The Logistic Regression model - Model selection and assessment

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Outline

Outline

- Model selection
- Model assessment
- A short intro to Decision Trees

Model selection

Model selection

Disclaimer

This is a very short introduction to model selection in the context of Logisitc Regression.

For a better coverage, chapter 7 `Model Assessment and Selection` of Hastie et al. (2009) discusses in depth the interplay between bias, variance and model complexity, in a general setting. Chapter 6 `Linear Model Selection and Regularization` of James et al. (2021) discusses methods to automatically perform variable selection in the context of linear models.

Also more developed in the Practical part of the Course.

Model selection

Manual selection - the old way

Usually a combination of:

- Single-variable analysis/screening: keep predictors showing individual association with the response
- Correlation analysis: remove redundant predictors that are highly correlated

see for example this excellent blog post

Very similar to Exploratory Data Analysis.

Model selection

Best subset selection

The "best subset" method evaluates all possible combinations of predictor variables, resulting in $2^p - 1$ models for p predictors, and selects the one that optimizes a specified criterion, such as the Akaike Information Criterion (AIC) or Bayesian Information Criterion (BIC). It is computationally intensive and usually restricted to low dimension data sets:

1. For $k = 1, \ldots, p$:
   - (a) Fit all $\binom{p}{k}$ models with exactly k predictors
   - (b) Pick the best among them and call it $\mathcal{M}_k$
     (largest log-likelihood or min deviance for Logistic Regression)

2. Select the single best model from $\mathcal{M}_1, \ldots, \mathcal{M}_p$
   using a chosen criterion (validation error, AIC, BIC, ...)

Model selection

Best subset - AIC / BIC

Given $|\mathcal{M}|$ we define the two following criteria which represent two way of penalizing the log-likelihood $\ell(Y, \hat{\beta})$:

$$\mathbf{AIC}(\mathcal{M}) = -2\ell(Y, \hat{\beta}) + 2|\mathcal{M}|$$

and

$$\mathbf{BIC}(\mathcal{M}) = -2\ell(Y, \hat{\beta}) + |\mathcal{M}| \log(n)$$

Model selection

Best subset - with R

The package **`bestglm`** allows best subset selection up to roughly 15 variables, by default it uses BIC. We use the Default data set to illustrate because Agriculture Farm Lending has around 30 variables:

```
BIC
BICq equivalent for q in (0.000417890560228229, 0.989405669357382)
Best Model:
                Estimate  Std. Error    z value      Pr(>|z|)
(Intercept) -10.749495878 0.369191361 -29.116326 2.230782e-186
studentYes   -0.714877620 0.147519010  -4.846003  1.259734e-06
balance       0.005738104 0.000231847  24.749526 3.136911e-135
```

Model selection

Stepwise Logistic Regression : Forward selection

Stepwise methods (Forward or Backward) iteratively add or remove variables based on a chosen criterion; once a variable is selected or dropped, it is fixed, and the process carries on, making them less computationally intensive than Best Subset selection. Below the Forward selection method:

1. For $k = 1, \ldots, p$:
   (a) Consider all $p + 1 - k$ models that augment the predictors in $\mathcal{M}_k$ with one additional predictor
   (b) Pick the best among these $p + 1 - k$ models and call it $\mathcal{M}_{k+1}$ (largest log-likelihood or min deviance for Logistic Regression)

2. Select the single best model from $\mathcal{M}_1, \ldots, \mathcal{M}_p$ using a chosen criterion (validation error, AIC, BIC, ...)

Model selection

Stepwise Logistic Regression : Backward selection

Below the Backward selection method:

1. Let $\mathcal{M}_p$ denote the full model containing all p predictors

2. For $k = p, \ldots, 1$:
   (a) Consider all k models that contain all but one of the predictors in $\mathcal{M}_k$ (total of $k - 1$
   (b) Pick the best among these k models and call it $\mathcal{M}_{k-1}$
   (largest log-likelihood or min deviance
   for Logistic Regression)

3. Select a single best model from $\mathcal{M}_1, \ldots, \mathcal{M}_p$
   using a chosen criterion (validation error, AIC, BIC, ...)

Additionally versions mixing forward and backward stepwise selection exist.

Model selection

Penalized Logistic Regression

As an alternative, penalized regression techniques:

- fit a Logistic Regression model with all p predictors but introducing constraints/penalization on coefficients (ie shrink coefficients toward zero)
- turns out to be an efficient means of variance reduction and/or variable selection

To estimate Logistic Regression model, we maximized in β the log-likelihood:

$$\ell(Y, \beta) = \log L(Y, \beta) = \sum_{i=1}^{n} \left(y_i \log(p_\beta(x_i)) + (1 - y_i) \log(1 - p_\beta(x_i))\right)$$

In the context of penalized Logistic Regression the idea is to minimize in β:

$$-\ell(Y, \beta) + \lambda_2 \|\beta\|_2 + \lambda_1 \|\beta\|_1$$

where λ_1, λ_2 are two constants.

Model selection

Penalized Logistic Regression

Having set λ_1, λ_2, minimize in β:

$$-\ell(Y, \beta) + \lambda_2 \|\beta\|_2 + \lambda_1 \|\beta\|_1$$

$\lambda_1 > 0, \lambda_2 = 0$: Lasso penalty. Promotes sparsity, selects some predictors while shrinking others to zero.

$\lambda_1 = 0, \lambda_2 > 0$: Ridge penalty.

$\lambda_1 > 0, \lambda_2 > 0$: Elastic Net penalty.

Model selection

Penalized Logistic Regression

Usually the following graphs are given in textbooks/slides to give some intuition about Ridge/Lasso:

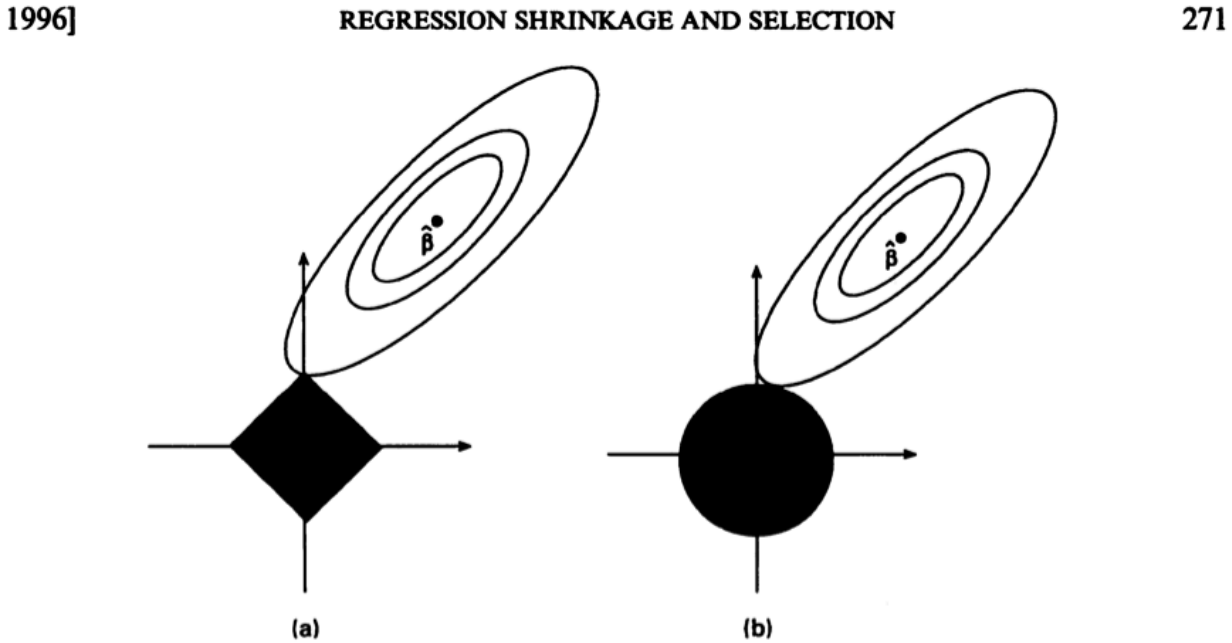


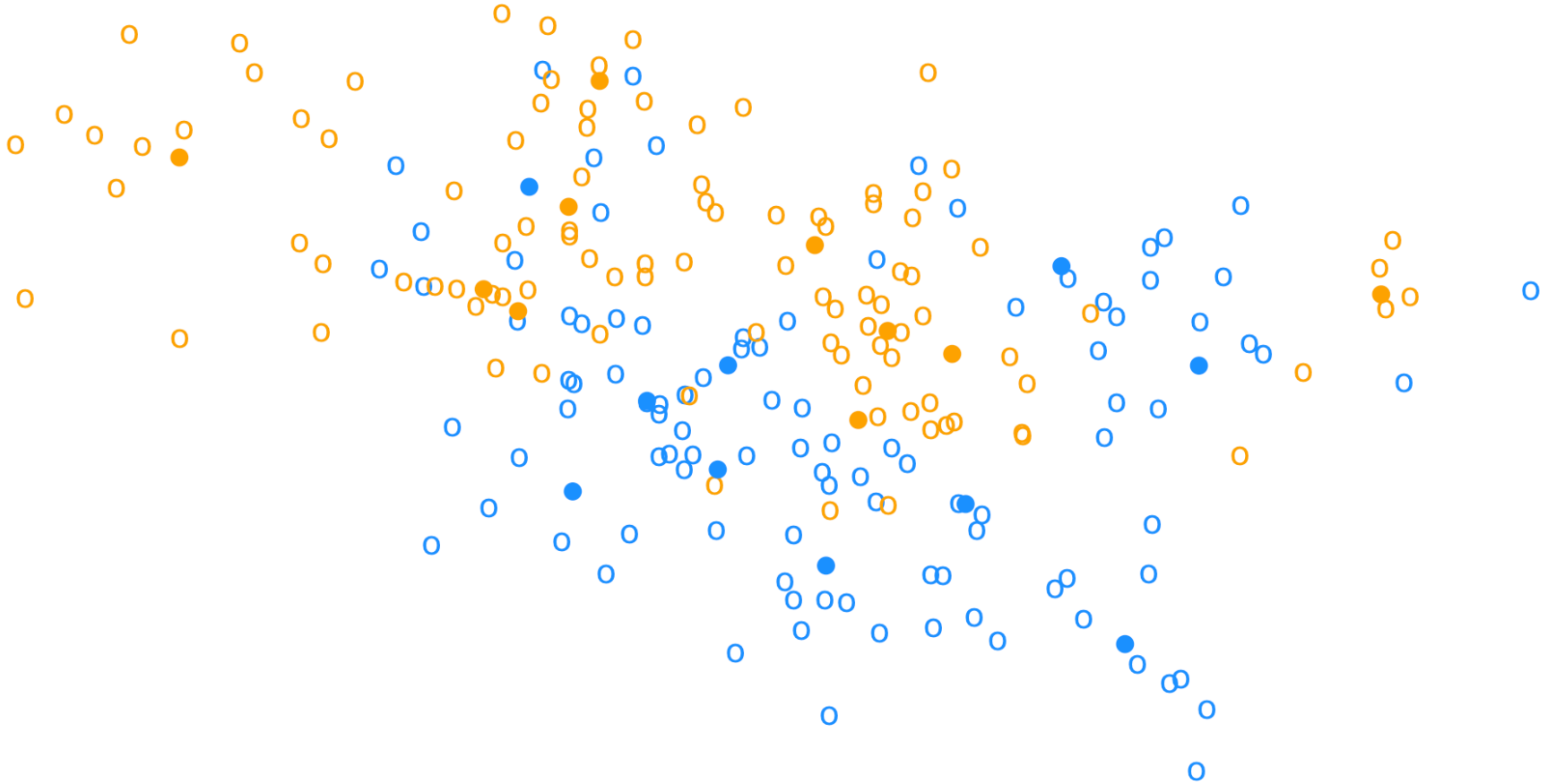
Fig. 2. Estimation picture for (a) the lasso and (b) ridge regression

The figure below is taken from the original Lasso article by Tibshirani published in 1996. Without entering to much details, Ridge does a proportional shrinkage of all coefficients while Lasso tends to truncates some of the coefficients at zero.

Model selection

Penalized Logistic Regression

Re-using here the 2D Mixture data set from introduction slides to give further intuition about Ridge/Lasso penalties:



Model selection

Ridge

Ridge estimator is:

$$\hat{\beta}_{ridge} = \underset{\beta}{\operatorname{argmin}} -\ell(Y, \beta) + \lambda ||\beta||_2$$

equivalently:

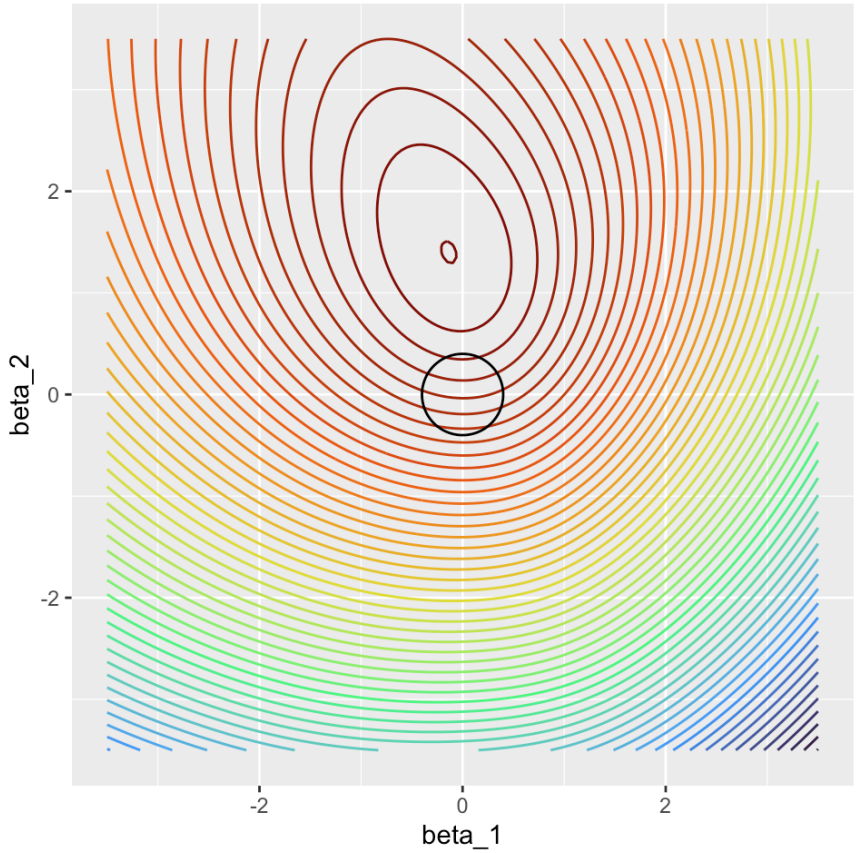
$$\hat{\beta}_{ridge} = \underset{\beta}{\operatorname{argmin}} -\ell(Y, \beta)$$

subject to $||\beta||_2 \leq t$, where t maps to λ (the higher λ, the lower t).

