WB2 - Praca domowa

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1 Dataset description

Let us start with the dataset analysis. Thanks to `mlr::summarizeColumns()` we may notice some pecularities in the dataset *sick*. Firstly, the columns **TBG** and **TBG_measured** contain no information about the samples, as they are consisted of a single value and no value respectively. It gives us a natural reason to remove them from the dataset. Moreover, trying to generate a simple model on the dataset returns an error signalizing a factor level of **hypopituitary** in the testing set with 0 occurrences in the training dataset. Whille more complex predictive models could have easily handled such difference, as we are limited to simple models, we therefore decide to remove **hypopituitary** from the dataset.

	name	type	na	mean	disp	median	mad	min	max	nlevs
1	age	numeric	0	51.5185676	18.905797370	54.00	22.23900	1.000	94.00	0
2	sex	factor	119	NA	NA	NA	NA	906.000	1991.00	2
3	on_thyroxine	factor	0	NA	0.122015915	NA	NA	368.000	2648.00	2
4	query_on_thyroxine	factor	0	NA	0.012599469	NA	NA	38.000	2978.00	2
5	on_antithyroid_medication	factor	0	NA	0.012267905	NA	NA	37.000	2979.00	2
6	sick	factor	0	NA	0.037466844	NA	NA	113.000	2903.00	2
7	pregnant	factor	0	NA	0.014588859	NA	NA	44.000	2972.00	2
8	thyroid_surgery	factor	0	NA	0.013594164	NA	NA	41.000	2975.00	2
9	I131_treatment	factor	0	NA	0.016246684	NA	NA	49.000	2967.00	2
10	query_hypothyroid	factor	0	NA	0.063992042	NA	NA	193.000	2823.00	2
11	query_hyperthyroid	factor	0	NA	0.062665782	NA	NA	189.000	2827.00	2
12	lithium	factor	0	NA	0.004641910	NA	NA	14.000	3002.00	2
13	goitre	factor	0	NA	0.009615385	NA	NA	29.000	2987.00	2
14	tumor	factor	0	NA	0.023872679	NA	NA	72.000	2944.00	2
15	hypopituitary	factor	0	NA	0.000000000	NA	NA	0.000	3016.00	1
16	psych	factor	0	NA	0.049734748	NA	NA	150.000	2866.00	2
17	TSH_measured	factor	0	NA	0.099801061	NA	NA	301.000	2715.00	2
18	TSH	numeric	301	5.2005672	26.407995825	1.30	1.48260	0.005	530.00	0
19	T3_measured	factor	0	NA	0.205901857	NA	NA	621.000	2395.00	2
20	T3	numeric	621	2.0174948	0.831273637	2.00	0.59304	0.050	10.60	0
21	TT4_measured	factor	0	NA	0.063328912	NA	NA	191.000	2825.00	2
22	TT4	numeric	191	108.5881416	35.591033048	104.00	26.68680	2.000	430.00	0
23	T4U_measured	factor	0	NA	0.104774536	NA	NA	316.000	2700.00	2
24	T4U	numeric	316	0.9963719	0.195110285	0.98	0.14826	0.250	2.32	0
25	FTI_measured	factor	0	NA	0.104111406	NA	NA	314.000	2702.00	2
26	FTI	numeric	314	110.5655811	32.879337473	107.00	22.23900	2.000	395.00	0
27	TBG_measured	factor	0	NA	0.000000000	NA	NA	3016.000	3016.00	1
28	TBG	numeric	3016	NaN	NA	NA	NA	Inf	-Inf	0
29	referral_source	factor	0	NA	0.420755968	NA	NA	29.000	1747.00	5
30	Class	factor	0	NA	0.061007958	NA	NA	184.000	2832.00	2

Figure 1: Training dataset summary

Many columns contain true/false labels as factors. To tidy up the dataset, we convert all the factor labels to numerical labels.

2 A simple model

Before any pre-processing, it is worth to check a simple model's performance. We will use a decision tree from **rpart** package.

```
tsk <- makeClassifTask(data = datTrainF, target = "Class", positive = "1")
lrn <- makeLearner("classif.rpart", predict.type = "prob")
resample(lrn, tsk, cv5, list(mlr::auc, auprc))
```

The above model - a simplest implementation with default hyperparameters - yields surprisingly good results: 96% AUC and 87% AUPRC. Although these number are quite big, we wish to improve the model nonetheless.

