Big Data Computing

Master's Degree in Computer Science

2021-2022

SAPIENZA
UNIVERSITÀ DI ROMA

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Recap from Last Lectures

- We presented 2 linear models: linear regression and logistic regression
- Those hypotheses work well whenever there exists a linear relationship between the features (input) and the response (output)
- Model's parameter estimation done either analytically (OLS) or iteratively (Gradient Descent)

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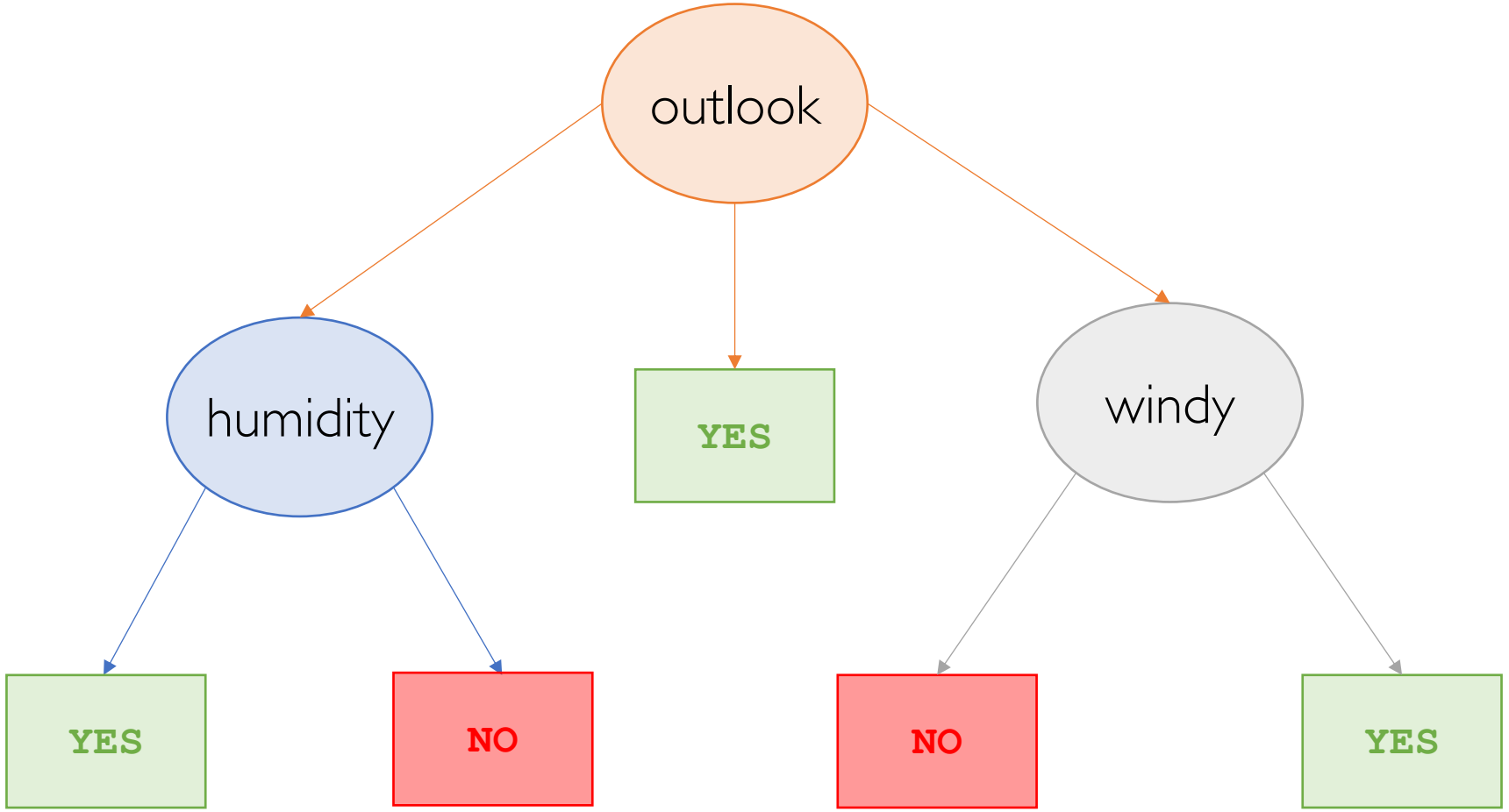
- The set of splitting rules can be represented as a tree (decision tree)
- Highly human-interpretable models

Decision Tree: An Example



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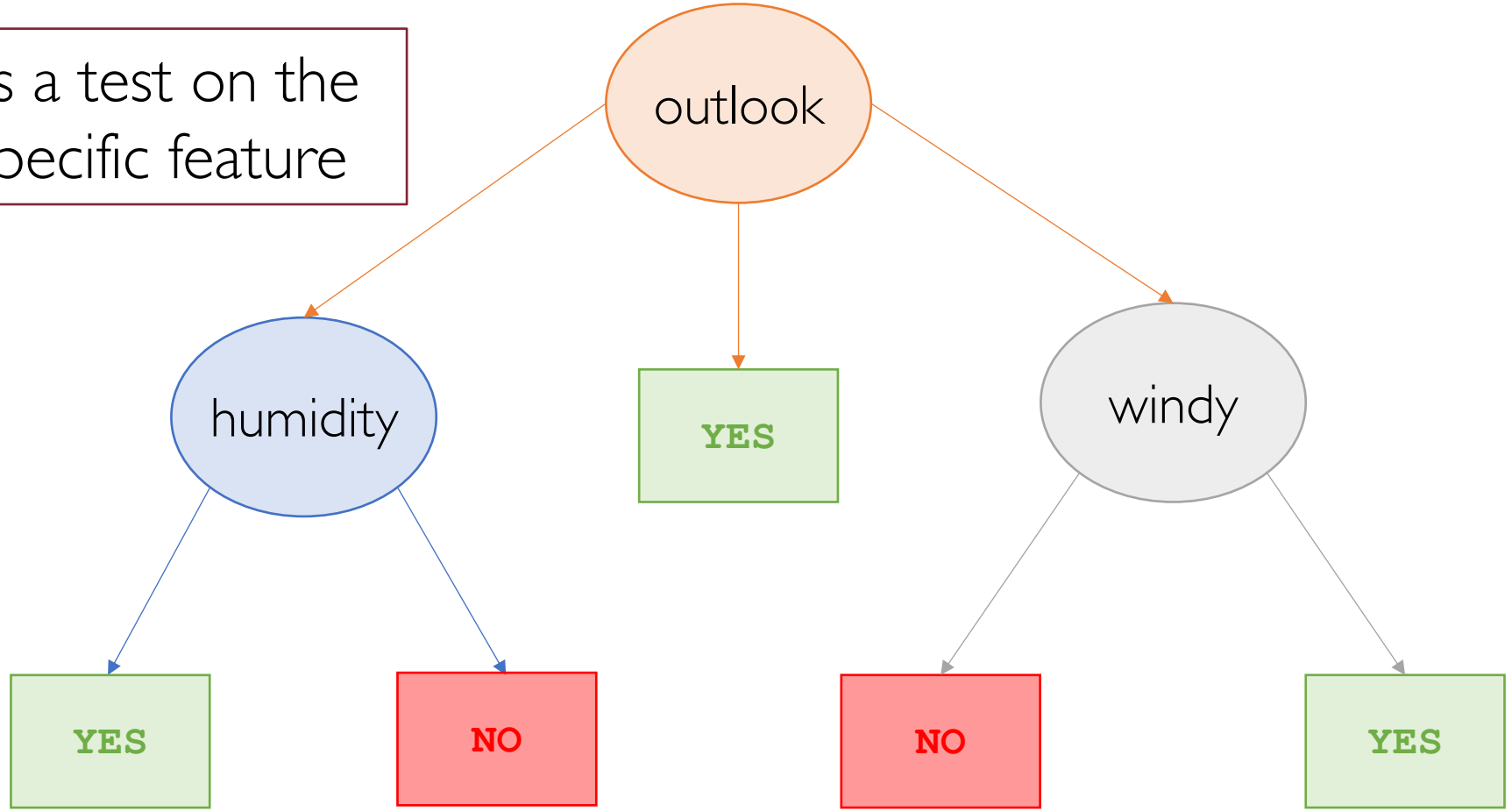
Each node is a test on the value of a specific feature



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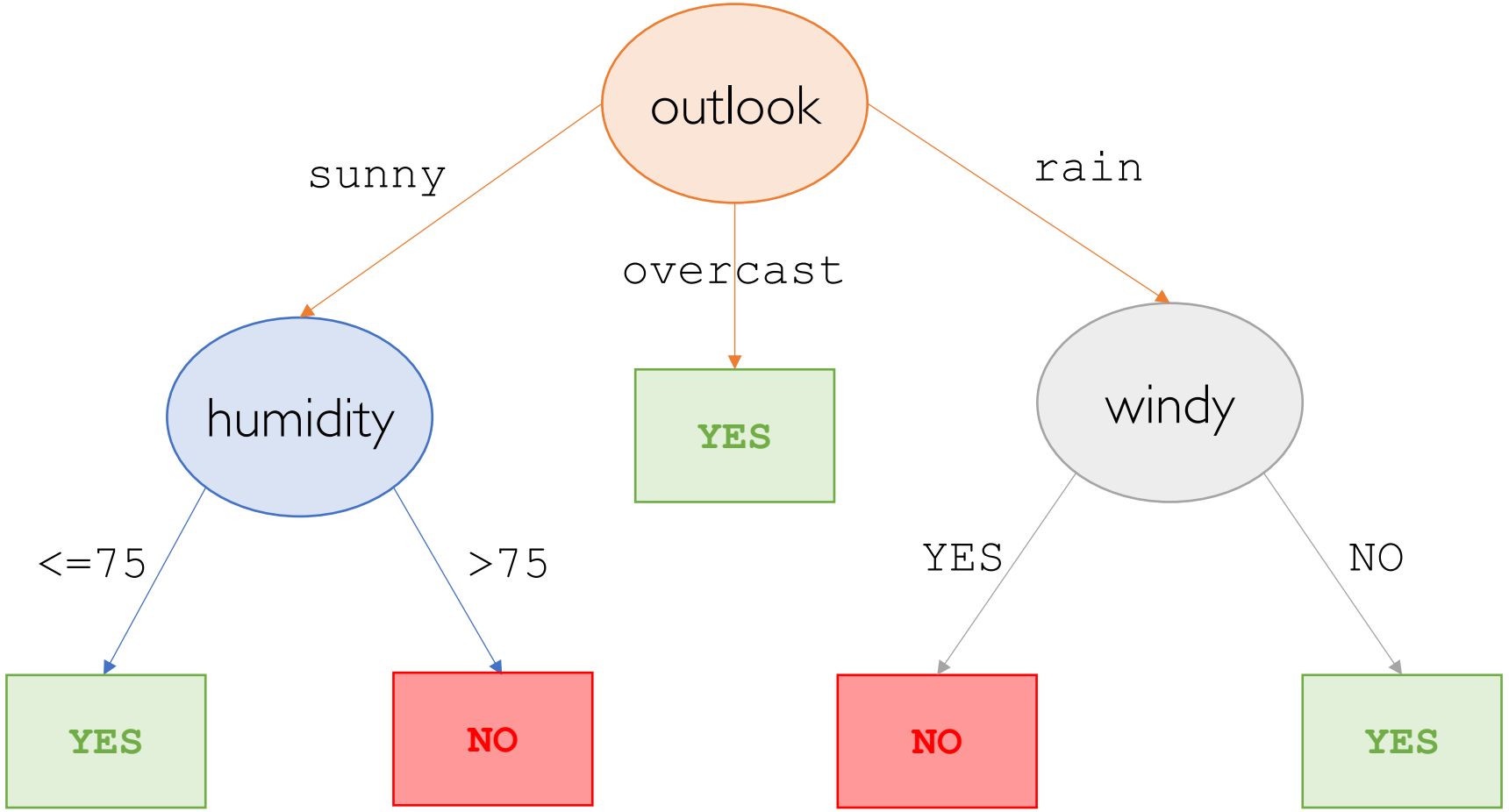

