Growing decision trees STAT 4710

Rolling into a new unit!

Unit 1: R for data mining



Unit 2: Prediction fundamentals



Unit 3: Regression-based methods

Unit 4: Tree-based methods

Unit 5: Deep learning

Lecture 1: Growing decision trees

Lecture 2: Tree pruning and bagging

Lecture 3: Random forests

Lecture 4: Boosting

Lecture 5: Unit review and quiz in class

Most methods covered so far based on $\hat{\beta}_0 + \hat{\beta}_1 X_1 + \cdots + \hat{\beta}_{p-1} X_{p-1}$:

- Linear regression
- Logistic regression
- Ridge, lasso, elastic net

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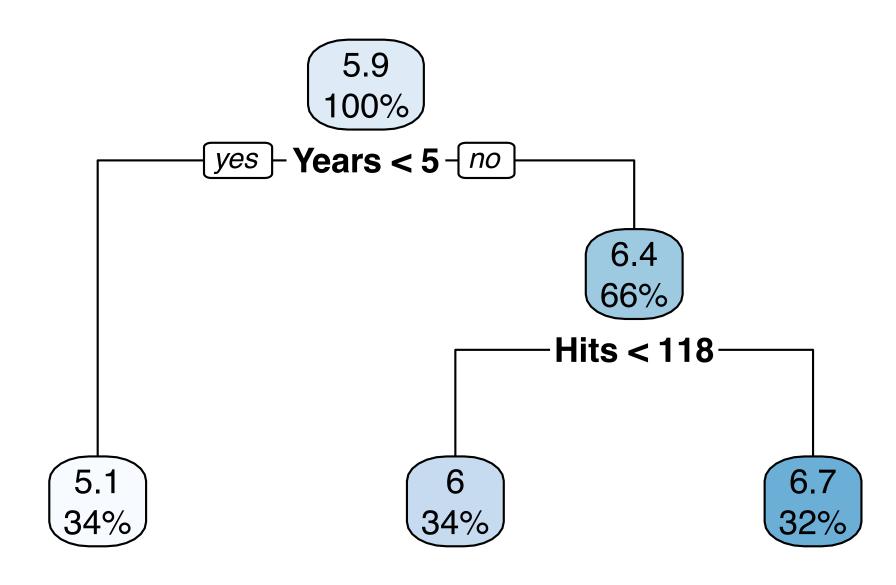
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In Unit 4 we will leave the land of linearity.

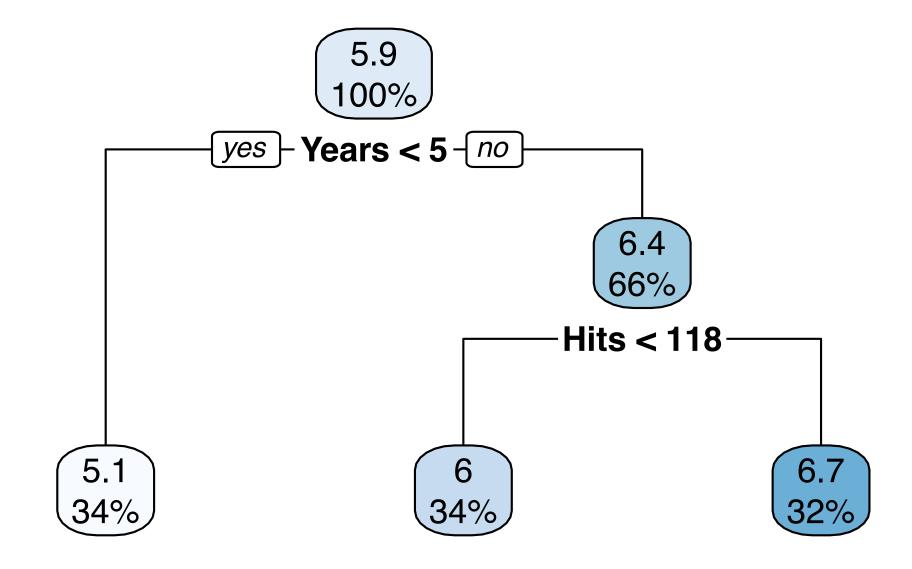
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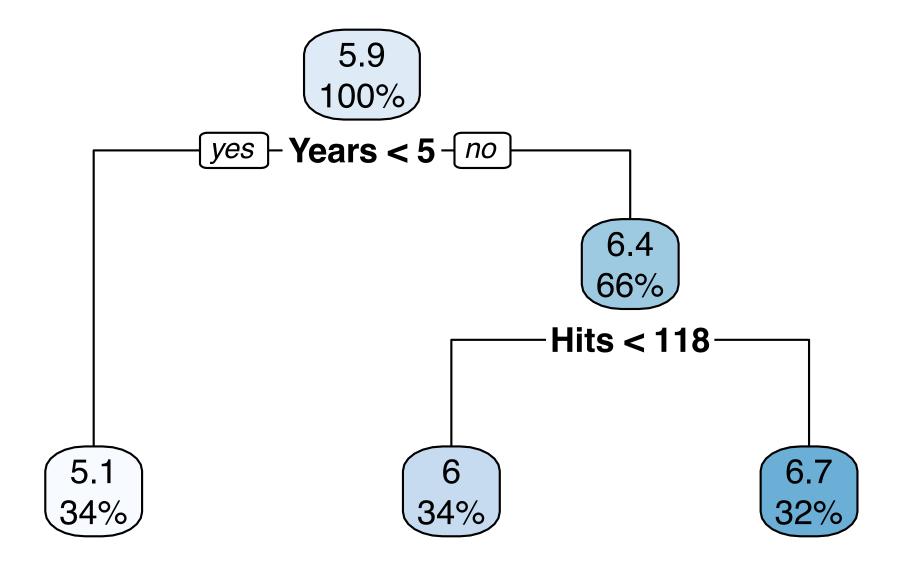
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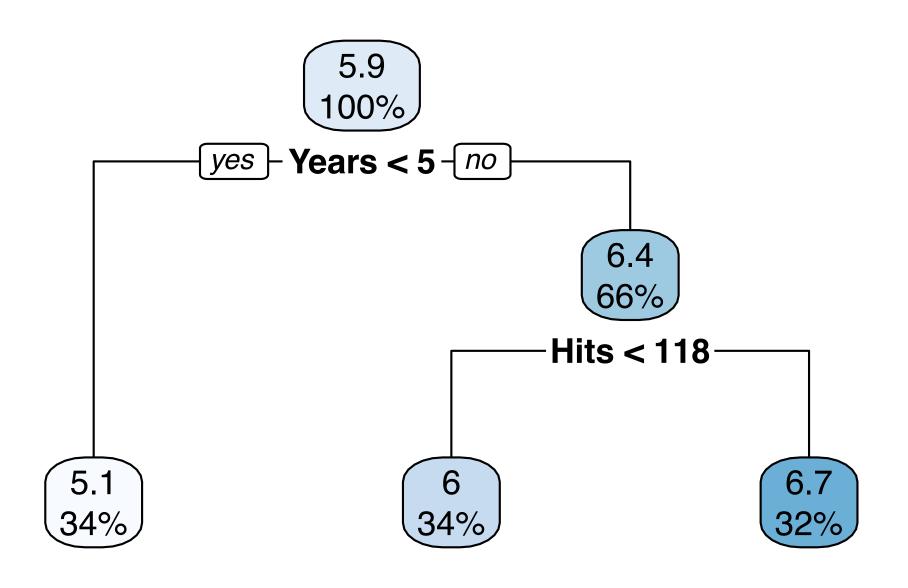
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However, trees are somewhat unstable and do not give the best prediction performance.

Nevertheless, trees can be used as building blocks for state-of-the-art prediction performance:

- Random forests (lecture 3)
- Boosting (lecture 4)



Tree-based models versus linear models

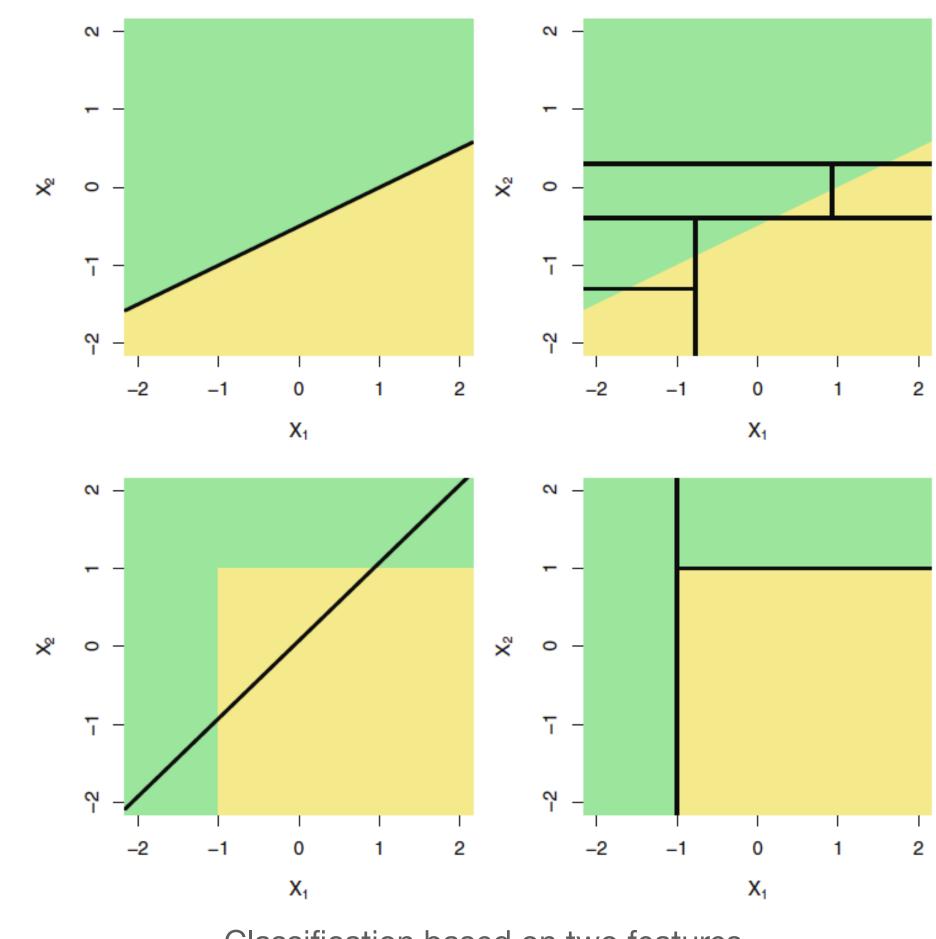
Which perform better?

Neither tree-based nor linear models dominate the other.

Each prediction method works better when the underlying trend in the data matches its modeling choice.

E.g. for classification:

- Linear model → linear decision boundary
- Decision tree → unions of rectangles



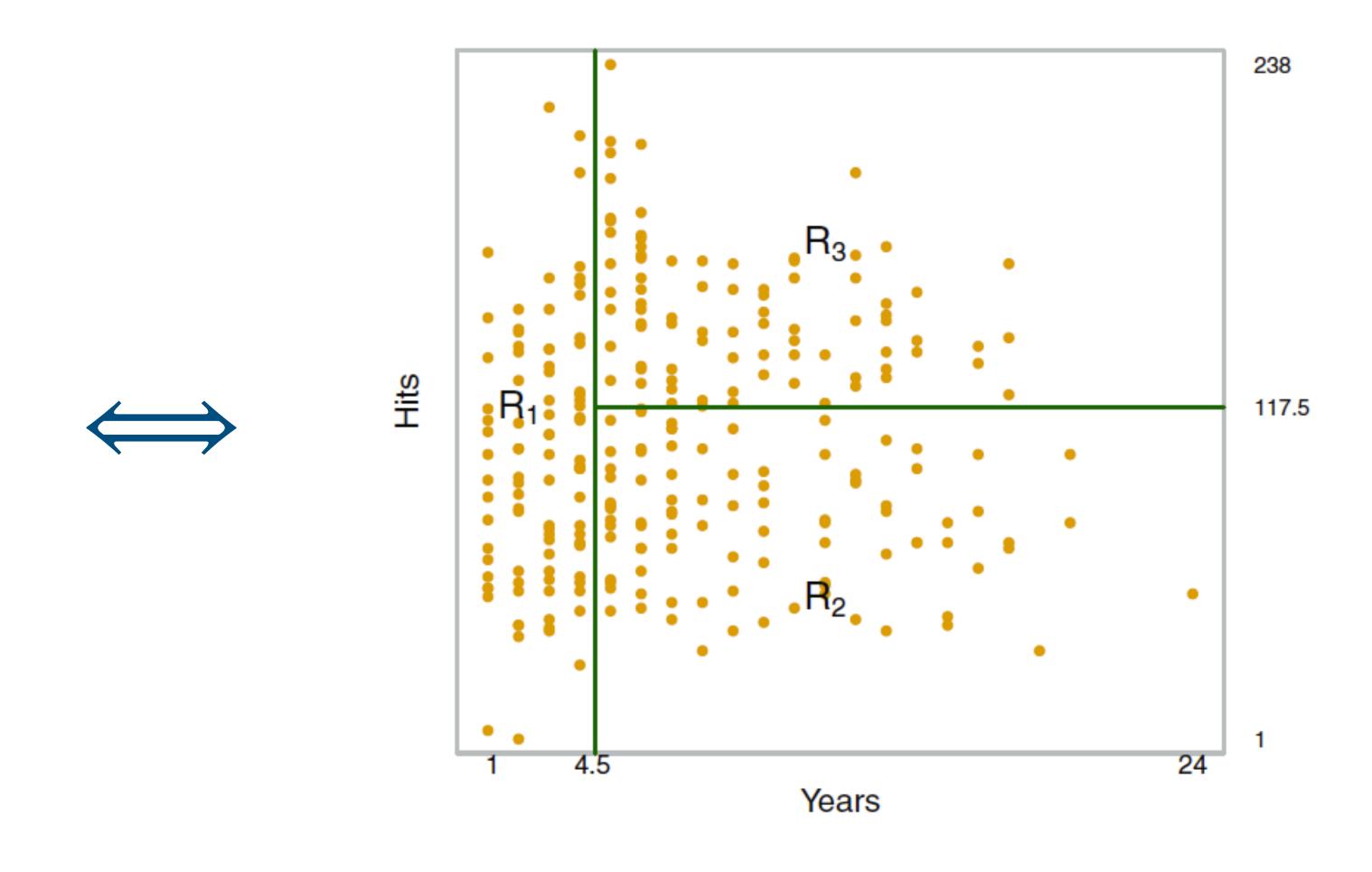
Classification based on two features (colors indicate the two classes).

