National Research Tomsk State University

Лаборатория анализа данных физики высоких энергий Томского государственного университета

Measurement of differential cross-sections of a single top quark produced in association with a W boson with ATLAS at $\sqrt{s} = 13$ TeV

Progress Report

Neda Firoz

Goal: separate **tW (top+anti-top)** from **$t\bar{t}$** in the **1j1b dilepton** region

•**Inputs (9 variables used):**
bdt_centrality_ll_recalc_NOSYS,
bdt_delta_pT_ll_MET_recalc_NOSYS,
bdt_delta_pT_llb_MET_recalc_NOSYS,
bdt_eta_llMetB_recalc_NOSYS,
bdt_m_l1b_recalc_NOSYS,
bdt_m_l2b_recalc_NOSYS,
bdt_pT_llMetB_recalc_NOSYS,
bdt_pT_llb_recalc_NOSYS,
bdt_sum_ET_recalc_NOSYS.

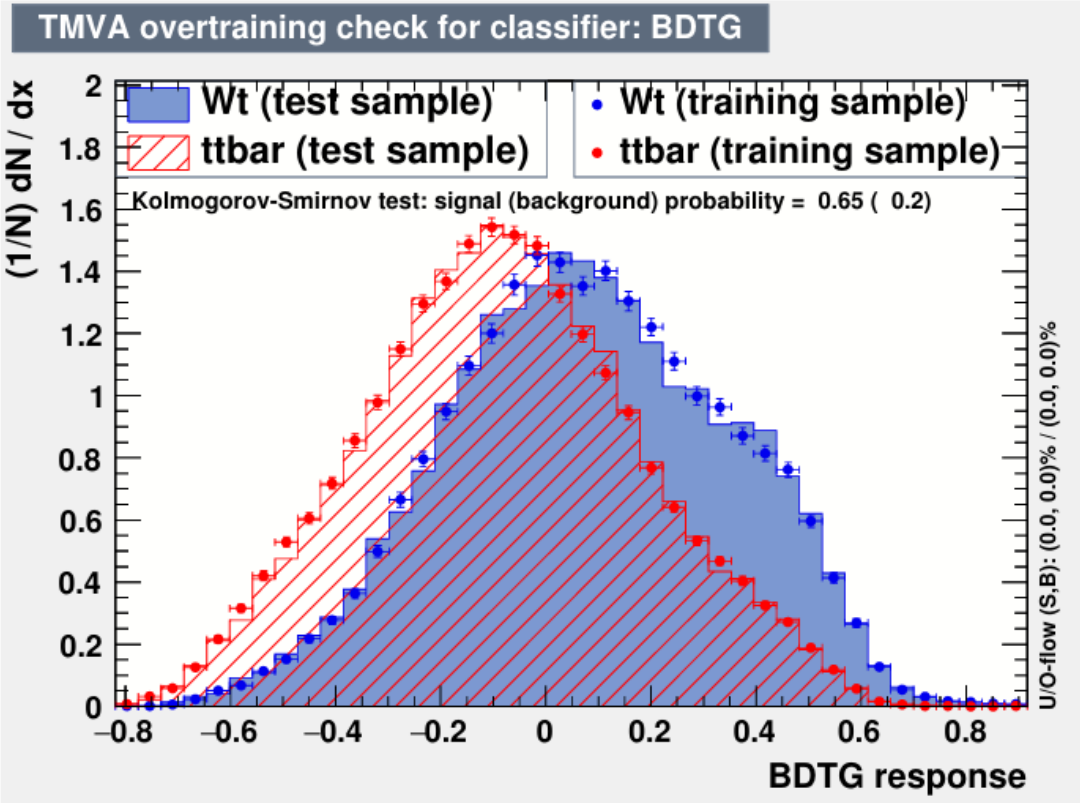
•**Samples / tree:** all files' tree name is analysis

Signal: tW (top) + $\bar{t}$W (anti-top)
Background: $t\bar{t}$ (non-all-had)

•**Event weights:** auto-resolved to weight_mc_NOSYS * weight_pileup_NOSYS * globalTriggerEffSF_NOSYS.

•**Bad values:** any variable ≤ **−990** or non-finite is masked per event.

Article's Report on BDT



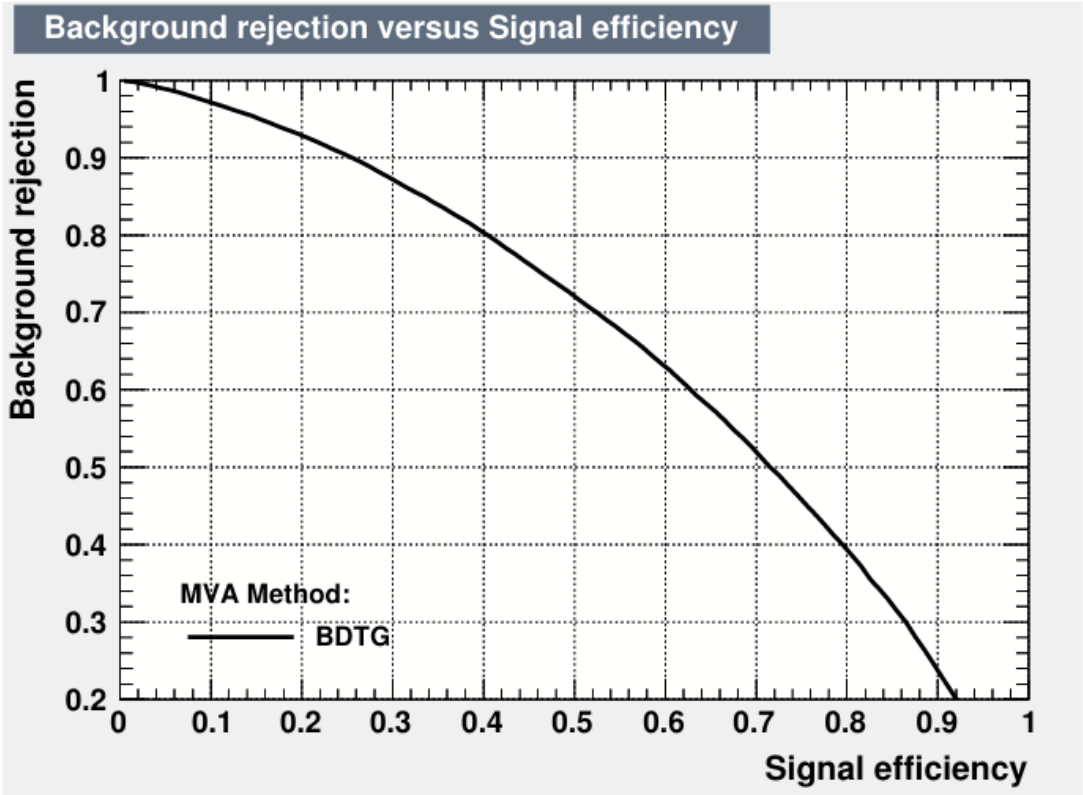


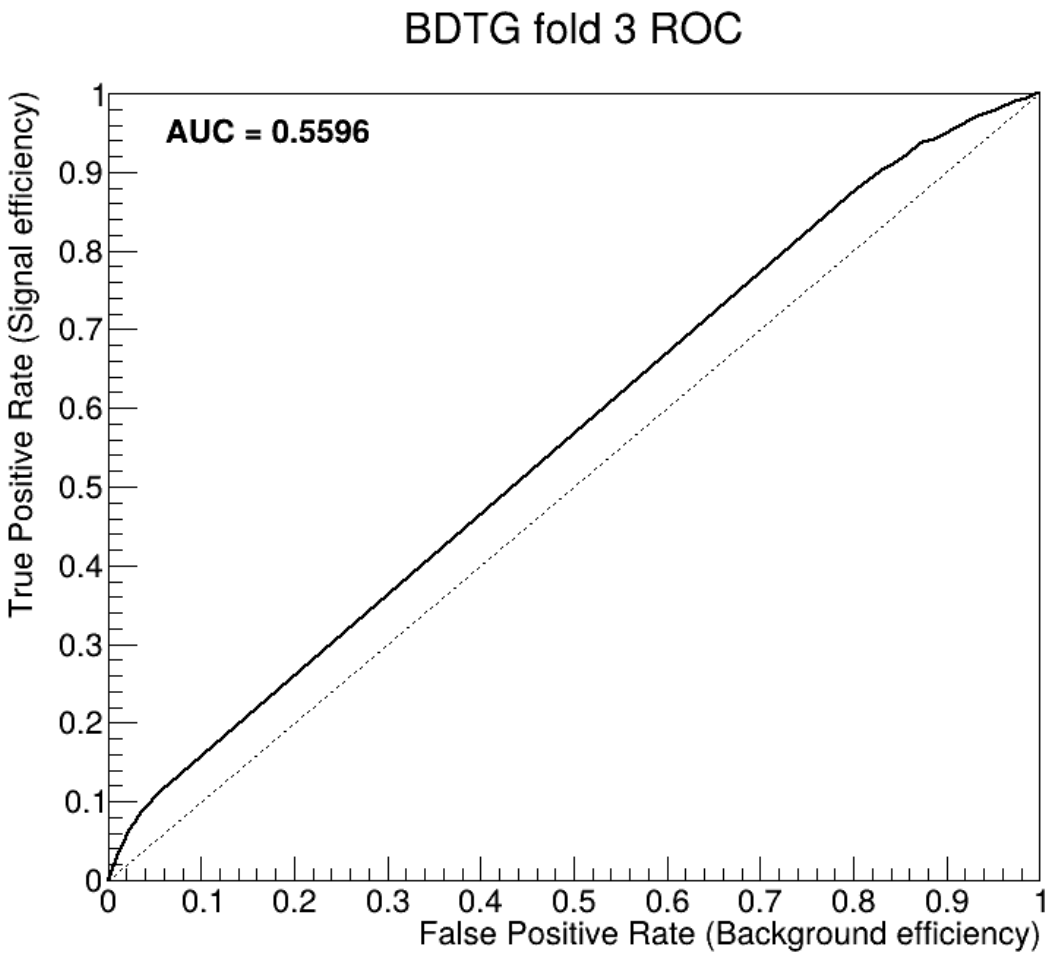
Figure 9: Comparison of test/training sample distributions and background rejection factor versus signal efficiency.

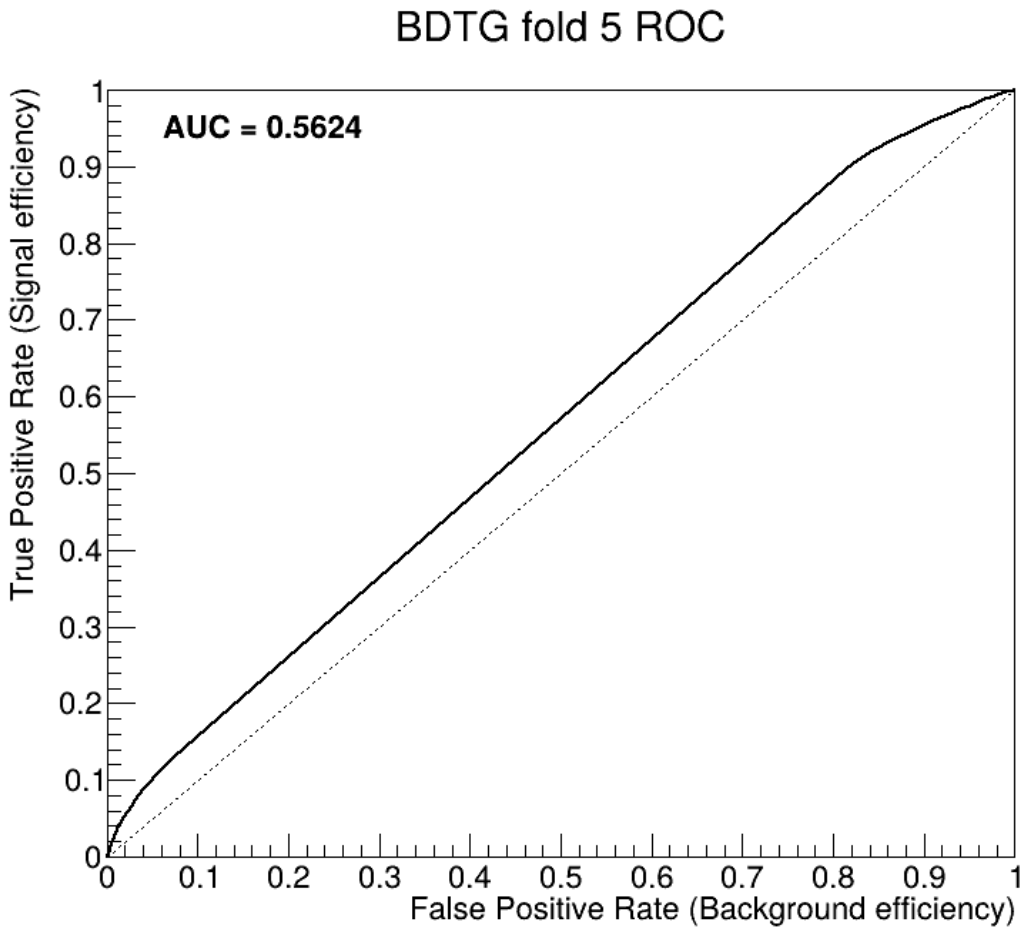
Results of Performance of ML Algorithms using K-fold on TMVA

