Classification tree, bagging, and random forest

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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**:

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

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

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

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Classification tree (algorithm)

Growing a tree (training)

Input:

- Training sample $\big((\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\big) = \mathcal{D}_n \in \mathbb{R}^d \times \{0, 1\}$.
- Measure of impurity $Q^{(m)}(T)$ for node m of tree T.
- Stopping criteria $S^{(m)}(T)$ for node m of tree T.

1. Define the root node by the region $R^{(0)}$ containing the entire sample, set $m = 0$.
2. If $S^{(m)}(T)$ is fulfilled then stop for this node (e.g., a lower bound for the # of obs. in a node).
3. Find a variable and a split (one-variable threshold) diving node region $R^{(m)}$ into two nodes with subregions $R^{(m_L)}$ and $R^{(m_R)}$ to minimize $Q^{(m)}(T)$.
4. Repeat steps 2–3 for all leaves until global stopping.

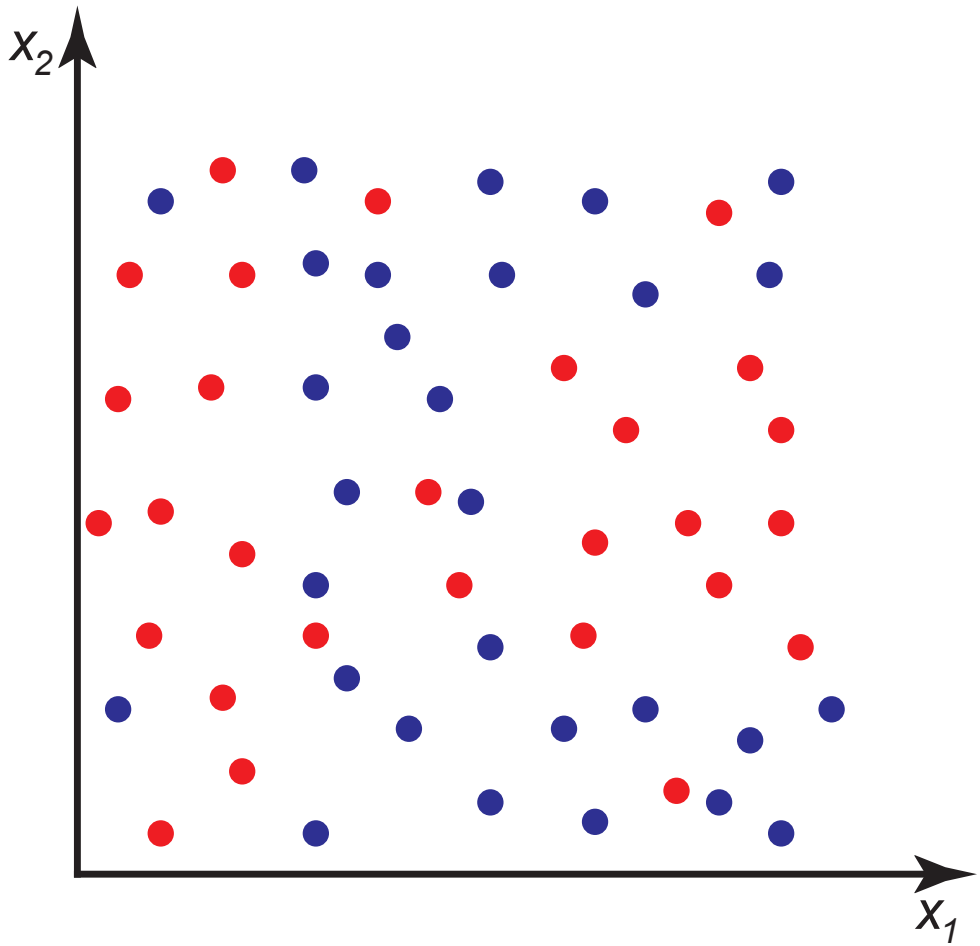
Output: The tree T.

Classification tree – Descending the tree

- *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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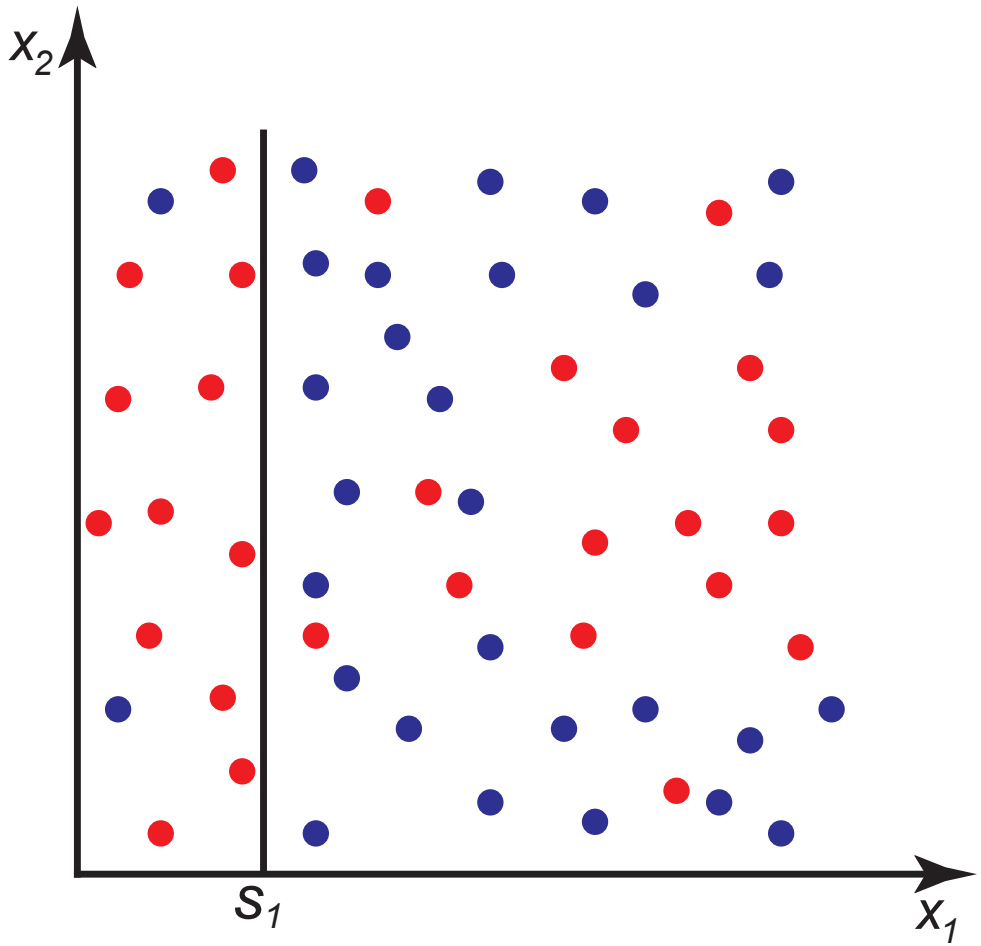

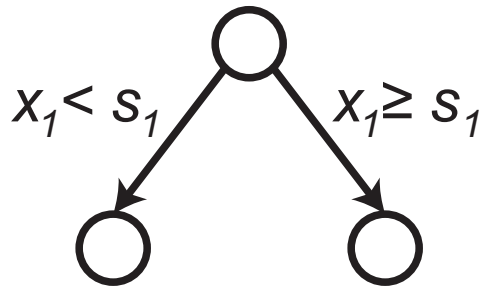

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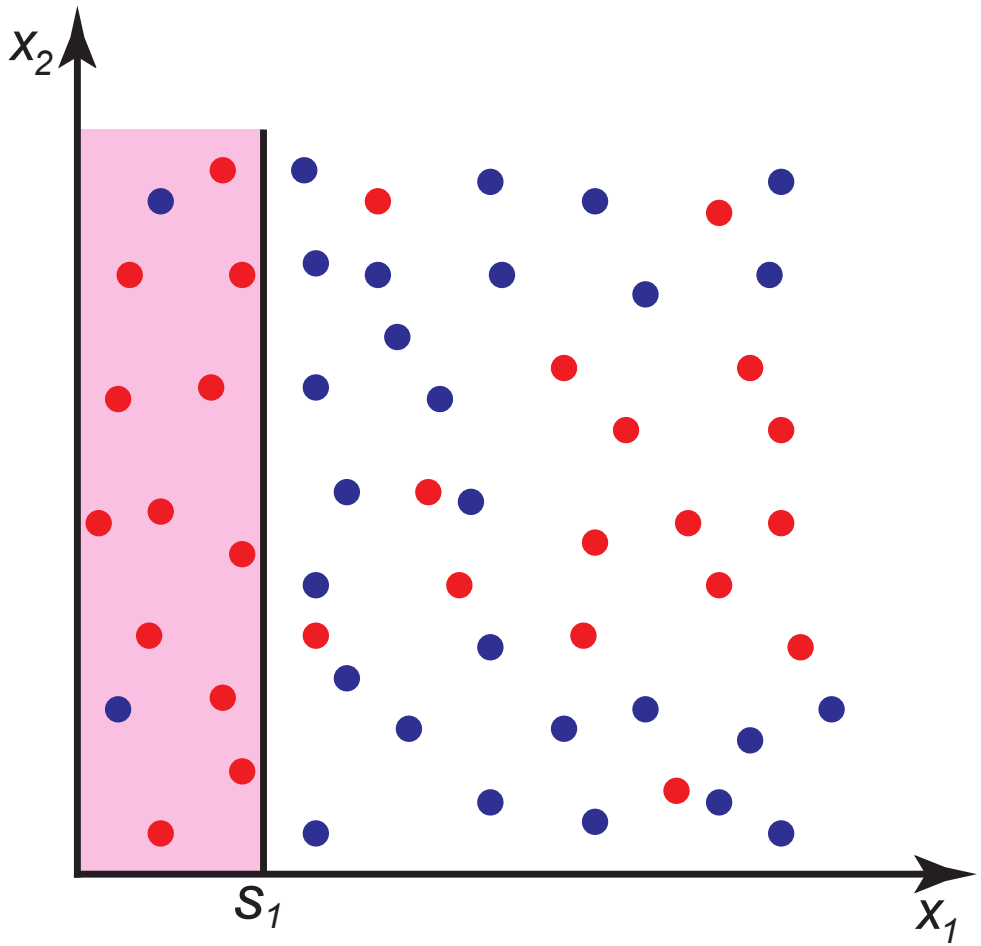

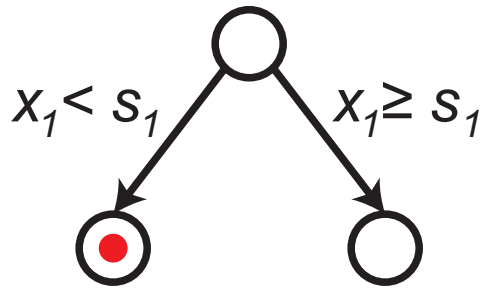

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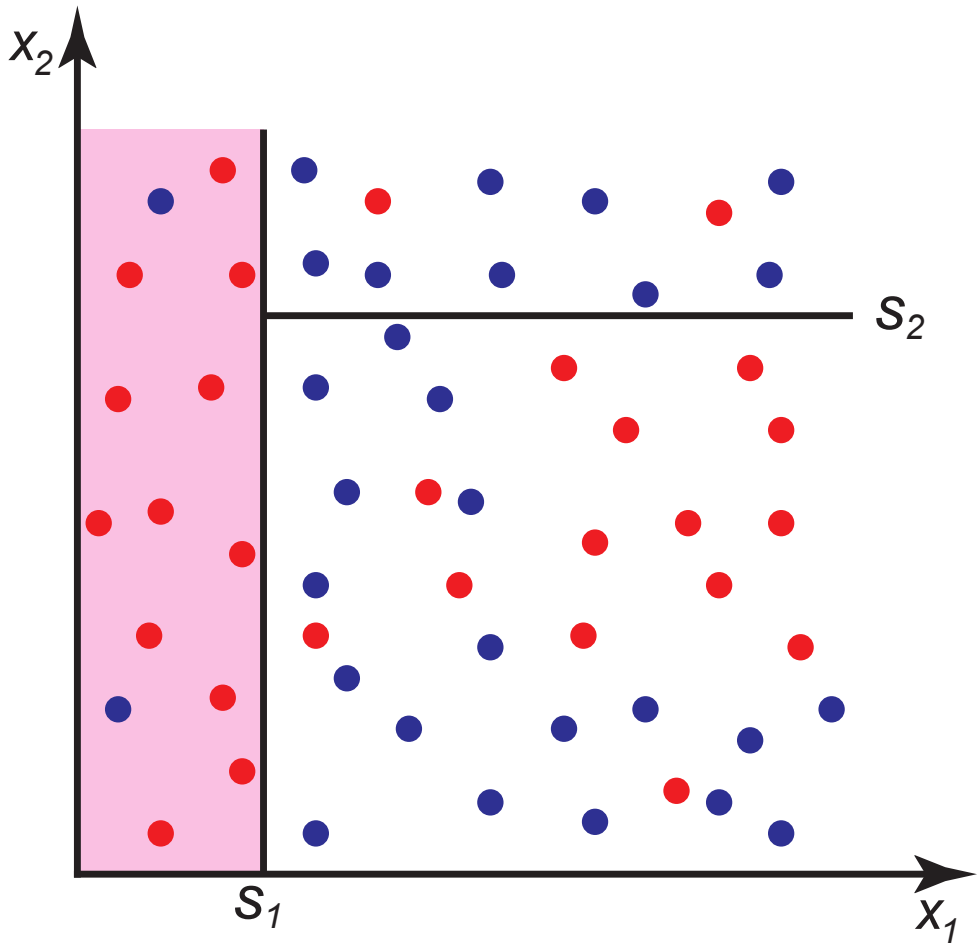

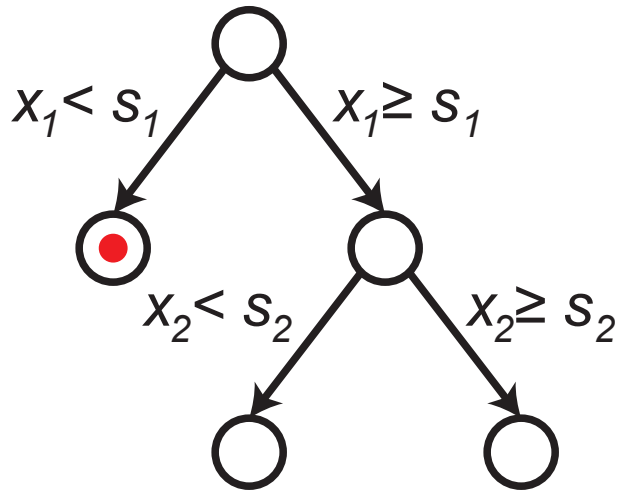

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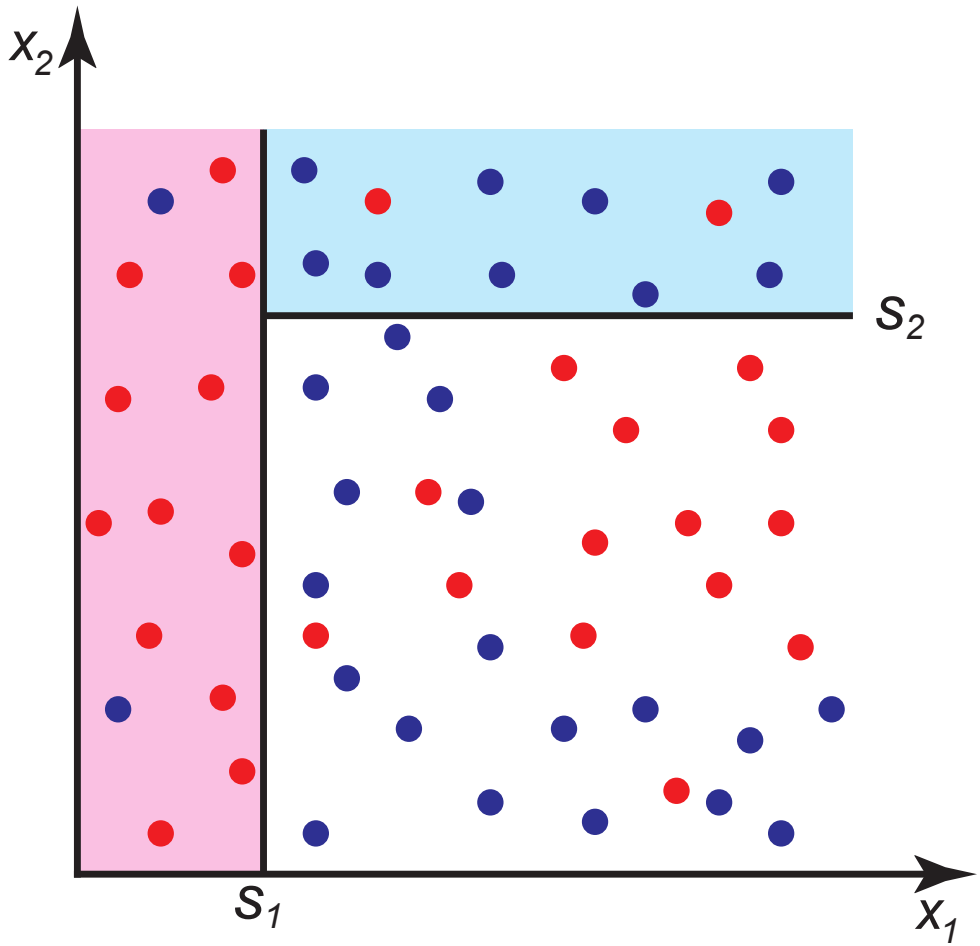

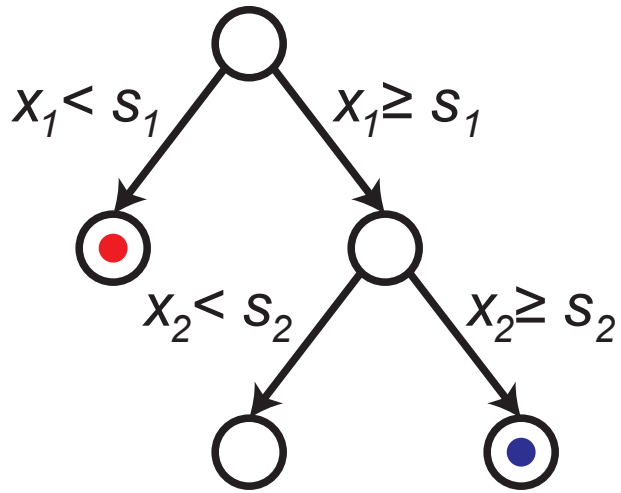

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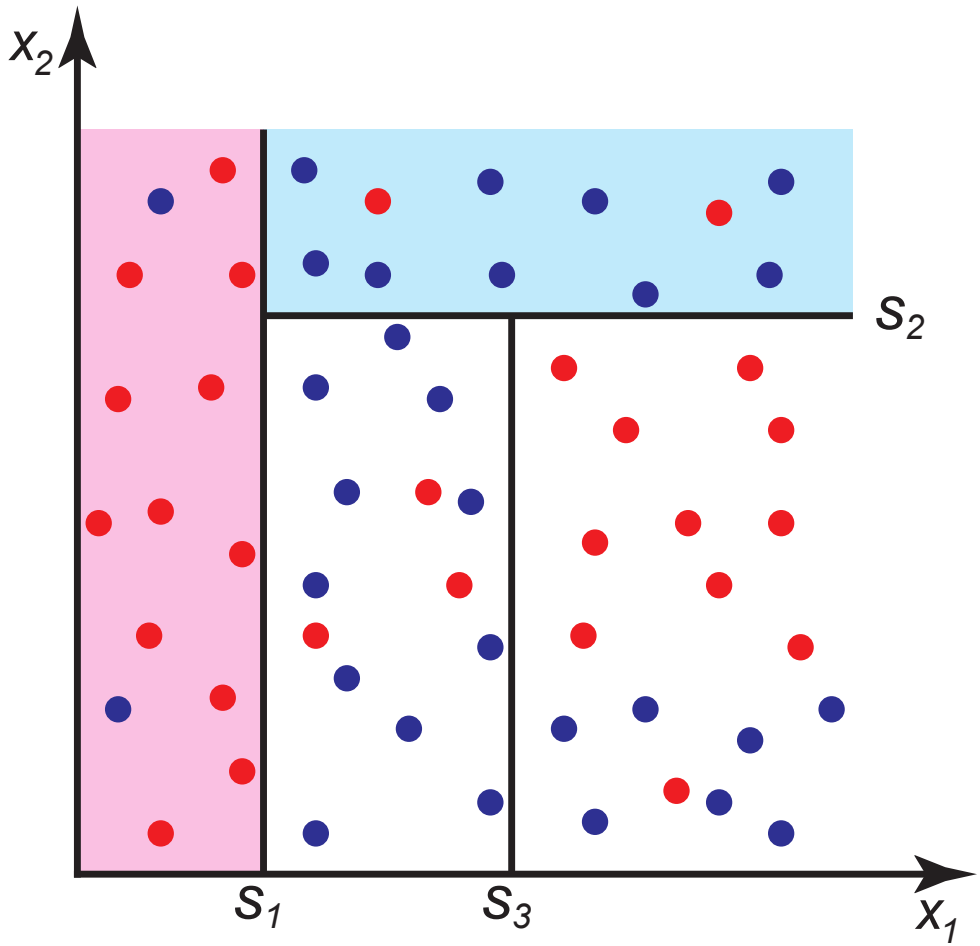

