Boosting algorithms

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Machine learning

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Today

AdaBoost
- Idea and the algorithm
- Properties and examples

Justification and generalization
- Minimization of the empirical risk
- Gradient boosting
- Tree-based gradient boosting
- LogitBoost

Literature

Learning materials include but are not limited to:

- Hastie, T., Tibshirani, R., and Friedman, J. (2009).
  The Elements of Statistics Learning: Data Mining, Inference, and Prediction (Second Edition).
  Springer.
  - Sections $10.\{1, 4, 5, 9\}$.

- Slides of the lecture.

- Schapire, R. E. and Freund, Y. (2012).
  Boosting: foundations and algorithms.
  MIT Press.

Binary supervised classification (reminder)

Notation:

- **Given:** for the random pair (X, Y) in $\mathbb{R}^d \times \{-1, 1\}$ consisting of a random observation X and its random binary label Y (class), a sample of n i.i.d.: $(\boldsymbol{x}_1, y_1), ..., (\boldsymbol{x}_n, y_n)$.
- **Goal:** predict the label of the new (unseen before) observation $\boldsymbol{x}$.
- **Method:** construct a classification rule:

$$g : \mathbb{R}^d \to \{-1, 1\}, \boldsymbol{x} \mapsto g(\boldsymbol{x}),$$

  so $g(\boldsymbol{x})$ is the prediction of the label for observation $\boldsymbol{x}$.
- **Criterion:** of the performance of g is the **error probability**:

$$R(g) = \mathbb{P}[g(X) \neq Y] = \mathbb{E}[\mathbb{1}(g(X) \neq Y)].$$

- **The best solution:** is to know the distribution of (X,Y):

$$g(\boldsymbol{x}) = \text{sign}\big(2\mathbb{E}[Y|X = \boldsymbol{x}] - 1 > 0\big).$$

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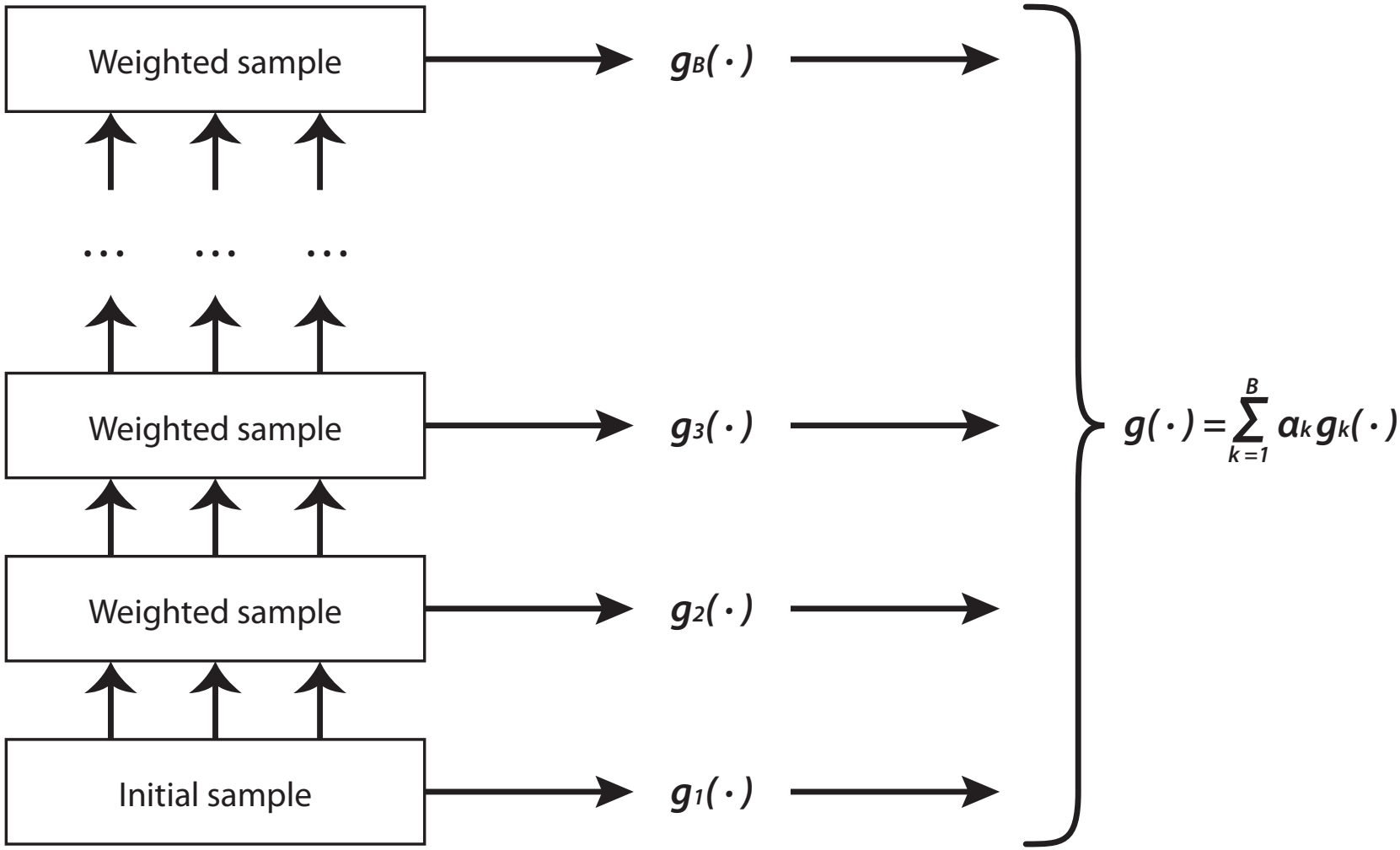
The principle

The principle underlying the boosting:

- **First** boosting algorithm has been introduced by Yoav Freund and Robert E. Schapire in 1996.
- Construct a **family of rules** (classifiers) and then aggregate them.
- **Recursive** process:
  - the rule constructed on the kth step depends on the rule constructed on step $k-1$.
- Use **classification error** for both constructing the next rule and weighting the current one when aggregating.

The principle



The principle

- Term **boosting** is used to describe the family of methods allowing for construction of a precise rule based on weak learners.

- A classification rule $g_\cdot(\cdot)$ is called a **weak learner** if it performs "slightly" better than a random guess:

$$\exists\, \epsilon > 0 \text{ such that } \mathbb{P}[g_\cdot(X) \neq Y] = \frac{1}{2} - \epsilon\,.$$

- **Examples** of weak learners:

  - $1NN$-classifier,

  - classification tree of low depth (*e.g.* with 2 leaves only = a stump).

AdaBoost (algorithm): Freund and Schapire (1997)

Constructing a committee (training)

Input:

- Training sample $\big((\boldsymbol{x}_1, y_1), ..., (\boldsymbol{x}_n, y_n)\big) \subset \mathbb{R}^d \times \{-1, 1\}$.
- Weak learner $g_\cdot(\cdot)$, number of iterations B.

1. Initialize weights $w_i = \frac{1}{n}$, $i = 1, ..., n$.
2. For $k = 1, ..., B$
   - 2.1 Learn a weak learner $g_k(\cdot)$ on $\mathcal{D}_n$ weighted by w_i, $i = 1, ..., n$.
   - 2.2 Calculate error rate:
   $$e_k = \sum_{i=1}^{n} w_i \mathbb{1}\big(g_k(\boldsymbol{x}_i) \neq y_i\big) .$$
   - 2.3 Calculate learner's weight: $\alpha_k = \log \frac{1-e_k}{e_k}$.
   - 2.4 Readjust observations' weights: $w_i = w_i e^{\alpha_k \mathbb{1}\left(g_k(\boldsymbol{x}_i) \neq y_i\right)}$, $i = 1, ..., n$; normalize to get $\sum_{i=1}^{n} w_i = 1$.

Output: The committee $g^{bst}(\cdot) = \text{sign}\Big(\sum_{k=1}^{B} \alpha_k g_k(\cdot)\Big)$.

Weighted majority voting (classification)

$$g^{bst}(\boldsymbol{x}) = \text{sign}\Big(\sum_{k=1}^{B} \alpha_k g_k(\boldsymbol{x})\Big) .$$

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AdaBoost: some comments

- The step of learning requires the weak learner to take into account the **weights** w_i, $i = 1, ..., n$ of observations.
- If weights cannot be taken into account, the weak learner can be trained on a **subsample** of $\mathcal{D}_n$ drawn (with replacement) with probabilities w_i, $i = 1, ..., n$.
- Observations' weights w_i, $i = 1, ..., n$ are updated on each iteration:
  - if the ith observation is **well classified**, then its weight is unchanged,
  - if the ith observation is **wrongly classified**, then its weight is increased.
- Learner's weight α_k **increases with performance of** $g_k(\cdot)$ calculated on (weighted) $\mathcal{D}_n$:
  - α_k increases with decreasing e_k;
  - anyway, $g_k(\cdot)$ **should not be "too weak"**: if $e_k > \frac{1}{2}$ then $\alpha_k < 0$.

AdaBoost: some properties

- The **error rate calculated for the training sample** e_k of the learner g_k is given by:

$$e_k = \frac{\sum_{i=1}^{n} w_i \mathbb{1}\big(g_k(\boldsymbol{x}_i) \neq y_i\big)}{\sum_{i=1}^{n} w_i} \,.$$

- Denote ϵ_k the **gain** of g_k **w.r.t. a purely random classifier**:

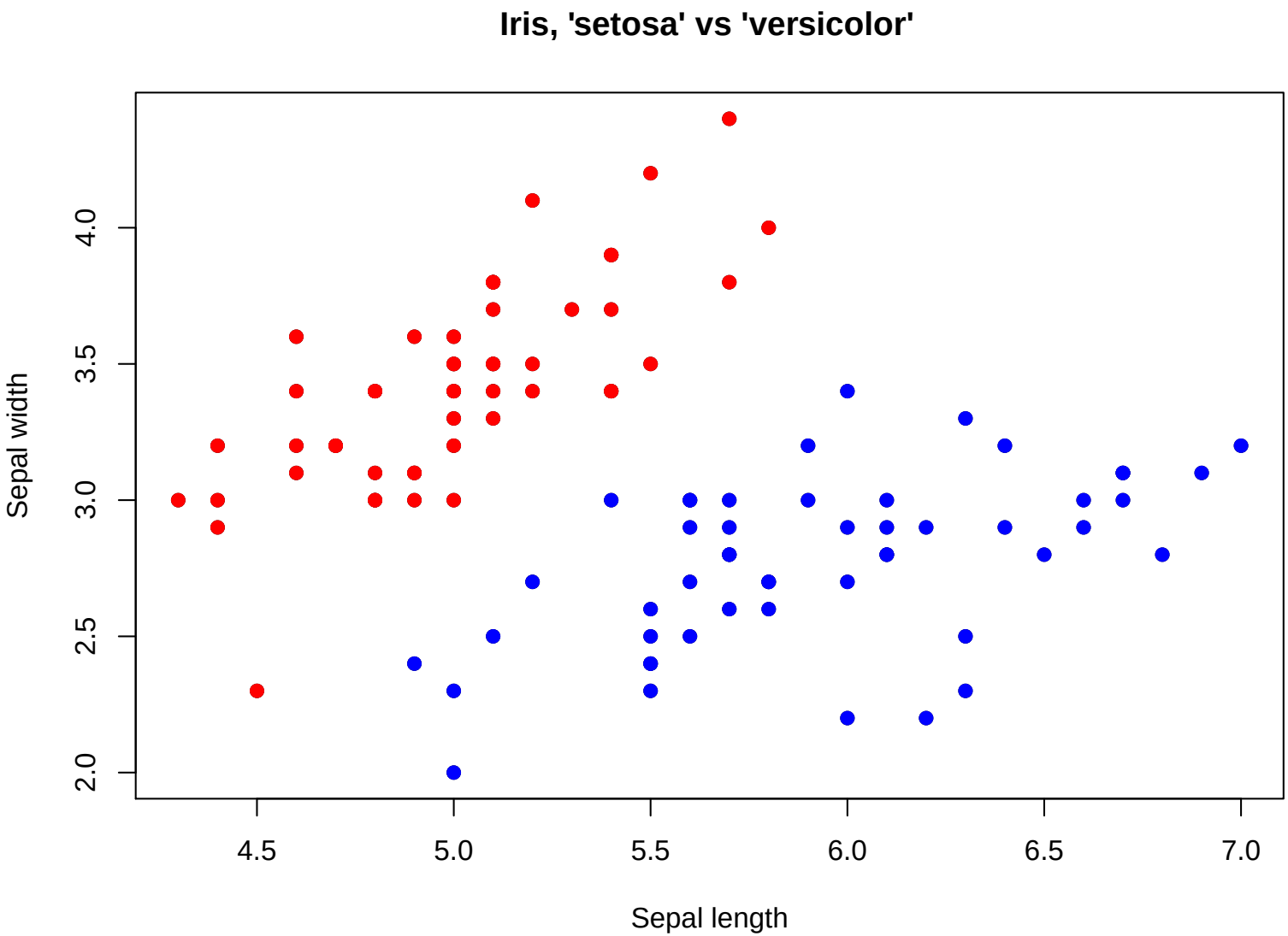
$$e_k = \frac{1}{2} - \epsilon_k \,.$$

- The empirical error (on training sample) is bounded by (Freund and Schapire, 1999):

$$L_n(g^{bst}) \leq e^{-2\sum_{k=1}^{B} \epsilon_k^2} \,.$$

- Consequently, the empirical error (on the training sample) **decreases to 0** with increasing B.
- Thus, if B is (too) large, AdaBoost tends to overfit the sample.

AdaBoost (Iris data, "setosa" *vs.* "versicolor")



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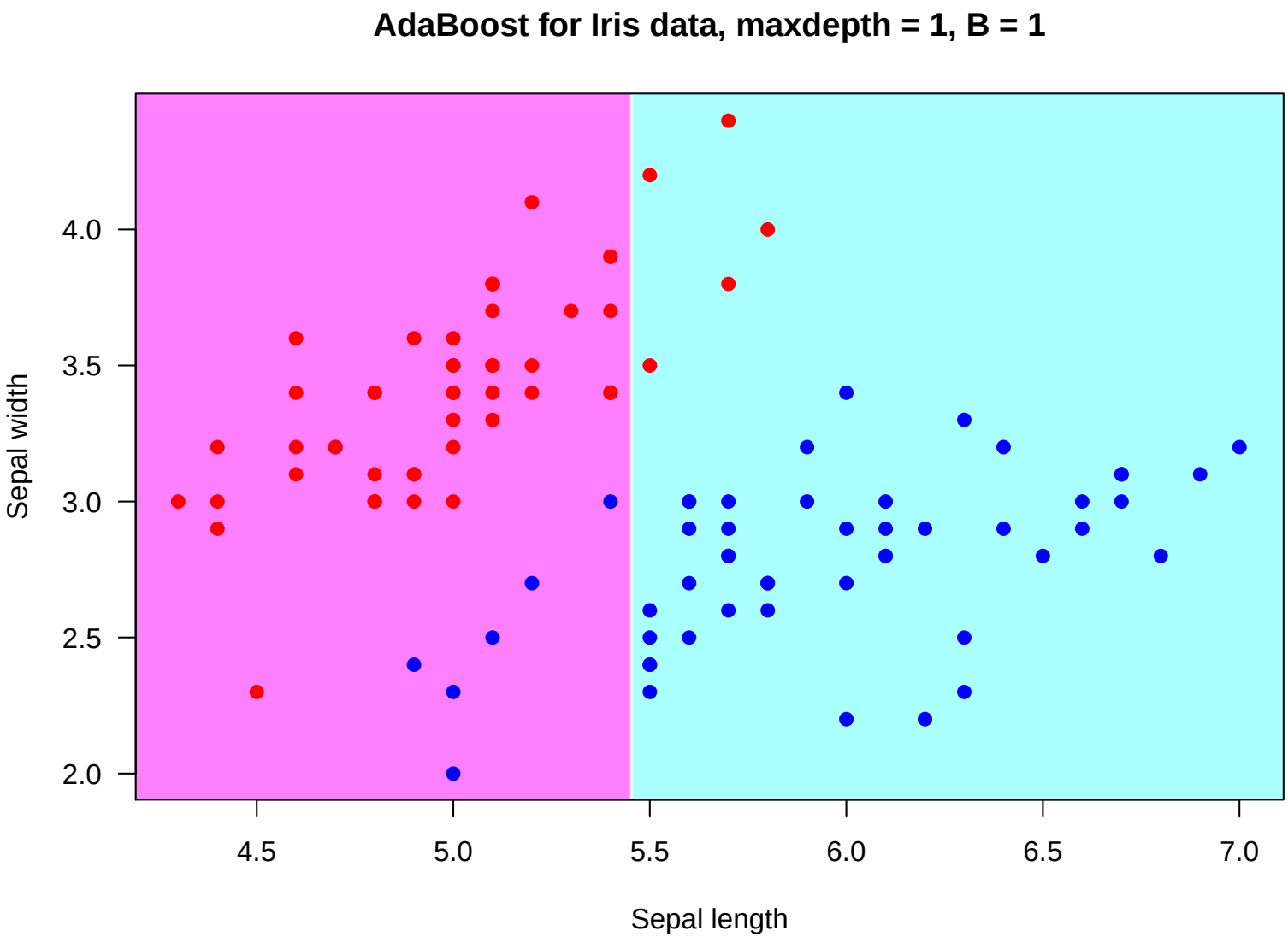