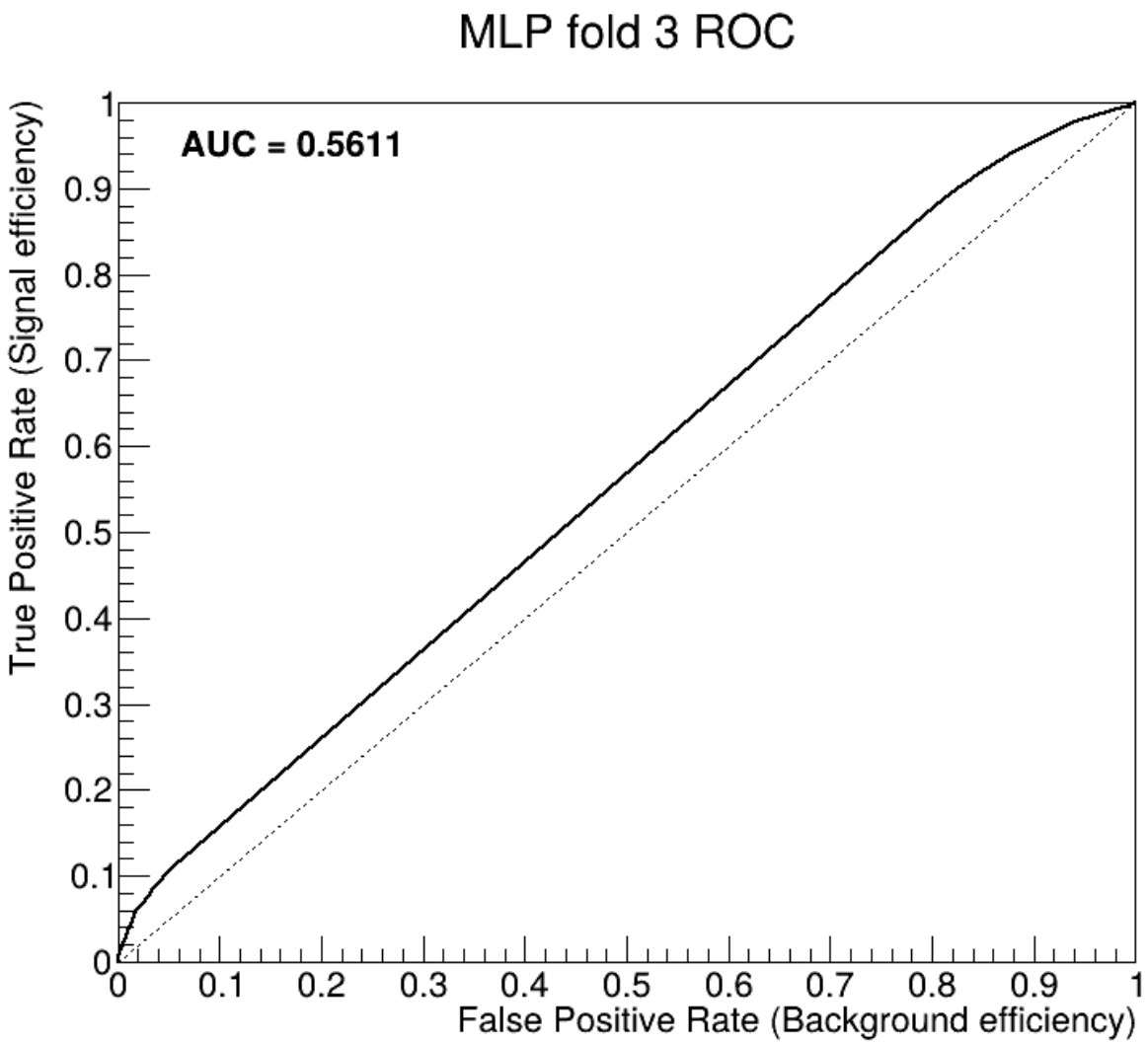
27th January 2026

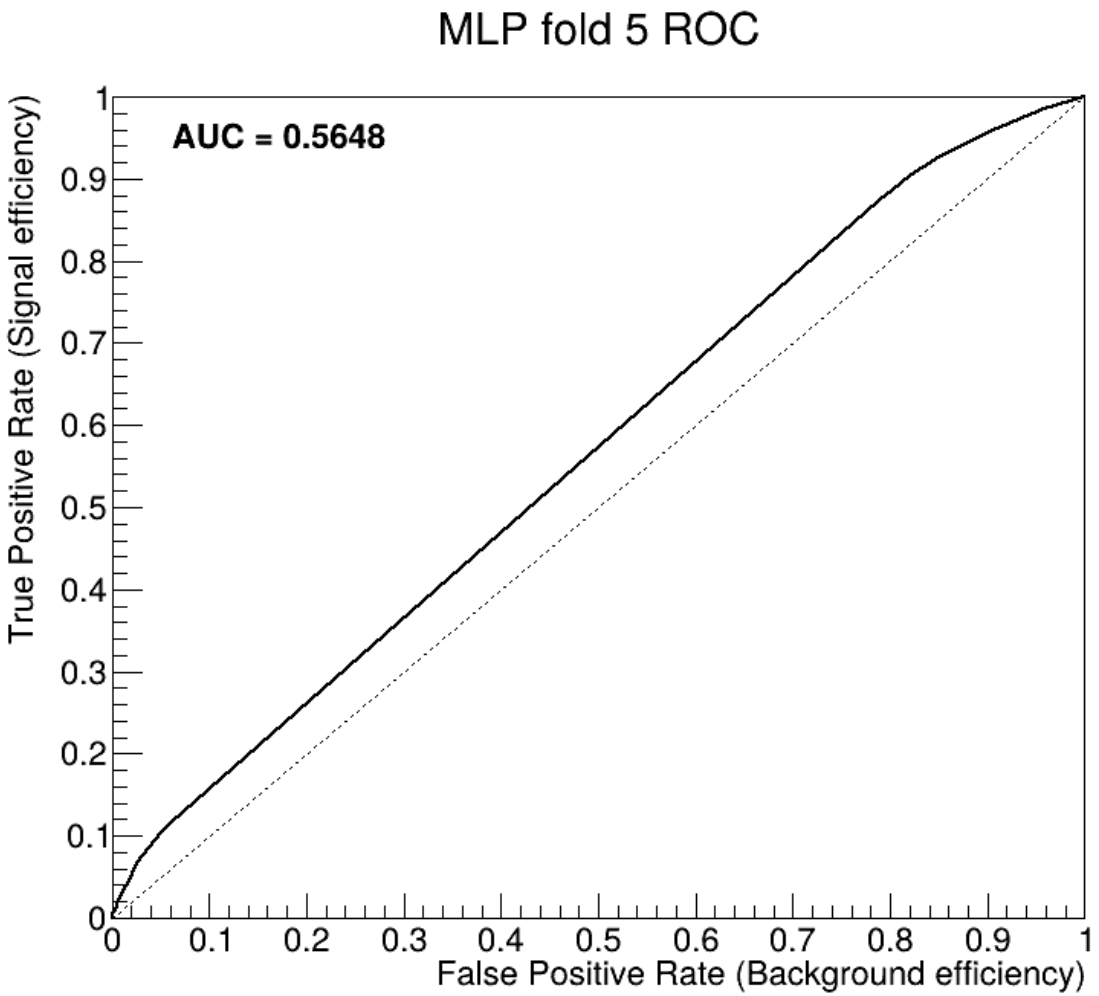
Algorithms	ROC_AUC_MEAN	ROC_AUC_STD	n_folds_used
BDTB	0.560854	0.003277	5
BDTG	0.55978	0.003049	5
Fisher	0.550102	0.00274	5
KNN	0.549632	0.003916	5
LD	0.547795	0.001821	5
Likelihood	0.523526	0.004158	5
MLP	0.561797	0.002013	5

I was doing an ordinary train/test split before cross-validation (CV).
So, CV was effectively training on (roughly) half the data, then splitting that again into folds. That alone could have pushed AUC down noticeably and make results unstable.
So, I faced three times unstable results on tmva. I am still trying to prepare correct code with kfold on TMVA.


BDTG fold 3 ROC
AUC = 0.5596
True Positive Rate (Signal efficiency)
False Positive Rate (Background efficiency)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

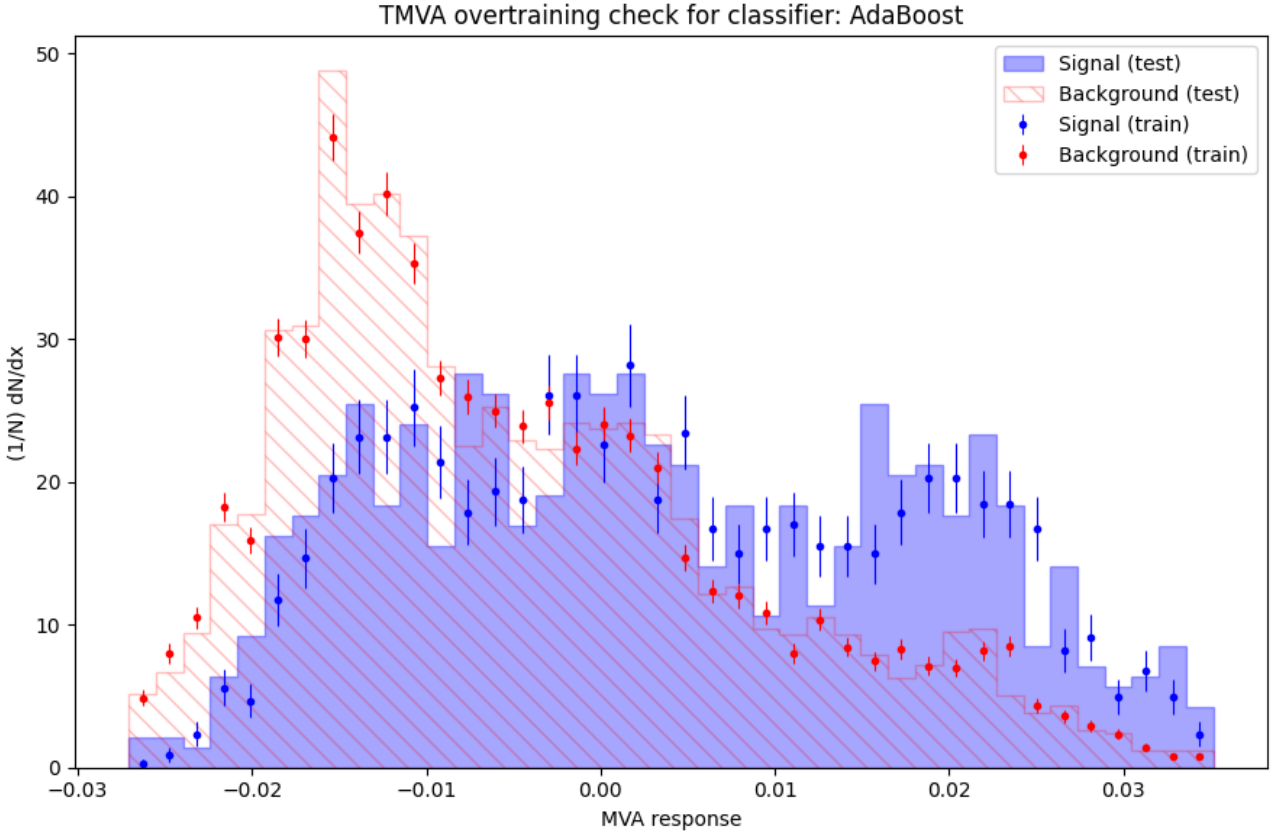

BDTG fold 5 ROC
AUC = 0.5624
True Positive Rate (Signal efficiency)
False Positive Rate (Background efficiency)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

