Growing decision trees

STAT 4710

October 26, 2023

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

Leaving the land of linearity

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

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In Unit 4 we will leave the land of linearity.

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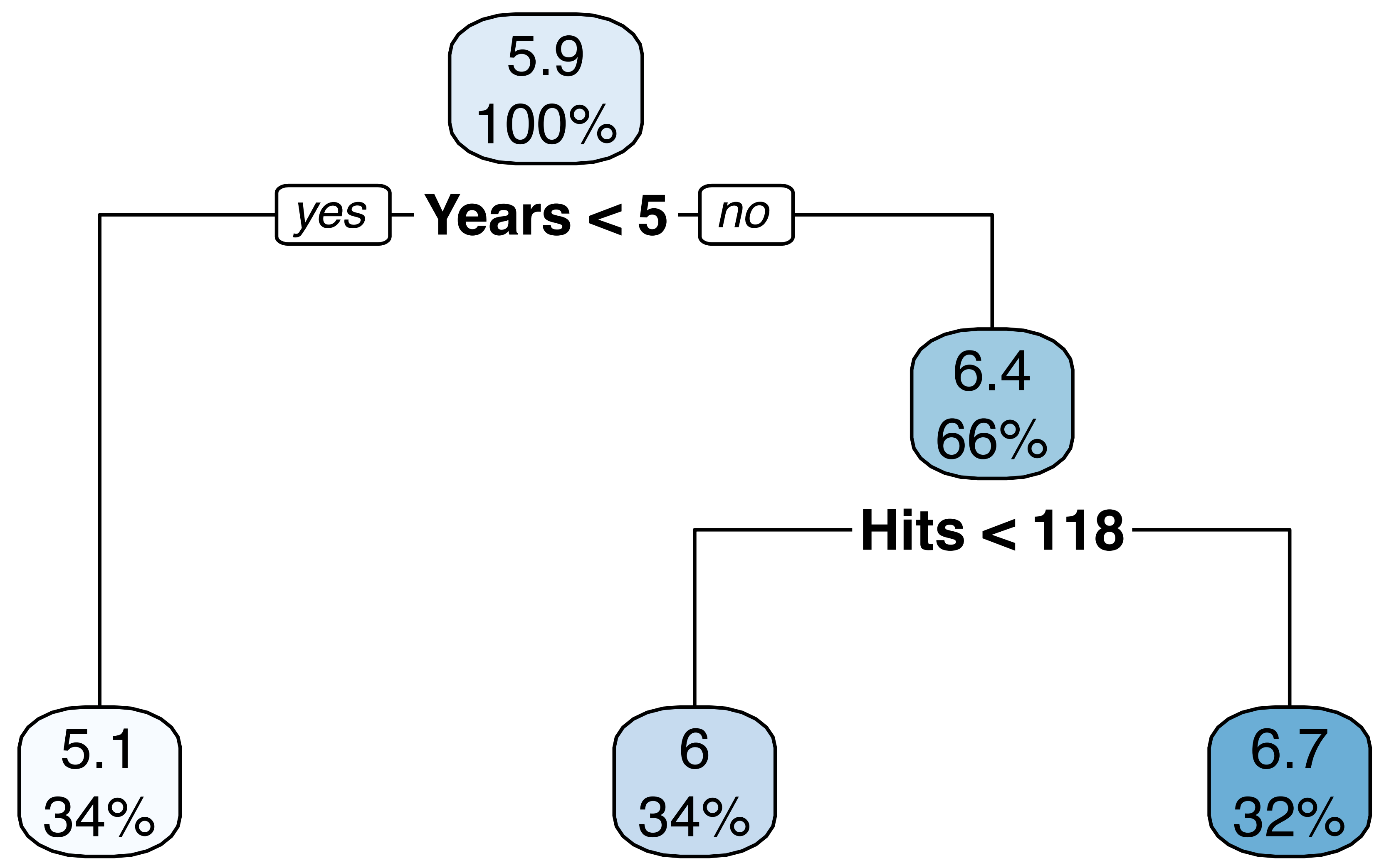

Predicting baseball players' salaries based on years played and number of hits in the previous year.

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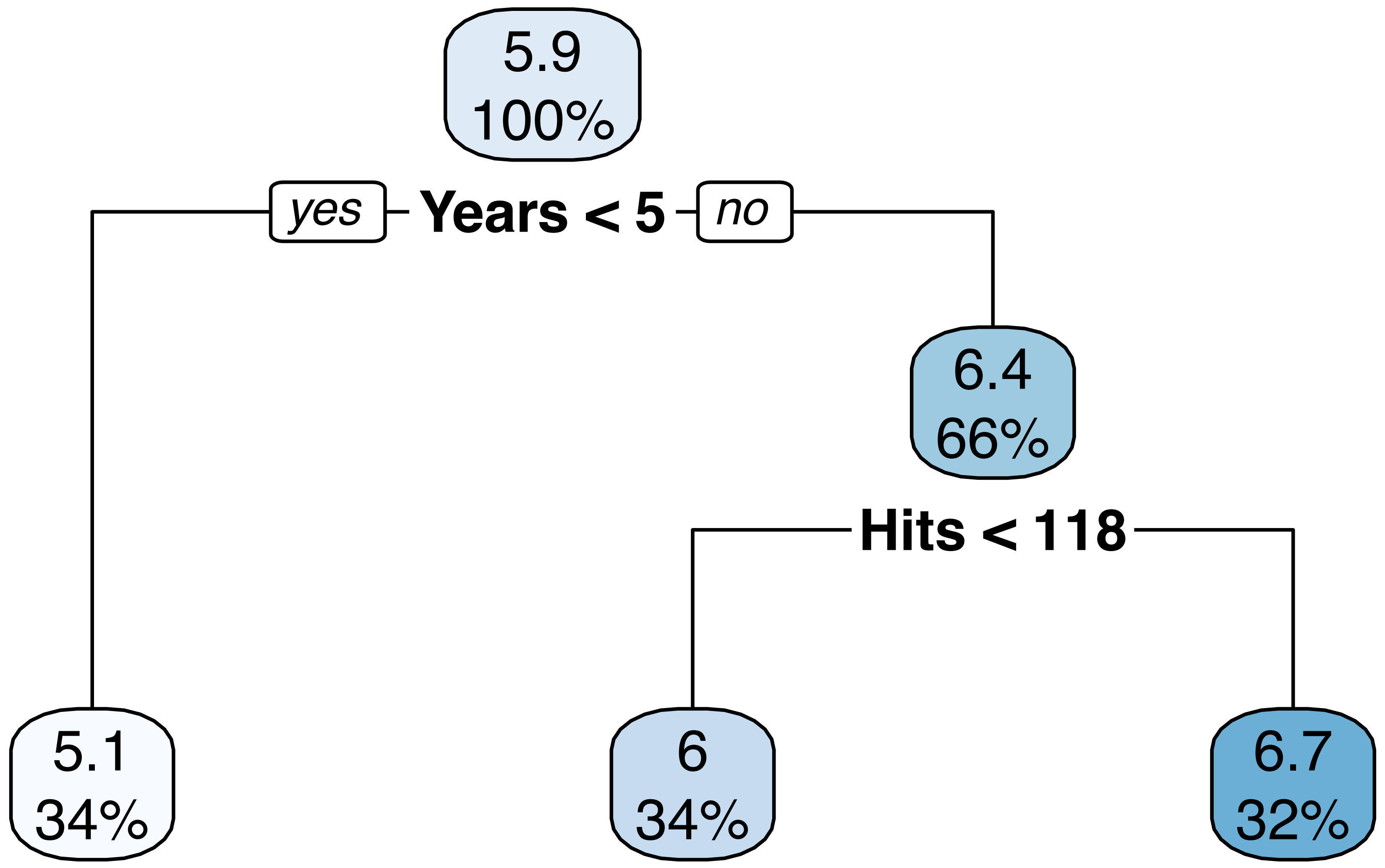
Their prediction rules can be nicely illustrated and are very interpretable.



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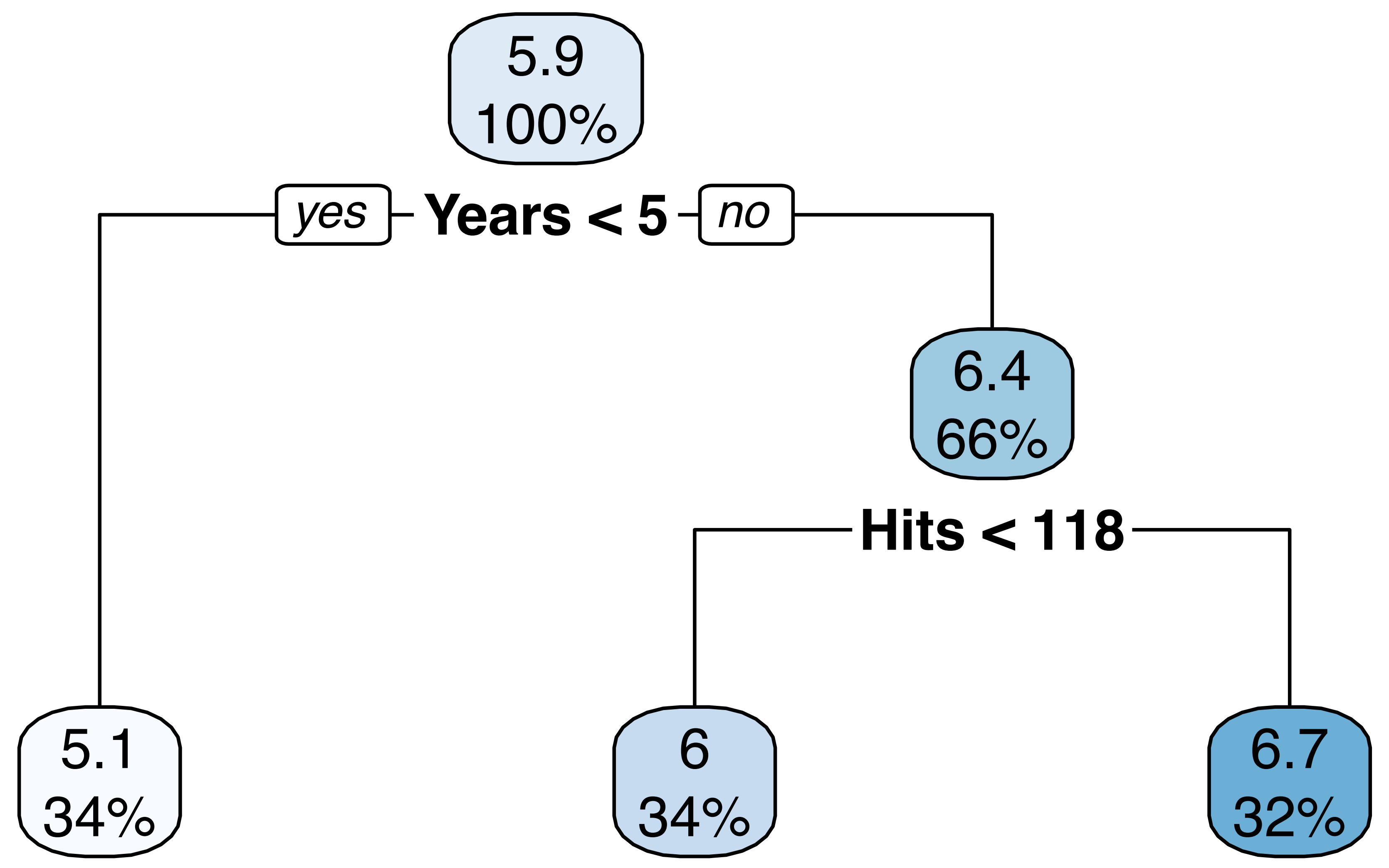

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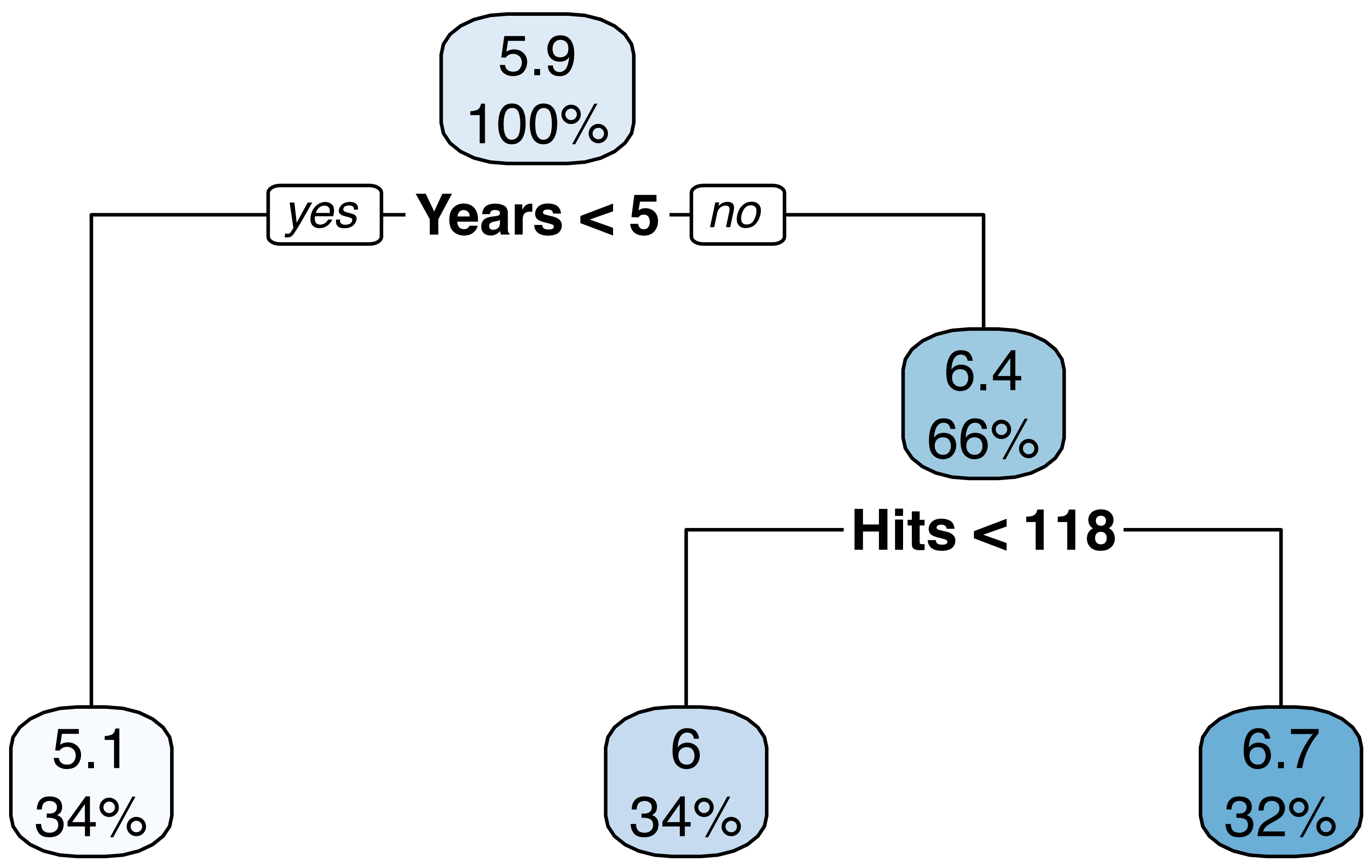
Nevertheless, trees can be used as building blocks for state-of-the-art prediction performance:

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



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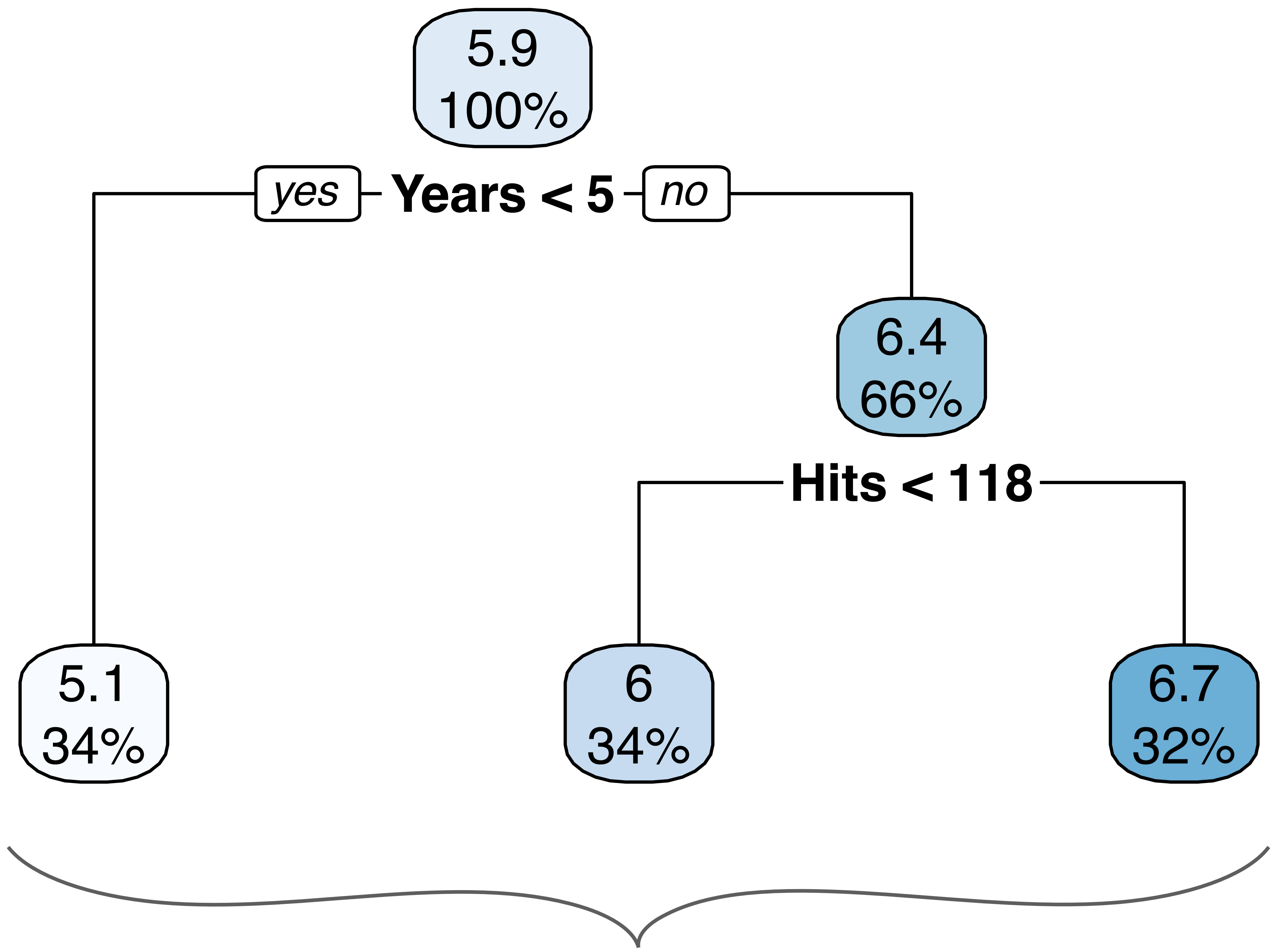
Hitters data

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)

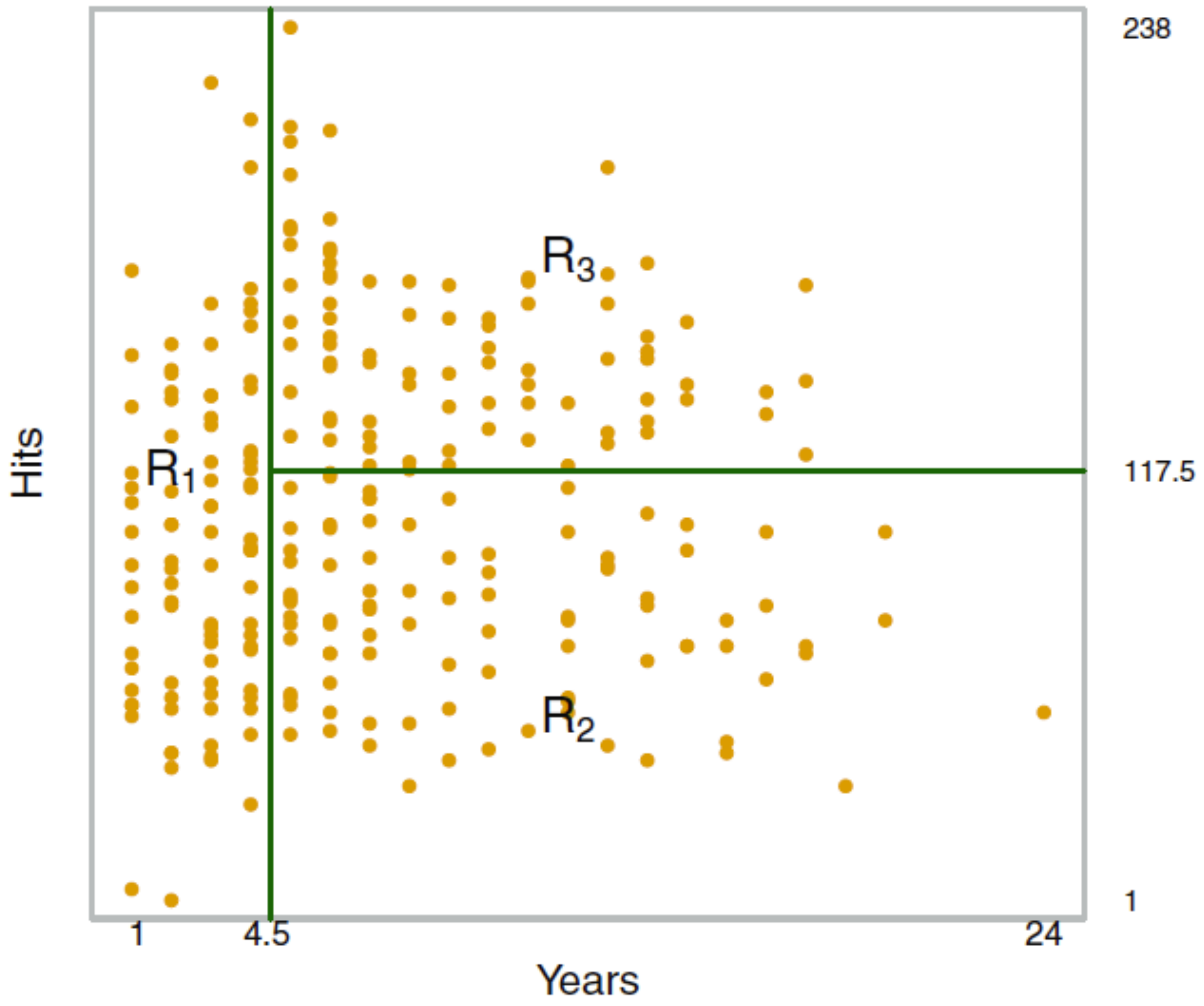
Image credit: DALL-E 3

Tree $\Longleftrightarrow$ Partition into nested, axis-aligned rectangles



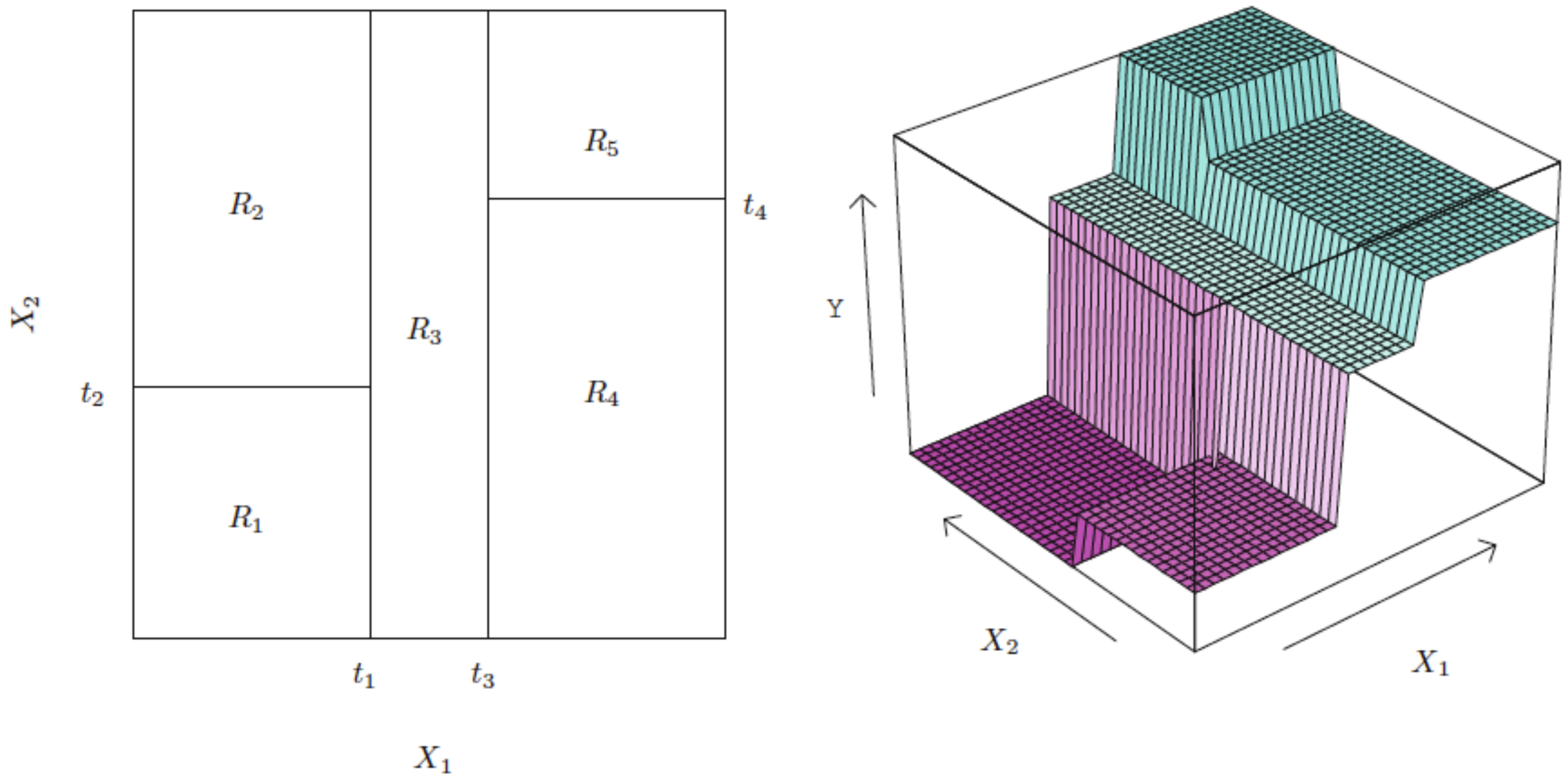
Nodes without any descendants called
leaf nodes or terminal nodes (equivalent)

$\Longleftrightarrow$



Each terminal node corresponds to a rectangular region of feature space.

Mathematical expression of the prediction rule



Mathematical expression of the prediction rule

A trained tree consists of:

- M regions $\widehat{R}_1, \ldots, \widehat{R}_M$
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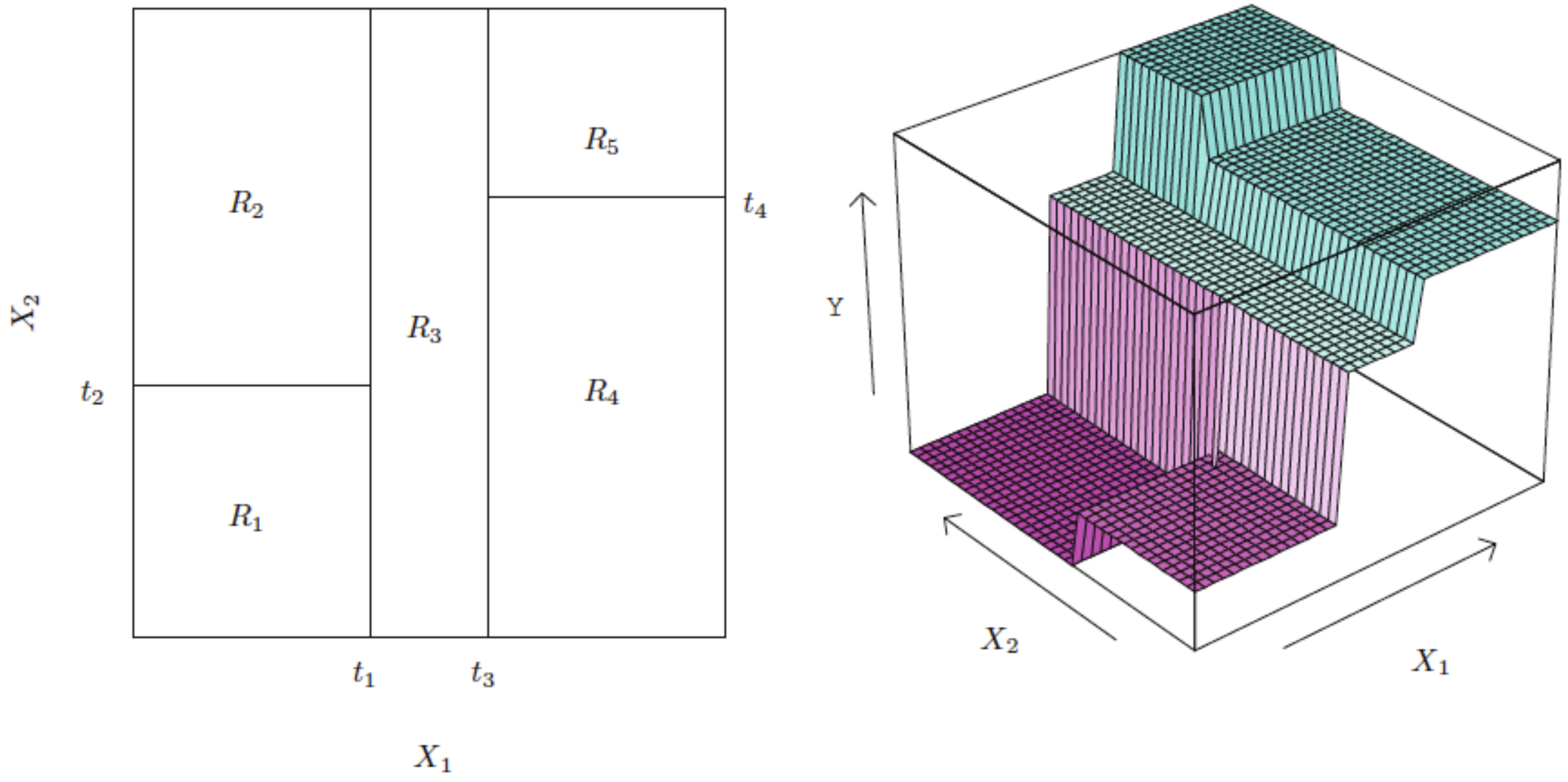

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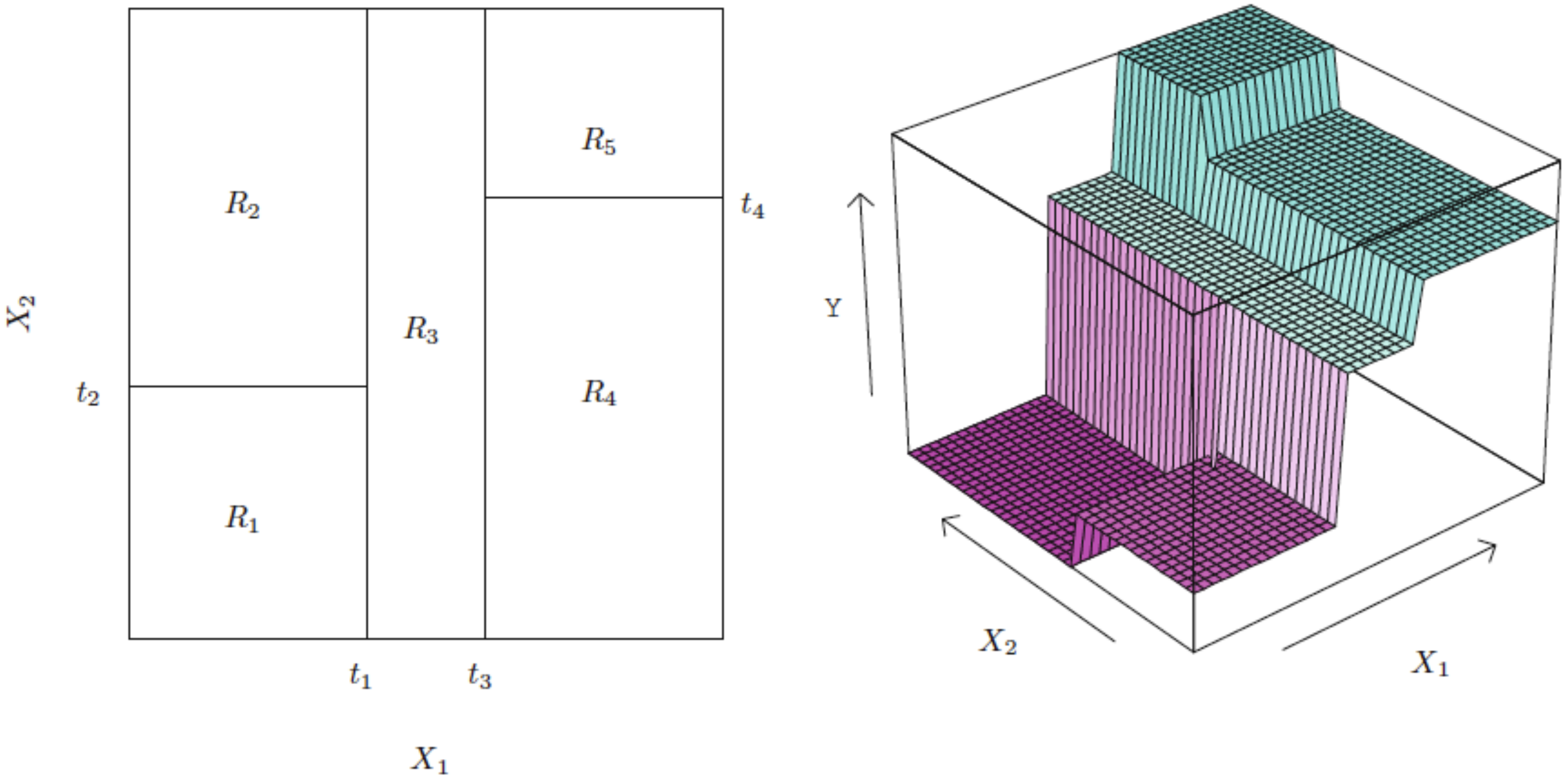
For a new feature vector X^{test}, predict the constant value $\widehat{c}_m$ for region $\widehat{R}_m$:

$$\widehat{Y}^{\text{test}} = \widehat{c}_m \text{ if } X^{\text{test}} \in \widehat{R}_m.$$

(continuous or categorical response)



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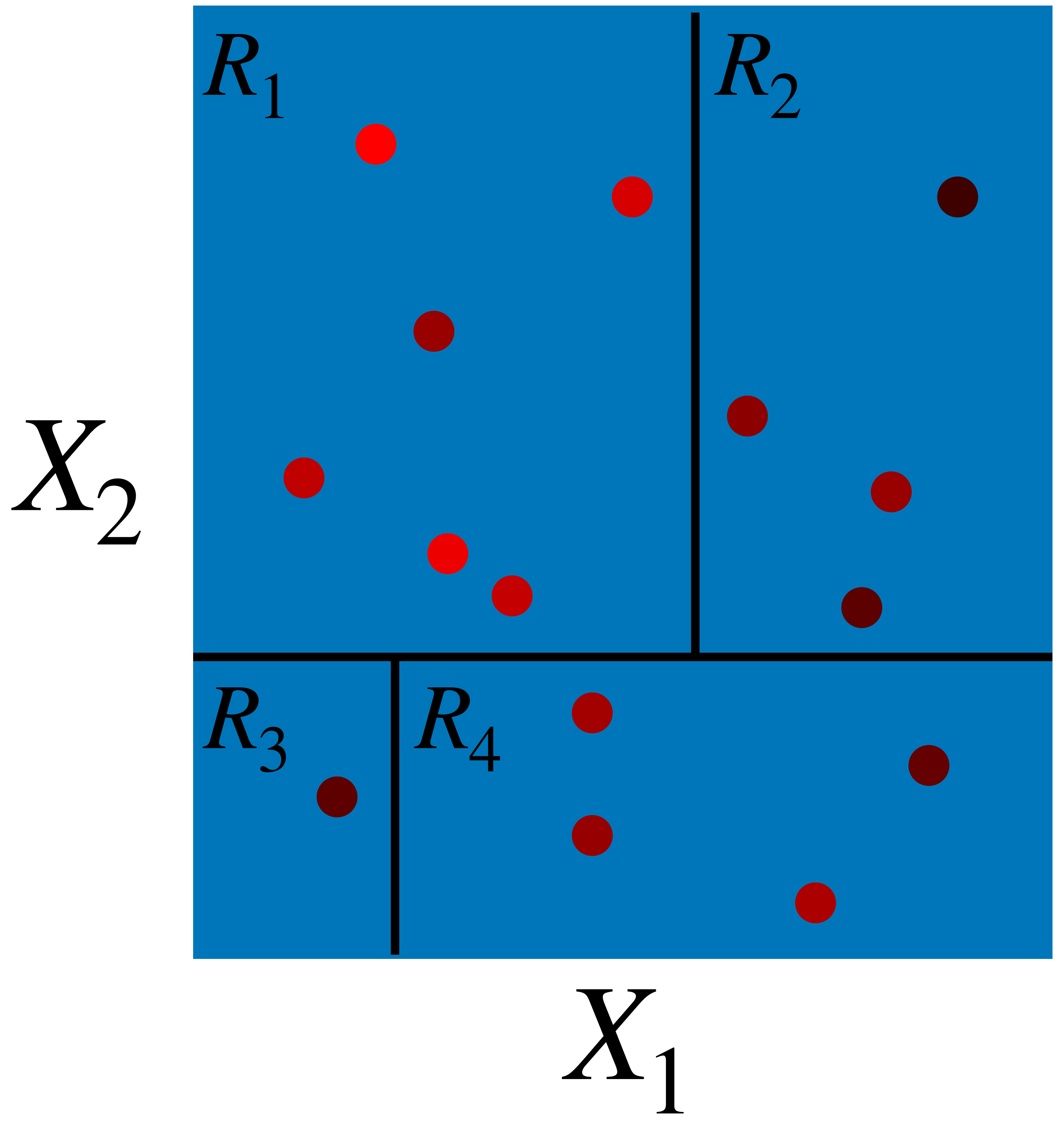
- If X_j is continuous, we just find a split point s and split into $\{X : X_j < s\}$ and $\{X : X_j \geq s\}$.
- If X_j is categorical, e.g. with levels $\{a, b, c, d, e\}$, then we need to split the levels into two groups, e.g. $\{a, c\}$ and $\{b, d, e\}$, giving the partitions $\{X : X_j \in \{a,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

Training a regression tree

The squared error objective



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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 (RSS):

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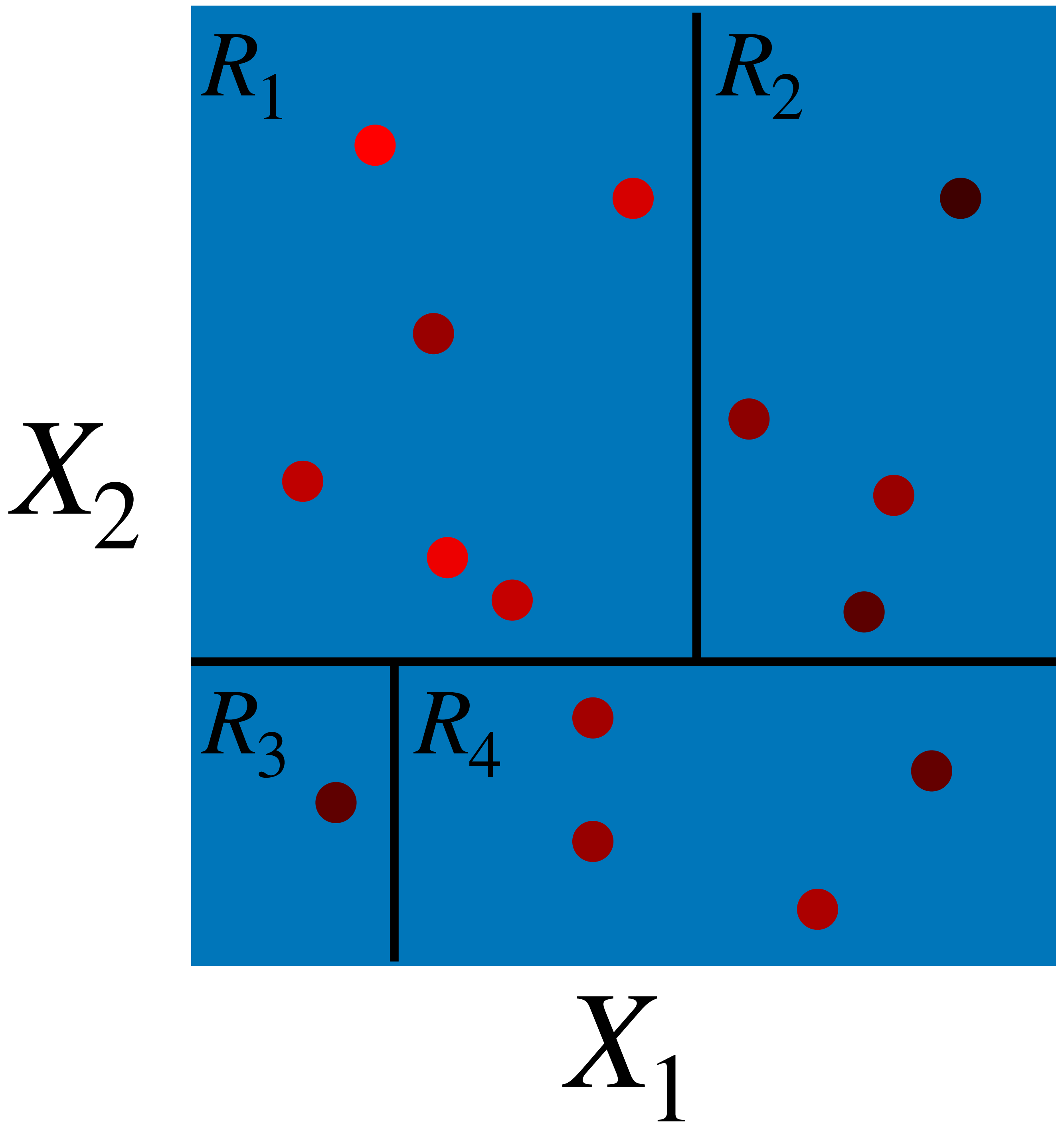

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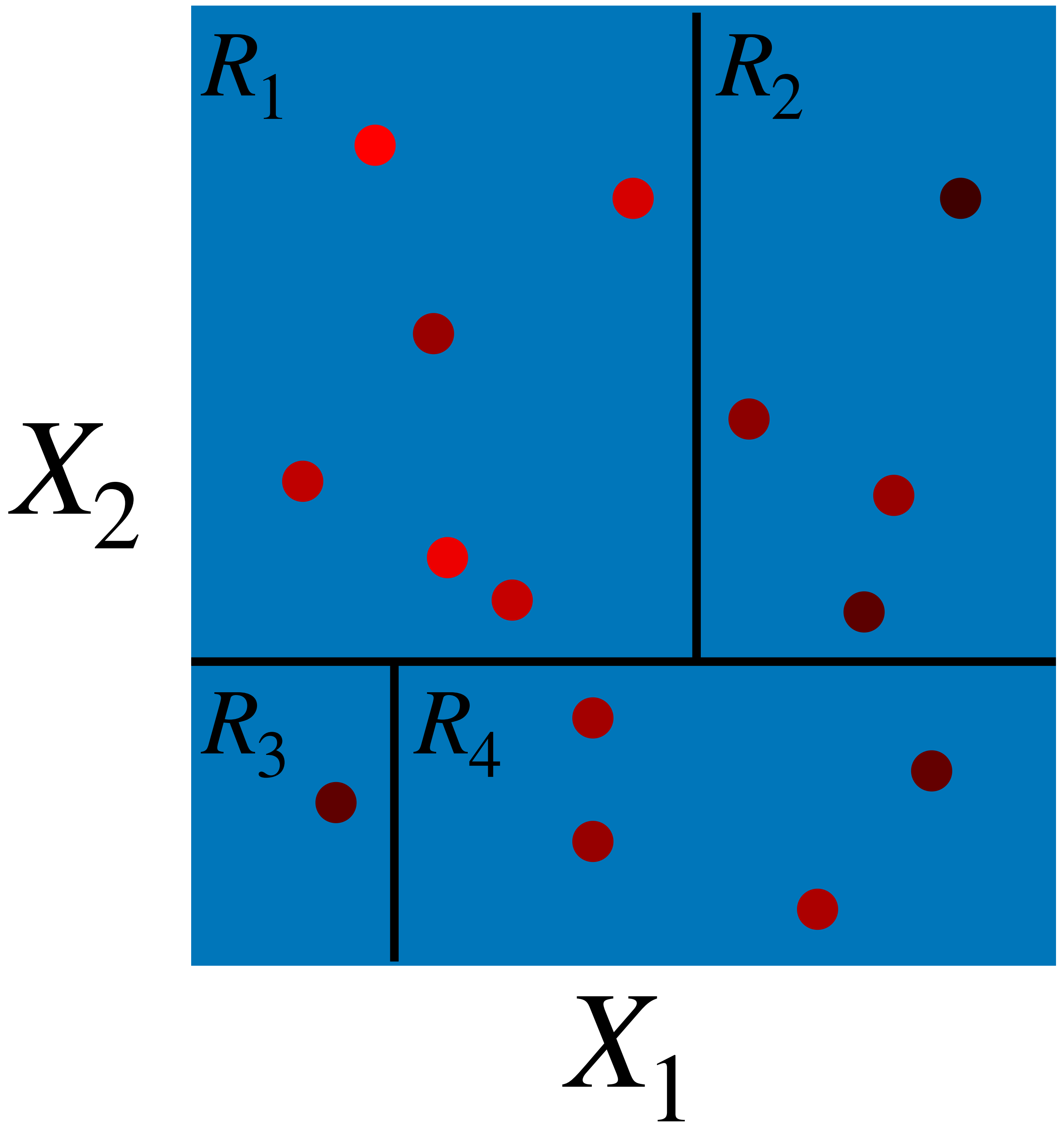

