Classification tree, bagging, and random forest

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(with contributions of Laurent Rouviere[2] and Valentin Patilea[3])

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Machine learning

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Today

Classification tree

- Algorithm
- Tuning

Bagging

- Motivation
- Algorithm
- An example

Random forest

- Algorithm
- Interpretation
- Consistency results

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.
  - Section 8.7.
  - Section 9.2.
  - Chapter 15.

- Slides of the lecture.

- Biau, Devroye, Lugosi (2008).
  Consistency of random forests and other averaging classifiers.
  Journal of Machine Learning Research, 9, 2015–2033.

Binary supervised classification (reminder)

Notation:

- **Given:** for the random pair (X, Y) in $\mathbb{R}^d \times \{0, 1\}$ consisting of a random observation X and its random binary label Y (class), a sample of n i.i.d.: $(\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)$.
- **Goal:** predict the label of the new (unseen before) observation $\mathbf{x}$.
- **Method:** construct a classification rule:

$$g : \mathbb{R}^d \to \{0, 1\}, \mathbf{x} \mapsto g(\mathbf{x}),$$

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

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

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

$$g(\mathbf{x}) = 1(\mathbb{E}[Y|X = \mathbf{x}] > 0.5).$$

Contents

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Classification tree (algorithm)

Growing a tree (training)

Input:

- Training sample $\big((\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\big) = \mathcal{D}_n \in \mathbb{R}^d \times \{0, 1\}$.

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Output: The tree T.

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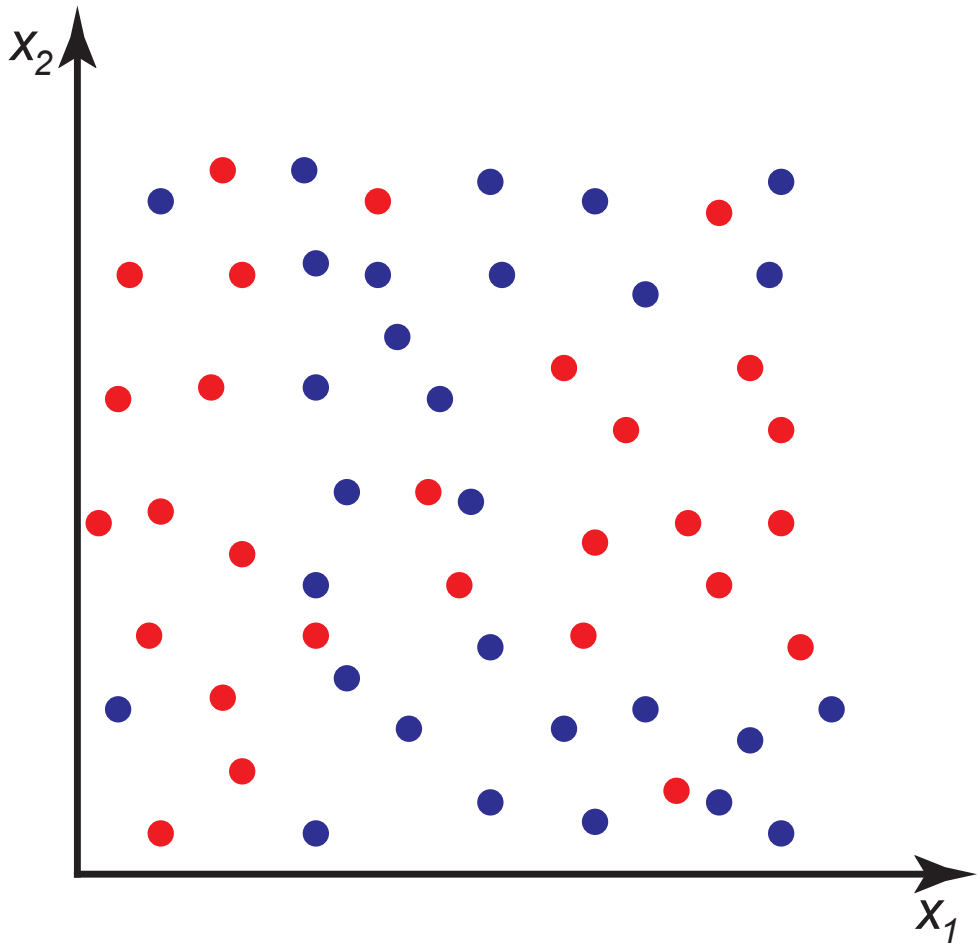
- *Descend the tree* until a terminal node.
- In each node m, classify the observations by choosing the *majority class*.
- That is, in node m *classify* the observations to class $c(m)$:

$$c(m) = \underset{k \in \{0,1\}}{\arg\max} \sum_{i \in R^{(m)}} I(y_i = k)\,.$$

Classification tree (illustration)



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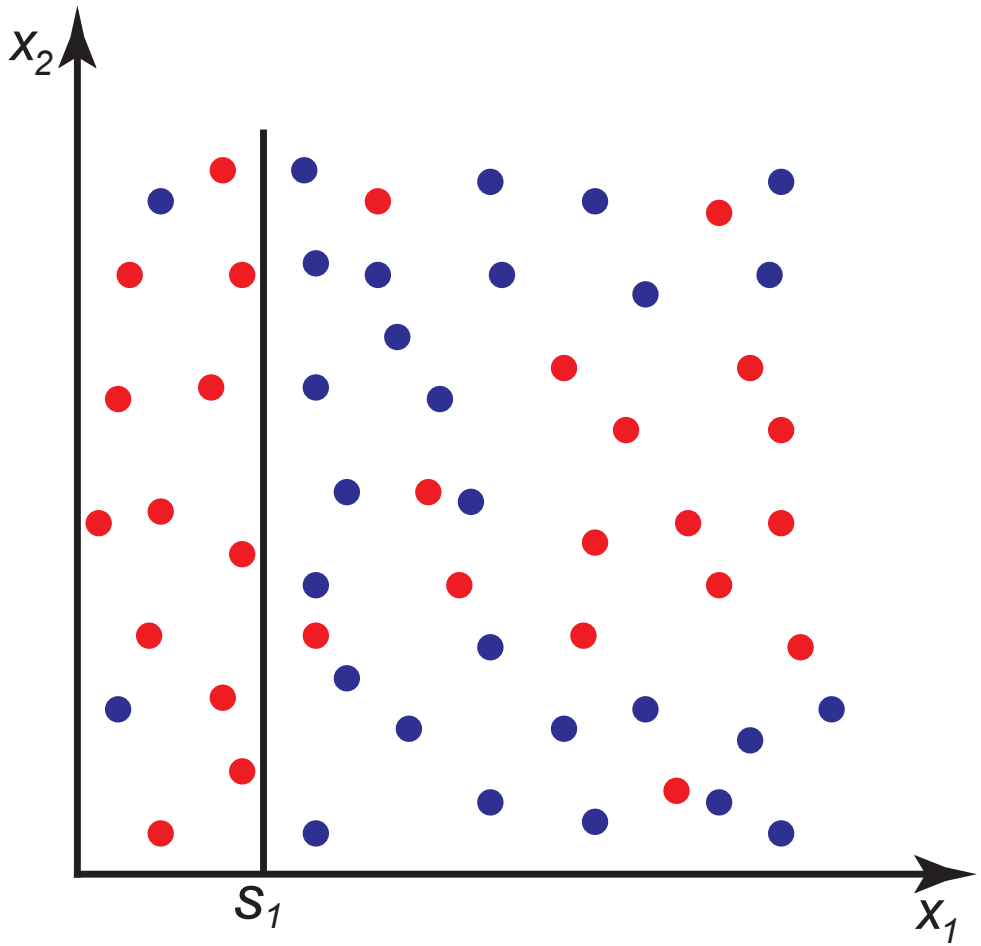

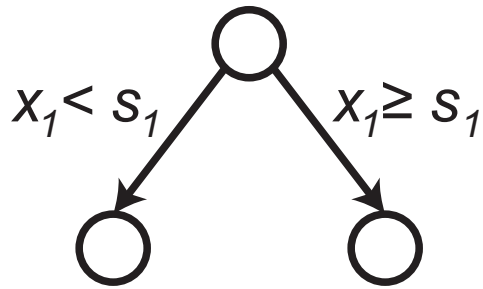

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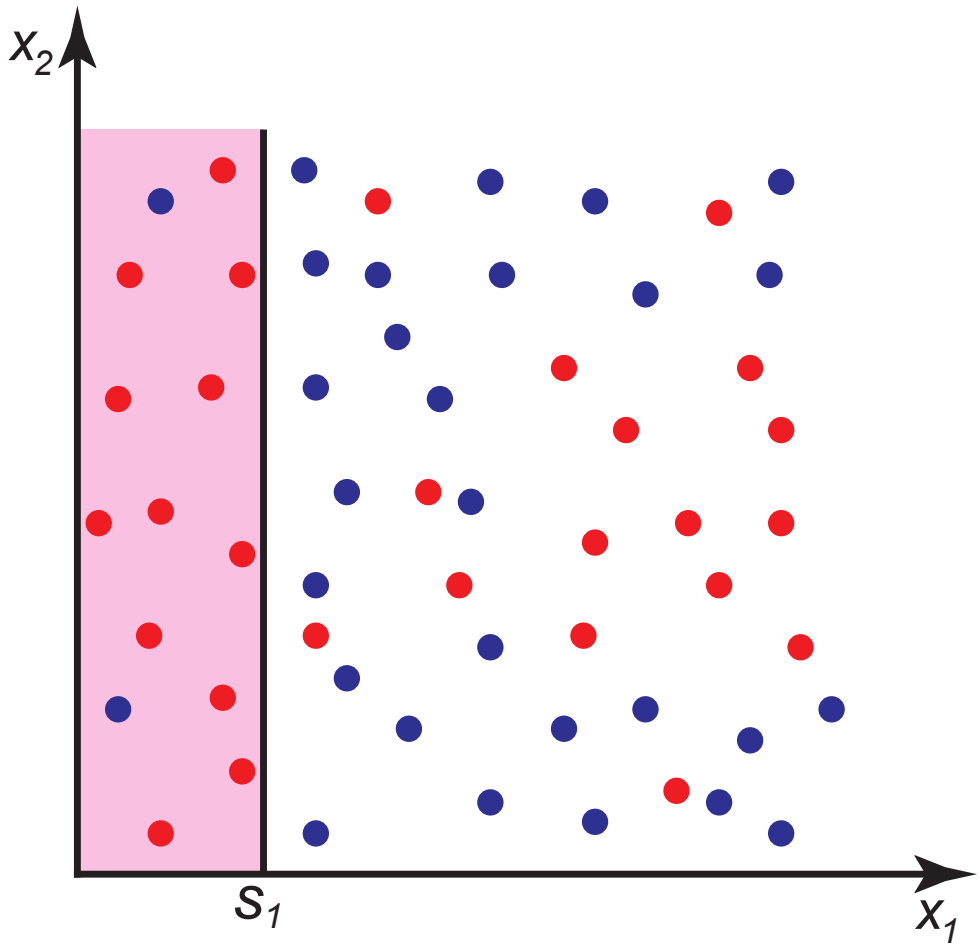

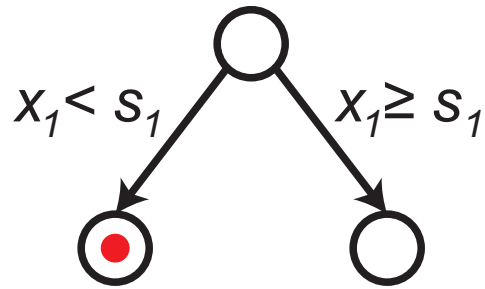

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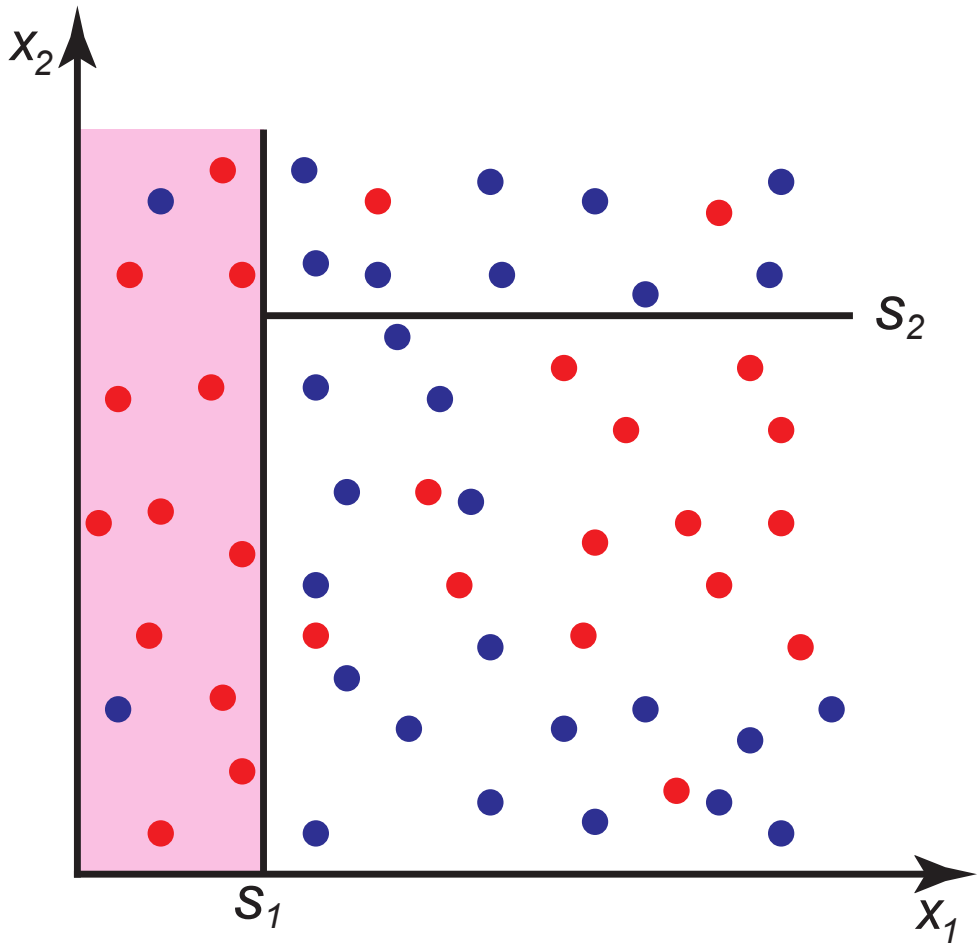

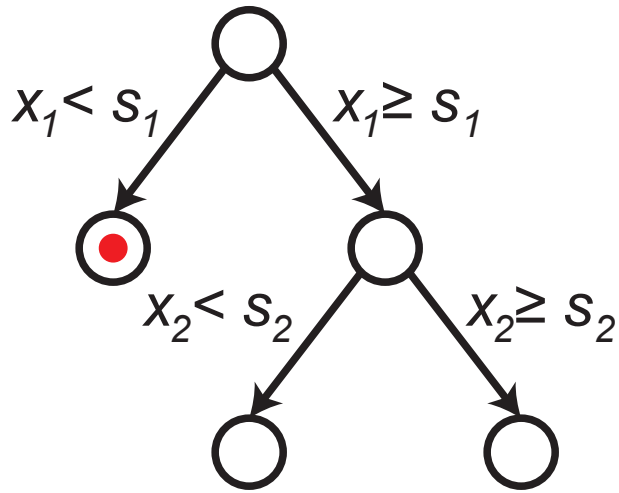

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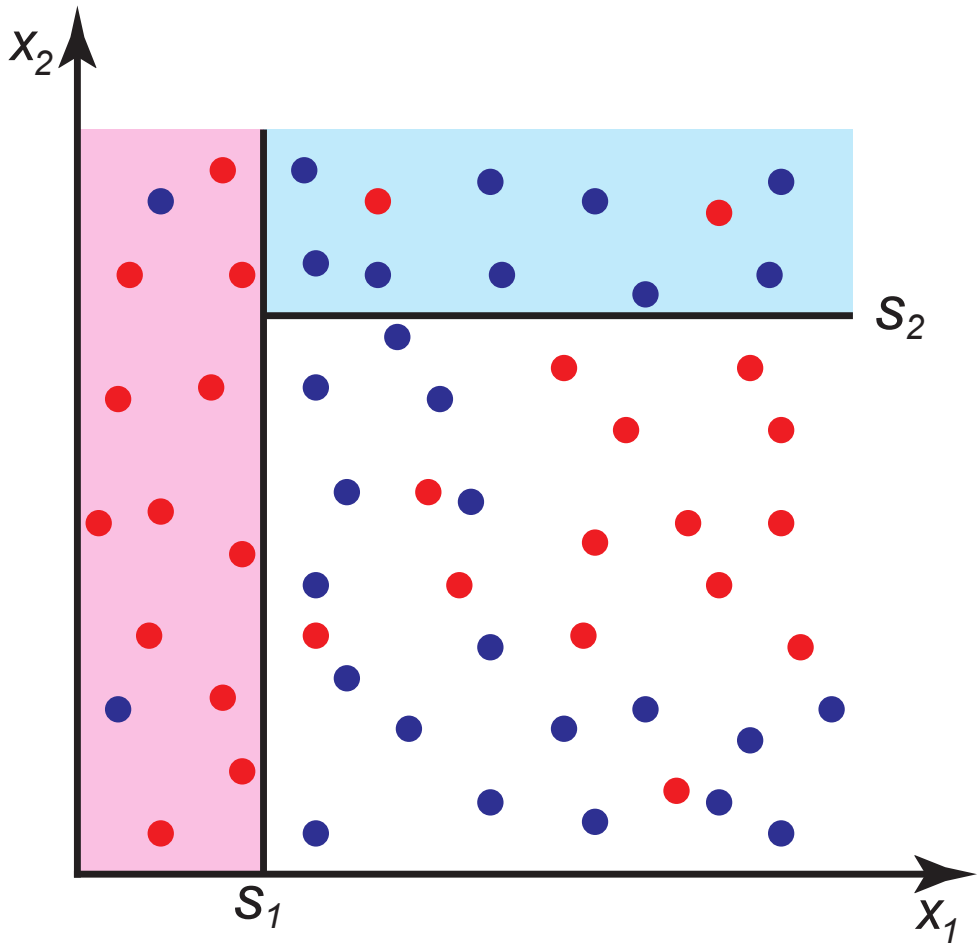

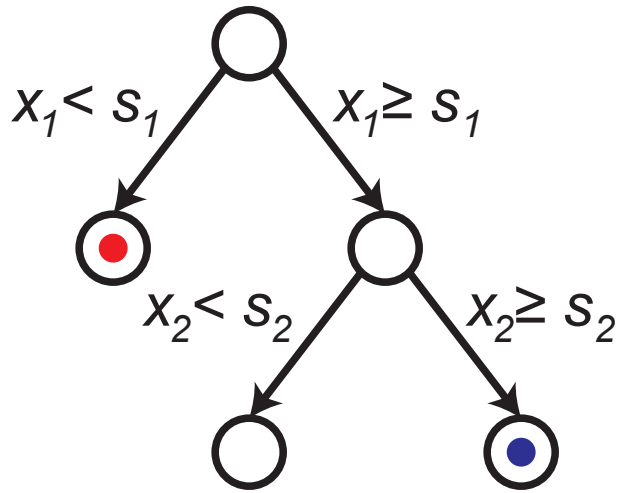

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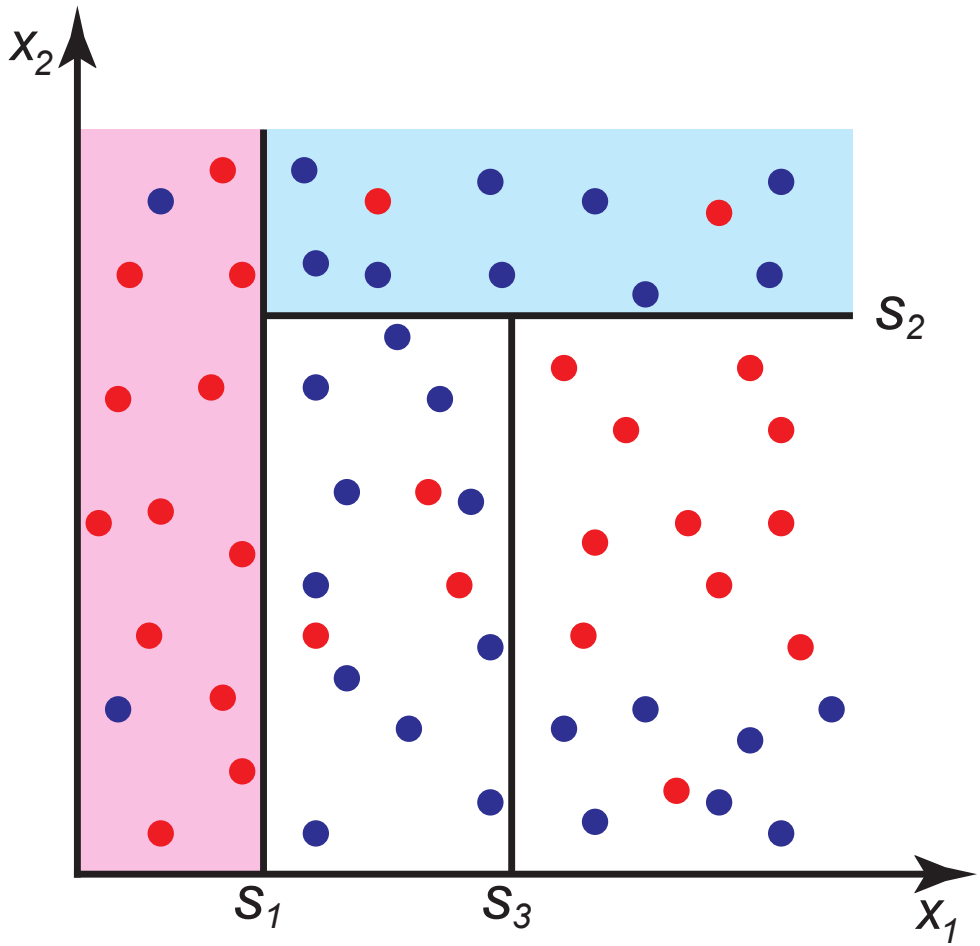

