Growing decision trees

STAT 4710

October 27, 2022

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 $\widehat{\beta}_0 + \widehat{\beta}_1 X_1 + \cdots + \widehat{\beta}_{p-1} X_{p-1}$:

- Linear regression
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In Unit 4 we will leave the land of linearity.

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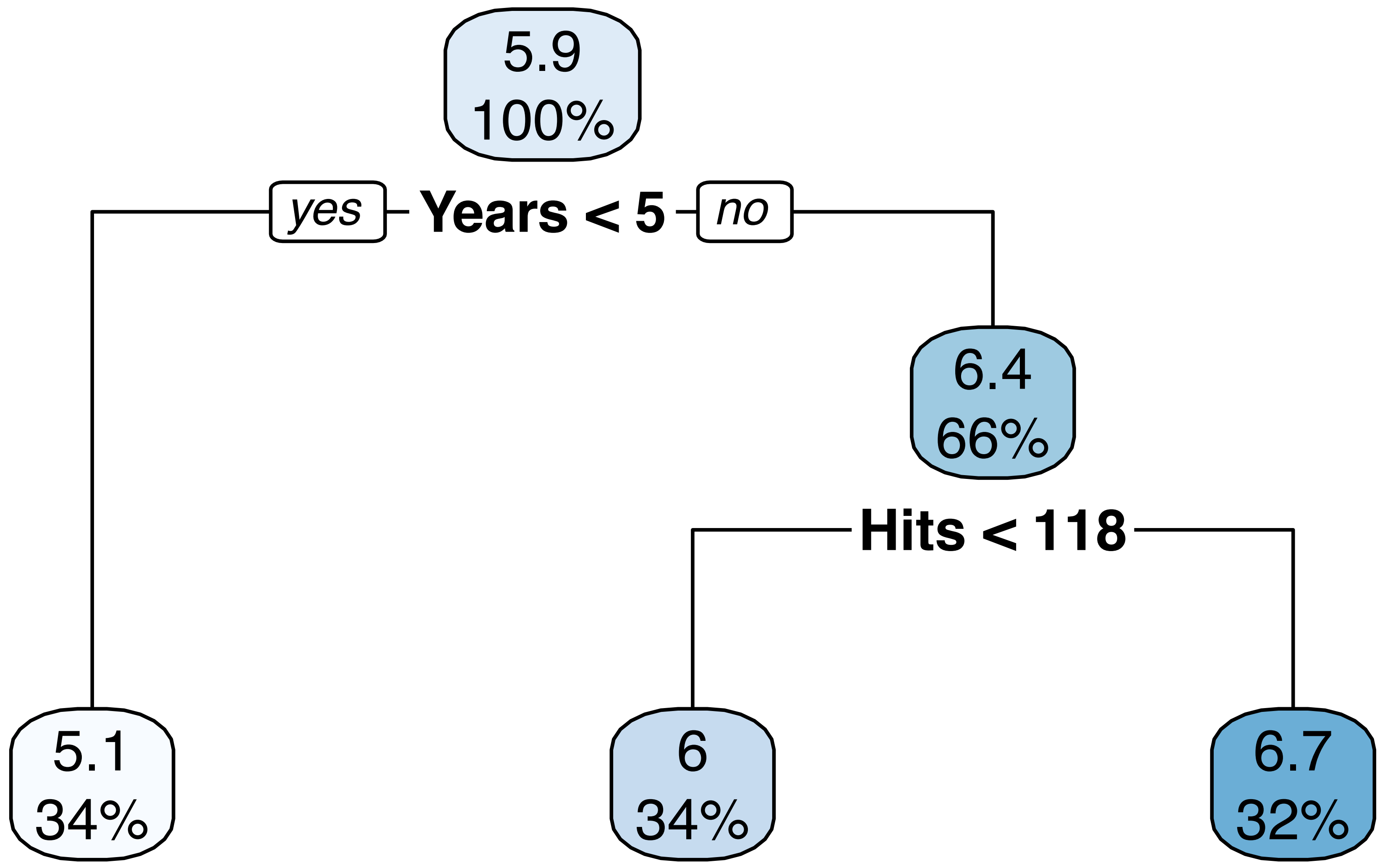

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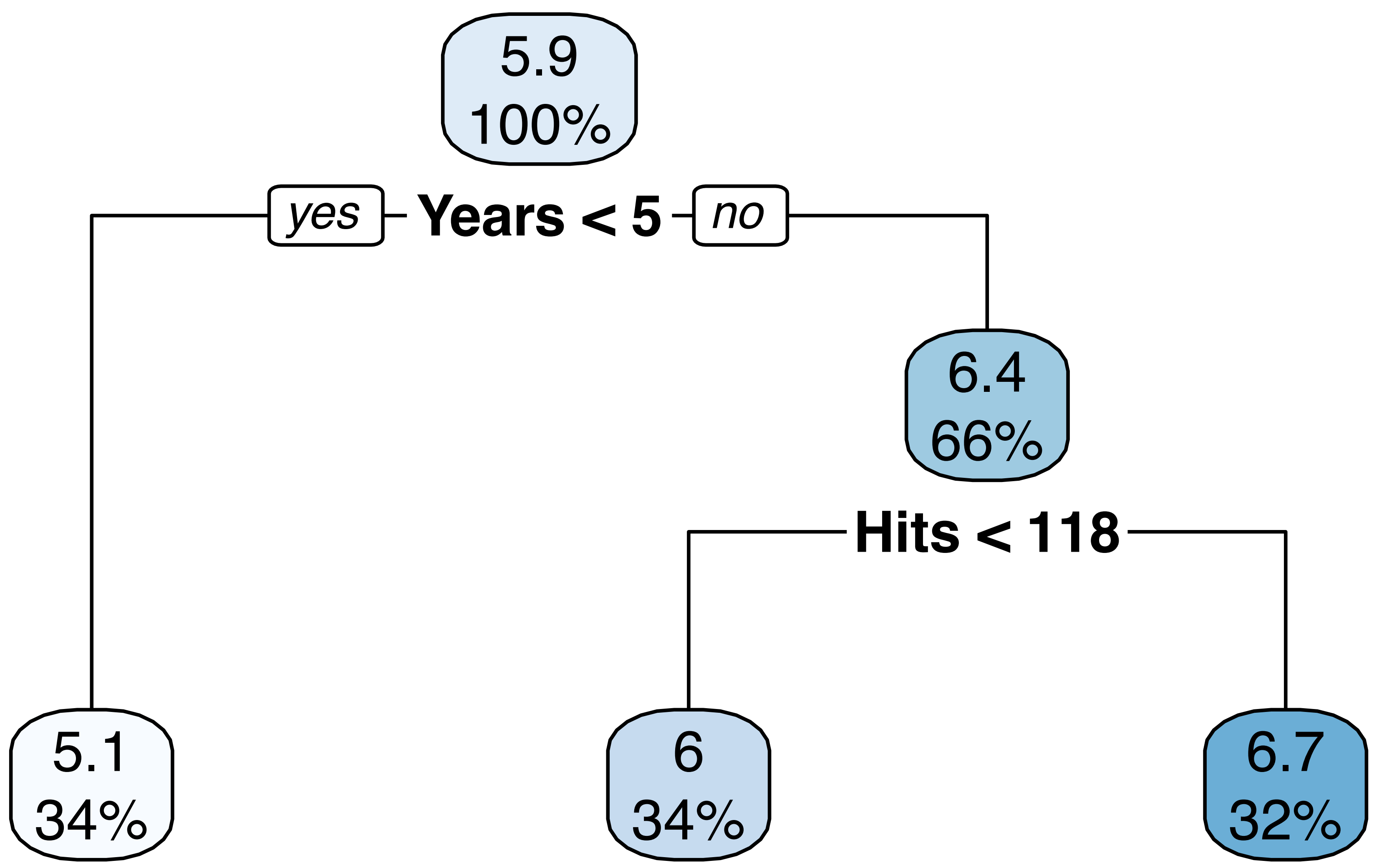
Their prediction rules can be nicely illustrated and are very interpretable.



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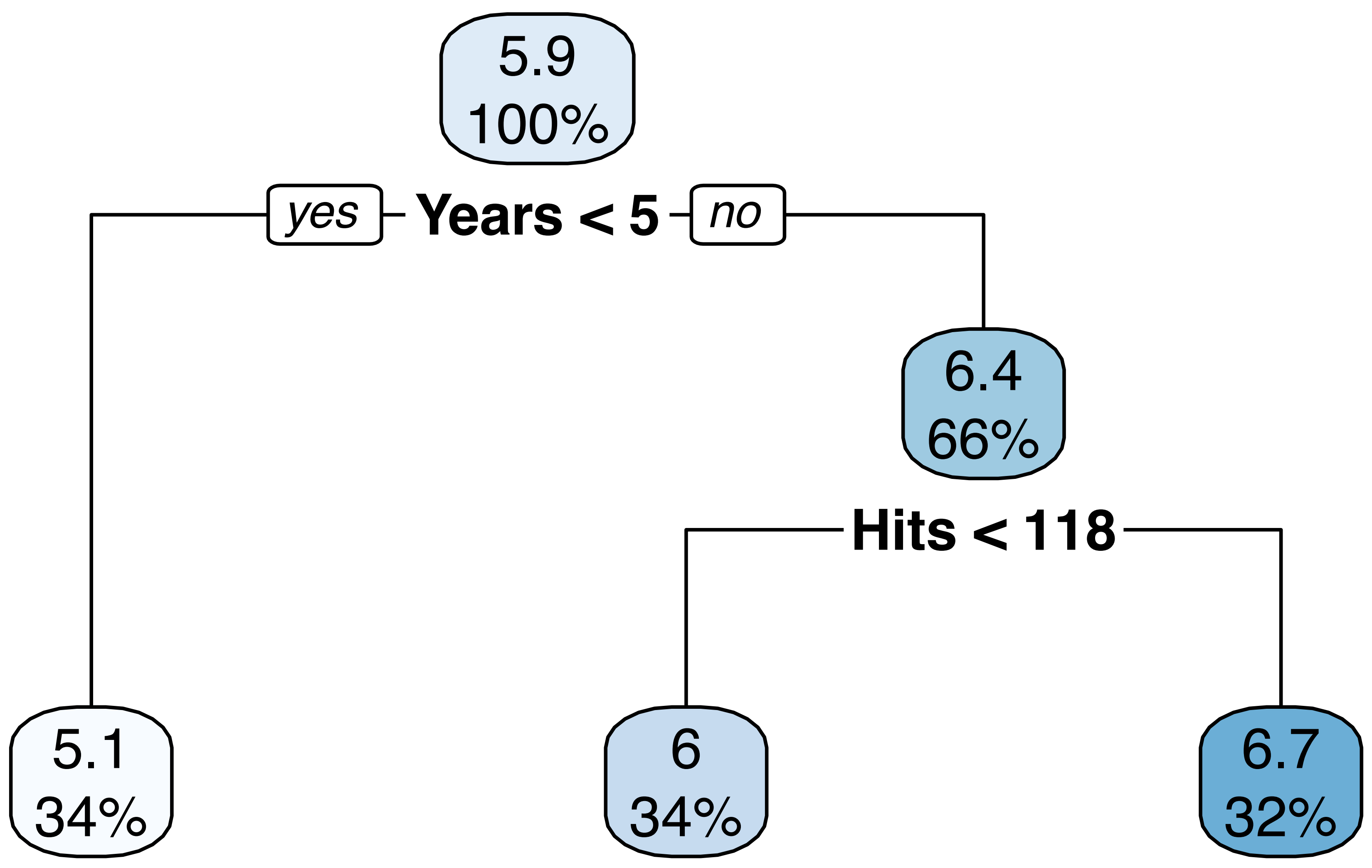

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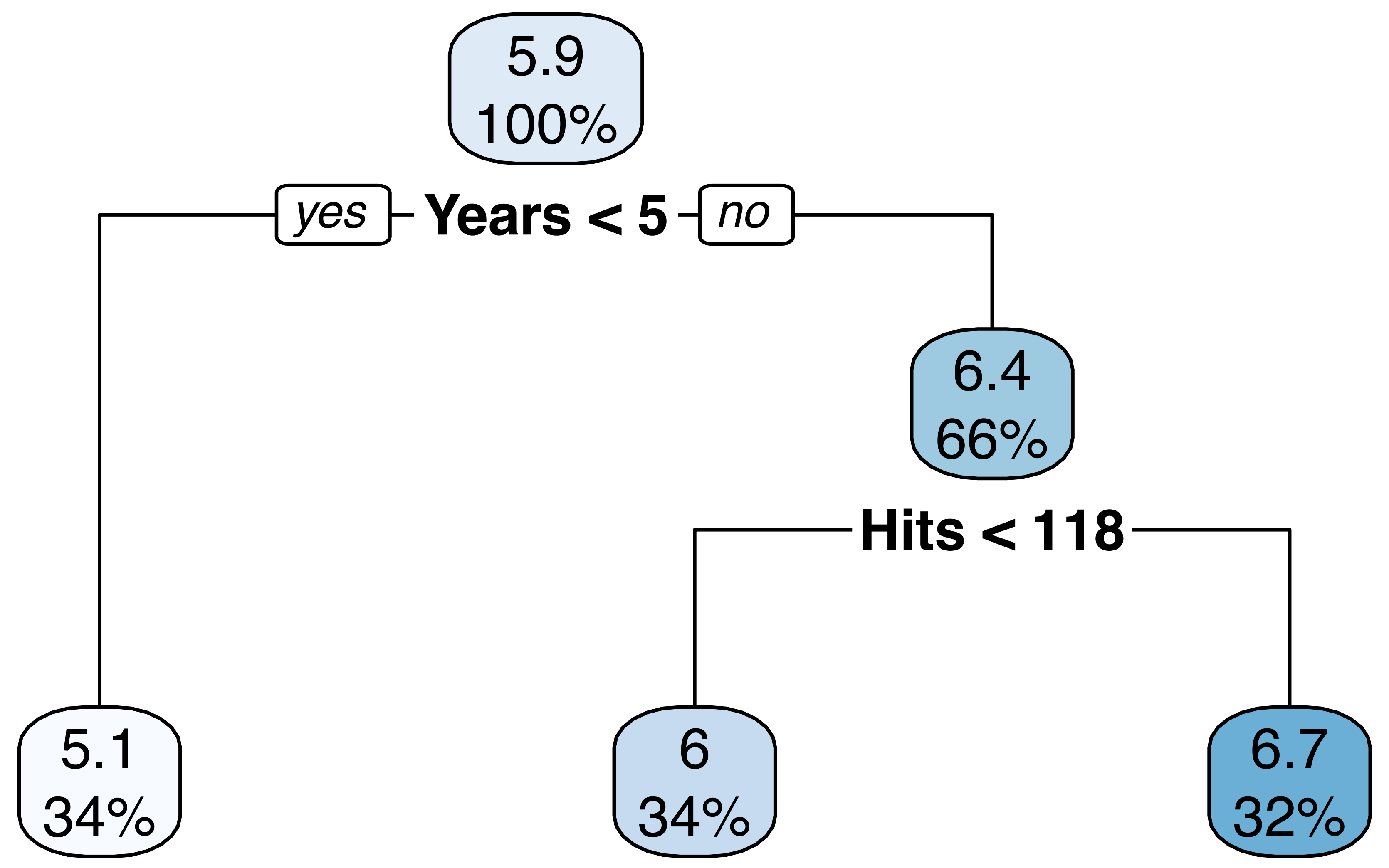
Nevertheless, trees can be used as building blocks for state-of-the-art prediction performance:

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



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Tree-based models versus linear models

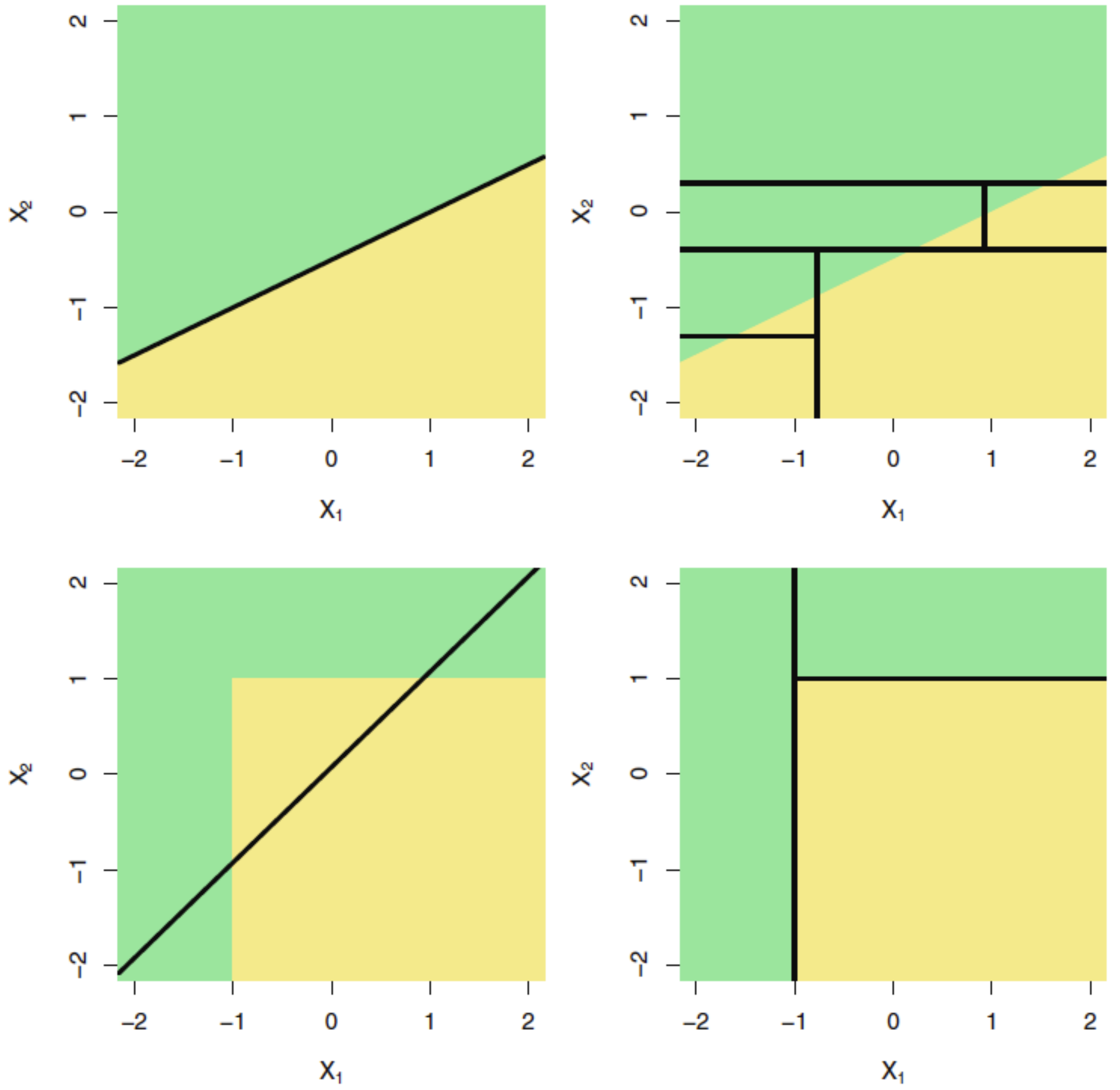
Which perform better?

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).

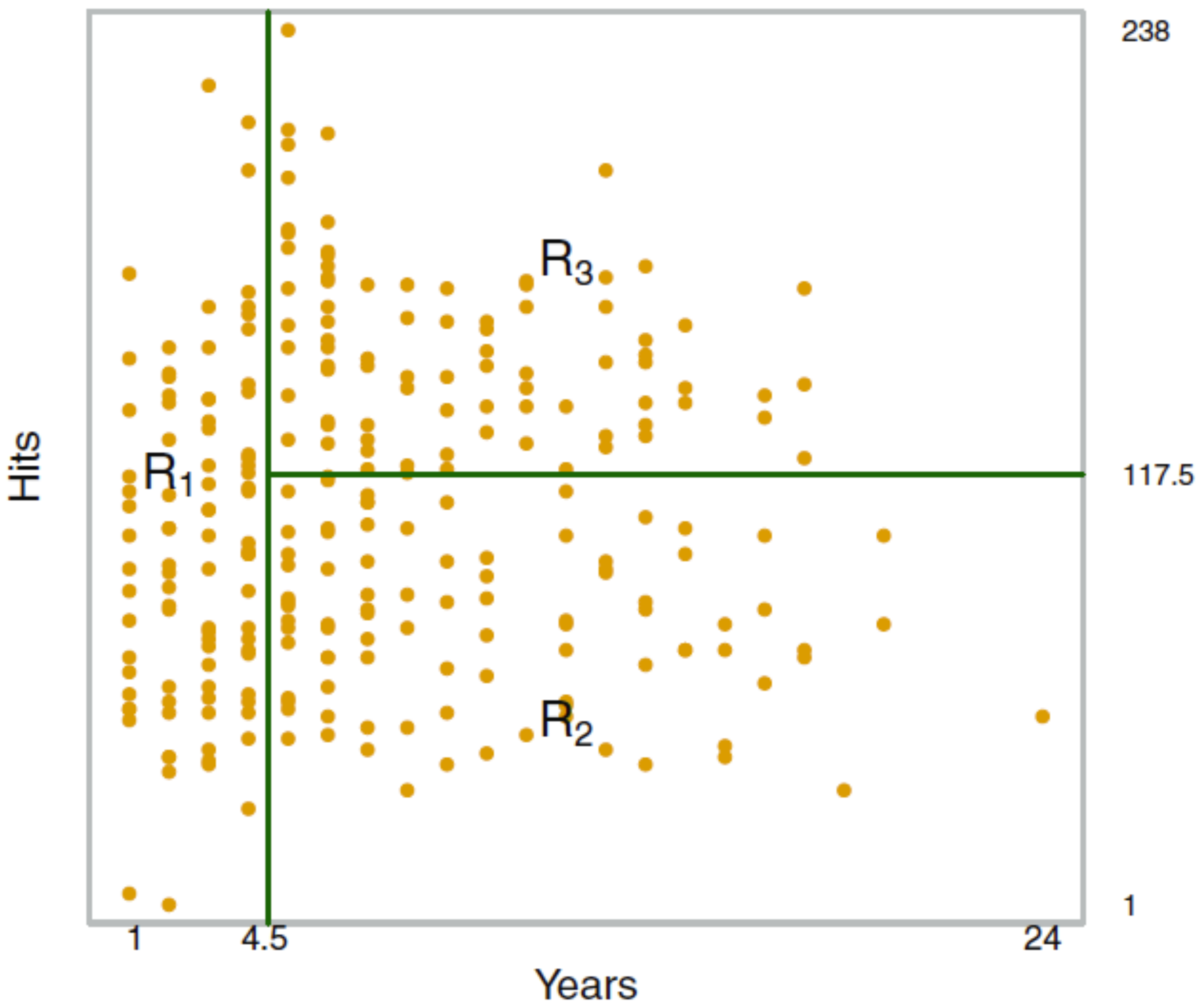
Hitters data

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

$\Longleftrightarrow$



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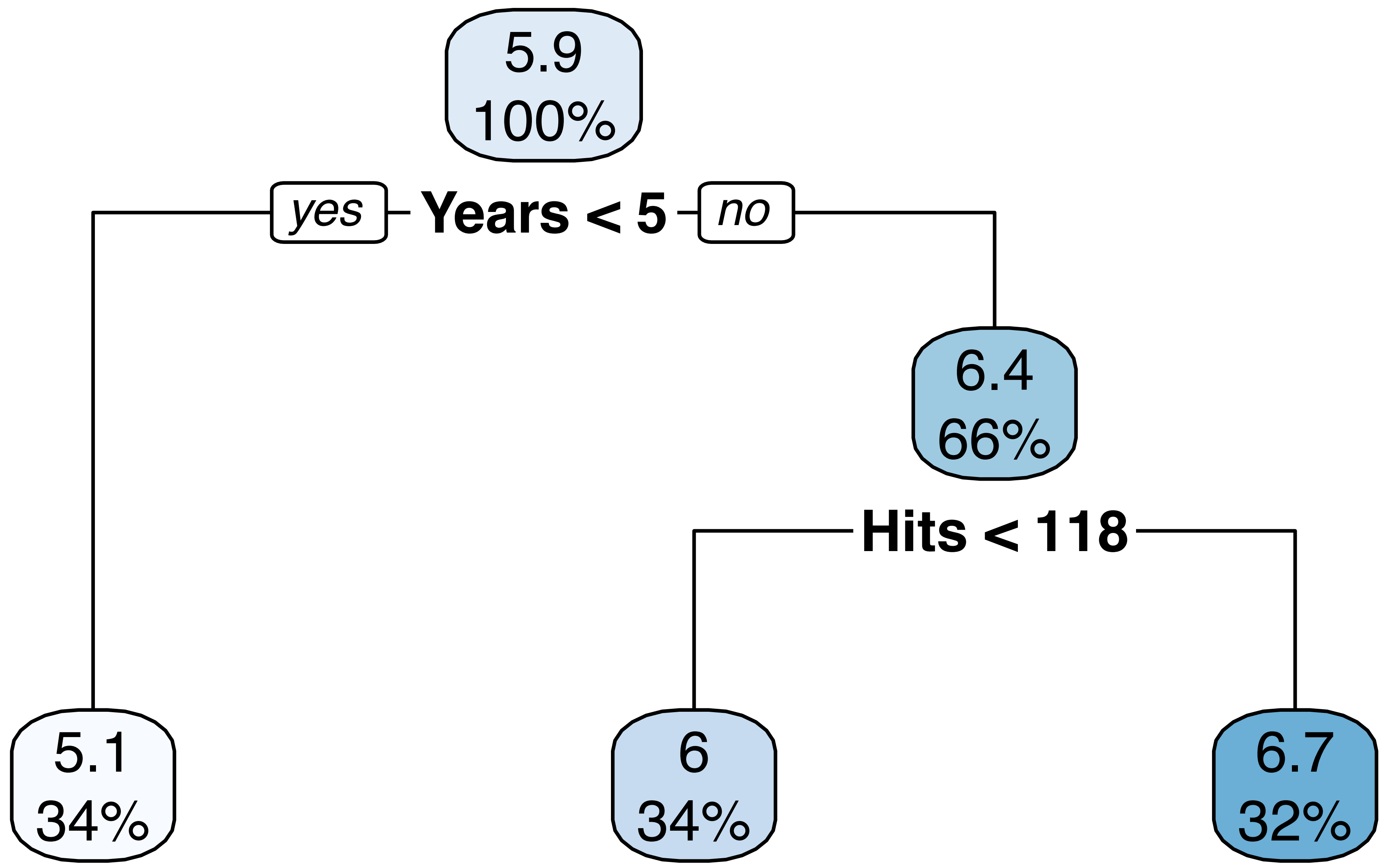

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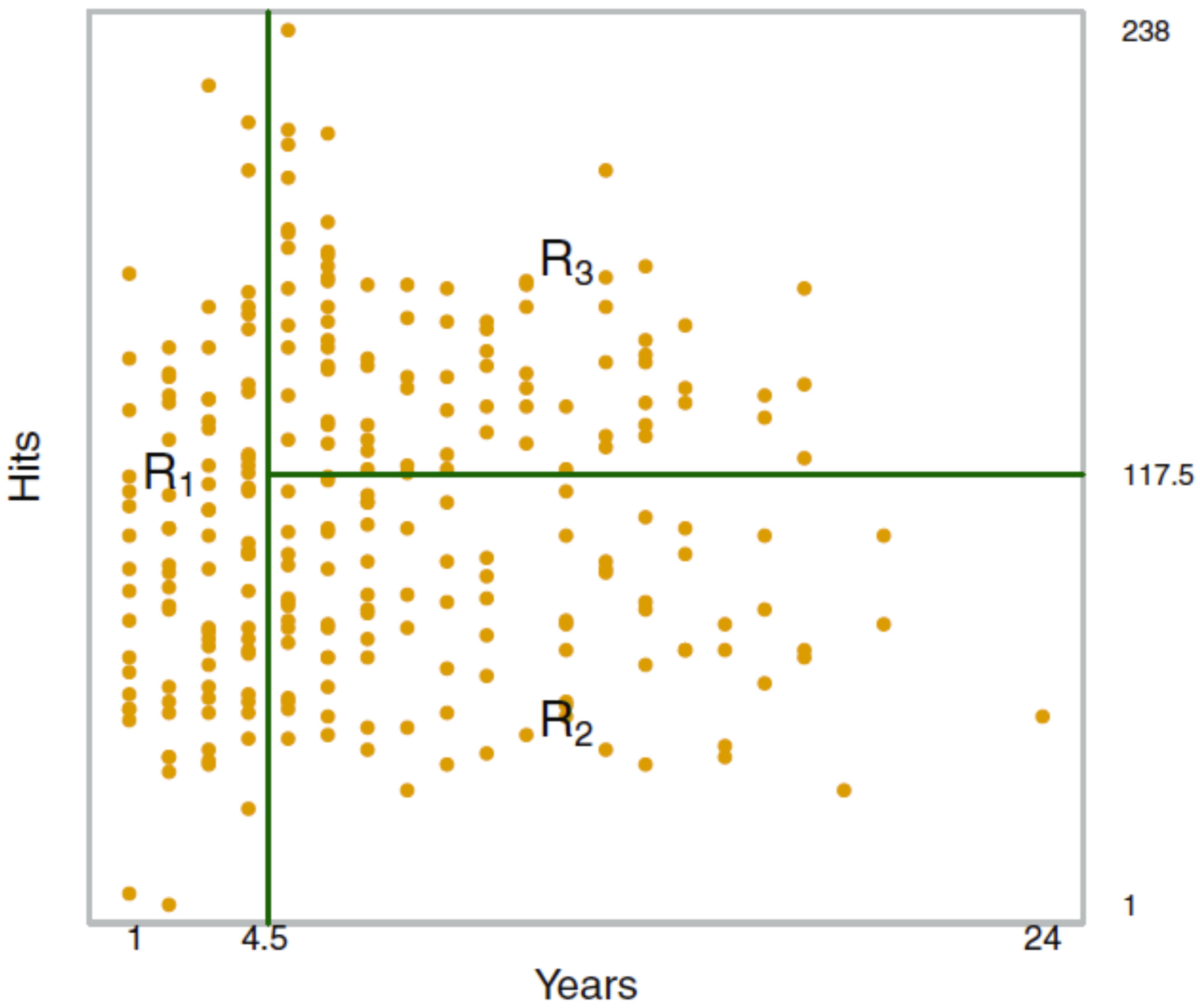


Mathematical expression of the prediction rule

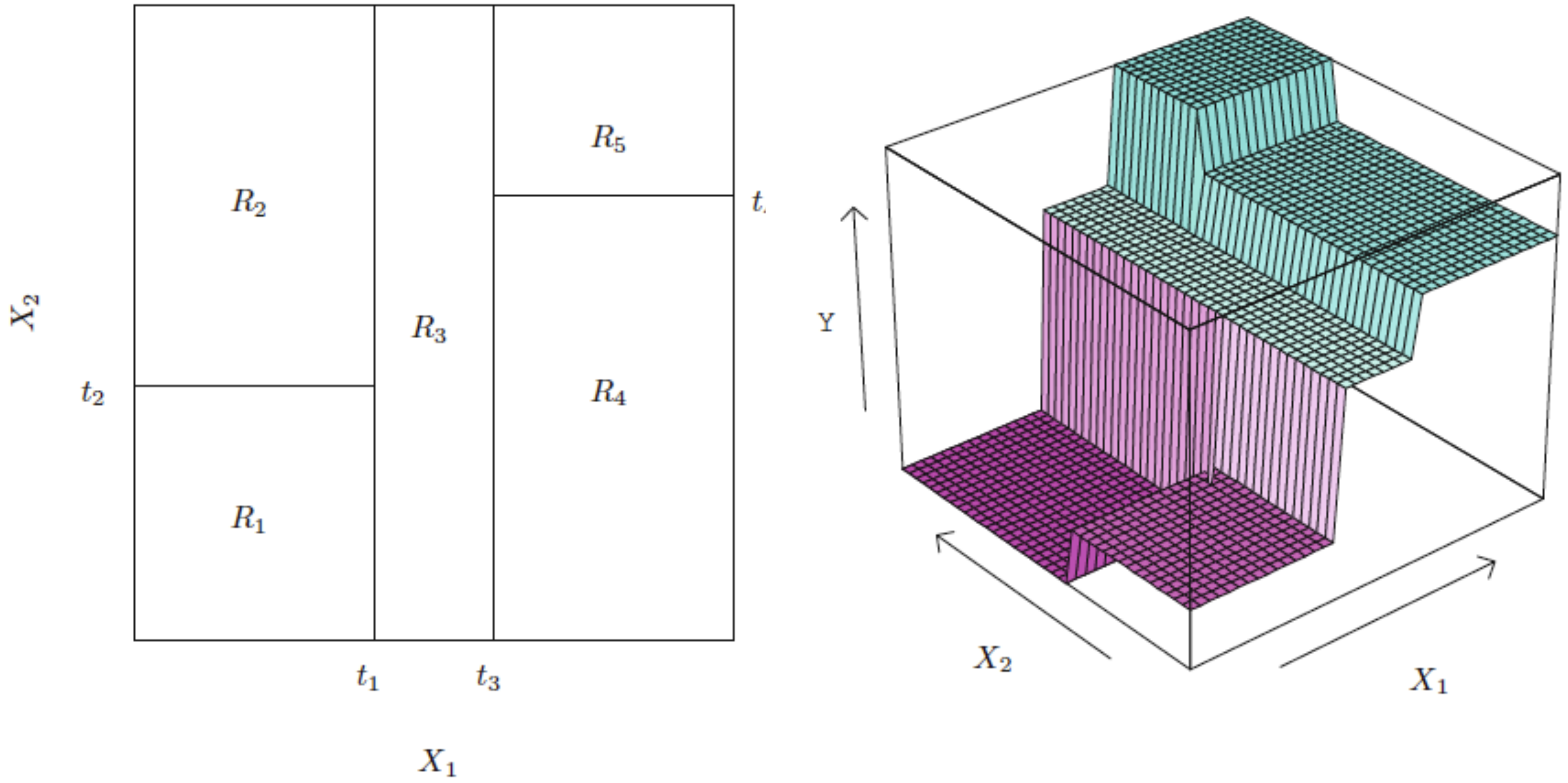
A trained tree consists of:

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

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

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

(continuous or categorical response)



Partitioning for continuous and categorical features

Suppose we partition on X_j.

