Decision Trees

Classification and Regression Trees, impurity functions, solution properties

Machine Learning and Data Mining, 2025

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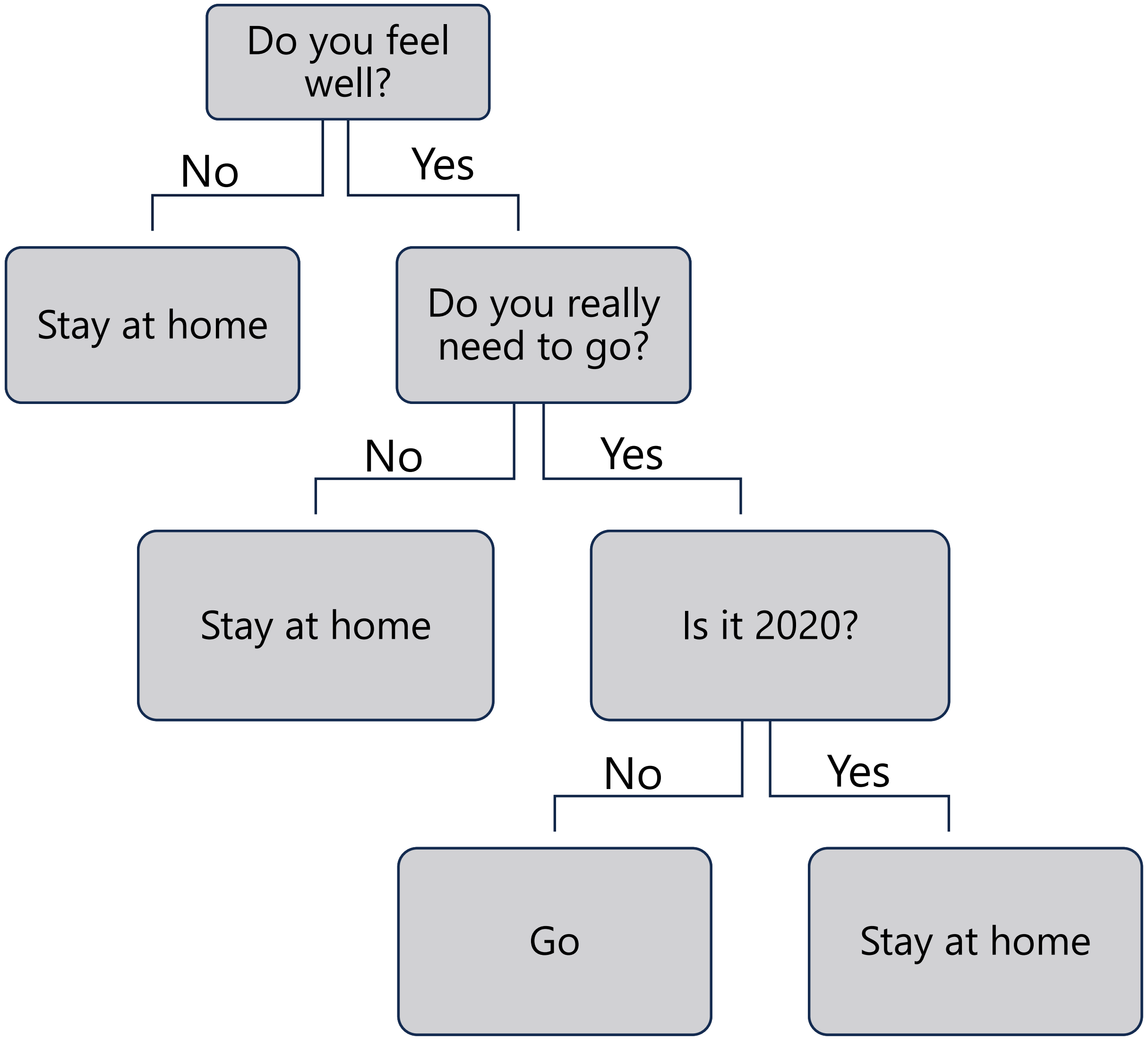
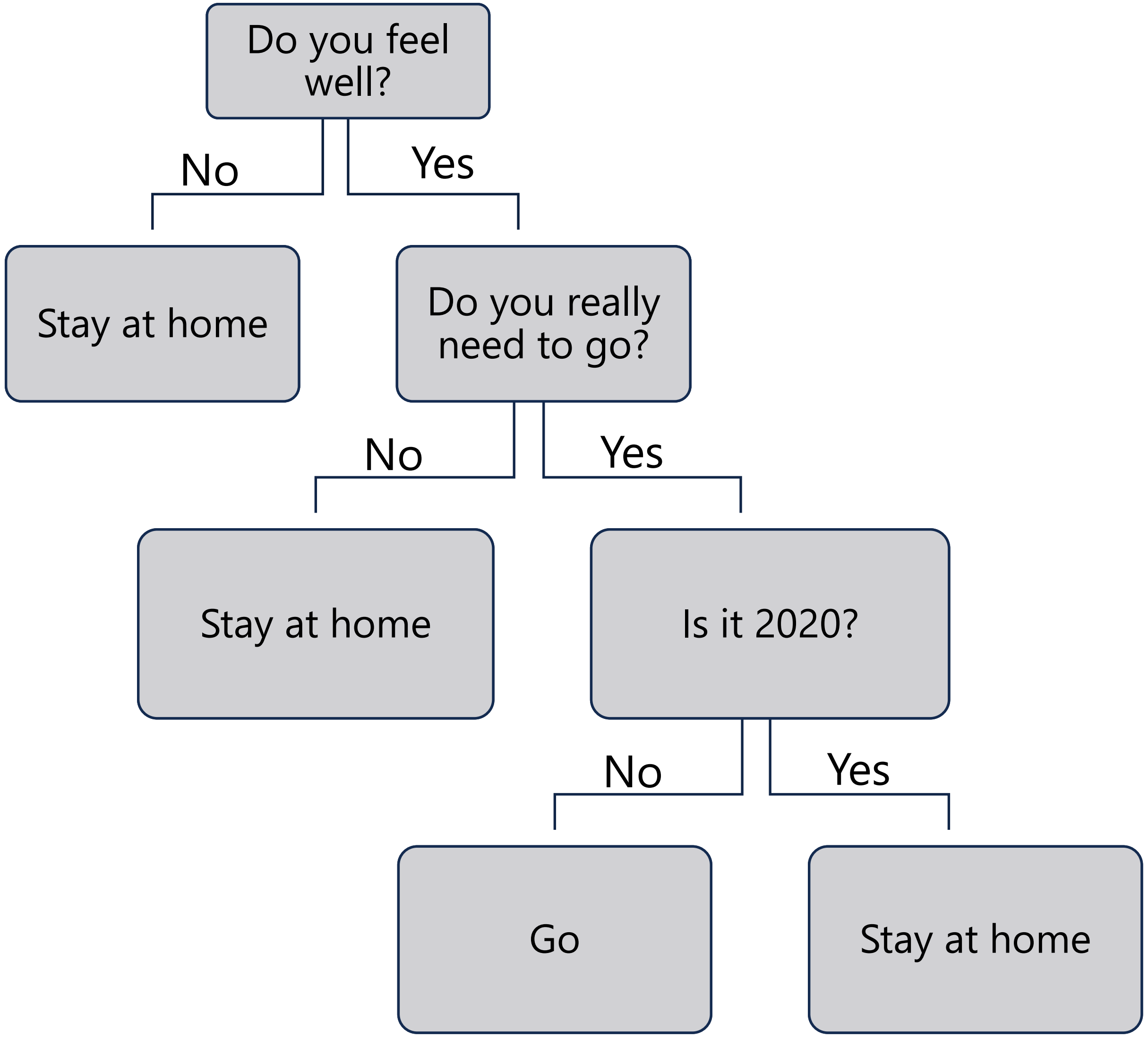
Basics

“Should you go to work?” chart



“Should you go to work?” chart

Directed graph



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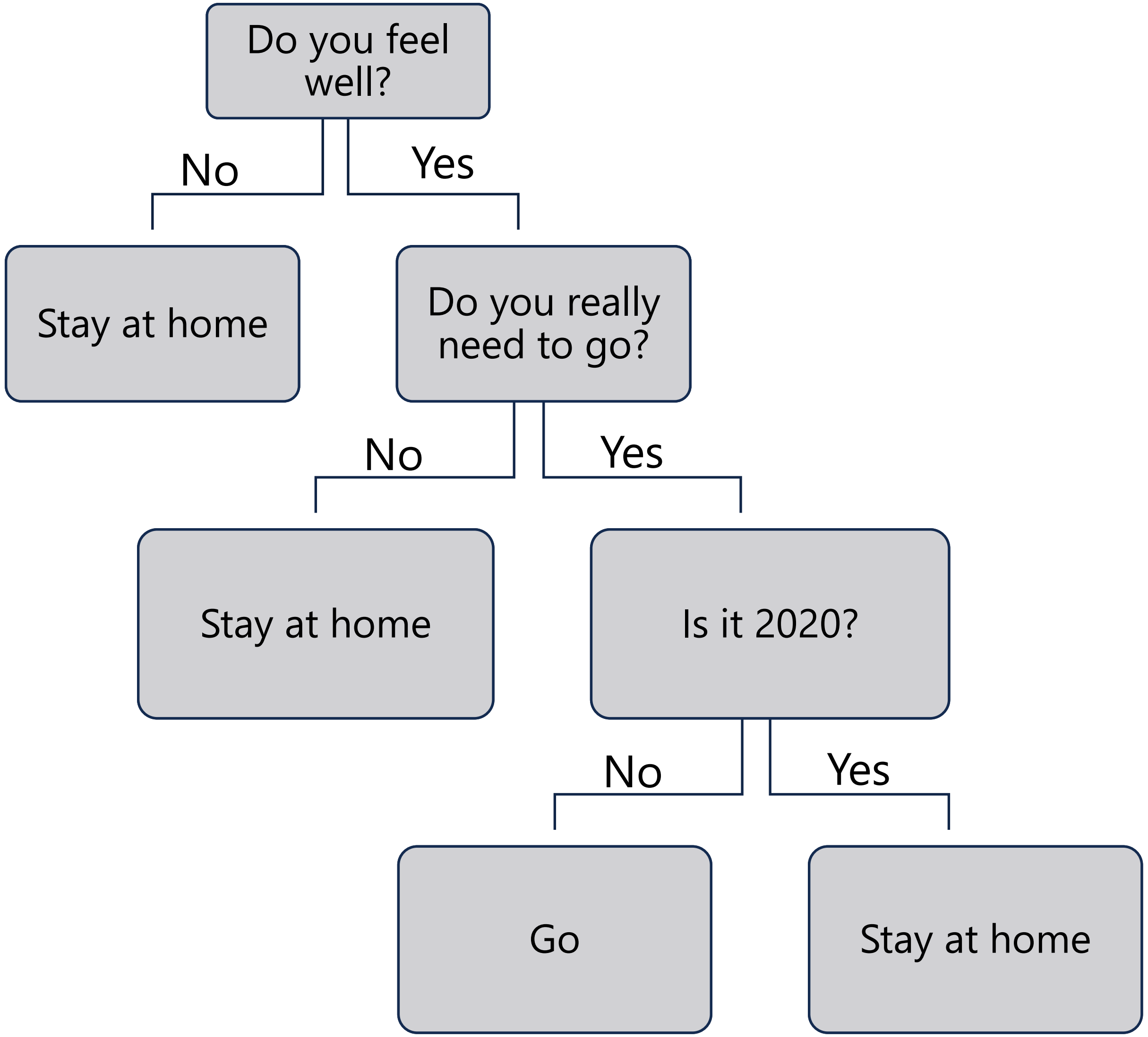
Directed graph