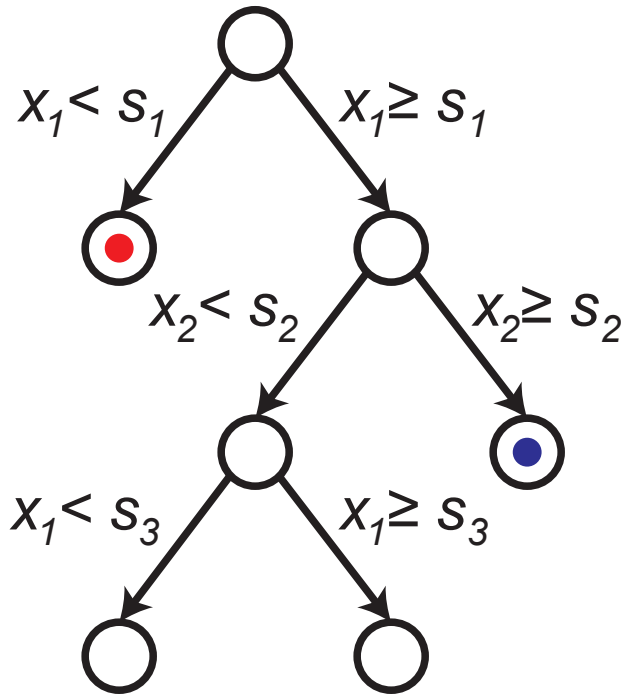

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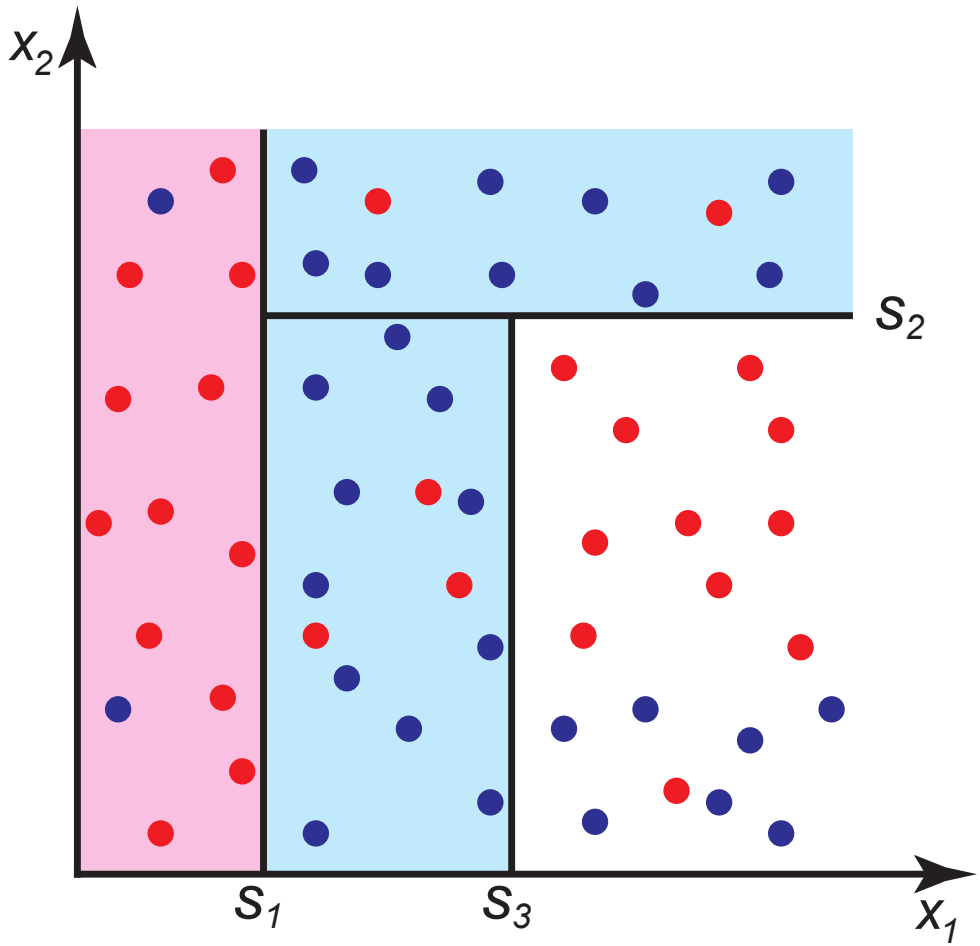

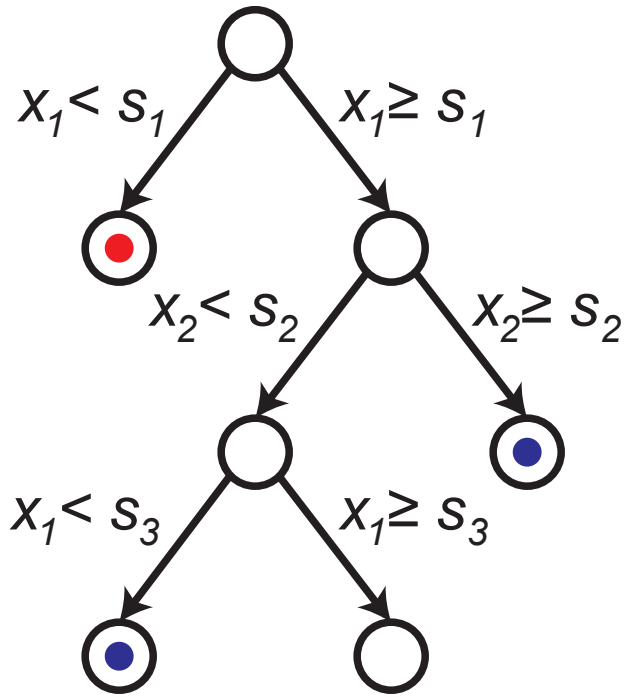

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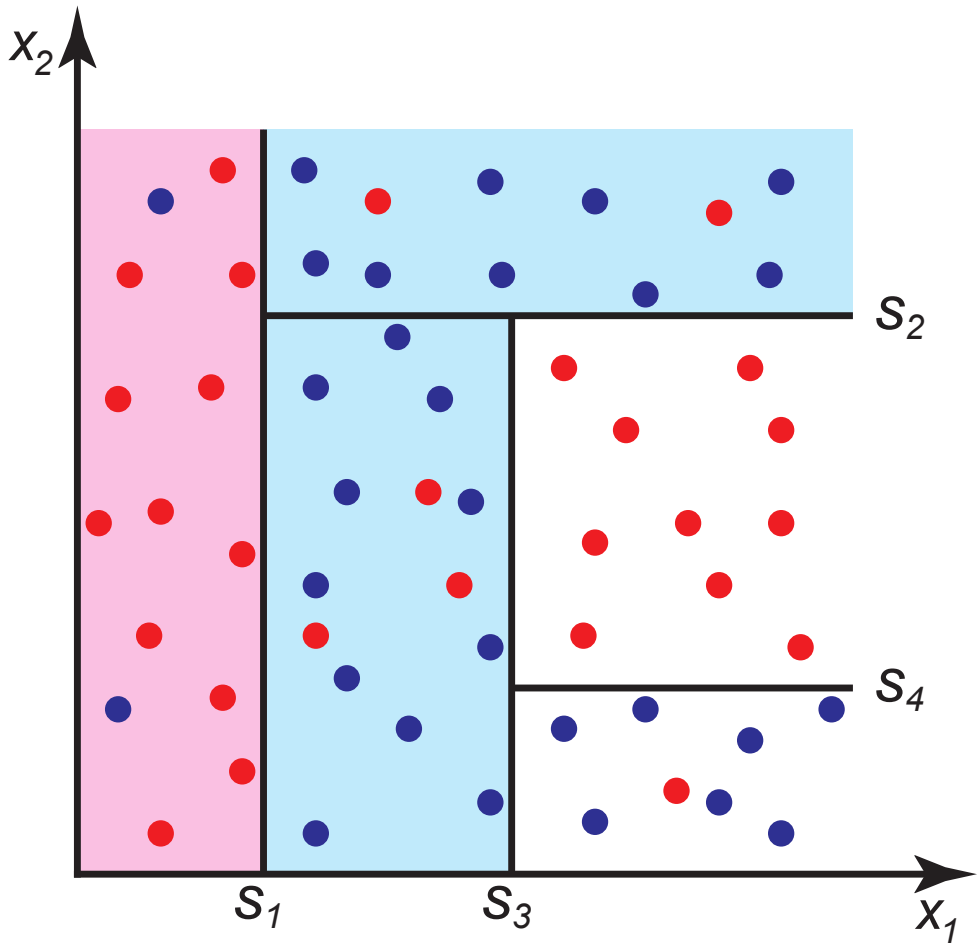

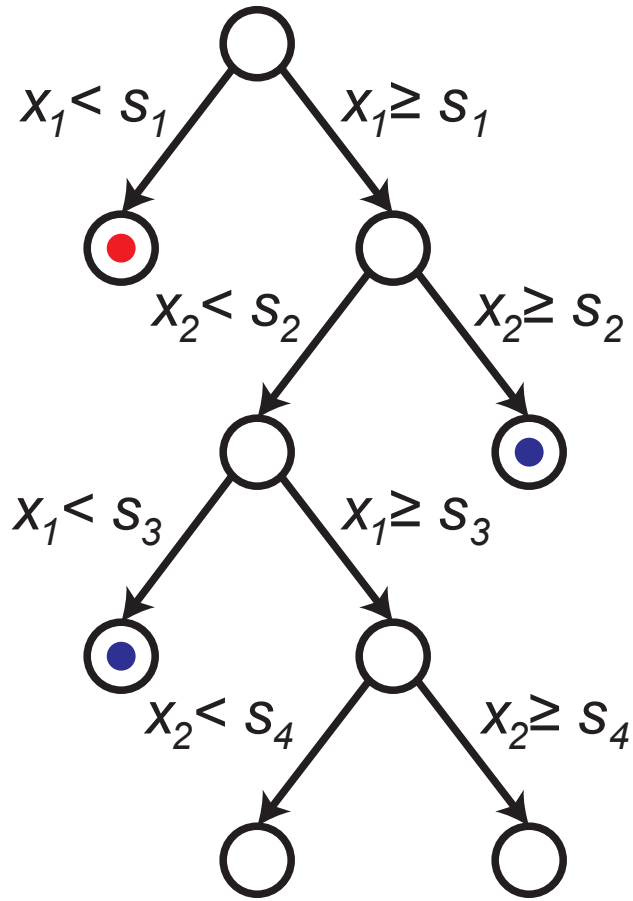

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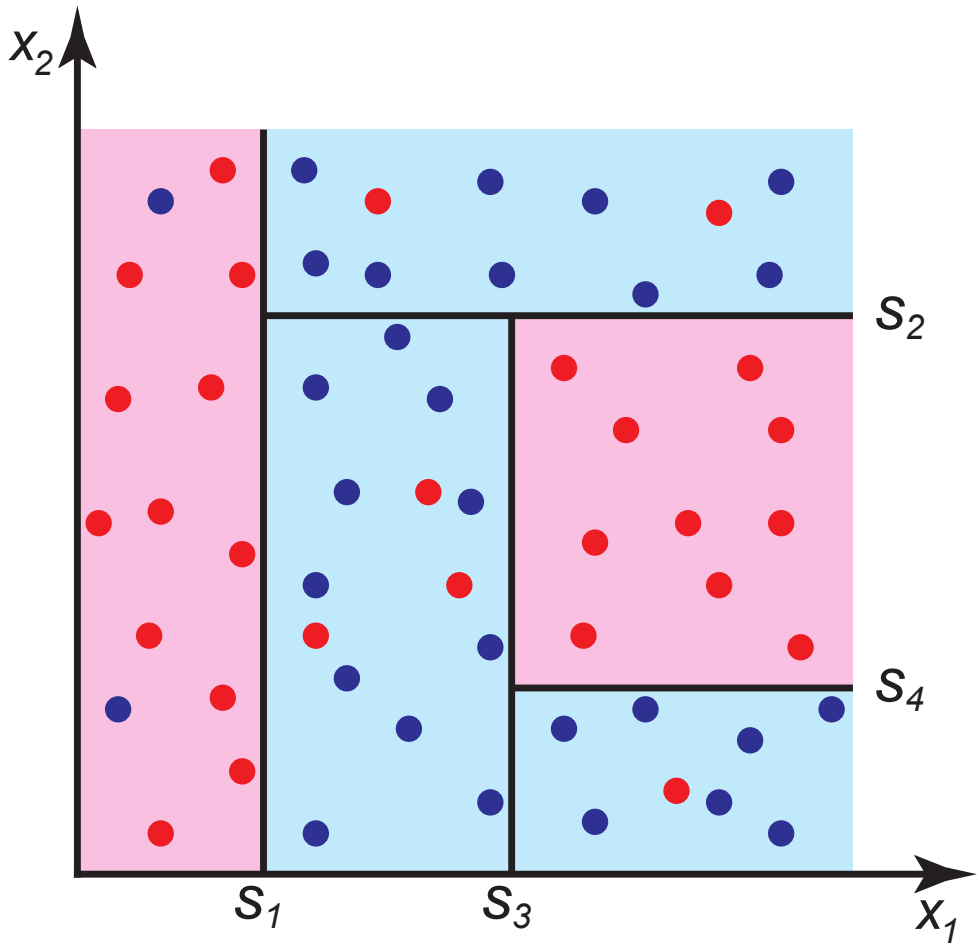

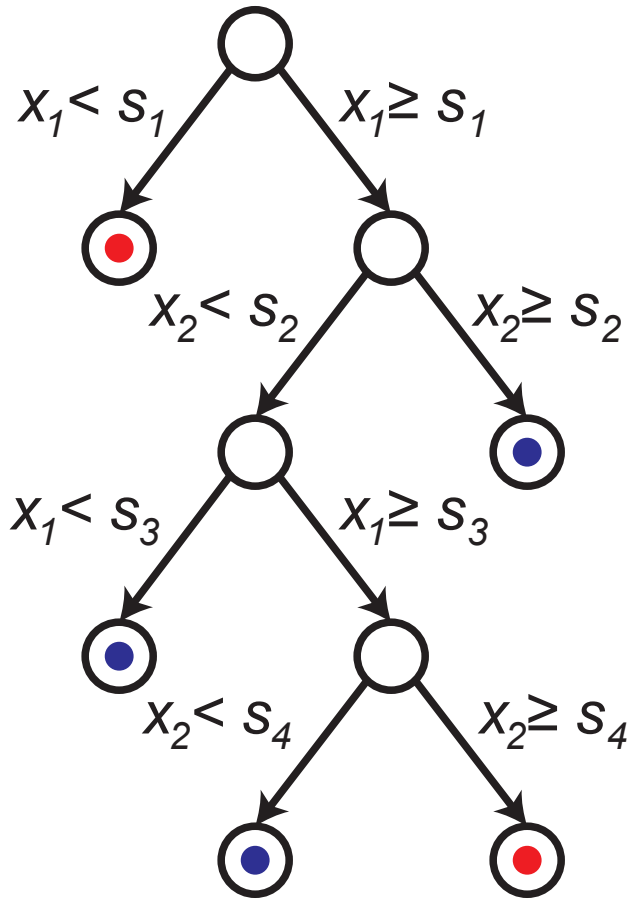

Classification tree: choice of impurity measure

Let $n^{(m)} = \#\{\mathbf{x} \,|\, \mathbf{x} \in R^{(m)}\}$ be the number of observations in region $R^{(m)}$. Then the classification accuracy of node m classifying to class k is

$$\hat{p}_k^{(m)} = \frac{1}{n^{(m)}} \sum_{\mathbf{x}_i \in R^{(m)}} I(y_i = k)\,.$$

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Possible choices for Q (the measure of impurity):

- Misclassification error:

$$Q^{(m)}(T) = \frac{n^{(m_L)}}{n^{(m)}}(1 - \hat{p}_{k(m_L)}^{(m_L)}) + \frac{n^{(m_R)}}{n^{(m)}}(1 - \hat{p}_{k(m_R)}^{(m_R)})\,,$$

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- Cross-entropy (deviance):

$$\begin{aligned} Q^{(m)}(T) = \; - \; \Big\{ & \Big(\frac{n^{(m_L)}}{n^{(m)}} \big(\hat{p}_k^{(m_L)} \log \hat{p}_k^{(m_L)} + (1 - \hat{p}_k^{(m_L)}) \log(1 - \hat{p}_k^{(m_L)})\big) \\ & + \frac{n^{(m_R)}}{n^{(m)}} \big(\hat{p}_k^{(m_R)} \log \hat{p}_k^{(m_R)} + (1 - \hat{p}_k^{(m_R)}) \log(1 - \hat{p}_k^{(m_R)})\big) \Big\}\,. \end{aligned}$$

Maximizing the gain

- Sometimes in the literature and in the textbooks, the minimization of $Q^{(m)}(T)$ is presented under the equivalent for of the *gain maximization*
- For instance, for the Gini index the gain is

$$2\hat{p}_k^{(m)}(1-\hat{p}_k^{(m)}) - Q_{Gini}^{(m)}(T)$$

- For instance, for the deviance the gain is

$$\hat{p}_k^{(m)} \log \hat{p}_k^{(m)} + (1-\hat{p}_k^{(m)}) \log(1-\hat{p}_k^{(m)}) - Q_{deviance}^{(m)}(T)$$

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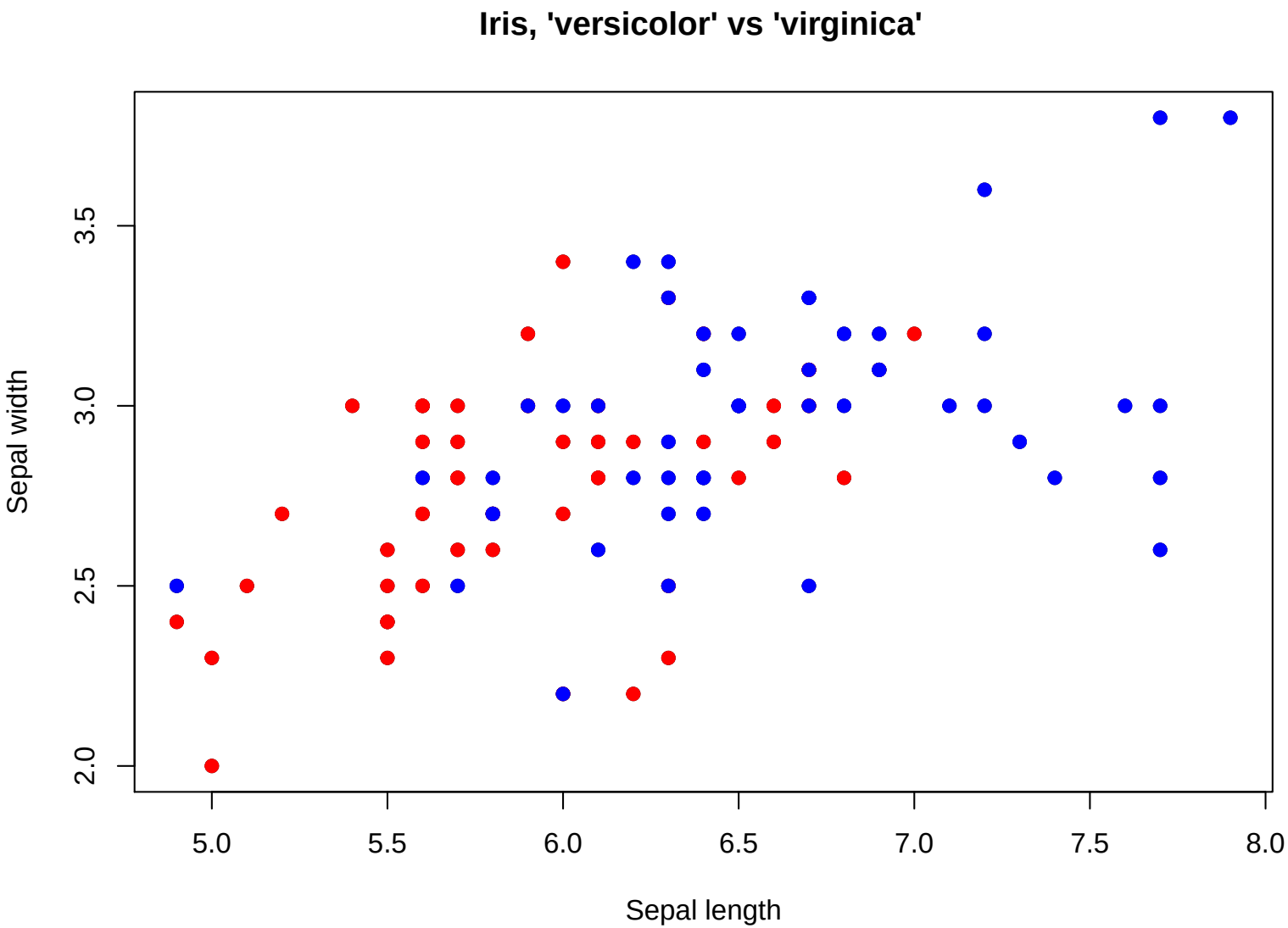

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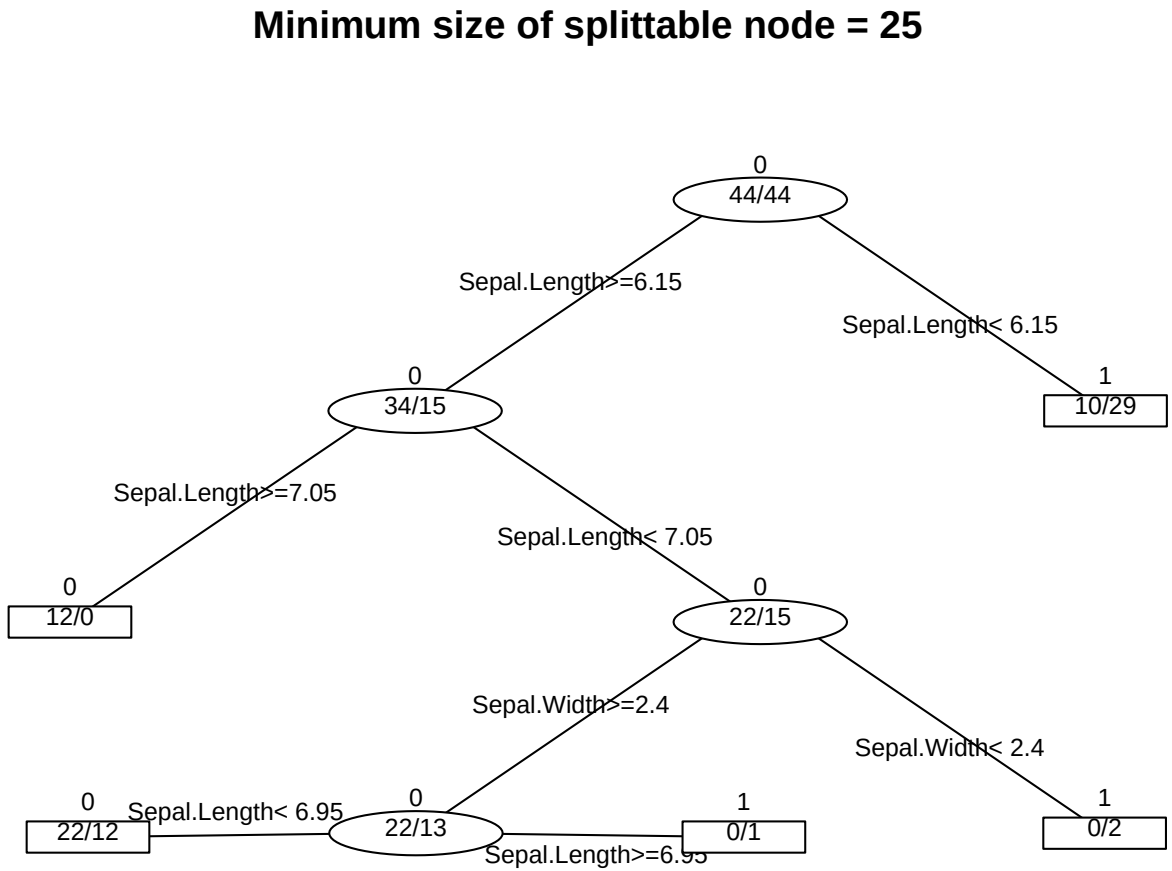