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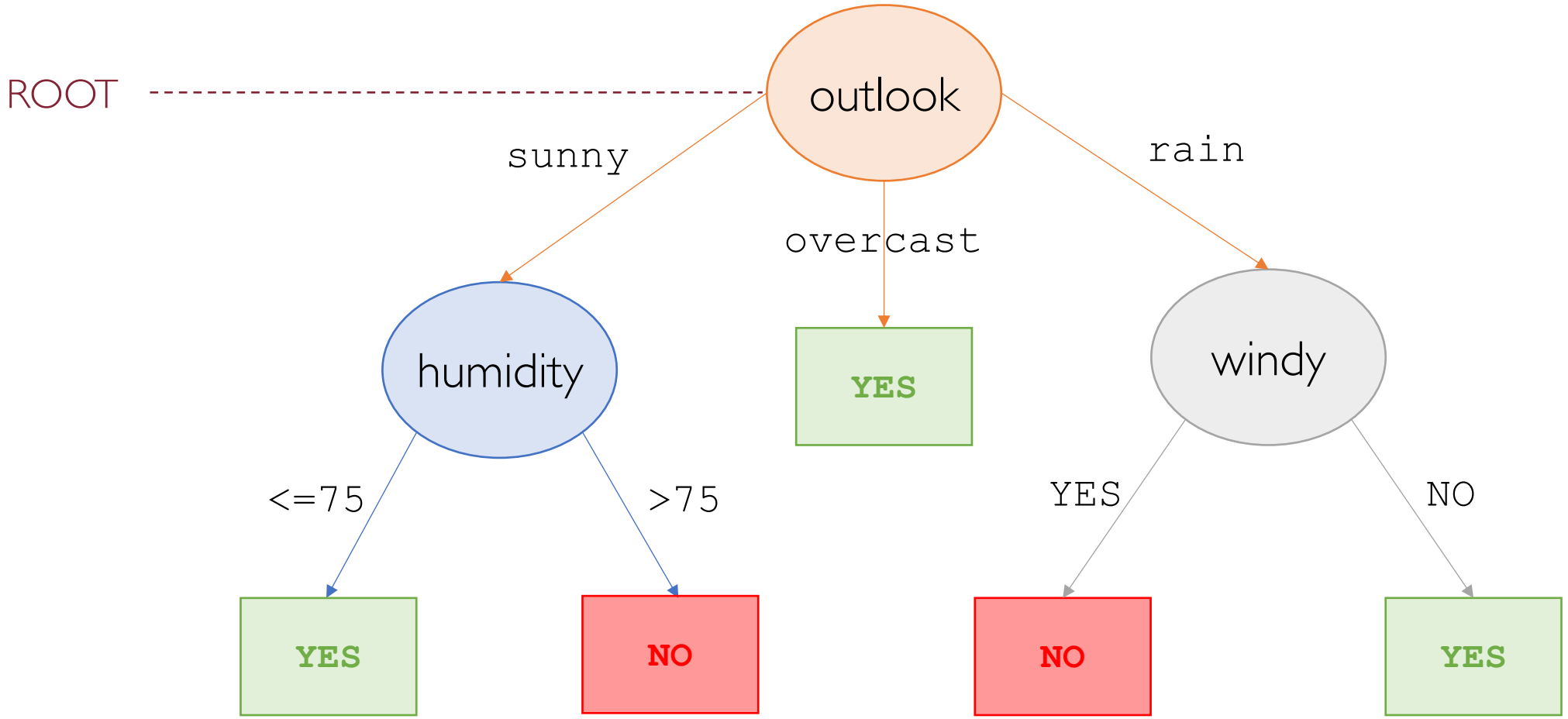

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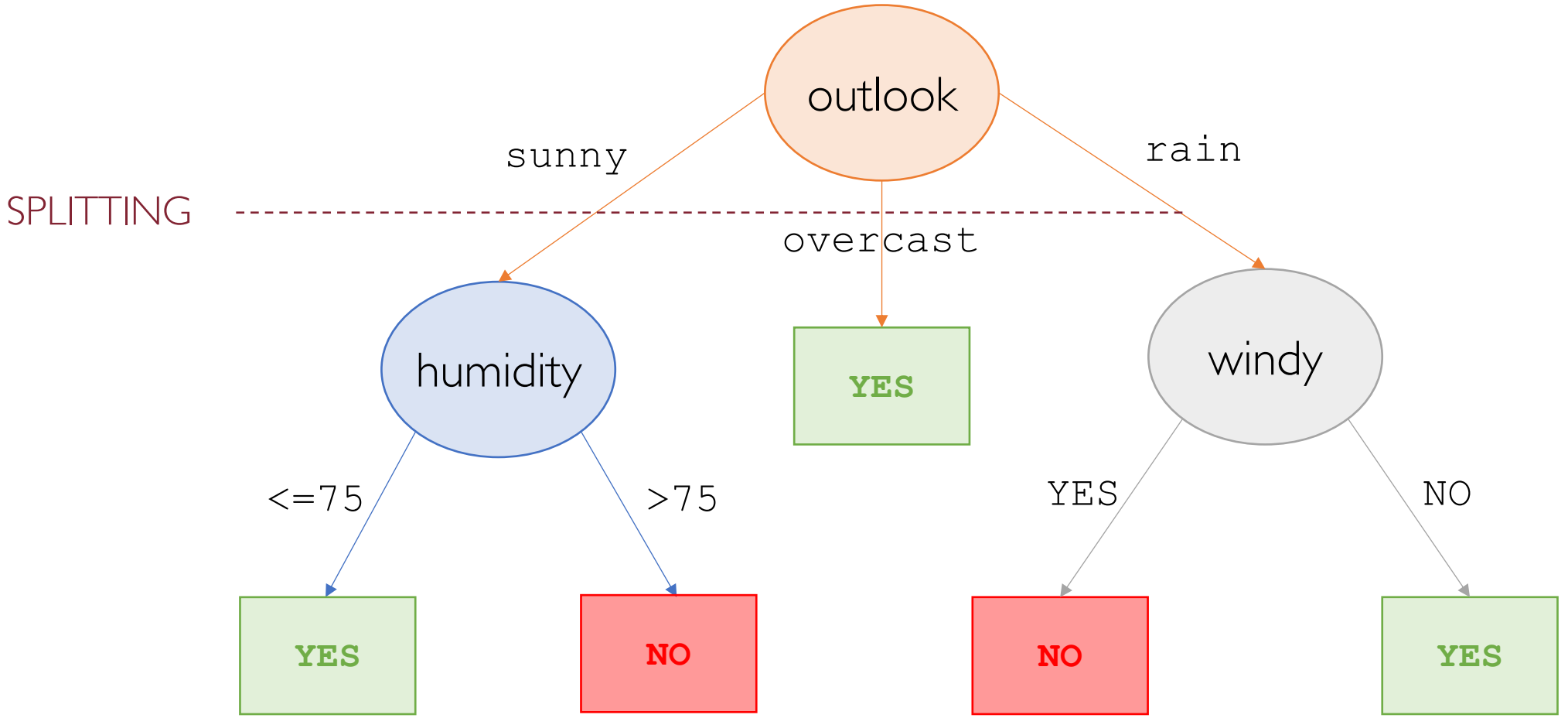

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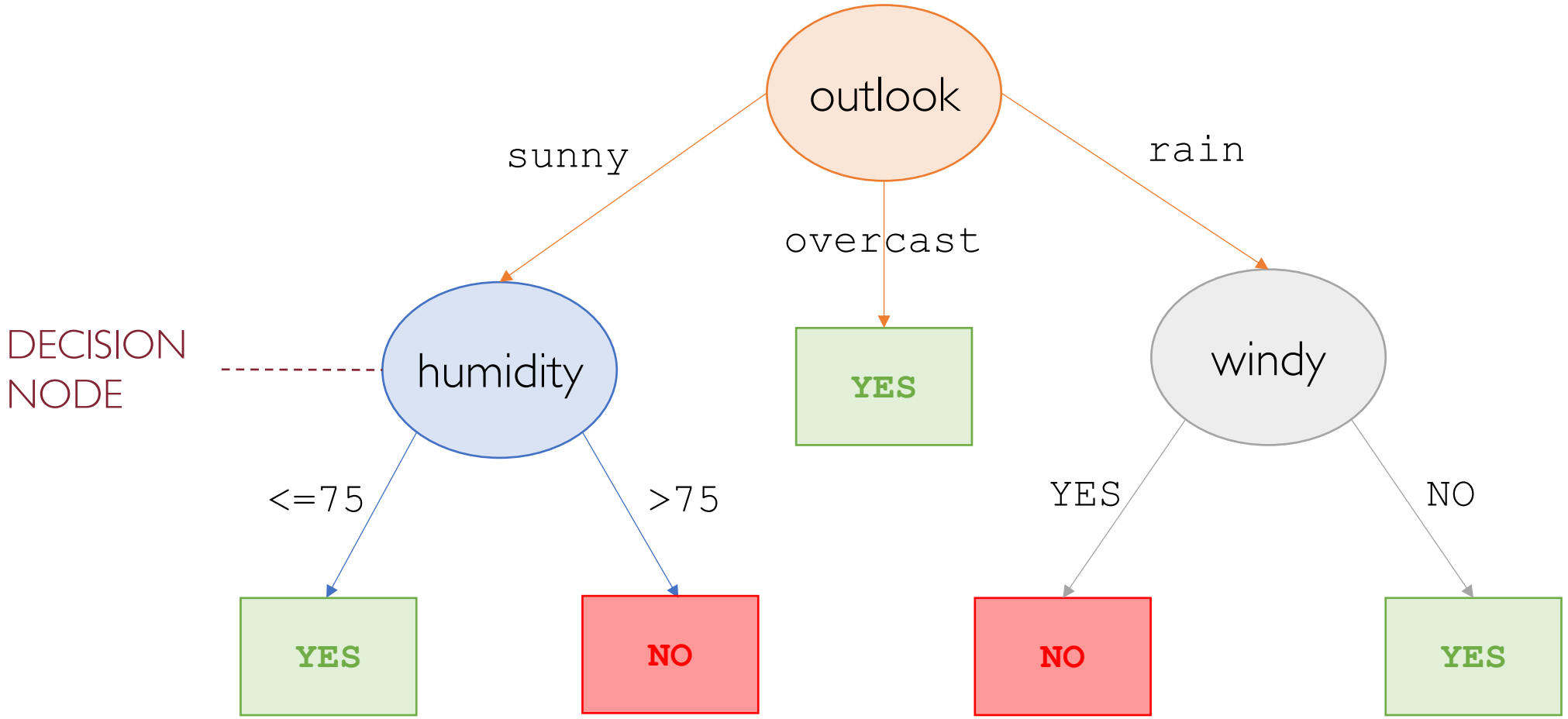