- 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

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:

$$\widehat{R}_1, \ldots, \widehat{R}_M, \widehat{c}_1, \ldots, \widehat{c}_M = \underset{R_1,\ldots,R_M,c_1,\ldots,c_M}{\arg\min} \sum_{i=1}^{n} (Y_i - \widehat{Y}_i)^2;$$

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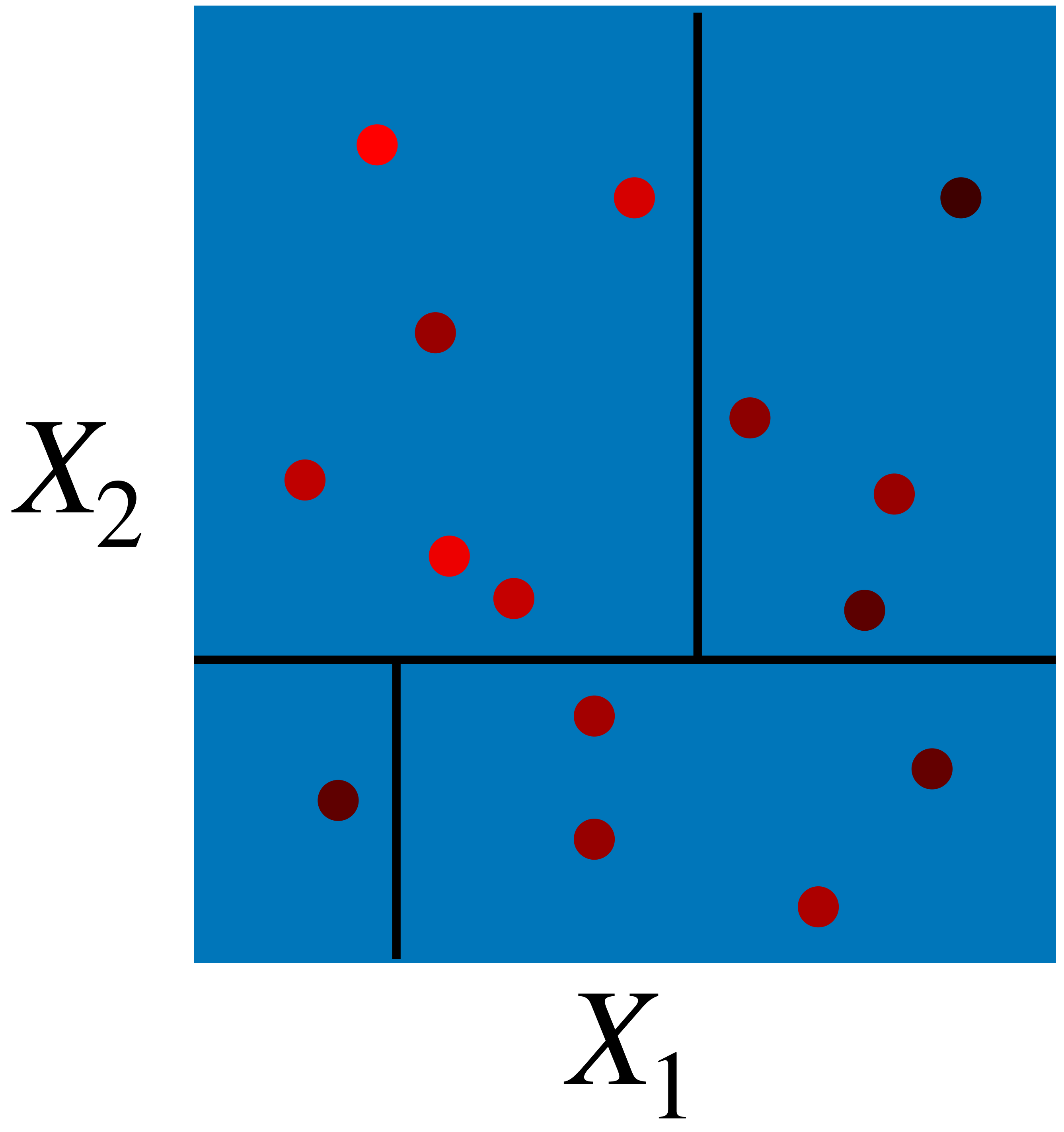

Training a regression tree

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

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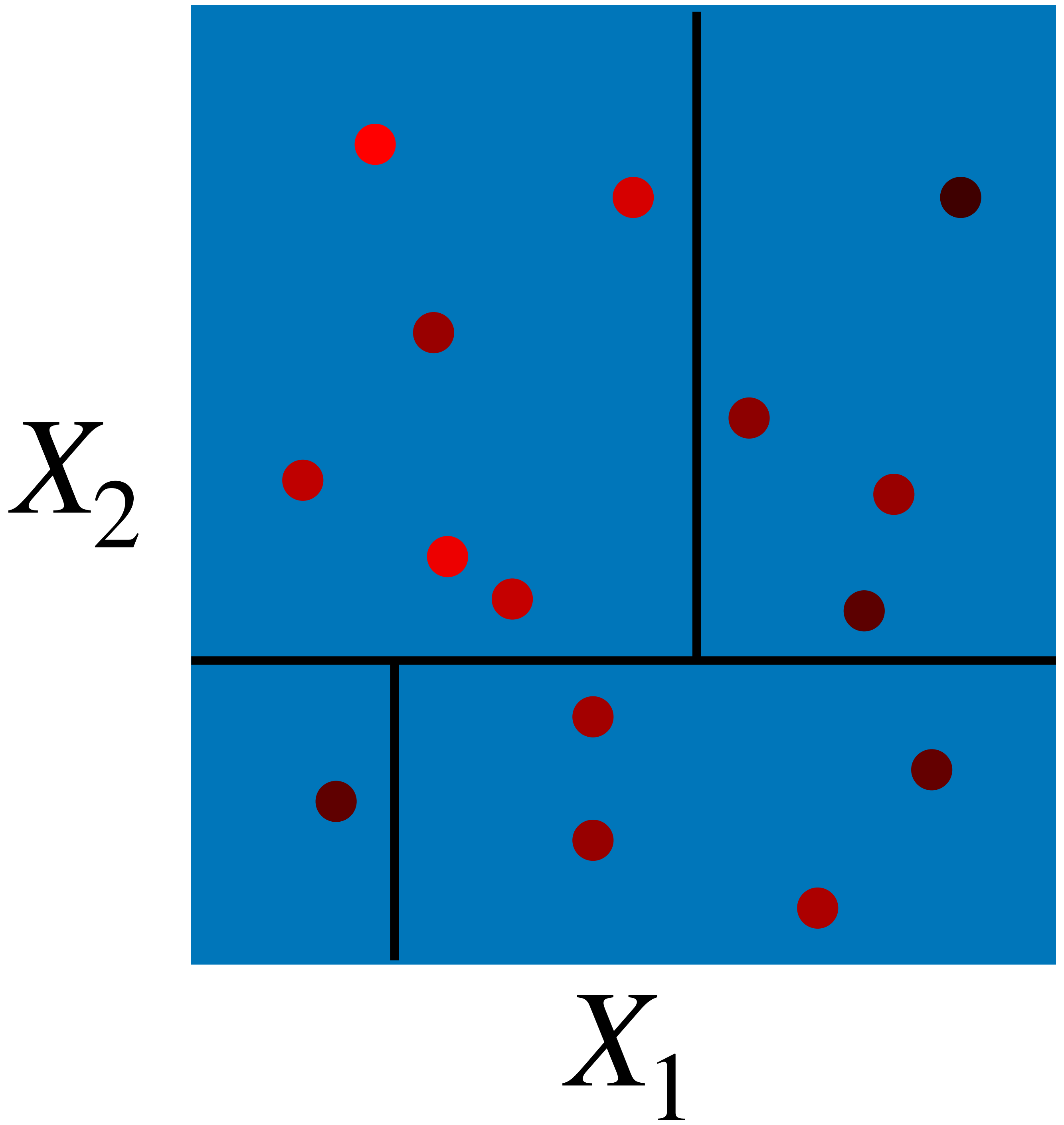
We're fitting a constant to each region, so the solution is

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



Training a regression tree

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:

1. Fit constant model to the entire space and calculate RSS.
2. Find split of the whole region that decreases RSS the most.
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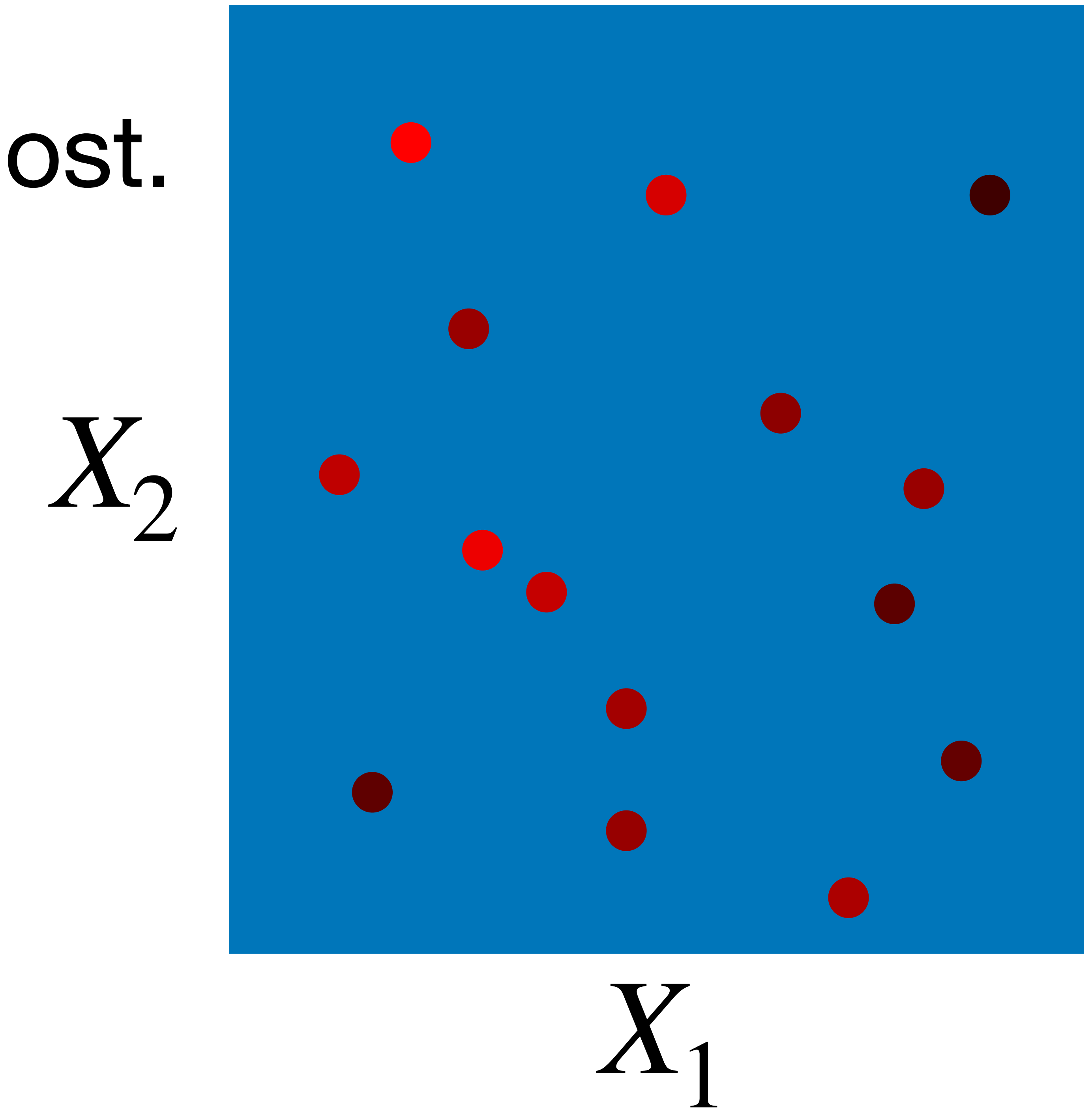
4. Repeat until there are M regions.



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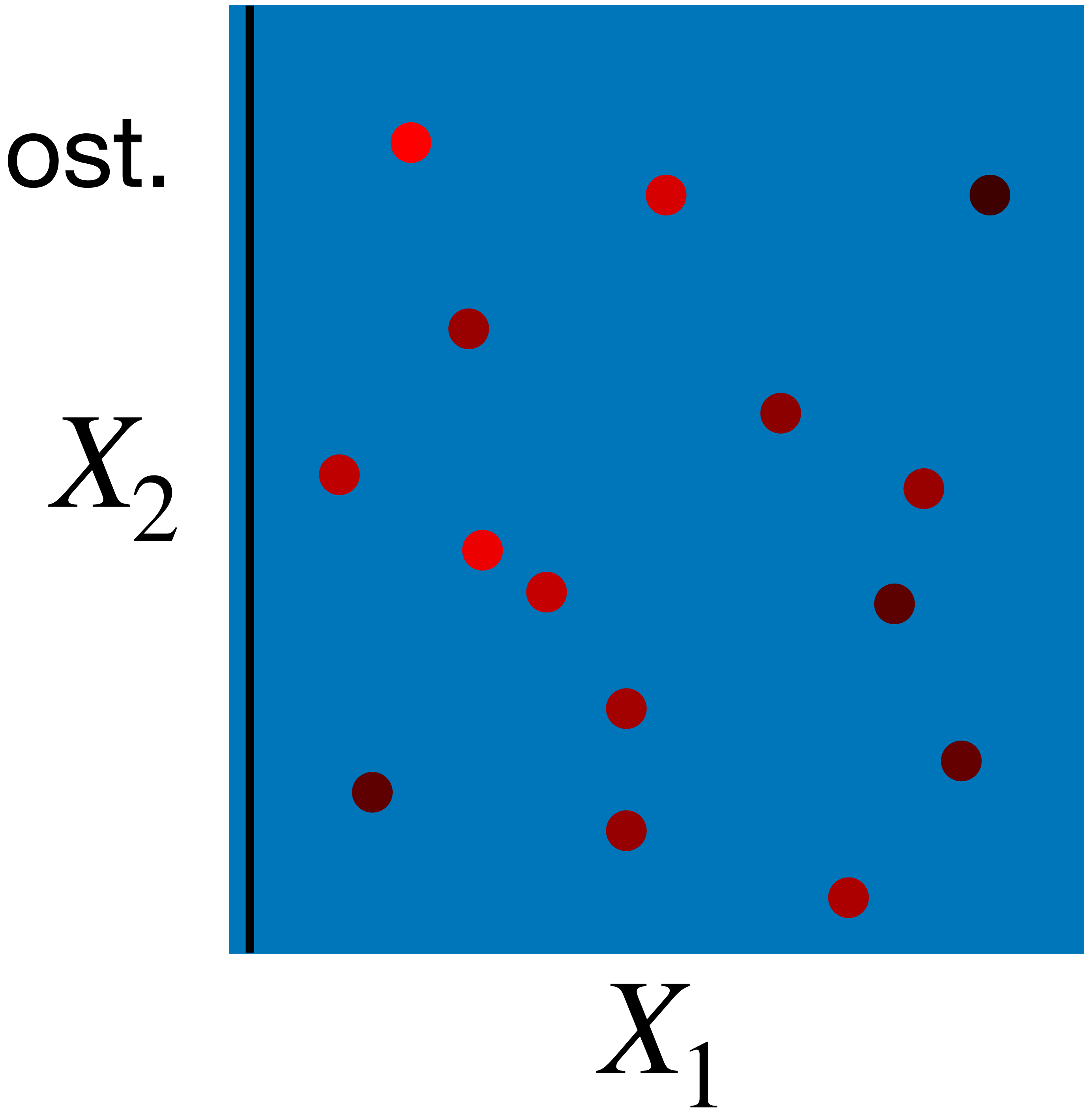

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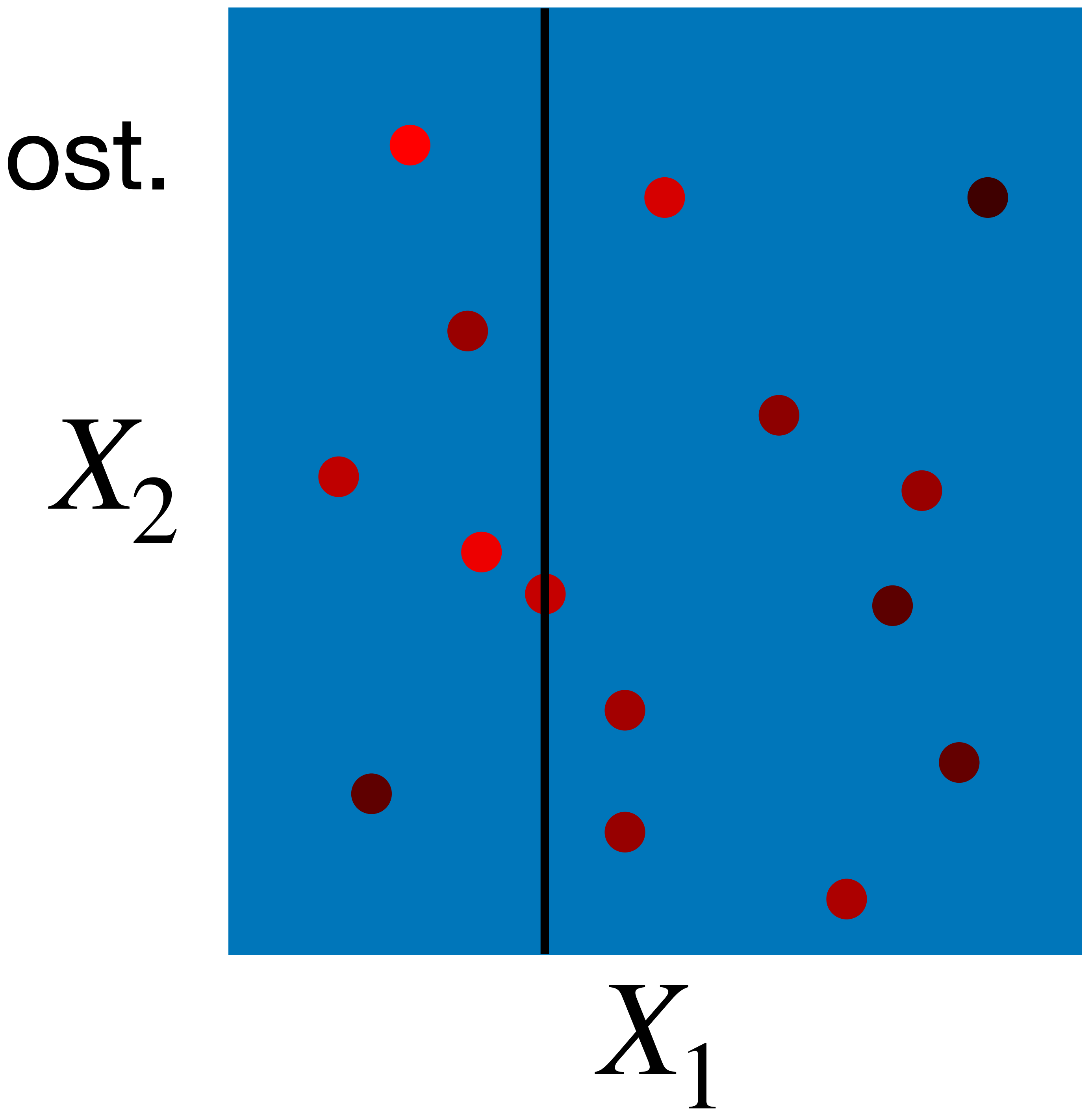

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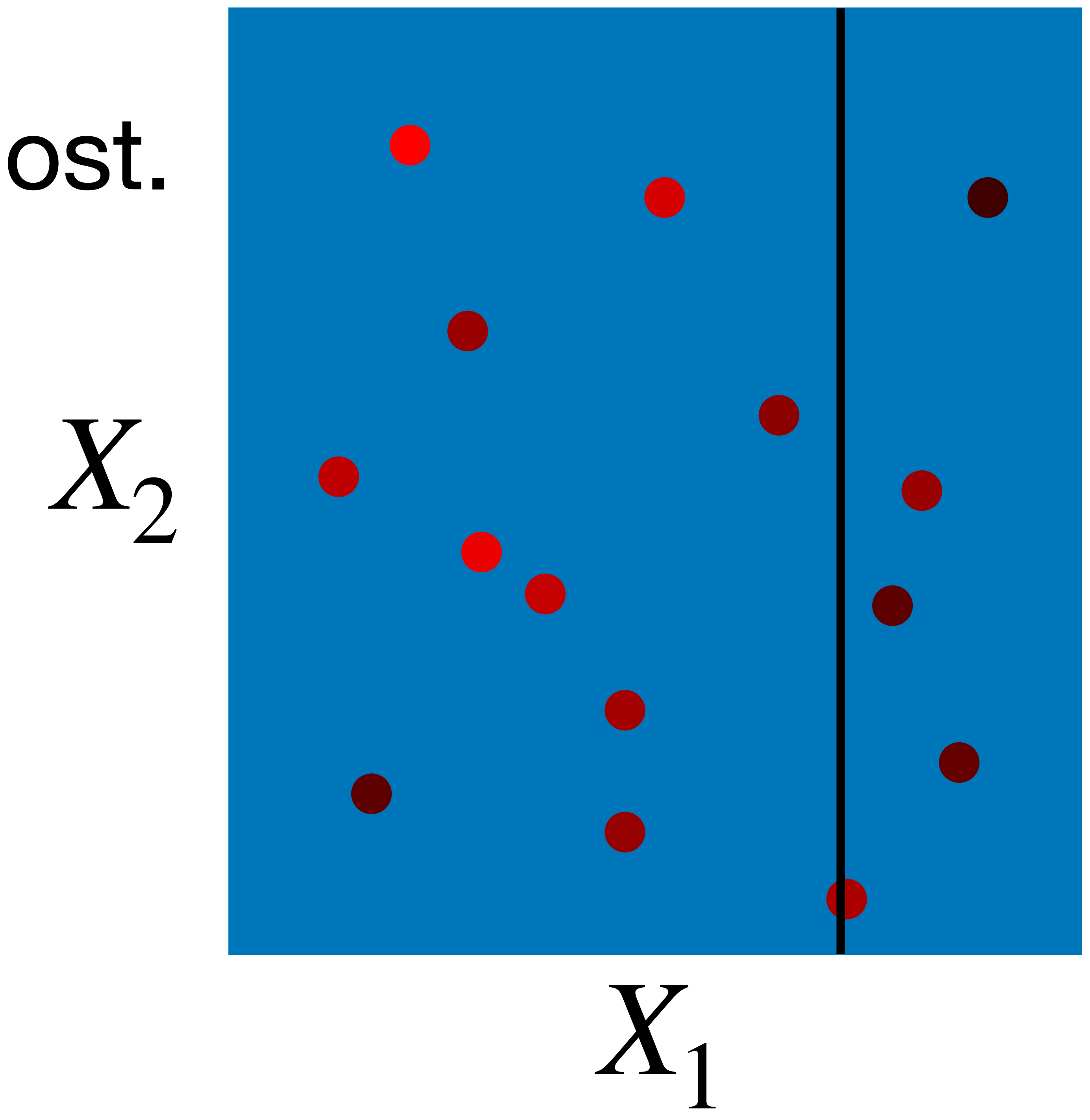

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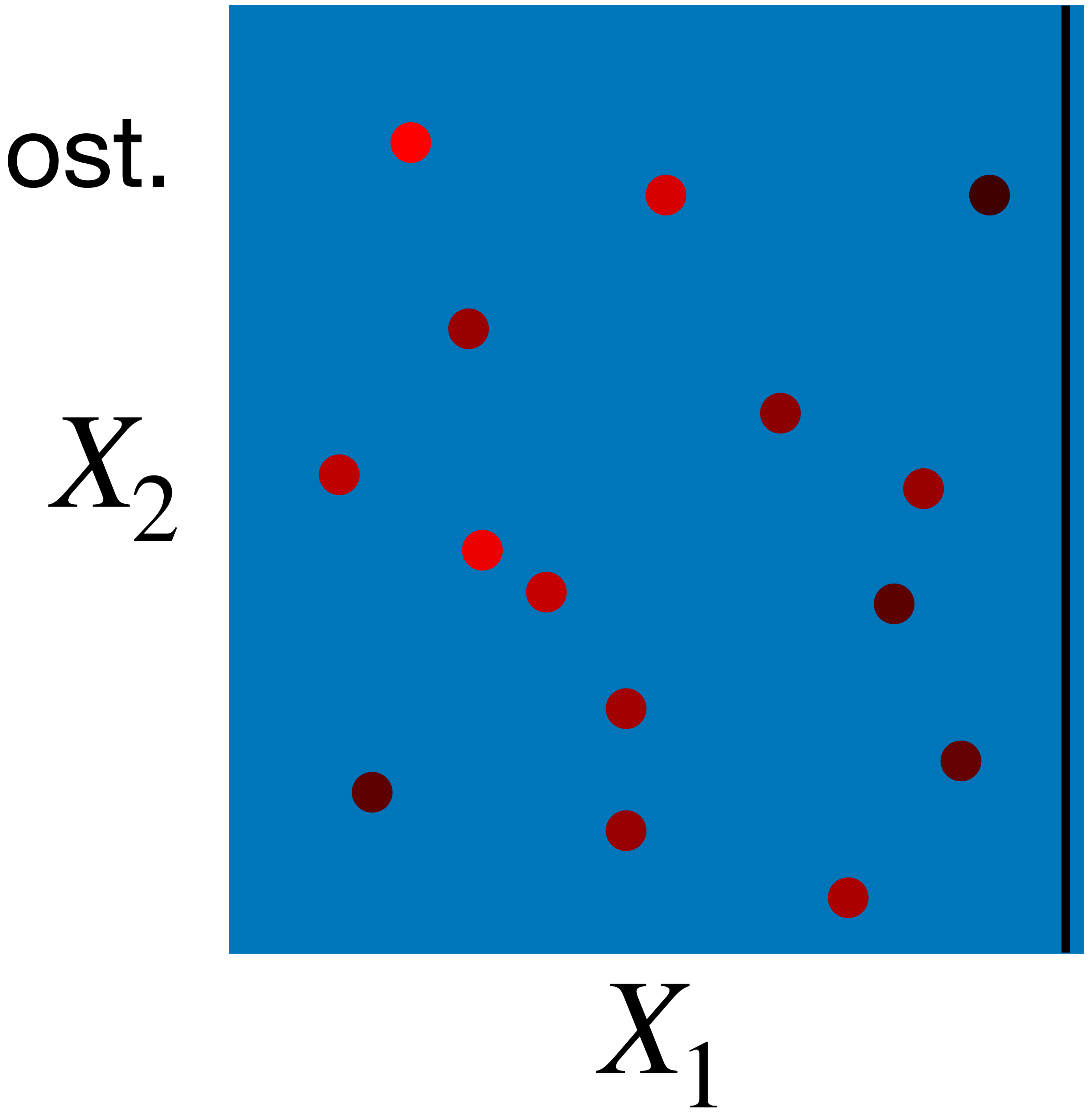

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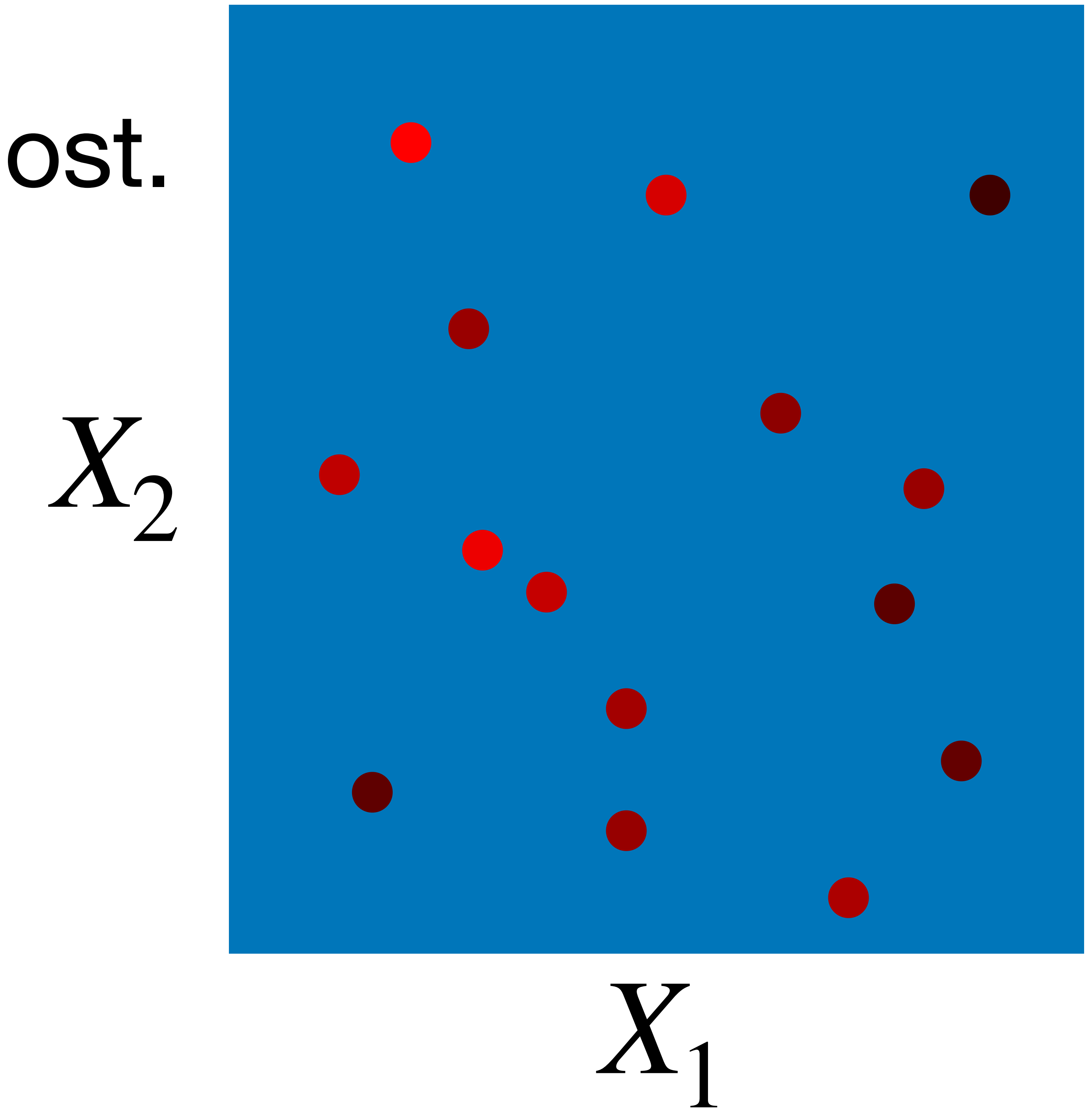