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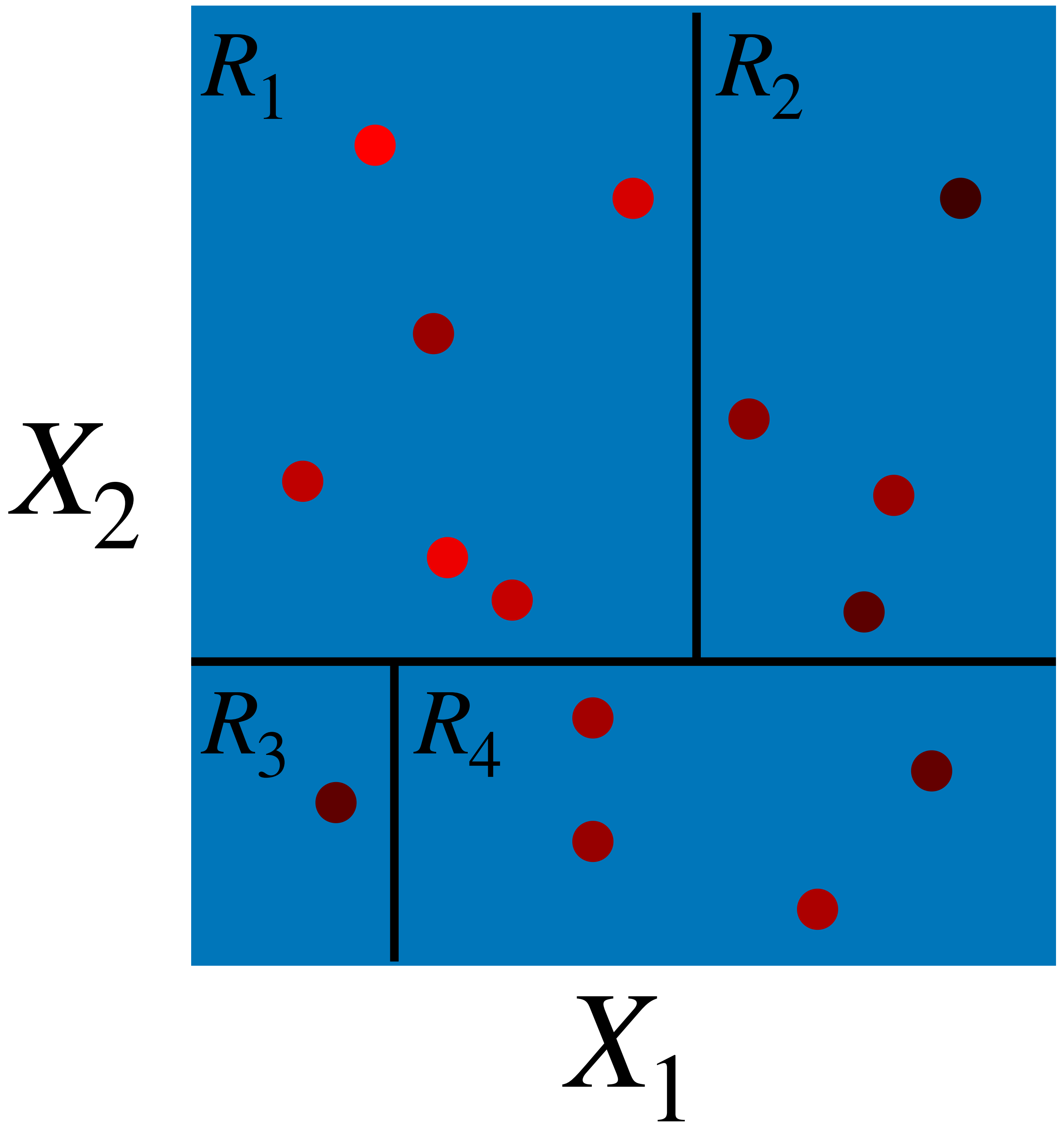

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Optimal $\widehat{c}_m$ given $\widehat{R}_m$

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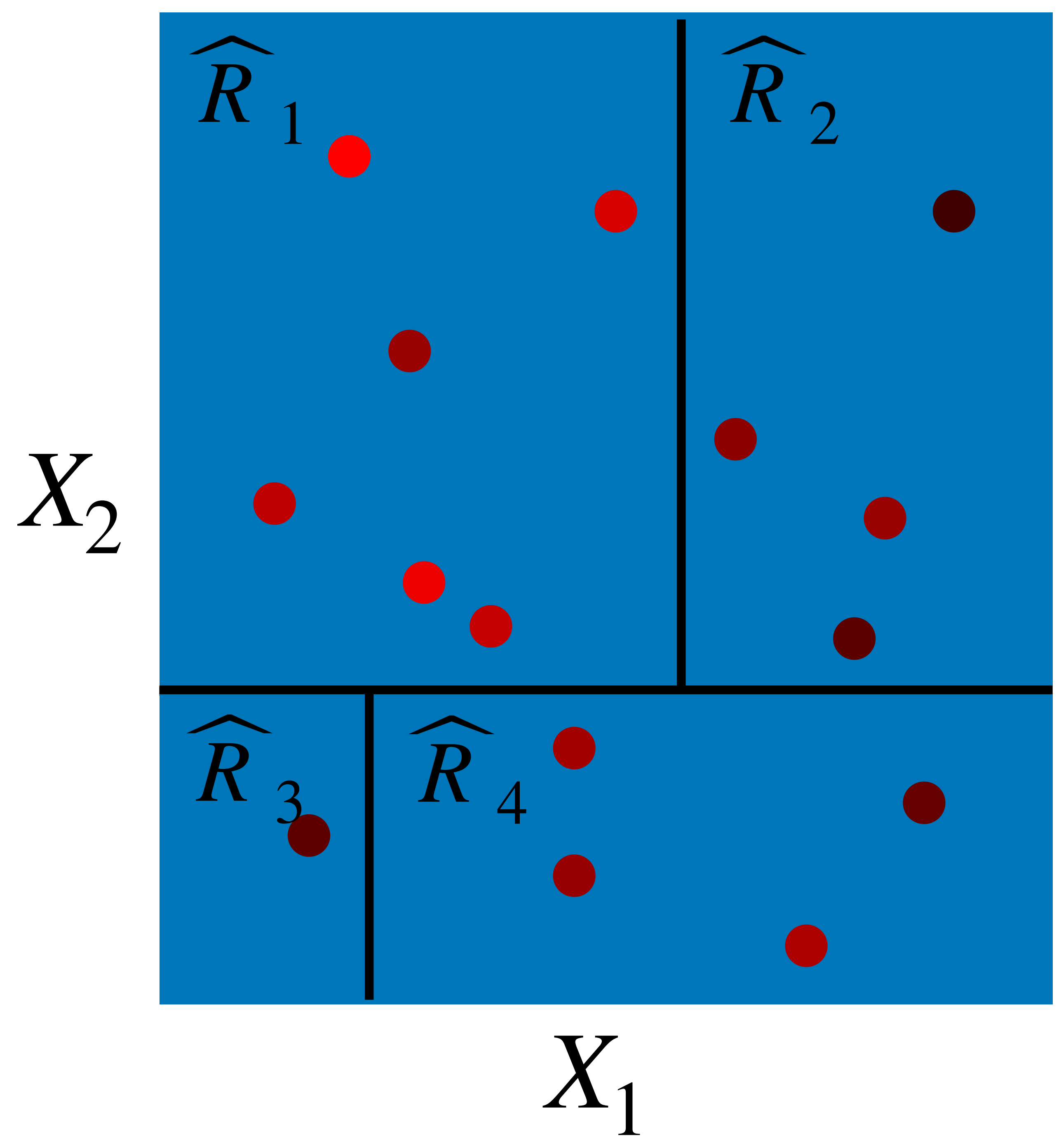

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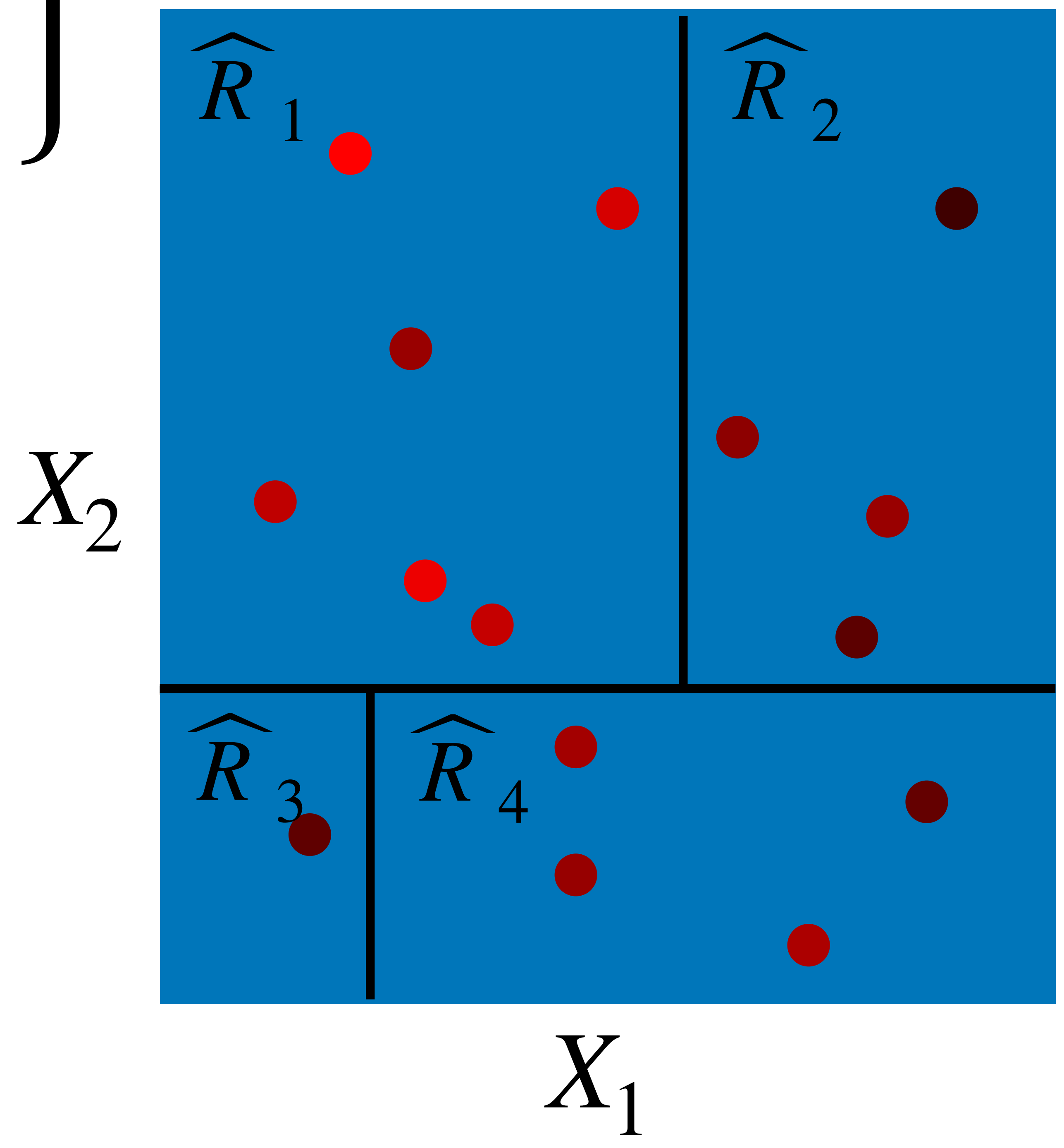

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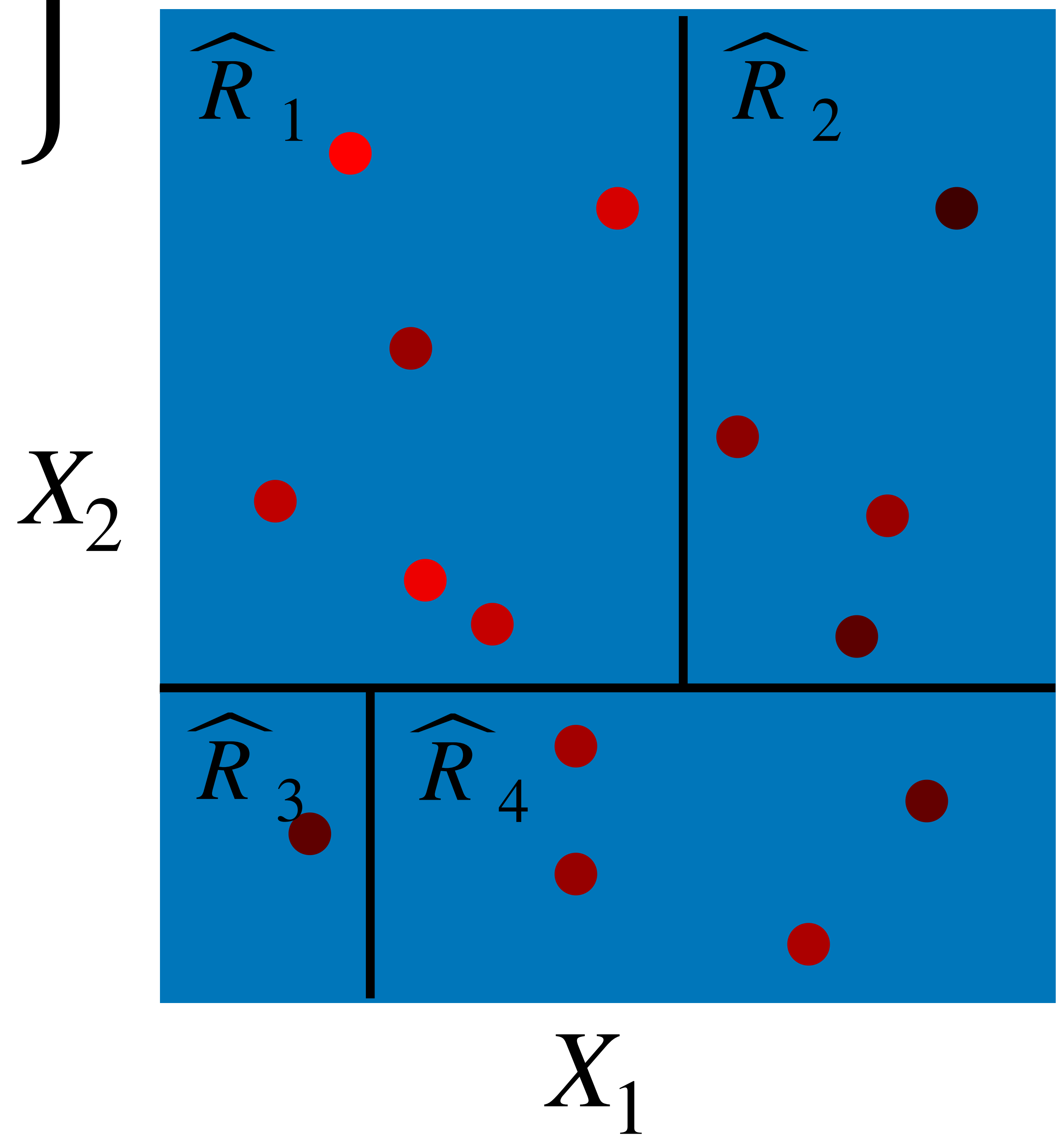
We're fitting a constant to each region, so the solution is

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



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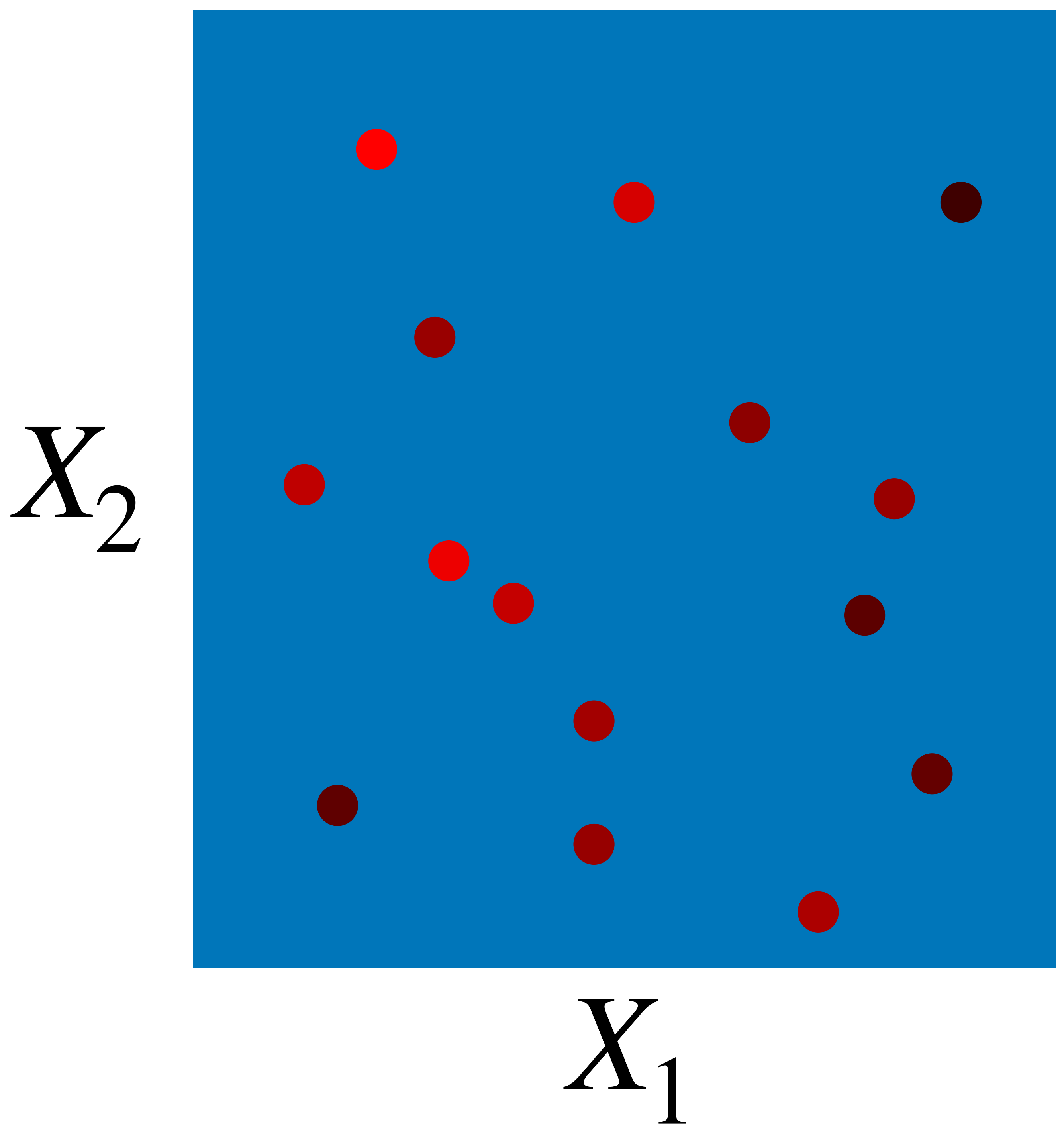

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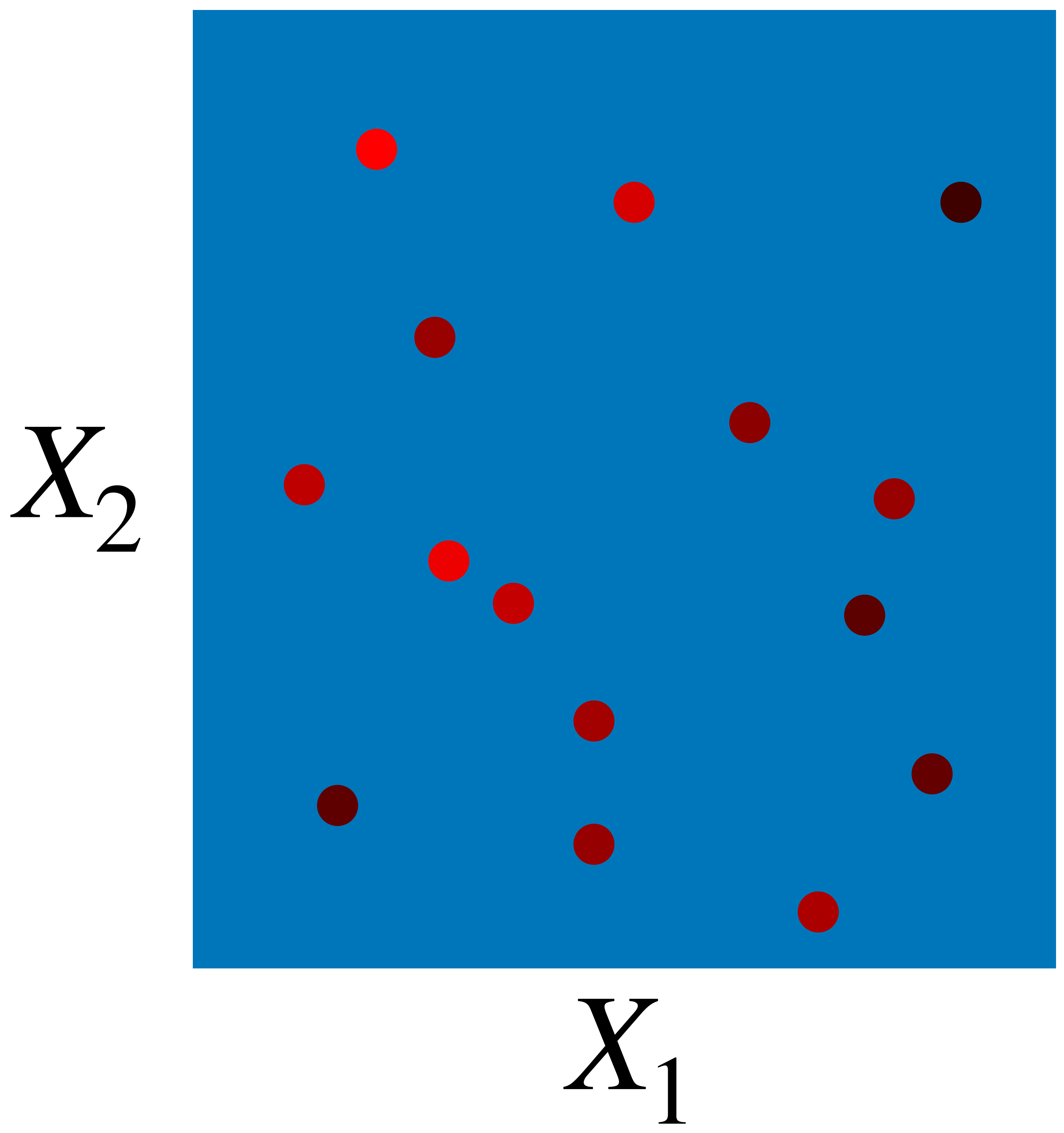

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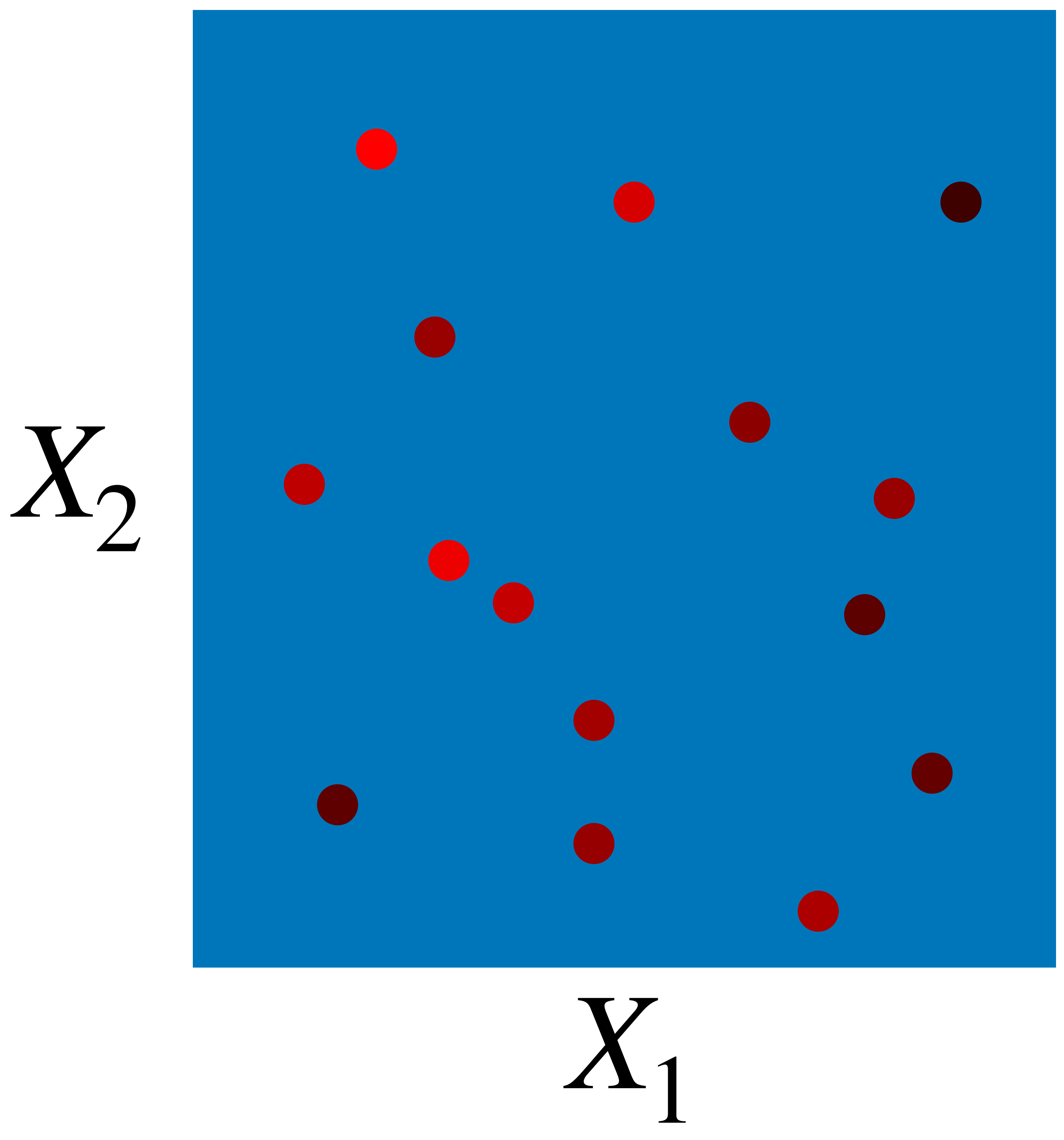

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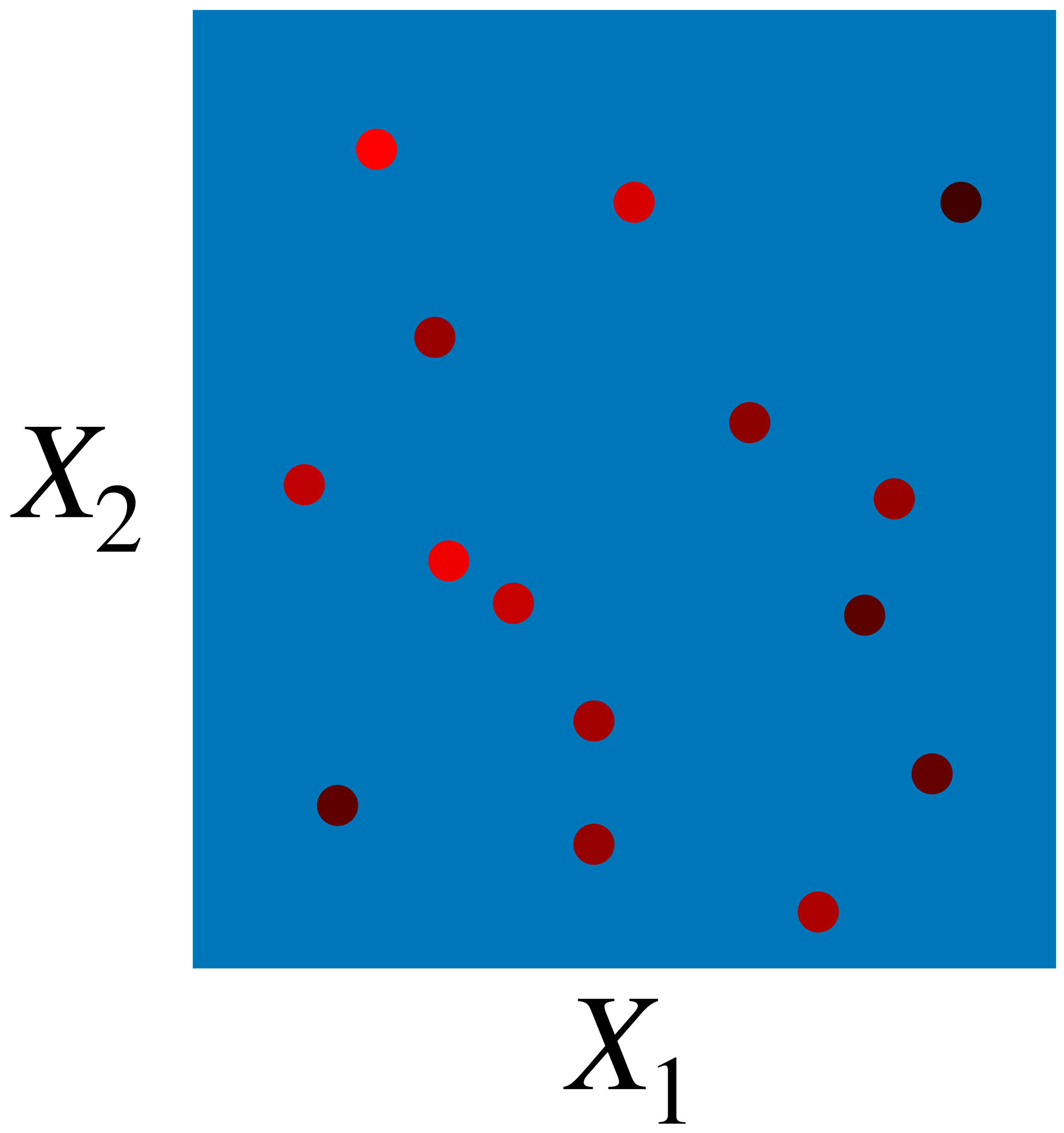

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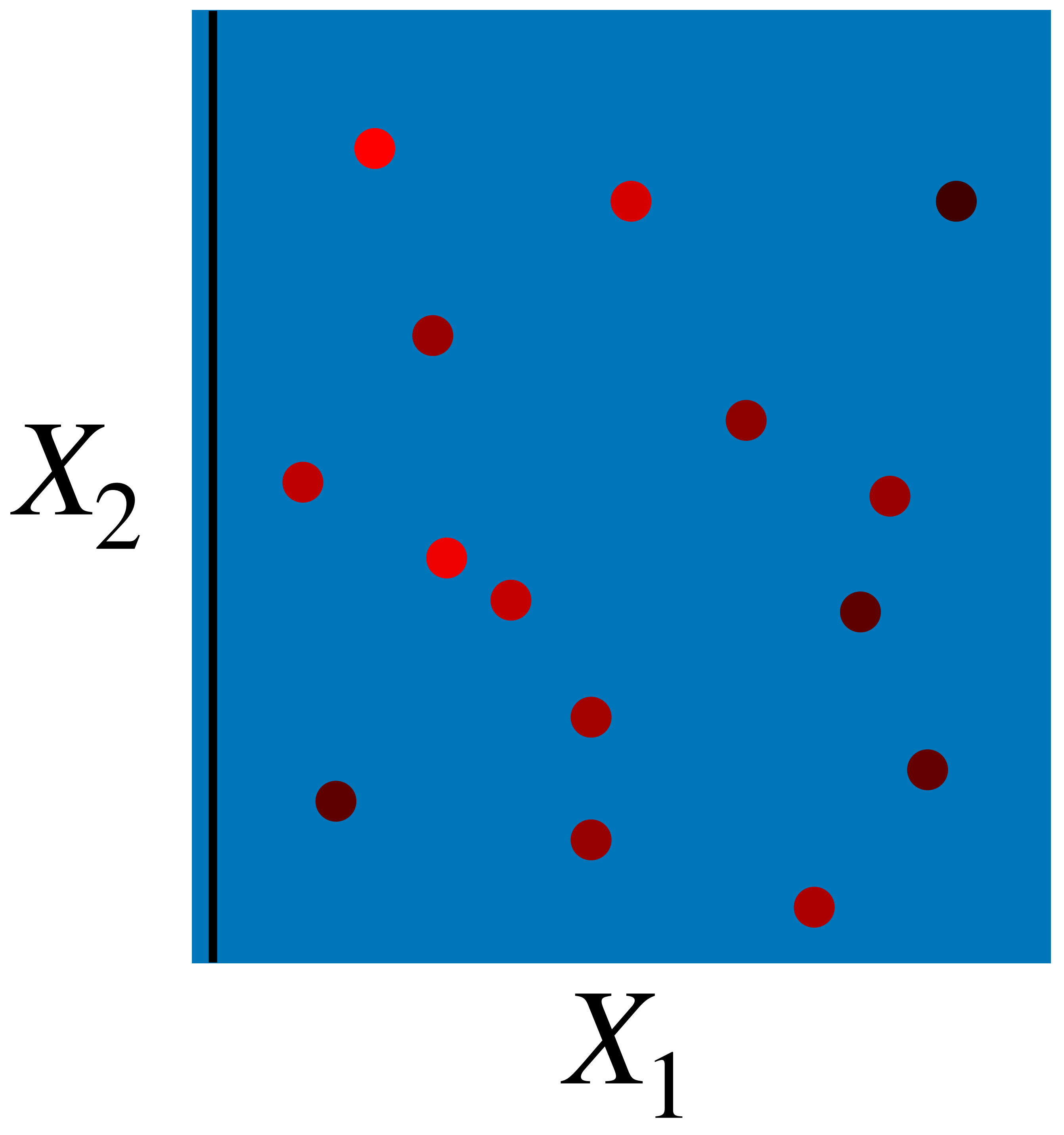

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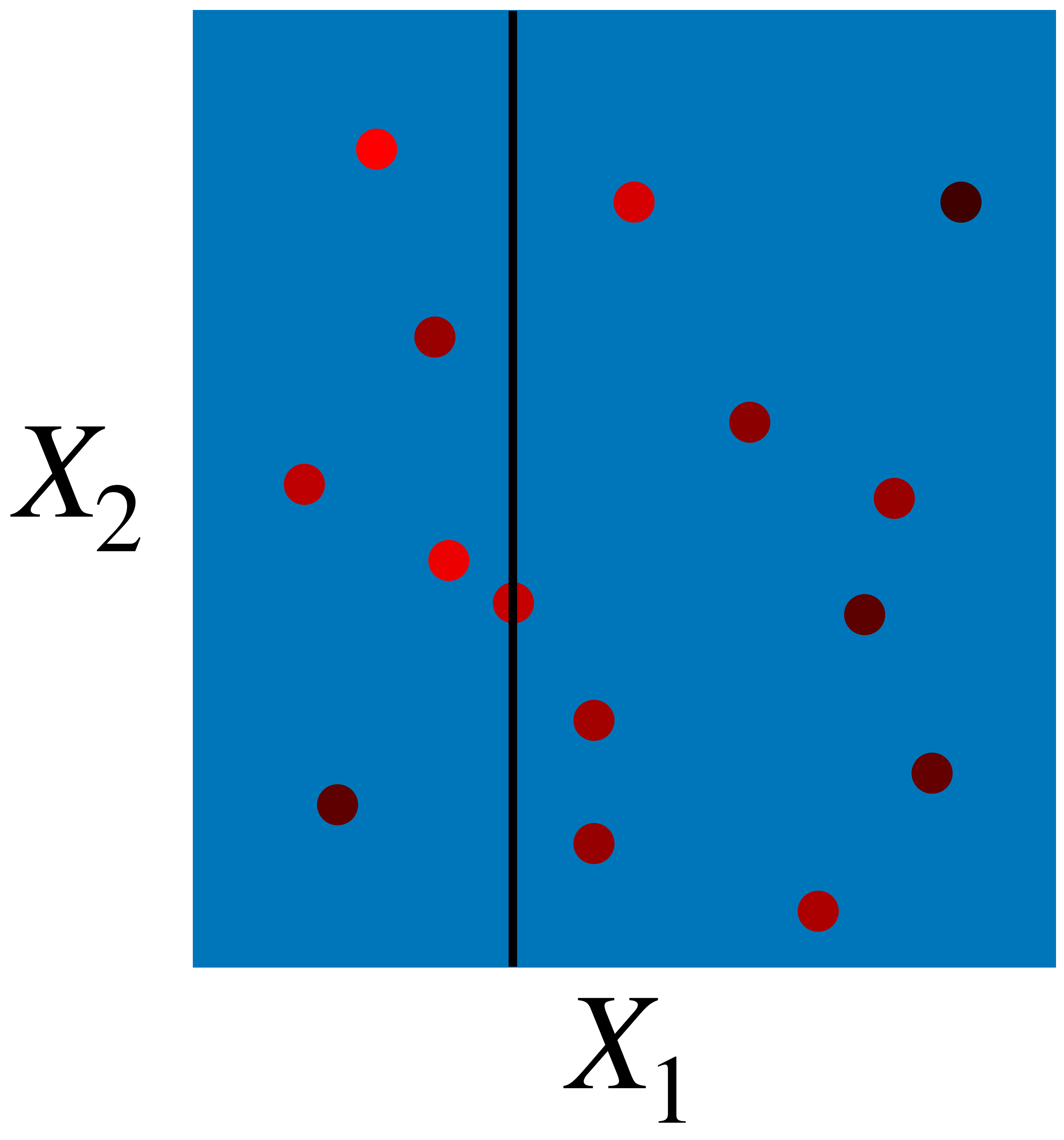

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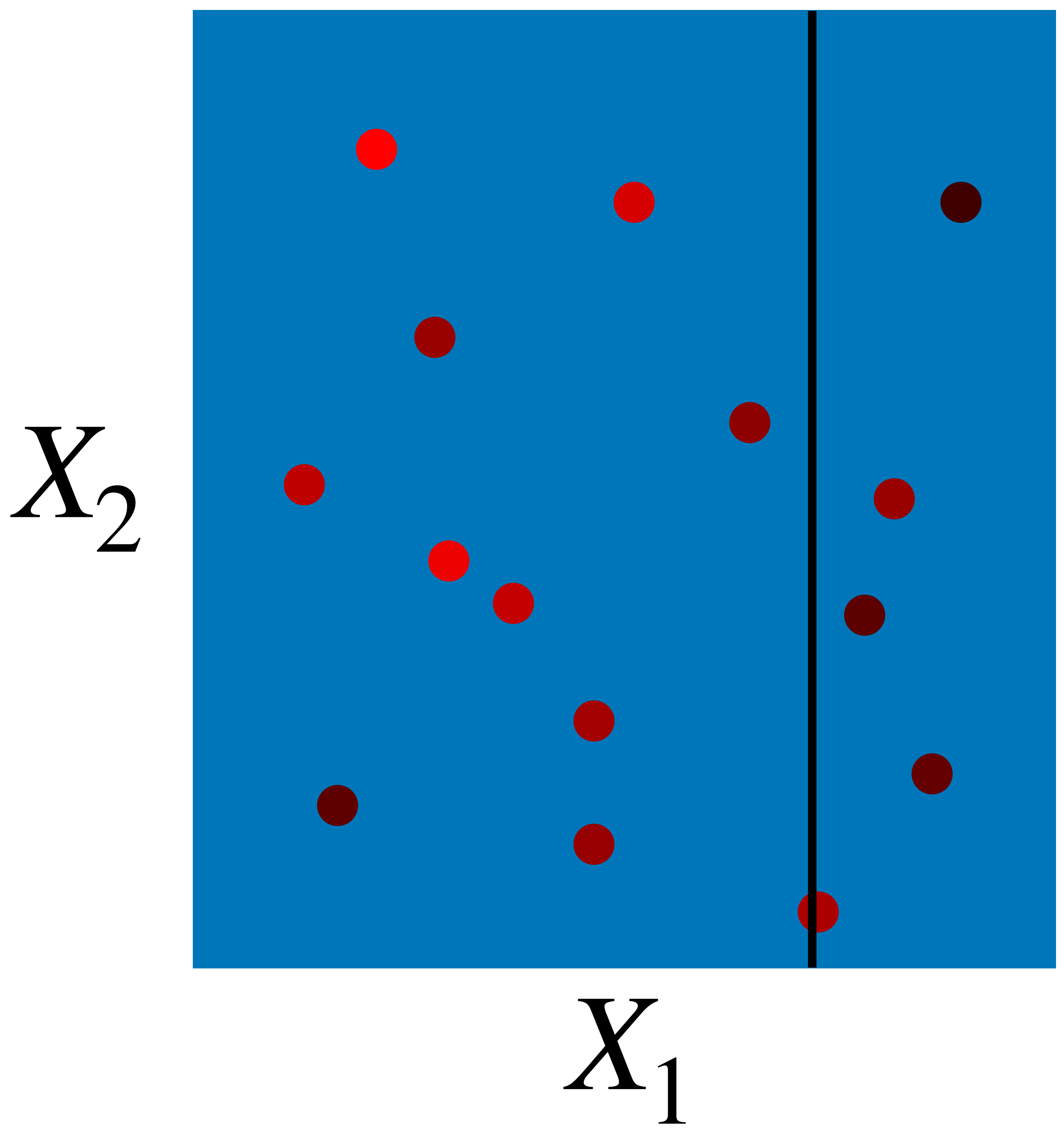

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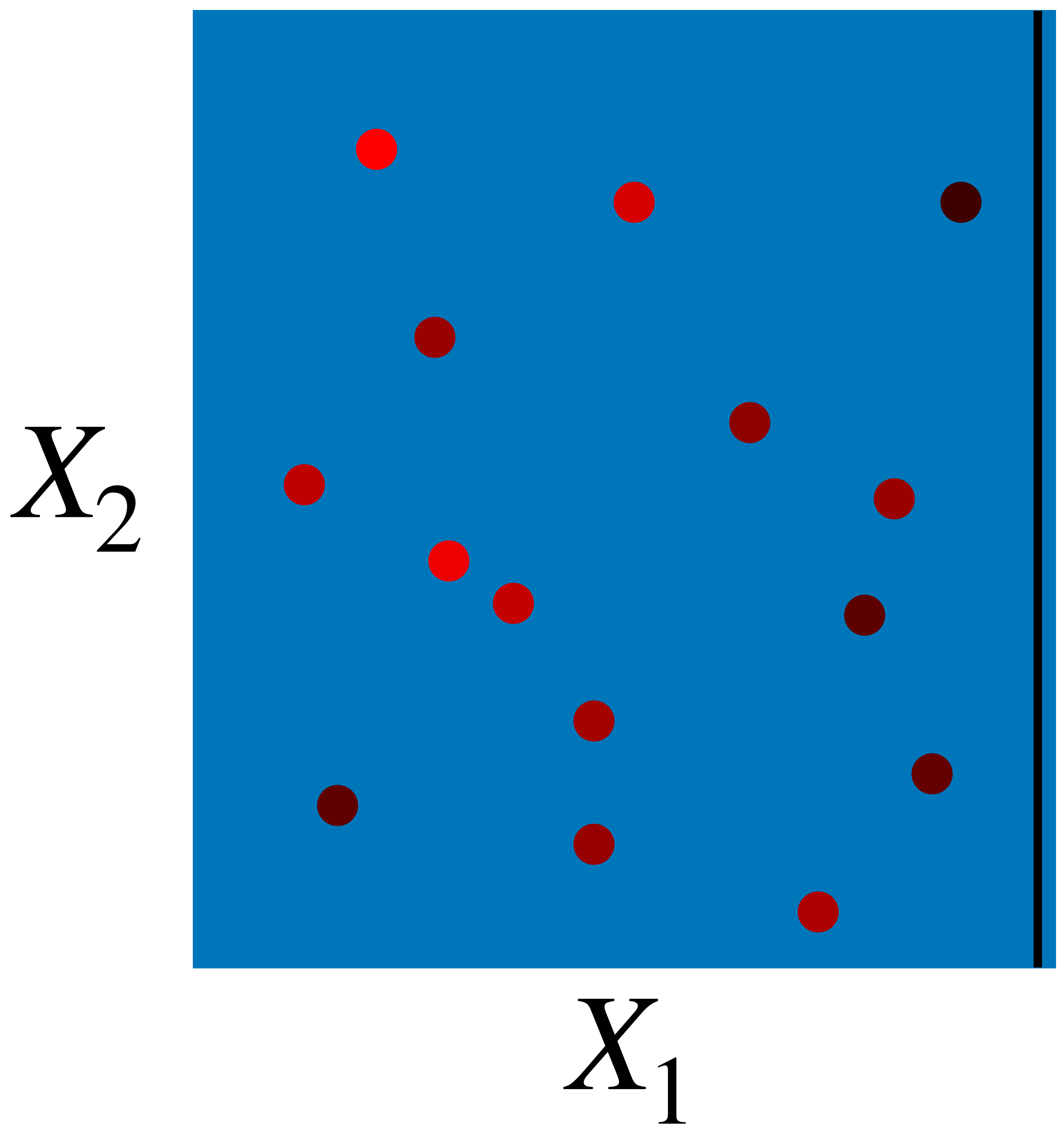

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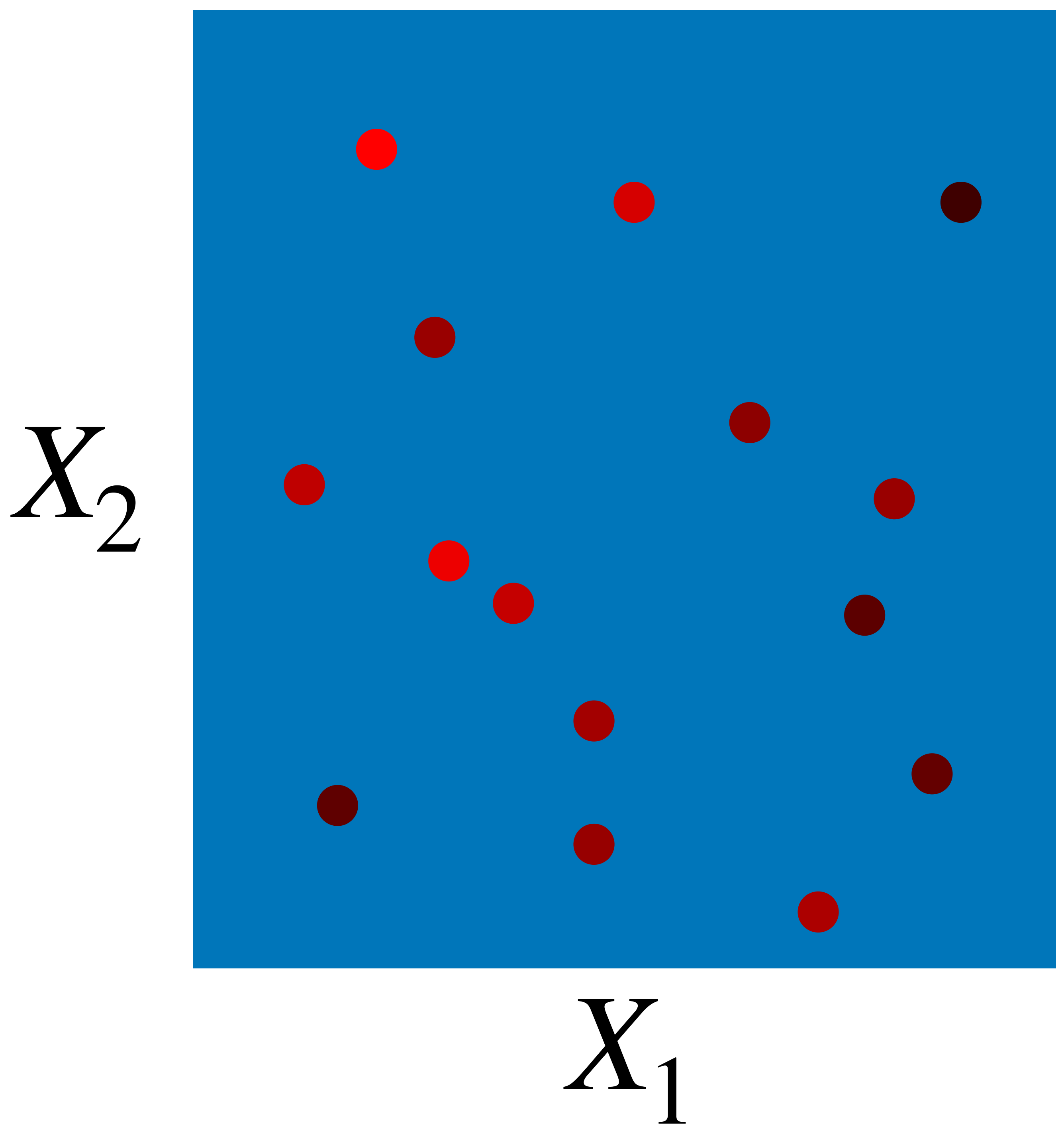