Hitters data

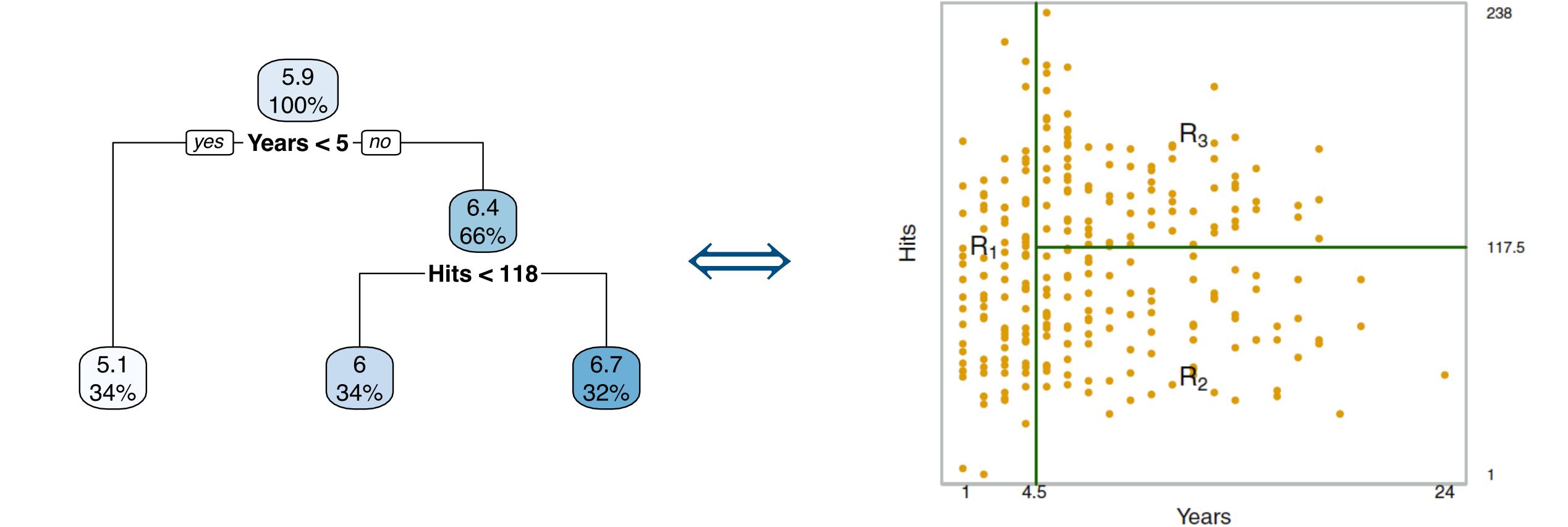
Major League Baseball Data from the 1986 and 1987 seasons.

- Observations: 322 MLB players
- Response: Salary (1987 annual salary on opening day in thousands of dollars)
- Features: Assists, AtBat,...,Hits,...,Years (19 total)

Tree \iff Partition into nested, axis-aligned rectangles



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Mathematical expression of the prediction rule

A trained tree consists of:

- M regions $\widehat{R}_1, ..., \widehat{R}_M$
- response values $\hat{c}_1, ..., \hat{c}_M$

For a new feature vector X^{test} , predict the constant value \widehat{c}_m for region \widehat{R}_m :

$$\widehat{Y}^{\text{test}} = \sum_{m=1}^{M} \widehat{c}_m \cdot I(X^{\text{test}} \in \widehat{R}_m).$$

 R_2 R_3 R_4 R_4 R_5 R_4 R_4 R_4 R_4 R_4 R_4 R_4 R_5 R_4 R_4 R_4 R_4 R_5 R_4 R_4 R_4 R_5 R_4 R_5 R_6 R_7 R_8 R_8 R_8 R_8

(continuous or categorical response)

Suppose we partition on X_j .

Suppose we partition on X_i .

• If X_j is continuous, we just find a split point s and split into $\{X: X_j < s\}$ and $\{X: X_j \geq s\}$.

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- If X_j is continuous, we just find a split point s and split into $\{X: X_j < s\}$ and $\{X: X_j \geq s\}$.
- If X_j is categorical, e.g. with levels $\{a,b,c,d,e\}$, then we need to split the levels into two groups, e.g. $\{a,c\}$ and $\{b,d,e\}$, giving the partitions $\{X:X_j\in\{a,c\}\}$ and $\{X:X_j\in\{b,d,e\}\}$.

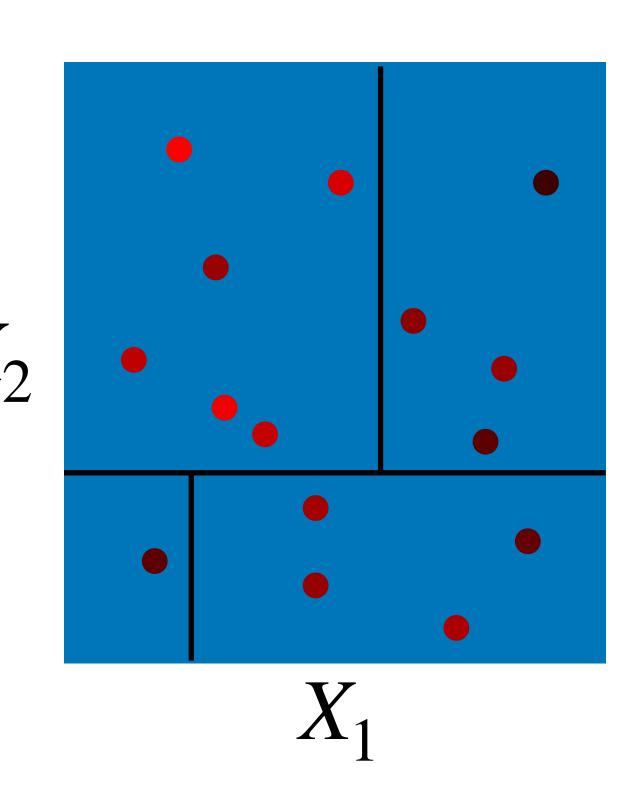
The squared error objective

As usual, we are given a training dataset $(X_1, Y_1), \ldots, (X_n, Y_n)$.

For a fixed M, we seek rectangles $\widehat{R}_1, \ldots, \widehat{R}_M$ and values $\widehat{c}_1, \ldots, \widehat{c}_M$ to minimize the residual sum of squares:

$$\widehat{R}_{1},...,\widehat{R}_{M},\widehat{c}_{1},...,\widehat{c}_{M} = \underset{R_{1},...,R_{M},c_{1},...,c_{M}}{\operatorname{arg min}} \sum_{i=1}^{n} (Y_{i} - \widehat{Y}_{i})^{2};$$

$$\widehat{Y}_i = \sum_{m=1}^{M} c_m \cdot I(X_i \in R_m).$$



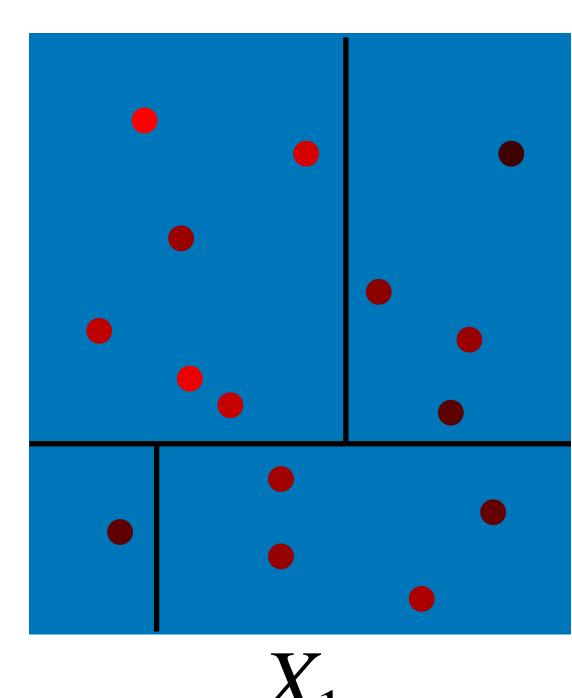
Optimal \hat{c}_m given \widehat{R}_m

First let's consider a simpler problem, where rectangles $\widehat{R}_1, ..., \widehat{R}_M$ are given:

$$\hat{c}_1, \dots, \hat{c}_M = \arg\min_{c_1, \dots, c_M} \sum_{i=1}^n (Y_i - \hat{Y}_i)^2; \quad \hat{Y}_i = \sum_{m=1}^M c_m \cdot I(X_i \in \widehat{R}_m).$$

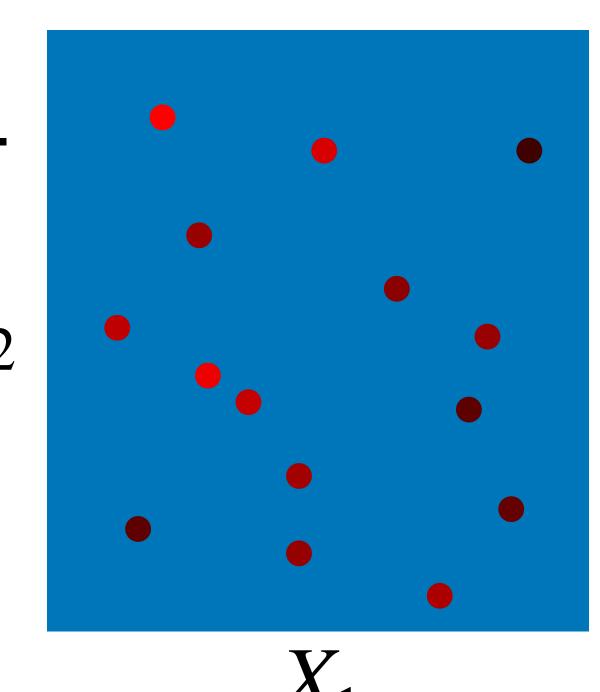
We're fitting a constant to each region, so the solution is

$$\widehat{c}_m = \operatorname{mean}\left(\{Y_i : X_i \in \widehat{R}_m\}\right).$$



Finding the rectangles \widehat{R}_m

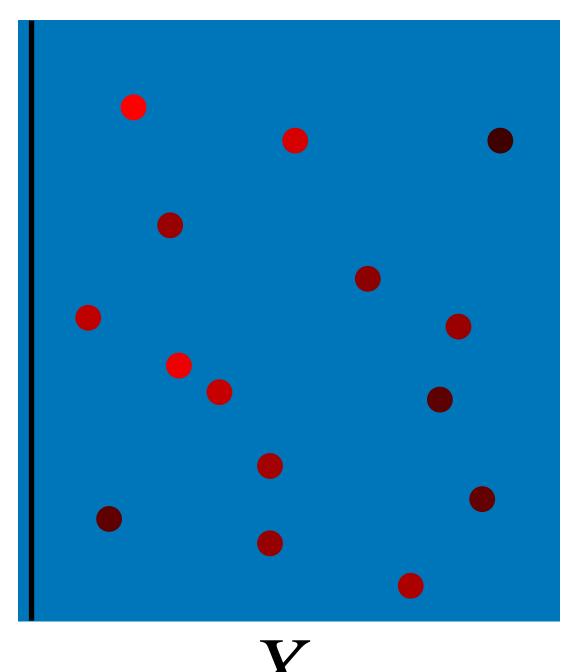
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- 2. Find split of the whole region that decreases RSS the most.
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- 4. Repeat until there are M regions.



Finding the rectangles \widehat{R}_m

The optimal set of rectangles is computationally intractable to find. In practice, we employ a greedy top-down algorithm:

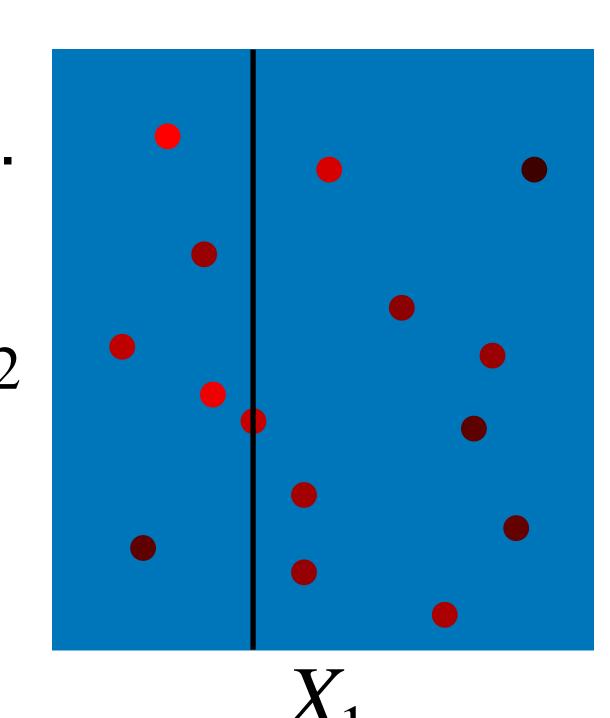
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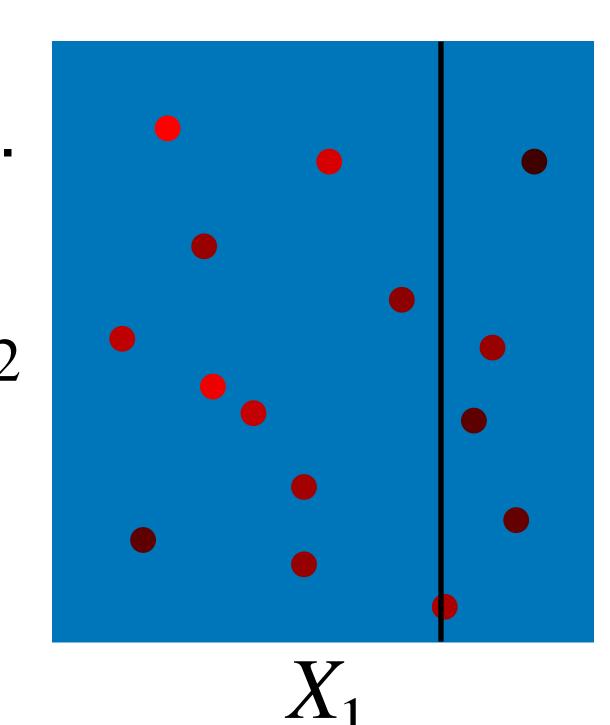
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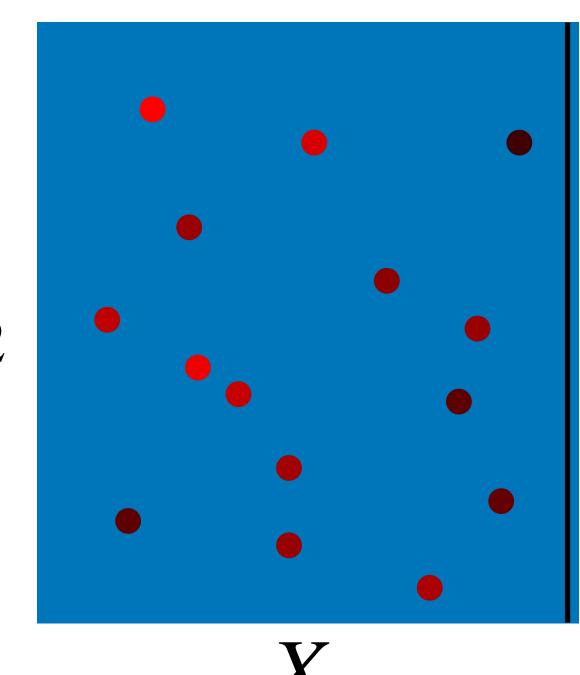
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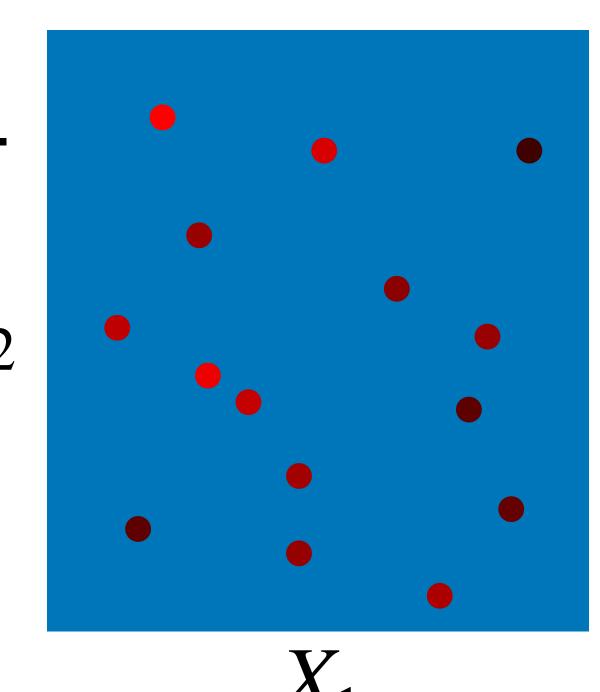
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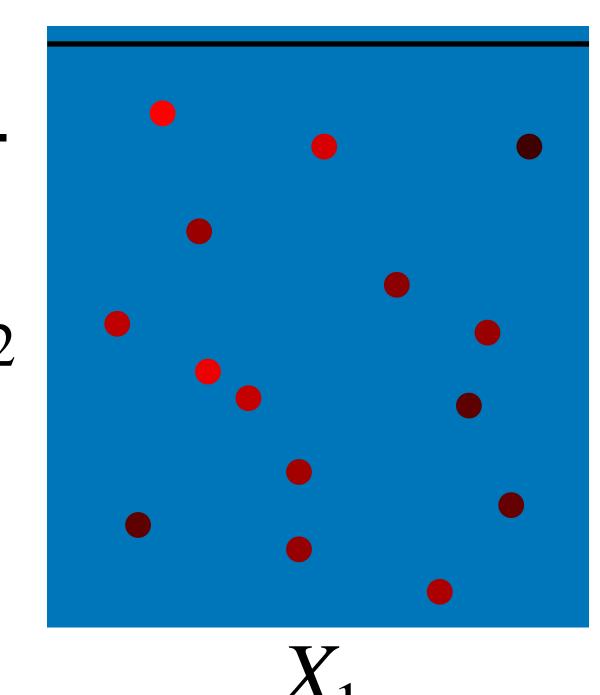
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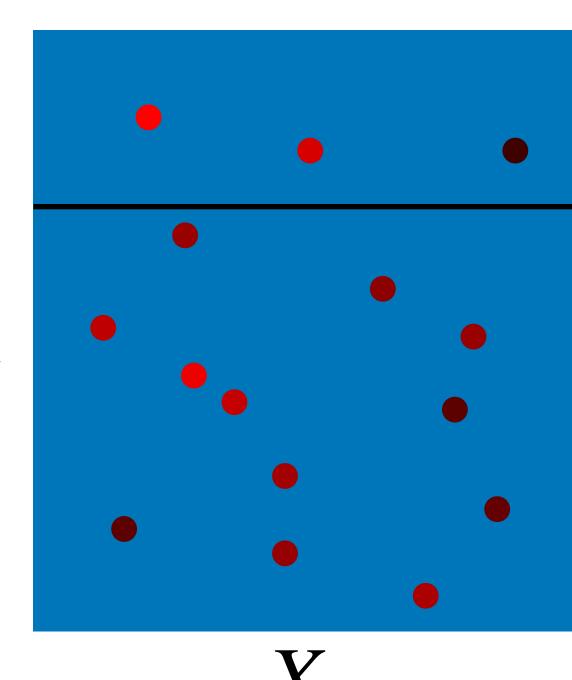
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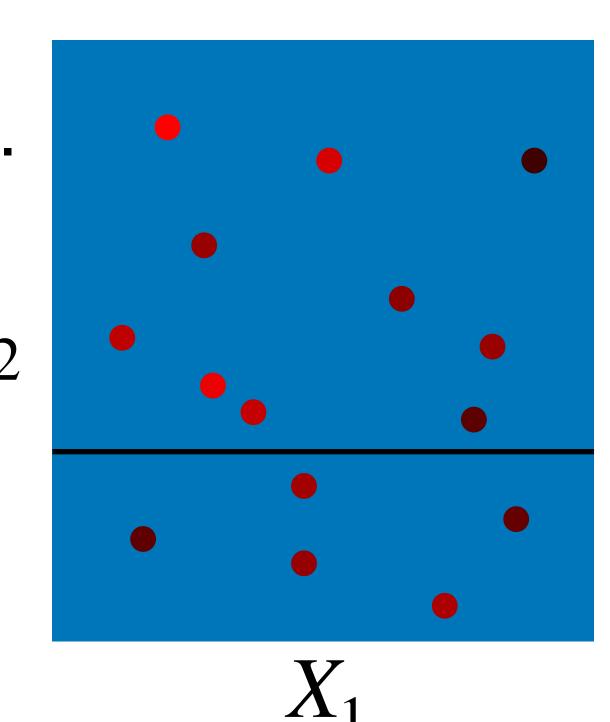
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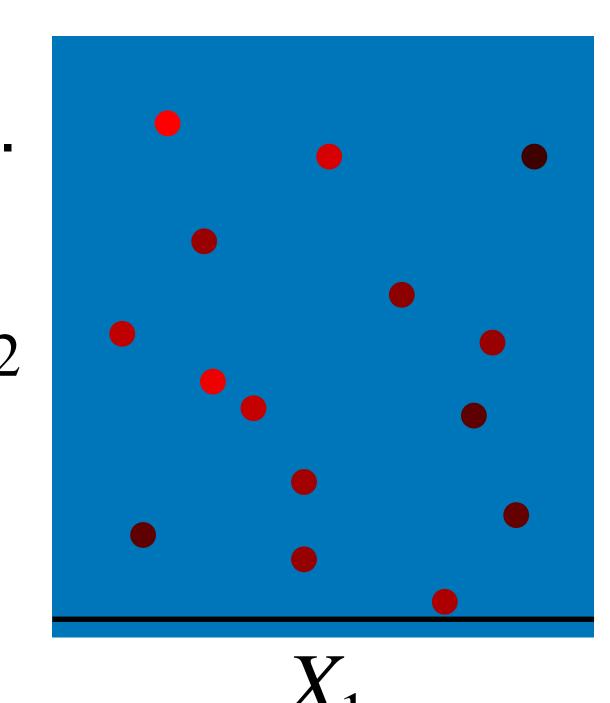
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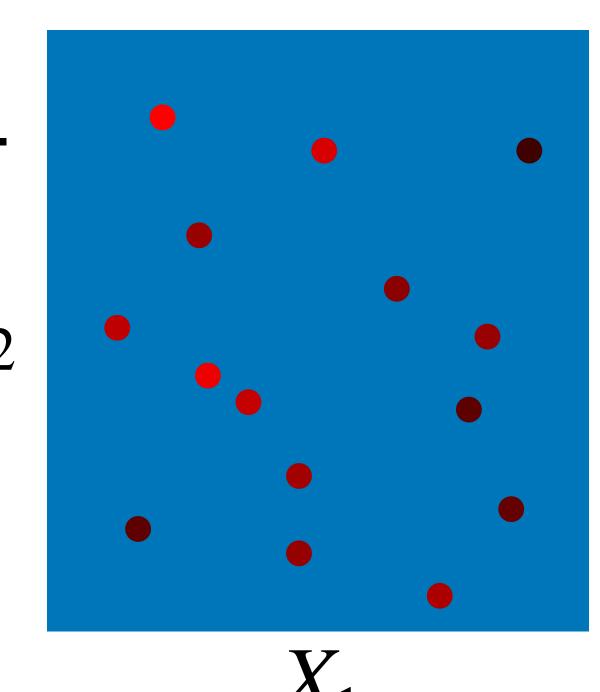