3 Feature selection

Let us check, whether there are features in the dataset having a negative impact on the prediction. We will use a natural Feature Importance measure for the decision tree based on the impurity measure.

```
validIX <- datTrainF$Class %>% createDataPartition(p = 0.8, list = FALSE)

train <- datTrainF[validIX,]
test <- datTrainF[-validIX,]

rp <- rpart(Class~., data = train, model = TRUE)
pred <- predict(rp, test)

s <- summary(rp)
```

The **summary** object returns the Feature Importance values for every variable. Since only 9 variables achieves the FI measure higher than 1, we may compare the prediction on a dataset without the rest of the columns with our previous prediction.

```
s$variable.importance
nm <- names(s$variable.importance[1:9])
nm[10] <- "Class"
datTrainN <- datTrainF[,nm]

tsk <- makeClassifTask(data = datTrainN, target = "Class", positive = "1")
lrn <- makeLearner("classif.rpart", predict.type = "prob")
resample(lrn, tsk, cv5, list(mlr::auc, auprc))
```

the above model, despite having removed 17 (1) columns, yields very similar results to the previous simple model **AUC** equal 95.8% and **AUPRC** equal 87.6%. Therefore, it suffices to continue our feature engineering on the smaller dataset, as we likely will reduce any noise in the dataframe without loss of efficiency. The variables left are: "T3", "TT4", "TSH", "FTI", "referral_source", "on_thyroxine", "T3_measured", "age", "T4U", "Class" (ordered by measured Feature Importance).

4 Data imputation

Next, we shall look into missing data, which is quite often on the dataset. Although the decision tree works fine on such datasets, imputing the data may improve models' accuracy. We will test two variants of the imputation - a classic, common one, and imputation with predictive models.

4.1 Classic imputation

In the classic imputation process with replace the missing values with:

- a mode - for categorical data,
- a mean - for numerical data.

```
datTrainI <- impute(datTrainN, classes = list(numeric = imputeMean(),
                                              factor = imputeMode()))$data
```

the above imputation has not yielded expected results: on the cross-validated dataset we achieved 95.5% **AUC** and 87.4% **AUPRC**. We might as well have done nothing.

4.2 Imputation with predicted values

The idea behind this variant is using predictive models to fill out the blank spots. For each column with missing data, we generate another decision tree model predicting the missing values. An important question is whether to start filling the data from the most important columns or inversely, from the least important. It is crucial due to the fact that the most important variable, namely **T3**, contains more 600 missing values. As the columns in the dataset are now ordered with the importance, we need to choose to start from either side. Both ideas have upsides and downsides; however, due to the fact that our most important variable nas so many NAs, we decide to start filling the dataset from the most important ones. This is because if we were to start from the least important ones, we would fill over 600 spots in **T3** with predictions based on predictions based on predictions .... We would therefore risk heavily biasing the data.

```
genData <- function(dat, name){
  datToImpute <- dat[is.na(dat[name]),]
  datFull <- dat[!is.na(dat[name]),]
  n <- nrow(datFull)


  if(class(unlist(c(datFull[name]))) == "factor"){
    print("Class: factor")
    tsk <- makeClassifTask(id = name, datFull, name,
                           fixup.data = "no", check.data = FALSE)
    lr <- makeLearner("classif.rpart")
  }else{
    print("Class: numeric")
```

```
    tsk <- makeRegrTask(id = name, datFull, name,
                        fixup.data = "no",check.data = FALSE)
    lr <- makeLearner("regr.rpart")
  }
  model <- mlr::train(lr, tsk)
  pred <- as.data.frame(predict(model,
                                newdata = datToImpute %>% select(-name)))
  colnames(pred) <- c(name)
  nd <- cbind(datToImpute %>% select(-name), pred)
  nd <- nd[colnames(datFull)]
  rbind(datFull, nd)
}
```

The above function generates a new dataset with imputed values of the "name" column. Iterating on the column set of the dataset, it allows us to fill all the blank spaces. Such imputation resulted in our first success, when it comes to improving the measures' values: **AUPRC** went up more than 1 percentage point, achieving 88.6%. **AUC** remains almost unchanged with 96.4%.