No loops



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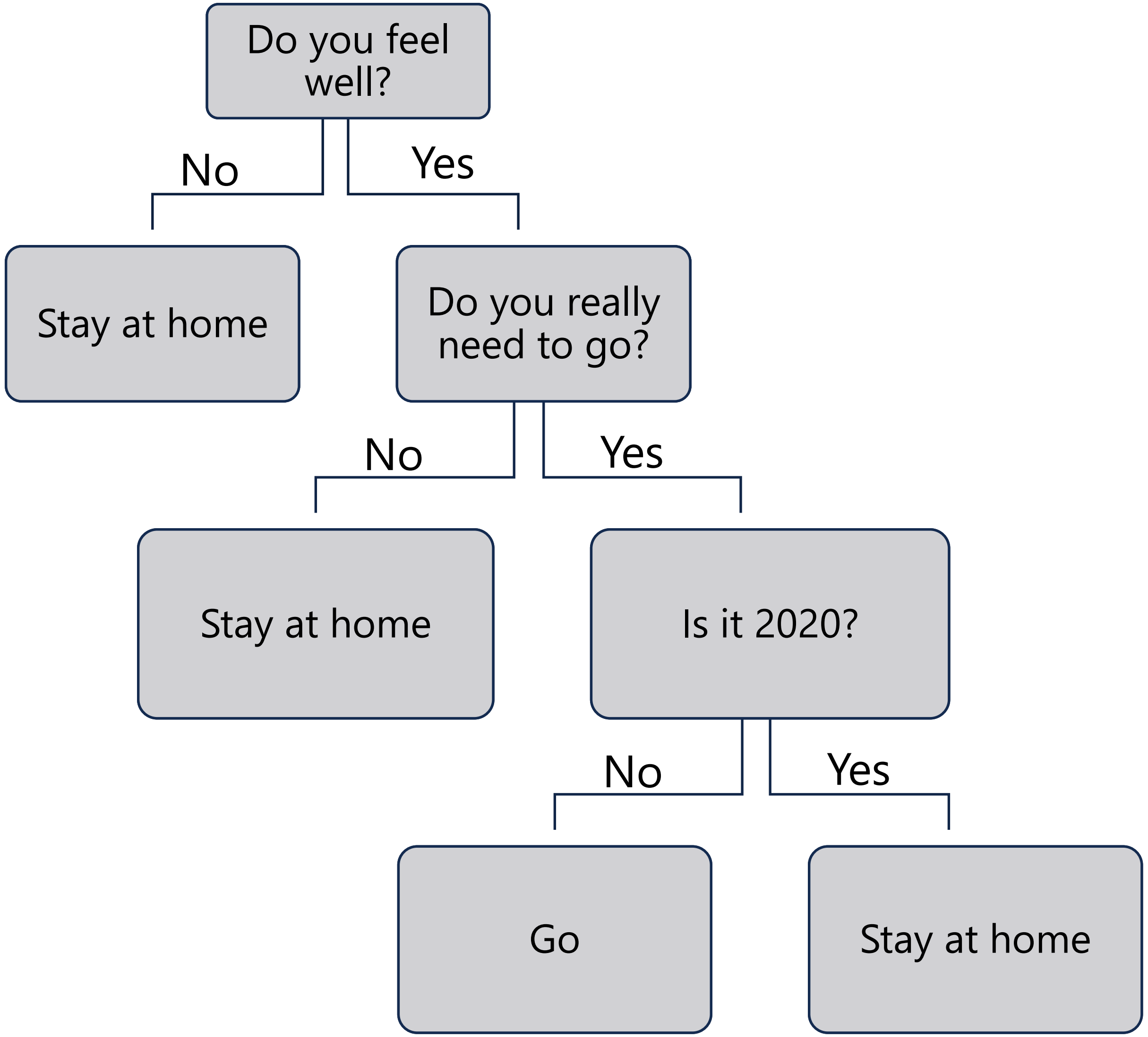
No loops

Single root node



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Directed graph

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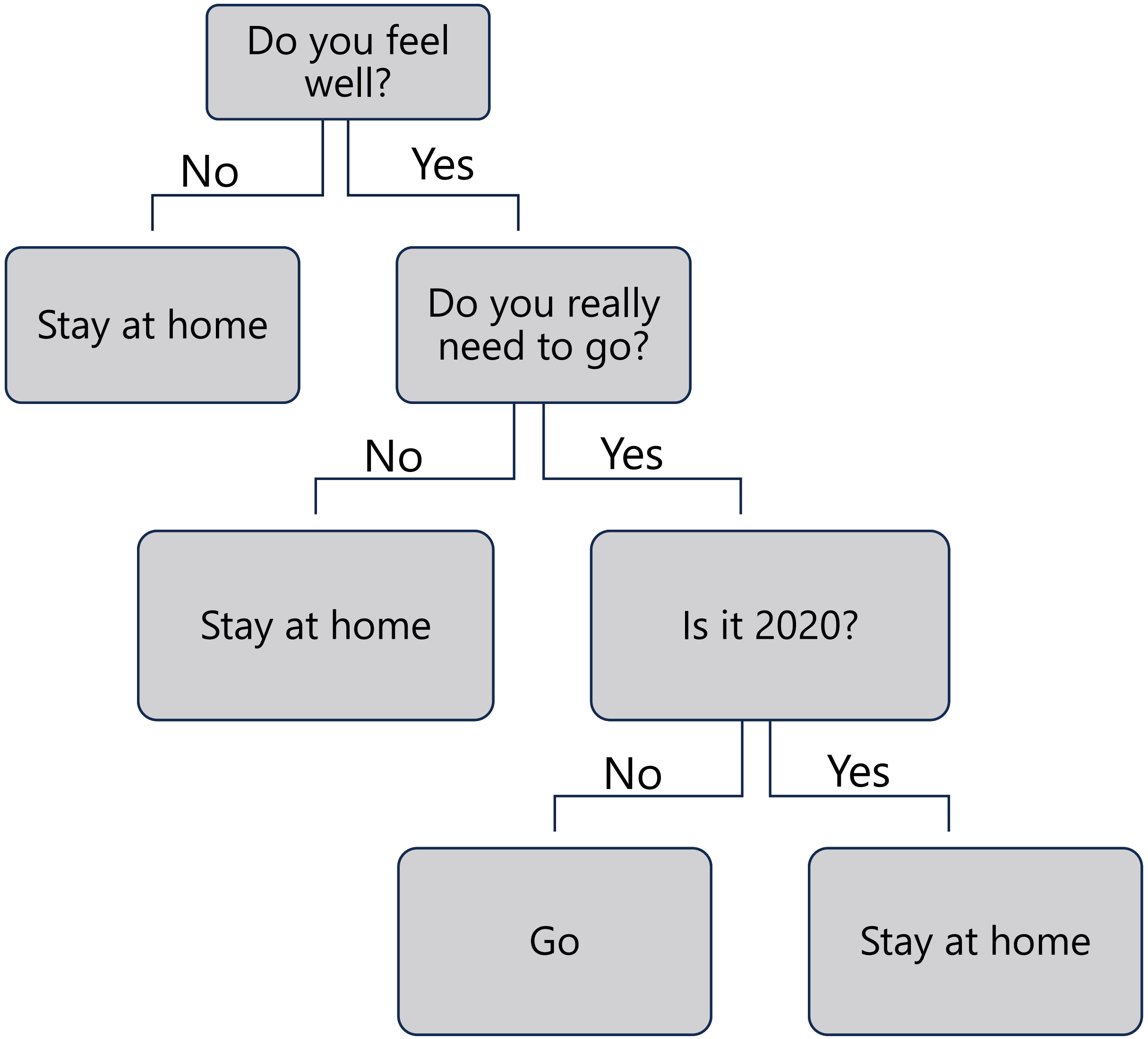
Single root node

Each node has:

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



“Should you go to work?” chart

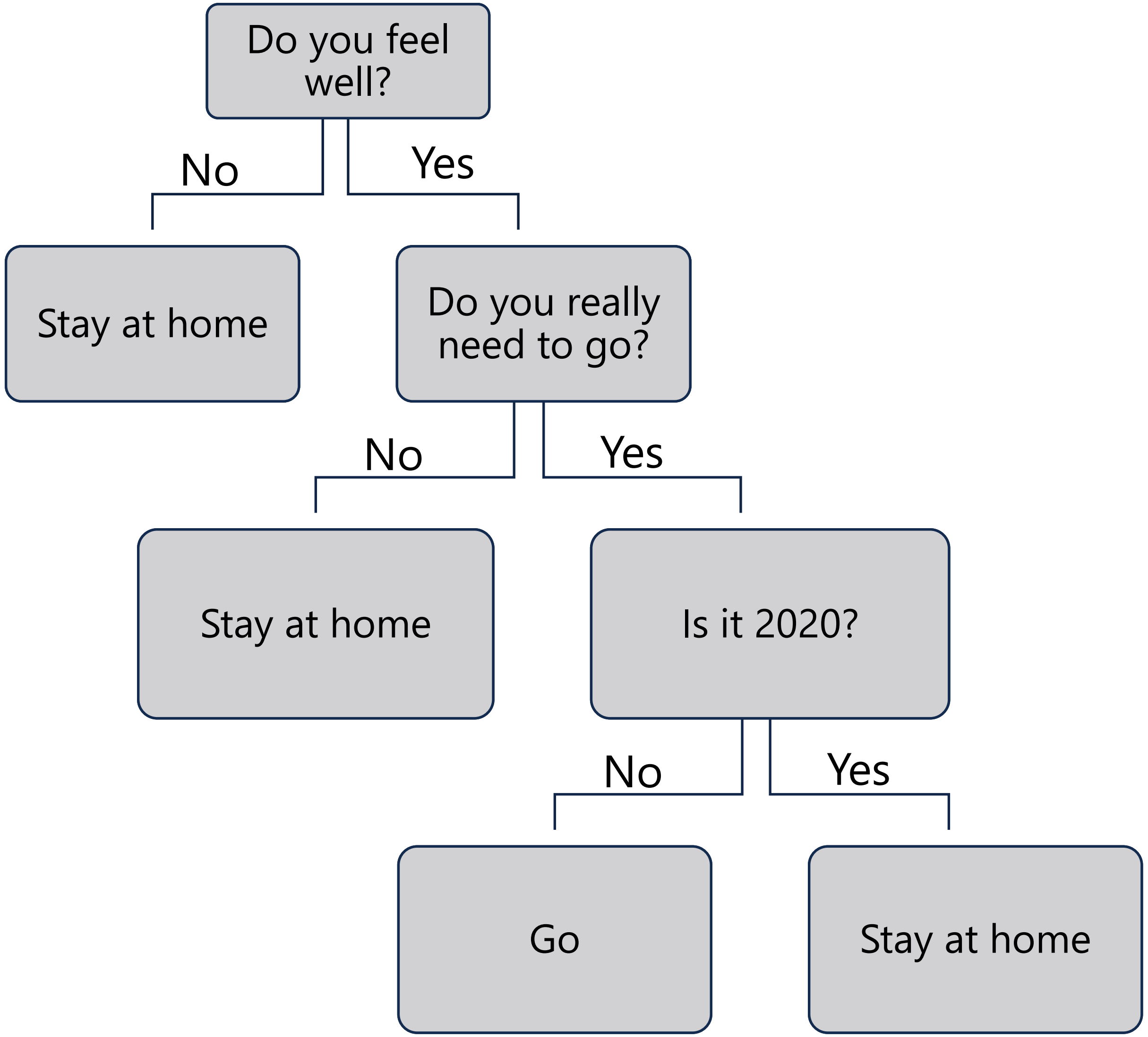
Directed graph

No loops

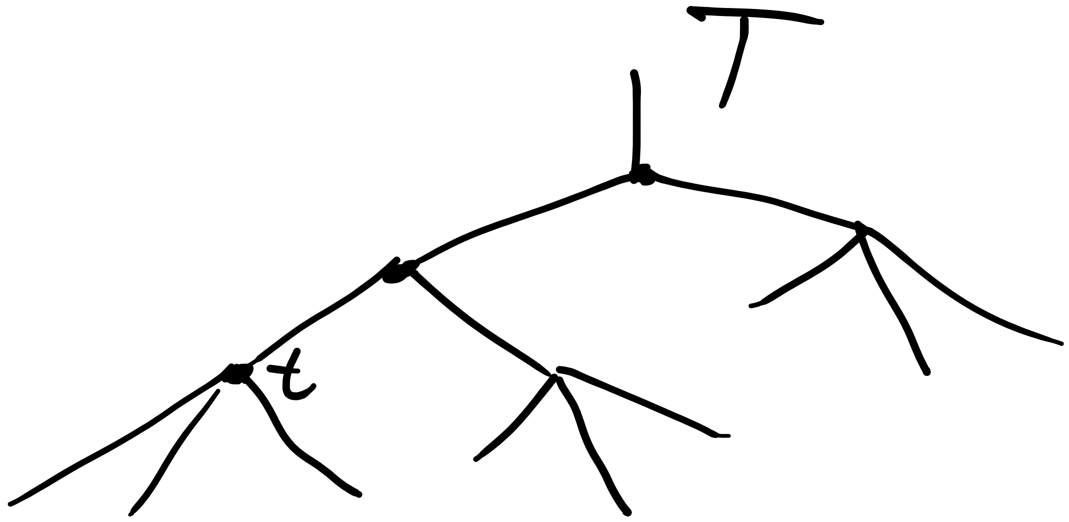
Single root node

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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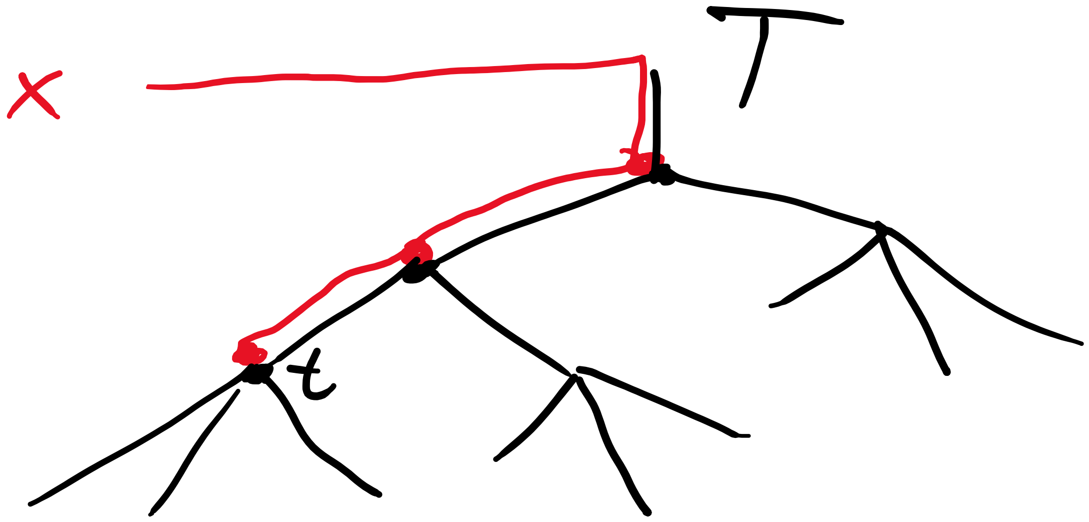

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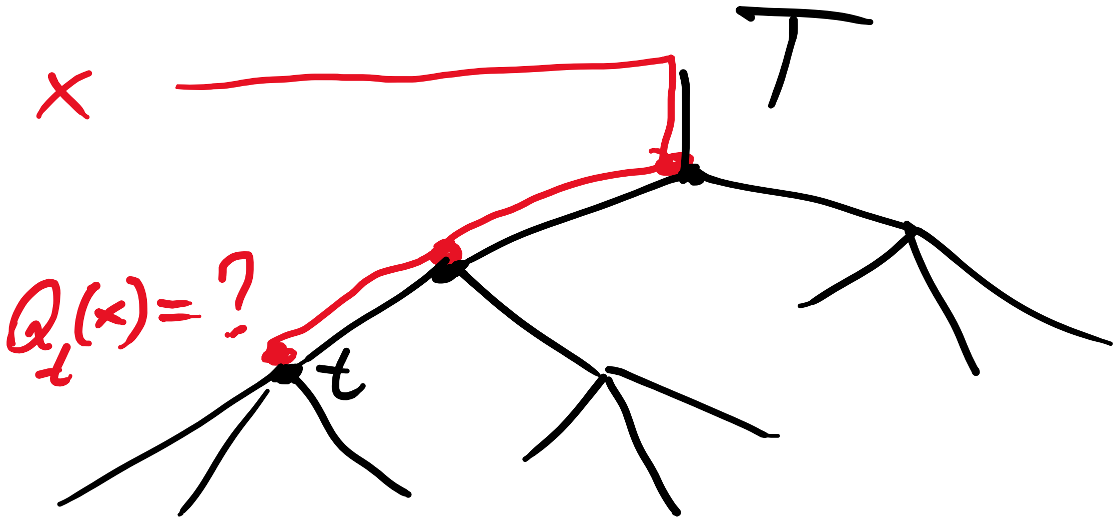

For each node $t \in T$ define a check function $Q_t(x)$

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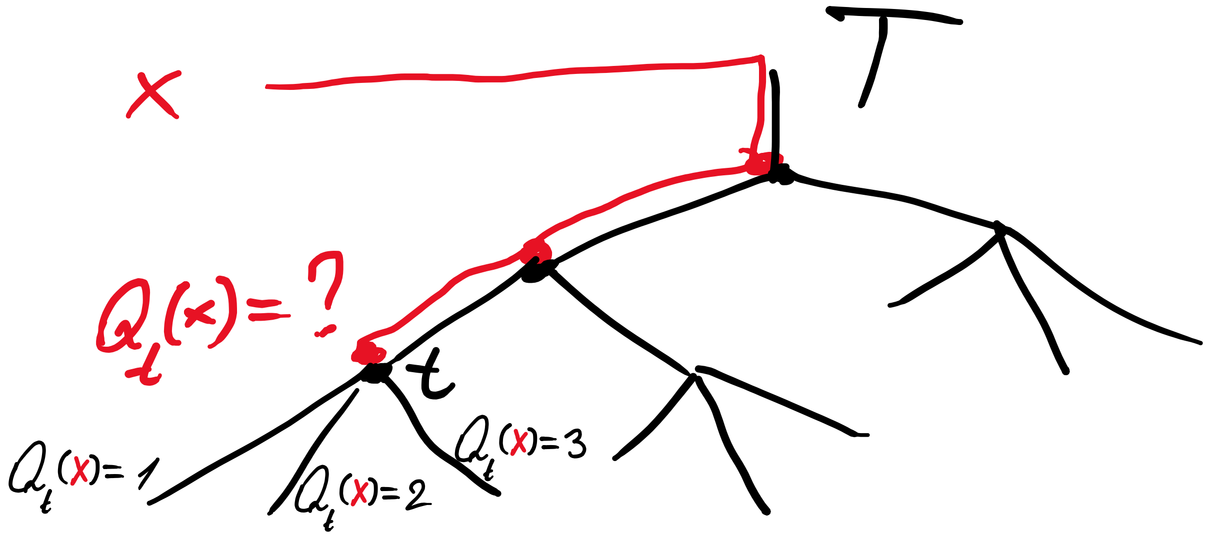