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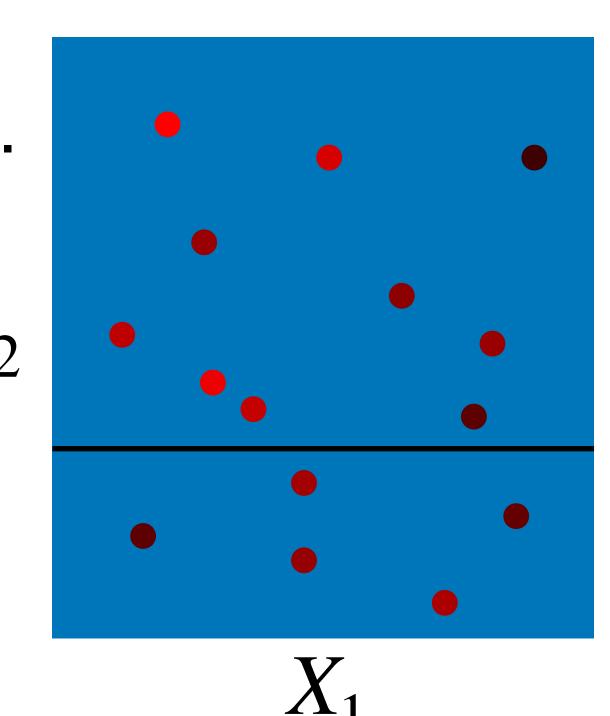
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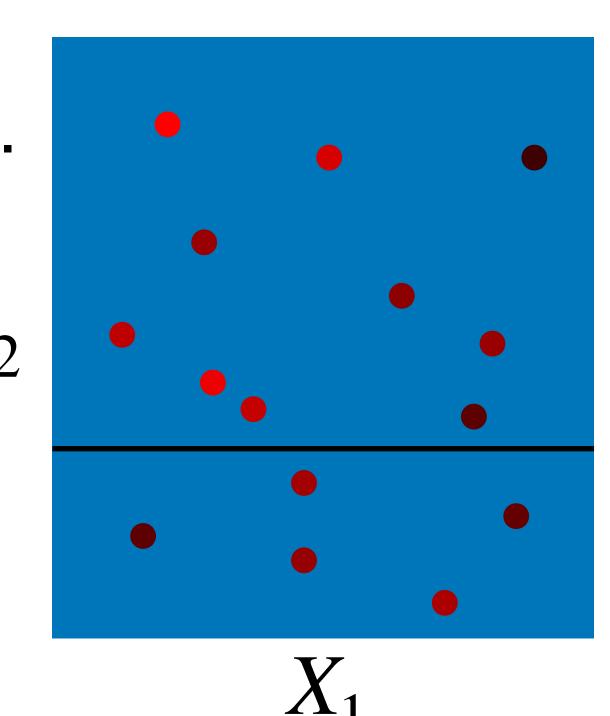
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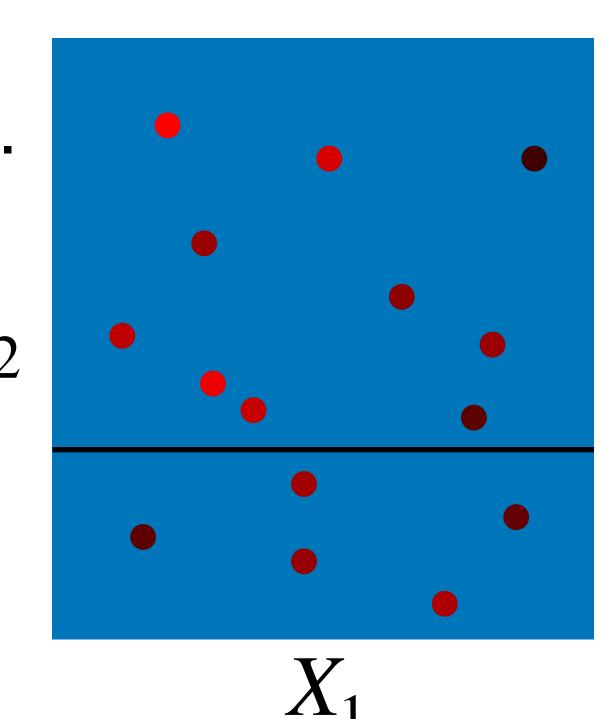
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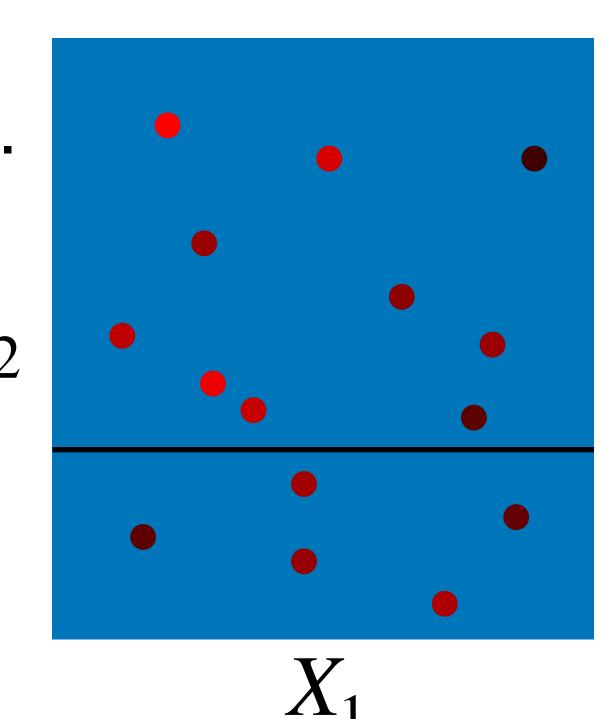
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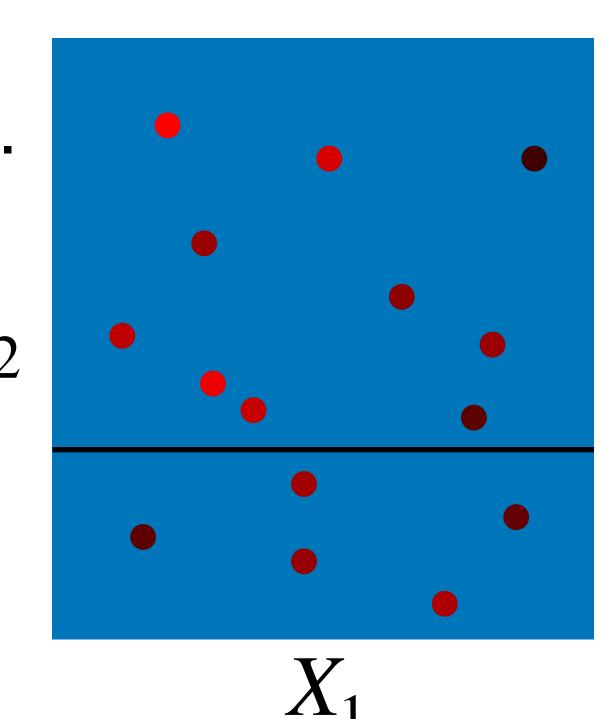
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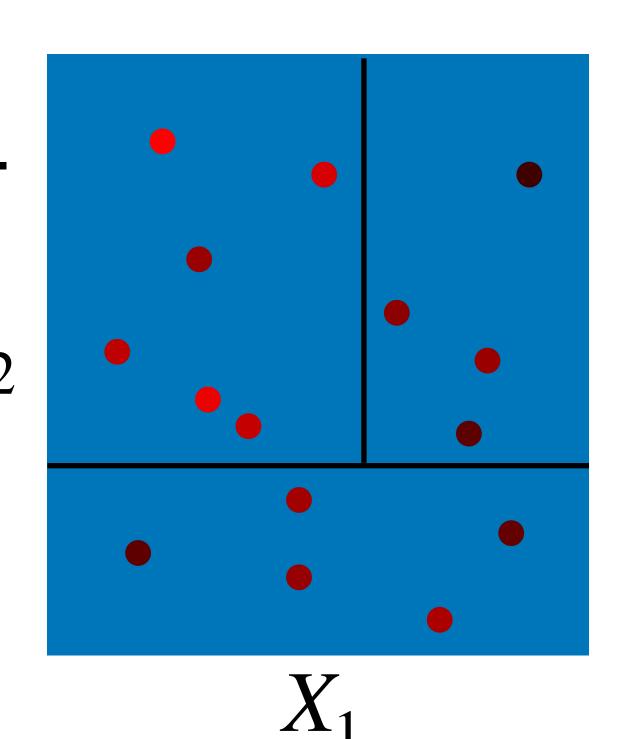
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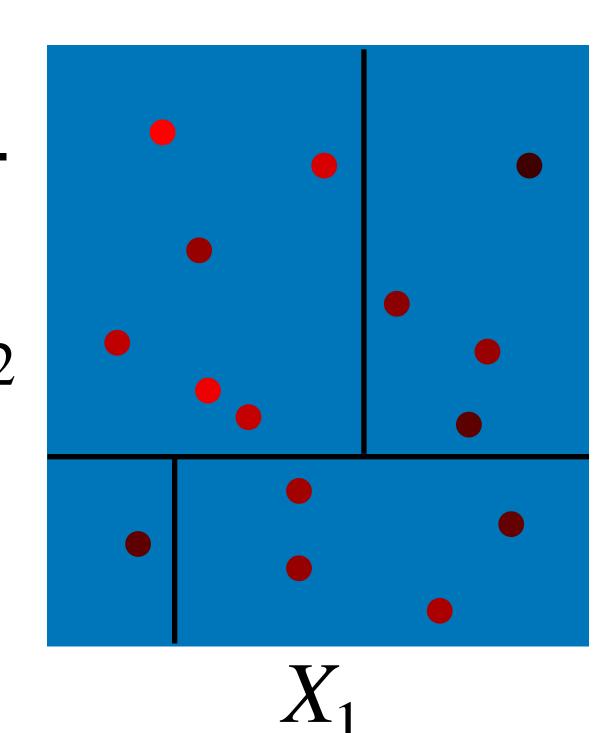
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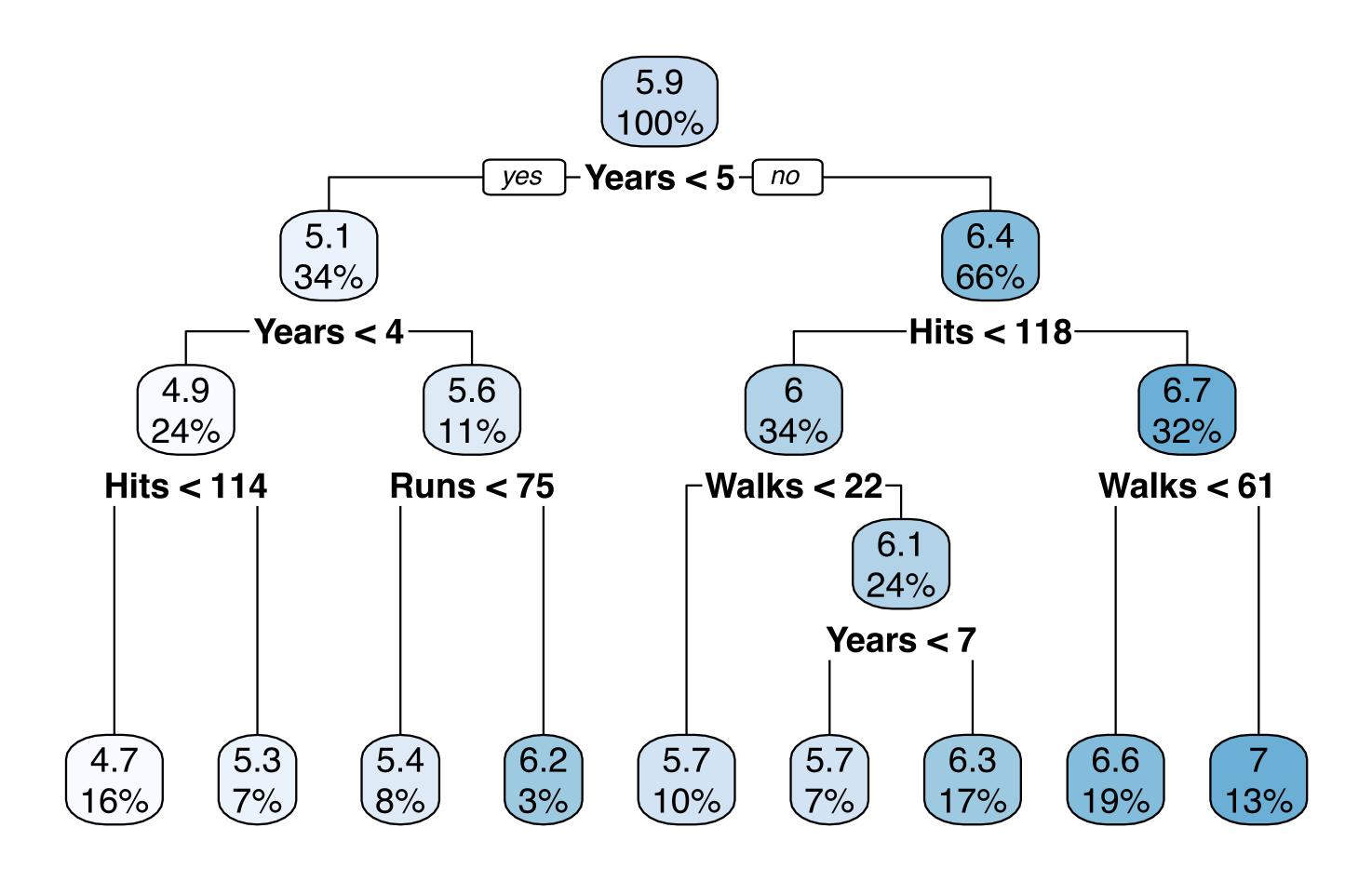