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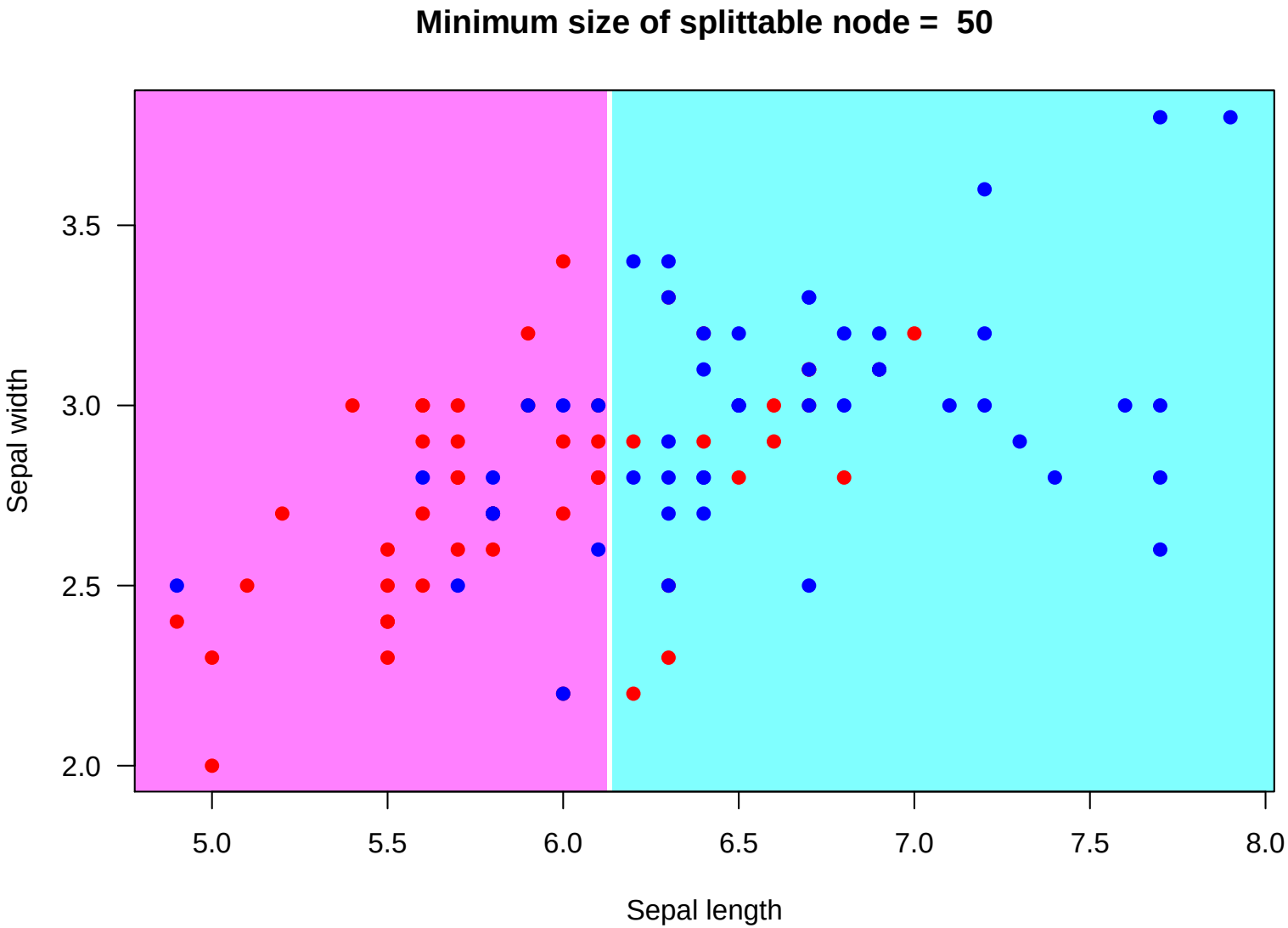

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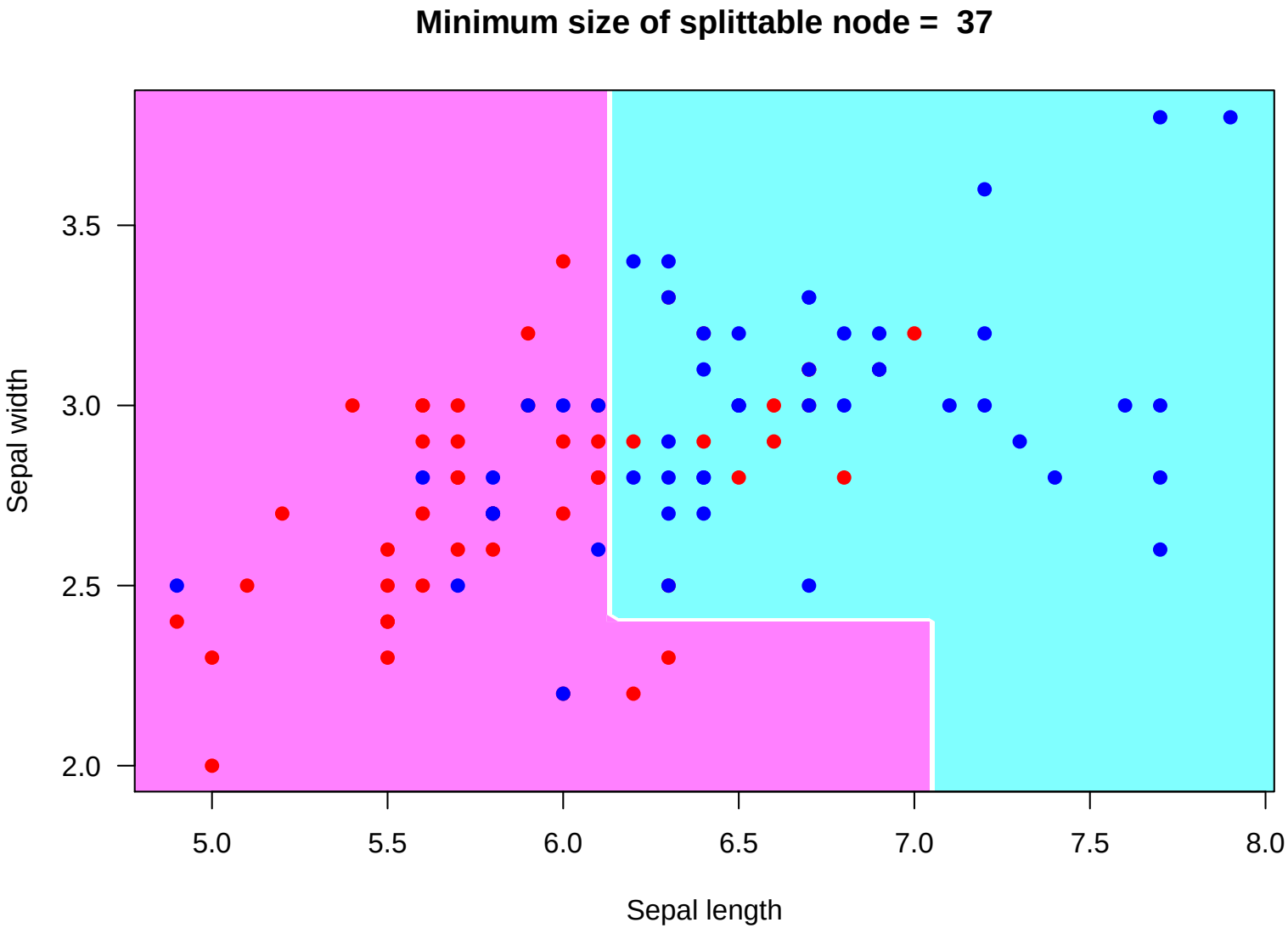

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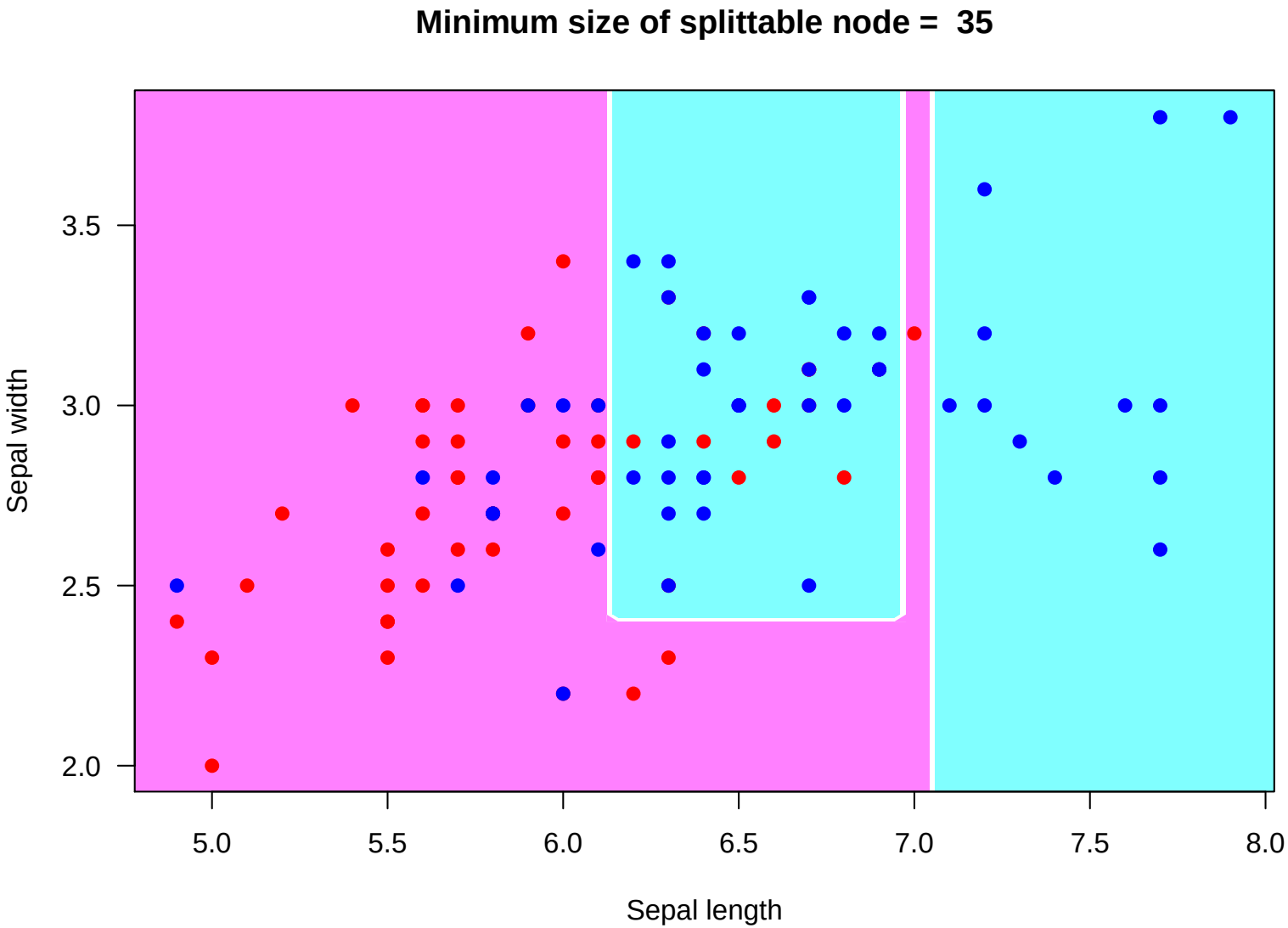

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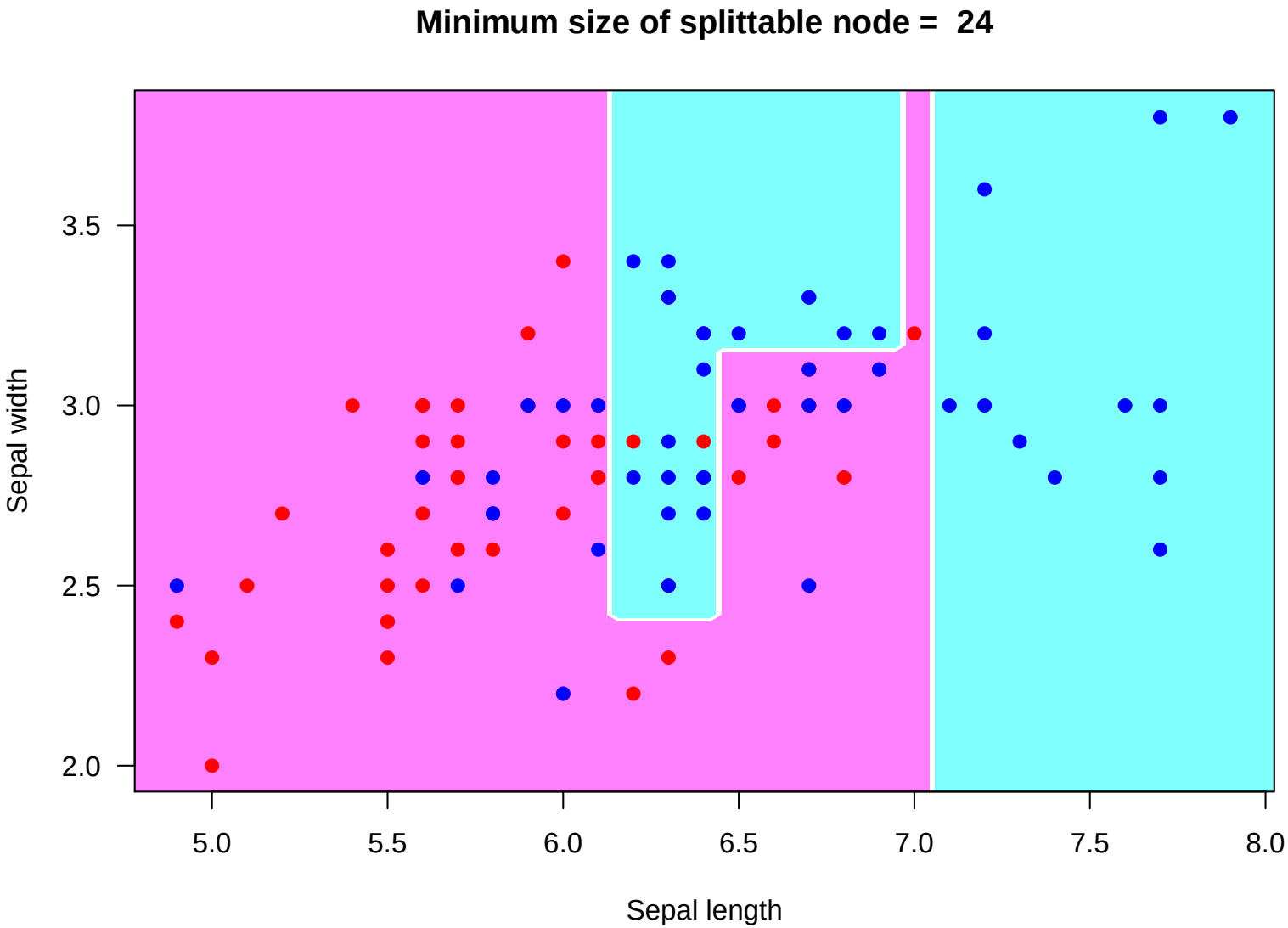

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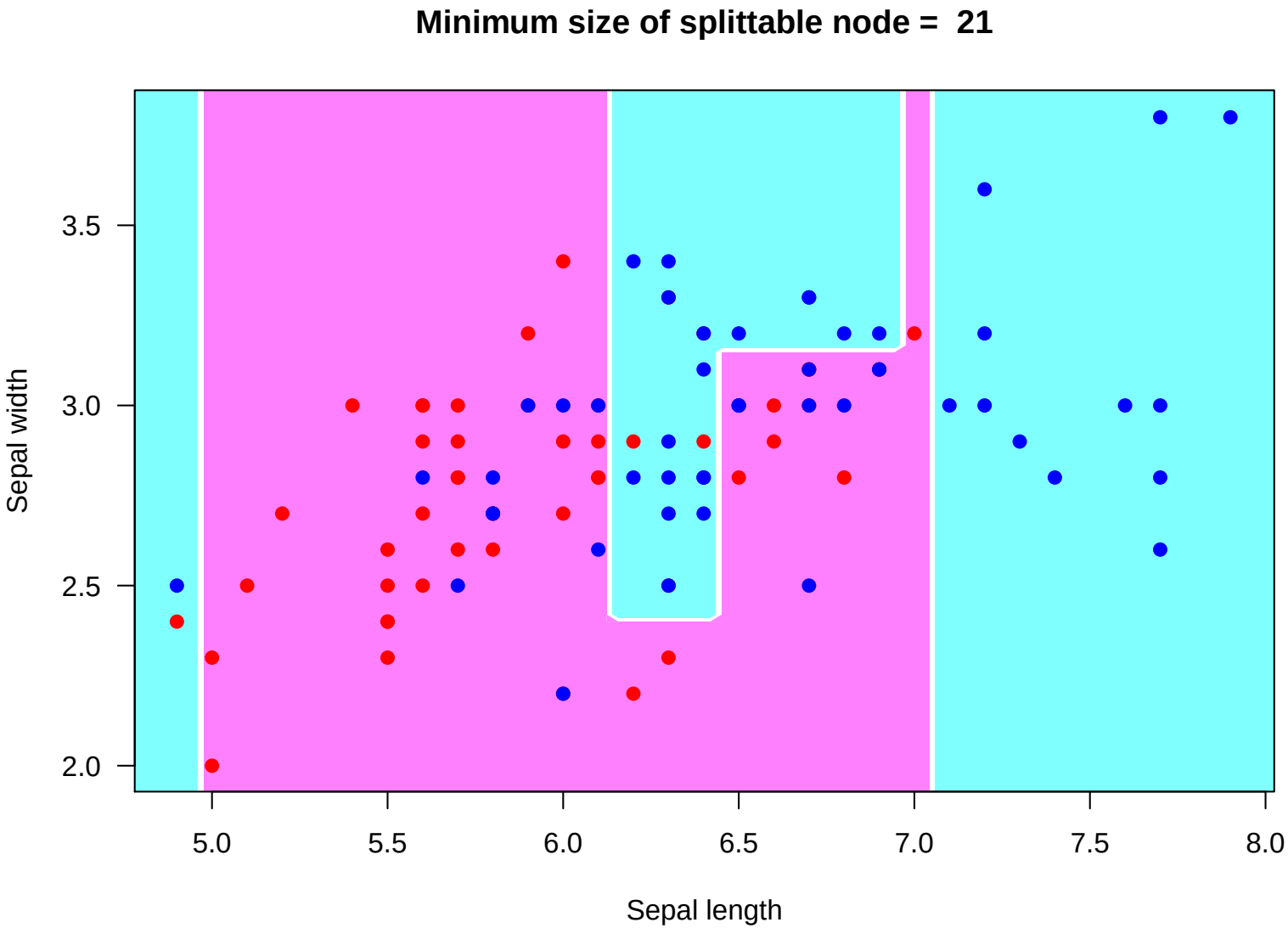

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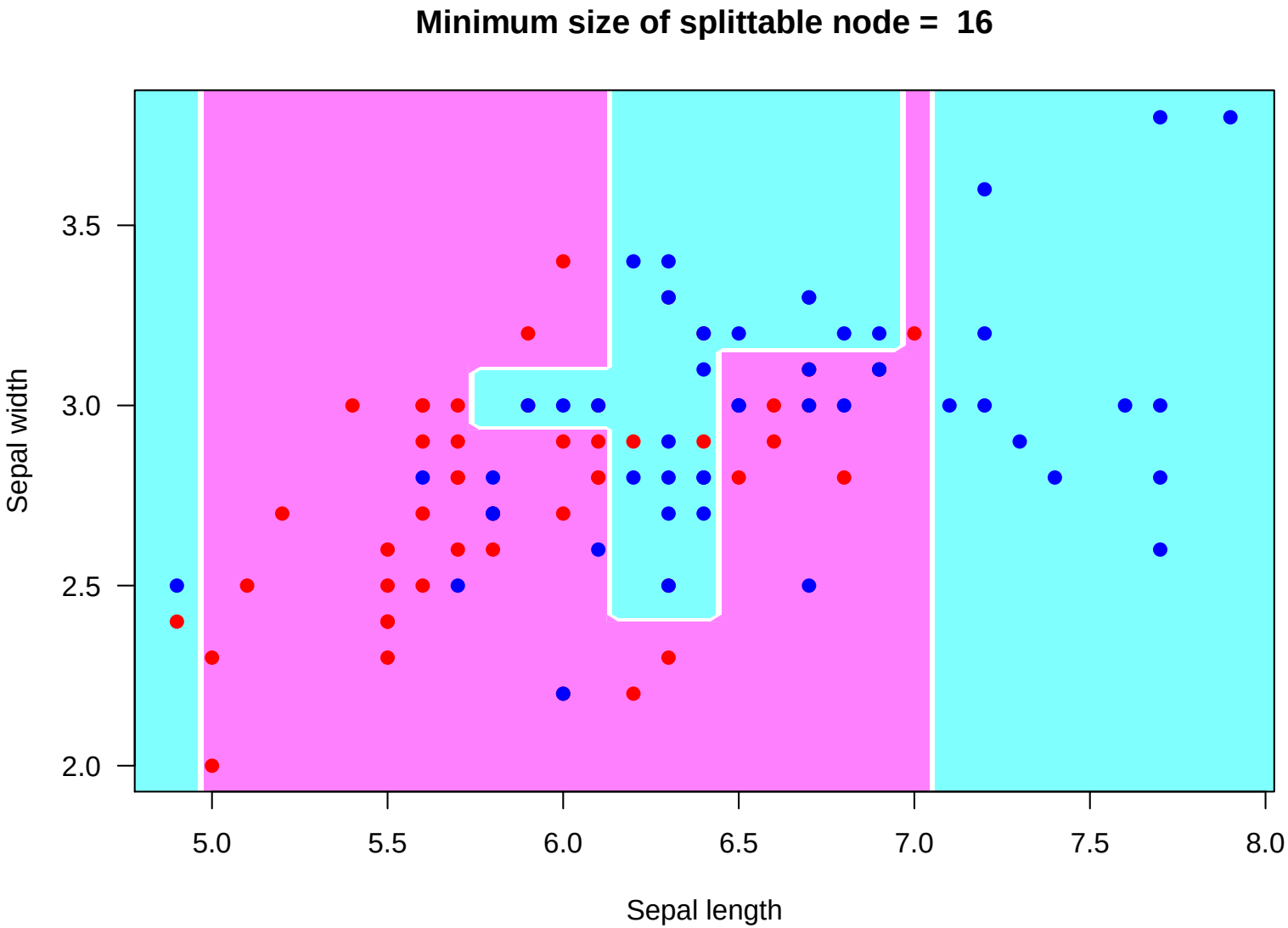