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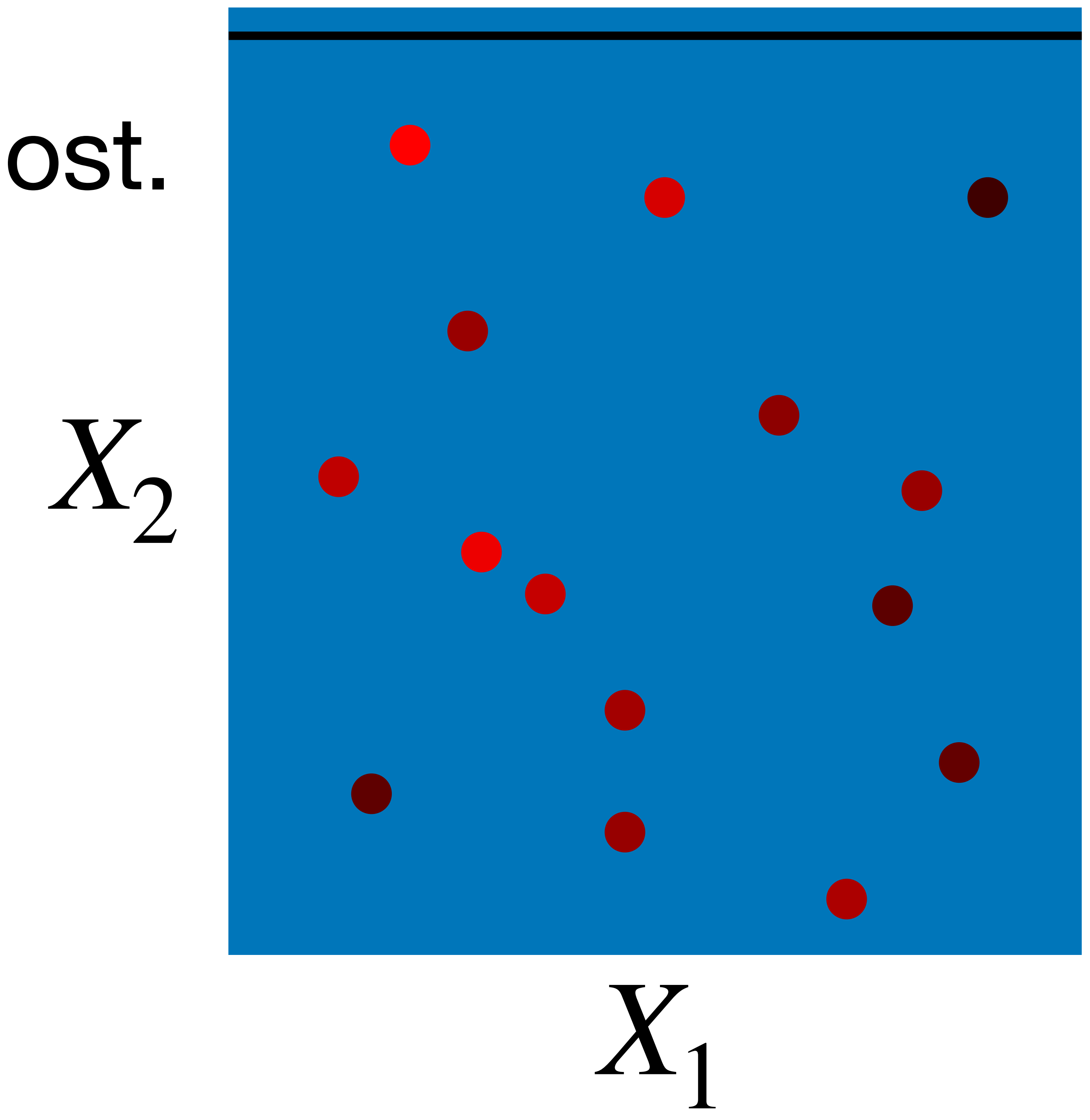

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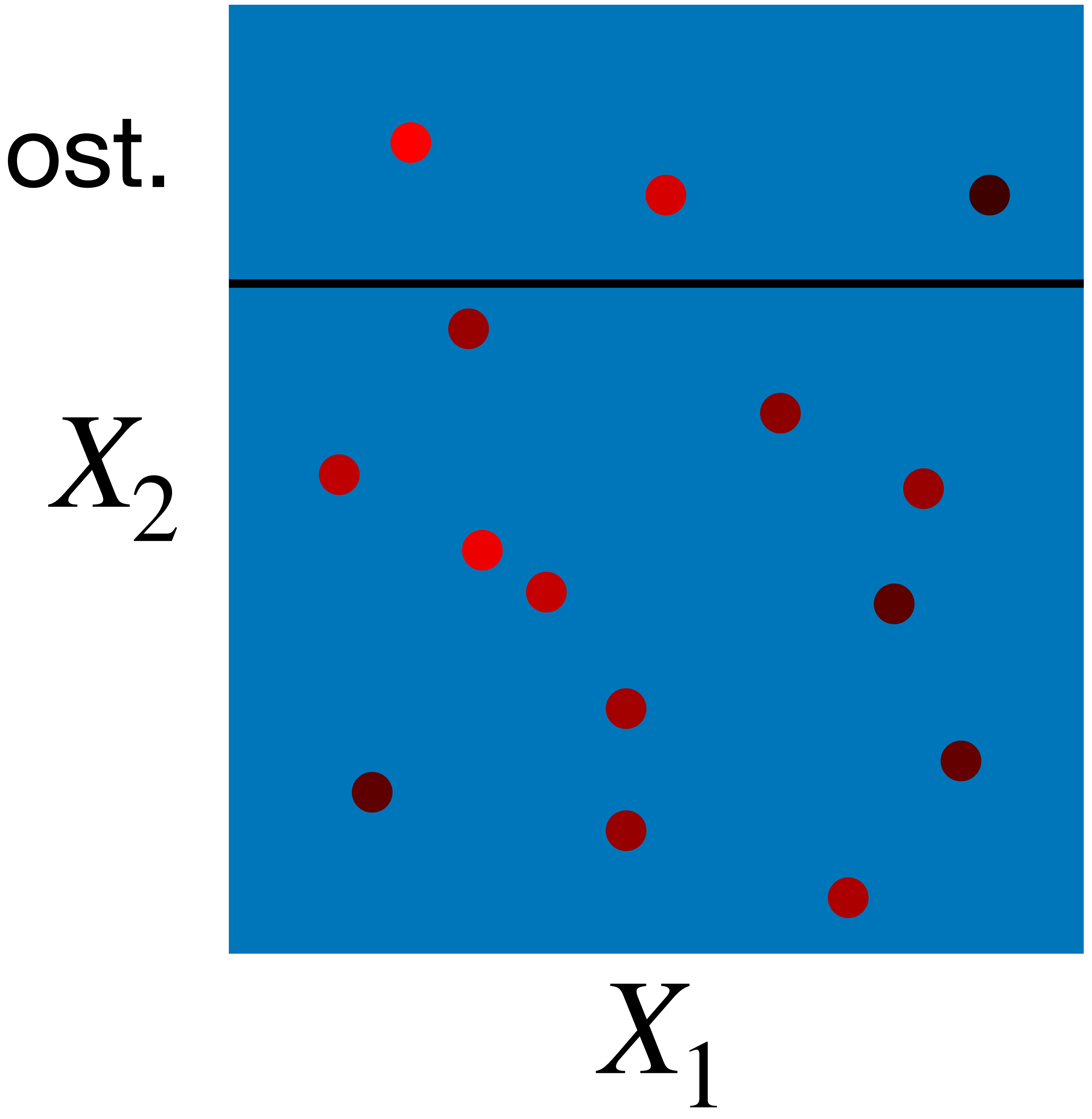

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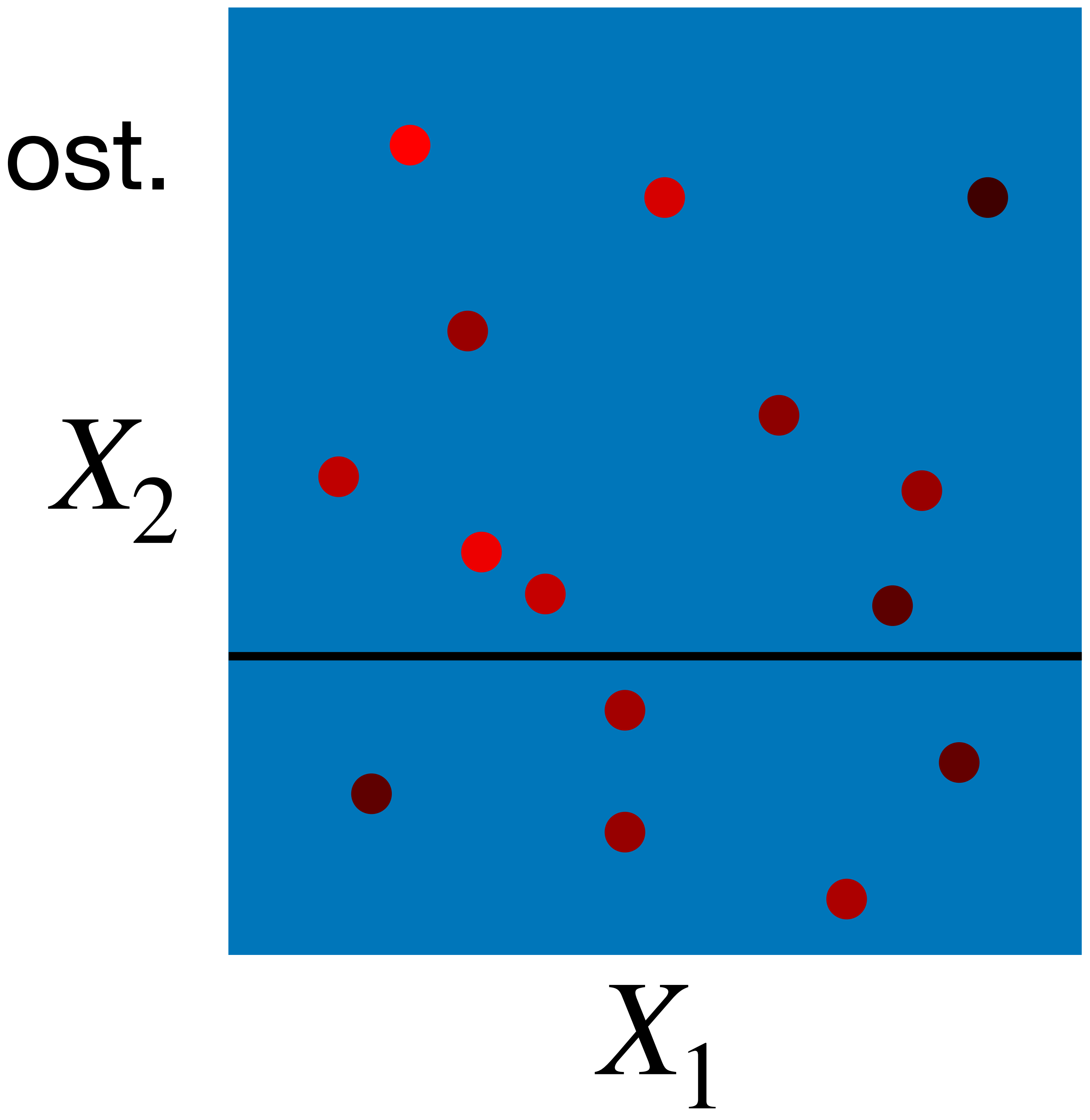

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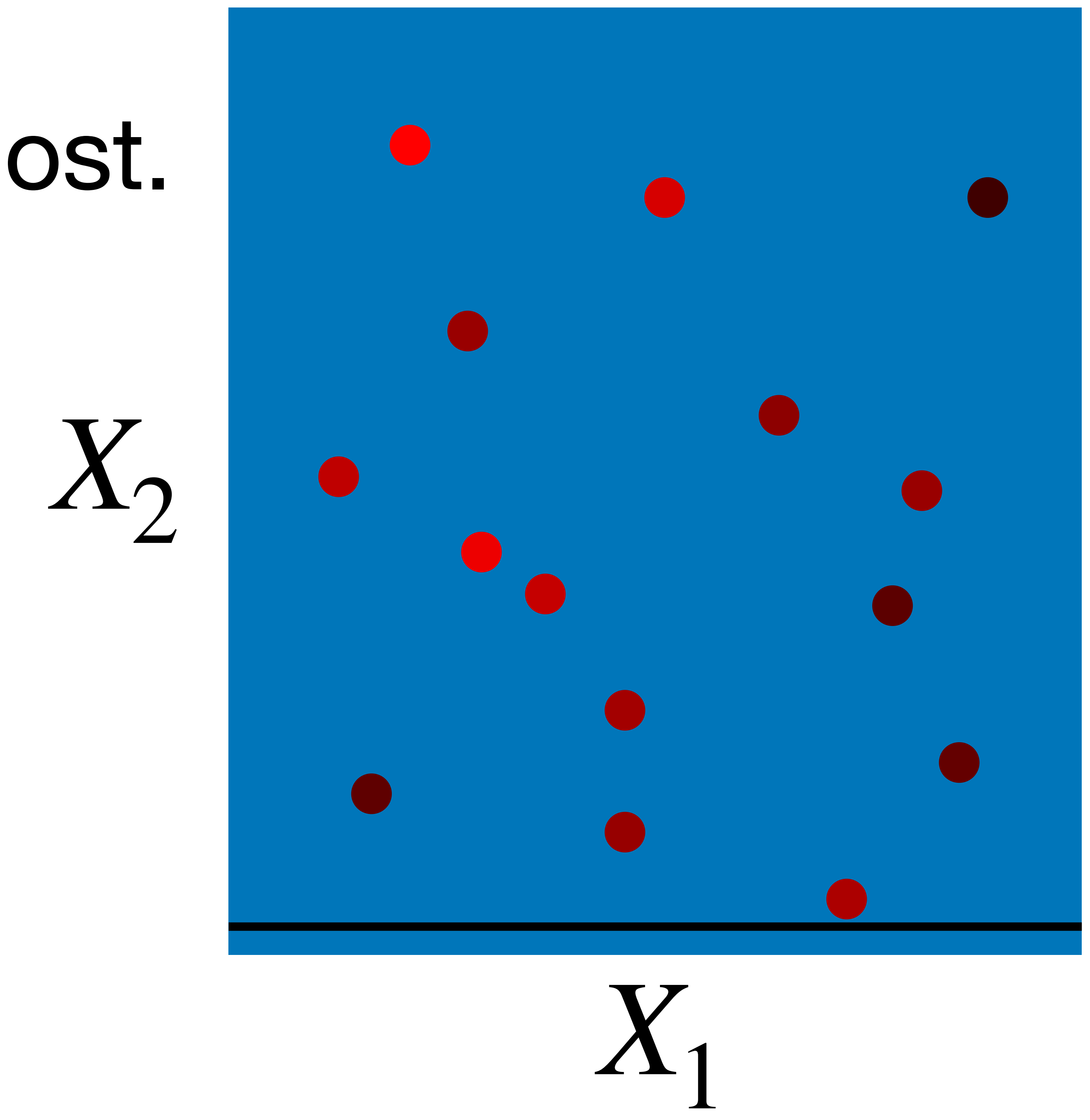

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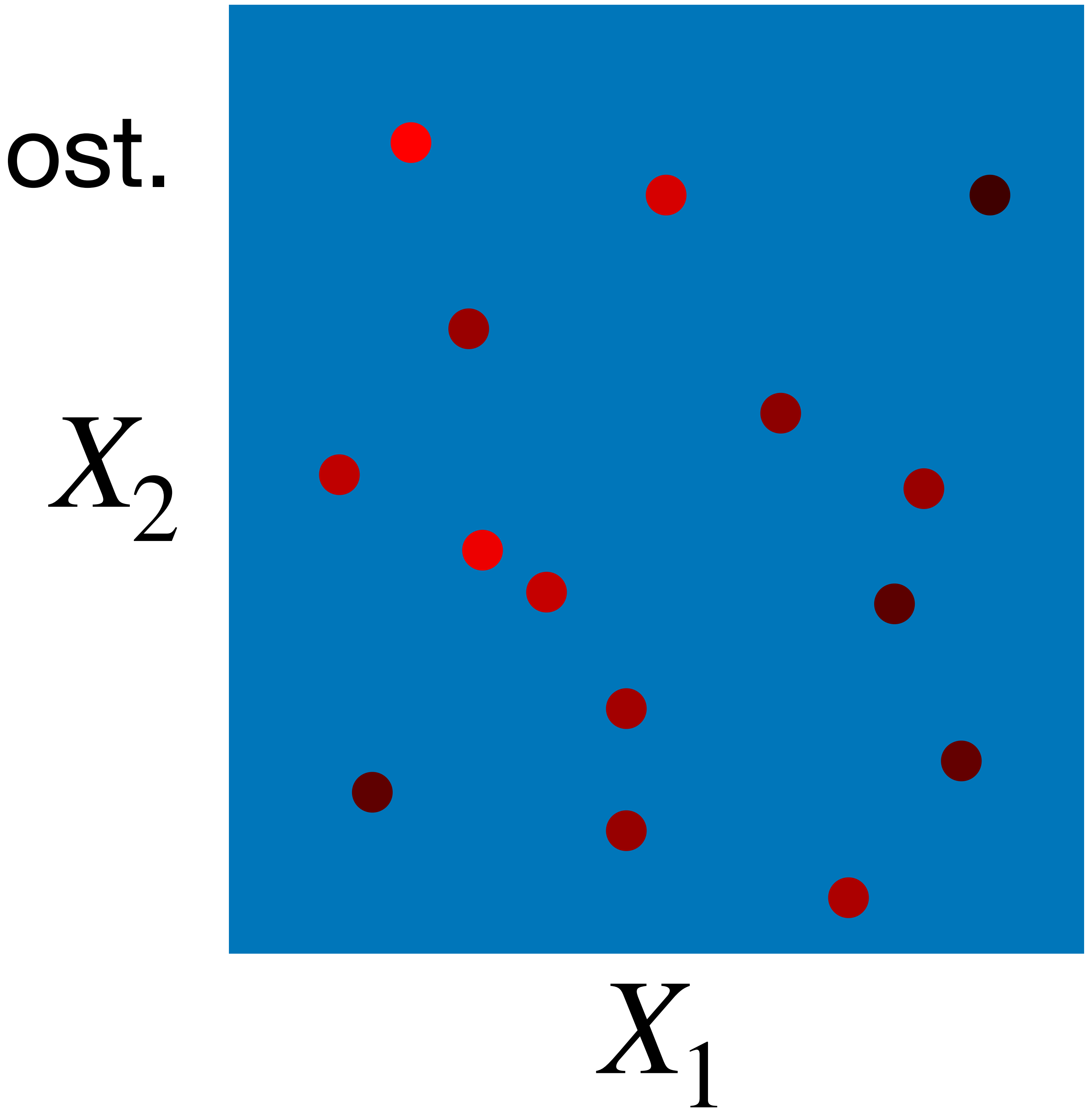

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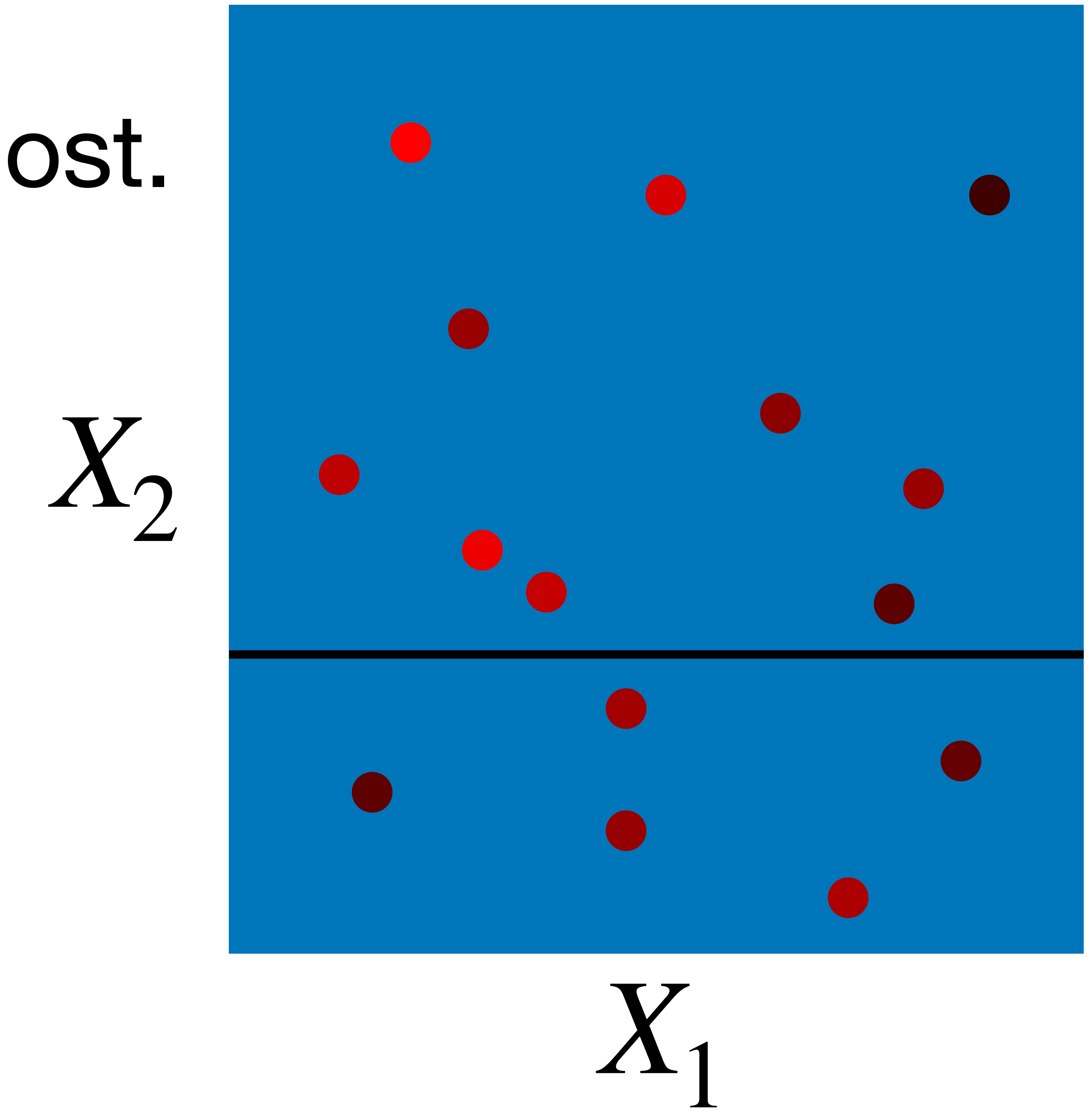

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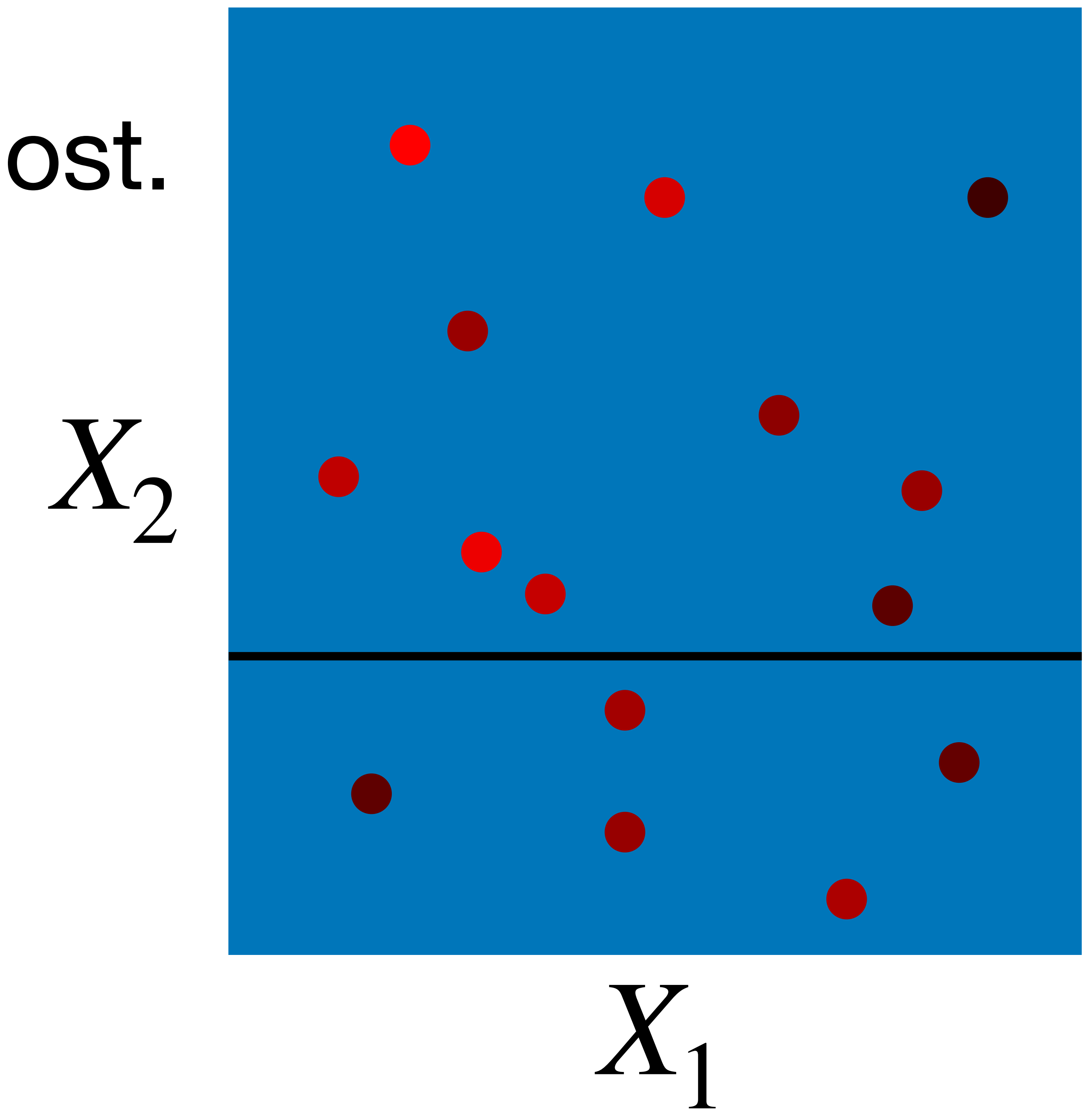

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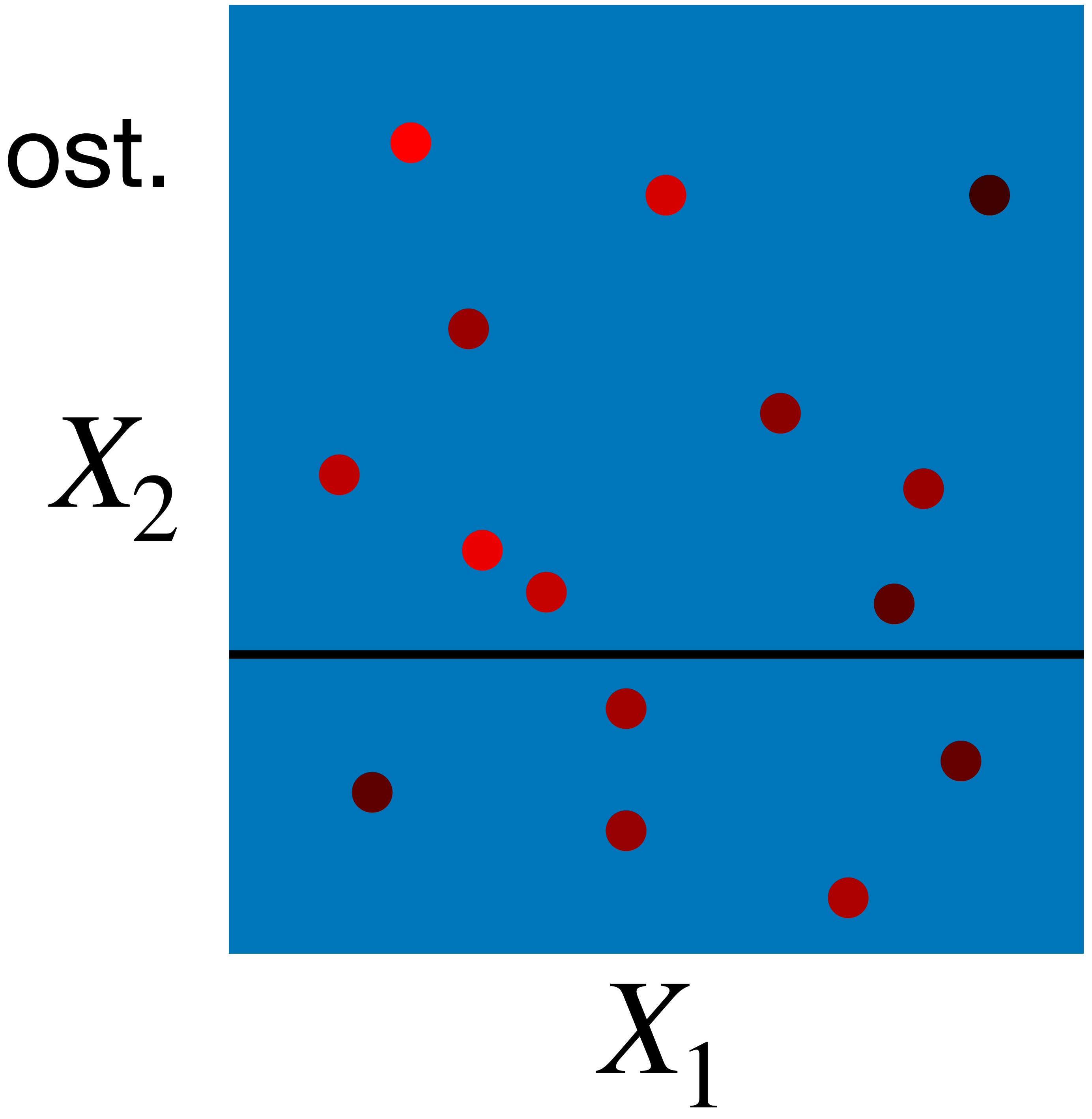

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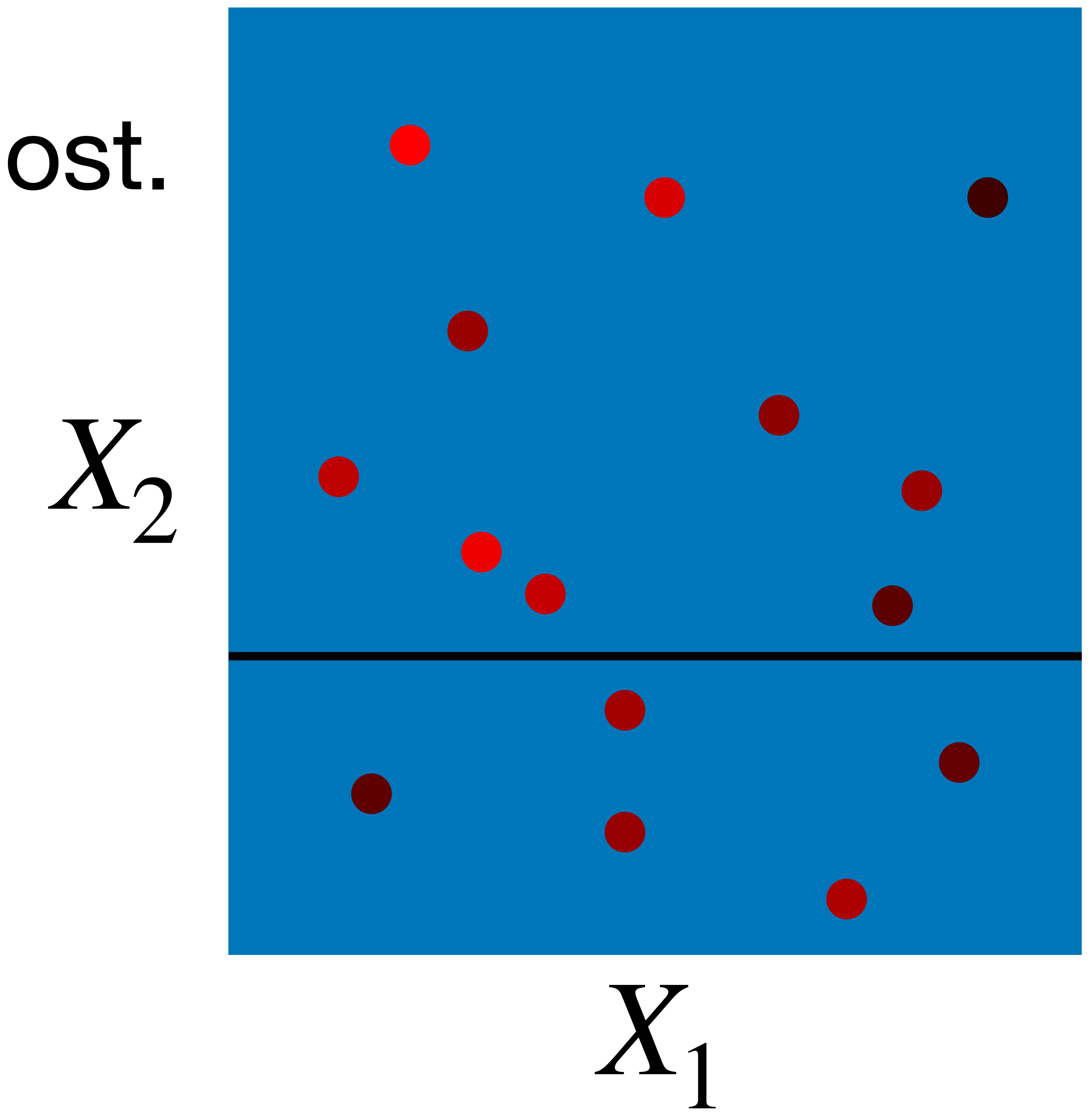