Model selection

Ridge

Log-likelihood of the Logistic Regression (colored levels lines centered around the MLE) for the Mixture data set, adding the Ridge constraint (the circle in black is the boundary $\|\beta\|_2 \leq t$) :



Model selection

Ridge - with R

In R the package **`glmnet`** implements the Lasso, Ridge and Elastic Net penalties in particular for Logistic Regression. Ridge Logistic Regression coefficients for x_1, x_2 as a function of λ:

▾ Code

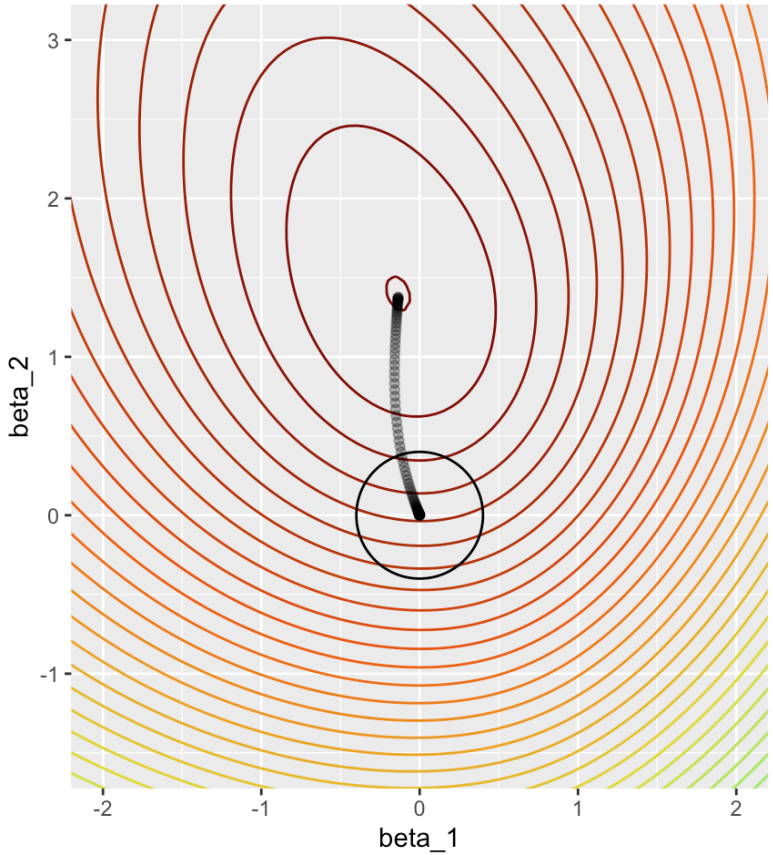
```
library(glmnet)
library(glmnetUtils) # convenient package allowing to use R formulas instead of glmnet sparse matrix
# Fitting Logistic Regression model with Ridge (alpha=0) penalty. Small lambda.min.ratio so that penalty is almost zero at start.
mixture_ridge <- glmnetUtils::glmnet(Y ~ ., data=data_mixture_example, family="binomial", alpha=0, lambda.min.ratio=0.000001)
# Extracting coefficients
ridge_result <- as_tibble(as.matrix(cbind(mixture_ridge$lambda, mixture_ridge$a0, t(mixture_ridge$beta))))
names(ridge_result) <-  c("lambda", "(Intercept)", row.names(mixture_ridge$beta))
# Showing results for very high/low values of lambda
bind_rows(ridge_result %>% head(),ridge_result %>% tail())
```

```
# A tibble: 12 × 4
      lambda `(Intercept)`        x1       x2
       <dbl>         <dbl>     <dbl>    <dbl>
 1 268.          -9.86e-32 -1.04e-37 2.64e-37
 2 233.          -5.00e- 4 -4.44e- 4 1.12e- 3
 3 202.          -5.75e- 4 -5.10e- 4 1.29e- 3
 4 176.          -6.61e- 4 -5.86e- 4 1.48e- 3
 5 153.          -7.59e- 4 -6.74e- 4 1.70e- 3
 6 133.          -8.73e- 4 -7.74e- 4 1.96e- 3
 7   0.00287     -9.42e- 1 -1.38e- 1 1.36e+ 0
 8   0.00250     -9.46e- 1 -1.37e- 1 1.36e+ 0
 9   0.00217     -9.50e- 1 -1.37e- 1 1.37e+ 0
10   0.00189     -9.54e- 1 -1.37e- 1 1.37e+ 0
11   0.00164     -9.57e- 1 -1.36e- 1 1.37e+ 0
12   0.00143     -9.59e- 1 -1.36e- 1 1.38e+ 0
```

Model selection

Ridge

Ridge Logistic Regression parameters β_1, β_2 path as λ increases. Starting from the Logistic Regression MLE for $\lambda = 0$ and then shrunken "uniformly" towards zero as λ increases.



Model selection

Lasso

Lasso Estimator is:

$$\hat{\beta}_{lasso} = \underset{\beta}{\operatorname{argmin}} -\ell(Y, \beta) + \lambda \|\beta\|_1$$

equivalently::

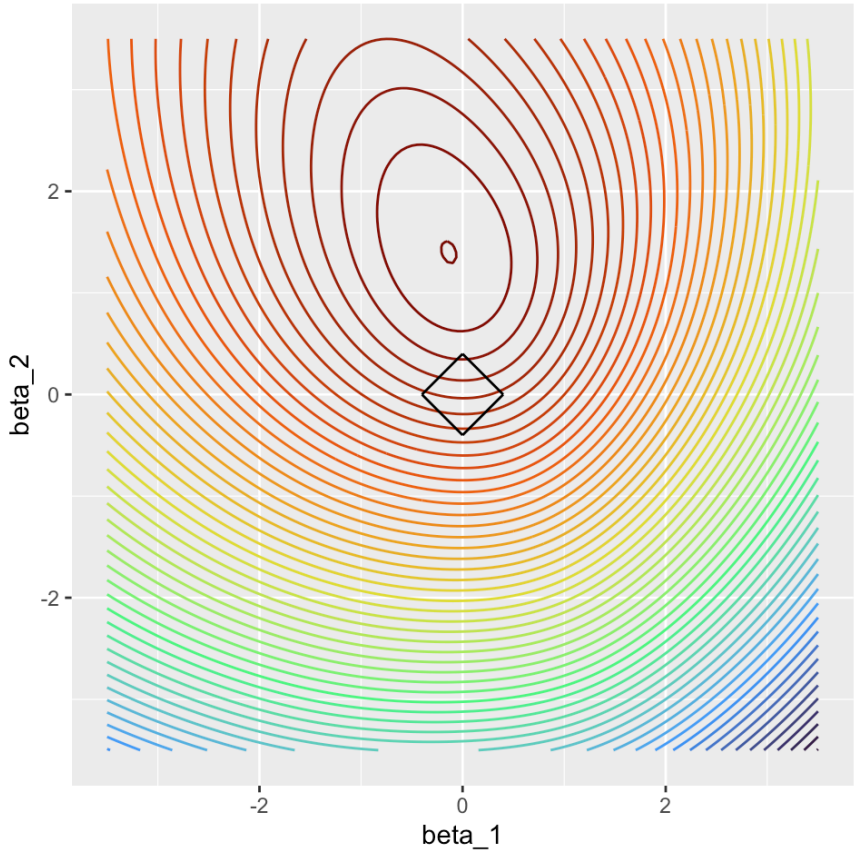
$$\hat{\beta}_{lasso} = \underset{\beta}{\operatorname{argmin}} -\ell(Y, \beta)$$

subject to $\|\beta\|_1 \leq t$, where t maps to λ.

Model selection

Lasso

Log-likelihood of the Logistic Regression (colored levels lines centered around the MLE) for the Mixture data set, adding the Lasso constraint (the diamond/square in black is the boundary $\|\beta\|_1 \leq t$) :



Model selection

Lasso

Lasso Logistic Regression parameters for $\boldsymbol{x_1}$, $\boldsymbol{x_2}$ as a function of $\boldsymbol{\lambda}$:

▾ Code

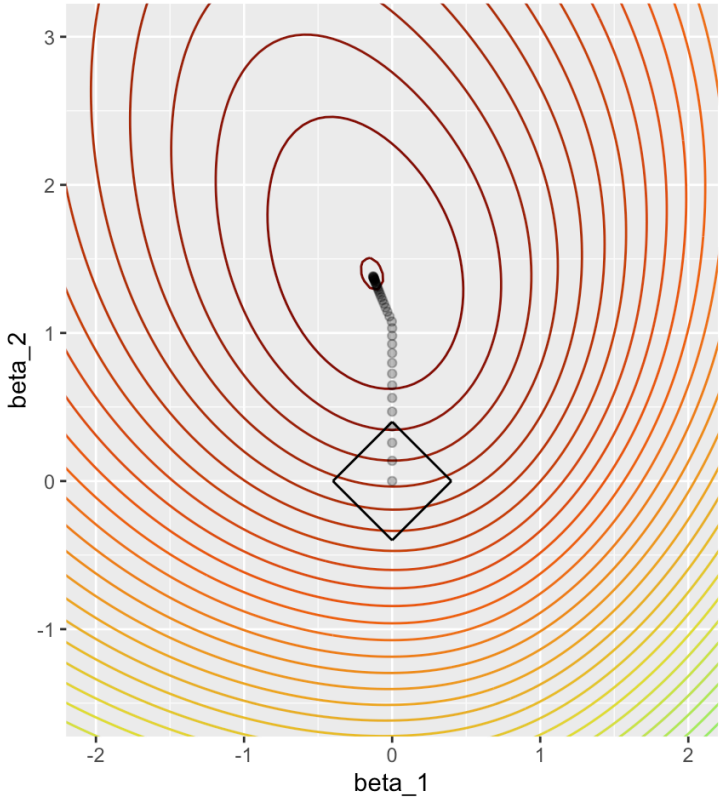
```r
# Fitting Logistic Regression model with Lasso (alpha=1) penalty. Small lambda.min.ratio so that penalty is almost zero at start.
mixture_lasso <- glmnetUtils::glmnet(Y ~ ., data=data_mixture_example, family="binomial", alpha=1, lambda.min.ratio=0.000001)
# Extracting coefficients
lasso_result <- as_tibble(as.matrix(cbind(mixture_lasso$lambda, mixture_lasso$a0, t(mixture_lasso$beta))))
names(lasso_result) <-  c("lambda", "(Intercept)", row.names(mixture_lasso$beta))
# Showing results for very high/low values of lambda
bind_rows(lasso_result %>% head(), lasso_result %>% tail())
```

```
# A tibble: 12 × 4
    lambda `(Intercept)`     x1    x2
     <dbl>         <dbl>  <dbl> <dbl>
 1 0.268       -9.86e-32  0     0
 2 0.233       -1.03e- 1  0     0.137
 3 0.202       -1.96e- 1  0     0.258
 4 0.176       -2.80e- 1  0     0.368
 5 0.153       -3.57e- 1  0     0.469
 6 0.133       -4.28e- 1  0     0.561
 7 0.00354     -9.63e- 1 -0.122 1.37
 8 0.00308     -9.65e- 1 -0.124 1.37
 9 0.00268     -9.67e- 1 -0.125 1.37
10 0.00233     -9.68e- 1 -0.126 1.38
11 0.00202     -9.69e- 1 -0.127 1.38
12 0.00176     -9.70e- 1 -0.128 1.38
```

Model selection

Lasso

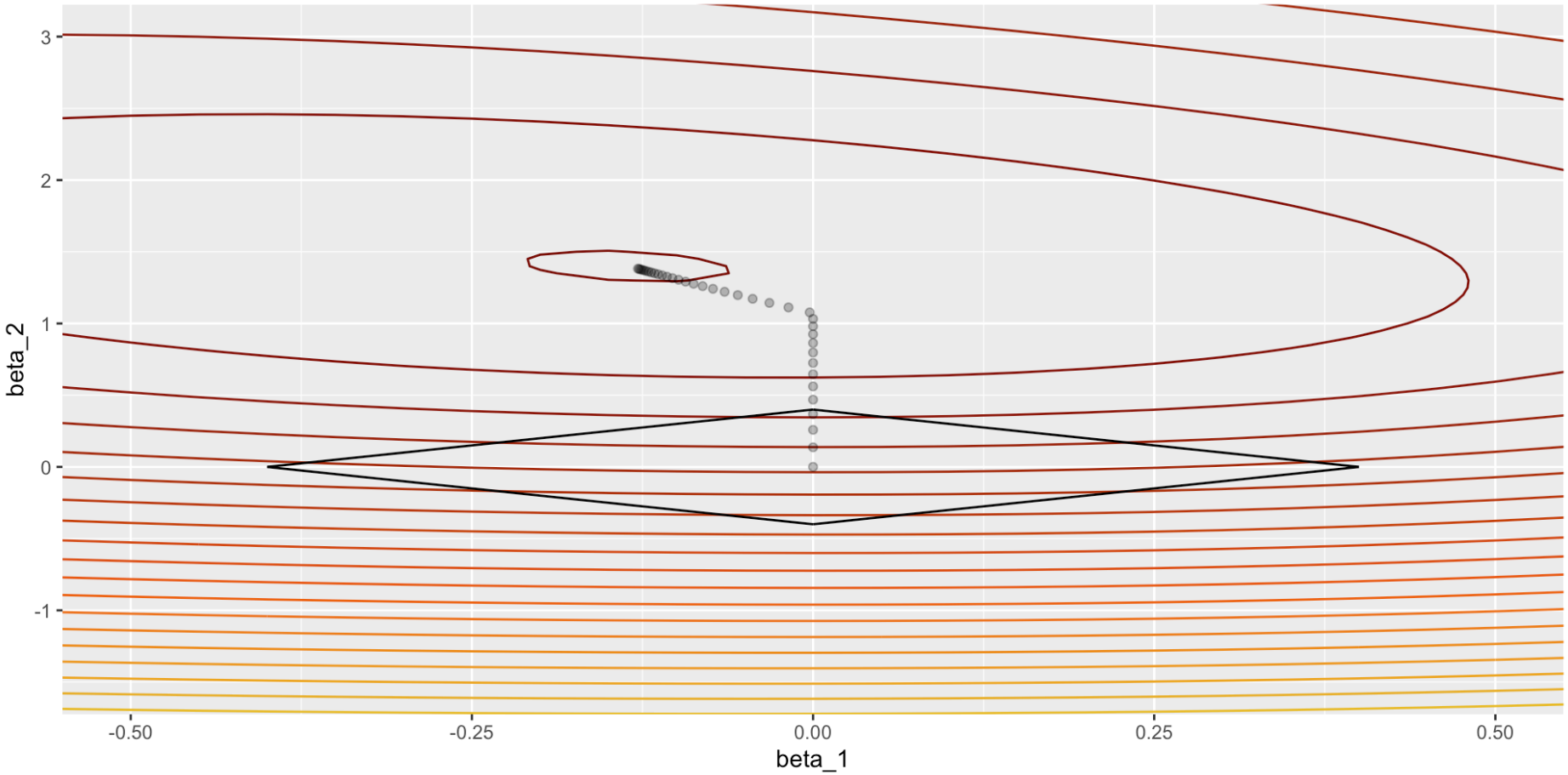
Lasso Logistic Regression parameters β_1, β_2 path as λ increases. Starting from the Logistic Regression MLE for $\lambda = 0$ and as λ increases and at some point the solution of the constrained optimization is likely to occur at one of the corners of the diamond.



Model selection

Lasso

Stretching the graph a little bit to better show the Lasso path, the β_1 parameter is the first shrunk to zero:



Model selection

Penalized Logistic Regression

- Reminding the aim of statistical learning: which method leads to better prediction accuracy?
- In practice, the true set of relevant predictors is unknown: only a few vs many variables possibly correlated)
- Resampling methods are to compare models on a given dataset given some criterion and may be used to select a good value of penalization parameters λ

Model assessment

Model assessment

Resampling methods

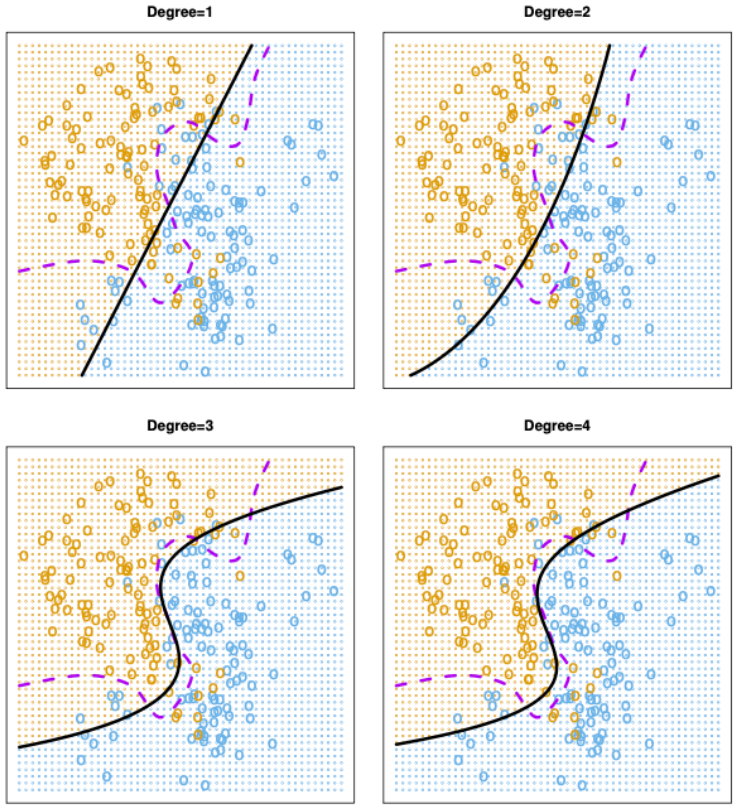


FIGURE 5.7. *Logistic regression fits on the two-dimensional classification data displayed in Figure 2.13. The Bayes decision boundary is represented using a purple dashed line. Estimated decision boundaries from linear, quadratic, cubic and quartic (degrees 1–4) logistic regressions are displayed in black. The test error rates for the four logistic regression fits are respectively* 0.201, 0.197, 0.160, *and* 0.162, *while the Bayes error rate is* 0.133.