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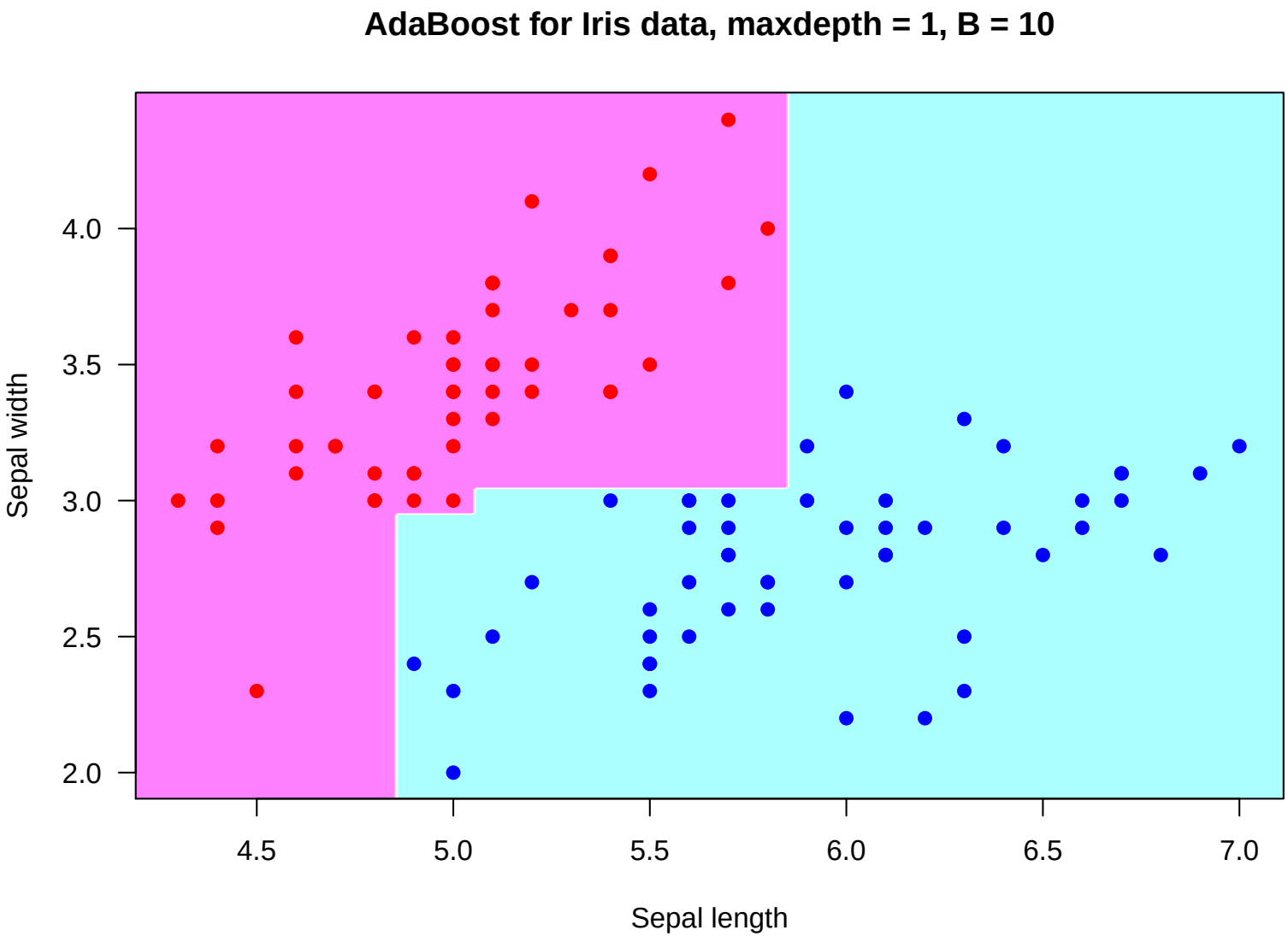

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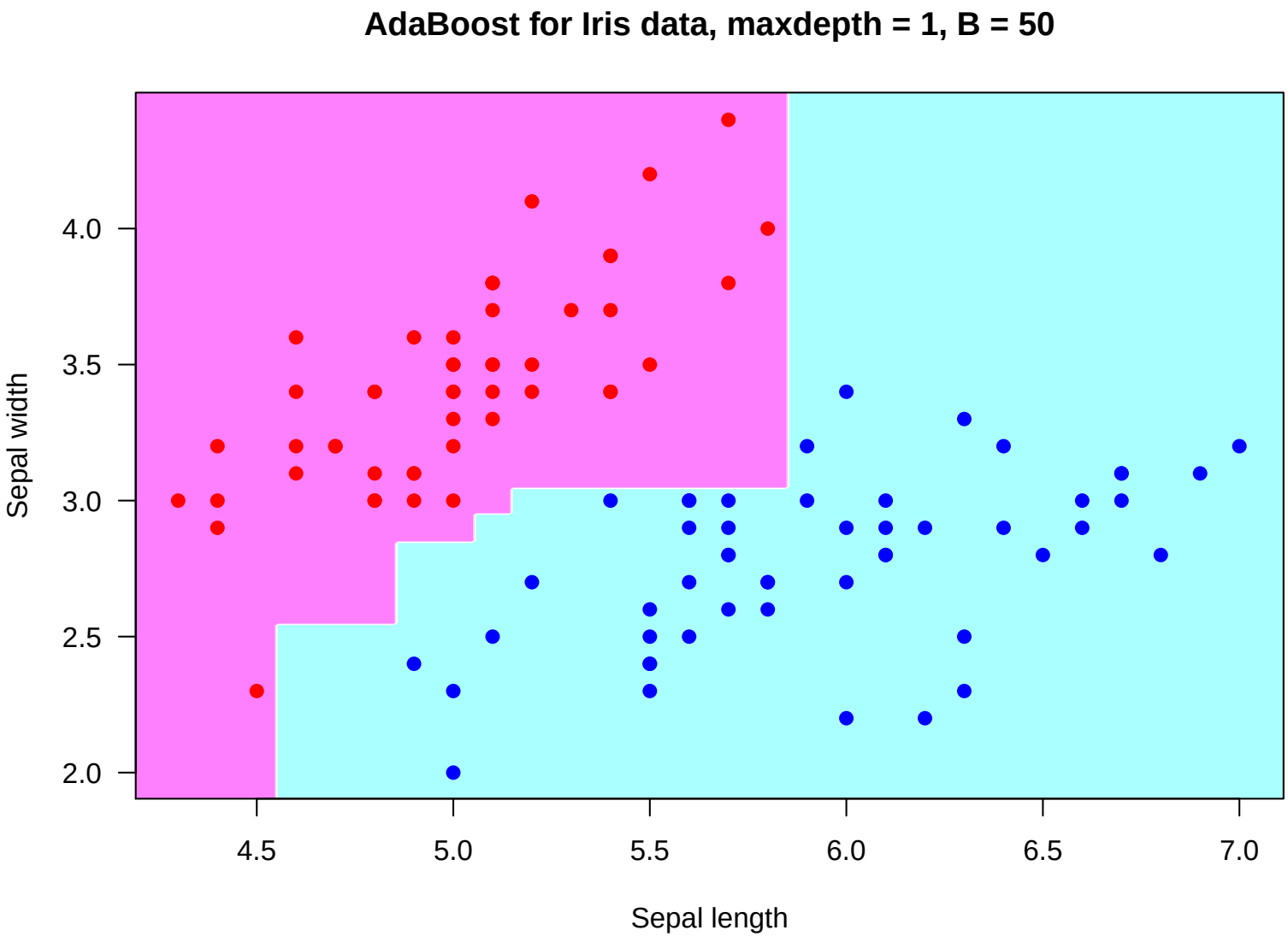

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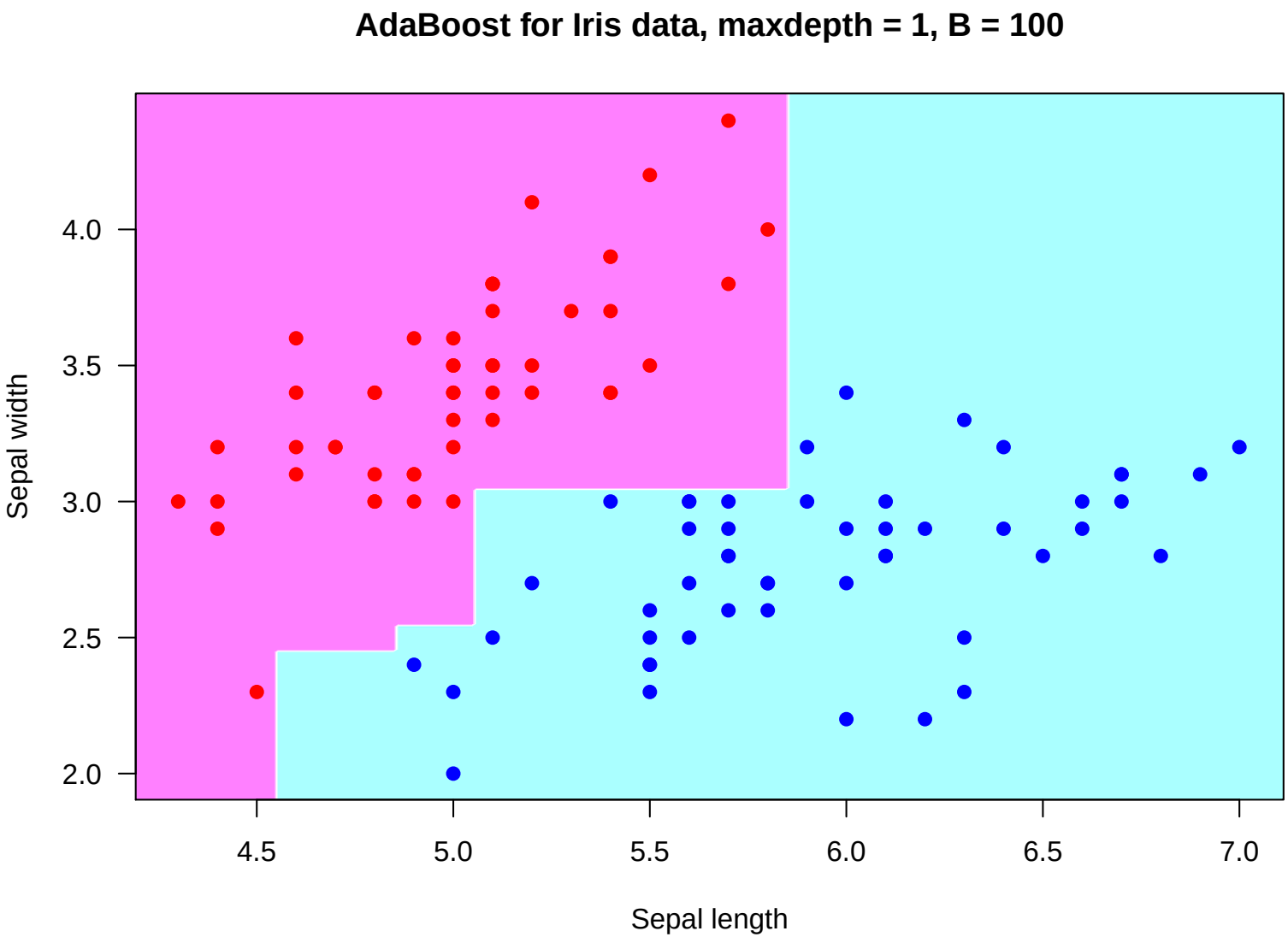

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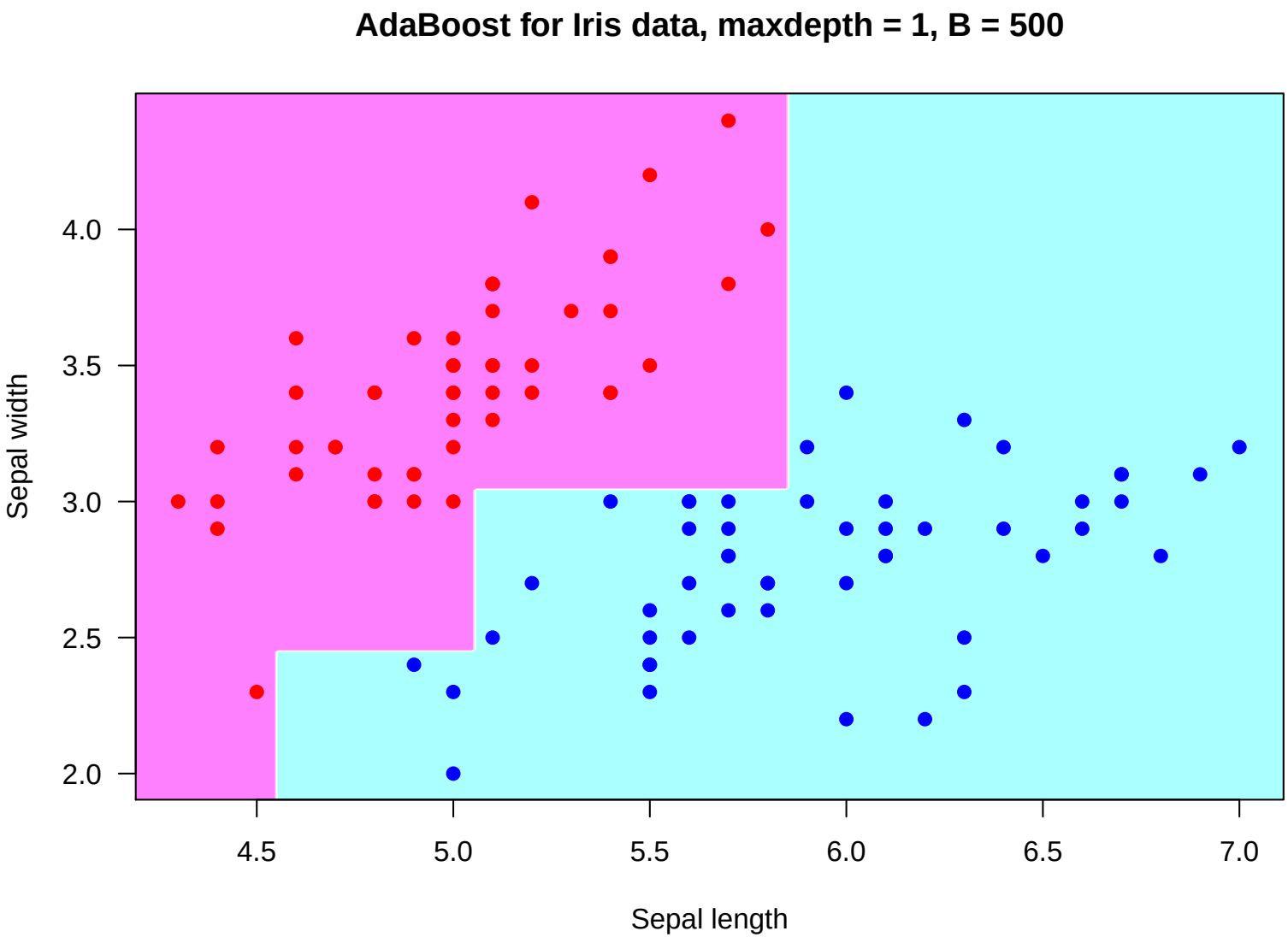
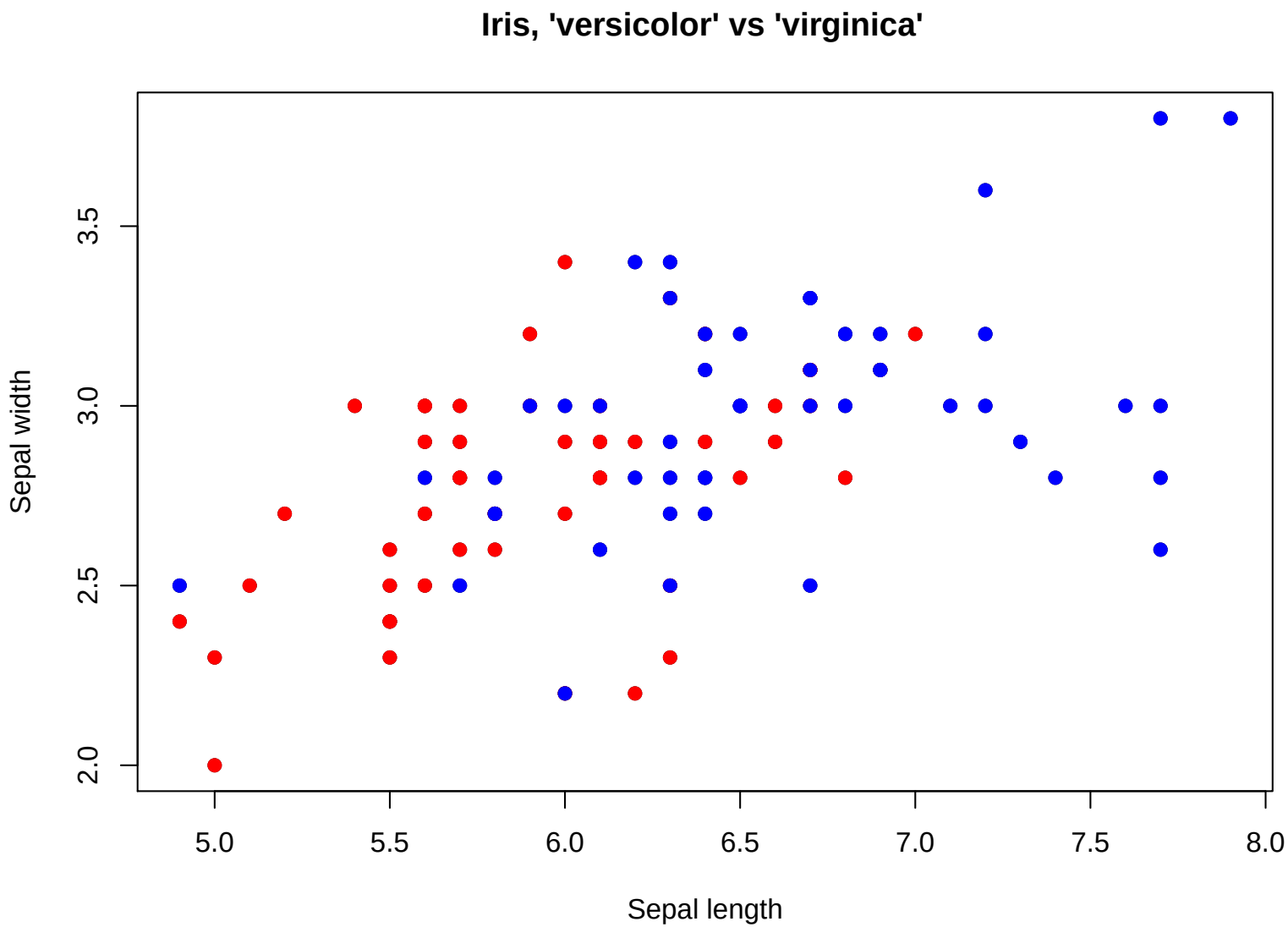