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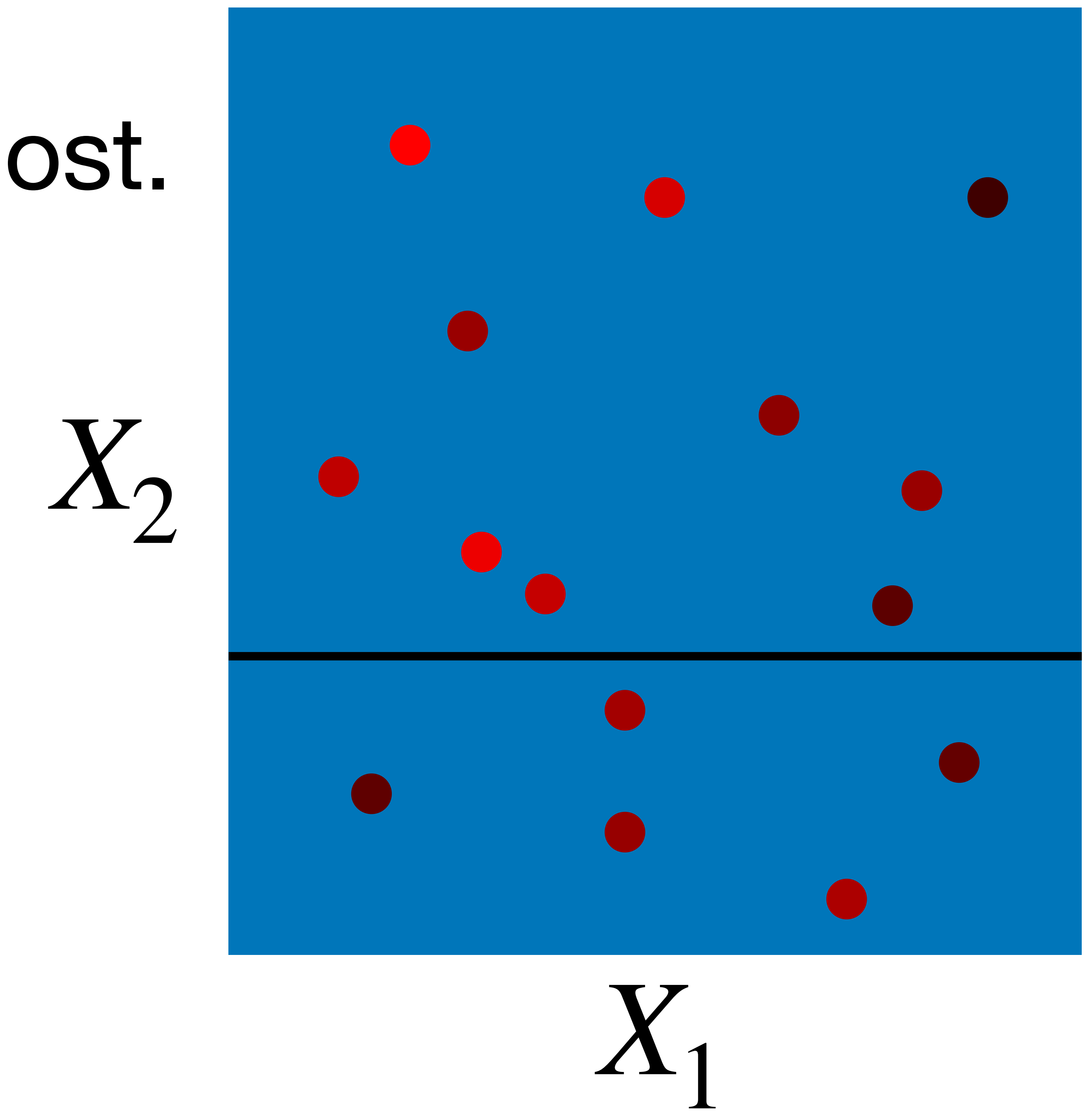

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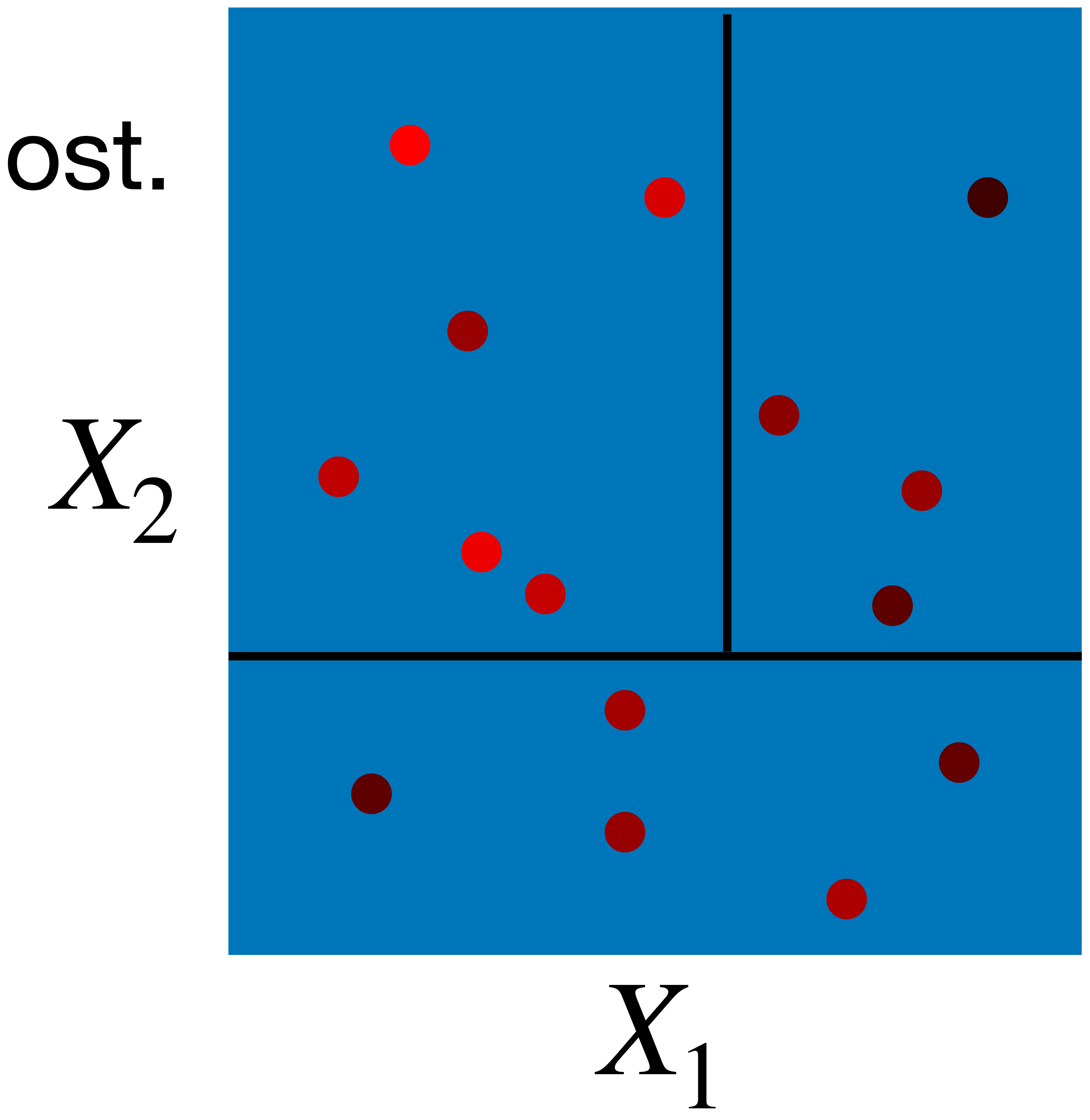

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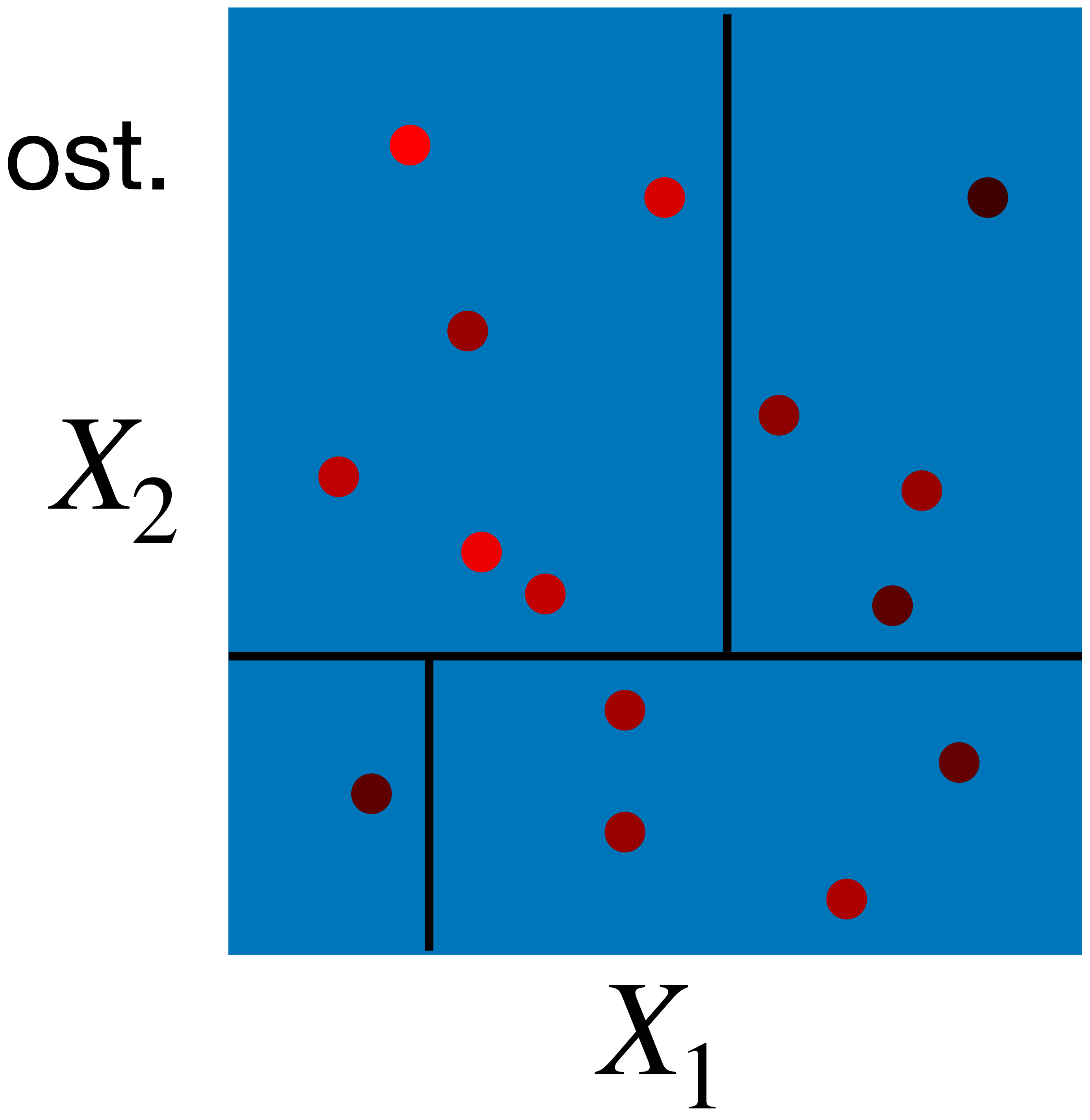
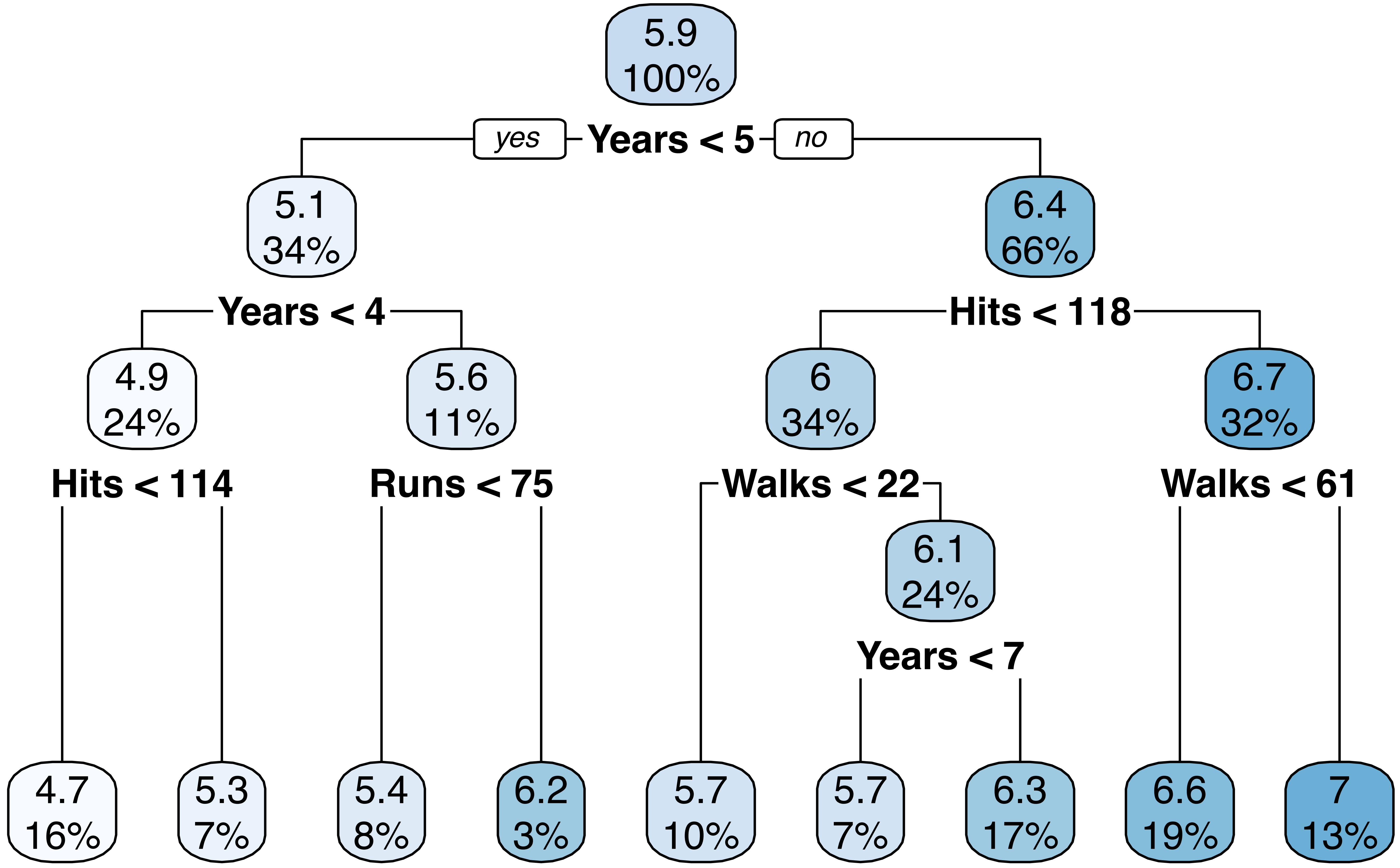


Training a regression tree

Final output



Training a classification tree

The misclassification error objective

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

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

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

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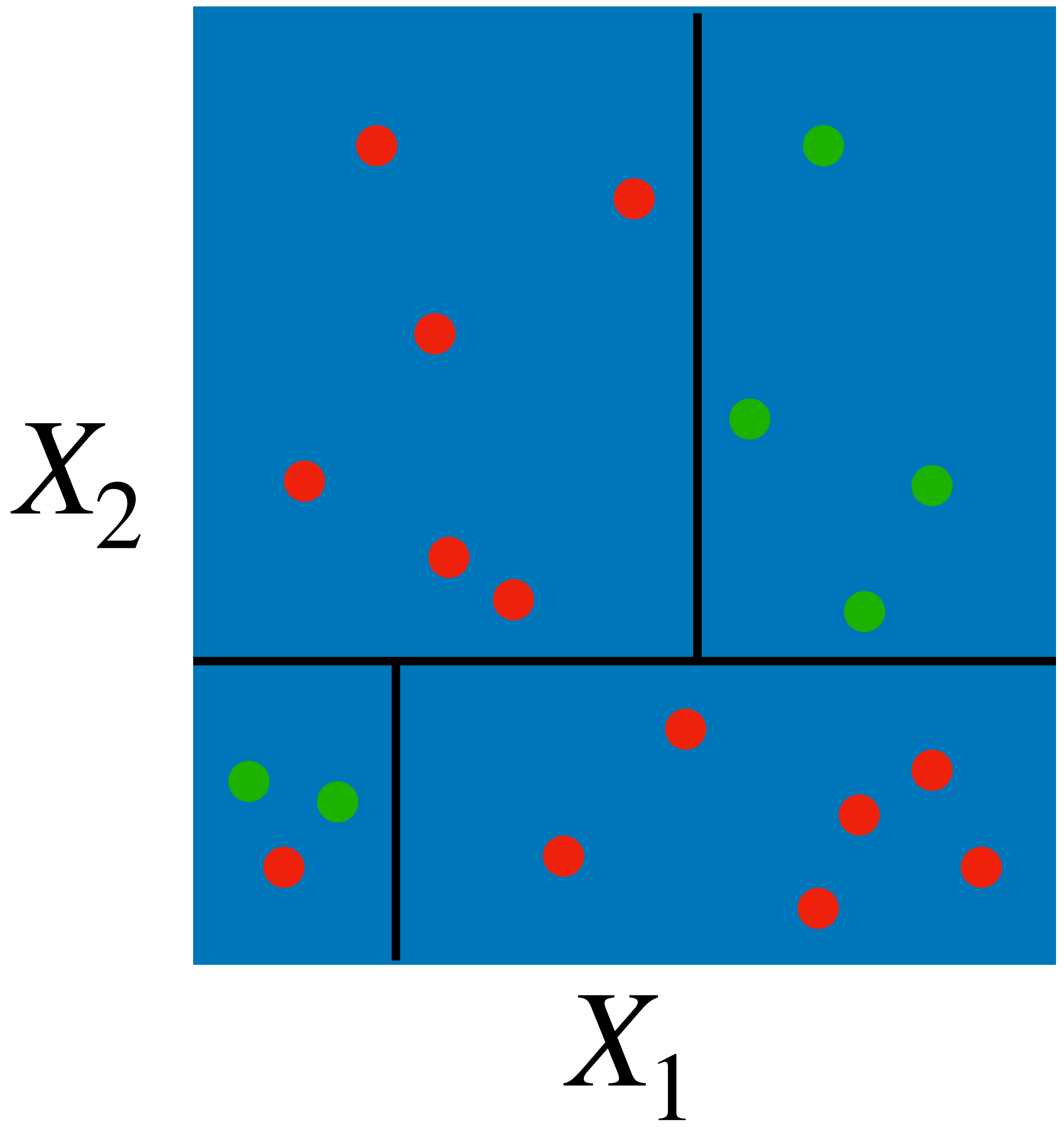

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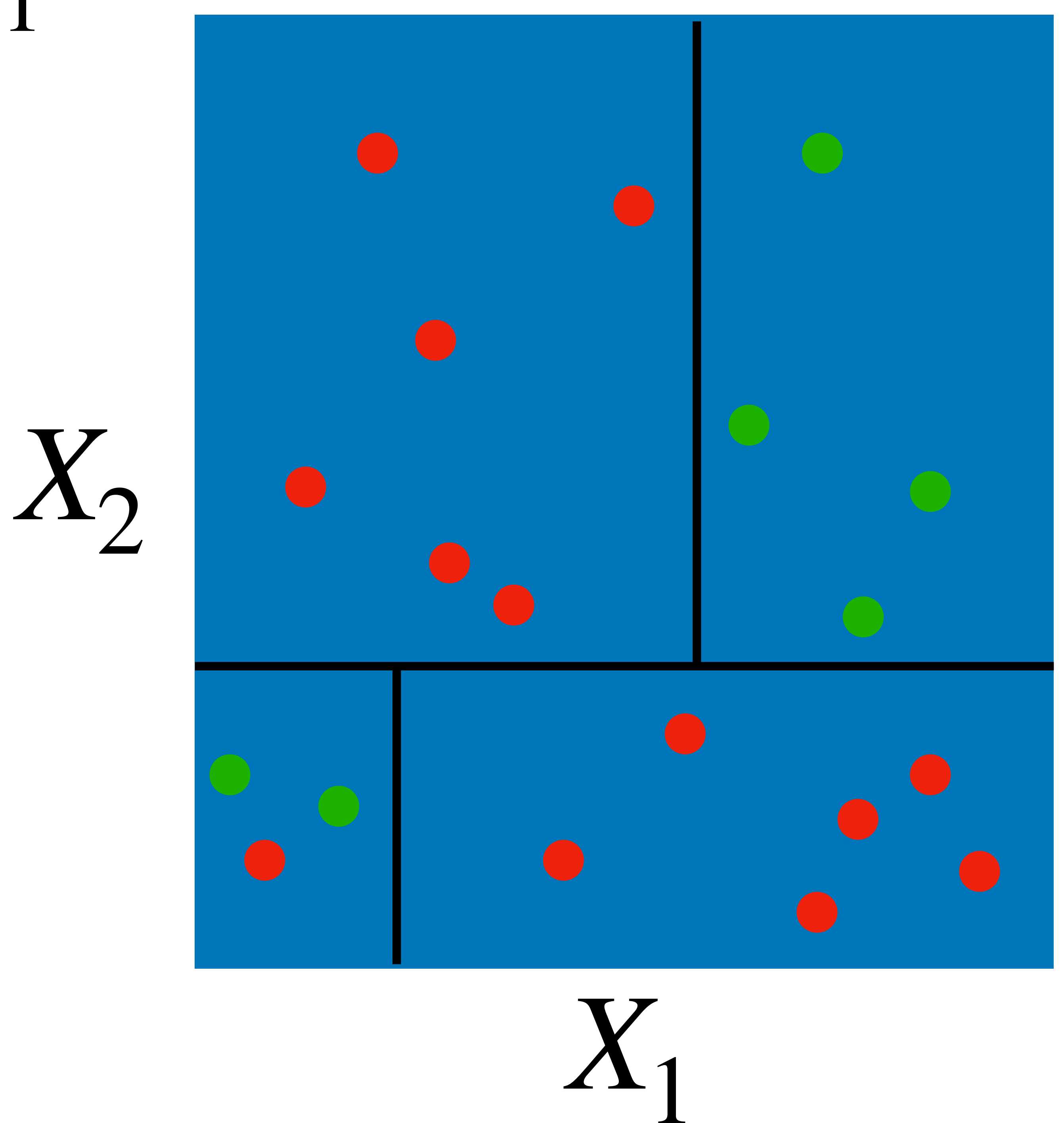
We're fitting the same category to each region, so the solution is the majority vote:

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



Training a classification tree

Finding the rectangles $\widehat{R}_m$

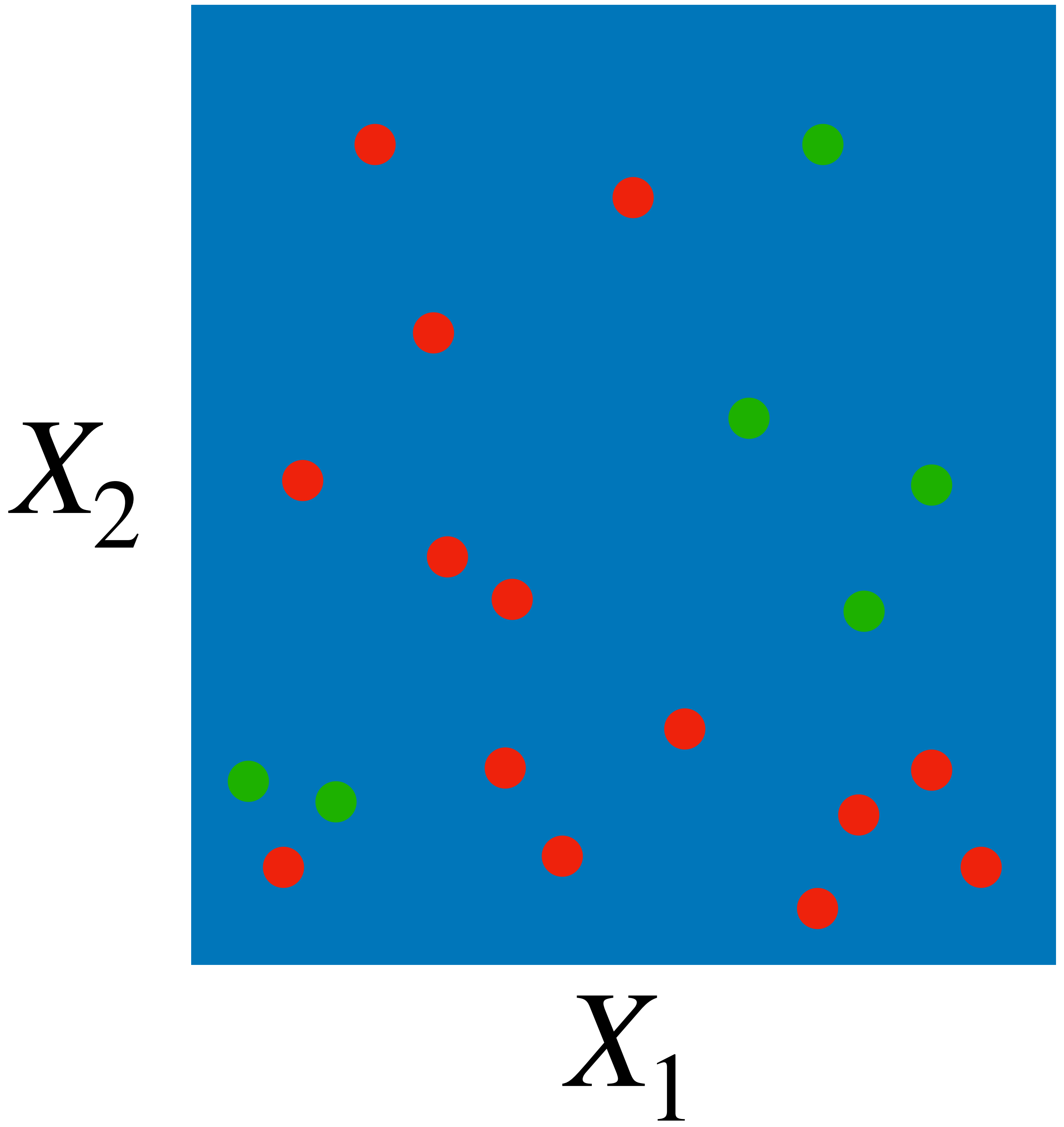
We use a very similar greedy recursive splitting algorithm.

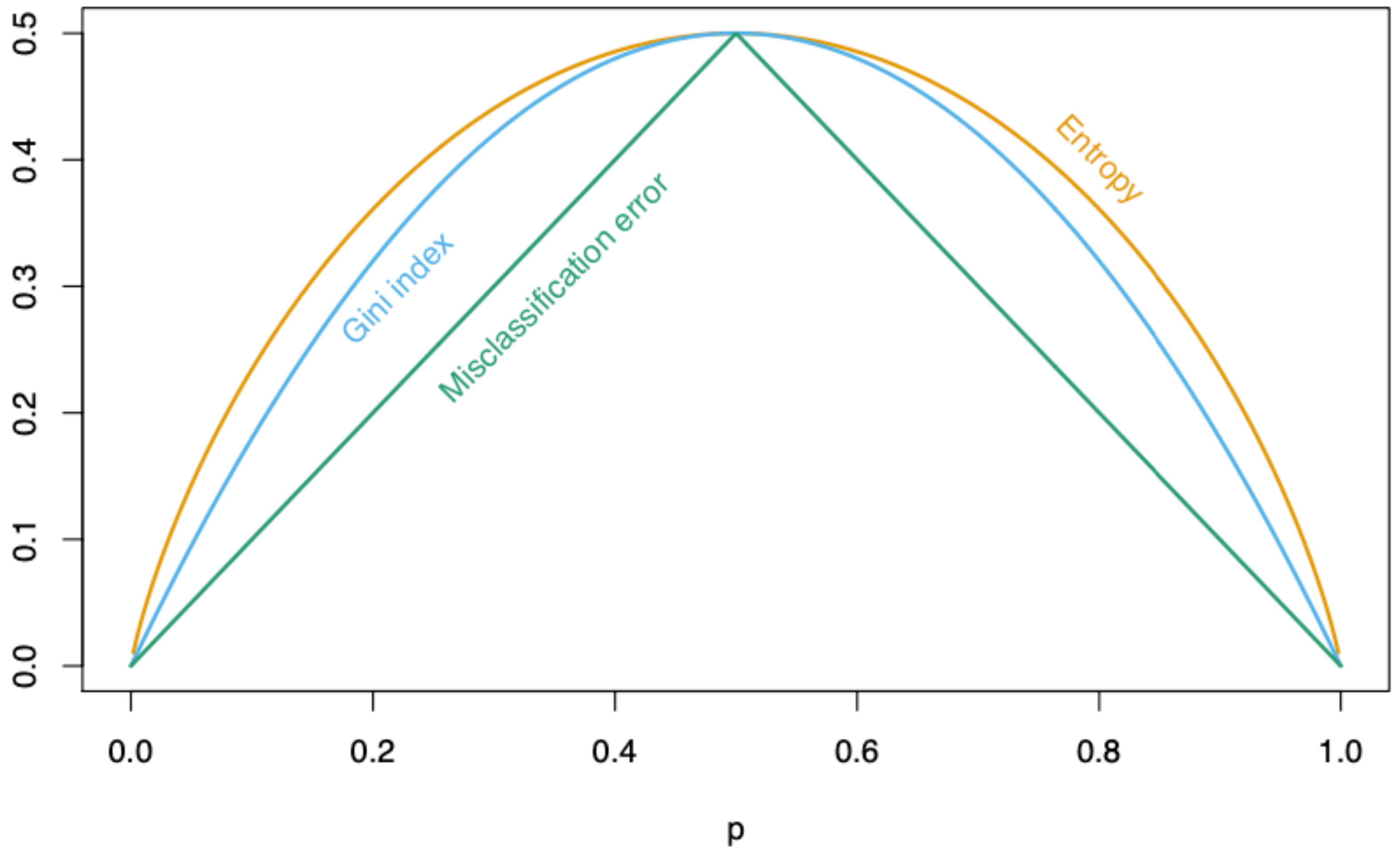
Let $\widehat{p}_m$ be proportion of class 1 in region m. The misclassification error in that region is $\min(\widehat{p}_m, 1 - \widehat{p}_m)$.

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

$$\text{Gini index} = 2\widehat{p}_m(1 - \widehat{p}_m).$$

Find split that minimizes the total impurity of the regions.