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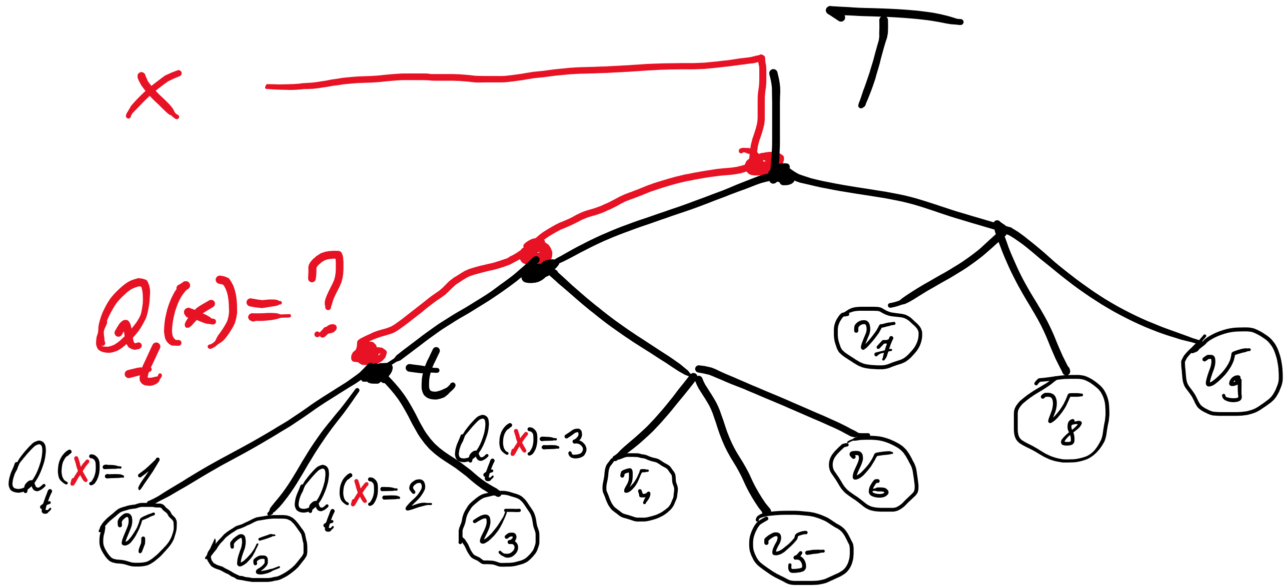
For each child node of t assign a set of unique values of $Q_t(x)$

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

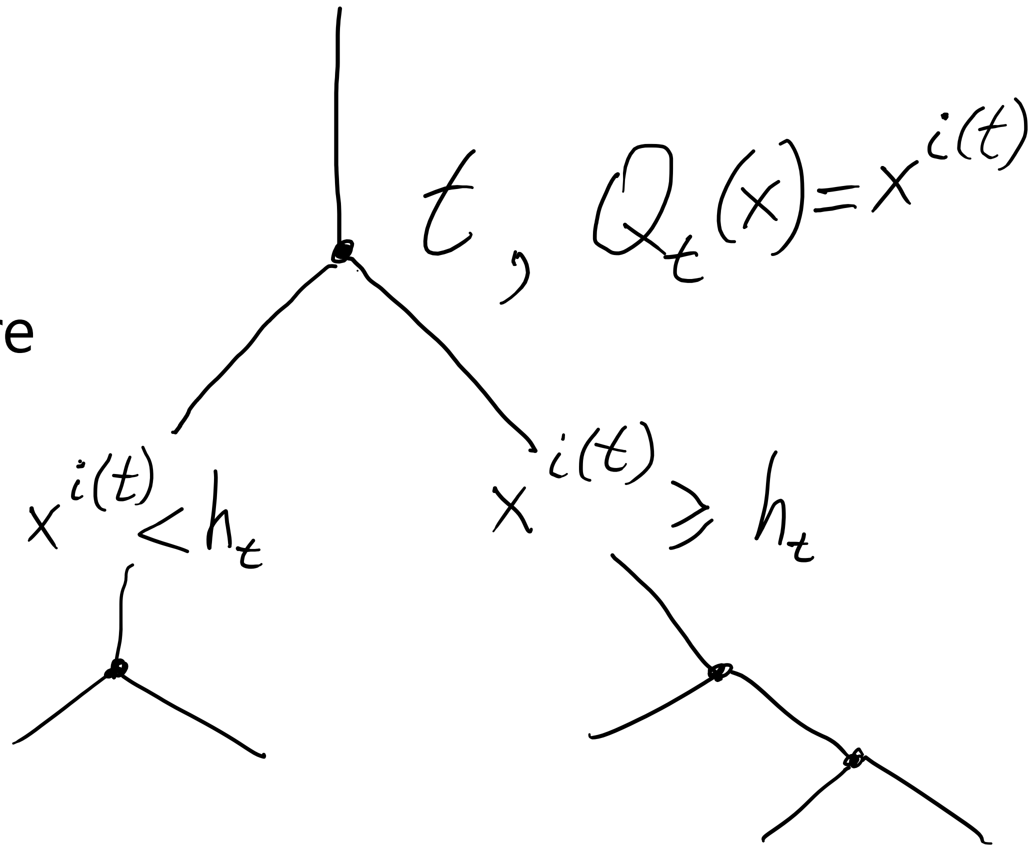
Binary trees

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 $D = \{(x_1, y_1), \ldots (x_N, y_N)\}$, 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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Find feature i and element $(x_k, y_k) \in D_t$, such that for the two subsets

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

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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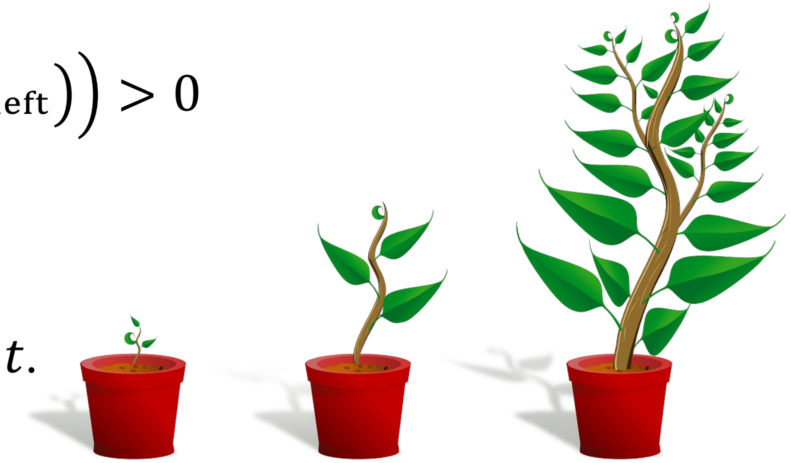
is maximized (over k and i).

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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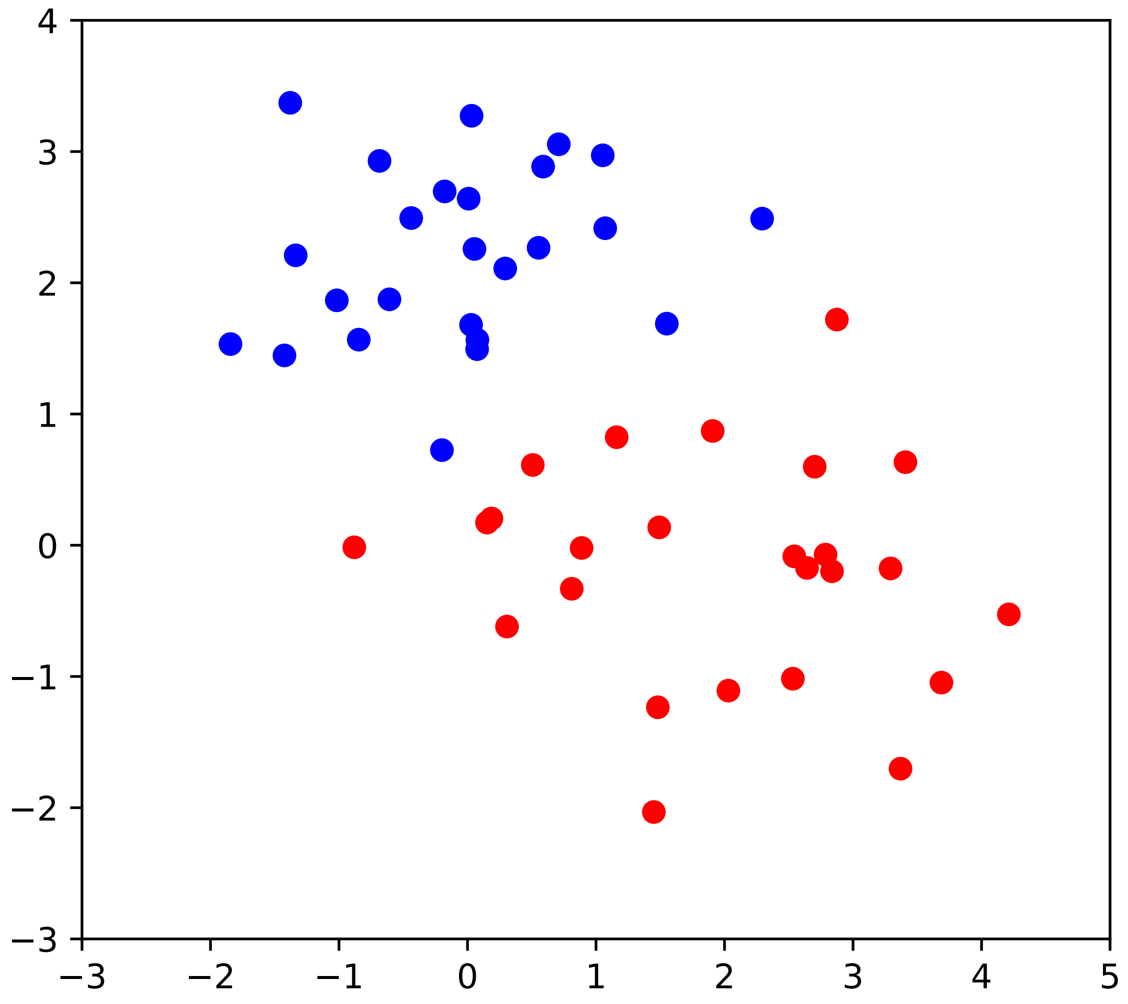