AdaBoost (Iris data, "versicolor" *vs.* "virginica")



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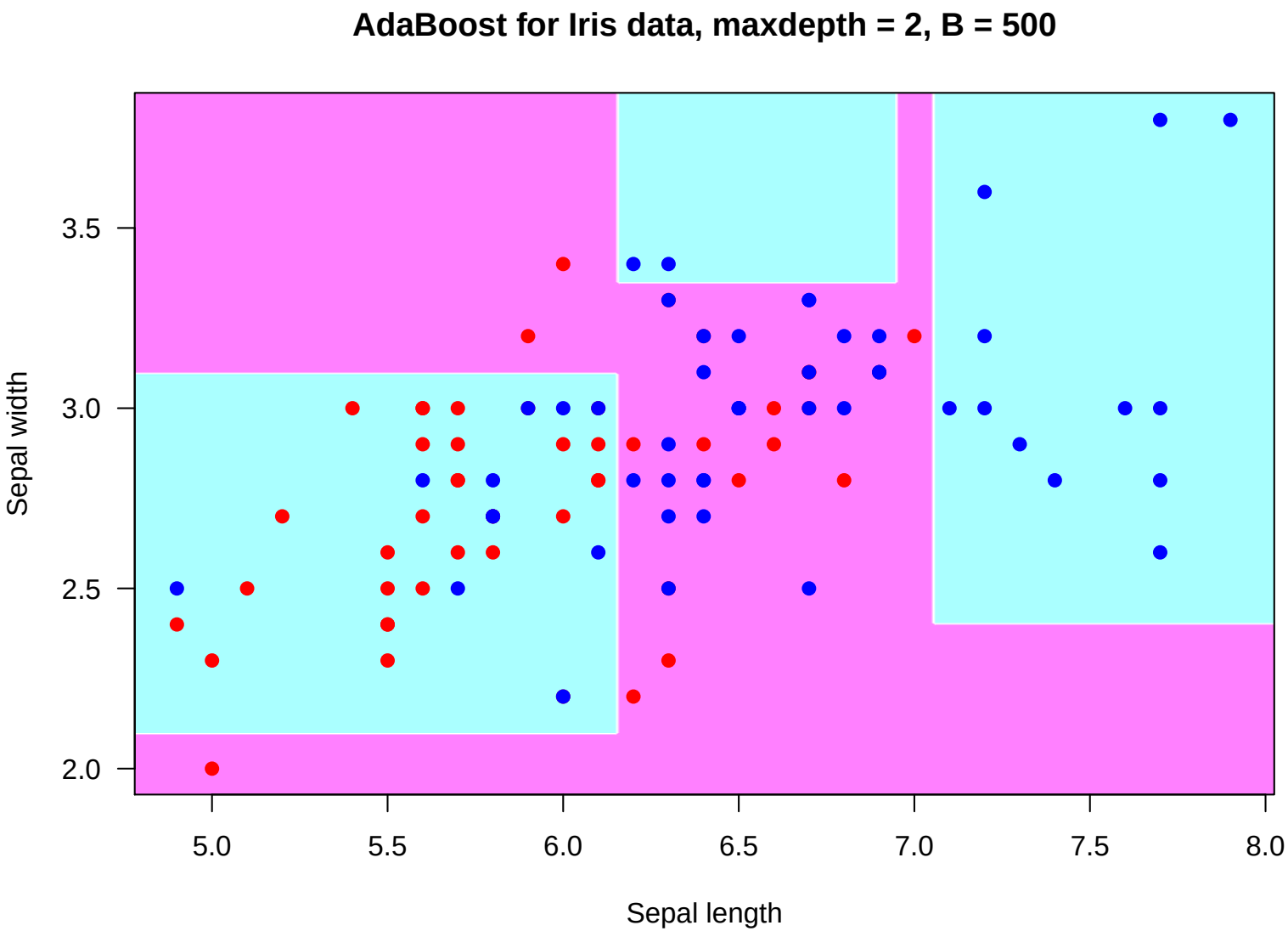

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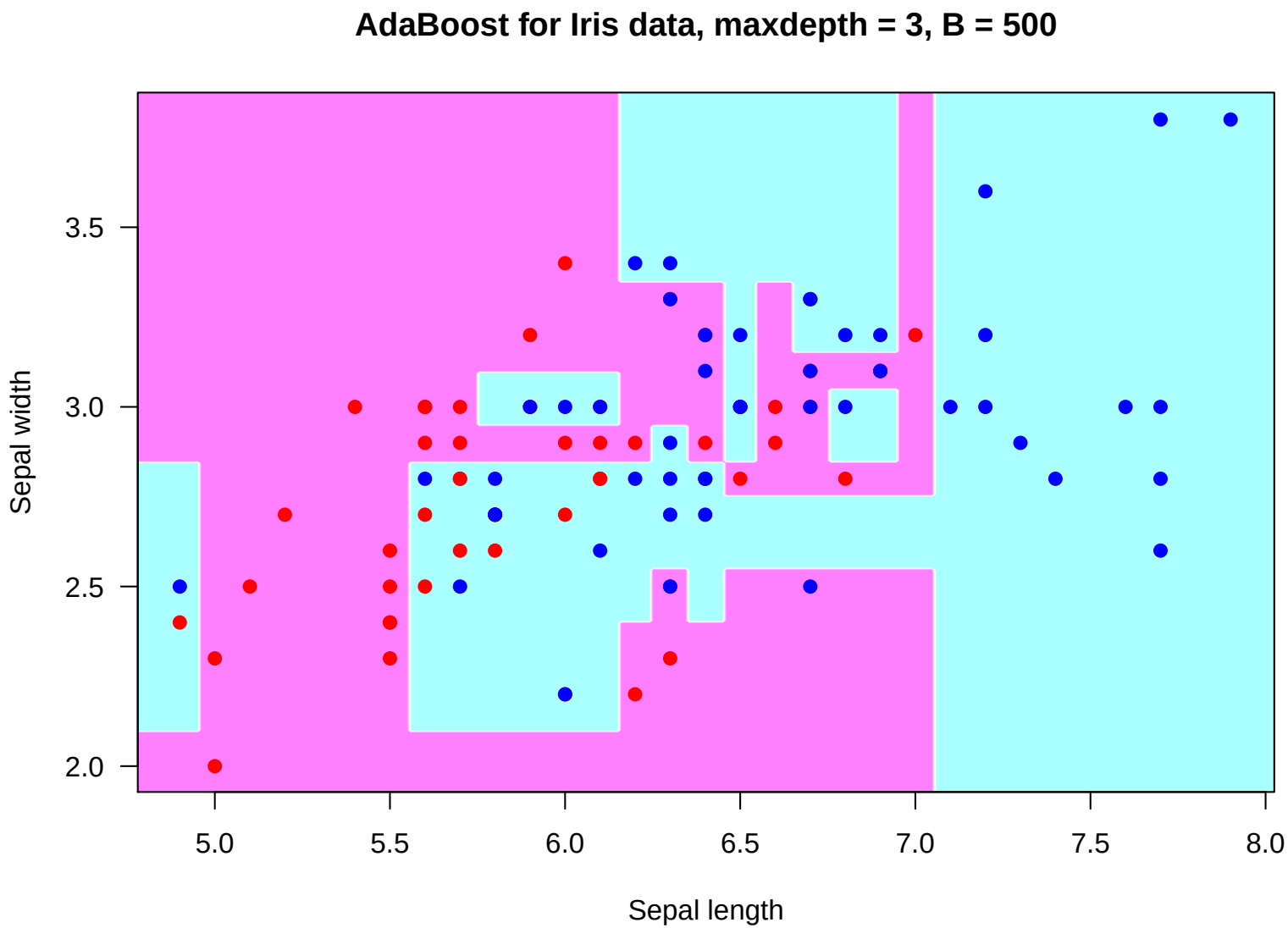

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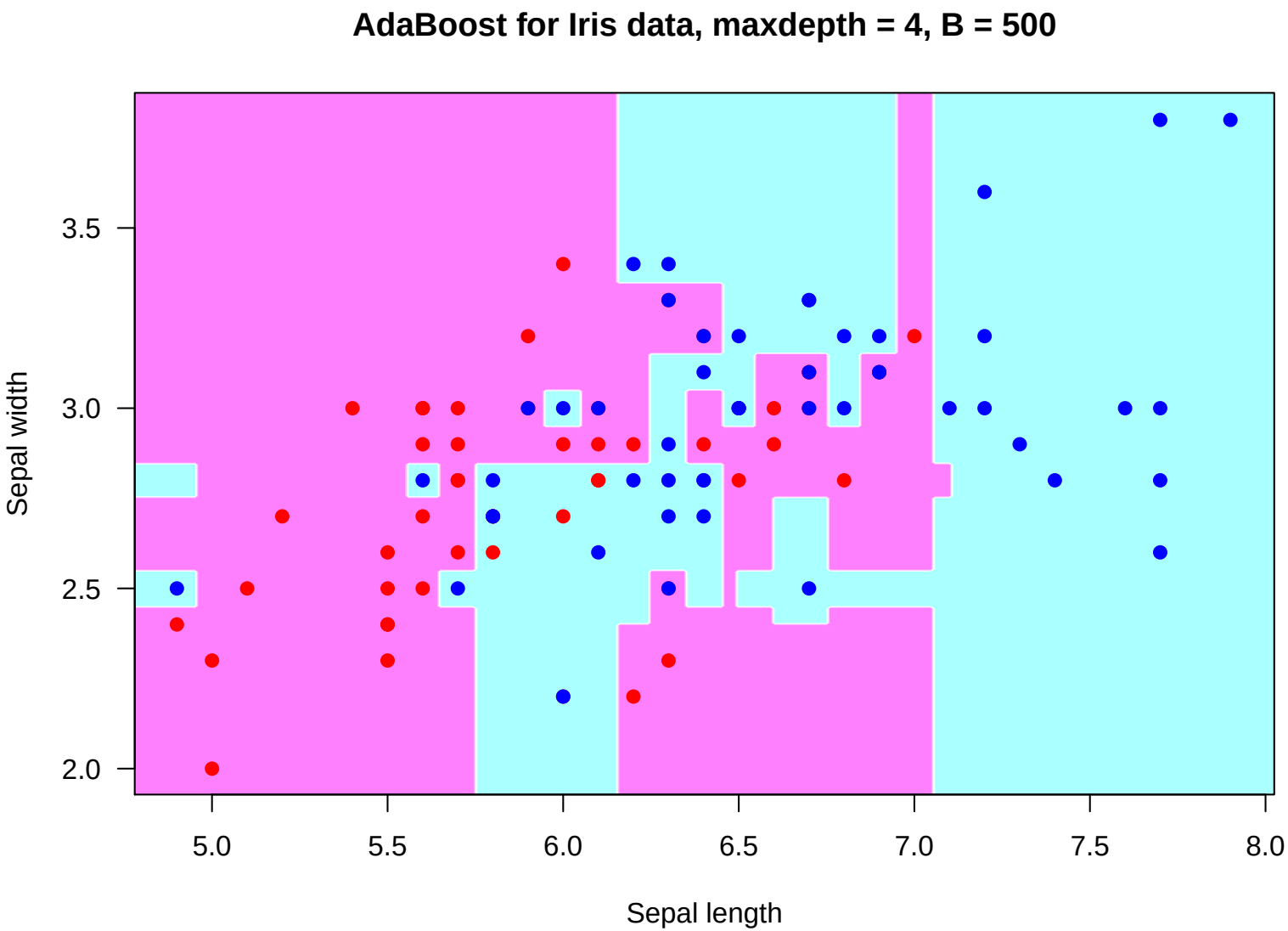

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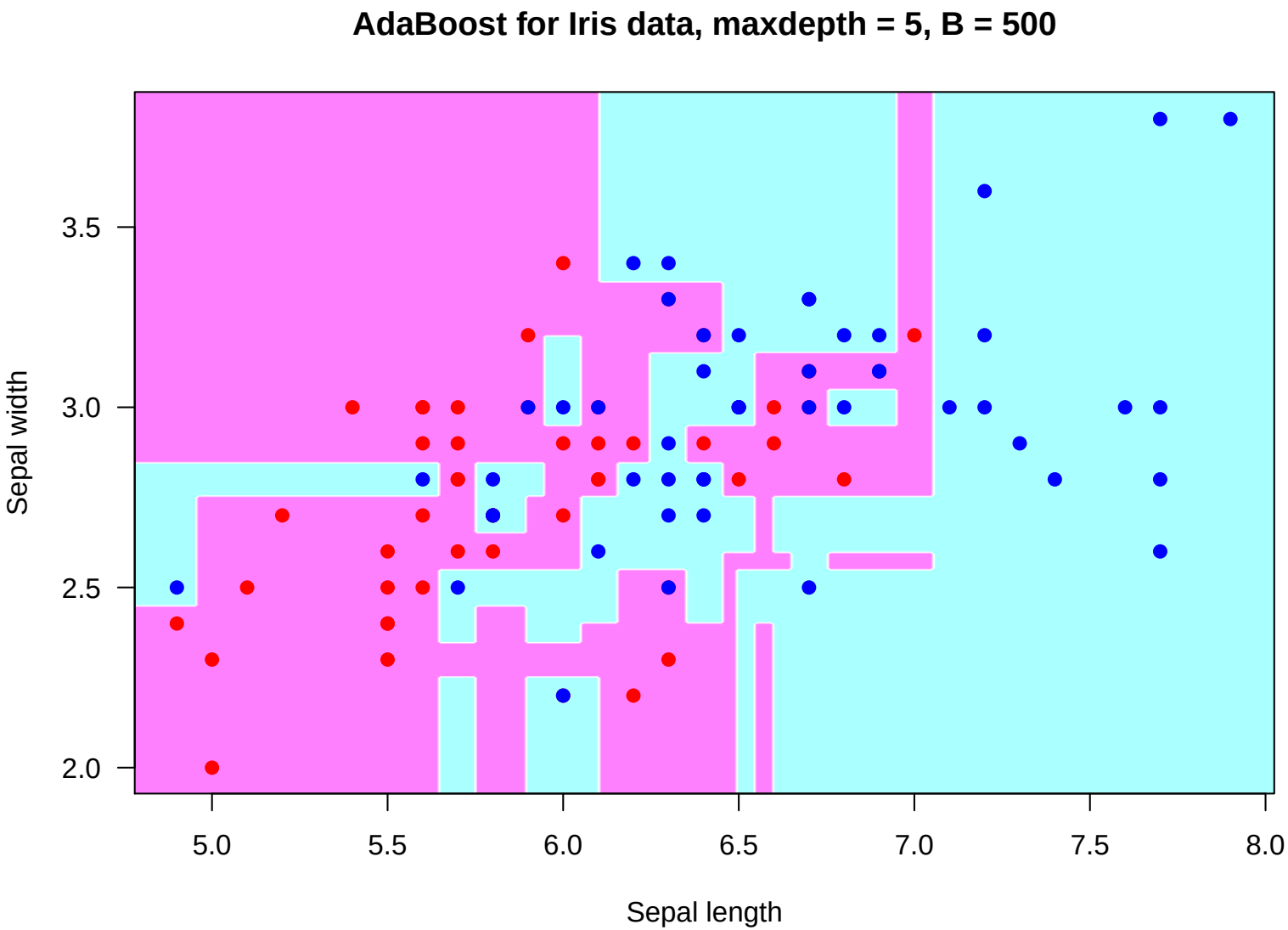
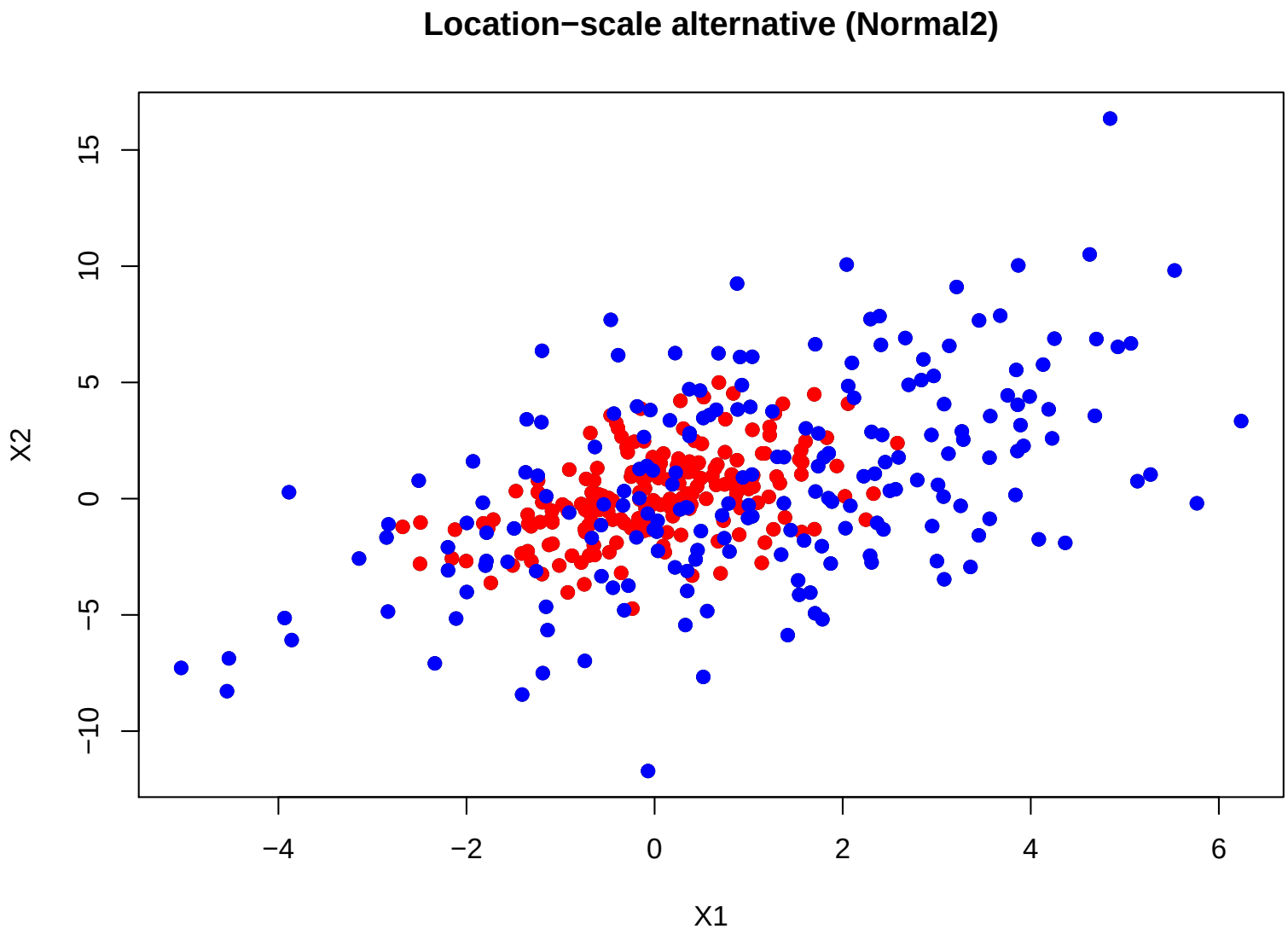