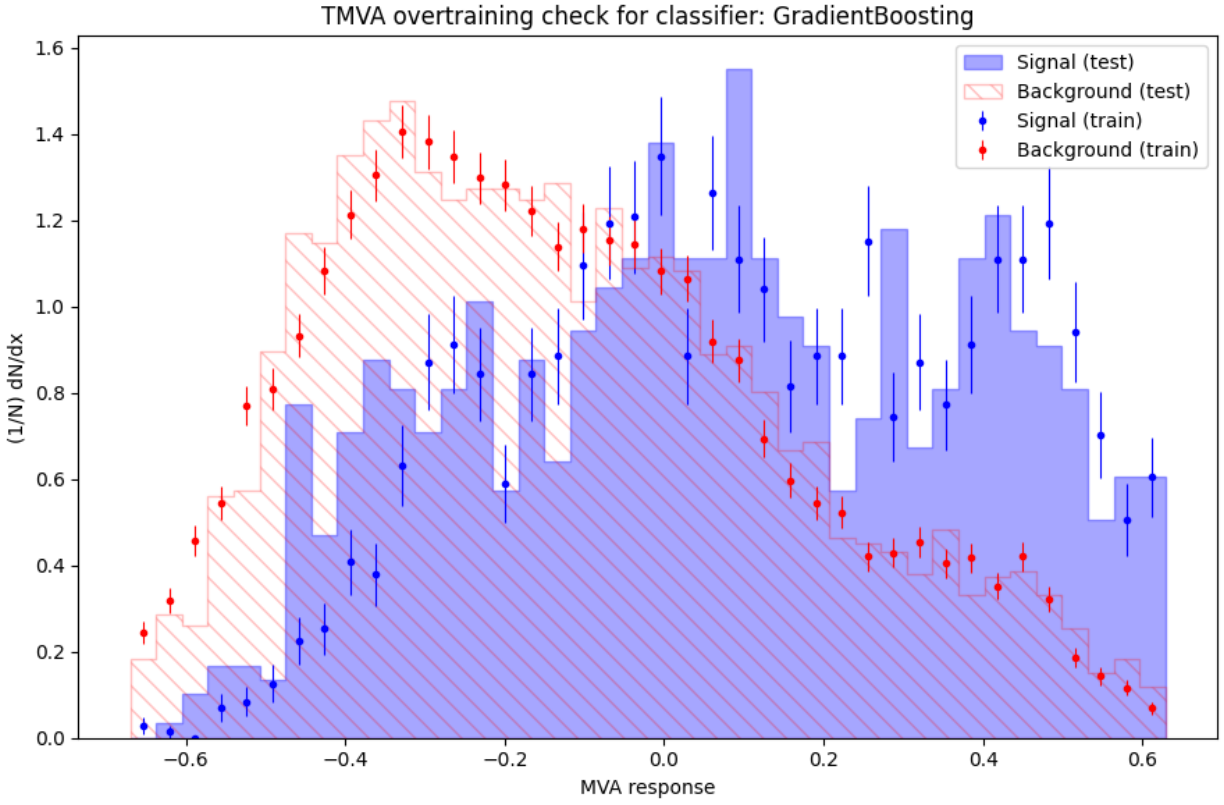

MLP fold 3 ROC
AUC = 0.5611
True Positive Rate (Signal efficiency)
False Positive Rate (Background efficiency)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

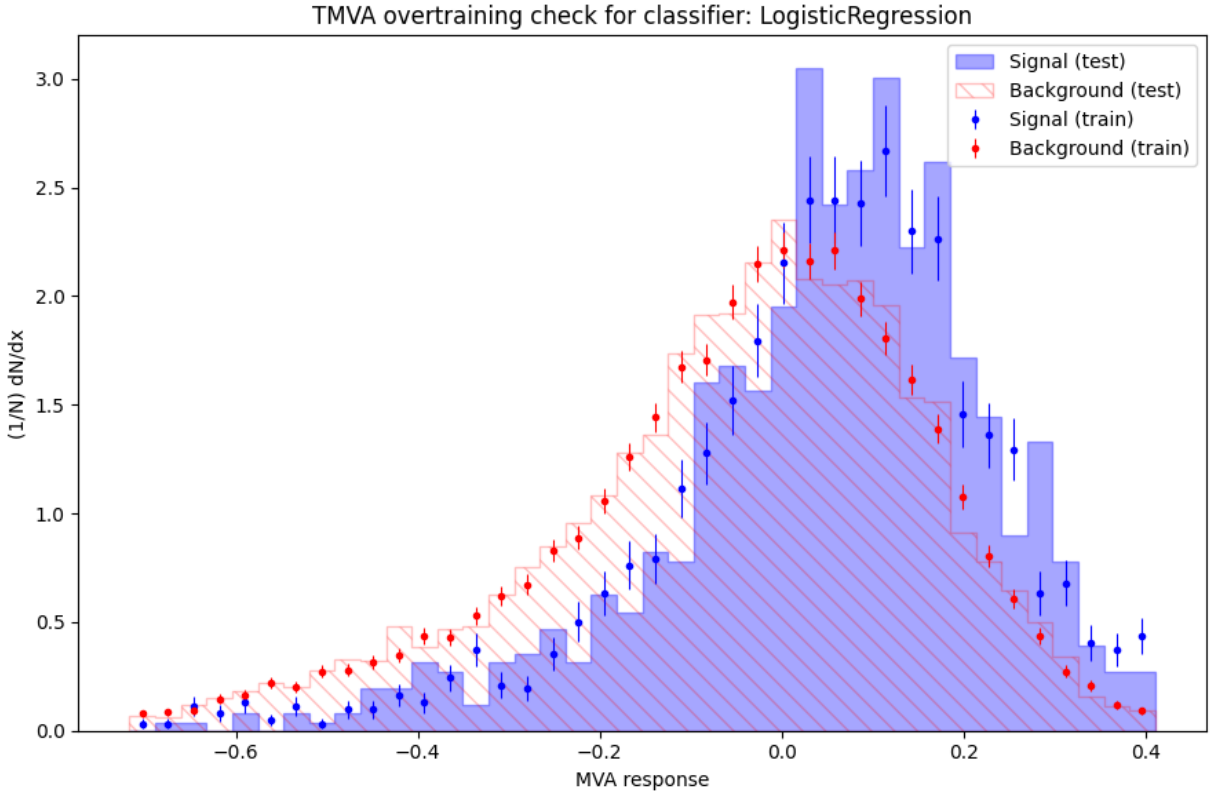

MLP fold 5 ROC
AUC = 0.5648
True Positive Rate (Signal efficiency)
False Positive Rate (Background efficiency)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

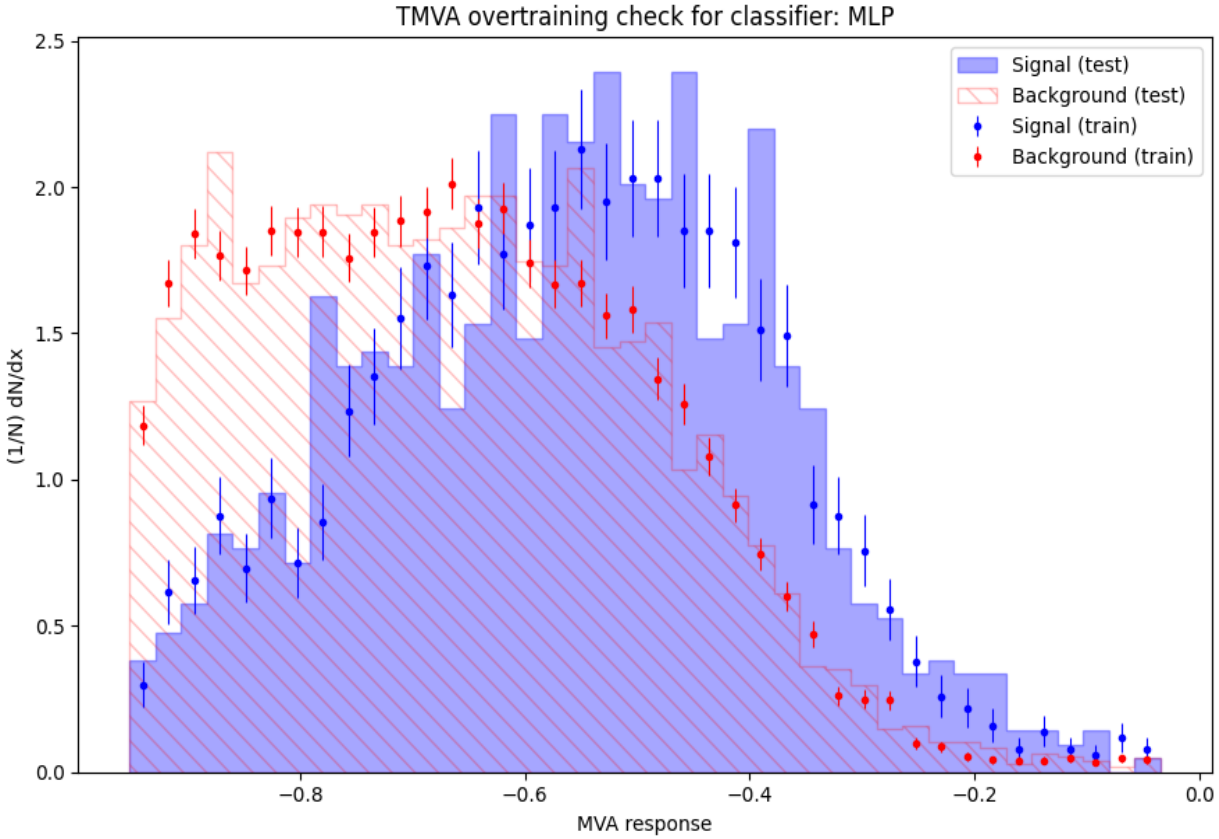
Results of Performance of ML Algorithms using K-fold on Python Trial 3
27th January 2026

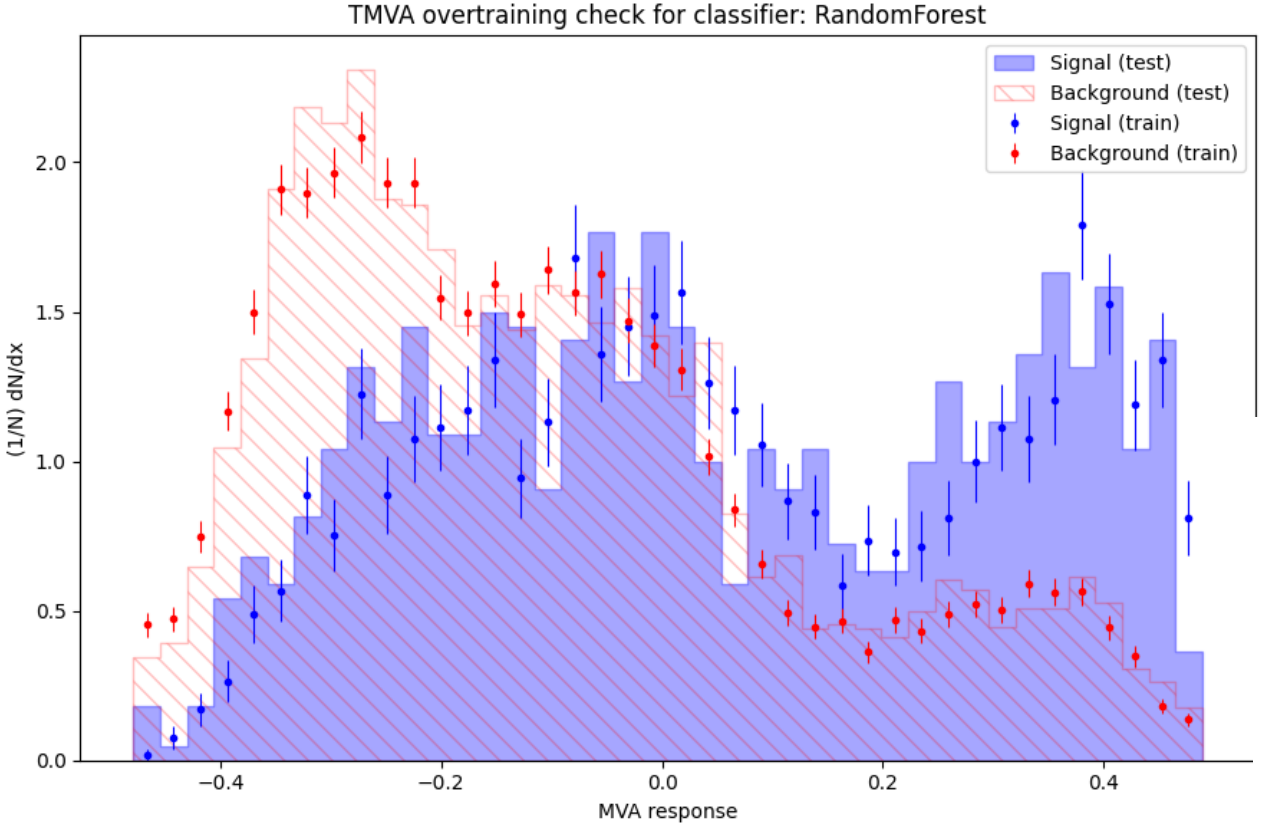
Algorithms	outer_k	inner_k	n_iters	mean_fold_auc	std_fold_auc	overall_oof_auc
AdaBoost	5	3	25	0.668024	0.008952	0.662409
Gaussian-NB	5	3	25	0.6407	0.006545	0.639867
Gradient Boosting	5	3	25	0.675134	0.01051	0.67482
KNN	5	3	25	0.643668	0.007173	0.643566
Logistic Regression	5	3	25	0.639506	0.011228	0.639507
MLP	5	3	25	0.665761	0.010691	0.664427
Random Forest	5	3	25	0.672187	0.010309	0.671608
SVC	5	3	10	0.676572	0.01301	0.676277