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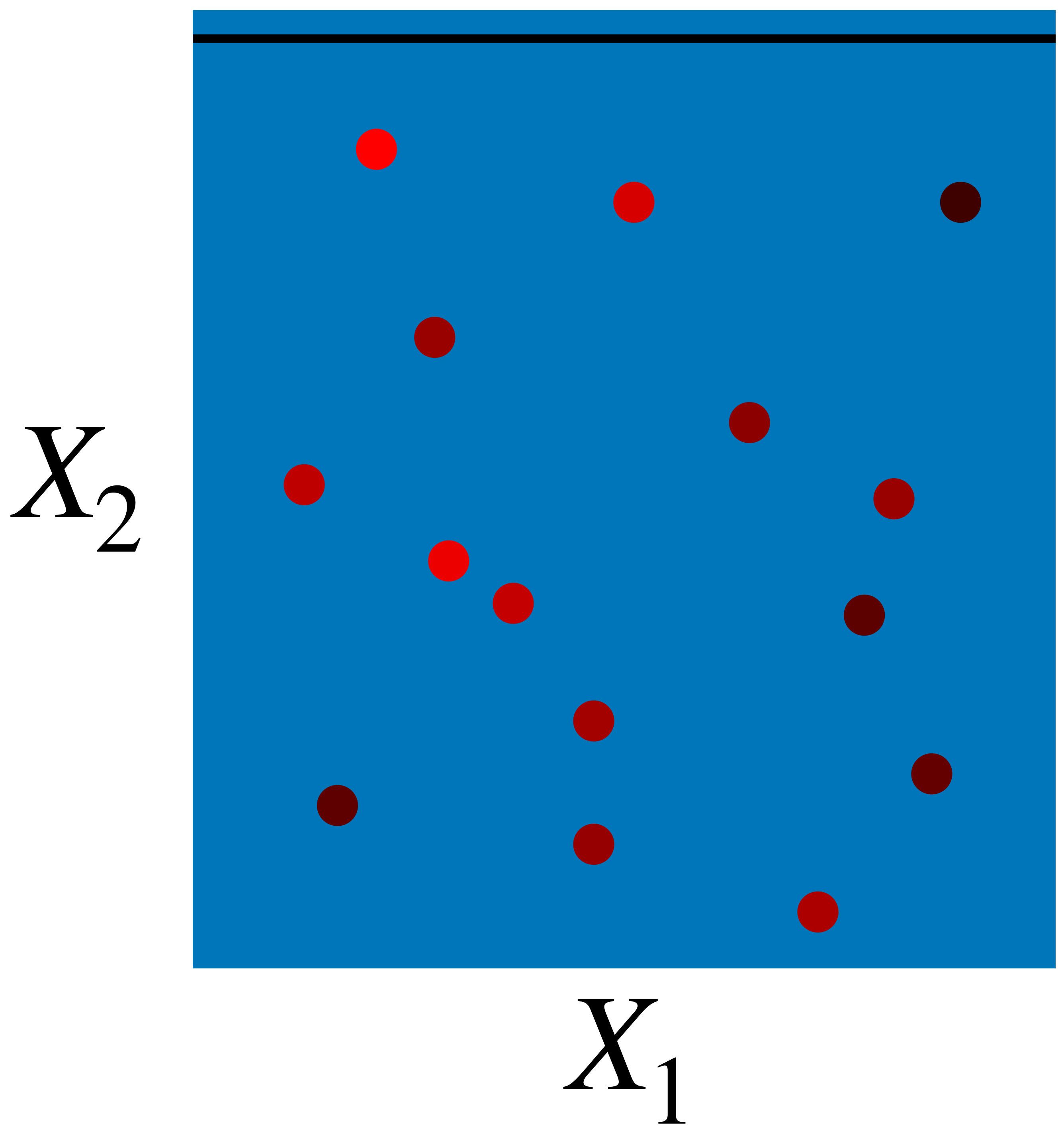

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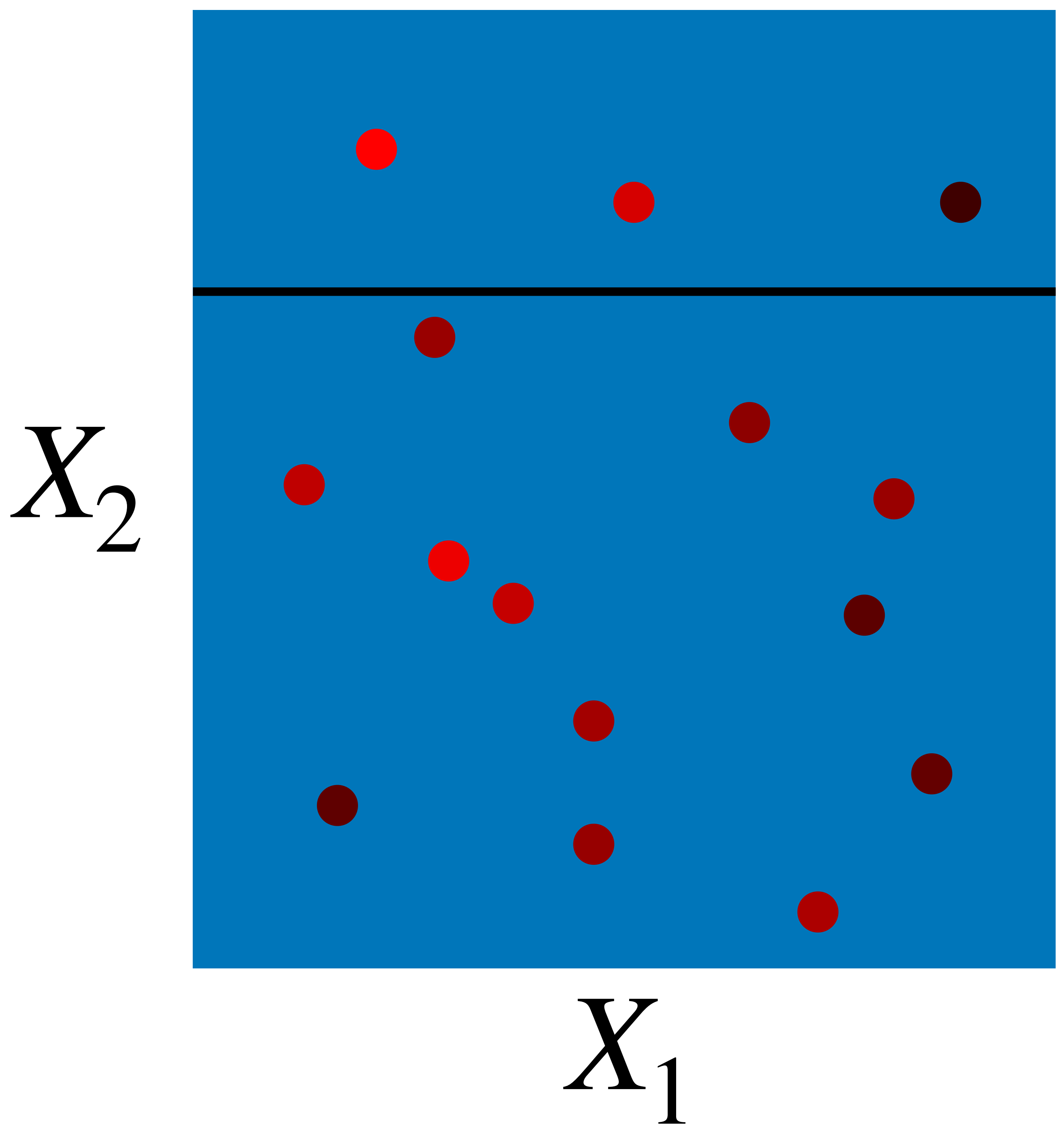

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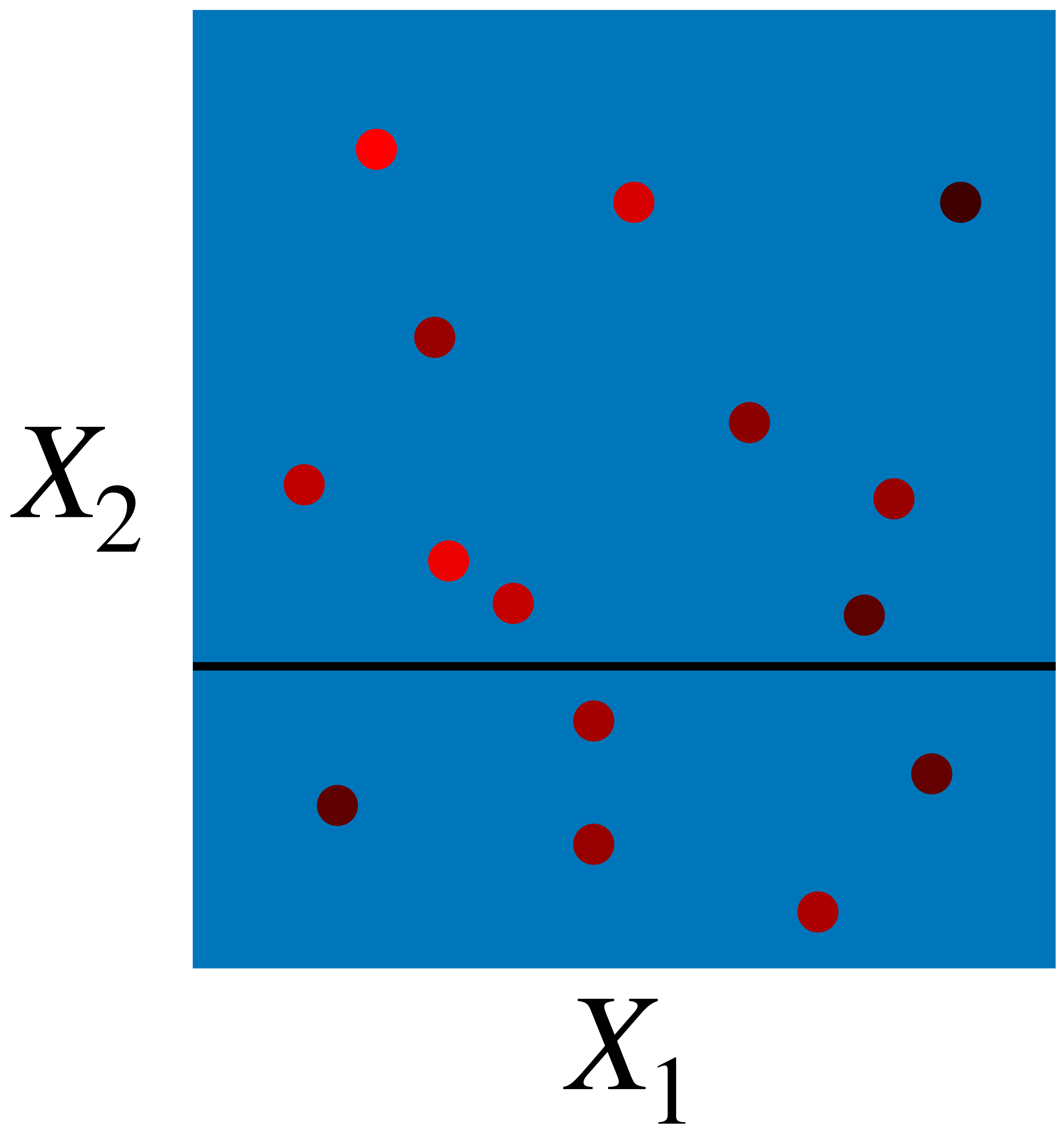

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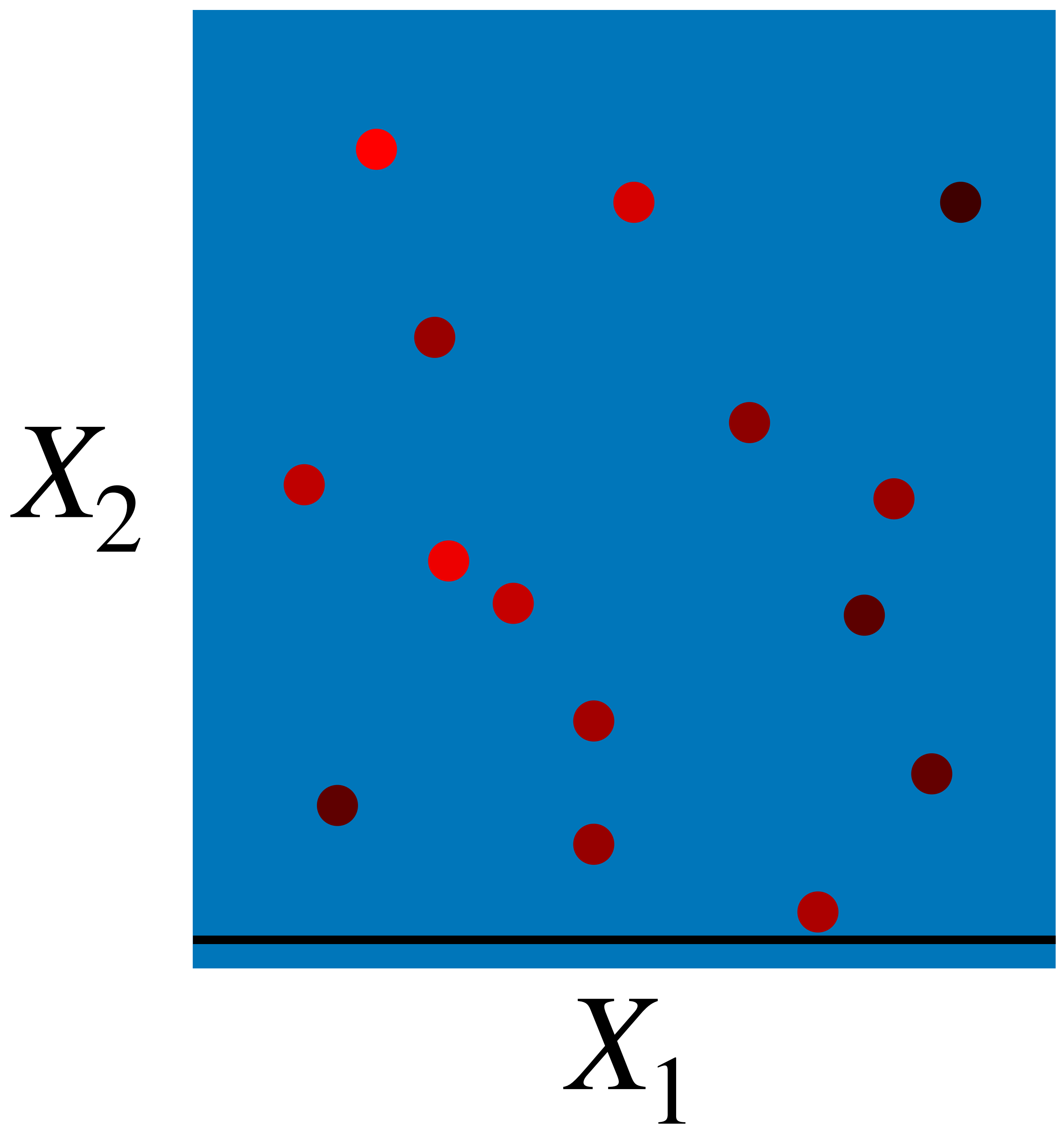

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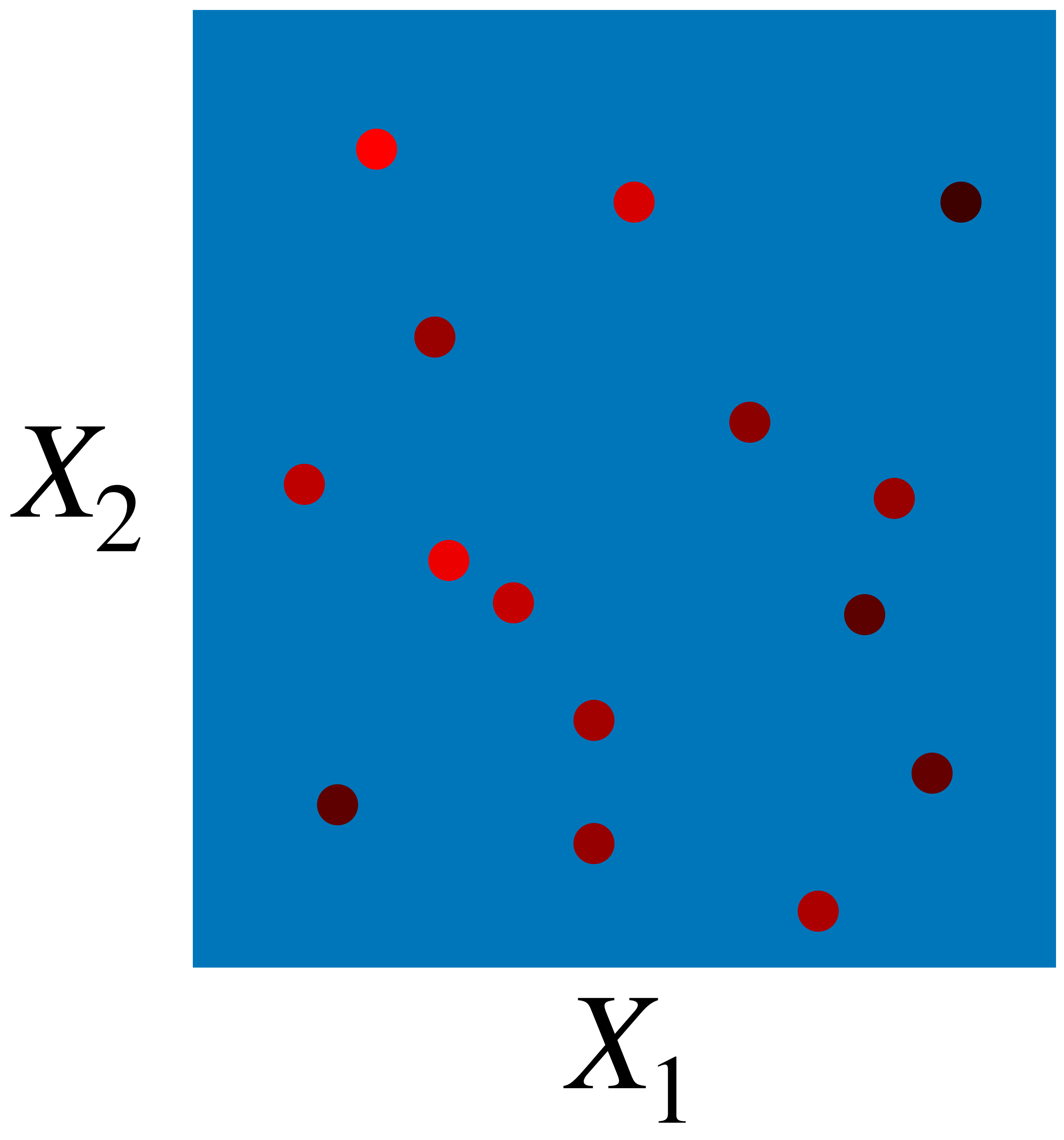

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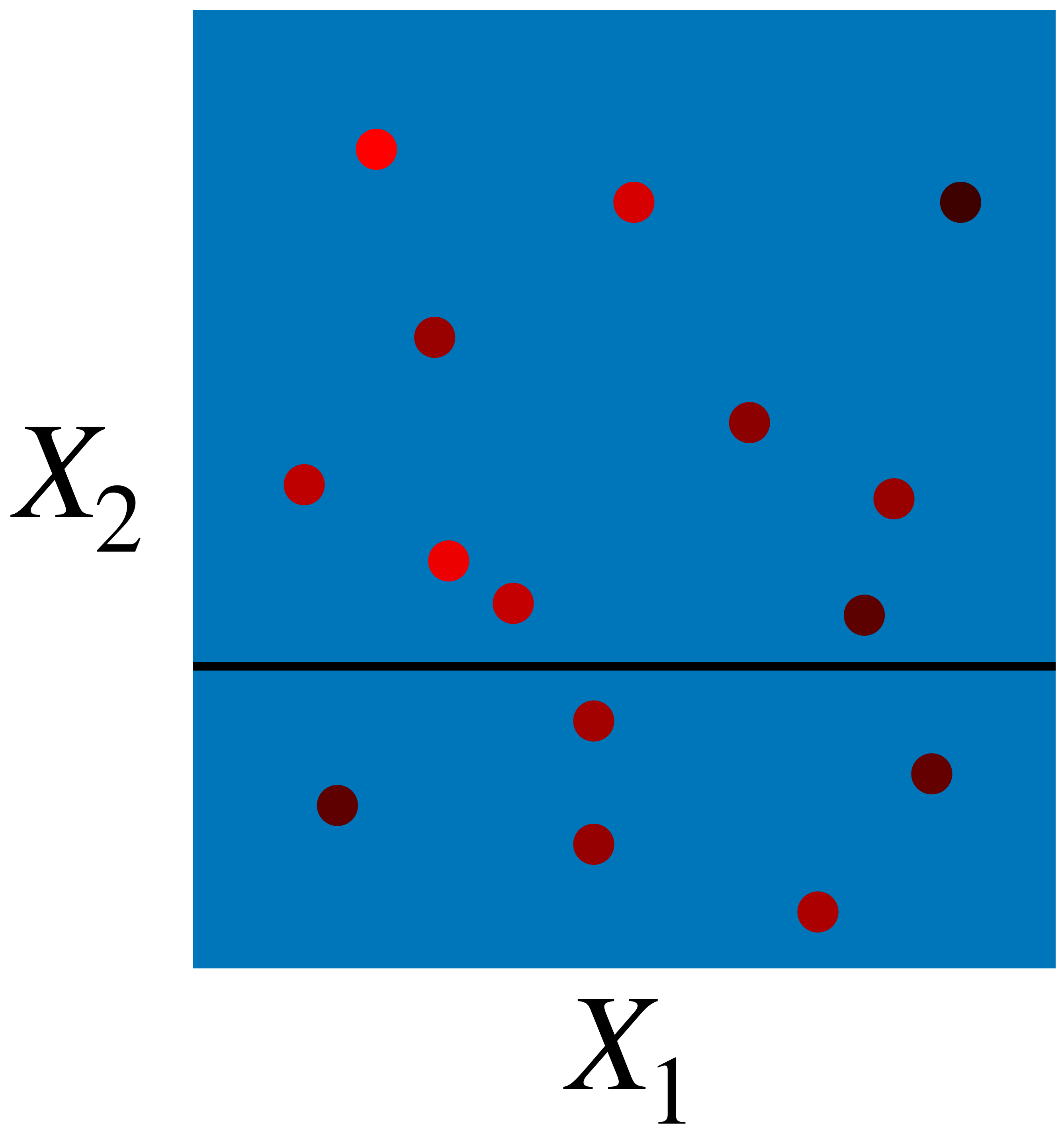

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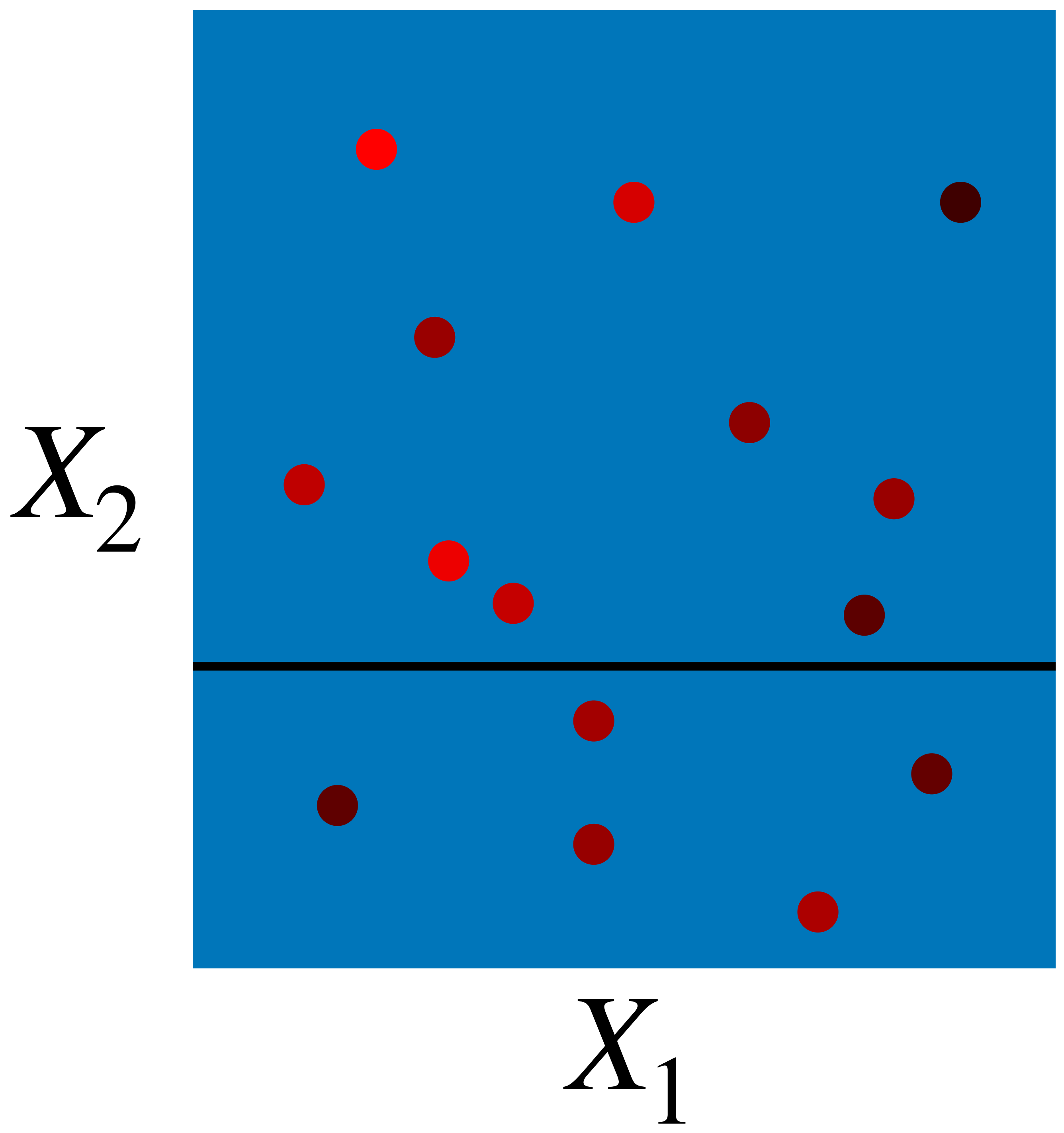
3. Find the split for each rectangle that decreases its RSS the most. Among these, choose best.



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

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1. Fit constant model to the entire space and calculate RSS.

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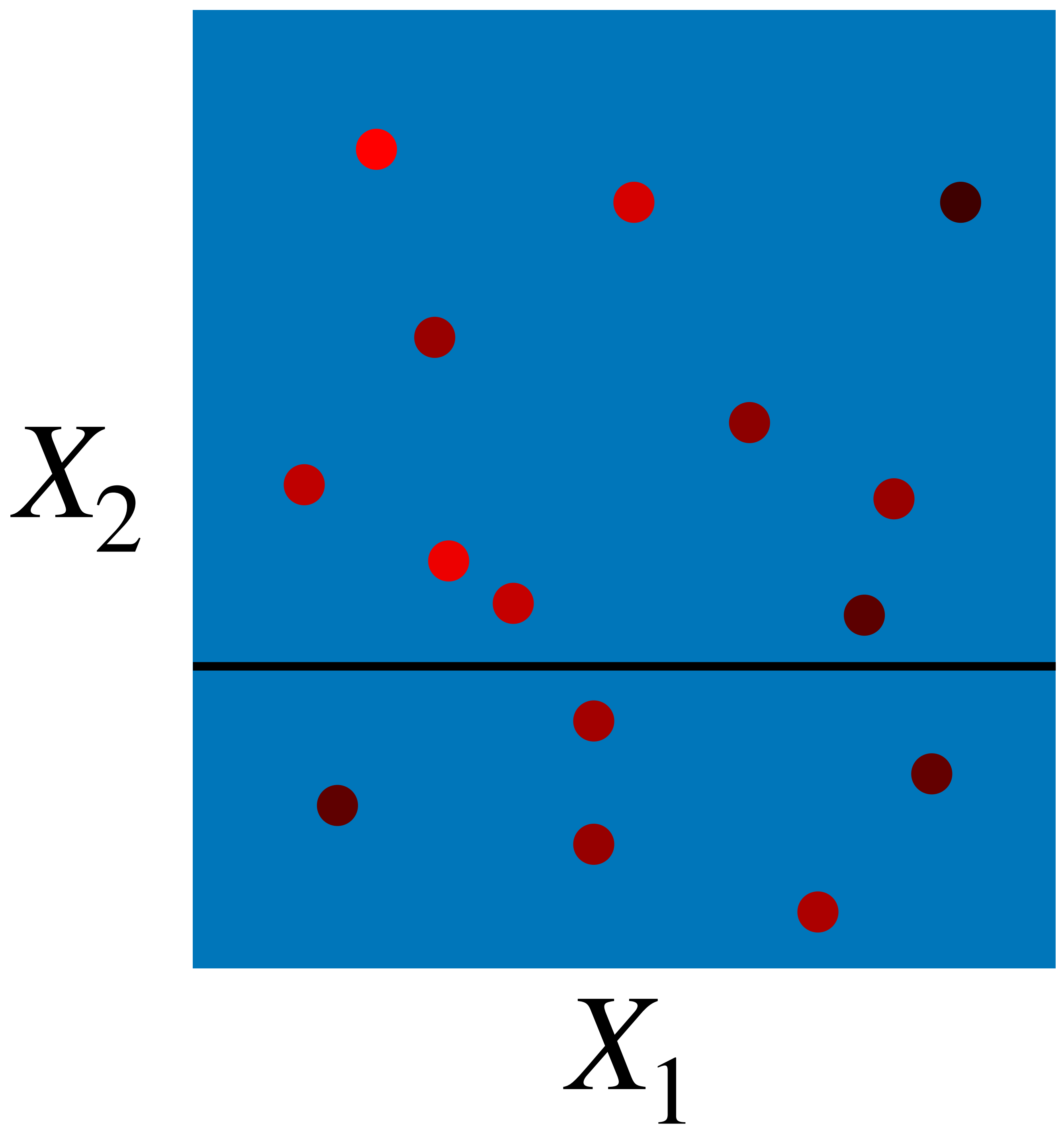
3. Find the split for each rectangle that decreases its RSS the most. Among these, choose best.



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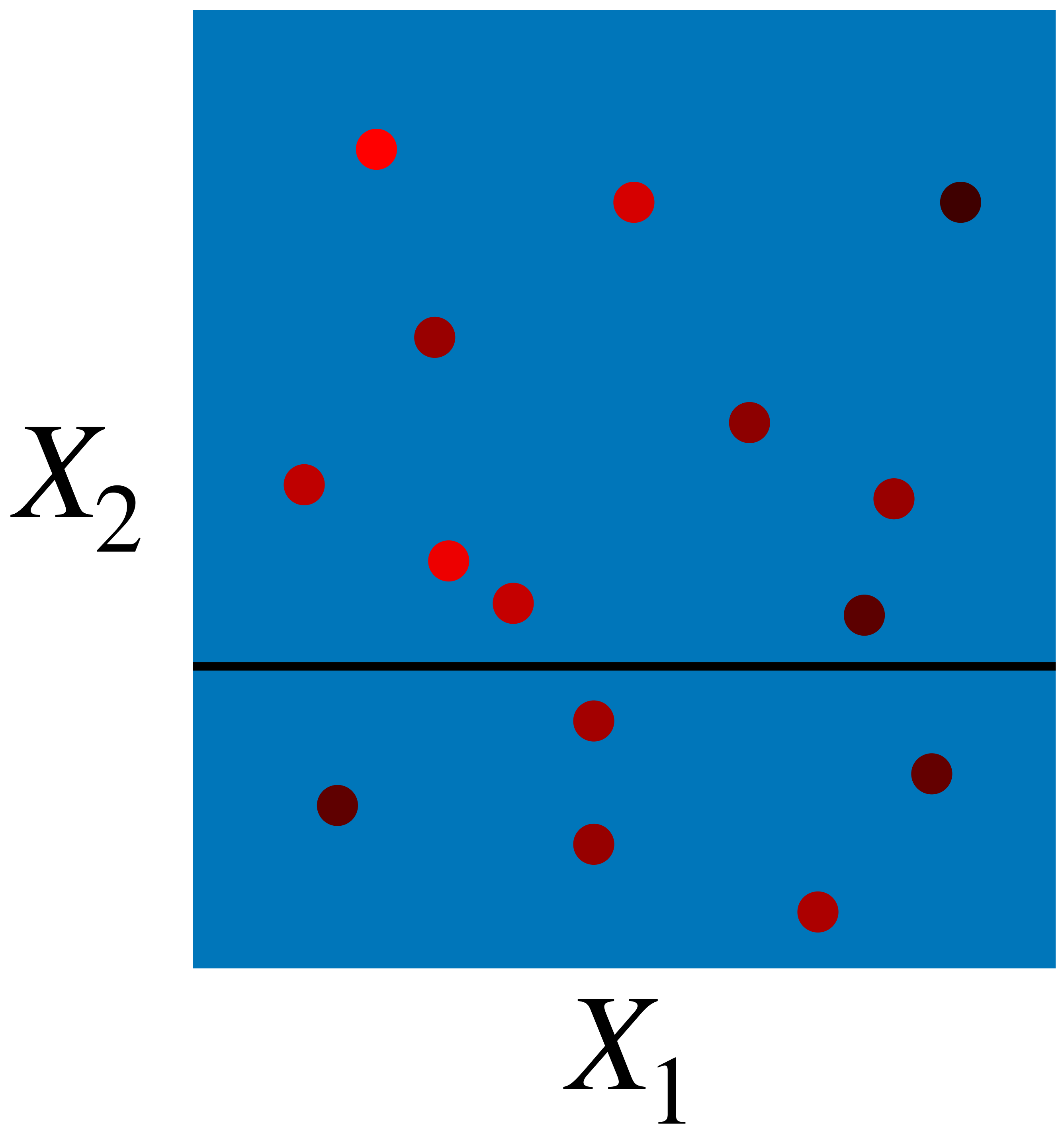

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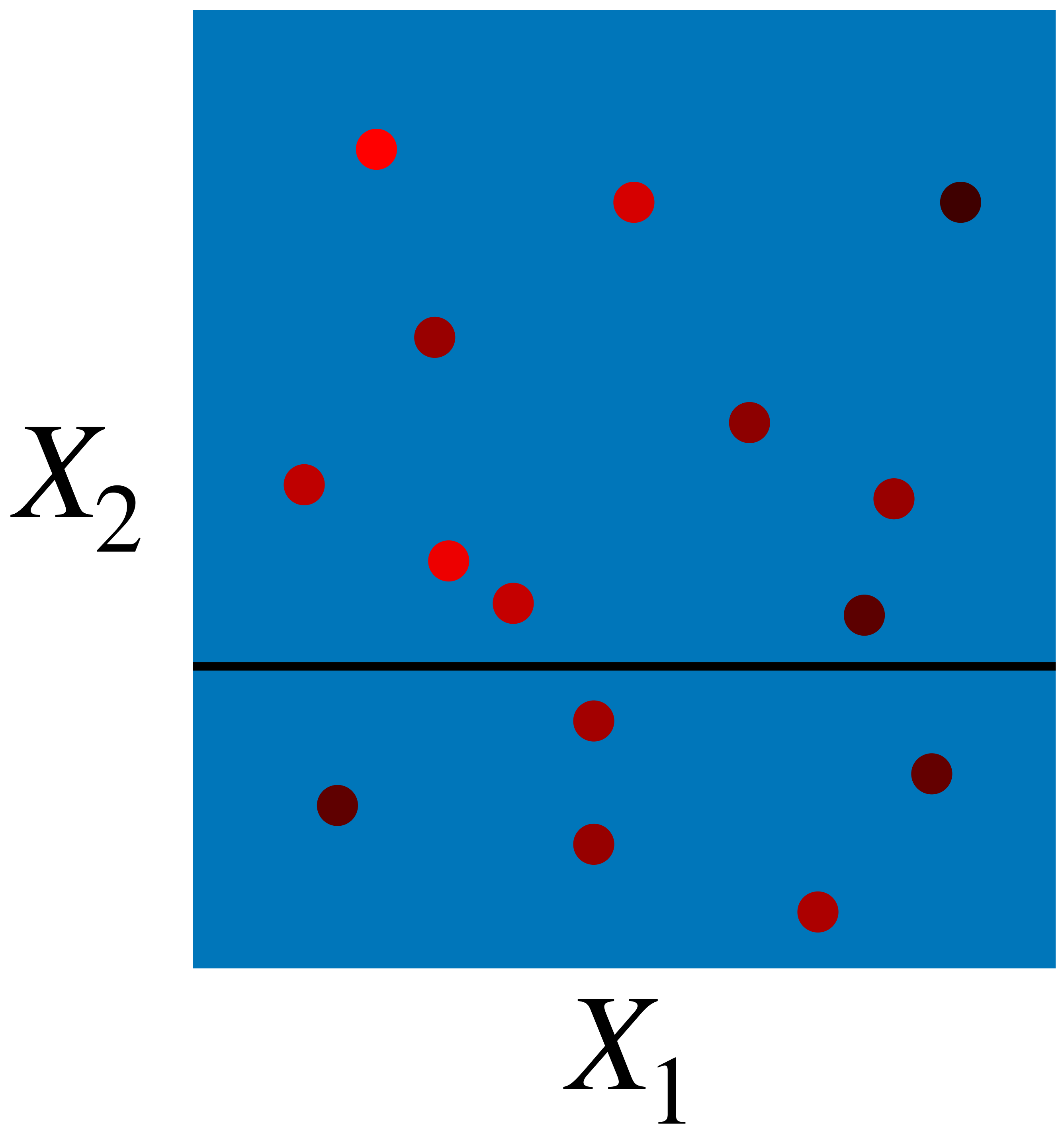

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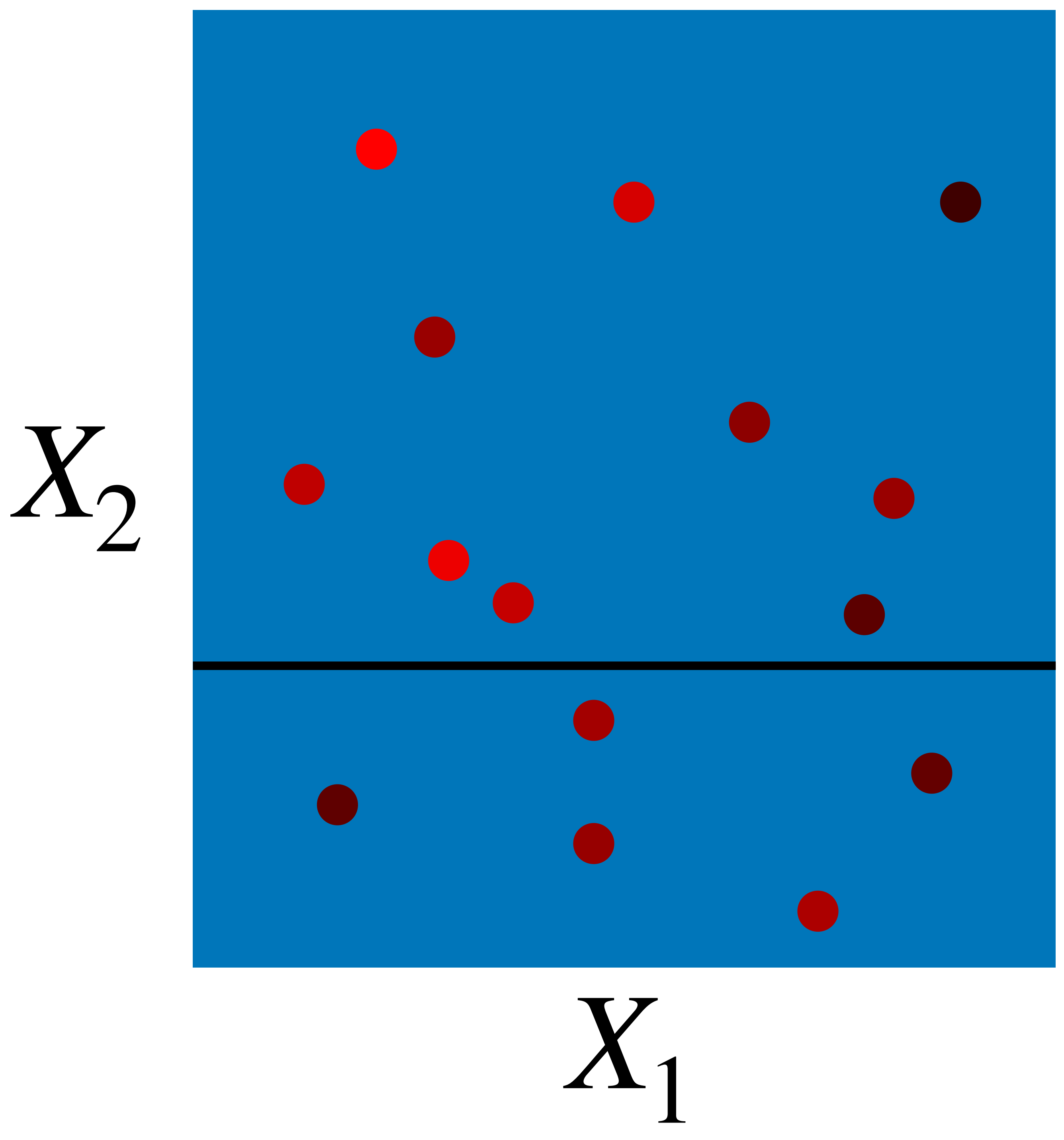

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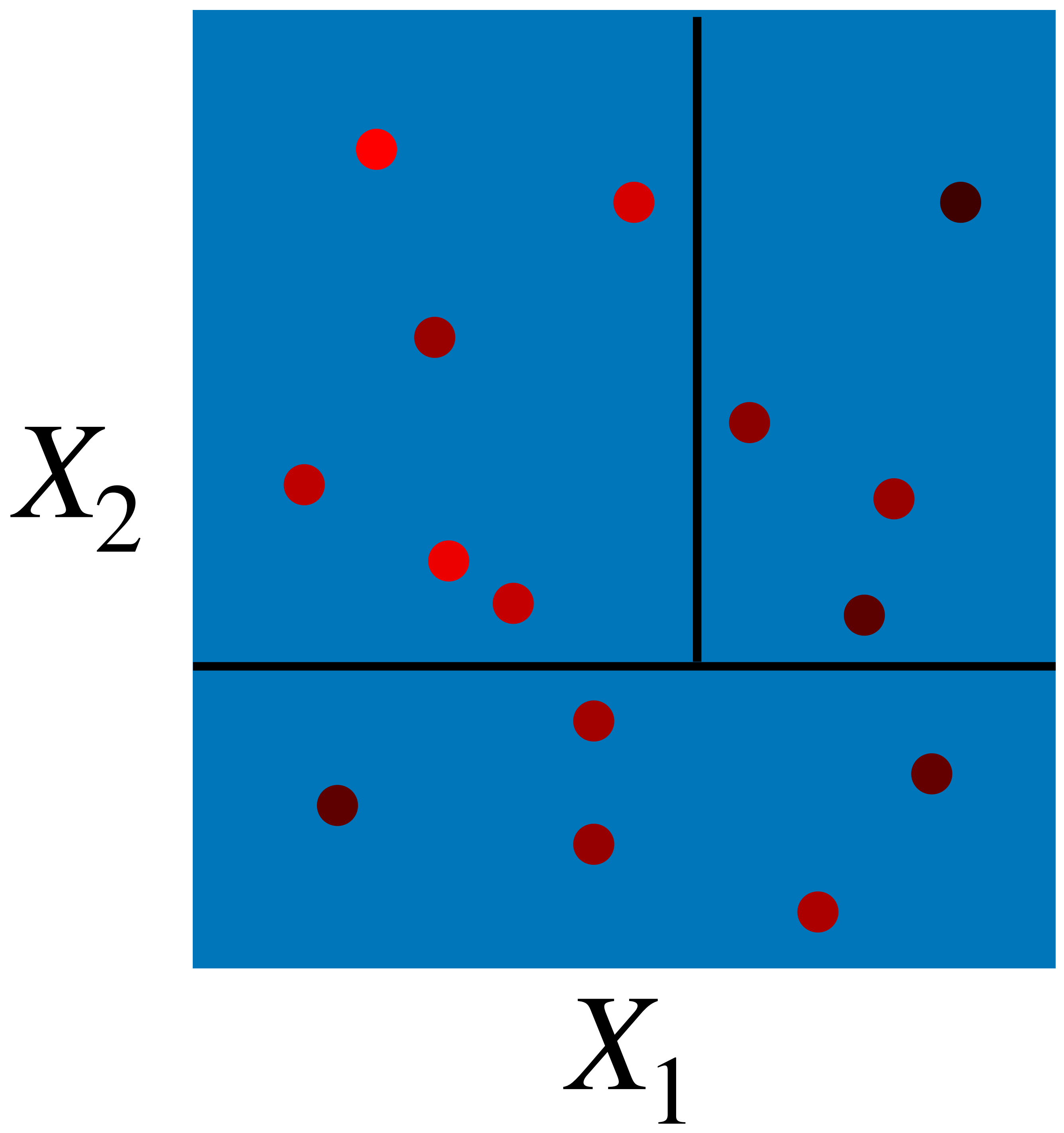

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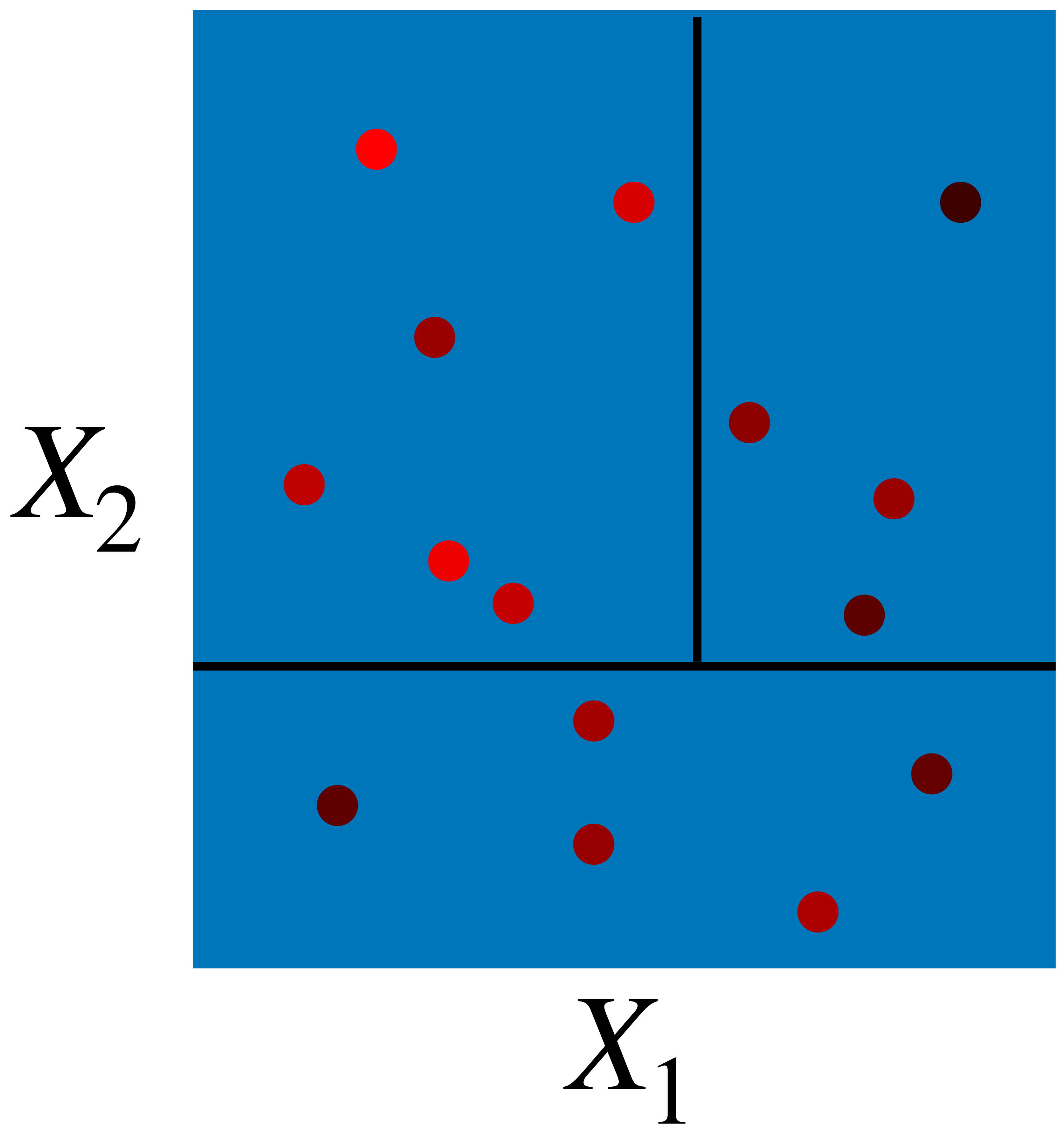