5 Variable discretization

Motivated with previous success we then proceed to data discretization - it may improve the model's efficiency, by transforming numerical data into categorical.

```
require(arules)
datTrainD <- datTrainI
datTrainD$age <- discretize(datTrainD$age, breaks = 5,
                            labels = c(0, 1, 2, 3, 4))
```

We present an example of **age** discretization. We repeated the above process for each numerical variable separately (only one variable was discretized at a time). We came to the conclusion that the idea was hopeless and yielded no positive results.

6 Hyperparameter tuning

What remains is hyperparameter tuning to maximize the **AUPRC** value. I use the bayesian optimisation from `mlrMBO` package. Our search space is following:

- `minsplit` - from 1 to 30,
- `cp` - from 0 to 1,
- `maxcompete` - from 0 to 10,
- `usesurrogate` - values: 0, 1 and 2,
- `maxdepth` - from 1 to 30

We use 100 iterations in the optimisation process

```
train <- datTrainI[validIX,]
test <- datTrainI[-validIX,]

tsk <- makeClassifTask(data = train, target = "Class", positive = "1")

rp <- makeSingleObjectiveFunction(name = "rpart.tuning",
                      fn = function(x) {
                      lrn <- makeLearner("classif.rpart",
                                      par.vals = x, predict.type = "prob")
                      m <- mlr::train(lrn, tsk)

                      pred <- predict(m, newdata = test)
                      prob <- getPredictionProbabilities(pred)

                      fg <- prob[test[,"Class"] == 1]
                      bg <- prob[test[,"Class"] == 0]
                      pr <- pr.curve(scores.class0 = fg,
                                      scores.class1 = bg, curve = F)
                      pr$auc.integral
                      },
                      par.set = par.set,
                      noisy = TRUE,
                      has.simple.signature = FALSE,
                      minimize = FALSE
)
ctrl = makeMBOControl()
ctrl = setMBOControlTermination(ctrl, iters = iters)
res = mbo(rp, control = ctrl, show.info = TRUE)
```

The above optimisation algorithm was not able to find a better set of parameters than the default one - the maximum of **AUPRC** found was 84%, significantly below our previous results.

7 Decision Tree Regressor

To finish our research, we propose to use a Decision Tree Regressor instead of Decision Tree Clasifier to predict the target values. As the values are convieniently mapped to 0 and 1 values and the DTR model won't produces values outside of the $[0, 1]$ interval in that dataset, we may therefore tahe the returned value for each sample as a probability of belonging the the positive class. We will produce the results for three variants of DTR optimisation:

7.0.1 Variant 1

In the first variant we minimize **AUPRC** for a prediction of separate testing subset of the training dataset, which is invariant to the optimising process iterations. While we

have achieved extremely high results (99% **AUPRC**), the model overfitted quite easily. We achieved much lower results on the testing dataset than the standard classification yielded.

7.0.2 Variant 2

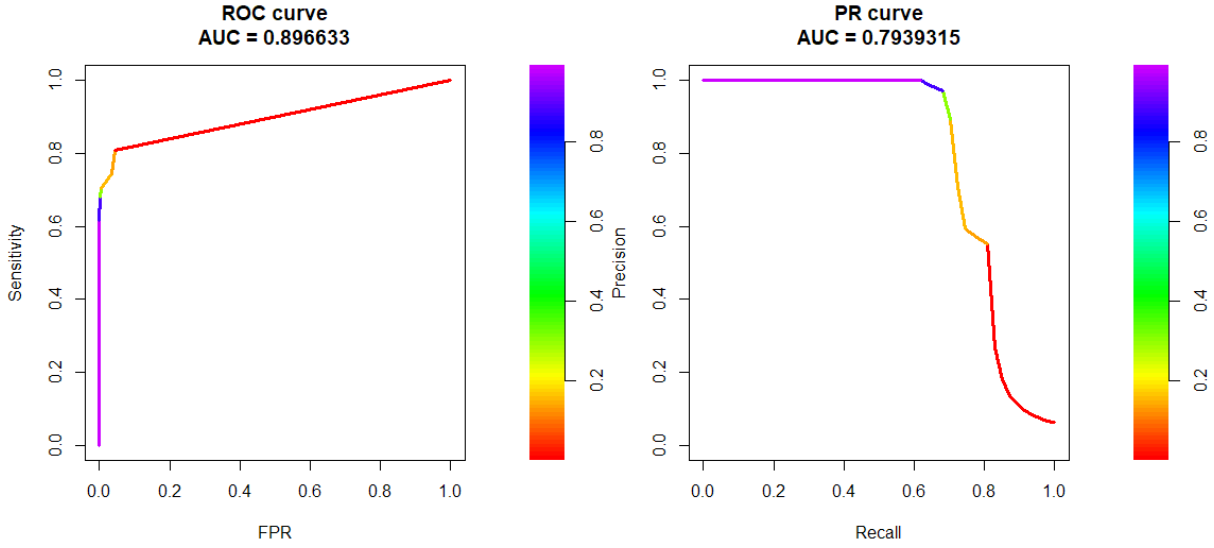
In the second variant we optimised the cross-validated measure on the training dataset. After optimisation, we have achieved almost 93% **AUPRC**; however, the model was poorly fit to the testing dataset, reaching 87.5% **AUPRC** - the overfitting happened once again.

