Big Data Computing

Master's Degree in Computer Science

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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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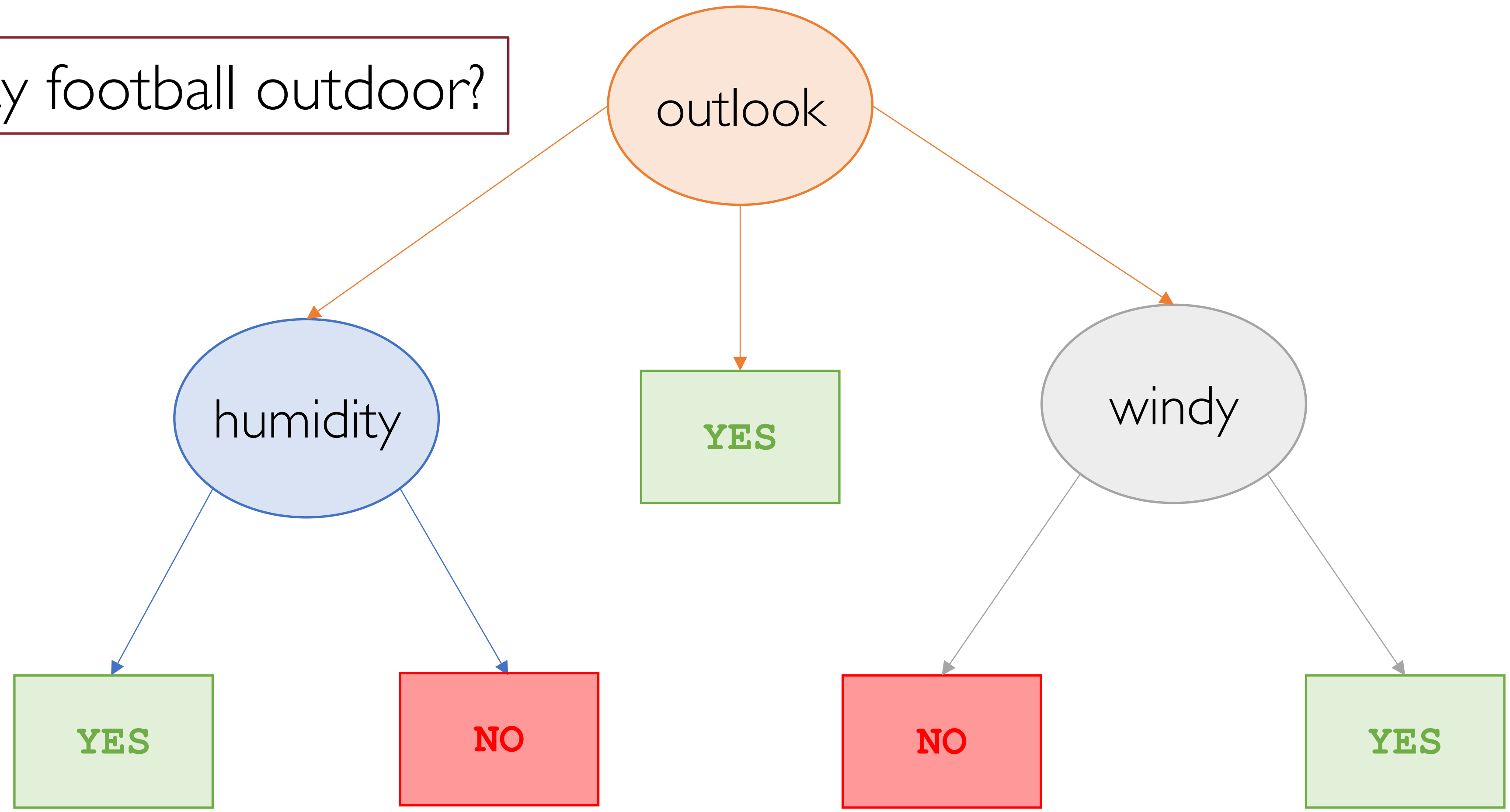
- A prediction is computed by taking the mean (regression) or the mode (classification) of the points in the region which the observation belongs
- The set of splitting rules can be represented as a tree (decision tree)
- Highly human-interpretable models

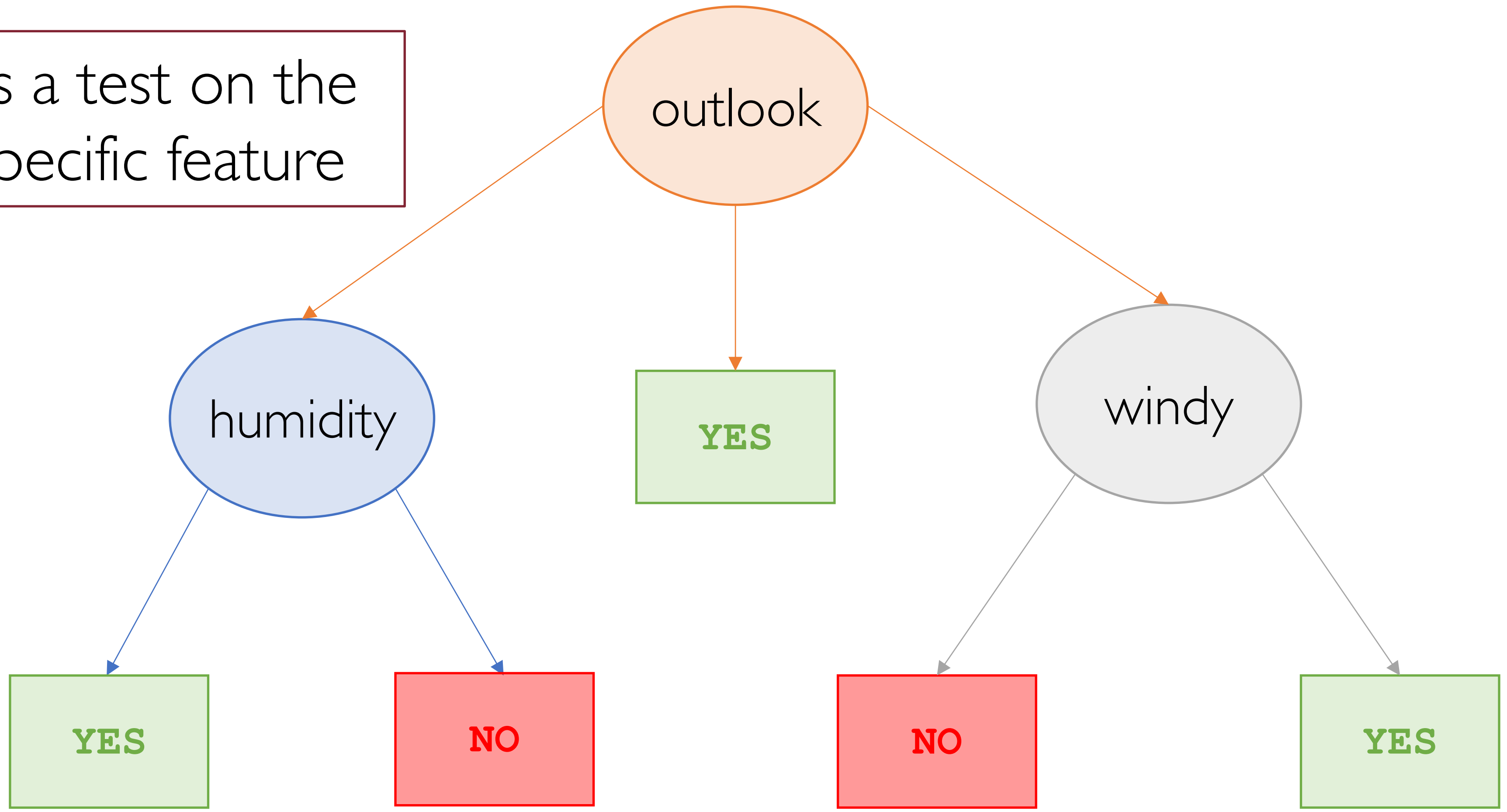
Decision Tree: An Example

Should we play football outdoor?



Decision Tree: An Example

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



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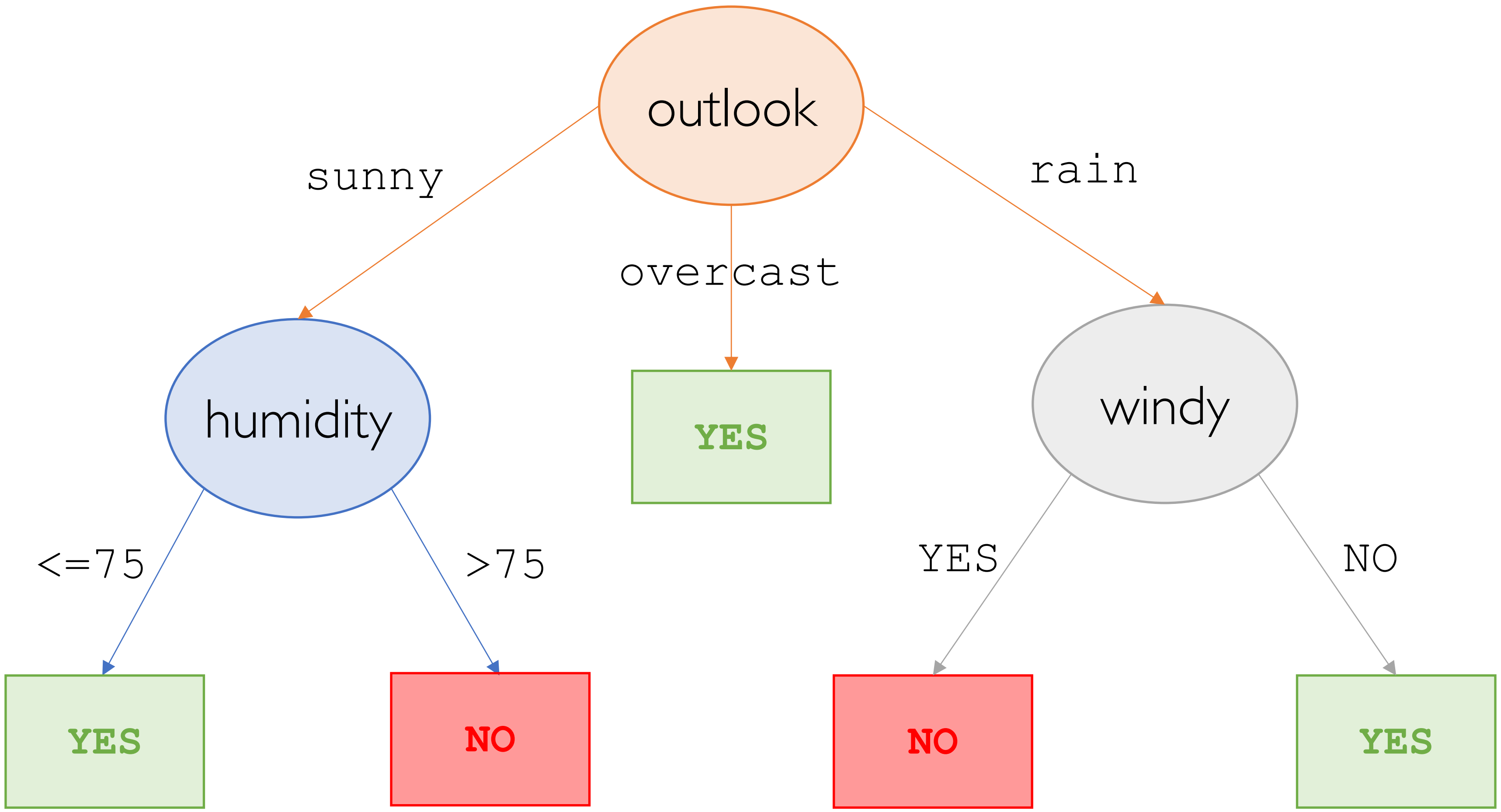