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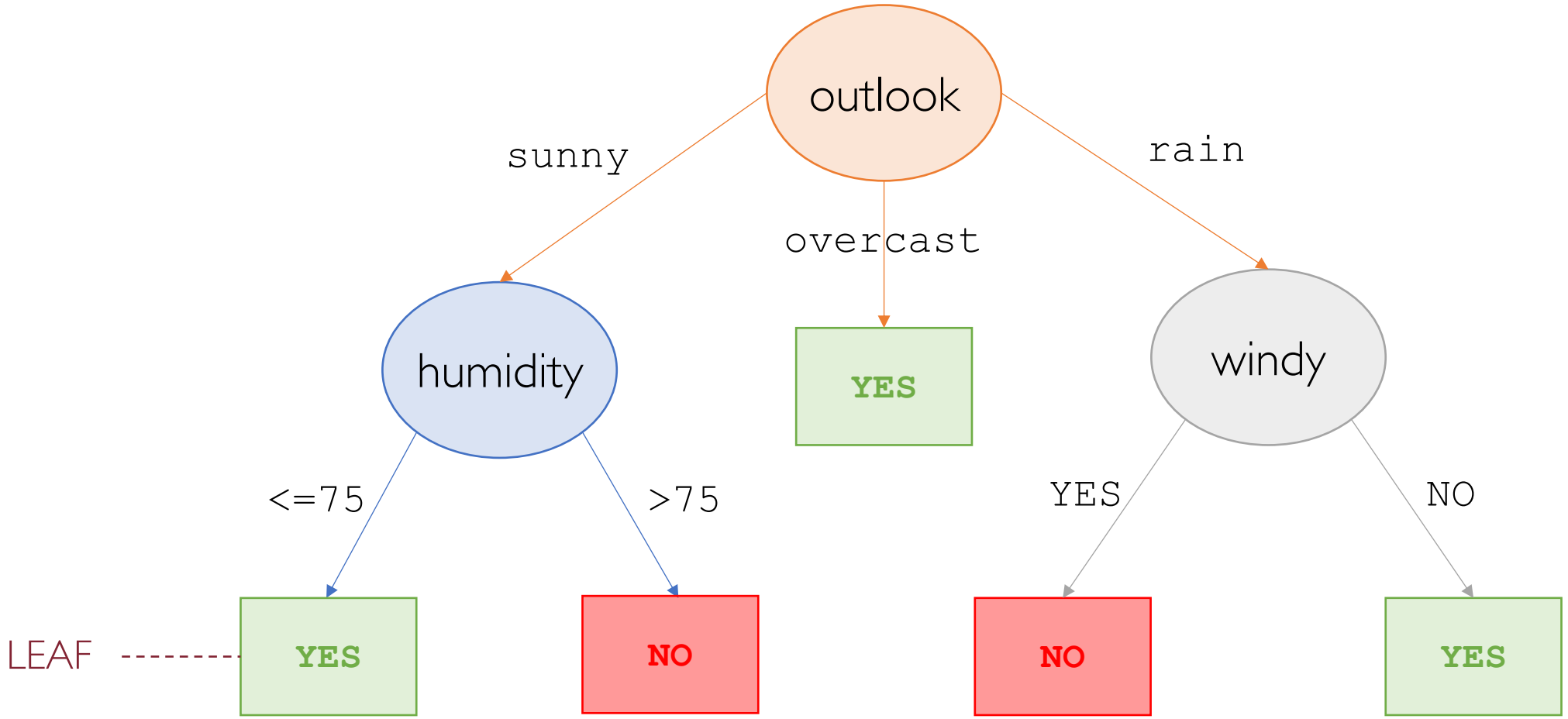

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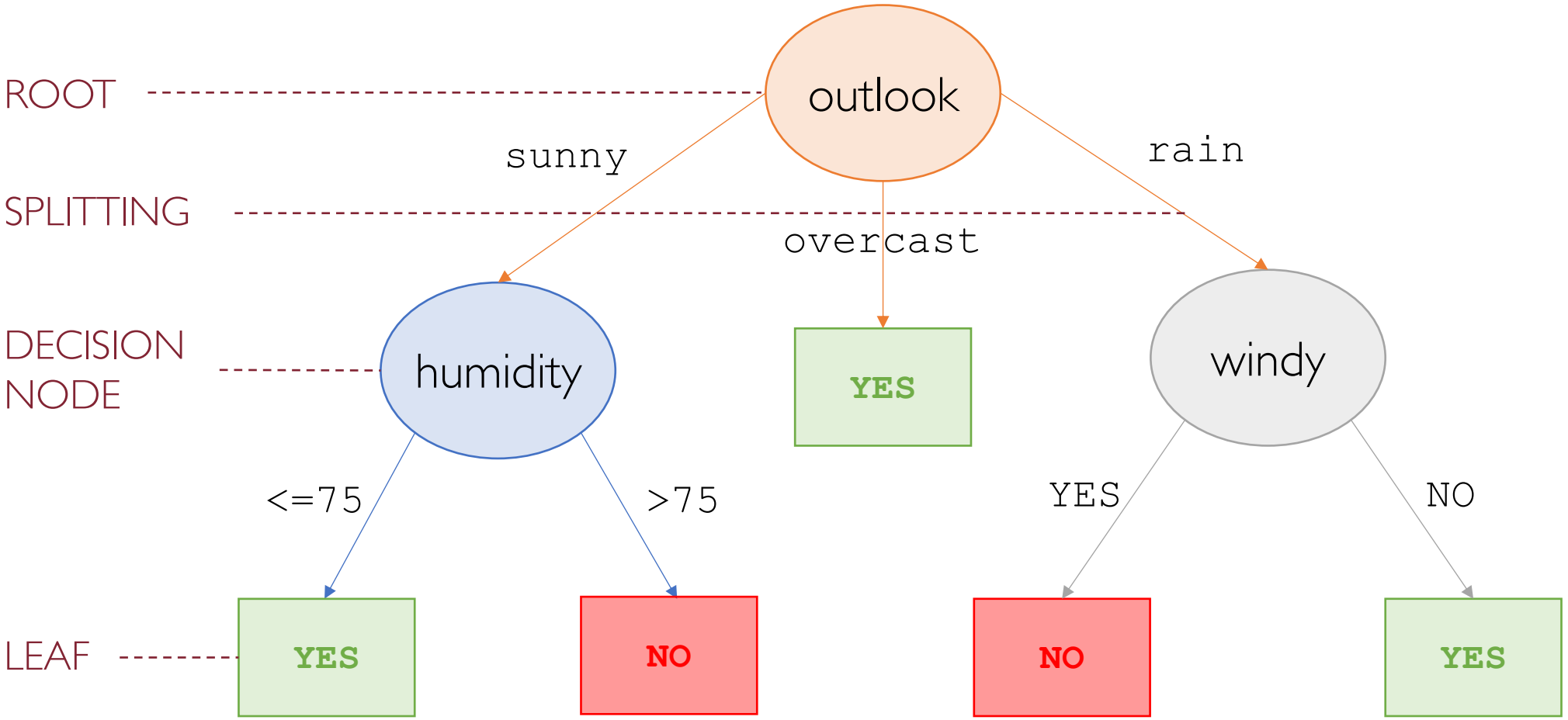
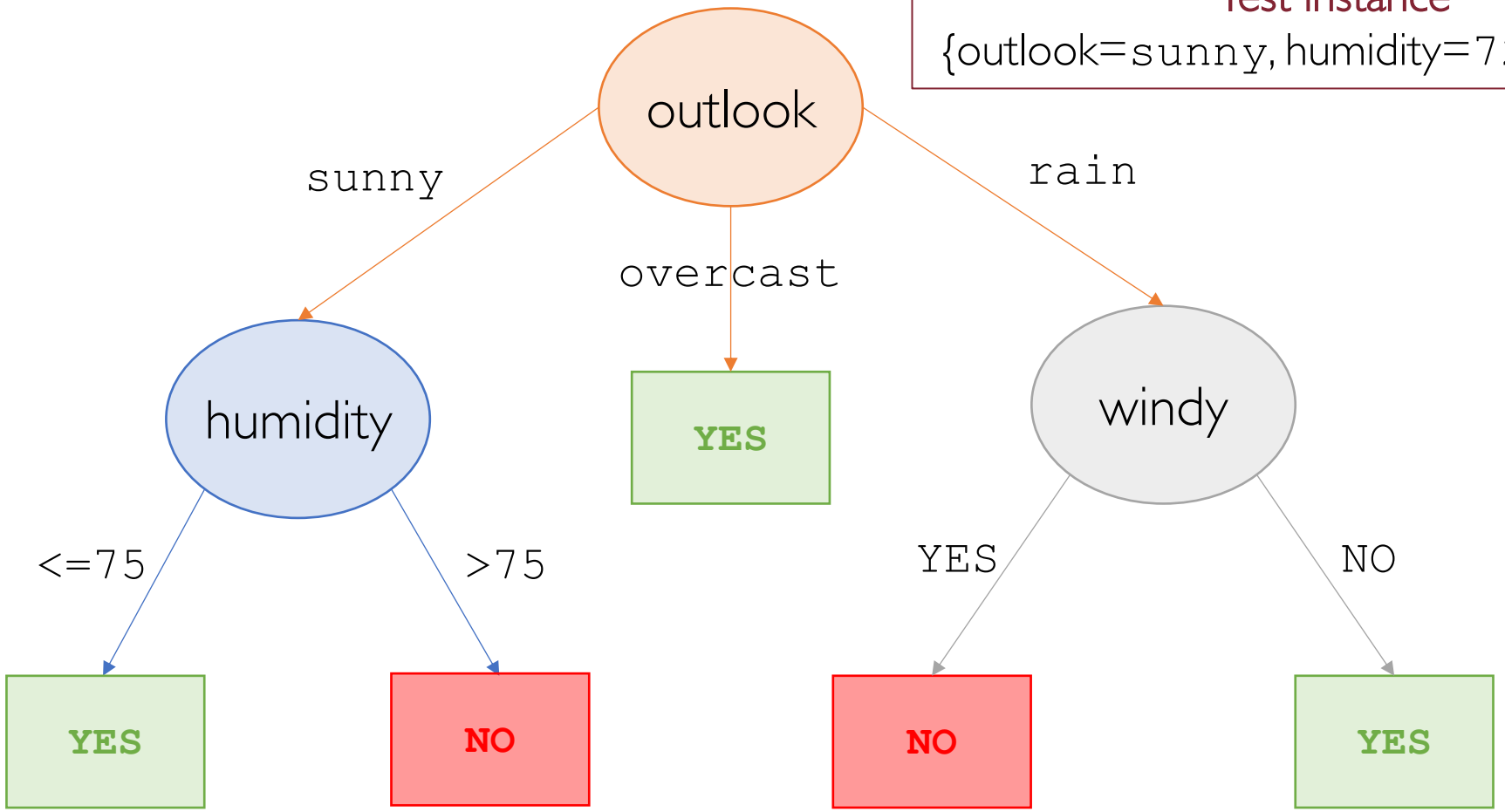