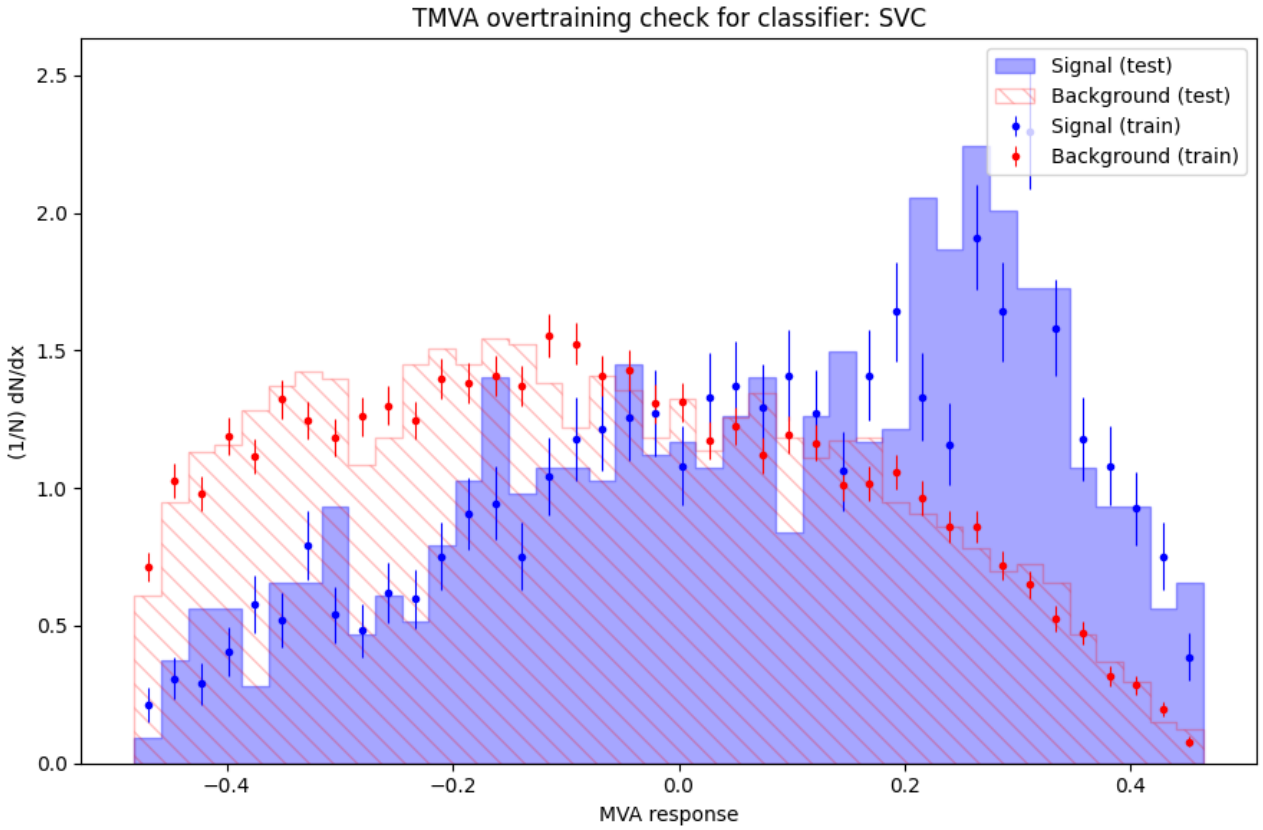

TMVA overtraining check for classifier: AdaBoost
Signal (test)
Background (test)
Signal (train)
Background (train)
(1/N) dN/dx
MVA response
0
10
20
30
40
50
−0.03
−0.02
−0.01
0.00
0.01
0.02
0.03

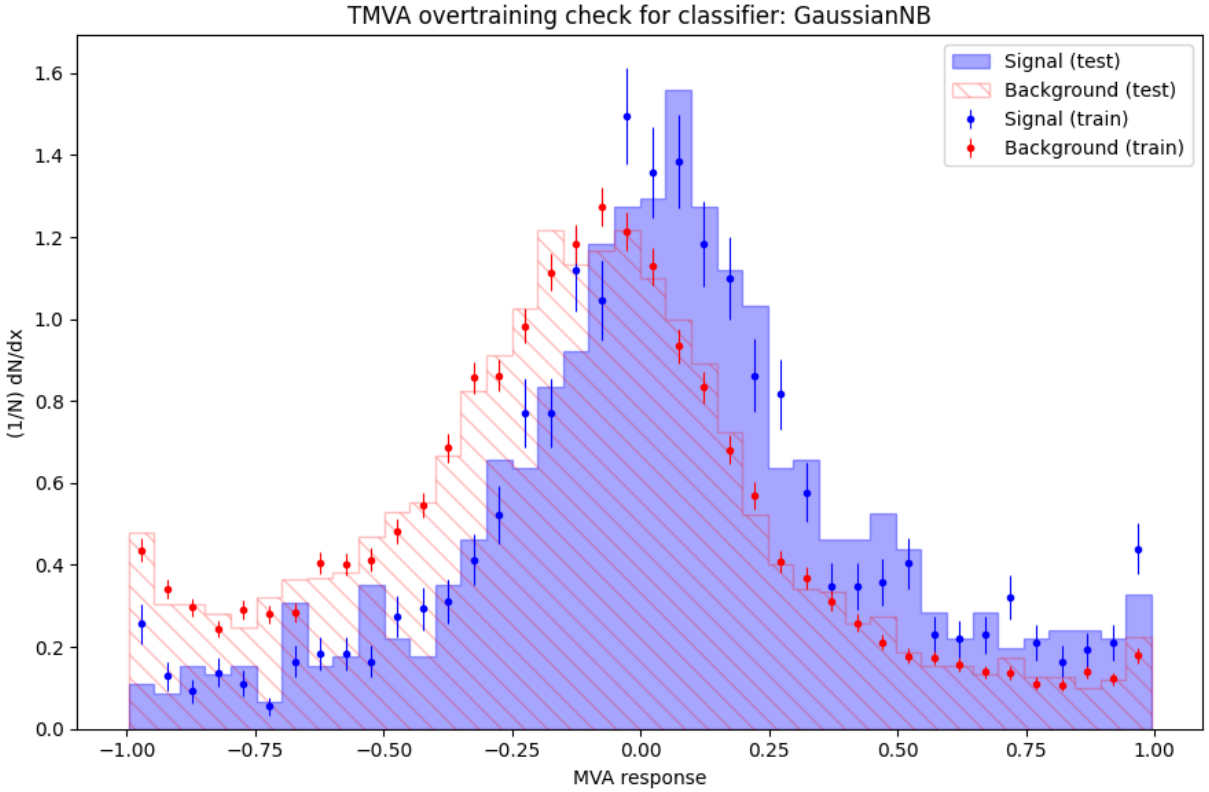

TMVA overtraining check for classifier: GradientBoosting
Signal (test)
Background (test)
Signal (train)
Background (train)
(1/N) dN/dx
MVA response
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
−0.6
−0.4
−0.2
0.0
0.2
0.4
0.6

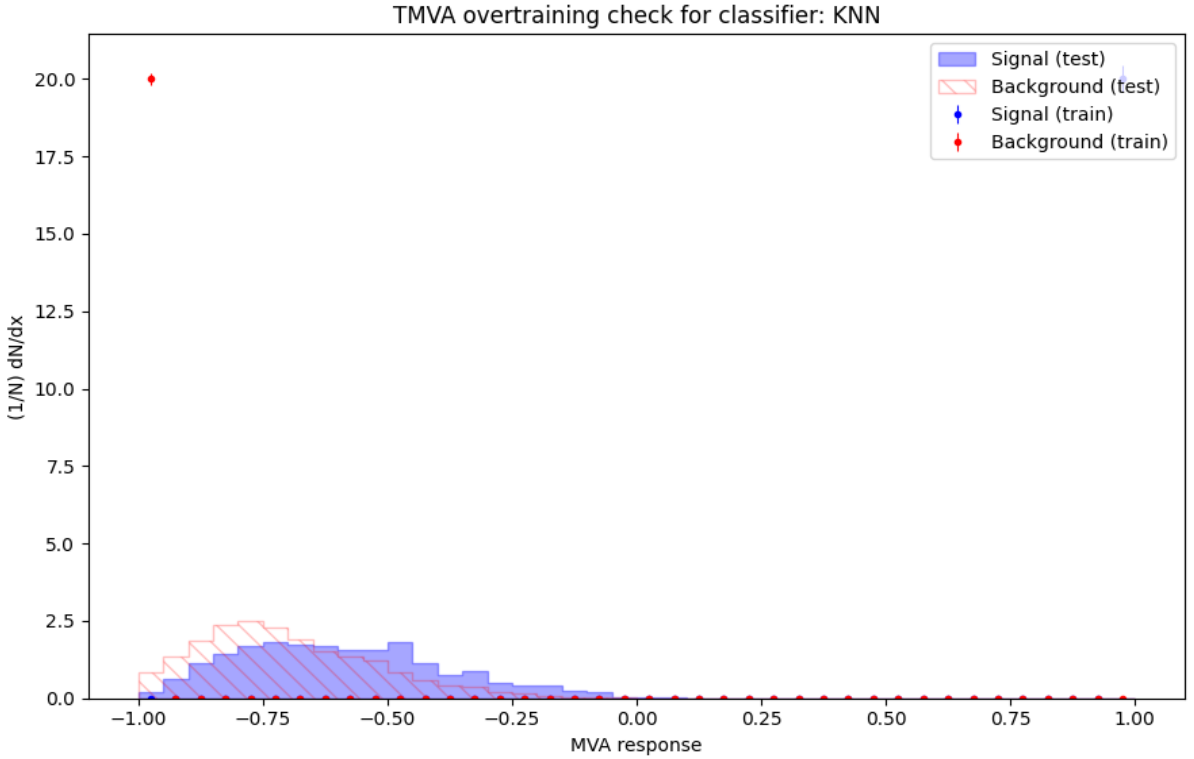

TMVA overtraining check for classifier: LogisticRegression
Signal (test)
Background (test)
Signal (train)
Background (train)
(1/N) dN/dx
MVA response
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.6
−0.4
−0.2
0.0
0.2
0.4