Fig 5.7 from James et al. (2021)

Model assessment

Resampling methods

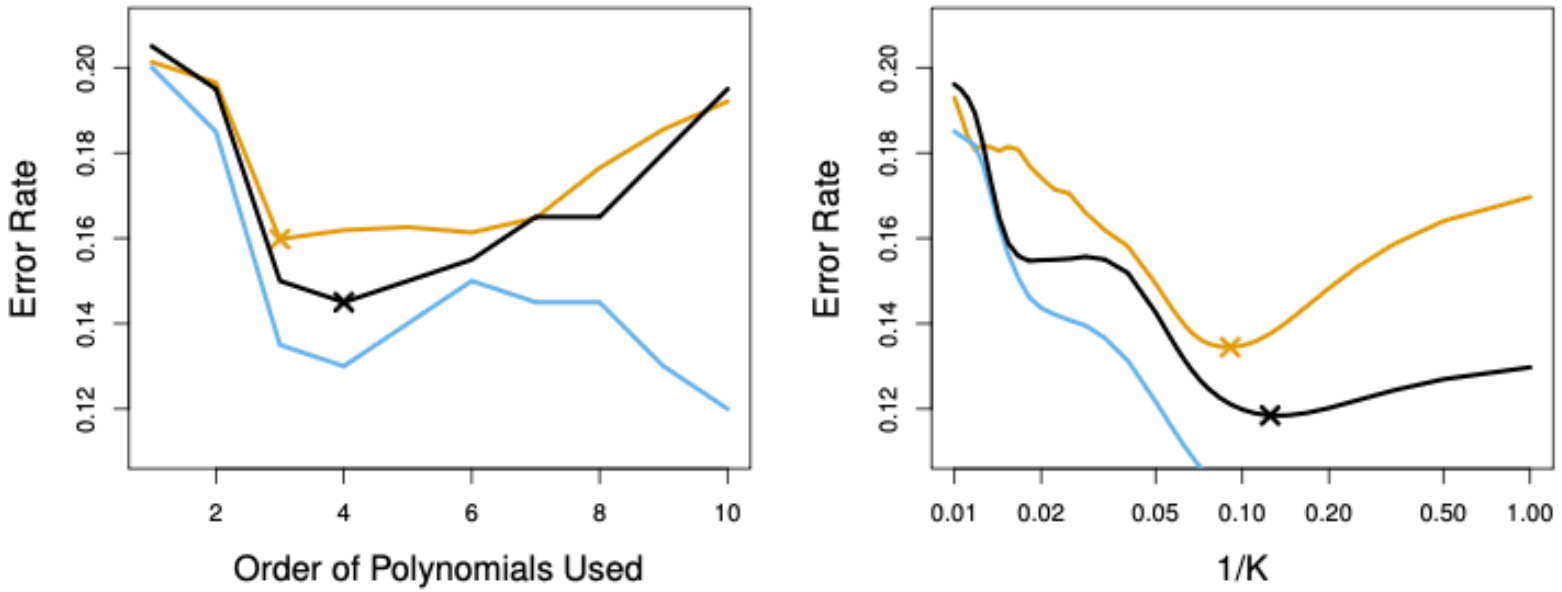


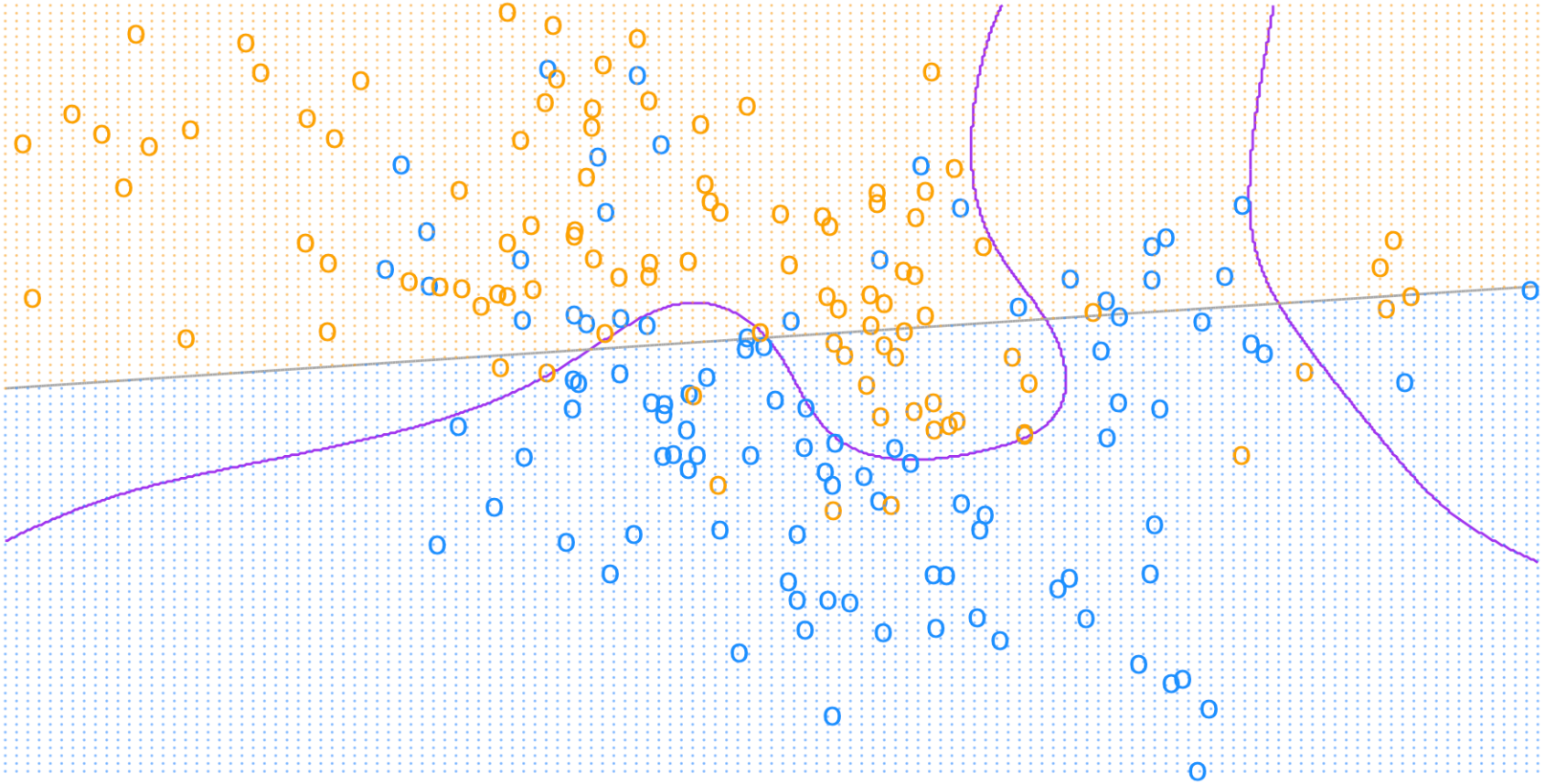
FIGURE 5.8. *Test error (brown), training error (blue), and* 10*-fold CV error (black) on the two-dimensional classification data displayed in Figure 5.7.* Left: *Logistic regression using polynomial functions of the predictors. The order of the polynomials used is displayed on the x-axis.* Right: *The KNN classifier with different values of K, the number of neighbors used in the KNN classifier.*

Fig 5.8 from James et al. (2021)

Model assessment

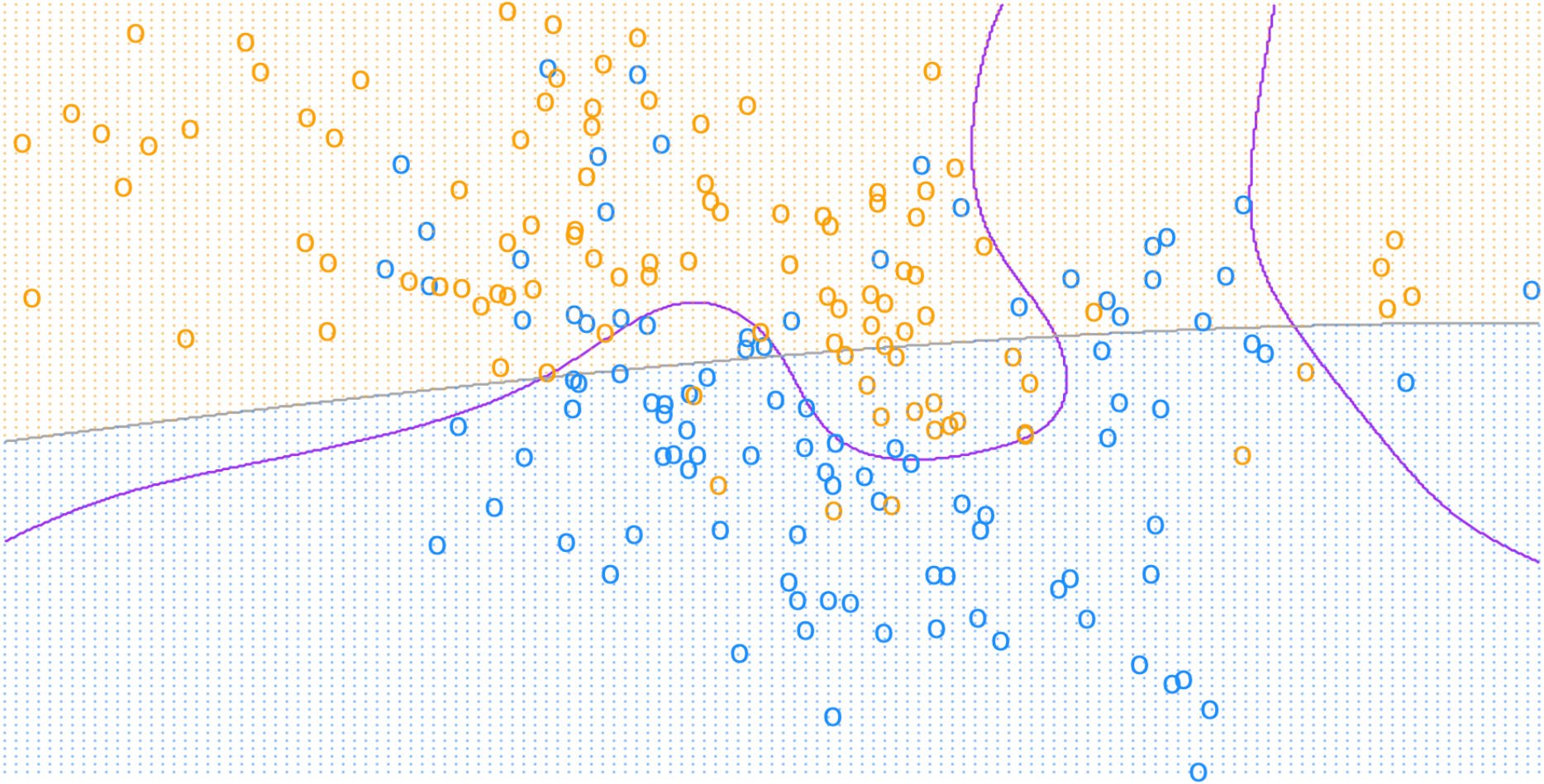
Original Mixture data set (d=1)

Tried to reproduce results form James et al. (2021) using Original Mixture data set with higher Bayes error



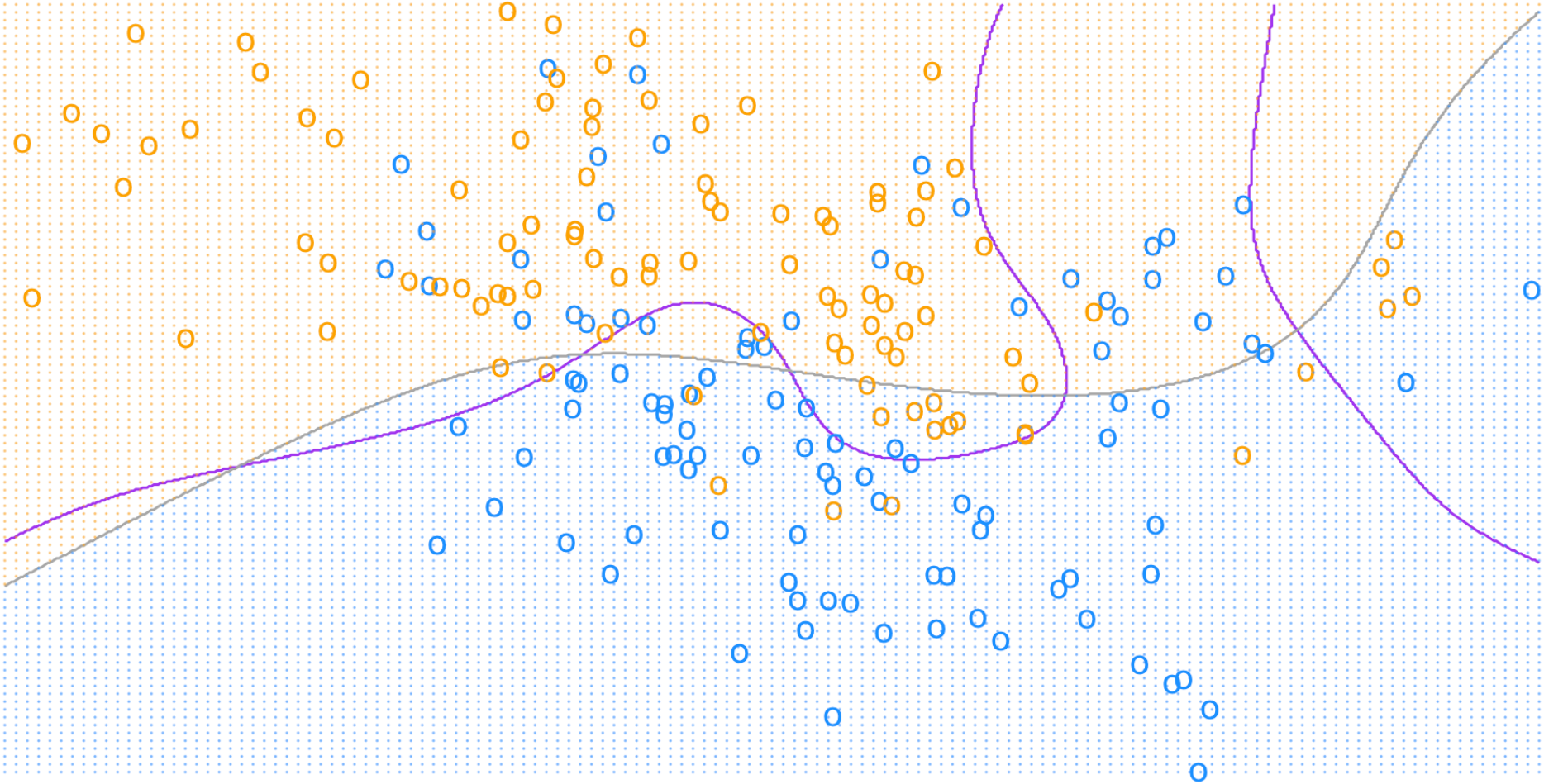
Model assessment

Original Mixture data set (d=2)



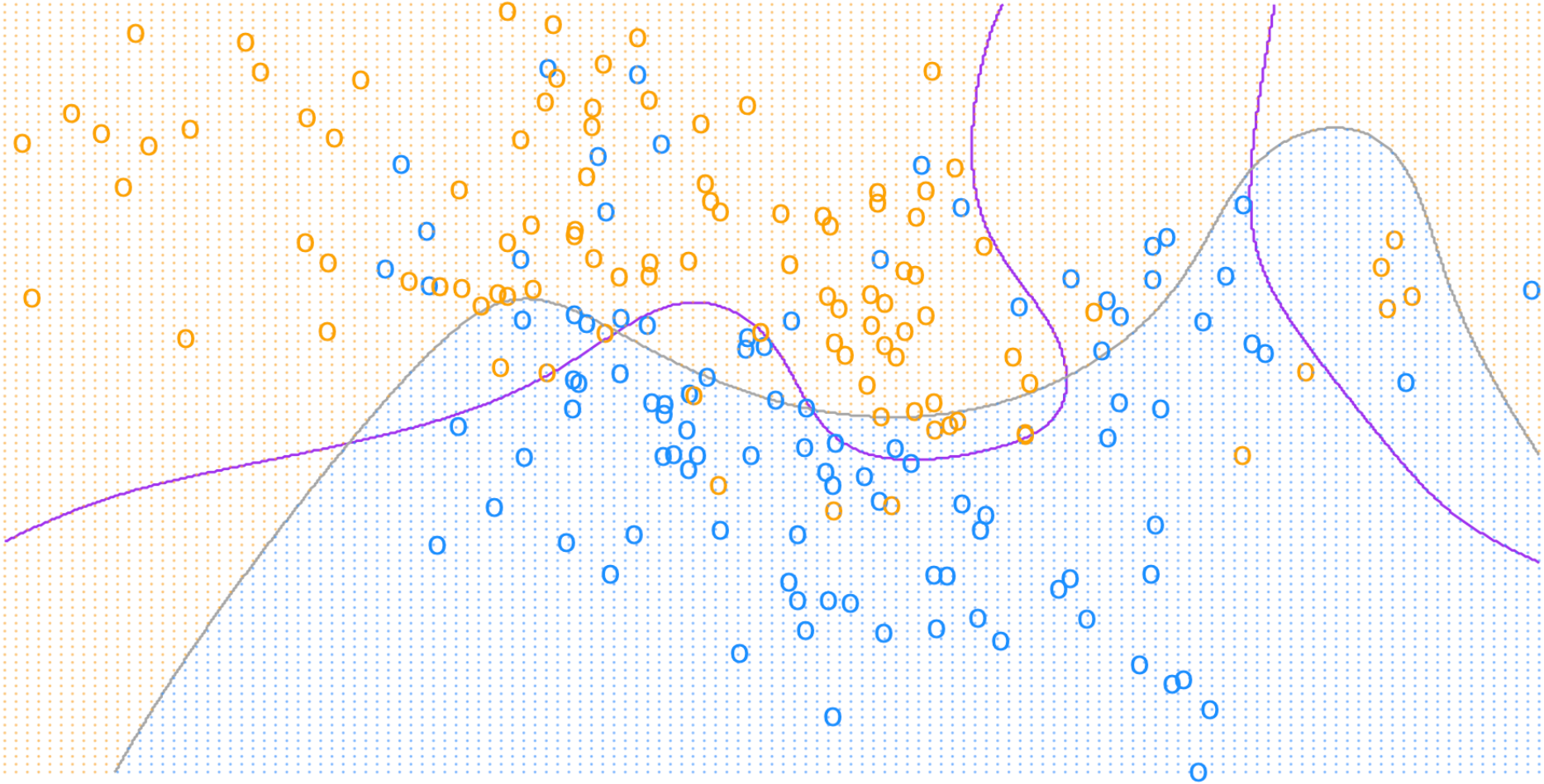
Model assessment

Original Mixture Mixture data set (d=3)