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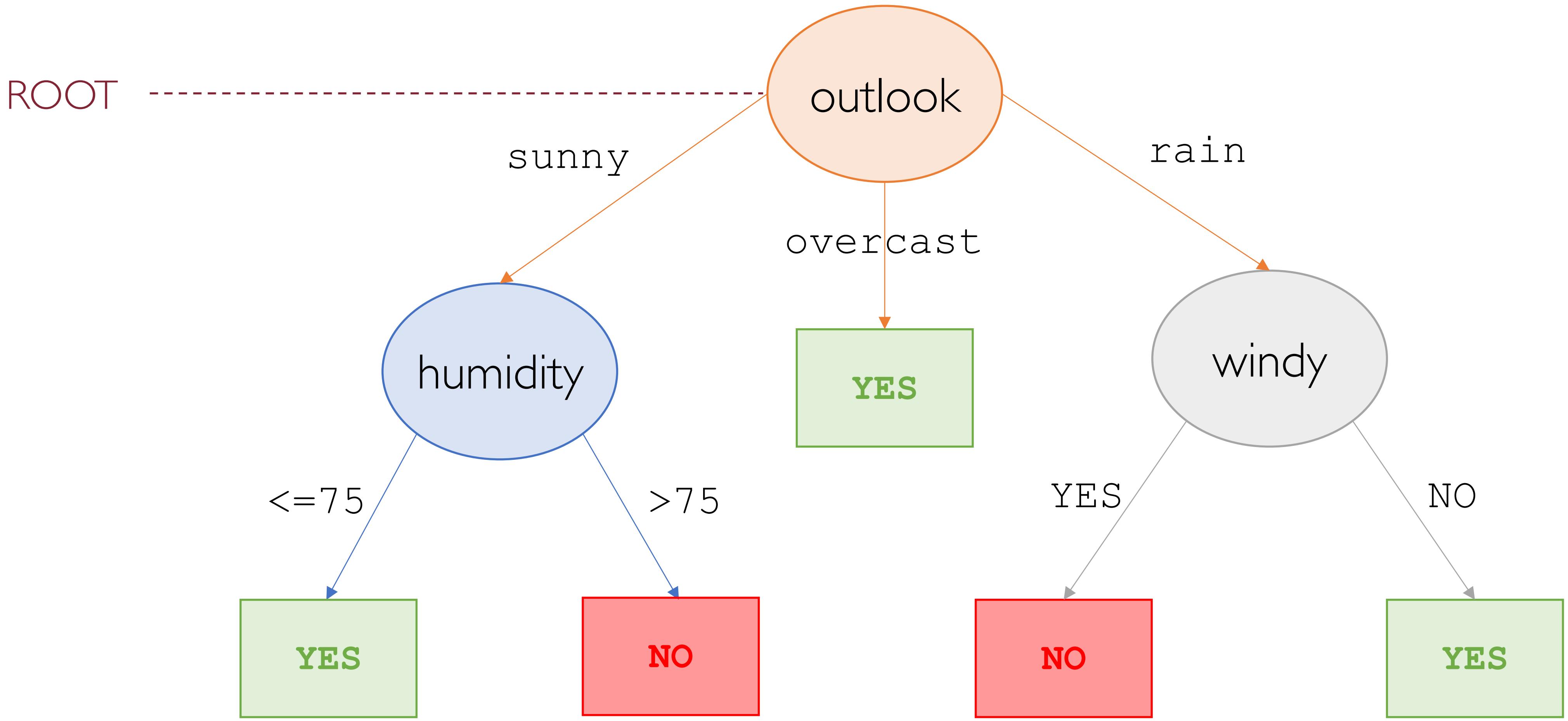

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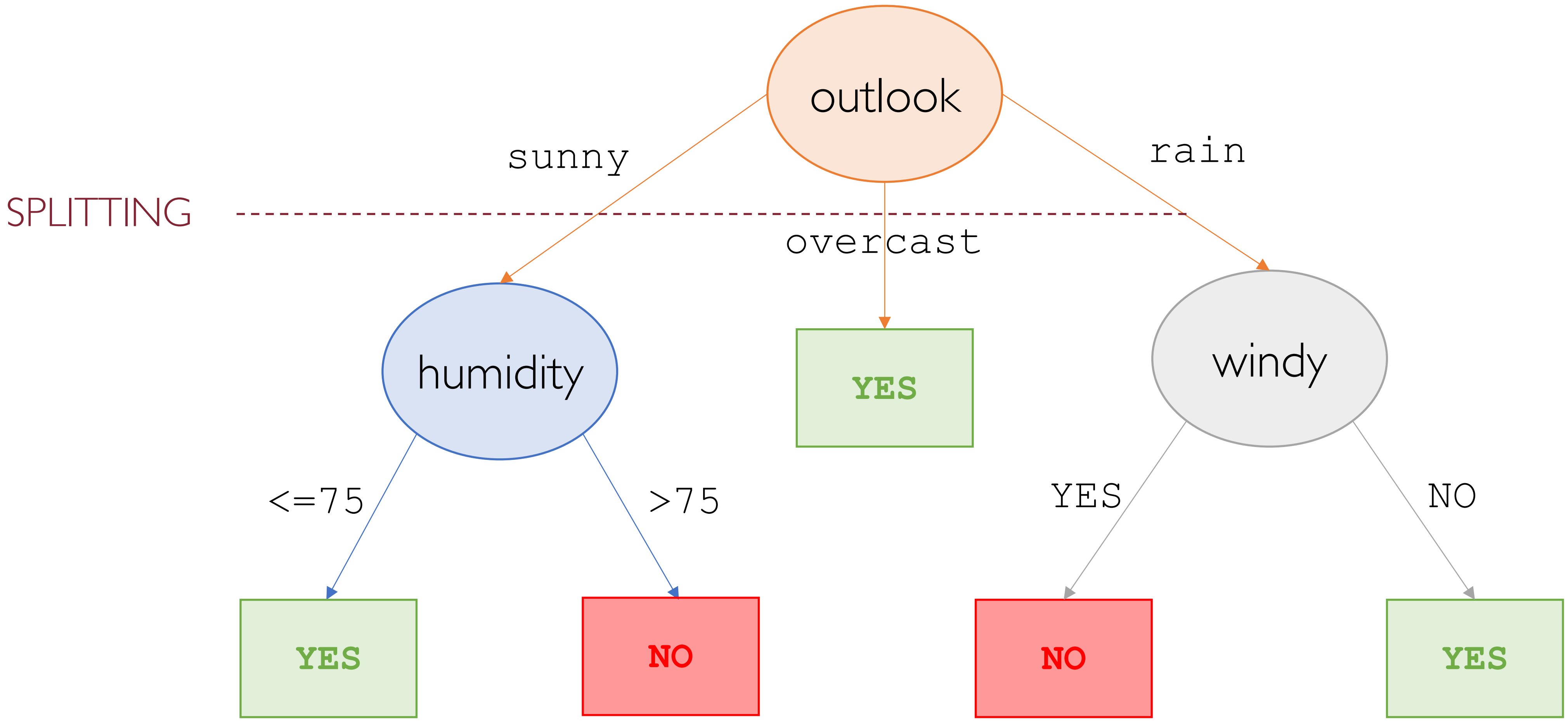