AdaBoost (normal location-scale alternative)



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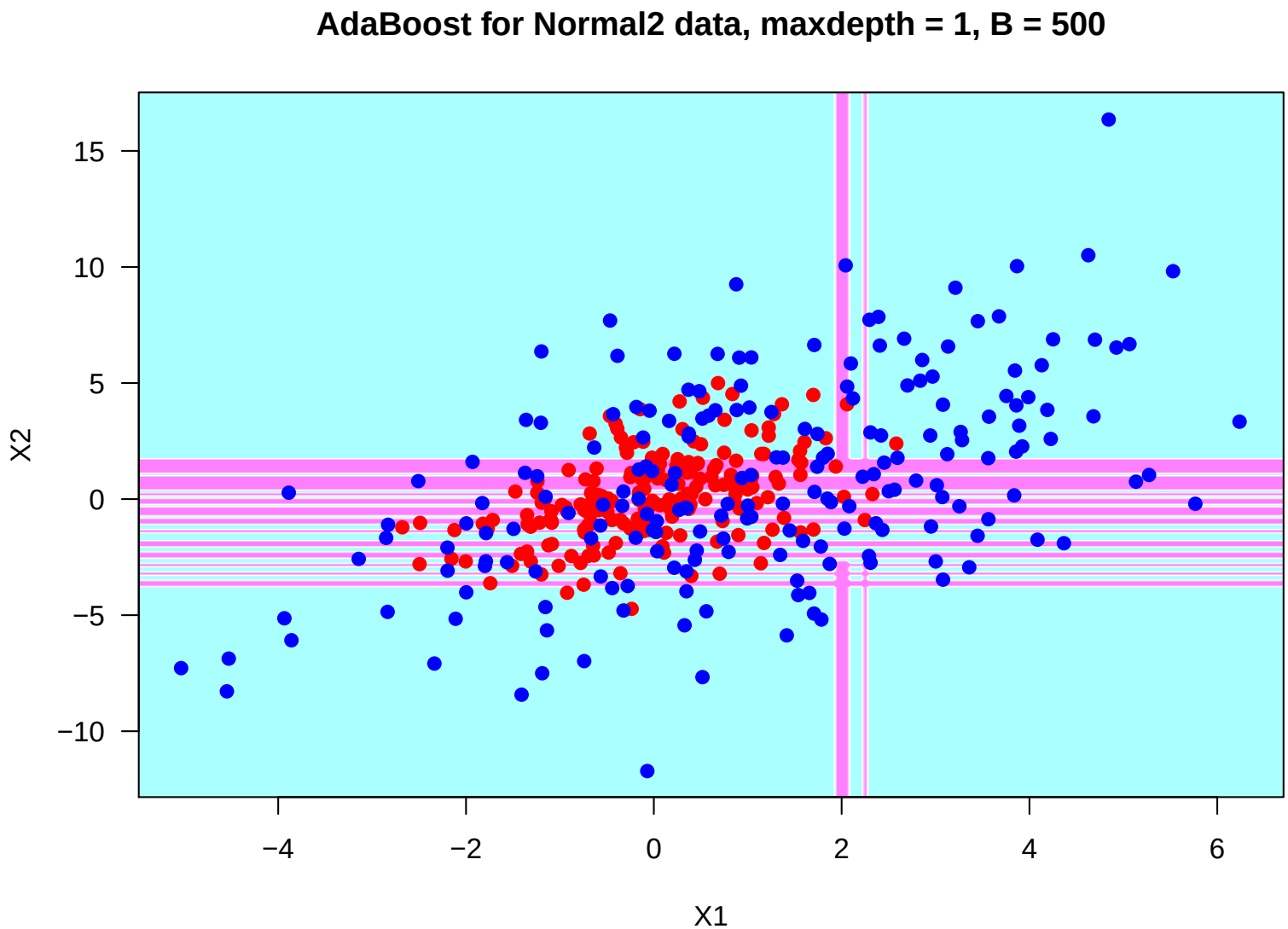

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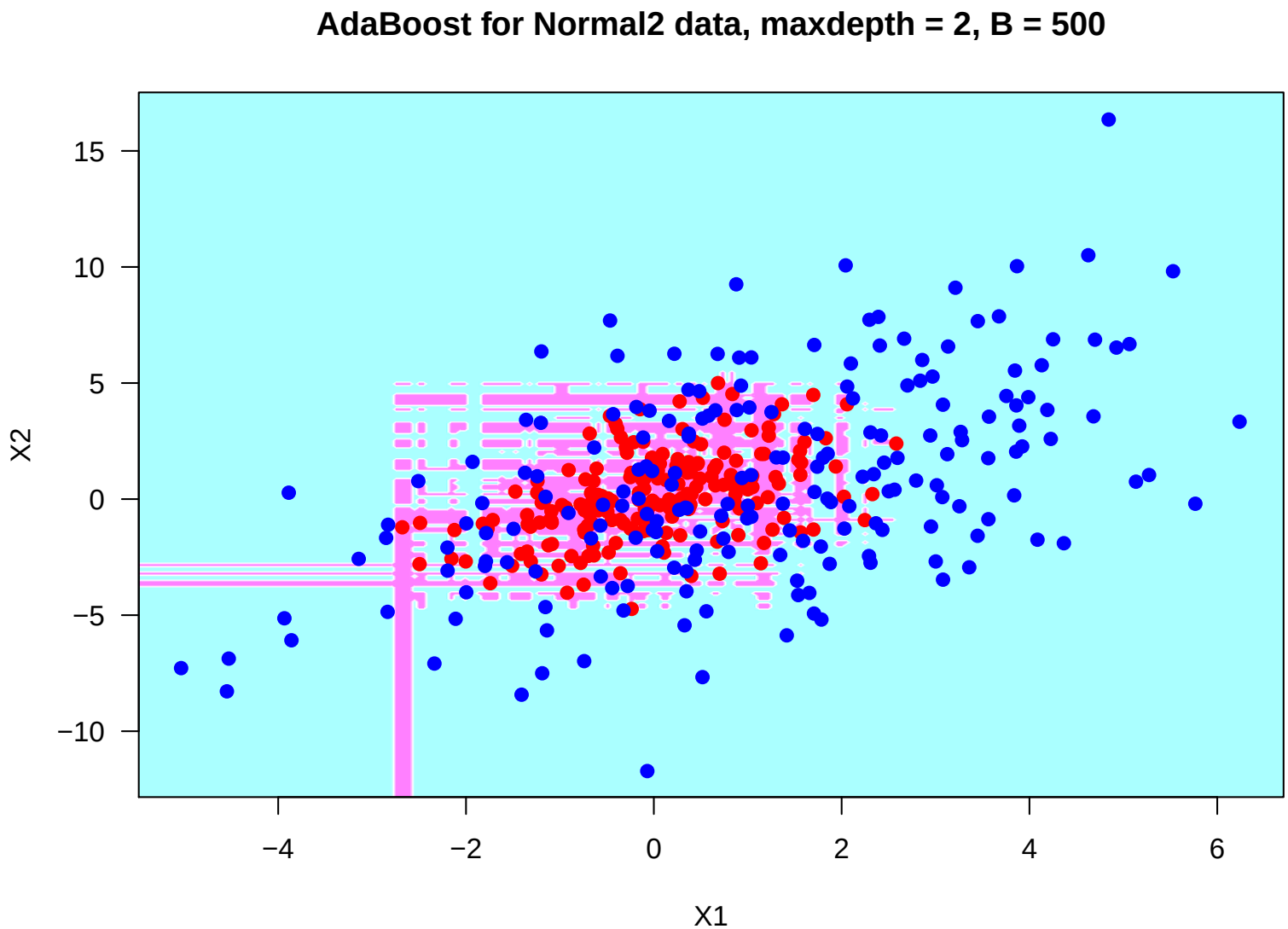

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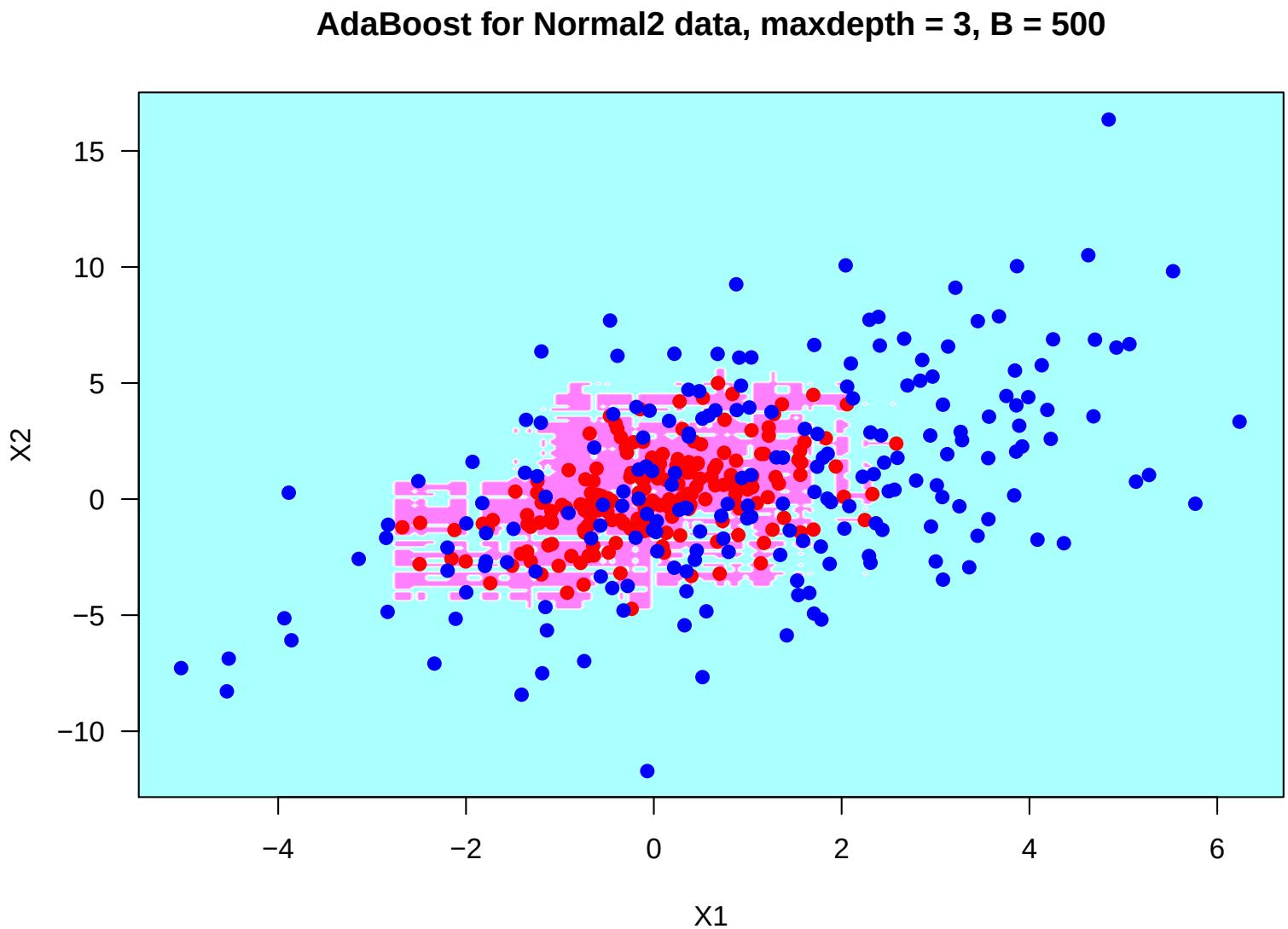

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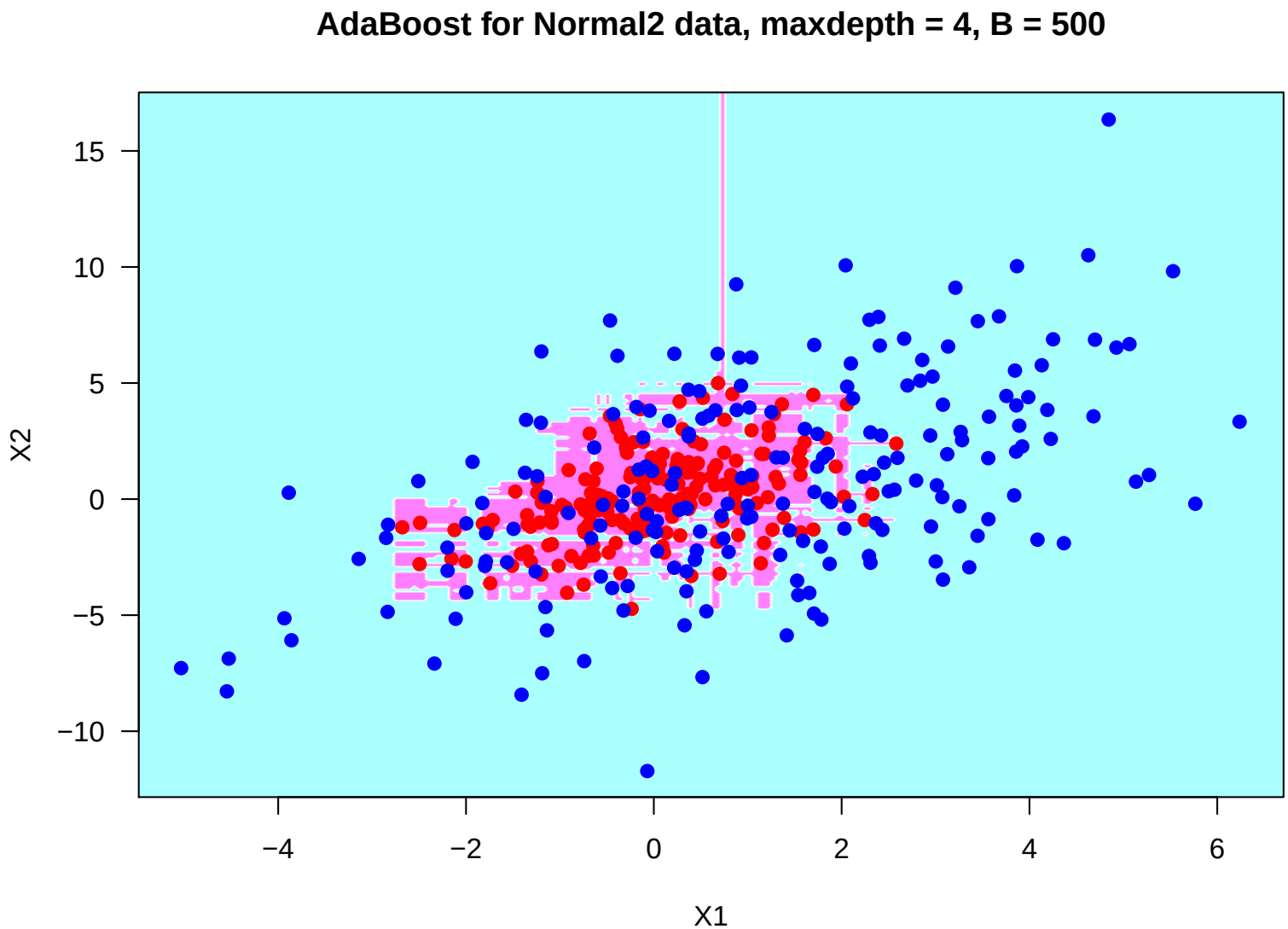