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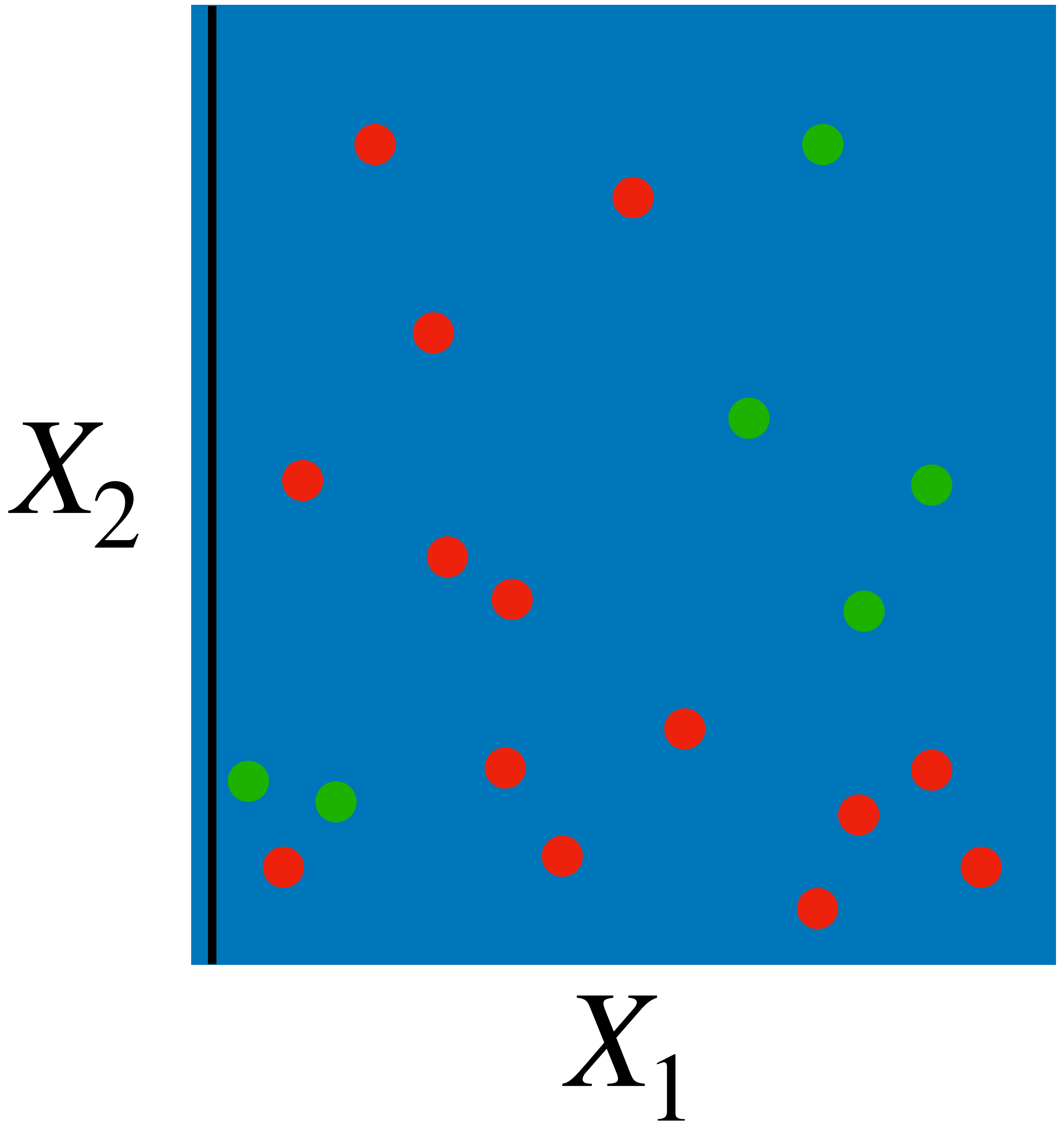

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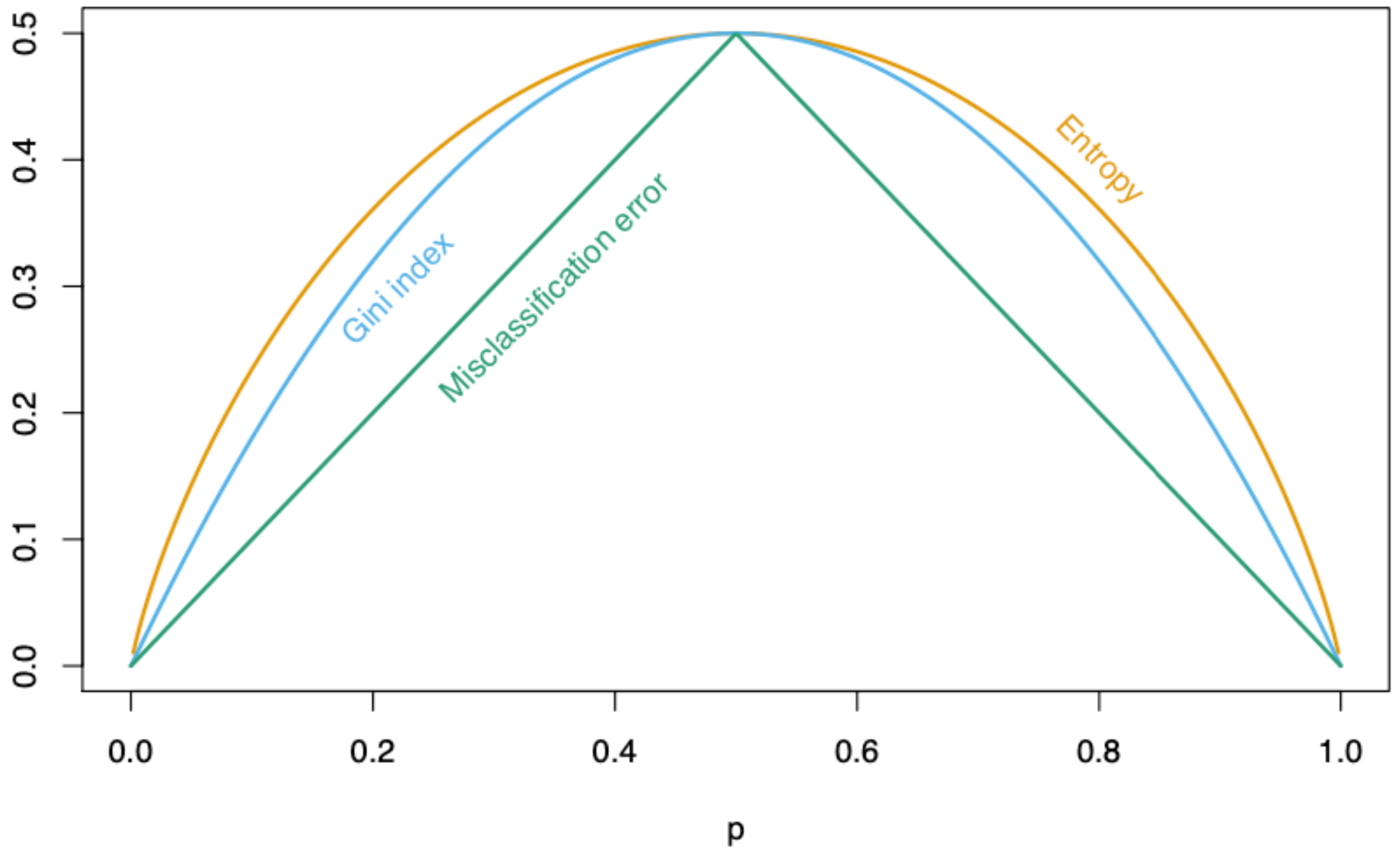

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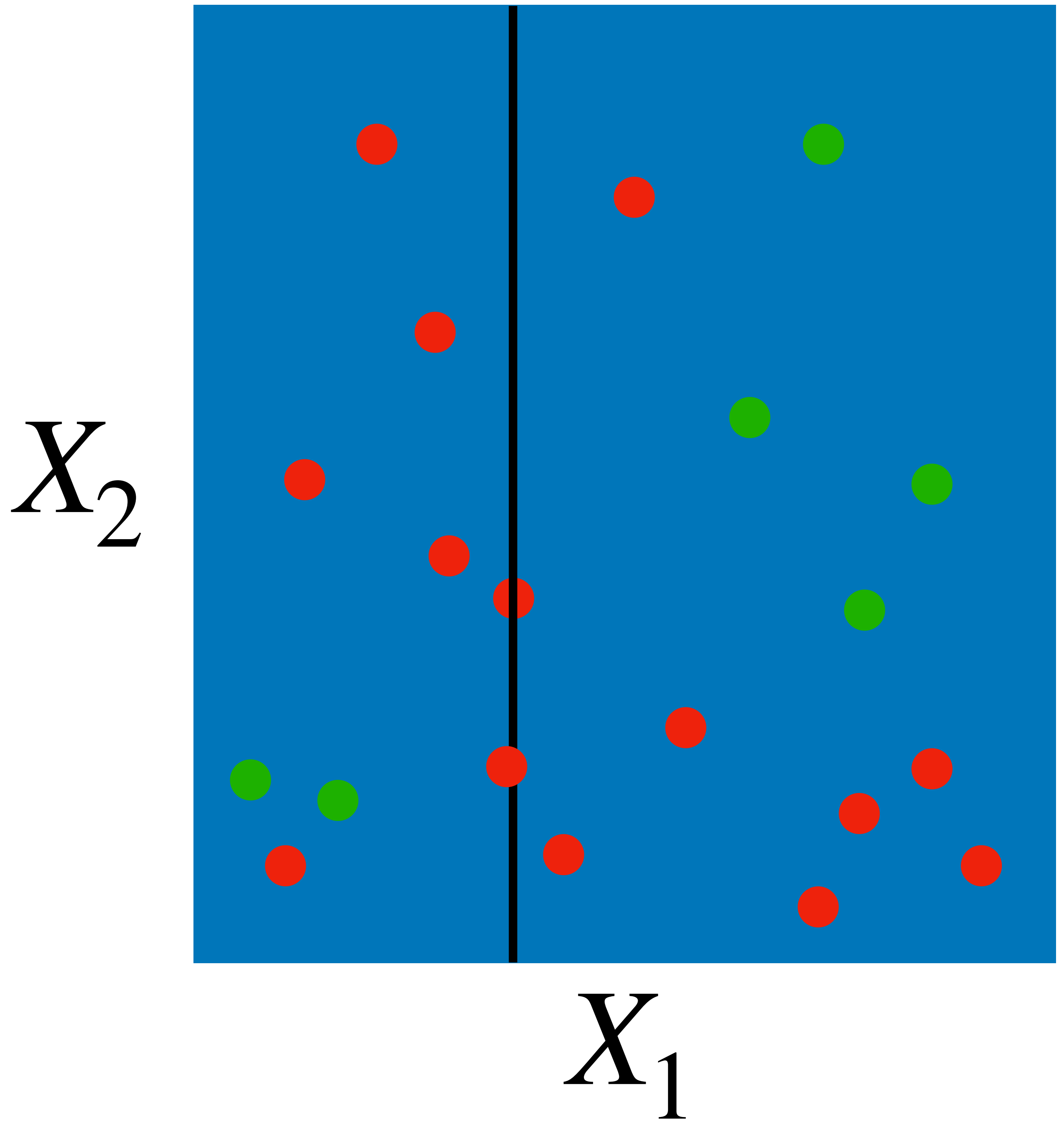

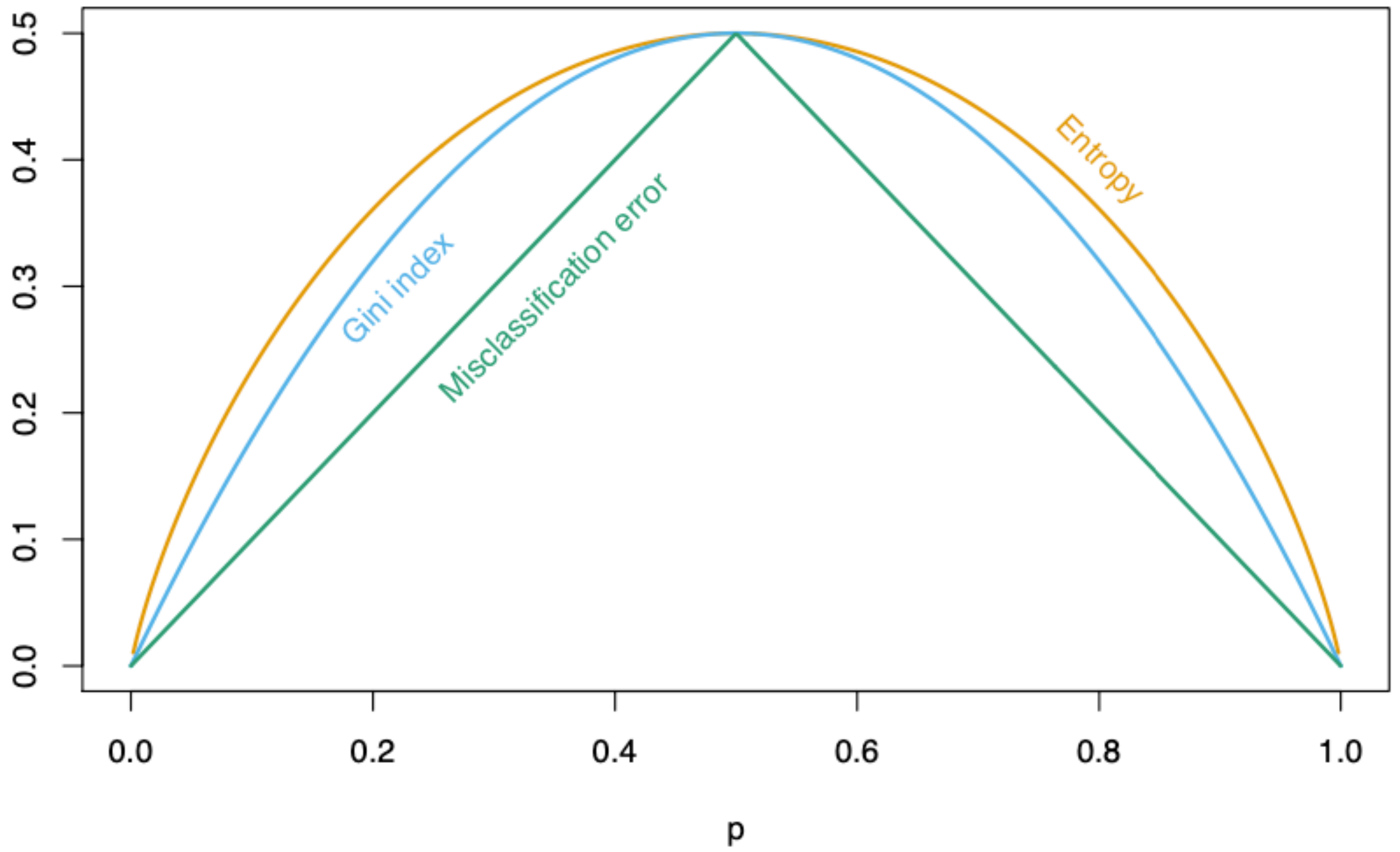

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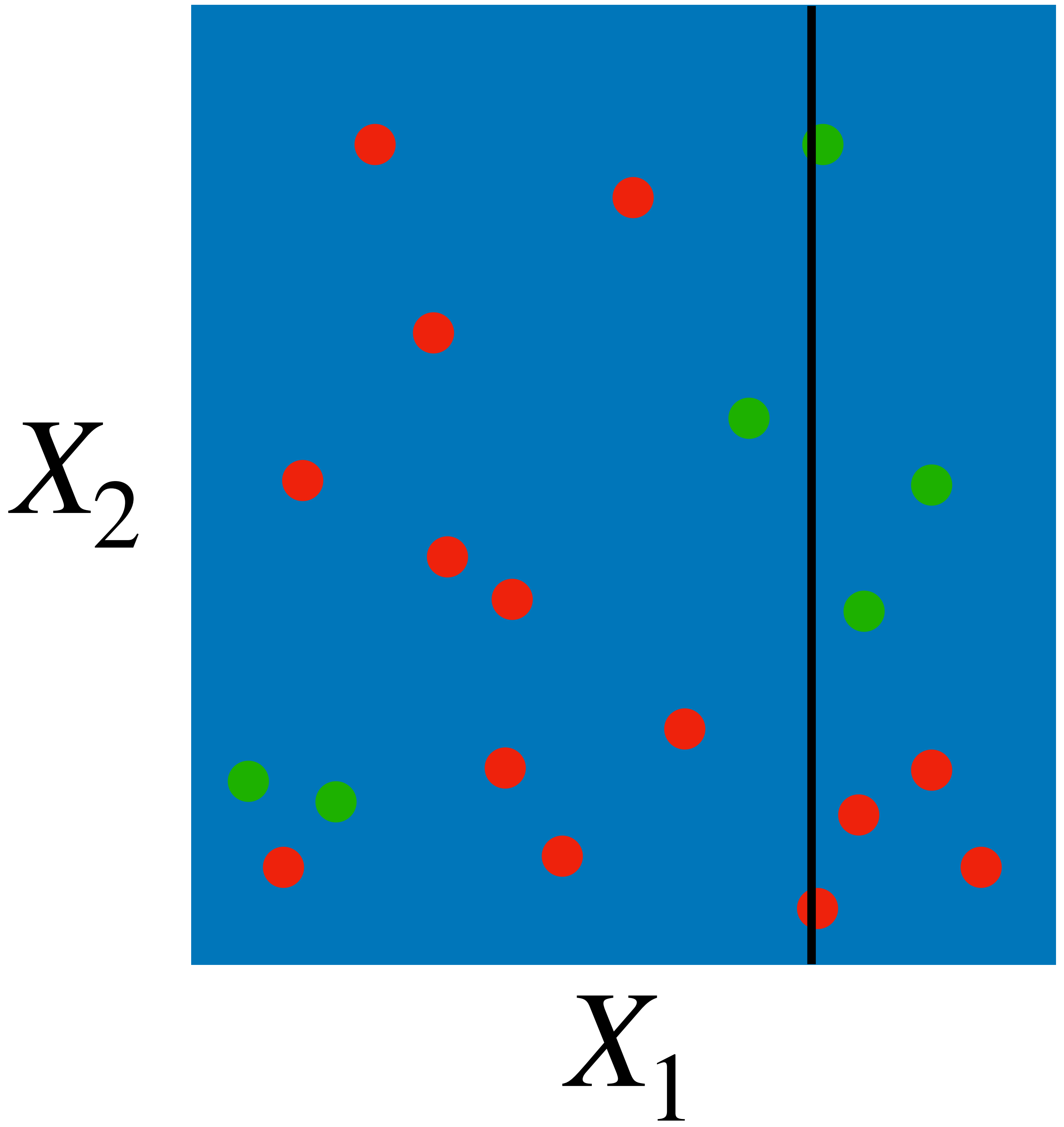

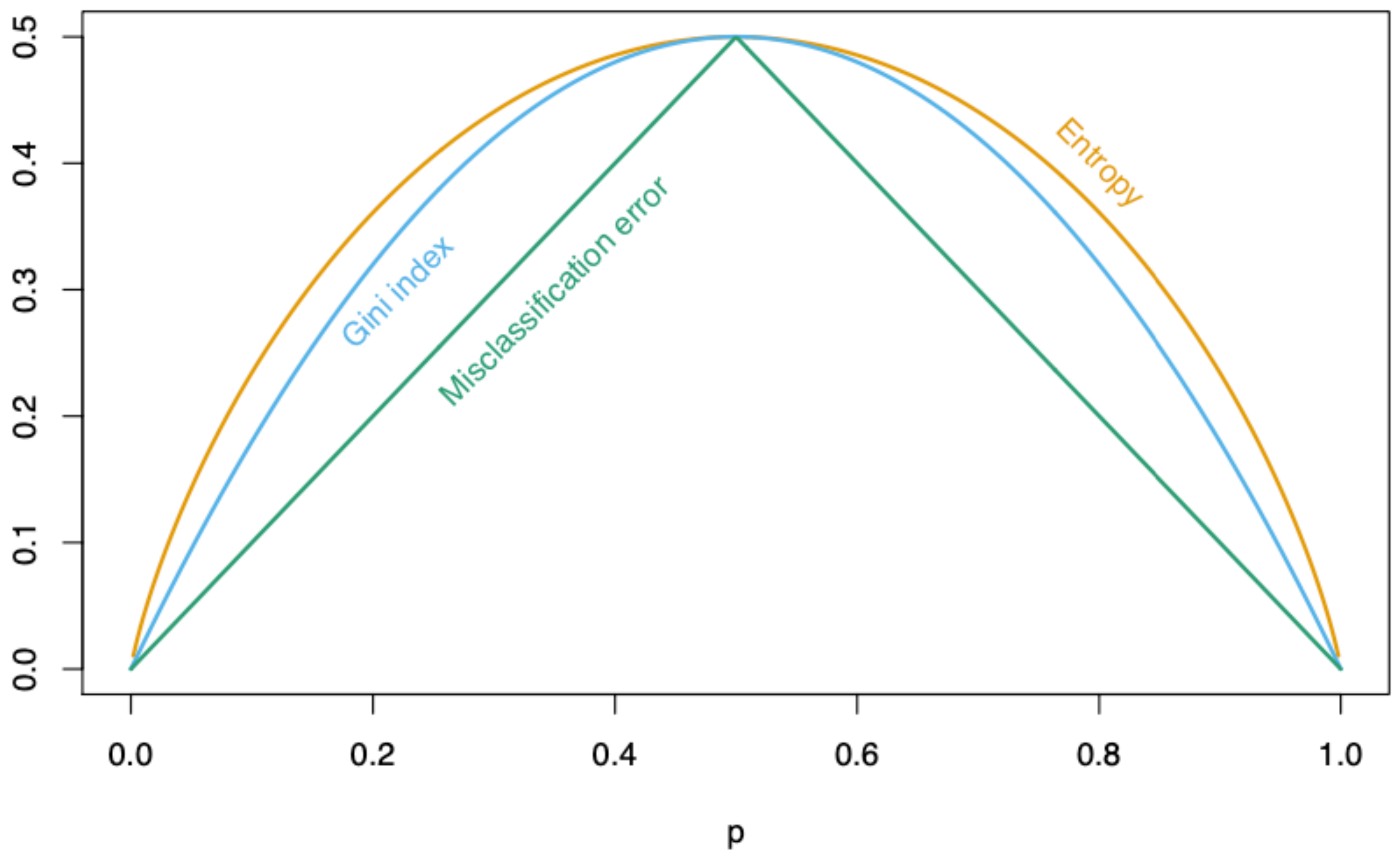

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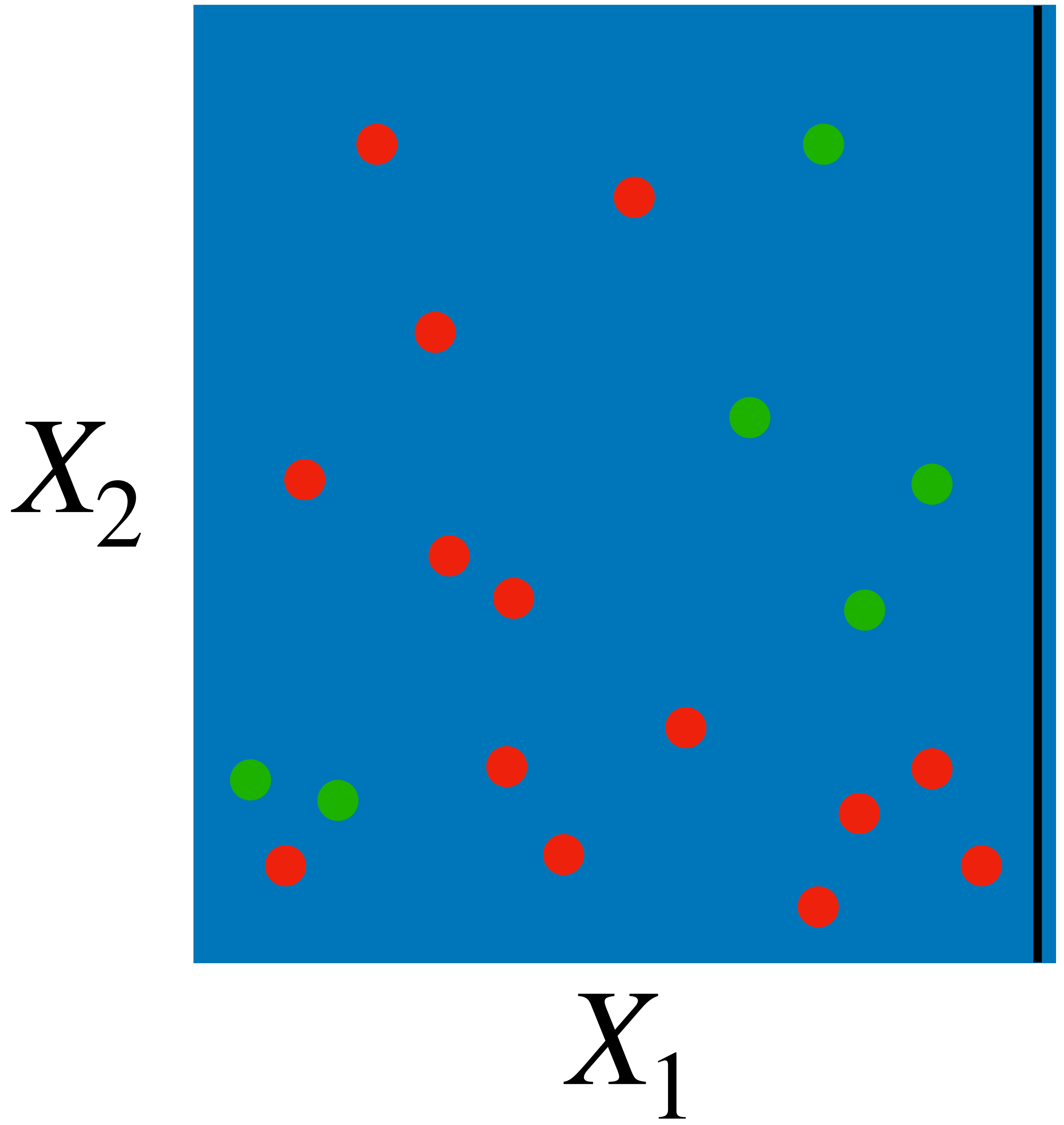

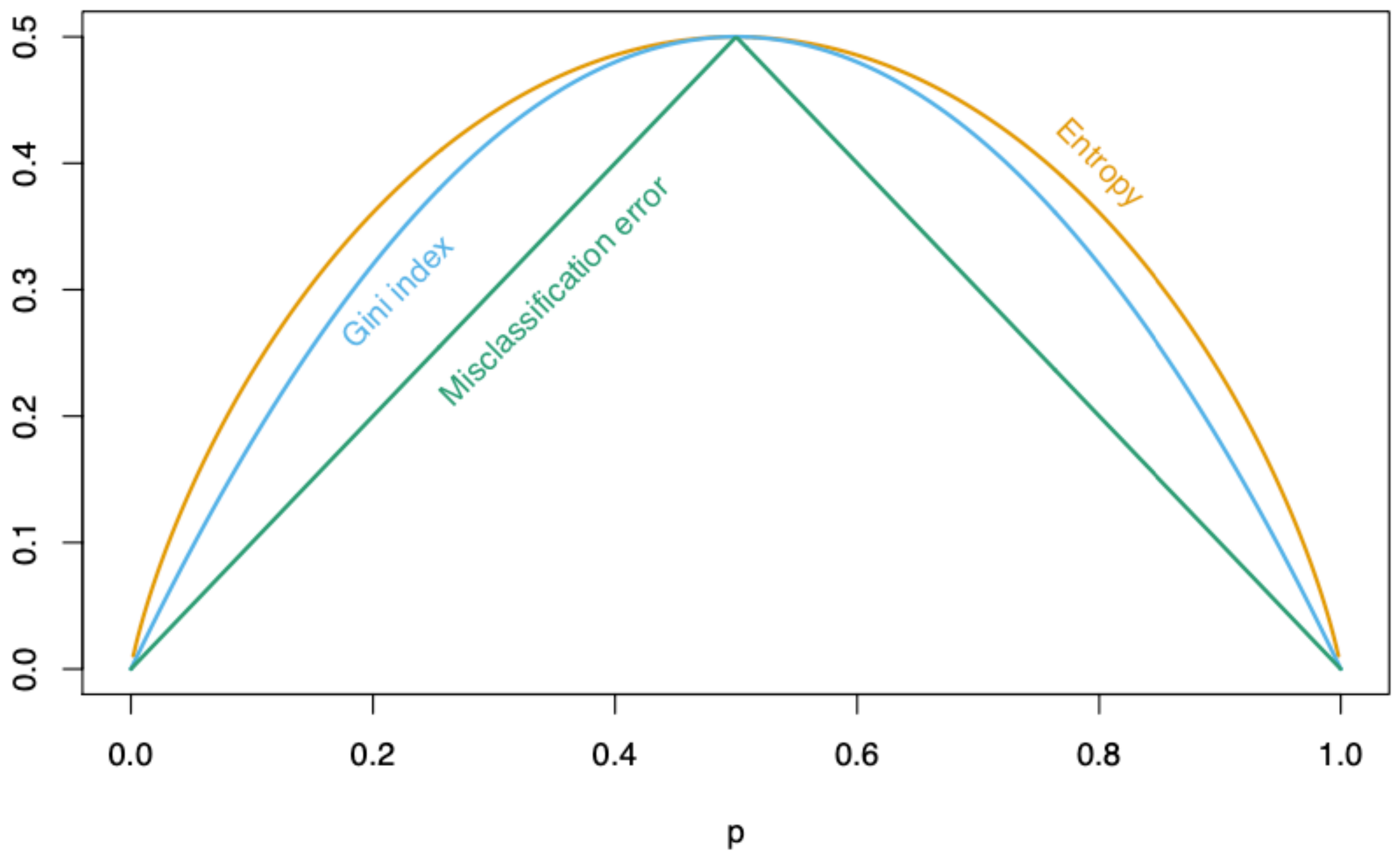

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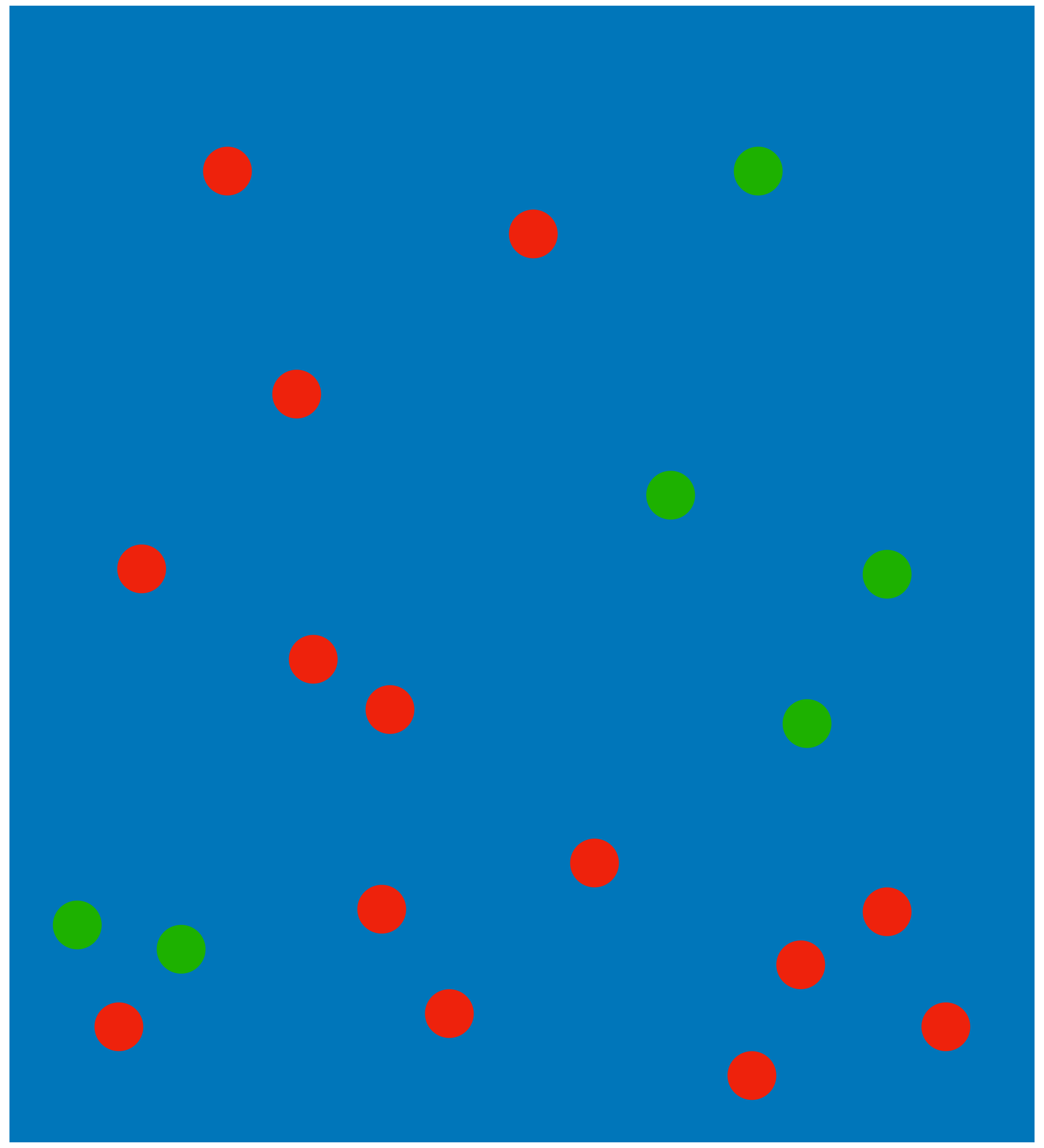
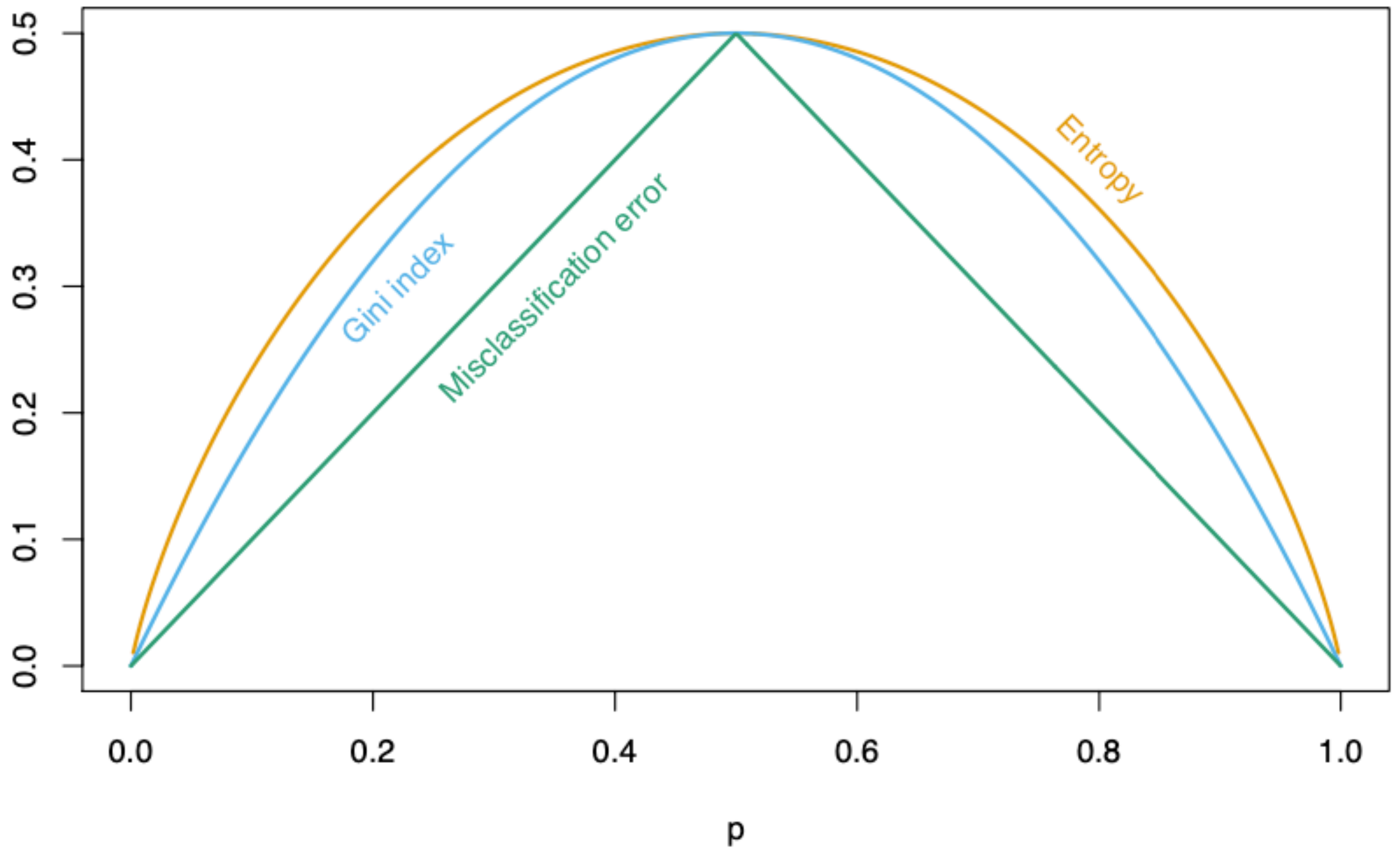
X_2