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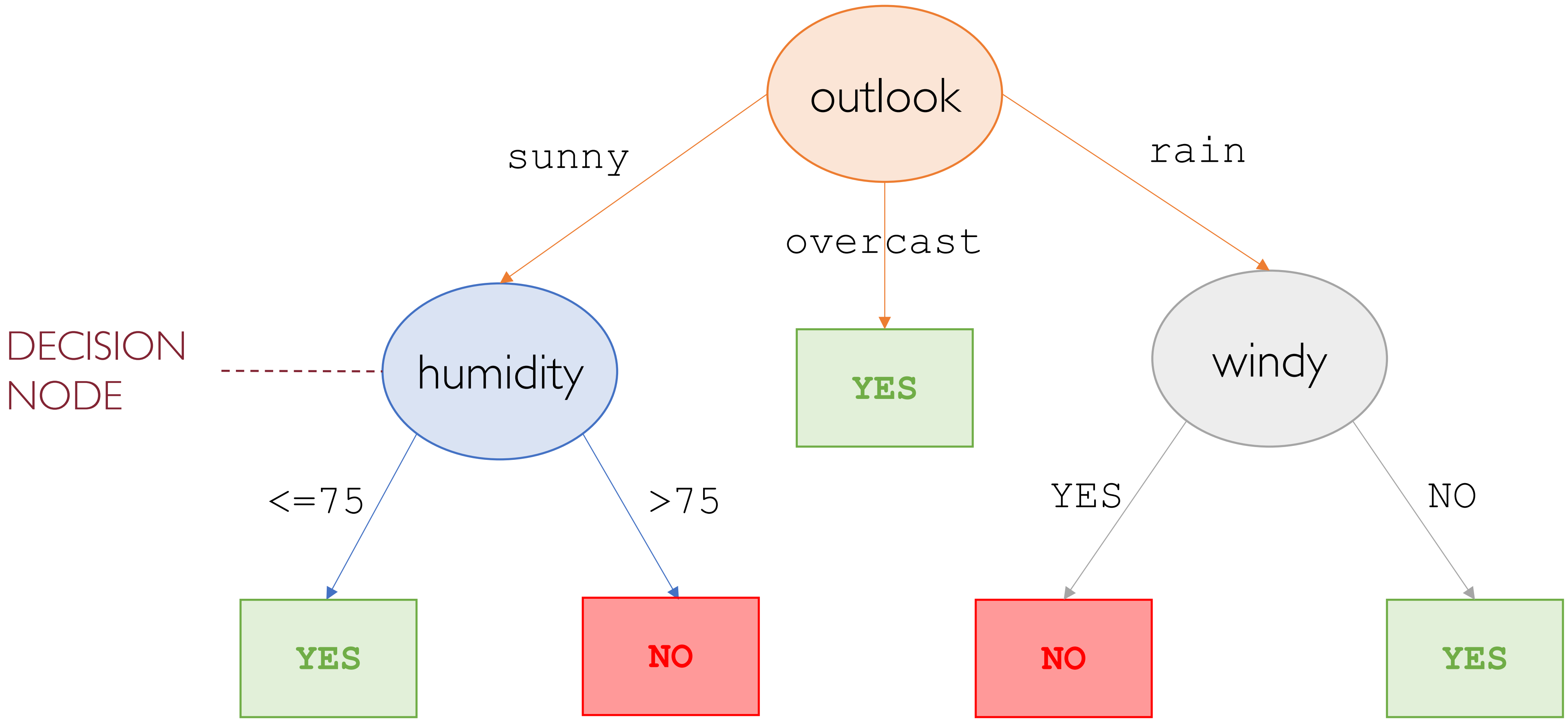

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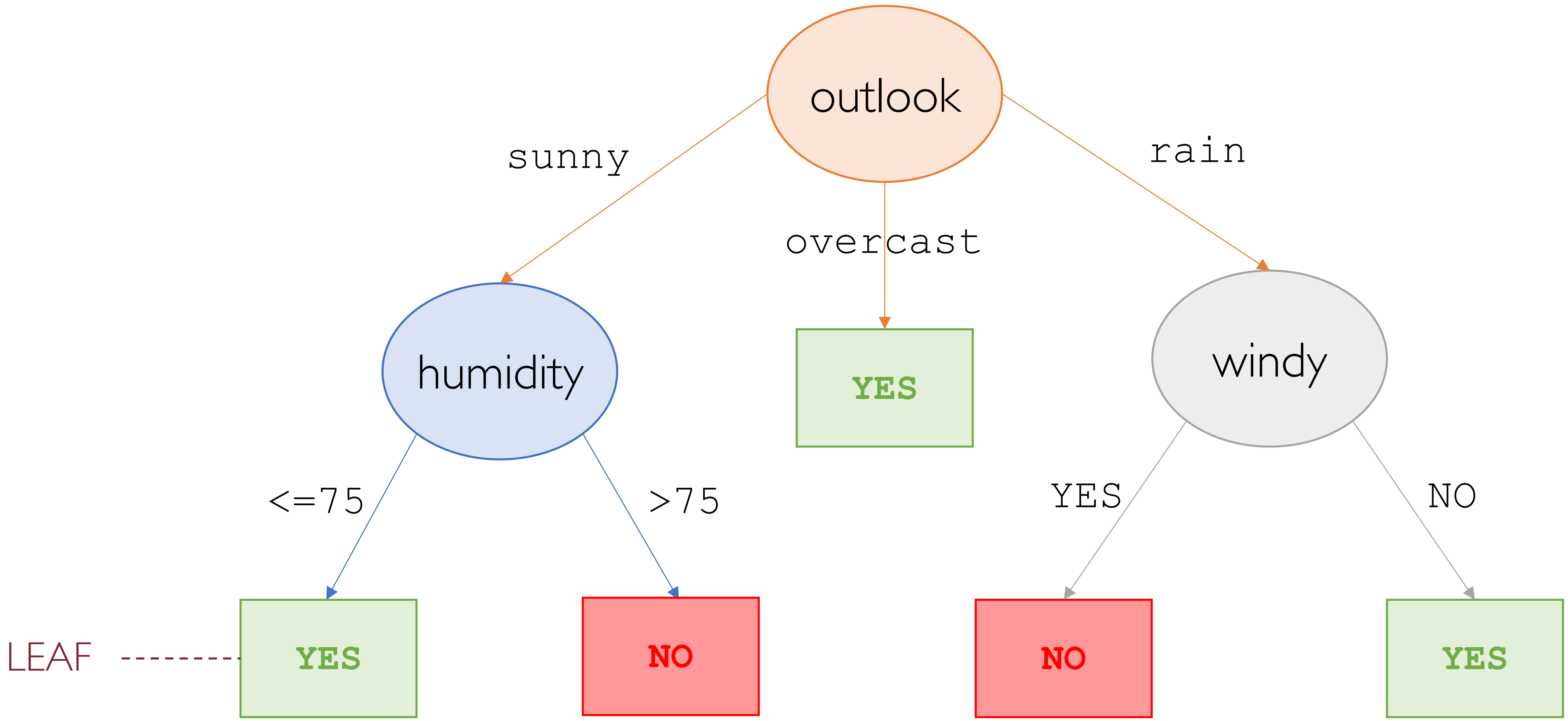

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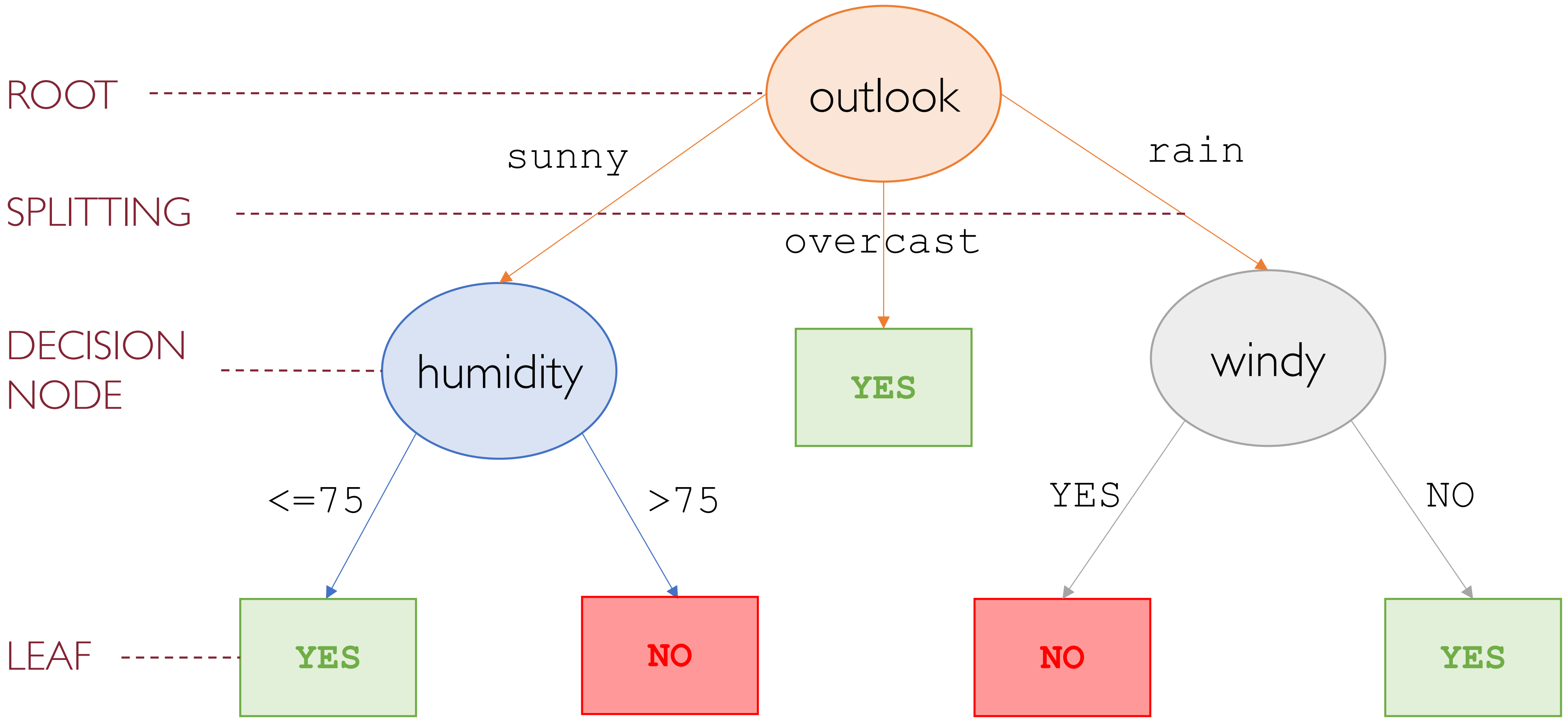