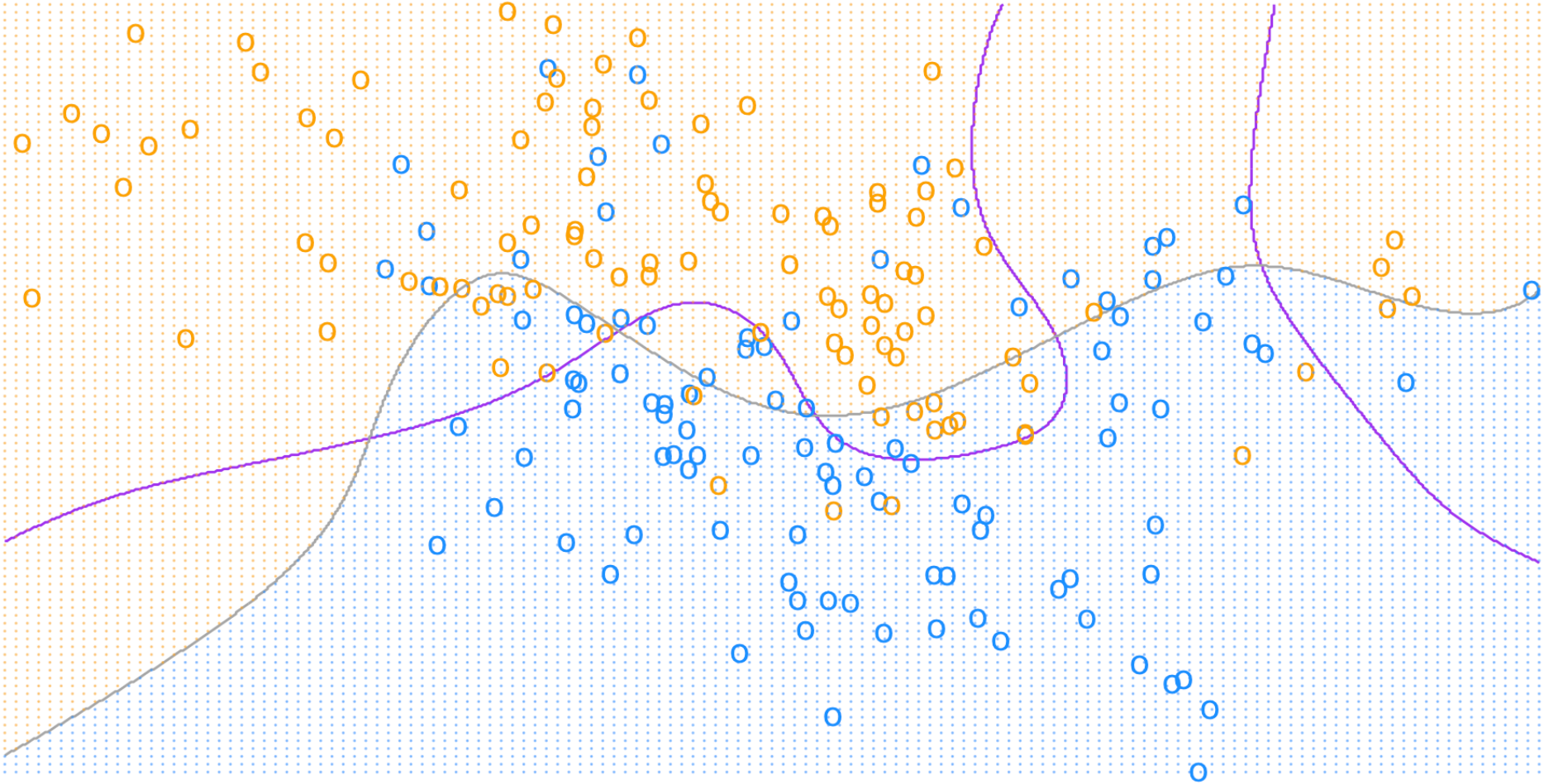
Model assessment

Original Mixture data set (d=4)



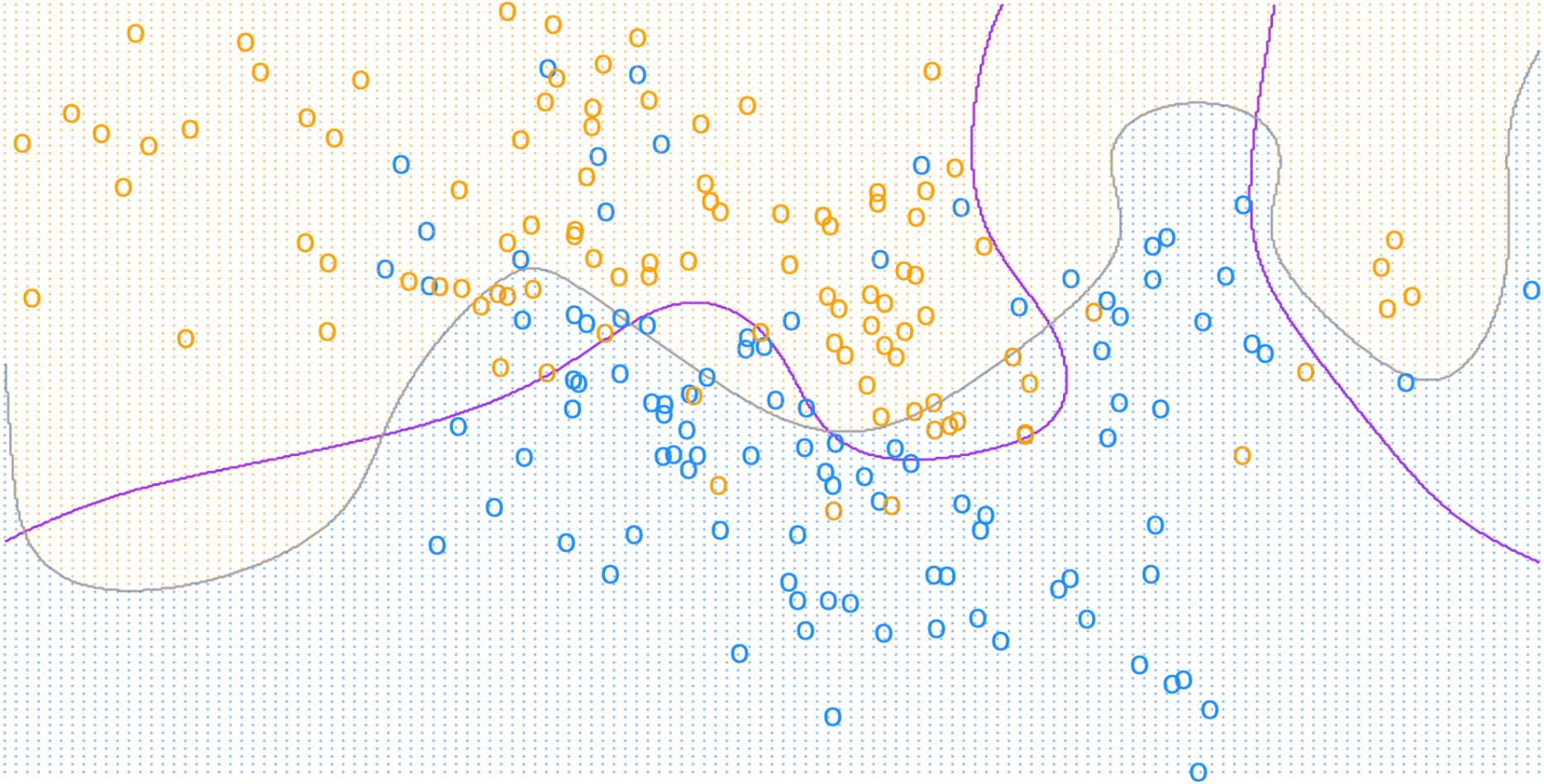
Model assessment

Original Mixture data set (d=5)



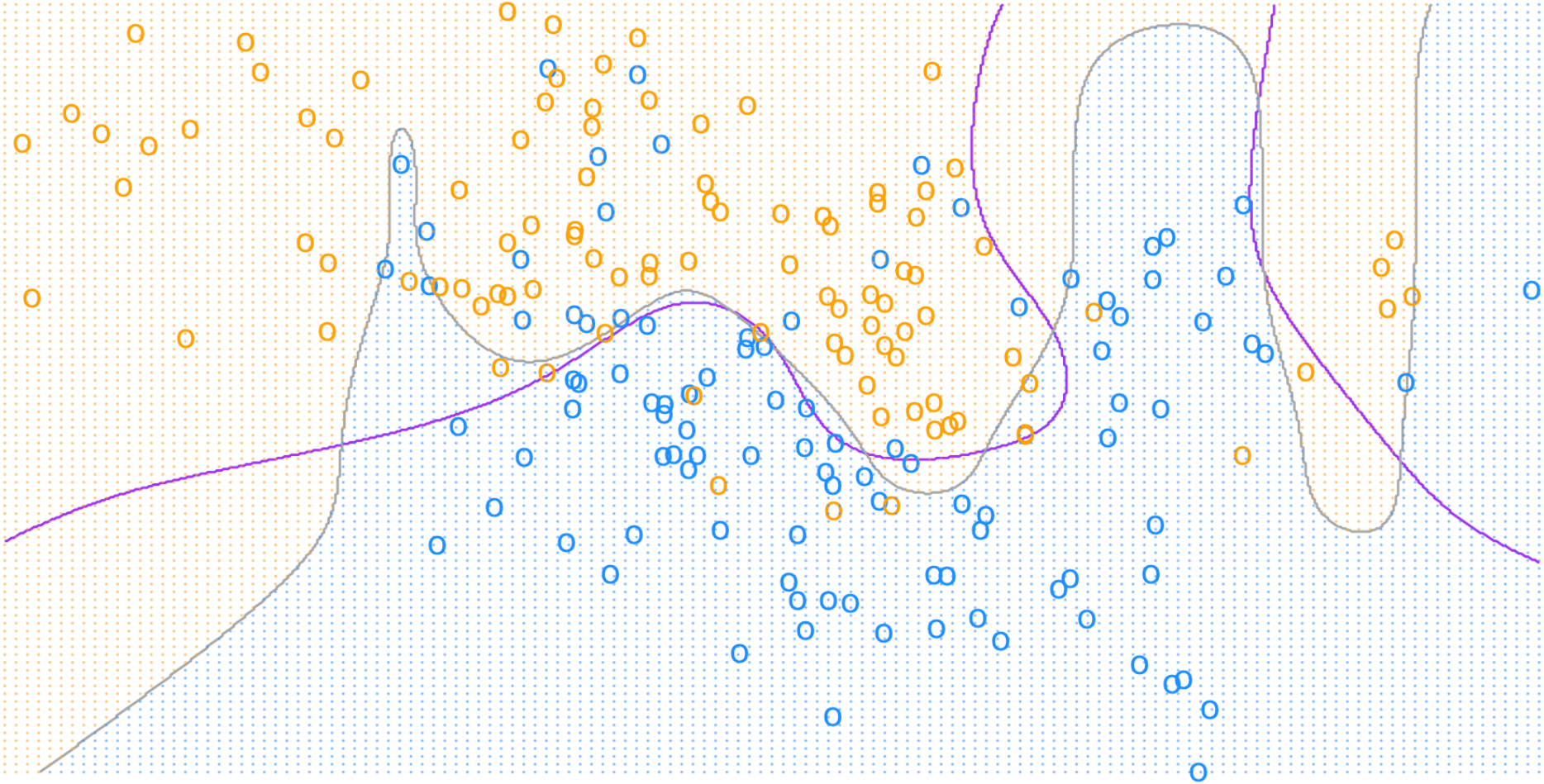
Model assessment

Original Mixture data set (d=6)



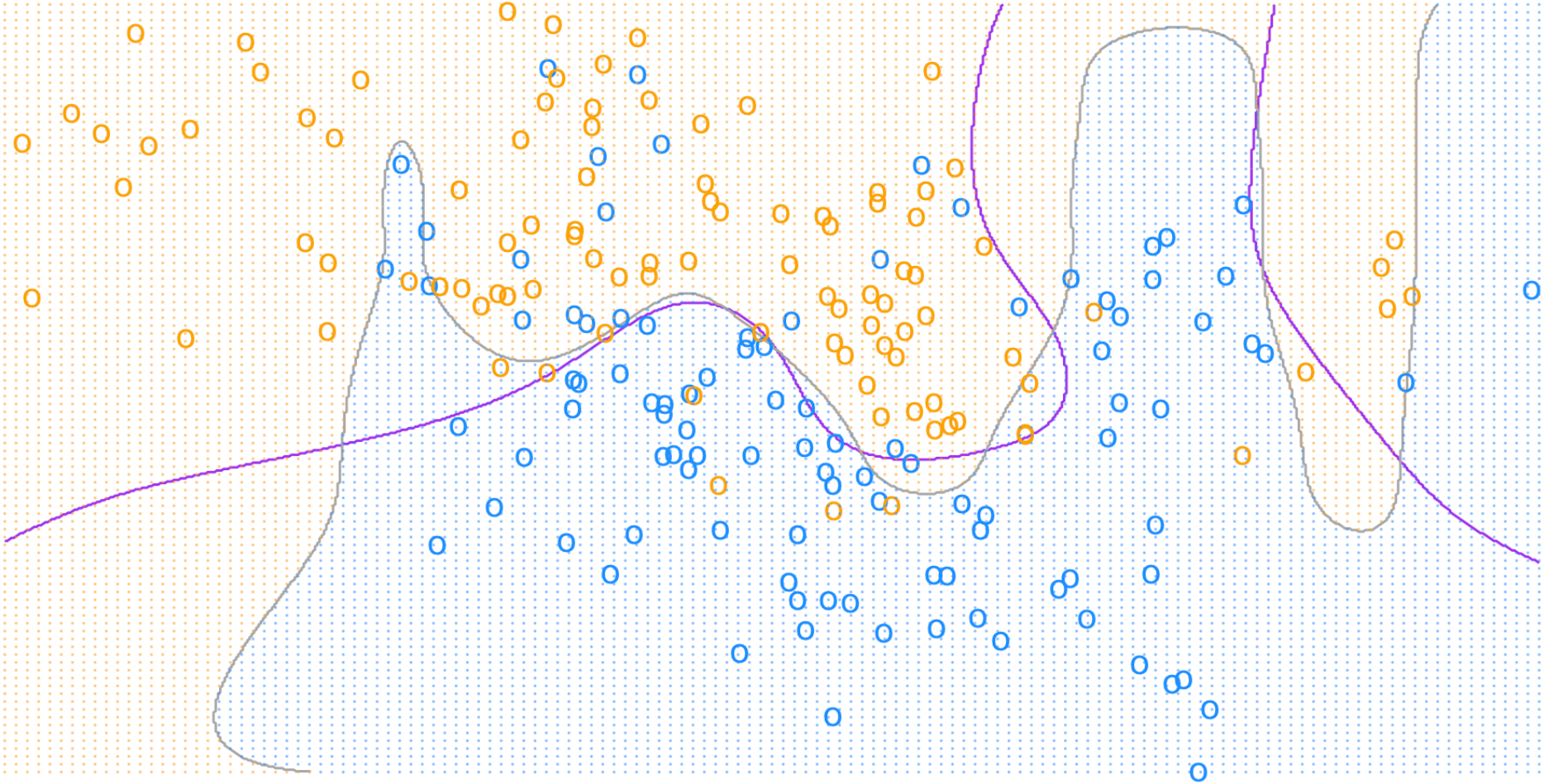
Model assessment

Original Mixture data set (d=7)