Decision Tree: An Example

Test instance
{outlook=sunny, humidity=72, windy=Y}



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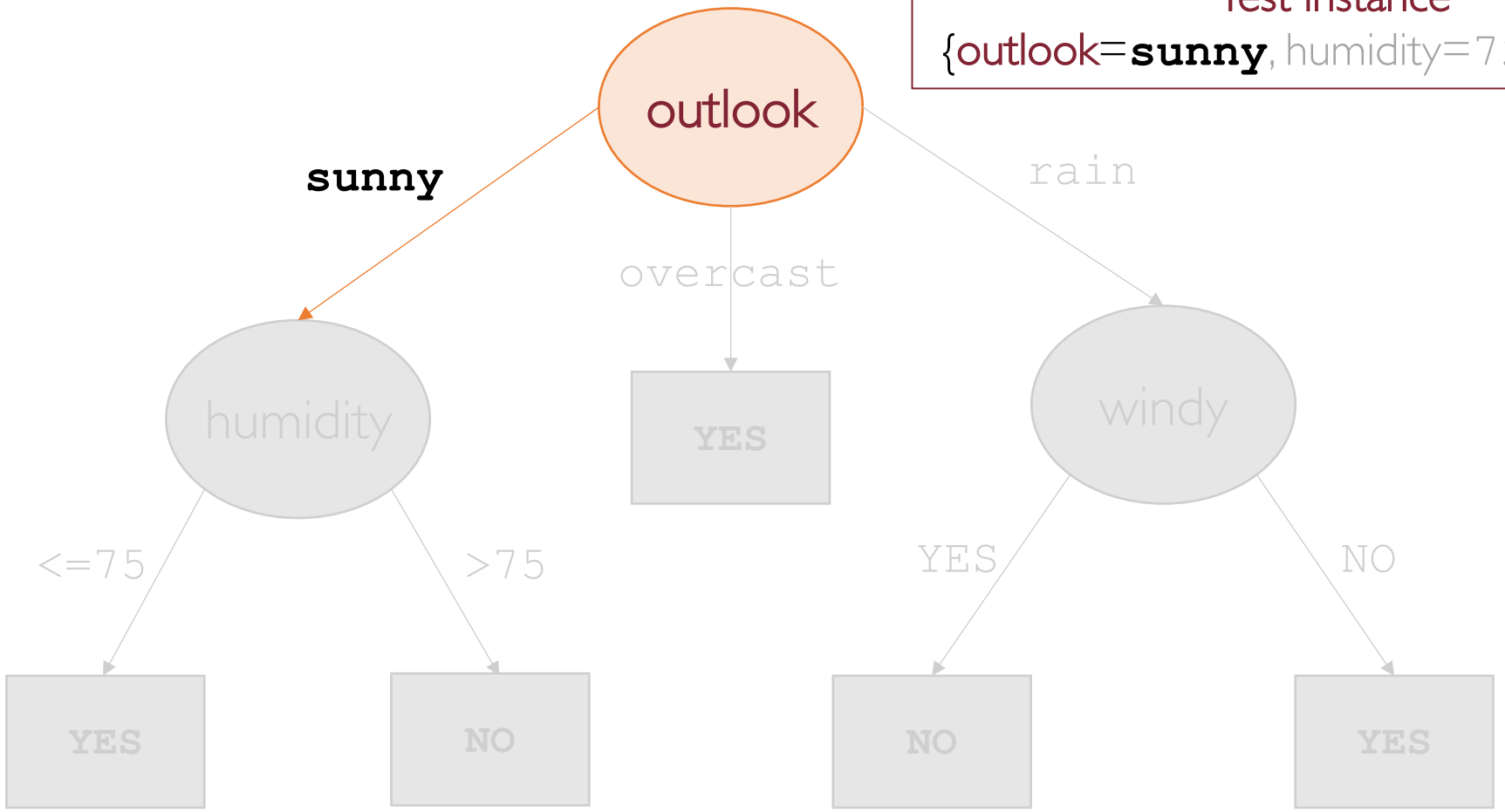

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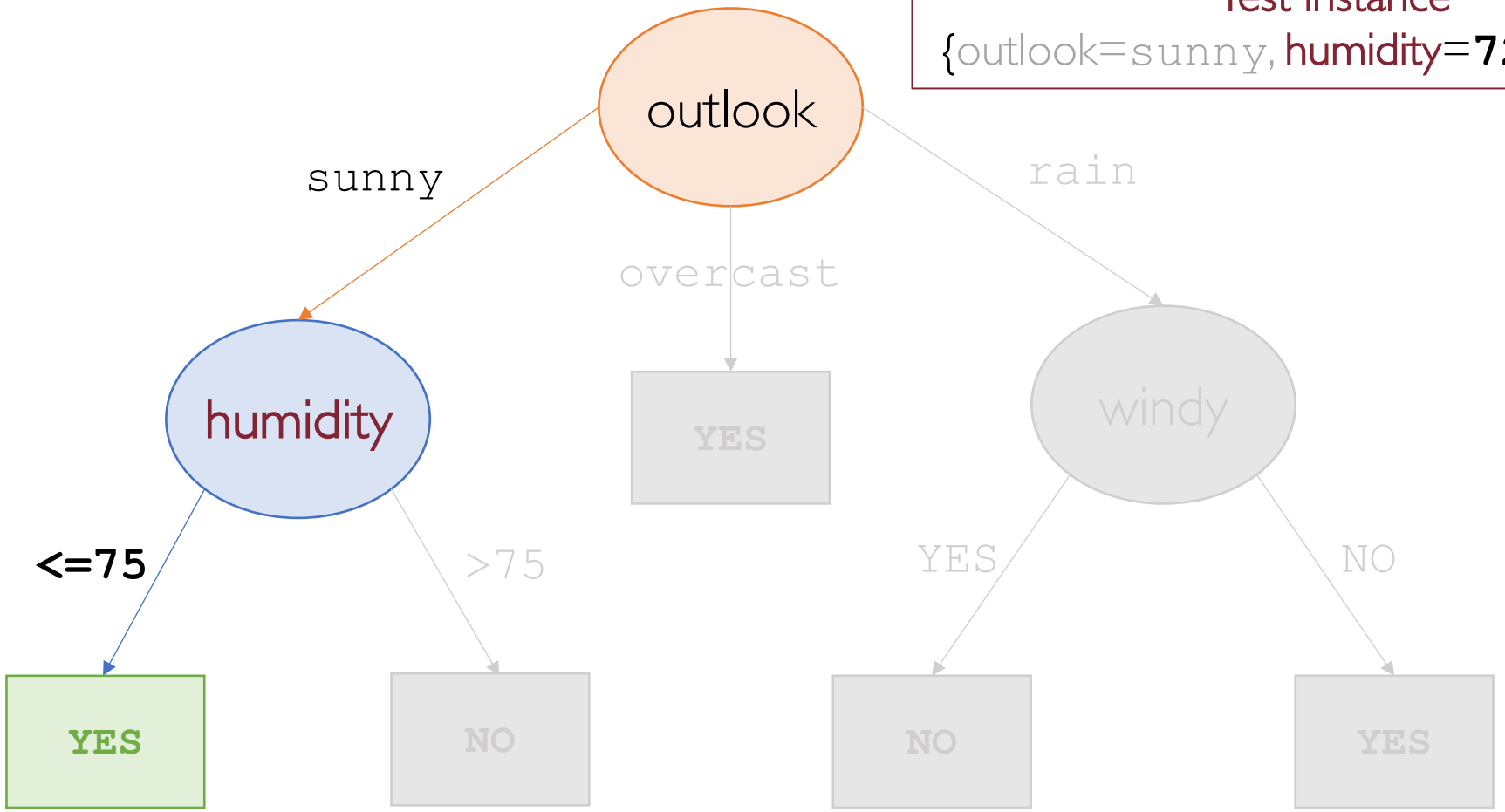

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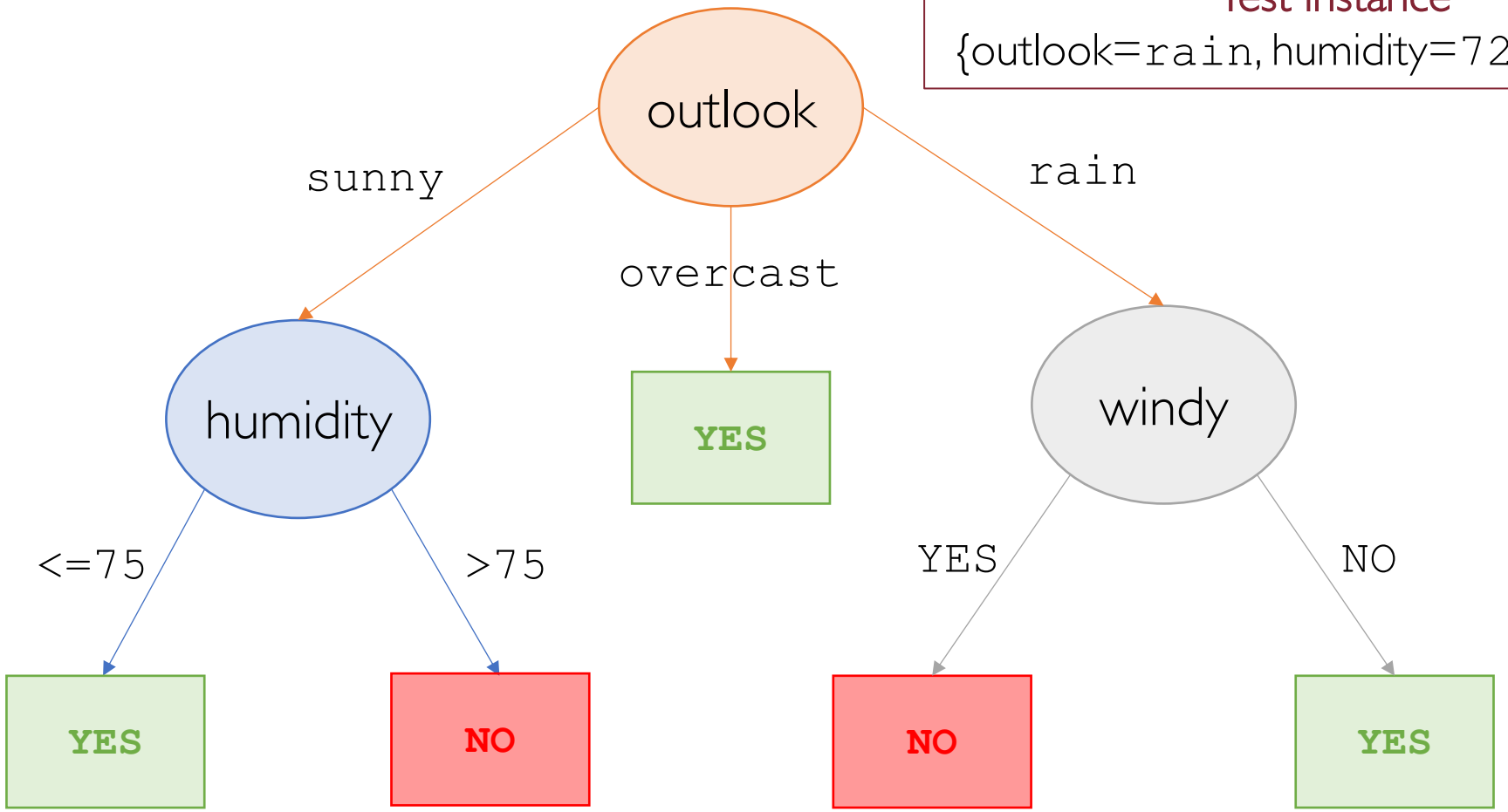