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Final output



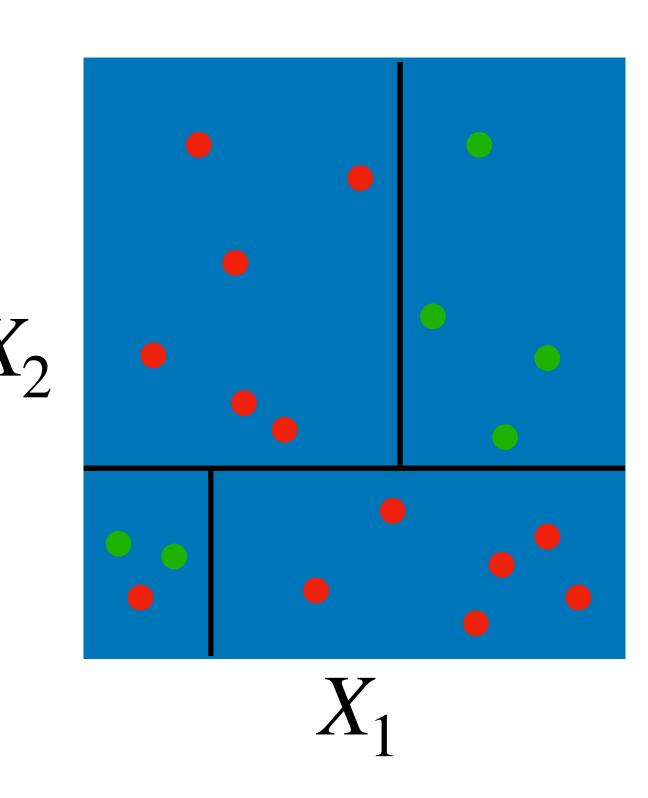
The misclassification error objective

As usual, we are given a training dataset $(X_1, Y_1), \ldots, (X_n, Y_n)$, where the response Y is binary.

For a fixed M, we seek rectangles $\widehat{R}_1, \ldots, \widehat{R}_M$ and values $\widehat{c}_1, \ldots, \widehat{c}_M$ to minimize the misclassification loss:

$$\widehat{R}_{1},...,\widehat{R}_{M},\widehat{c}_{1},...,\widehat{c}_{M} = \underset{R_{1},...,R_{M},c_{1},...,c_{M}}{\operatorname{arg min}} \frac{1}{n} \sum_{i=1}^{n} I(Y_{i} \neq \widehat{Y}_{i});$$

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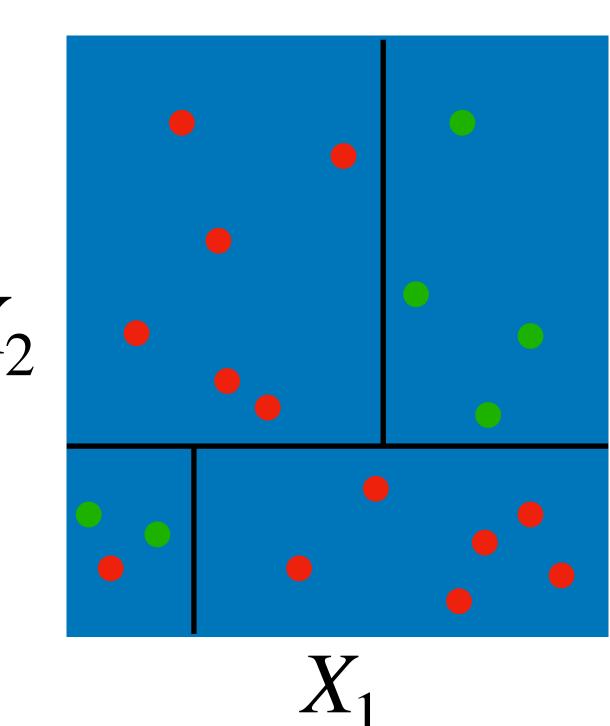
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We're fitting the same category to each region, so the solution is the majority vote:

$$\widehat{c}_m = \operatorname{mode}\left(\{Y_i : X_i \in \widehat{R}_m\}\right).$$



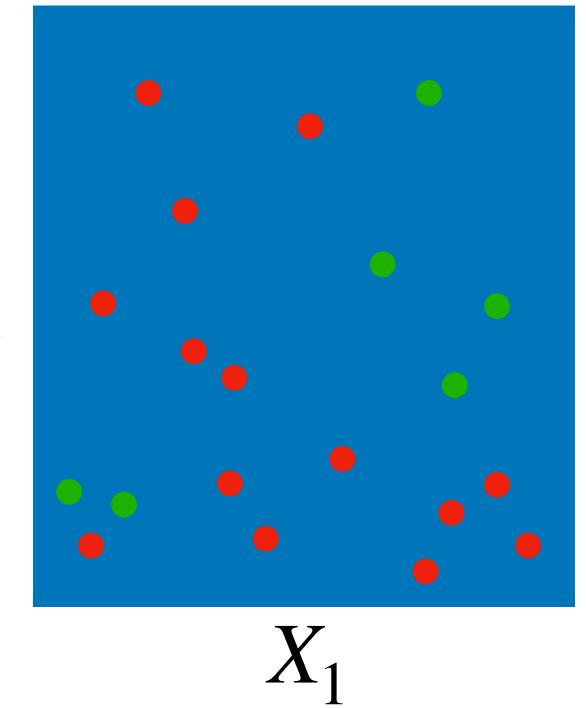
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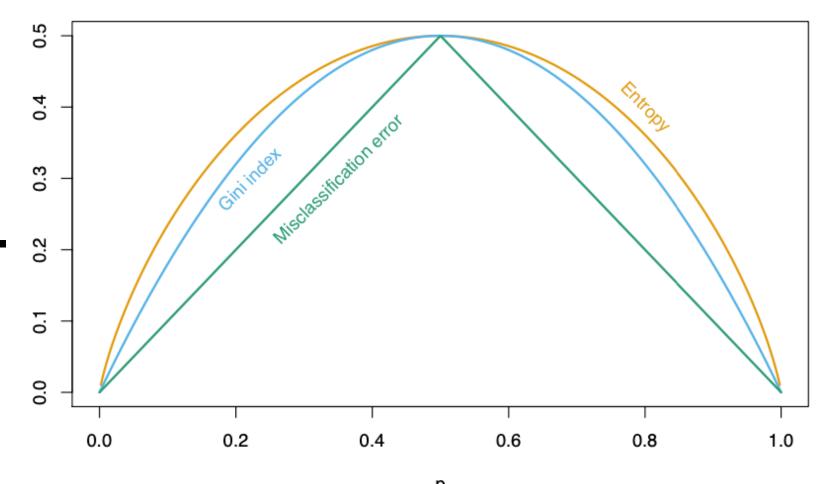
We use a very similar greedy recursive splitting algorithm.