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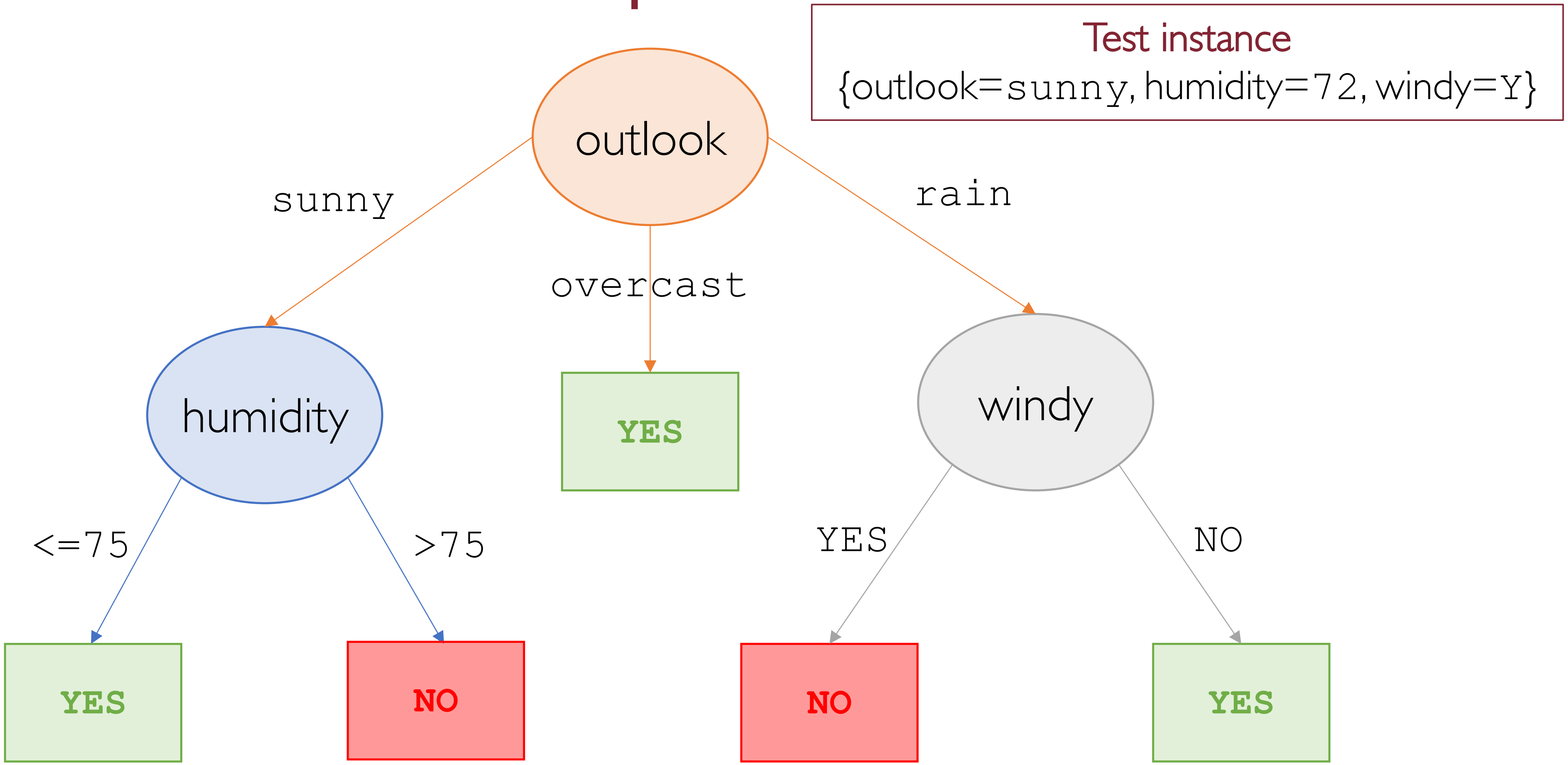

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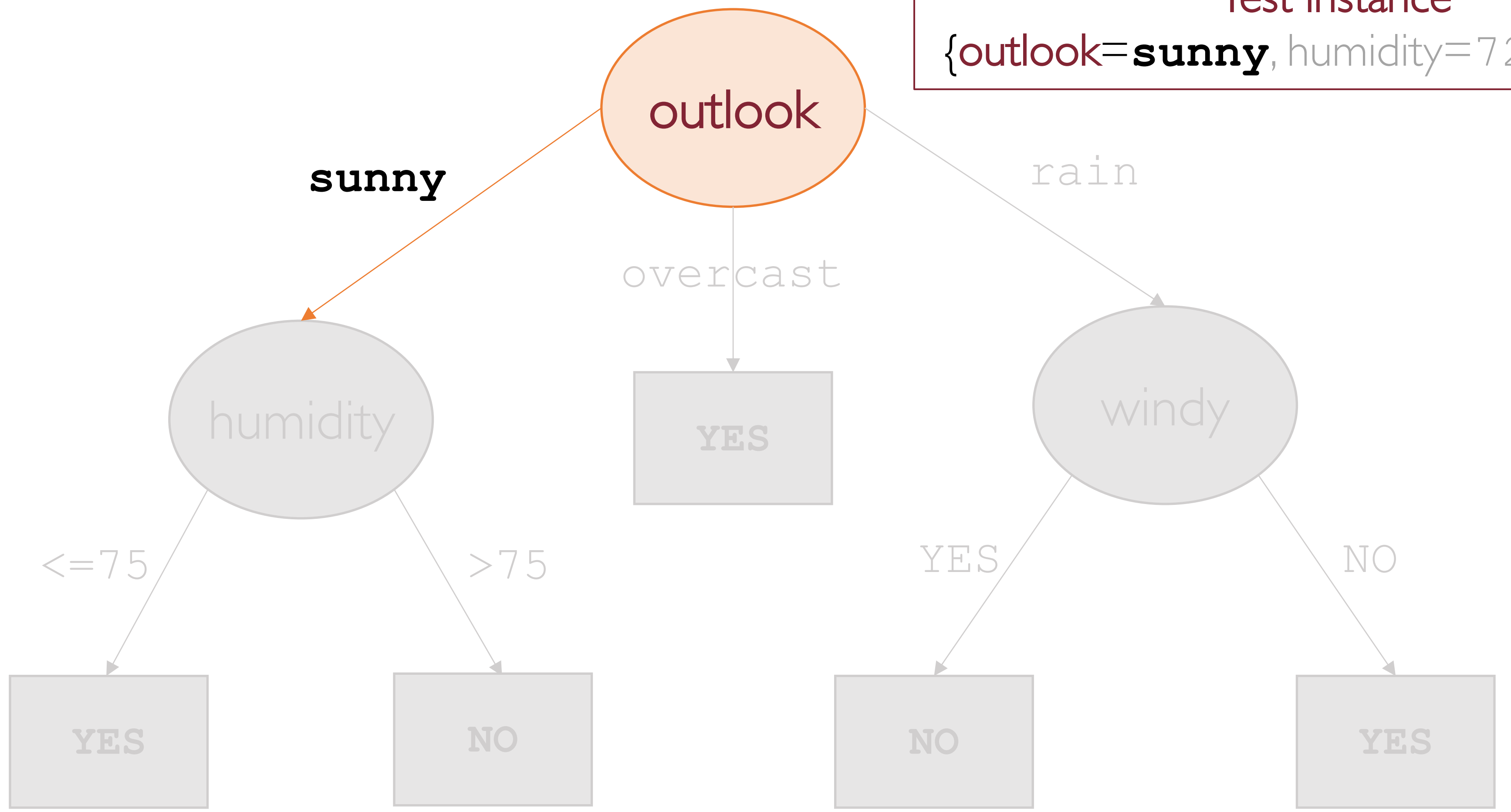

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{outlook=**sunny**, humidity=72, windy=Y}