7.0.3 Variant 3

In the third variant we do not optimise the parameters and generate a model on almost raw data achieved after the basic pre-processing. It gave absolutely best effect on the testing dataset: 92.4% **AUPRC** and 97.6% **AUC**

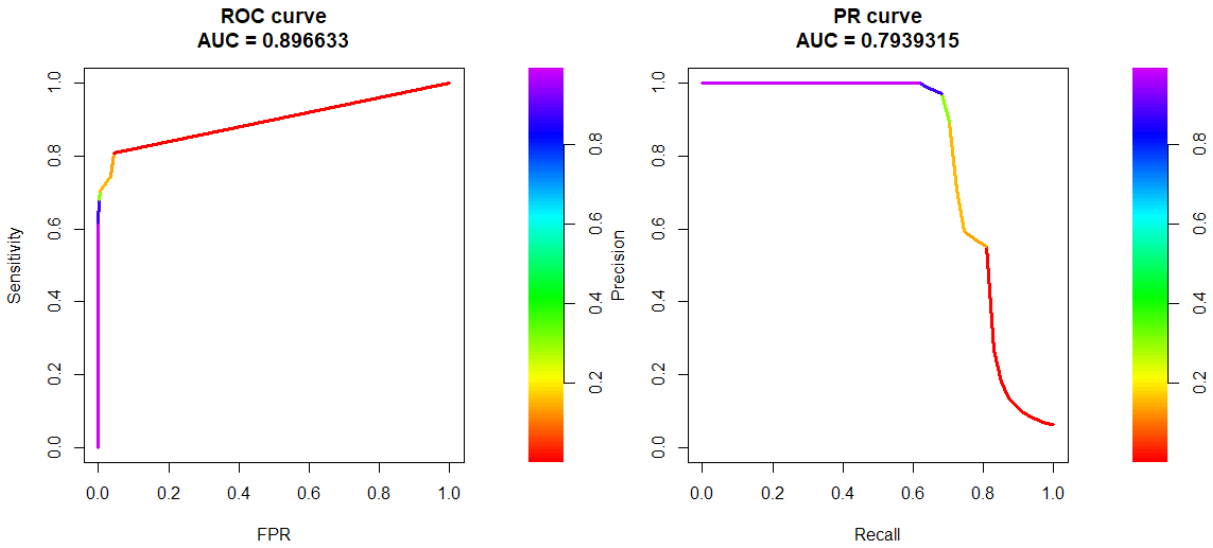
8 Combined results

For each above-presented engineering and processing operation we may now summarize achieved results on the testing dataset.