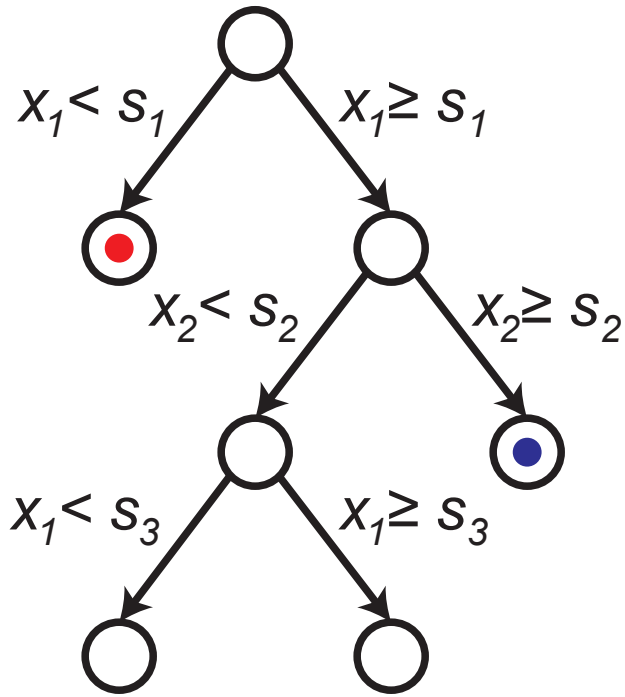

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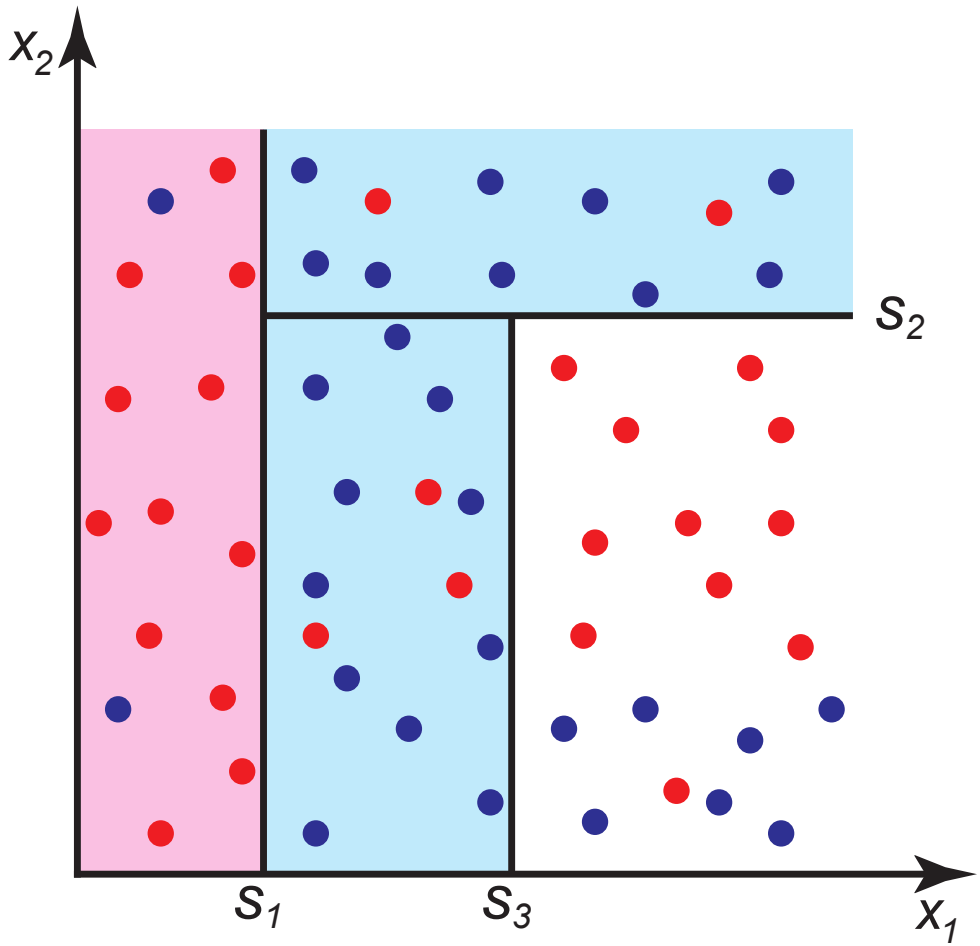

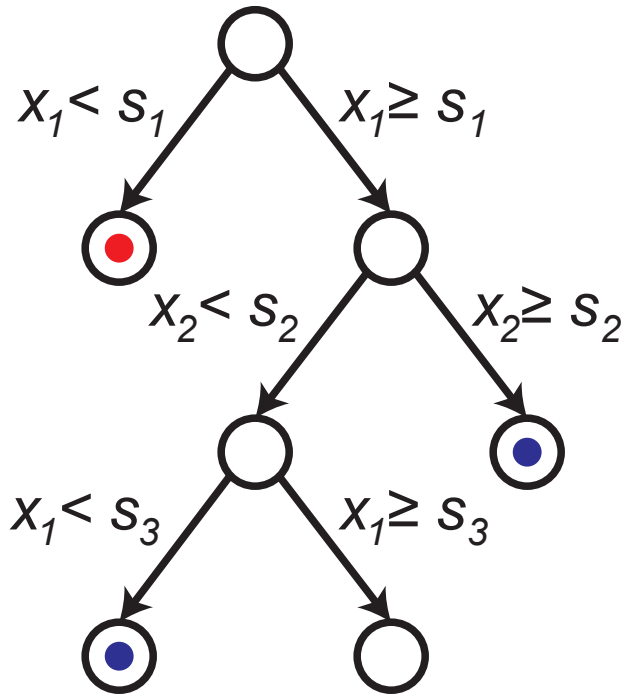

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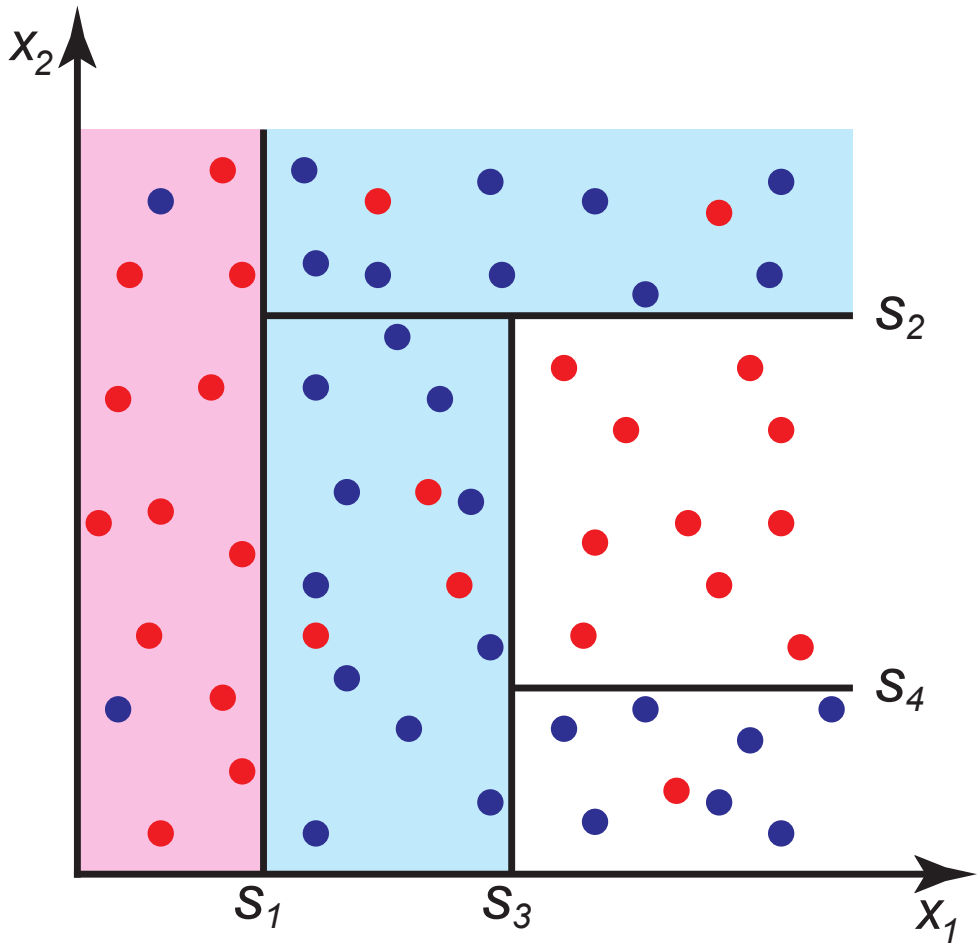

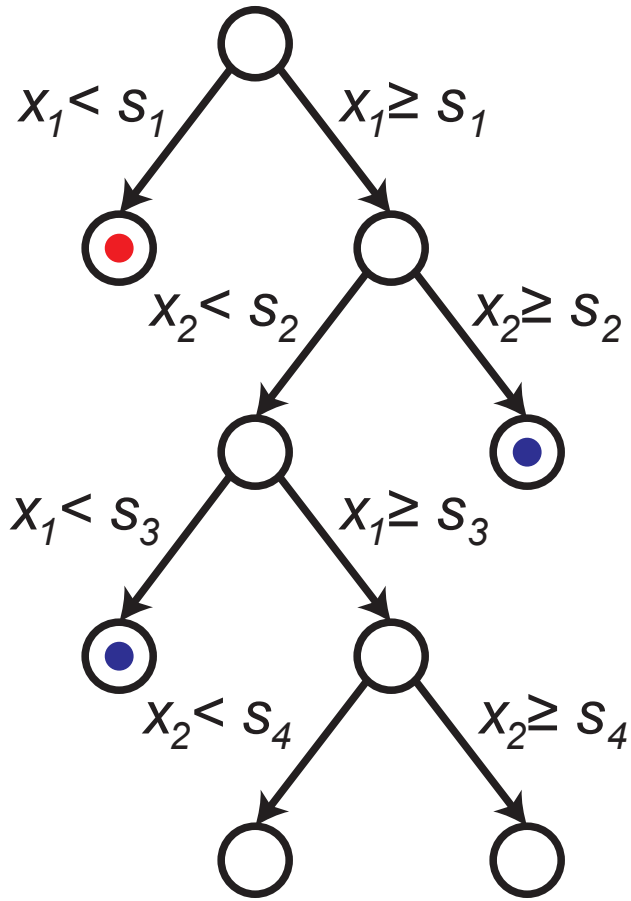

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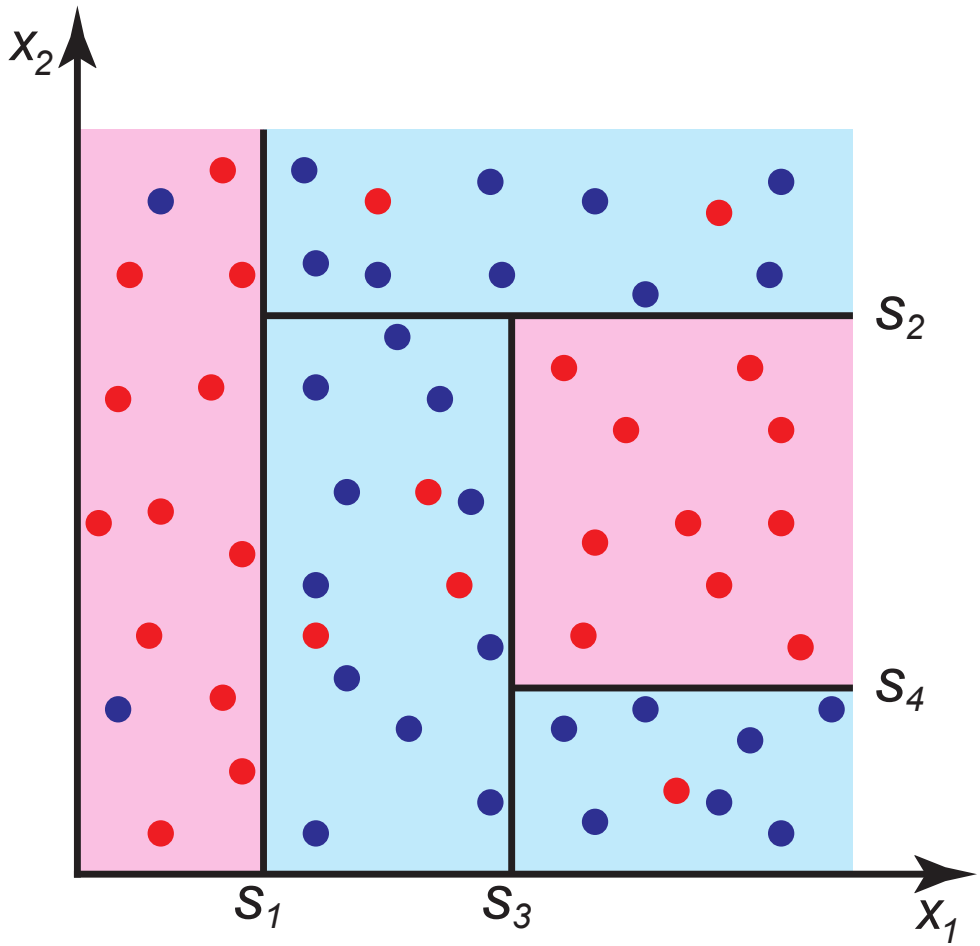
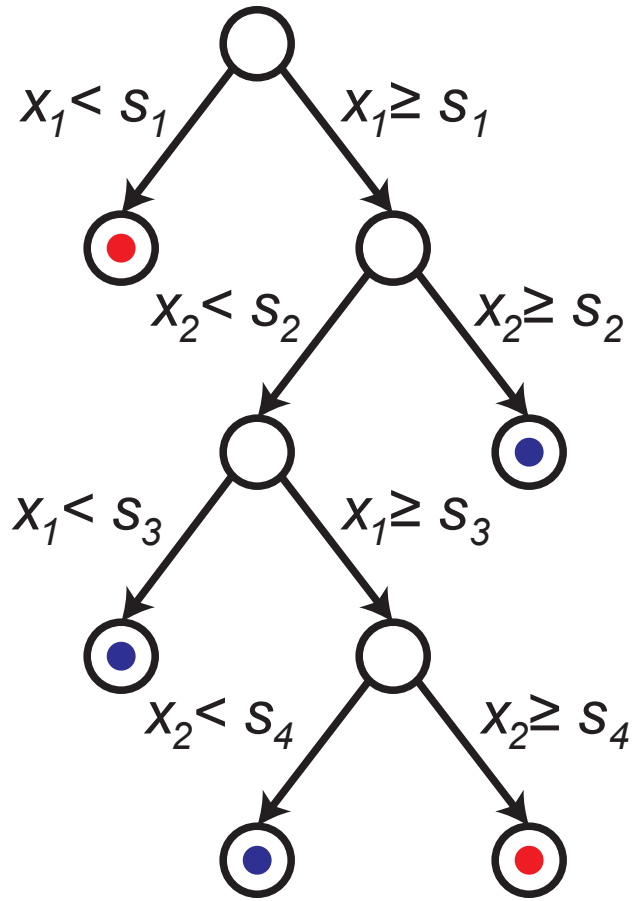




Classification tree: choice of impurity measure

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

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

Possible choices for Q (the measure of impurity):

- Misclassification error:

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

- Gini index:

$$Q^{(m)}(T) = \frac{n^{(m_L)}}{n^{(m)}} 2\hat{p}_k^{(m_L)}(1 - \hat{p}_k^{(m_L)}) + \frac{n^{(m_R)}}{n^{(m)}} 2\hat{p}_k^{(m_R)}(1 - \hat{p}_k^{(m_R)})\,,$$

- 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

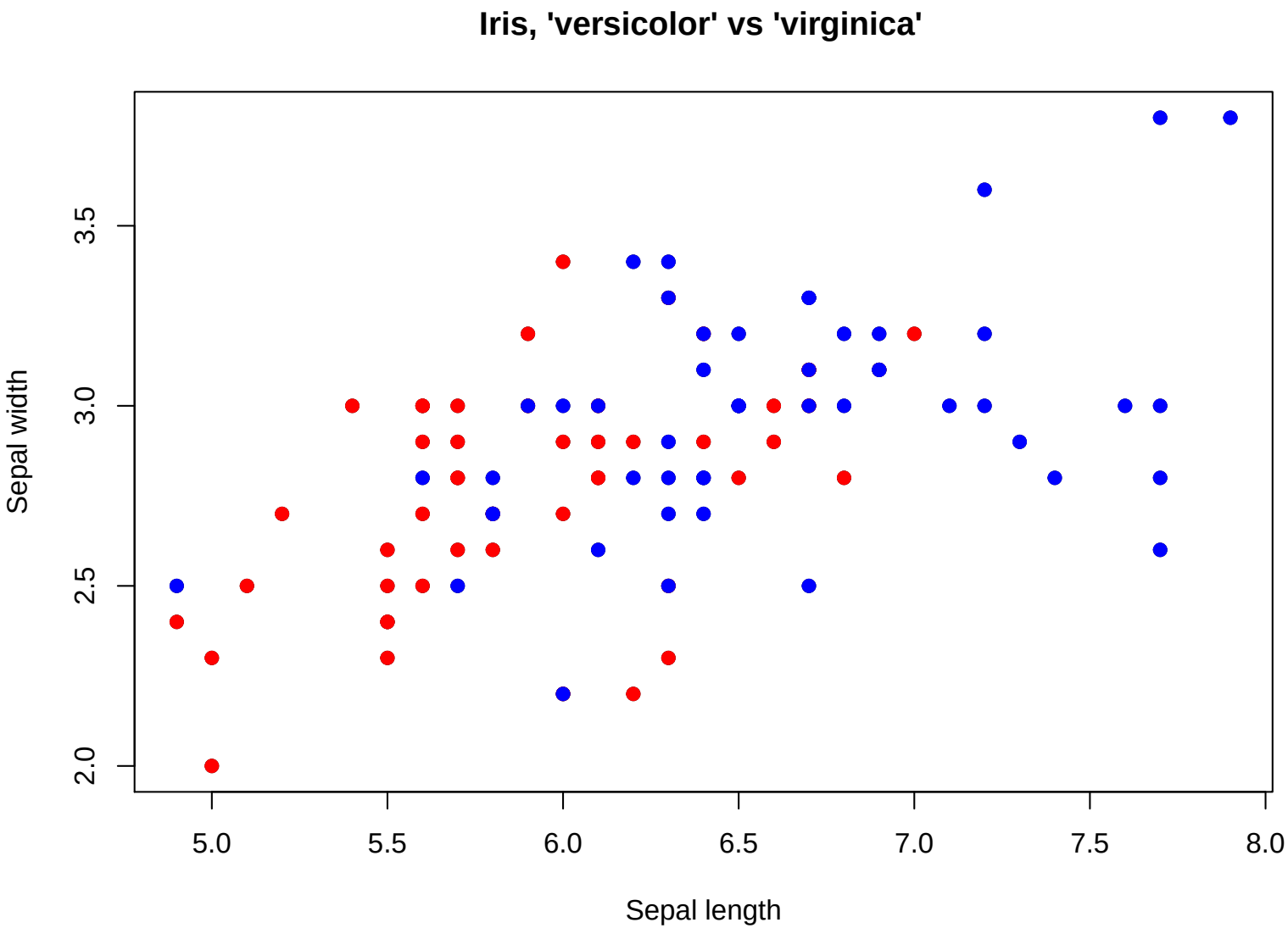
- Sometimes in the literature and in the textbooks, the minimization of $Q^{(m)}(T)$ is presented under the equivalent for of the *gain maximization*
- For instance, for the Gini index the gain is

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

- For instance, for the deviance the gain is

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

Classification tree: iris data



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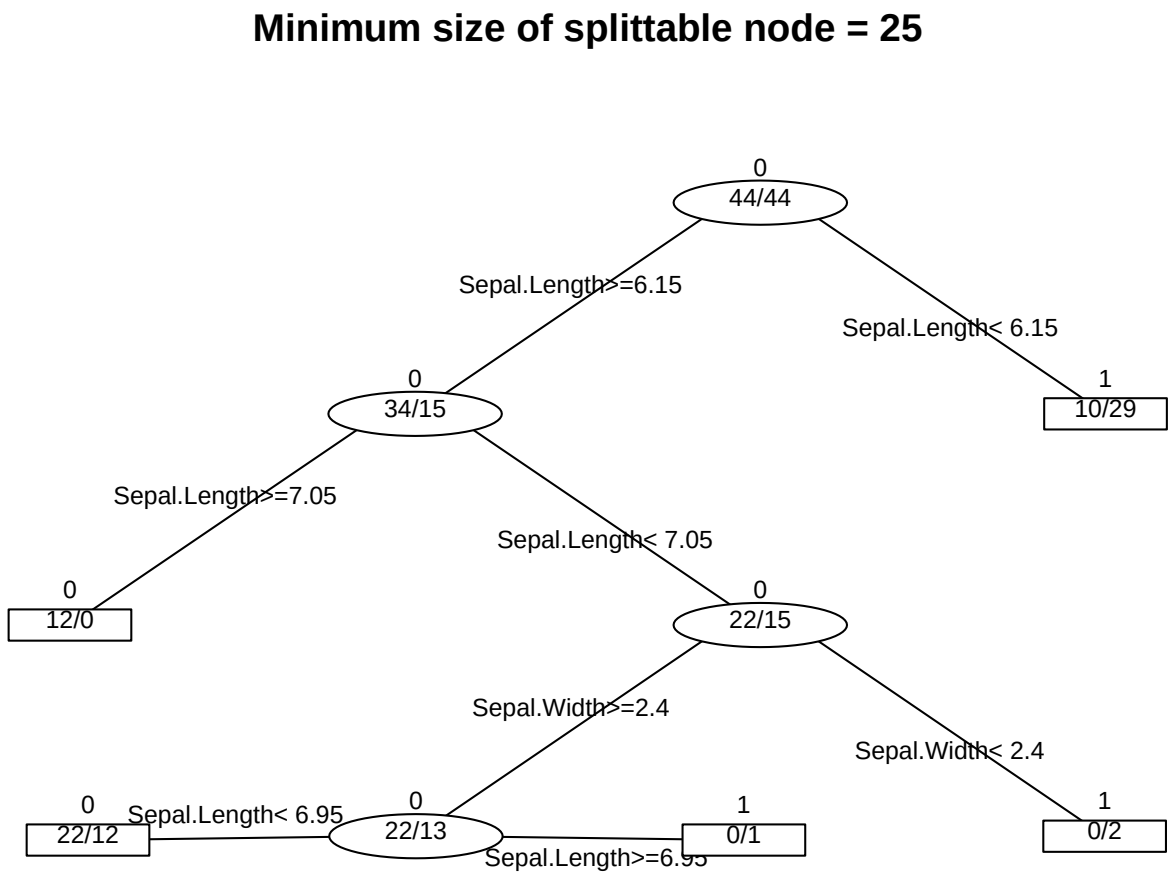