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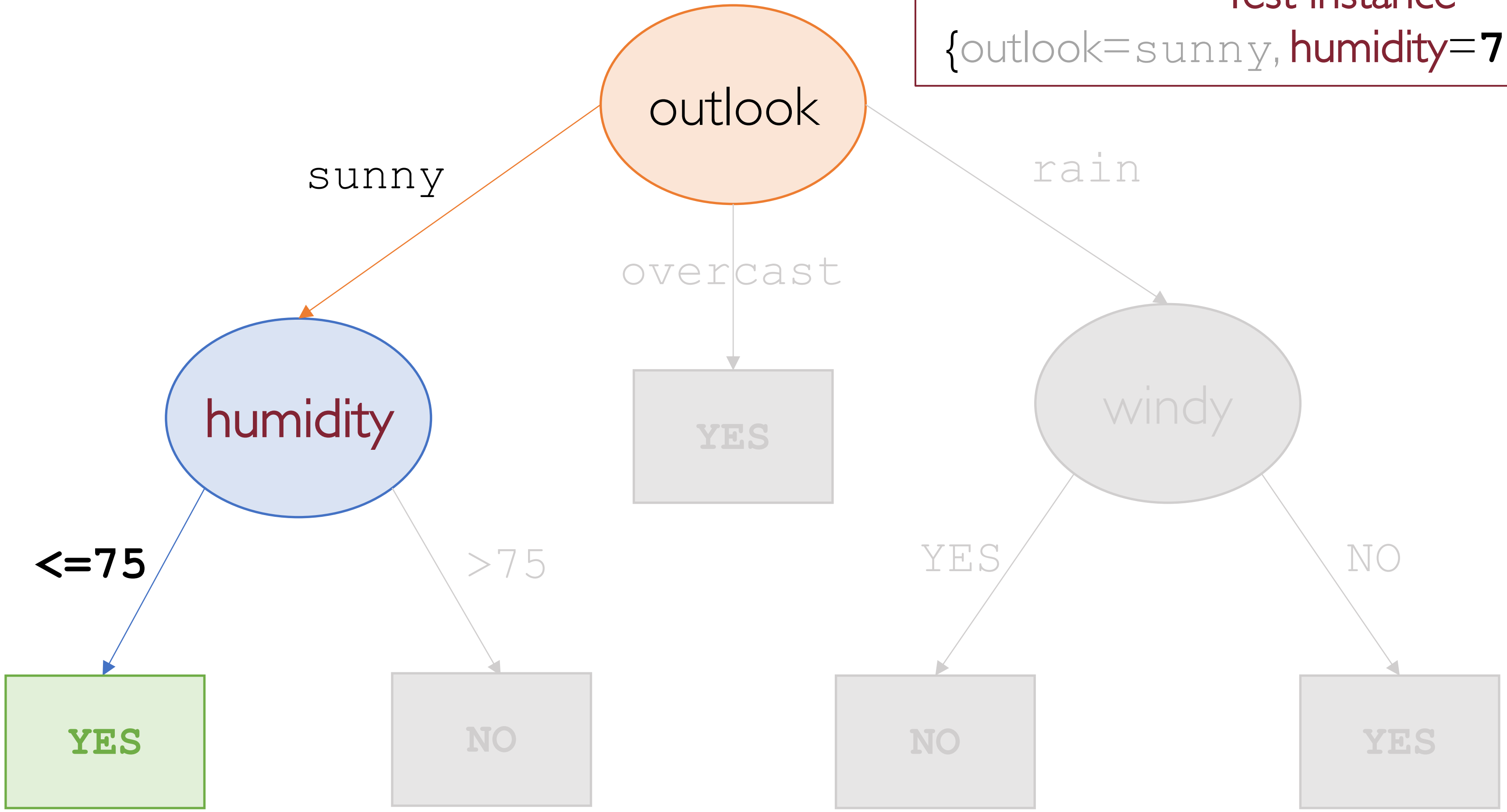
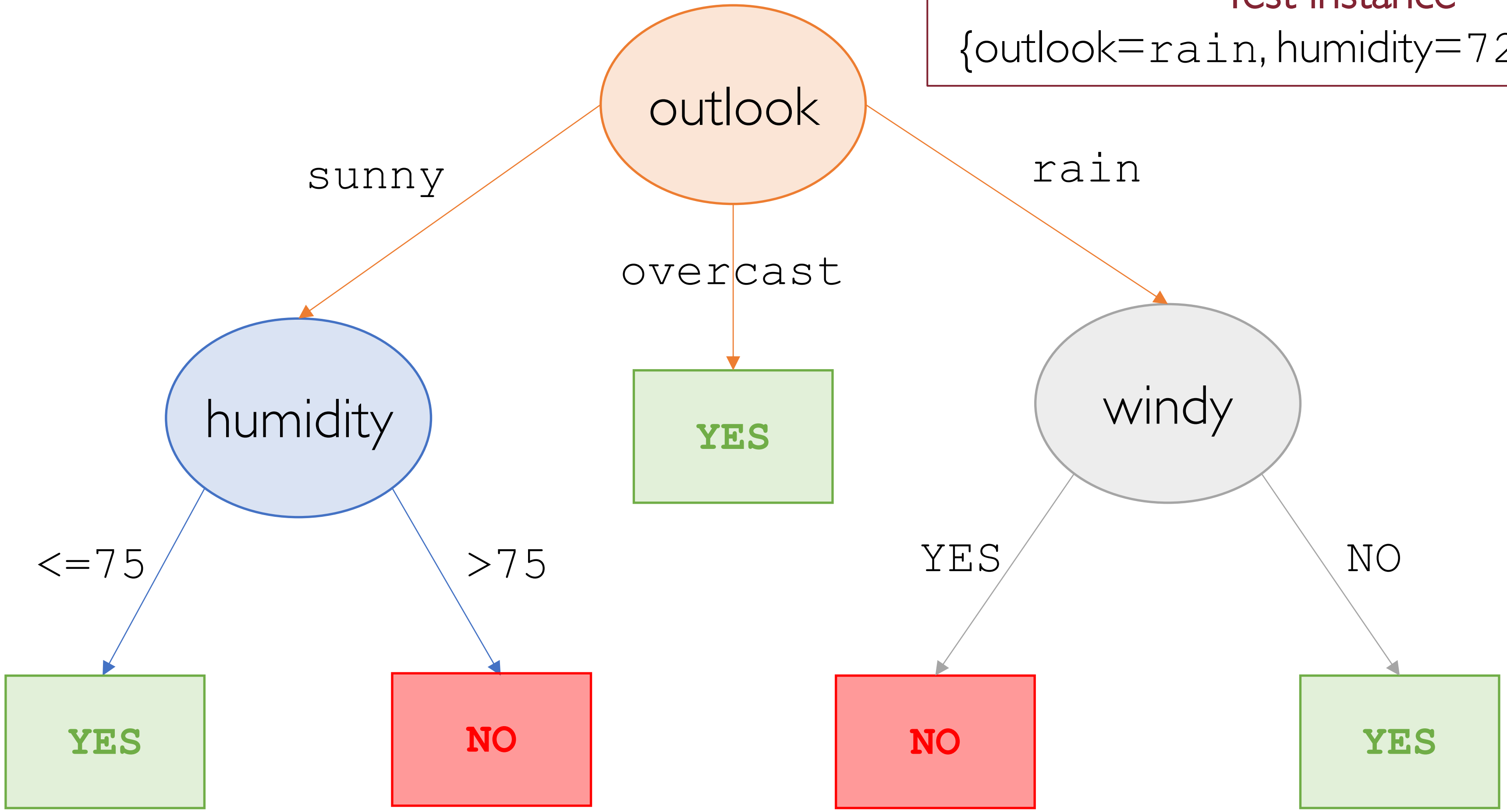


Decision Tree: An Example

Test instance
{outlook=`rain`, humidity=`72`, windy=`Y`}



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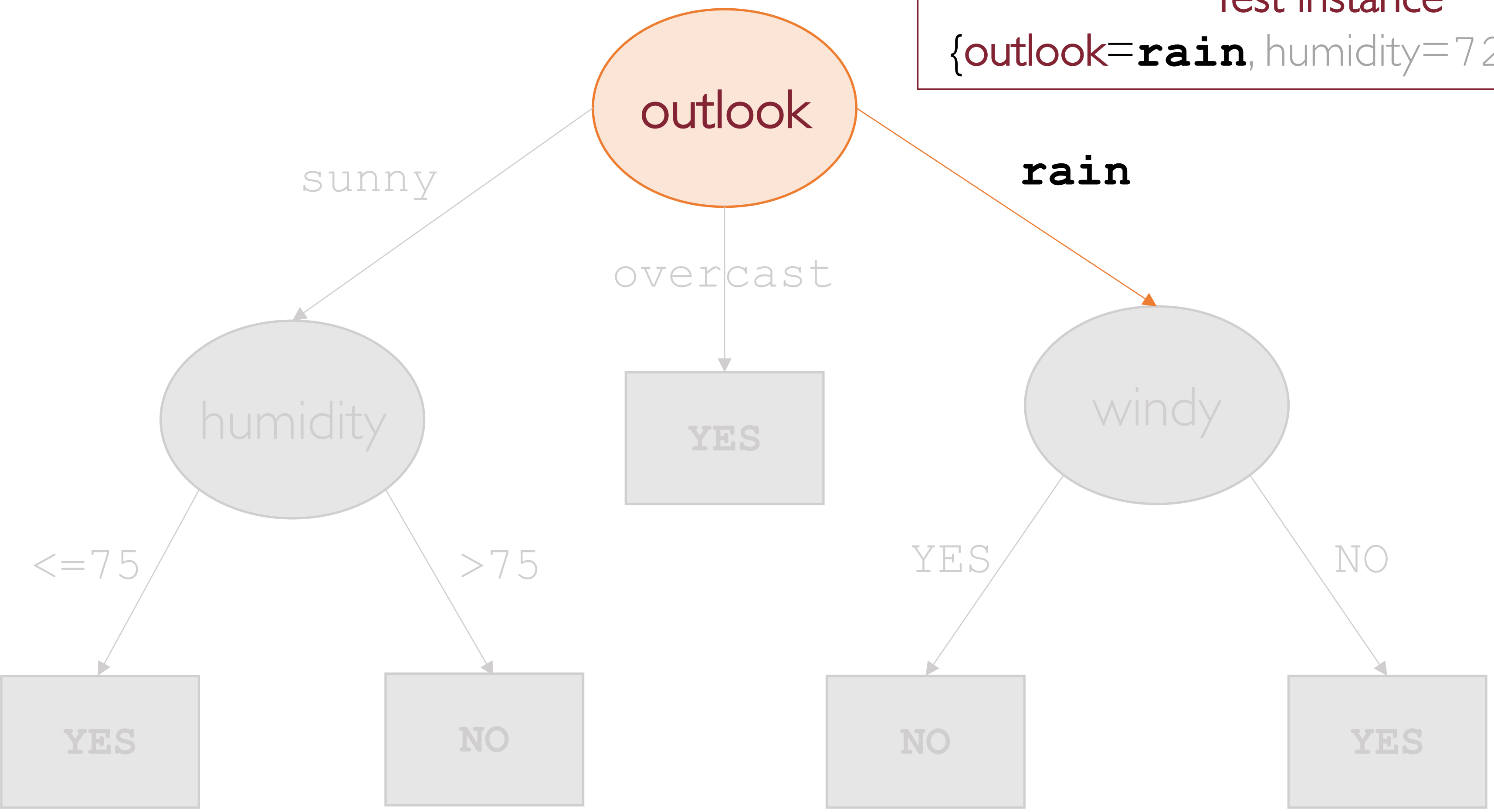