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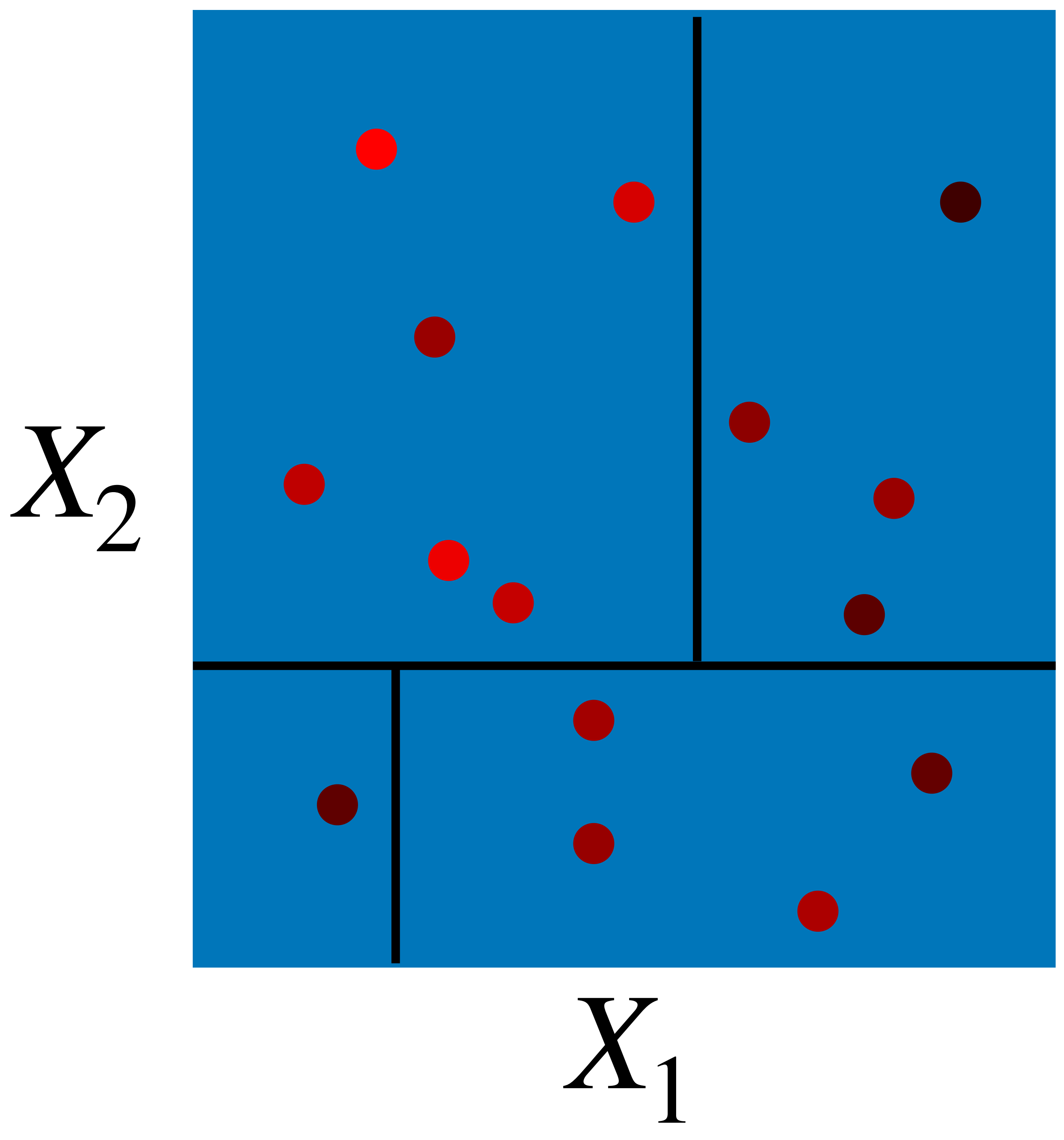
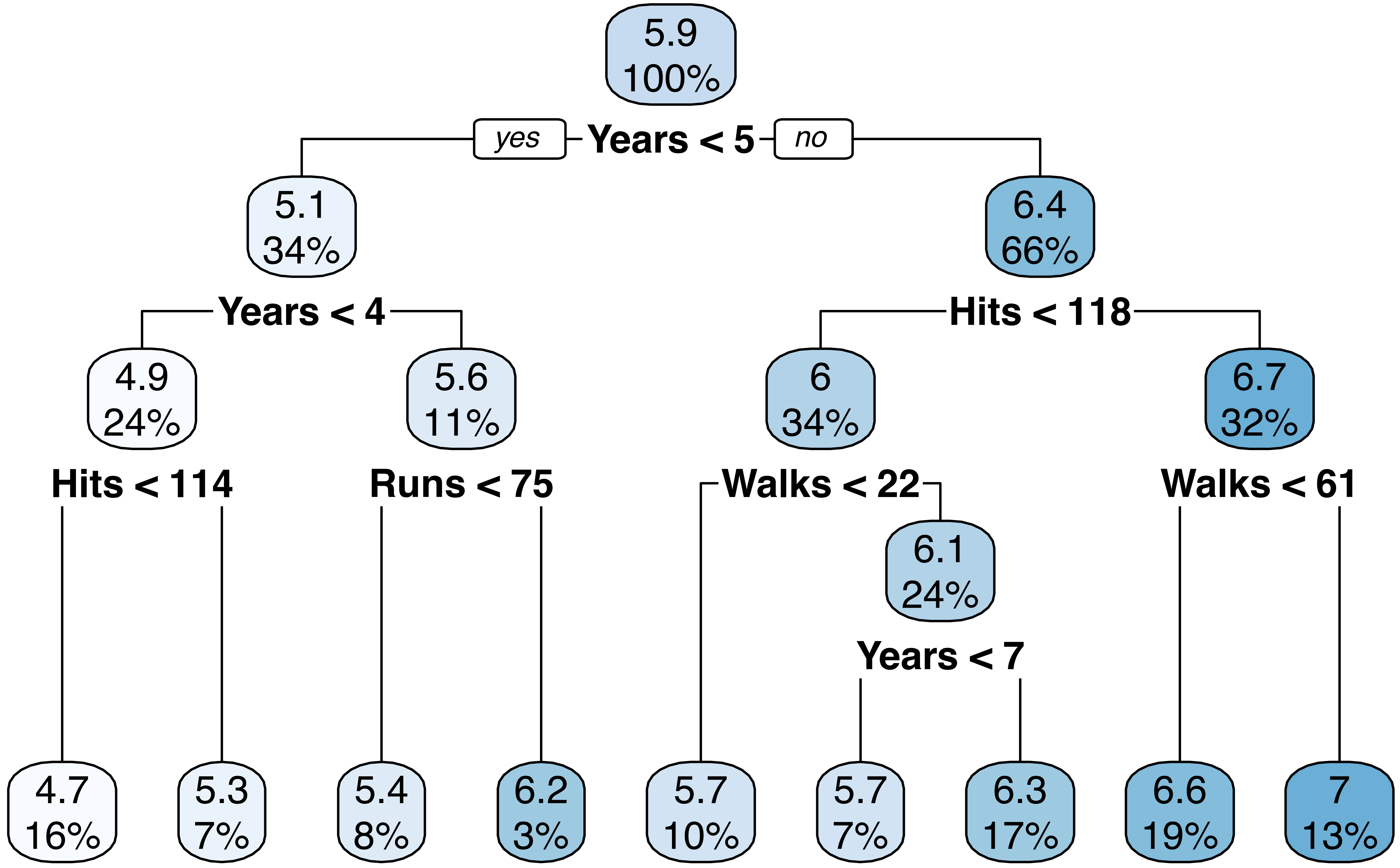


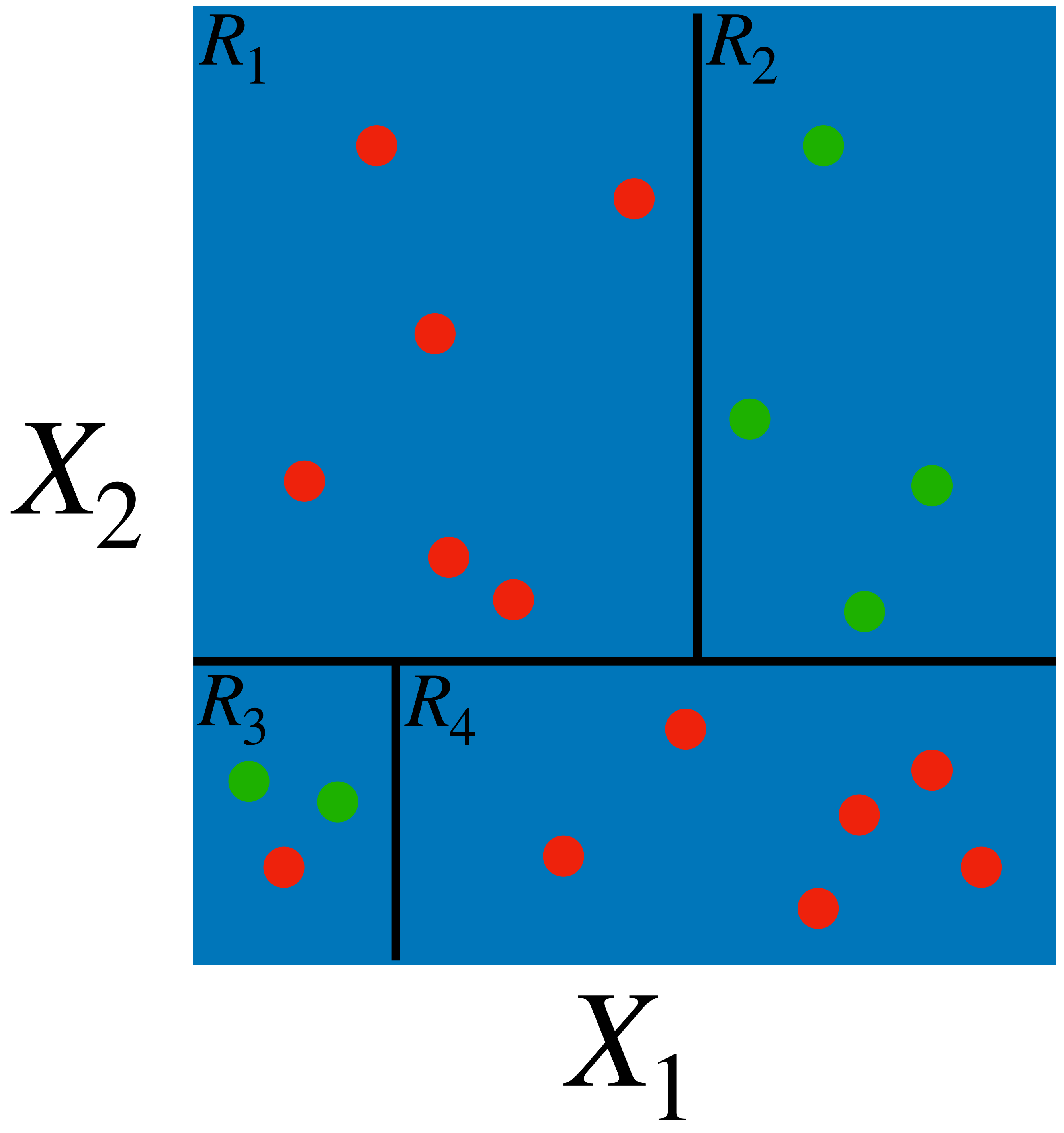
Training a regression tree

Final output



Training a classification tree

The misclassification error objective



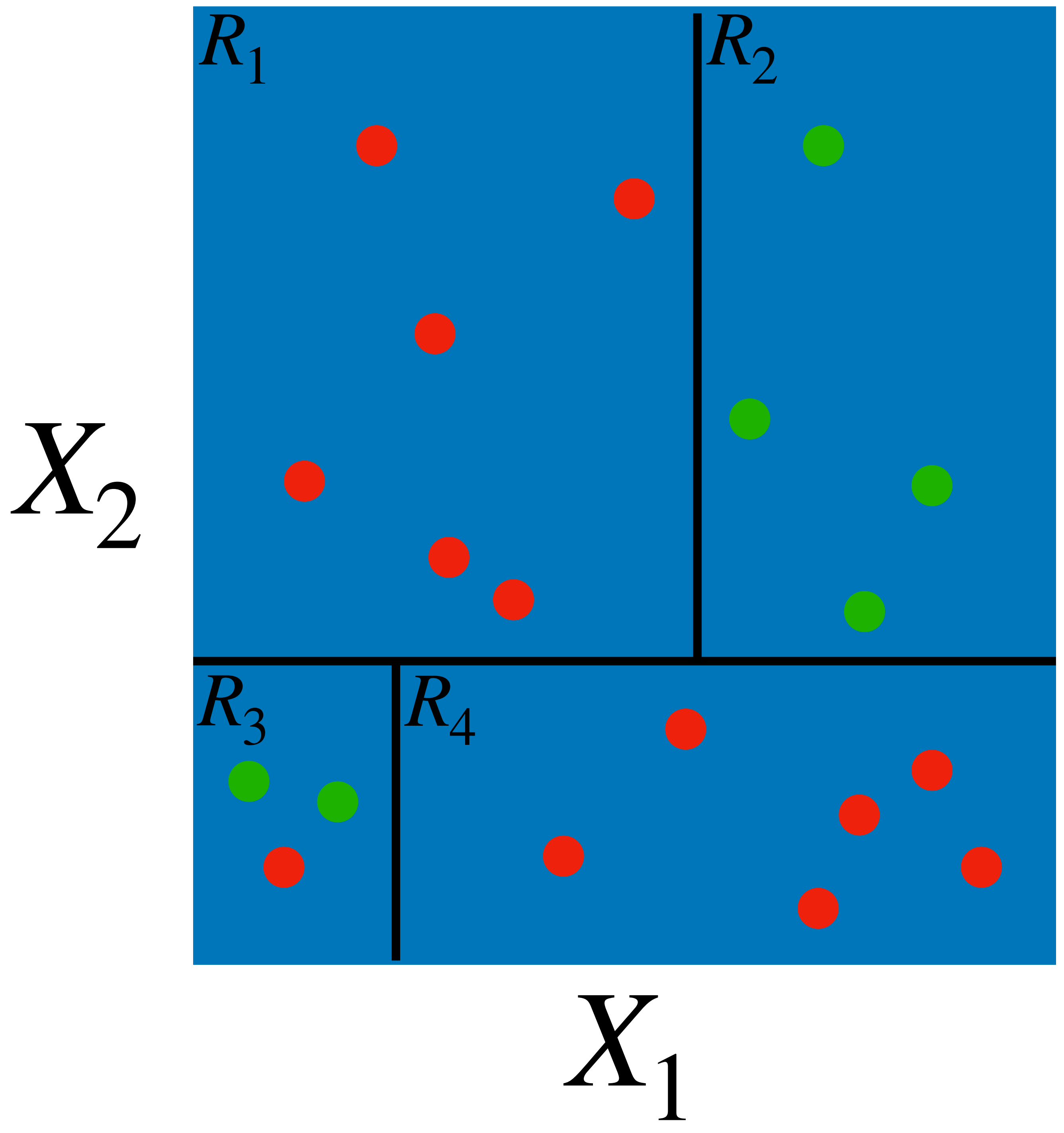
Training a classification tree

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 error:

$$\widehat{R}_1, \ldots, \widehat{R}_M, \widehat{c}_1, \ldots, \widehat{c}_M = \underset{R_1,\ldots,R_M,c_1,\ldots,c_M}{\arg\min} \frac{1}{n}\sum_{i=1}^{n} I(Y_i \neq \widehat{Y}_i)$$



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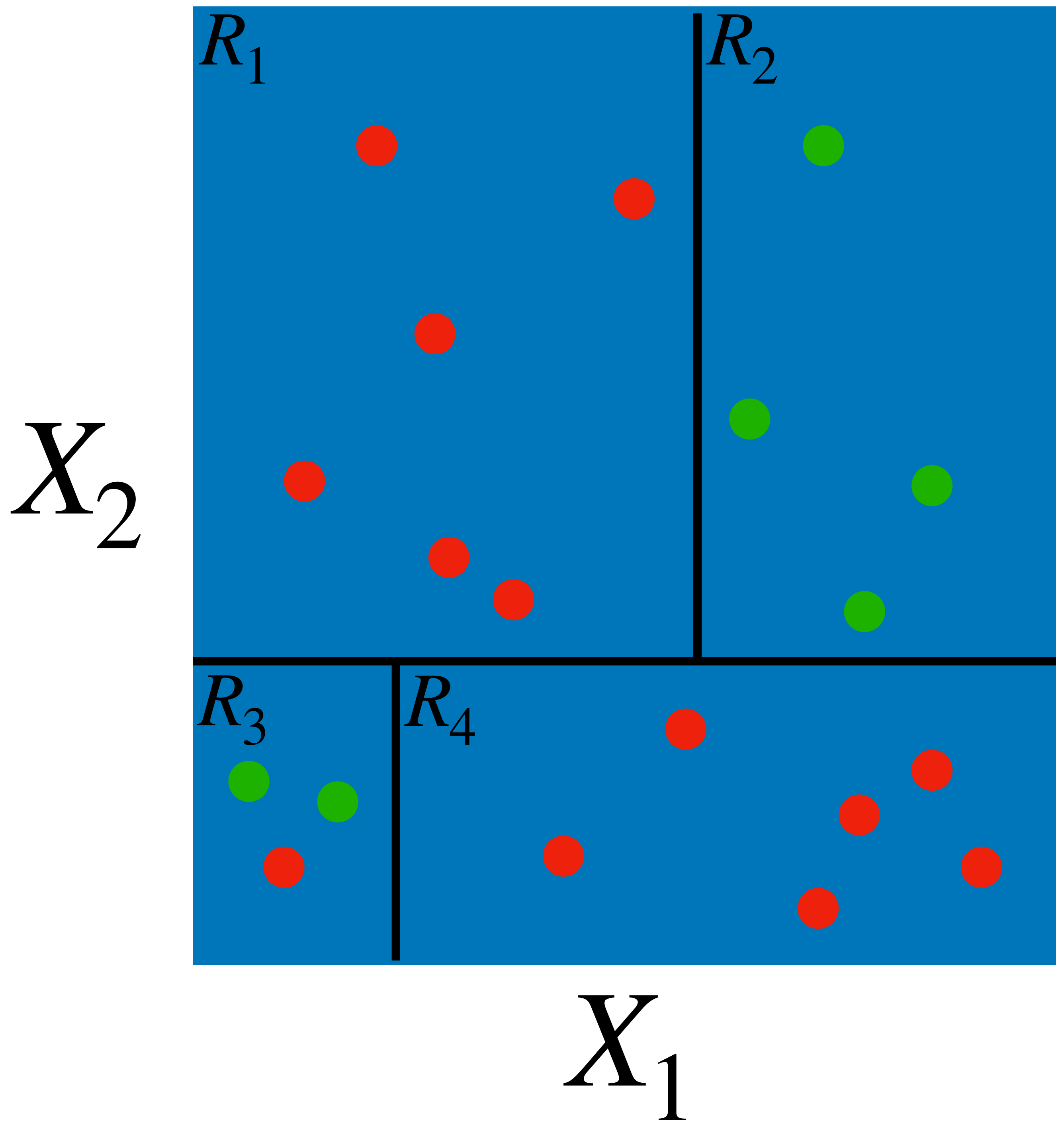

Training a classification tree

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

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

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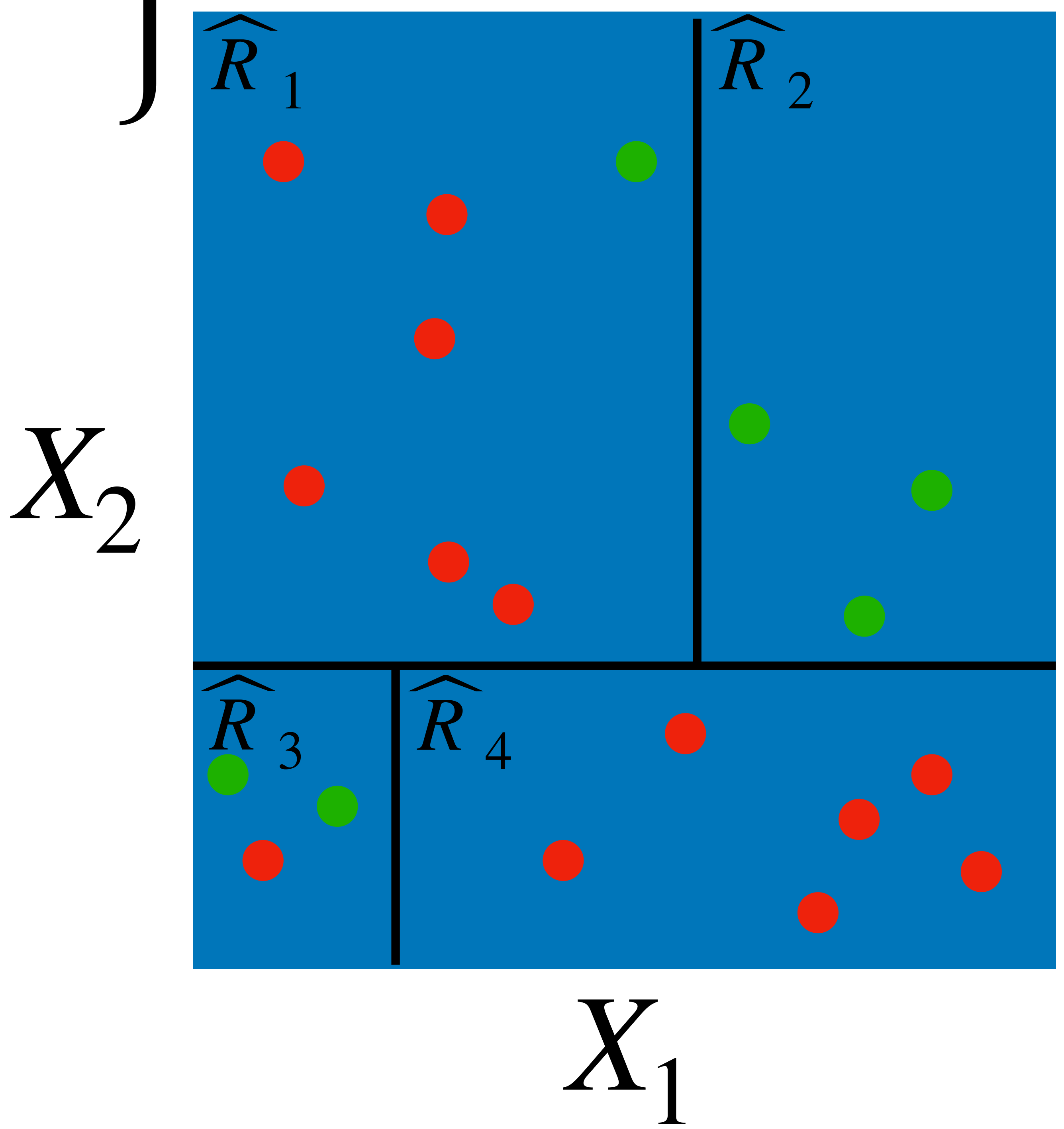

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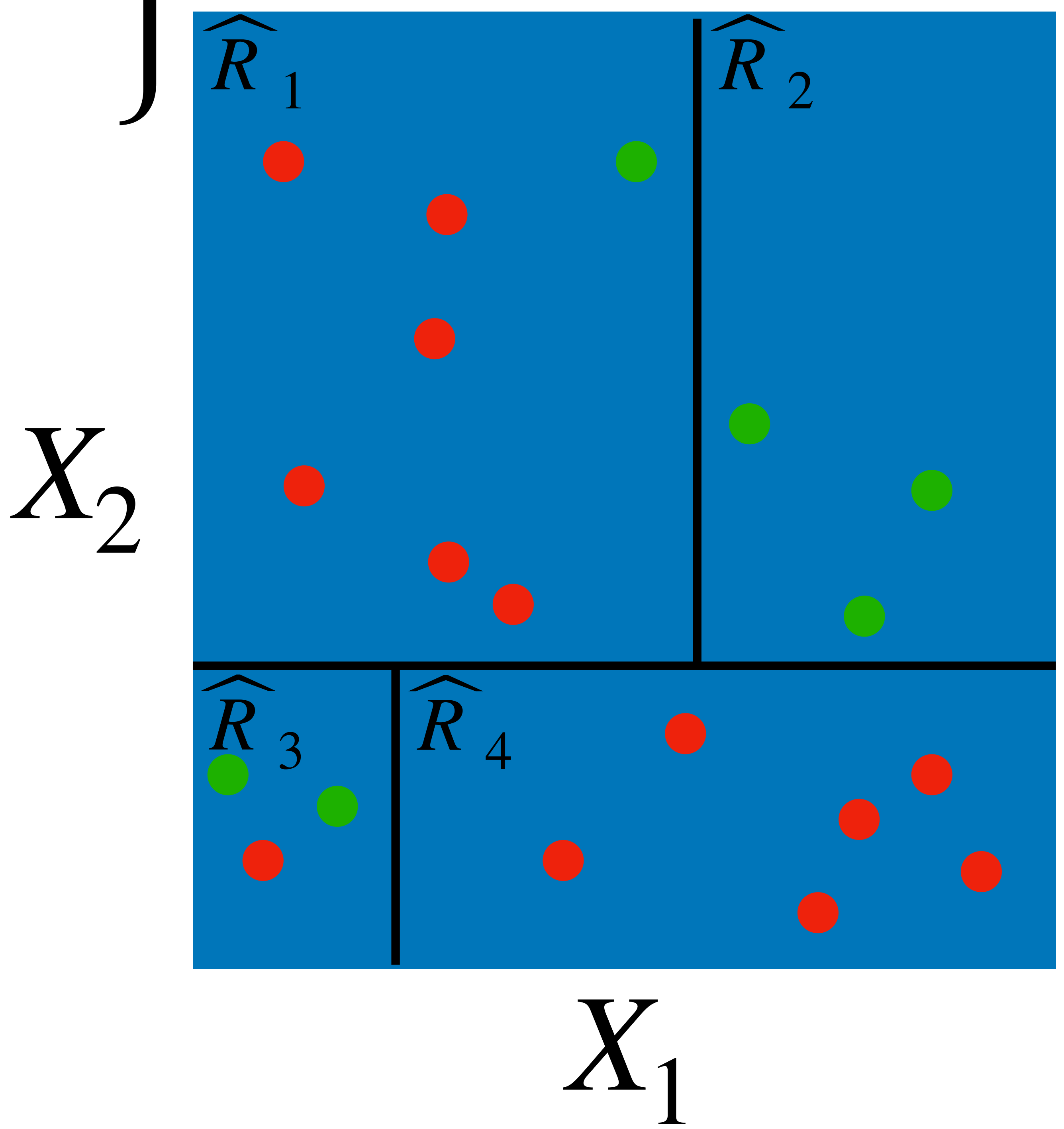
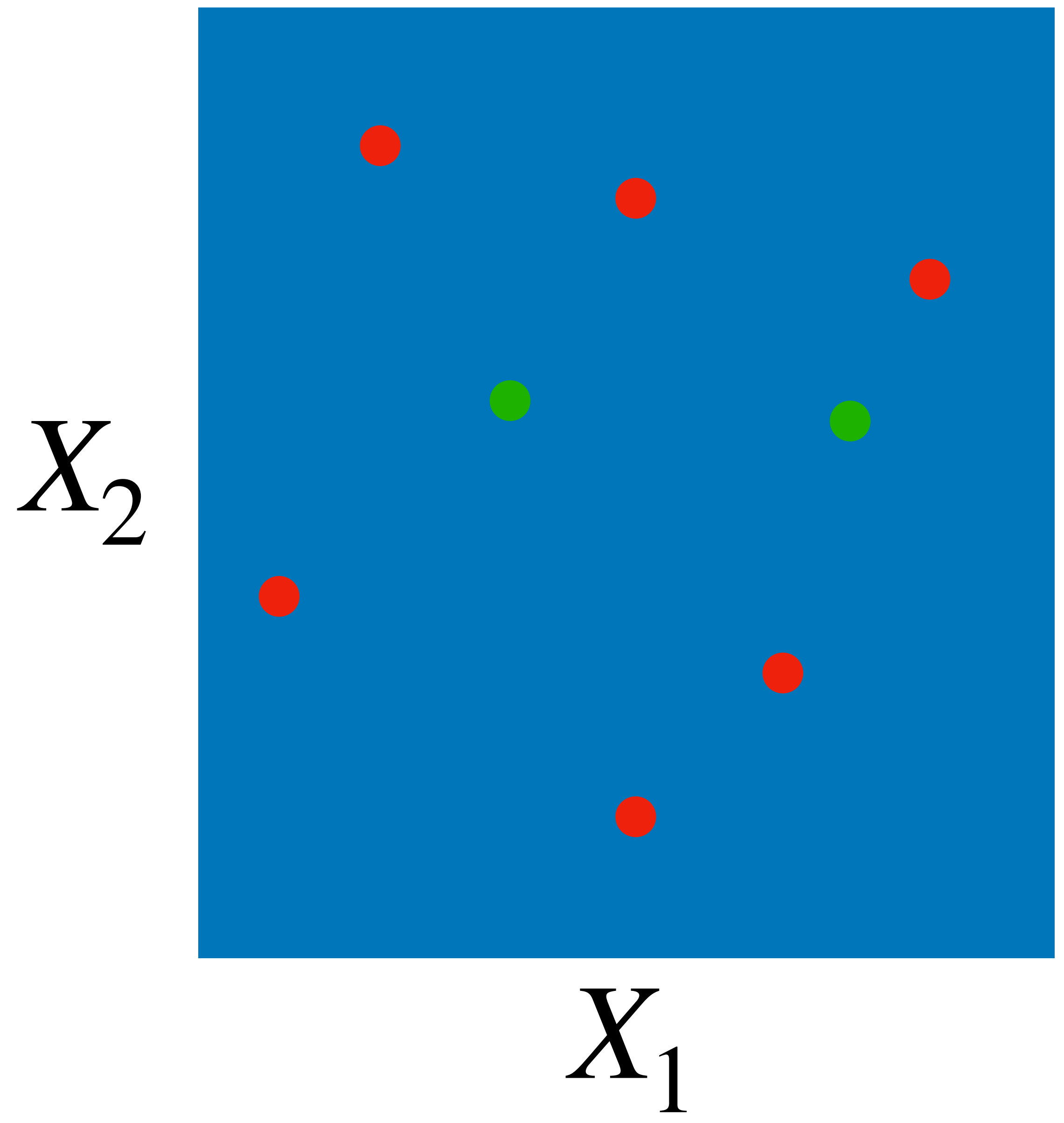
We're fitting the same category to each region, so the solution is the majority vote:

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



Training a classification tree

Finding the rectangles $\widehat{R}_m$: Inadequacy of misclassification error

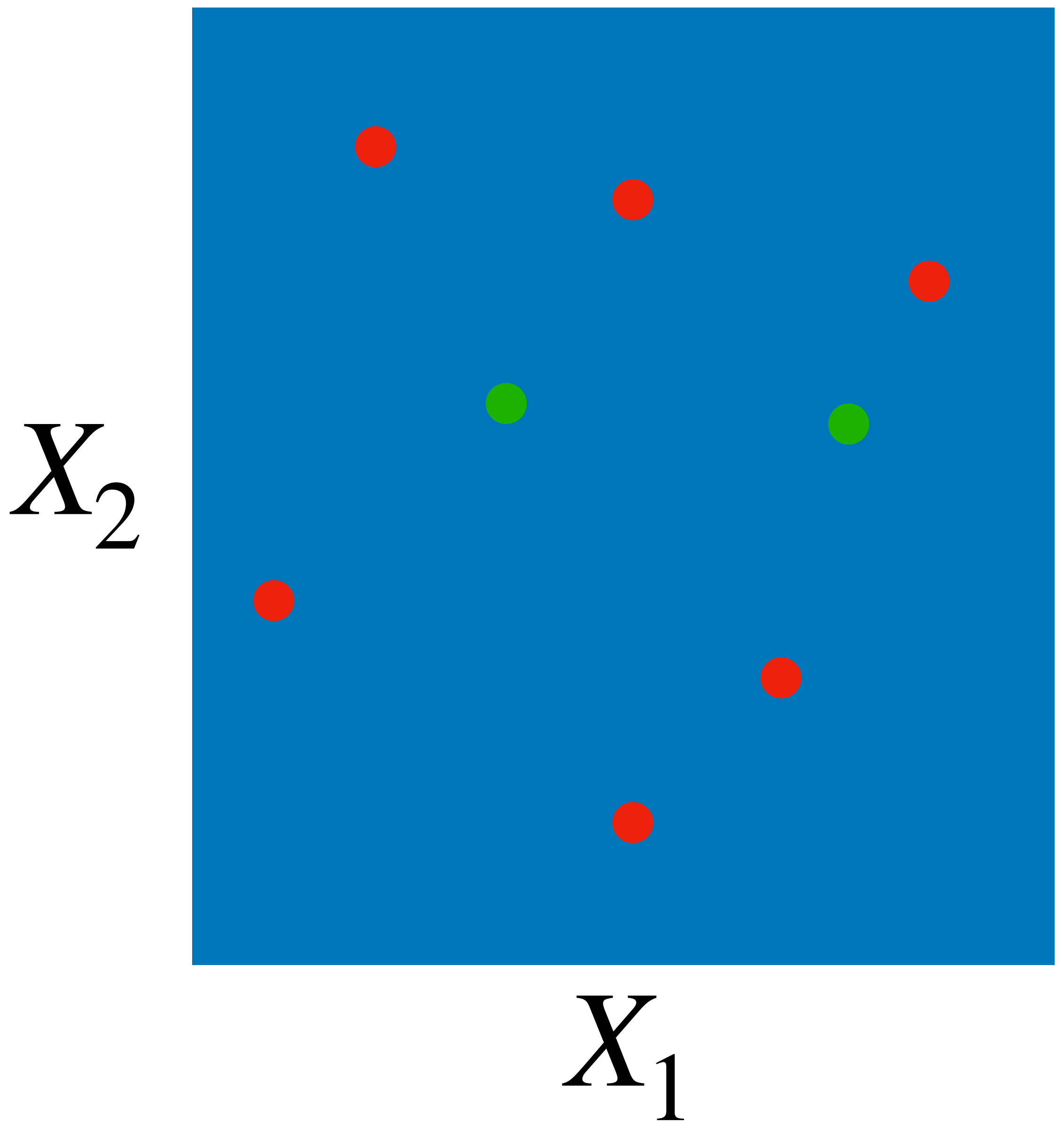


Training a classification tree

Finding the rectangles $\widehat{R}_m$: Inadequacy of misclassification error

Misclassification error:

$$\frac{1}{n}\left\{\sum_{i:X_i\in R_1} I(Y_i \neq c_1) + \cdots + \sum_{i:X_i\in R_M} (Y_i \neq c_M)\right\}$$



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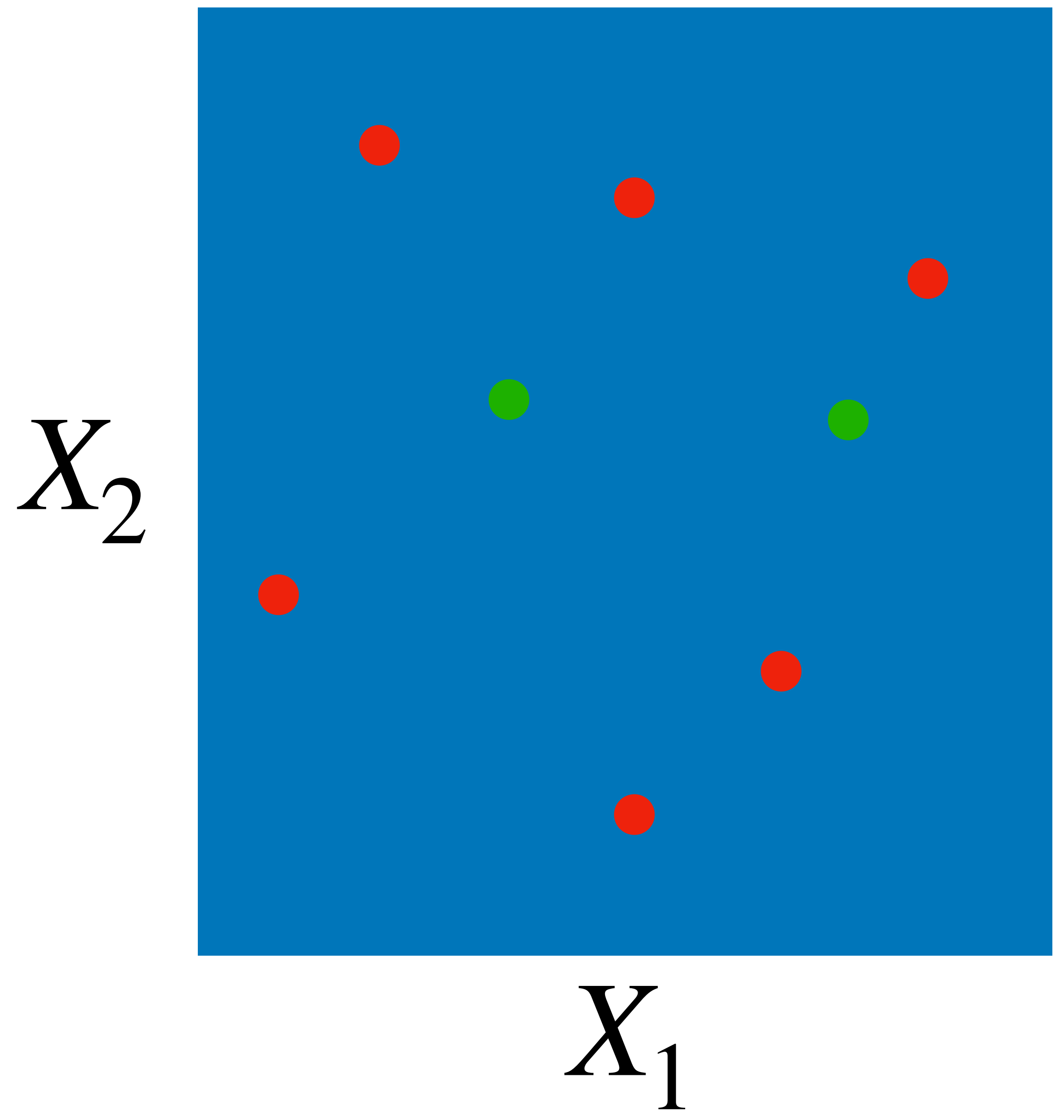

In example at right, no choice of split point decreases misclassification error.

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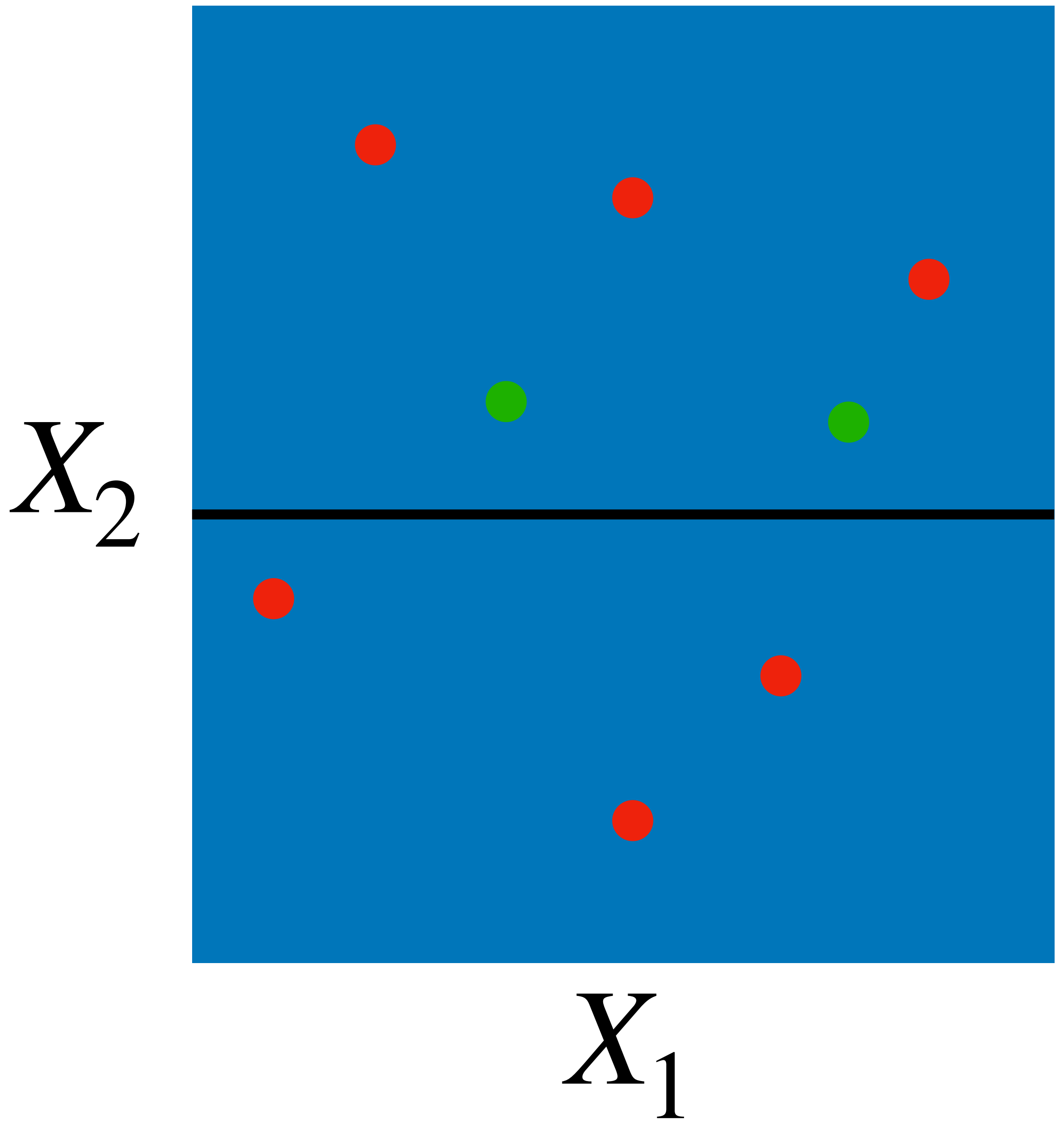

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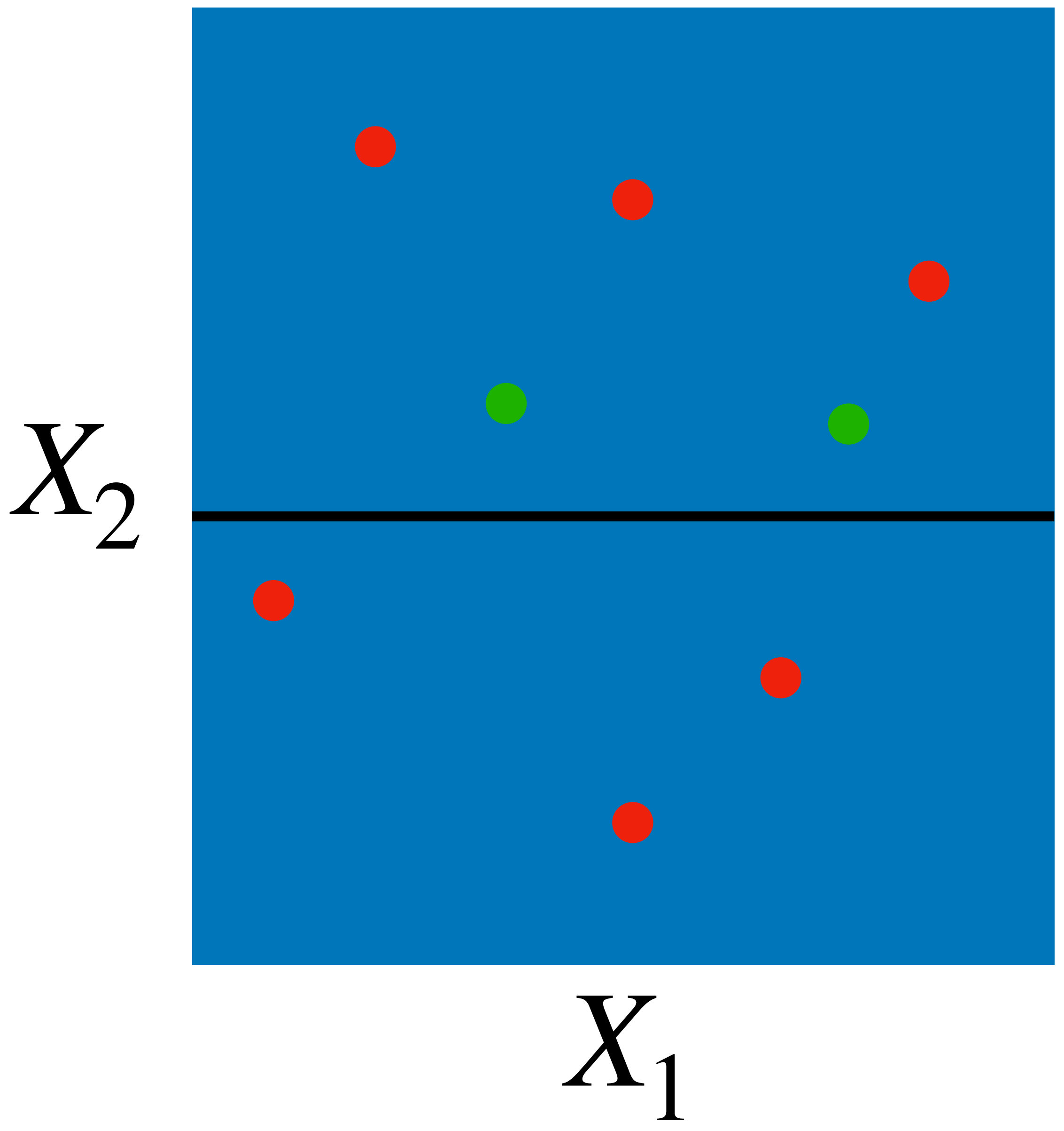

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Misclassification error not sensitive enough to find good split points at each step.