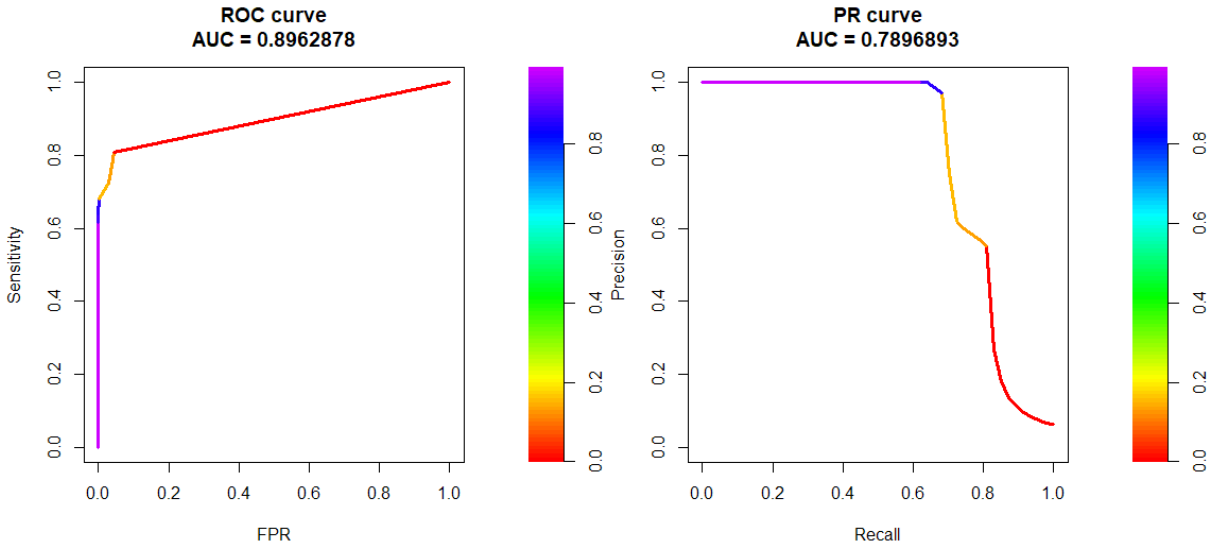
(a) ROC of the basic model

(b) PRC of the basic model



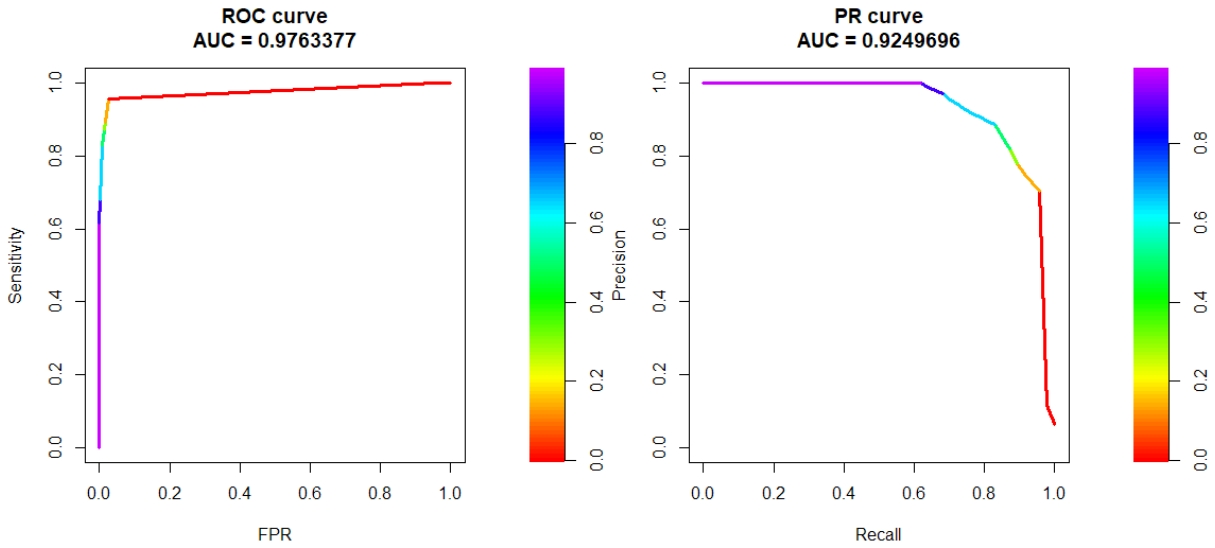
(a) ROC after feature removal

(b) PRC after feature removal



(a) ROC after imputation

(b) PRC after imputation



(a) ROC of DTR

(b) PRC of DTR

Having completed the analysis, we conclude that the decision tree classicator achieved its possible maximal efficiency, since the differences between presented models are almost insignificant. However, treating the problem as a regression problem instead of classification yields surprisingly high results. Although the model exhibited a tendency to overfit easily, it is worth to research it further, as it seems to be an unexpected ally in anomaly detection.

9 Black box models' comparison

We will now proceed to comparing our previous model with more advanced black box models. We will look into four models' performances, namely: Bayesian Additive Regression Trees (BART), Gradient Boosting Machine (GBM), Random Forest (RF), and Propositional Rule Learner (JRip). We will conduct the research in three variants: in the first variant, the models are trained on the default parameters; in the second variant, we use Bayesian optimization process to maximize the AUPRC; in the third variant, we use train the models as if the task was a regression problem instead of classification one. In case of Decision Tree, it yielded surprisingly good results - we shall check whether the improvement happens for the black box models as well.