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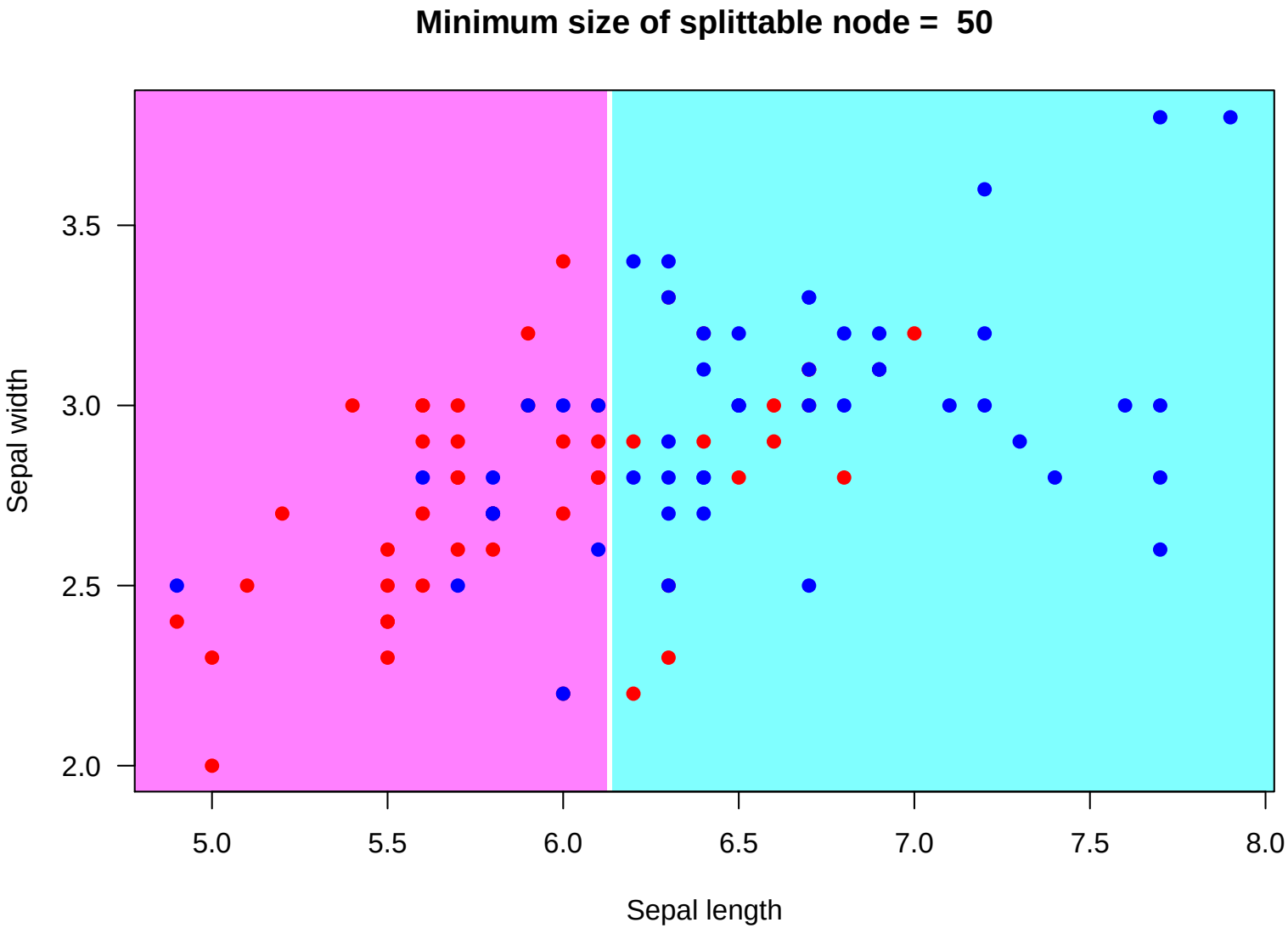

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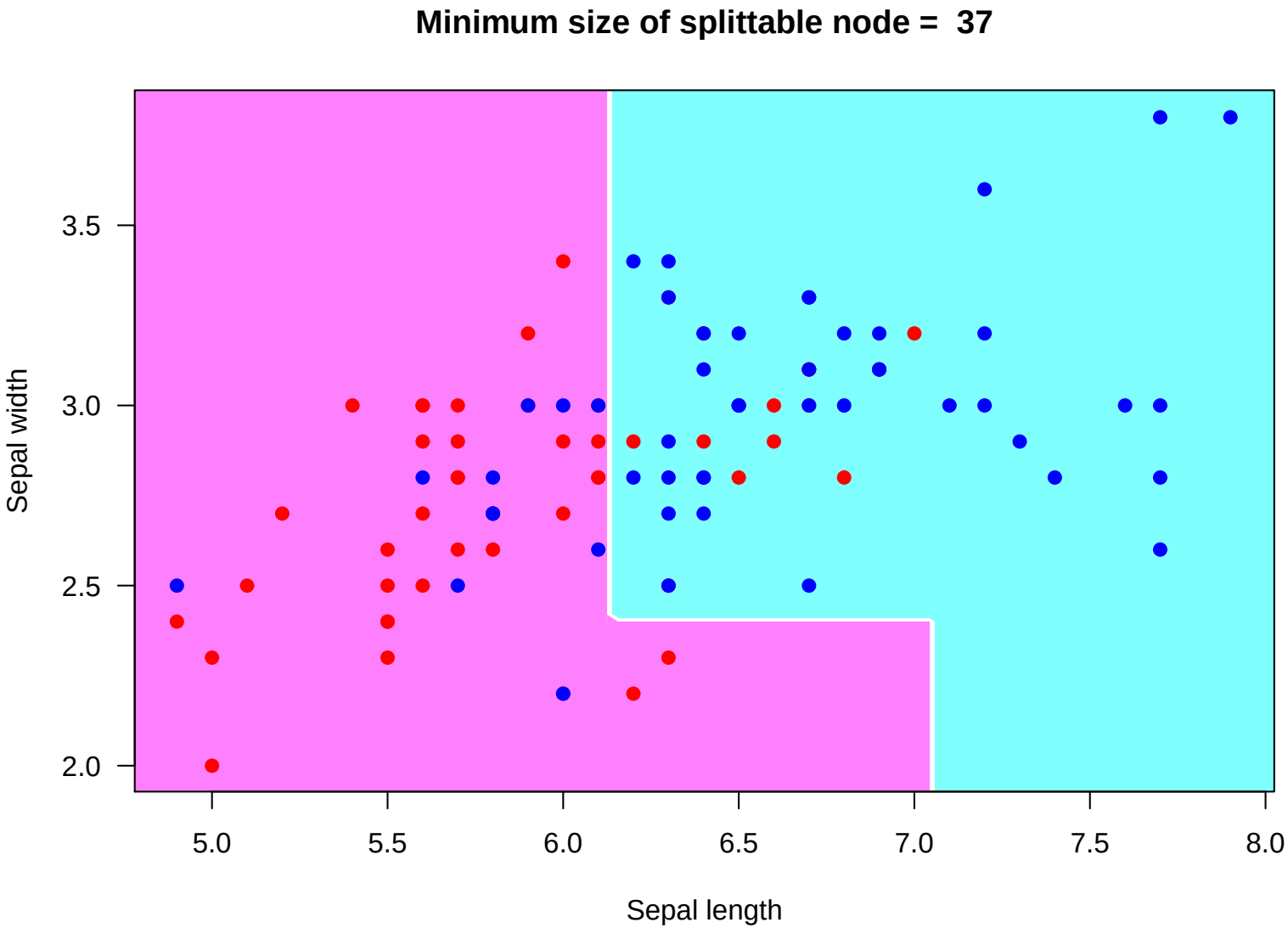

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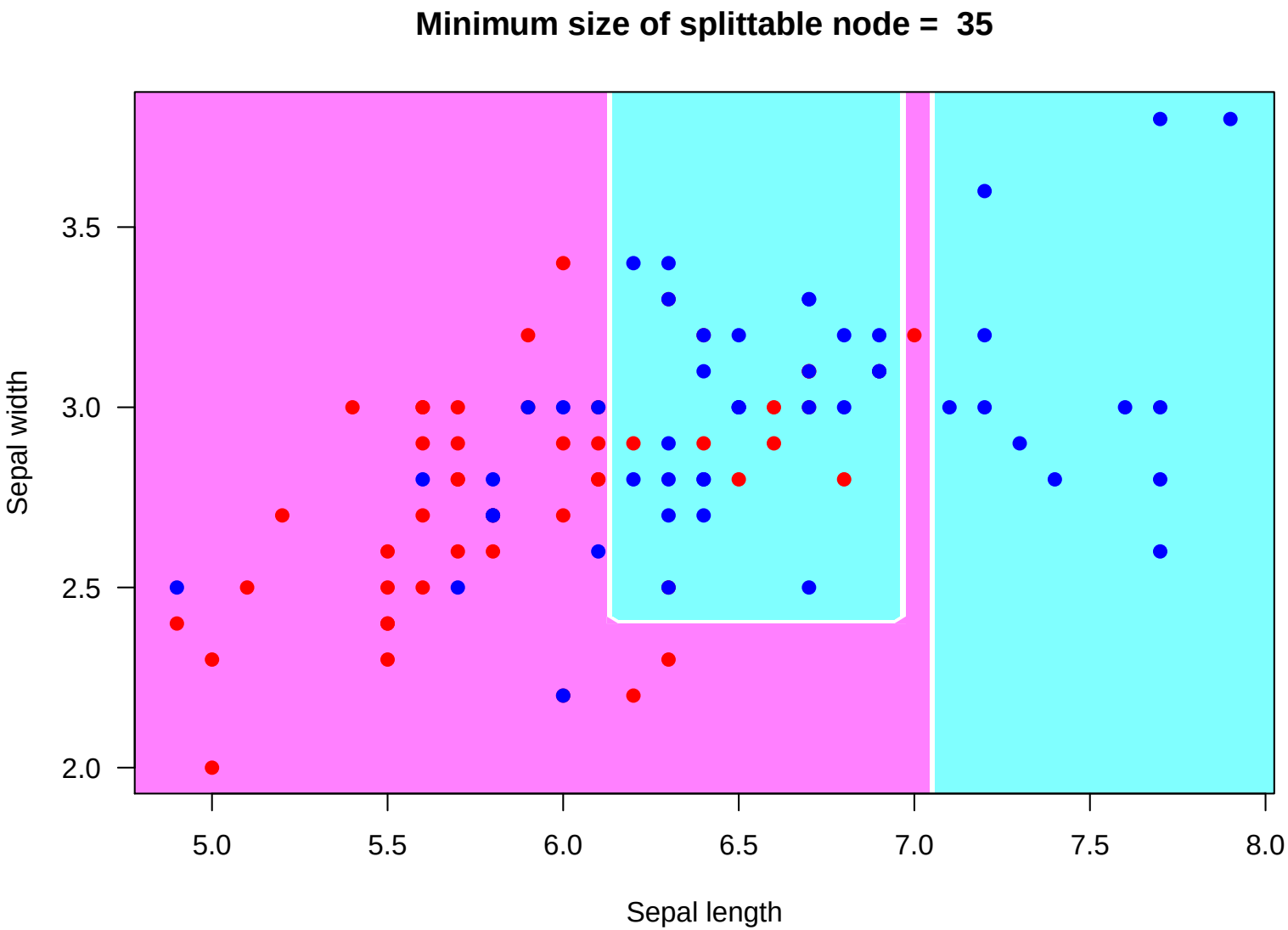

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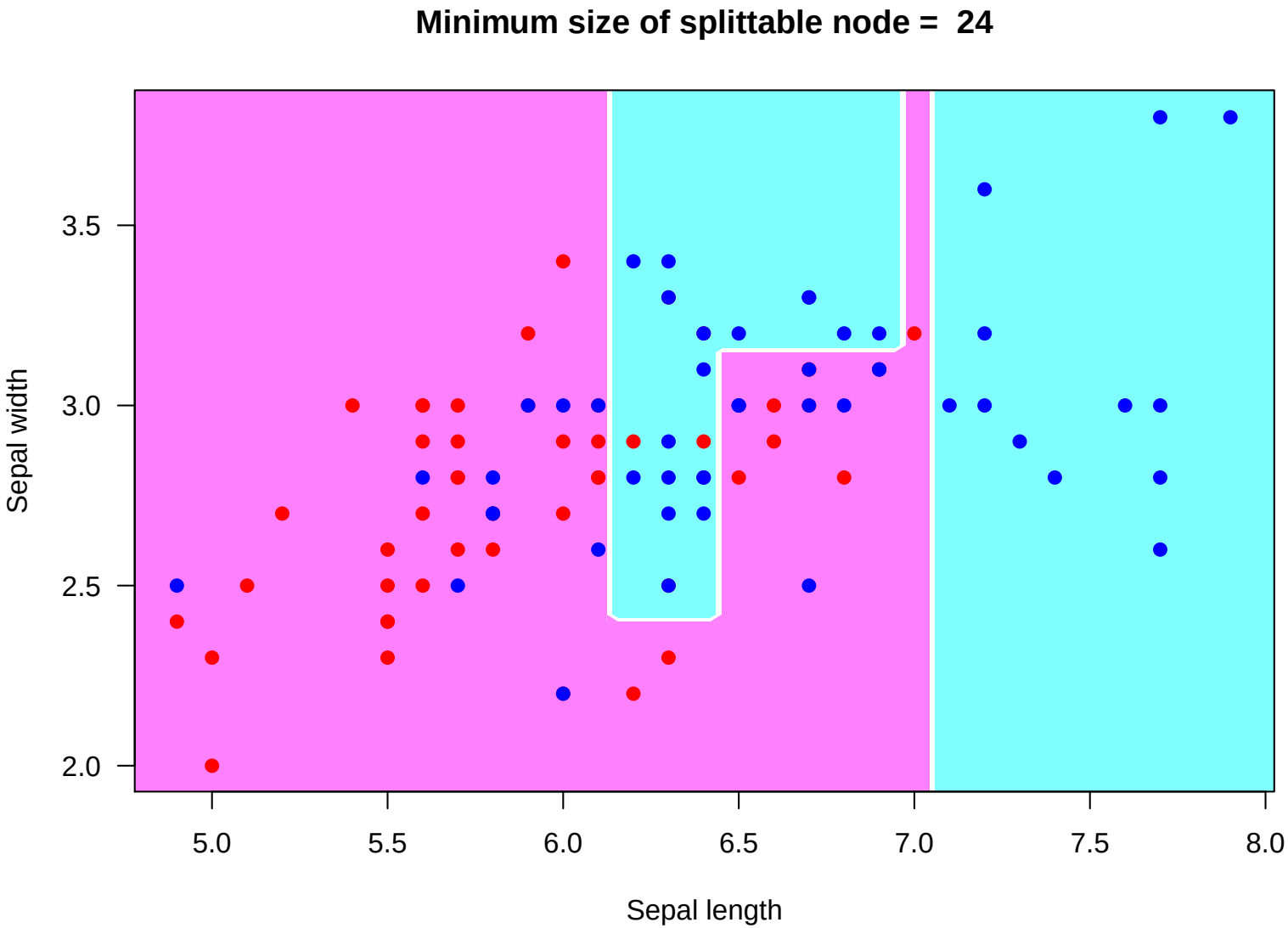

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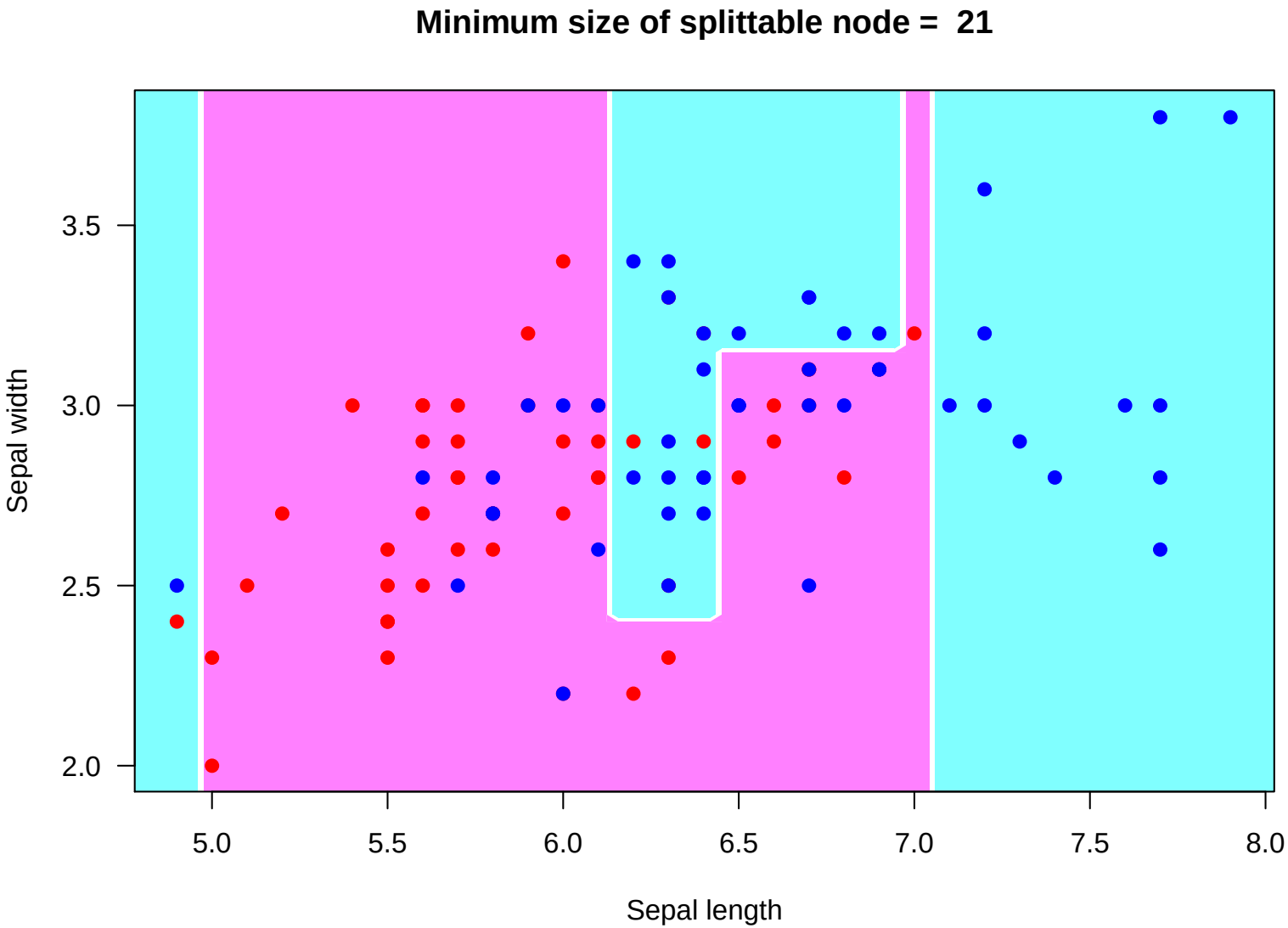

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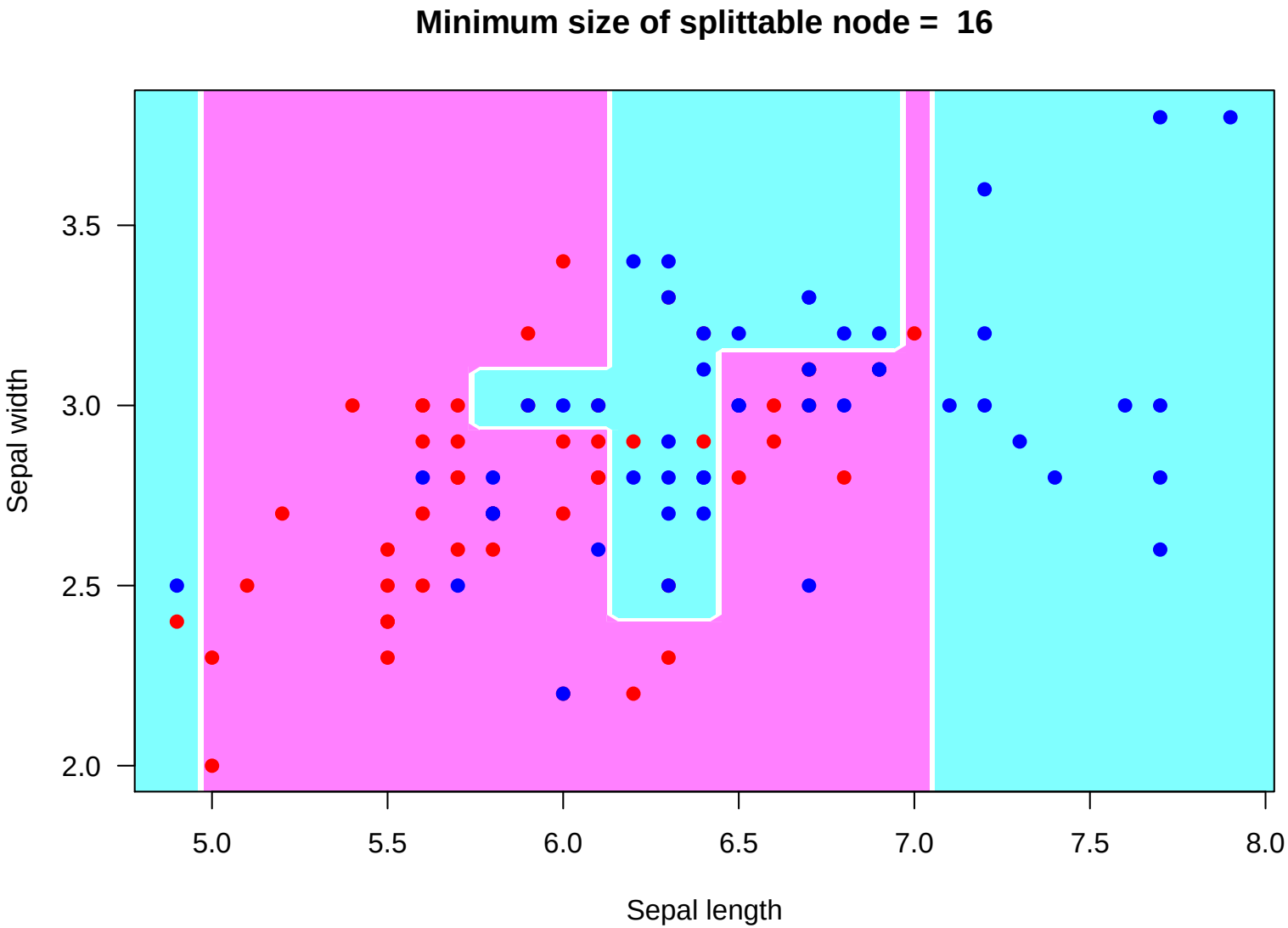