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Finding the rectangles $\widehat{R}_m$: The Gini index (measure of node impurity)

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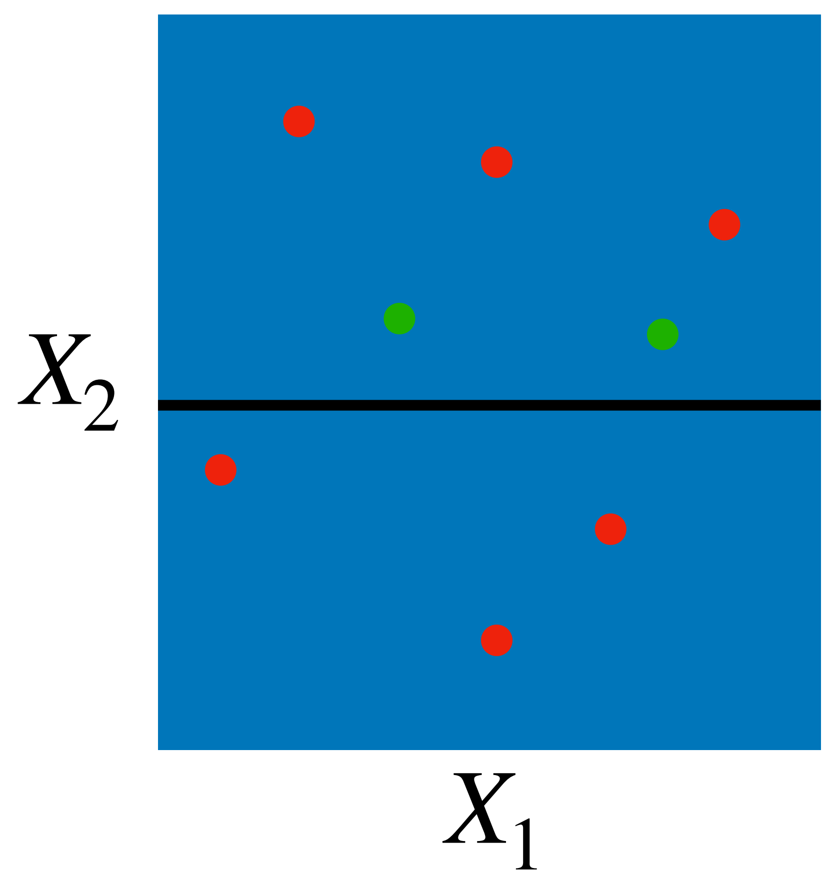
If $\hat{p}_m$ is region m class 1 proportion, misclassification error in that region is $\min(\hat{p}_m, 1 - \hat{p}_m)$.



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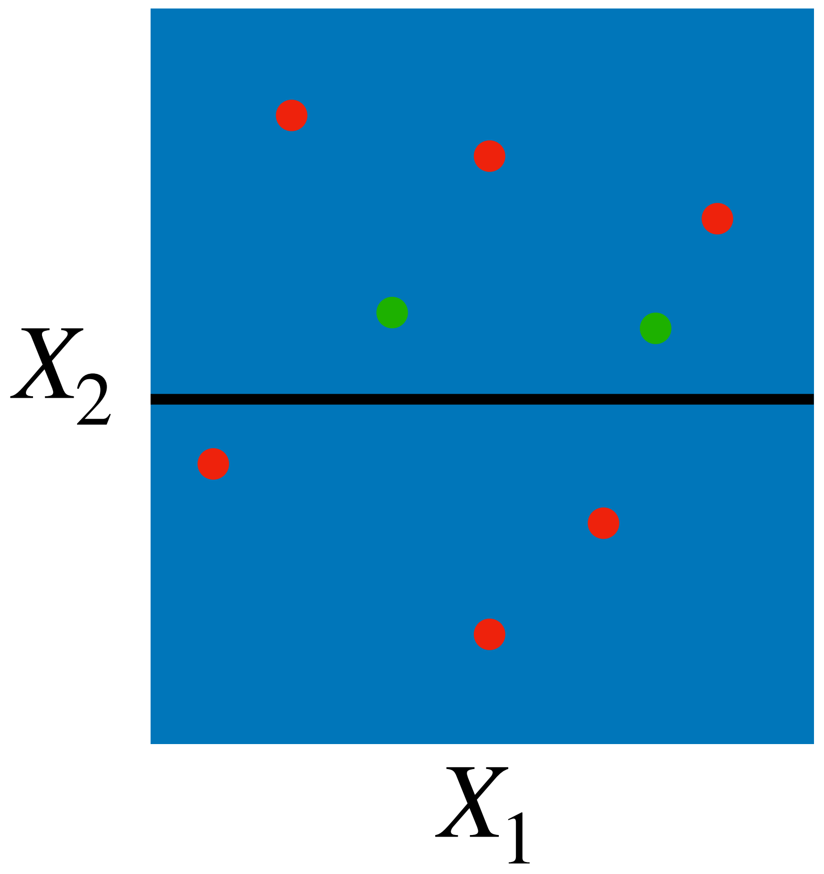
If n_m is the number of training observations in that region, then

$$\text{Total misclassification error} = \frac{1}{n}\left\{ \sum_{i:X_i \in R_1} I(Y_i \neq c_1) + \cdots + \sum_{i:X_i \in R_M} (Y_i \neq c_M) \right\}$$



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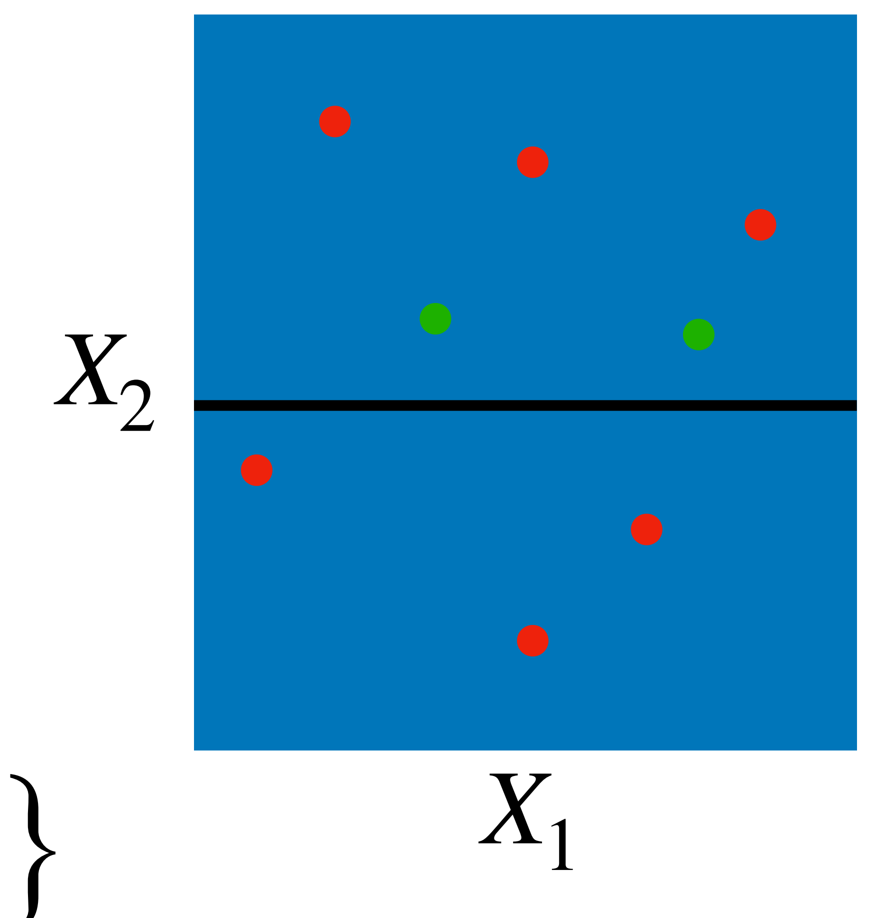
$$= \frac{1}{n}\left\{ n_1 \min(\hat{p}_1, 1 - \hat{p}_1) + \cdots + n_M \min(\hat{p}_M, 1 - \hat{p}_M) \right\}$$



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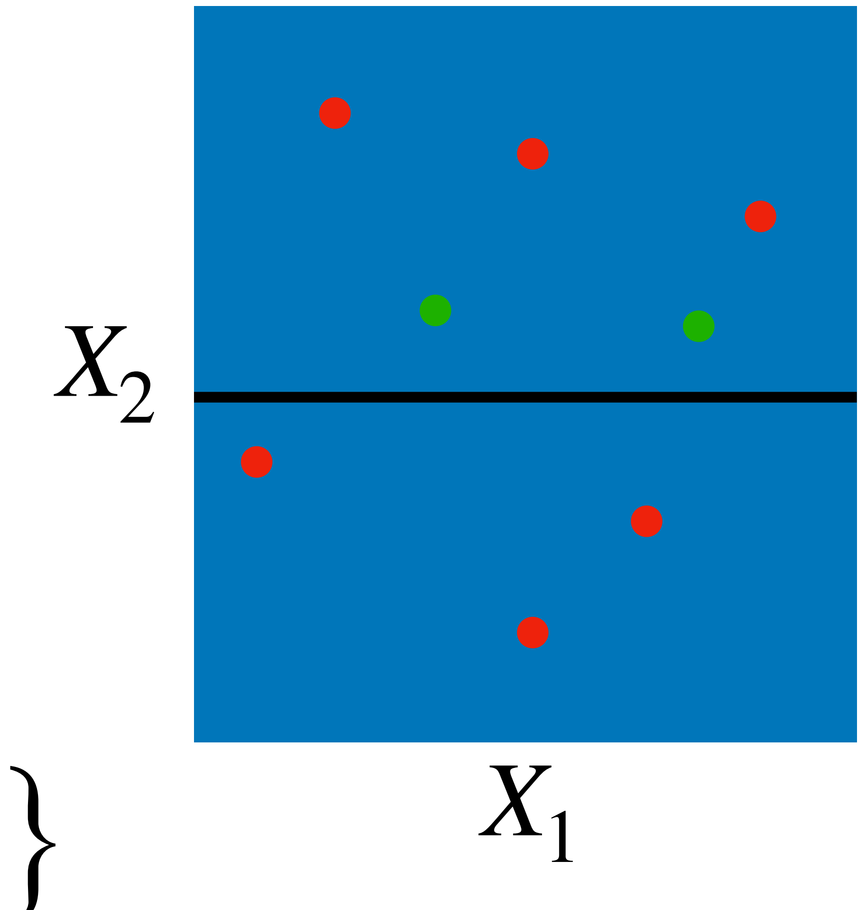

Replace misclassification error $\min(\widehat{p}_m, 1 - \widehat{p}_m)$ by the Gini index $= 2\widehat{p}_m(1 - \widehat{p}_m)$:

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Finding the rectangles $\widehat{R}_m$: The Gini index (measure of node impurity)

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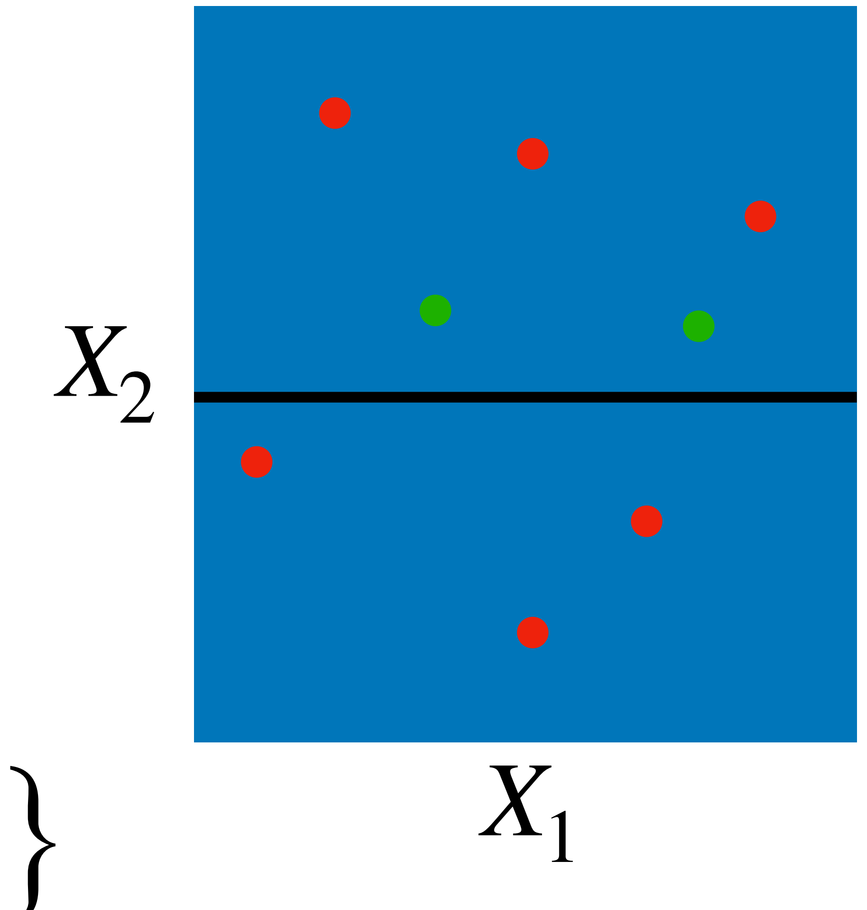

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Finding the rectangles $\widehat{R}_m$: Gini index versus misclassification error

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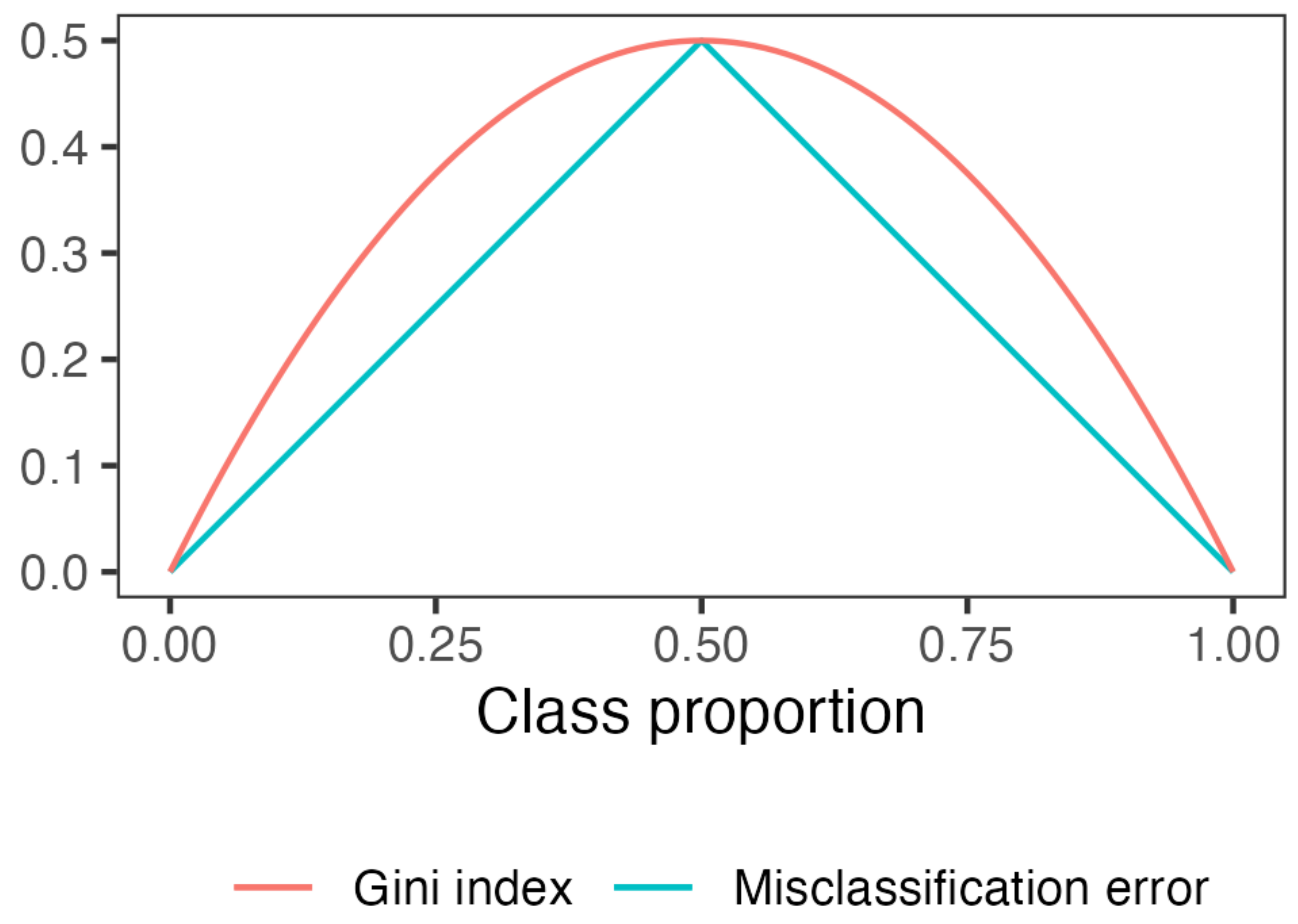
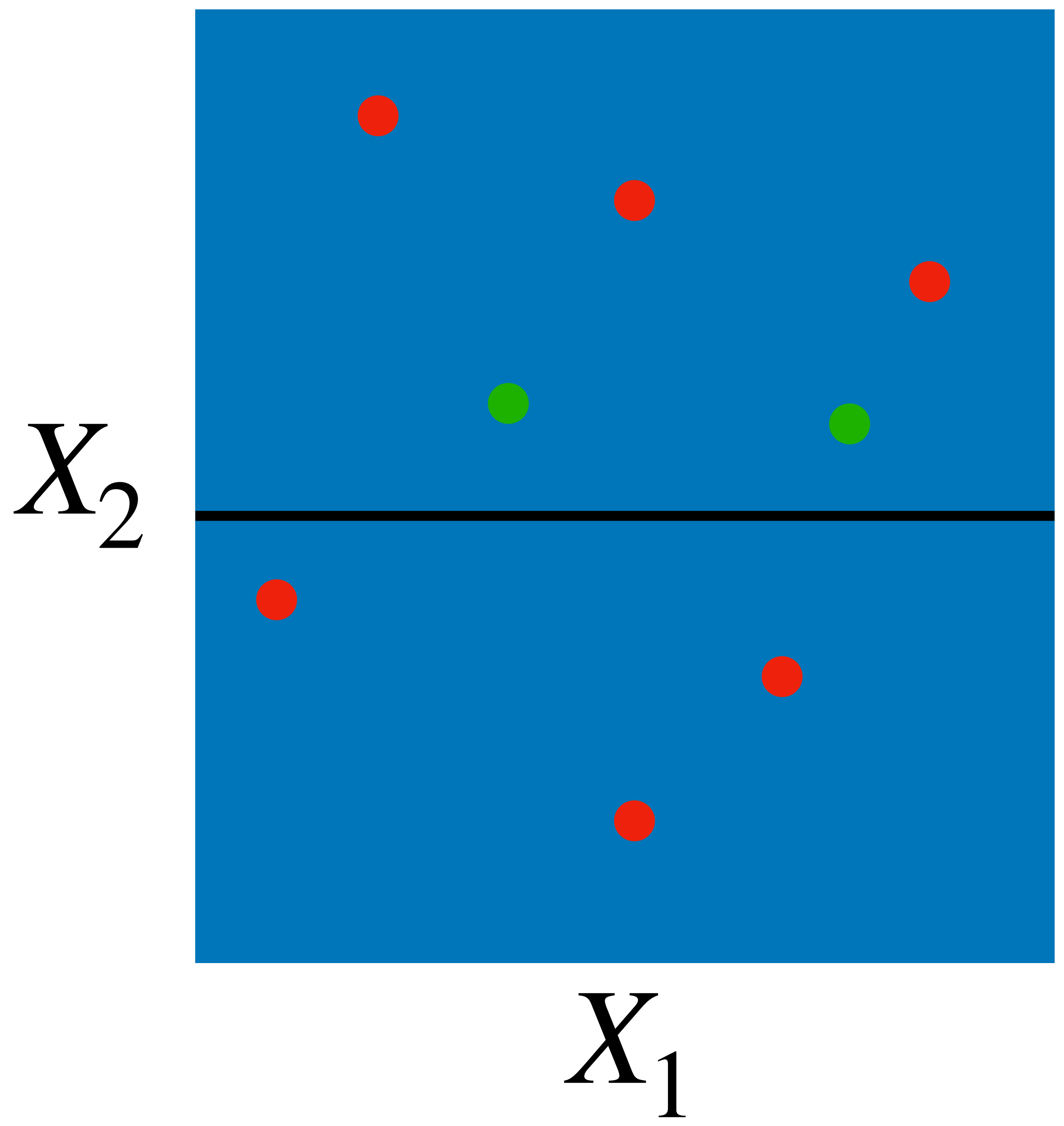
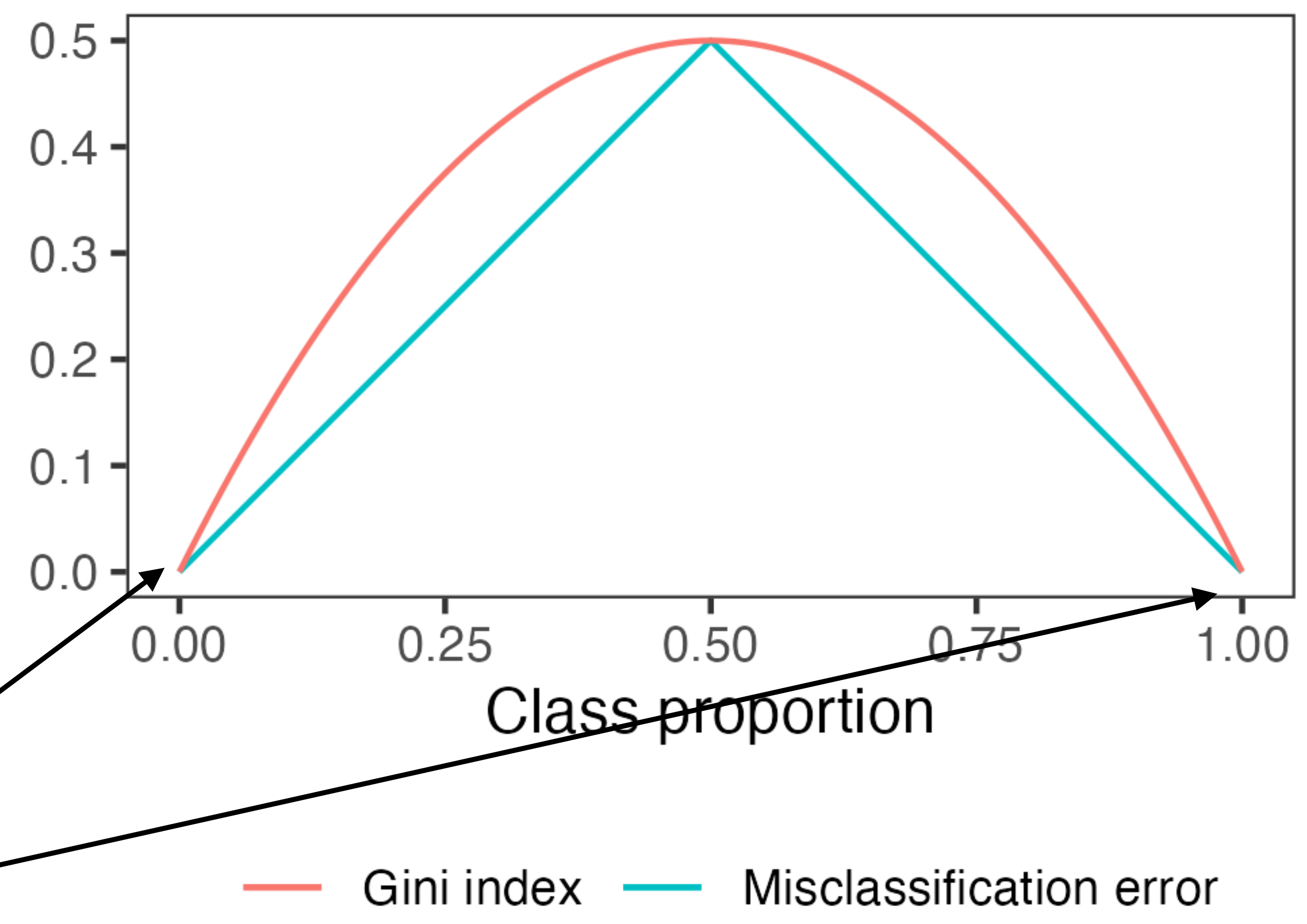


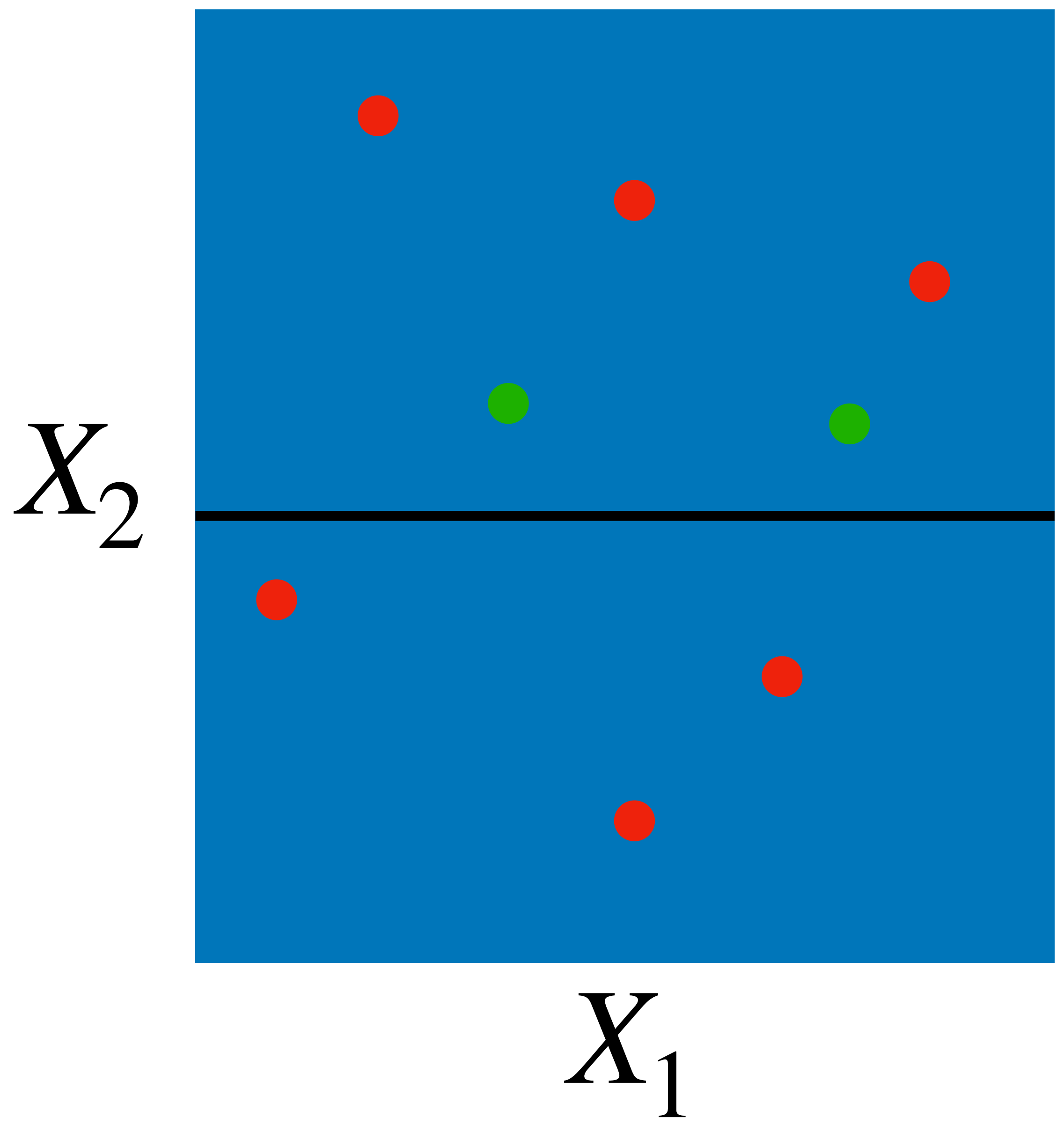


Training a classification tree

Finding the rectangles $\widehat{R}_m$: Gini index versus misclassification error



Rises more sharply away from 0 and 1, promoting node purity



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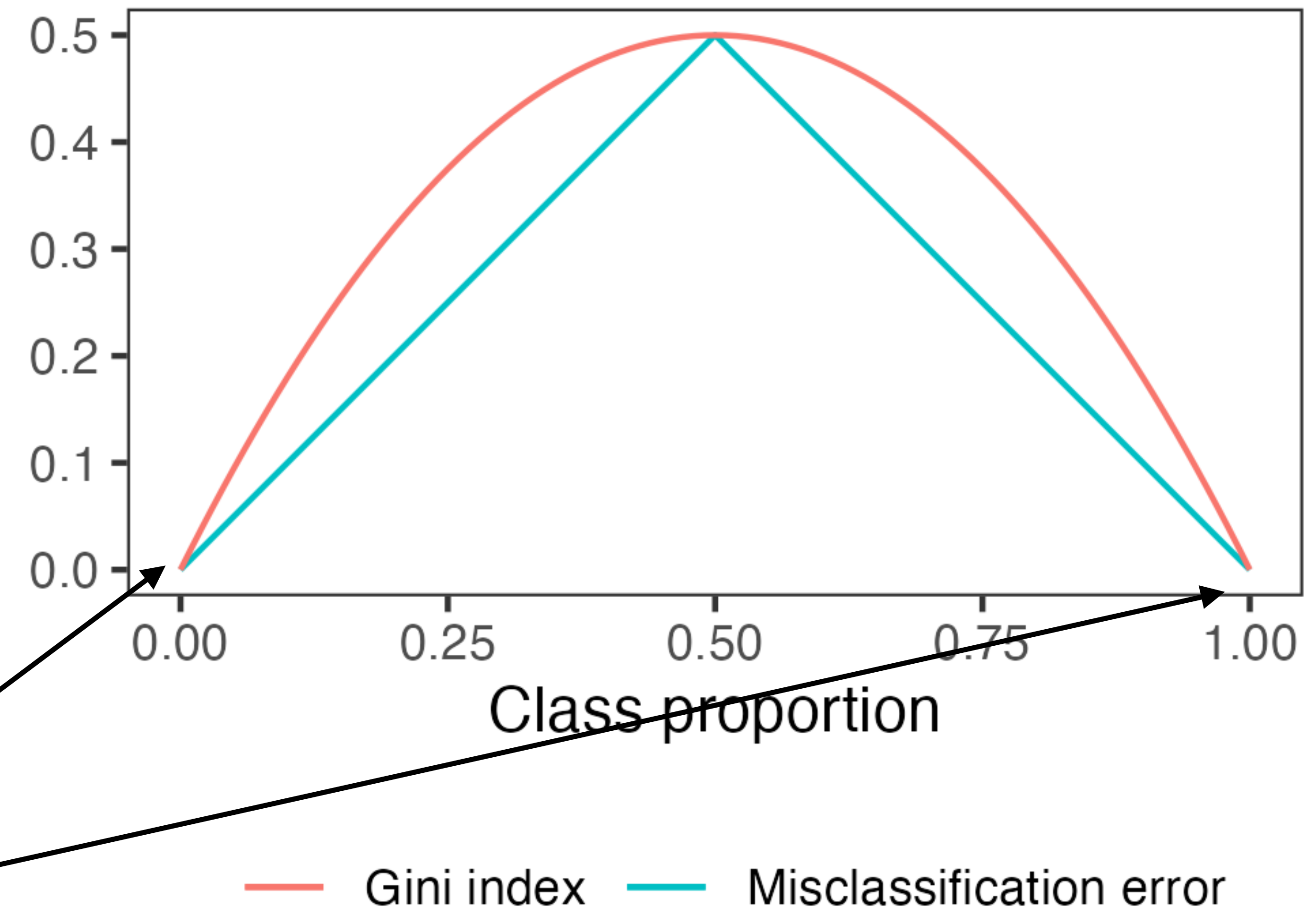

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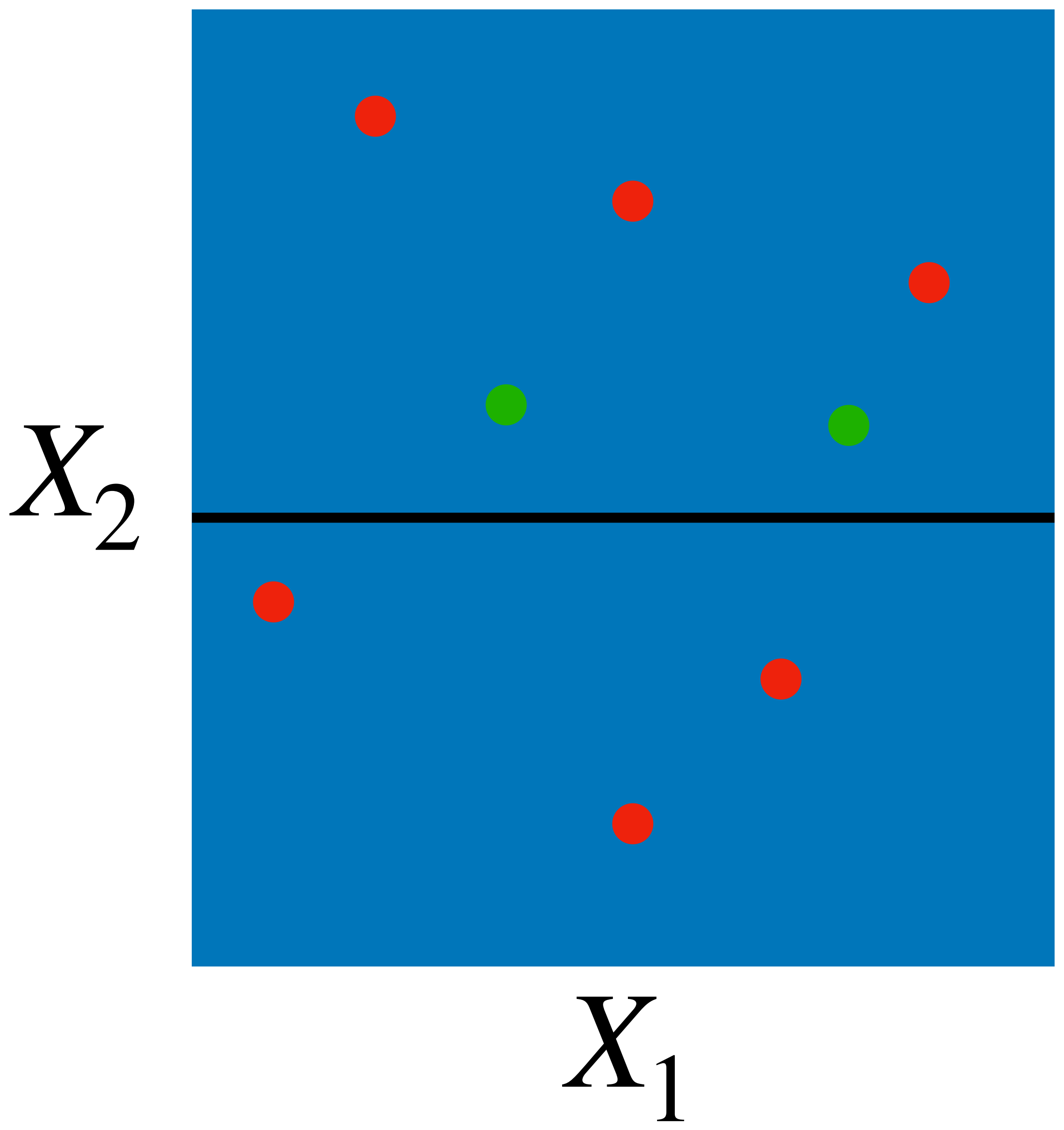
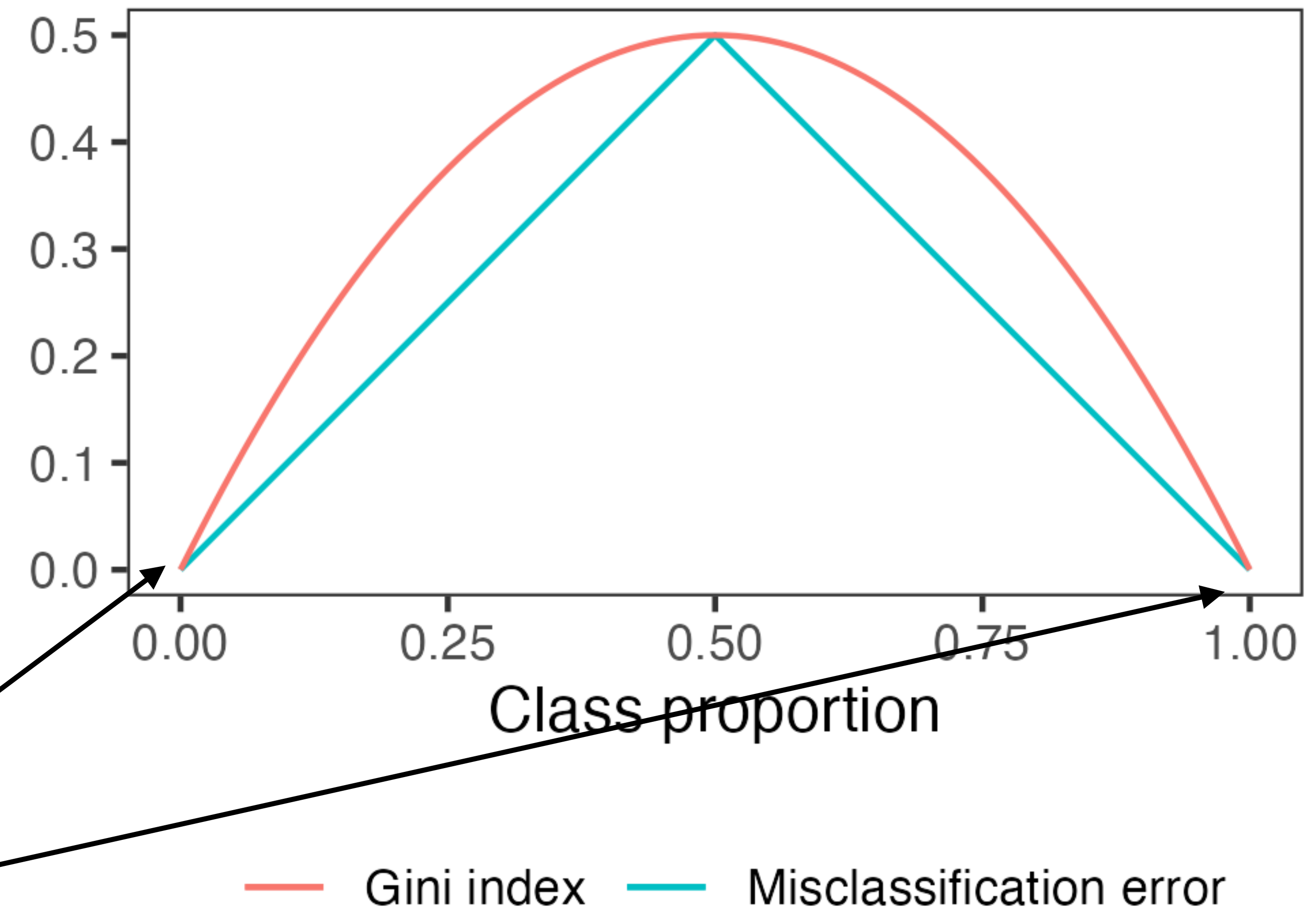


Tree	Total Misclass. error

Training a classification tree

Finding the rectangles $\widehat{R}_m$: Gini index versus misclassification error



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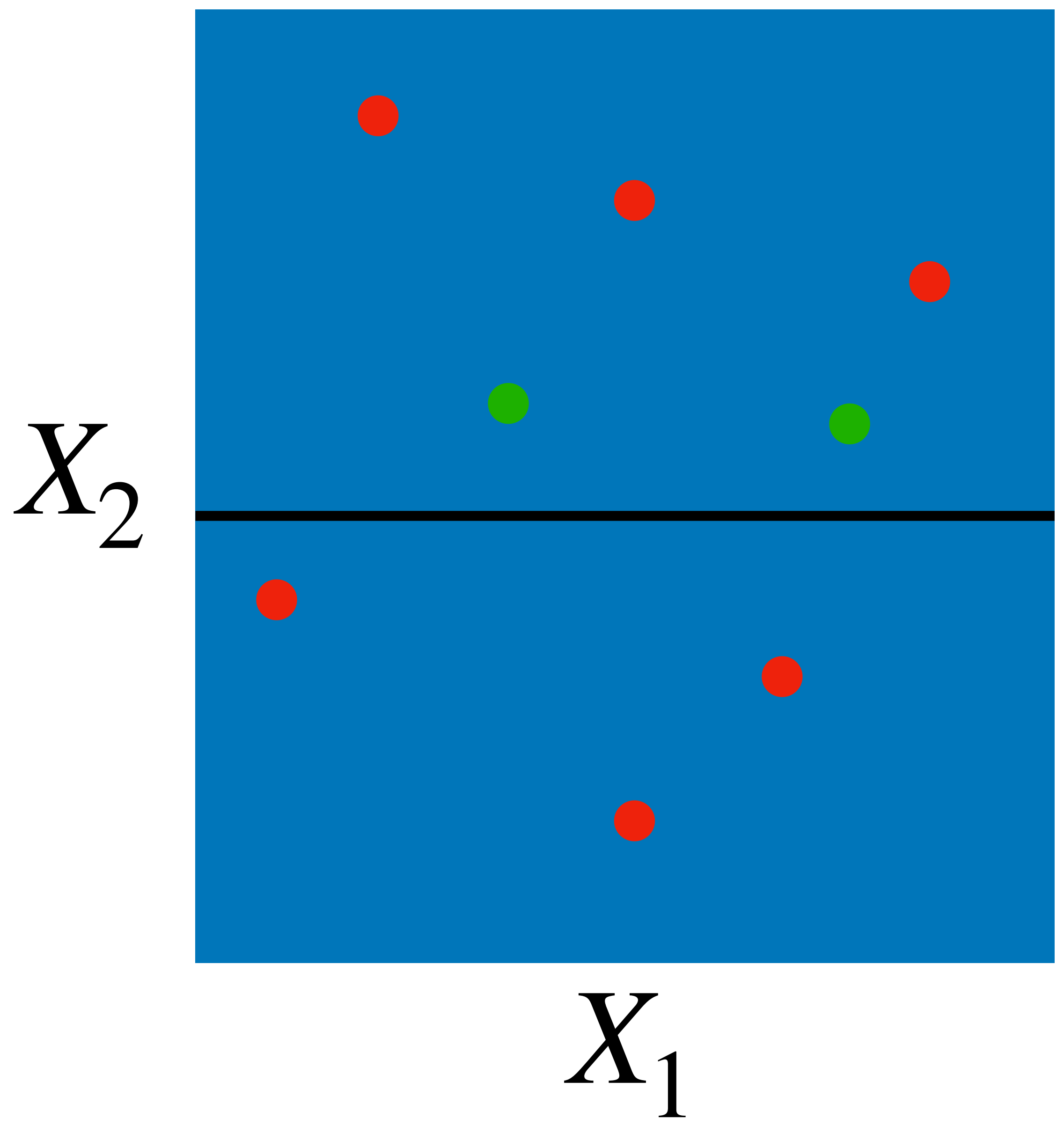
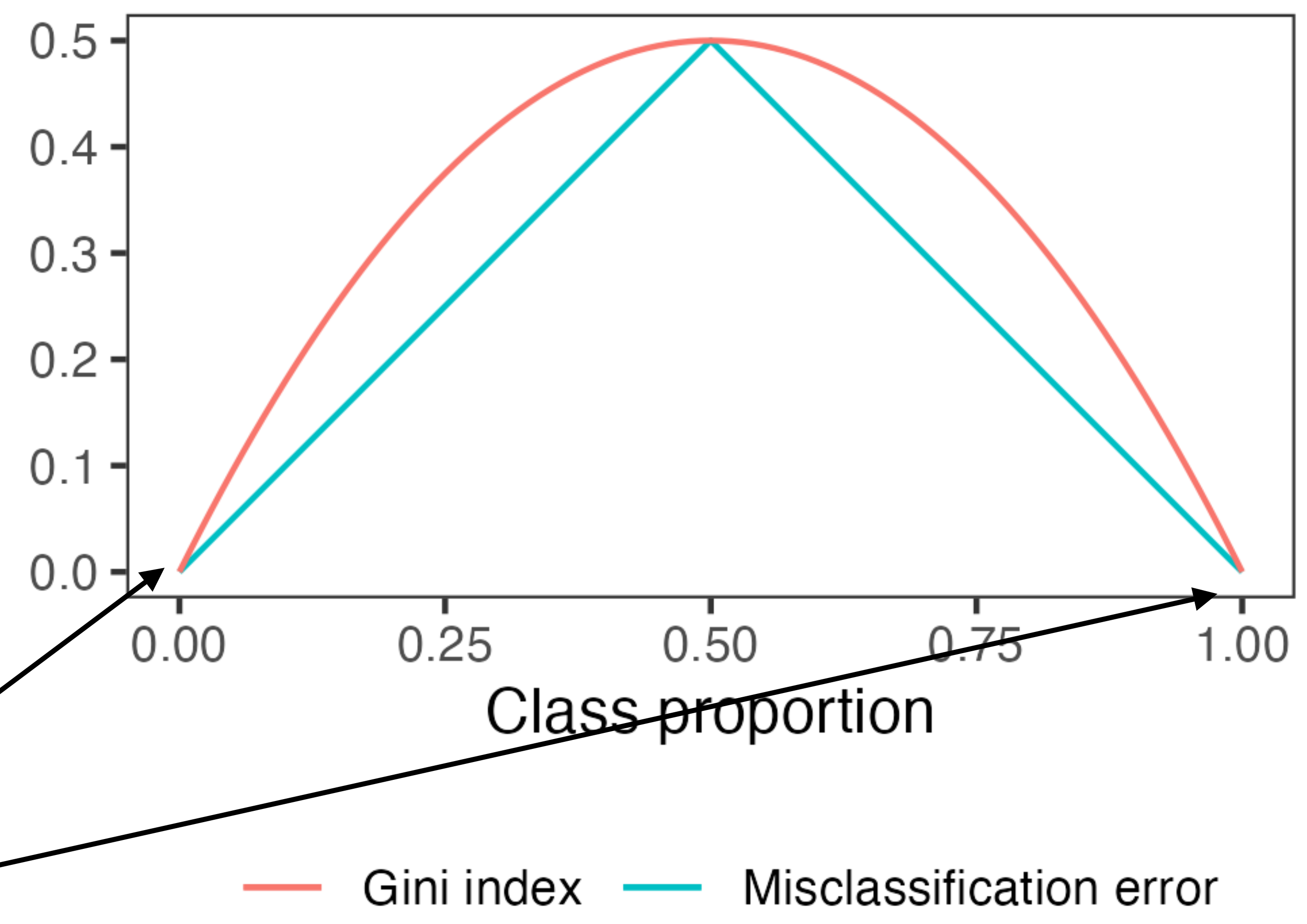


Tree	Total Misclass. error
No splits	

Training a classification tree

Finding the rectangles $\widehat{R}_m$: Gini index versus misclassification error