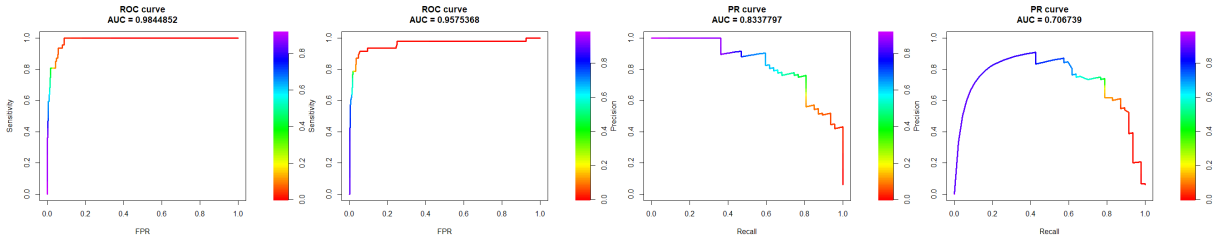
10 Variant I

In the first variant, we train the black box models without any hyperparameter tuning. It will serve as a starting point to in-between variants comparison, as well as a basic experiment to verify their superiority over the Decision Tree Classifier presented previously. Curiously, only the Random Forest achieved higher values of AUC and AUPRC than the previous DTR model. Bart machine achieved a bit higher AUC, however the AUPRC value is lower; nonetheless, all the black boxes but JRip achieved significantly higher AUPRC value on the cross-validated set than the decision tree classifiers, while JRip yielding comparable results. Let us look into the models' ROC and PR curve on the

	AUC	AUPRC
DTR	0.976	0.927
BART	0.982	0.885
GBM	0.953	0.861
RF	0.996	0.956
JRip	0.940	0.774

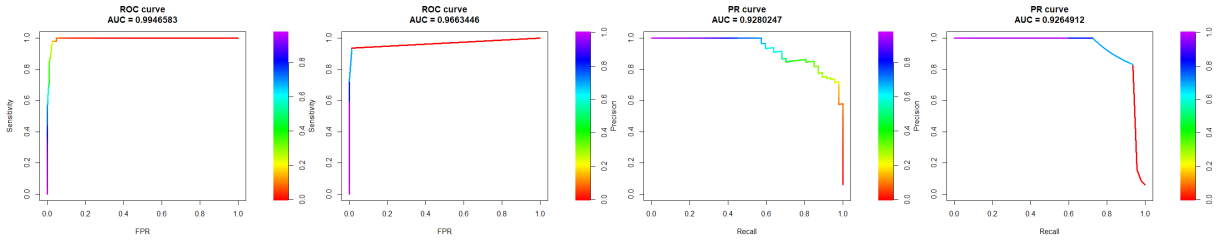
Table 1: Comparison of the black box models' performances on cross-validation with the previous DTR model

testing dataset.



(a) BART ROC AUC = 0.984 (b) GBM ROC AUC = 0.958 (c) BART PR AUPRC = 0.834 (d) GBM PR AUPRC = 0.707

Figure 6: BART and GBM on the testing dataset



(a) RF ROC AUC = 0.995 (b) JRip ROC AUC = 0.966 (c) RF PR AUPRC = 0.928 (d) JRip PR AUPRC = 0.926

Figure 7: RF and JRip on the testing dataset

Interestingly, BART and GBM, the models which performed quite nicely on the resampled training dataset, yielded much worse results on the testing dataset when it comes to the AUPRC measure. Additionally, the GBM model behaves unexpectedly out of order for low recall values. Moreover, JRip model, which gave the worst results on the cross-validation, is now head to head with RF on the testing dataset. We also prefer the JRip model over RF due to much more regular behaviour of the PR curve. In comparison with DTR, we see that RF model is only slightly better: 99.5% AUC and 92.8% AUPRC compared to 97.6% AUC and 92.4%.