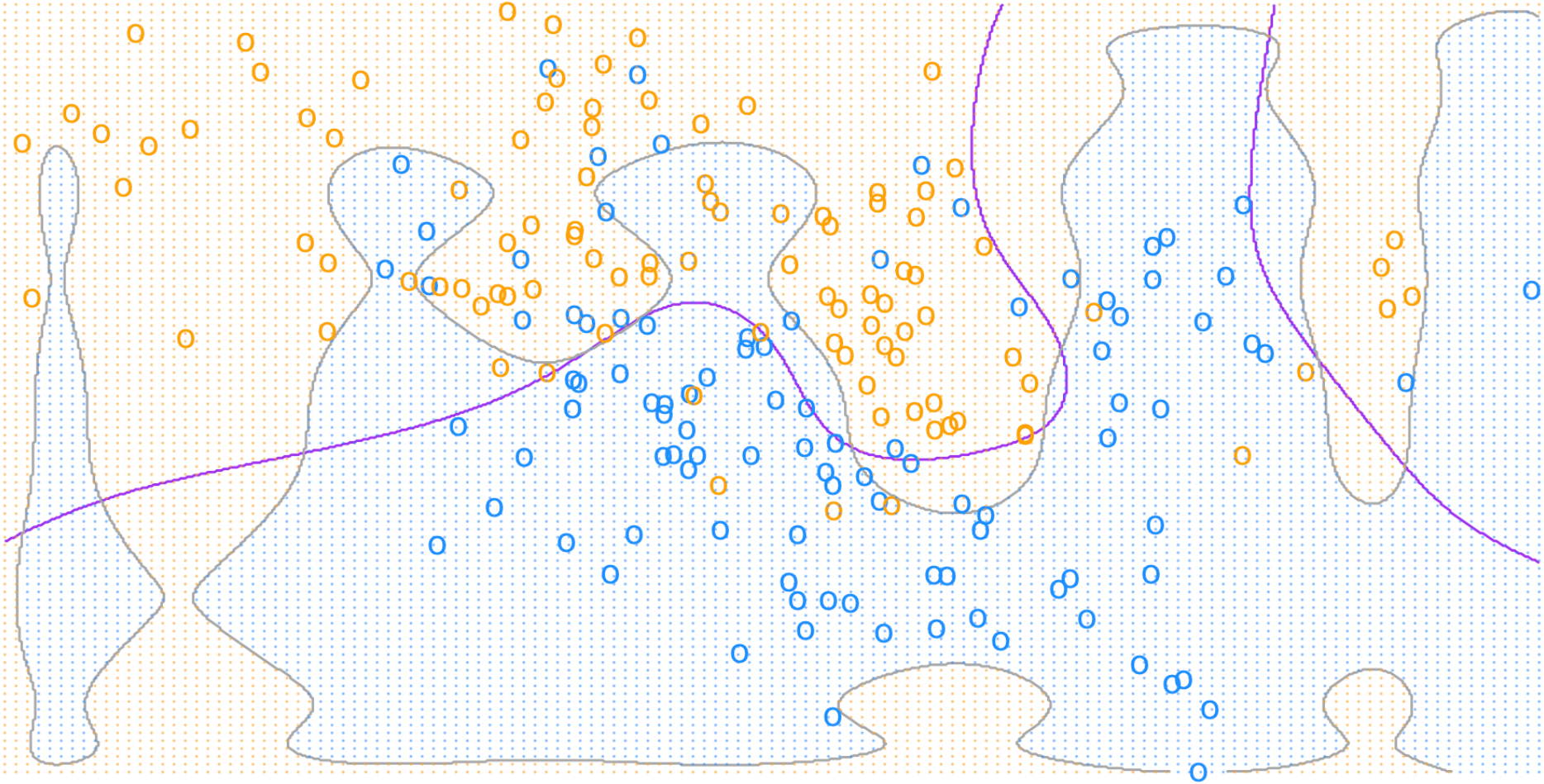
Model assessment

Original Mixture data set (d=8)



Model assessment

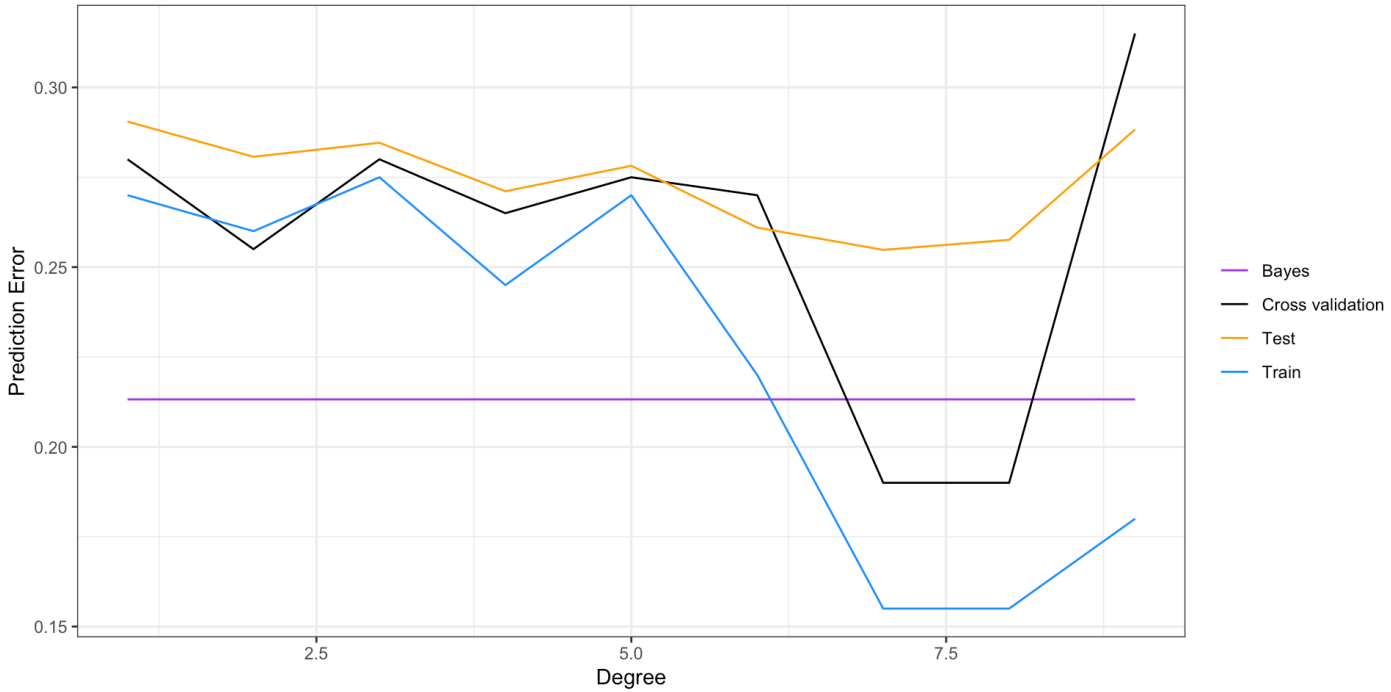
Original Mixture data set (d=10)



Model assessment

Original Mixture data set, misclassification curve

We plot below the misclassification curve, comparing the misclassification error estimated on a large testing set using the generating distribution (in orange, testing set generated knowing the oracle) with misclassification estimated using a resampling method on the training set (in black, 10-fold Cross Validation, defined later). In our case, we see that misclassification using a resampling method, although optimistic, behaves roughly like misclassification using large testing set:



Model assessment

The Hold-out approach

It consists in splitting the data set into:

- a learning or training set used to train the classifier or the Score ;
- a validation or test set used to estimate the empirical risk of the classifier or any other metric (ROC curve, AUC).

1. Using a partition of the dataset $\mathcal{D}$ into training and validation sets $\{\mathcal{T}, \mathcal{V}\}$:
   (a) Fit the classifiers $f_1, \ldots, f_m$ on $\mathcal{T}$
   (b) Compute the empirical risk on the validation set:
   $$\hat{\mathrm{R}}(f) = \frac{1}{n_{\mathcal{V}}} \sum_i \ell(y_i, f_m(x_i))$$
   or any other chosen metric

2. Select the single best model f_{m^*} with respect to the empirical risk or metric

Model assessment

The Hold-out approach

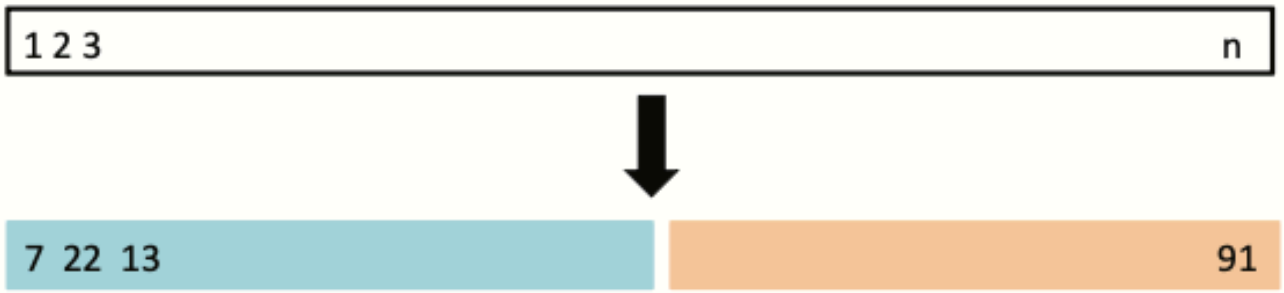


FIGURE 5.1. *A schematic display of the validation set approach. A set of n observations are randomly split into a training set (shown in blue, containing observations 7, 22, and 13, among others) and a validation set (shown in beige, and containing observation 91, among others). The statistical learning method is fit on the training set, and its performance is evaluated on the validation set.*

Fig 5.1 from James et al. (2021)

The main drawback using a single split of data is the possible variability of empirical risk, which is more pregnant when the data set size reduces. Against this issue an alternative approach is to repeat this process on multiple splits of the data.

Model assessment

The K-fold Cross-Validation approach

It consists in splitting randomly the data set into K blocks of folds then repeating K times the Hold-out approach, each time using a different block as validation set.

1. Partition the dataset $\mathcal{D}$ randomly into K blocks $\{\mathcal{D}_1, \ldots, \mathcal{D}_K\}$

2. For $k = 1, \ldots, K$:
   (a) Define training and validation sets: $\mathcal{V}_k = \mathcal{D}_k,\ \mathcal{T}_k = \mathcal{D} \setminus \mathcal{D}_k$
   (b) Fit the classifiers $f_1, \ldots, f_m$ on $\mathcal{T}_k$
   (c) Compute the empirical risk on the validation set:

   $$\hat{\mathrm{R}}(f) = \frac{1}{n_{\mathcal{V}_k}} \sum_i \ell(y_i, f_m(x_i))$$

   or any other chosen metric

3. Select the single best model f_{m^*} using the average empirical risk or metric

Model assessment

The K-fold Cross-Validation approach

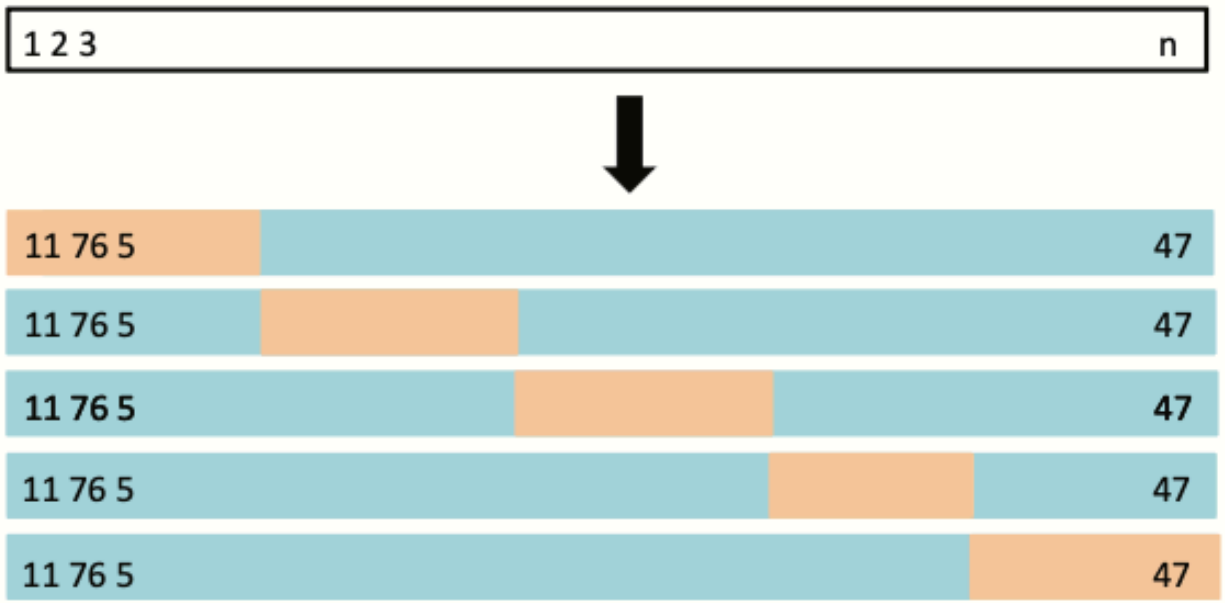


FIGURE 5.5. *A schematic display of 5-fold CV. A set of n observations is randomly split into five non-overlapping groups. Each of these fifths acts as a validation set (shown in beige), and the remainder as a training set (shown in blue). The test error is estimated by averaging the five resulting MSE estimates.*

Fig 5.5 from James et al. (2021)

Model assessment

The K-fold Cross-Validation approach

A variant is to first split the data set into a training and validation set. Perform K-fold Cross-Validation on the training set, for example to select some classifier hyper parameter (number of variables or model specification in logistic regression, penalty, etc), then assess the best "optimized" models on the validation set.

Another variant is to repeat the K-fold CV 5 or 10 times to improve the accuracy of the estimated performance and provide and estimate on its variability.

This book chapter gives a practical overview on these methods (how to implement it in R) and also gives references discussing their validity and limitations.

This recent blog by NVIDIA Kaggle grandmasters advocates resampling techniques (cross-validation) as a foundation for any supervized learning problem.

A short intro to Decision Trees

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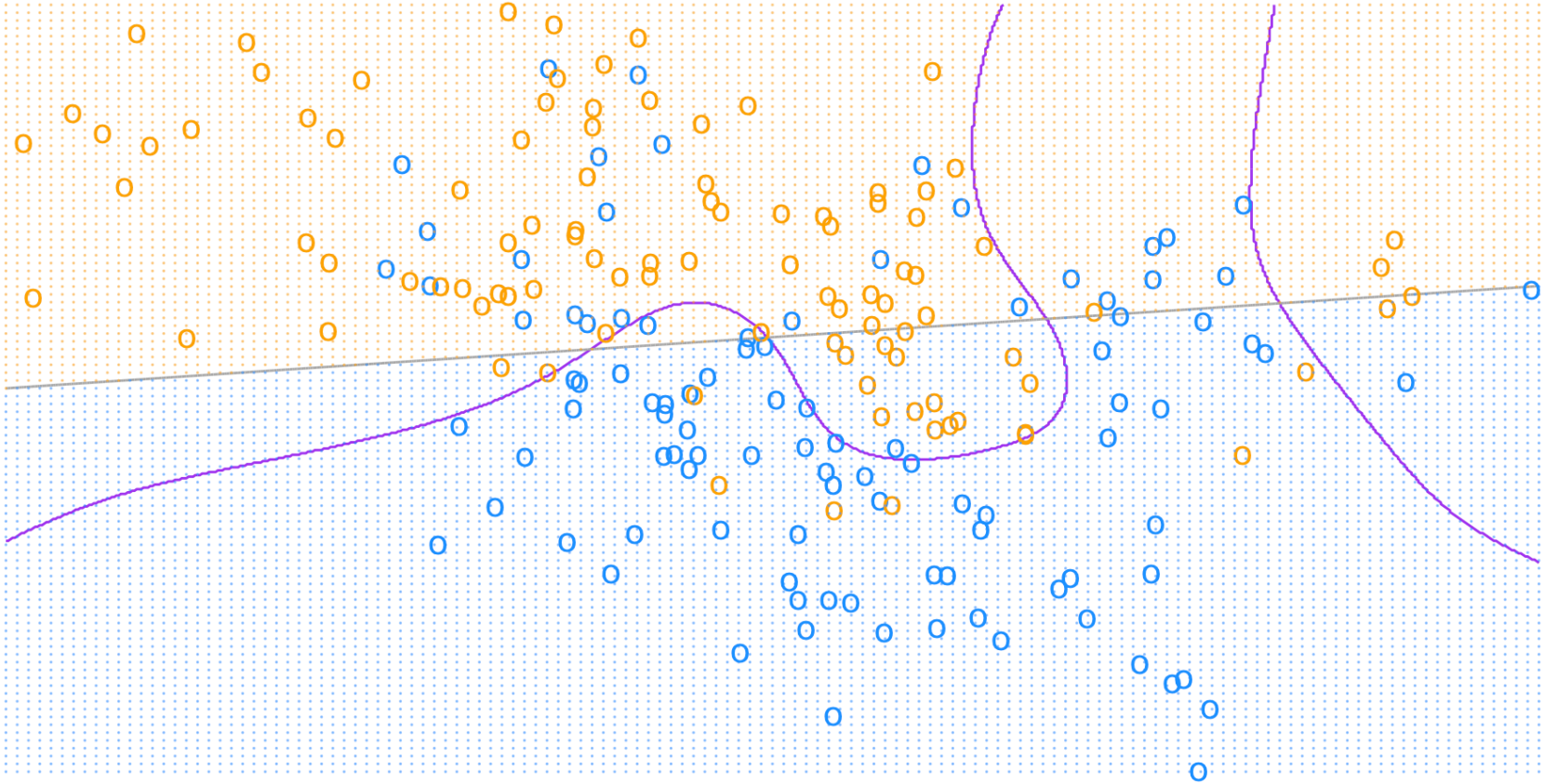
Mixture data set: Logistic Regression



The empirical risk on testing set is 0.291.