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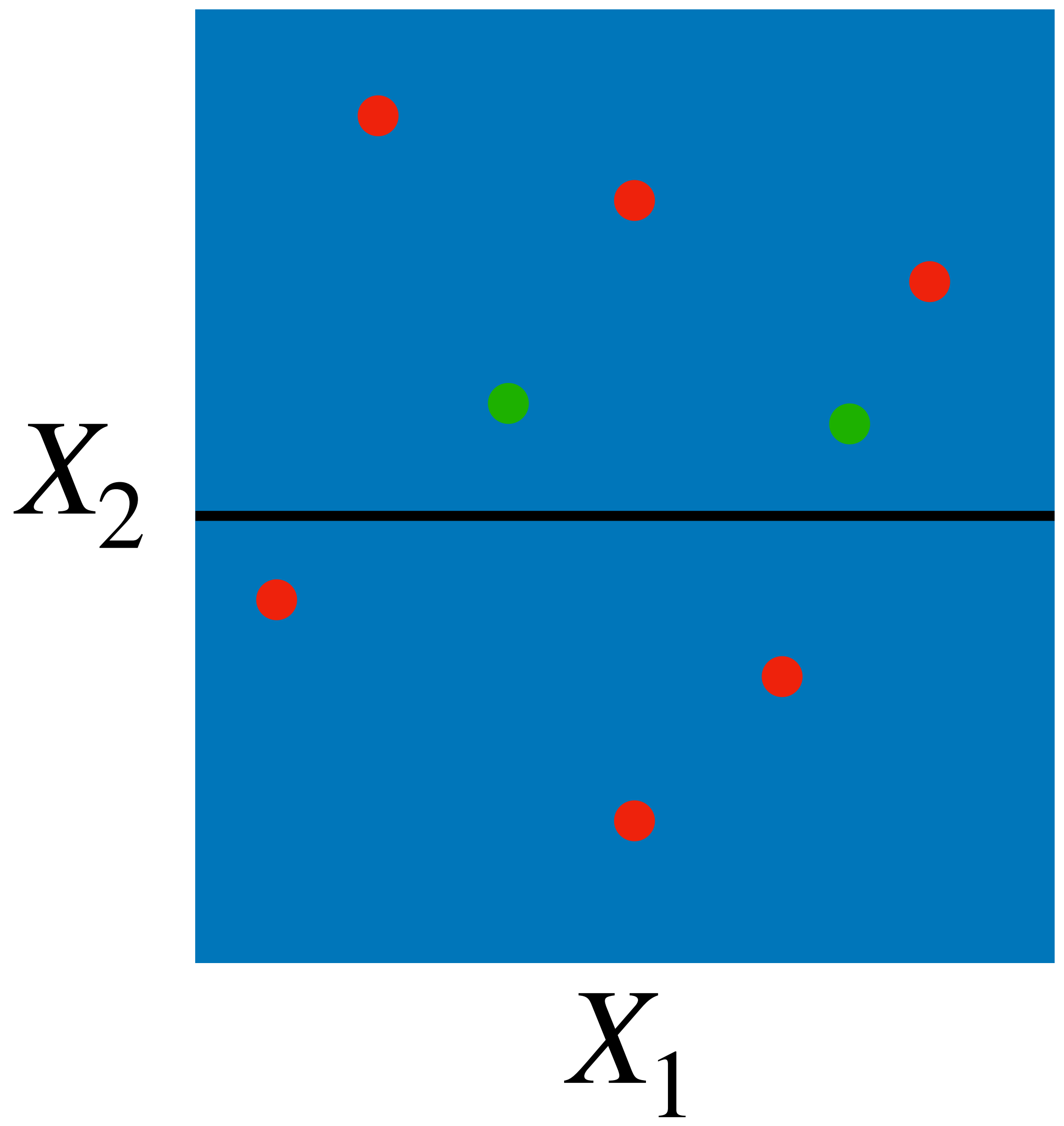
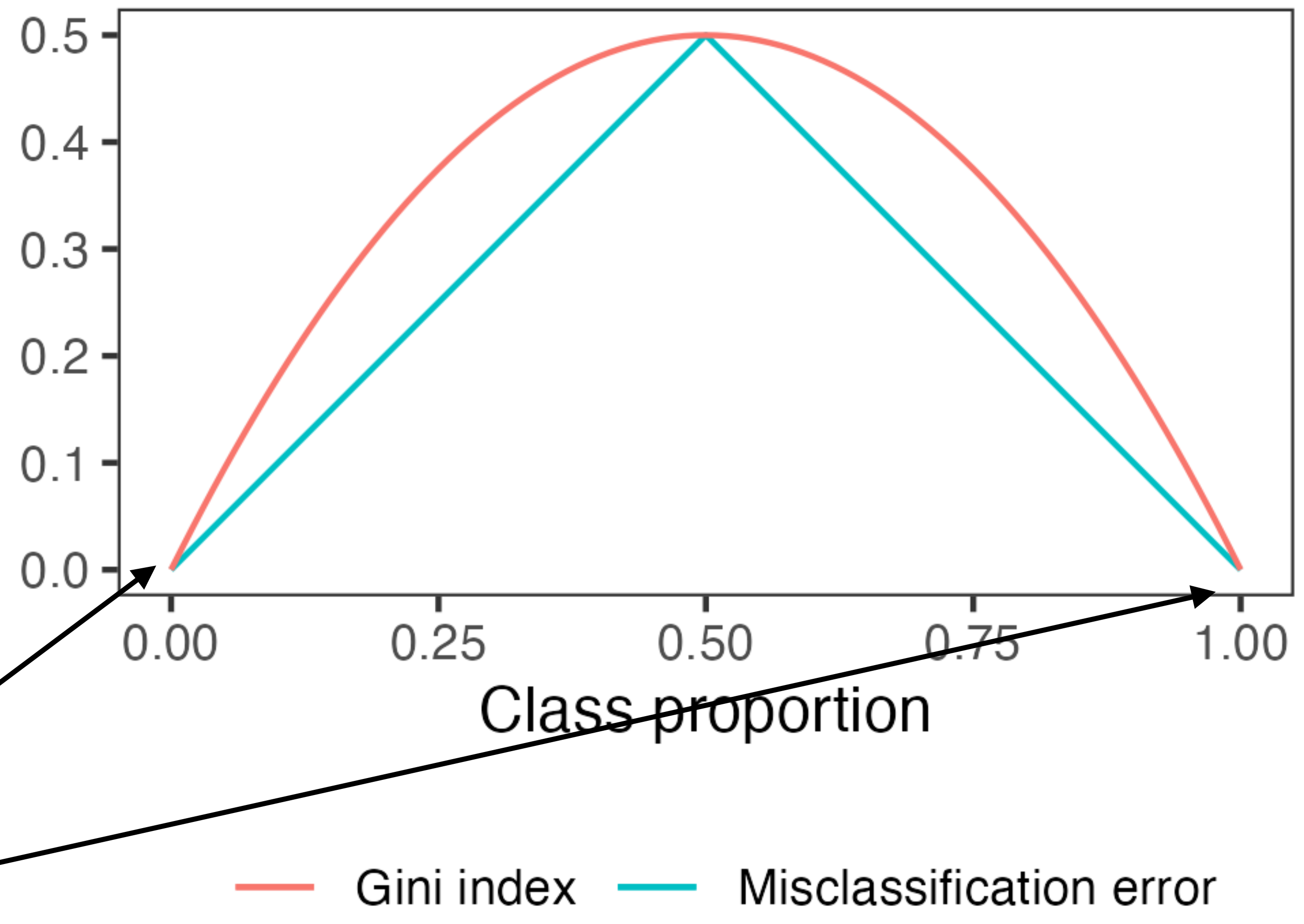


Tree	Total Misclass. error
No splits	$\frac{1}{4}$

Training a classification tree

Finding the rectangles $\widehat{R}_m$: Gini index versus misclassification error



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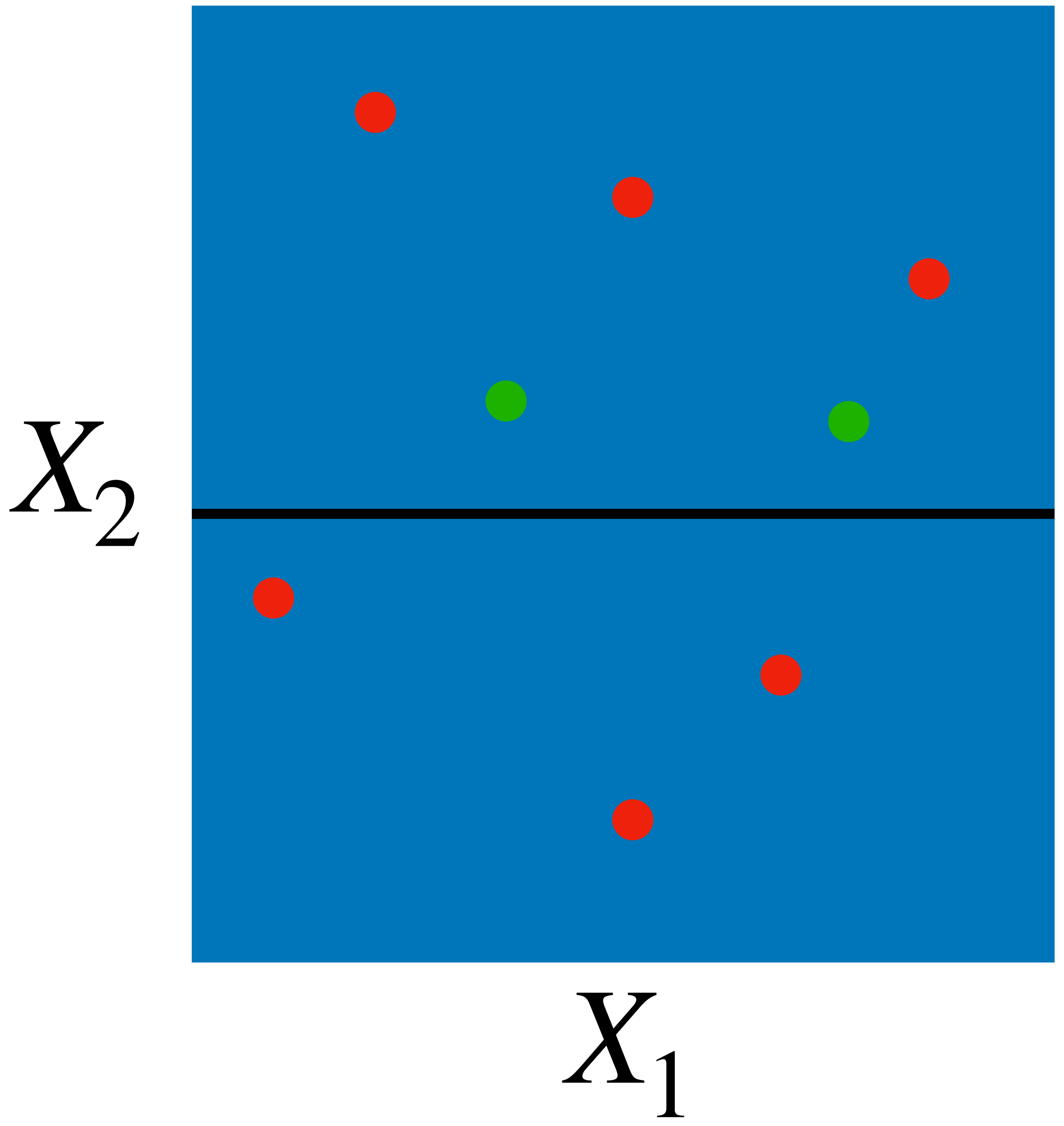
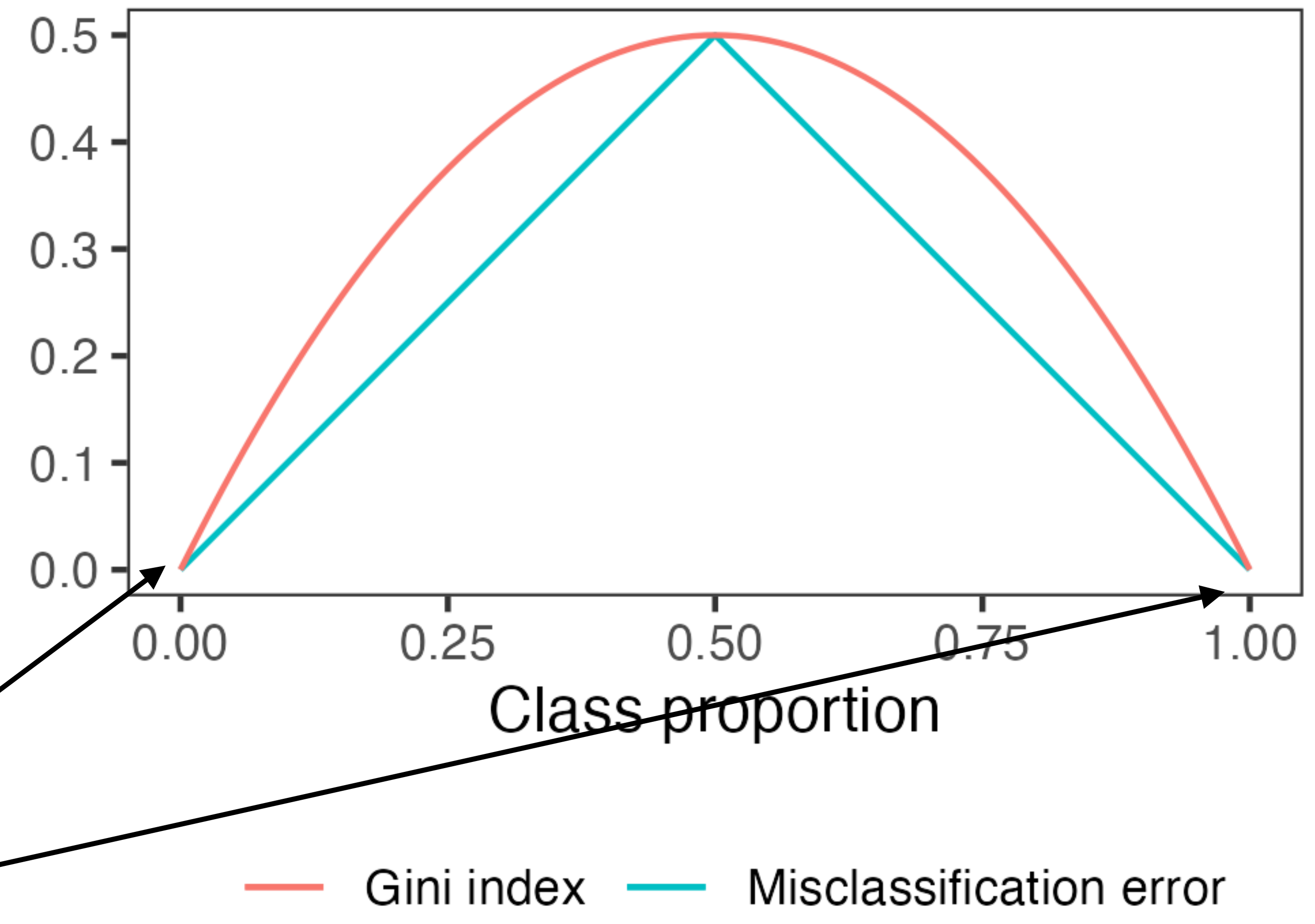


Tree	Total Misclass. error
No splits	$\frac{1}{4}$
One split	

Training a classification tree

Finding the rectangles $\widehat{R}_m$: Gini index versus misclassification error



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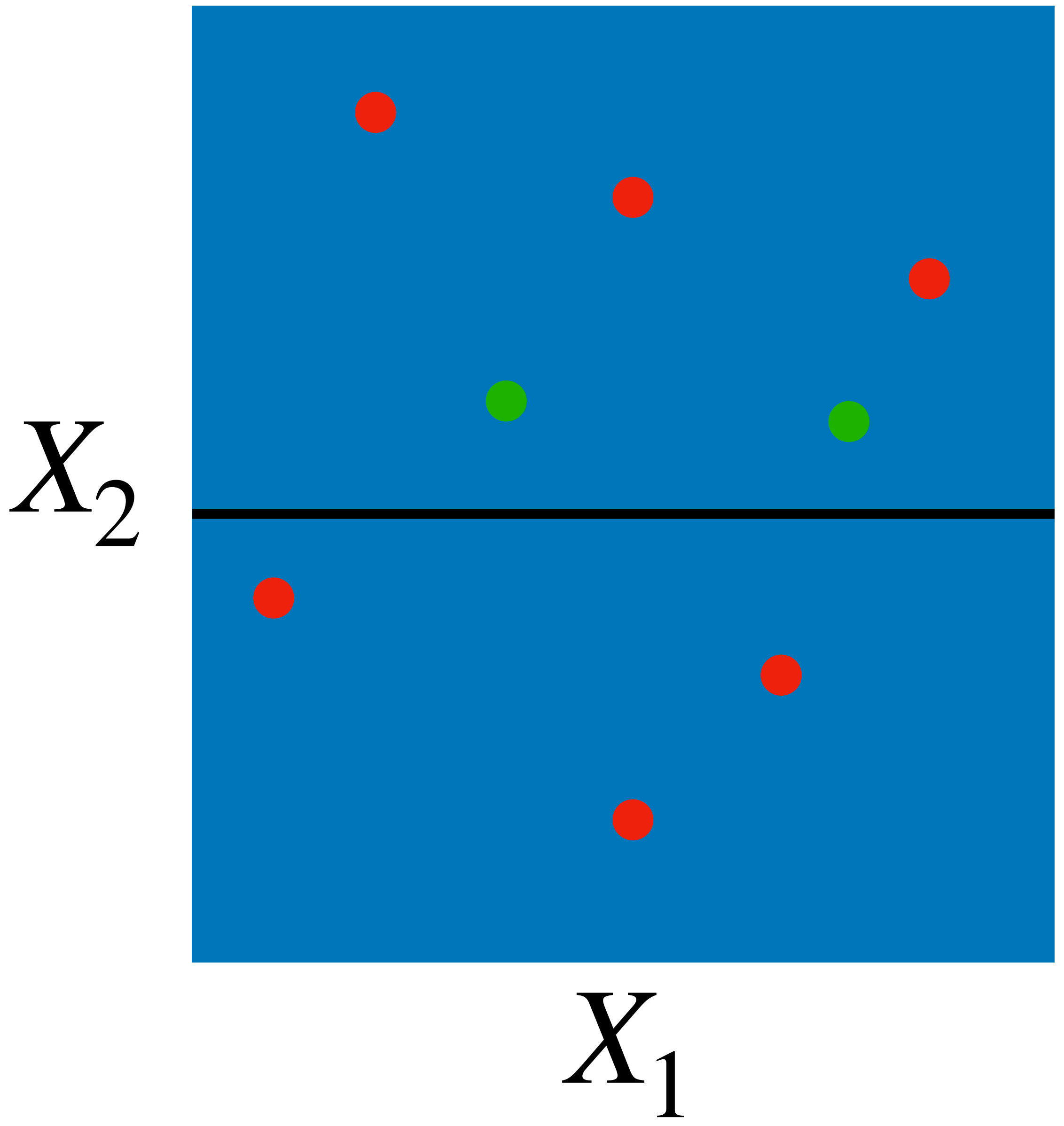

Tree	Total Misclass. error
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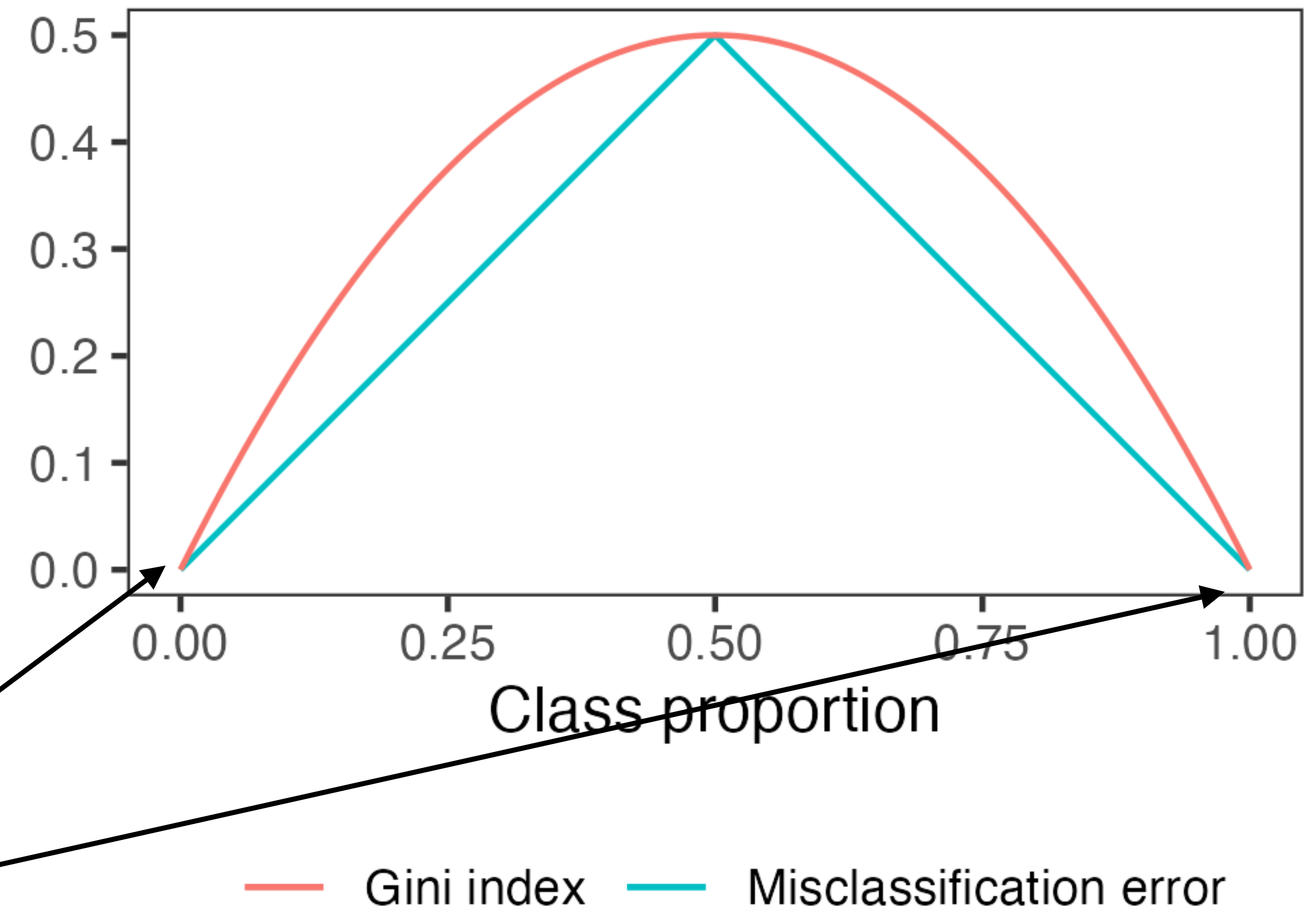

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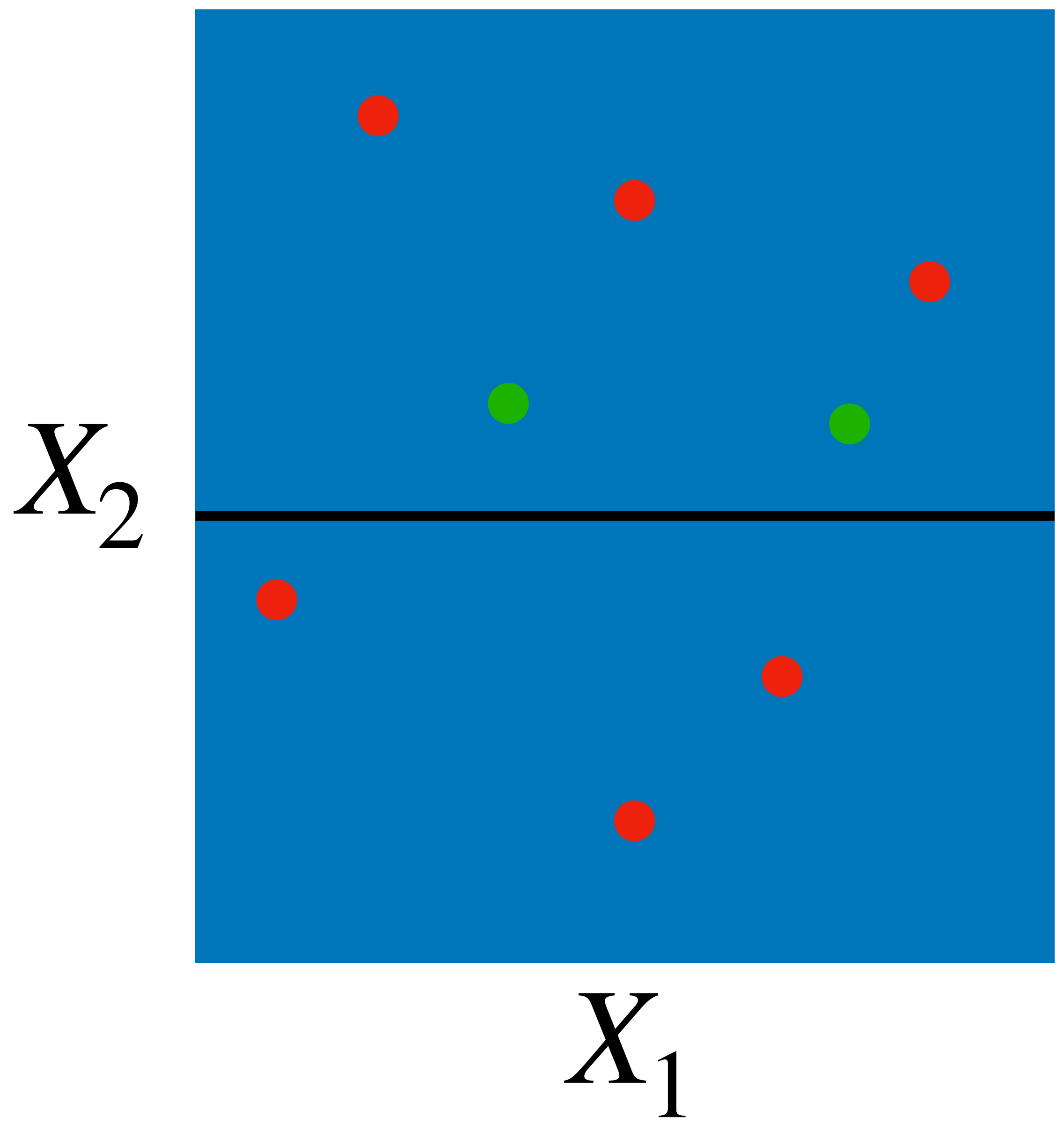
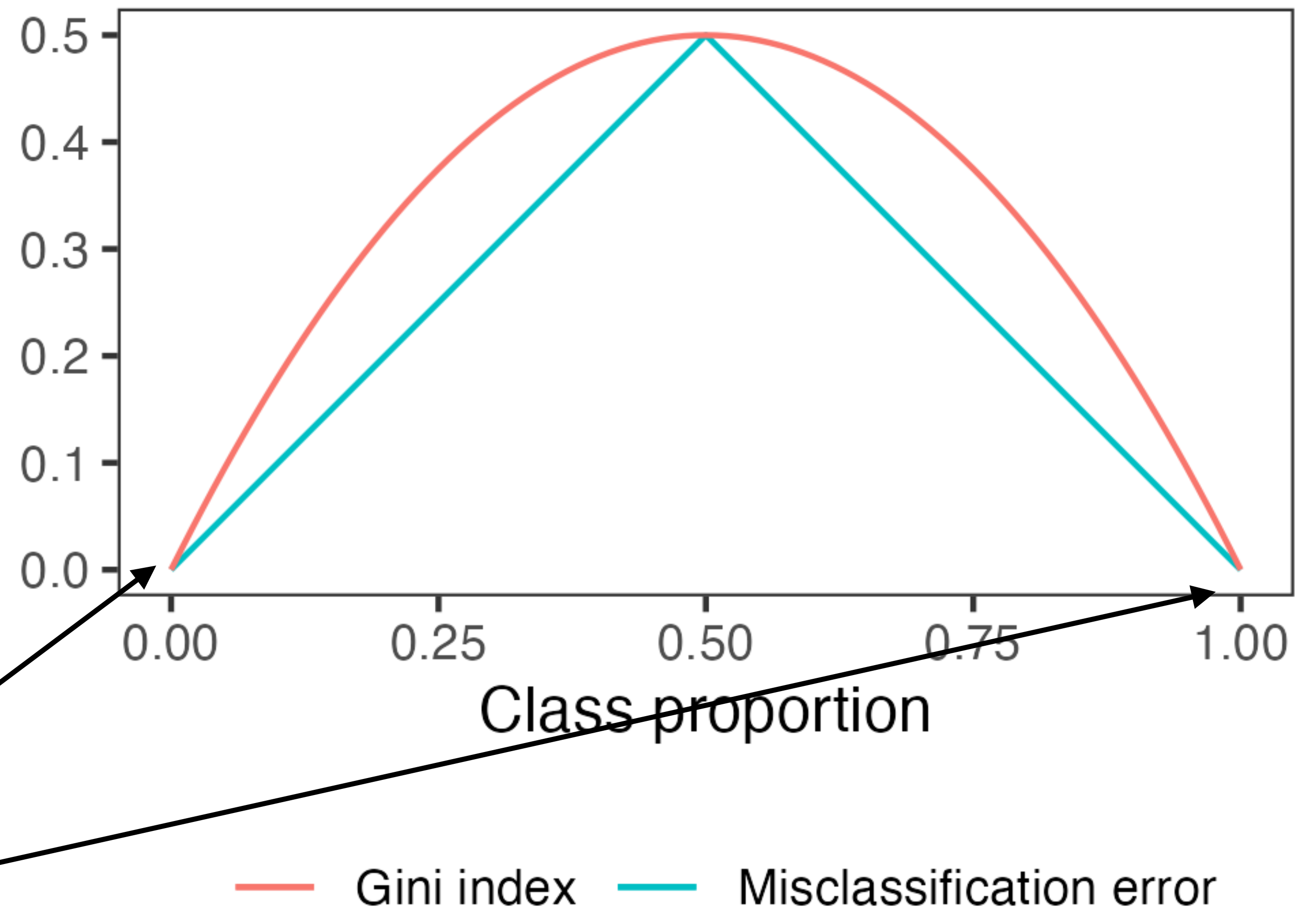


Tree	Total Misclass. error	Total Gini index
No splits	$\frac{1}{4}$	
One split	$\frac{1}{4}$	

Training a classification tree

Finding the rectangles $\widehat{R}_m$: Gini index versus misclassification error



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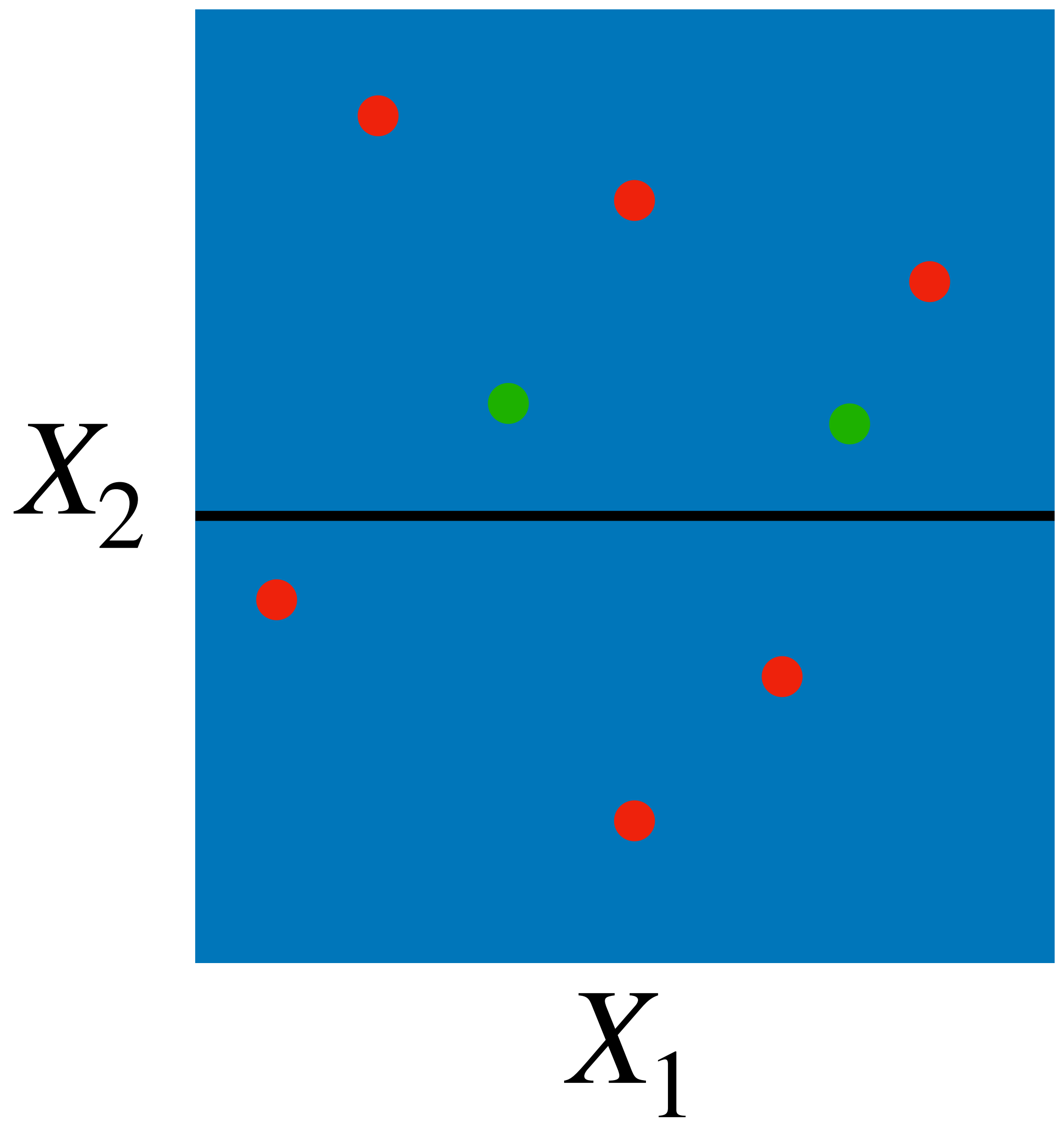

Tree	Total Misclass. error	Total Gini index
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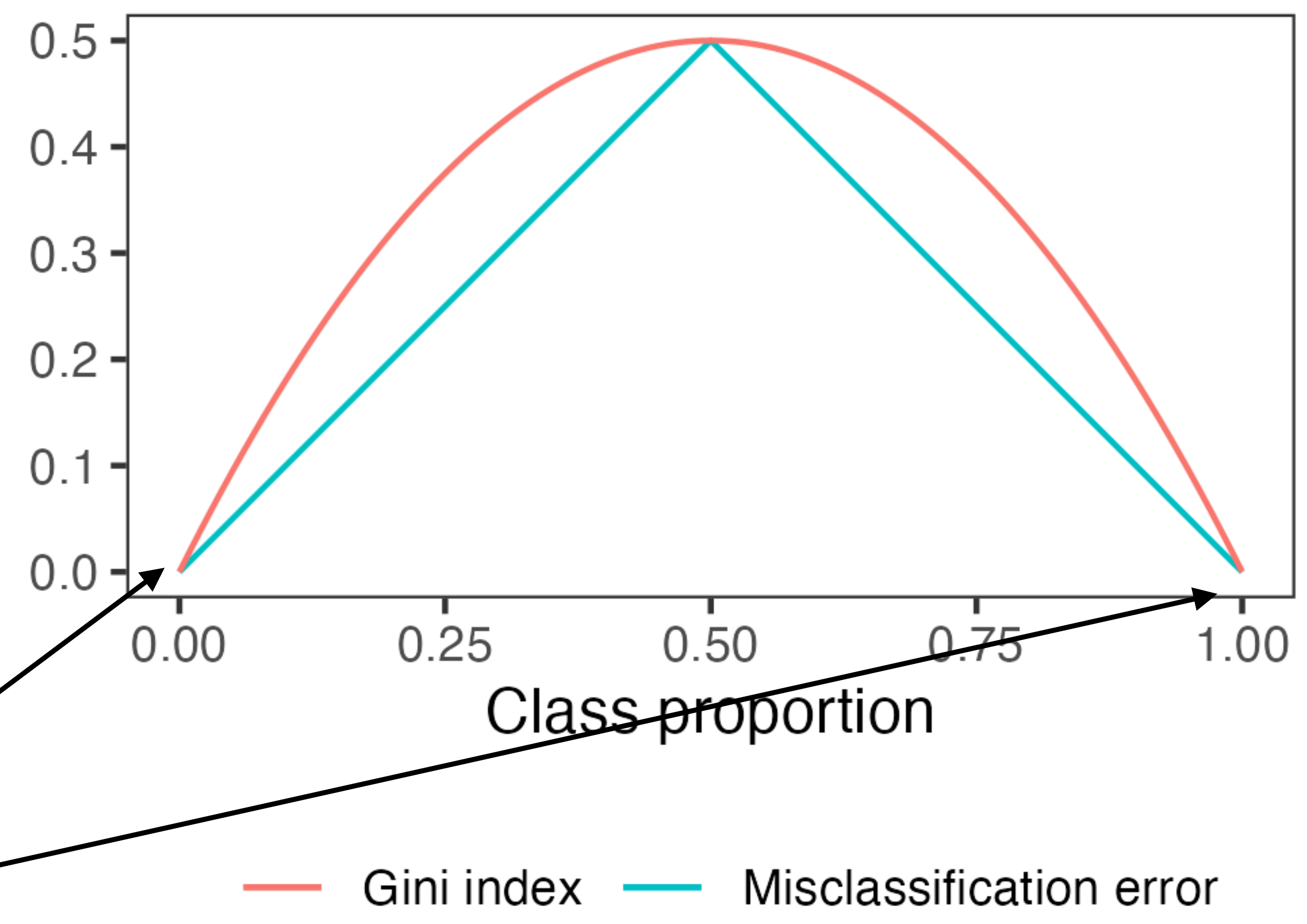

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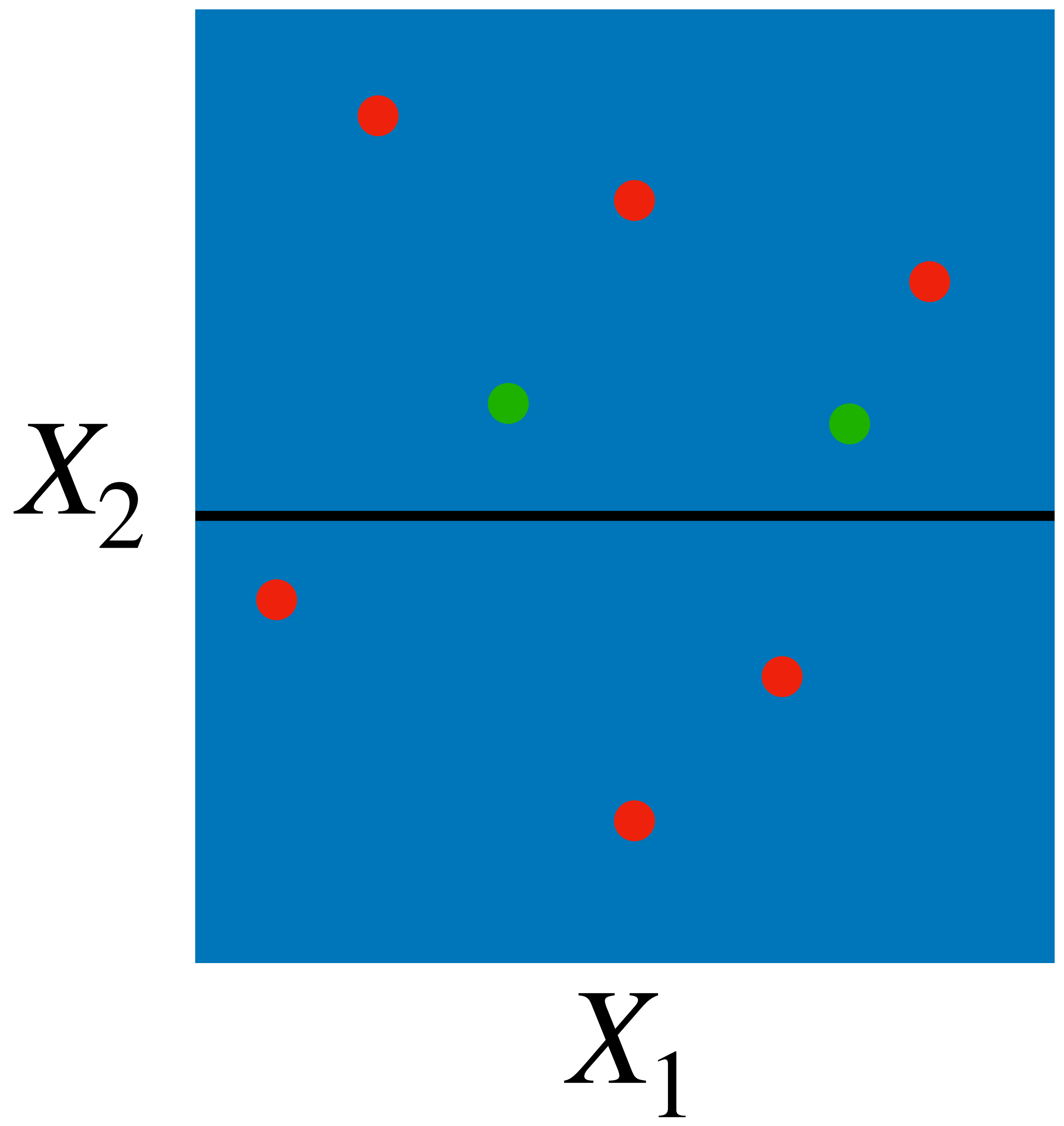

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Finding the rectangles $\widehat{R}_m$

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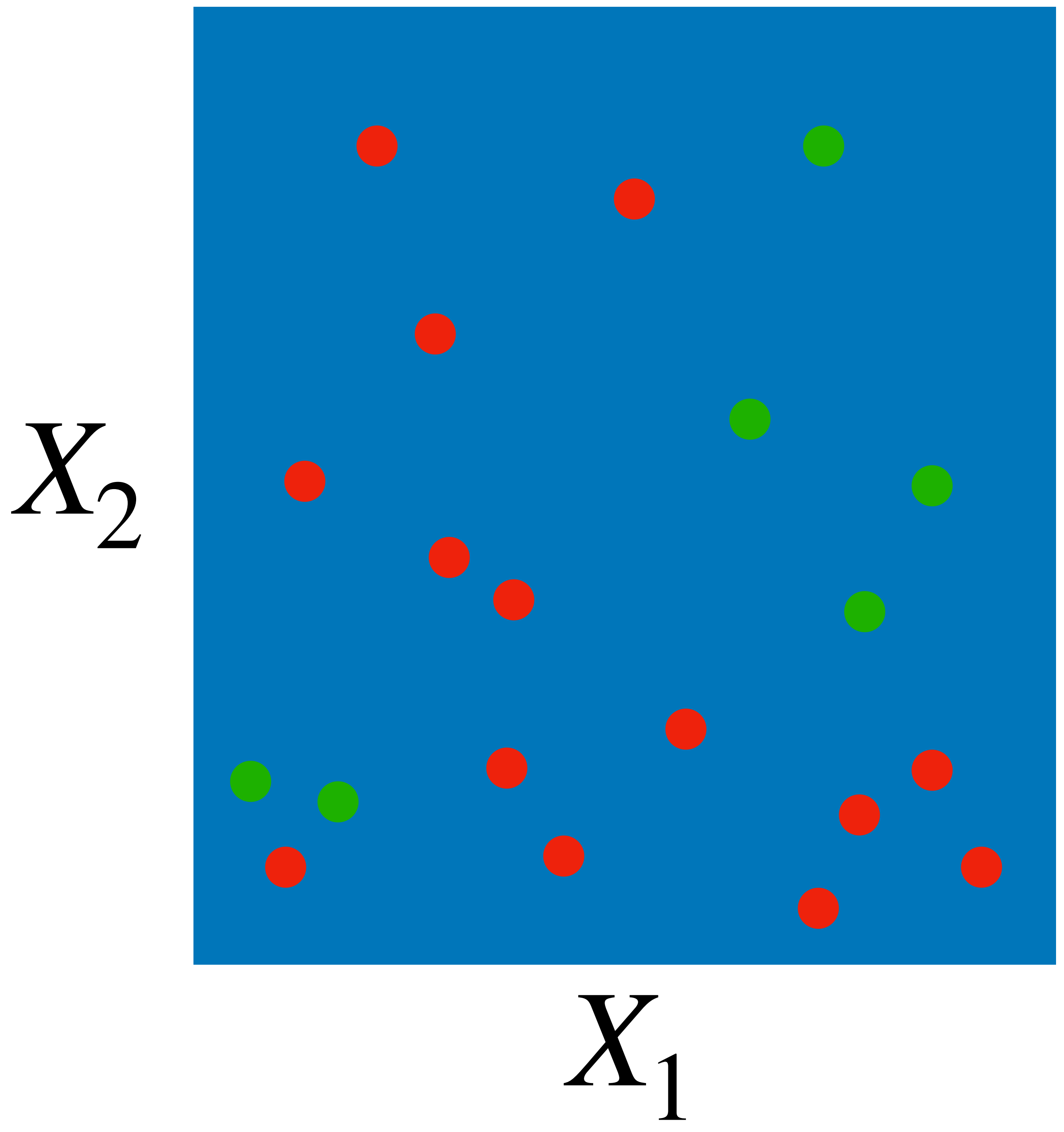

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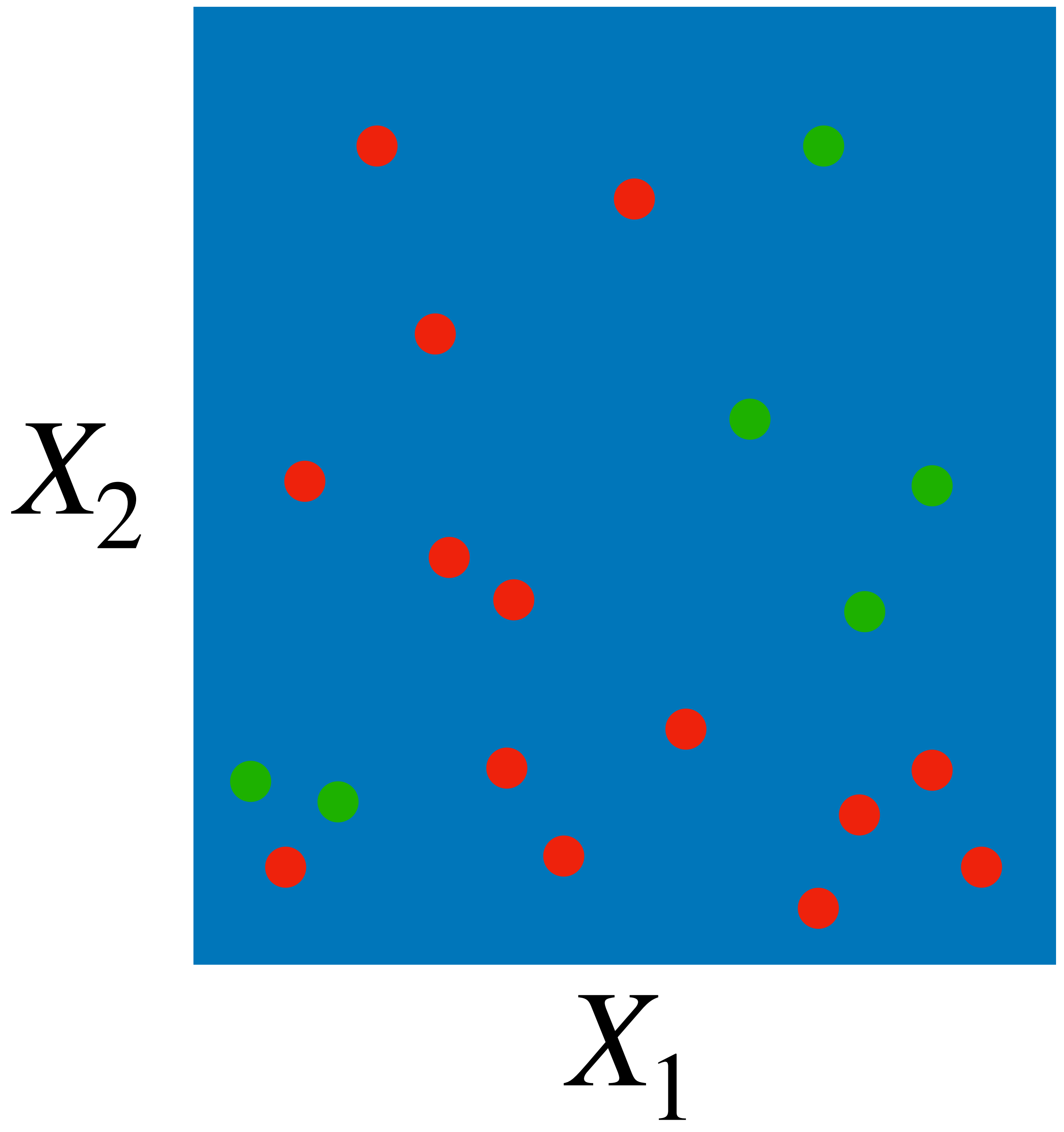