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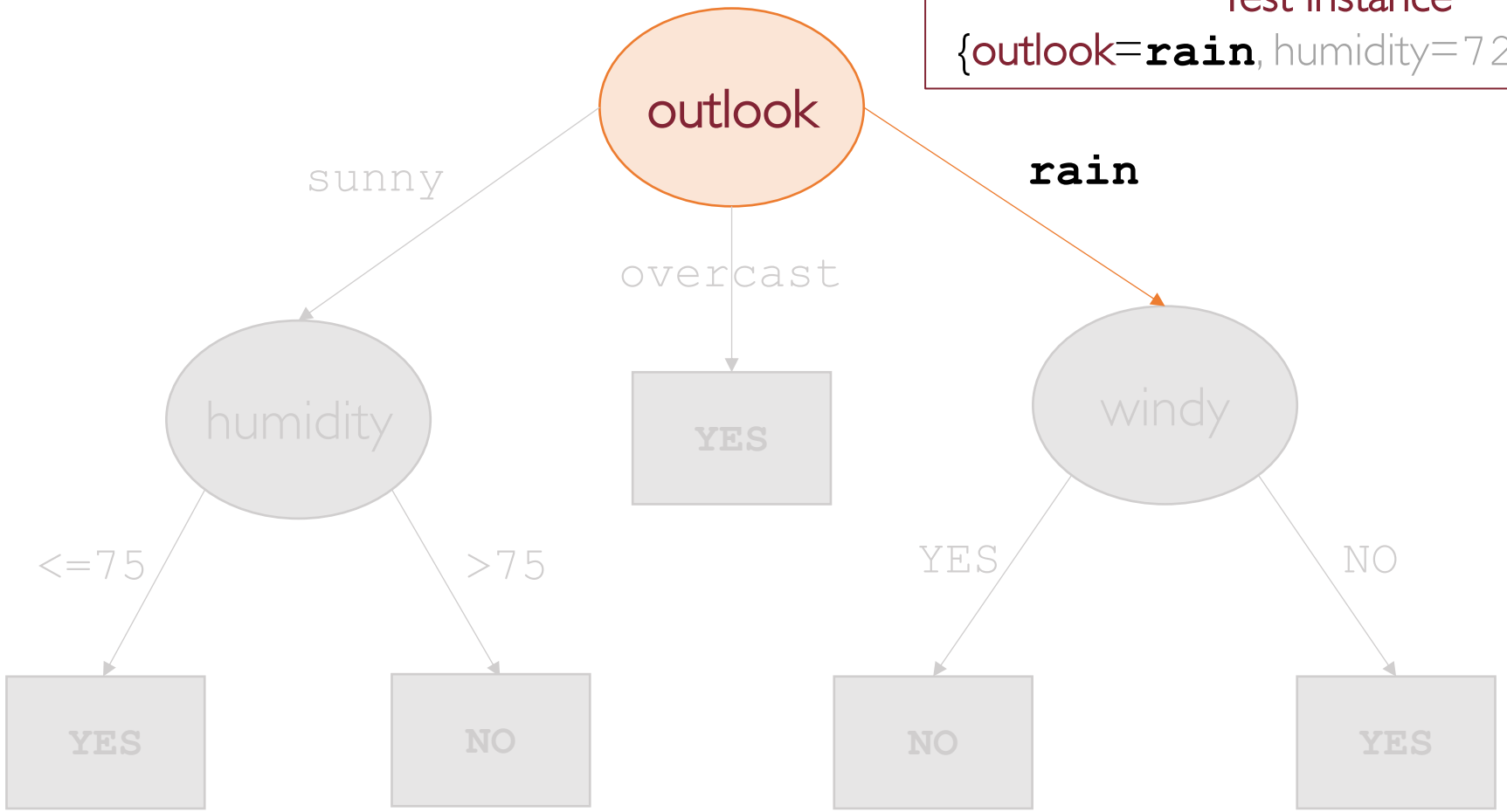

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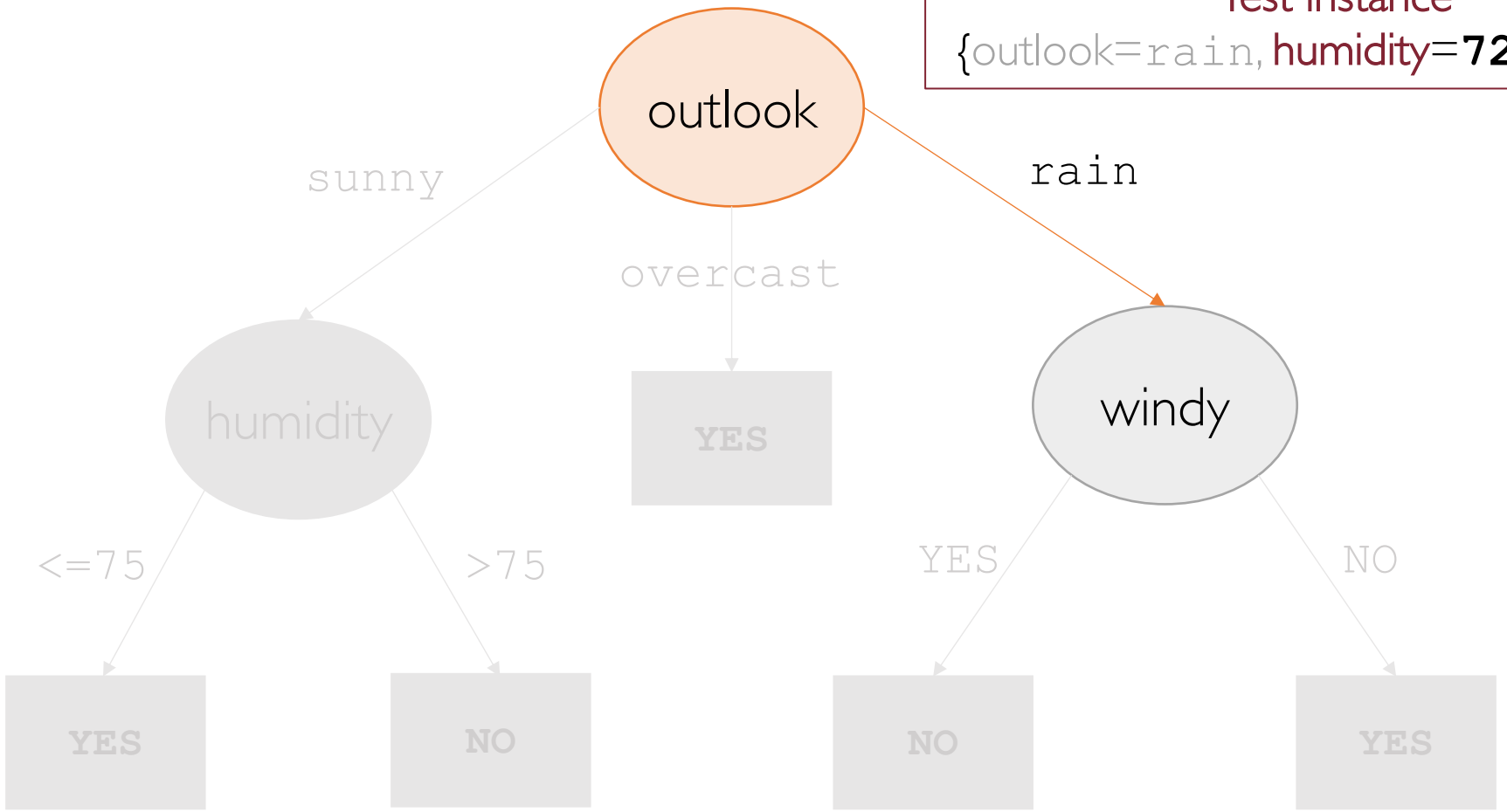