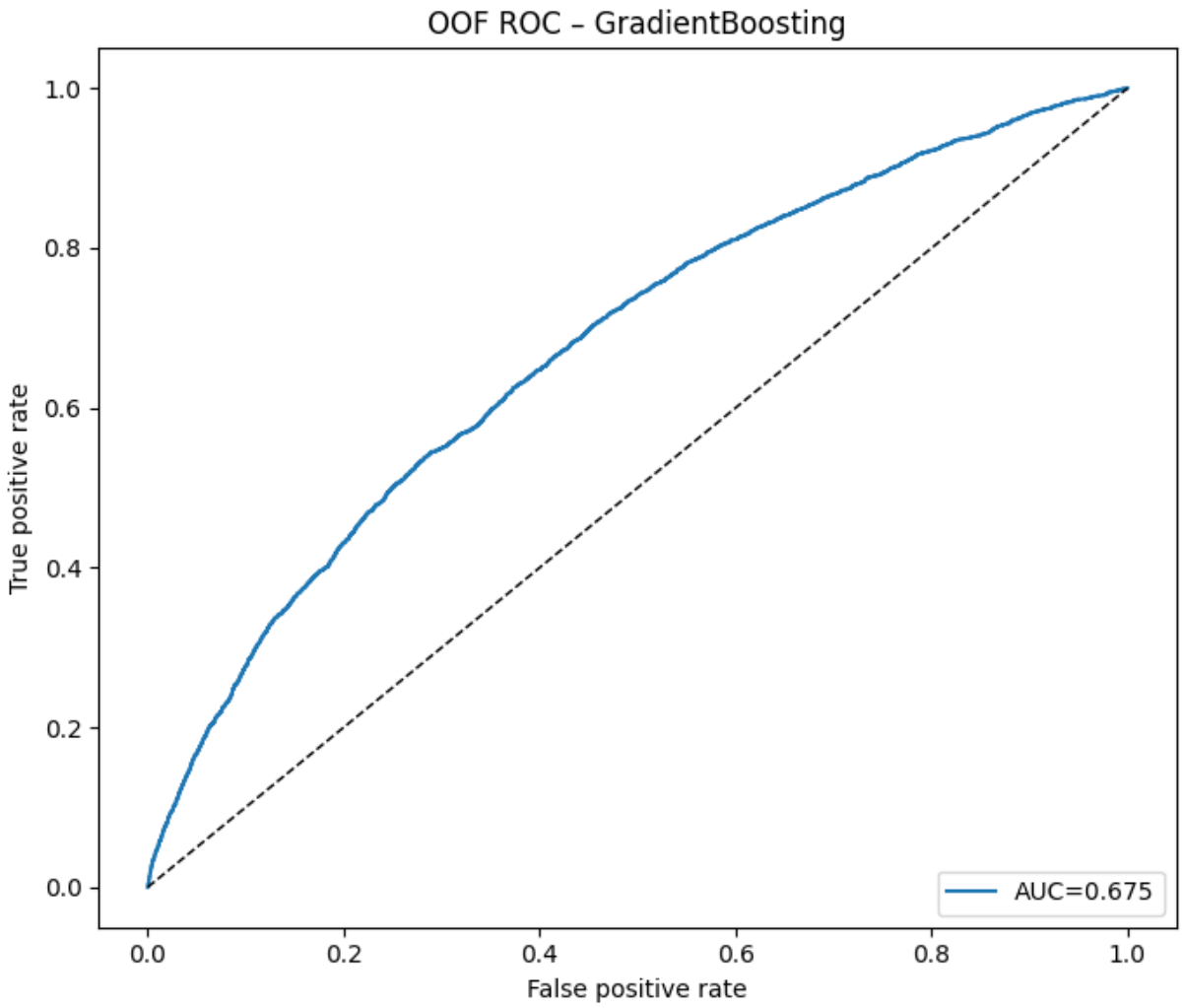

TMVA overtraining check for classifier: MLP
Signal (test)
Background (test)
Signal (train)
Background (train)
(1/N) dN/dx
MVA response
2.5
2.0
1.5
1.0
0.5
0.0
−0.8
−0.6
−0.4
−0.2
0.0

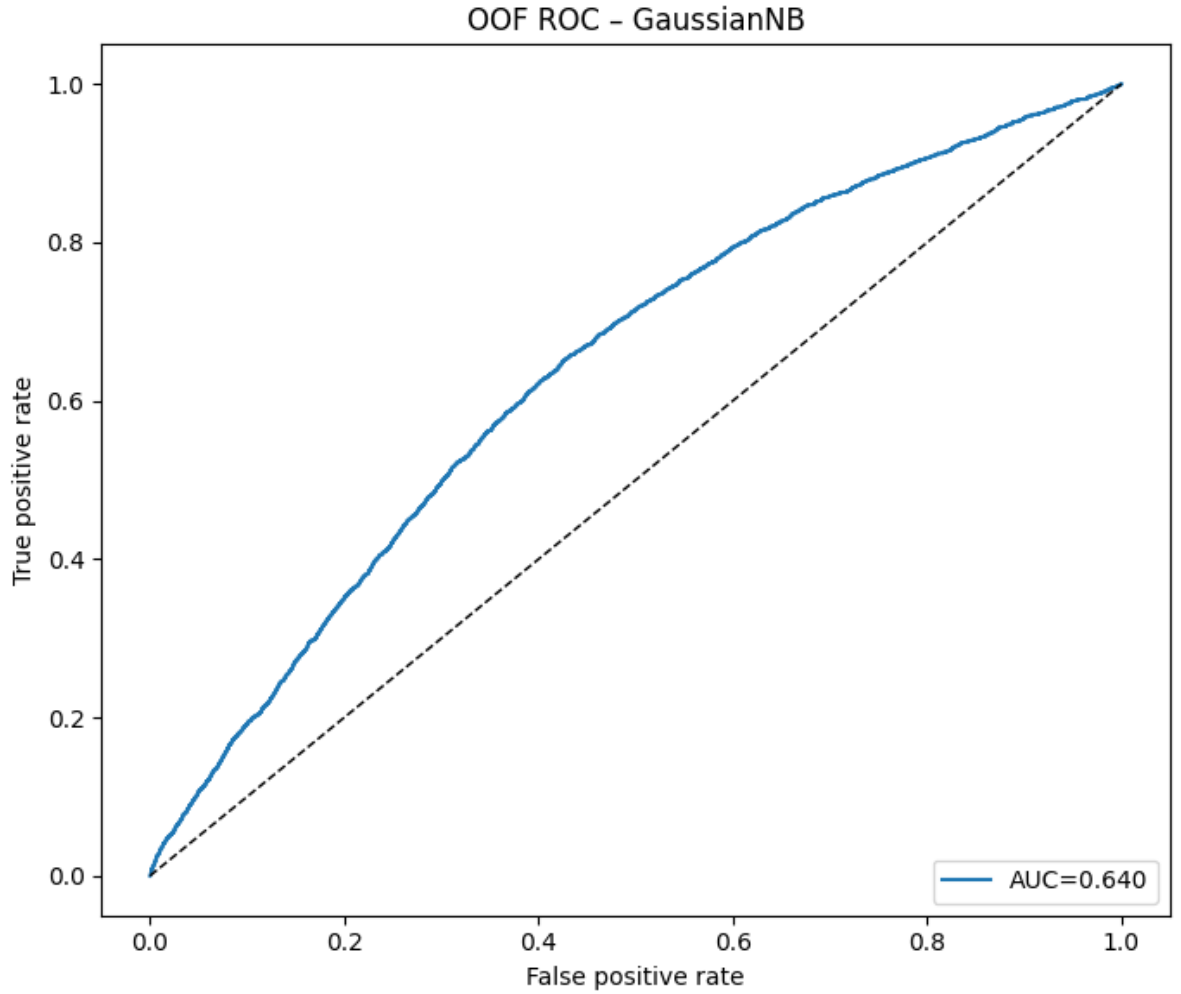

TMVA overtraining check for classifier: RandomForest
Signal (test)
Background (test)
Signal (train)
Background (train)
(1/N) dN/dx
MVA response
0.0
0.5
1.0
1.5
2.0
−0.4
−0.2
0.0
0.2
0.4

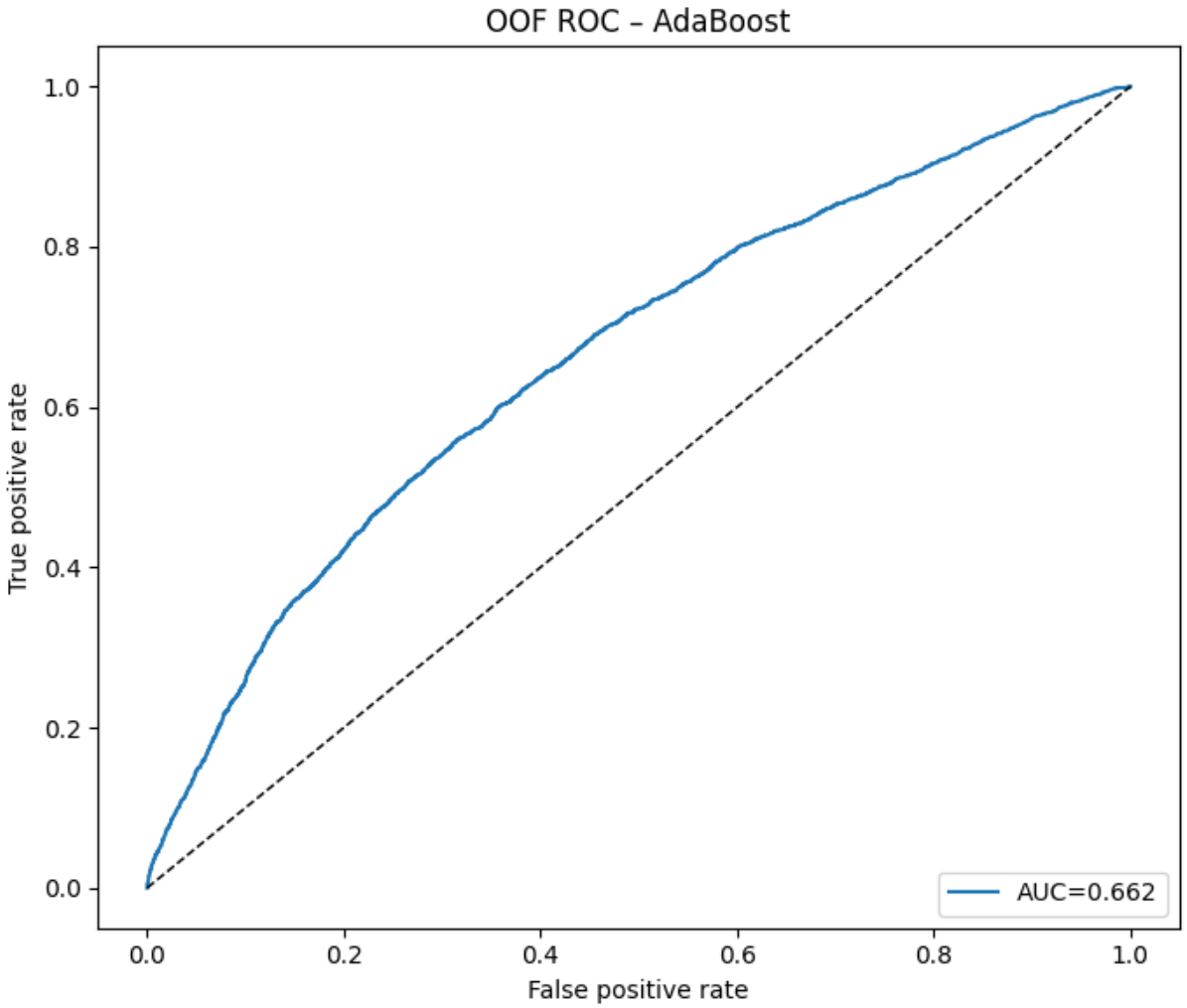

TMVA overtraining check for classifier: SVC
Signal (test)
Background (test)
Signal (train)
Background (train)
(1/N) dN/dx
MVA response
0.0
0.5
1.0
1.5
2.0
2.5
−0.4
−0.2
0.0
0.2
0.4