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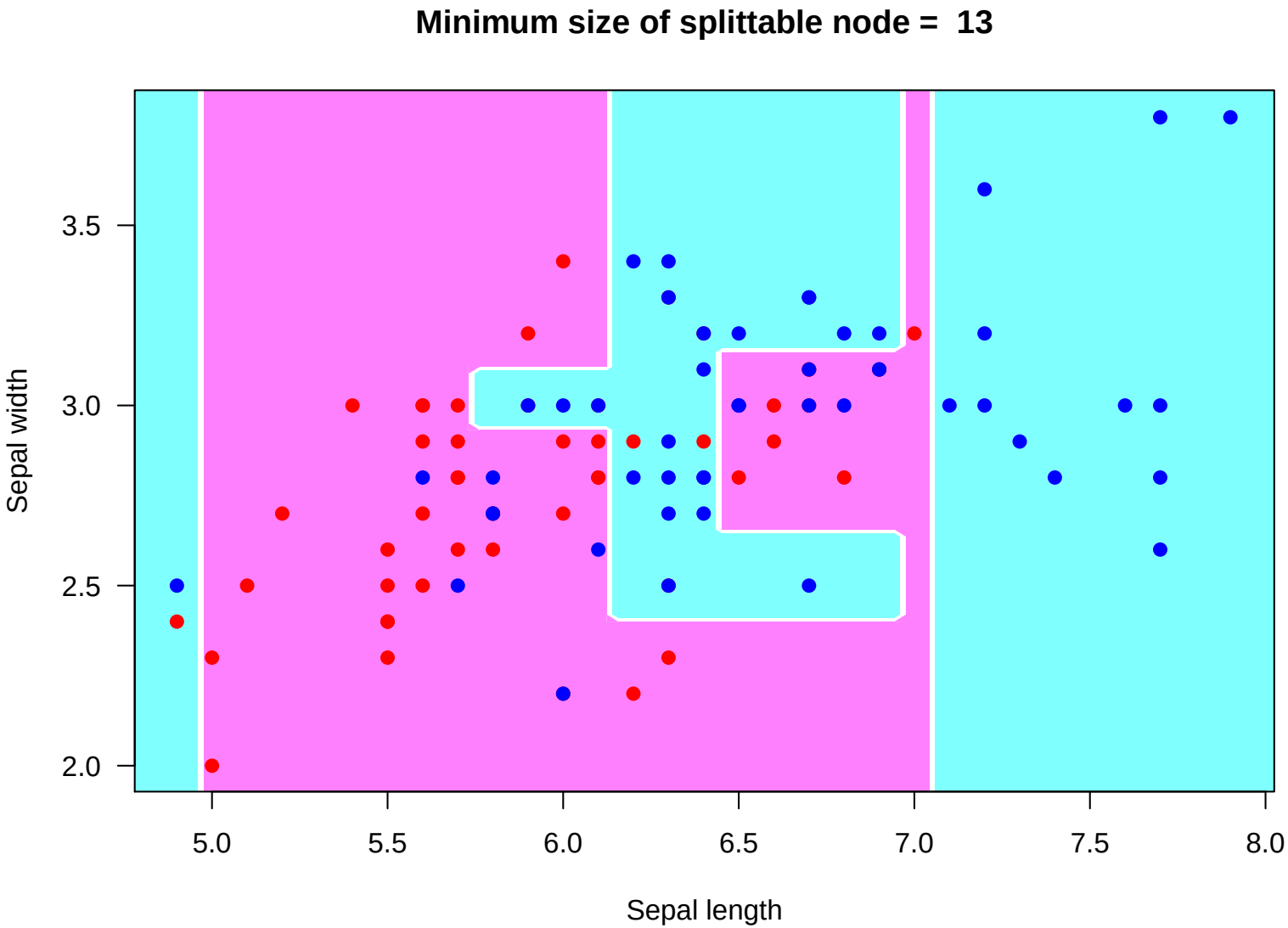

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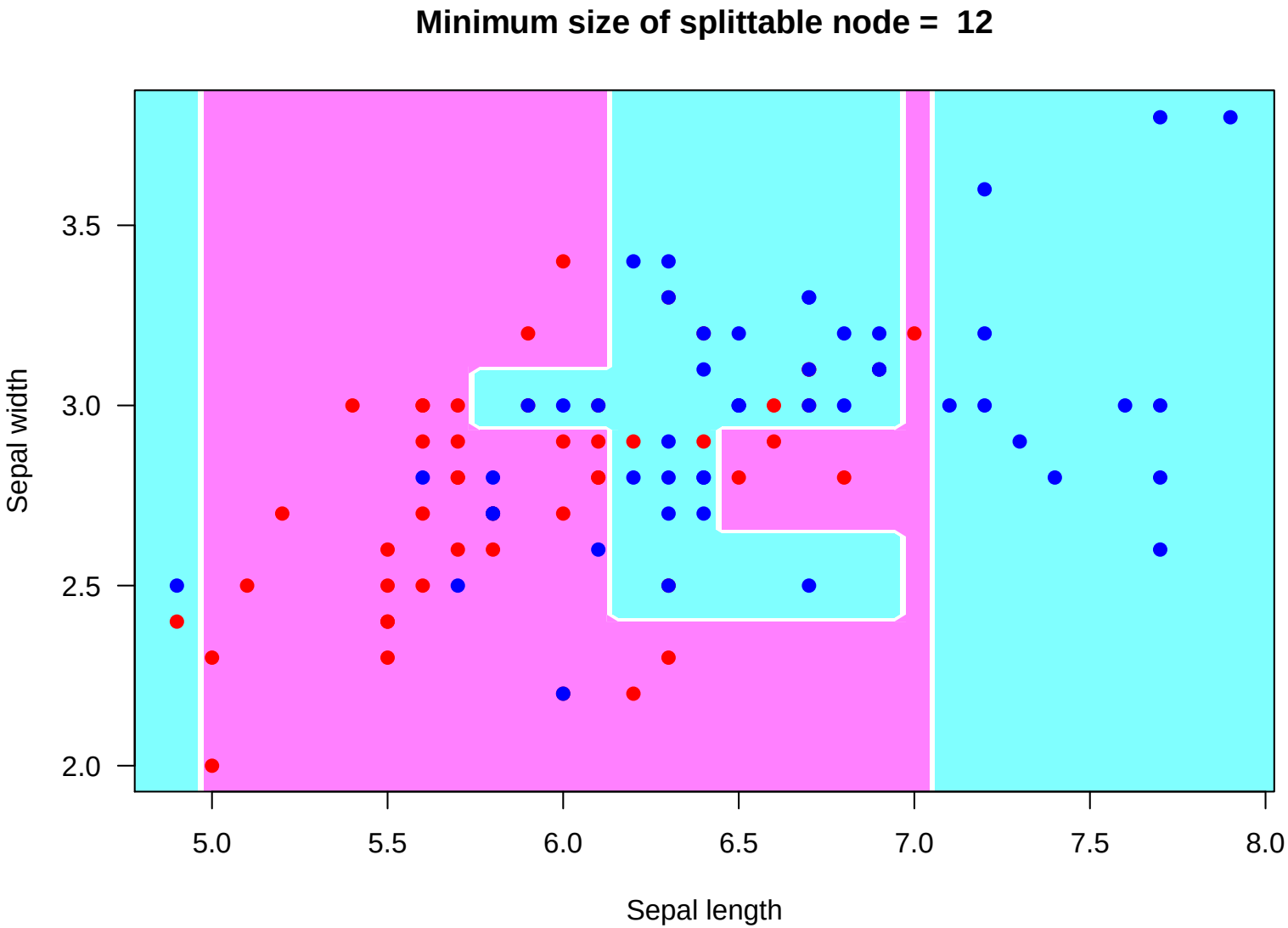

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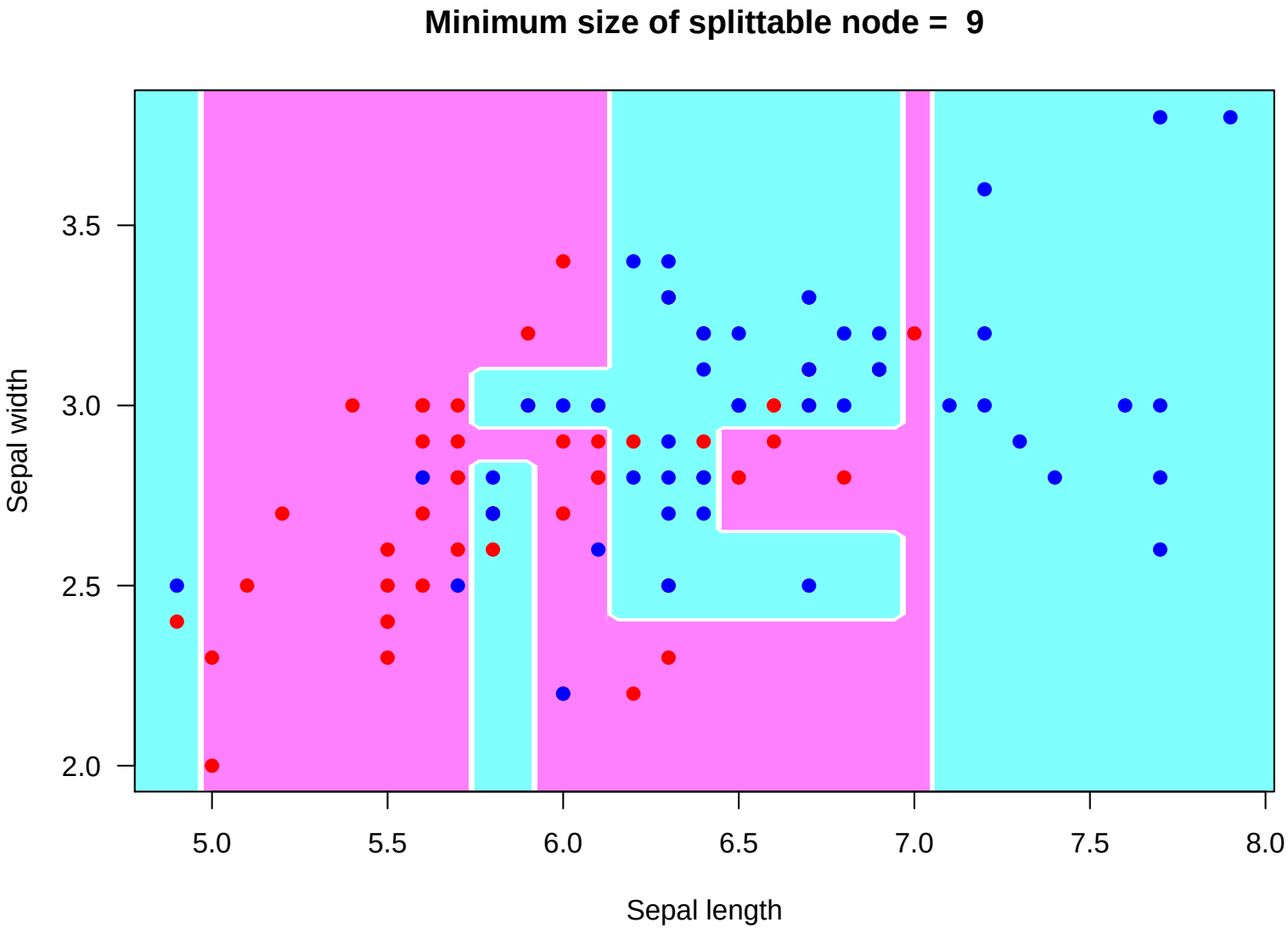

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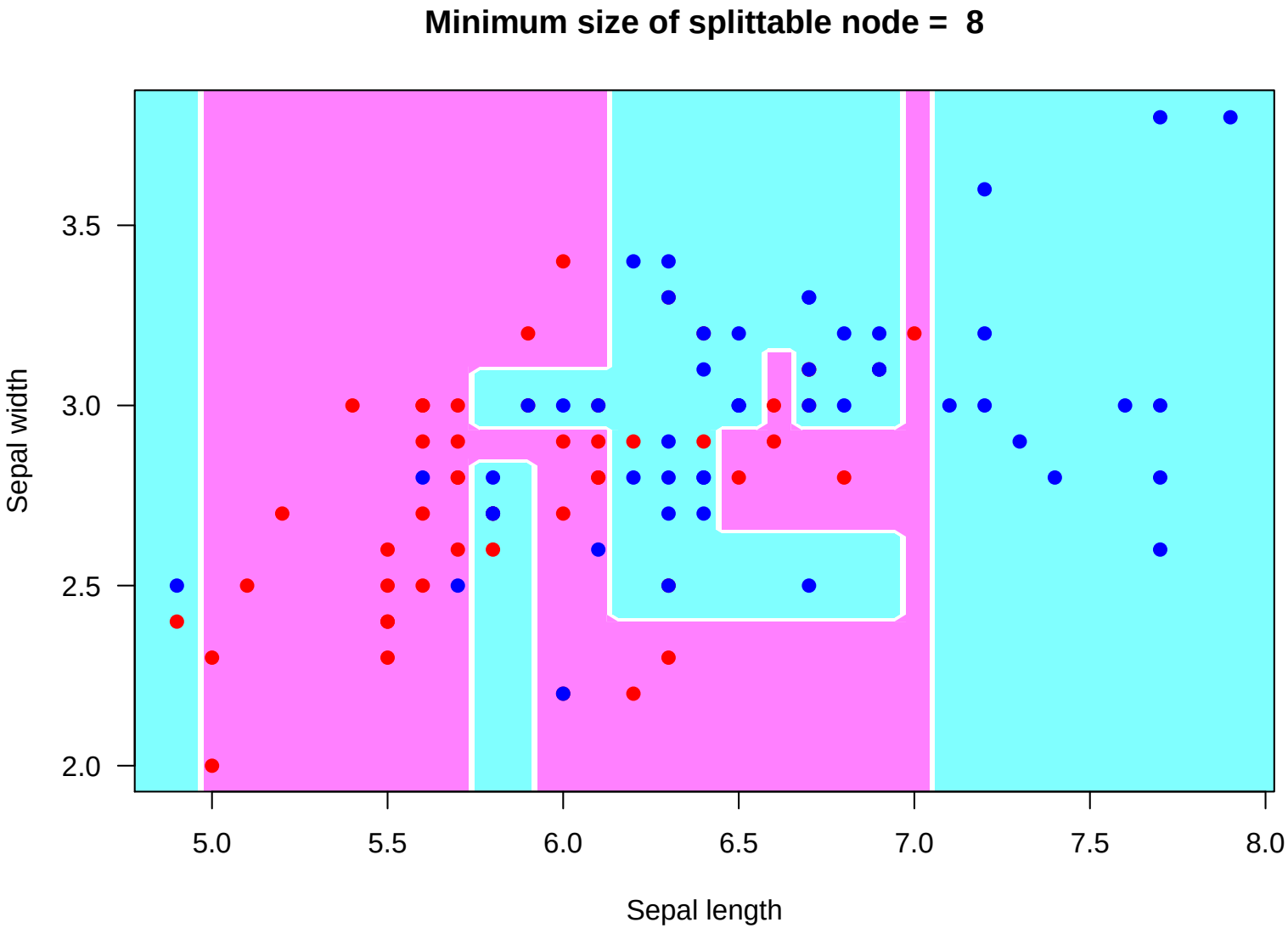

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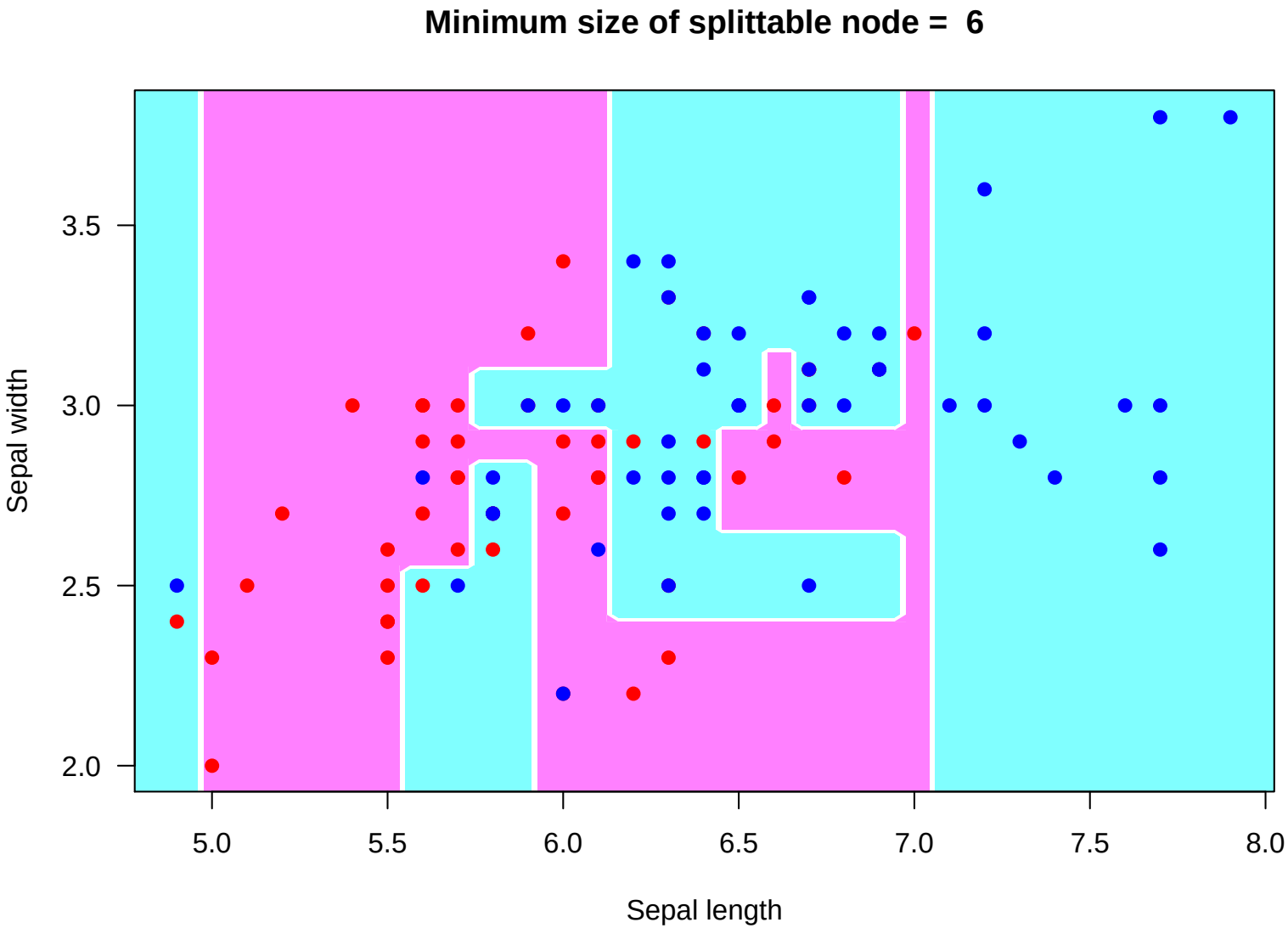

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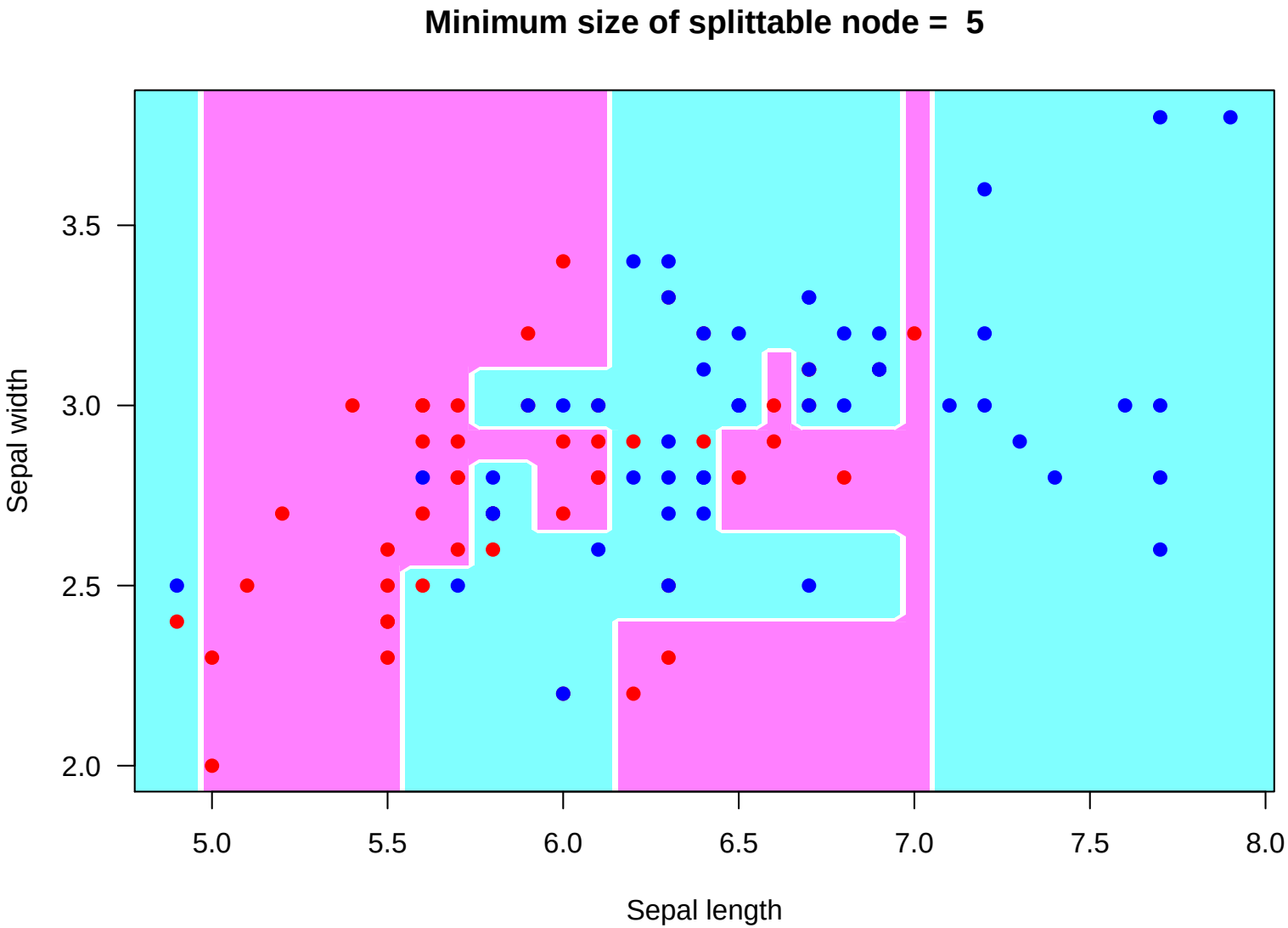