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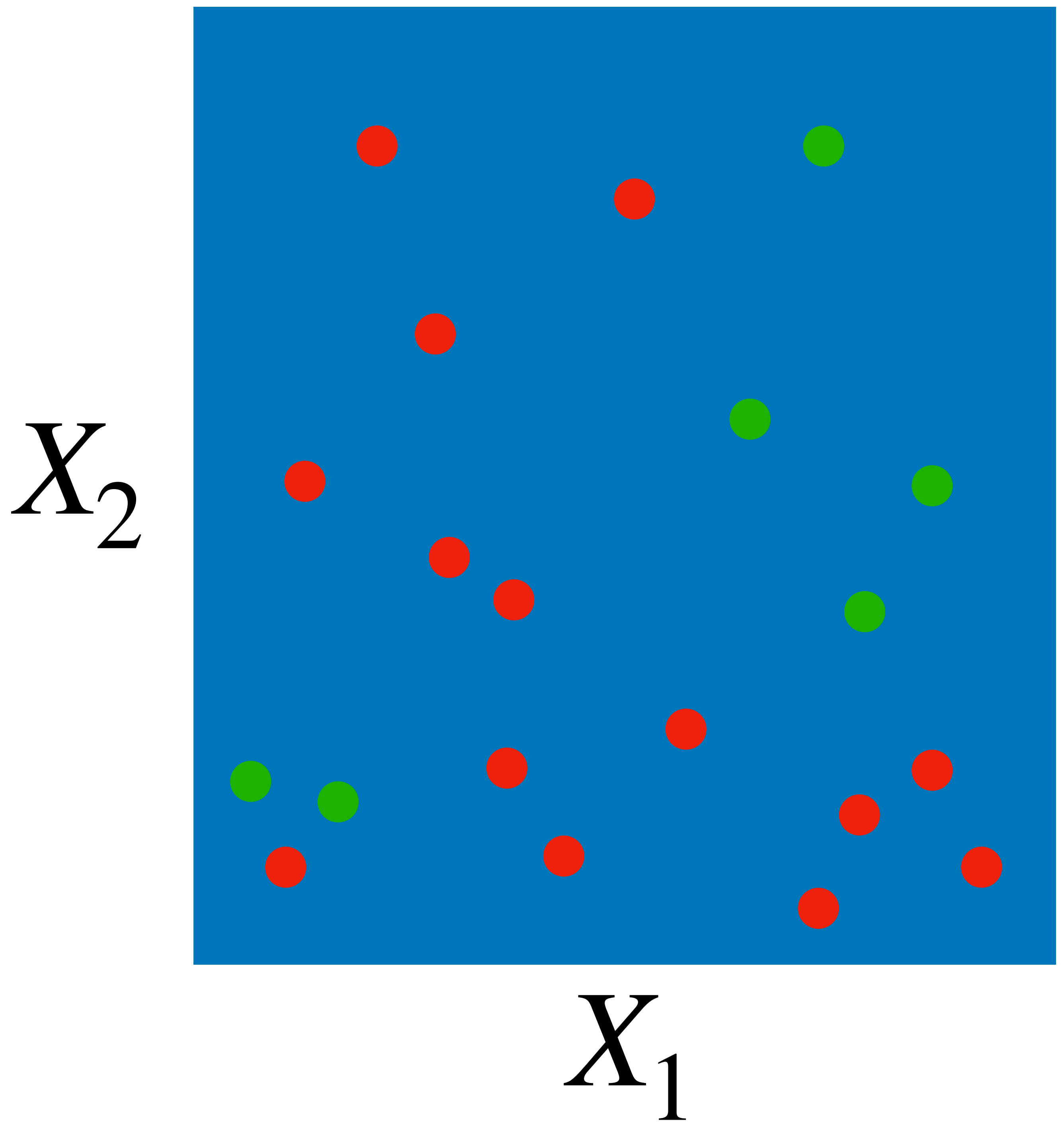

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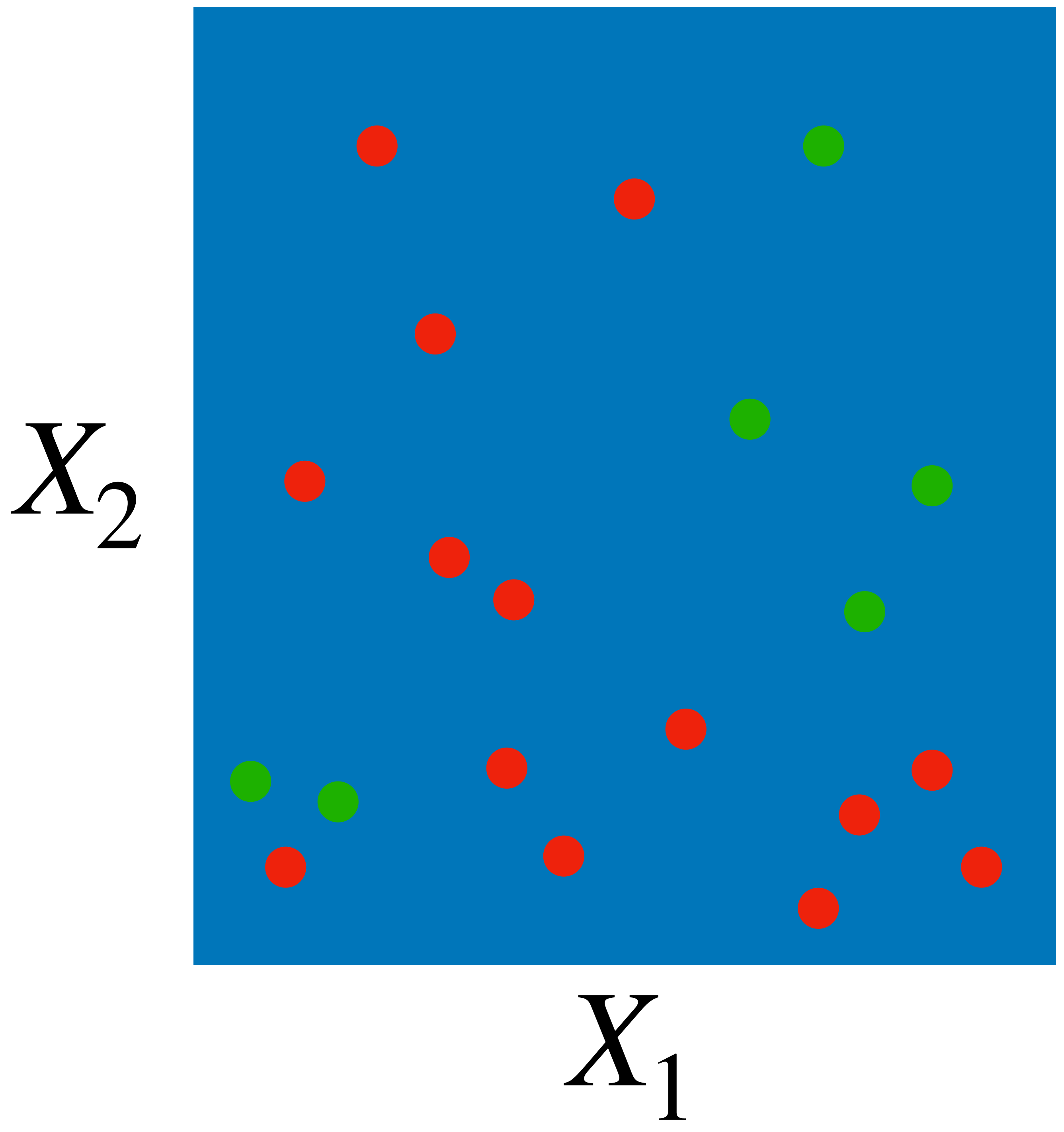

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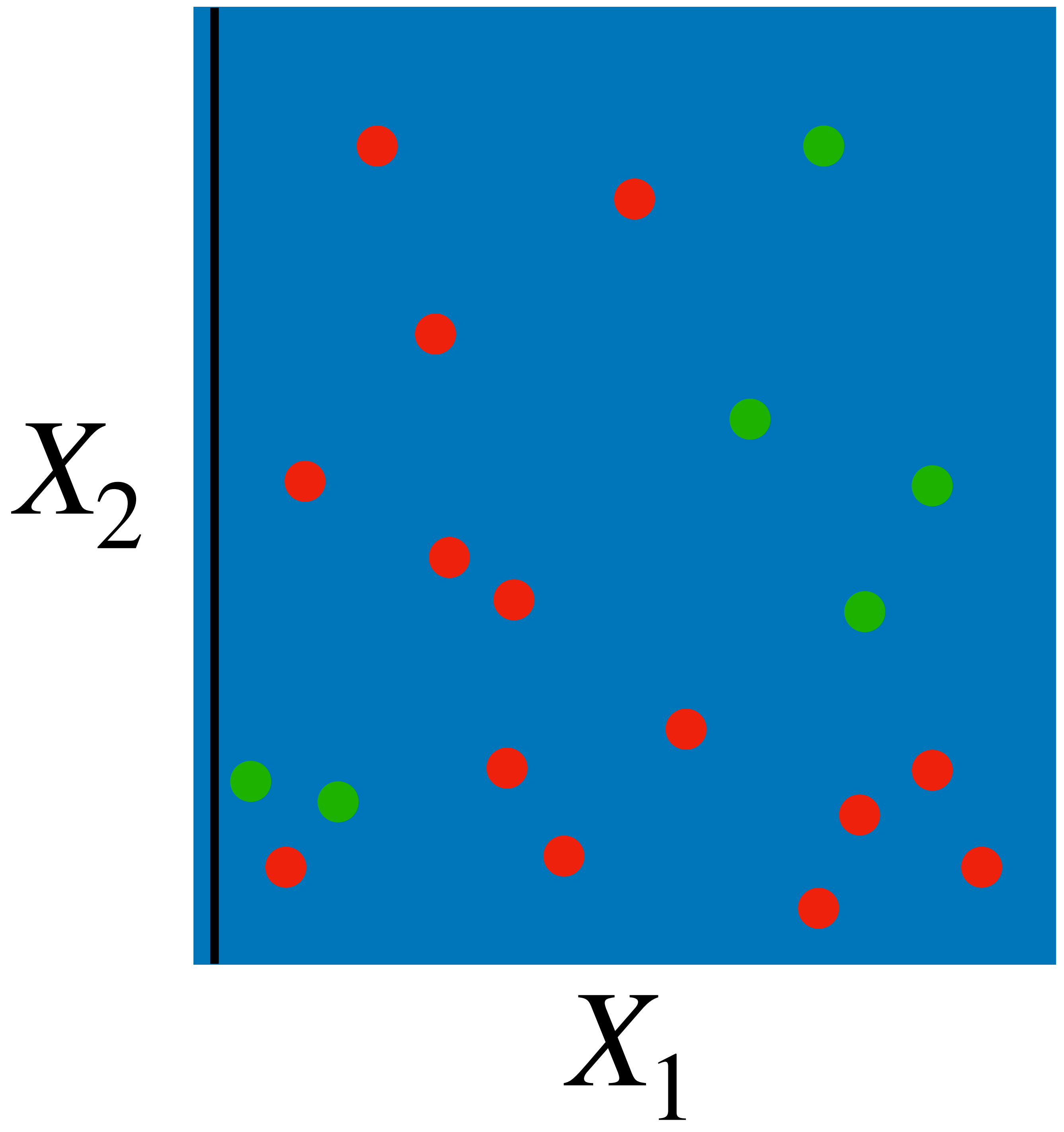

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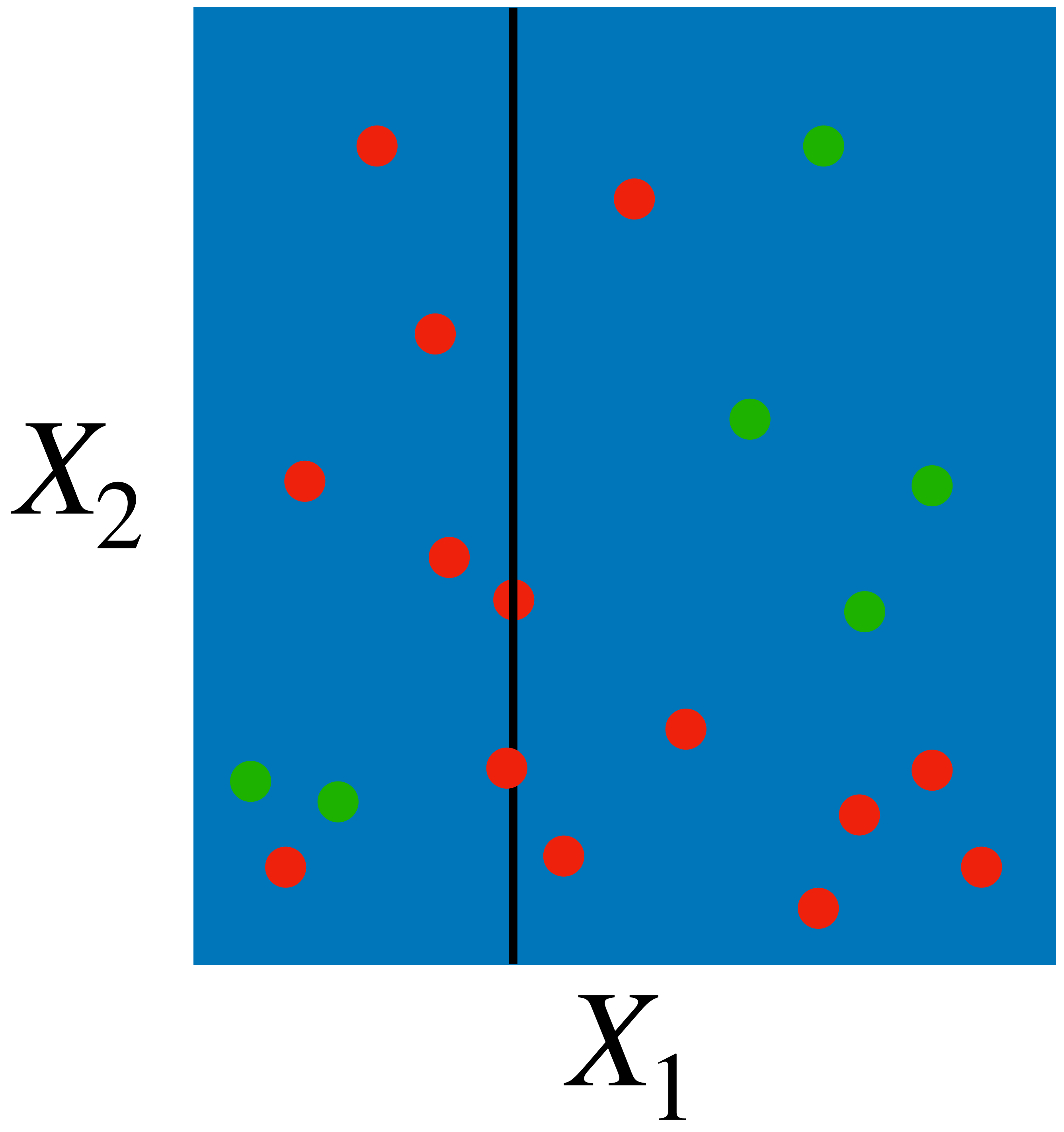

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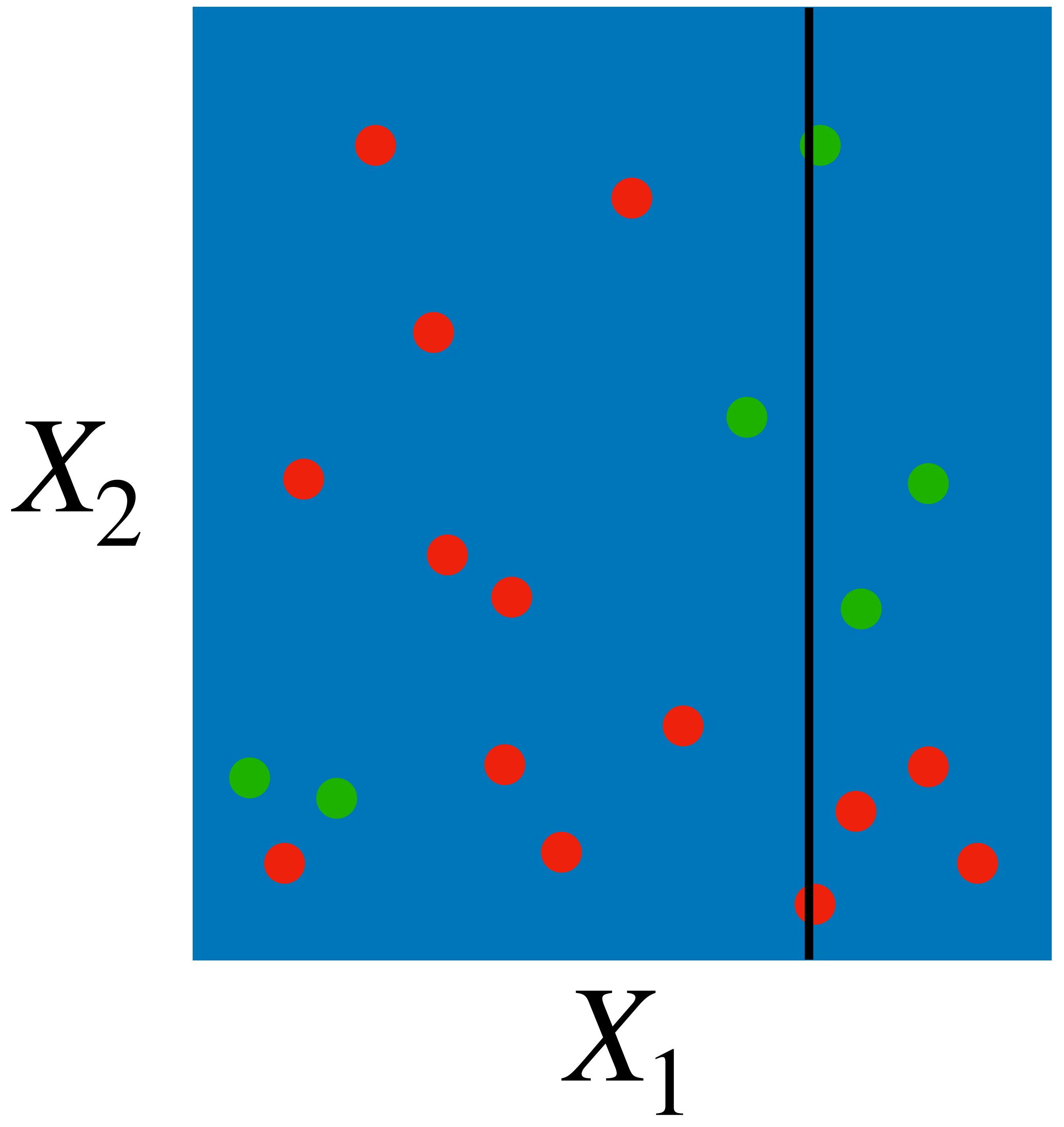

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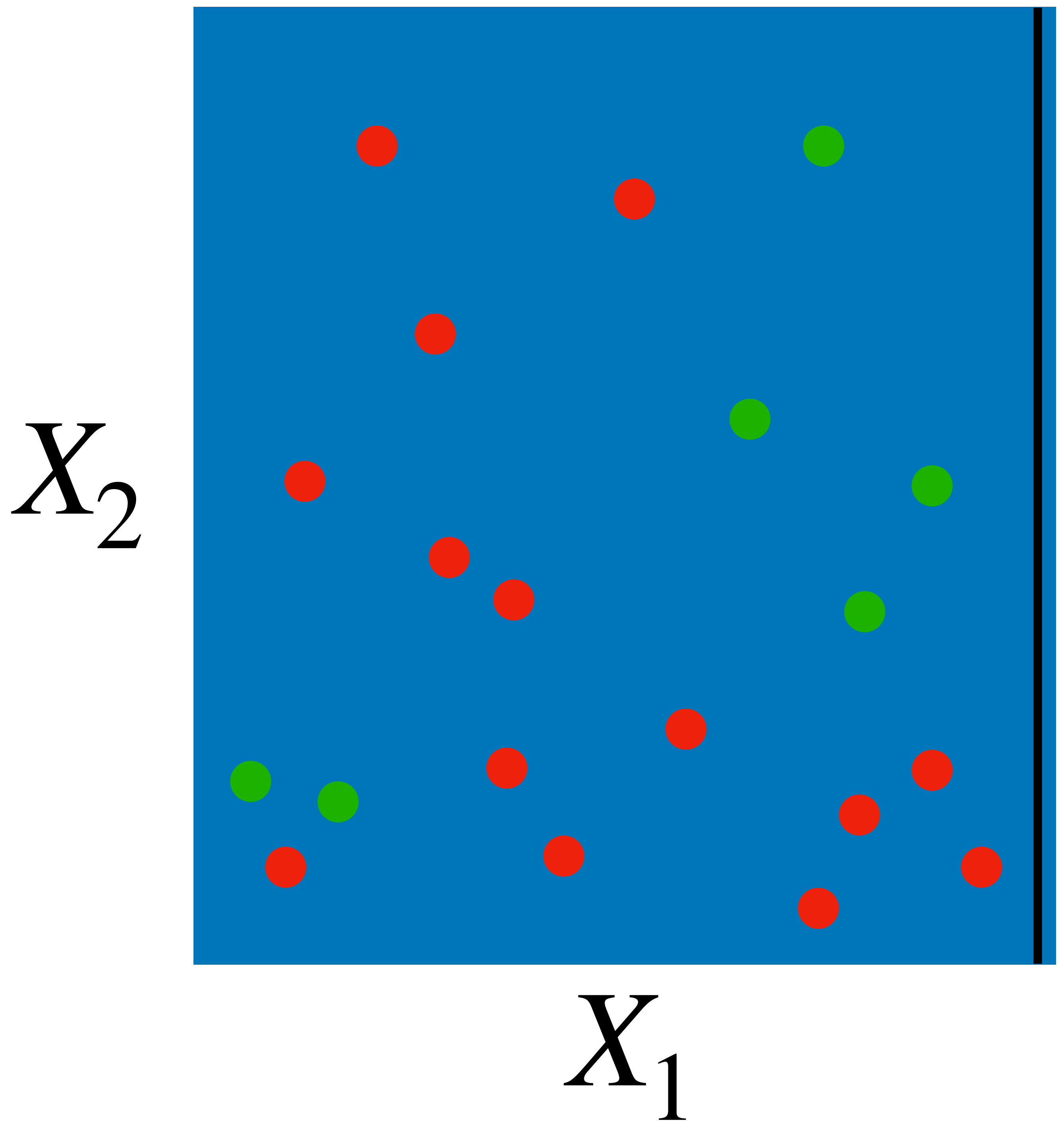

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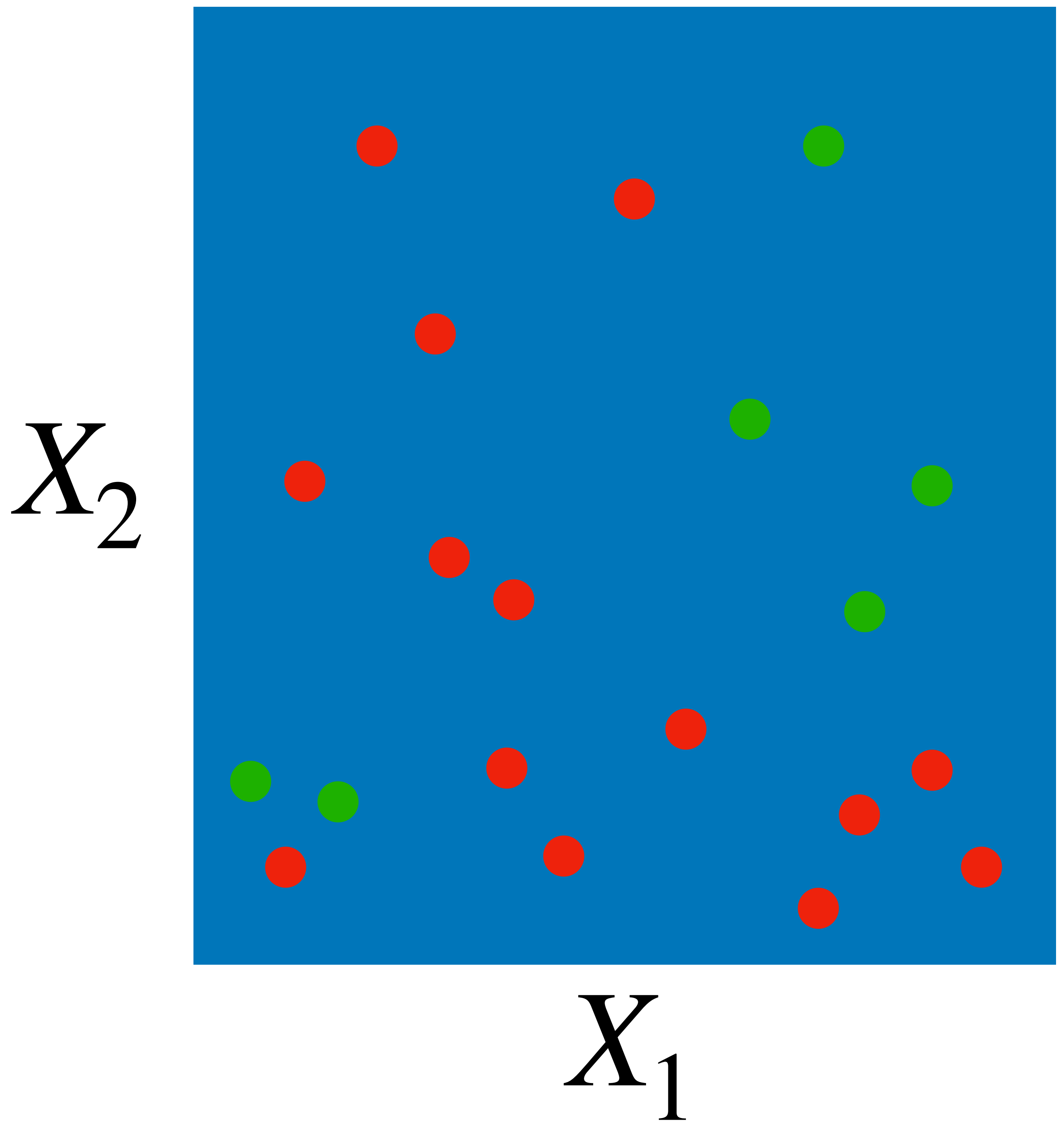

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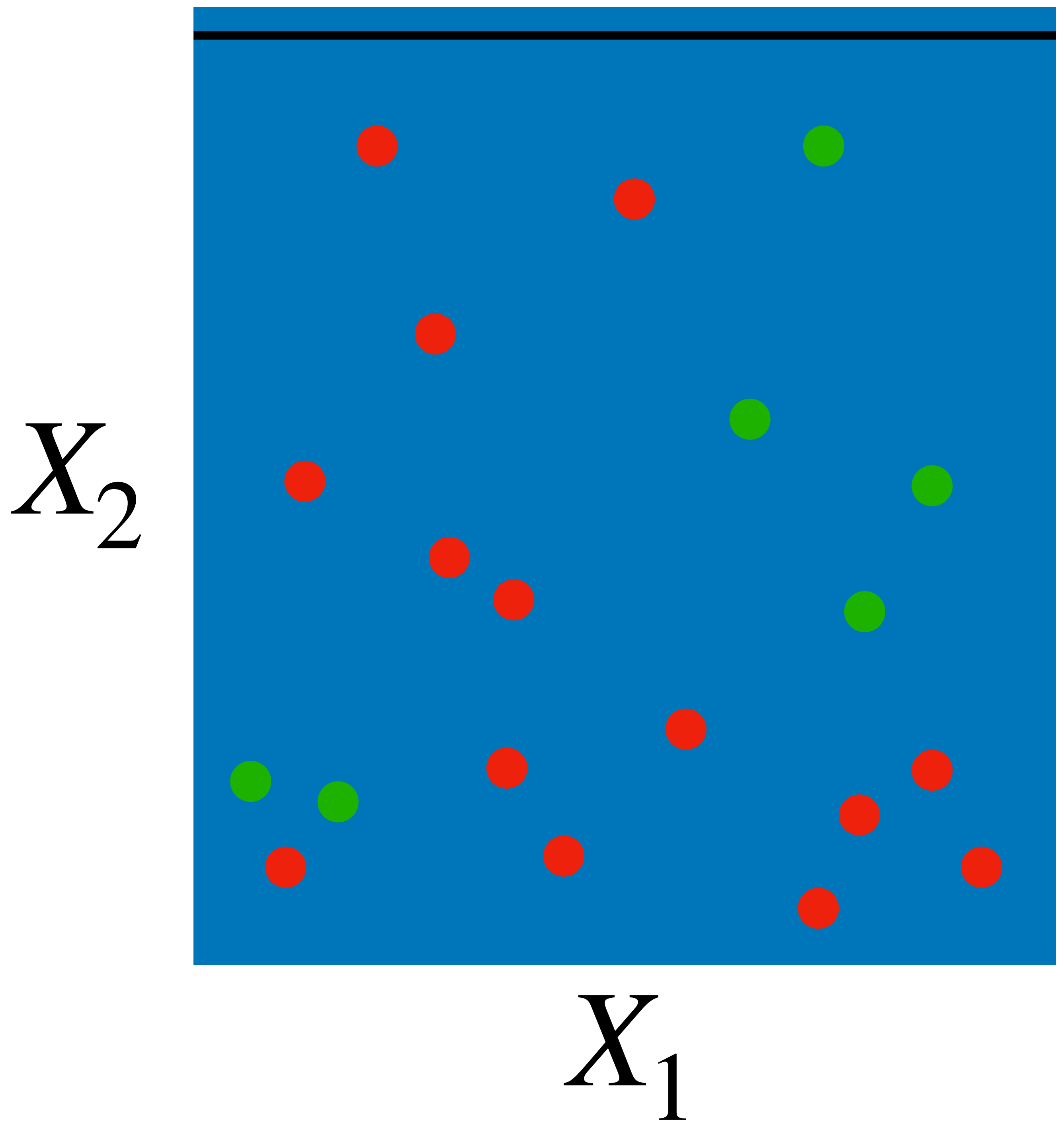

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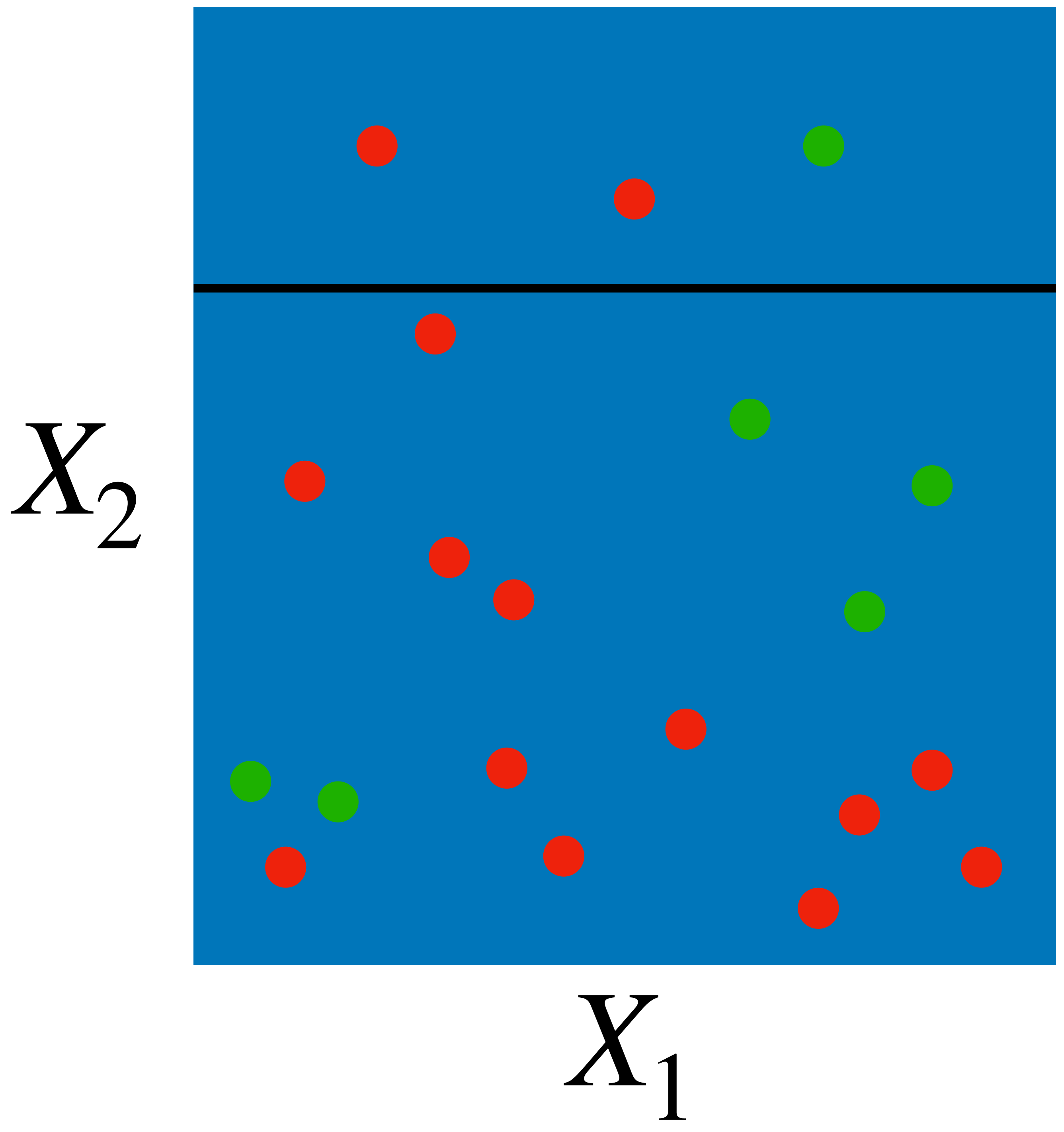

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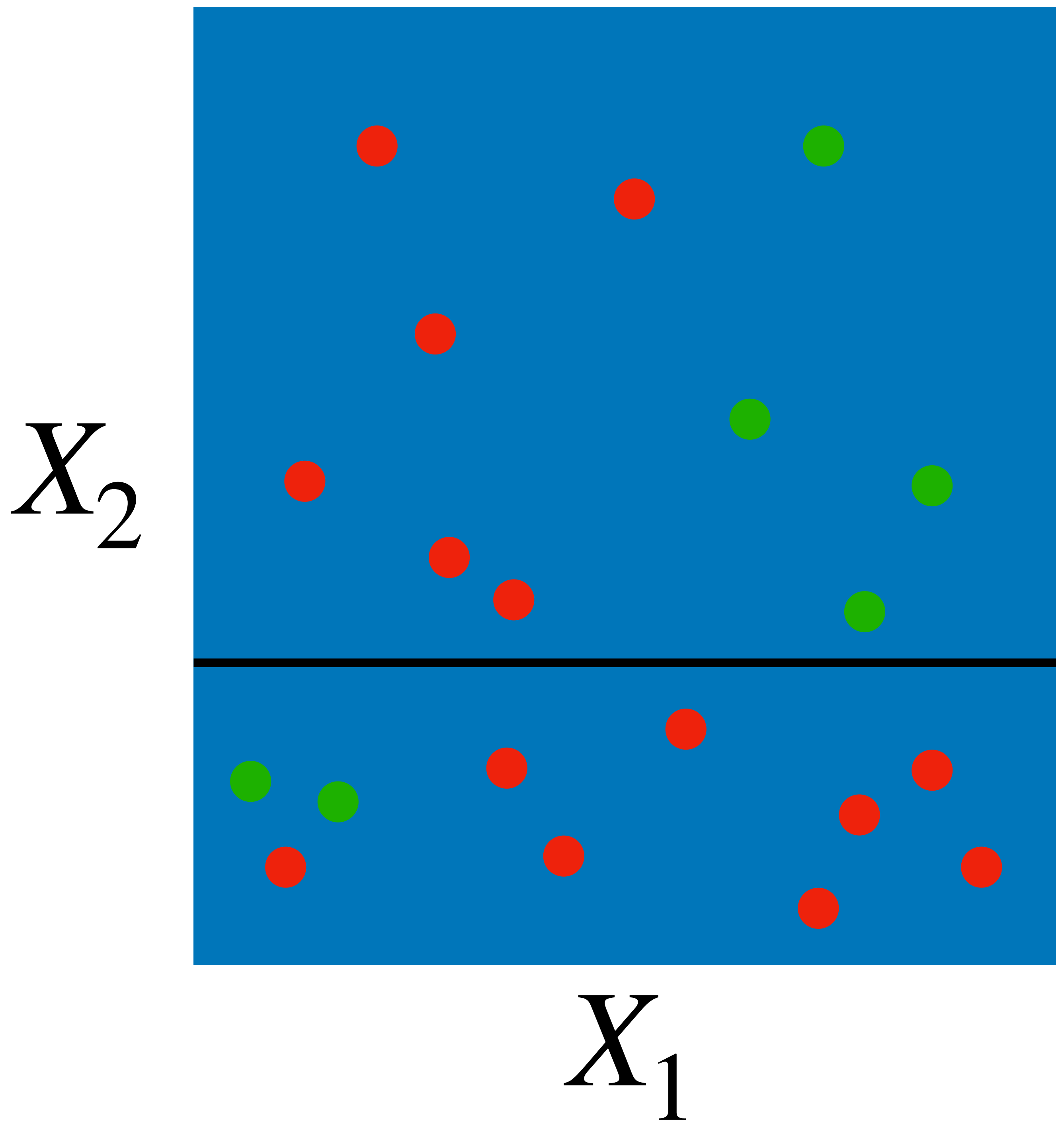

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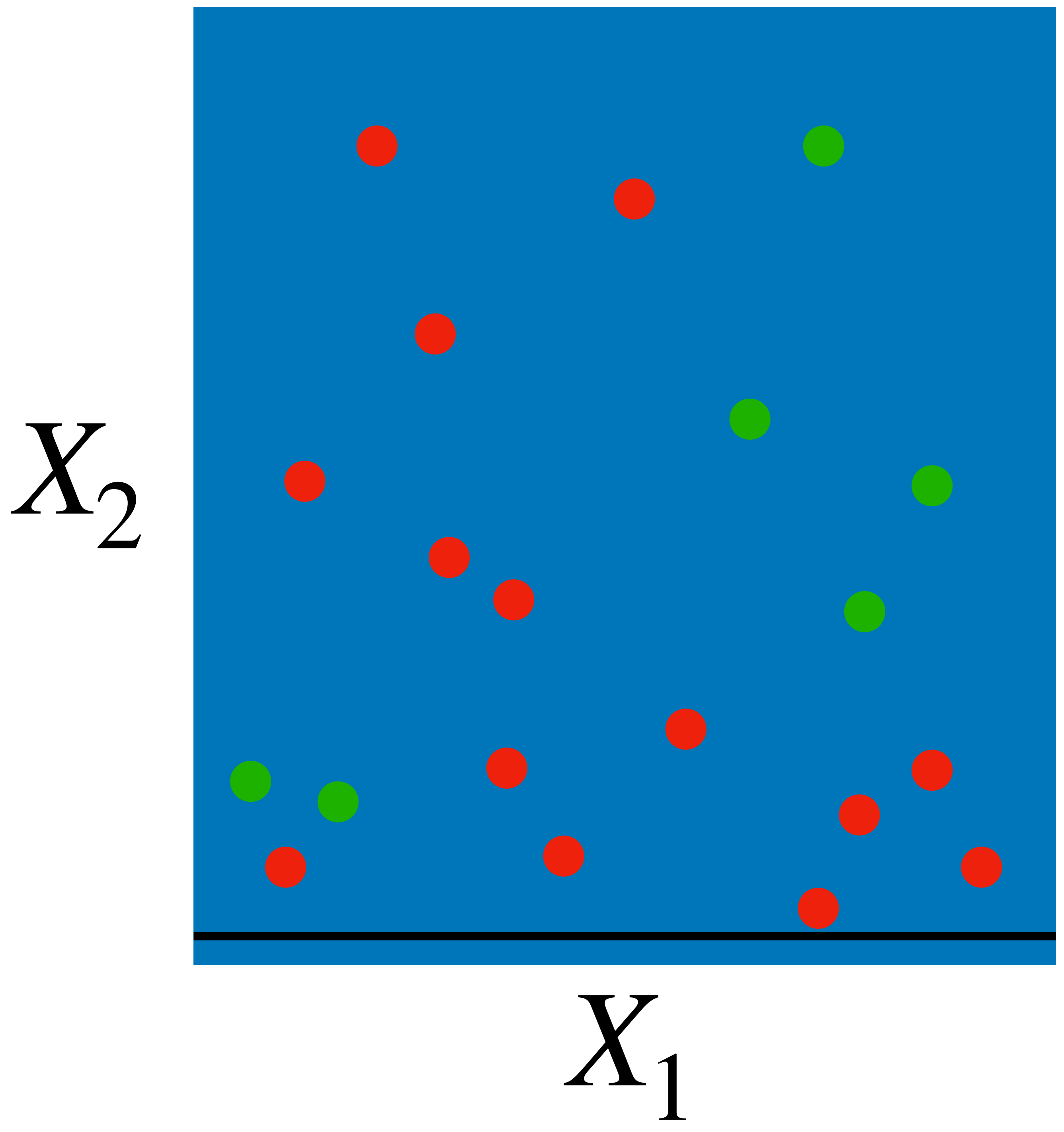

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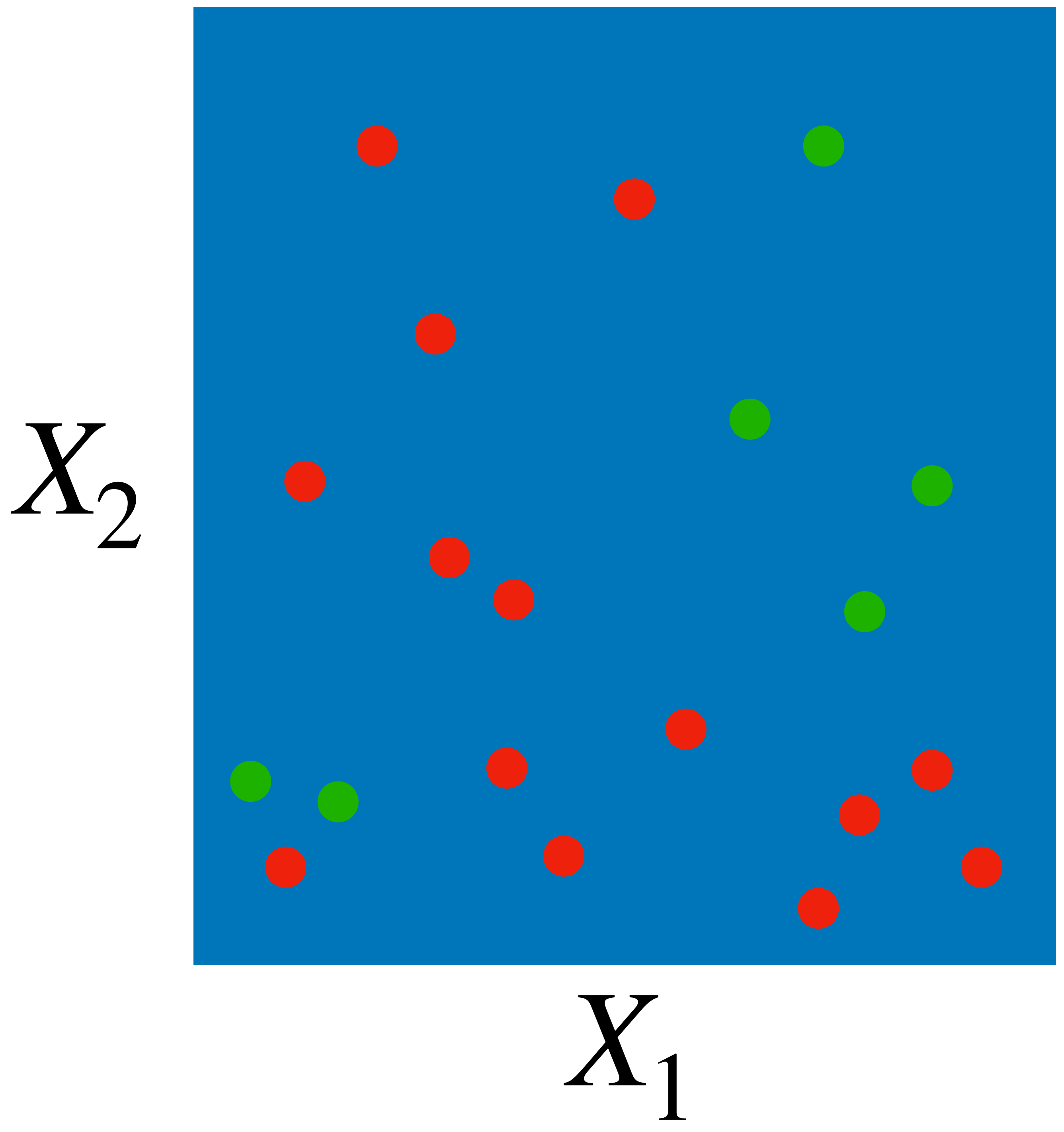