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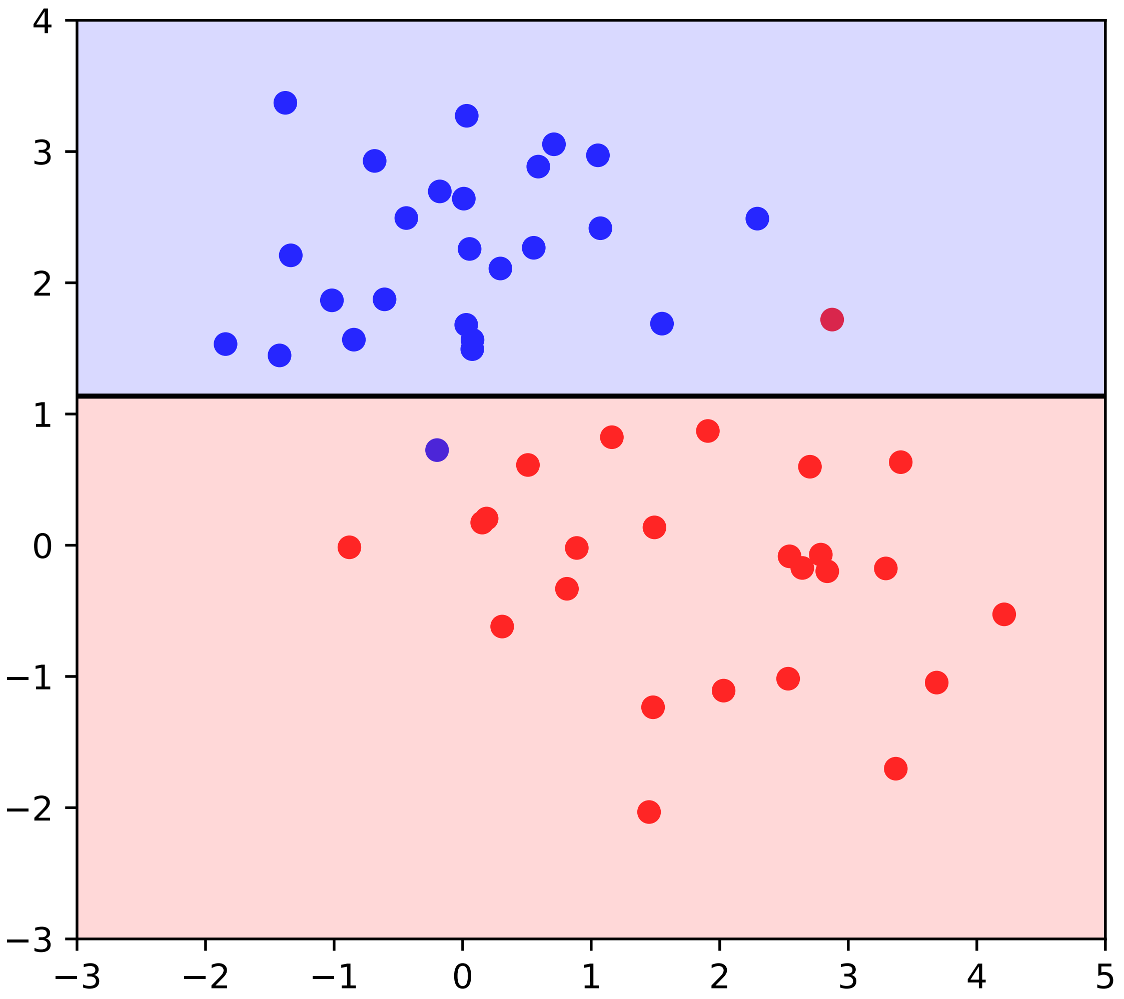

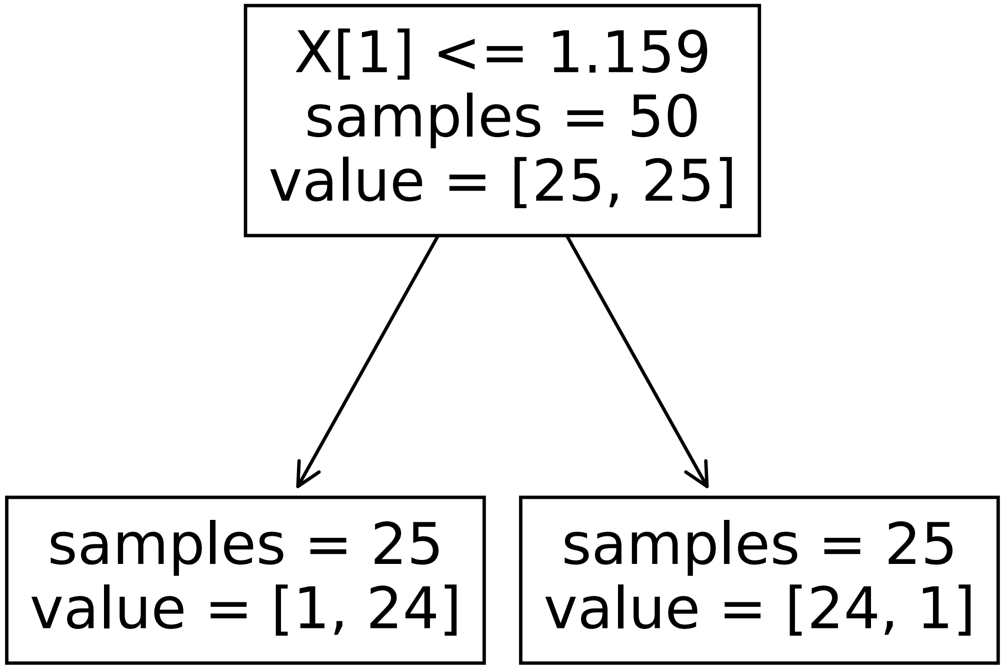

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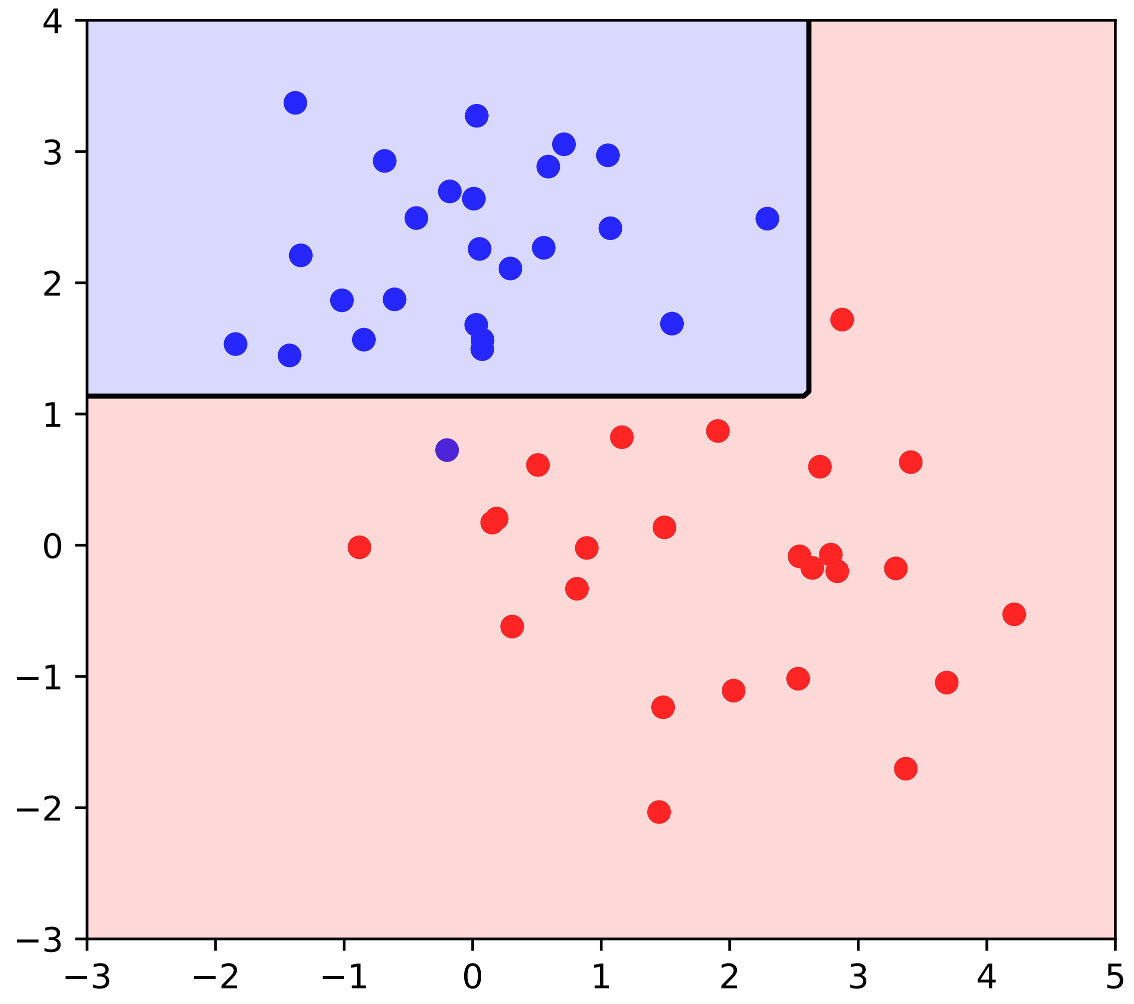