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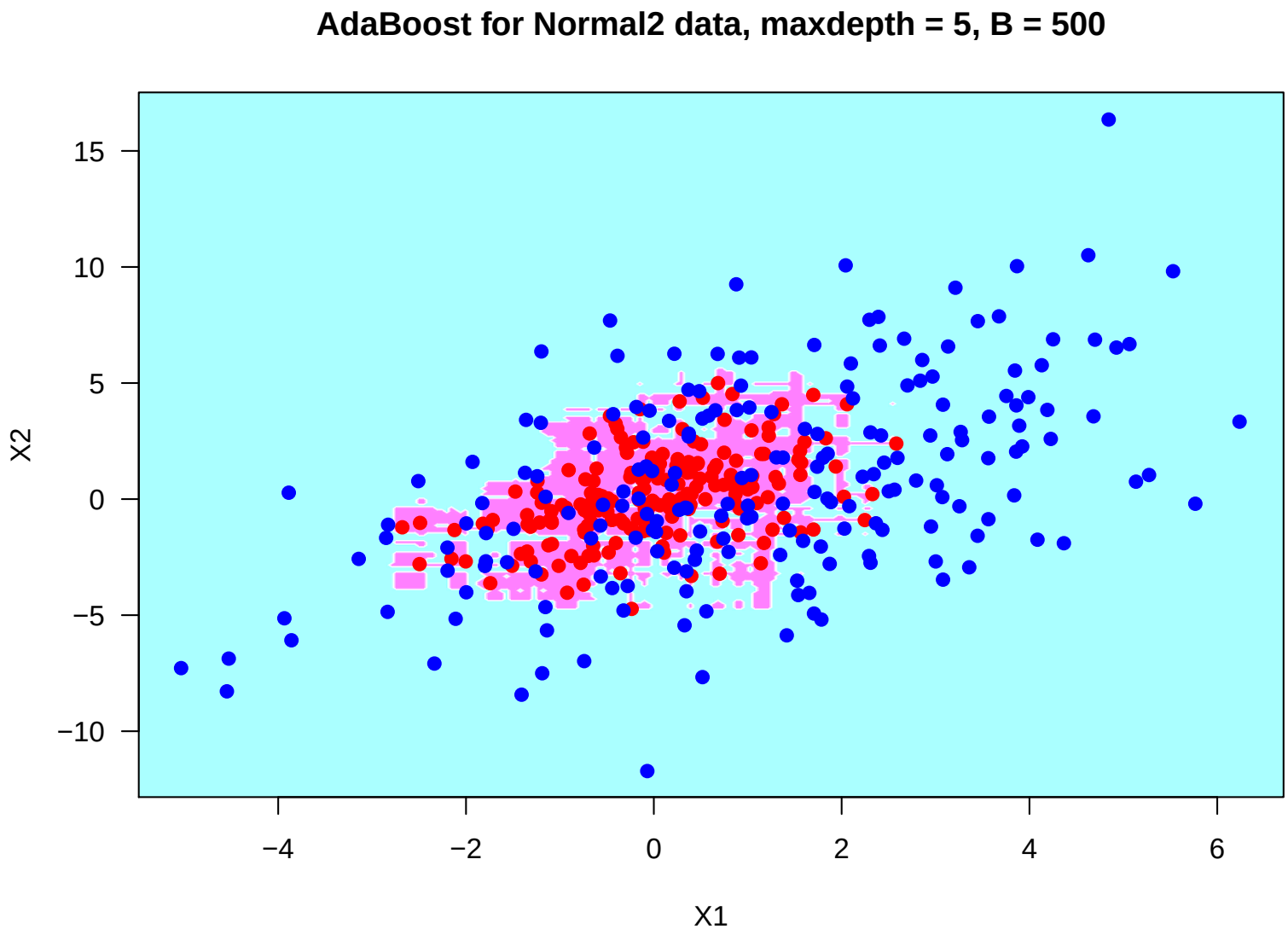

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Minimization of the empirical risk

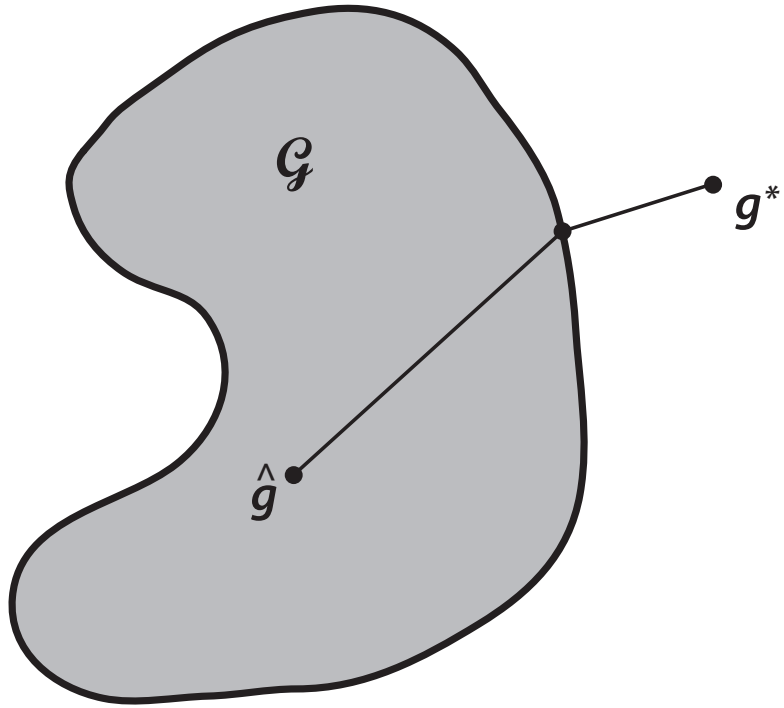
- Regard a **random pair** (X, Y) taking values in $\mathbb{R}^d \times \{-1, 1\}$.
- Consider a **class of** classification **rules** $\mathcal{G}$:
  - one attempts to find **the best rule** in $\mathcal{G}$.
- **Try:** Choose the rule which minimizes a loss function, for example:

$$L(g) = \mathbb{P}\big[g(X) \neq Y\big] .$$

- **Problem:** As we cannot calculate $\mathbb{P}$, we cannot calculate $L(g)$ as well.
- **Idea:** Choose a rule that minimizes the empirical version (*i.e.* on the training sample) of the loss function — the **empirical risk**:

$$L_n(g) = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}\big(g(\boldsymbol{x}_i) \neq y_i\big) .$$

Minimization of the empirical risk



$$L(\hat{g}) - L(g^*) = \underbrace{L(\hat{g}) - \inf_{g \in \mathcal{G}} L(g)}_{} + \underbrace{\inf_{g \in \mathcal{G}} L(g) - L(g^*)}_{} .$$

- These two terms (usually) vary in inverse sense.

Risk convexification

- **Problem:** The function

$$\mathcal{G} \to \mathbb{R}, \quad g \mapsto \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}\big(g(\boldsymbol{x}_i) \neq y_i\big)$$

  is (usually) **difficult to minimize**.

- **Idea:** Find another loss function $\ell : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ such that

$$\mathcal{G} \to \mathbb{R}, \quad g \mapsto \frac{1}{n} \sum_{i=1}^{n} \ell\big(g(\boldsymbol{x}_i), y_i\big)$$

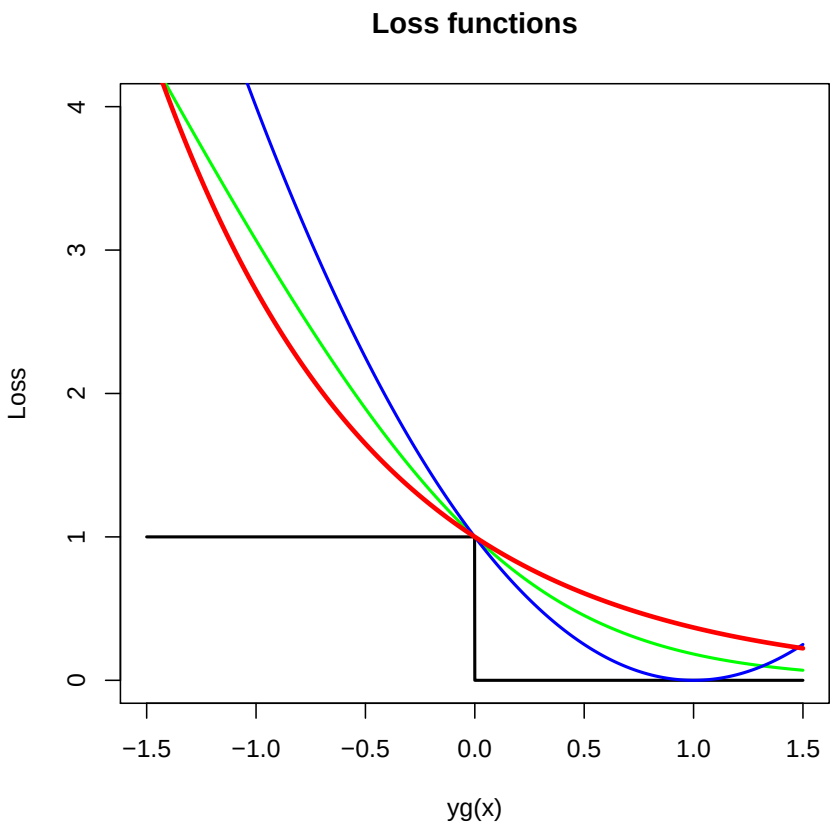
  is **"easy" to minimize**, *e.g.* a **differentiable** one.

- This is even more the case if the function $u \mapsto \ell(u, v)$ is **convex**.

- The loss function $\ell\big(g(\boldsymbol{x}), y\big)$ should **measure the difference** between the value to be predicted $y \in \{-1, 1\}$ and $g(\boldsymbol{x})$.

- Thus $\ell\big(g(\boldsymbol{x}), y\big)$ should take:
  - **large** values if $yg(\boldsymbol{x}) < 0$,
  - **small** values if $yg(\boldsymbol{x}) > 0$.

Loss functions



— Misclassification:

$$\ell\big(g(\boldsymbol{x}), y\big) = \mathbb{1}\big(yg(\boldsymbol{x}) < 0\big)\,.$$

— Exponential:

$$\ell\big(g(\boldsymbol{x}), y\big) = e^{-yg(\boldsymbol{x})}\,.$$

— Binomial log-likelihood:

$$\ell\big(g(\boldsymbol{x}), y\big) = -\log(1+e^{-2yg(\boldsymbol{x})})\,.$$

— Squared error:

$$\ell\big(g(\boldsymbol{x}), y\big) = \big(1 - yg(\boldsymbol{x})\big)^2\,.$$

Summary

- For:
  - a random pair (X, Y) taking values in $\mathbb{R}^d \times \{-1, 1\}$,
  - a loss function $\ell : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$
  one seeks a classifier close to:

$$g^* = \arg\min_g \mathbb{E}[\ell(g(X), Y)] \,.$$

- **Strategy:** Given a training sample $(\boldsymbol{x}_1, y_1), (\boldsymbol{x}_2, y_2), ..., (\boldsymbol{x}_n, y_n)$ of (X, Y), one minimizes the empirical version of $\mathbb{E}[\ell(g(X), Y)]$:

$$\frac{1}{n} \sum_{i=1}^{n} \ell\big(g(\boldsymbol{x}_i), y_i\big) \,.$$

- **Recursive approach:** Approximate g^* by $\hat{g}(\cdot) = \sum_{k=1}^{B} g_k(\cdot)$, where $g_k(\cdot)$s are constructed recursively.

- **Method:** Numerical optimization, *e.g.*, **gradient descent**.

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Functional gradient descent (FGD)

- Let $\boldsymbol{g}_k = \big(g_k(\boldsymbol{x}_1), g_k(\boldsymbol{x}_2), ..., g_k(\boldsymbol{x}_n)\big)$, and

$$J(\boldsymbol{g}_k) = \frac{1}{n}\sum_{i=1}^{n} \ell\big(g_k(\boldsymbol{x}_i), y_i\big)\,.$$

- The gradient descent algorithm can be expressed by the recursive formula:

$$\boldsymbol{g}_k = \boldsymbol{g}_{k-1} - \lambda \nabla J(\boldsymbol{g}_{k-1})$$

  with $\lambda > 0$ being the step size of the gradient descent.

Such an approach possesses certain disadvantages:

- The regularity of the estimated function is not taken into account:
  - if $\boldsymbol{x}_i$ is close to $\boldsymbol{x}_j$ then $\hat{g}(\boldsymbol{x}_i)$ is close to $\hat{g}(\boldsymbol{x}_j)$.
- The estimator is calculated at the points of the training sample only $\boldsymbol{x}_1, ..., \boldsymbol{x}_n$.

Gradient boost (algorithm): Friedman (2001)

Constructing a classifier (training)

Input:

- Training sample $\big((\boldsymbol{x}_1, y_1), ..., (\boldsymbol{x}_n, y_n)\big) \subset \mathbb{R}^d \times \{-1, 1\}$.
- Weak learner $g_\cdot(\cdot)$.
- Number of iterations B.
- Regularization parameter $\lambda \in (0, 1]$.

1. Initialization: $g_0(\cdot) = \arg\min_{c \in \mathbb{R}} \frac{1}{n} \sum_{i=1}^{n} \ell\big(c, y_i\big)$.
2. For $k = 1, ..., B$
   - 2.1 Calculate the negative gradient $-\frac{\partial}{\partial g(\boldsymbol{x}_i)} \ell\big(g(\boldsymbol{x}_i), y_i\big)$ and evaluate it at points $g_{k-1}(\boldsymbol{x}_i)$:

$$v_i = -\frac{\partial}{\partial g(\boldsymbol{x}_i)} \ell\big(g(\boldsymbol{x}_i), y_i\big)\Big|_{g(\boldsymbol{x}_i)=g_{k-1}(\boldsymbol{x}_i)}, \quad i = 1, ..., n\,.$$

   - 2.2 Learn a weak learner $h_k(\cdot)$ on $(\boldsymbol{x}_1, v_1), (\boldsymbol{x}_2, v_2), ..., (\boldsymbol{x}_n, v_n)$.
   - 2.3 Update the classifier: $g_k(\cdot) = g_{k-1}(\cdot) + \lambda h_k(\cdot)$.

Output: The classification rule $\hat{g}(\cdot) = g_k(\cdot)$.

Gradient boost: some comments

- The output of $\hat{g}(\cdot)$ is a **real number**. To predict the class label one should use the "sign" operator:

$$\hat{y} = \text{sign}\big(\hat{g}(\boldsymbol{x})\big) \,.$$

- The algorithm (almost) **coincides with AdaBoost** for:
  - $\ell\big(g(\boldsymbol{x}), y\big) = e^{-yg(\boldsymbol{x})}$,
  - $\lambda = 1$.

- The **choice of the regularization parameter** λ is connected to the number of iterations B.
  It "controls" the speed of minimization of function

$$\frac{1}{n}\sum_{i=1}^{n} \ell\big(g(\boldsymbol{x}_i), y_i\big) \,.$$

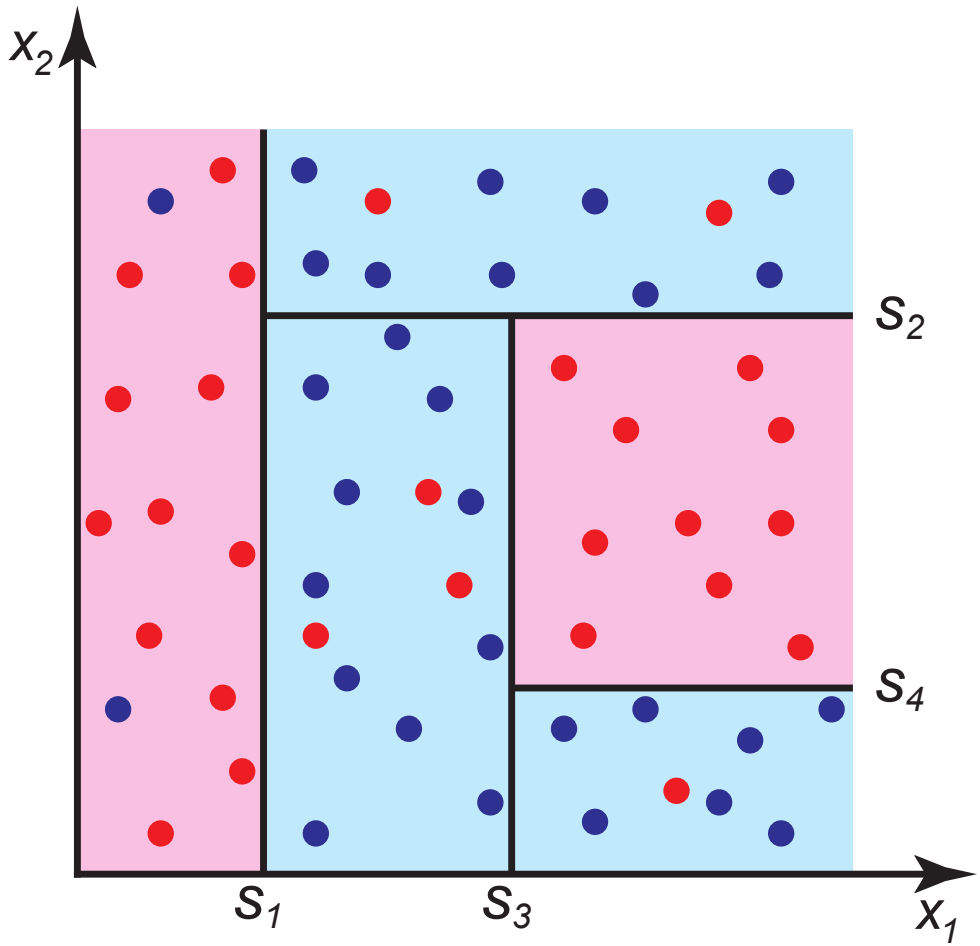
- Larger values of λ correspond to smaller values of B, and *vice versa*.

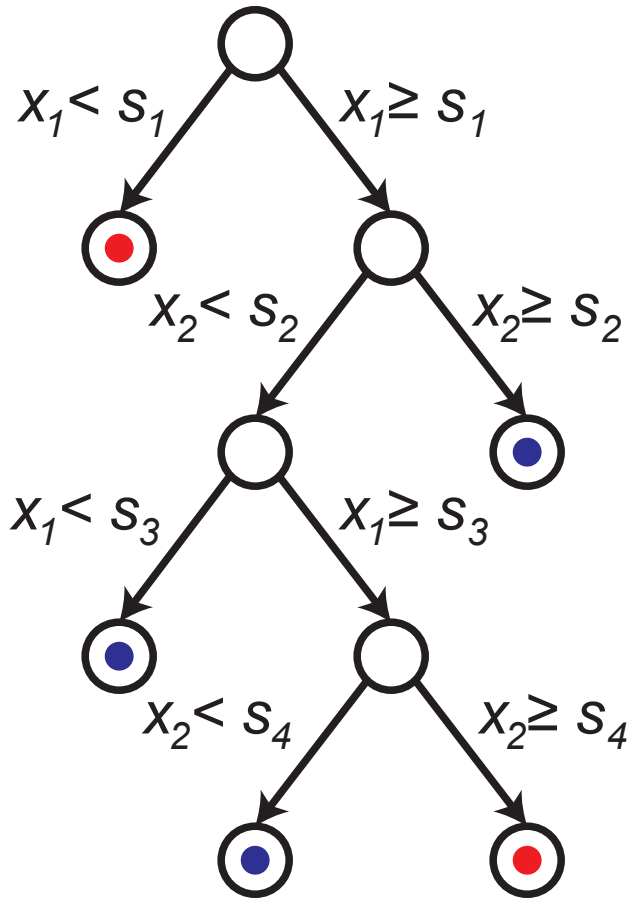
Contents

Weak learners

- For Gradient boost, as well as for AdaBoost, the classification rule used in the algorithm should be **weak** (slightly better than the purely random choice).
- Boosting a **non-weak** classification **rule** usually delivers **poor performance** increase.
- It is recommended to use a classification rule with **high bias** but **small variance** (boosting allows to reduce bias and not variance).
- Often **tree** is used as a weak learner. For high bias one usually chooses **trees with a few leaves only** (*i.e.*, of low depth).
- In numerous implementations of boosting **regression trees** are used.