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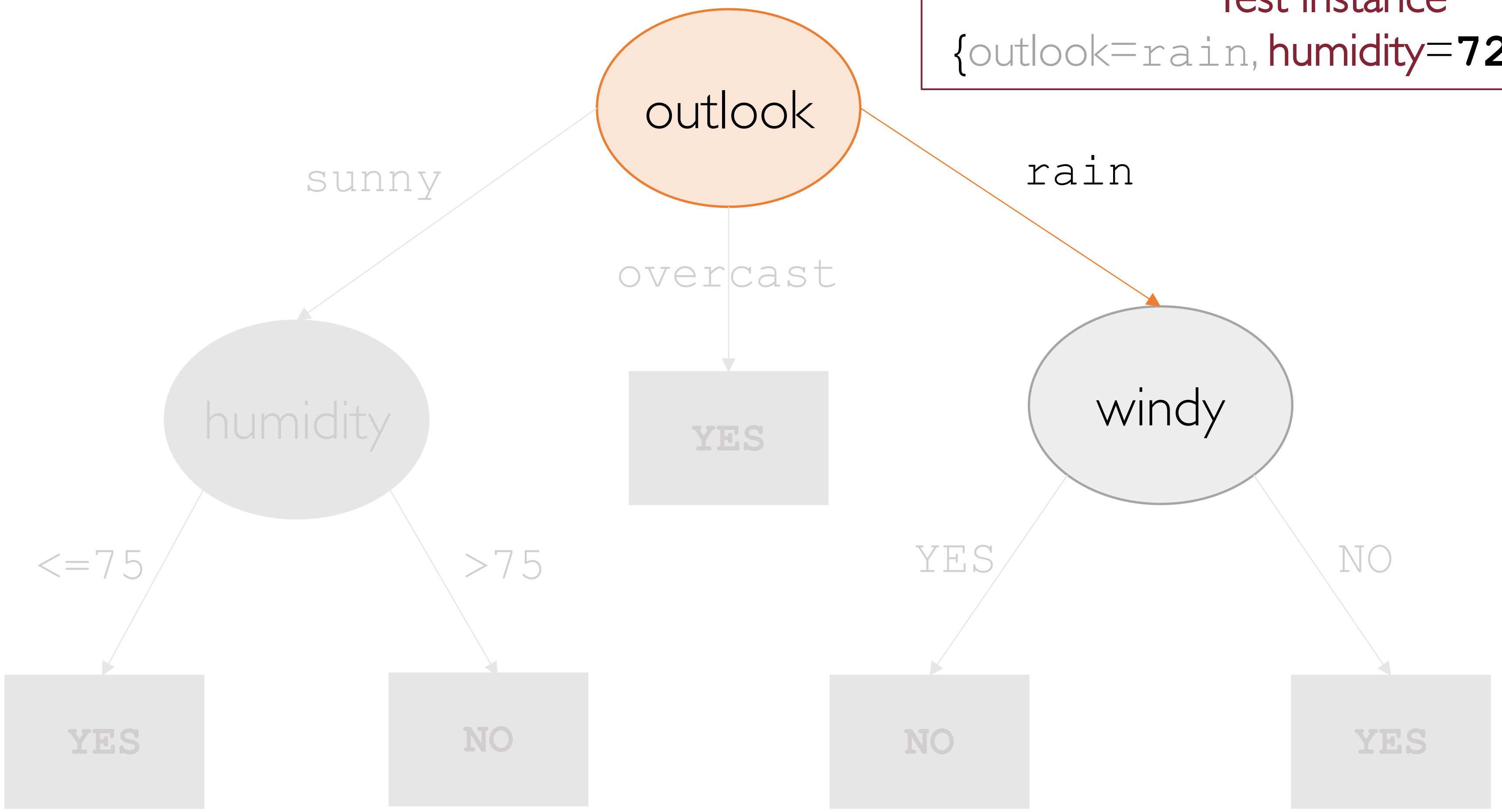

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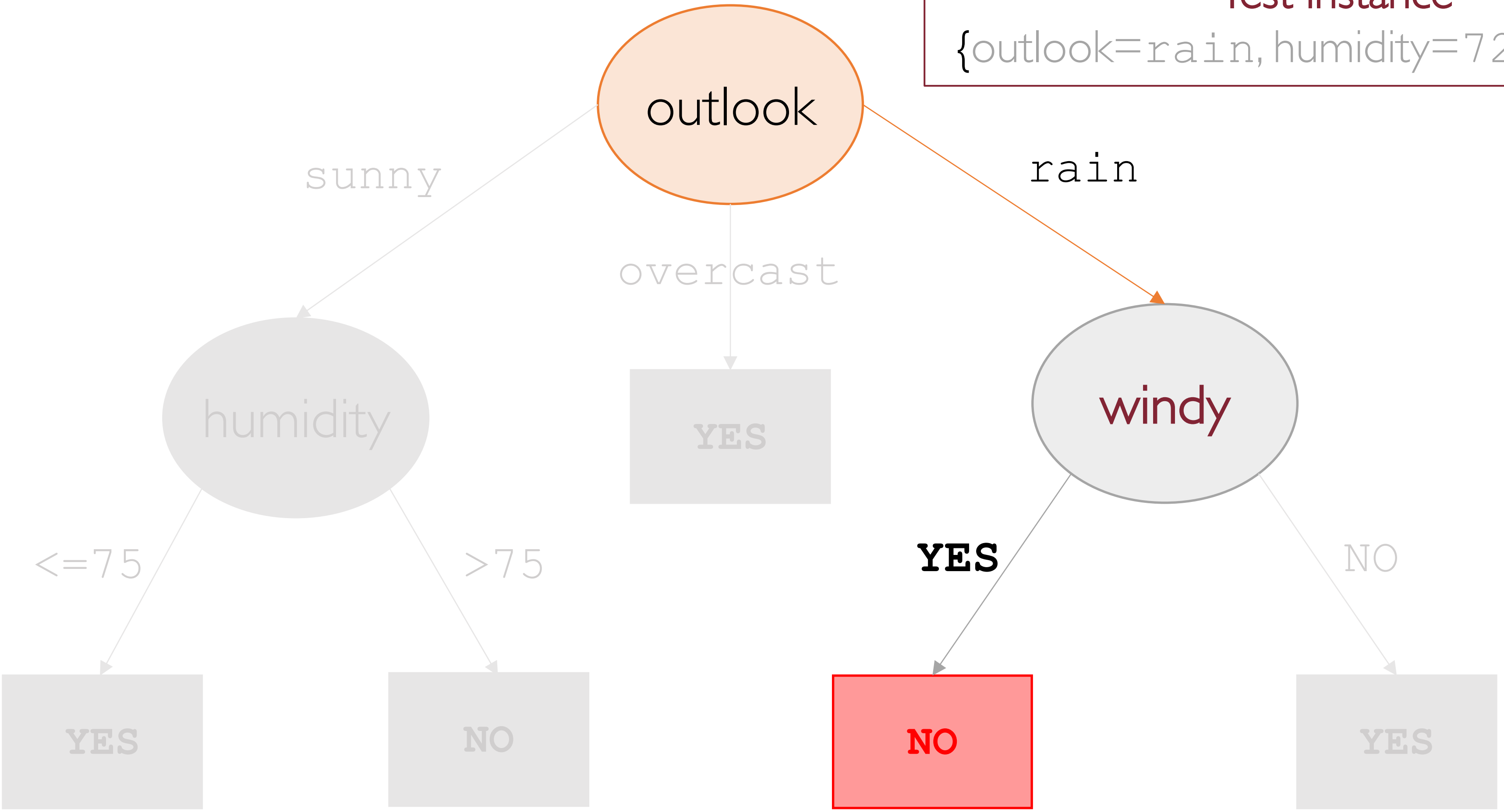

A Bit of Notation

$\mathcal{X} \subseteq \mathbb{R}^n$	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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- Split the input feature space (i.e., the set of possible values observed for each feature x_i) into a set of non-overlapping regions $R_1, R_2, \ldots, R_J$

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- For every observation that falls into the region R_j, we make the same prediction, i.e., the mean of the response values in R_j
- 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)

Partitioning the Input Space

- In theory, partitions could have *any* shape

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The mean computed from observations in R_j

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(e.g., boolean)

One branch for each value

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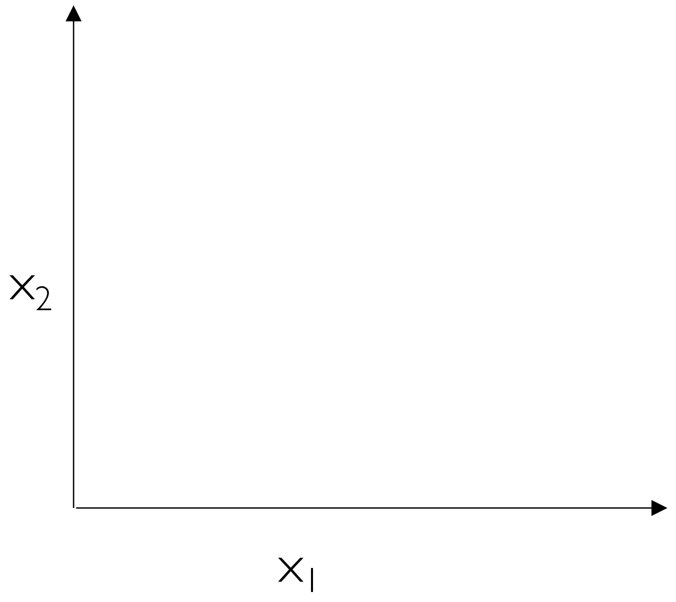

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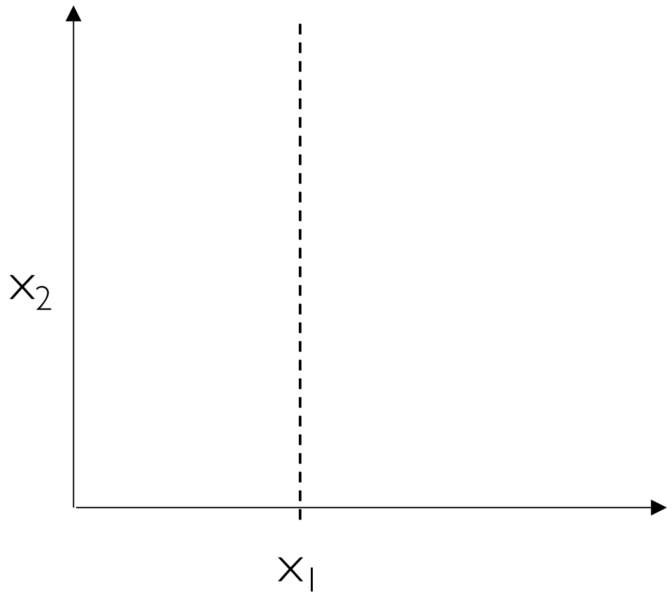