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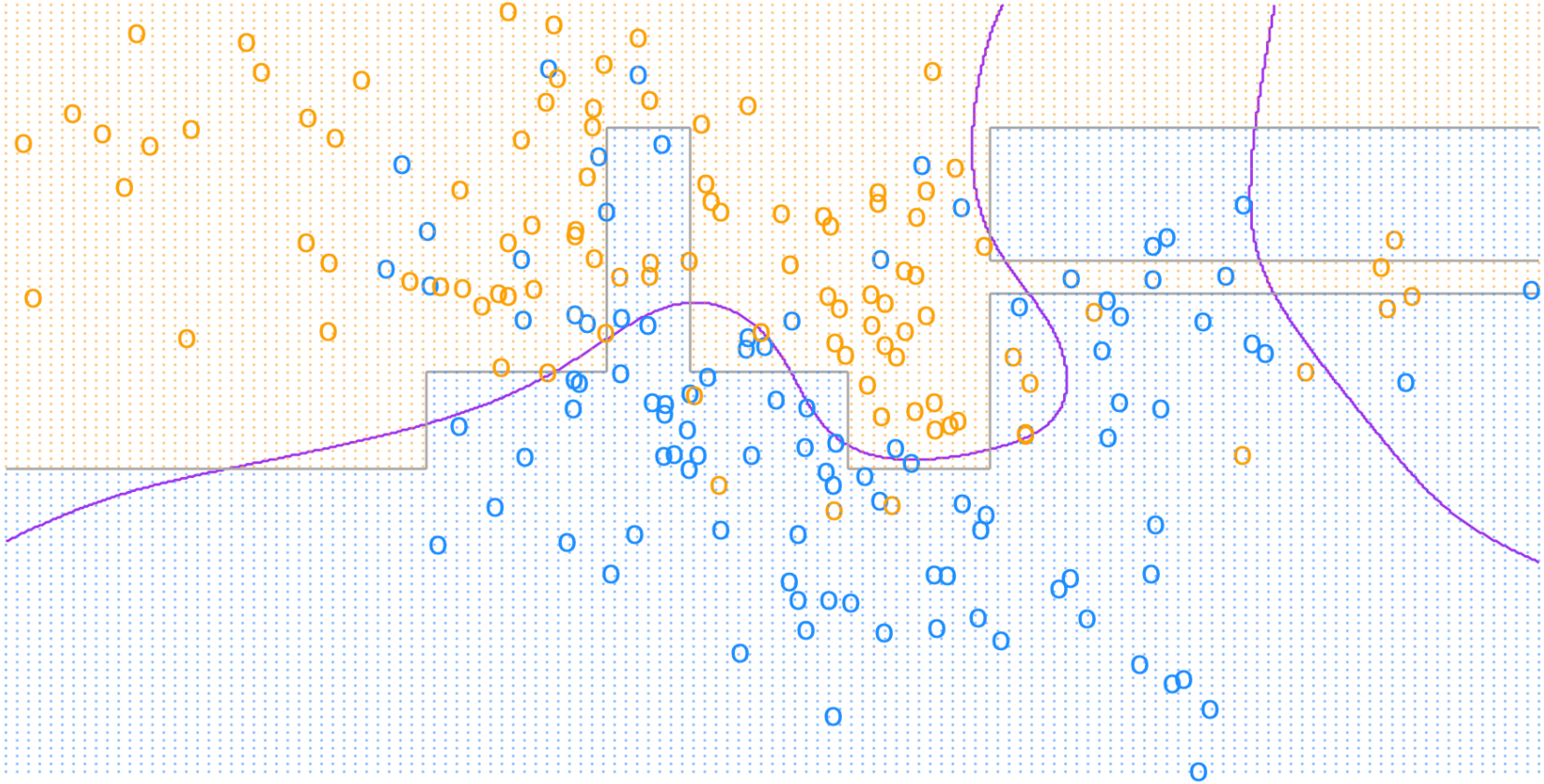
Toy example - Logistic Regression - binning



The empirical risk on testing set is 0.265.

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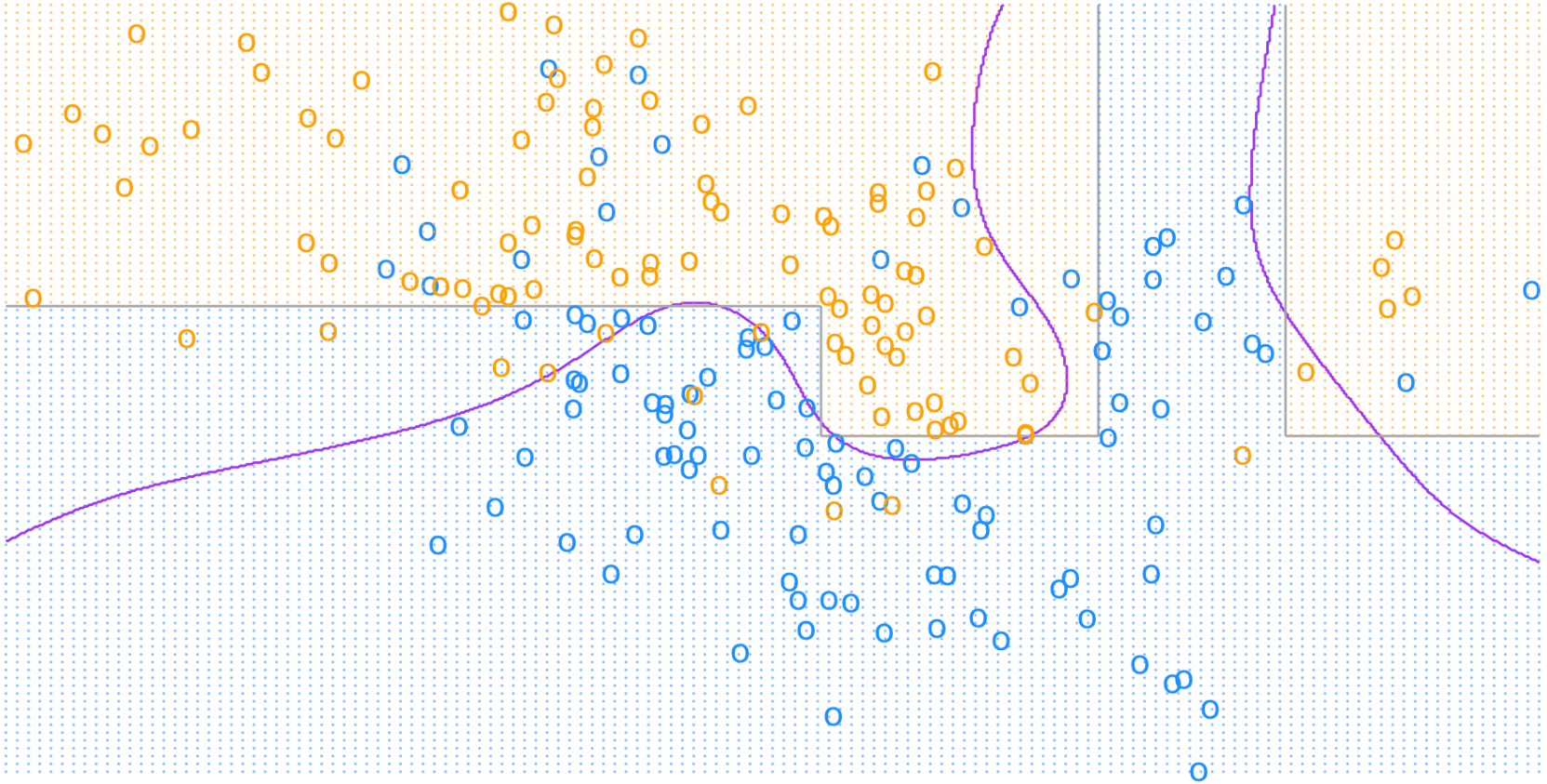
Toy example - Decision Trees



The empirical risk on testing set is 0.247.

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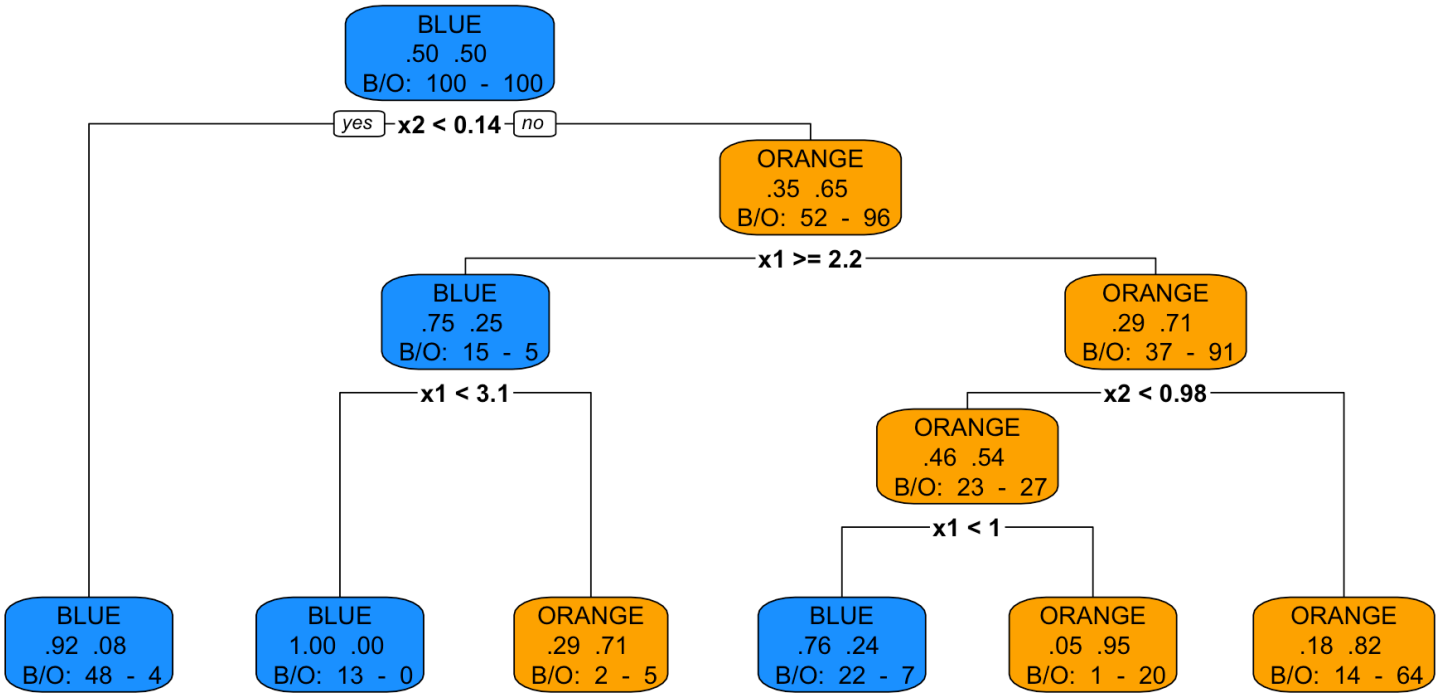
Scoring Toy example - Decision Trees

We show below the previously fitted Decision tree:



How to fit such a tree? What criterion is used?

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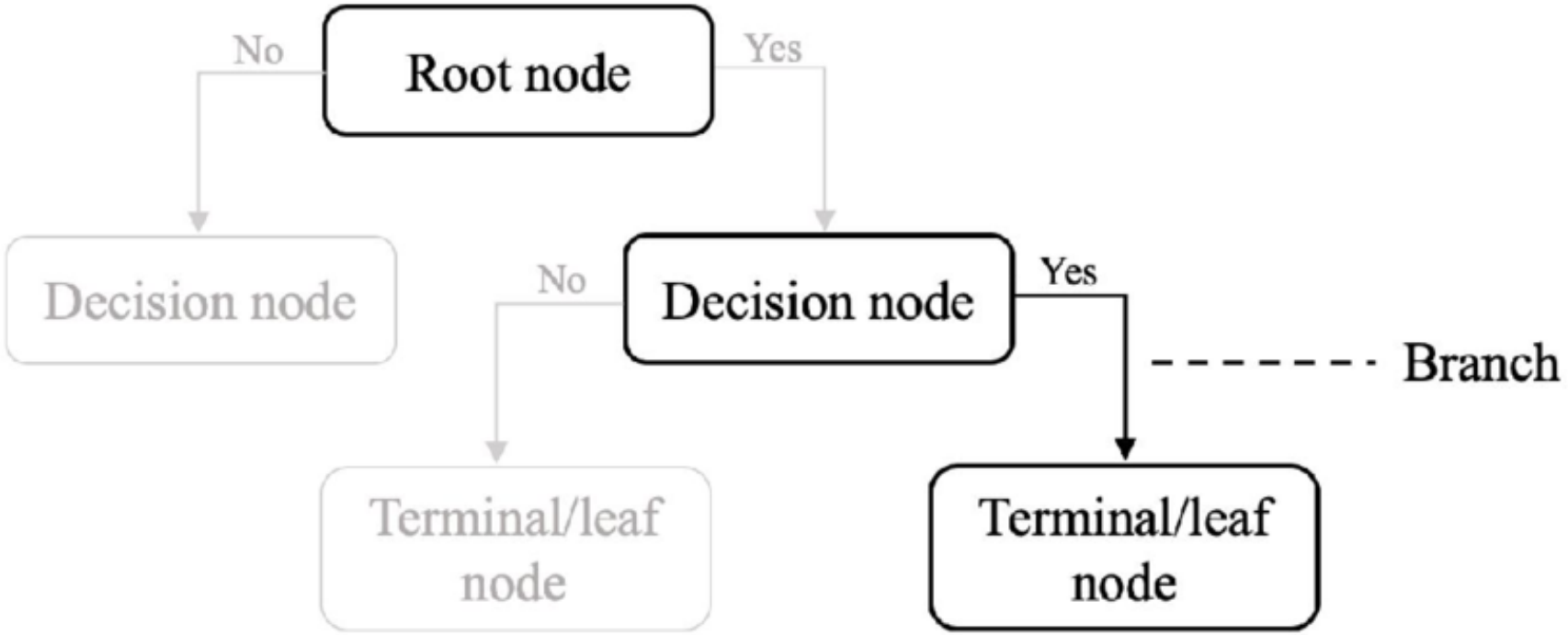
Trees Terminology

Decision trees recursively partition the data by applying specific cutoff values to the features. This process creates various subsets of the data set, with each data point belonging to one of these subsets. The final subsets are known as Terminal or Leaf nodes, while the intermediate ones are referred to as Internal, Split or Decision nodes.



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CART

Classification And Regression Tree (CART) (Breiman et al. (1983)), is a recursive method:

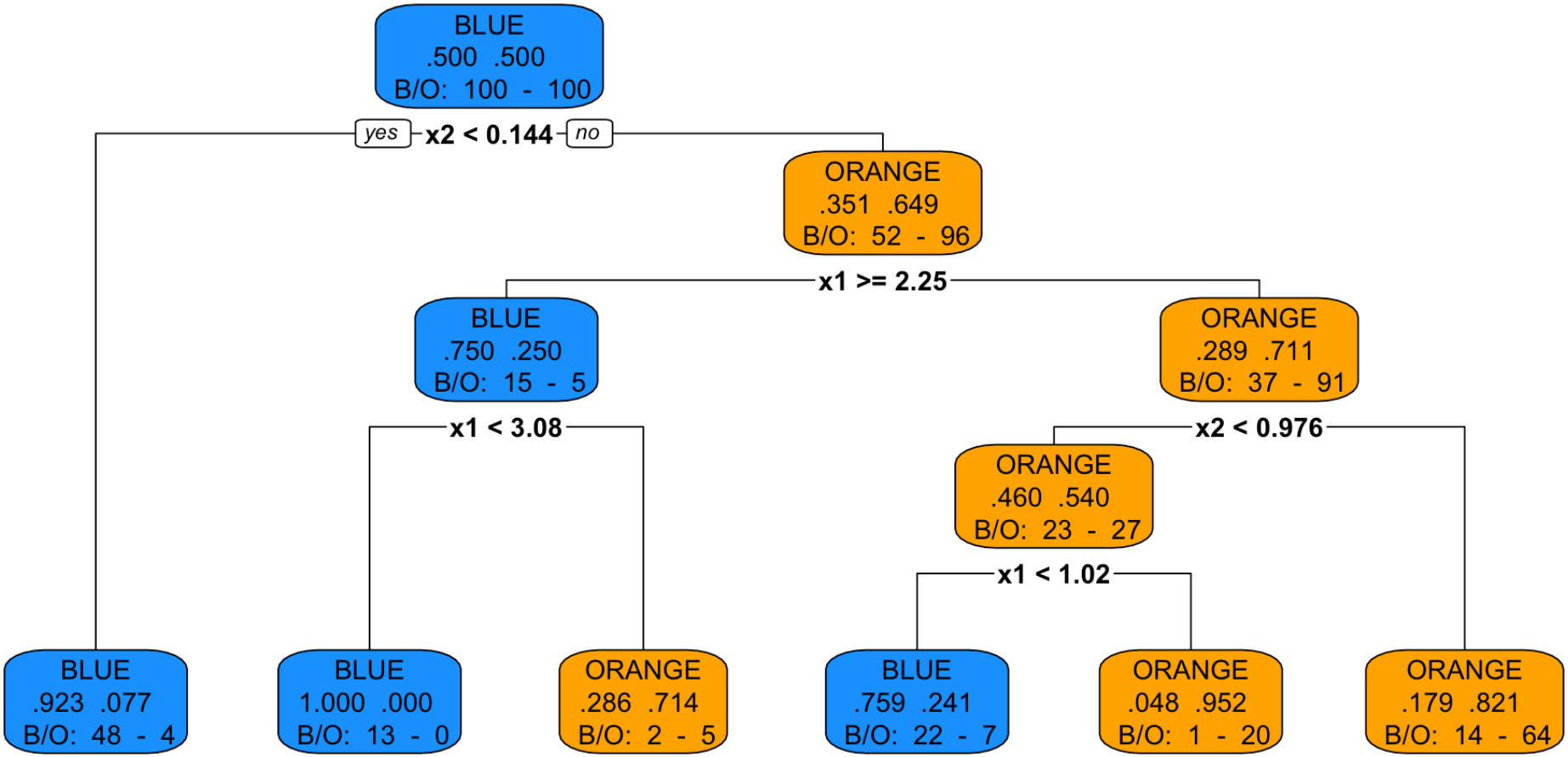
- At the root of the tree we find the entire sample.
- Each node of the tree divides the sample into 2 branches, according to a feature variable (discrete, continuous or ordinal variable (threshold) or a nominal variable (set of categories)).
- A terminal node is called a leaf. Usually the tree is represented upside down with its root at the top

The tree is built by the following process:

- First find the single variable which 'best' **splits** the data into two groups ('best' will be defined later).
- The data is separated, and then this process is applied separately to each sub-group, and so on recursively until a **stopping rule** occurs (either no improvement can be made or the subgroups reach a minimum size).