Reminder: classification tree





Regression tree

- Regression tree is grown in a **(very) similar to the classification tree manner** with slight changes:
- Suppose that **a partition** into M regions $R_1, R_2, ..., R_M$ **is given**.
- The **response is** then modeled as **a constant** c_m **in each region**:

$$f(\boldsymbol{x}) = \sum_{m=1}^{M} c_m \mathbb{1}(\boldsymbol{x} \in R_m) \,.$$

- Adopt **sum of squares as impurity measure**:

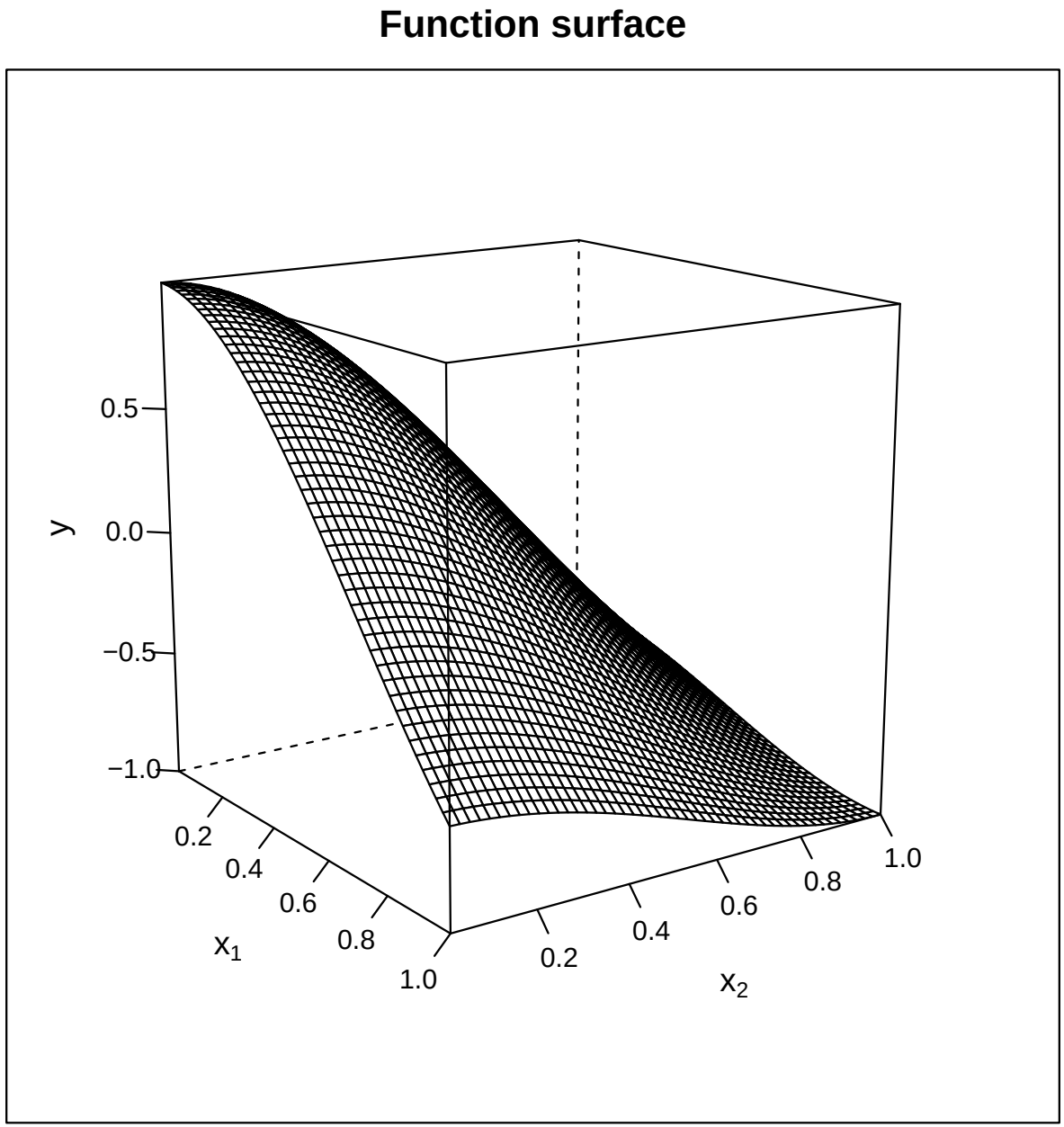
$$Q^{(m)}(T) = \frac{n^{(m_L)}}{n^{(m)}} \sum_{\boldsymbol{x}_i \in R_{m_L}} (y_i - \hat{c}_{m_L})^2 + \frac{n^{(m_R)}}{n^{(m)}} \sum_{\boldsymbol{x}_i \in R_{m_R}} (y_i - \hat{c}_{m_R})^2 \,.$$

- One can check that the **optimal choice of** $\hat{c}_m$ for region R_m **is the average over** R_m:

$$\hat{c}_m = \frac{1}{n^{(m)}} \sum_{\boldsymbol{x}_i \in R_m} y_i \,,$$

with $n^{(m)}$ being the number of observations $\boldsymbol{x}_i \in \mathcal{D}_n$ in region R_m.

Regression tree (illustration)



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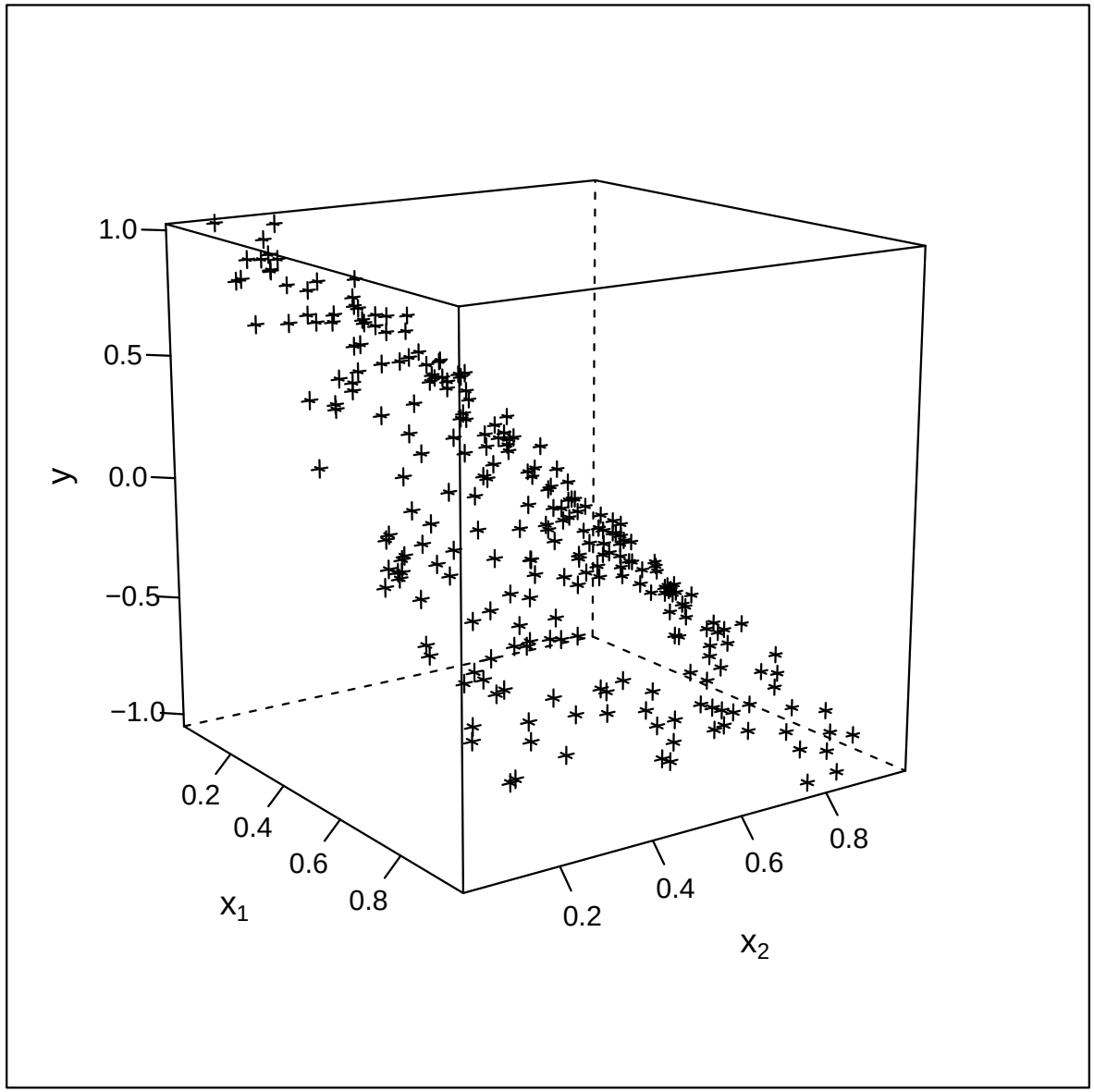

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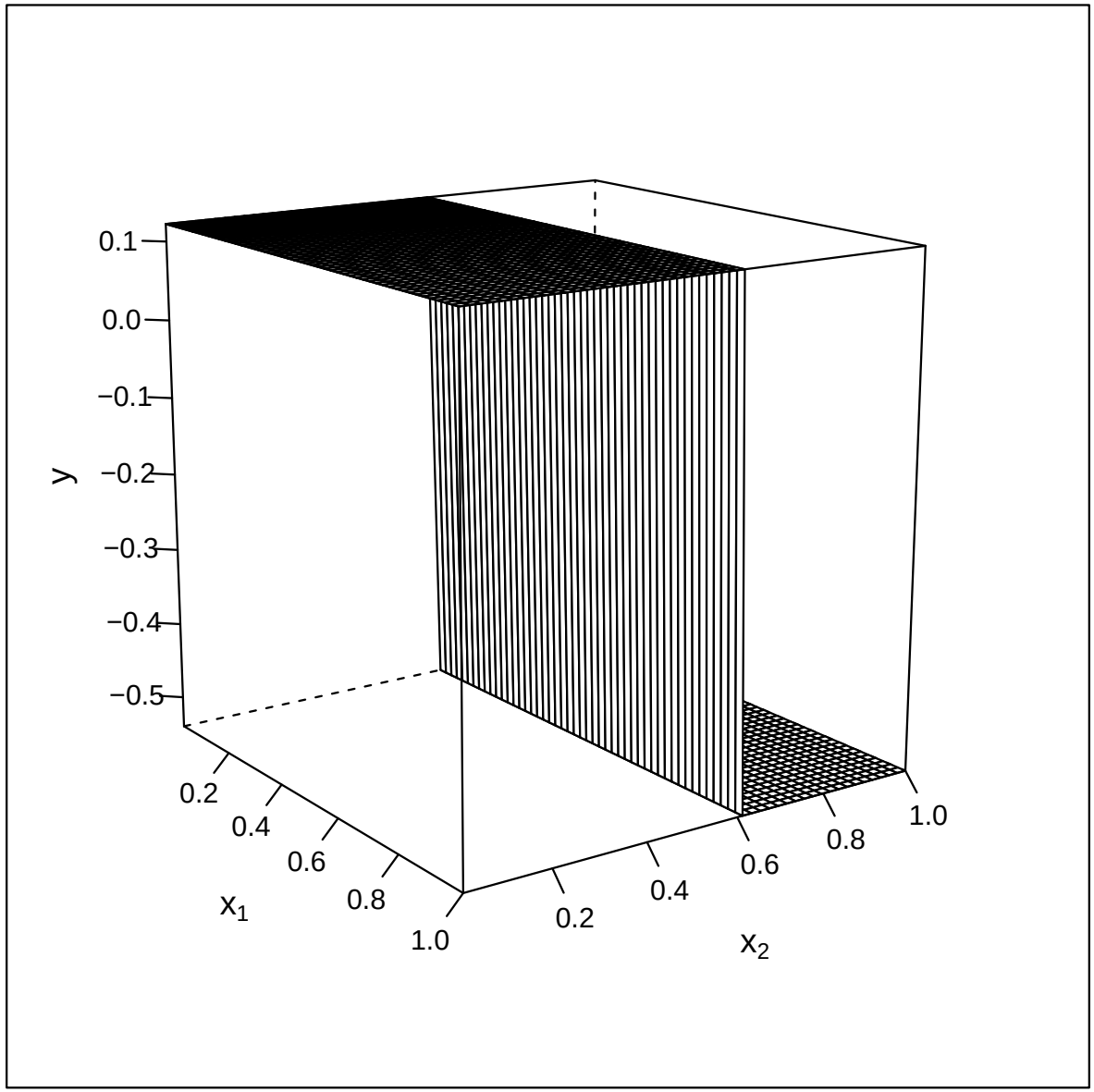

