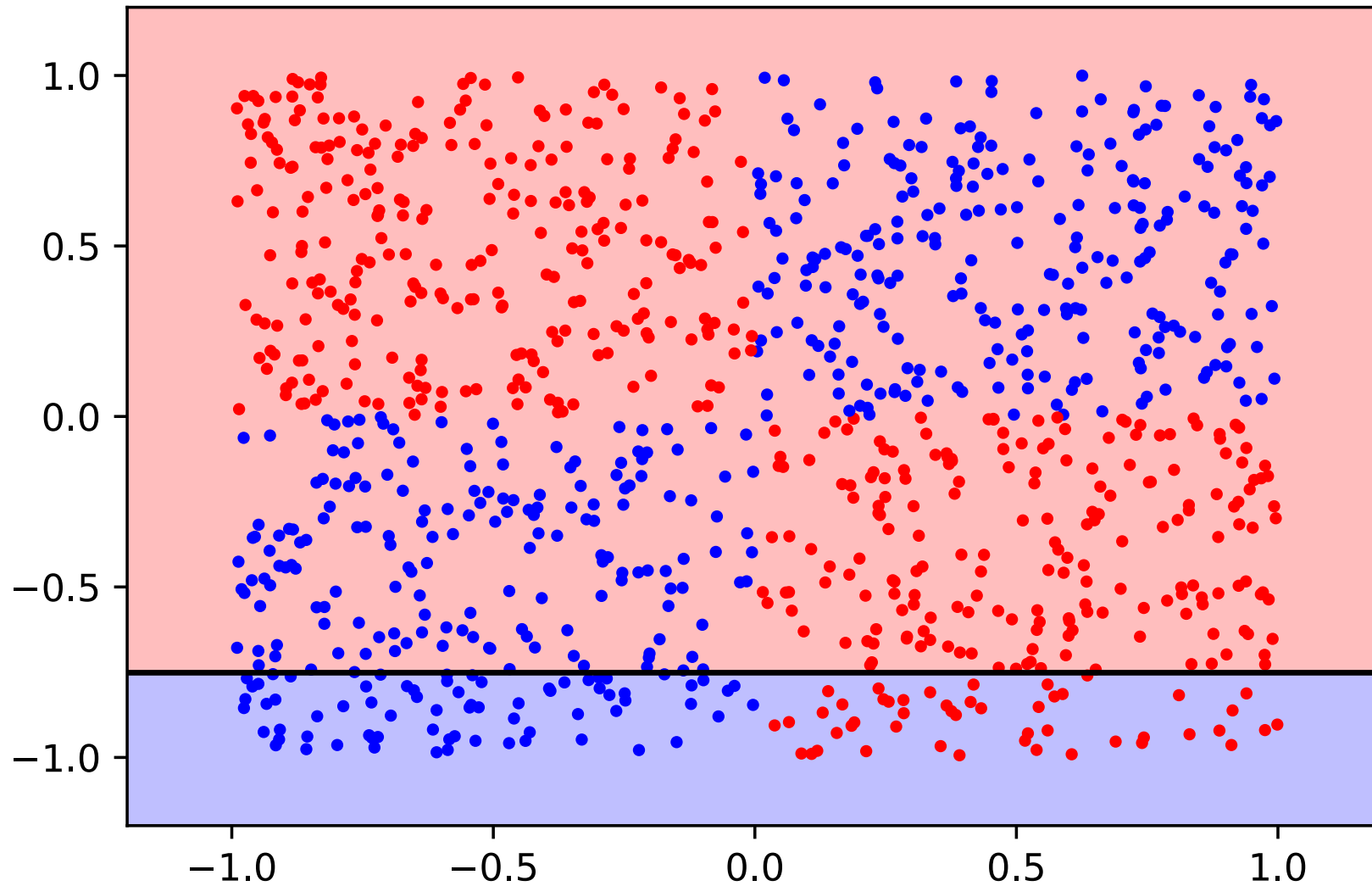
Resulting function is a
piecewise constant