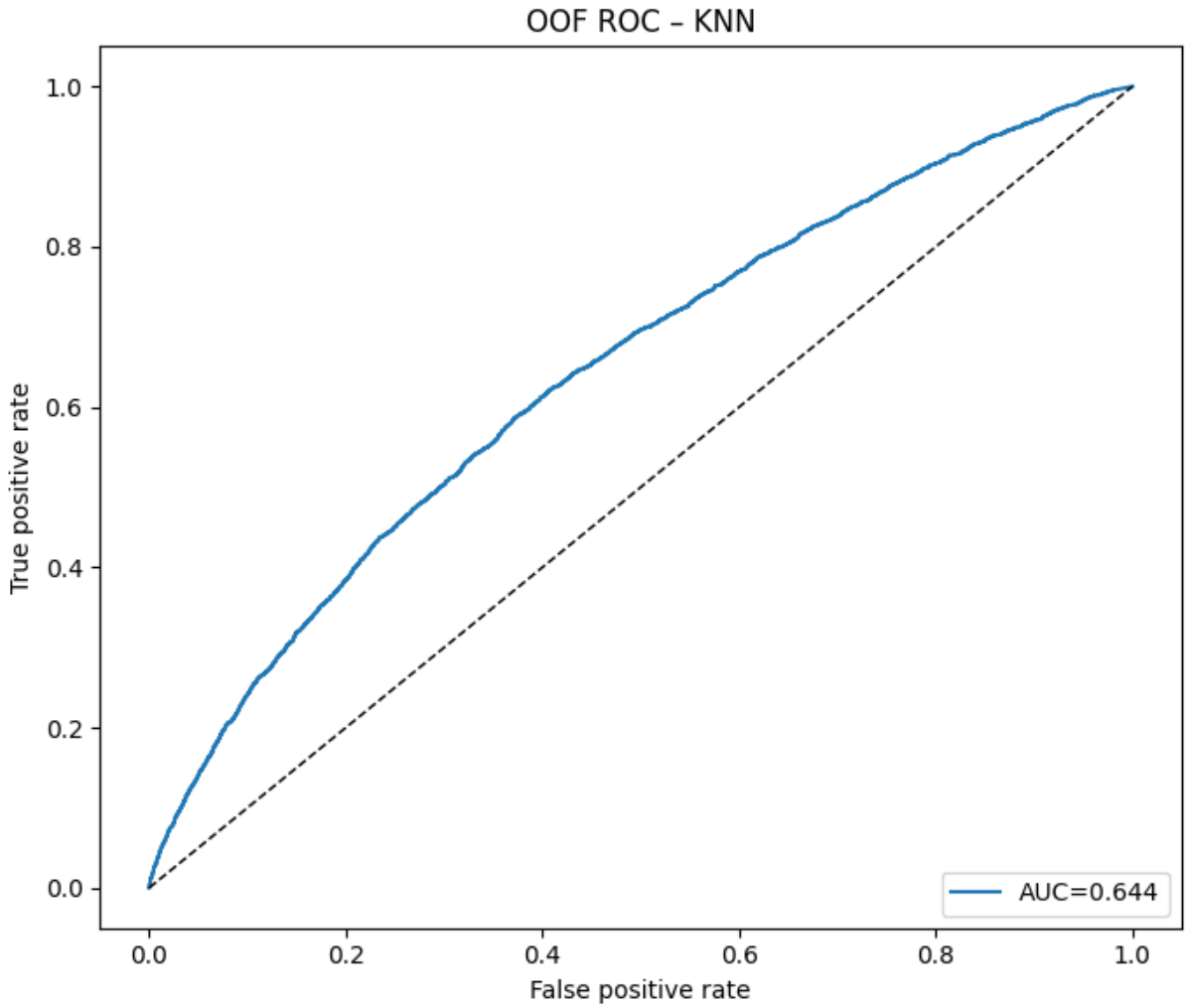

TMVA overtraining check for classifier: GaussianNB
Signal (test)
Background (test)
Signal (train)
Background (train)
(1/N) dN/dx
MVA response
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

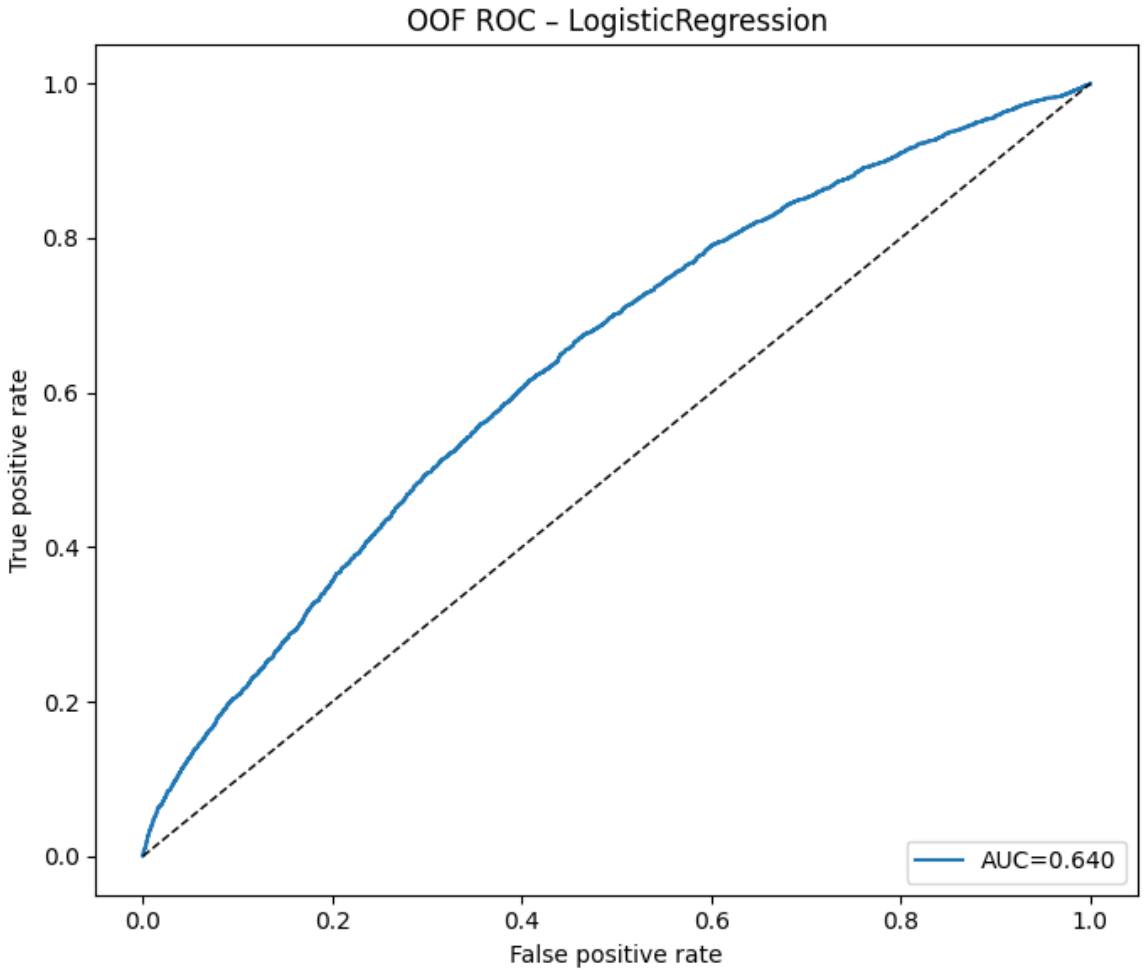

TMVA overtraining check for classifier: KNN
Signal (test)
Background (test)
Signal (train)
Background (train)
(1/N) dN/dx
MVA response
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

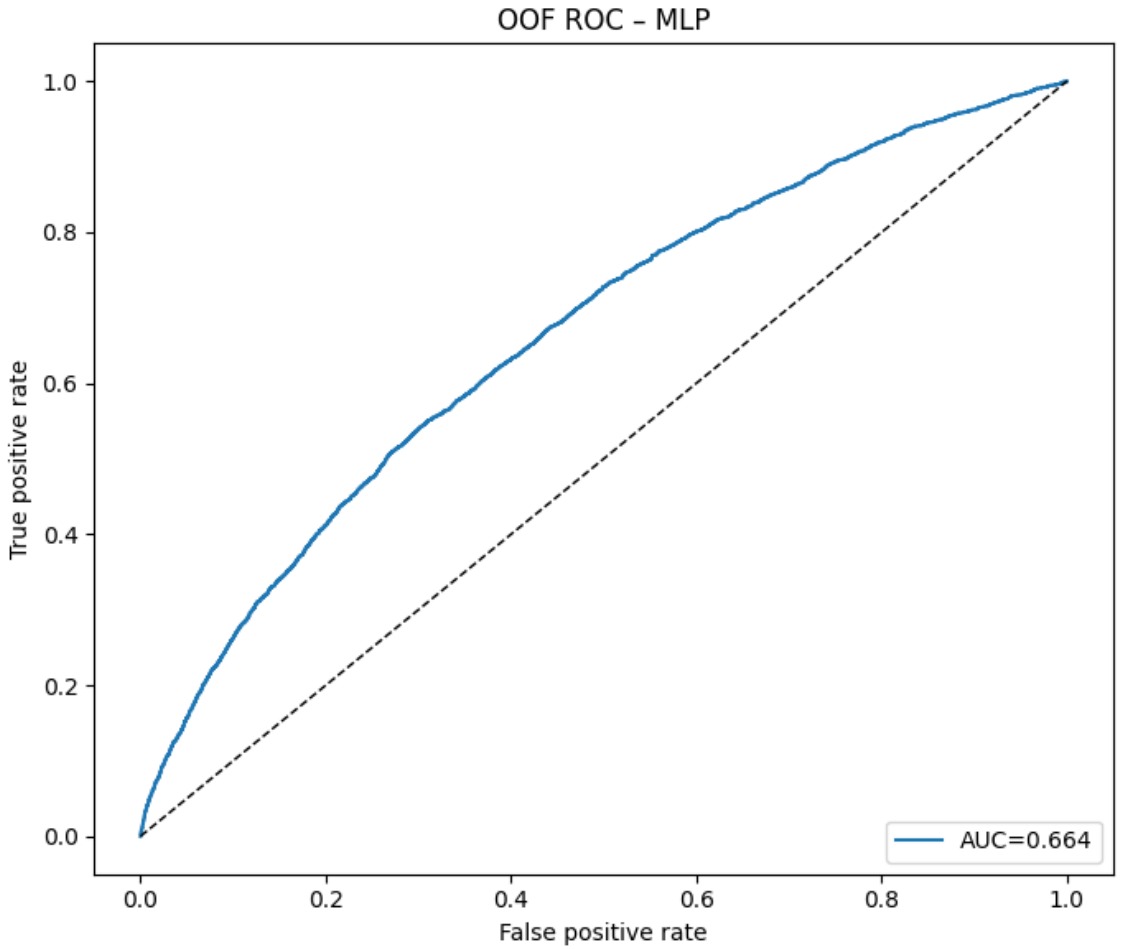

OOF ROC – GradientBoosting
True positive rate
False positive rate
AUC=0.675
0.0
0.2
0.4
0.6
0.8
1.0

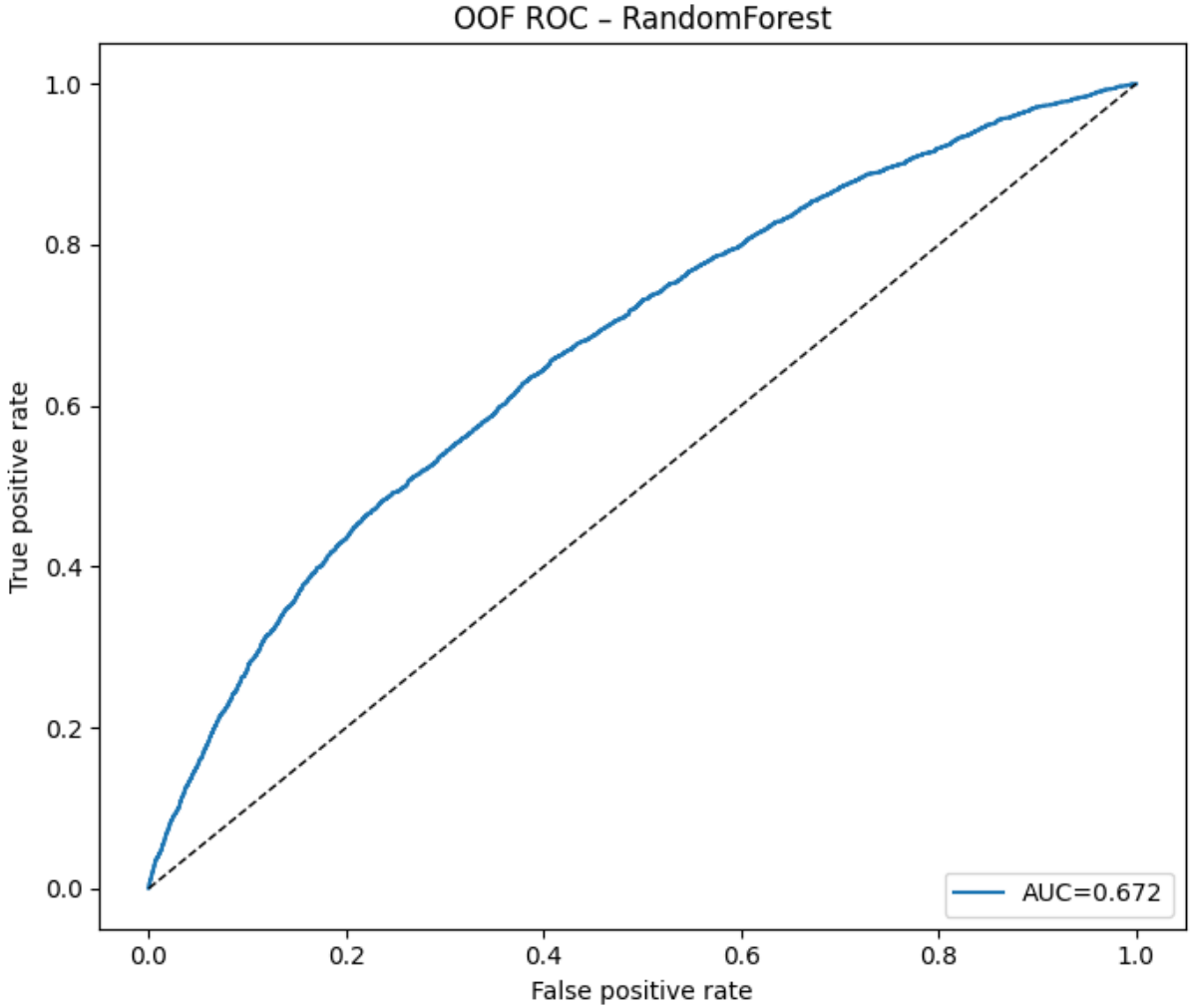

OOF ROC – GaussianNB
True positive rate
False positive rate
AUC=0.640
0.0
0.2
0.4
0.6
0.8
1.0