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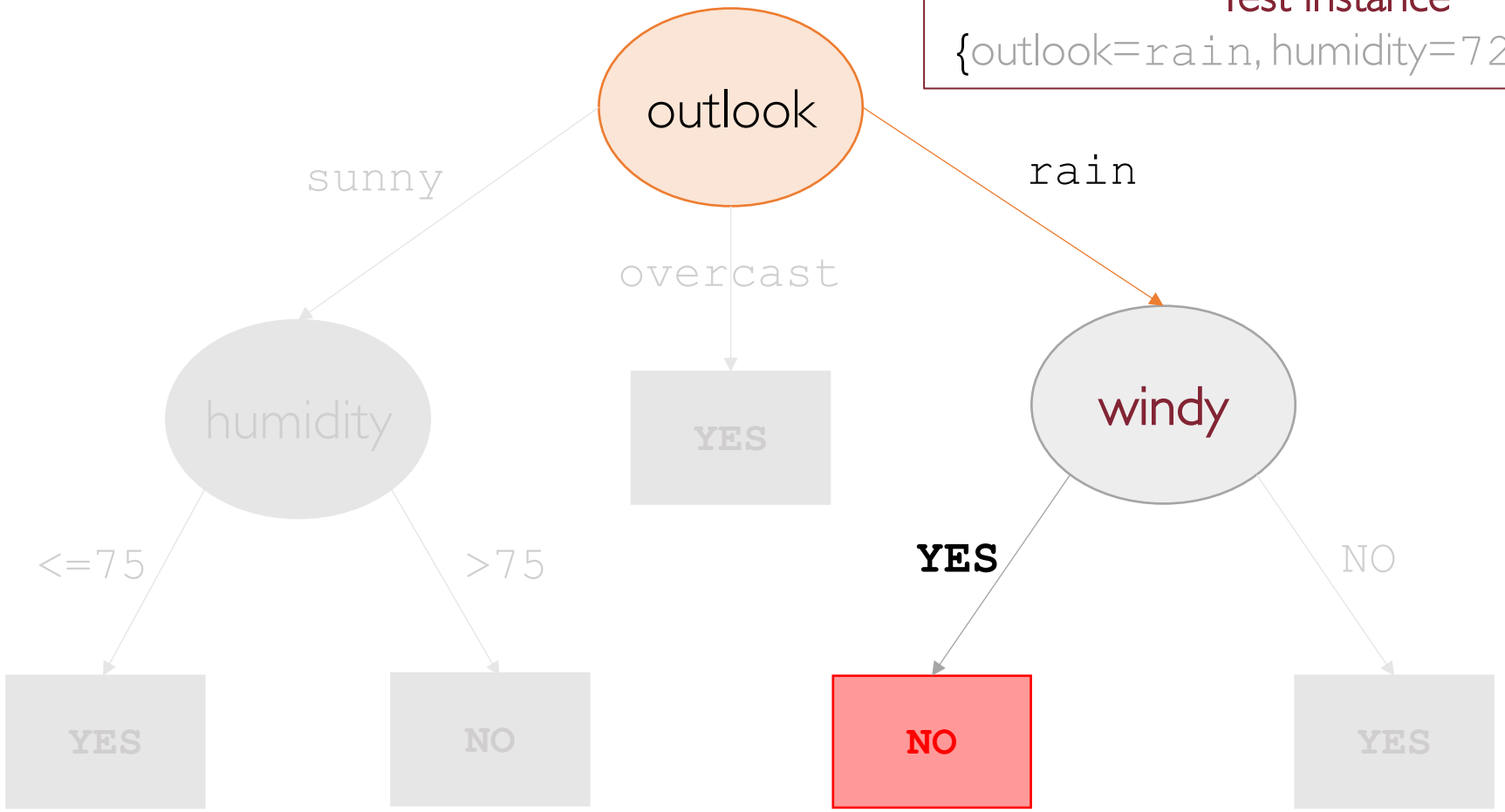

A Bit of Notation

$\mathcal{X} \subseteq \mathbb{R}^n$ input feature space

$\mathcal{Y}$ output space

$\mathcal{Y} \subseteq \mathbb{R}$ real-value label (regression)

$\mathcal{Y} = \{1, \ldots, k\}$ discrete-value label (k-ary classification)

$(\mathbf{x}_i, y_i)$ *i*-th labeled instance

$\mathbf{x}_i = (x_{i,1}, \ldots, x_{i,n}) \in \mathcal{X}$ *n*-dimensional feature vector of the *i*-th instance

$y_i \in \mathcal{Y}$ label of the *i*-th instance

$\mathcal{D} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$ dataset of *m* i.i.d. labeled instances

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- Example:
  - Suppose we split the input feature space in 2 regions: R_1 and R_2 and the response mean as computed from $R_1 = 10$ and $R_2 = 20$
  - For any $\mathbf{x}$ belonging to R_1 (R_2) will be predicted 10 (20)

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- In theory, partitions could have *any* shape

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$$\text{RSS} = \sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2$$

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The mean computed from observations in R_j

Discrete vs. Continuous Inputs

Discrete Inputs

(e.g., boolean)

One branch for each value

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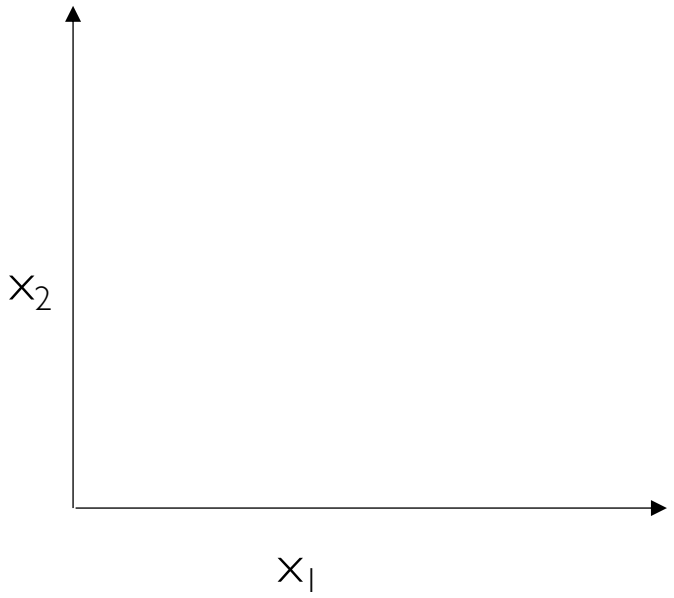

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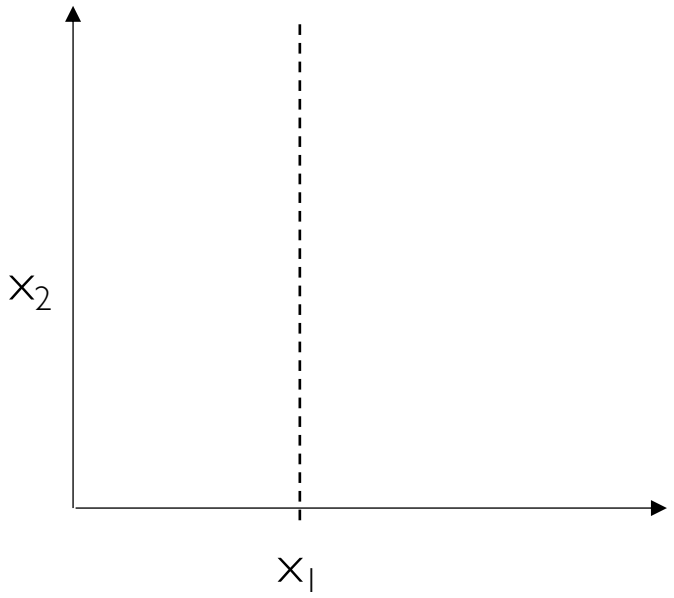

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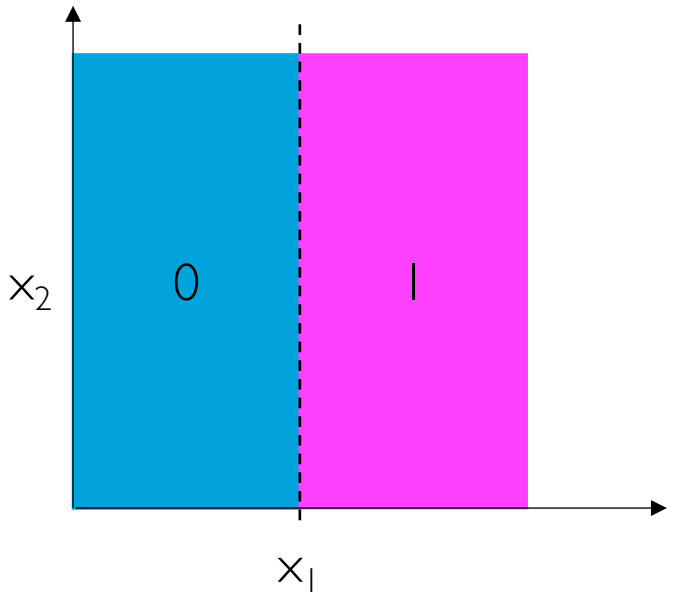

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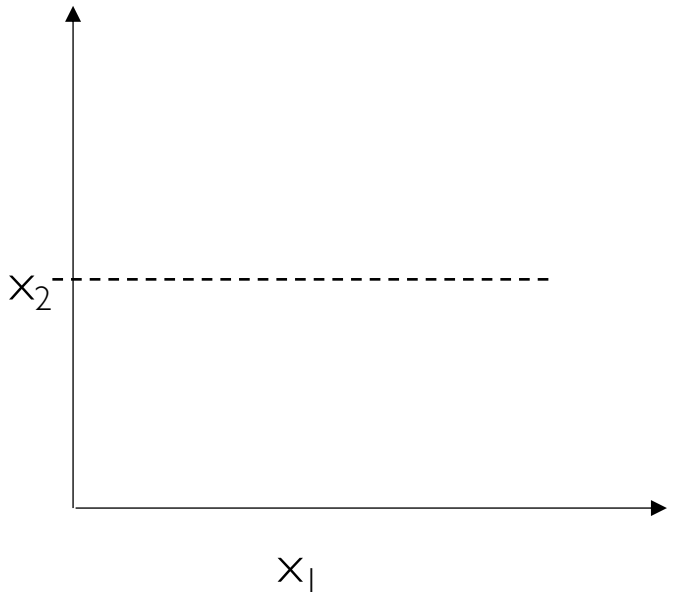

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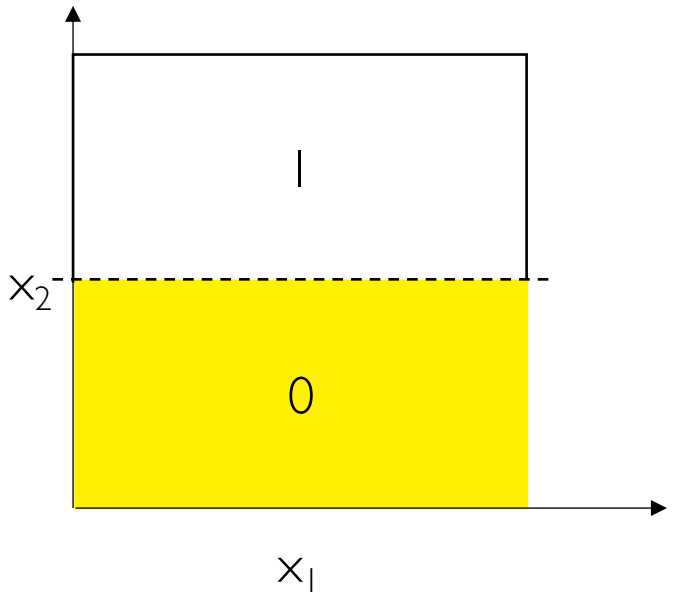