Let \hat{p}_m be proportion of class 1 in region m. The misclassification error in that region is $\min(\hat{p}_m, 1 - \hat{p}_m)$.

Misclassification error not sensitive enough to find good split points at each step; instead, evaluate impurity using

Gini index =
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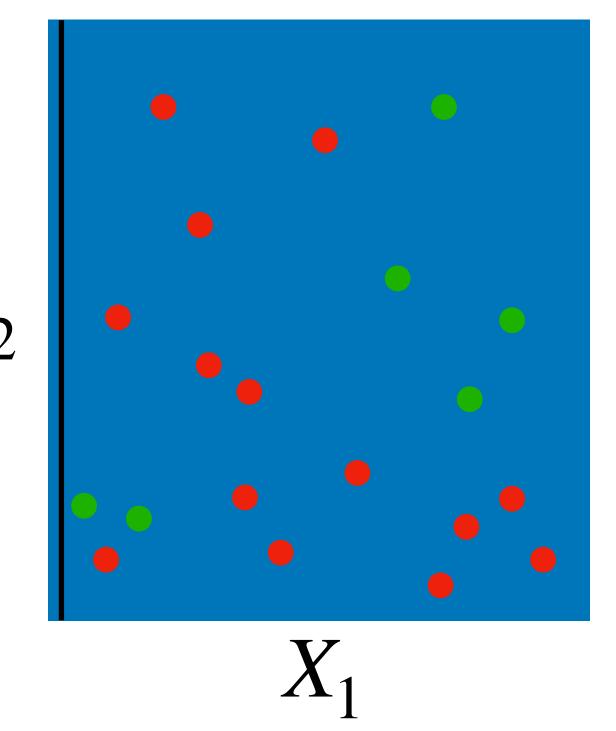
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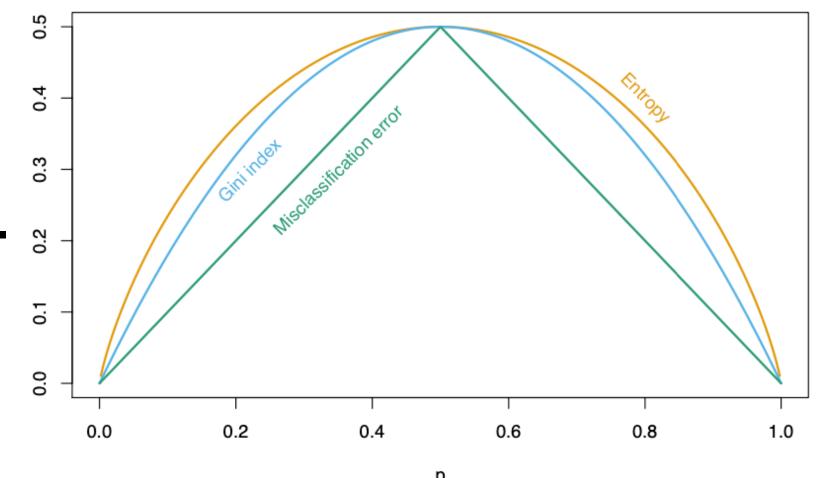
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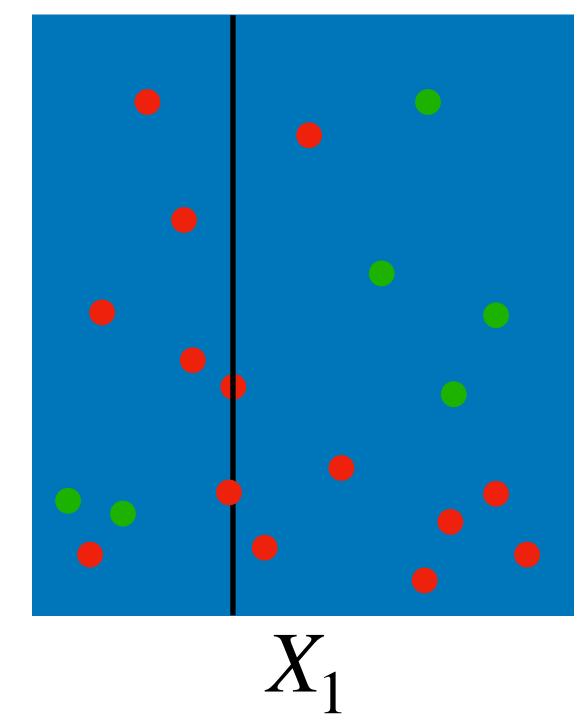
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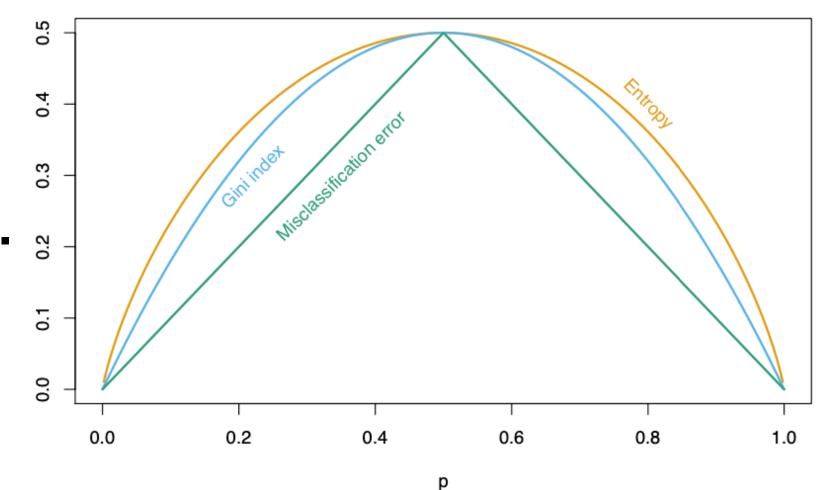
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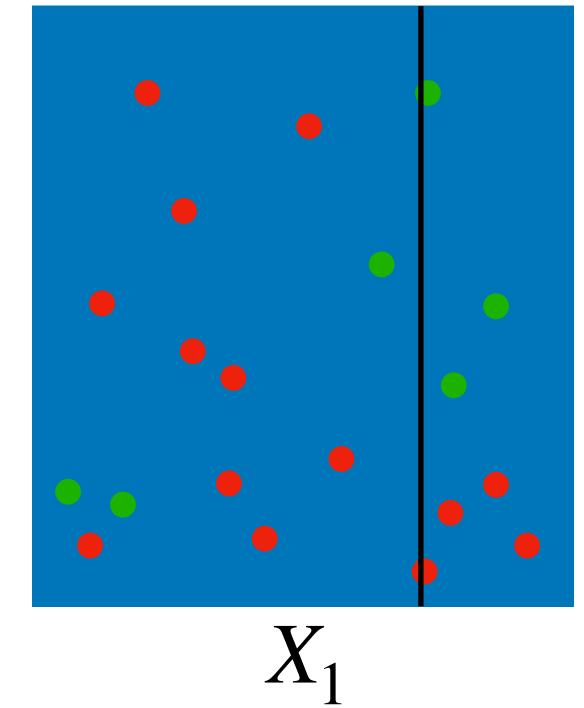
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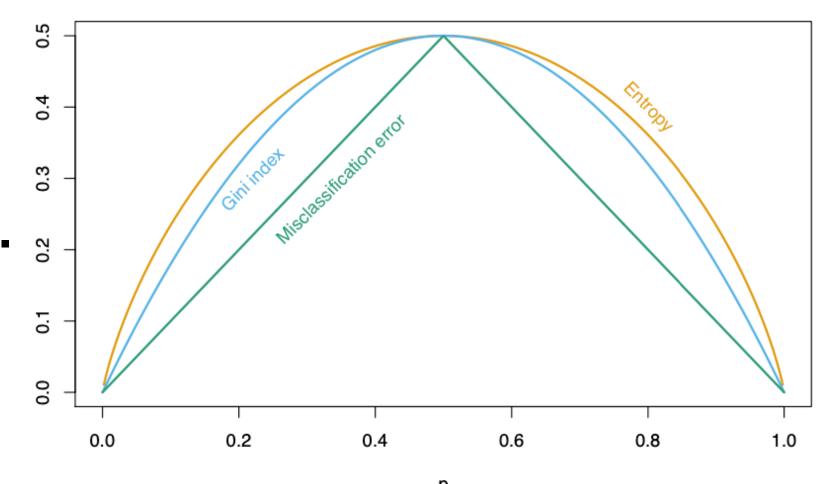
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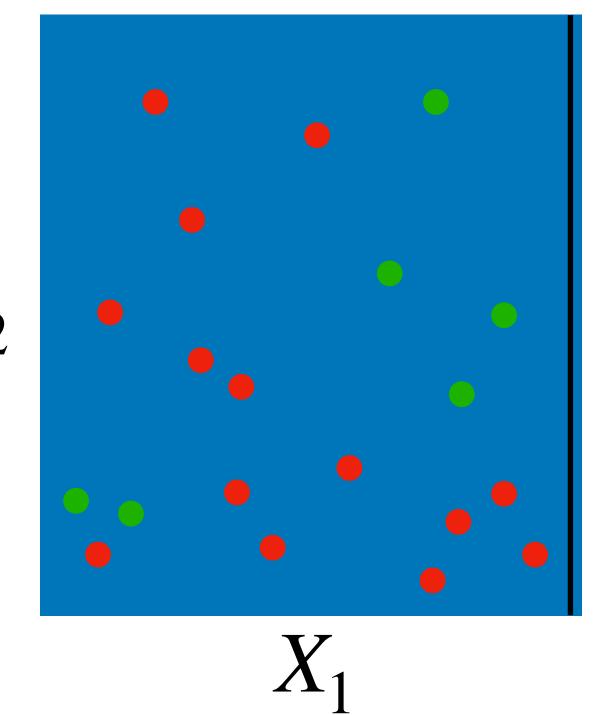
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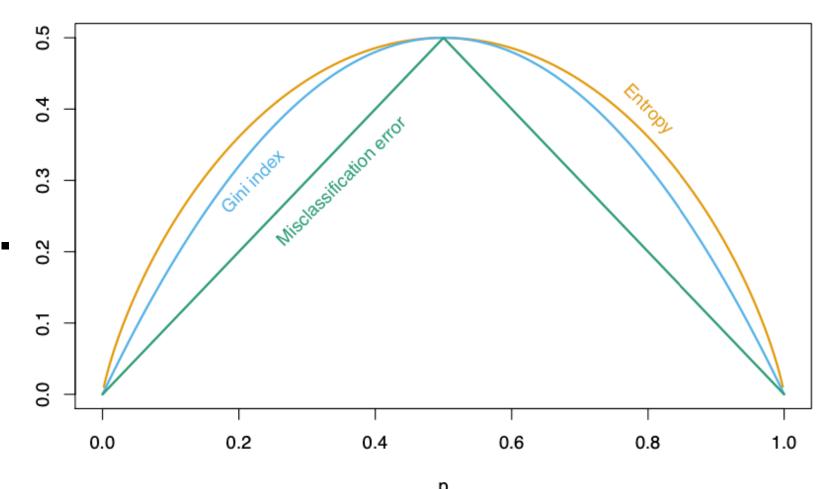
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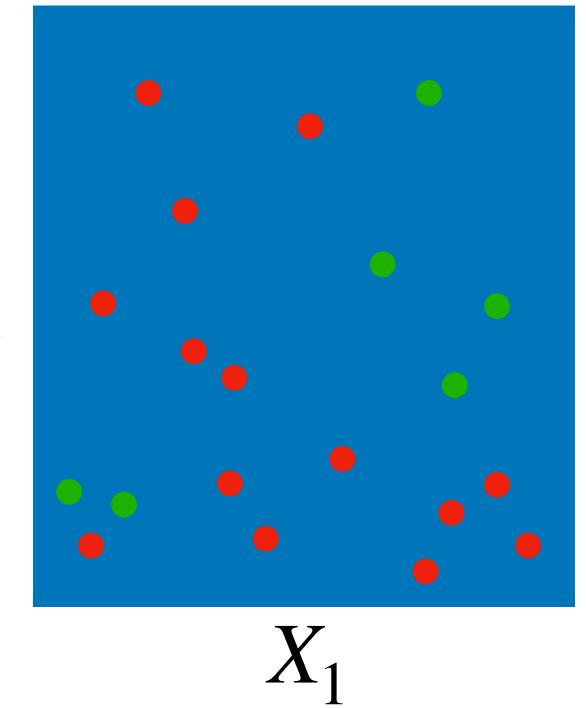
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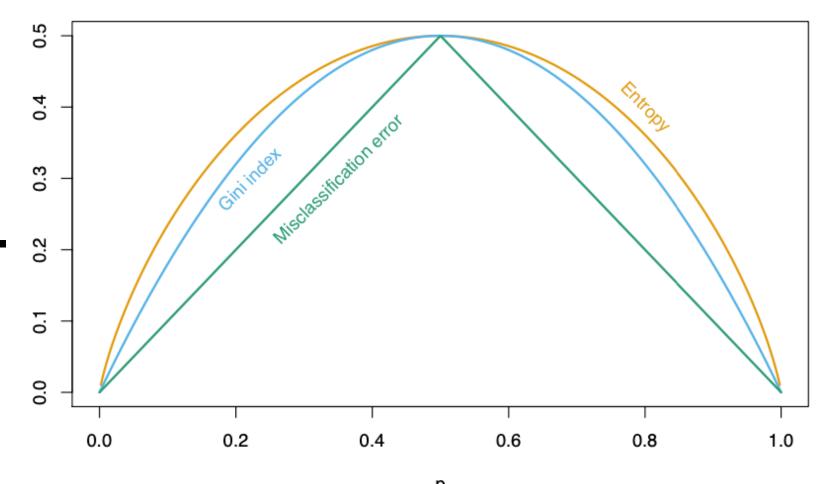
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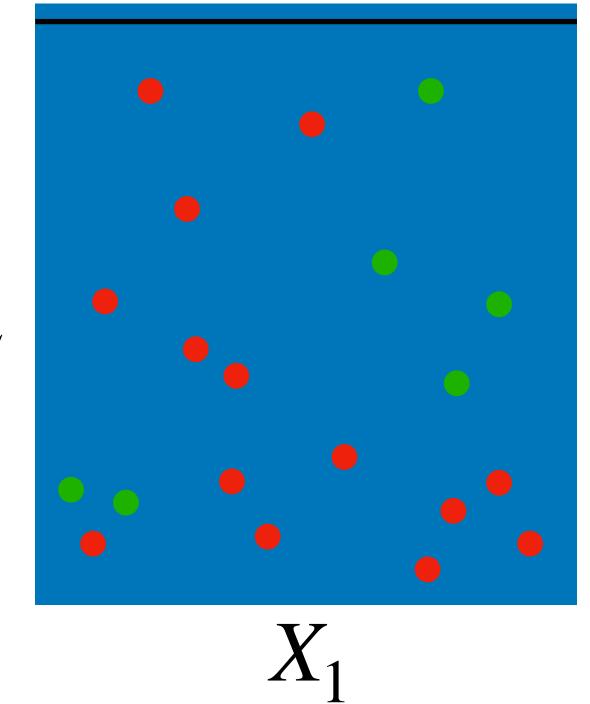
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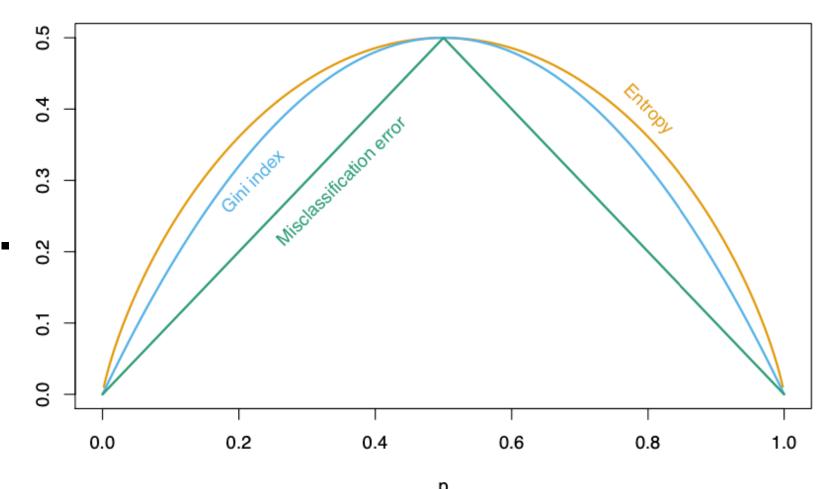
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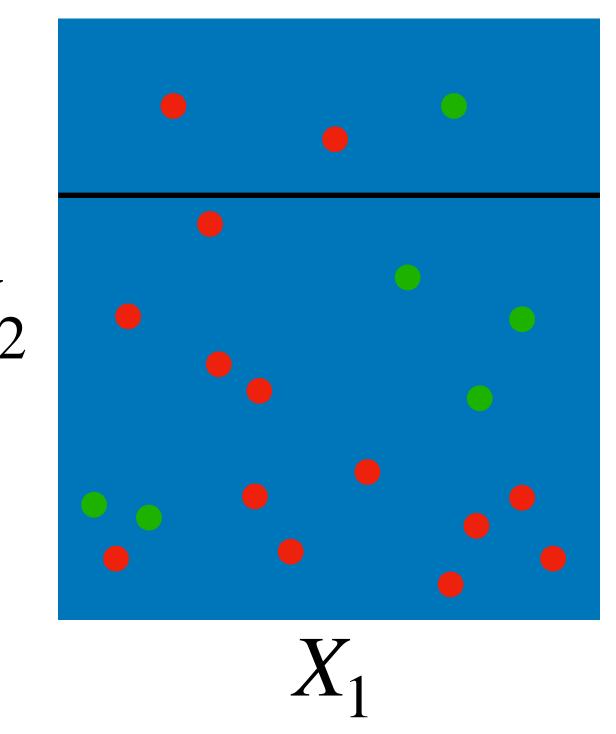
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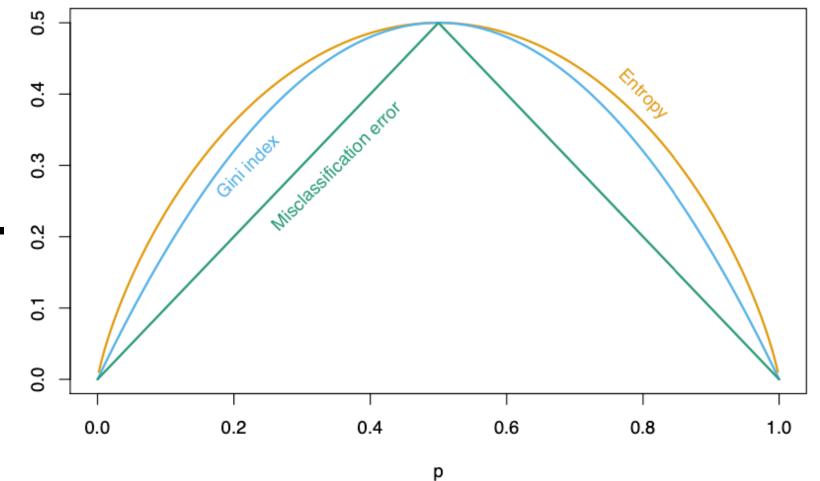
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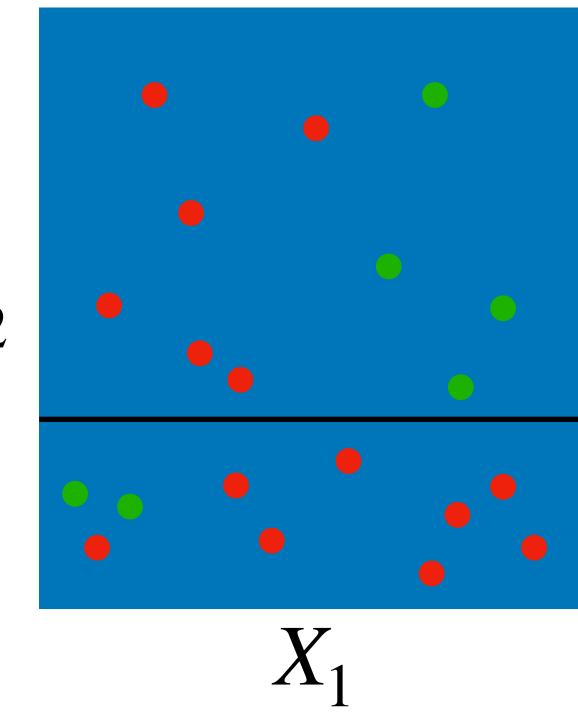
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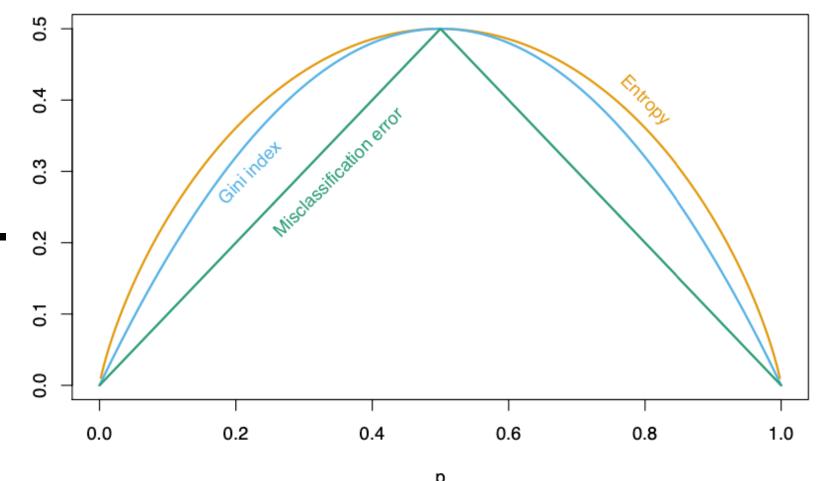
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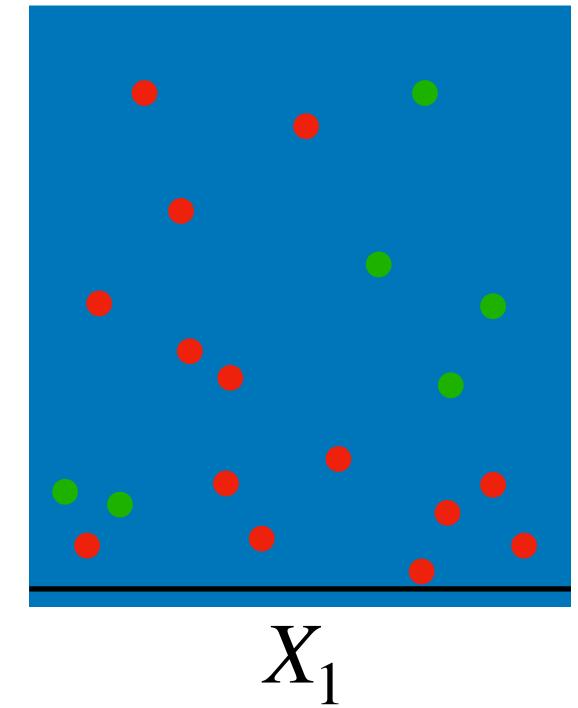
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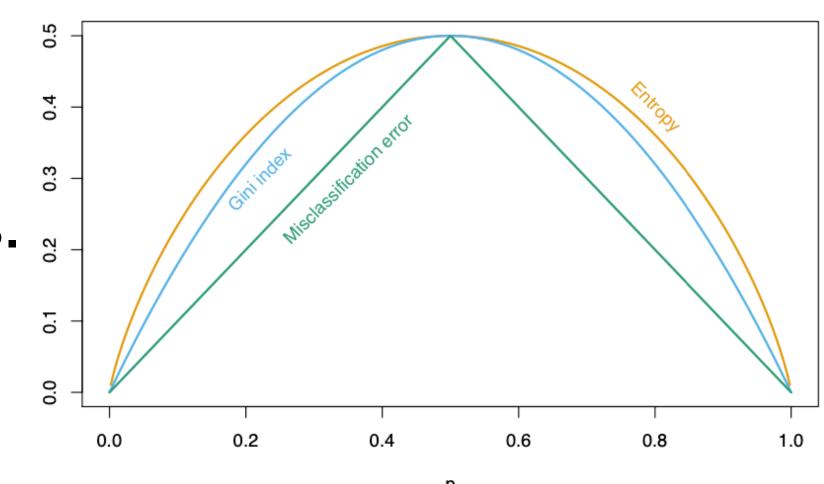
We use a very similar greedy recursive splitting algorithm.

Let \hat{p}_m be proportion of class 1 in region m. The misclassification error in that region is $\min(\hat{p}_m, 1 - \hat{p}_m)$.