X_1



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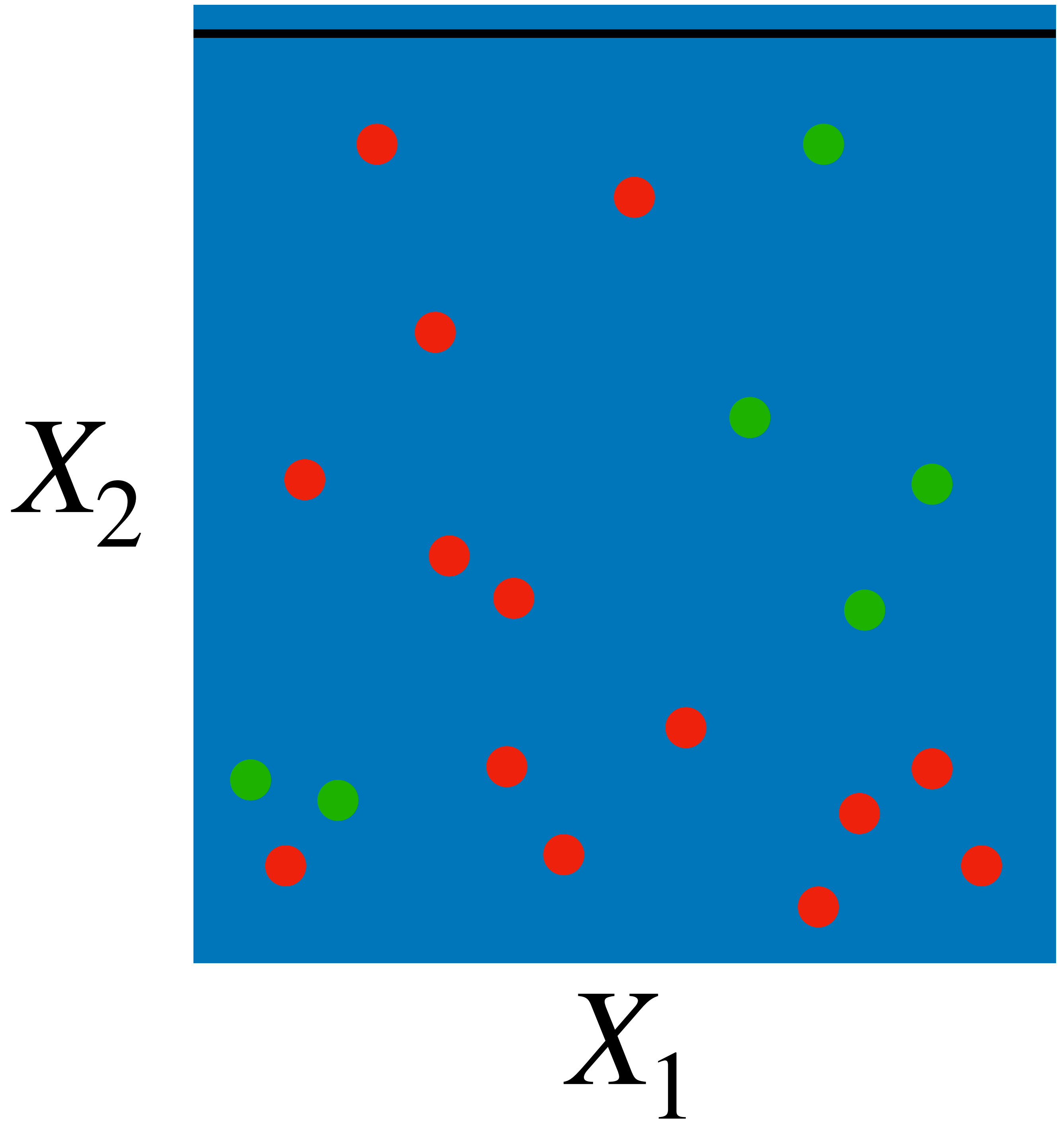

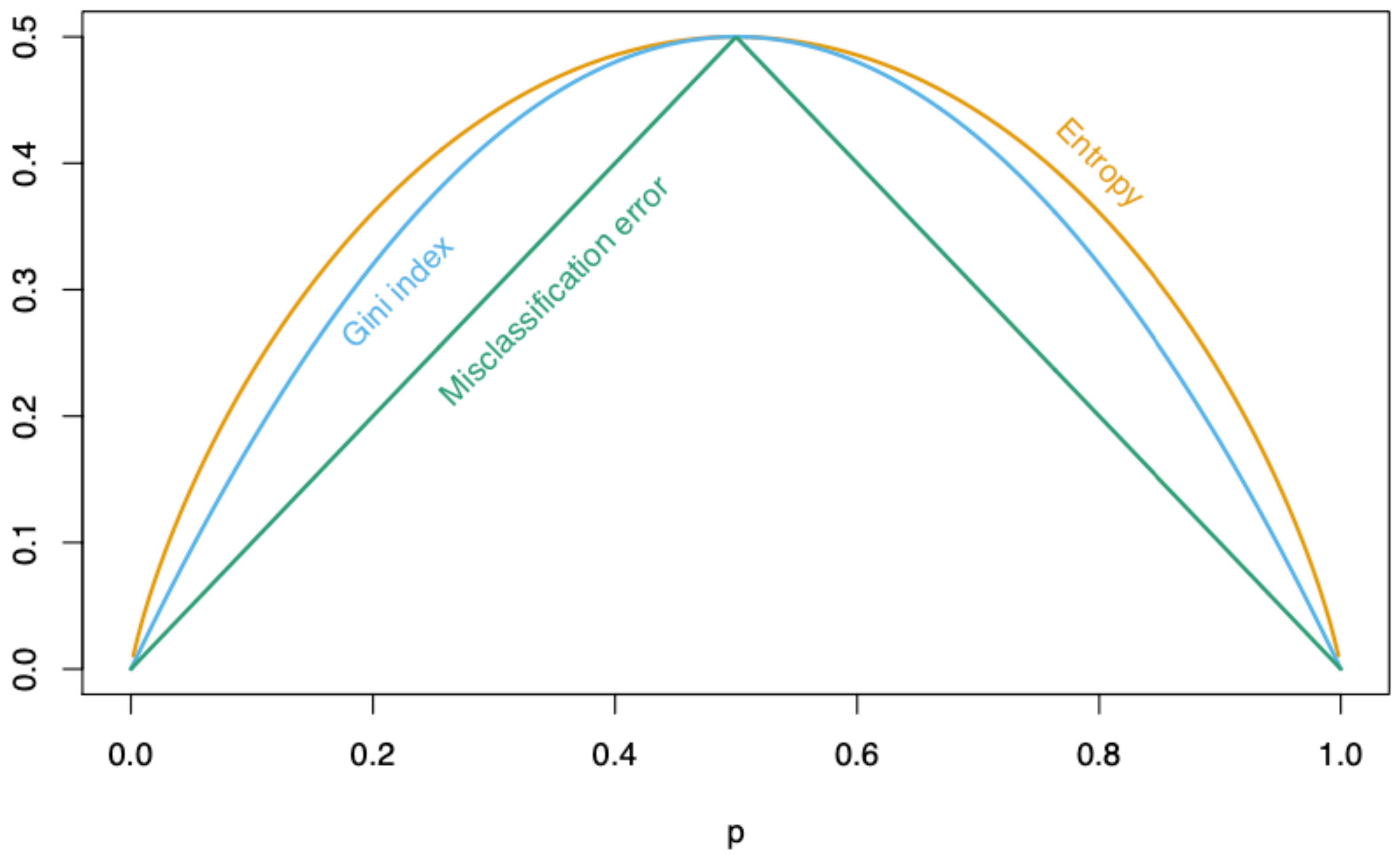

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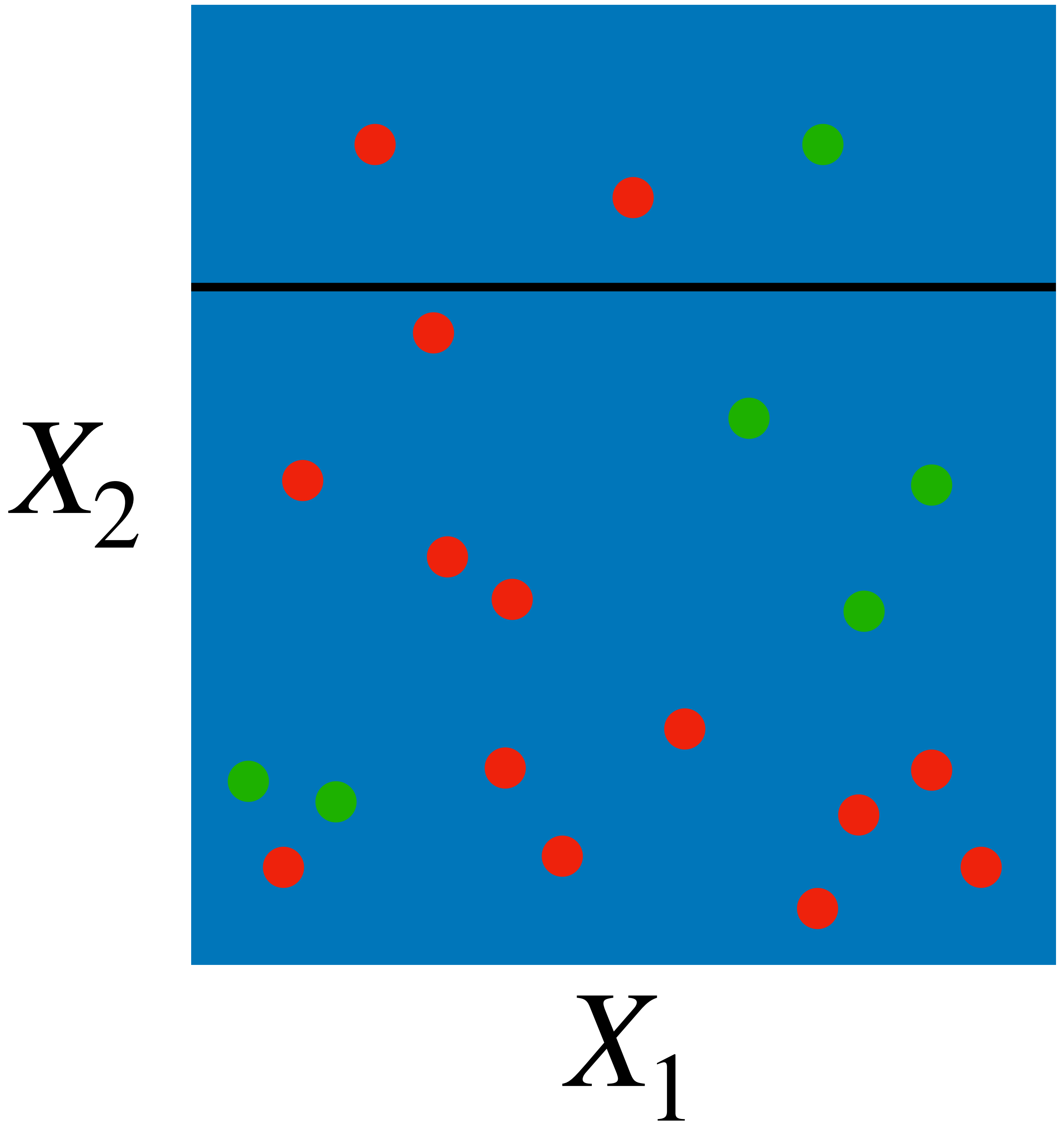

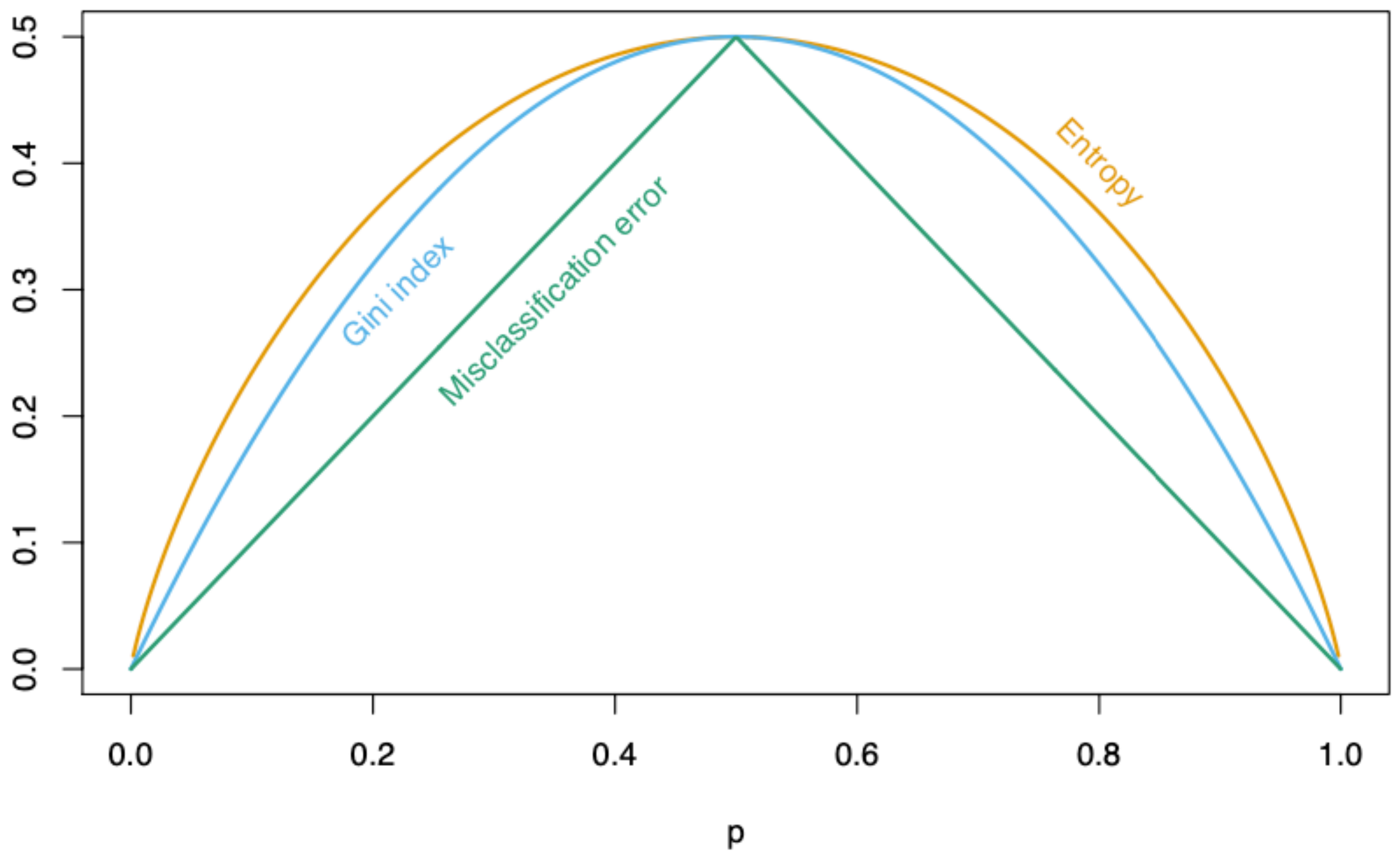

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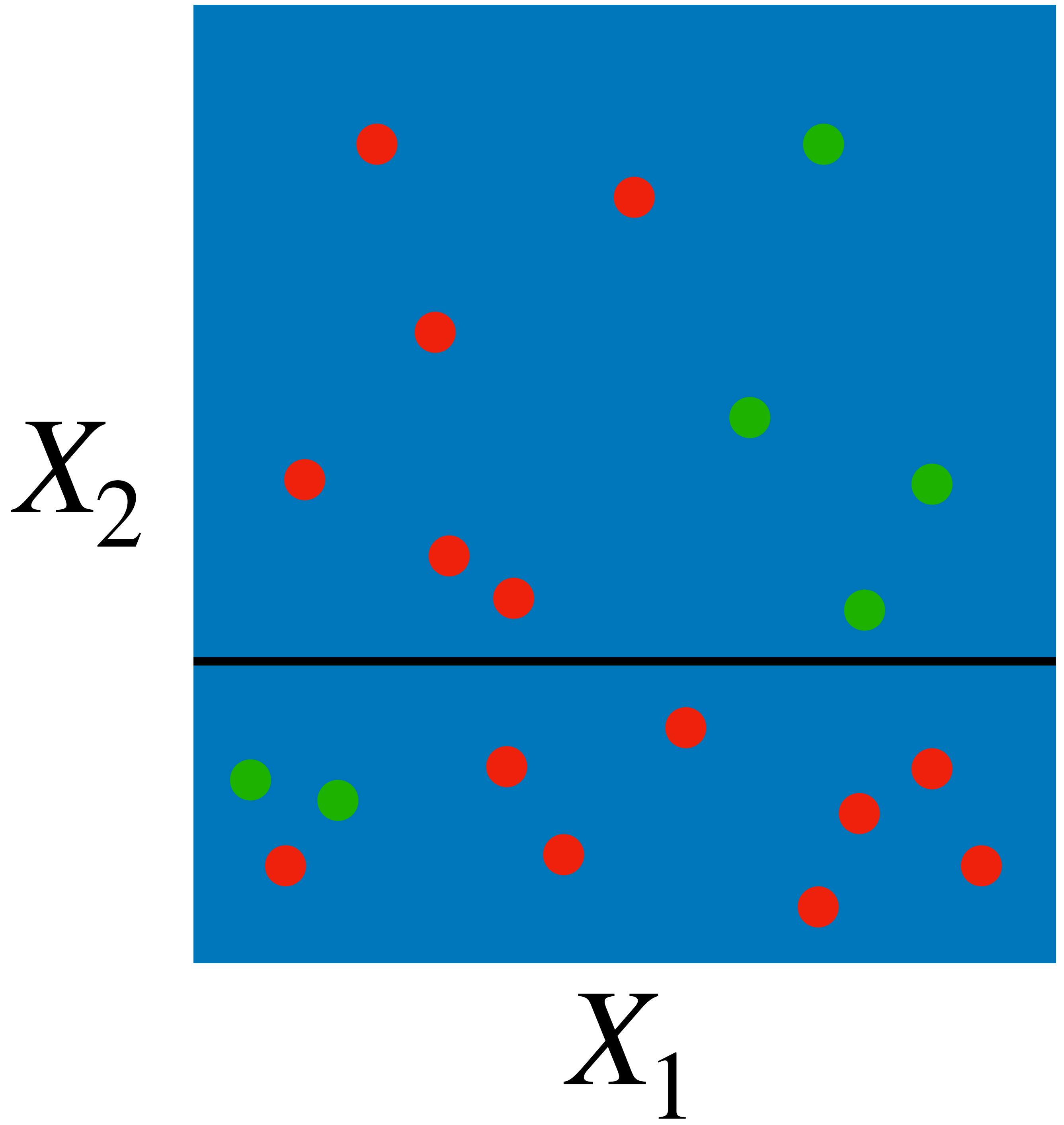

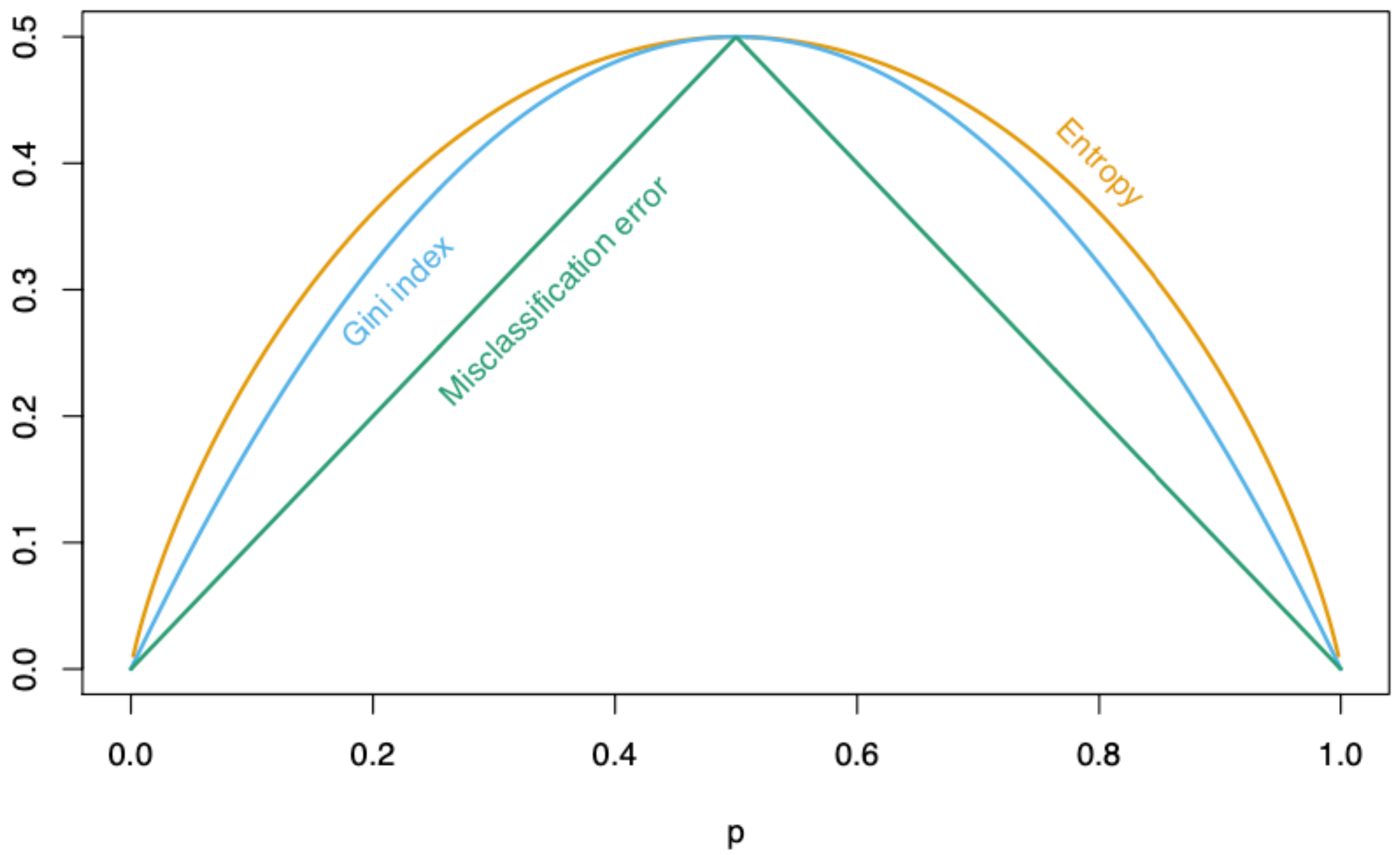

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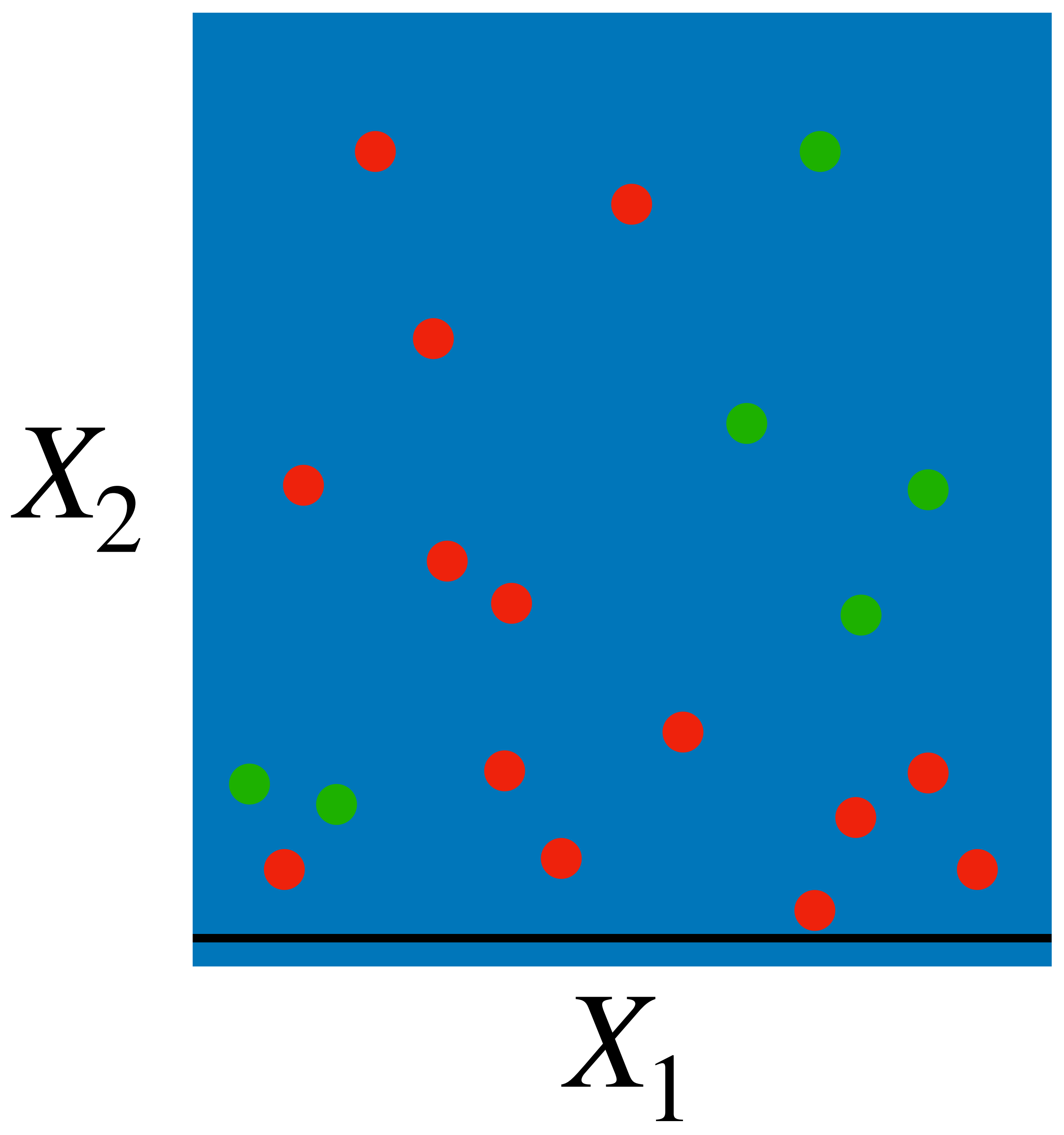

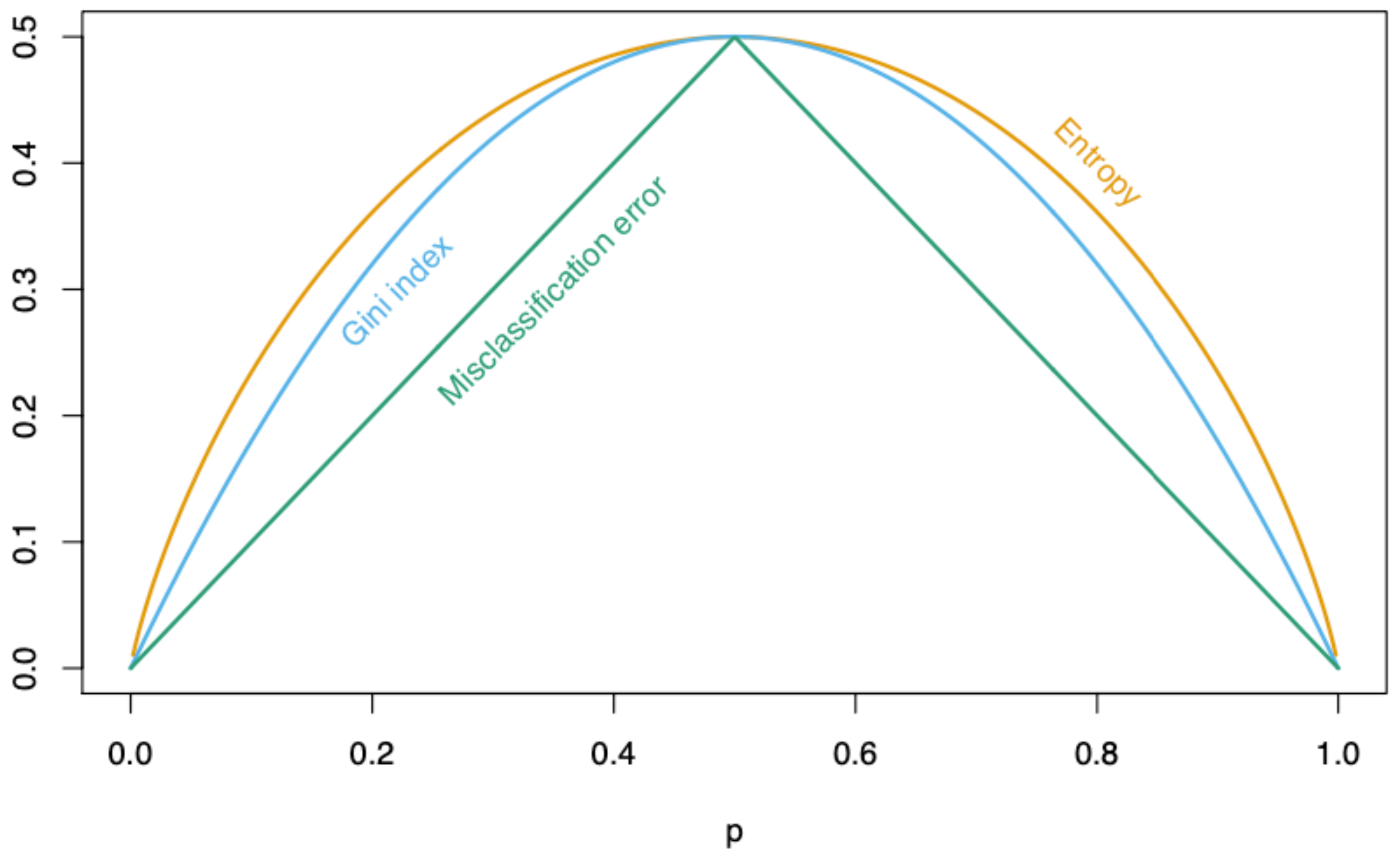

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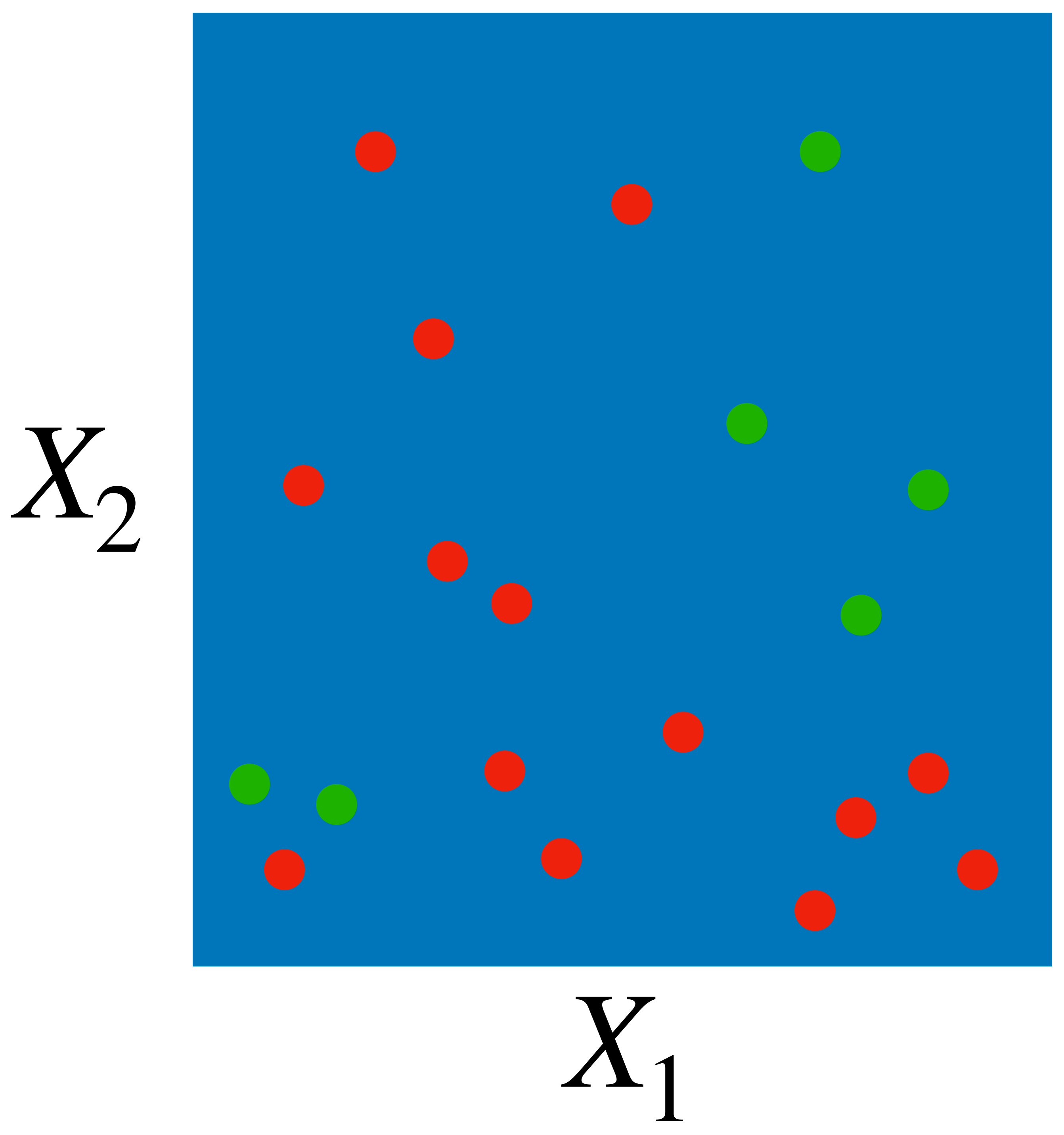