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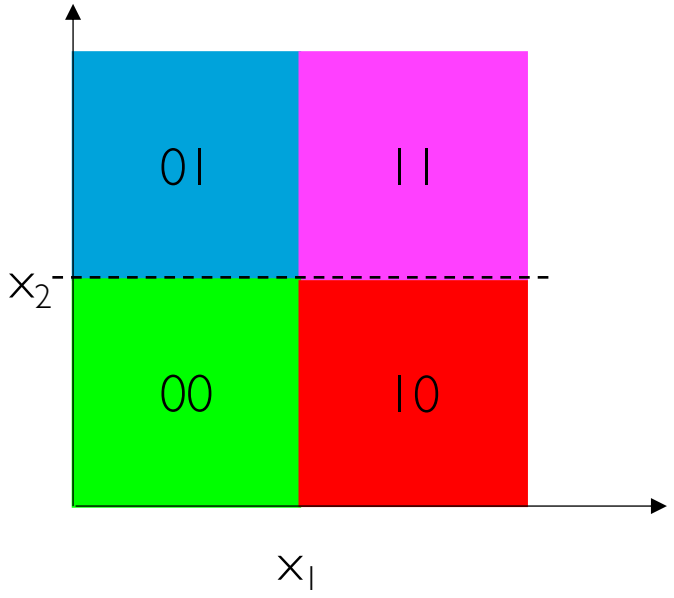

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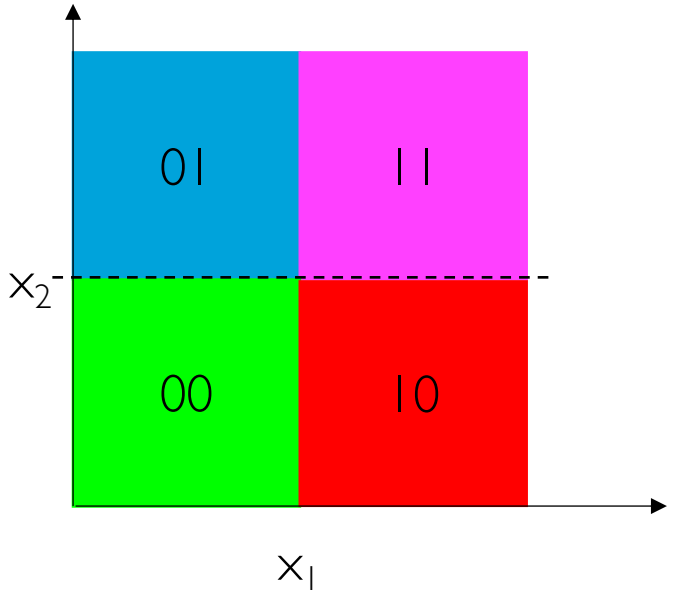

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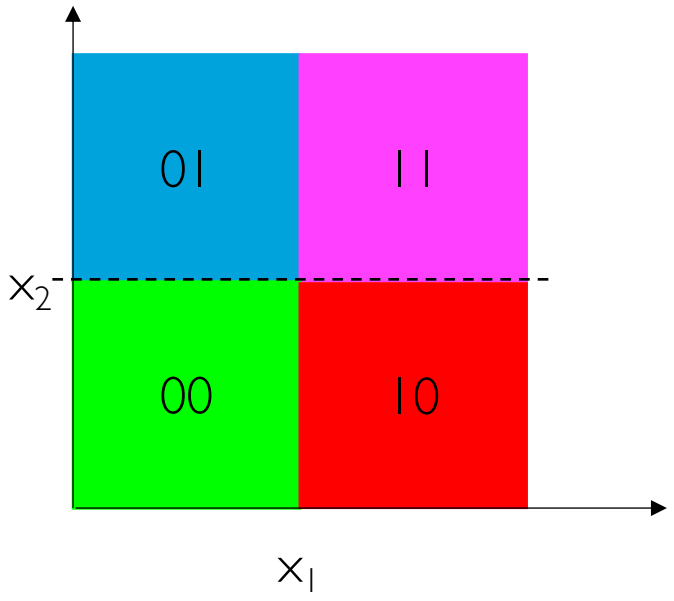

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Test x_j <= s and create 2 branches

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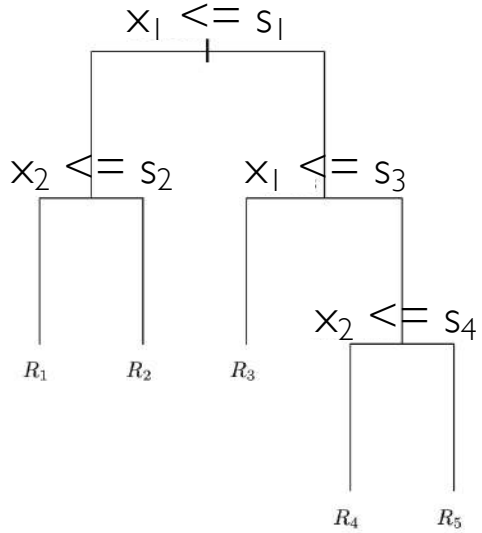

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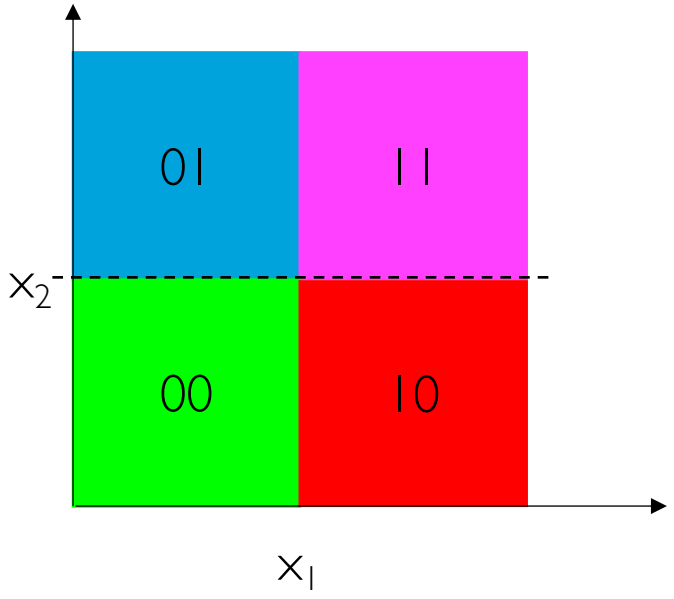

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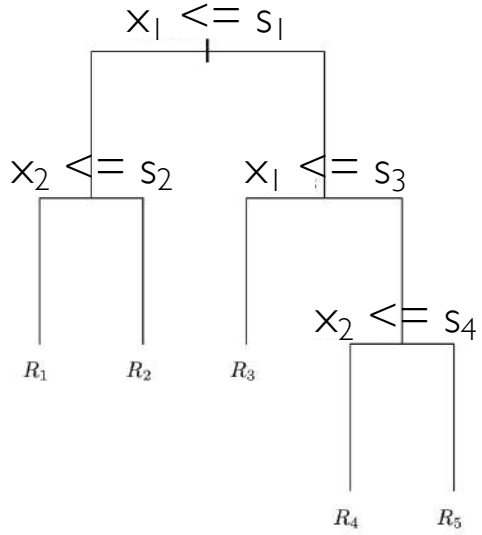

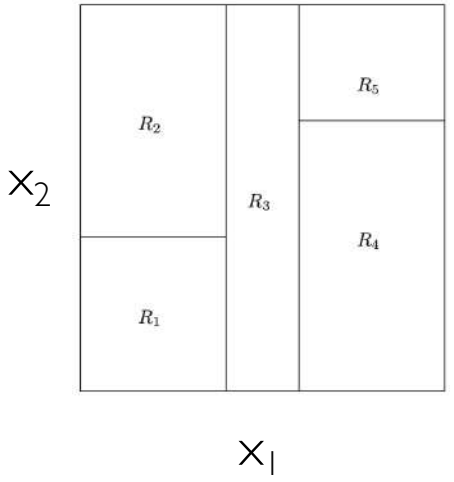

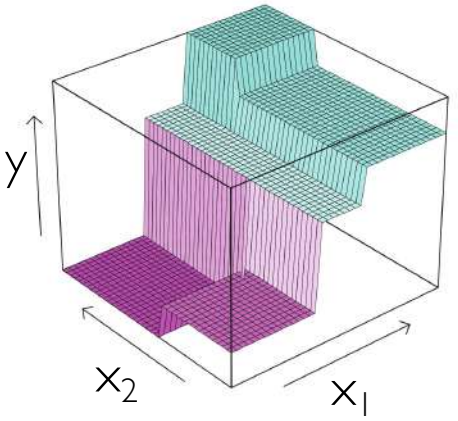

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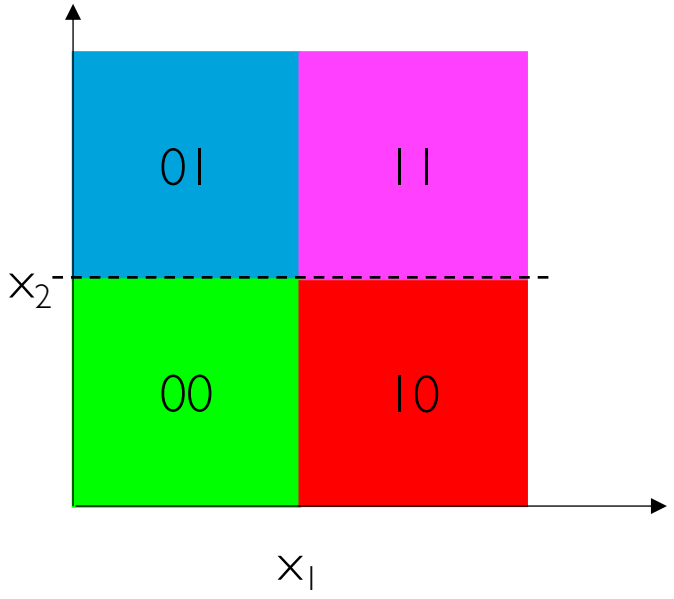

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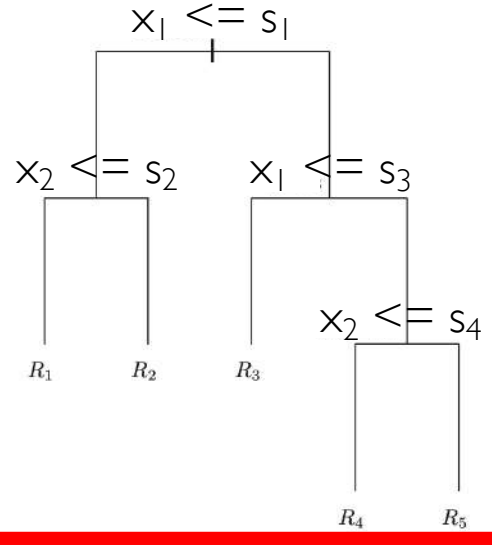