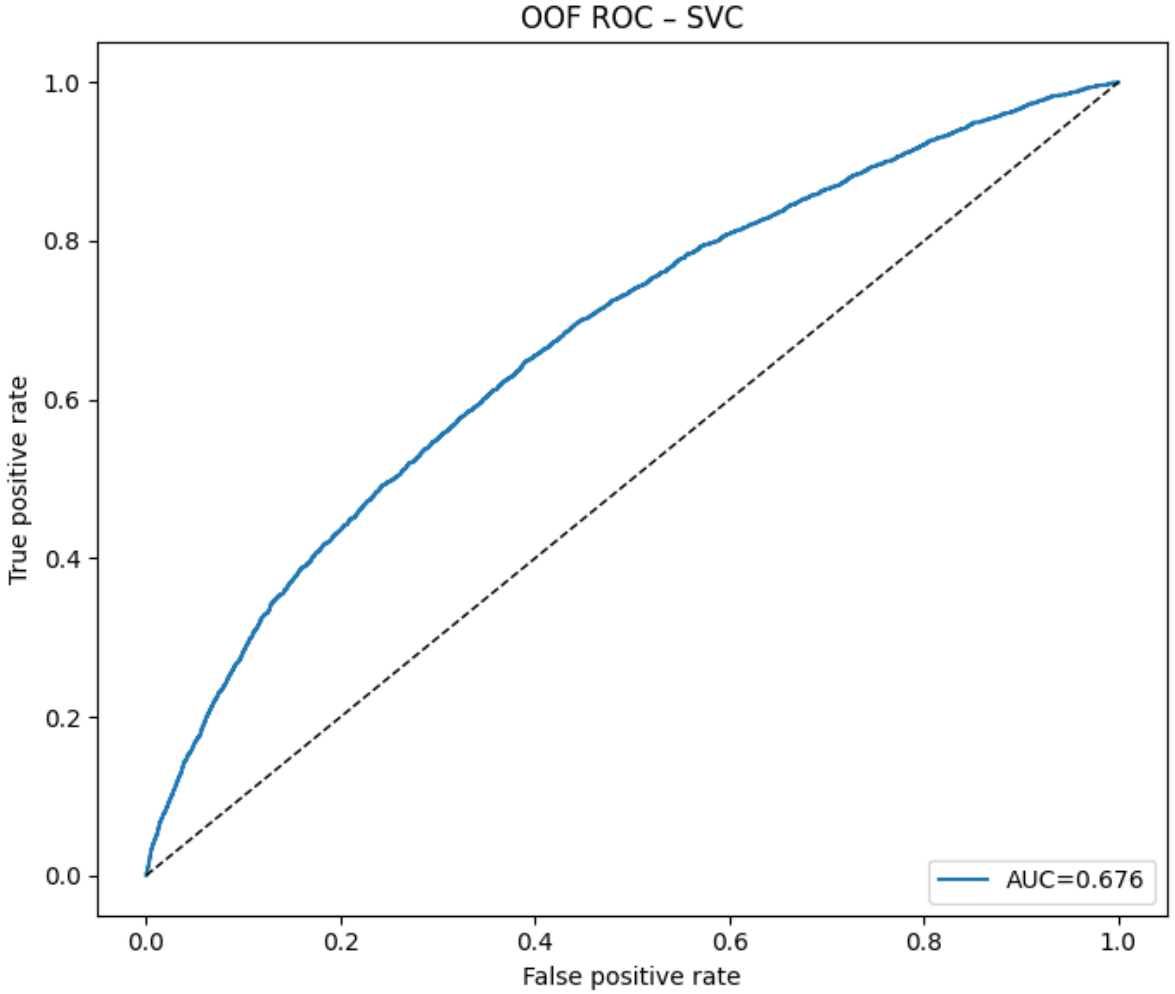

OOF ROC – AdaBoost
True positive rate
False positive rate
AUC=0.662
0.0
0.2
0.4
0.6
0.8
1.0


OOF ROC – KNN
True positive rate
False positive rate
AUC=0.644
0.0
0.2
0.4
0.6
0.8
1.0


OOF ROC – LogisticRegression
True positive rate
False positive rate
AUC=0.640
0.0
0.2
0.4
0.6
0.8
1.0


OOF ROC – MLP
True positive rate
False positive rate
AUC=0.664
0.0
0.2
0.4
0.6
0.8
1.0


OOF ROC – RandomForest
True positive rate
False positive rate
AUC=0.672
0.0
0.2
0.4
0.6
0.8
1.0

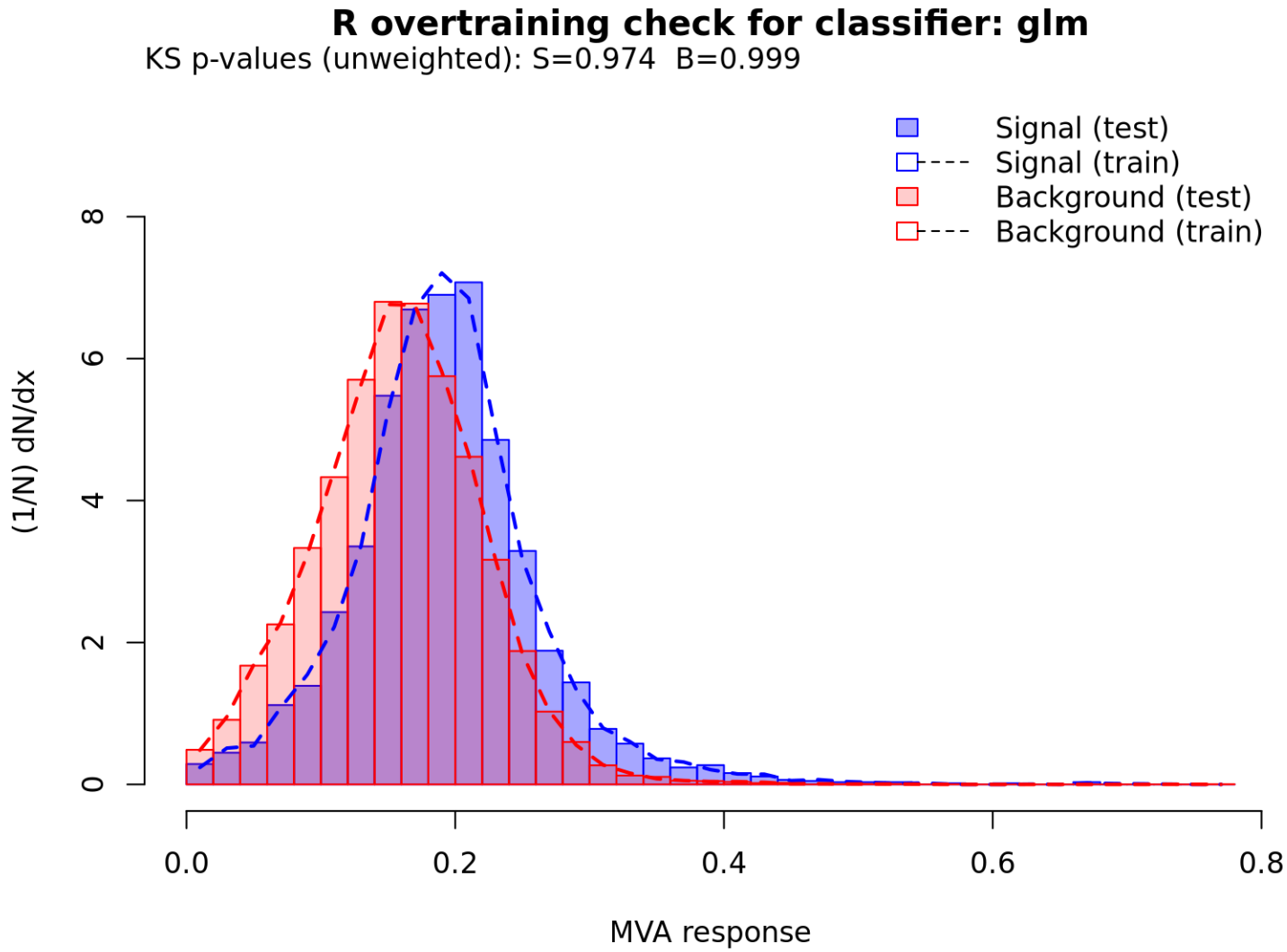

OOF ROC – SVC
True positive rate
False positive rate
AUC=0.676
0.0
0.2
0.4
0.6
0.8
1.0

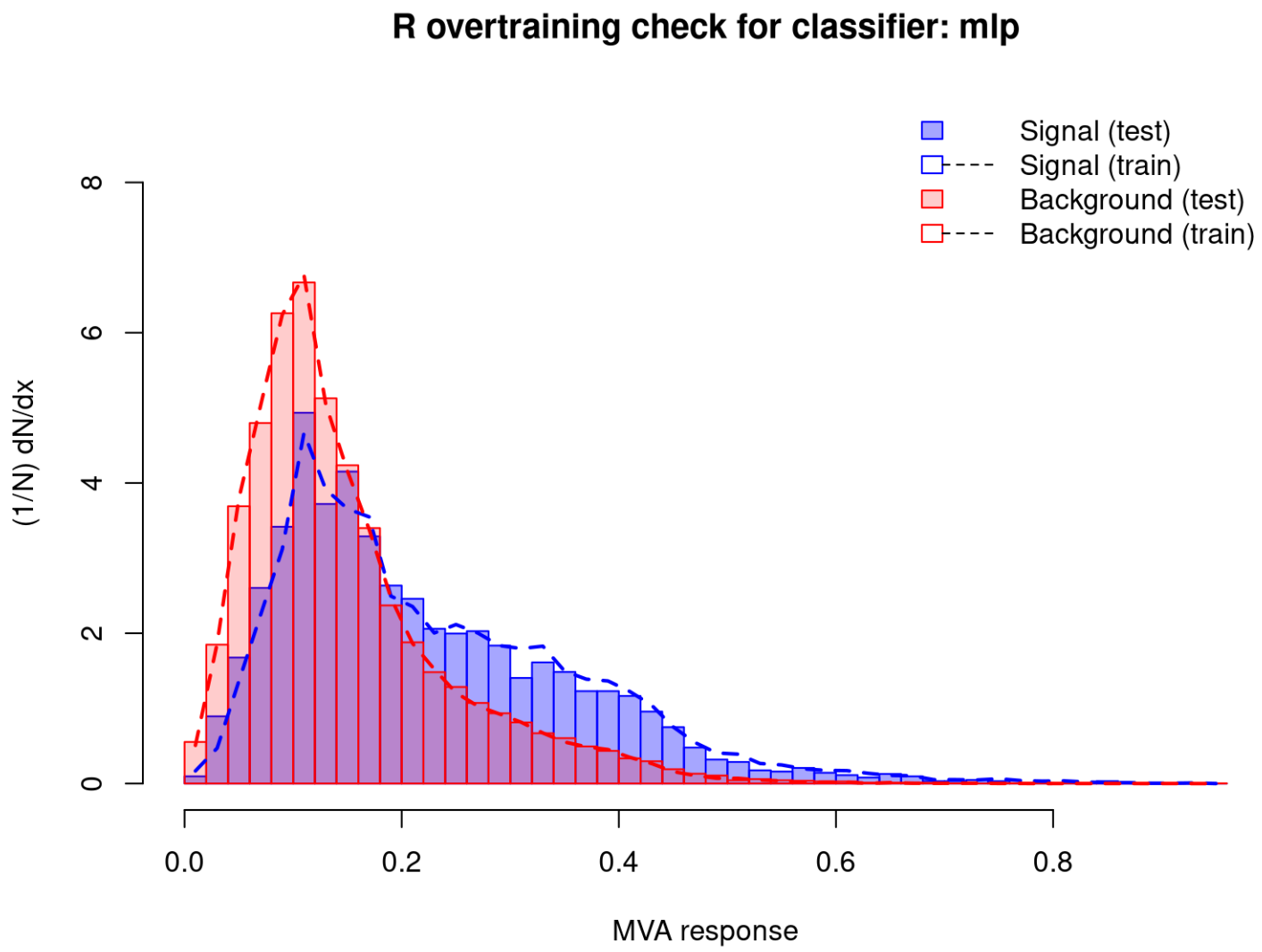
Results of Performance of ML Algorithms using K-fold on R without caret package.
03 Feb 2026