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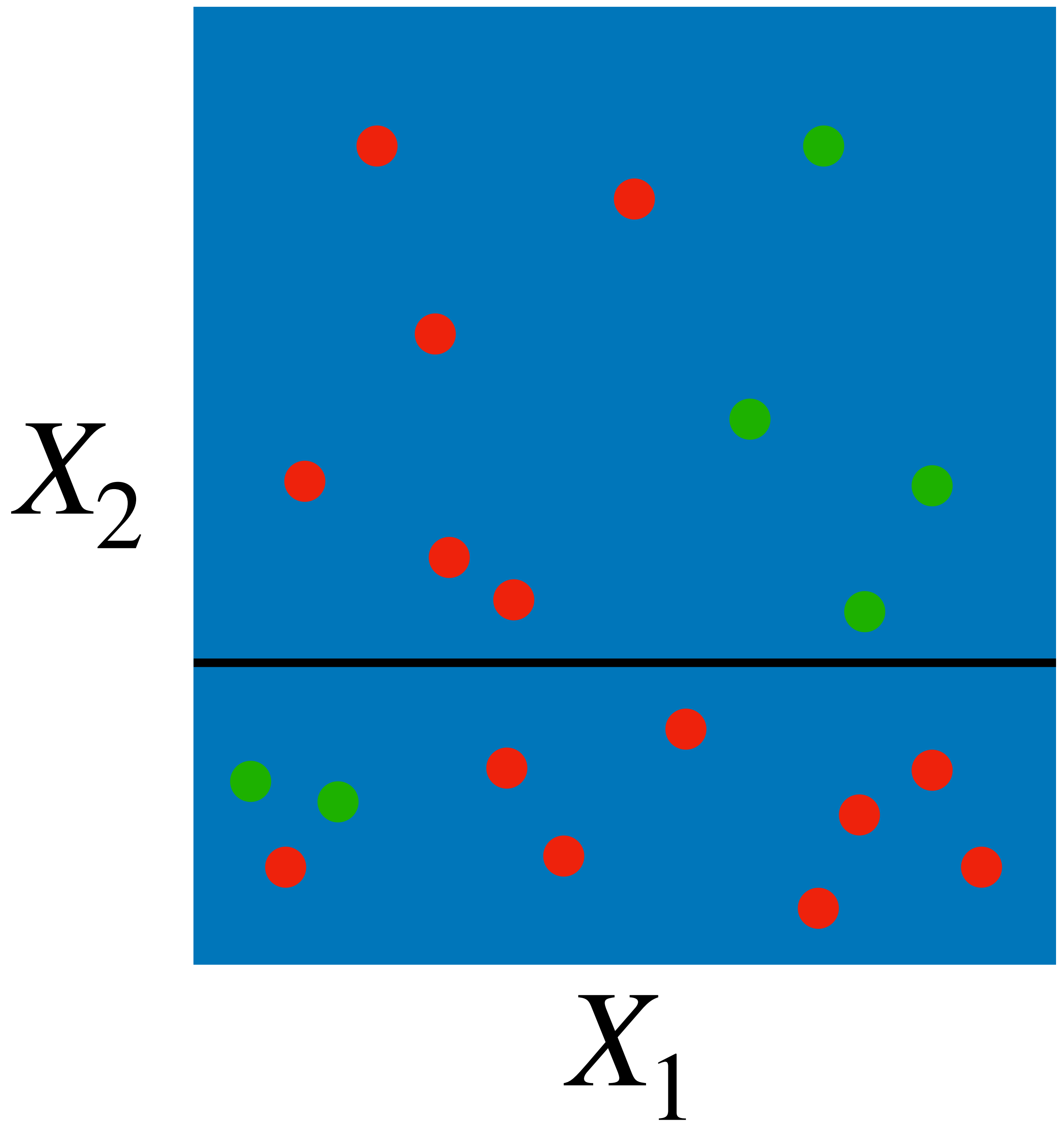

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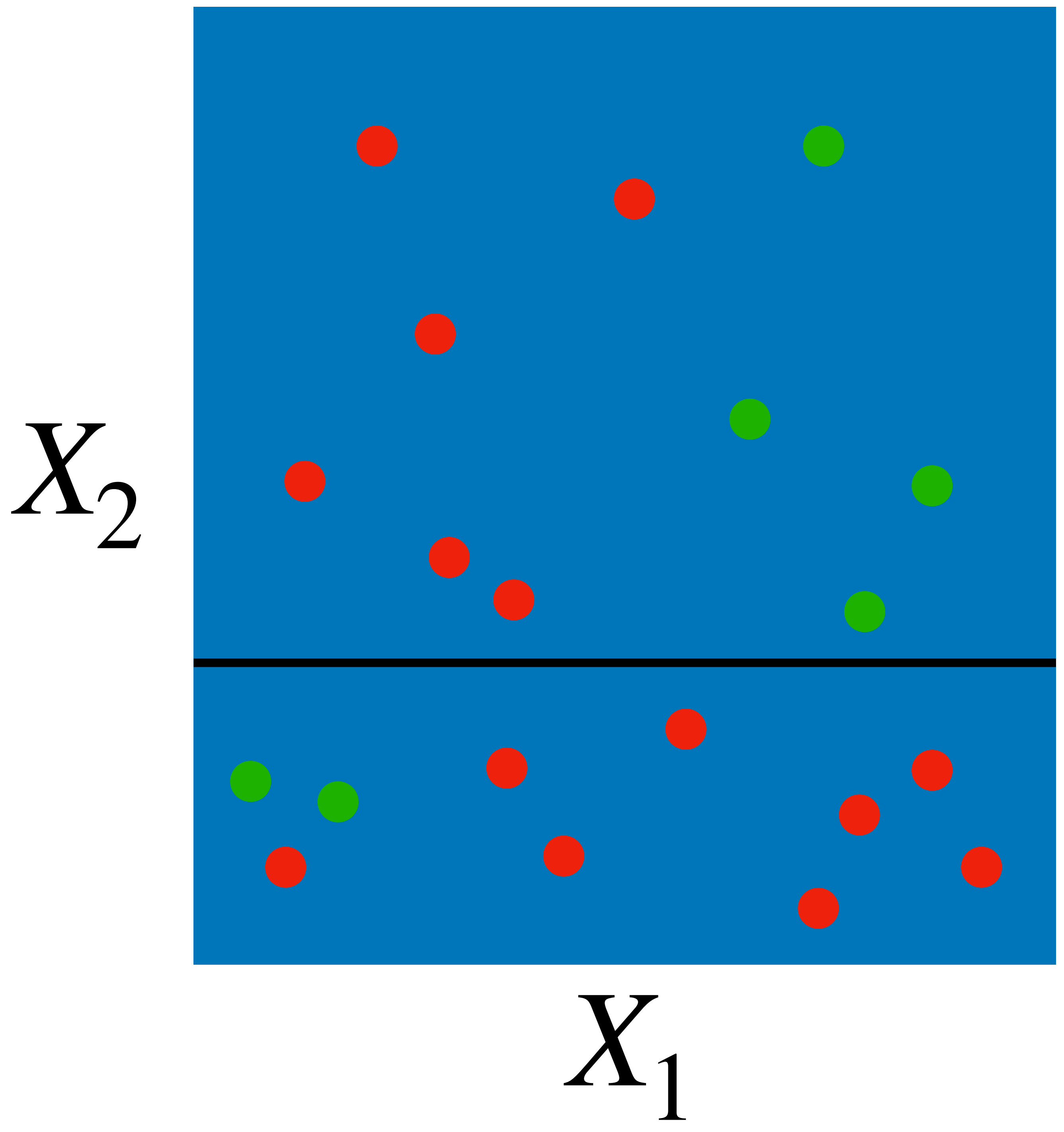

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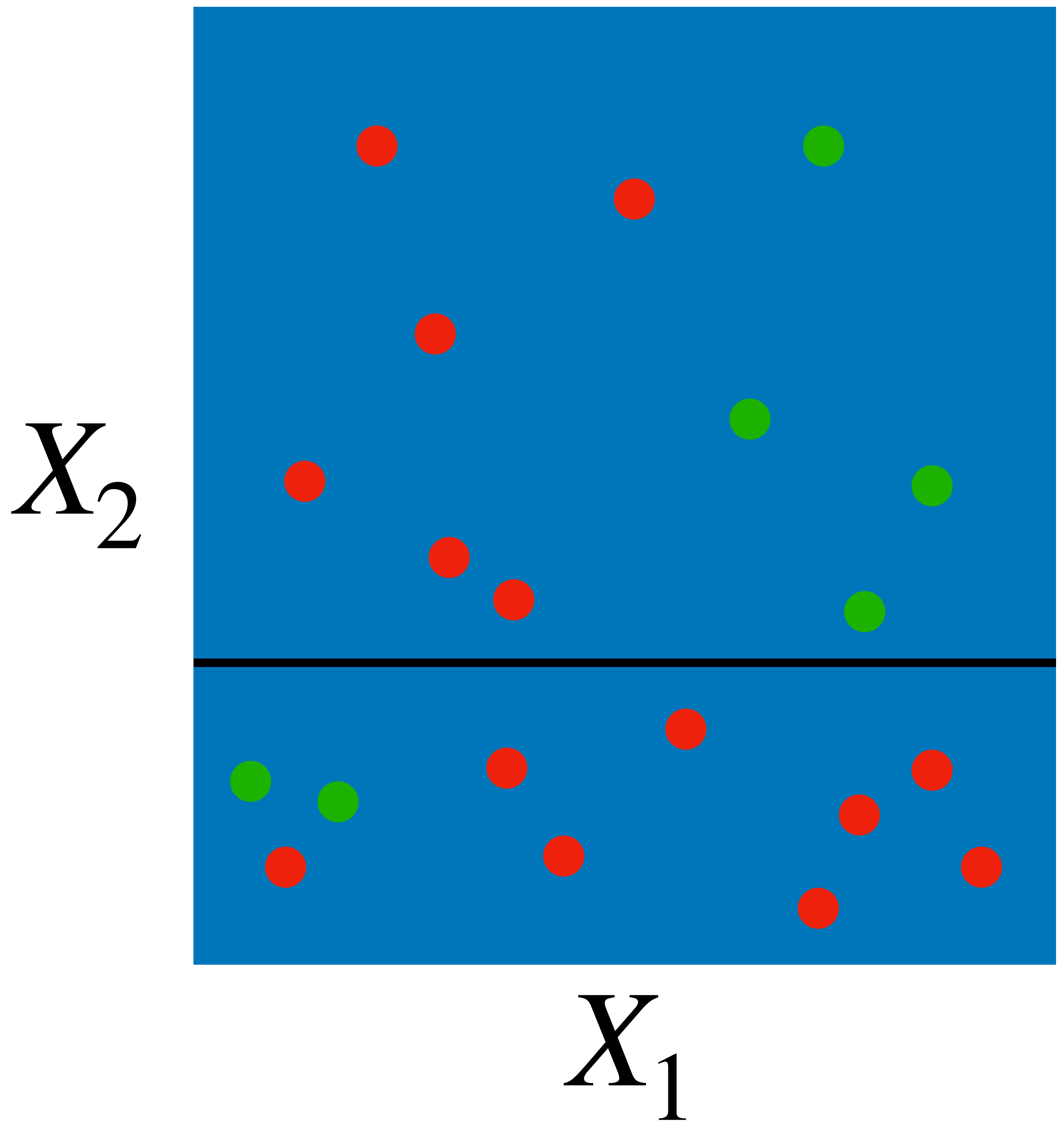

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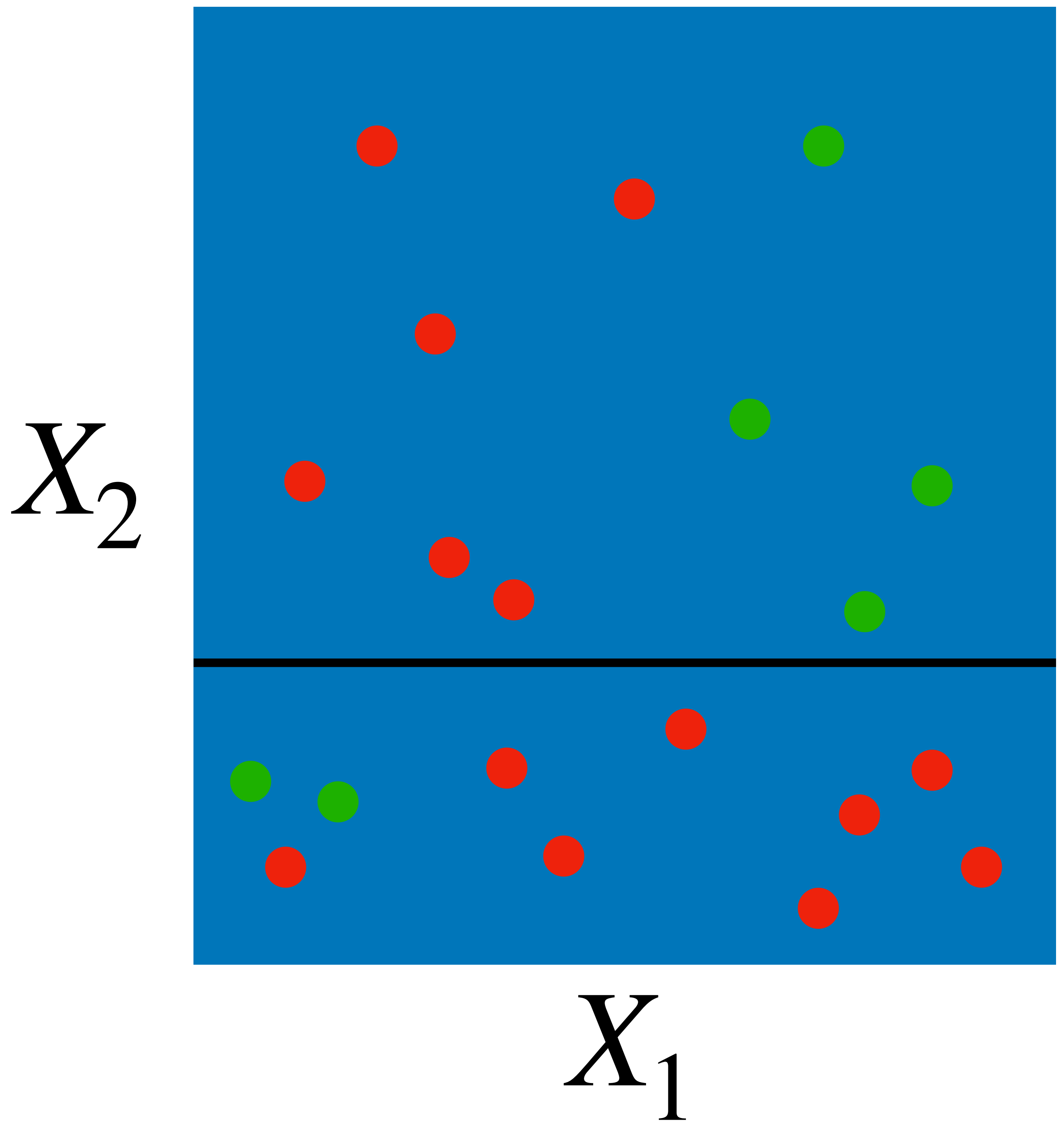

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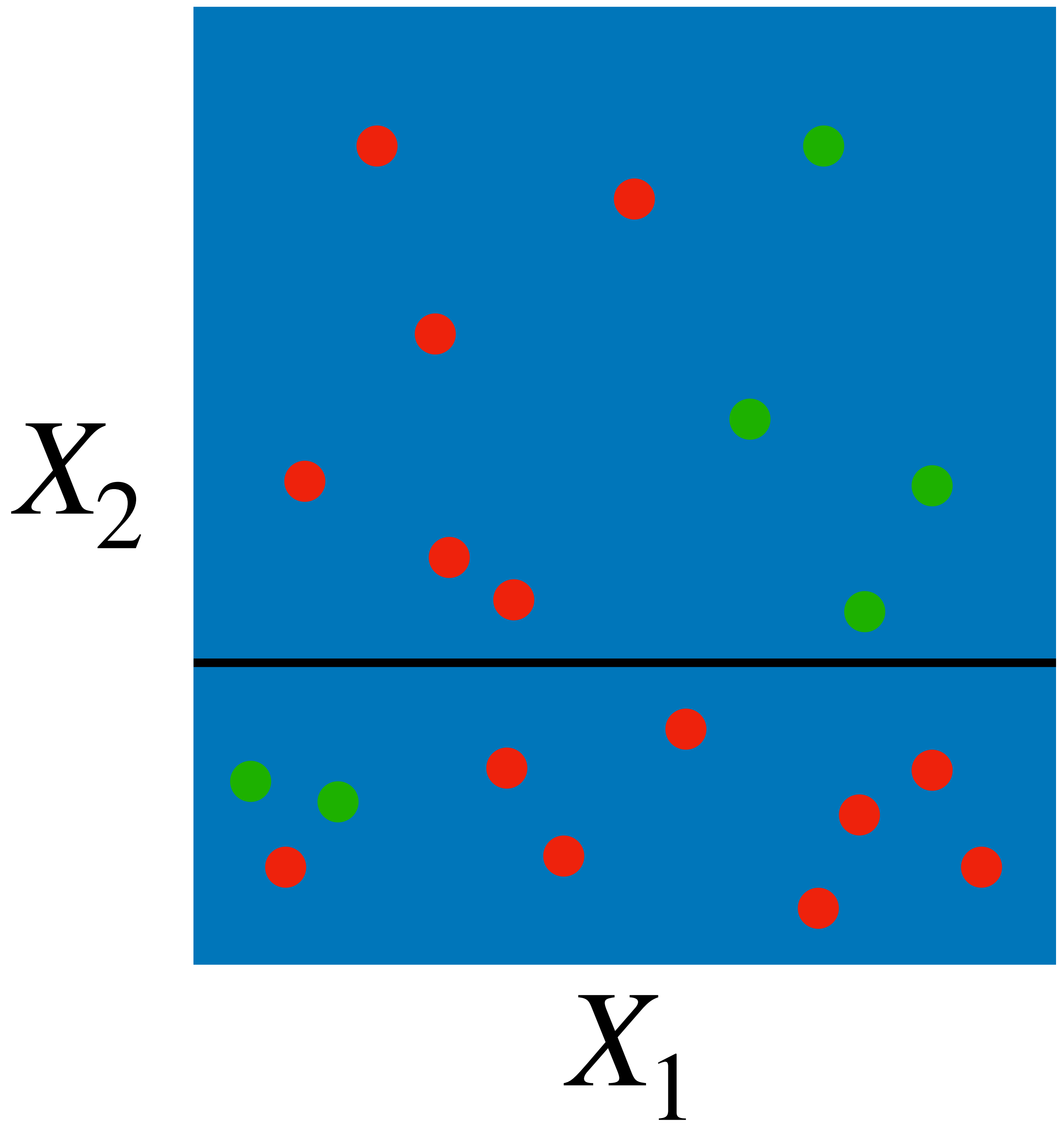

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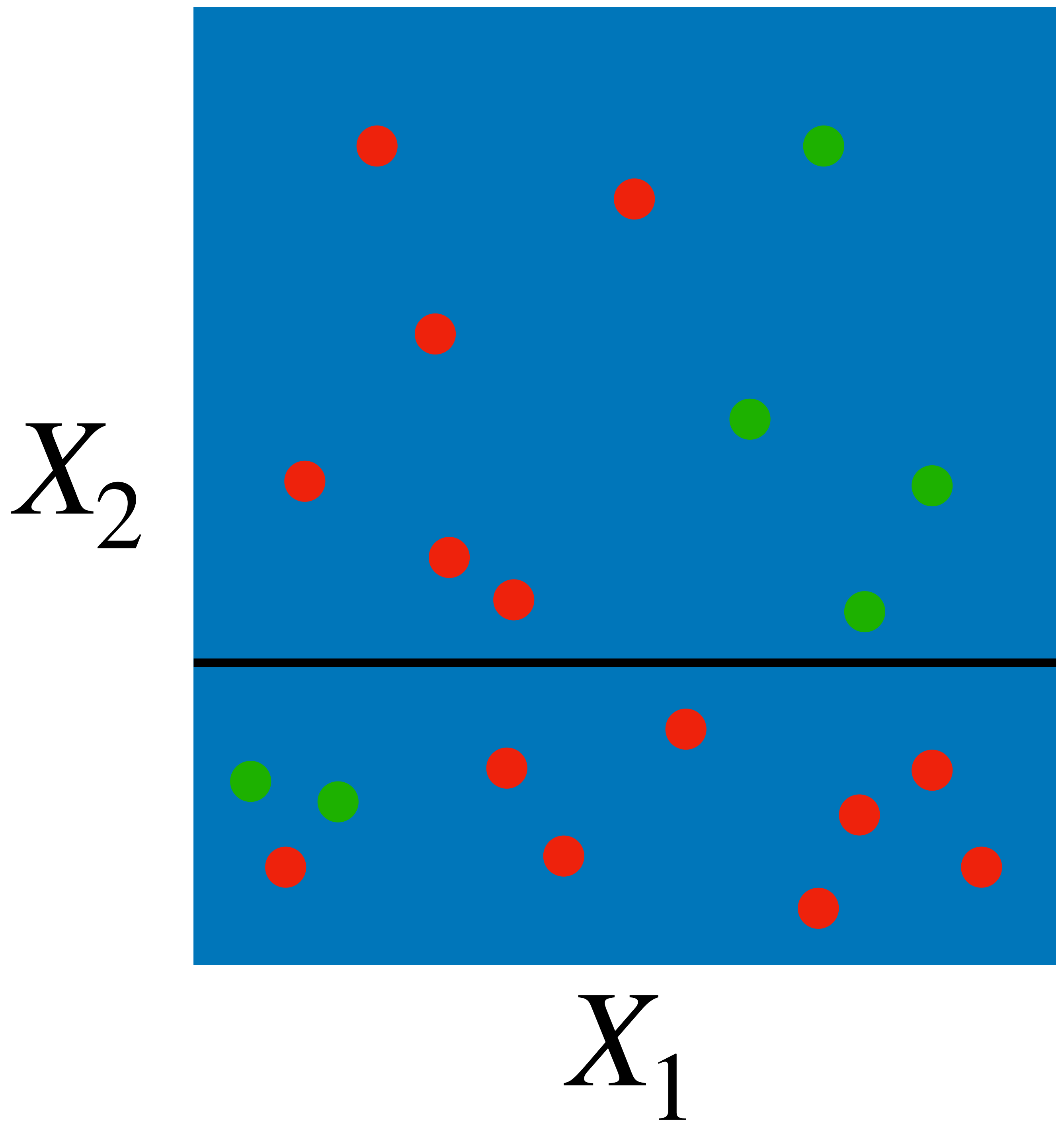

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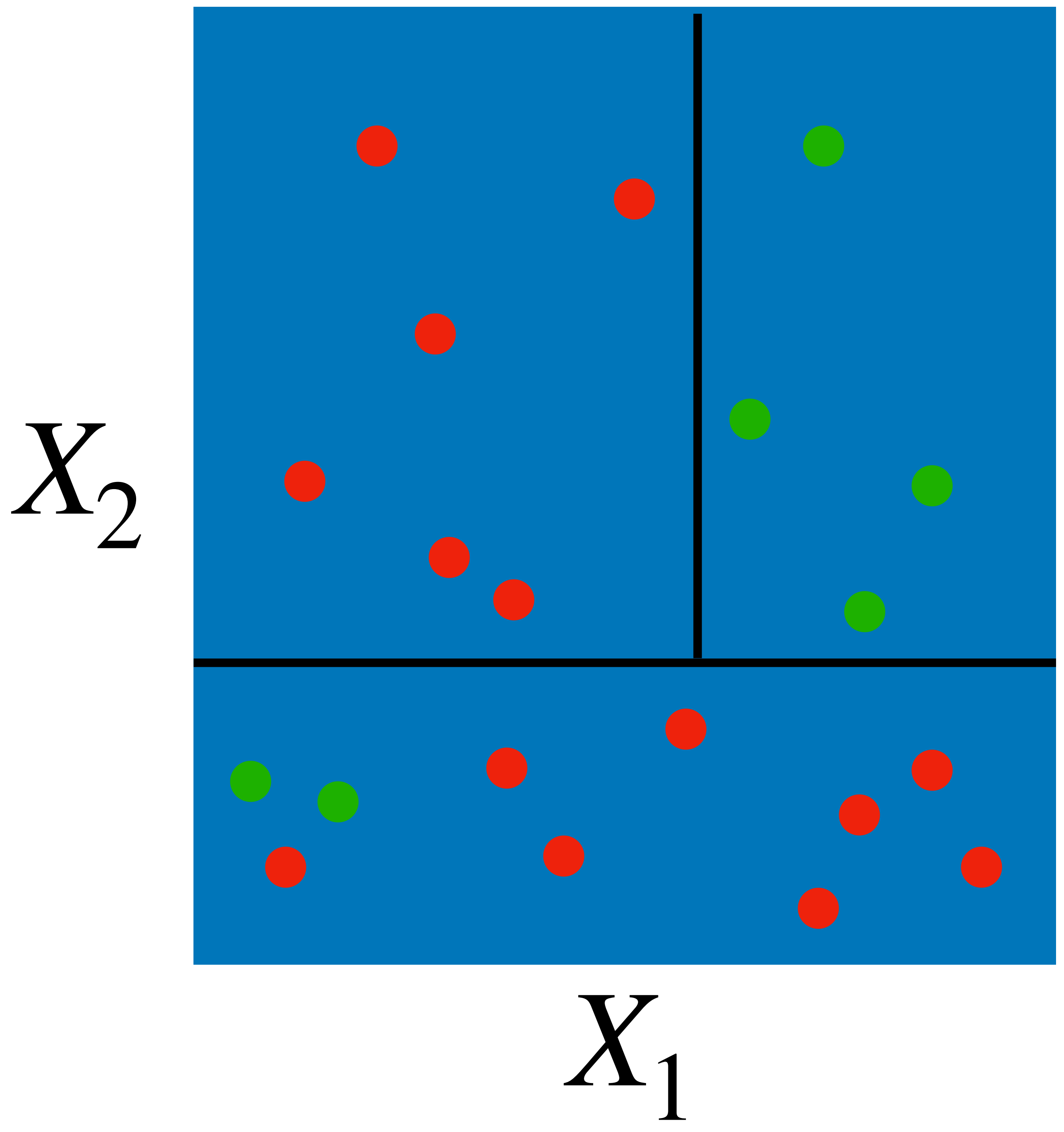

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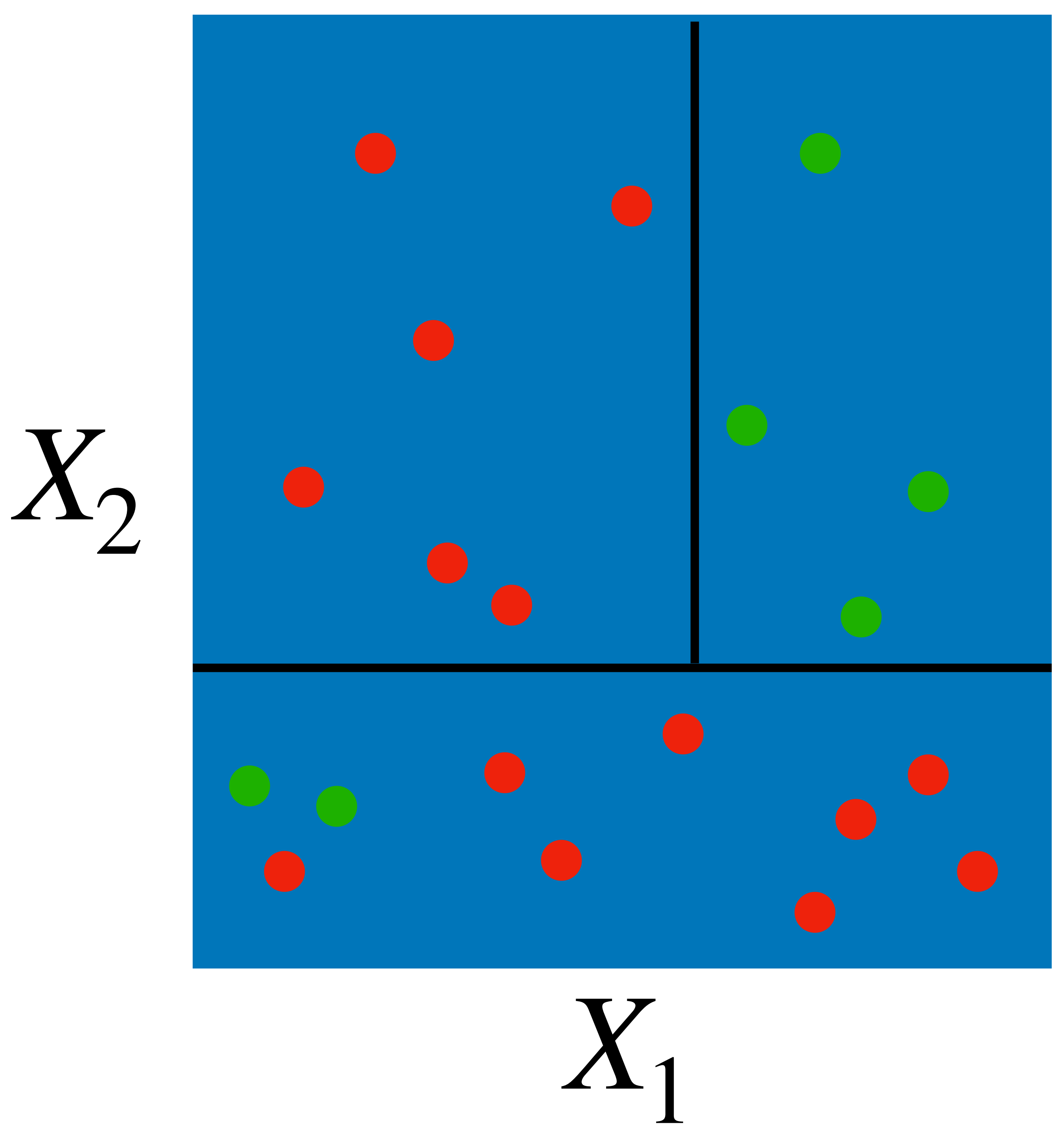

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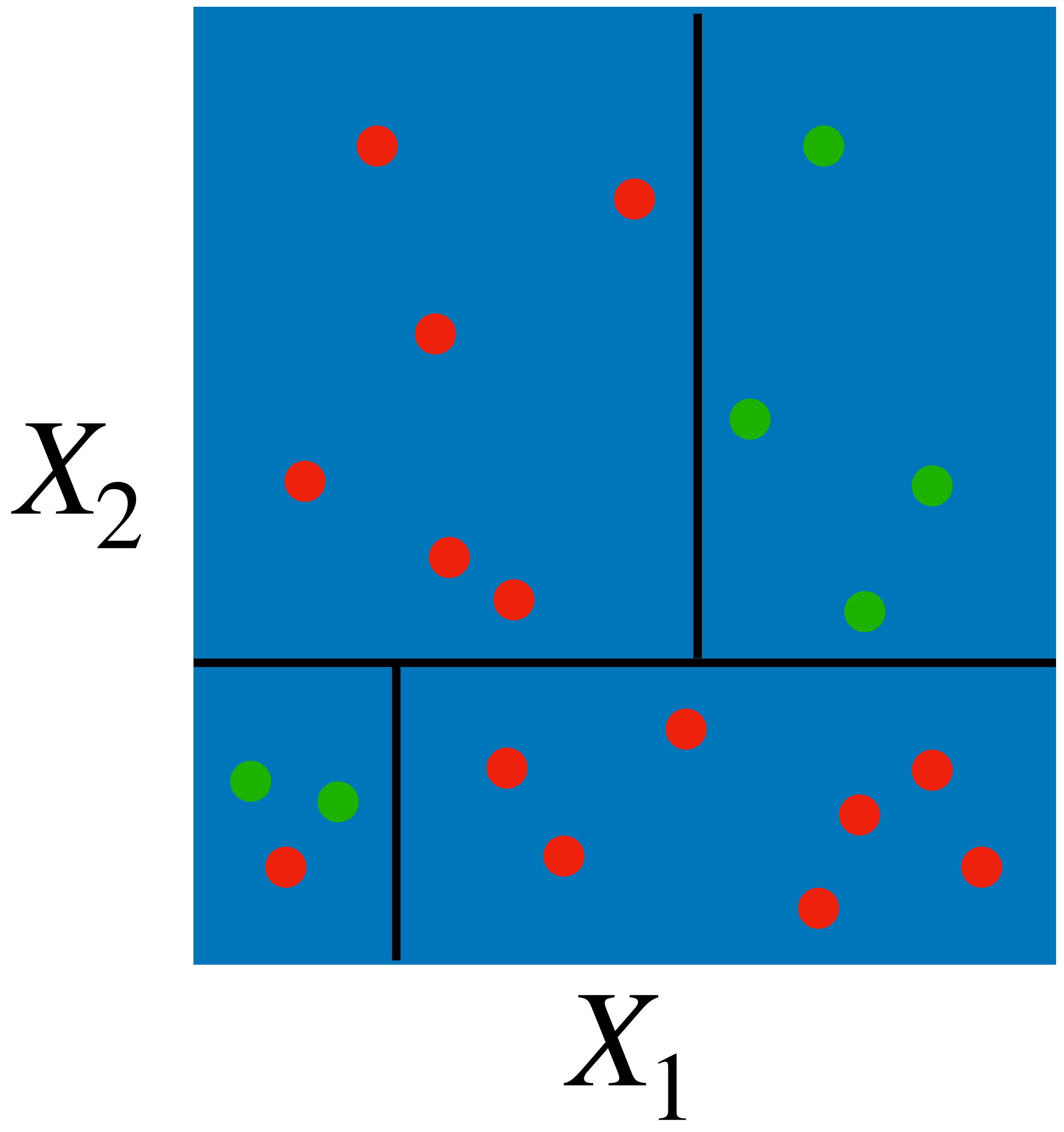
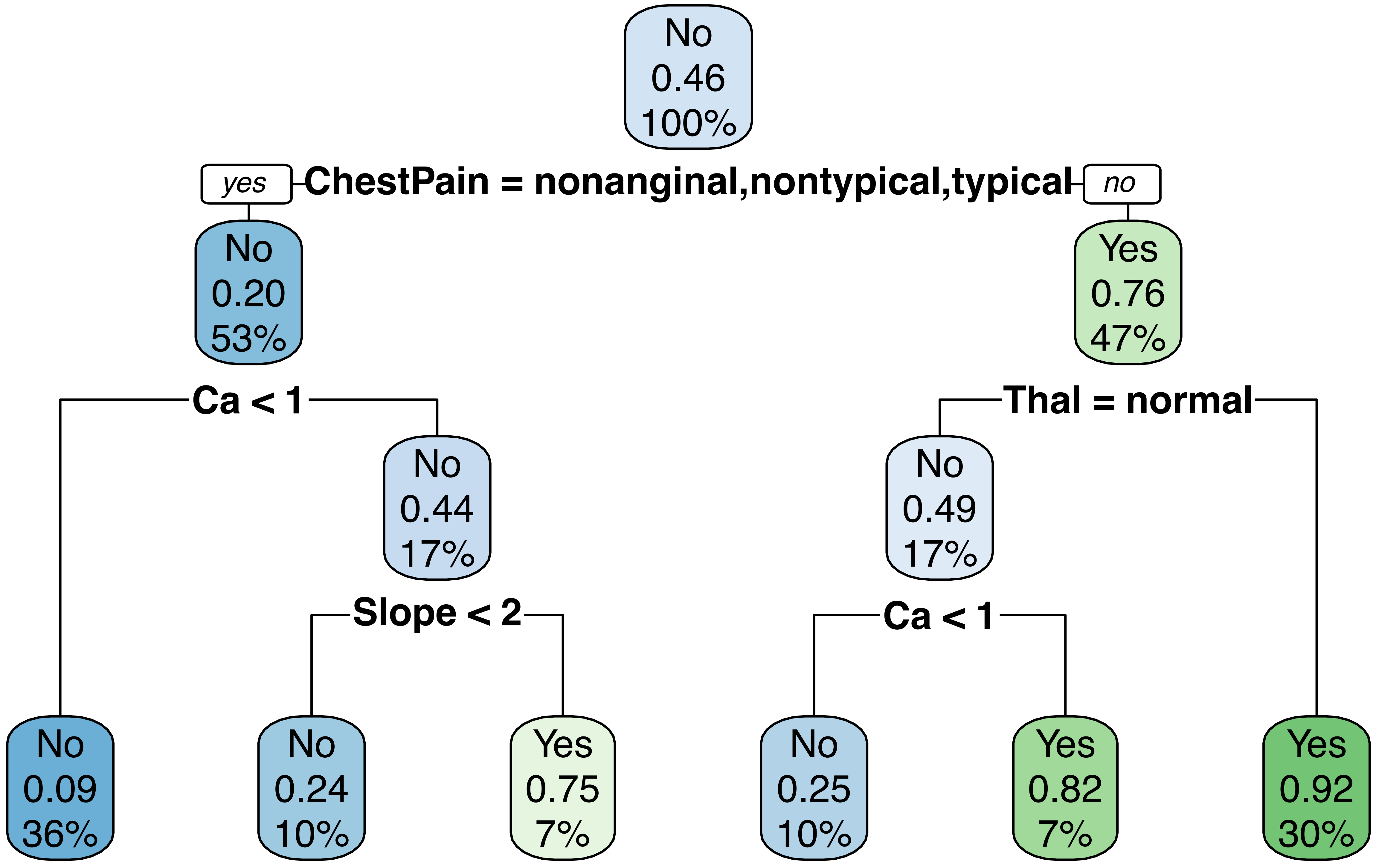


Training a classification tree

Final output

Example: Heart disease data set.

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



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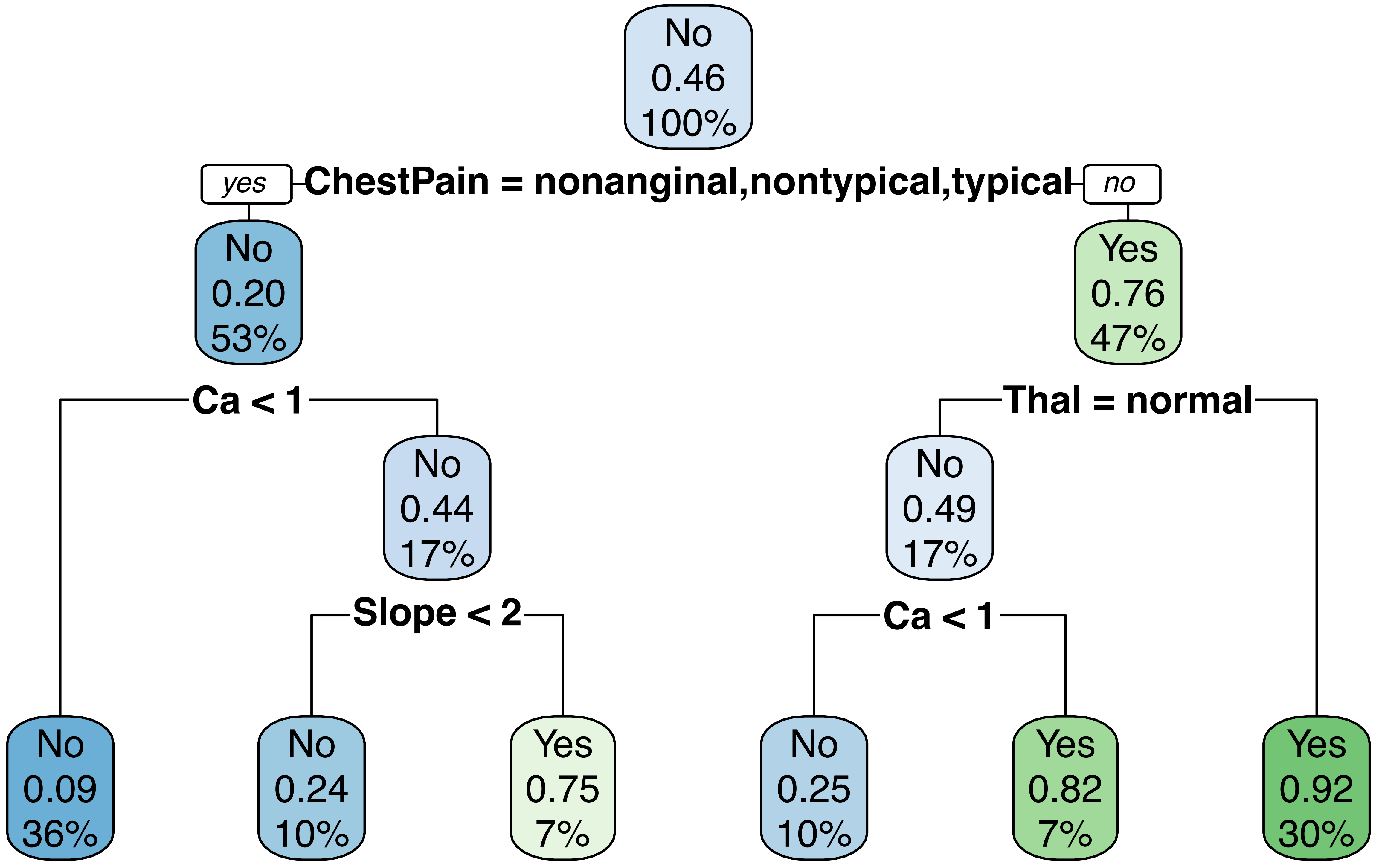

Note: Classification trees extend seamlessly to more than two classes!

Tree-based models versus linear models

Which perform better?

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Neither tree-based nor linear models dominate the other.

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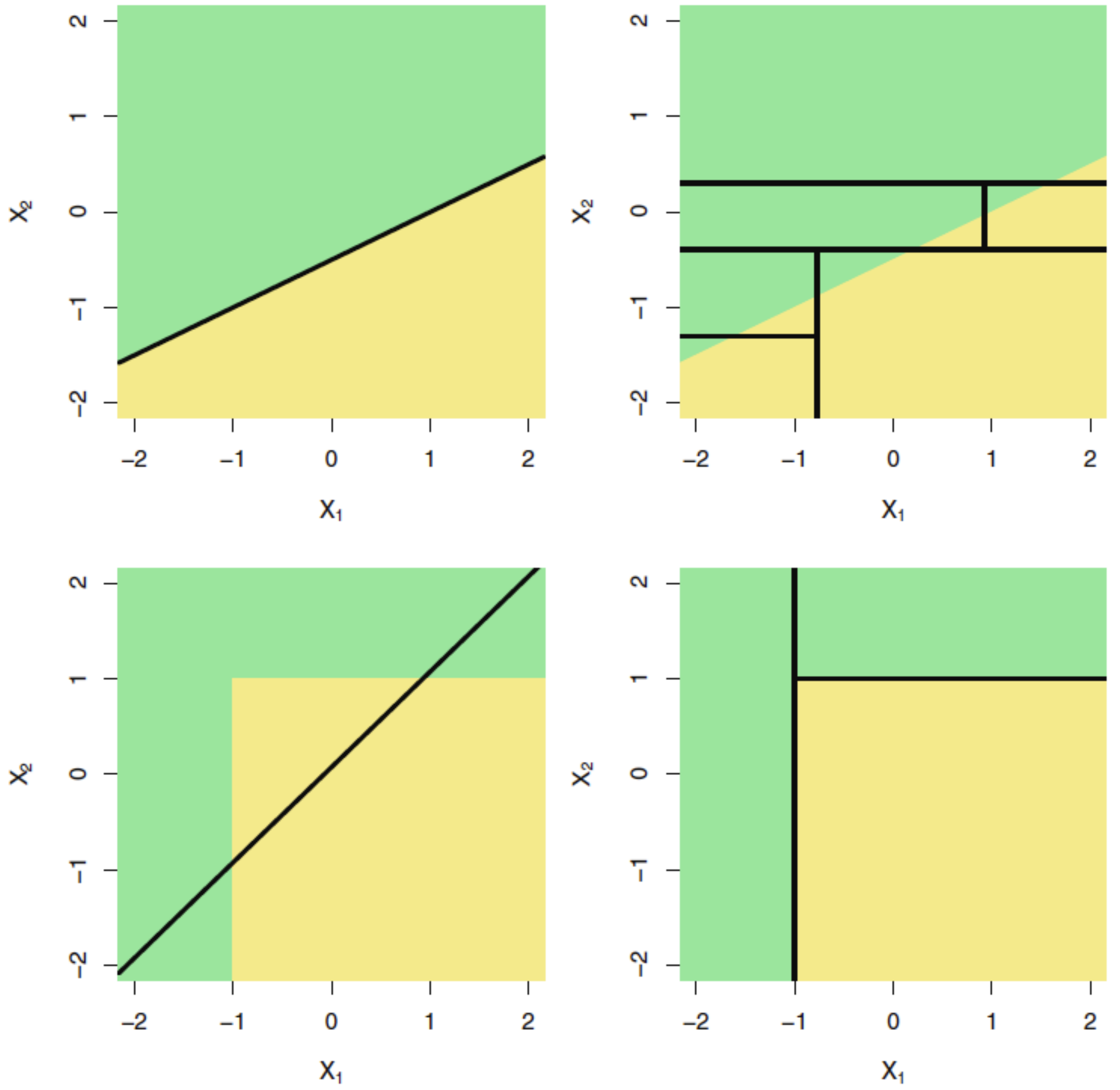

Classification based on two features (colors indicate the two classes).

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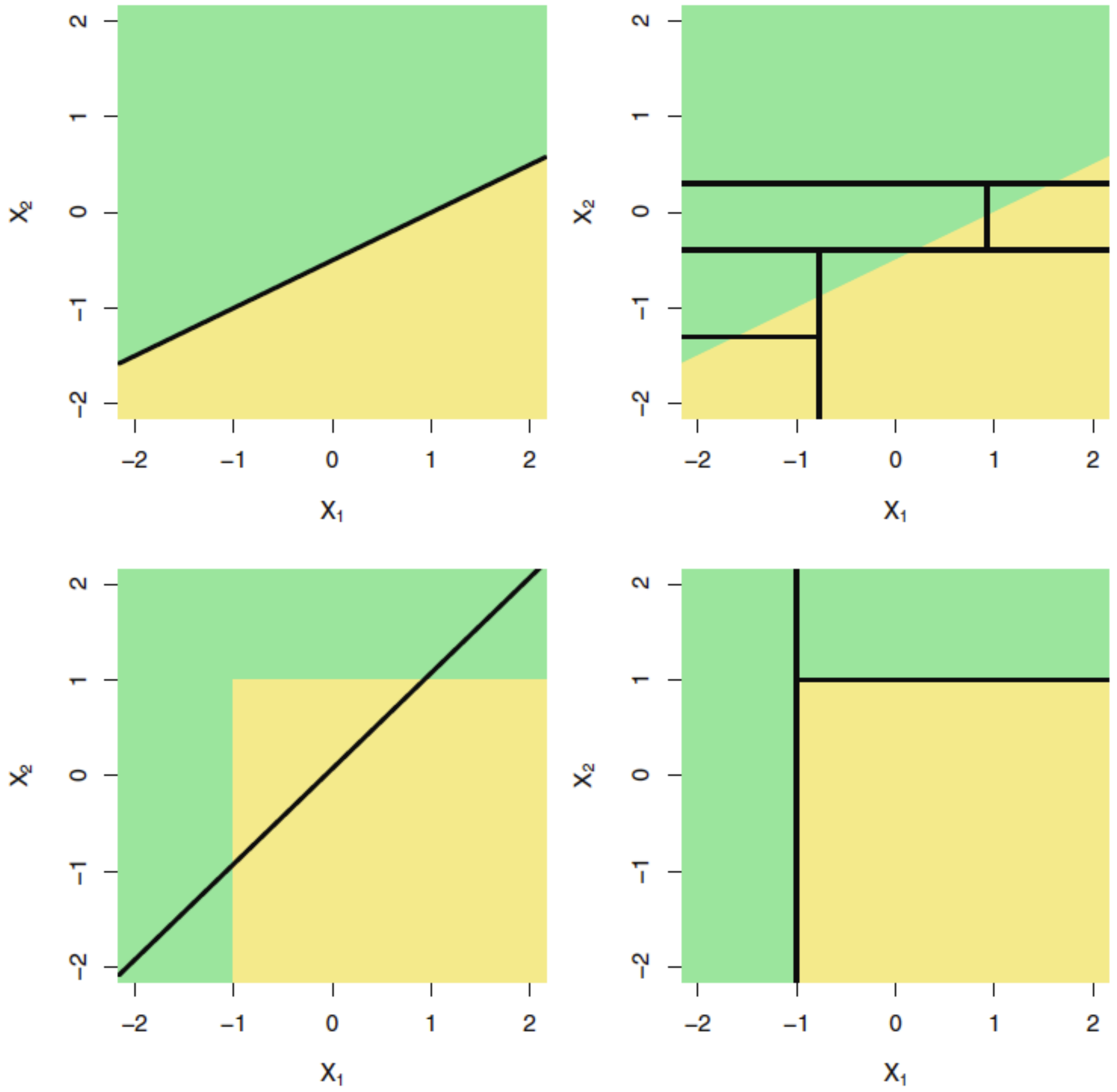
E.g. for classification:

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



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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 error, respectively.