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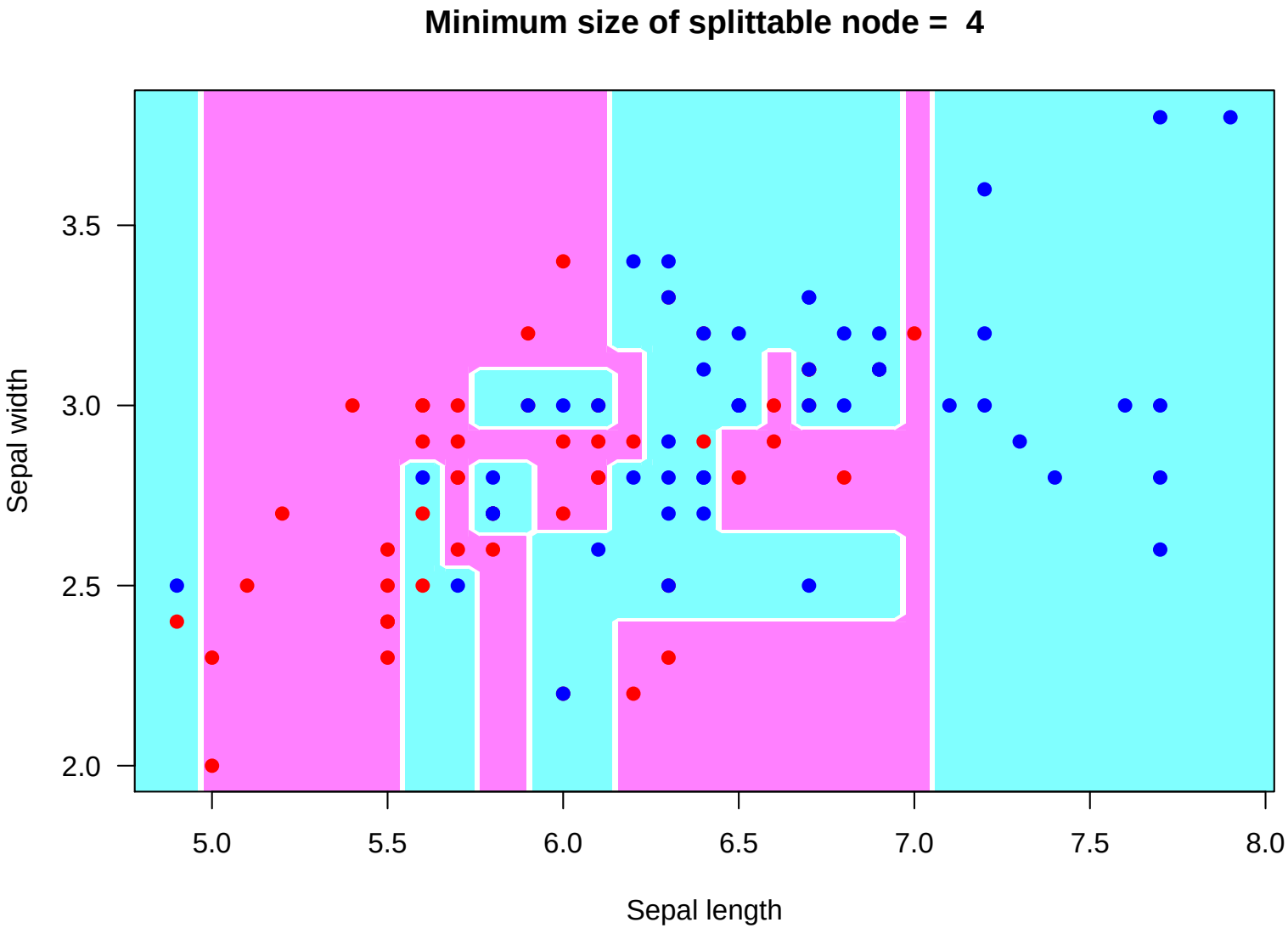

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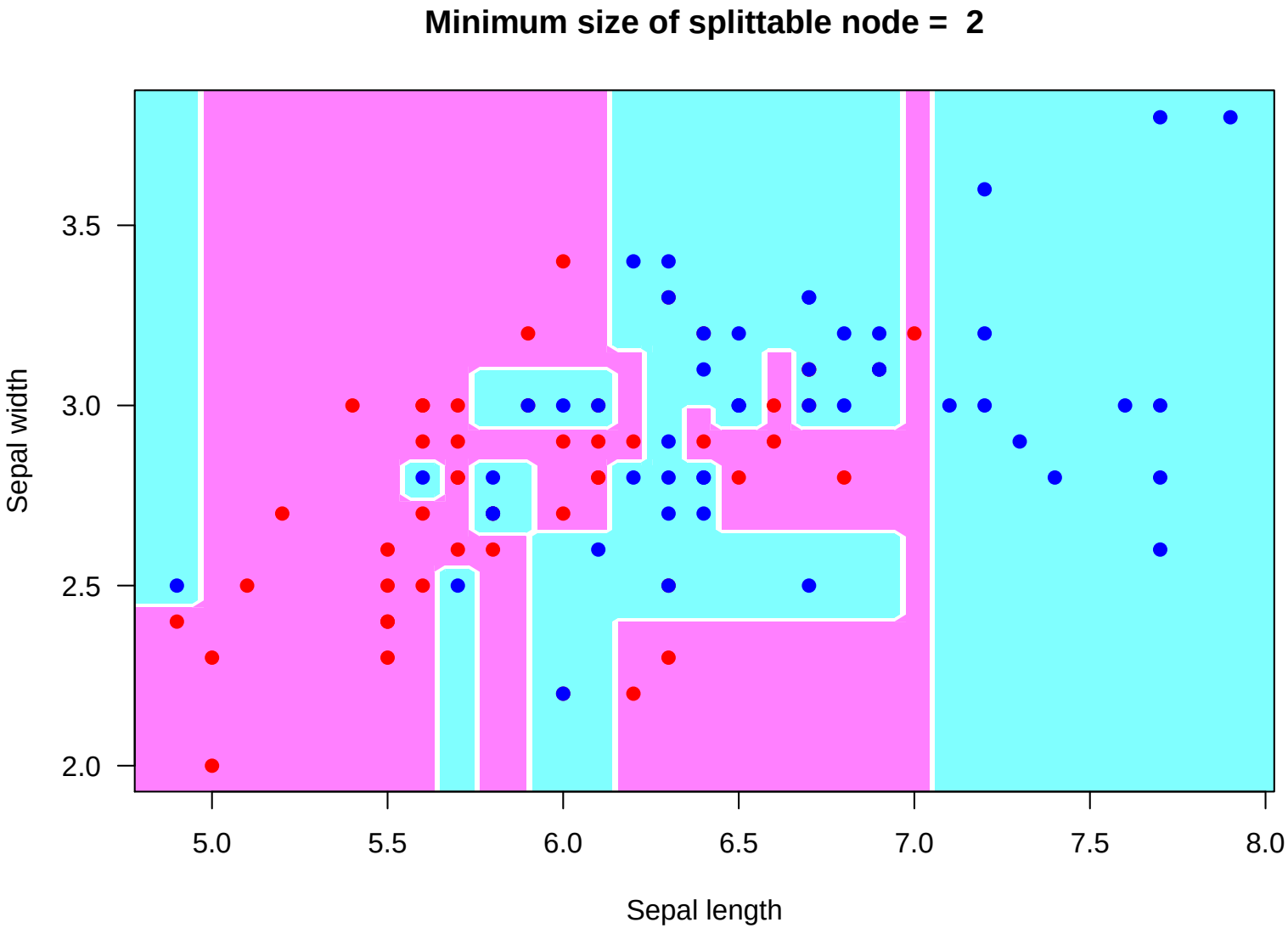

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Classification tree: tuning and properties

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$$S^{(m)}(T) = I(n^{(m)} < n_{min}).$$

- Often the classification tree is constructed in two stages:
  1. n_{min} **is set very small** and the tree is grown to T_0.

Classification tree: tuning and properties

- A possible (and wide-spread) choice for the stopping criteria S is to restrict **the number of points in region** $R^{(m)}$ to be split to some constant n_{min}:

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For each α, it can shown that there is a unique smallest subtree T_α that minimizes $C_\alpha(T)$.
Pruning parameter α is chosen by the means of **cross-validation**.

Some more comments

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- The key **advantage** of the classification tree is its **interpretability**, as the feature space partition is fully described by a single tree.

- Some **disadvantage** are the *instability* (trees have high variance, a small change in the data can result in a quite different series of splits – see bagging for a solution) and the *difficulty in capturing additive structures*.

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The key idea

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- **Bagging** is a shortcut for **B**ootstrap **Agg**regat**ing**.

- The main idea is to construct a single estimator that consists of **a number of basic classifiers** (weak learners) (taught on a bootstrapped samples) aggregated by averaging (voting).

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- $g_k(\mathbf{x}) = g_k(\mathbf{x}; (X_1, Y_1), ..., (X_n, Y_n))$ as well as $\hat{g}_B(\mathbf{x}) = \hat{g}_B(\mathbf{x}; (X_1, Y_1), ..., (X_n, Y_n))$ are random variables.

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- One can measure the improvement of aggregating by comparing performance of $\hat{g}_B(\mathbf{x})$ and those of $g_k(x)$, $k = 1, ..., B$ in terms of **bias** and **variance**.

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(the conclusion here is obtained under the unfeasible assumption of i.i.d. property of $g_1, ..., g_B$).

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If $X_1, ..., X_n$ are i.i.d. random variables taking values in $\{0, 1\}$, then for any $\eta > 0$ it holds

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Applying the Chernoff-Hoeffding inequality gives

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- Resort to the idea of the **bootstrap**.

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$$\begin{aligned}
\lim_{B\to\infty} g^{agg}(\mathbf{x}) &= \lim_{B\to\infty} 1\Big(\frac{1}{B}\sum_{k=1}^{B} g_k^*(\mathbf{x}) > 0.5\Big) \\
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- So $g^{agg}(\mathbf{x})$ stabilizes with increasing B converging to the **bagging estimator** $1\big(\mathbb{E}^*[g_k^*(\mathbf{x}) \mid \mathcal{D}_n] > 0.5\big)$.

Choice of the parameters

- There are two choices to be done:
  - **base classifier** $g(\cdot)$,
  - **number of** bootstrap **iterations** B.

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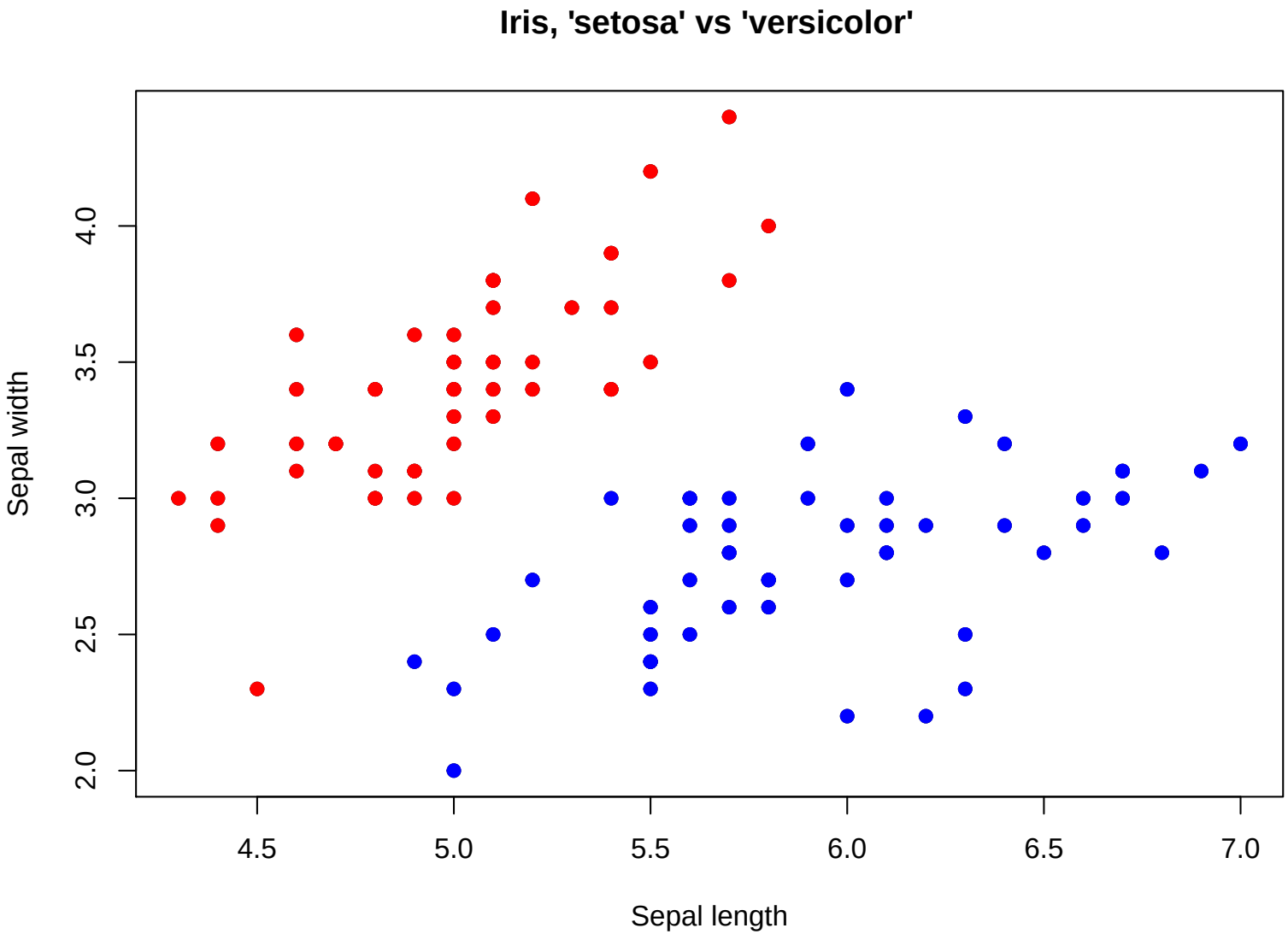
- Thus, B should be chosen as large as possible, regarding computational capabilities.

Bagging classification tree: iris data



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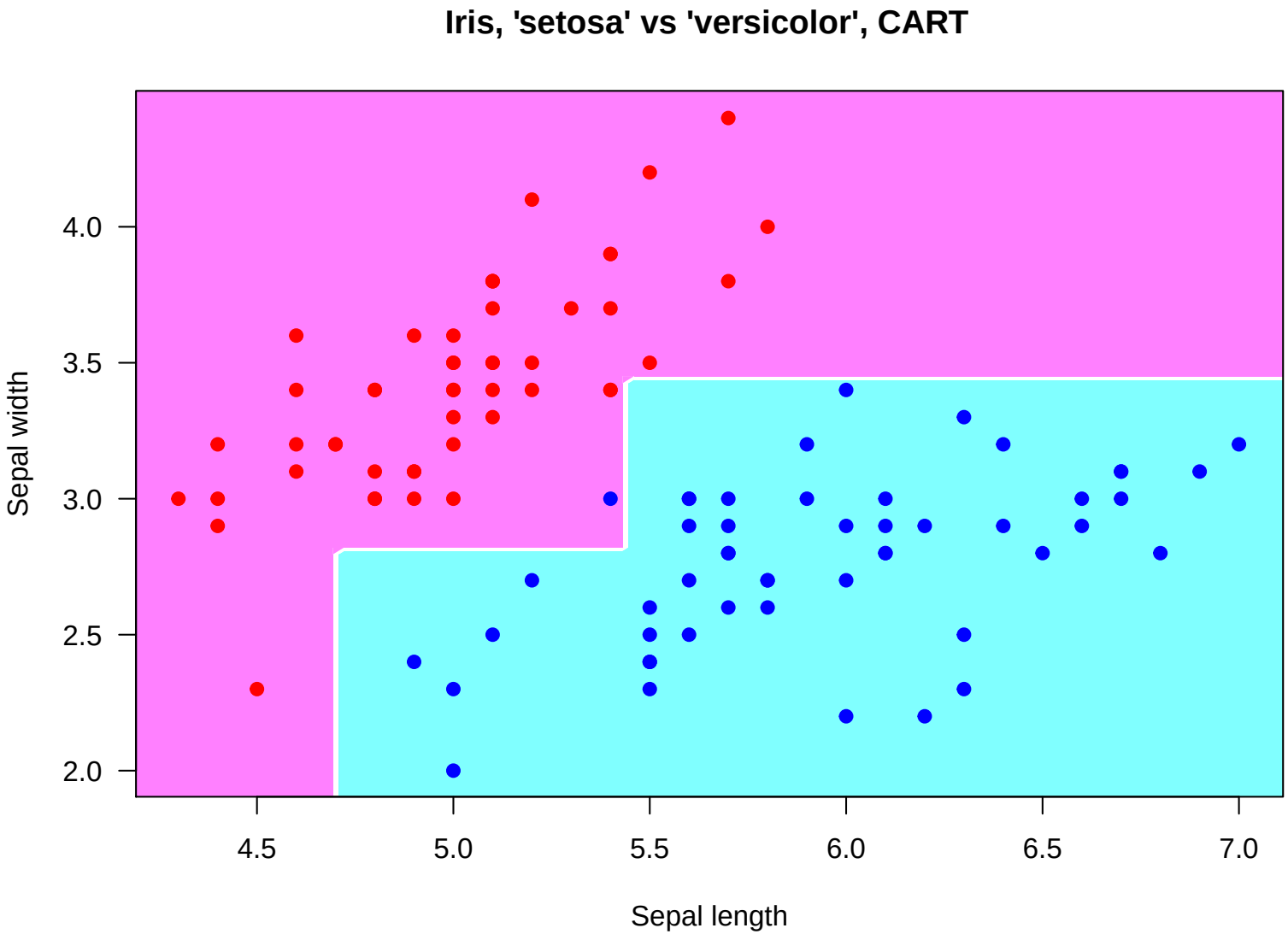

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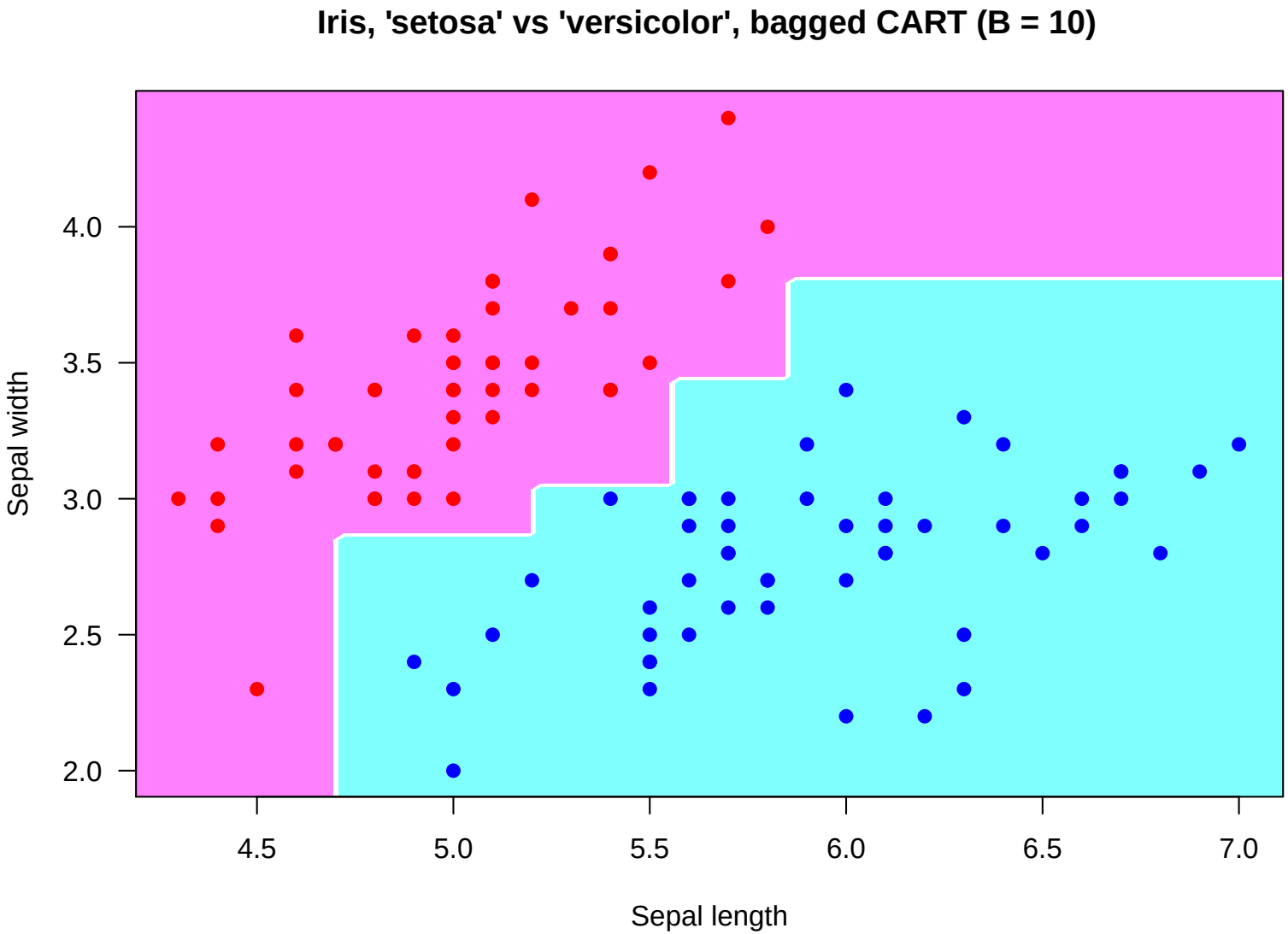