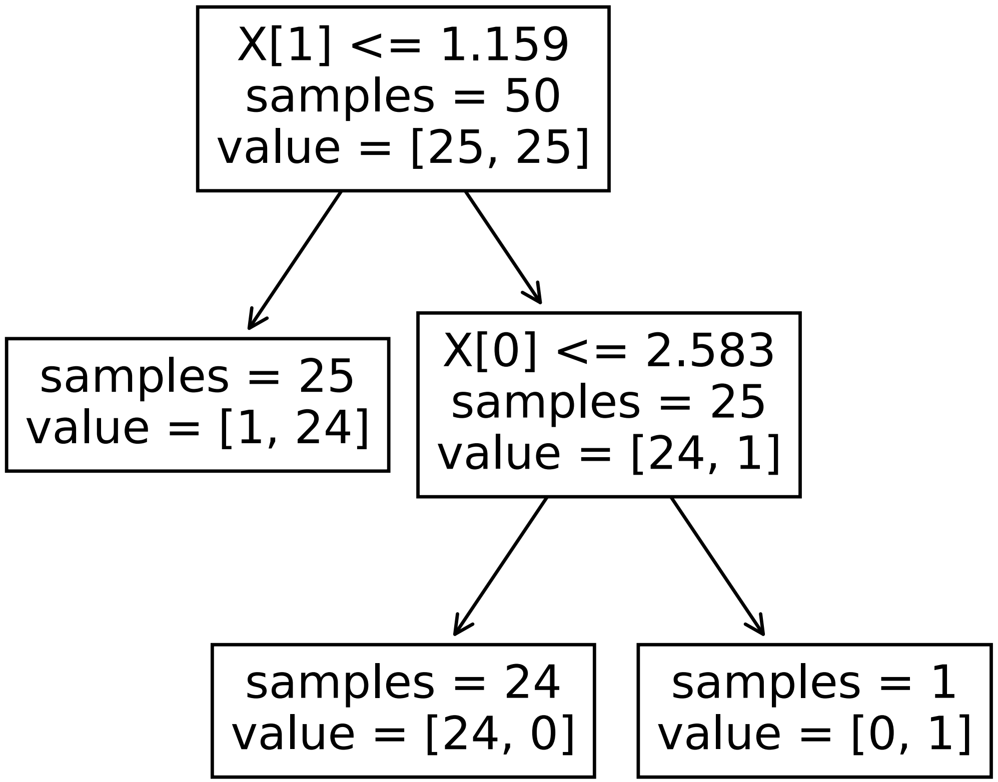

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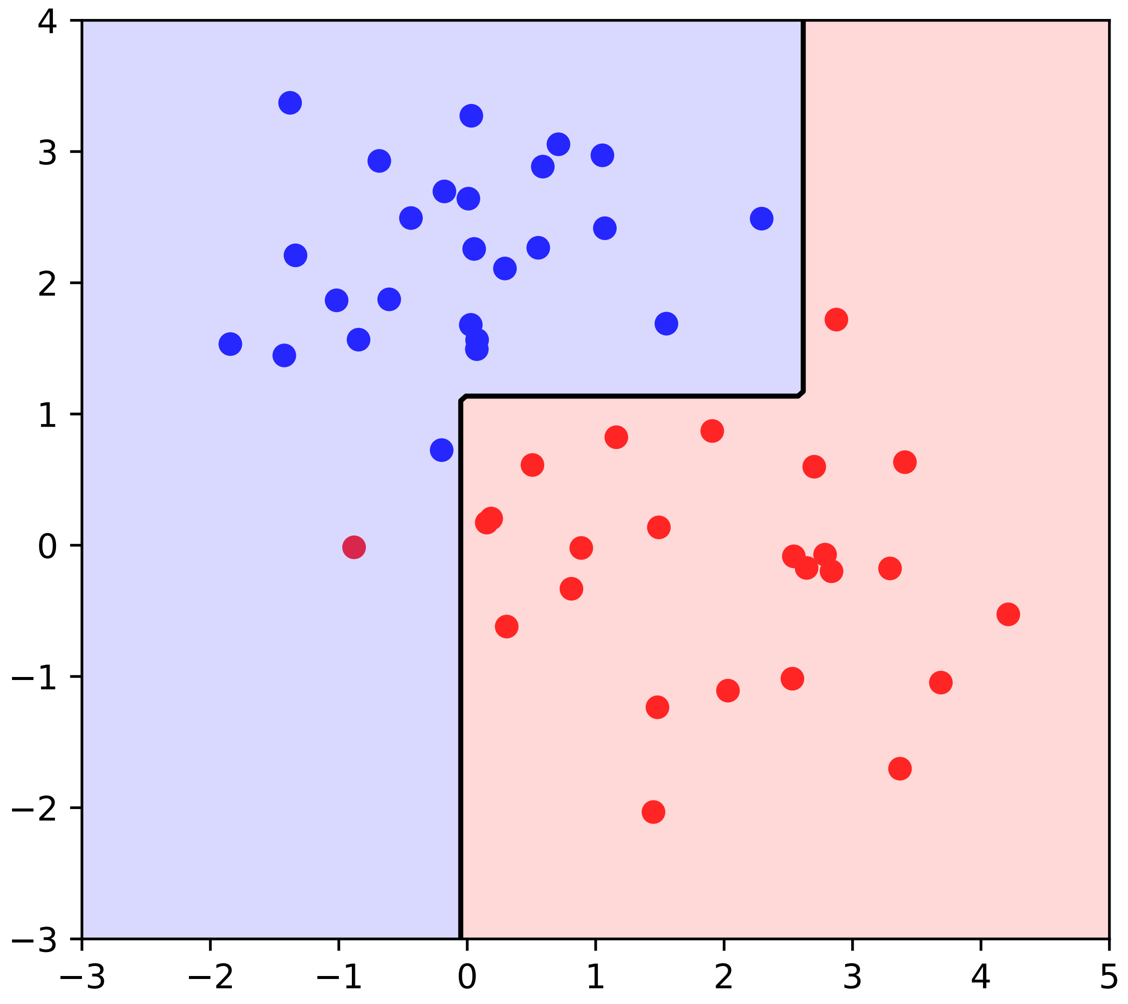