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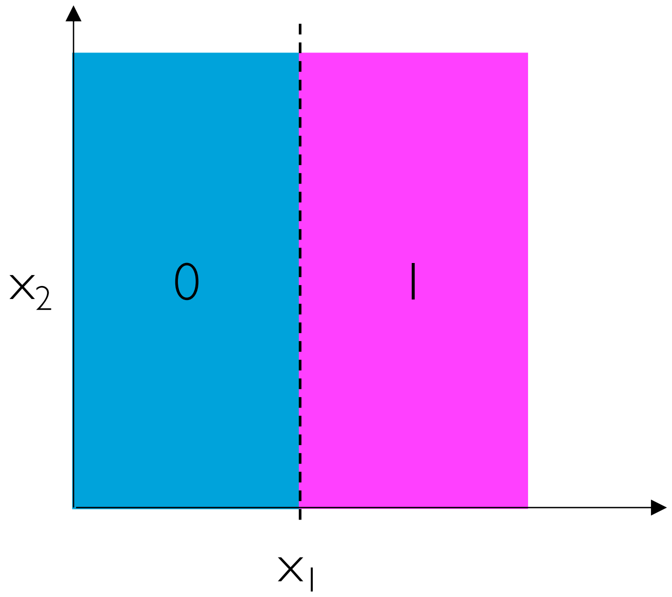

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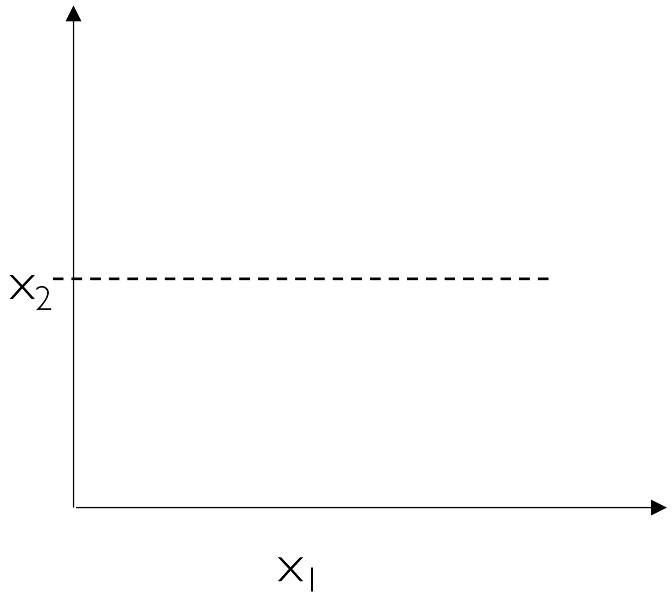

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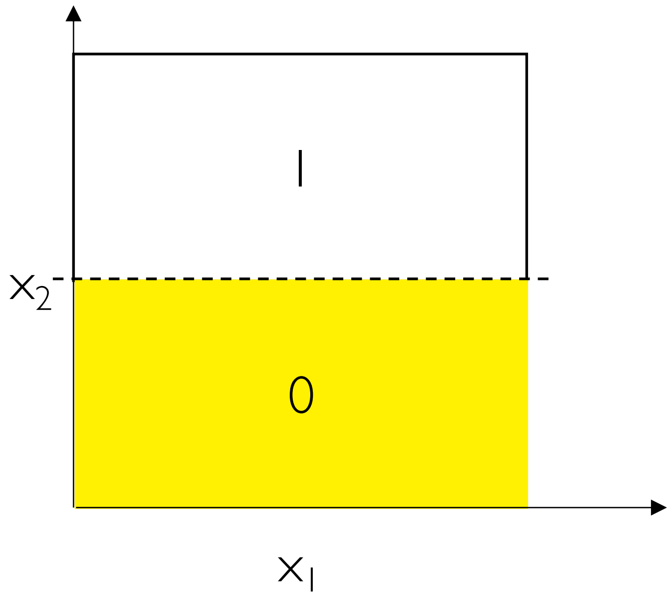

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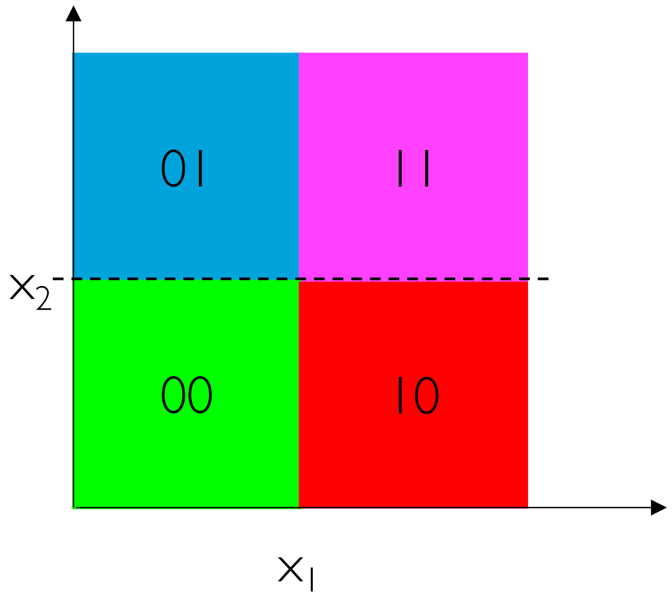

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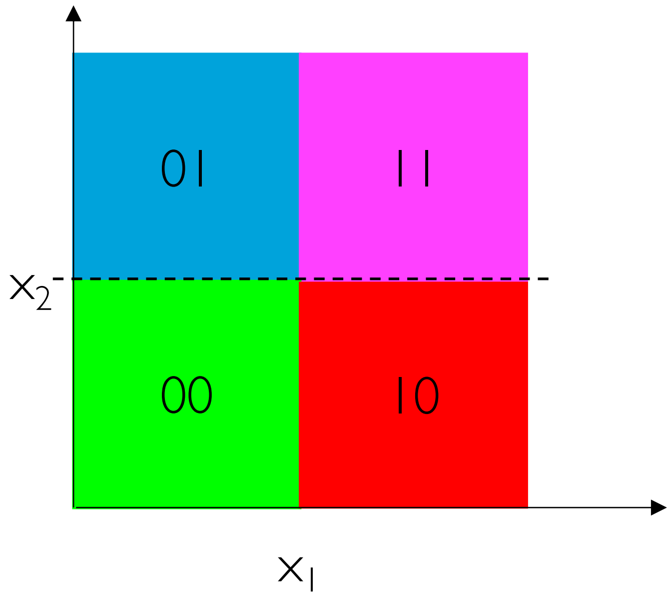

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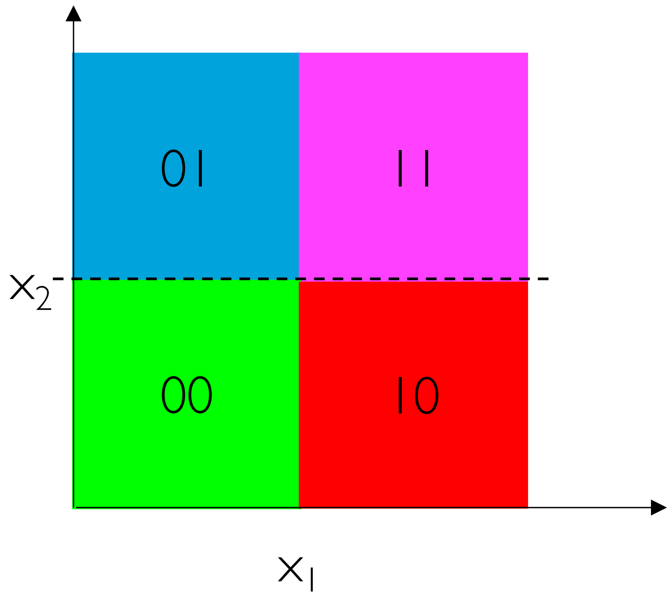

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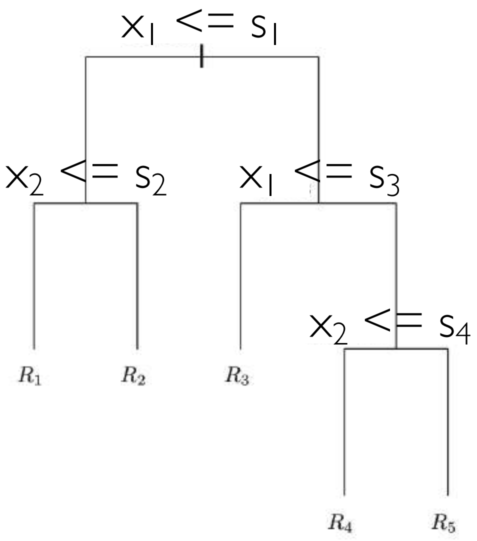
For each attribute, find a splitting point s

Test x_j <= s and create 2 branches

The same attribute may be further split in each subtree



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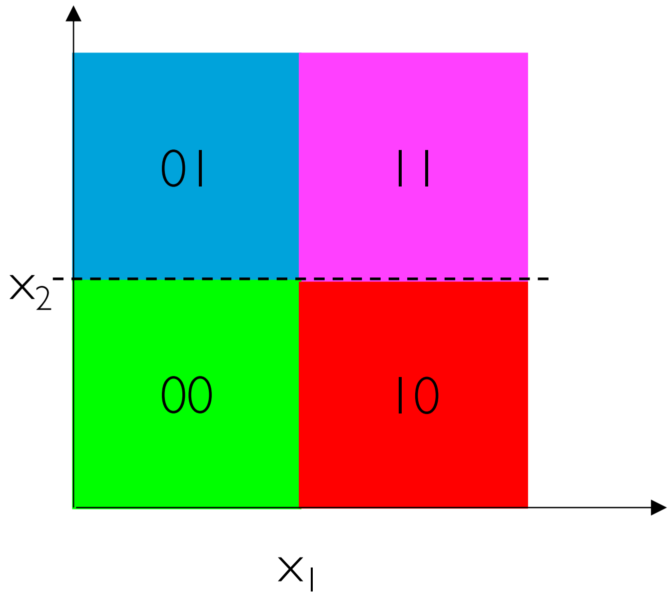