11 Variant II

We now proceed to tuning the black box models with the Bayesian optimization on a three-fold cross-validation. We again use the `mlrMBO` package, restricting the possible parameters' values to:

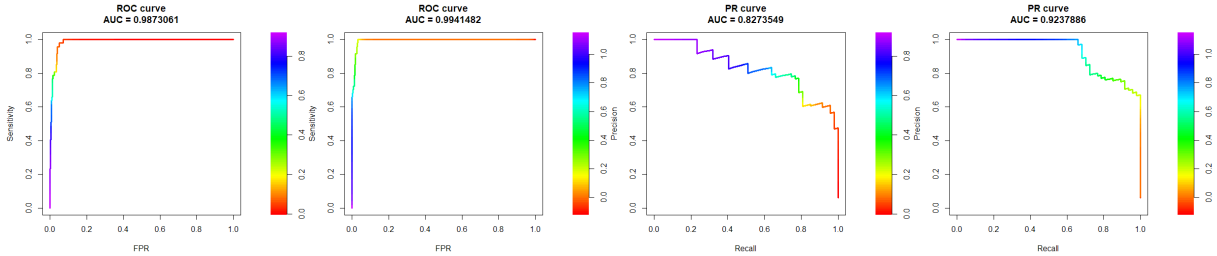
- BART:
  - `num_trees` - from 50 to 80,
  - `alpha` - from 0.5 to 1,
  - `beta` - from 1 to 3,
  - `prob_rule_class` - from 0.4 to 0.6
- GBM:
  - `distribution` - bernoulli or gaussian,
  - `interaction.depth` - from 1 to 3,
  - `shrinkage` - from 0.05 to 0.2,
- RF:
  - `nodesize` - from 1 to 3,
  - `nsplit` - from 0 to 2,
- JRip:
  - `F` - from 2 to 10,
  - `N` - from 1 to 10,
  - `O` - from 1 to 10.

After the optimization process, the models achieved following results (DTR for comparison): We may observe that almost all of the results are at least slightly better than before.

	AUC	AUPRC
DTR	0.976	0.927
BART	0.985	0.906
GBM	0.992	0.961
RF	0.997	0.961
JRip	0.936	0.800

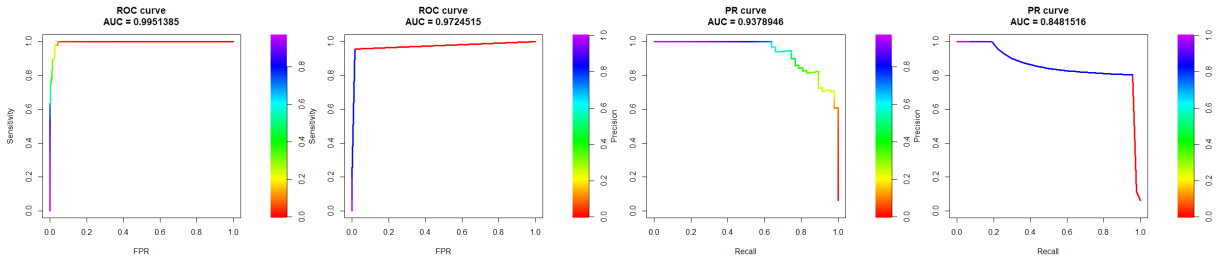
Table 2: Comparison of the black box models' performances after Bayesian optimization on cross-validation with the previous DTR model

We should especially note the ten percentage points increase in the GBM's AUPRC value, as well as four percentage points increase in its AUC value. However, this deos not yet indicate that the models will perform better on the testing dataset. Let us take a look at ROC and PR curve on the testing datasets:



(a) BART ROC AUC = 0.987 (b) GBM ROC AUC = 0.994 (c) BART PR AUPRC = 0.827 (d) GBM PR AUPRC = 0.924

Figure 8: BART and GBM on the testing dataset



(a) RF ROC AUC = 0.995 (b) JRip ROC AUC = 0.972 (c) RF PR AUPRC = 0.938 (d) JRip PR AUPRC = 0.848

Figure 9: RF and JRip on the testing dataset

While the RF model remains a clear winner, having achieved almost 94% AUPRC on the testing dataset, we should note the big switch between GBM and JRip. GBM has achieved over 99% AUC and over 92% AUPRC, while the JRip model fell harshly from 92.6% AUPRC to only 84.8%. The optimization process did not help with fixing the PR curve of BART model, it still presents high irregularity.