Misclassification error not sensitive enough to find good split points at each step; instead, evaluate impurity using

Gini index =
$$2\hat{p}_m(1 - \hat{p}_m)$$
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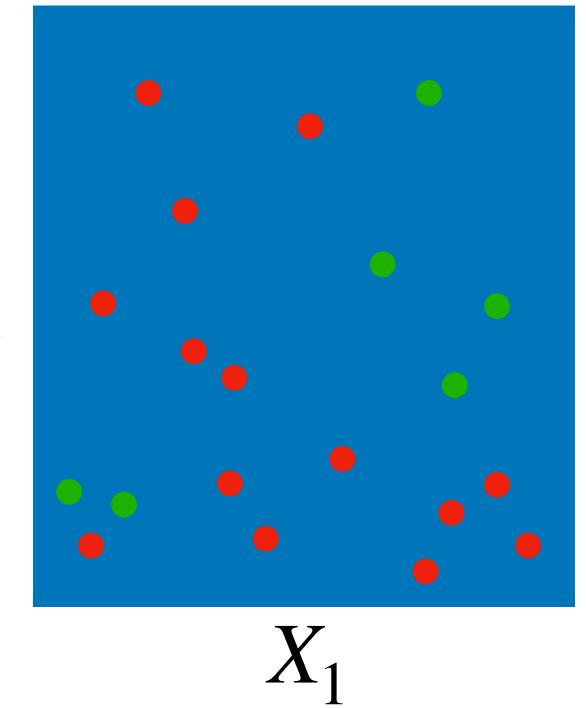
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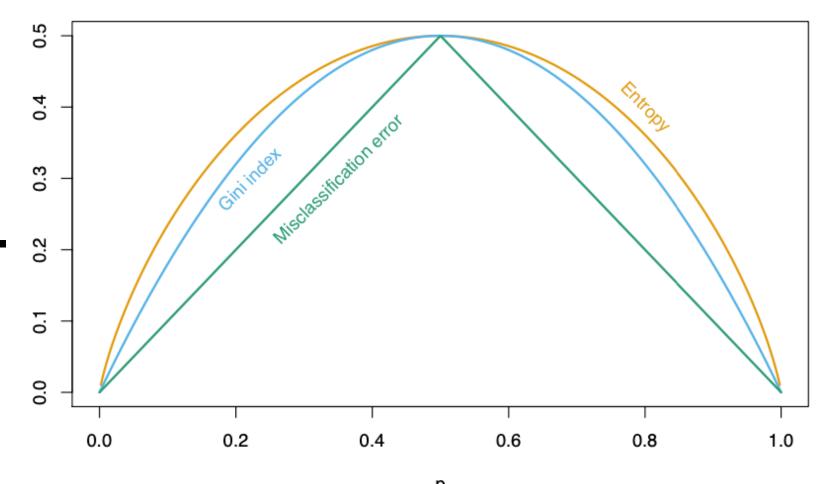
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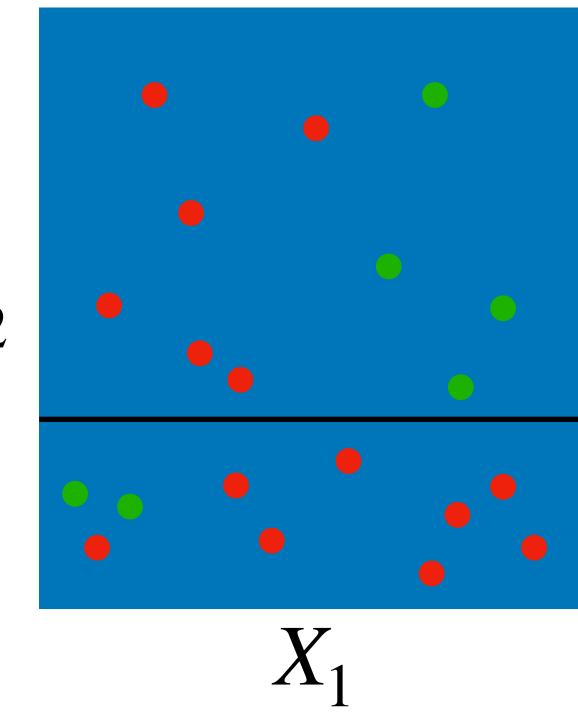
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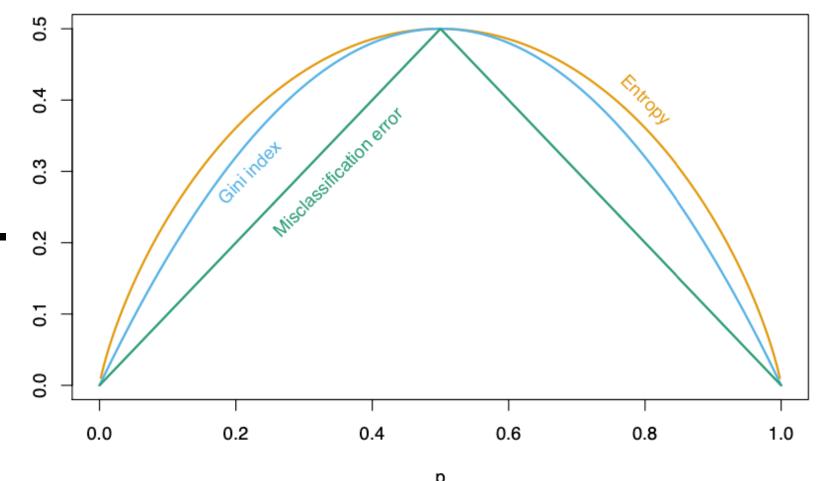
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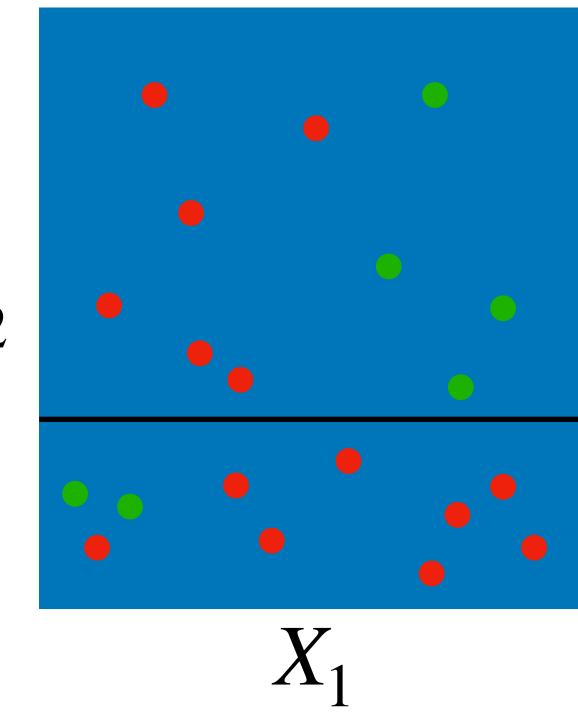
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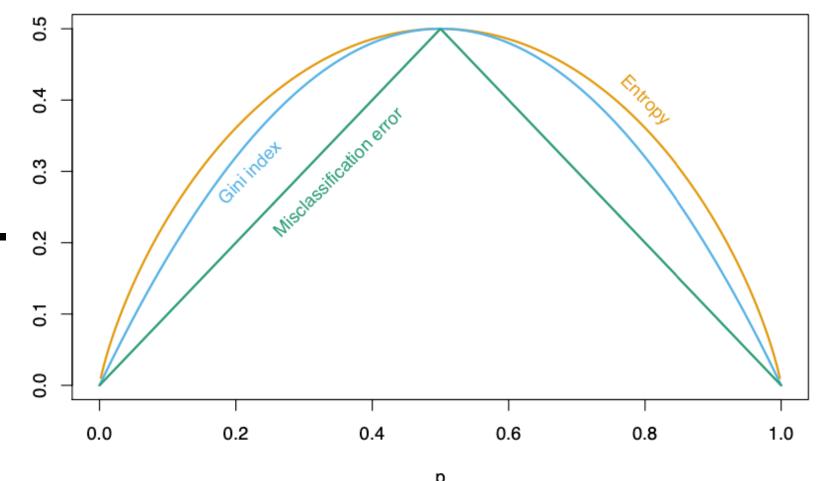
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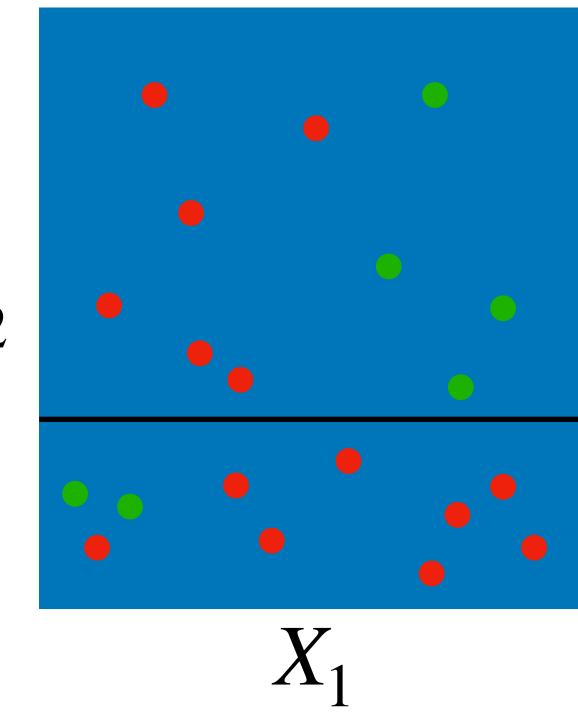
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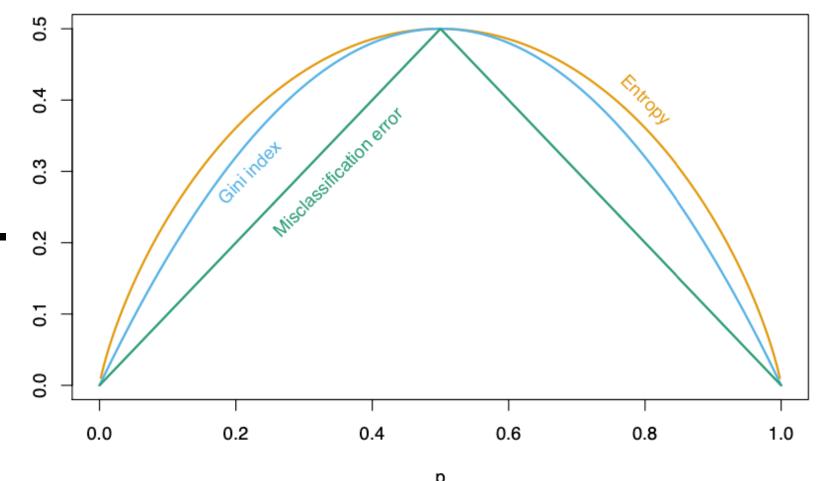
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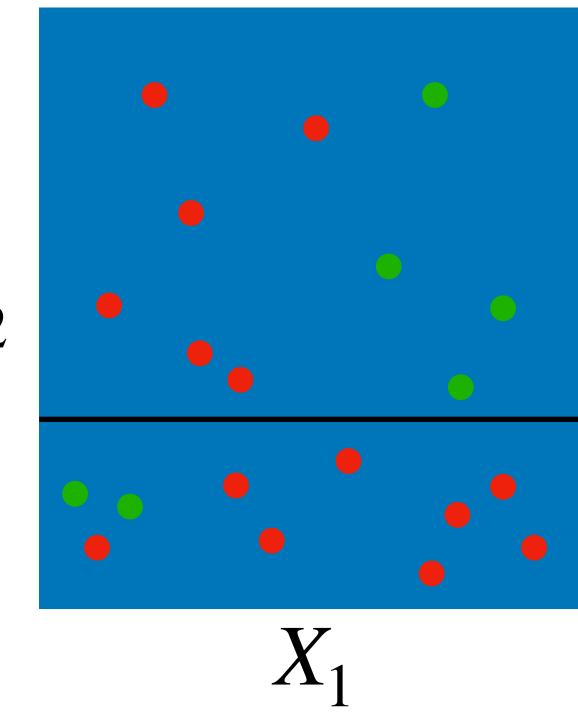
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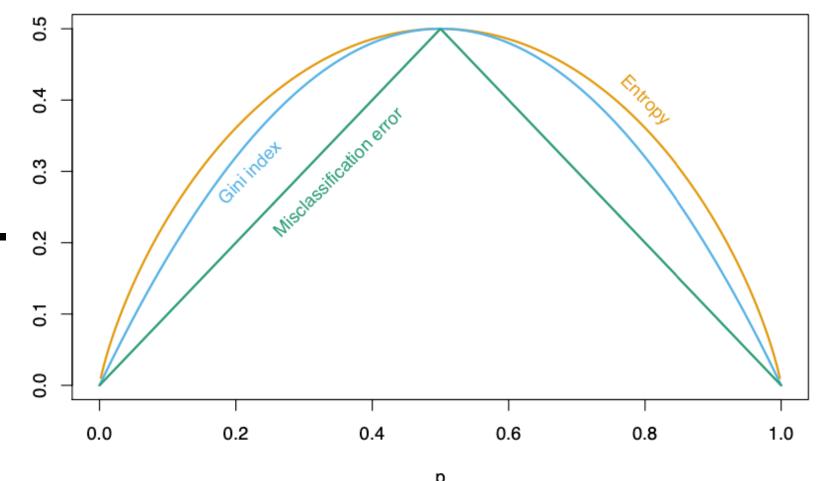
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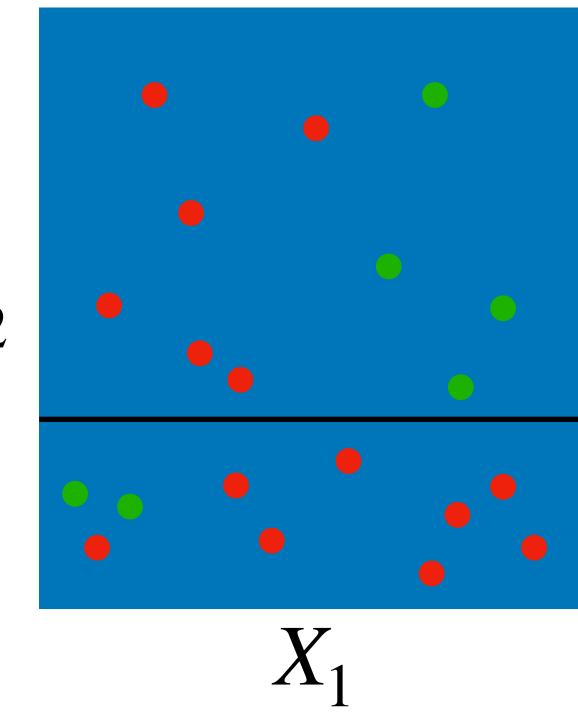
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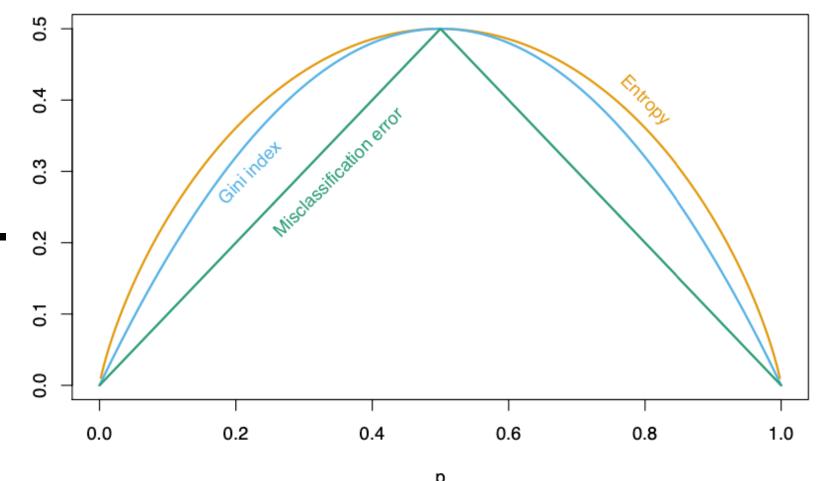
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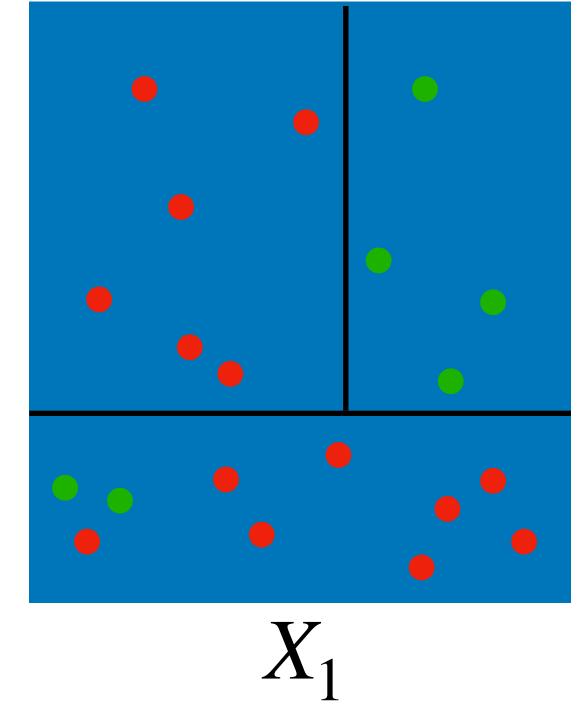
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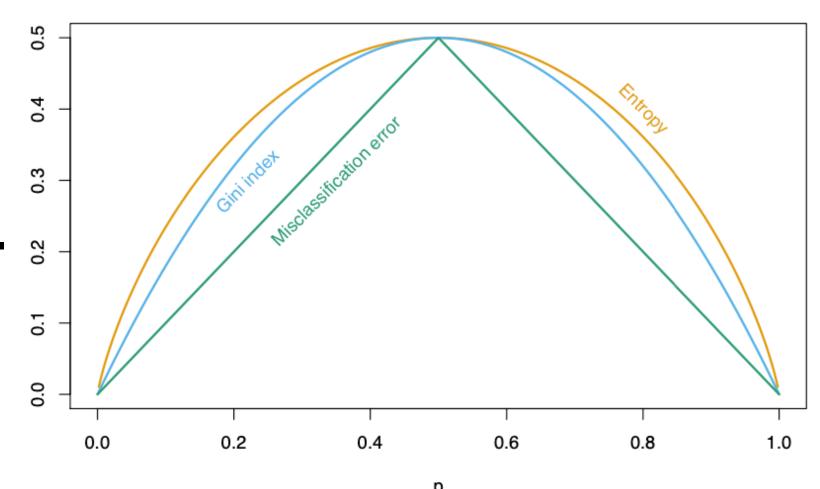
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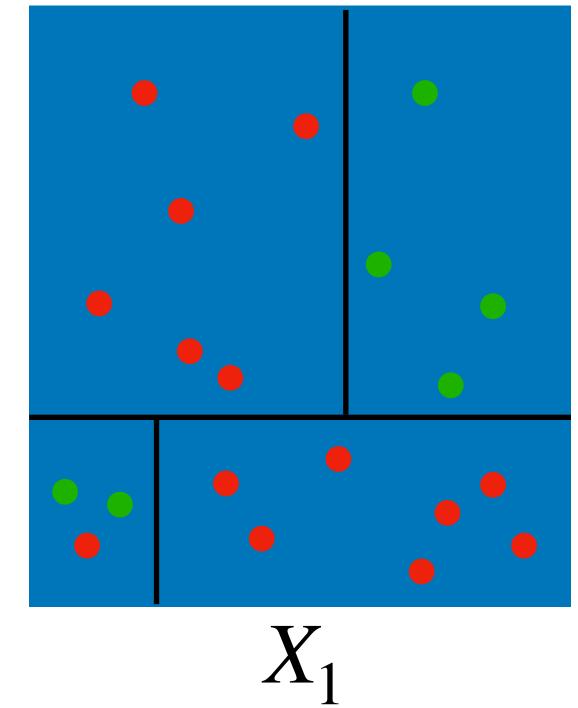
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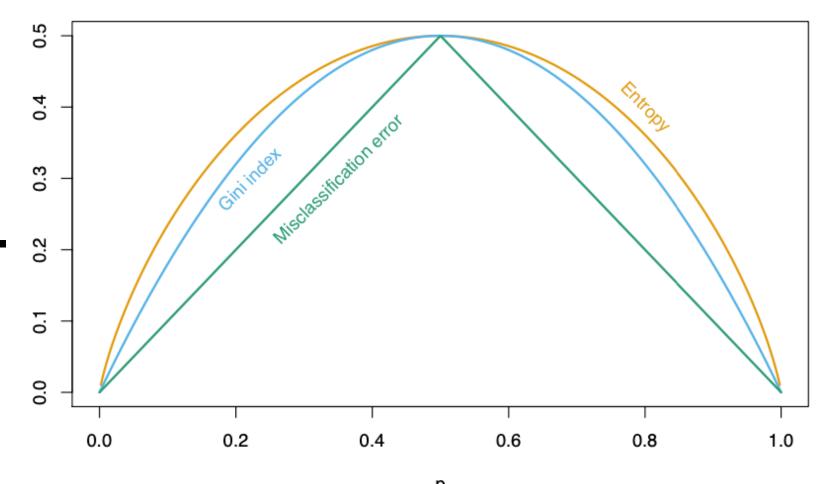
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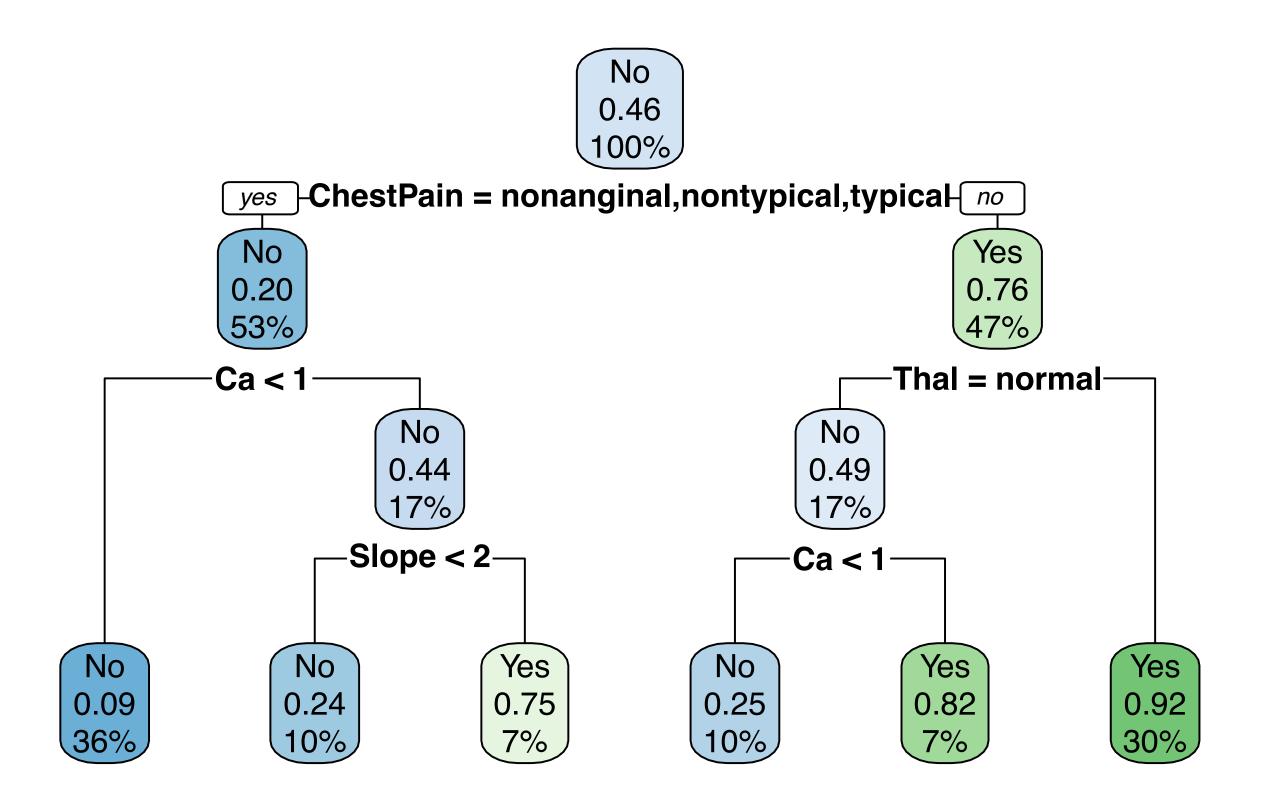