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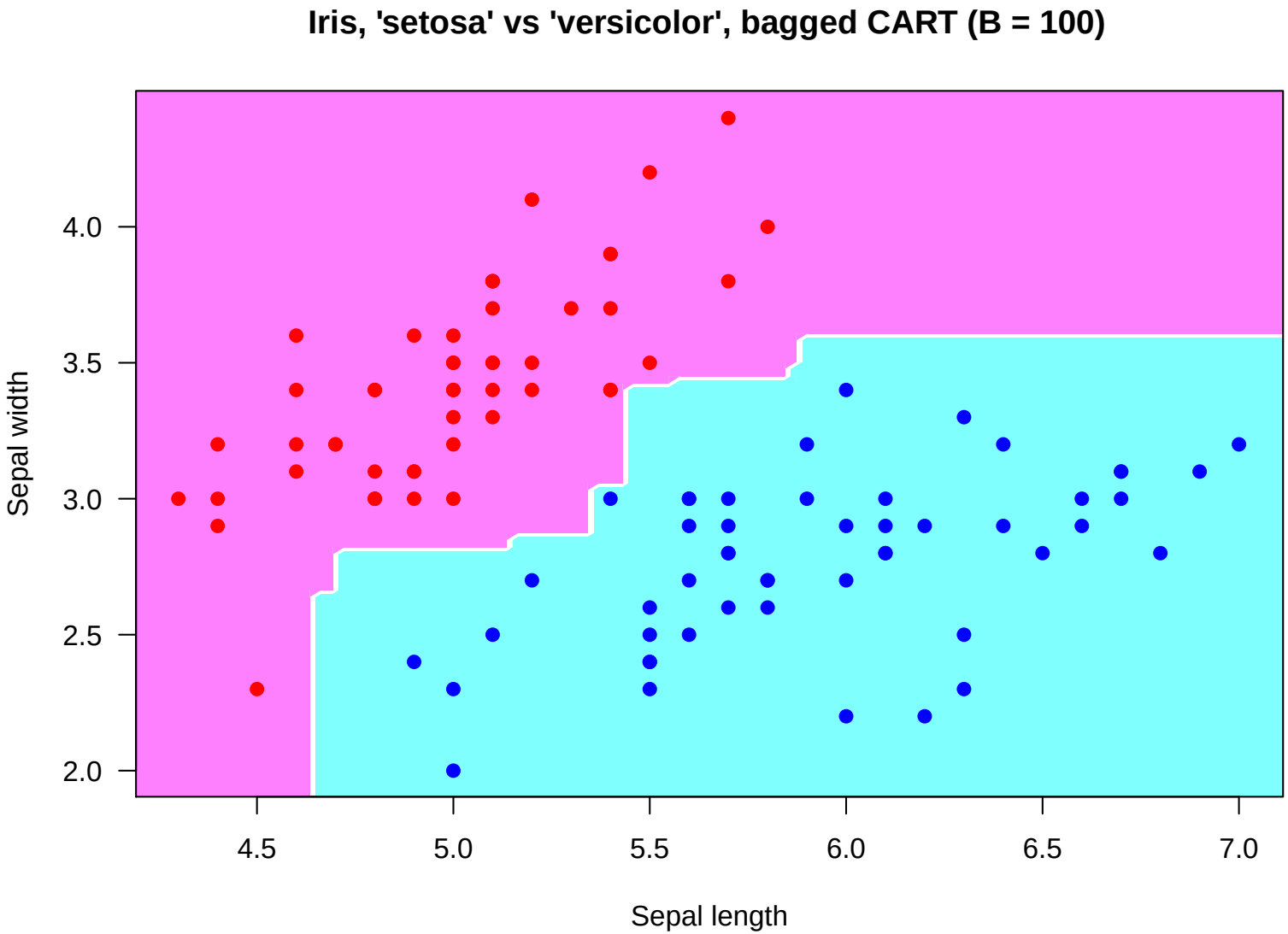

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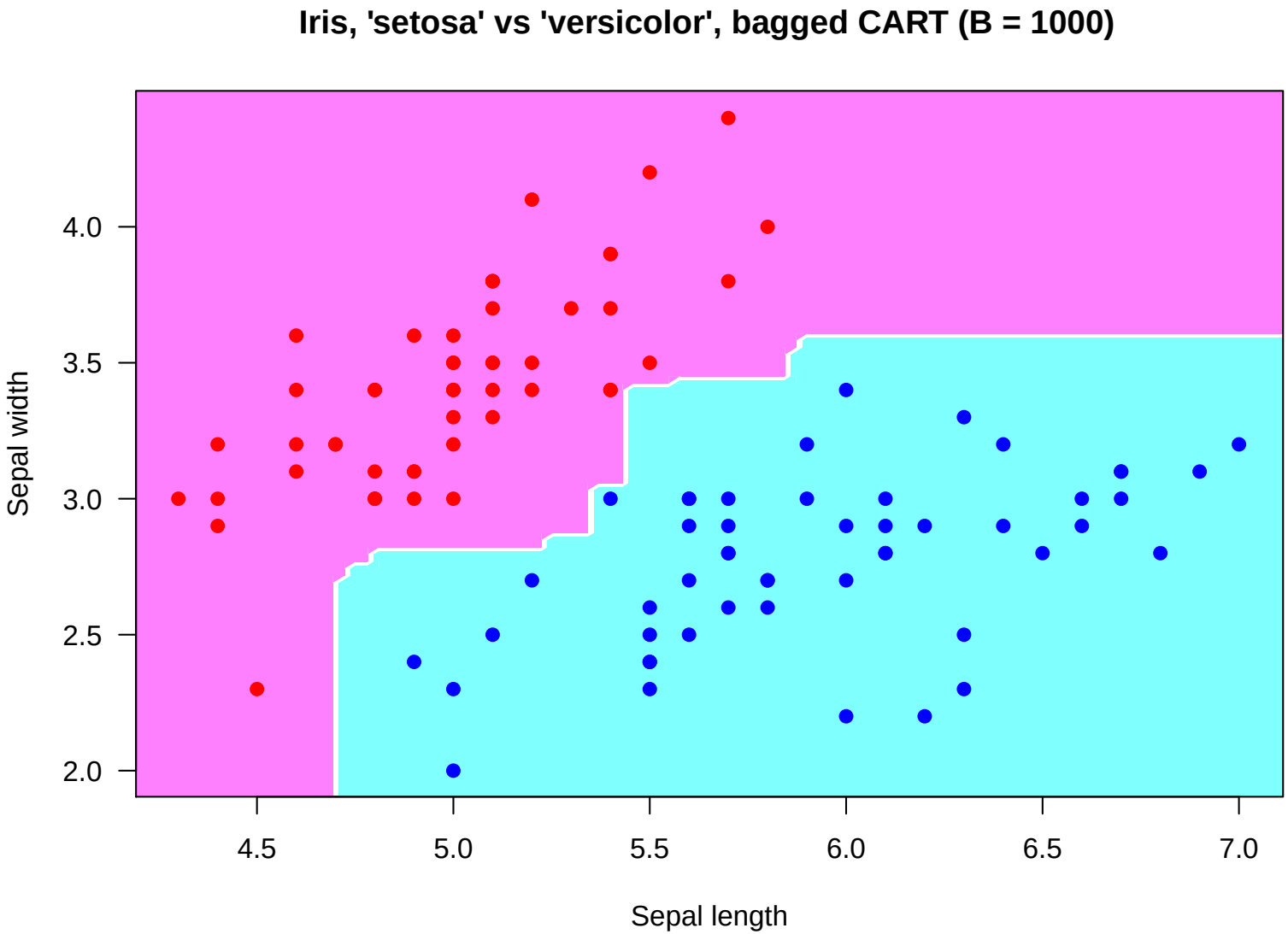

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- Bagging reduces interpretability of the classifier because any simple structure in the model is lost.

Contents

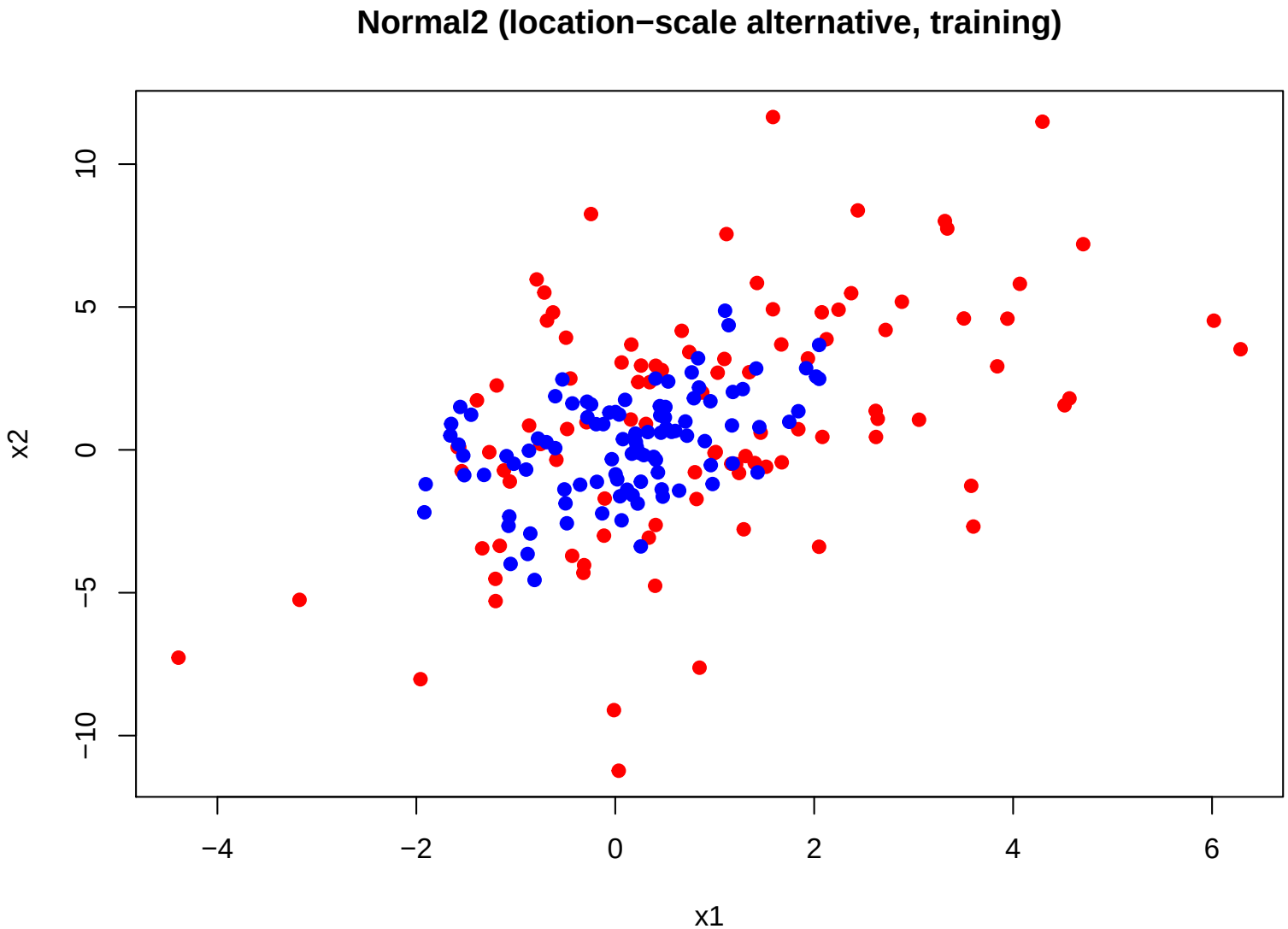
Normal2 data generation

- Generate independent copies of a bivariate normal vector:
  - for $Y = 0$ mean $(0, 0)$ and

$$\Sigma = \begin{pmatrix} 1 & 1 \\ 1 & 4 \end{pmatrix}$$

  - for $Y = 1$ mean $(0, 0)$ and the variance is equal to 4Σ

Normal2 data



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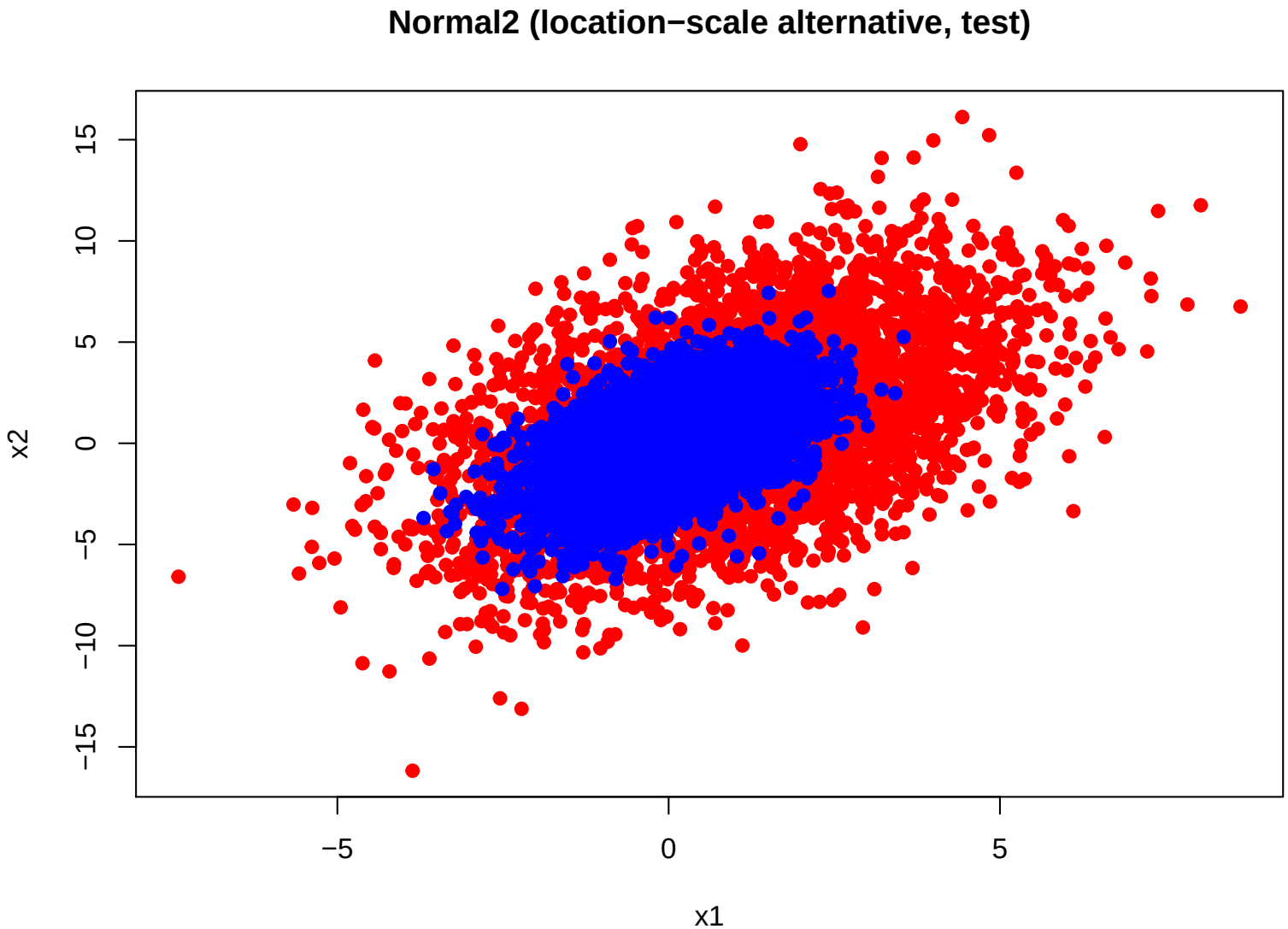
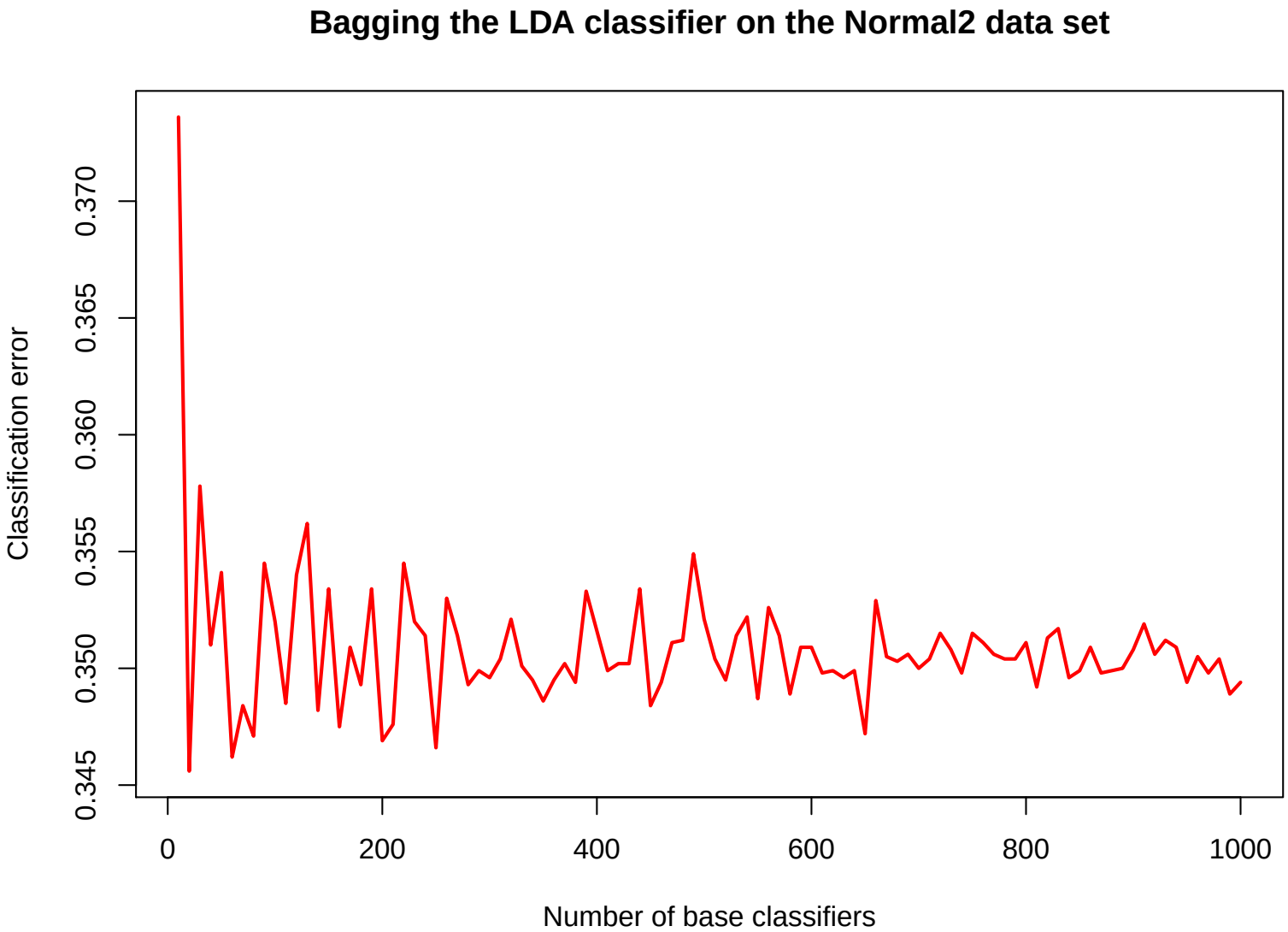
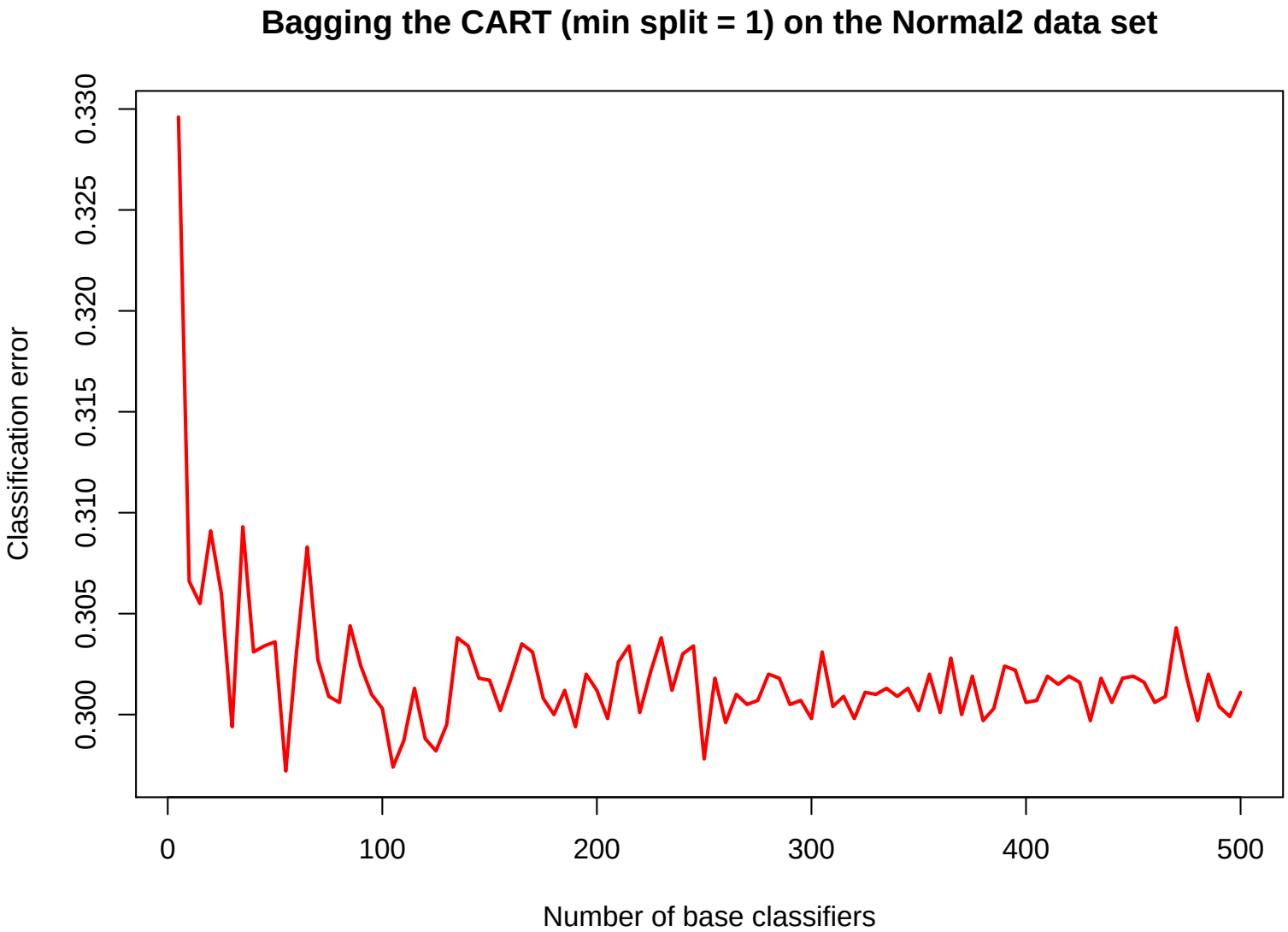