XOR example



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

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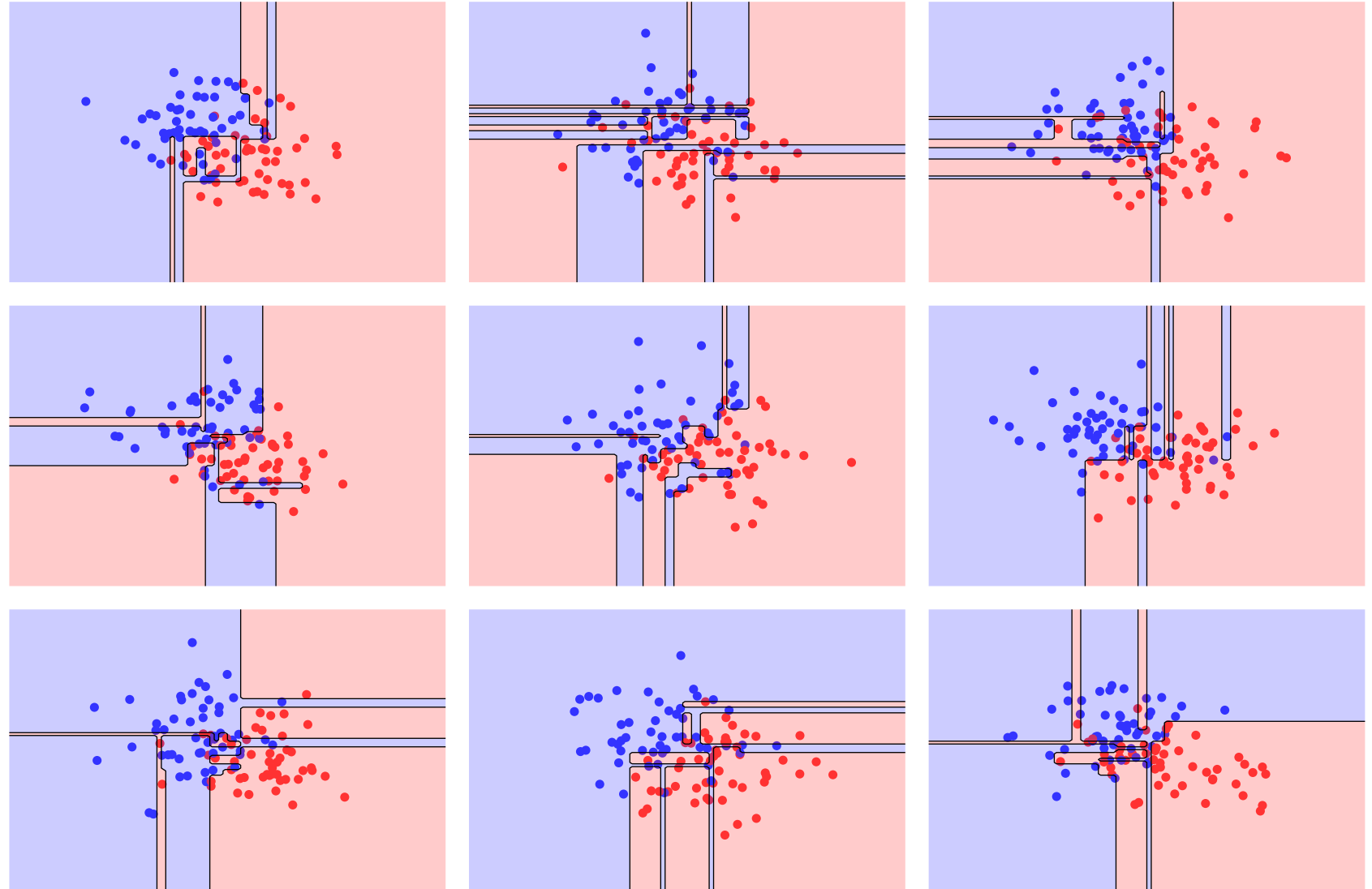


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High Variance

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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