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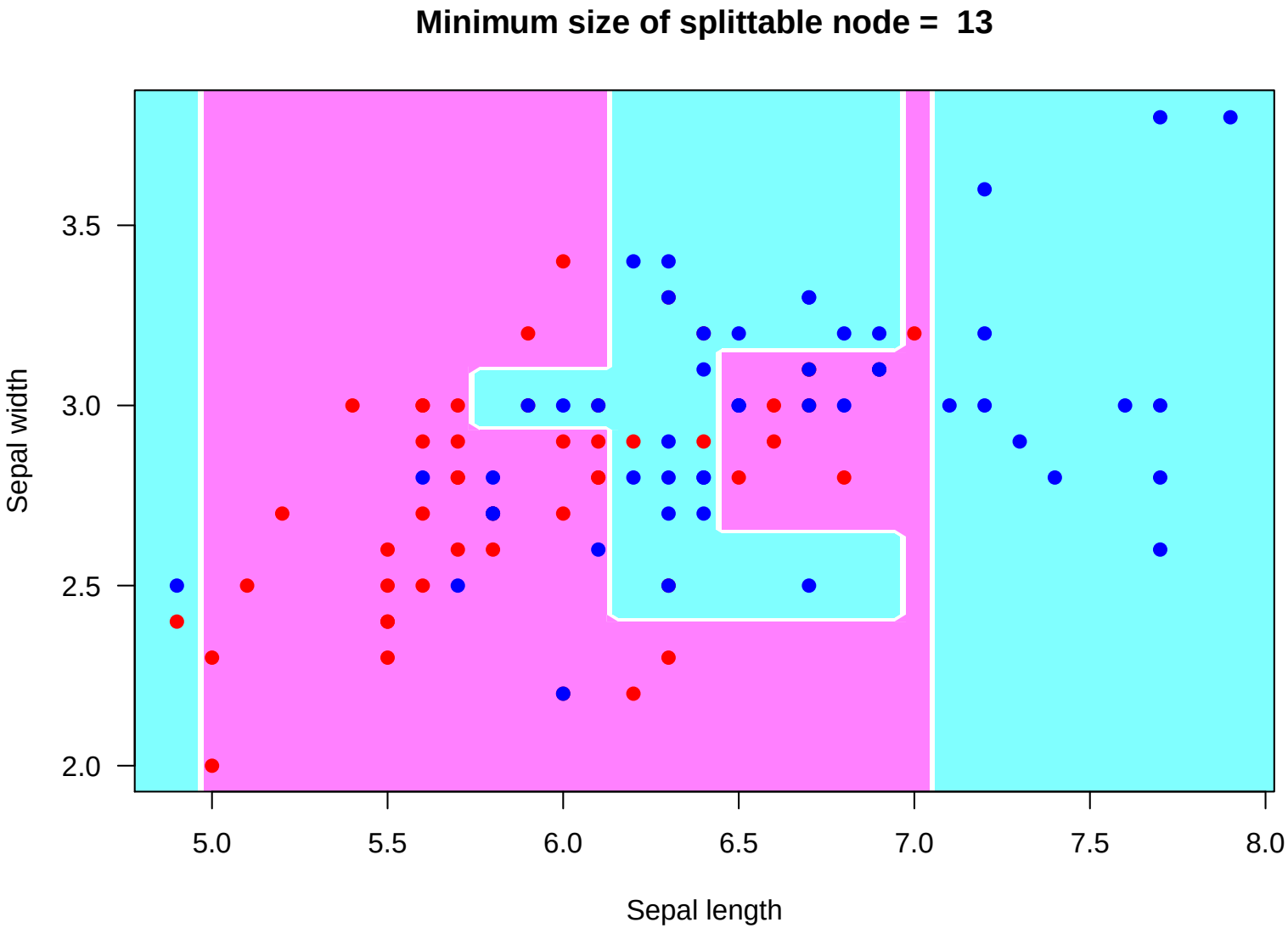

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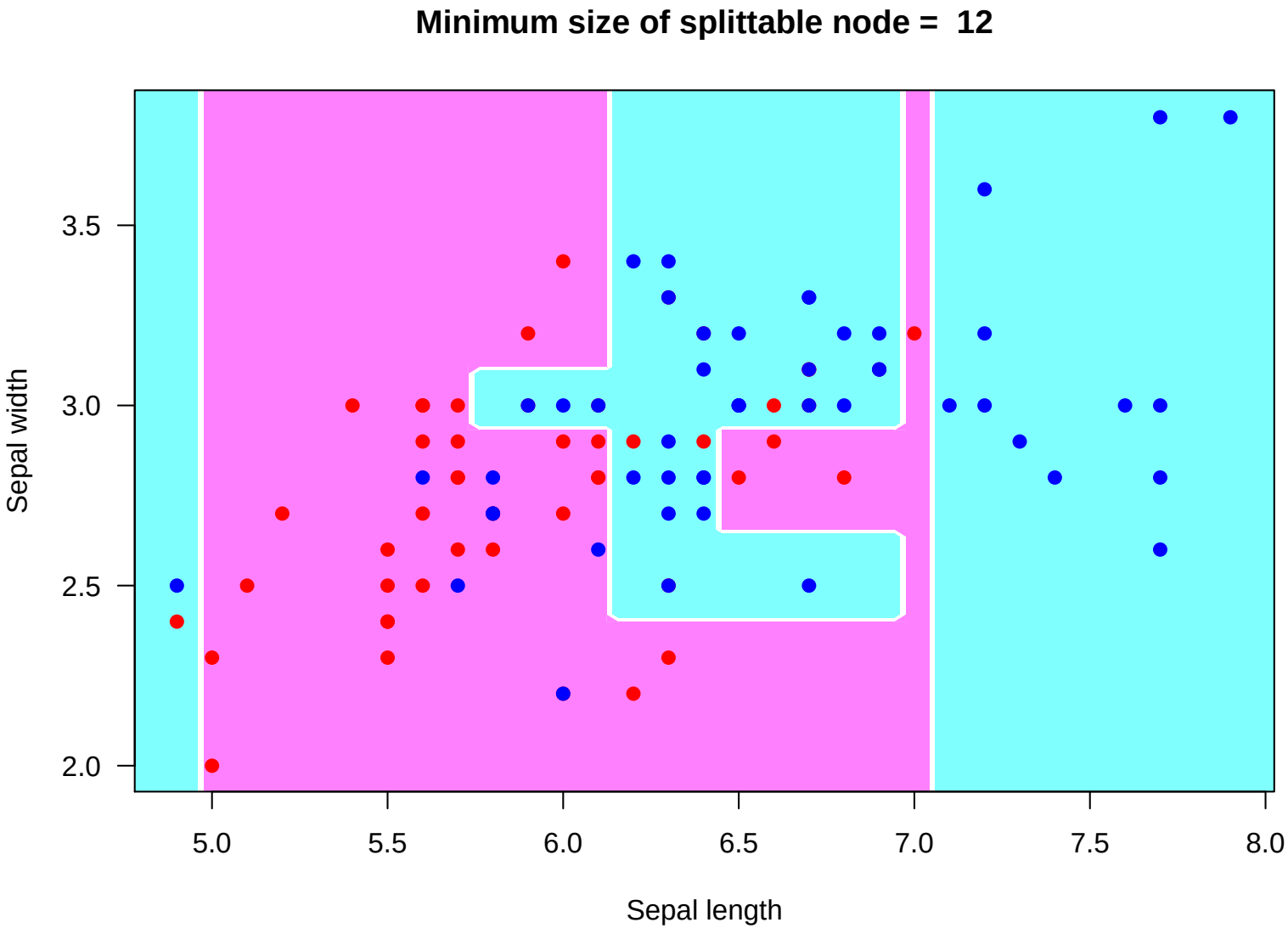

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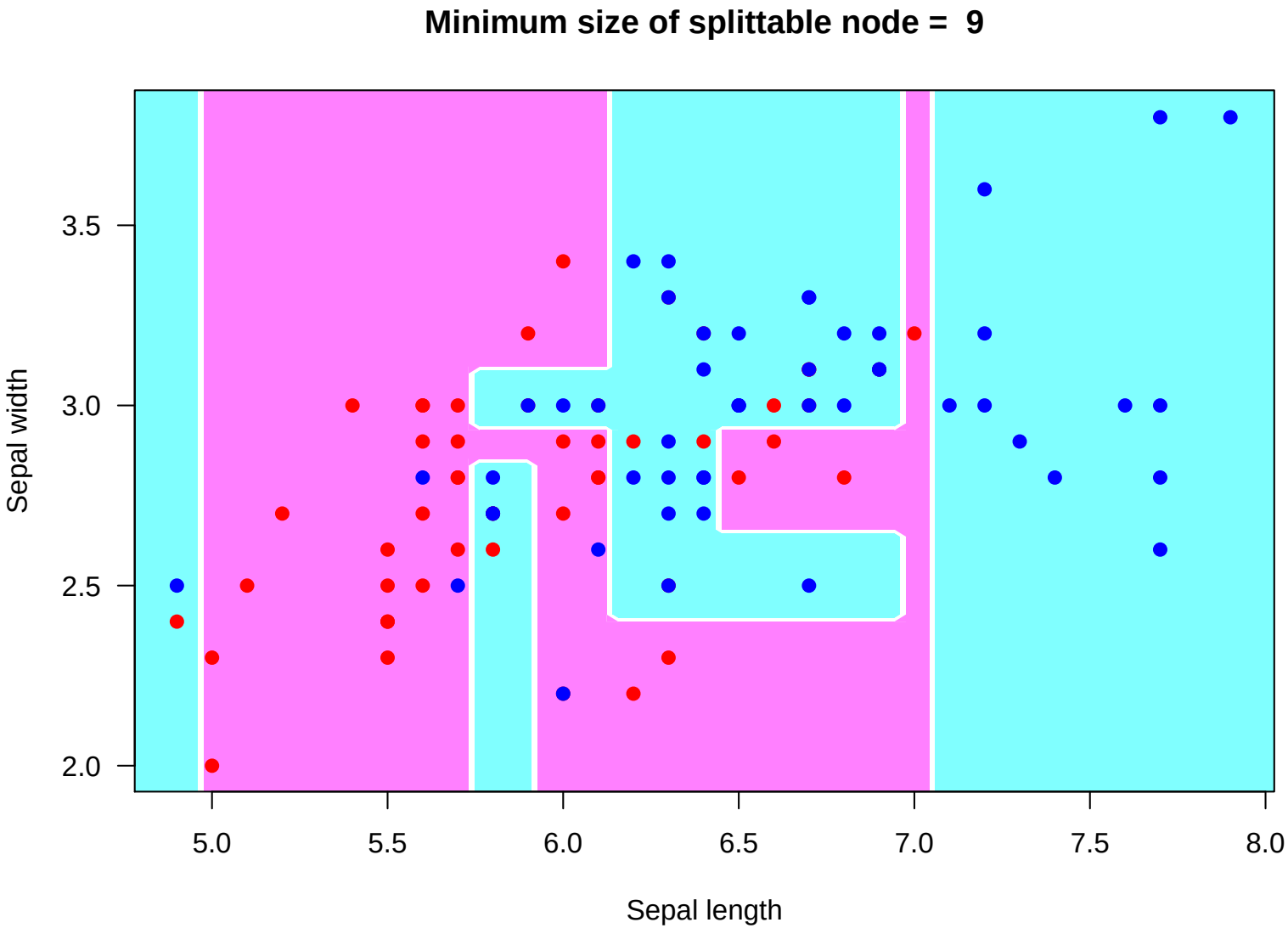

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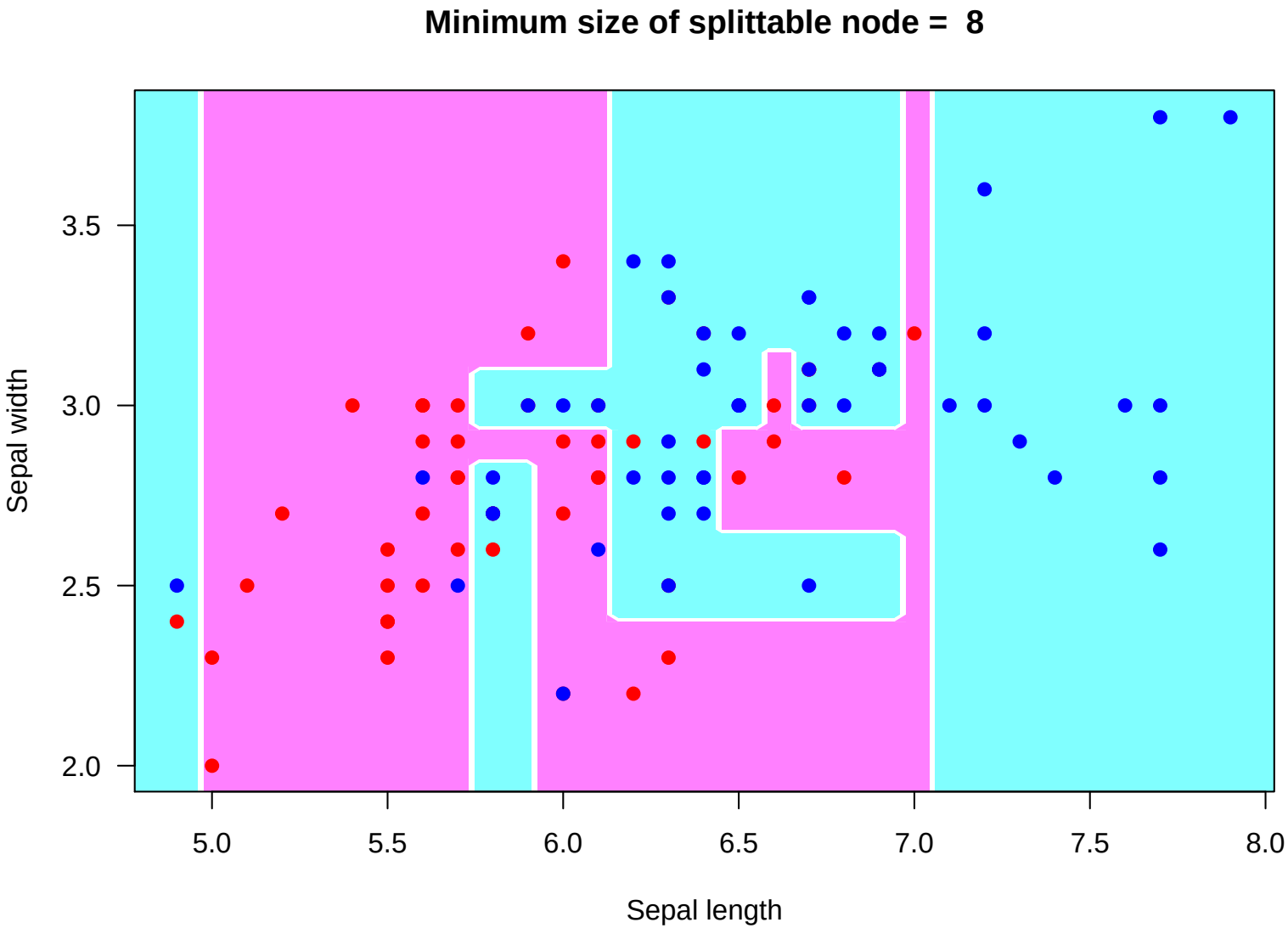

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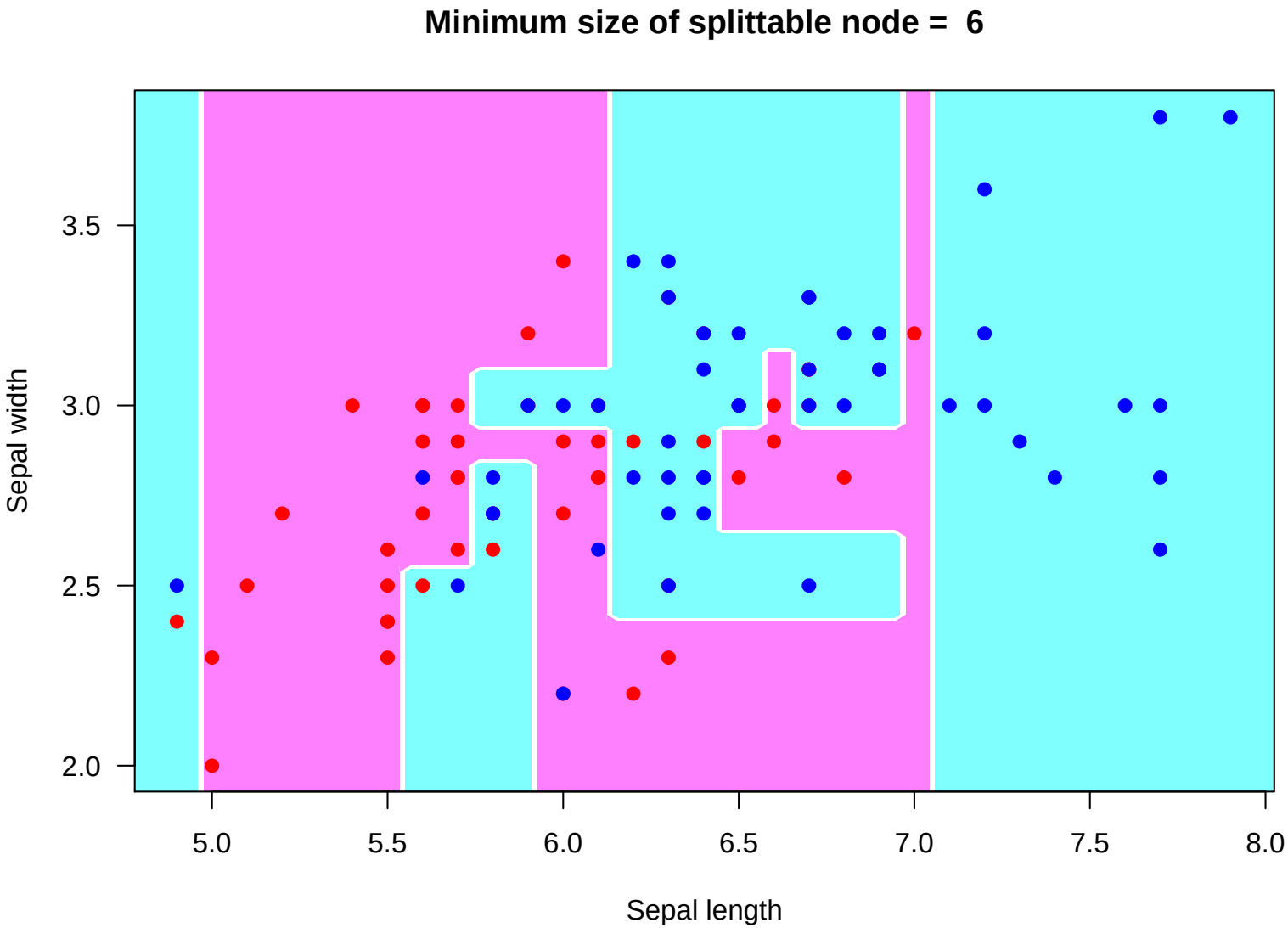

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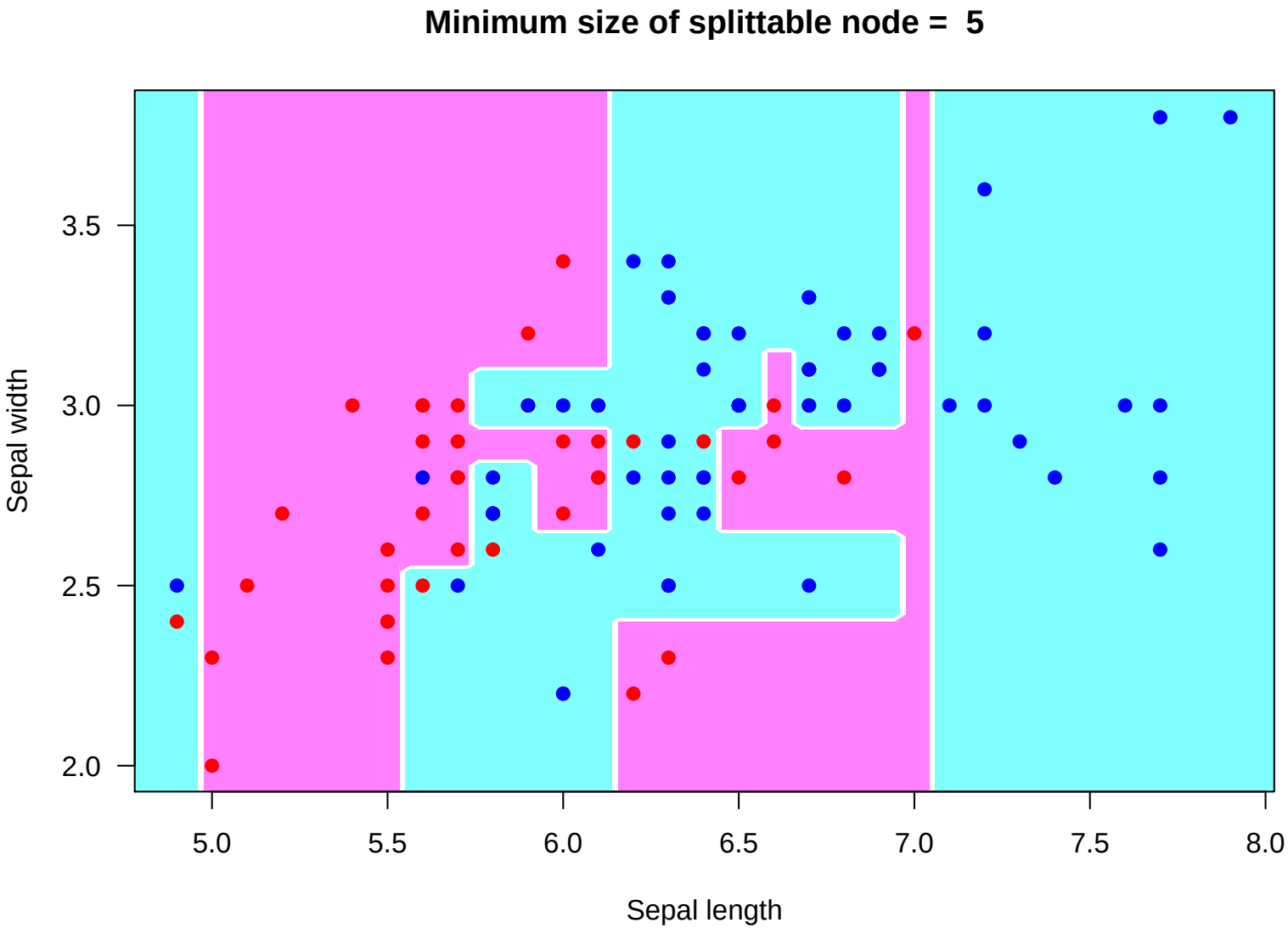