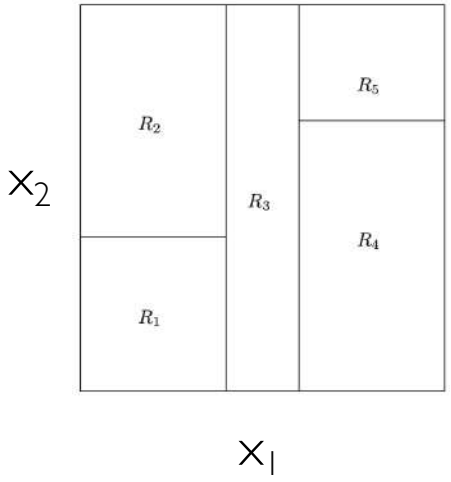

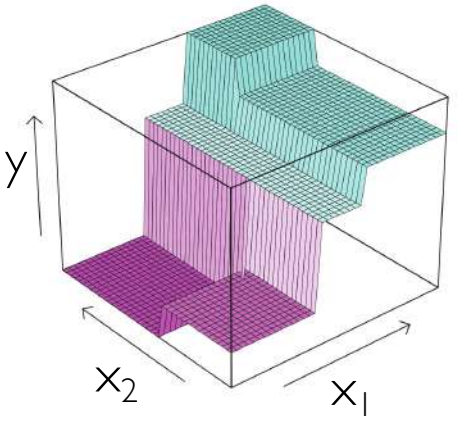

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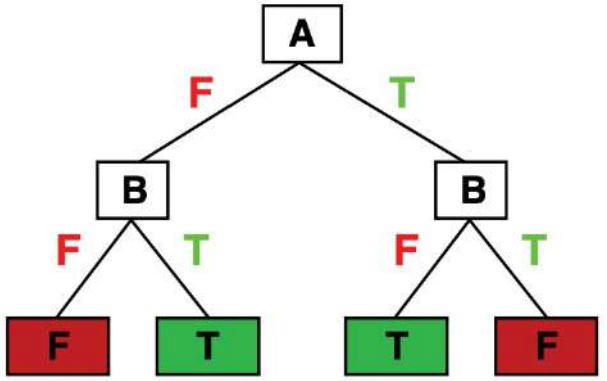

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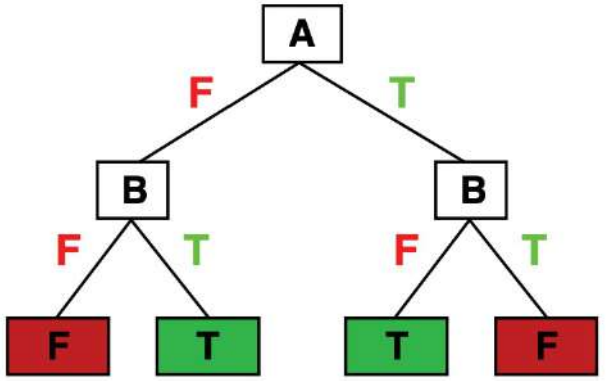

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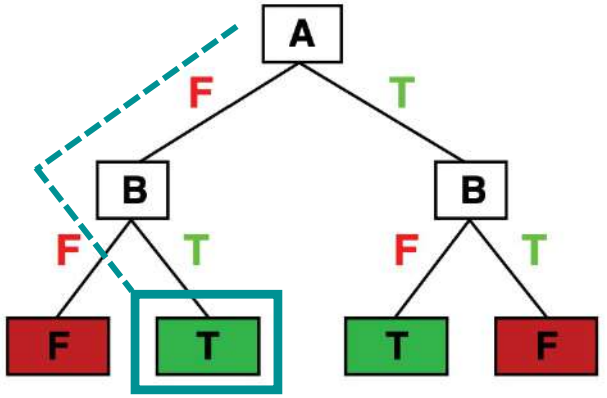

Each row of the truth table maps to a root-to-leaf path on the tree

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Such a tree will have one dedicated root-to-leaf path for each training instance

Expressiveness

Continuous Inputs/Continuous Outputs

Decision Trees can *approximate* any function arbitrarily closely

Trivially, there exists a consistent decision tree for any training set

Such a tree will have one dedicated root-to-leaf path for each training instance

Of course, this tree clearly overfits the training data and it will not generalize to unseen examples (needs regularization)

Hypothesis Space

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Each boolean function of n boolean inputs is represented by a truth table

x_1	x_1	…	x_n	y
0	0	…	0	
1	0	…	0	
1	1	…	0	
…	…	…	…	
…	…	…	…	
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2^n rows

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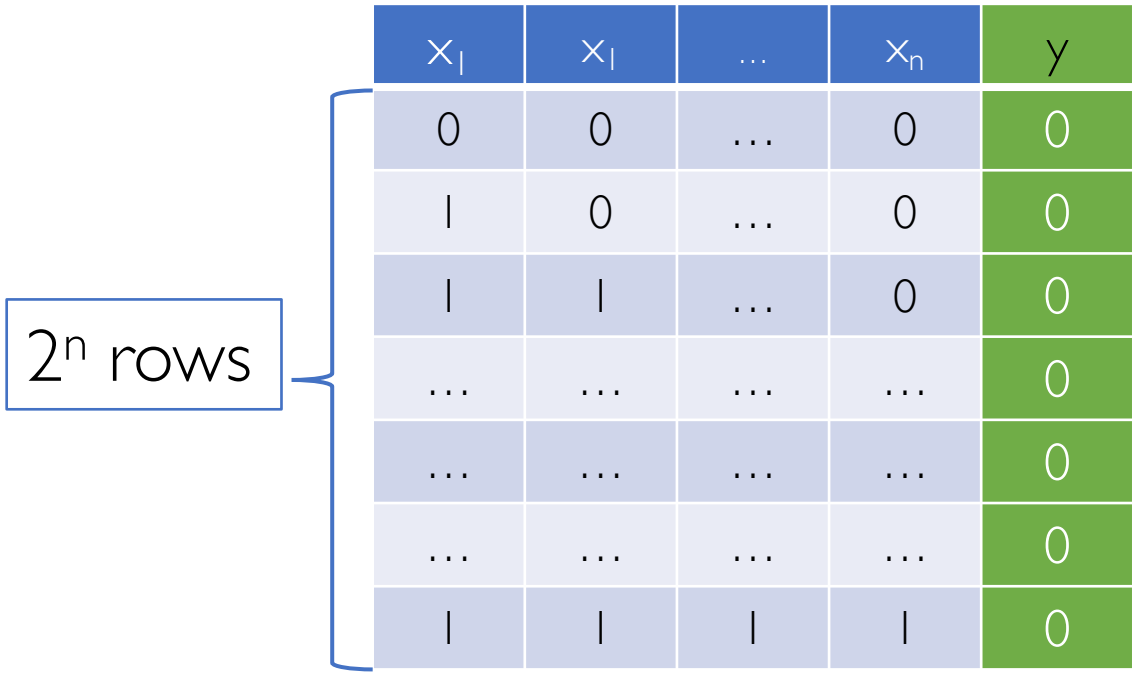
2^n rows

For each input y = 0 or 1

Hypothesis Space

A possible boolean function is the one which will output all 0s



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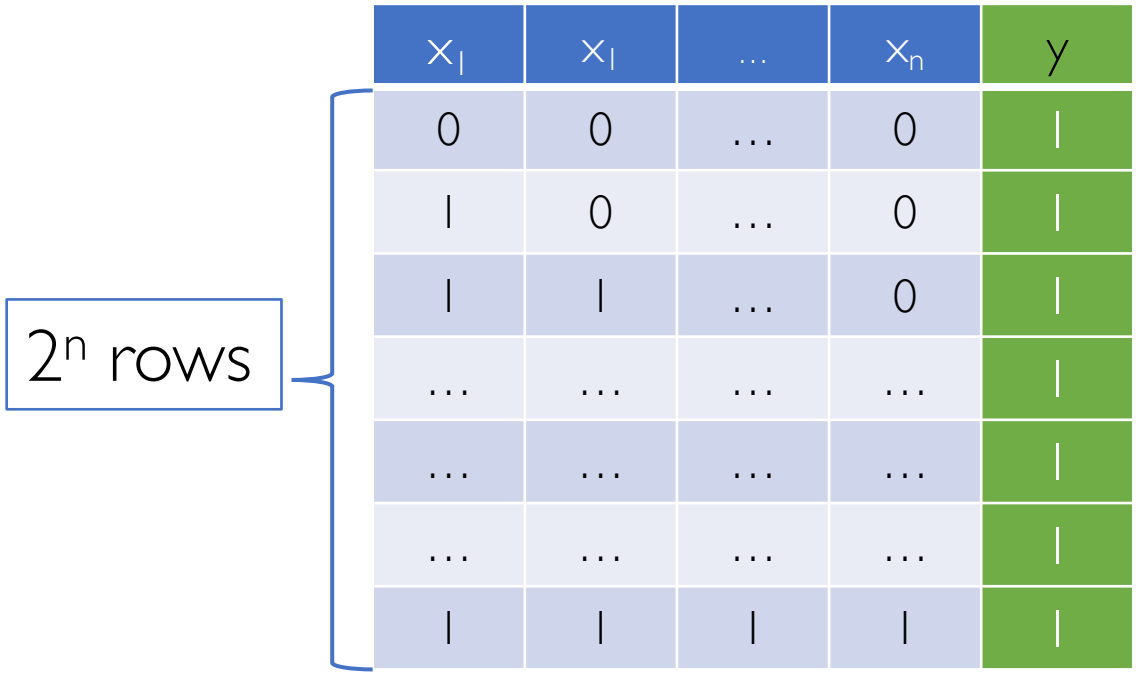
Hypothesis Space

Another possible boolean function is the one which will output all 1s



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Larger hypothesis space means also it is generally harder for the learning algorithm to find the best hypothesis (larger space to explore)

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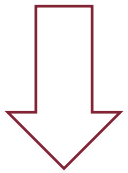

Solution

Top-Down greedy heuristic Recursive Binary Splitting

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- Greedy strategy:
  - At each step, the best "local" split is made
  - Looking ahead might result in a different split, which leads to a better tree

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$$\{x_{i,f} \leq s\}$$

is the region of the feature space in which the *f*-th feature takes on values less than or equal to *s*

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Goal: find the pair (f, s) which minimizes the following

$$\sum_{i:\ \mathbf{x}_i \in R_{\text{left}}(f,s)} (y_i - \hat{y}_{R_{\text{left}}})^2 + \sum_{i:\ \mathbf{x}_i \in R_{\text{right}}(f,s)} (y_i - \hat{y}_{R_{\text{right}}})^2$$

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- Each time, we reduce the RSS

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  - That would correspond to an overfitted tree
- Possible stopping criteria (tree grows until):
  - no region contains more than *N* observations
  - max depth of the tree is *D*
  - RSS is reduced by at least a threshold value *t*

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- At test time, an unseen instance follows a root-to-leaf path on the tree and ends up into a region R_j
- The prediction for that test instance will be the mean of the region R_j

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- Learning the optimal DT is NP-Complete: Recursive Binary Splitting algorithm is an effective greedy training heuristic
- Regression Trees:
  - Use Residual Sum of Squares (RSS) as splitting criterion
  - At inference time, predictions are the mean of the leaf observations