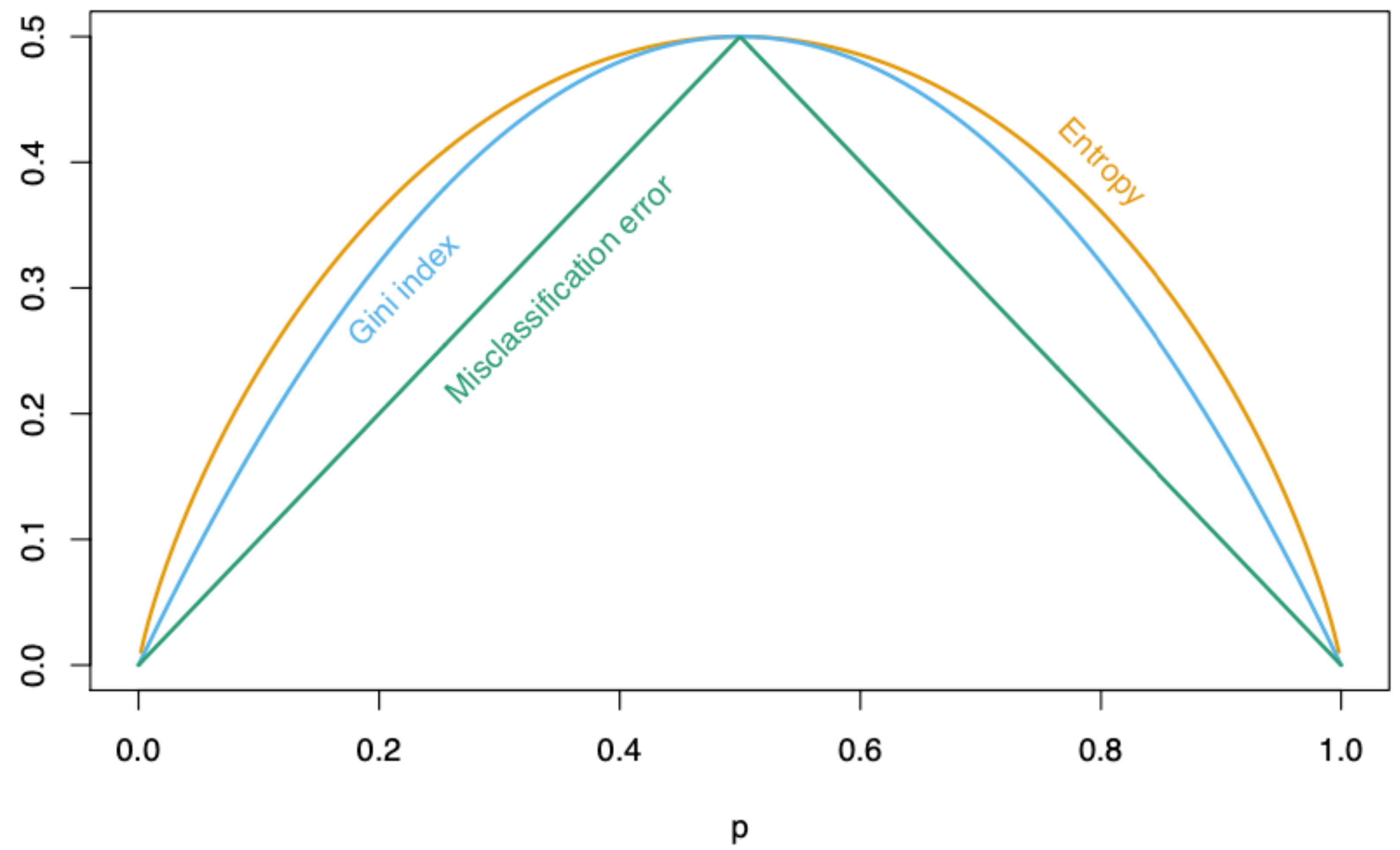

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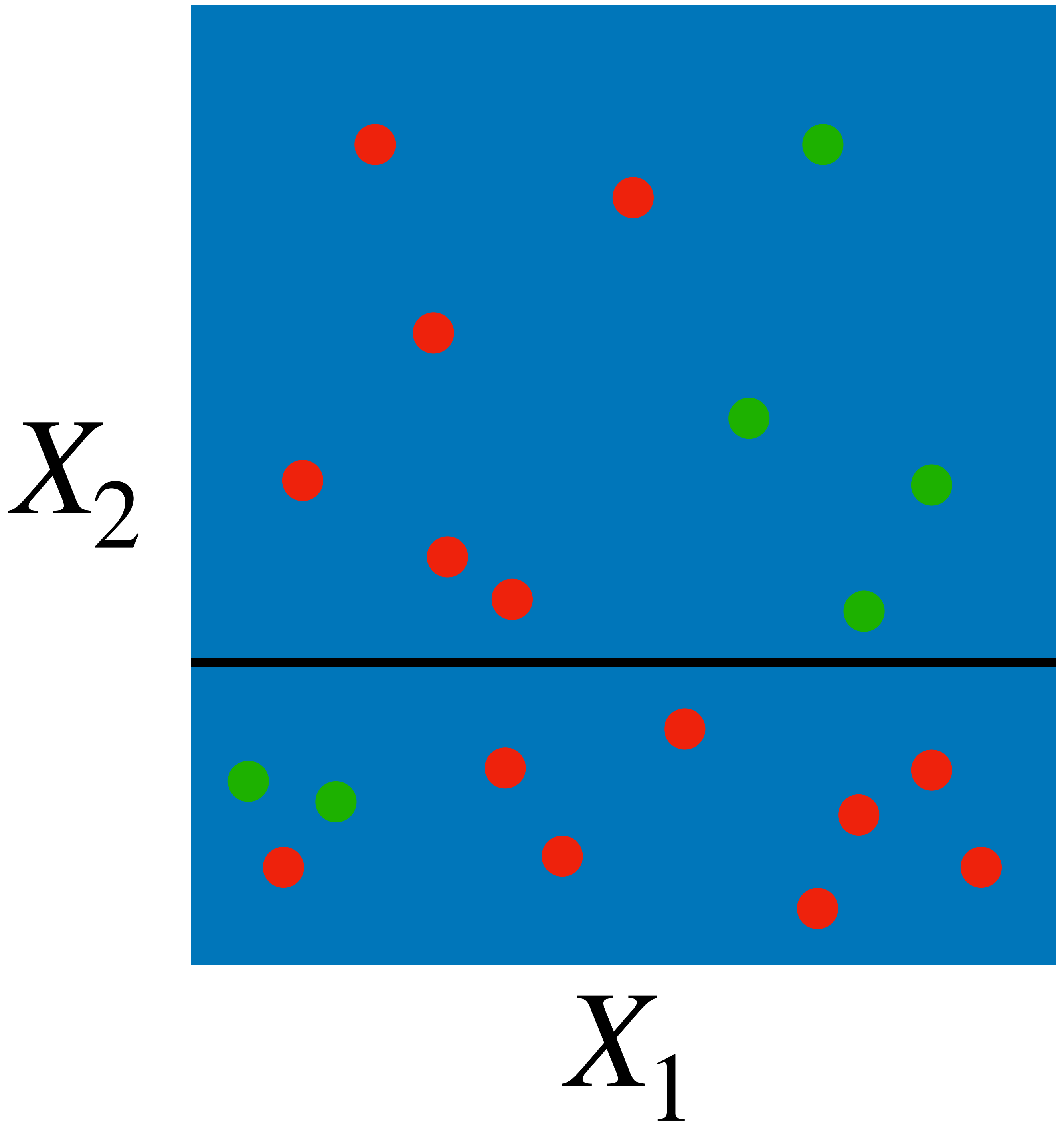

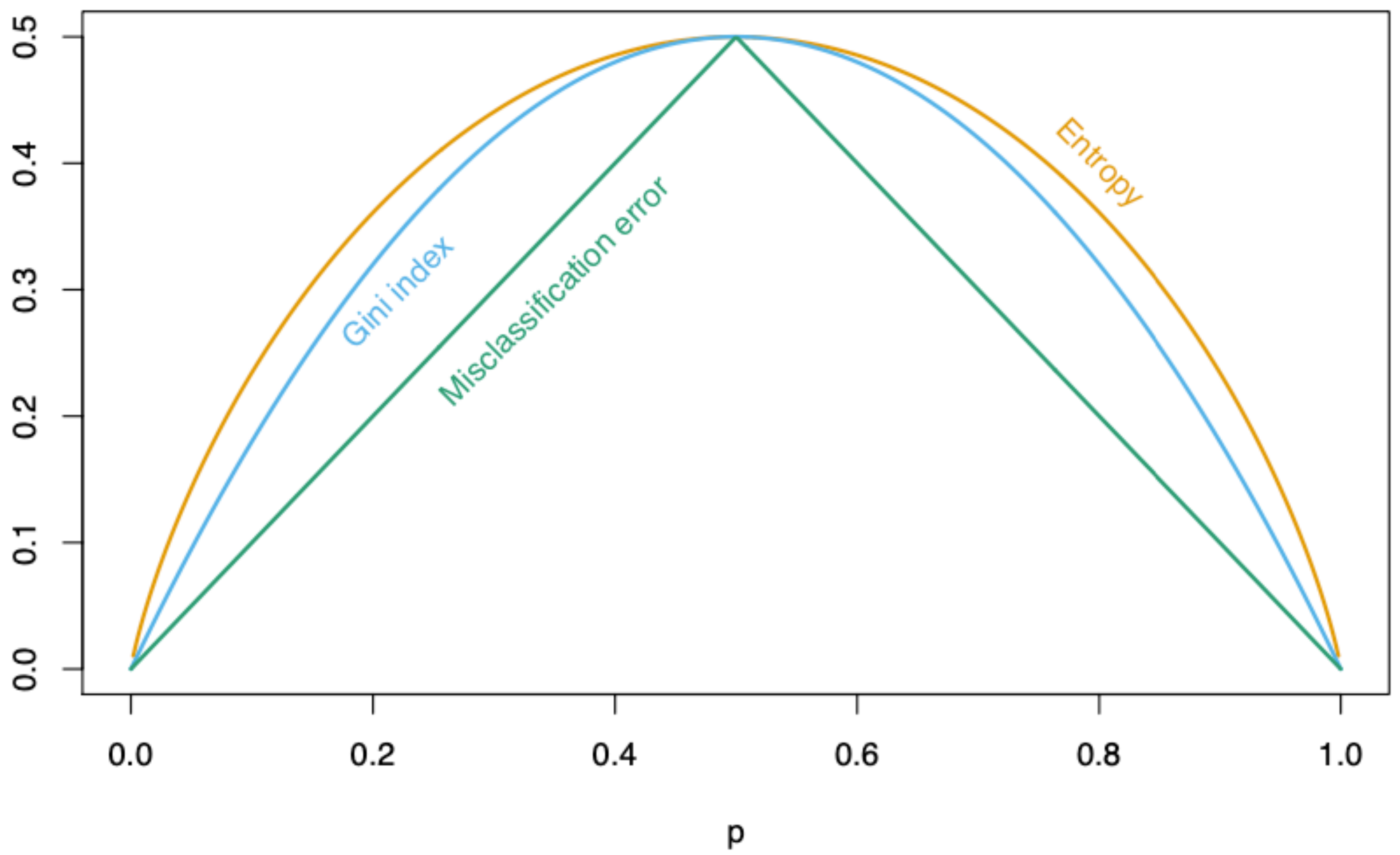

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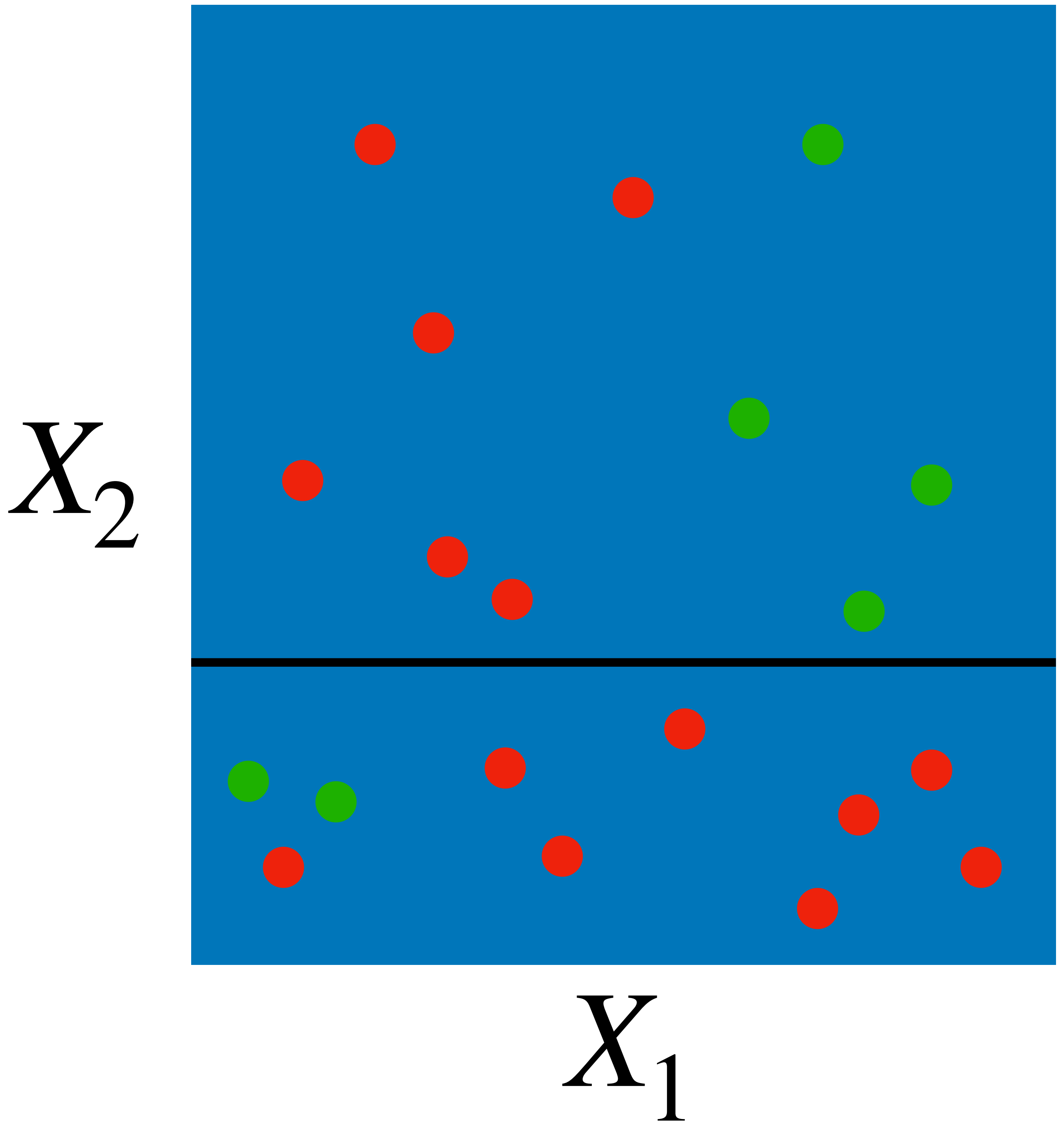

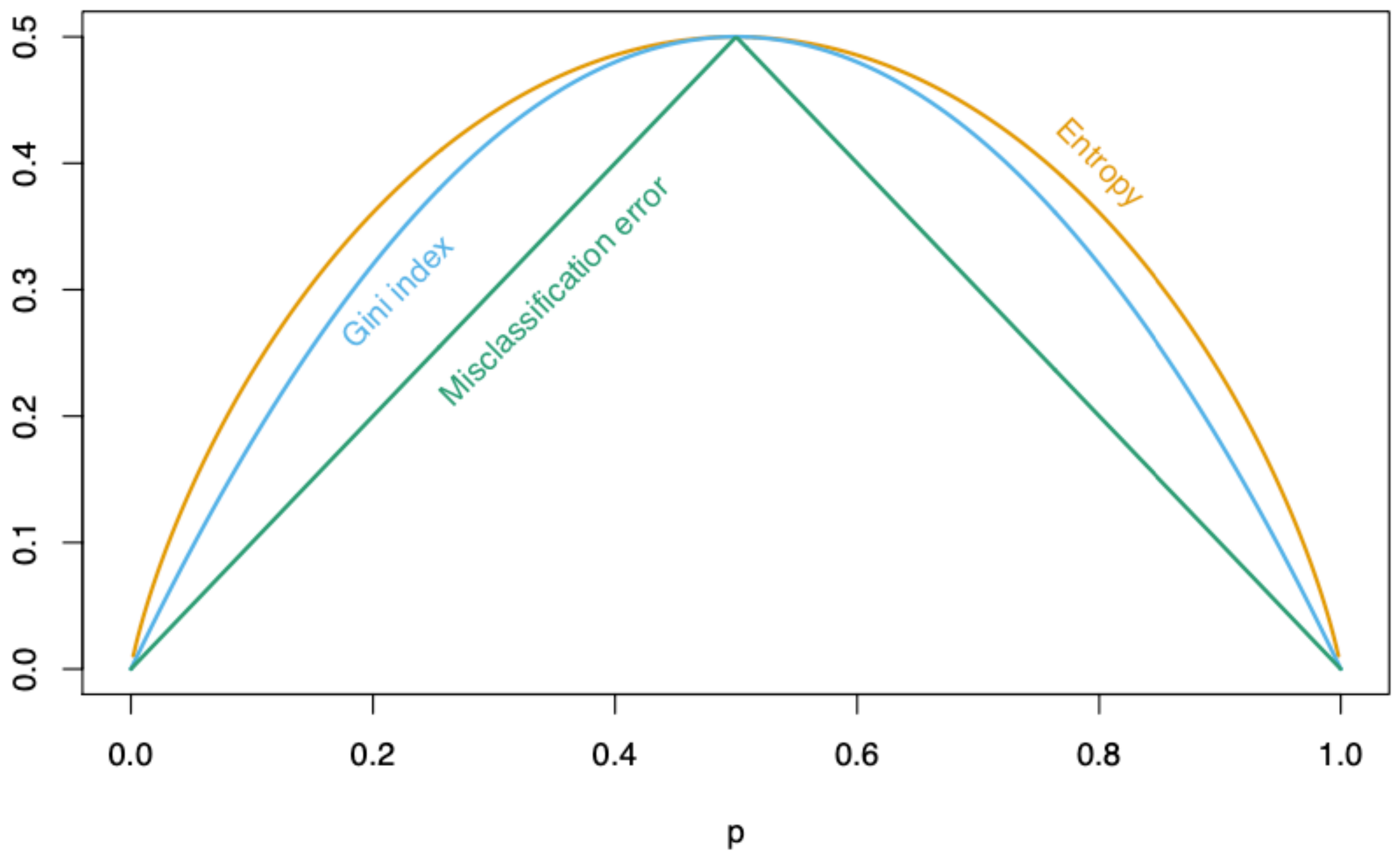

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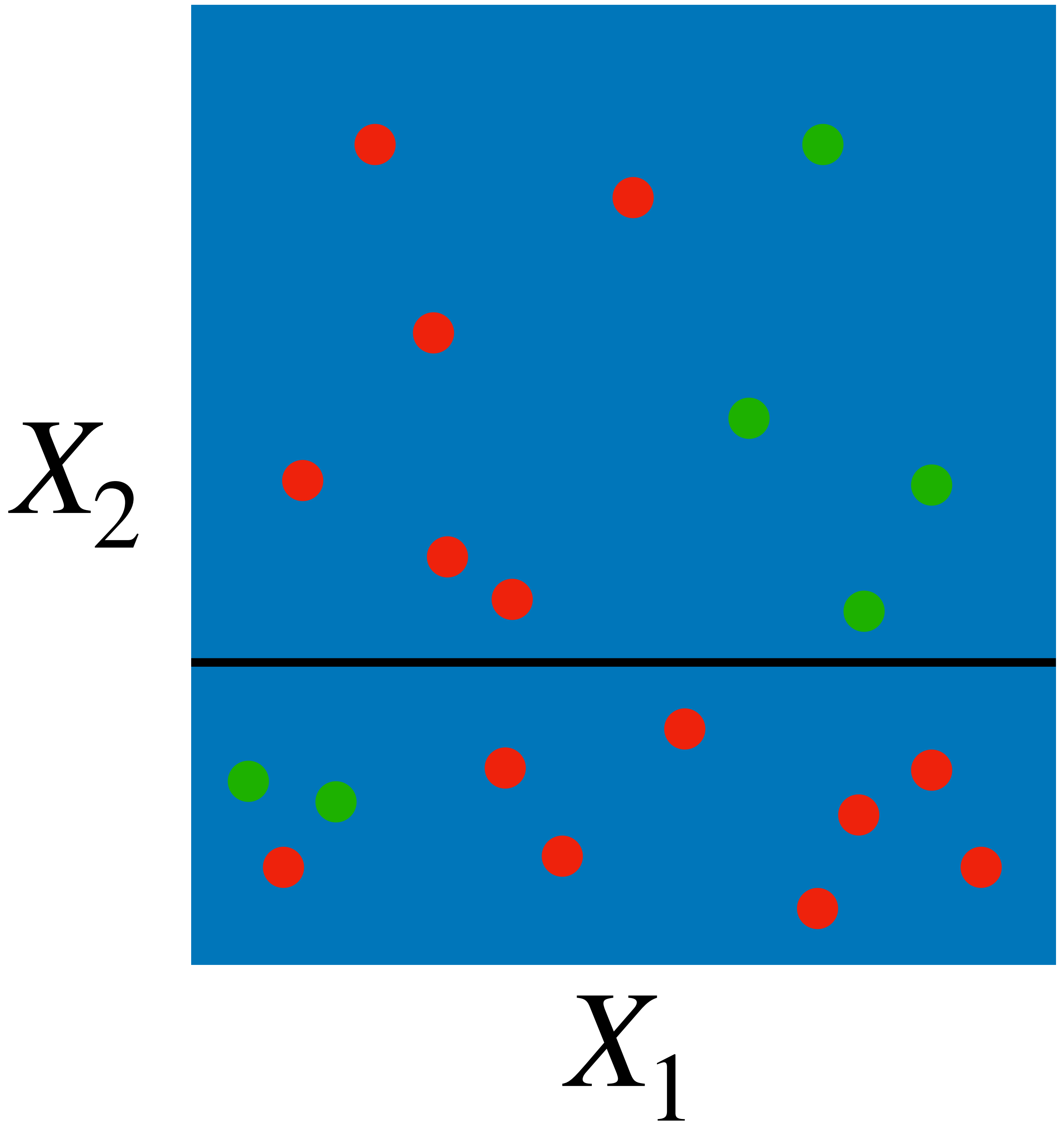

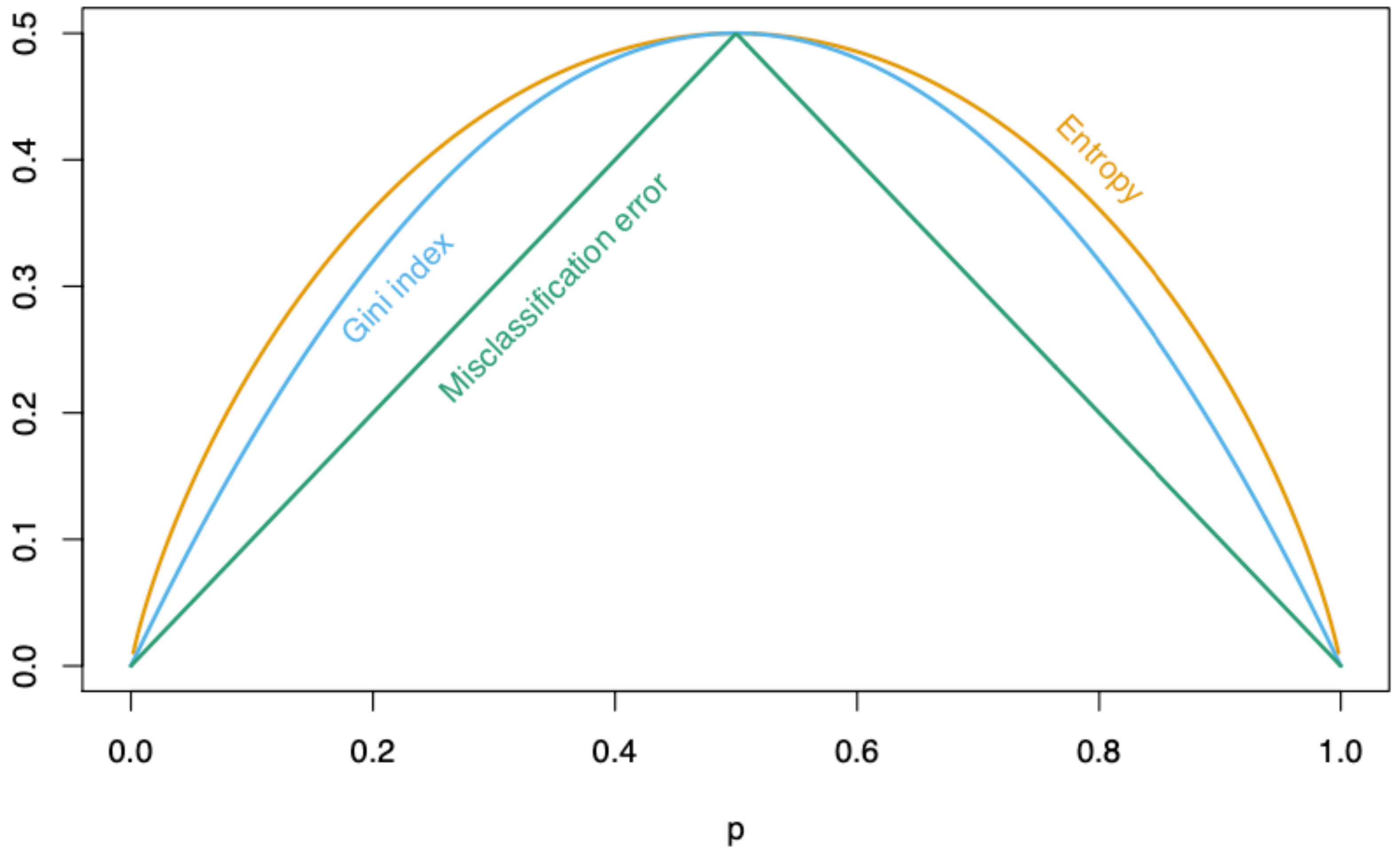

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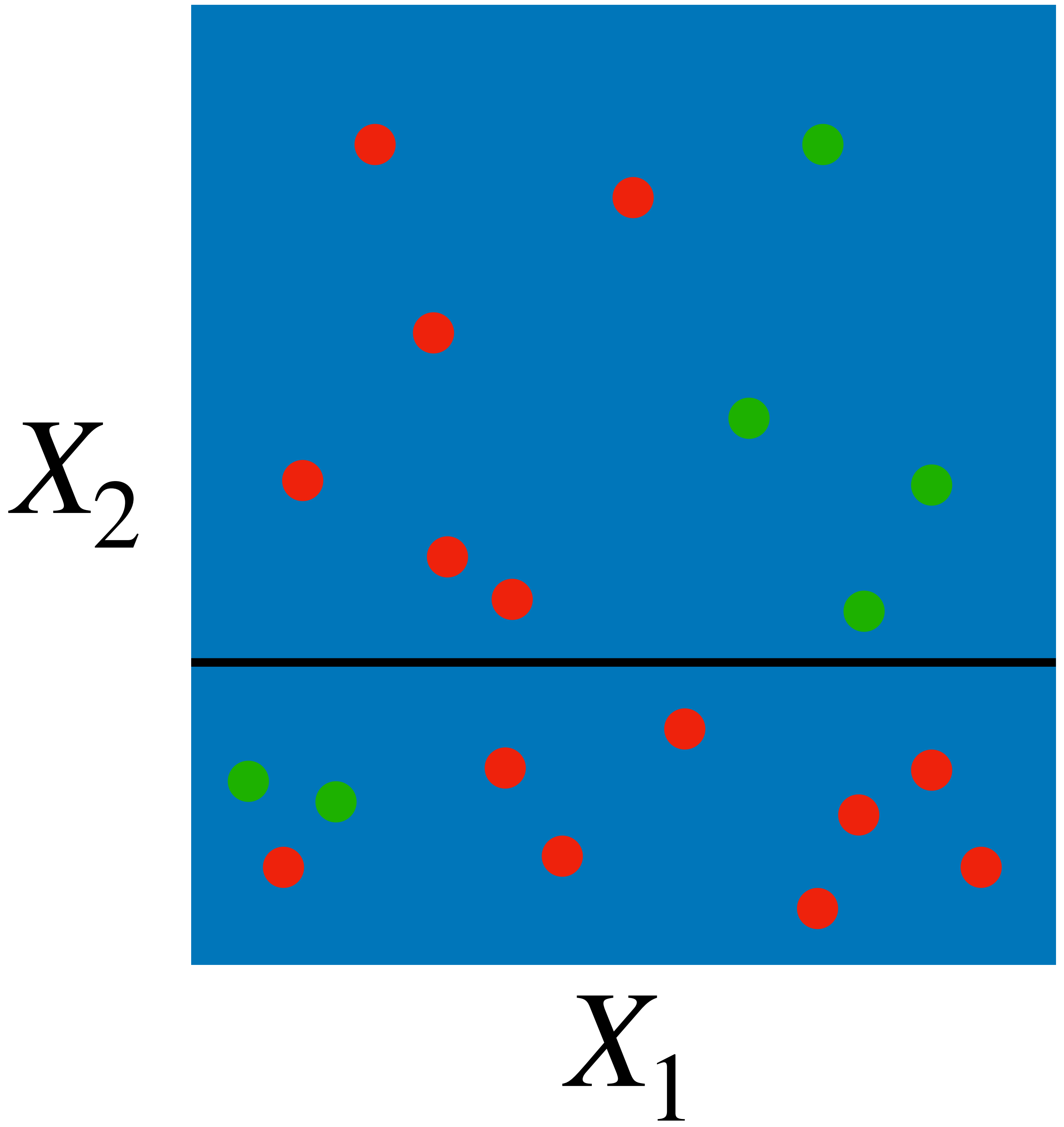