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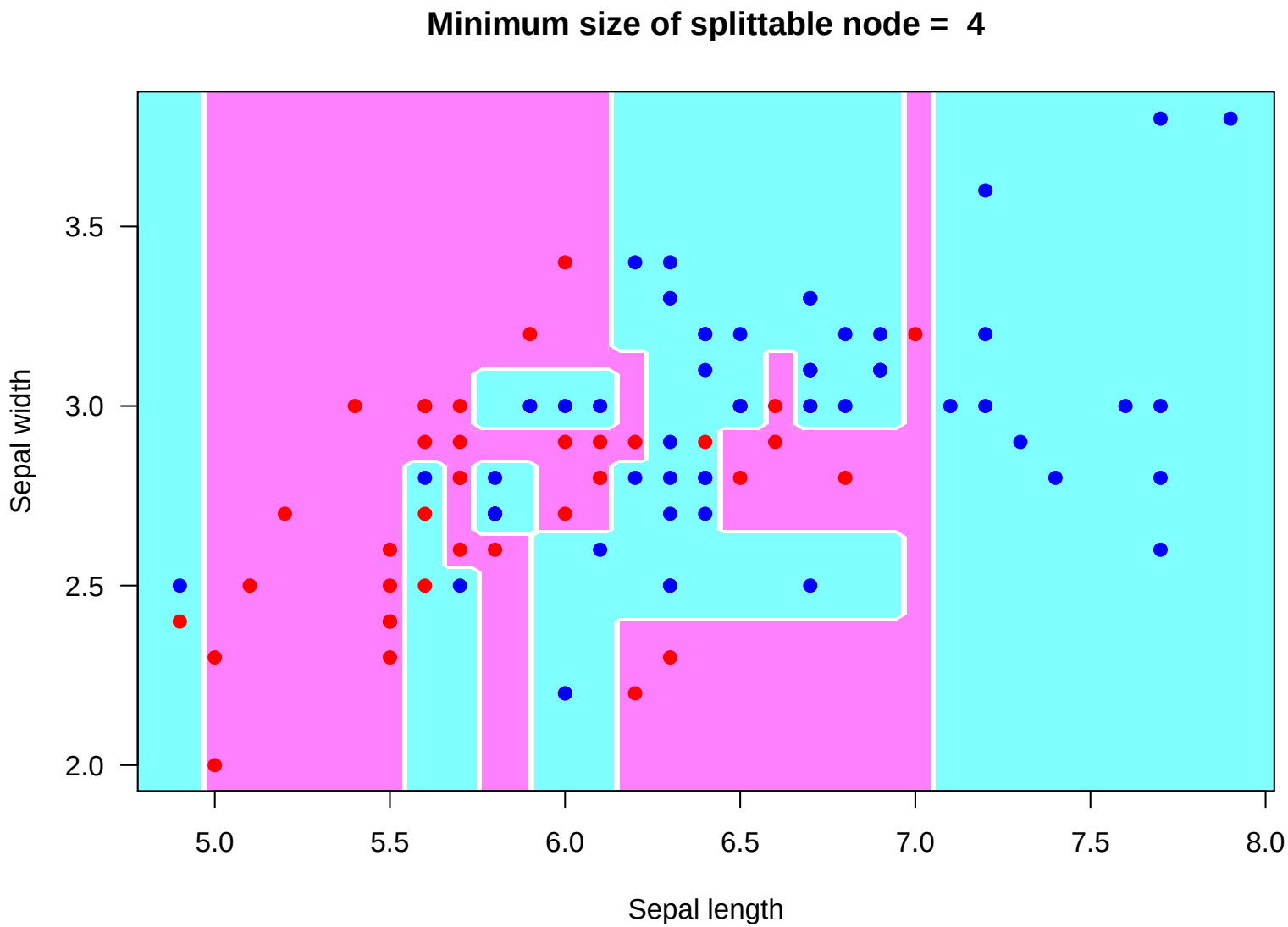

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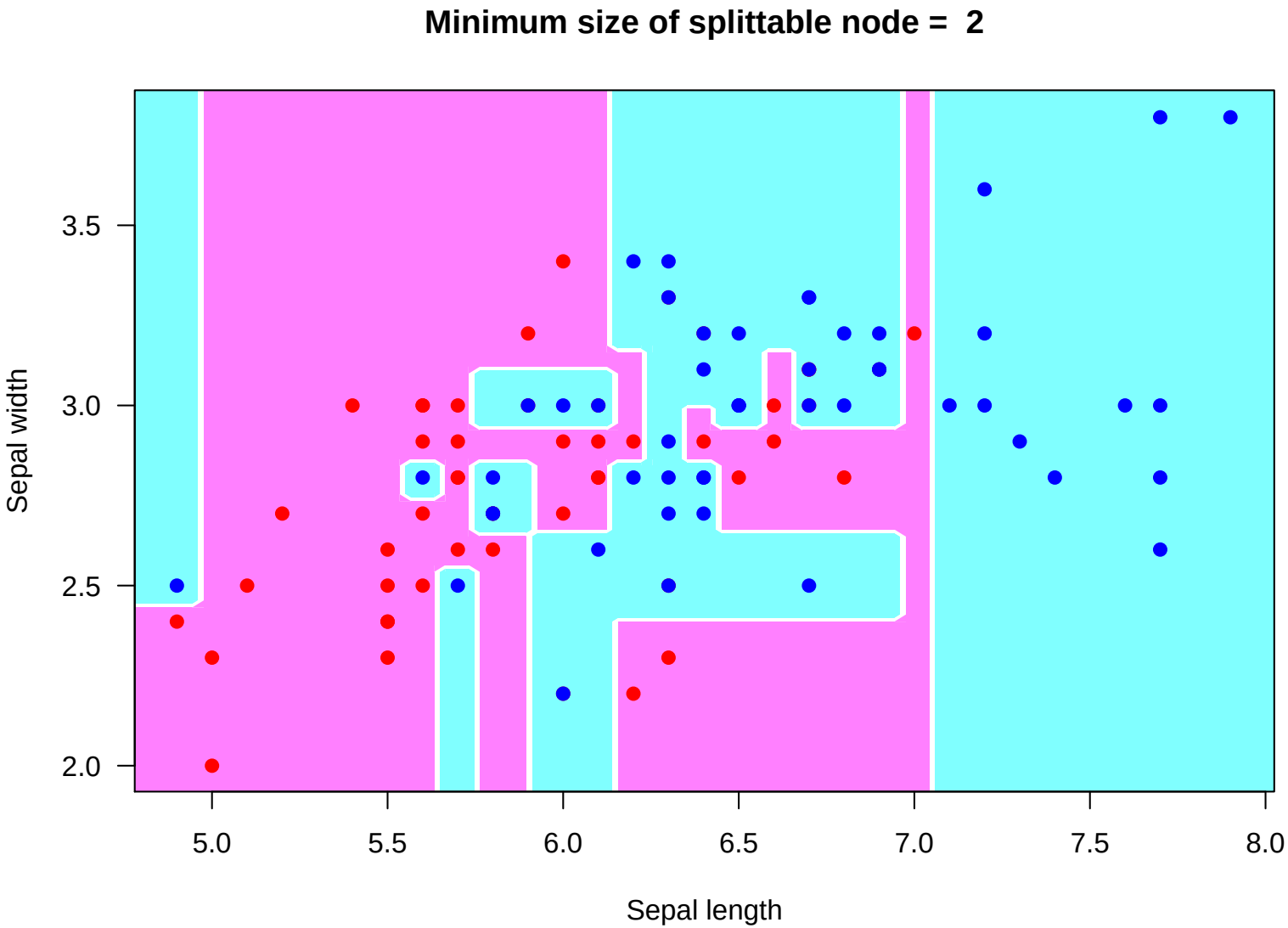

Contents

Classification tree
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Bagging
- Motivation
- Algorithm
- An example

Random forest
- Algorithm
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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}:

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

- Often the classification tree is constructed in two stages:
  1. n_{min} **is set very small** and the tree is grown to T_0.
  2. **Pruning** of tree (*i.e.*, collapsing any number of its non-terminal nodes) is conducted based on some parameter α, which consists in choosing a **subtree** $T \subset T_0$ that **minimizes** a **cost-complexity** criterion, *e.g.*

$$C_\alpha(T) = \sum_{m=1}^{\#T} n^{(m)} Q^{(m)}(T) + \alpha \#T ,$$

  where $\#T$ stands for the number of nodes in the tree.
  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

- To handle *predictors with unordered values* when the outcome is of 0-1 type, one can simply order the predictor classes according to the proportion falling in outcome class 1.

- To handle *missing predictor values* there are two recommended approaches
  - if the predictor is categorical, create a new category 'missing';
  - a more general approach is the construction of surrogate variables (see Hastie *et al.* (2009, section 9.2) for the details).

- 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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Classification tree
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Classification tree
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The key idea

- The "Wisdom of Crowds" (Surowiecki, 2004): The **collective knowledge** of a diverse and **independent** body of people typically exceeds the knowledge of any single individual, and can be harnessed by voting.

- **Bagging** implements this way of thinking standing for a range of methods following the general idea introduced by Léo Breiman (1996).

- **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).

Motivation (regression)

- Consider the standard regression setting

$$Y = g(X) + \epsilon.$$

- The single bagged estimator

$$\hat{g}_B(\mathbf{x}) = \frac{1}{B}\sum_{k=1}^{B} g_k(\mathbf{x})$$

  is the estimator of g obtained by aggregating estimators $g_1, ..., g_B$.

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

- 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**.

Bias and variance (regression)

- **Assumption (unfeasible):** Random variables $g_1, ..., g_B$ are i.i.d.

- **Bias:**

$$\mathbb{E}[\hat{g}_B(\mathbf{x})] = \mathbb{E}[g_k(\mathbf{x})]\,.$$

Conclusion

Aggregation does not modify the bias.

- **Variance:**

$$\mathbb{V}[\hat{g}_B(\mathbf{x})] = \frac{1}{B}\mathbb{V}[g_k(\mathbf{x})]\,.$$

Conclusion

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

Motivation (classification)

- Let $g_1, ..., g_B$ be an ensemble of **basic classifiers**.
- **Assumption:** Each basic classifier has an independent error $\epsilon < 0.5$ for predicting the correct decision $y = 1$ for some value $\mathbf{x}$:

$$\mathbb{P}\big(g_k(\mathbf{x}) \neq 1\big) = \epsilon < 0.5 \quad \text{for} \quad k = 1, ..., B\,,$$
$$g_1(\mathbf{x}), ..., g_B(\mathbf{x}) \quad \text{are still assumed } \textbf{i.i.d}\,.$$

- Further, let the aggregated classifier be

$$g^{agg}(\mathbf{x}) = \mathbb{1}\Big(\frac{1}{B}\sum_k g_k(\mathbf{x}) > 0.5\Big)\,.$$

- Then $\sum_k g_k(\mathbf{x})$ will have binomial distribution

$$\sum_k g_k(\mathbf{x}) \sim Bin(B, 1-\epsilon)$$

and classification error of $\mathbf{x}$ will decrease with increasing B:

$$\mathbb{P}\big(g^{agg}(\mathbf{x}) \neq 1\big) = \sum_{k=1}^{B/2} \binom{B}{k} (1-\epsilon)^k \epsilon^{B-k} \xrightarrow[B\to\infty]{} 0\,.$$

Motivation (classification)

Theorem (Chernoff-Hoeffding, Bernoulli scheme)

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

$$\mathbb{P}\Big(\mathbb{E}[X_i] - \frac{1}{n}\sum_{i=1}^{n} X_i > \eta\Big) < \exp(-2\eta^2 n)\,.$$

One can express classification error as

$$\mathbb{P}\big(g^{agg}(\mathbf{x}) \neq 1\big) = \mathbb{P}\Big(\frac{1}{B}\sum_{k=1}^{B} g_k(\mathbf{x}) < 0.5\Big)\,.$$

By a sequence of simple transformations we obtain

$$\underbrace{(1-\epsilon)}_{\mathbb{E}[g_1(\mathbf{x})]} - \frac{1}{B}\sum_{k=1}^{B} g_k(\mathbf{x}) > 0.5 - \epsilon\,.$$

Applying the Chernoff-Hoeffding inequality gives

$$\mathbb{P}\big(g^{agg}(\mathbf{x}) \neq 1\big) < \exp\Big(-\frac{1}{2}B(1-2\epsilon)^2\Big)\,.$$

Motivation

- The derivations from above exploit the **assumption** that random variables $g_1(\mathbf{x}), ..., g_B(\mathbf{x})$ are **independent and identically distributed**.

- As the classifiers $g_1, ..., g_B$ are constructed using the same training sample $\mathcal{D}_n$, the assumption of **independence** is not really credible.

- **Remark:** If the variables $g_1, \ldots, g_B$ identically distributed with variance σ^2, but not necessarily independent, with positive pairwise correlation ρ, then

$$\mathbb{V}\left[\frac{1}{B}\sum_{k=1}^{B} g_k\right] = \rho\sigma^2 + \frac{1-\rho}{B}\sigma^2 \,.$$

- The idea is thus to **introduce a source of randomness** into the sample used to train each single classifier g_k , $k = 1, ..., B$ to render the pairwise correlation of the g_k's as small as possible.

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

Contents

Classification tree
- Algorithm
- Tuning

Bagging
- Motivation
- Algorithm
- An example

Random forest
- Algorithm
- Interpretation
- Consistency results

Bagging (algorithm)

Training

Input:

- Training sample $\big((\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\big) = \mathcal{D}_n \in \mathbb{R}^d \times \{0, 1\}$.
- Basic classifier $g(\cdot)$.
- Number of estimators to aggregate B.

For $k = 1, ..., B$

1. Draw a sample $\mathcal{D}^*_{n,k}$ from $\mathcal{D}_n$ using bootstrap.
2. Learn g^*_k on $\mathcal{D}^*_{n,k}$.

Output: The aggregated classifier $g^{agg}(\cdot) = \mathbb{1}\Big(\frac{1}{B}\sum_{k=1}^{B} g^*_k(\cdot) > 0.5\Big)$.

Classification

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

$$g^{agg}(\mathbf{x}) = \mathbb{1}\left(\frac{1}{B}\sum_{k=1}^{B} g^*_k(\mathbf{x}) > 0.5\right).$$

Drawing bootstrap samples

- **Bootstrap** is a technique based on random sampling, which allows for estimating the sampling distribution of almost any statistics.
- Bootstrap drawings are represented by B random variables θ_k, $k = 1, ..., B$.
- In general for the sample consisting of n observations, two techniques are used to draw bootstrap samples:
  - draw (choose randomly) n **observations with replacements**,
  - draw (choose randomly) $l < n$ **observations without replacement**.
- Thus aggregated classifiers contain two sources of randomness:
  - due to the $\mathcal{D}_n$ being a random draw from distribution of (X, Y),
  - due to the bootstrap drawing.

Choice of the parameters

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

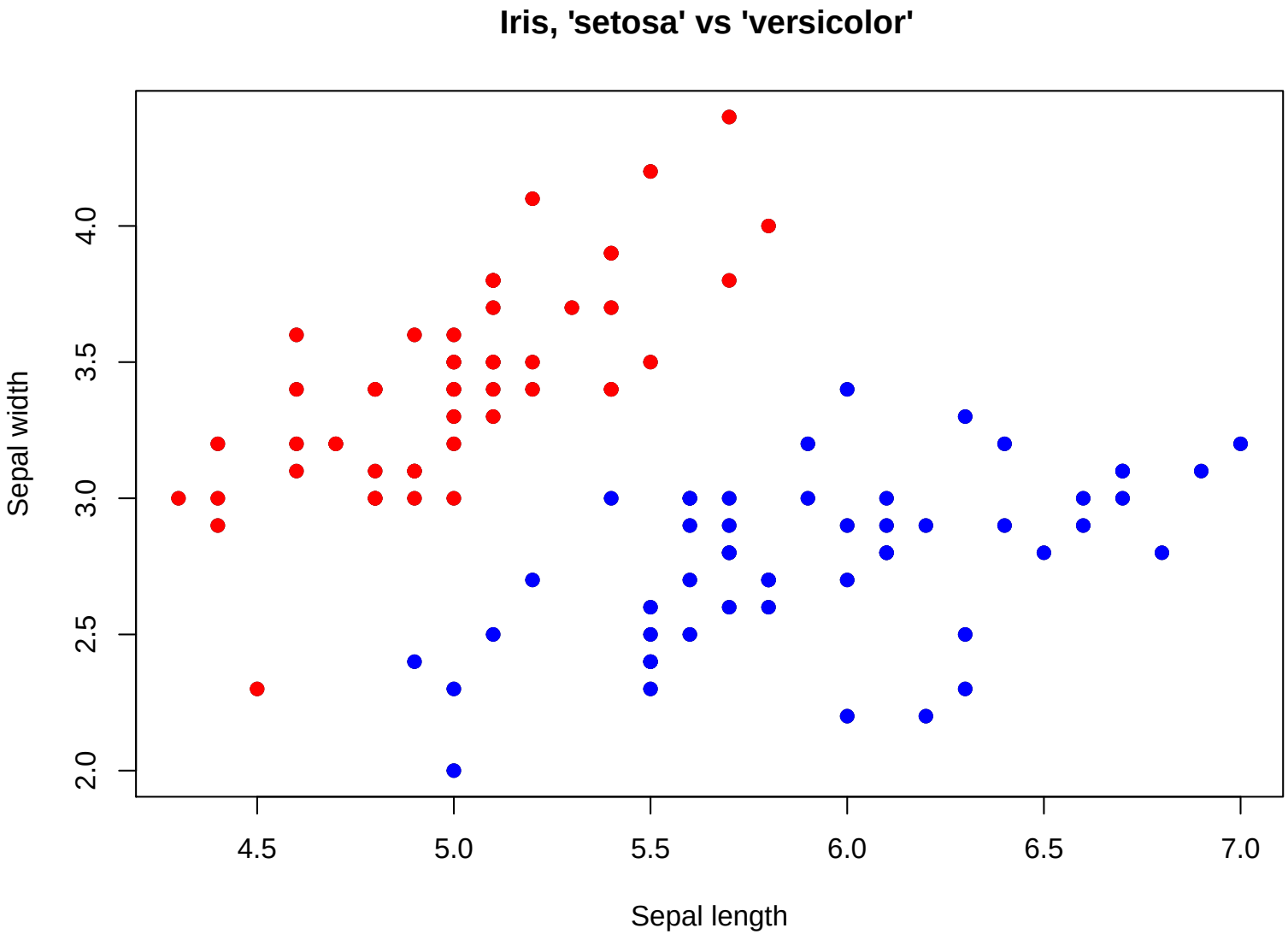
- Under suitable conditions, given the original sample $\mathcal{D}_n$, by the law of large numbers we have, almost surely

$$\begin{aligned}
\lim_{B\to\infty} g^{agg}(\mathbf{x}) &= \lim_{B\to\infty} \mathbb{1}\Big(\frac{1}{B}\sum_{k=1}^{B} g_k^*(\mathbf{x}) > 0.5\Big) \\
&= \mathbb{1}\Big(\lim_{B\to\infty} \frac{1}{B}\sum_{k=1}^{B} g_k^*(\mathbf{x}) > 0.5\Big) \\
&= \mathbb{1}\big(\mathbb{E}^*[g_k^*(\mathbf{x}) \mid \mathcal{D}_n] > 0.5\big)\,.
\end{aligned}$$

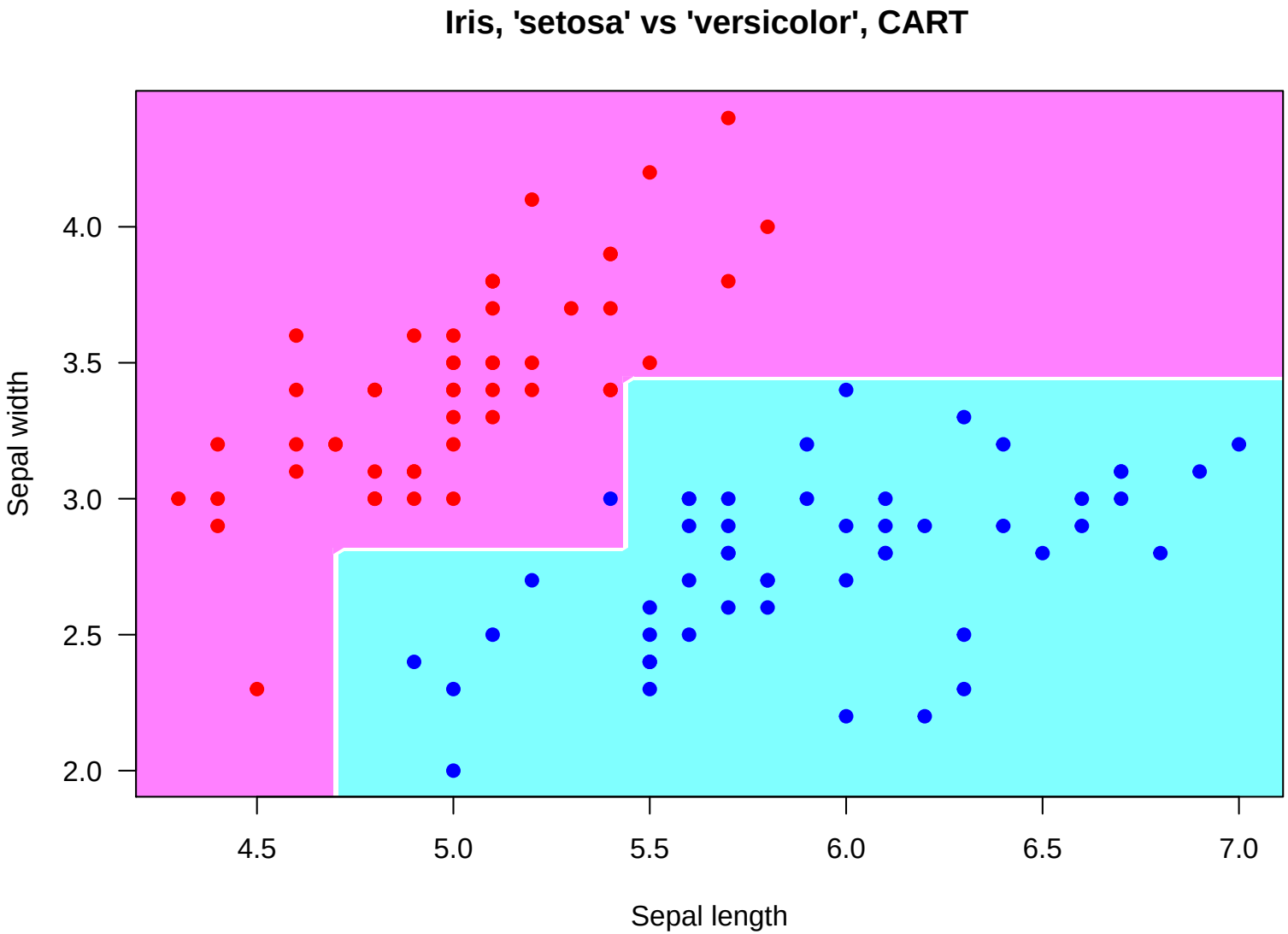
- So $g^{agg}(\mathbf{x})$ stabilizes with increasing B converging to the **bagging estimator** $\mathbb{1}\big(\mathbb{E}^*[g_k^*(\mathbf{x}) \mid \mathcal{D}_n] > 0.5\big)$.