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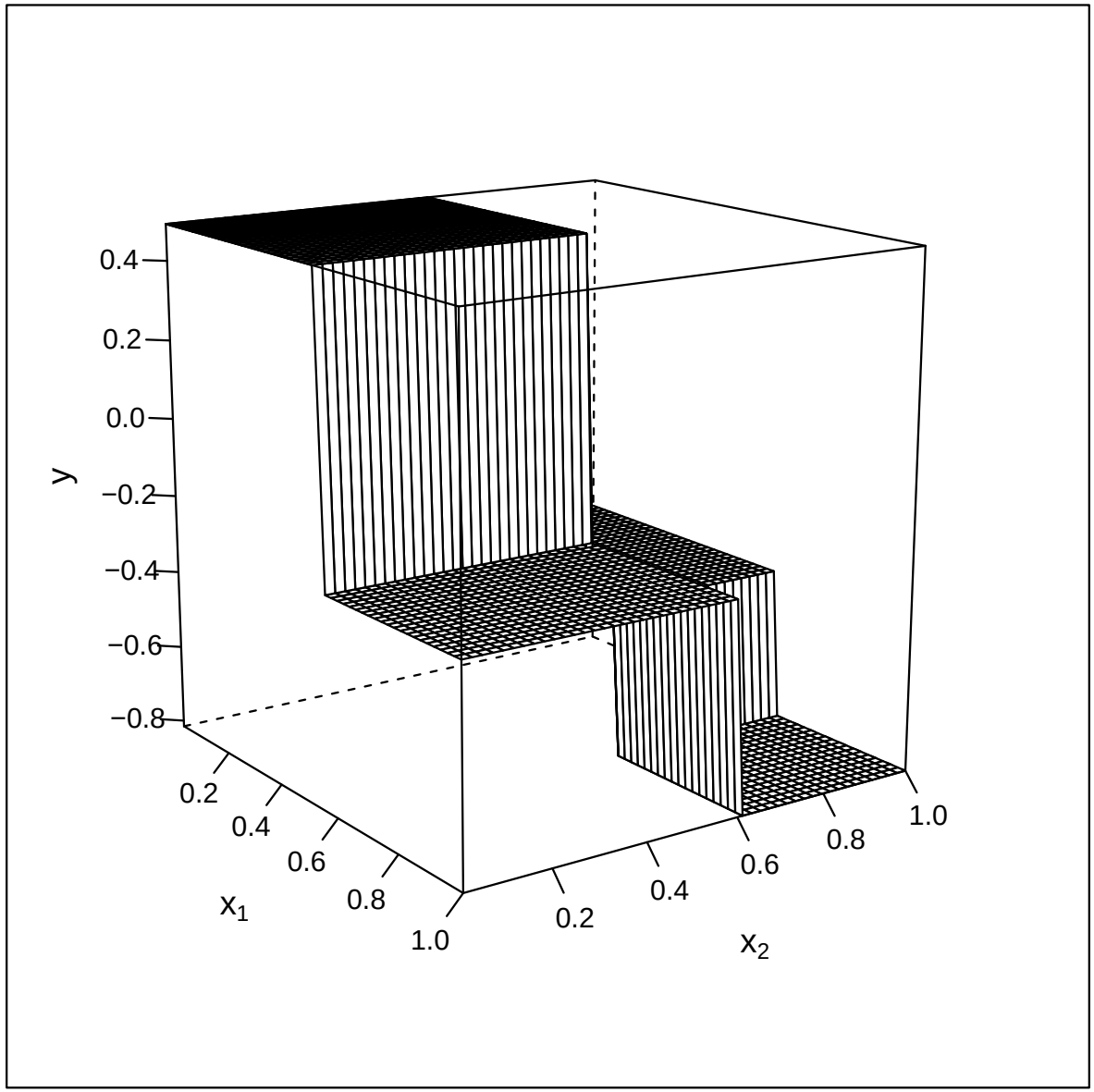
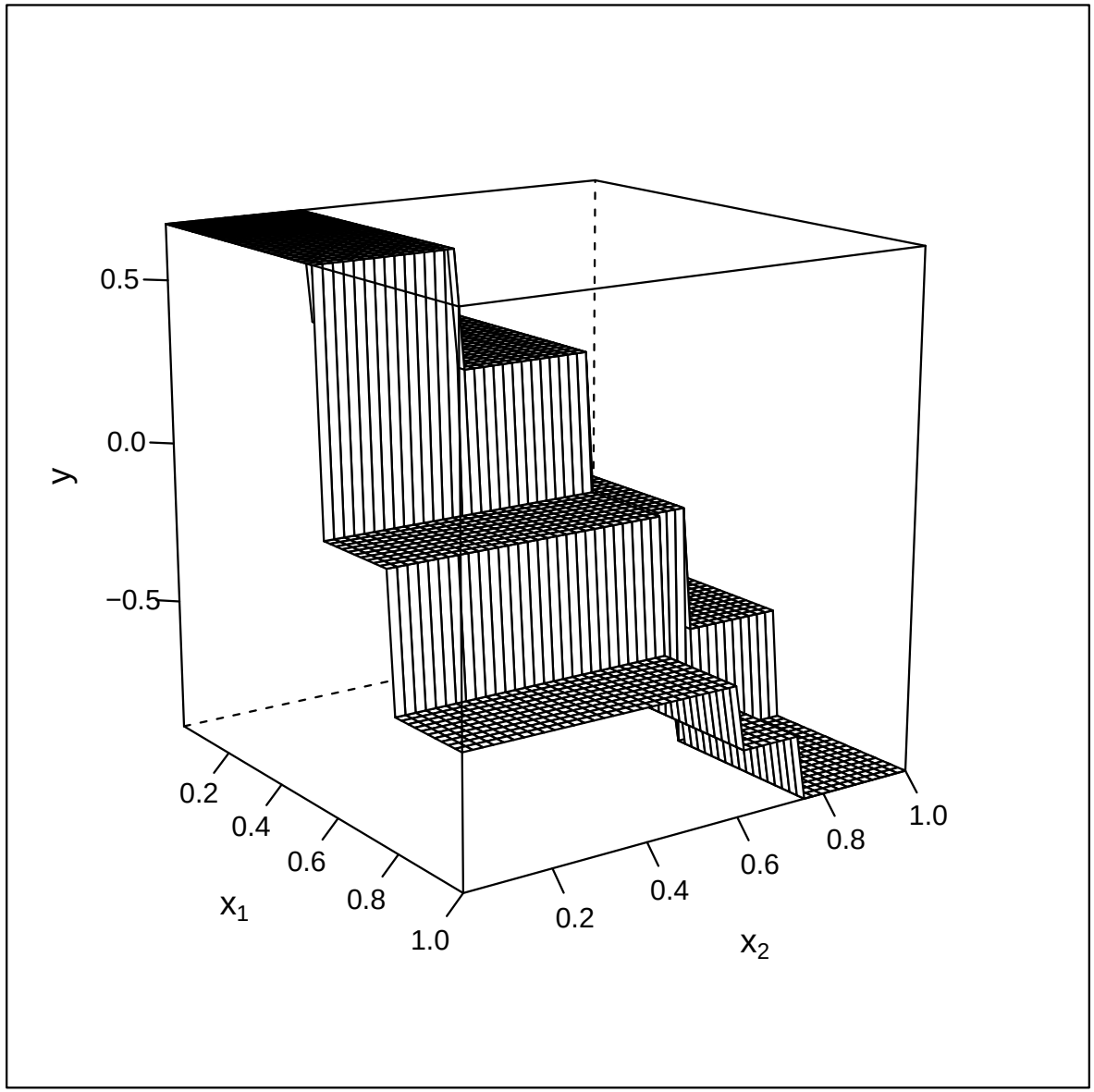
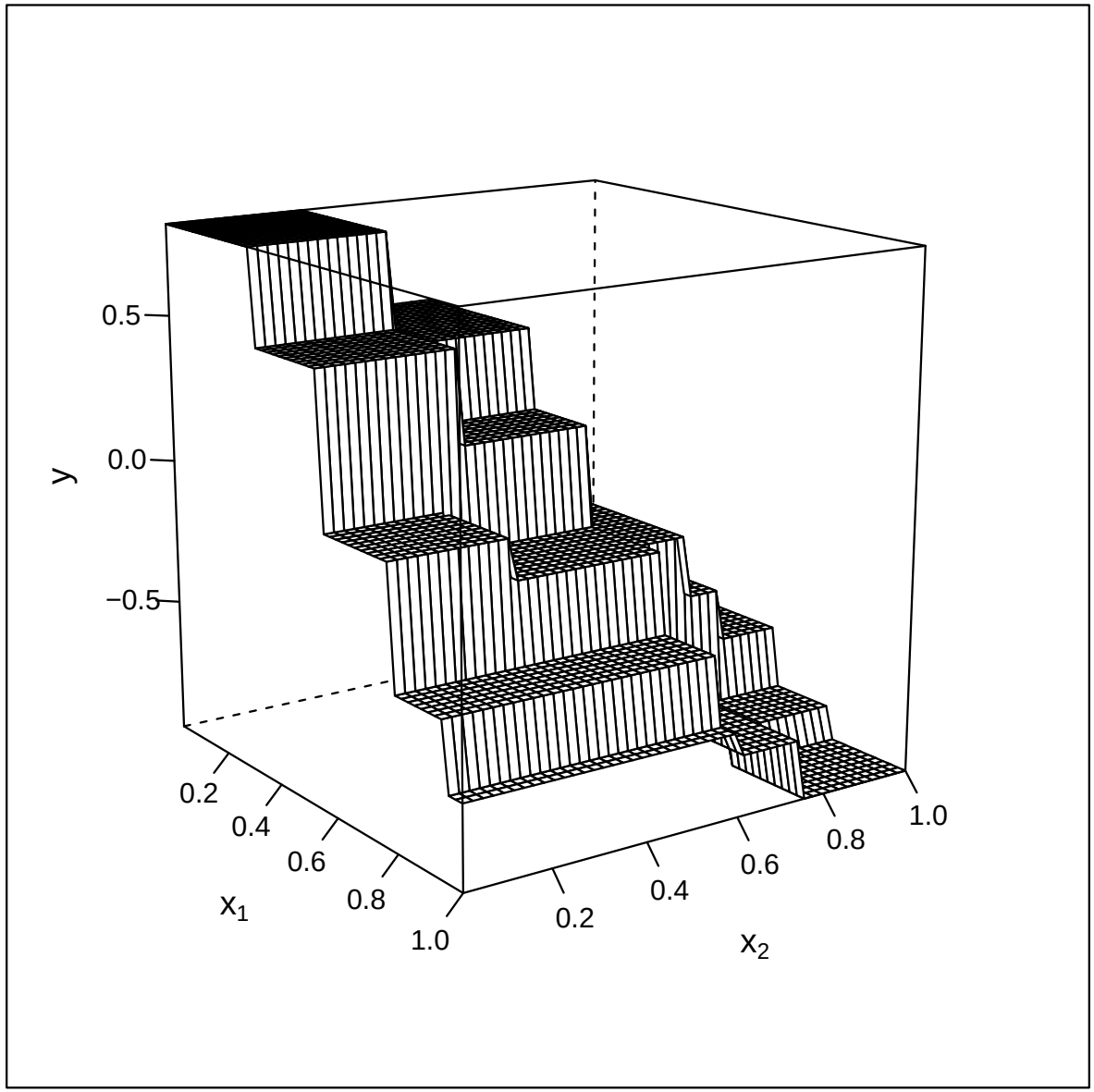


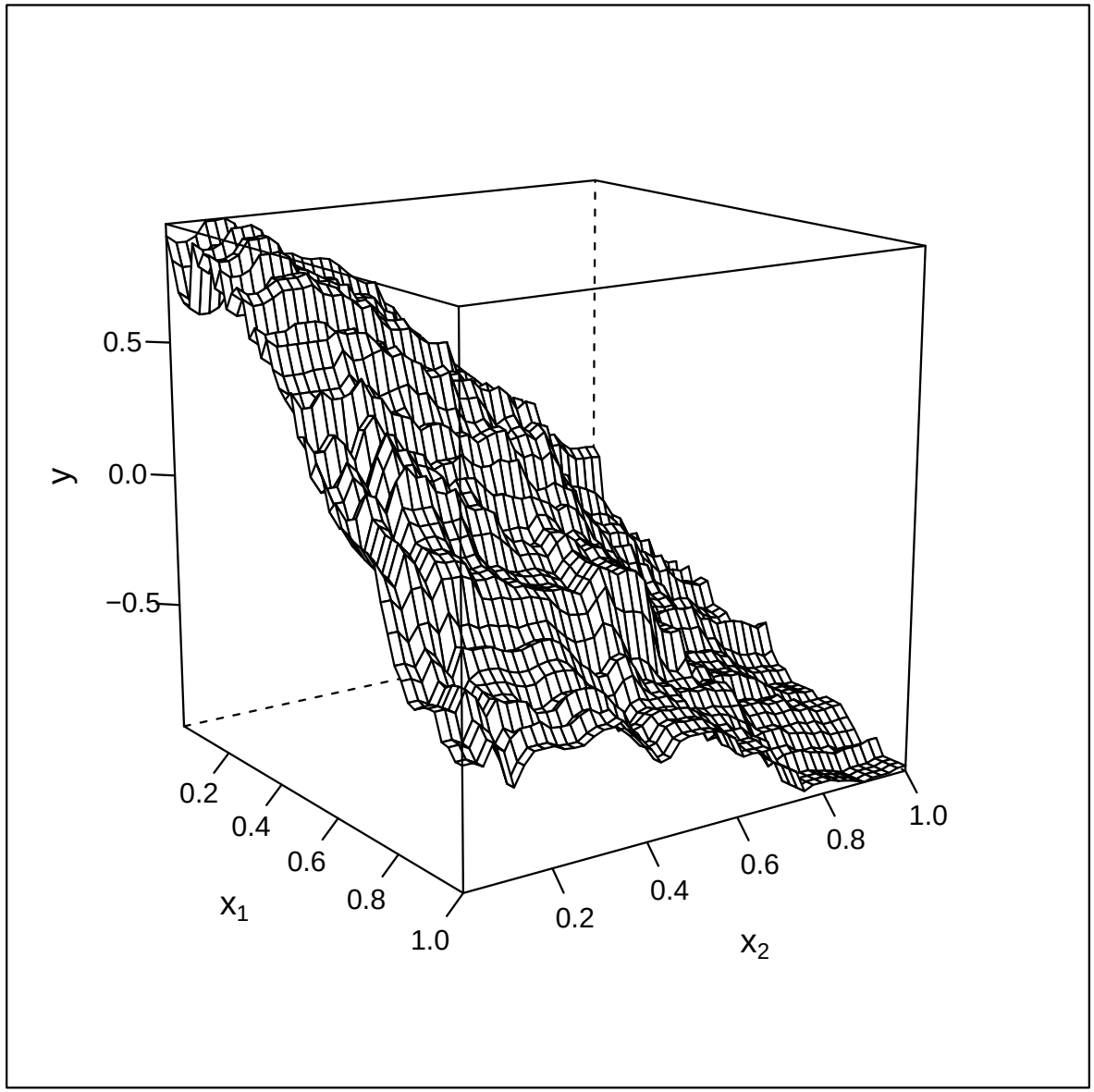
Regression tree (illustration)



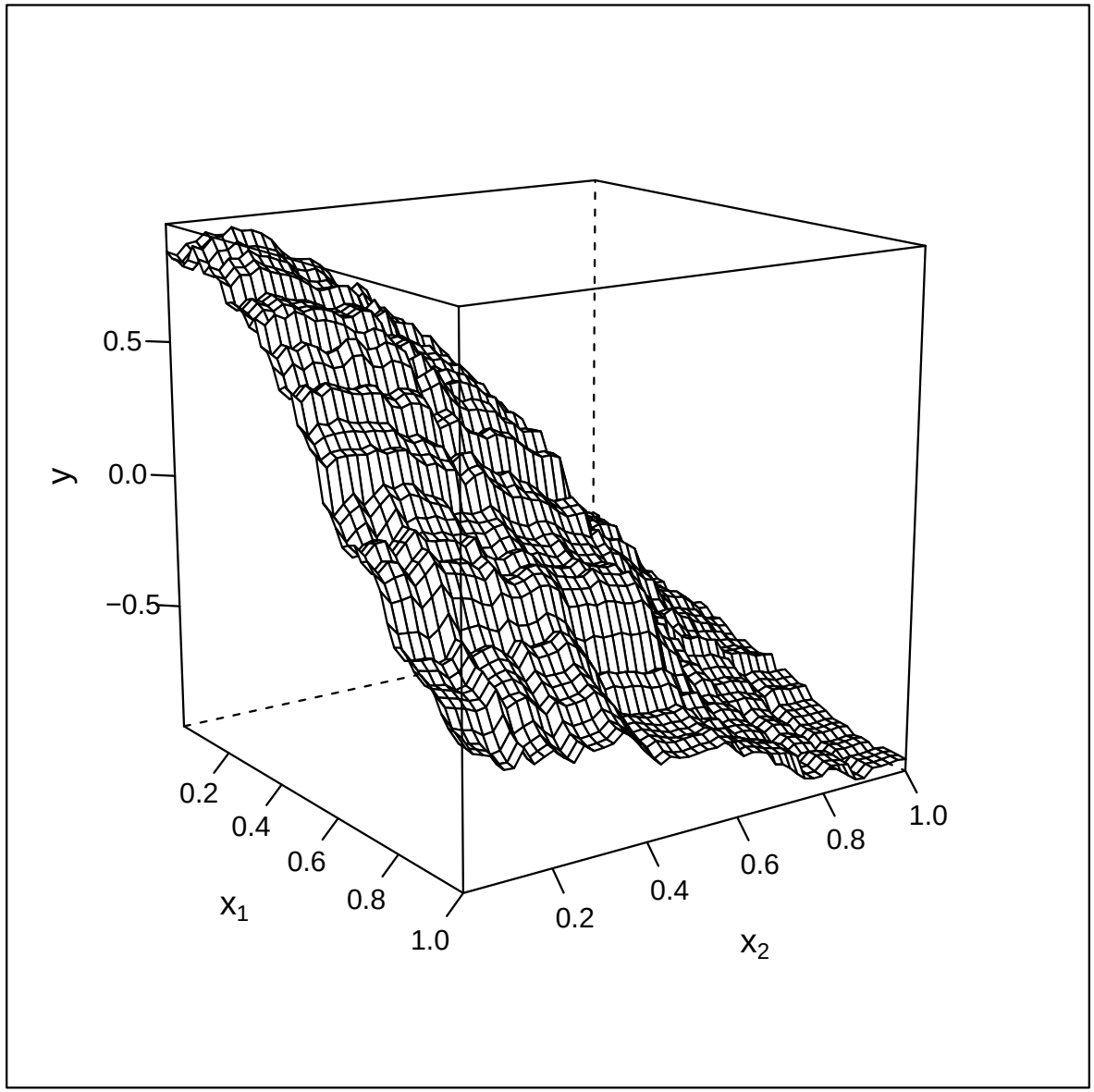
Regression tree (illustration)



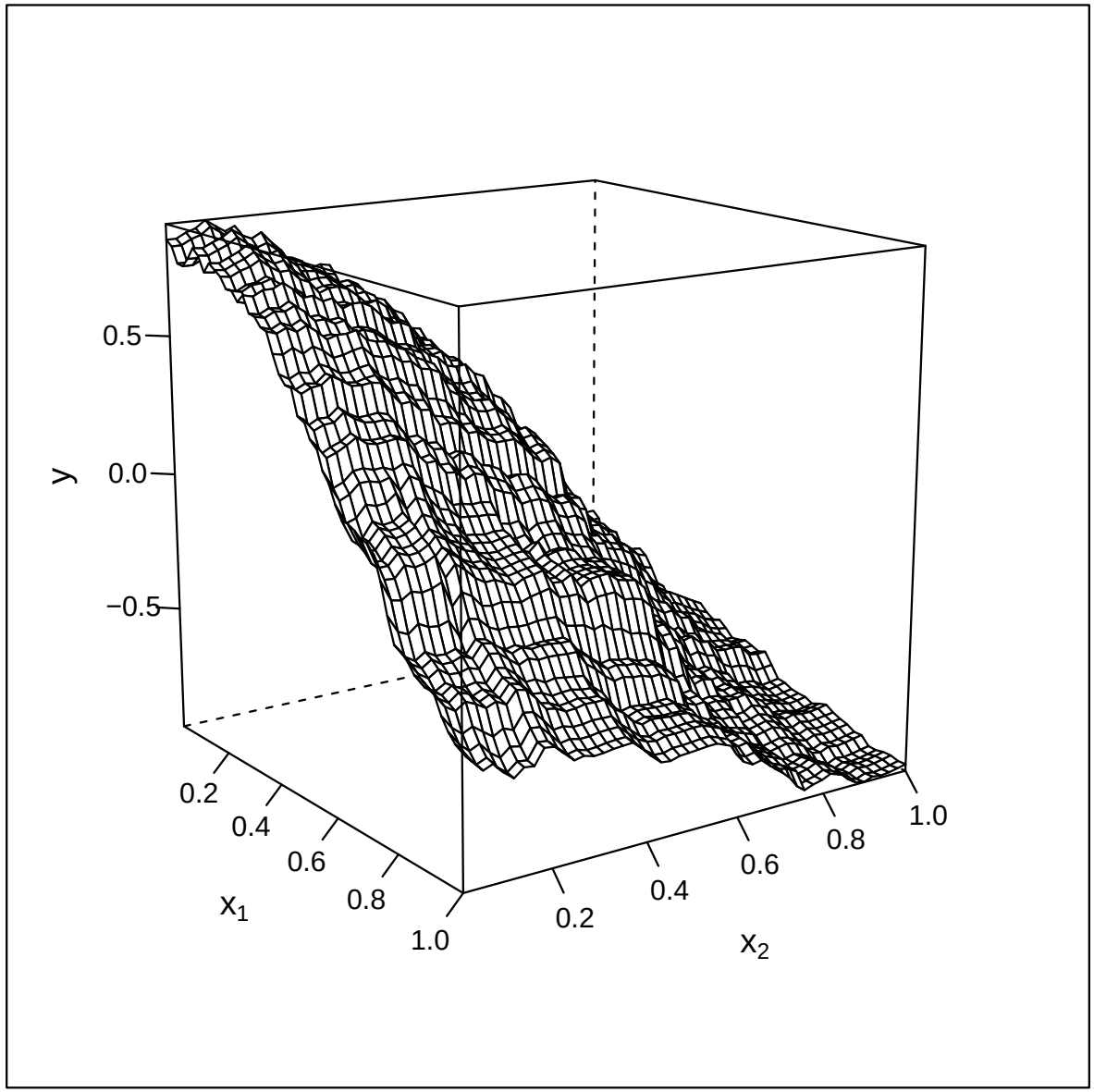
Regression tree (illustration)