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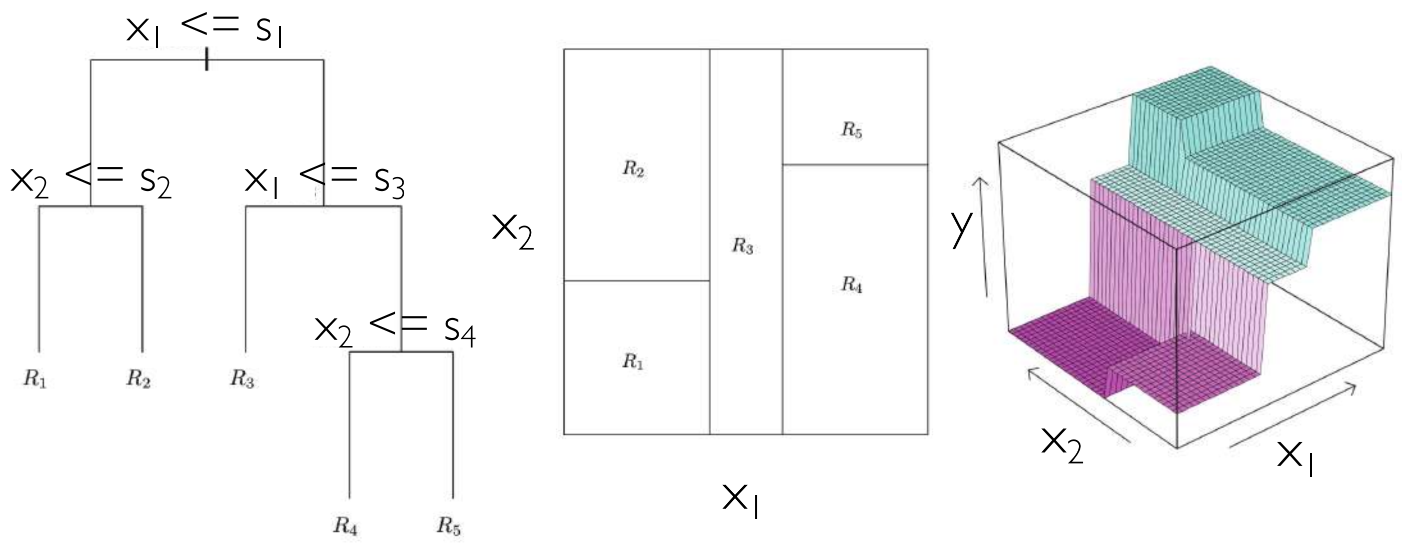

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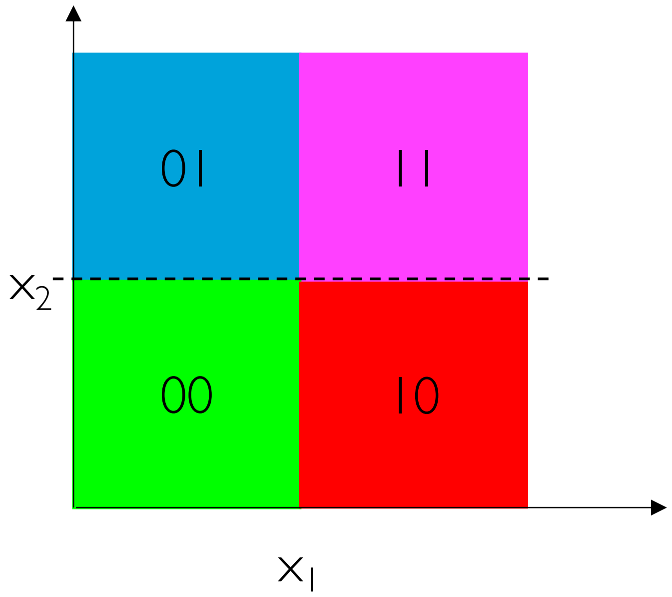

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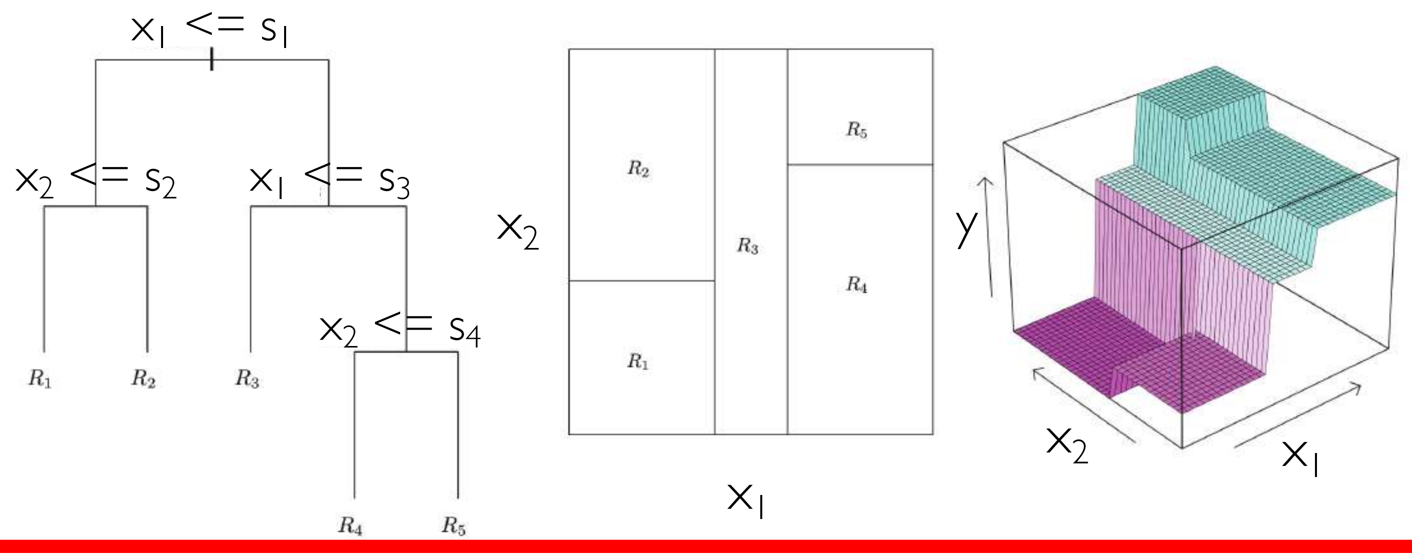

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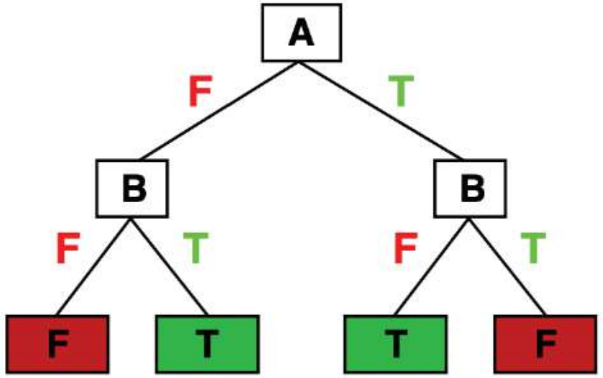
F	F	F
F	T	T
T	F	T
T	T	F



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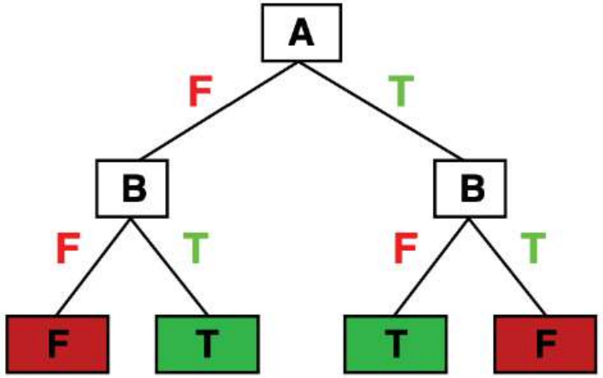

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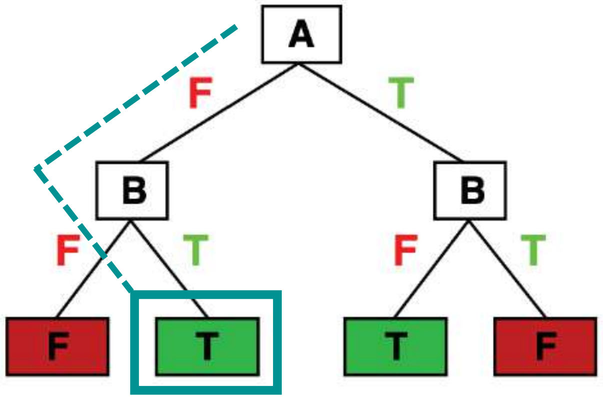

Each row of the truth table maps to a root-to-leaf path on the tree

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

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

Hypothesis Space

How many distinct decision trees can be built out of n boolean attributes?

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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

2^n rows

x_1	x_1	…	x_n	y
0	0	…	0	0
1	0	…	0	0
1	1	…	0	0
…	…	…	…	0
…	…	…	…	0
…	…	…	…	0
1	1	1	1	0

Hypothesis Space

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

2^n rows

x_1	x_1	...	x_n	y
0	0	...	0	1
1	0	...	0	1
1	1	...	0	1
...	...	...	...	1
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The hypothesis space defined by decisions tree is very expressive because there are a lot of different functions it can represent

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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top-down

- 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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$$\boxed{R_{\text{left}}(f, s) = \{\mathbf{x}_i \mid x_{i,f} \leq s\} \quad R_{\text{right}}(f, s) = \{\mathbf{x}_i \mid x_{i,f} > s\}}$$

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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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$$R_{\text{left}}(f, s) = \{\mathbf{x}_i \mid x_{i,f} \leq s\} \quad R_{\text{right}}(f, s) = \{\mathbf{x}_i \mid x_{i,f} > s\}$$

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

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

Growing the Tree

- Finding the pair (f, s) which minimizes the quantity below can be done "easily", especially when the number of features d is not too large

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- Each time, we reduce the RSS

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- 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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- The prediction for that test instance will be the **mean** of the region R_j

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- Regression Trees:
  - Use Residual Sum of Squares (RSS) as splitting criterion
  - At inference time, predictions are the mean of the leaf observations