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

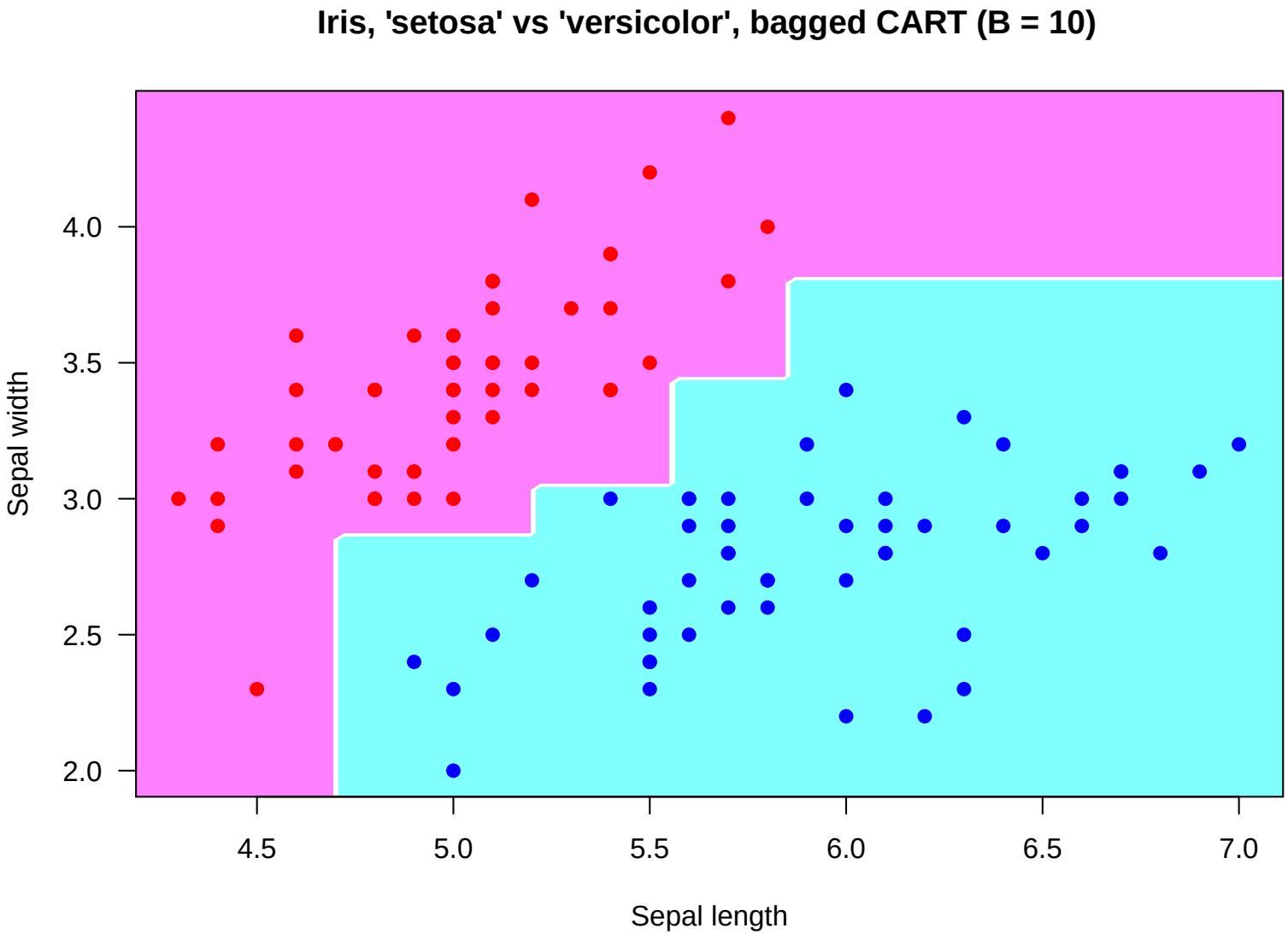
Bagging classification tree: iris data



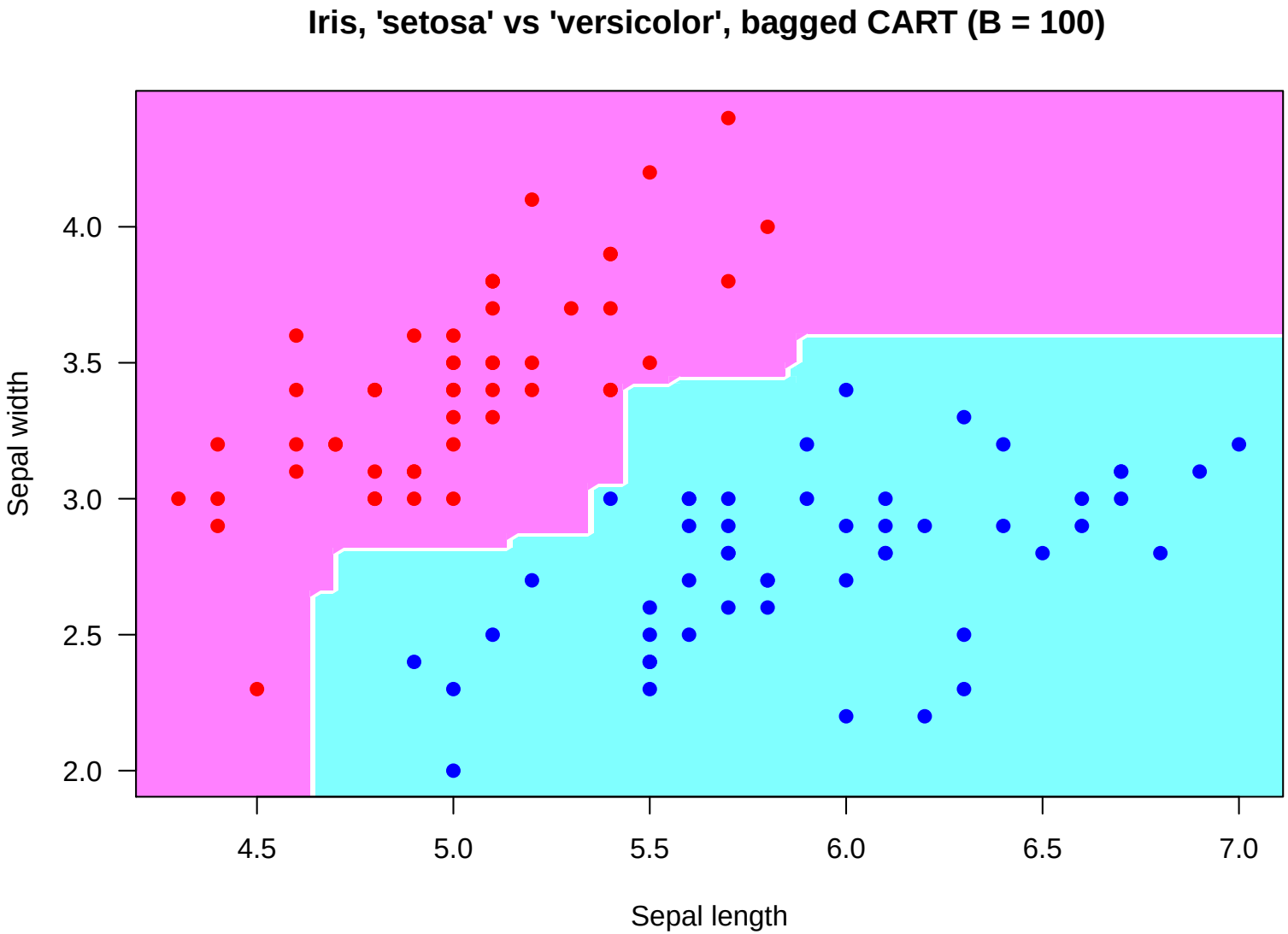
Bagging classification tree: iris data



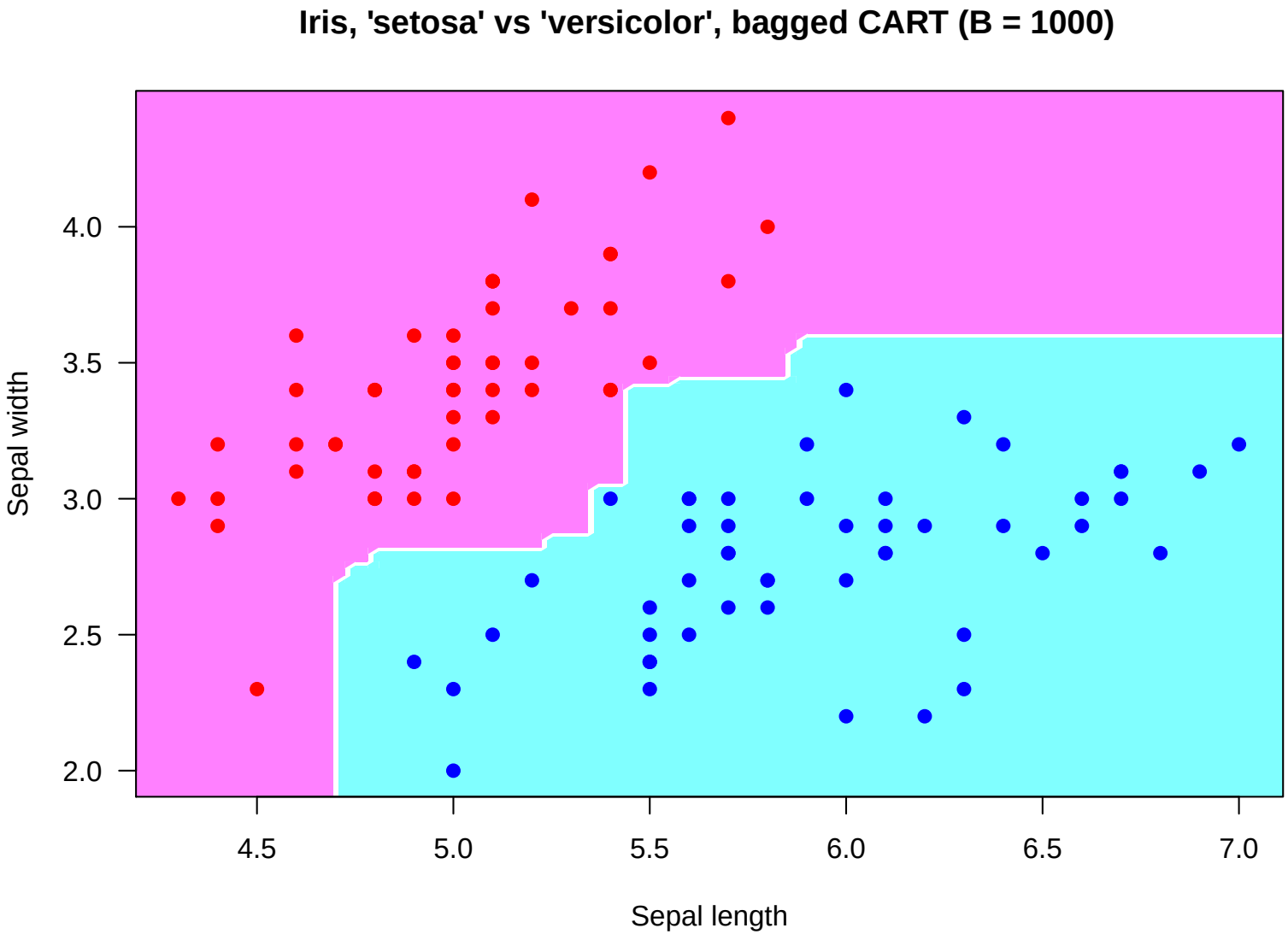
Bagging classification tree: iris data



Bagging classification tree: iris data



Bagging classification tree: iris data



Properties and recommendations

- Bagging a good classifier can make it better, bagging a bad classifier can make it worse.
- Significant improvement by bagging is not expected on large data sets because there bootstrap samples are very similar. Subsampling is expected to improve things.
- Bagging could be improved by using a robust location estimator instead a mean over the B bootstrapped classifiers. Taking the median yields the so-called *bragging* (Buhlmann, 2003). Trimmed means is another option.
- Bagging reduces interpretability of the classifier because any simple structure in the model is lost.

Contents

Classification tree
- Algorithm
- Tuning

Bagging
- Motivation
- Algorithm
- An example

Random forest
- Algorithm
- Interpretation
- Consistency results

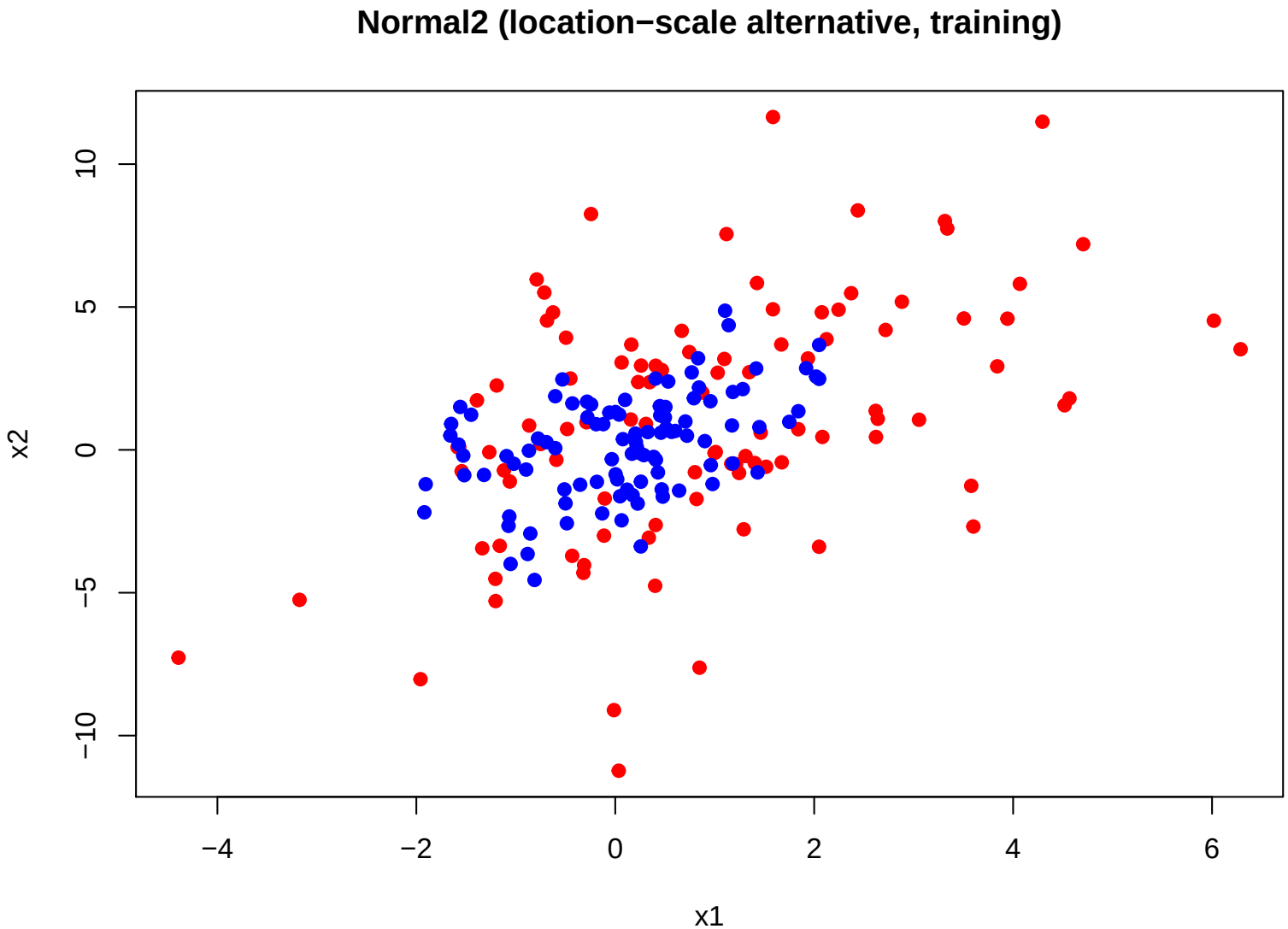
Normal2 data generation

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

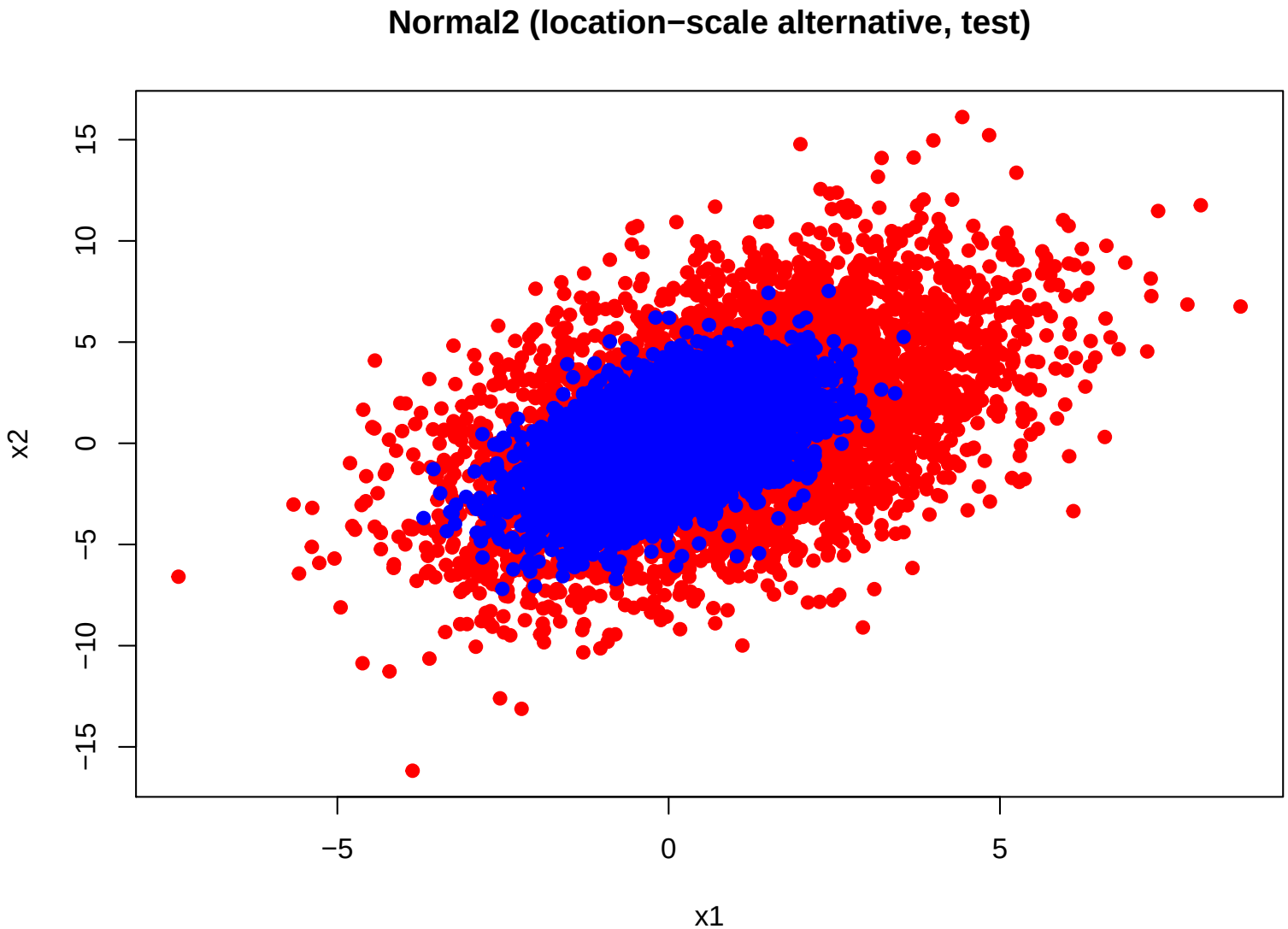
$$\Sigma = \begin{pmatrix} 1 & 1 \\ 1 & 4 \end{pmatrix}$$