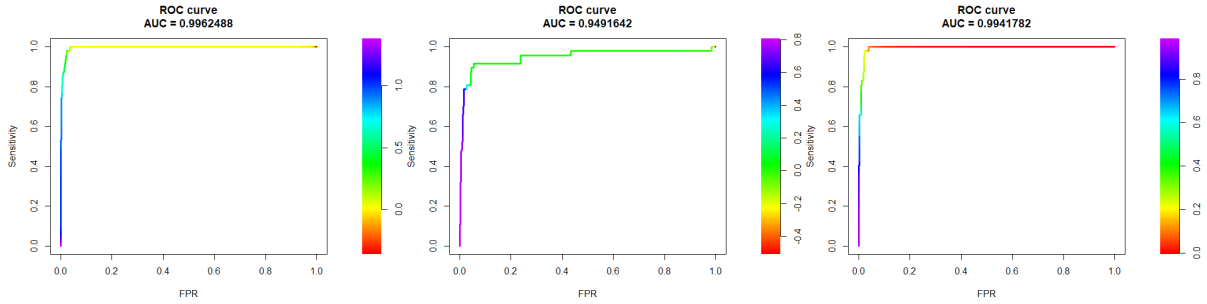
12 Variant III

Lastly, we shall create predictive models trained as if the task was a regression instead of classification. We should note that the JRip model does not have a direct equivalent solving regressive task, therefore we are restricted to the remaining three models: Random Forest Regressor, BART Regressor and GBM Regressor. We present the results in the table below (wth DTR for comparison):

	AUC	AUPRC
DTR	0.976	0.927
BART	0.990	0.948
GBM	0.959	0.835
RF	0.996	0.948

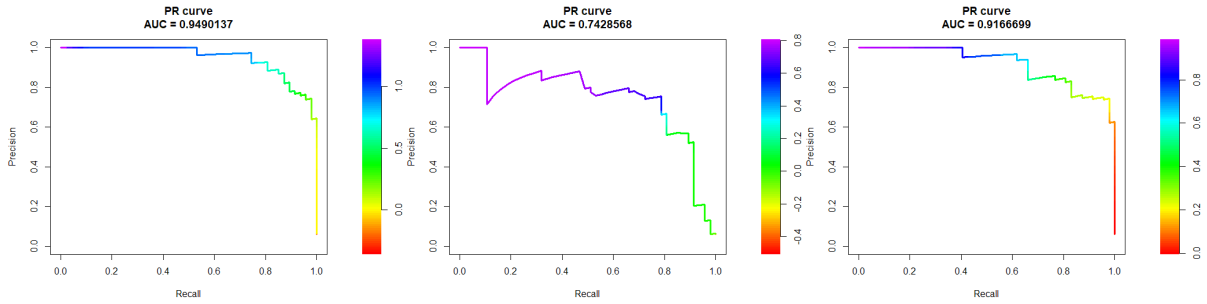
Table 3: Comparison of the regressive black box models' performances on cross-validation with the previous DTR model

The effect of using regressive models may be clearly seen - while it provided no increase in the results of GBM model, we may notice very high values of AUPRC and AUC of the BART machine, as well as high values of these measures for RF model. We may therefore hope for an increase in performance on the testing dataset.



(a) BART ROC AUC = 0.996 (b) GBM ROC AUC = 0.949 (c) RF ROC AUC = 0.994

Figure 10: ROC and AUC of the regressive models



(a) BART PRC AUPRC = 0.949 (b) GBM PRC AUPRC = 0.743 (c) RF PRC AUPRC = 0.917

Figure 11: PRC and AUPRC of the regressive models

While the GBM model clearly is not fit to be used as a regressive model in a classification task, achieving only 74% AUPRC, the remaining two models did better - BART's AUPRC equal to 94.9% is the highest result so far, proving the efficiency of tree-based predictive models in such odd setup. The RF Regressor, although the model proved its efficiency before, now has achieved slightly worse results, pointing toward possible overfitting; as we noted in the previous sections, the Decision Tree Regressors were highly prone to overfitting. However, it seems that Bayesian Additive Regressive Trees are invulnerable to the effect, yielding surprisingly good results.

To summarize all the experiments, we may expect sligtly better results from the black box models than from the Decision Tree Regressor, however the differences in AUPRC are low - our best black box model has achieved 94.9% AUPRC in comparison to DTR's 92.7% on the testing dataset. Nonetheless, an important observation is that not only decision trees, but also other tree-based models tend to yield better results in two-valued classification tasks when used as regressive models.

Potwierdzam samodzielność powyższej pracy oraz niekorzystanie przeze mnie z niedozwolonych źródeł - Łukasz Brzozowski