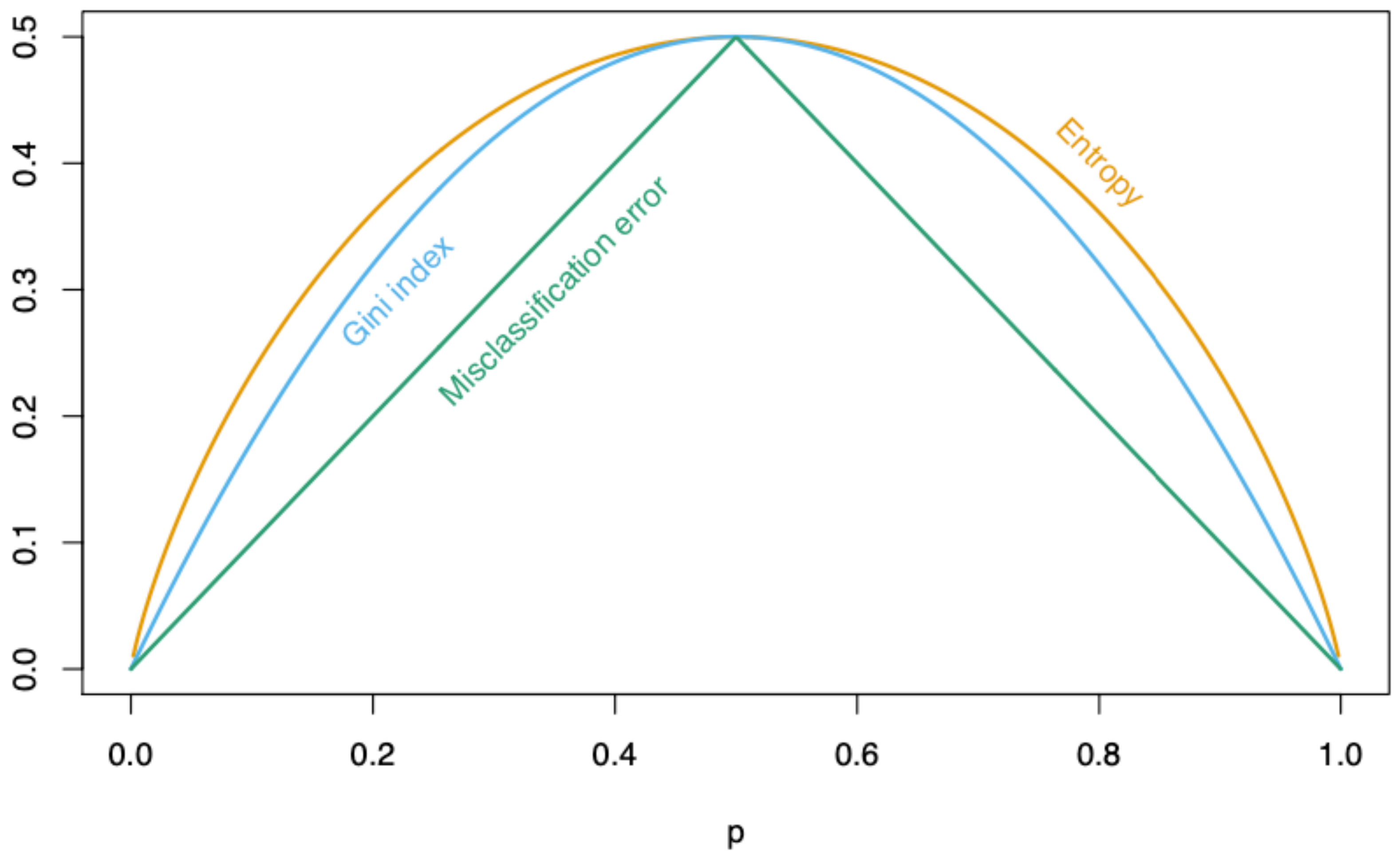

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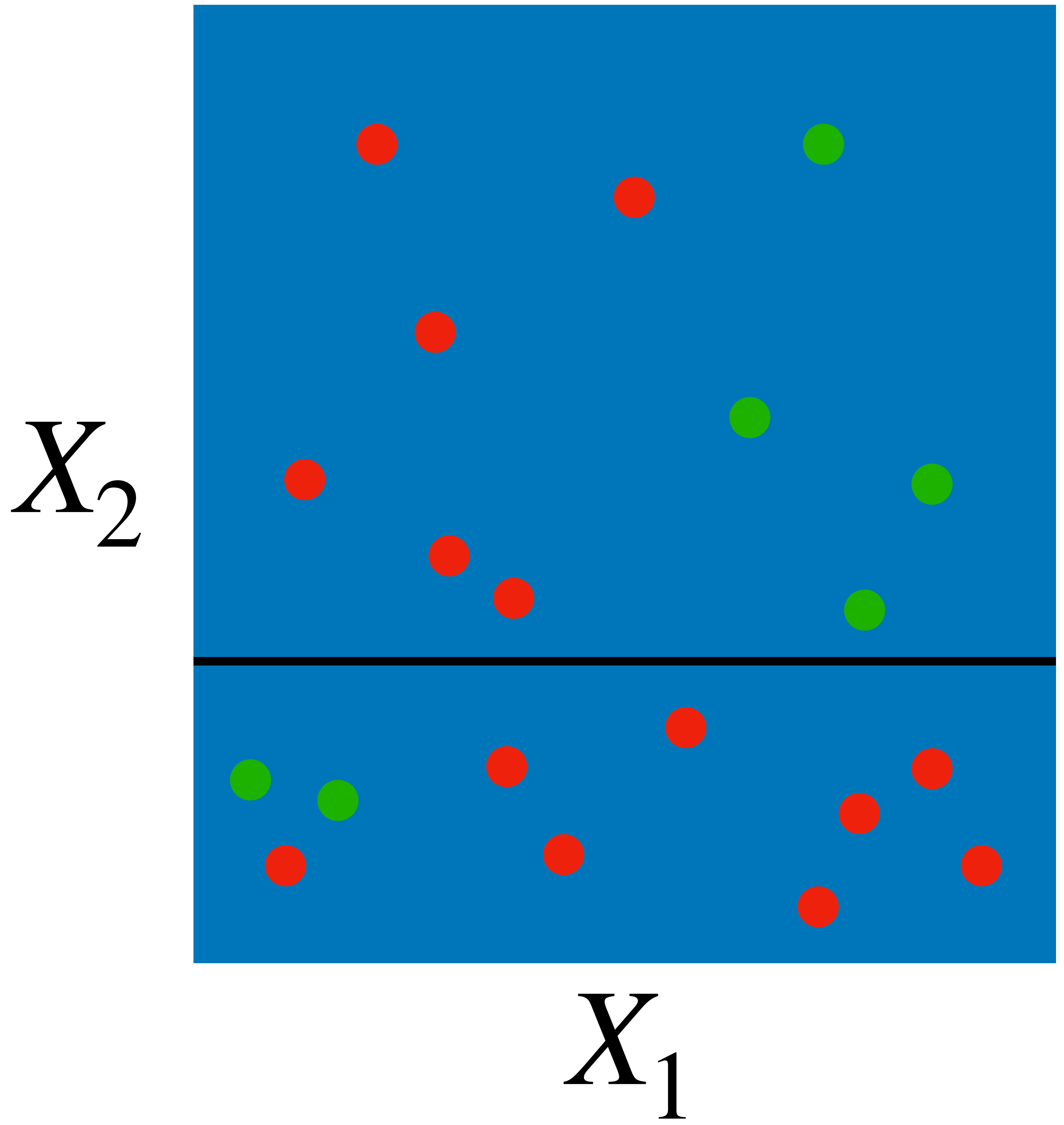

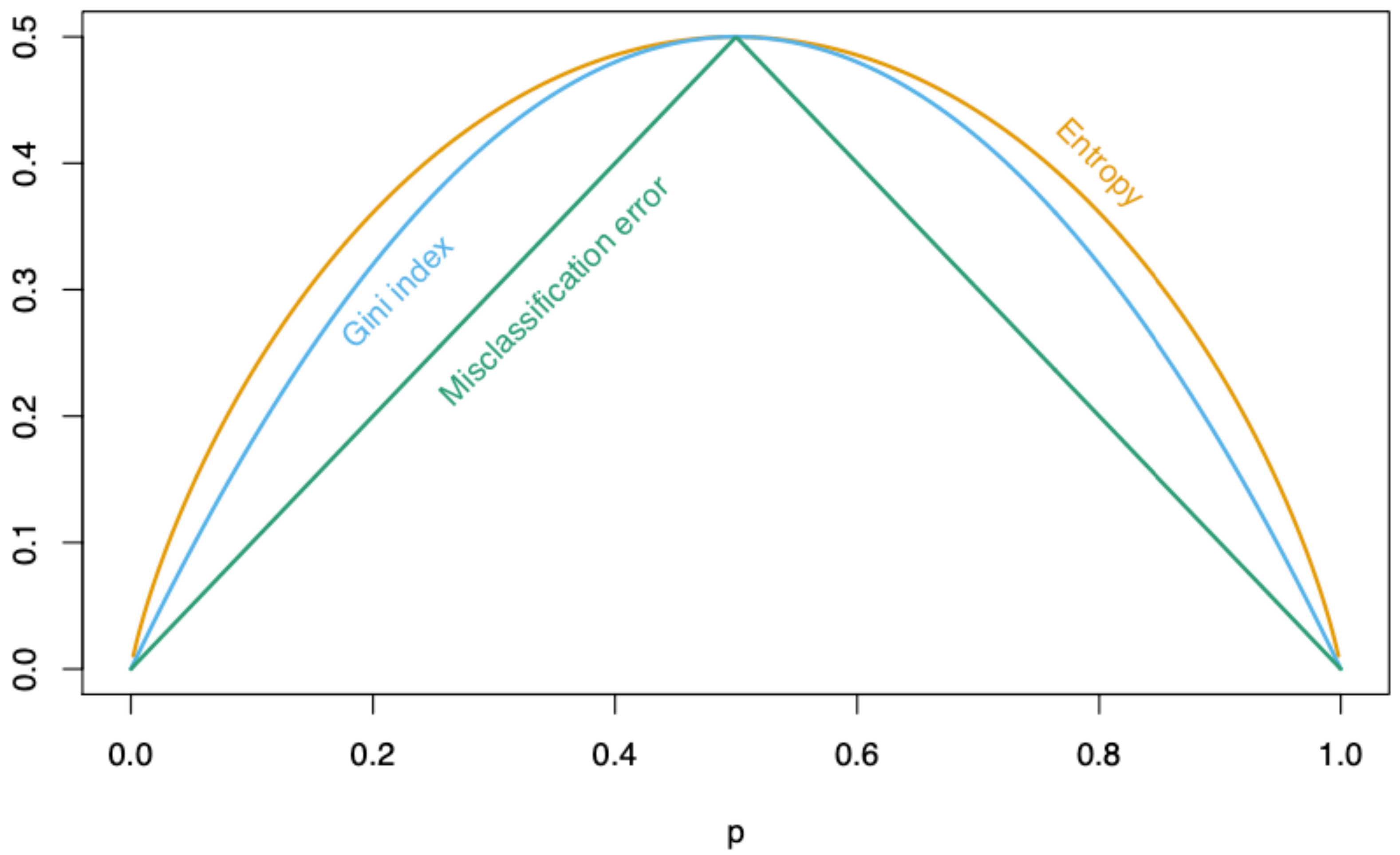

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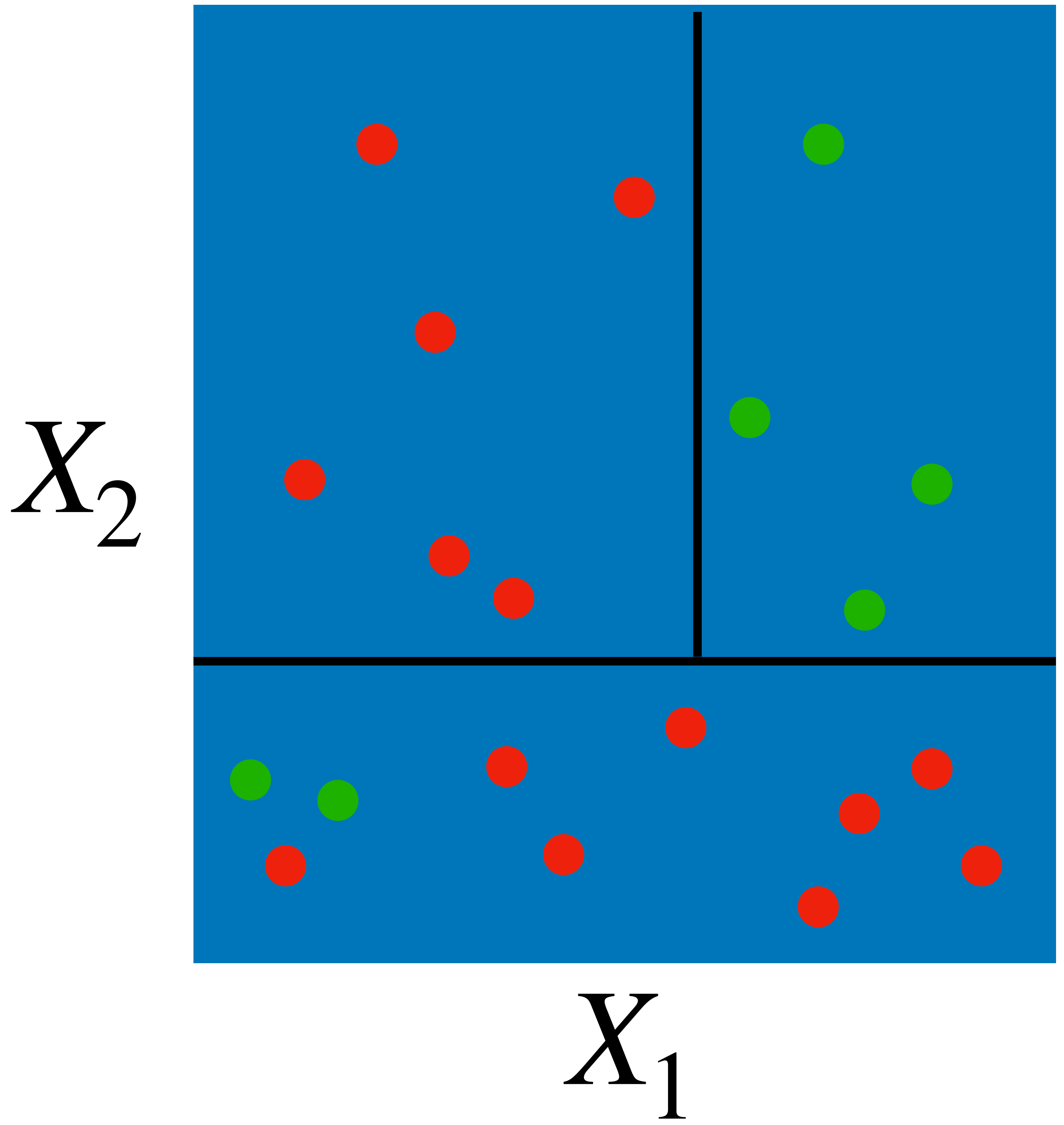

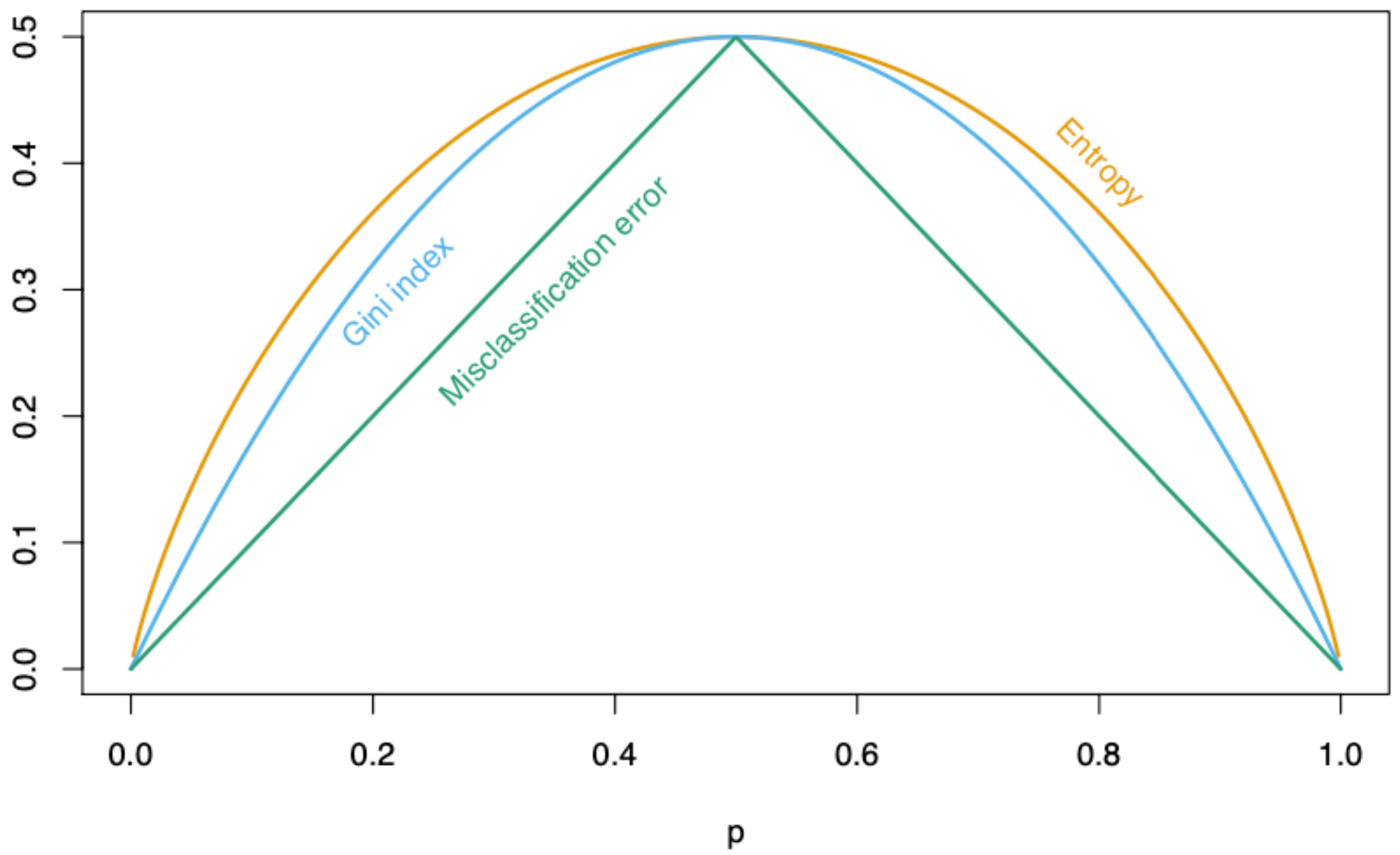

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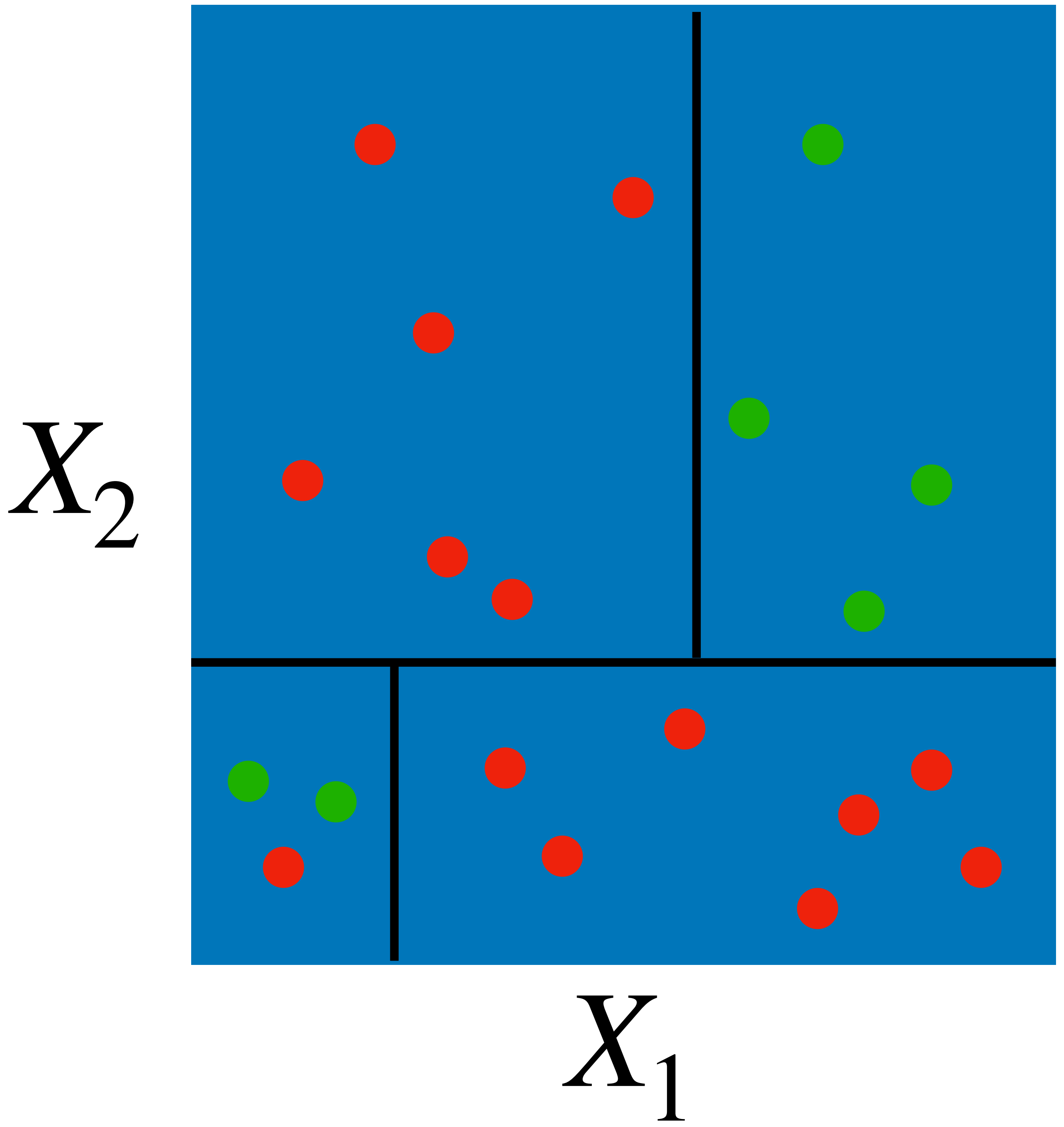

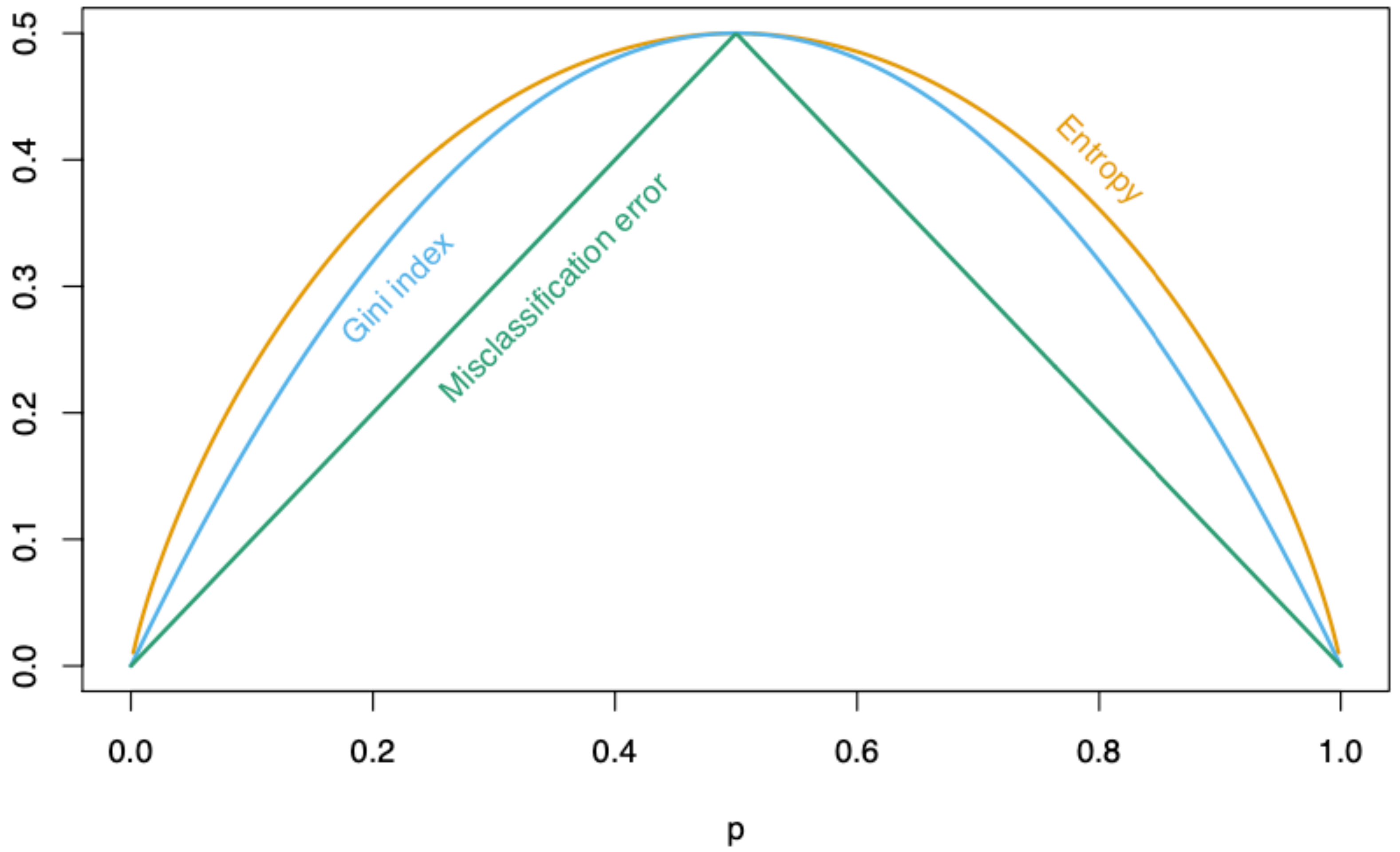

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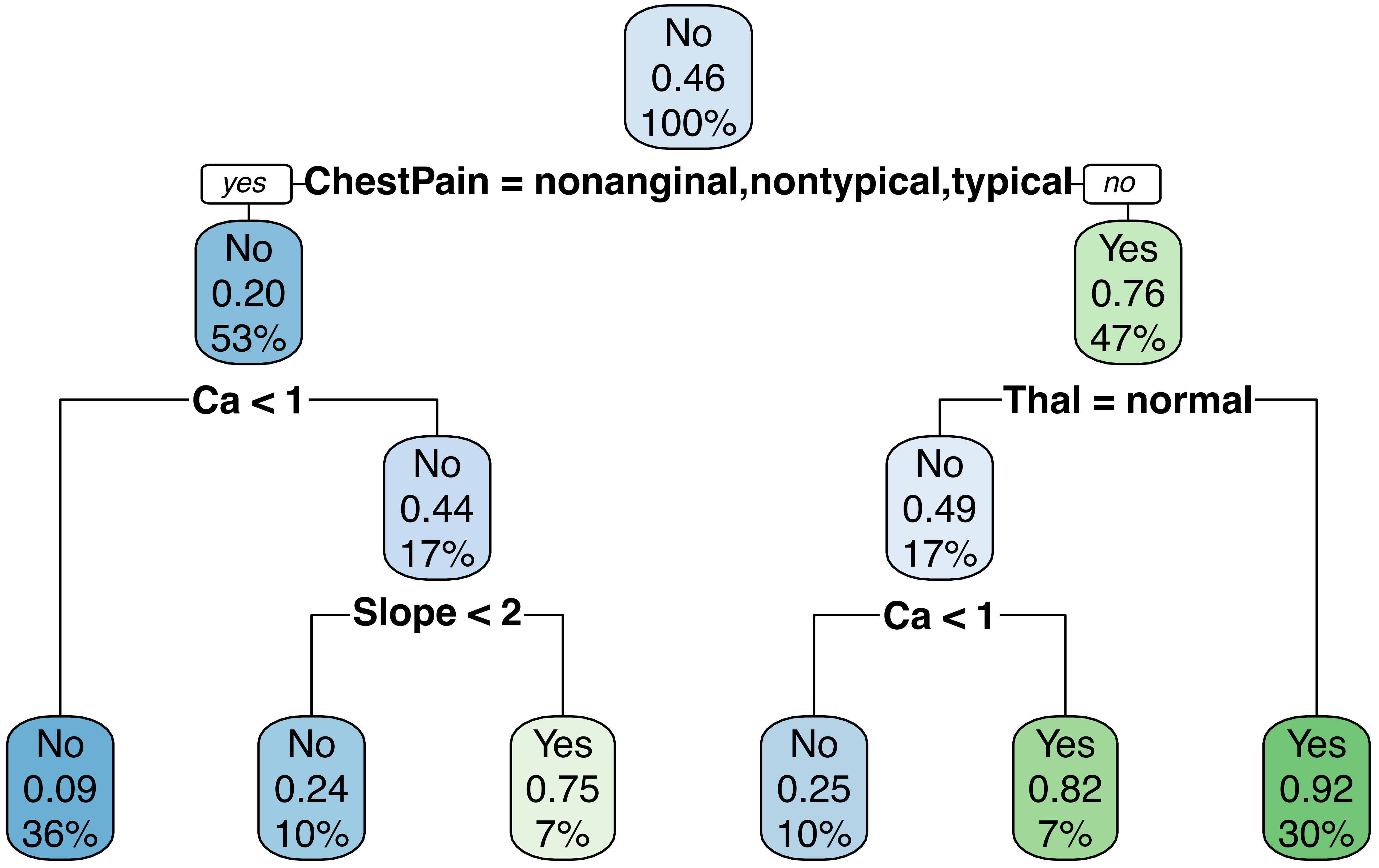
Final output

Example: Heart disease data set.

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



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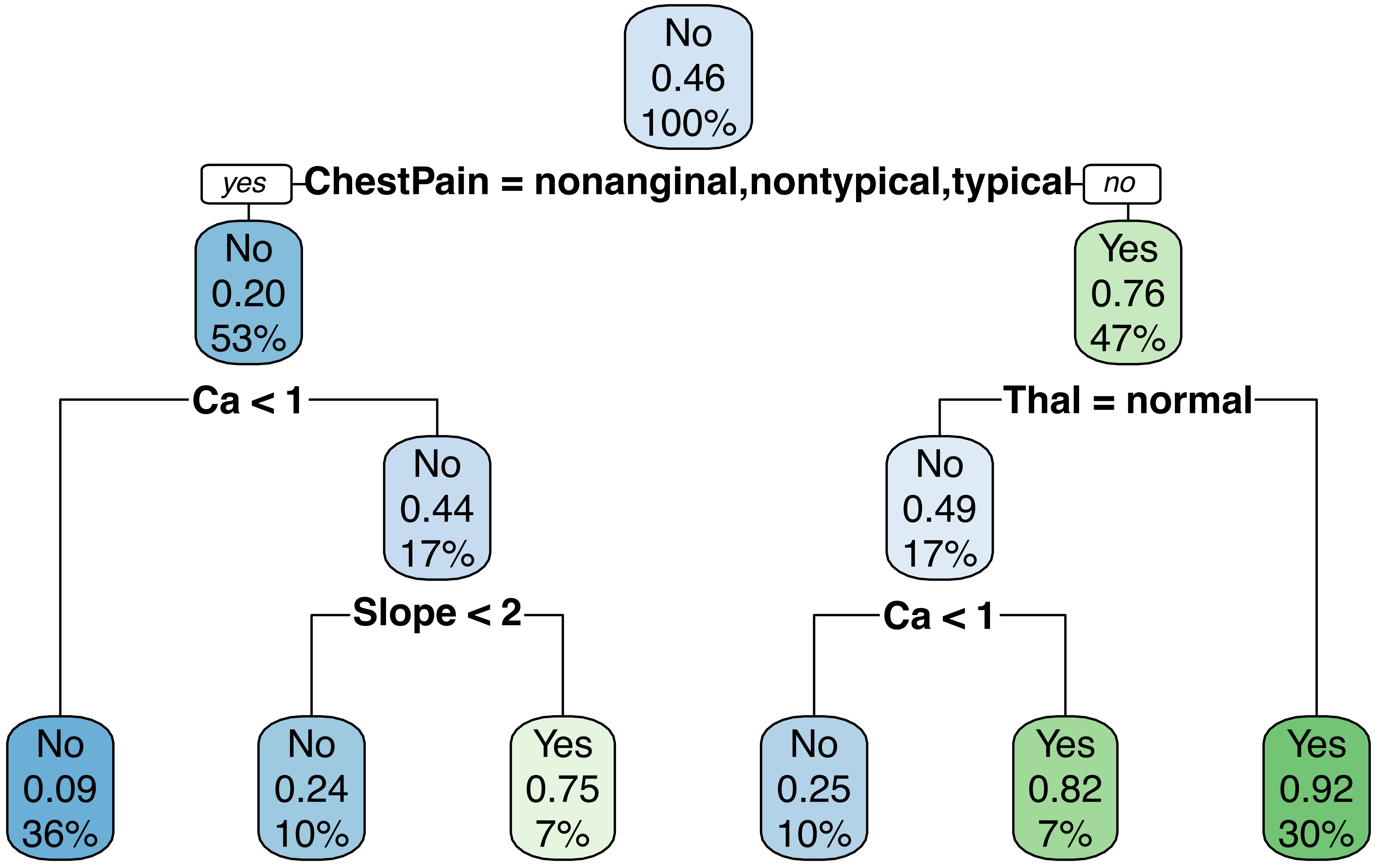

Note: Classification trees extend seamlessly to more than two classes!

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.