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

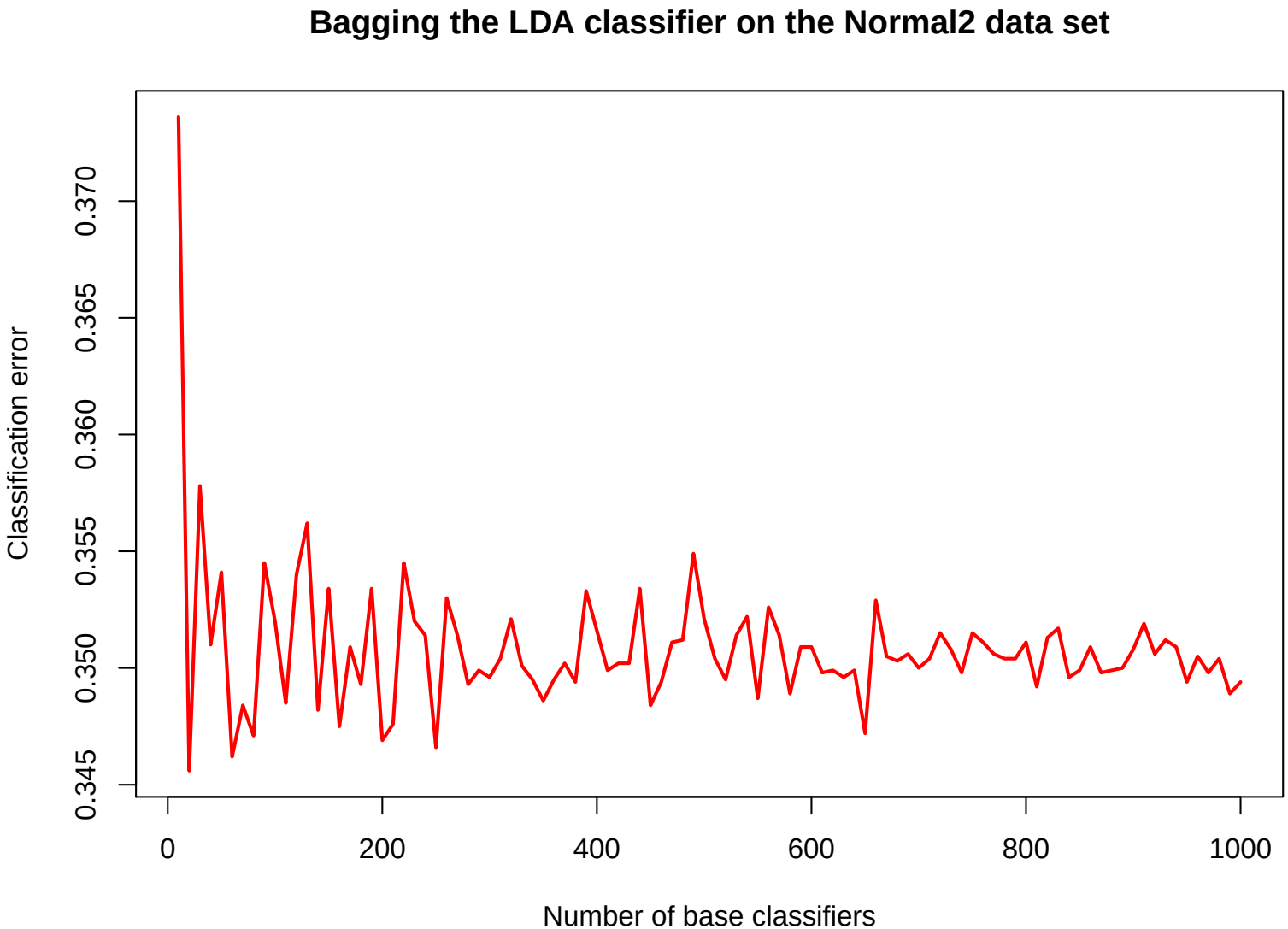
Normal2 data



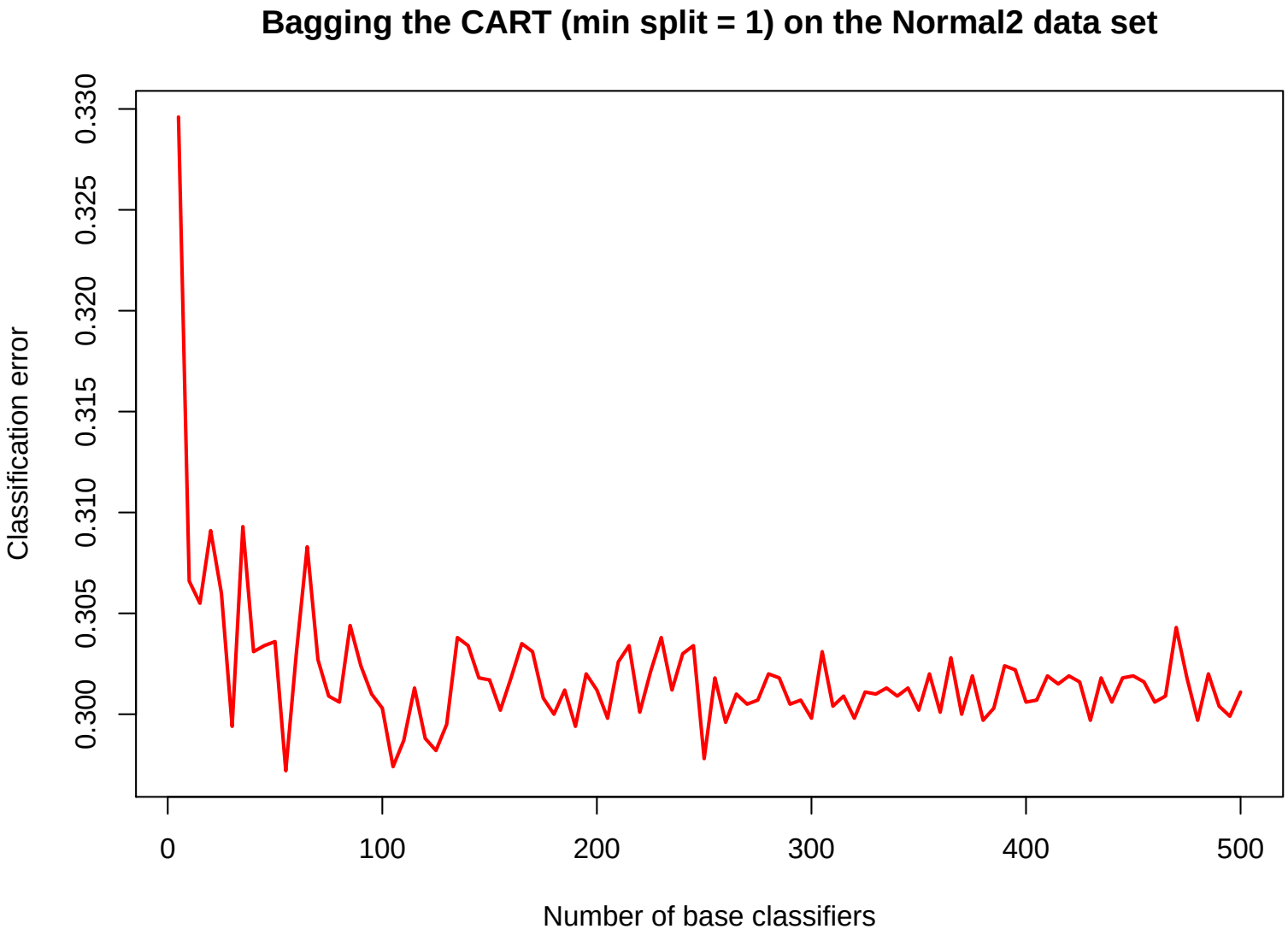
Normal2 data



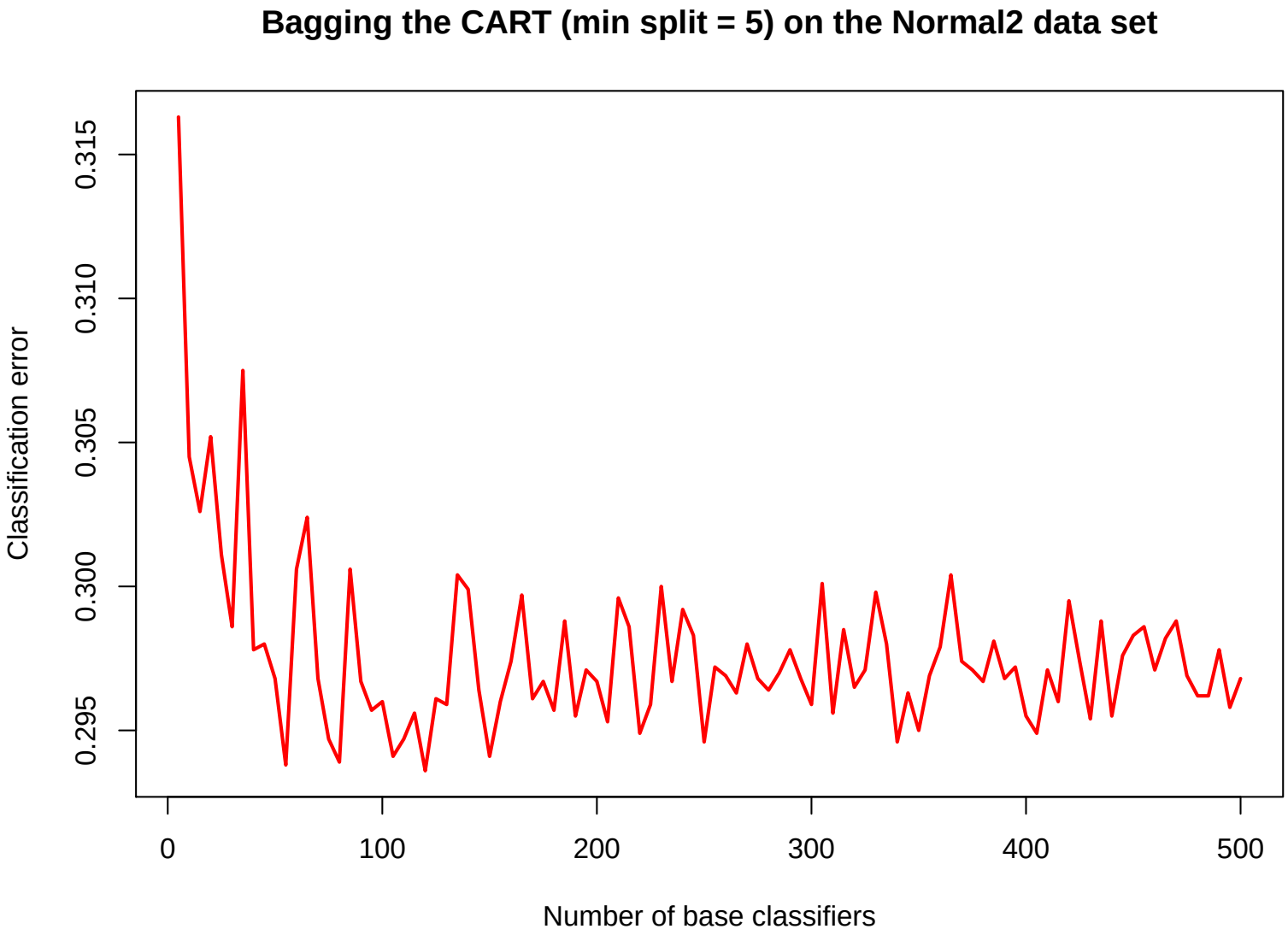
Bagging LDA: Normal2 data



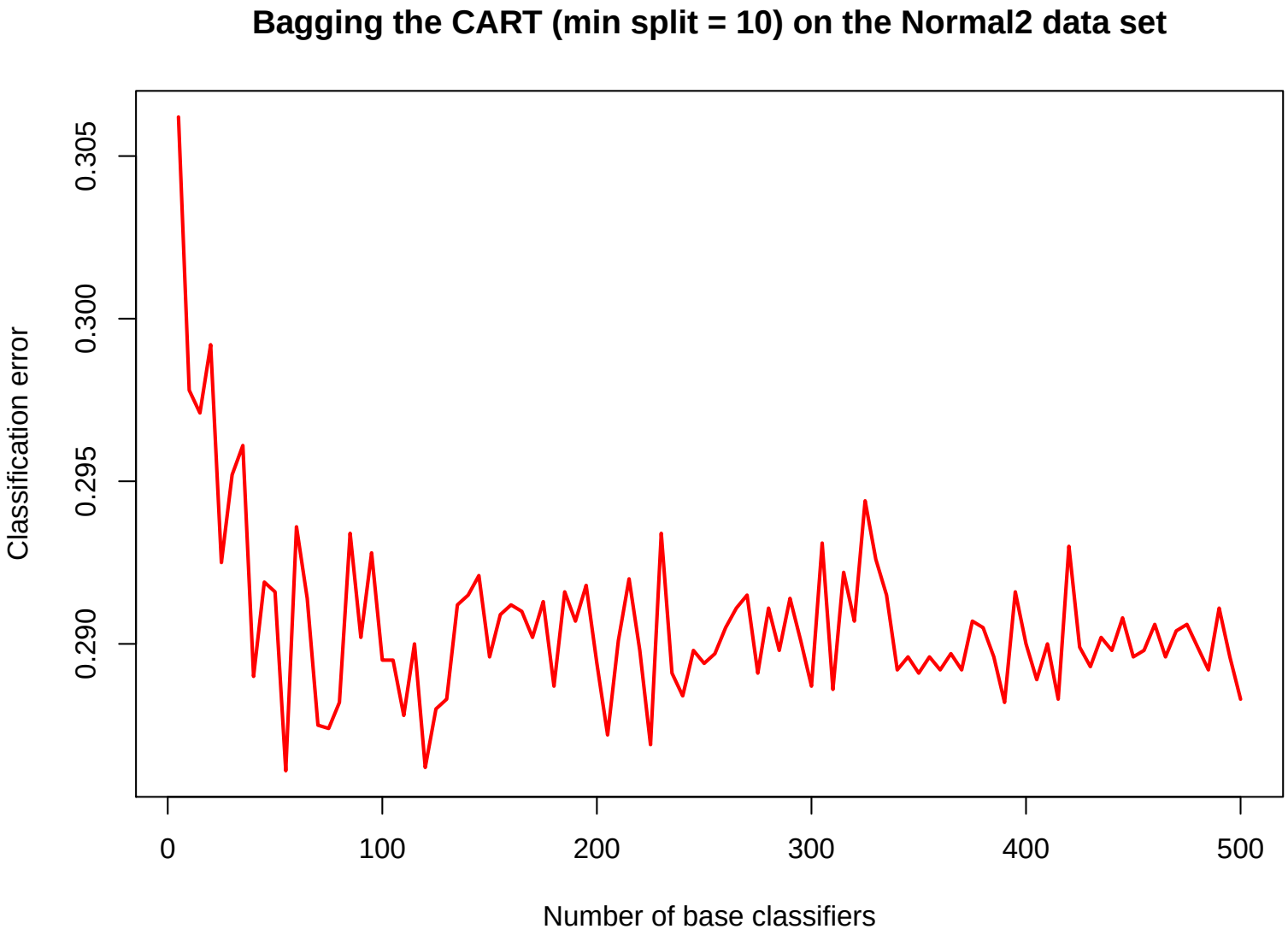
Bagging classification tree: Normal2 data



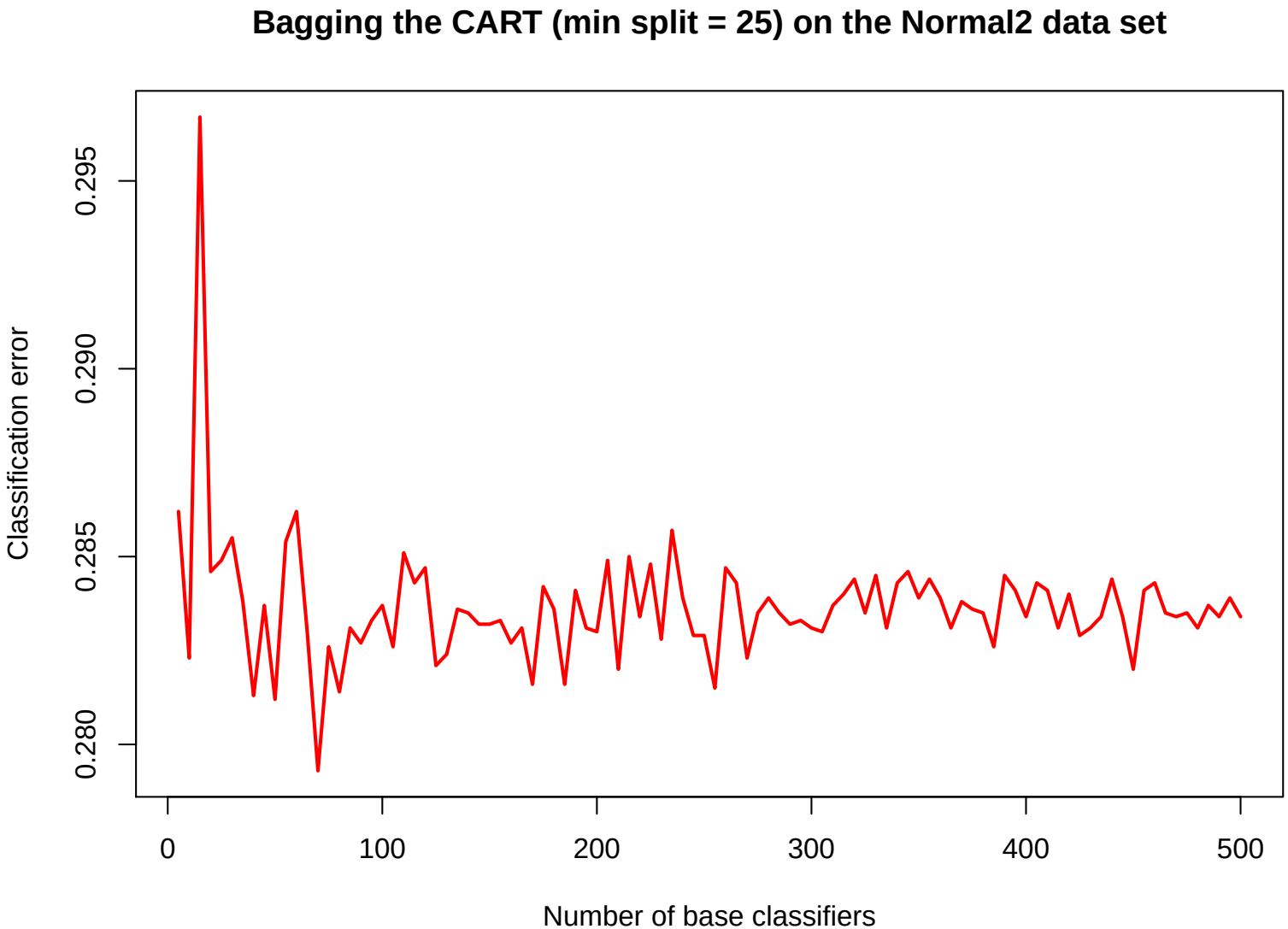
Bagging classification tree: Normal2 data



Bagging classification tree: Normal2 data



Bagging classification tree: Normal2 data



Contents

Classification tree
- Algorithm
- Tuning

Bagging
- Motivation
- Algorithm
- An example

Random forest
- Algorithm
- Interpretation
- Consistency results

Contents

Classification tree
- Algorithm
- Tuning

Bagging
- Motivation
- Algorithm
- An example

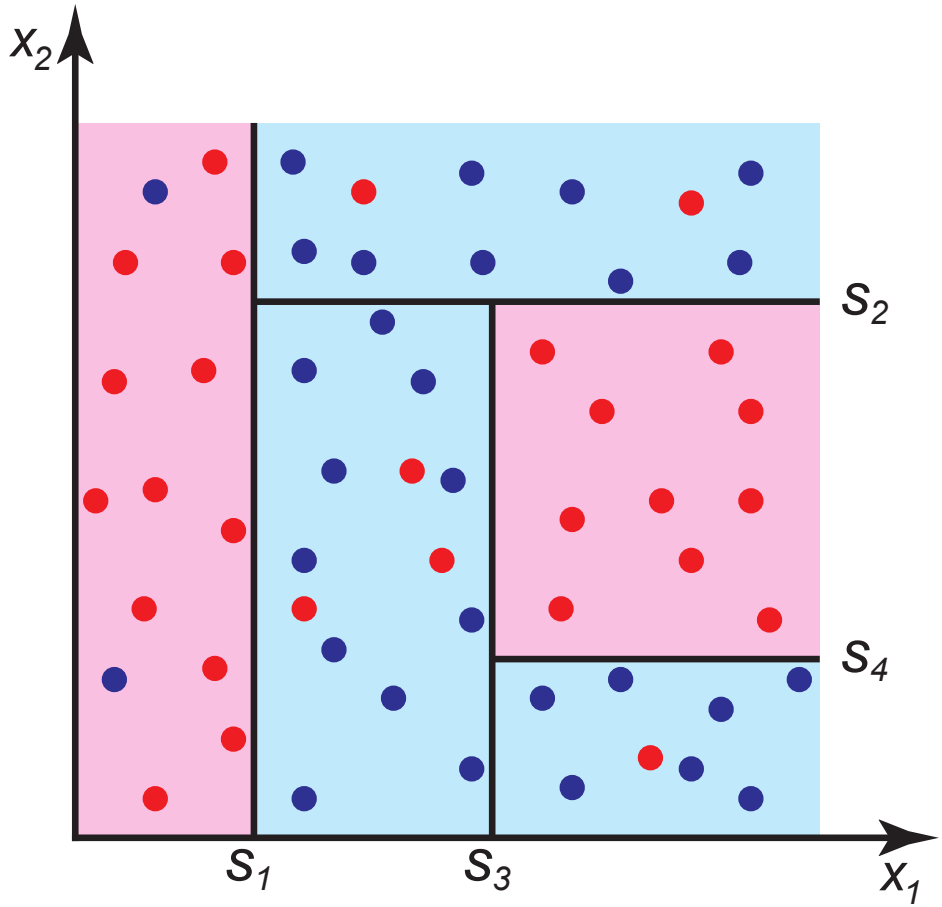
Random forest
- Algorithm
- Interpretation
- Consistency results

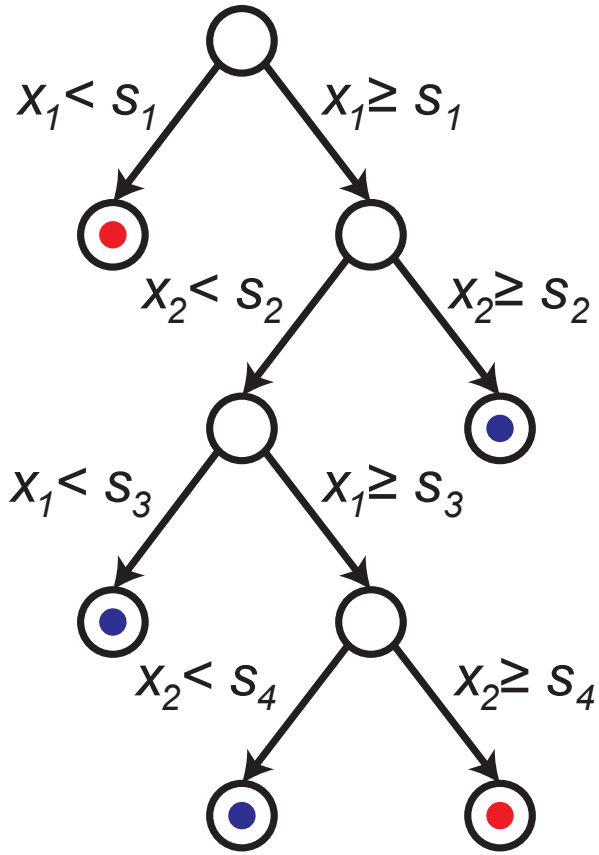
The key idea

- Random forest is a **collection of trees**.
- Random forests have been introduced by **Léo Breiman** in the early 2000s. The following web-page is dedicated to random forests: `http://www.stat.berkeley.edu/~breiman/RandomForests/`
- Random forests can be seen as a **modified version of bagging** as they also aggregate trees taught on the bootstrap samples.
- 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:

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

The key idea





- **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 $\big((\mathbf{x}_1, y_1), ..., (\mathbf{x}_n, y_n)\big) = \mathcal{D}_n \in \mathbb{R}^d \times \{0, 1\}$.
- Number of trees B; minimum number of observations for a node to be split n_{min}; impurity criterion Q.
- number of variables to use when splitting $m \in \{1, ..., d\}$.

For $k = 1, ..., B$

1. Draw a sample $\mathcal{D}^*_{n,k}$ from $\mathcal{D}_n$ using bootstrap.
2. Learn the classification tree T^*_k on $\mathcal{D}^*_{n,k}$; each time when splitting a node, search optimal variable among m variables randomly chosen out of all d variables.

Output: The aggregated classifier $T^{RF}(\cdot) = \mathbb{1}\Big(\frac{1}{B}\sum_{k=1}^{B} T^*_k(\cdot) > 0.5\Big)$.