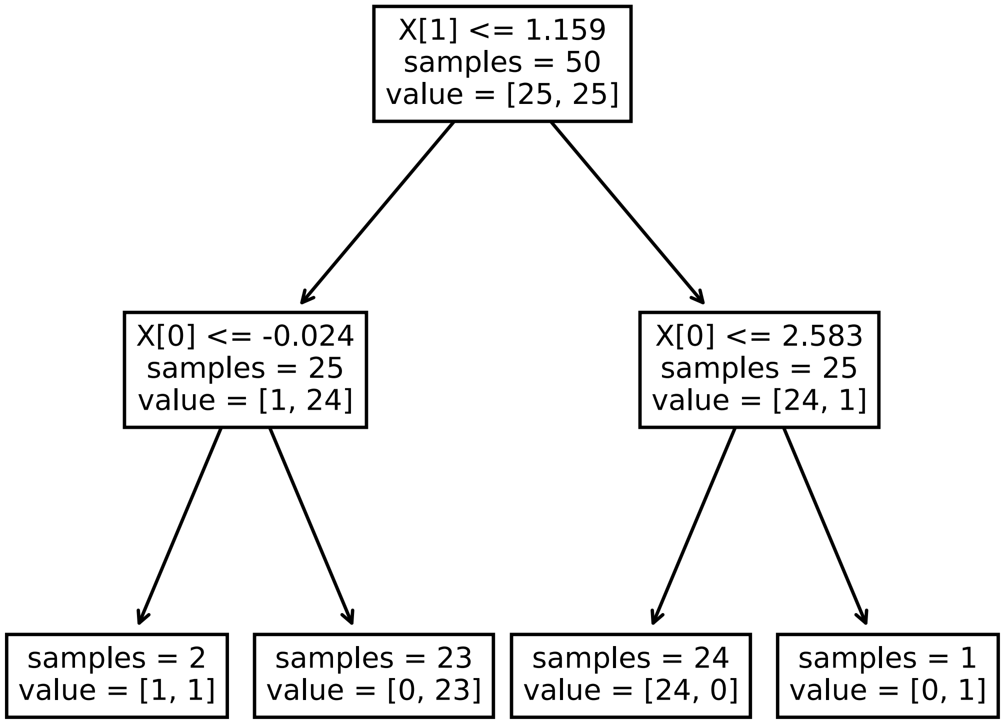

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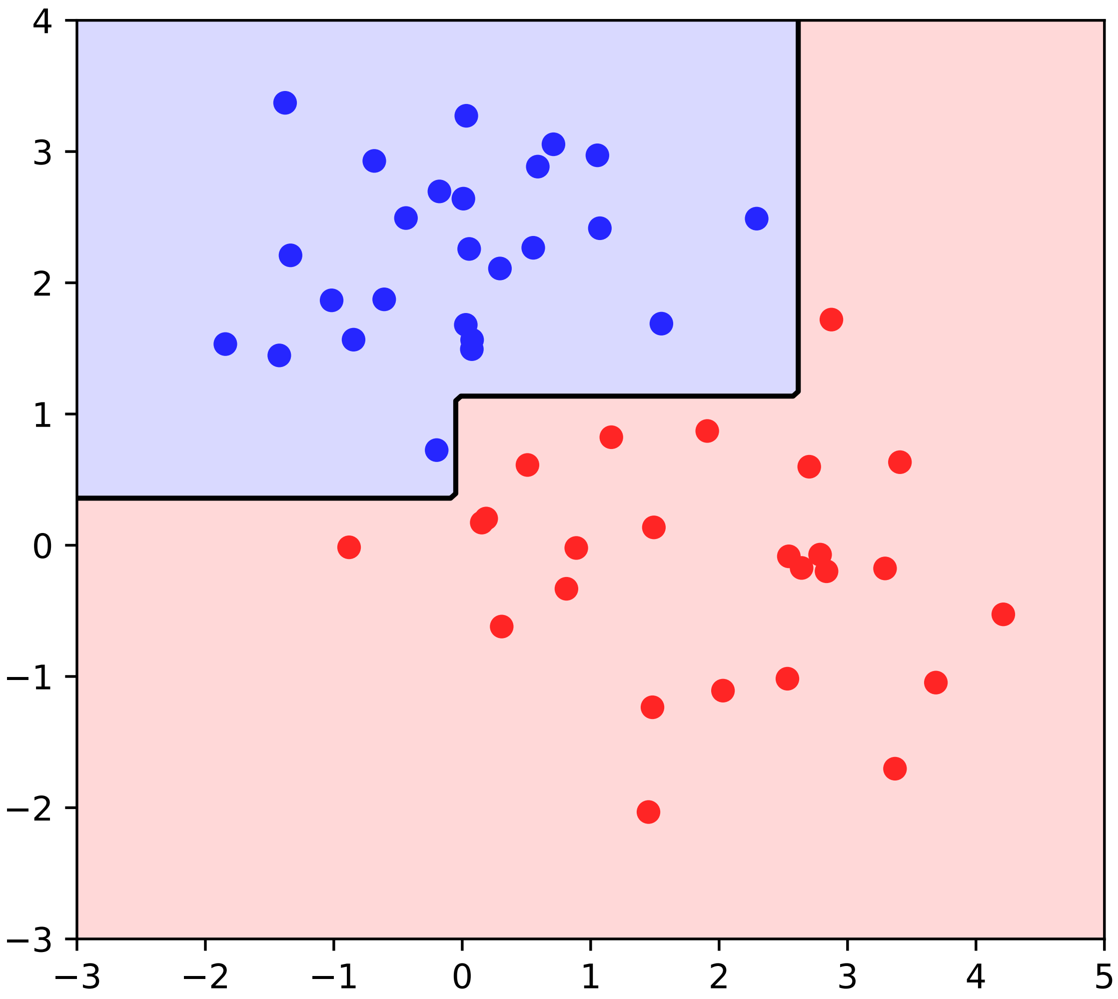

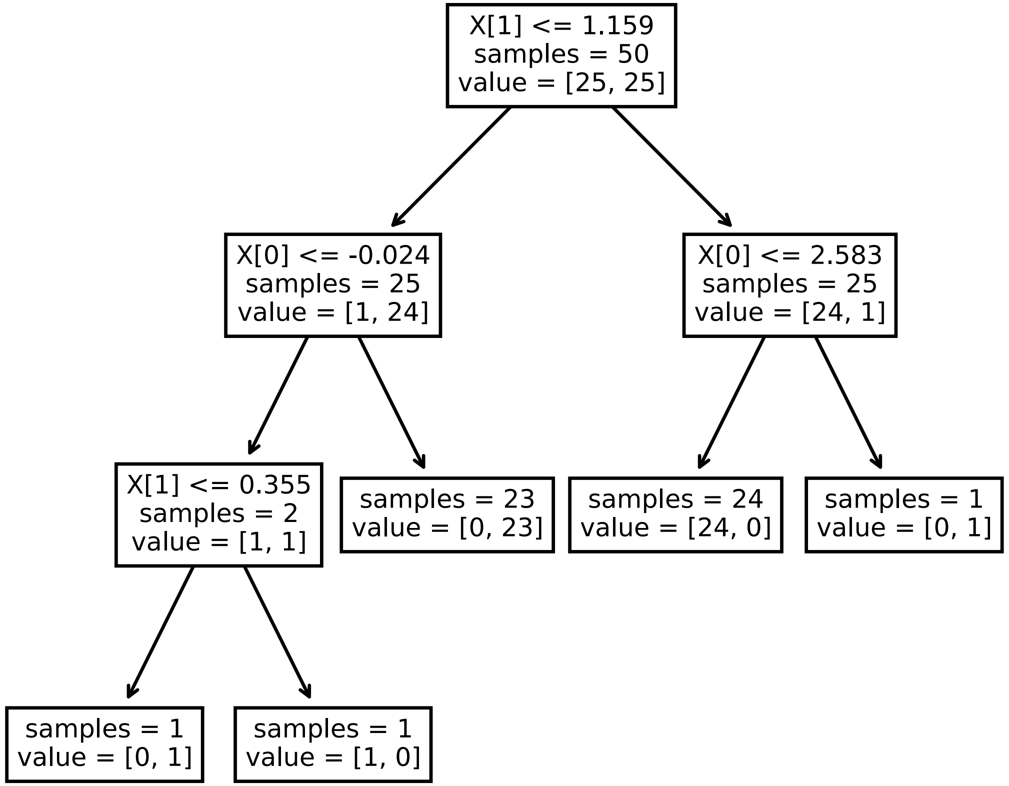

Impurity measures

Regression

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:

Impurity measures

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

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

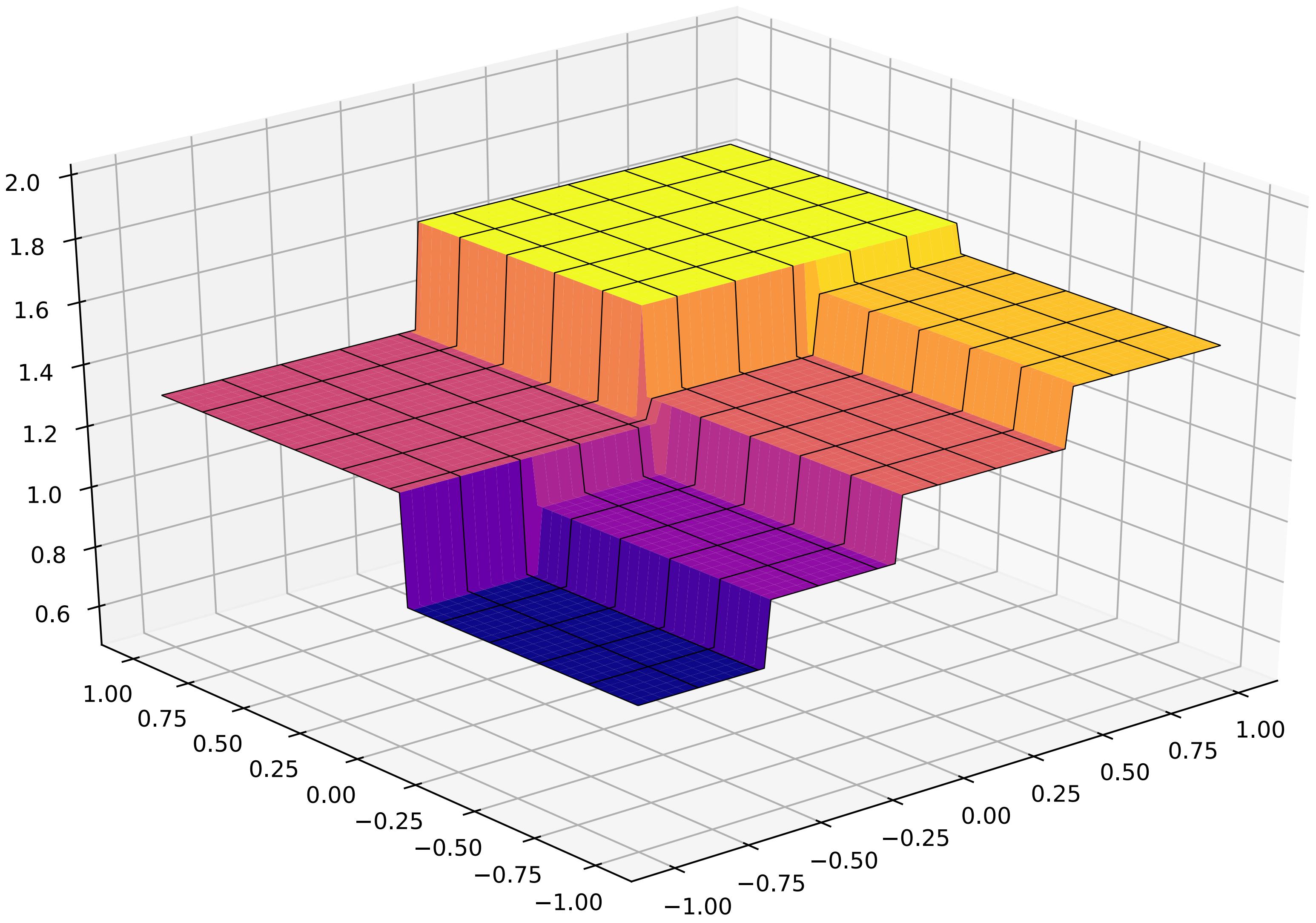
Minimum number of samples in a leaf

Minimum impurity gain

You name it…

Solution properties

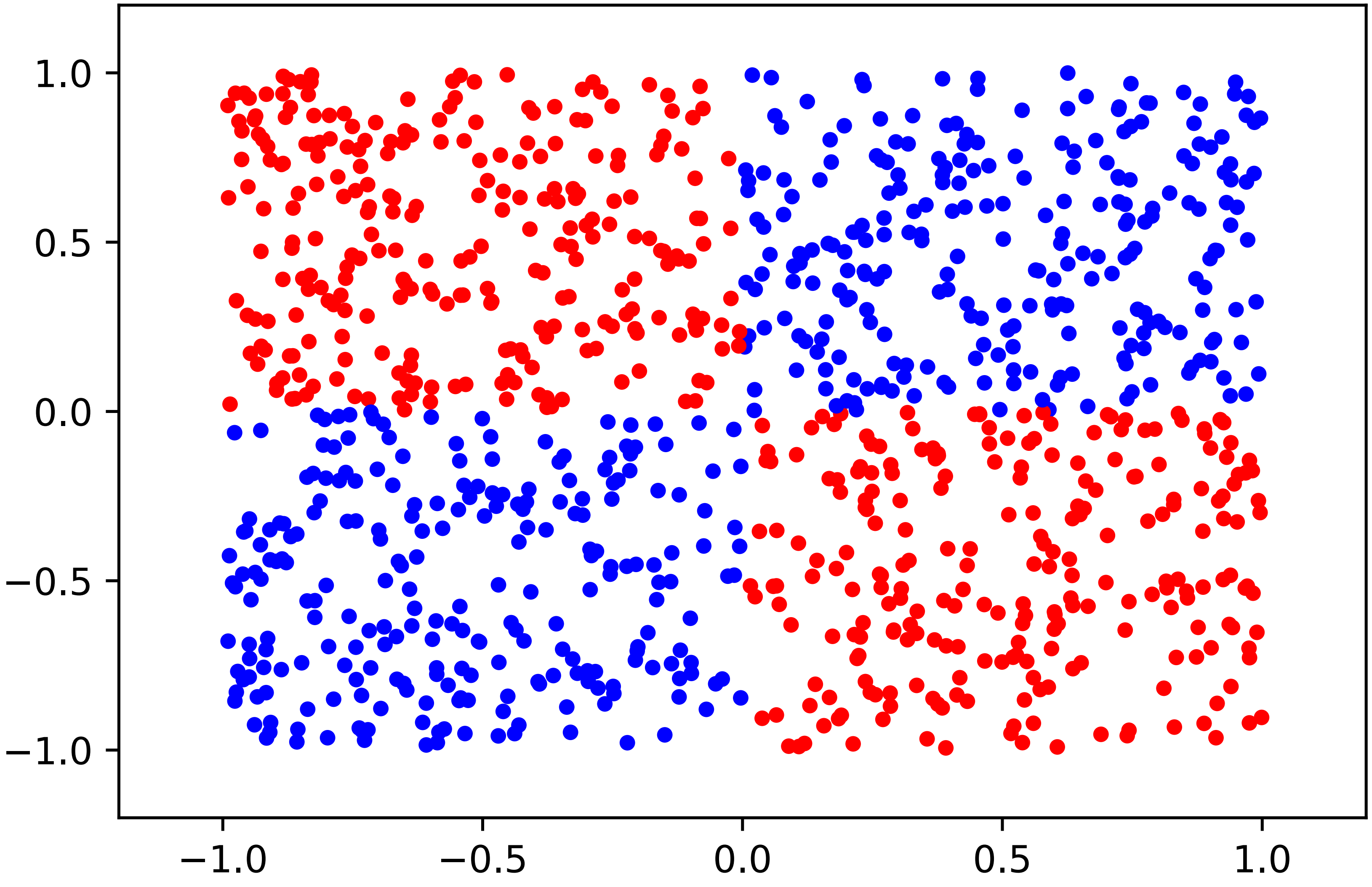
Prediction function



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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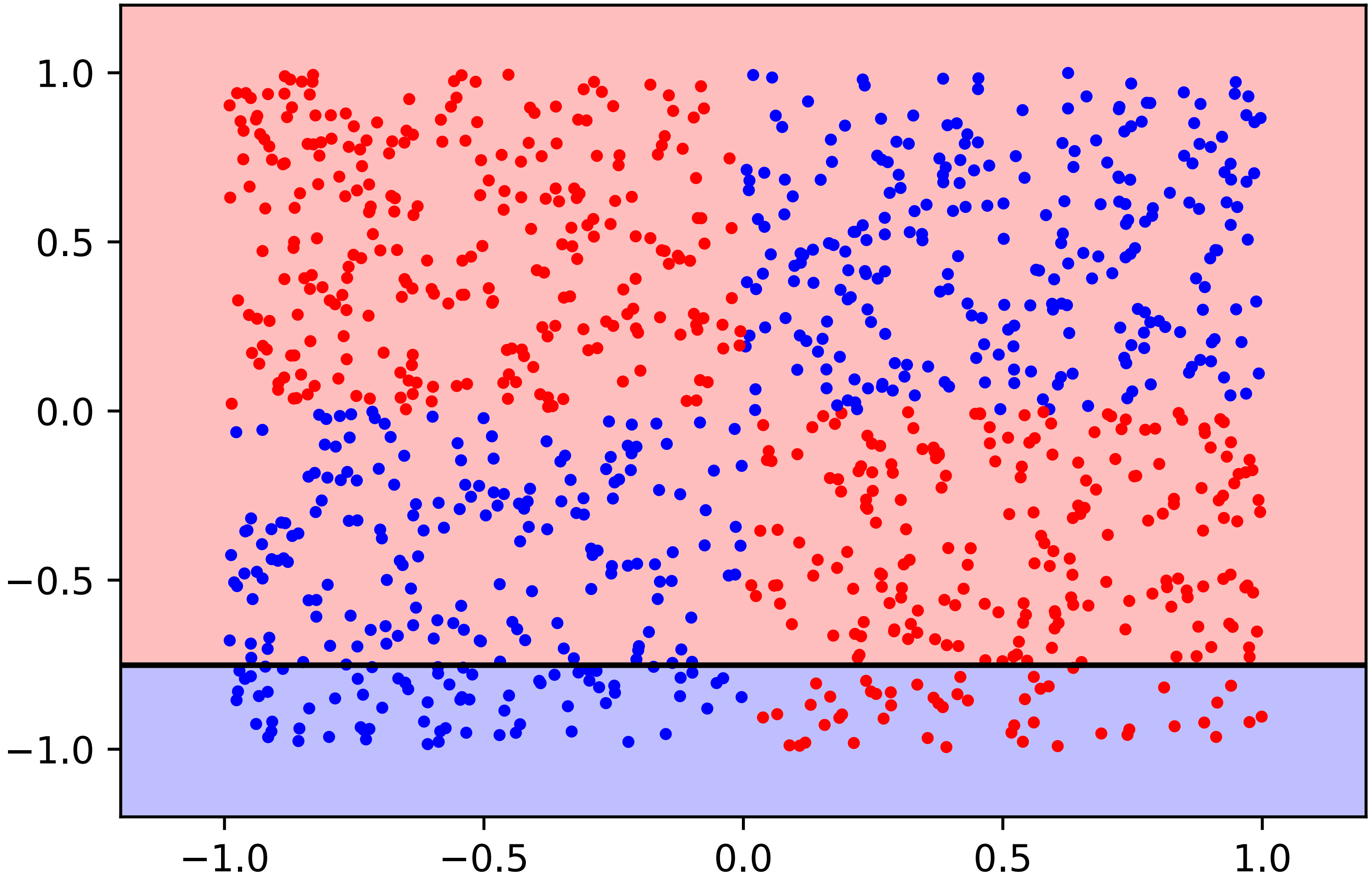

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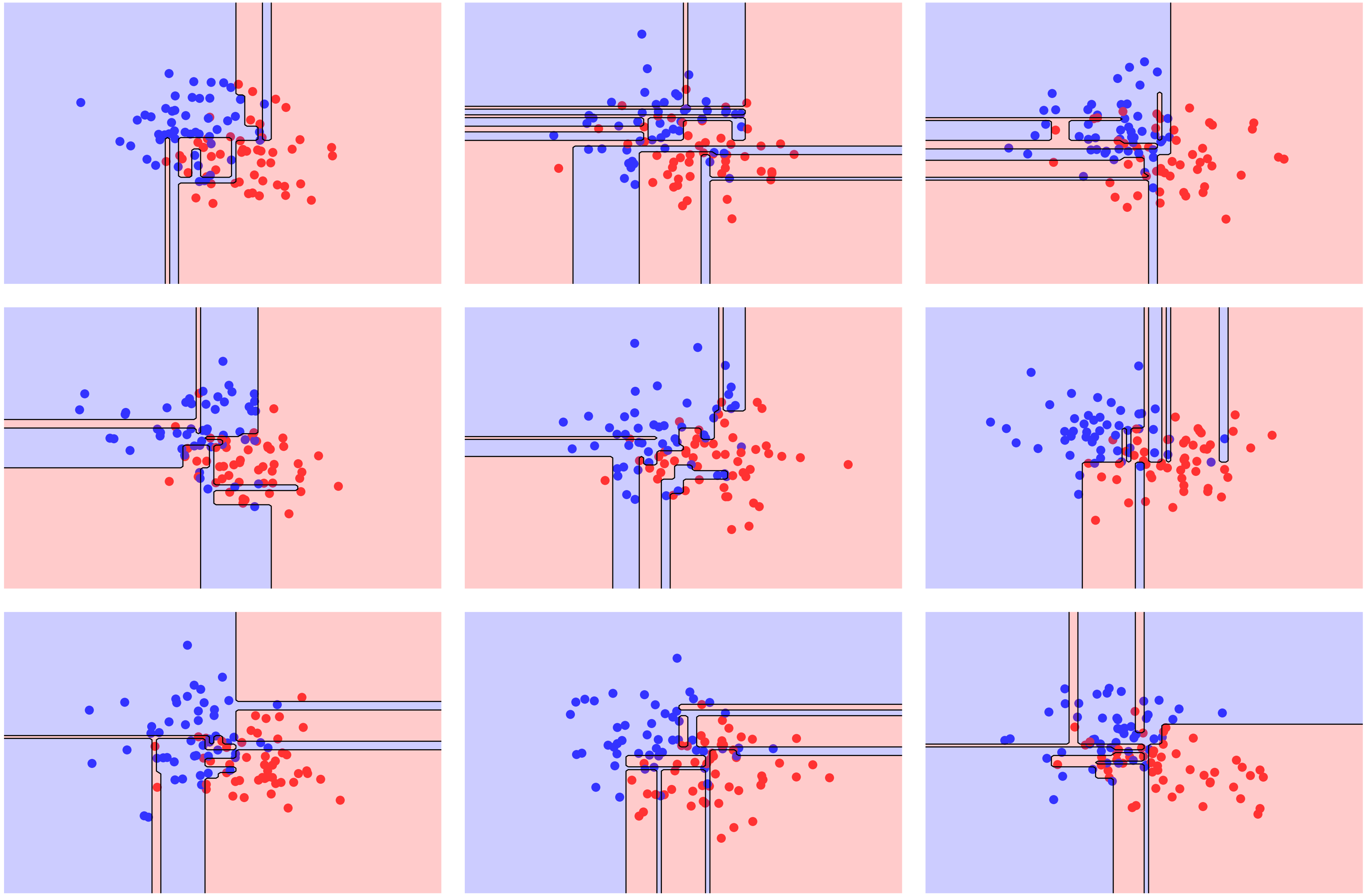
High Variance

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 ∈ 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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