Bagging LDA: Normal2 data



Bagging classification tree: Normal2 data



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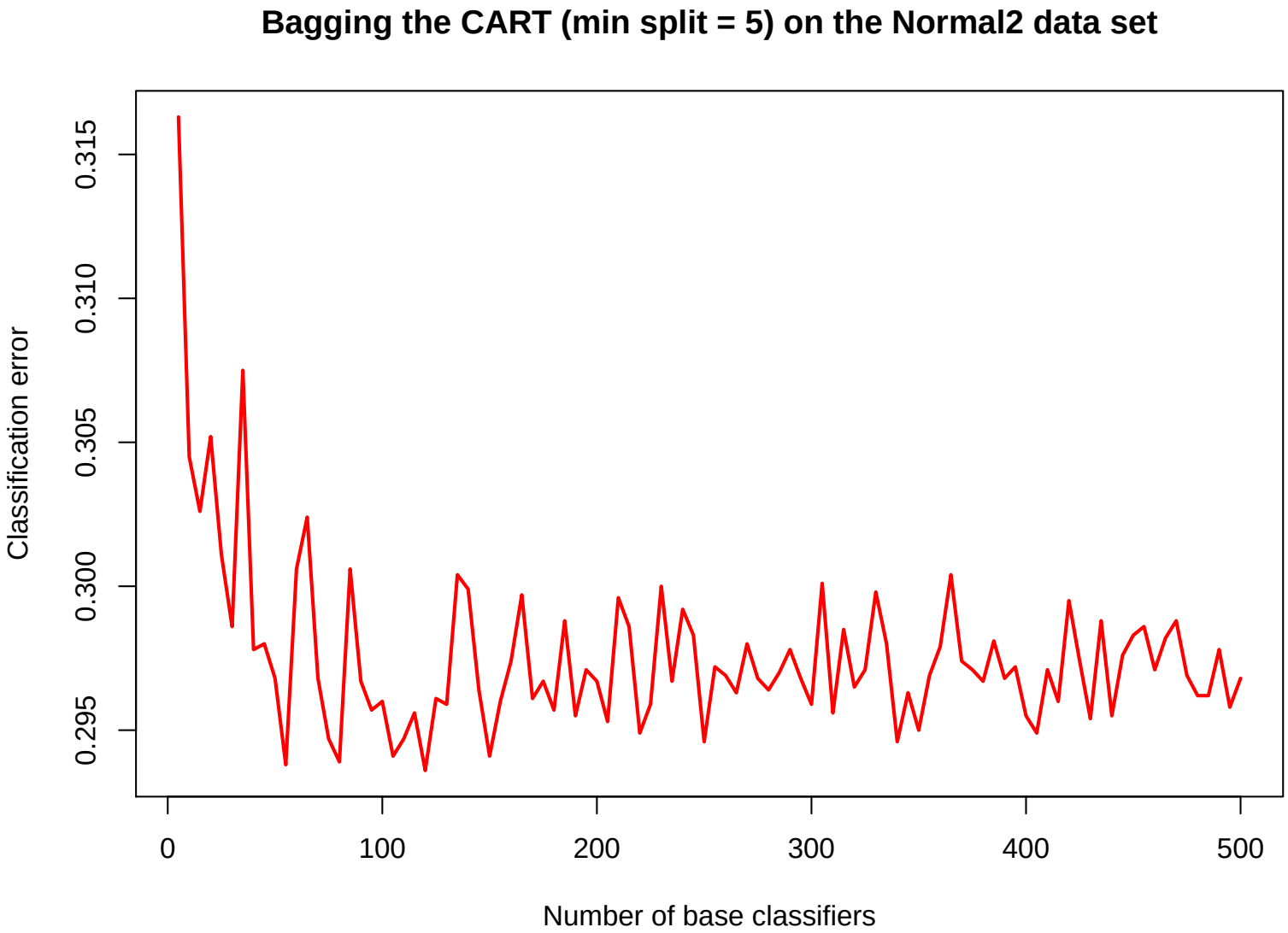

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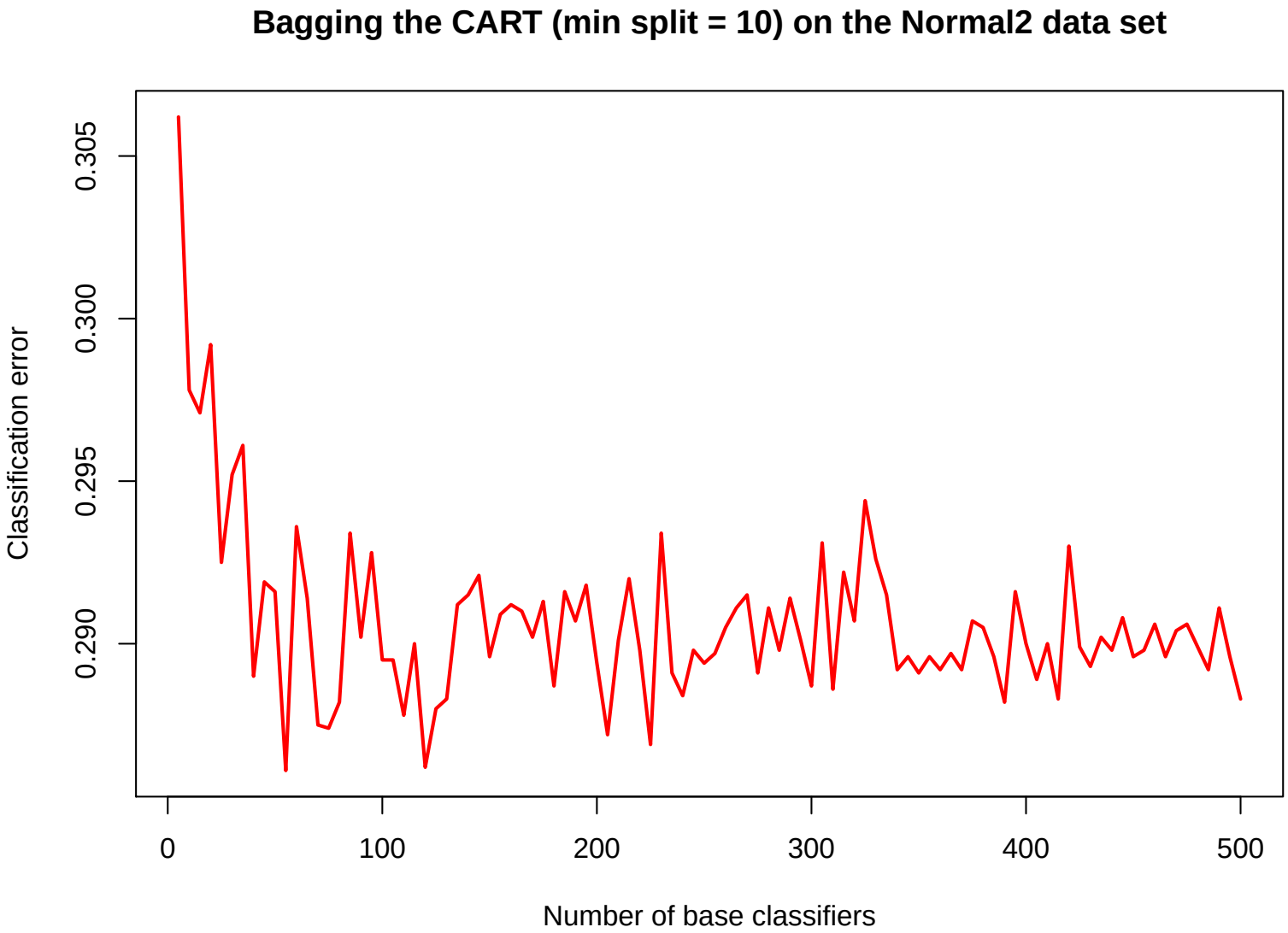

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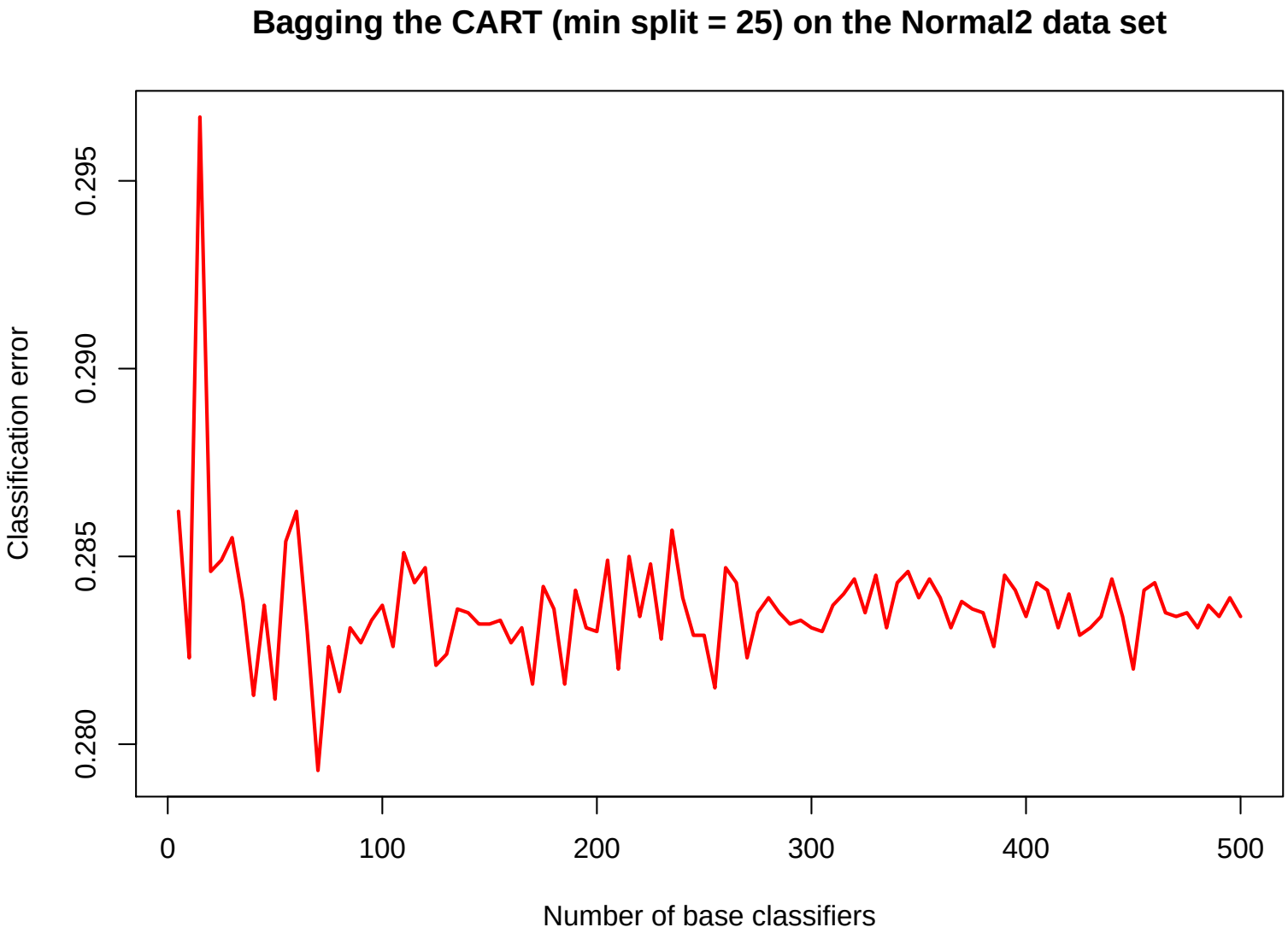

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- However, random forests introduce a substantial modification of bagging that builds a large collection of *de-correlated* trees.
- Let $T_k(\mathbf{x})$, $k = 1, ..., B$ be tree-similar classifiers ($T_k : \mathbb{R}^d \to \{0, 1\}$). The **random forest** classifier assigns new observation $\mathbf{x}$ by aggregating these:

$$T^{RF}(\mathbf{x}) = 1\Big(\frac{1}{B}\sum_{k=1}^{B} T_k(\mathbf{x}) > 0.5\Big).$$

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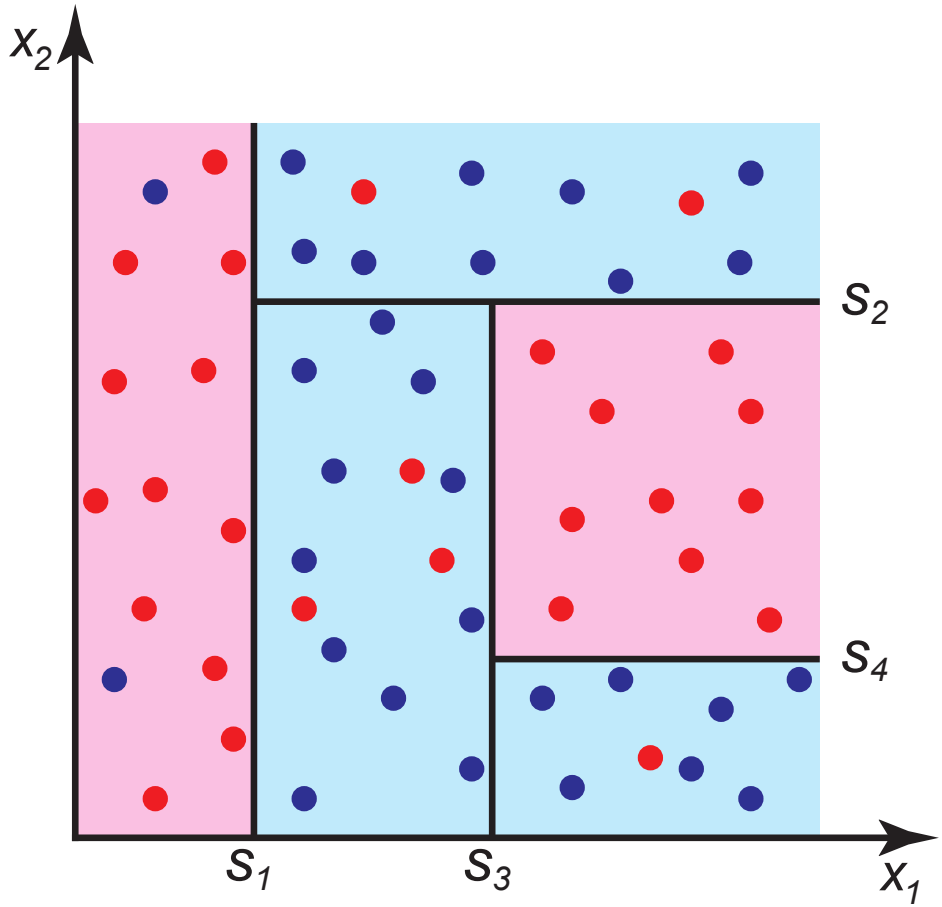
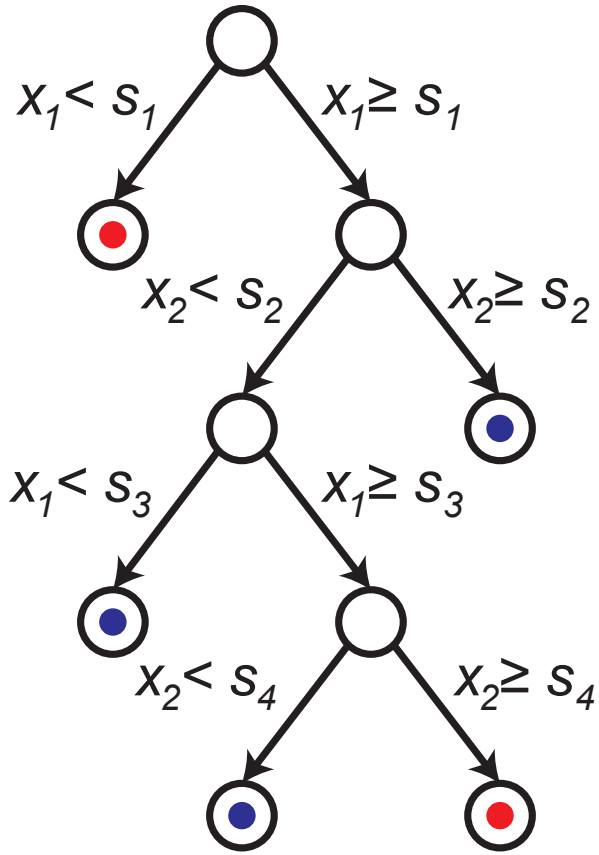

x_2
s_2
s_4
s_1
s_3
x_1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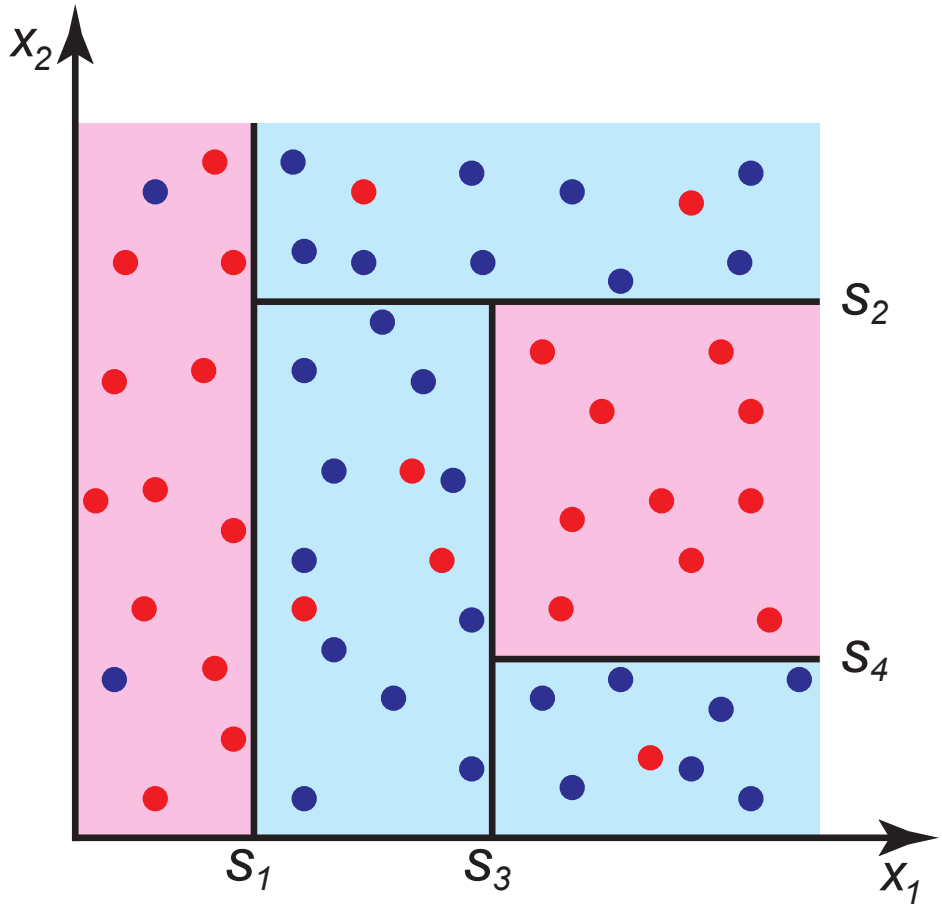

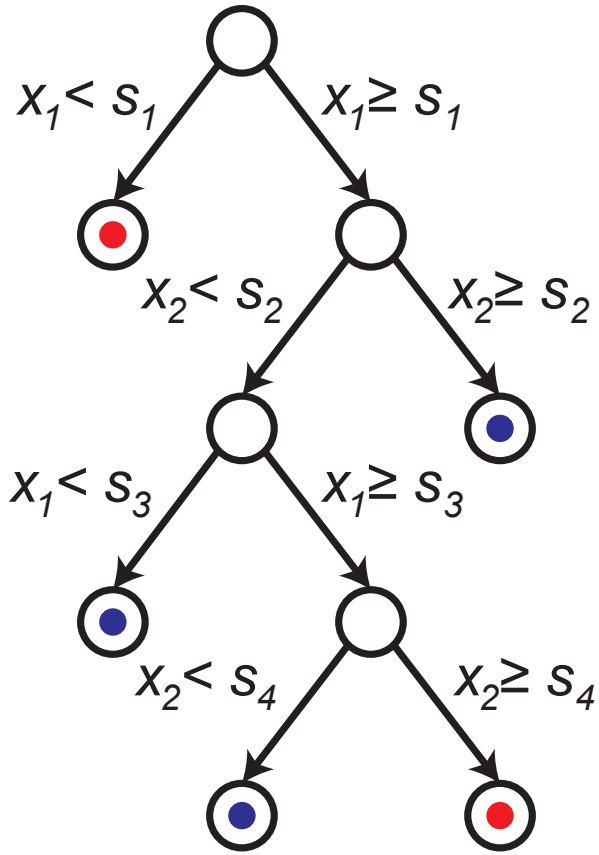

- **To reduce correlation between trees**, Breiman proposes
  - first, **randomly select** m variables out of all d variables,
  - next, pick the best variable/split-point among the m.

Random forests (algorithm)

Training

Input:

- Training sample $\big((\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\big) = \mathcal{D}_n \in \mathbb{R}^d \times \{0, 1\}$.