Decision Trees

CART for Mixture data set



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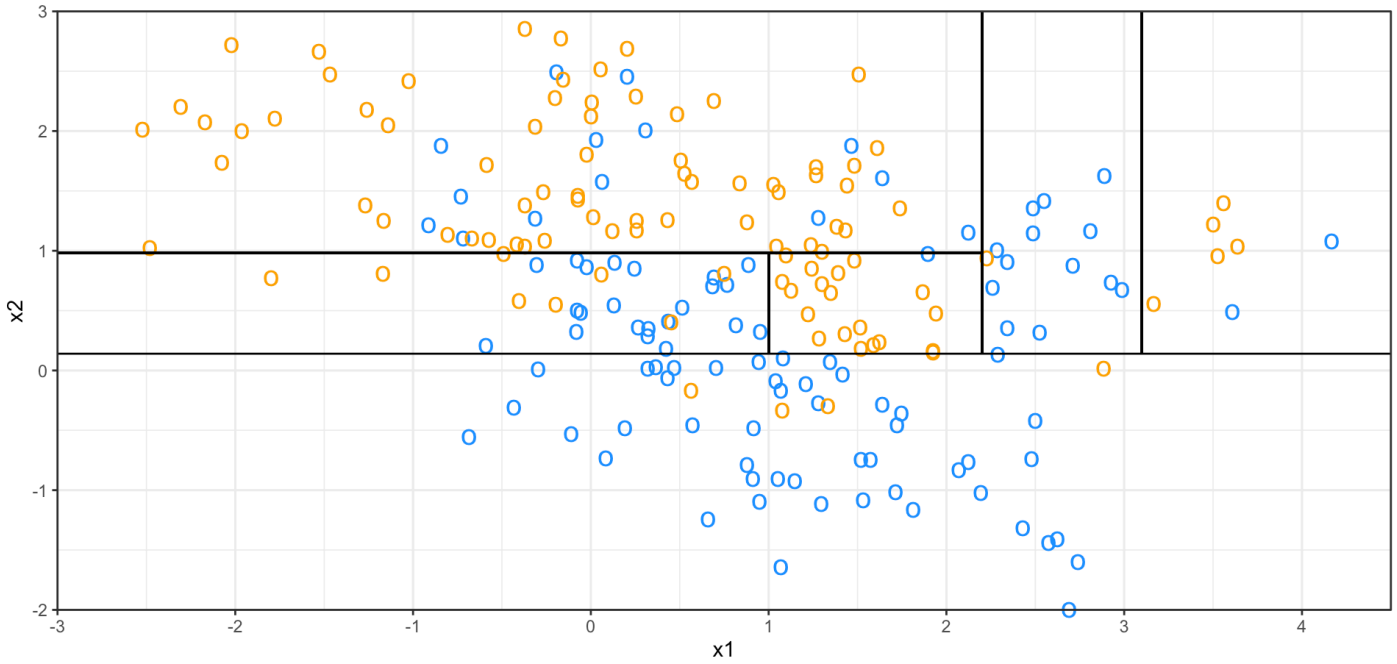
CART for Mixture data set

Starting from the top of the tree and going down the `CART/rpart` algorithm splits at each node according to a binary decision.

It ends up splitting the space into six regions, and then models the output by the mode/majority (classification) or proportion (scoring/probability) of Y in each region:



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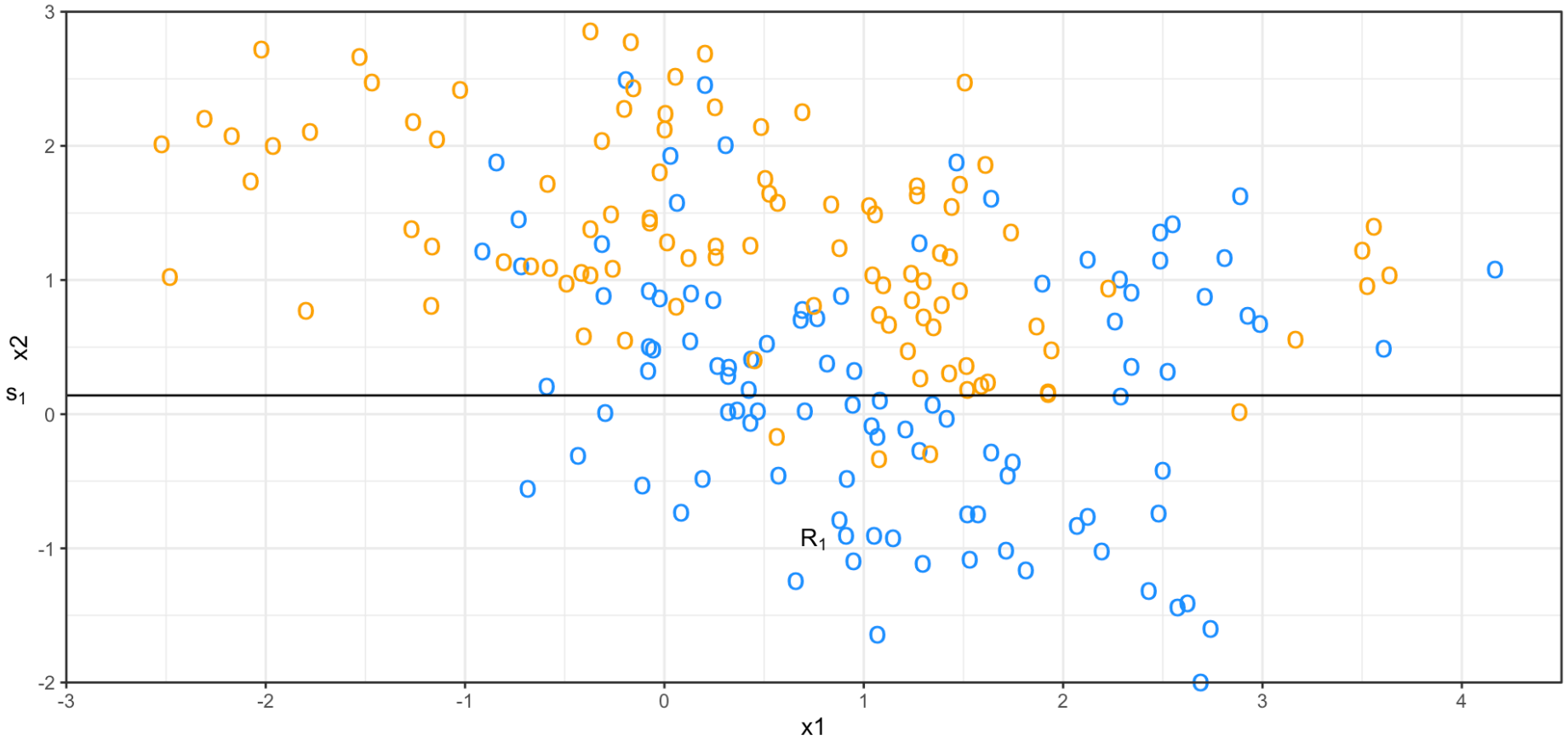
CART for Mixture data set

For example, with the Mixture data, `CART/rpart` first splits at $x_2 = s_1 = 0.14$:



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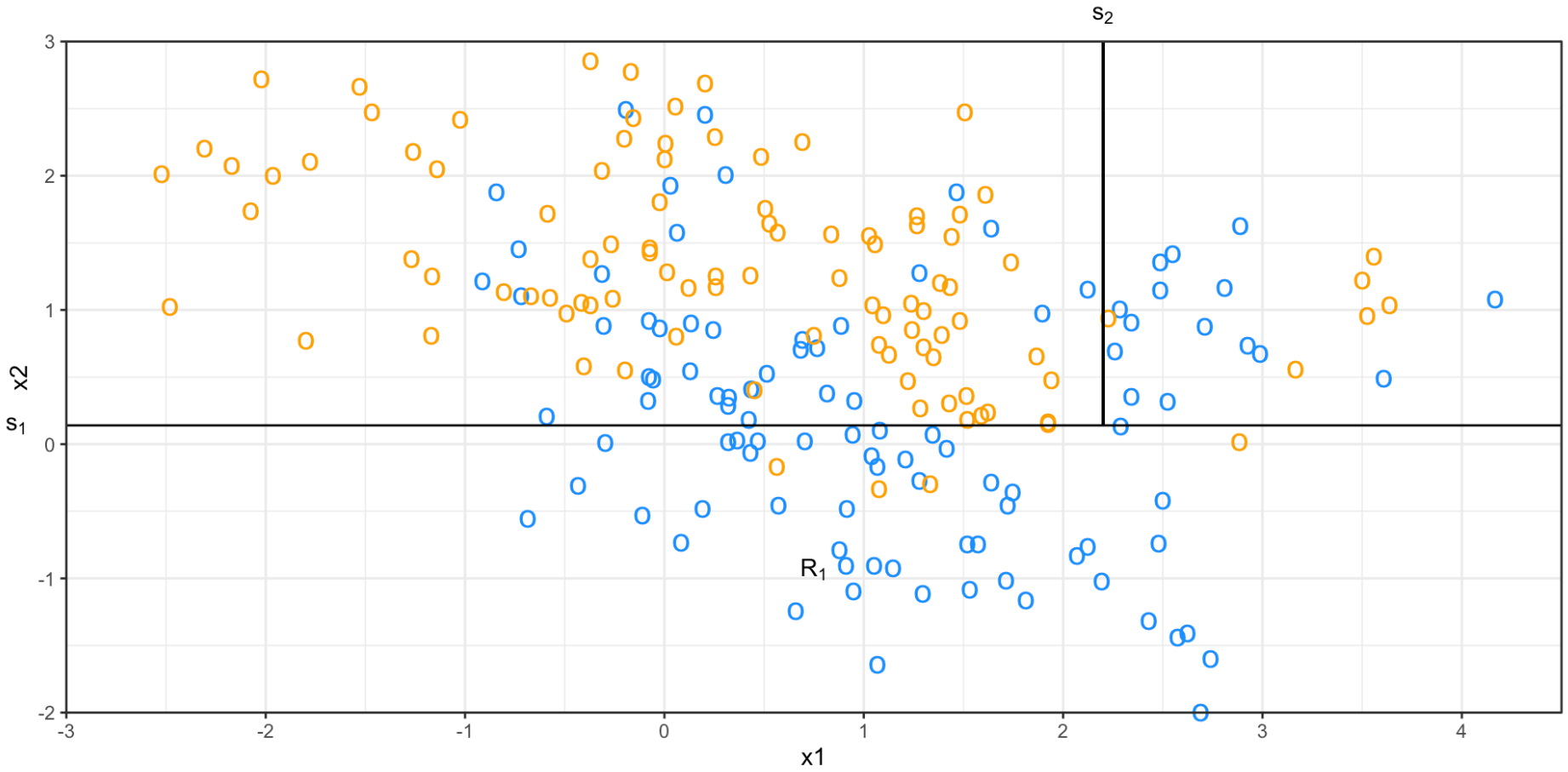
CART for Mixture data set

Then, the region $x_2 \geq s_1$ is split at $x_1 = s_2 = 2.2$:



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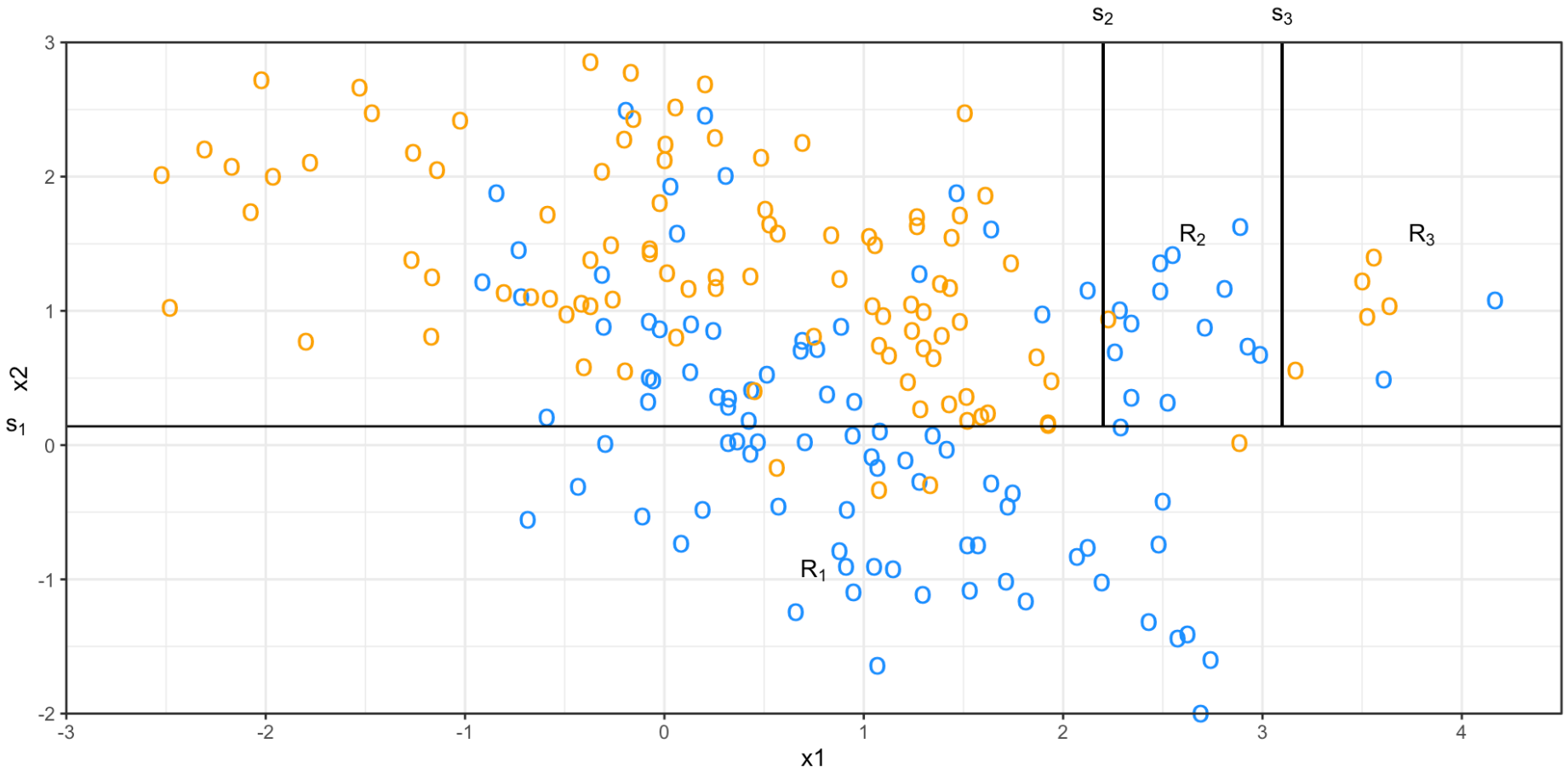
CART for Mixture data set

Then, the region $x_2 \geq s_1,\ x_1 > s_2$ is split at $x_1 = s_3 = 3.1$:



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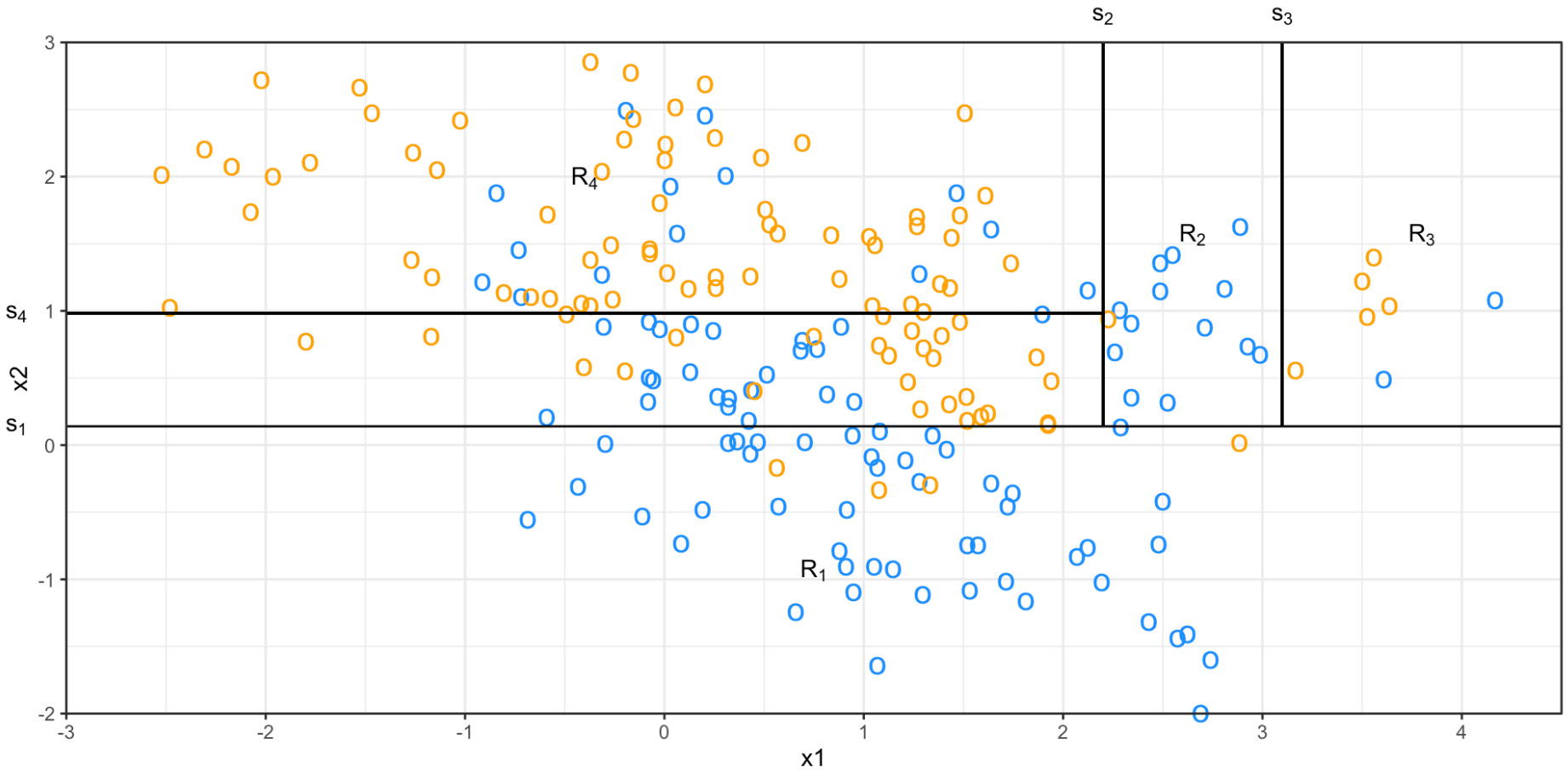
CART for Mixture data set

And the region $x_2 \geq s_1,\ x_1 \leq s_2$ is split at $x_2 = s_4 = 0.98$:



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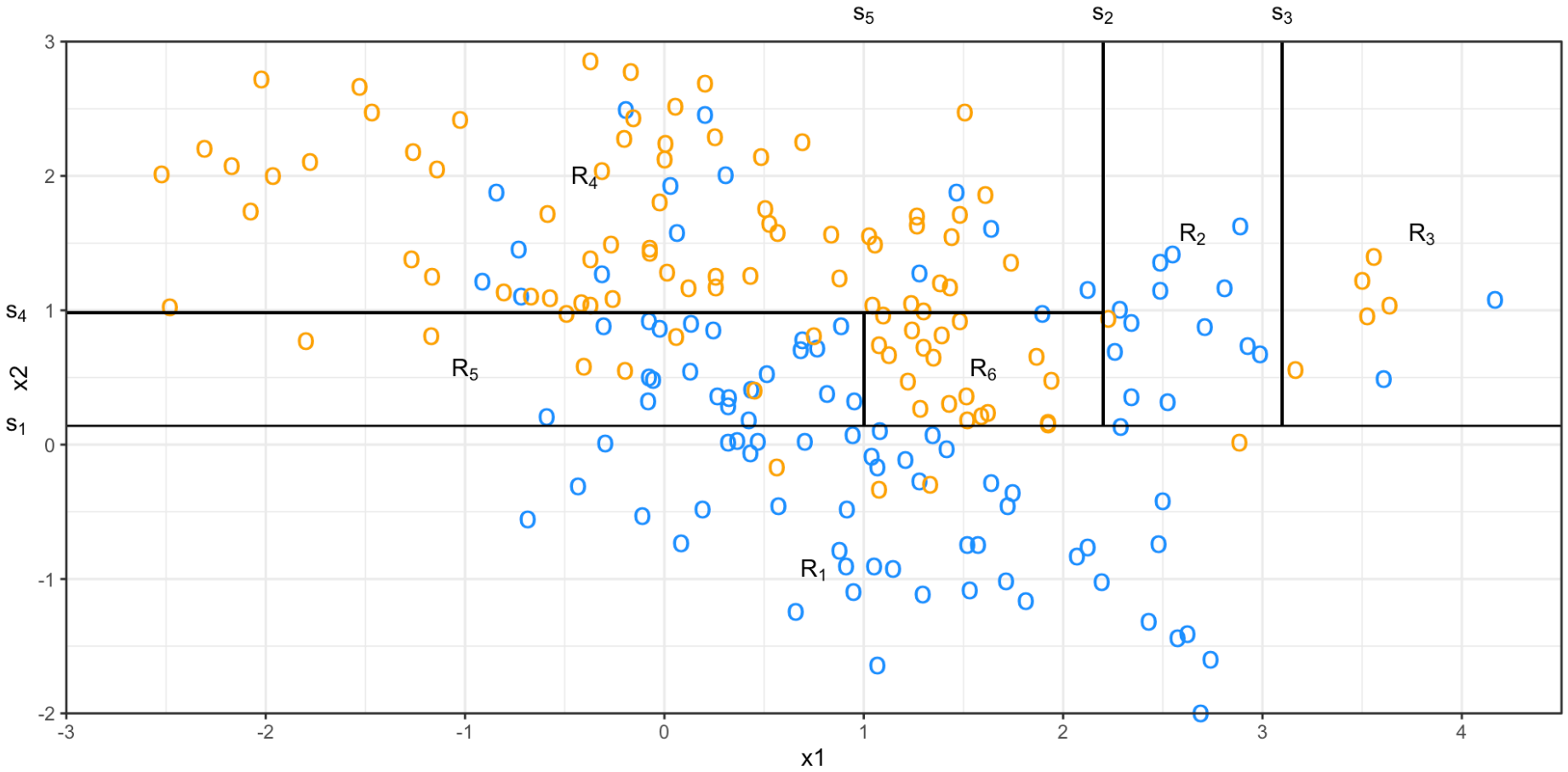
CART for Mixture data set

Finally the region $x_2 \geq s_1,\ x_1 \leq s_2,\ x_2 < s_4$ is split at $x_1 = s_5 = 1$. Resulting in $R_1, R_2, \ldots, R_6$ shown below:



Decision Trees

Splitting criterion

In order to classify well the data, CART seeks as much as possible to obtain pure leaf nodes (i.e. high probability for one class).

At each step CART selects a predictor X_j and a split-point s such that splitting the current region $\mathcal{R}$ into the regions $\mathcal{R}_L(j,s) = \{X|Xj < s\}$ and $\mathcal{R}_R(j,s) = \{X|Xj \geq s\}$ leads to the greatest possible reduction in a well chosen measure of impurity.

Given a leaf node m representing a region R_m containing n_m observations we denote $\mathcal{I}_m$ a measure of node impurity, three measures are usually retained:

- the misclassification error: $\mathcal{I}_m = \frac{1}{n_m} \sum_{x_i \in R_m} \mathbb{1}_{y_i \neq \hat{C}_m} = 1 - \hat{p}^m_{\hat{C}_m} = 1 - \max(\hat{p}^m, 1 - \hat{p}^m)$ the fraction of observations in the region that do not belong to the most common class
- the Gini index: $\mathcal{I}_m = \sum_k \hat{p}^m_k (1 - \hat{p}^m_k) = 2\hat{p}^m(1 - \hat{p}^m)$
- the cross-entropy or deviance: $\mathcal{I}_m = -\sum_k \hat{p}^m_k \log(1 - \hat{p}^m_k) = -\hat{p}^m \log(\hat{p}^m) - (1 - \hat{p}^m) \log(1 - \hat{p}^m)$

where we have denoted $\hat{p}^m = \hat{p}^m_1 = 1 - \hat{p}^m_0$

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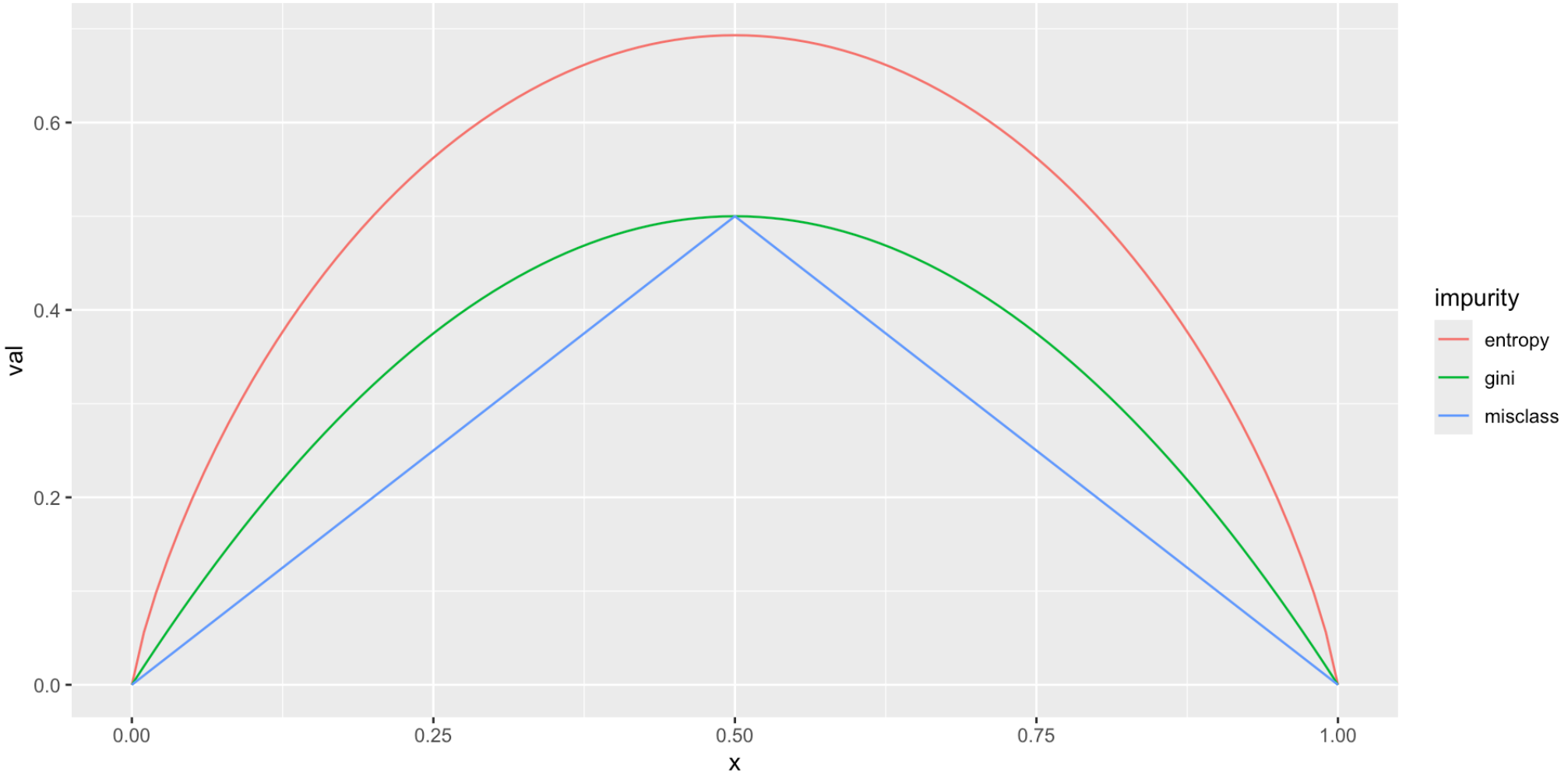
Impurity measures



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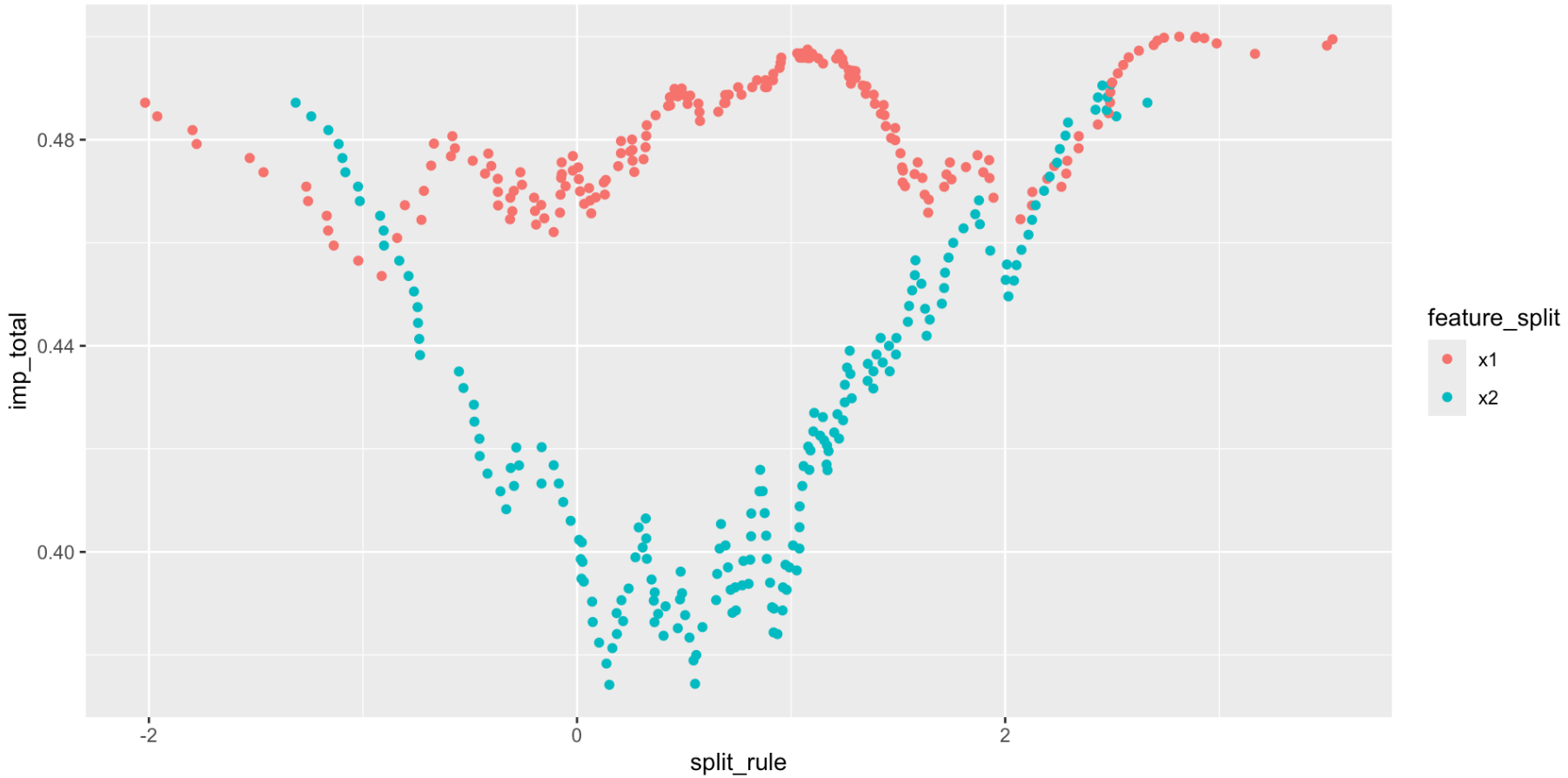
A split example

```
# A tibble: 1 × 6
  feature_split split_rule imp_left imp_right imp_total imp_node
  <chr>              <dbl>    <dbl>     <dbl>     <dbl>    <dbl>
1 x2                 0.151    0.142     0.456     0.374      0.5
```



References

Breiman, L., Friedman, J. H., Olshen, R. A., & Stone, C. J. and. (1983). *Classification and regression trees*. Wadsworth.

Hastie, T., Tibshirani, R., & Friedman, J. (2009). *The elements of statistical learning*. Springer New York. https://doi.org/10.1007/978-0-387-84858-7

James, G., Witten, D., Hastie, T., & Tibshirani, R. (2021). *An introduction to statistical learning: With applications in r*. Springer US. https://doi.org/10.1007/978-1-0716-1418