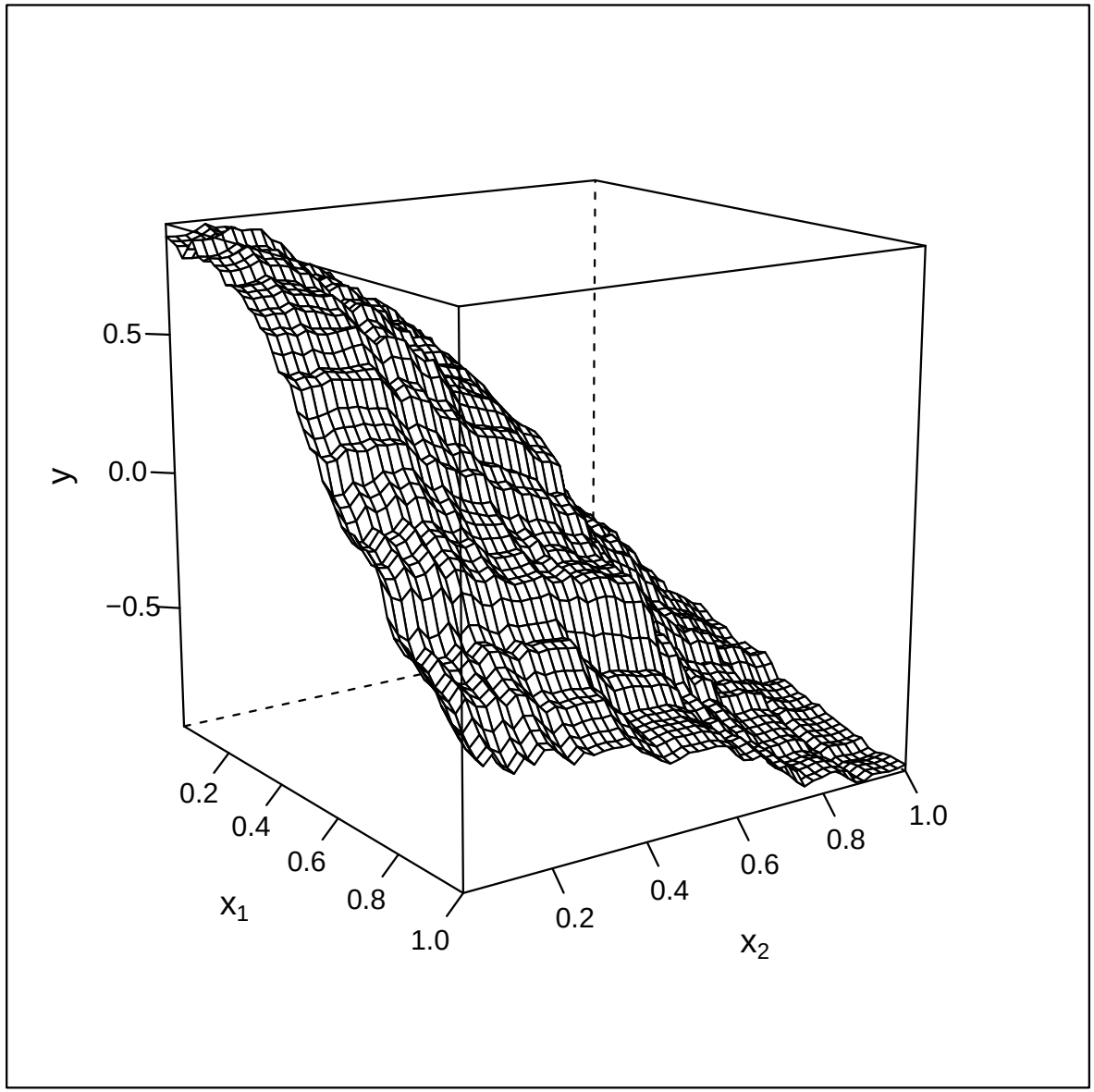
Regression tree (illustration)



Regression tree (illustration)



Regression tree (illustration)



Boosting regression trees in R

- Function `gbm` of `R`-package `gbm` by Ridgeway (2006).

Input parameters (arguments):

- loss function ℓ (`distribution`),
- number of iterations B (`n.trees`),
- depth of the grown three K (`interaction.depth`),
- regularization parameter λ (`shrinkage`).

FGD-trees (algorithm): Friedman (2001), Ridgeway (2006)

Constructing a classifier (training)

Input: Training sample $\big((\boldsymbol{x}_1, y_1), ..., (\boldsymbol{x}_n, y_n)\big) \subset \mathbb{R}^d \times \{-1, 1\}$.

1. Initialization: $g_0(\cdot) = \arg\min_{c \in \mathbb{R}} \frac{1}{n} \sum_{i=1}^{n} \ell\big(c, y_i\big)$.
2. For $k = 1, ..., B$
   - 2.1 Calculate the negative gradient $-\frac{\partial}{\partial g(\boldsymbol{x}_i)} \ell\big(g(\boldsymbol{x}_i), y_i\big)$ and evaluate it at points $g_{k-1}(\boldsymbol{x}_i)$:

$$v_i = -\frac{\partial}{\partial g(\boldsymbol{x}_i)} \ell\big(g(\boldsymbol{x}_i), y_i\big)\Big|_{g(\boldsymbol{x}_i)=g_{k-1}(\boldsymbol{x}_i)}, \quad i = 1, ..., n\,.$$

   - 2.2 Grow the regression tree of maximal depth K based on the sample

$$(\boldsymbol{x}_1, v_1),\ (\boldsymbol{x}_2, v_2),\ ...,\ (\boldsymbol{x}_n, v_n)\,.$$

   - 2.3 For each leaf $m = 1, ..., M$ calculate the optimal prediction:

$$\rho_m = \arg\min_{\rho \in \mathbb{R}} \sum_{\boldsymbol{x}_i \in R_m} \ell\big(g_{k-1}(\boldsymbol{x}_i) + \rho, y_i\big)\,.$$

   - 2.4 Update the classifier: $g_k(\boldsymbol{x}) = g_{k-1}(\boldsymbol{x}) + \lambda \rho_{m(\boldsymbol{x})}$ with $m(\boldsymbol{x})$ being a leaf containing $\boldsymbol{x}$.

Output: The classification rule $\hat{g}(\boldsymbol{x}) = g_k(\boldsymbol{x})$.

Contents

Connection to AdaBoost

- One can show (Hastie, Tibshirani, Friedman, 2000) that the AdaBoost algorithm is a gradient descent method for minimizing

$$\mathbb{E}\big[\ell\big(g(X), Y\big)\big]\,.$$

  with $\ell\big(g(\boldsymbol{x}), y\big) = e^{-yg(\boldsymbol{x})}$.

- Thus the output $\hat{g}(\boldsymbol{x})$ is an estimator of

$$g^*(\boldsymbol{x}) = \frac{1}{2}\log\frac{\mathbb{P}[Y=1|X=\boldsymbol{x}]}{\mathbb{P}[Y=-1|X=\boldsymbol{x}]}\,.$$

- Hence:

$$\mathbb{P}[Y=1|X=\boldsymbol{x}] = \frac{e^{g^*(\boldsymbol{x})}}{e^{-g^*(\boldsymbol{x})}+e^{g^*(\boldsymbol{x})}}\,,$$

$$\mathbb{P}[Y=-1|X=\boldsymbol{x}] = \frac{e^{-g^*(\boldsymbol{x})}}{e^{-g^*(\boldsymbol{x})}+e^{g^*(\boldsymbol{x})}}\,.$$

- The **gradient descent** algorithm can be applied to **further loss functions**.

LogitBoost

- Suppose (here) that Y takes values from $\{0, 1\}$.
- The conditional random variable $Y|X = \boldsymbol{x}$ follows the Bernoulli distribution with parameter $p(\boldsymbol{x}) = \mathbb{P}[Y = 1|X = \boldsymbol{x}]$, and its **likelihood as a function of** $p(\boldsymbol{x})$ for an observation $(\boldsymbol{x}, y)$ can be written as:
$$p(\boldsymbol{x})^y \left(1 - p(\boldsymbol{x})\right)^{1-y}.$$
- The **logistic regression model** assumes:
$$p(\boldsymbol{x}) = \frac{1}{1 + e^{-(\beta_0 + \boldsymbol{\beta}^T \boldsymbol{x})}} = \frac{e^{\beta_0 + \boldsymbol{\beta}^T \boldsymbol{x}}}{1 + e^{\beta_0 + \boldsymbol{\beta}^T \boldsymbol{x}}},$$
where $(\beta_0, \beta^T)^T$ is estimated by maximizing the likelihood.
- One can use the functional gradient descent method to **overcome the linearity assumption** on parameters of $(1, \boldsymbol{x}^T)^T$ in $p(\boldsymbol{x})$.

LogitBoost

- One can rewrite:

$$p(\boldsymbol{x}) = \frac{1}{1 + e^{-2f(\boldsymbol{x})}} = \frac{e^{f(\boldsymbol{x})}}{1 + e^{f(\boldsymbol{x})}}$$

  with $f : \mathbb{R}^d \to \mathbb{R}$ being an unknown function.

- As it is done in logistic regression, one can **estimate $f(\boldsymbol{x})$ based on the likelihood**.

- **Choice of the loss function:** the negative log-likelihood (which will be minimized):

$$-\Big(y \log p(\boldsymbol{x}) + (1-y) \log\big(1 - p(\boldsymbol{x})\big)\Big) = \log(1 + e^{-2\tilde{y} f(\boldsymbol{x})})$$

  with $\tilde{y} = 2y - 1 \in \{-1, 1\}$.

- One can simply verify convexity of:

$$v \mapsto \log(1 + e^{-2\tilde{y}v})\,.$$

LogitBoost

- The functional gradient descent algorithm applied to the loss function:

$$\begin{aligned} \ell : \mathbb{R} \times \{-1, 1\} &\to \mathbb{R} \\ \left(f(\boldsymbol{x}), \tilde{y}\right) &\mapsto \log(1 + e^{-2\tilde{y}f(\boldsymbol{x})}) \end{aligned}$$

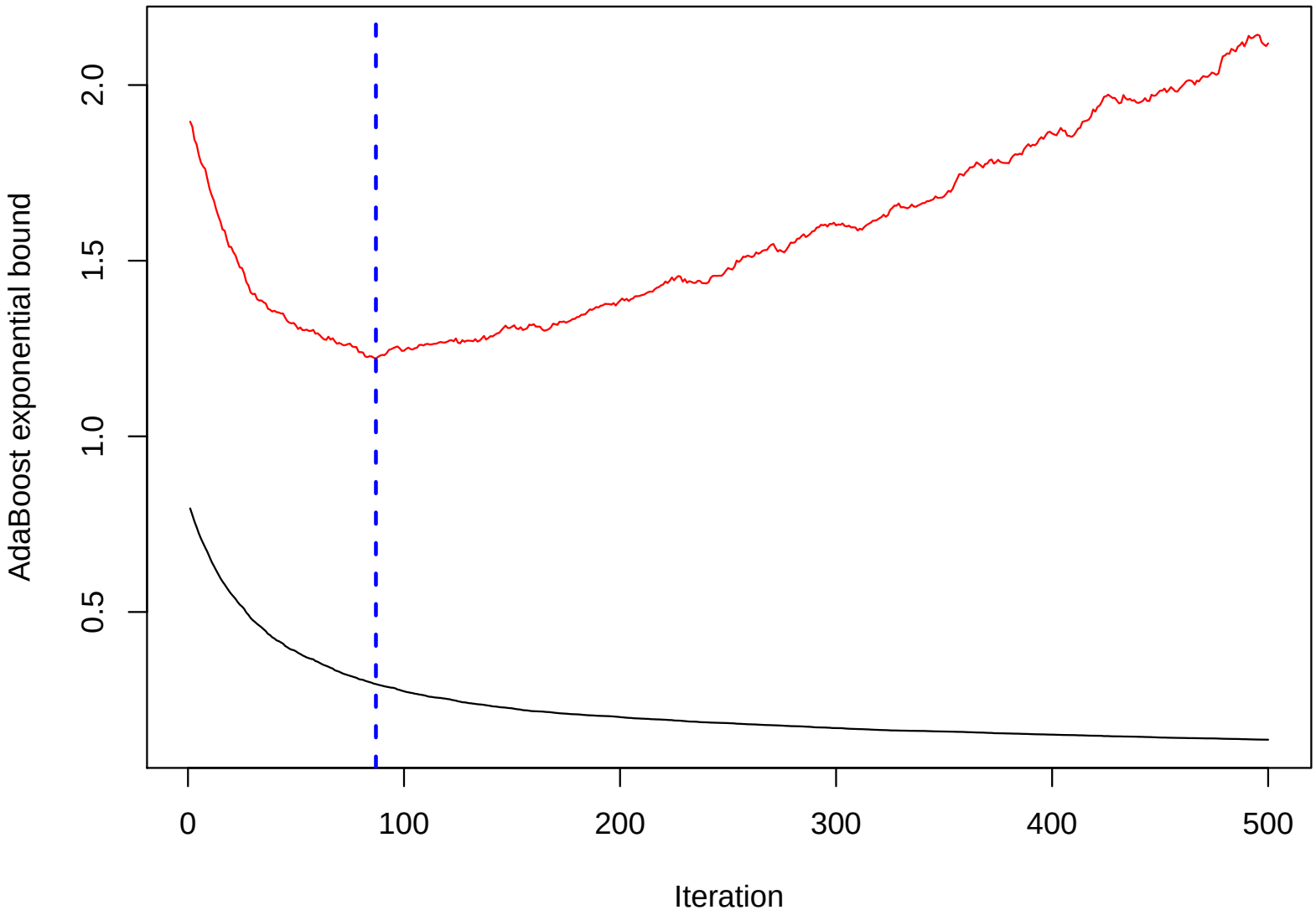
  is called **LogitBoost**.

- For this loss function, the function $\mathbb{E}\left[\ell\left(f(X), Y\right)\right]$ is minimized at:

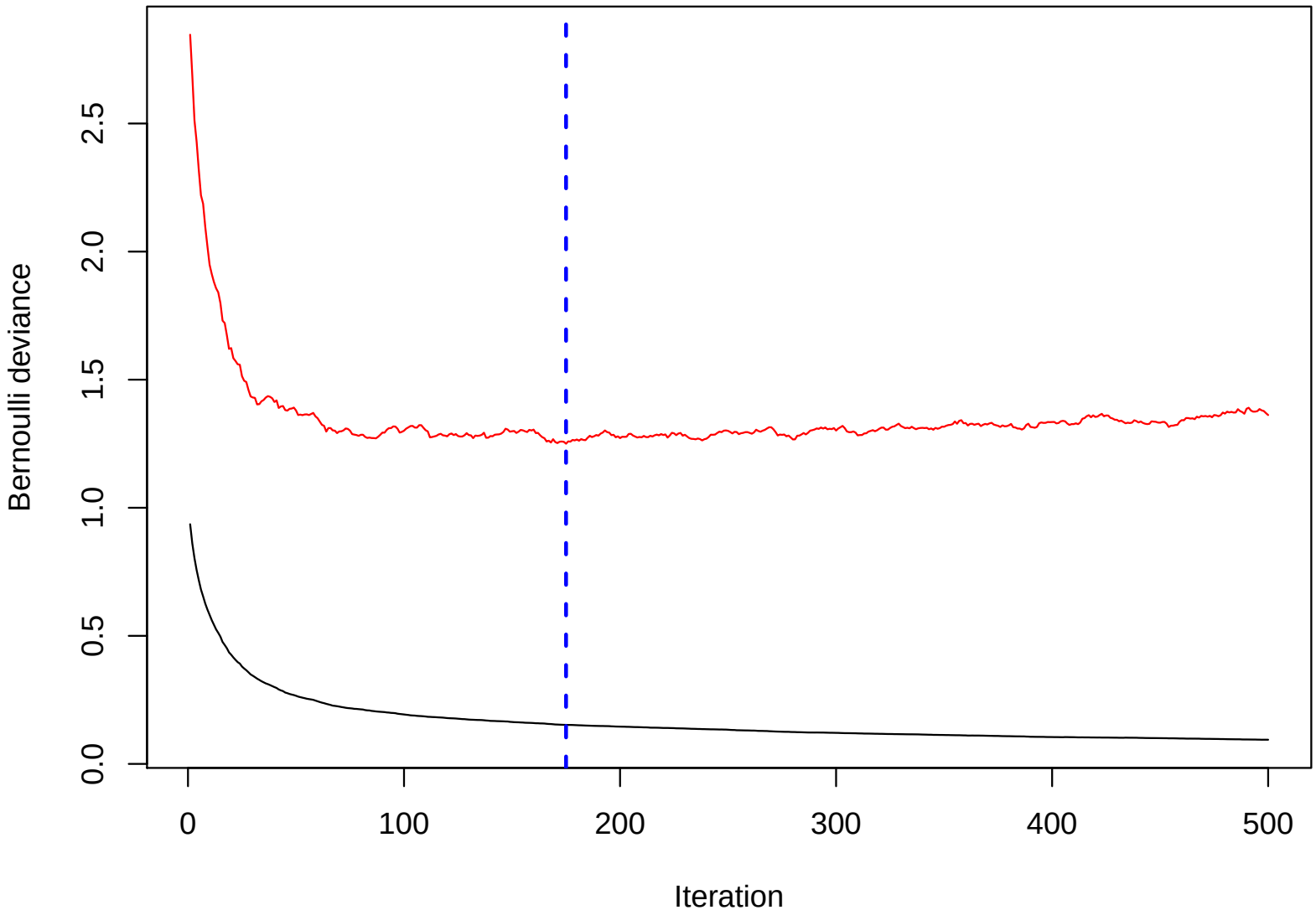
$$f^*(\boldsymbol{x}) = \frac{1}{2} \log \frac{\mathbb{P}[Y = 1 | X = \boldsymbol{x}]}{\mathbb{P}[Y = -1 | X = \boldsymbol{x}]} .$$

- Thus, AdaBoost and LogitBoost provide an estimator of the same quantity.

Performance validation, spam data (AdaBoost, FGD)



Performance validation, spam data (LogitBoost, FGD)



Thank you for your attention!

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And some references

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