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Classification

- Classify the new observation $\mathbf{x}$ as

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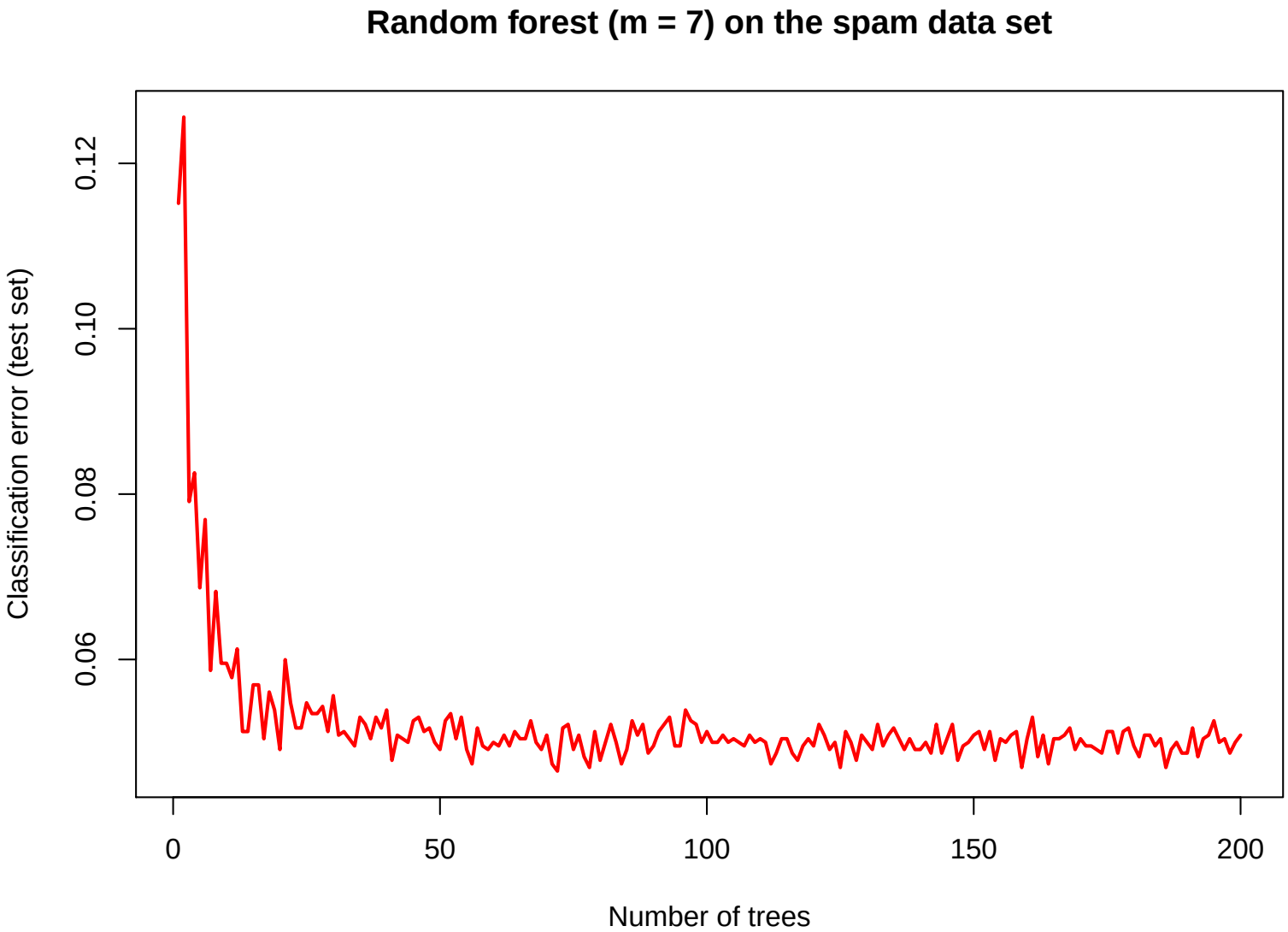
Spam data

- See Hastie *et al.* (2009, ch.1)
- A standard data set consisting of information from 4601 email messages
- The purpose is to predict if the email message is a spam or not
- For all 4601 email messages, the following information is available
  - the true outcome (email type) email or spam is available
  - the relative frequencies of 57 of the most commonly occurring words and punctuation marks in the email message.

Random forests: spam data



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- The **inventors recommend** $m = \lfloor \sqrt{d} \rfloor$
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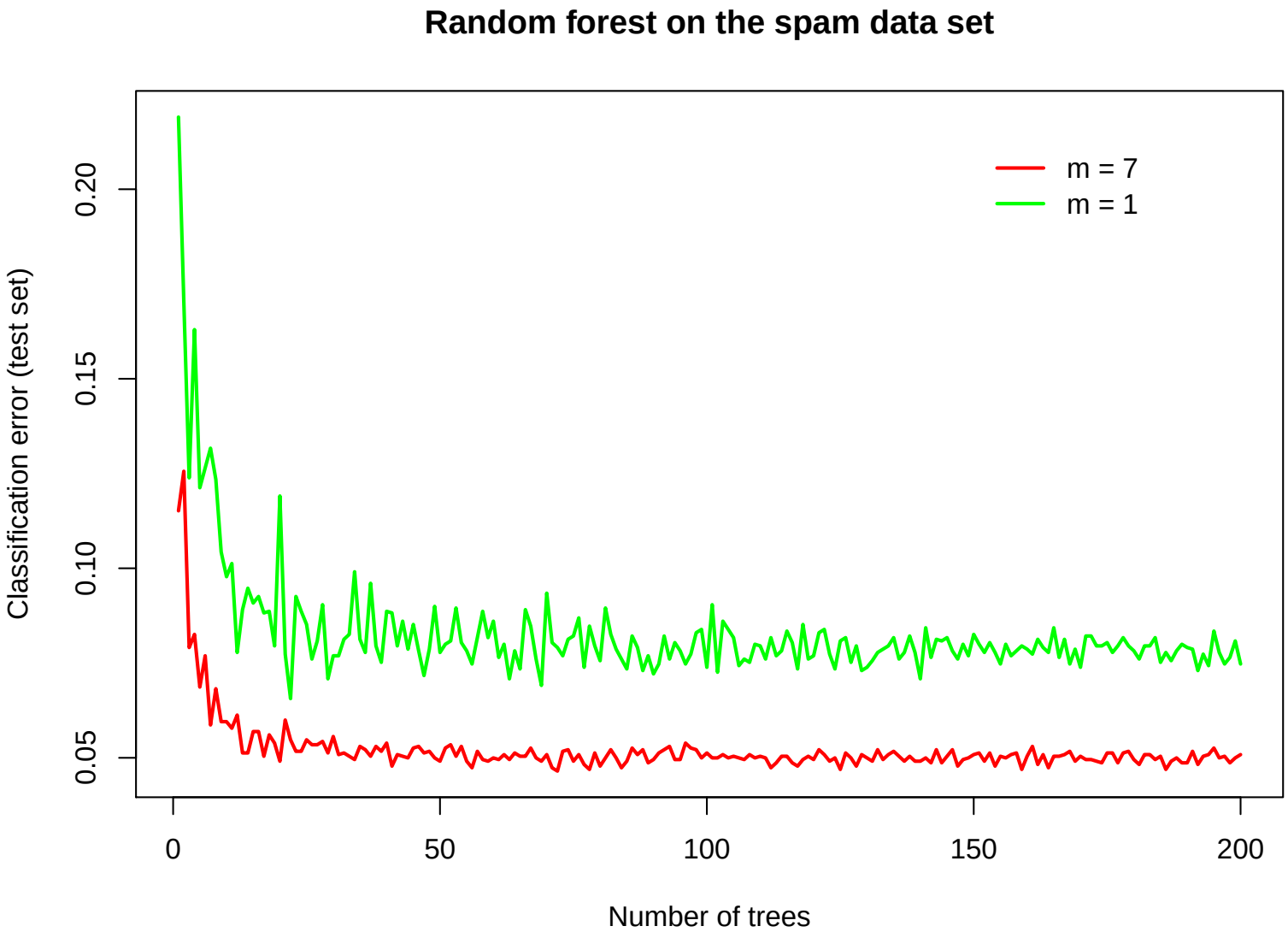
Random forests: spam data



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- Random forests offer an additional possibility to directly estimate classification error exploiting the **out-of-bag (OOB)** principle.
- The same idea can be extended from sample points to variables allowing to measure **variable importance**.

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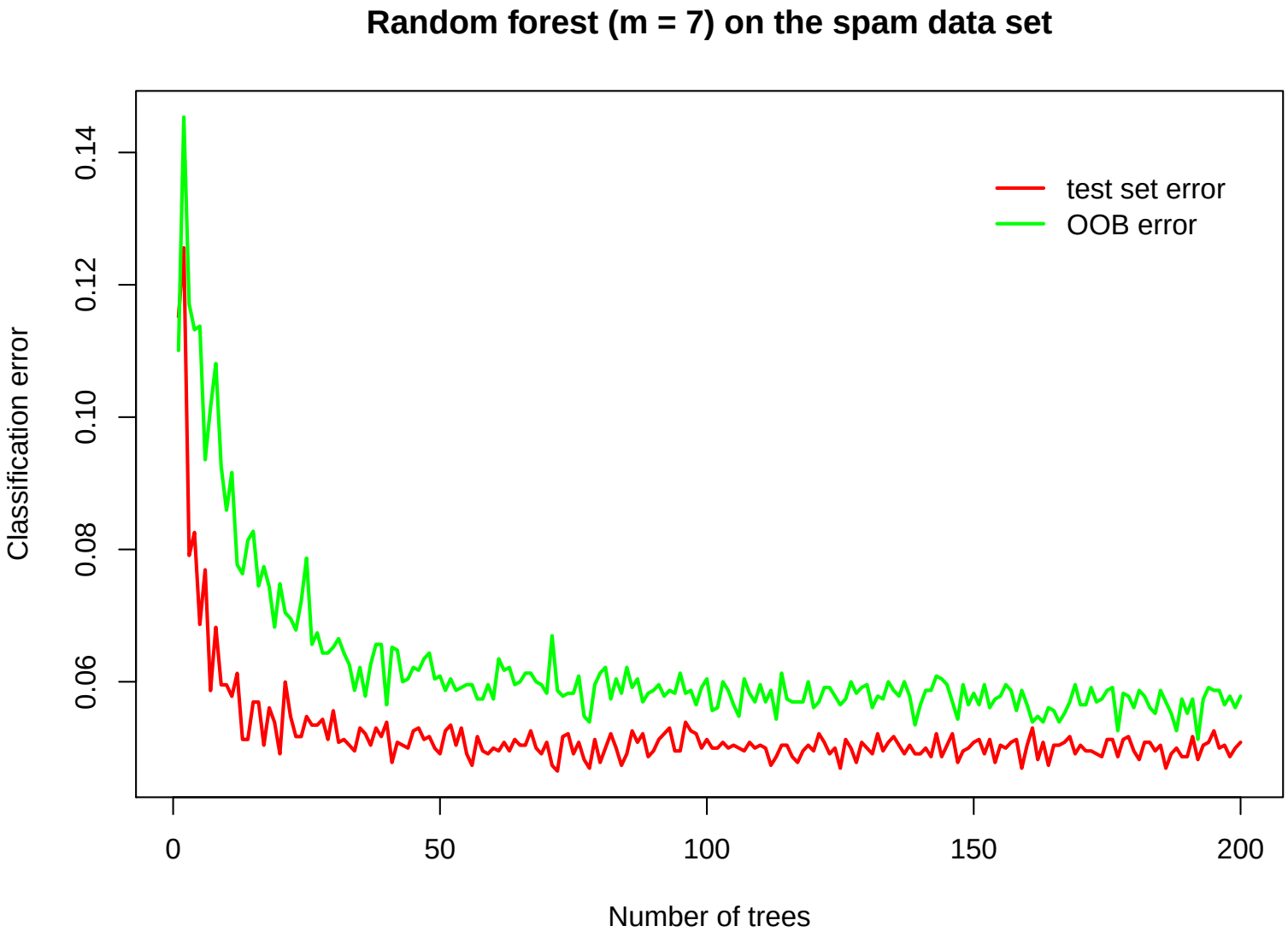
- Averaging over all observations $\mathbf{x}_i$, $i = 1, ..., n$ from $\mathcal{D}_n$ gives the out-of-bag estimate of the error rate:

$$R_{OOB} = \frac{1}{n} \sum_{i=1}^{n} 1\big(\hat{y}_i \neq y_i\big) \,.$$

Random forests: spam data



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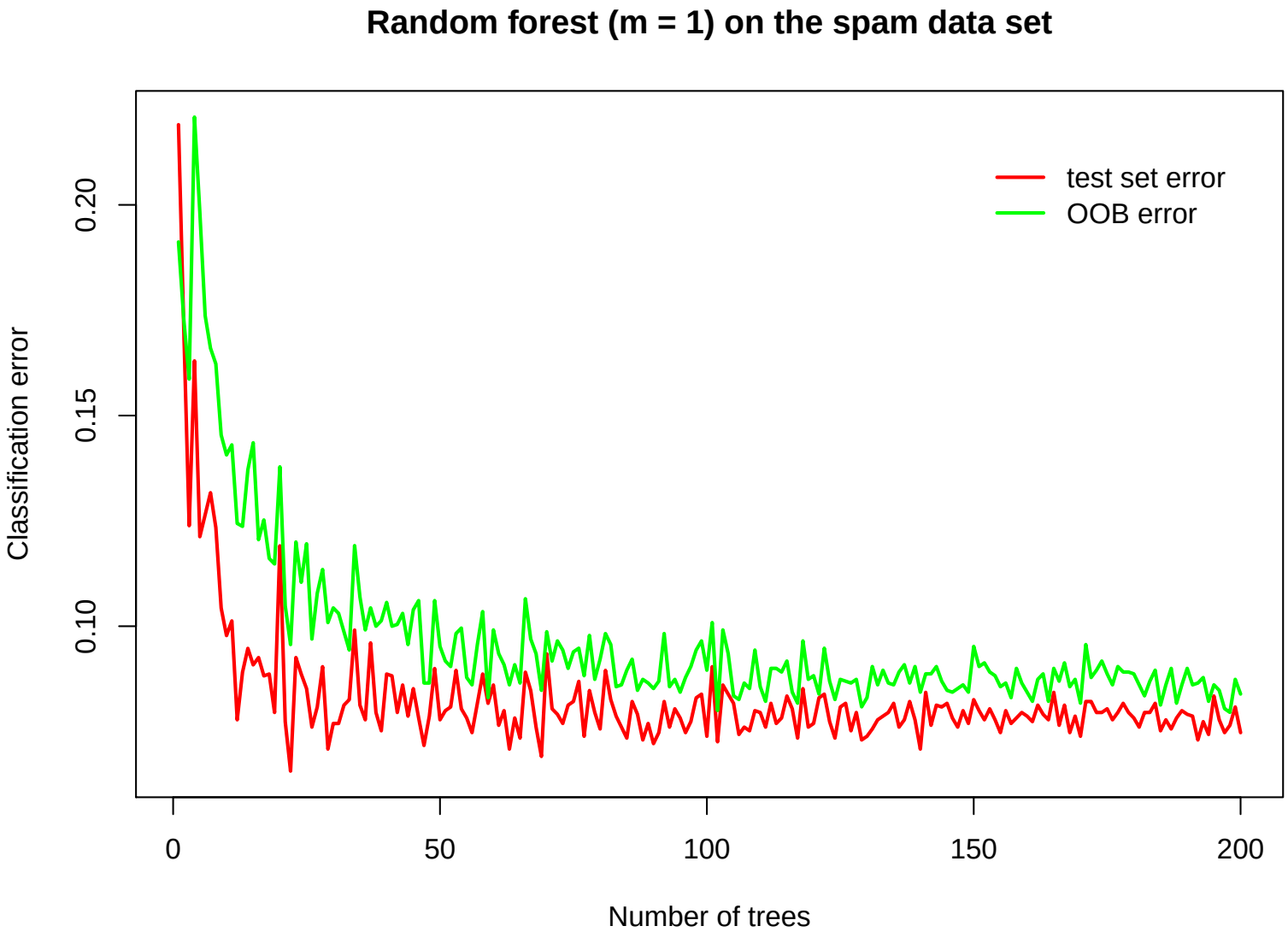

Importance of a variable

- For a bootstrap sample $\mathcal{D}^*_{n,k}$, let $\mathcal{D}^{*-}_{n,k}$ be the **subset of training sample not contained in** $\mathcal{D}^*_{n,k}$, *i.e.* it holds $\mathcal{D}^*_{n,k} \cup \mathcal{D}^{*-}_{n,k} = \mathcal{D}_n$ and $\mathcal{D}^*_{n,k} \cap \mathcal{D}^{*-}_{n,k} = \emptyset$.

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- Further, let $\mathcal{D}^{*-}_{n,k}(j)$ be the same subset $\mathcal{D}^{*-}_{n,k}$ where the **values of variable** $j \in \{1, ..., d\}$ have been **randomly perturbed**, and measure the error from above on this perturbed subset:

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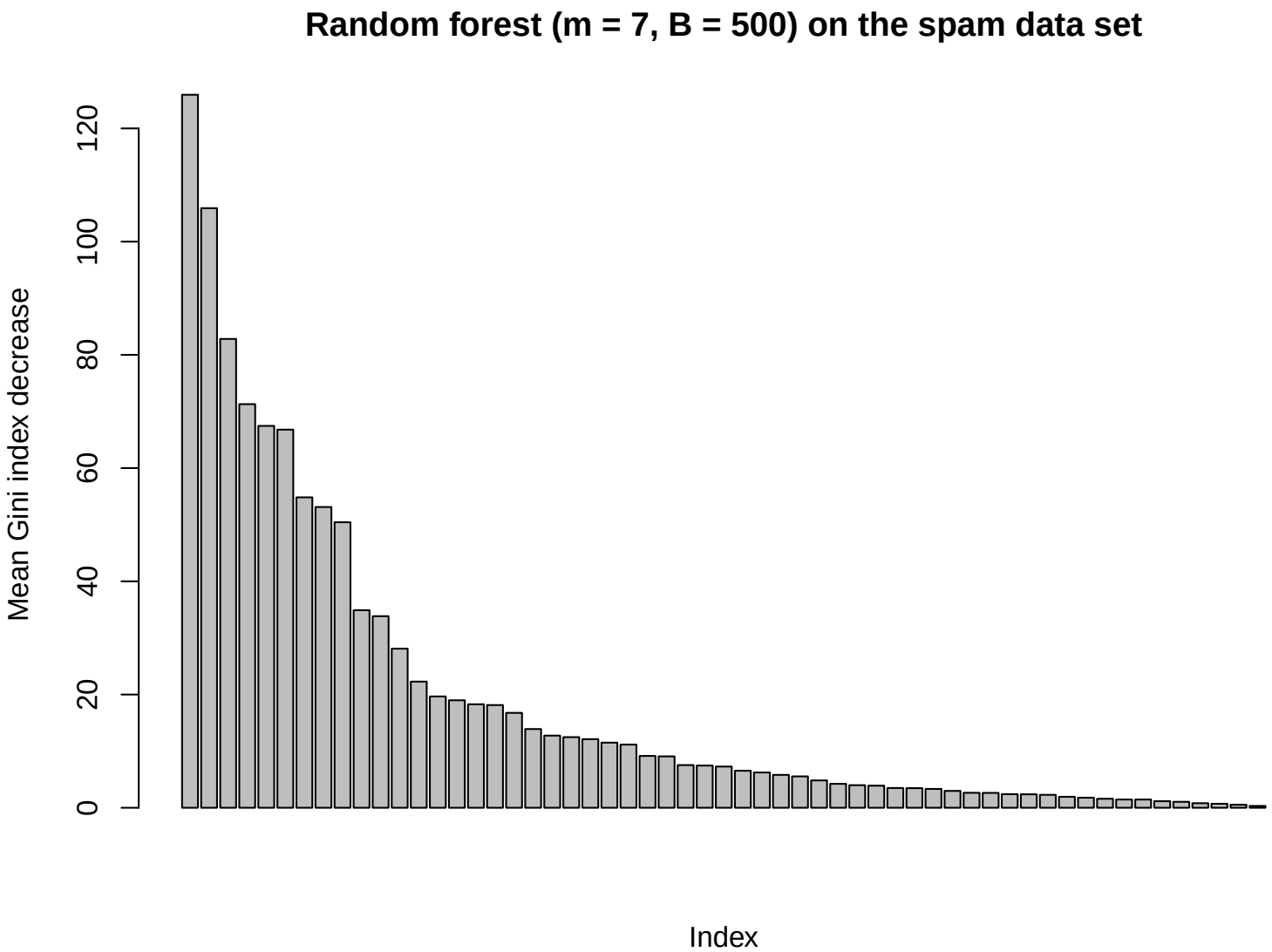
- The **importance of variable** j can thus be measured (by averaging over all B trees) as:

$$Imp(X_j) = \frac{1}{B} \sum_{k=1}^{B} \left(R_{OOB(k,j)} - R_{OOB(k)}\right).$$

Random forests: importance of the variables using the Gini index decrease



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Theorem (Biau, Devroye, Lugosi, 2008; Th. 1)

Assume that the distribution of X is supported on $[0,1]^d$. Then the purely random forest classifier $T_B^{prRF} = 1\big(\frac{1}{B}\sum_{k=1}^{B} T^{pr}(\cdot, \mathcal{D}_n)\big)$ (as well as $\lim_{B\to\infty} T_B^{prRF}$) is consistent whenever $k \to \infty$ and $k/n \to 0$ as $k \to \infty$.

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Theorem (Biau, Devroye, Lugosi, 2008)

Assume that the distribution of X has non-atomic marginals in $\mathbb{R}^d$. Then the scale-invariant random forest classifier $T_B^{siRF} = 1\big(\frac{1}{B}\sum_{k=1}^{B} T^{si}(\cdot, \mathcal{D}_n)\big)$ (as well as $\lim_{B\to\infty} T_B^{siRF}$) is consistent whenever $k \to \infty$ and $\frac{k}{n} \to 0$ as $k \to \infty$.

Consistency of bagging

Remind:

- Bagging classifier:

$$g_B^{agg}(\mathbf{x}) = 1\Big(\frac{1}{B}\sum_{k=1}^{B} g_k^*(\mathbf{x}) > 0.5\Big)\,.$$

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Theorem (Biau, Devroye, Lugosi, 2008; Th. 6)

Assume that the classifier g is consistent for a certain distribution (X, Y). Then the bagging classifier g_B^{agg} and its limit $1\big(\mathbb{E}[g_k^*(\mathbf{x}) \mid \mathcal{D}_n)] > 0.5\big)$ are also consistent if $nq_n \to \infty$ as $n \to \infty$.

Thank you for your attention!

And some more references

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