Final output

Example: Heart disease data set.

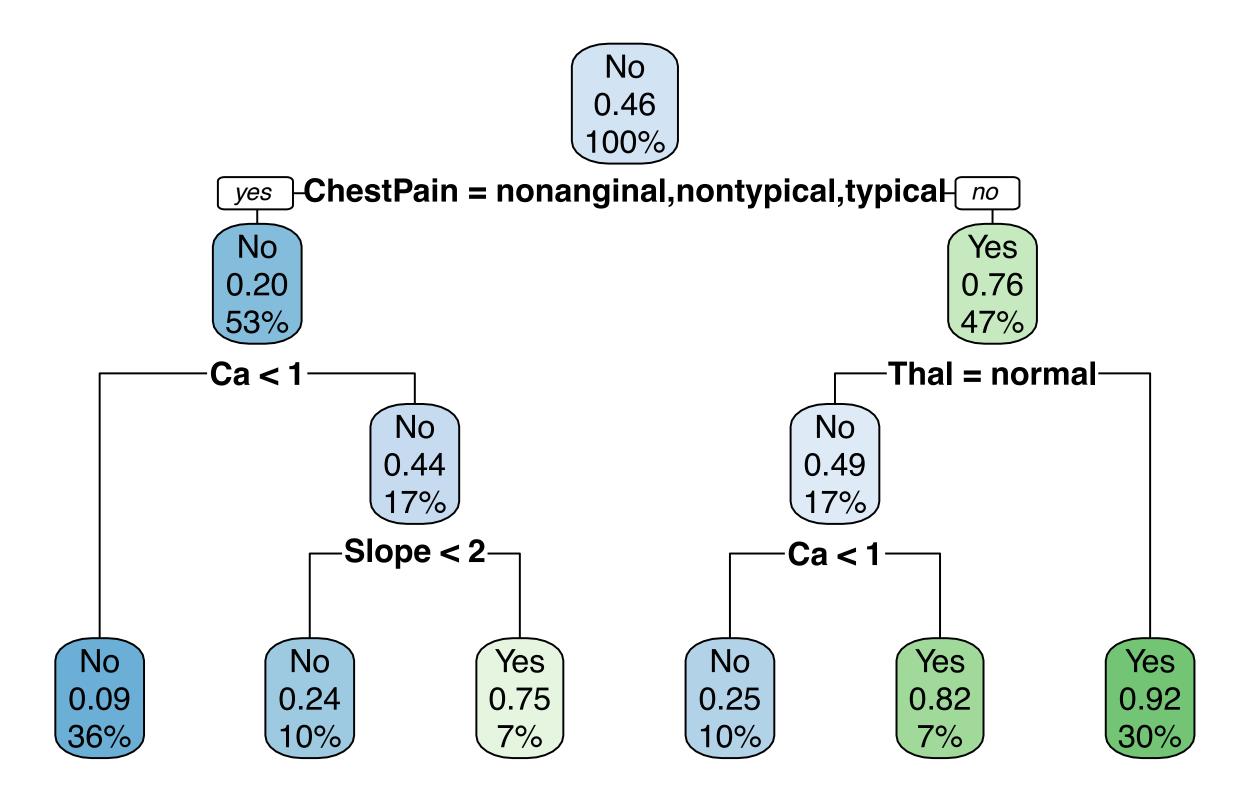
- 303 patients with chest pain
- Binary response HD (heart disease)
- 13 demographic and clinical features



Final output

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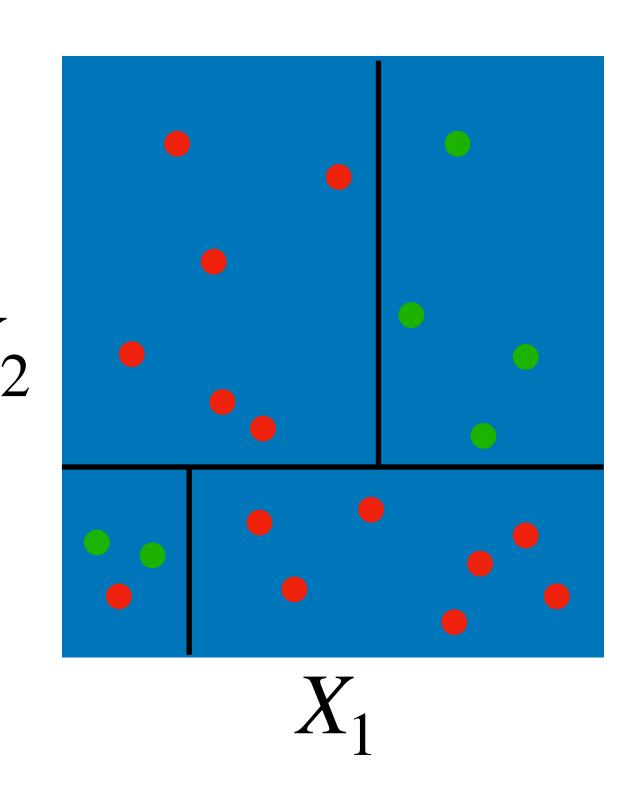
- 303 patients with chest pain
- Binary response HD (heart disease)
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Note: Classification trees extend seamlessly to more than two classes!

Summary

- Decision trees partition the feature space into axis-aligned nested rectangles, producing a constant prediction for feature vectors in each rectangle.
- Decision trees are built by recursively choosing
 - The optimal rectangle to split
 - The optimal feature to split that rectangle on
 - The optimal split-point for that feature
- Regression and classification trees aim to minimize squared error and misclassification losses, respectively.



Quiz Practice