Classification

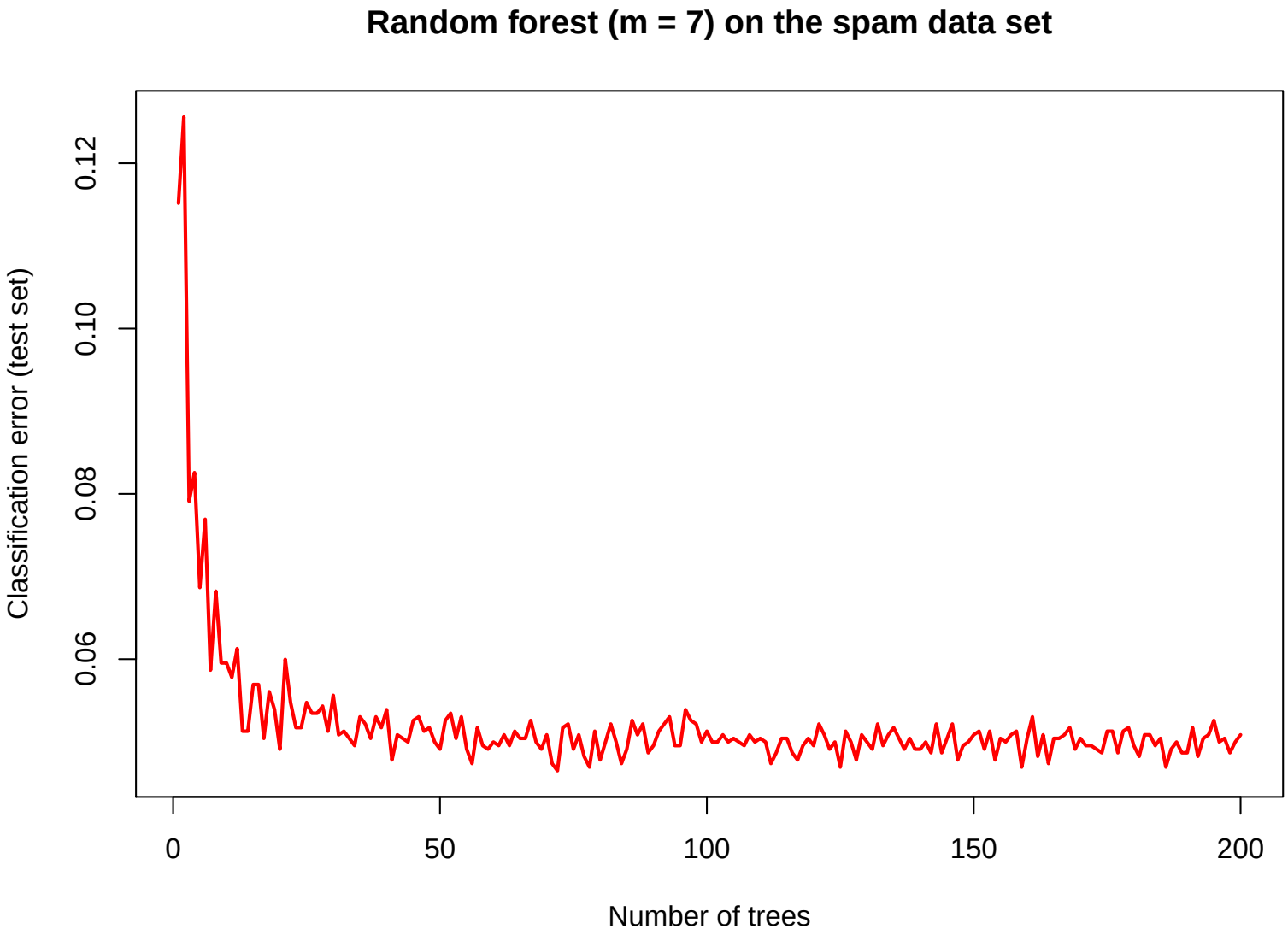
- Classify the new observation $\mathbf{x}$ as

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

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



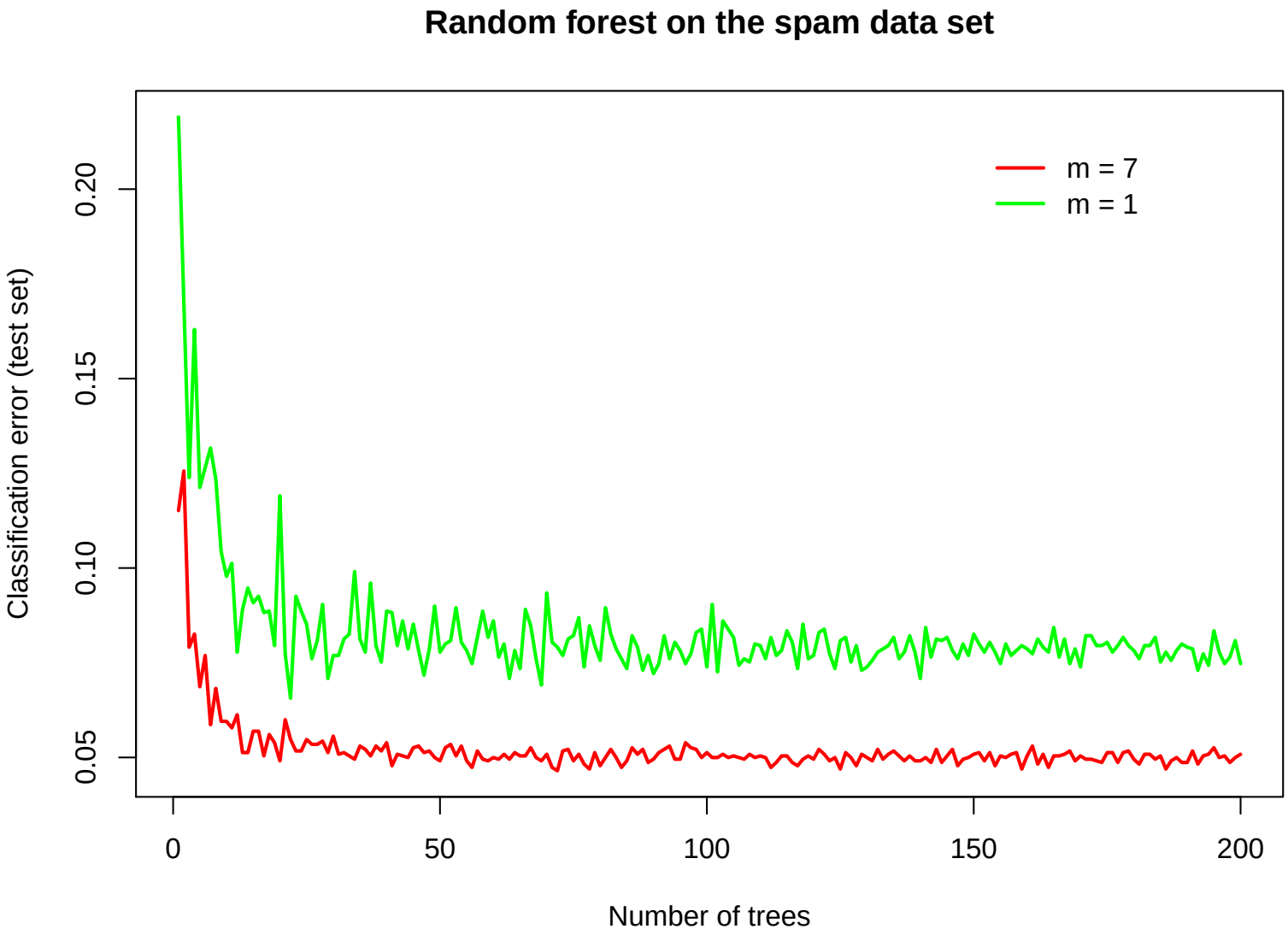
Properties

- There are **two** introduced **sources of randomness**:
  - B **bootstrap samples**,
  - m **variables randomly chosen** out of d when splitting each tree node.
- The method is simple, implementations are available in numerous software, *e.g.* `R`-package `randomForest`.
- The classifier is known for relatively **high speed** of training and classification.
- The classifier is known for its relatively **precise prediction on complex data**, *i.e.* those including many variables, missing entries, *etc*.
- Classifier has **limited sensibility w.r.t. to the choice of parameters**: B, m, n_{min}.

Choice of number m of variables for a node

- Parameter m is related to the **dependence between** single **trees**.
- The **lower** is m:
  - to larger extent the variables at which to split each node **are chosen randomly**,
    thus the more **different** are single **trees**,
    thus the more **independent** are single **trees**,
  - the **lower** is the **prediction accuracy of** each single **tree**,
    and thus of the entire forest as well.
- The **higher** is m: *vice versa*.
- It is recommended to check the performance of the random forests for **different choices of** m.
- The **inventors recommend** $m = \lfloor \sqrt{d} \rfloor$
  (the default value in `R`-package `randomForest`).

Random forests: spam data



Contents

Classification tree
- Algorithm
- Tuning

Bagging
- Motivation
- Algorithm
- An example

Random forest
- Algorithm
- Interpretation
- Consistency results

Performance and interpretation

- It is desirable to measure the performance of the random forests, as of any other classification technique, in terms of the error probability:

$$R(T^{RF}) = \mathbb{P}\left(T^{RF}(X) \neq Y\right).$$

- As usual, the error can be measured:
  - For a **probability distribution**: by a **simulation study**, *i.e.* train T^{RF} and measure its classification error for a number of simulated data sets.
  - For **given data**: by **splitting data** into training and test subsets, by **iterating this splitting** if data are small, or by **cross-validation**.
- 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**.

Out-of-bag error

- For each pair $(\mathbf{x}_i, y_i)$ from $\mathcal{D}_n$, let I_i be the **set of indices of trees** whose bootstrap samples $\mathcal{D}_n^*$ **do not contain this observation**.

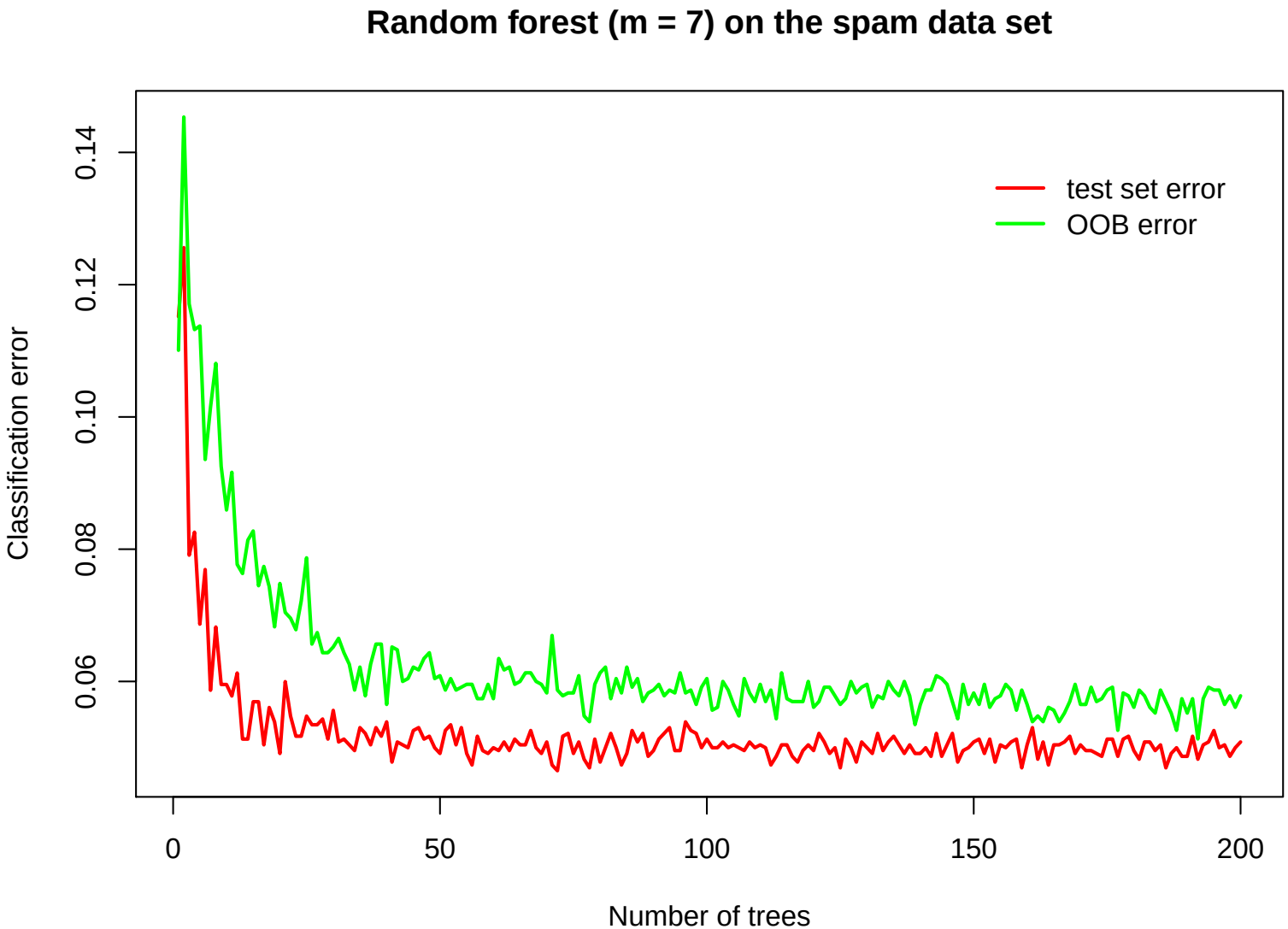
- By these trees, observation $\mathbf{x}_i$ is then classified as

$$\hat{y}_i = \frac{1}{\#I_i} \sum_{k \in I_i} T_k^*(\mathbf{x}_i) \,.$$

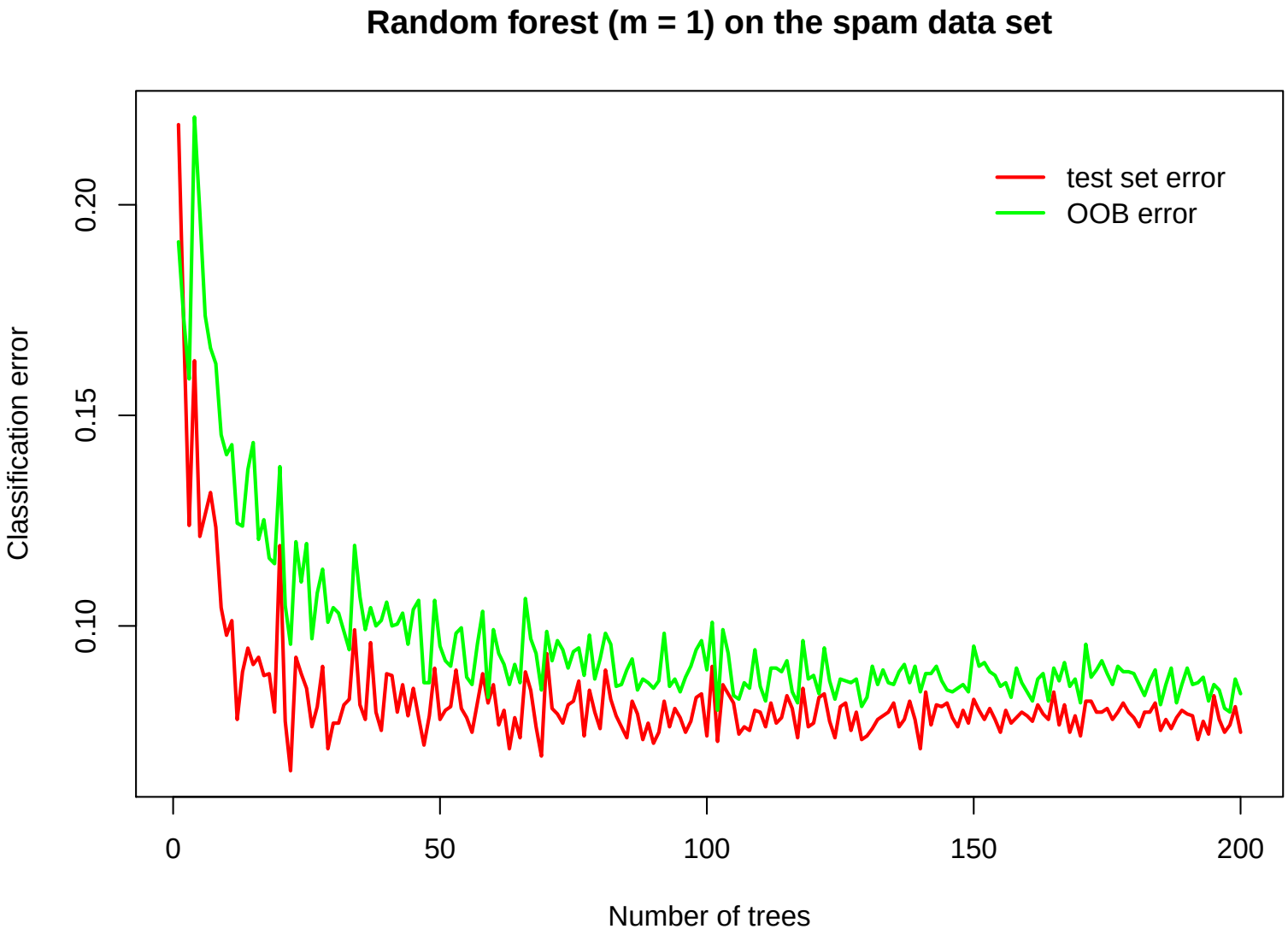
- Averaging over all observations $\mathbf{x}_i$, $i = 1, ..., n$ from $\mathcal{D}_n$ gives the out-of-bag estimate of the error rate:

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

Random forests: spam data



Random forests: spam data



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 $\mathcal{D}^*_{n,k} \cap \mathcal{D}^{*-}_{n,k} = \emptyset$.
- Then, let $R_{OOB(k)}$ be the classification error estimated on $\mathcal{D}^{*-}_{n,k}$:

$$R_{OOB(k)} = \frac{1}{\#\mathcal{D}^{*-}_{n,k}} \sum_{\mathbf{x} \in \mathcal{D}^{*-}_{n,k}} \mathbb{1}\left(T^*_k(\mathbf{x}) \neq y_i\right).$$

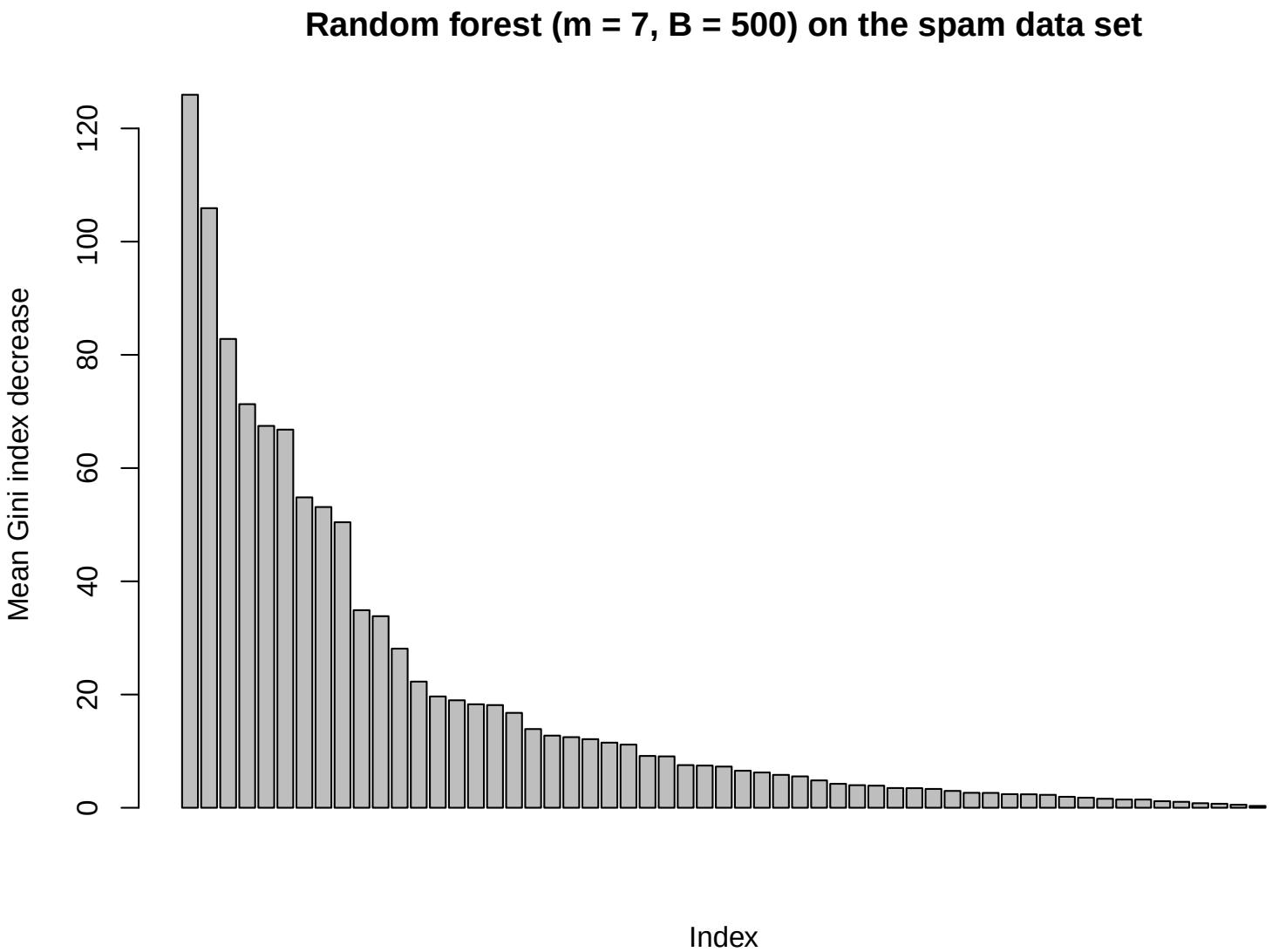
- Further, let $\mathcal{D}^{*-}_{n,k}(j)$ be the same subset $\mathcal{D}^{*-}_{n,k}$ where the **values of variable** $j \in \{1, ..., d\}$ have been **randomly perturbed**, and measure the error from above on this perturbed subset:

$$R_{OOB(k,j)} = \frac{1}{\#\mathcal{D}^{*-}_{n,k}(j)} \sum_{\mathbf{x} \in \mathcal{D}^{*-}_{n,k}(j)} \mathbb{1}\left(T^*_k(\mathbf{x}) \neq y_i\right).$$

- 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



Contents

Classification tree
- Algorithm
- Tuning

Bagging
- Motivation
- Algorithm
- An example

Random forest
- Algorithm
- Interpretation
- Consistency results

Consistency of the purely random forest classifier

Define the **purely random tree classifier** T^{pr} as follows:

- The support of X (and thus the root node of T^{pr}) is $[0,1]^d$.
- At each step, the leaf is chosen uniformly at random among all existing leaves.
- At each node, the split variable j is chosen uniformly at random among $1, ..., d$.
- The selected cell is split at a random location, chosen according to a uniform random variable on the length of the chosen side of the selected cell.
- The procedure is repeated k times where $k \geq 1$ is fixed in advance.
- The only data driven element is the class label of the leaf, chosen due to the majority of the observations contained in it.

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 $T_B^{prRF} = \mathbb{1}\big(\frac{1}{B}\sum_{k=1}^{B} T^{pr}(\cdot, \mathcal{D}_n)\big)$ (as well as $\lim_{B\to\infty} T_B^{prRF}$) is consistent whenever $k \to \infty$ and $k/n \to 0$ as $k \to \infty$.

Consistency of the scale-invariant random forest classifier

Define the **scale-invariant random tree classifier** T^{si} as follows:

- Take the **purely random tree classifier**.
- Let the root node be the entire space $\mathbb{R}^d$.
- Define the node-cutting procedure as follows:
  if the cell (node) m contains n_m points $\mathbf{x}_1, ..., \mathbf{x}_{n_m}$, then the random index I is chosen uniformly from the set $\{0, 1, ..., n_m\}$, and the cut is performed in the chosen variable between the points $\mathbf{x}_I$ and $\mathbf{x}_{I+1}$.

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 $T_B^{siRF} = \mathbb{1}\left(\frac{1}{B}\sum_{k=1}^{B} T^{si}(\cdot, \mathcal{D}_n)\right)$ (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:

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

- Averaged classifier (the limit of the bagging classifier):

$$\lim_{B\to\infty} g_B^{agg}(\mathbf{x}) = \mathbb{1}\big(\mathbb{E}^*[g_k^*(\mathbf{x}) \mid \mathcal{D}_n) > 0.5]\big)\,.$$

with θ being a random variable delivering a bootstrap sample of size $Bin(n, q_n)$ (without replacement), and $q_n \in [0, 1]$.

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 $\mathbb{1}\big(\mathbb{E}[g_k^*(\mathbf{x}) \mid \mathcal{D}_n)] > 0.5\big)$ 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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