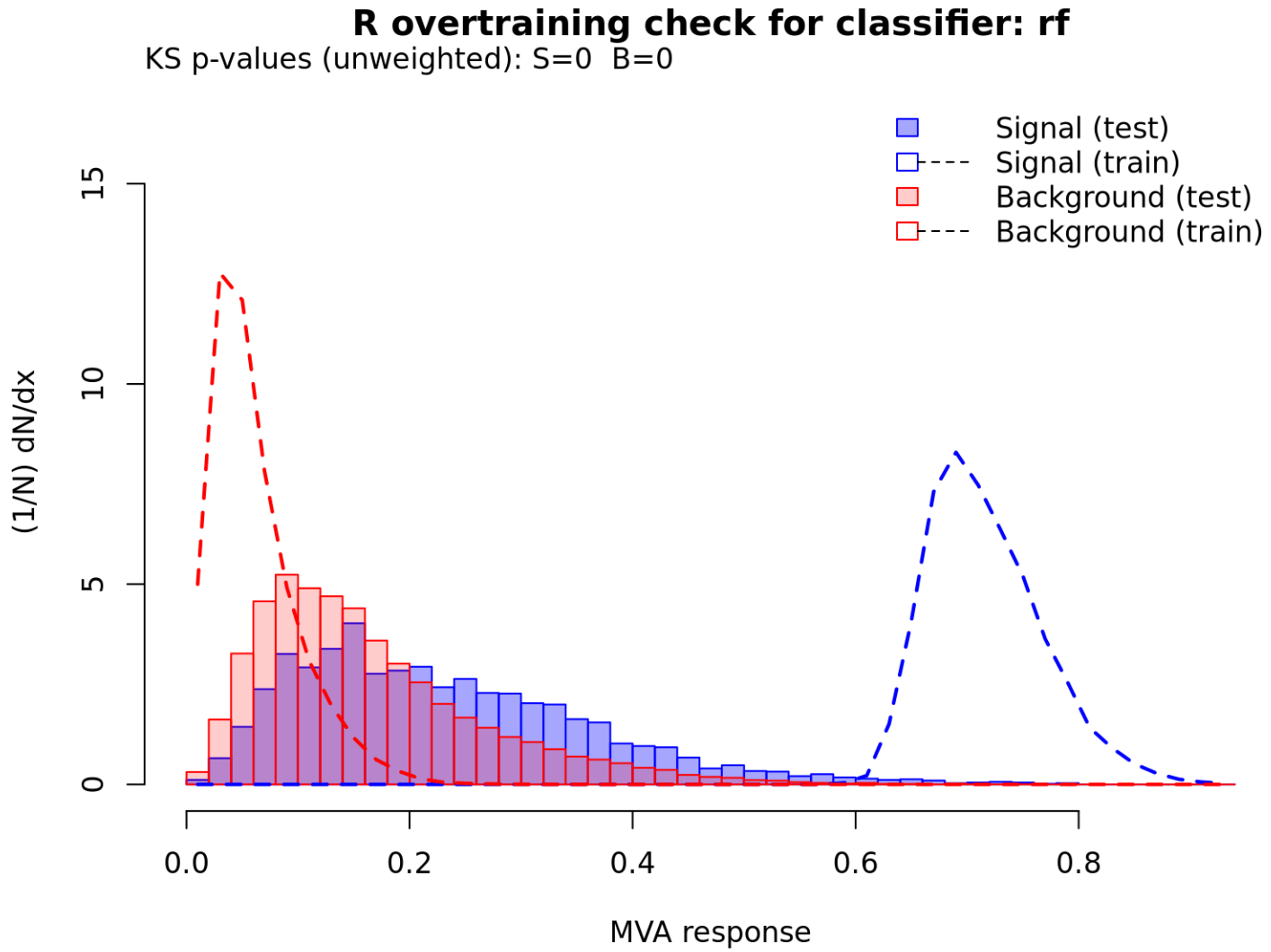
Methods: glm, rf, gbm, xgboost, svm, knn, nb, mlp

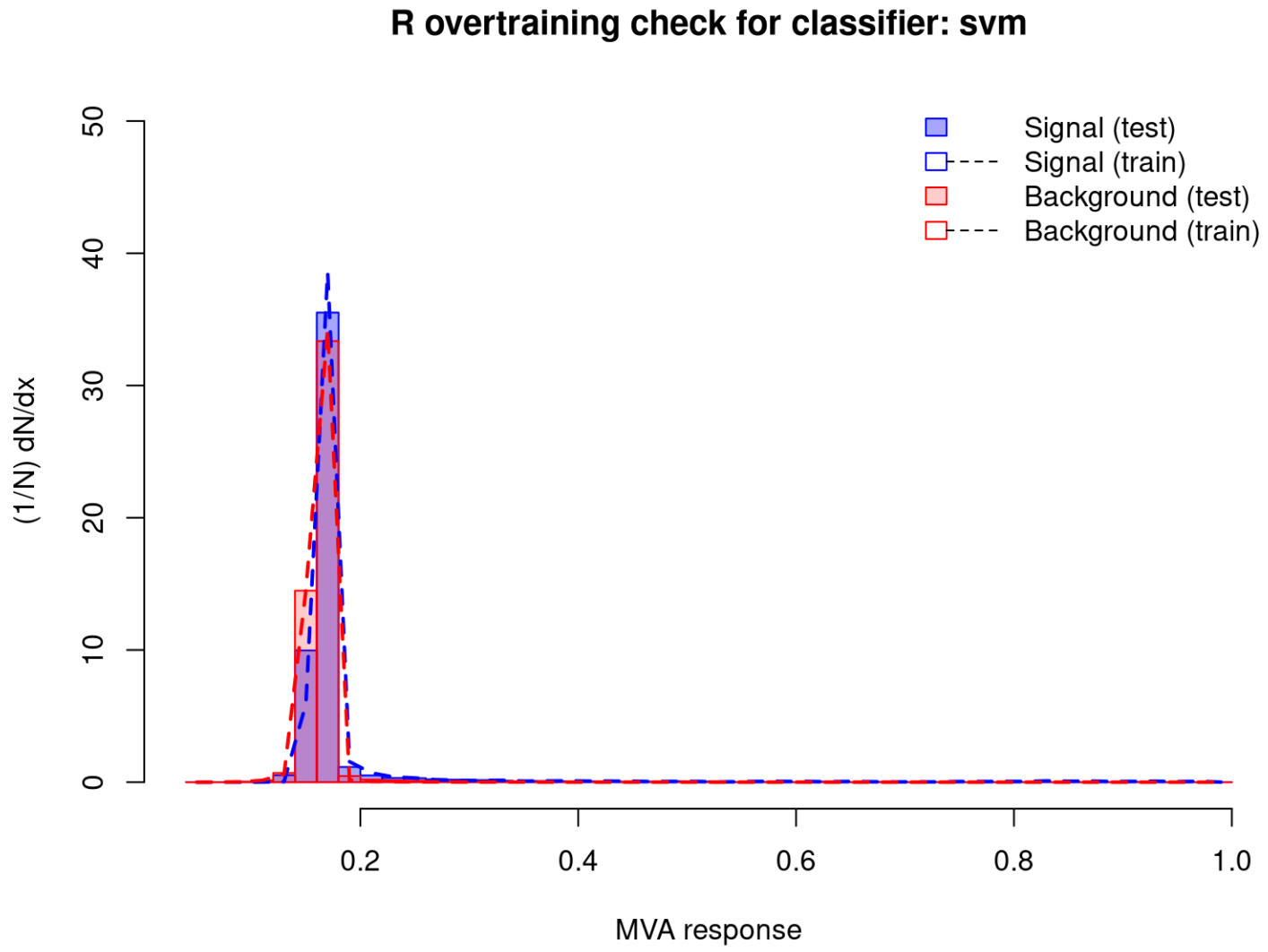
R-Platform (k-fold) Results on New Data

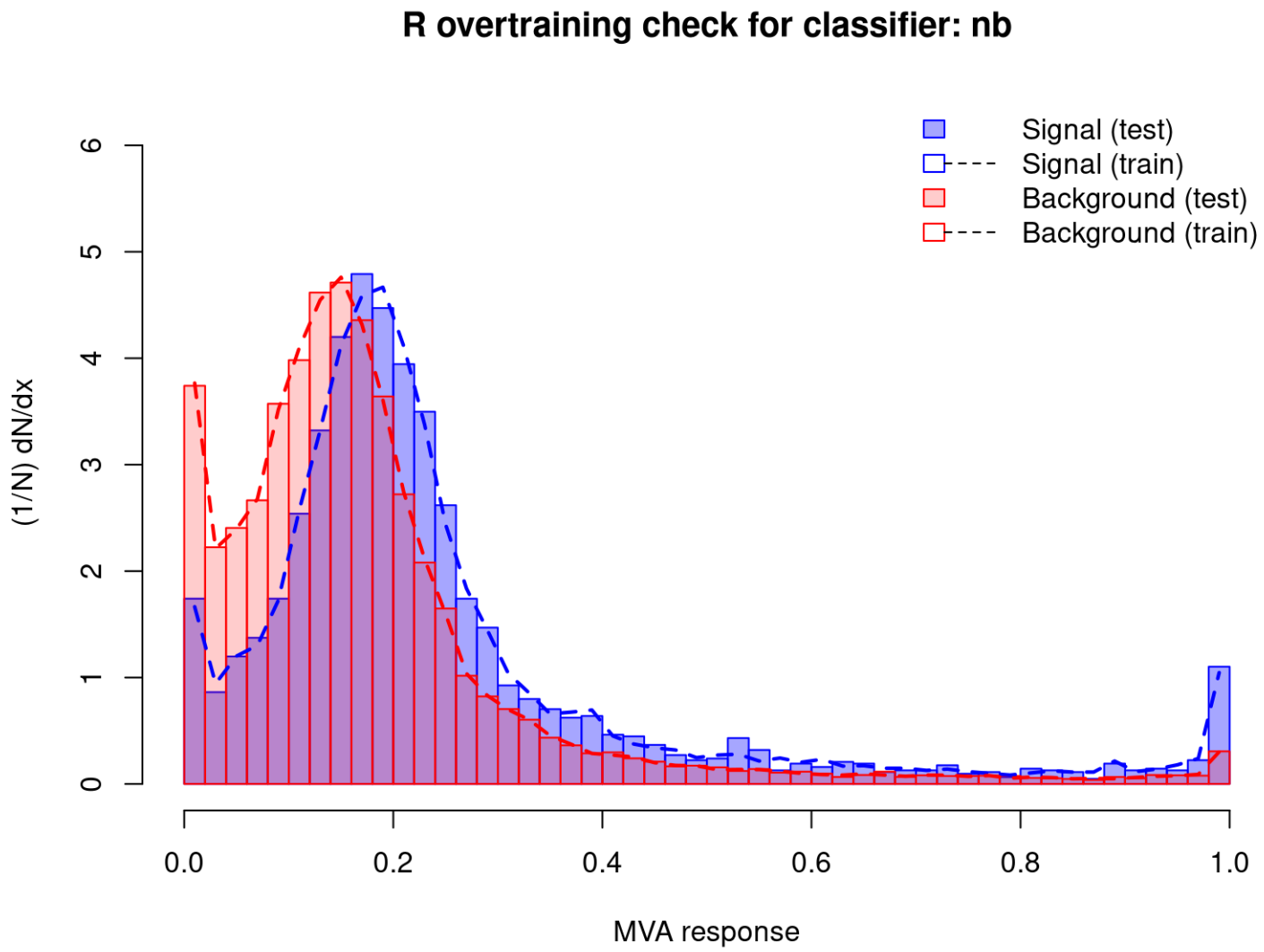
METHOD	*auc_oof_weighted*	*acc_oof_weighted*
GBM	1	1
MLP	0.660152	0.836995
XGBOOST	0.659179	0.835844
RF	0.656103	0.835792
GLM	0.643484	0.836315
NB	0.640344	0.813926
SVM	0.590384	0.836263

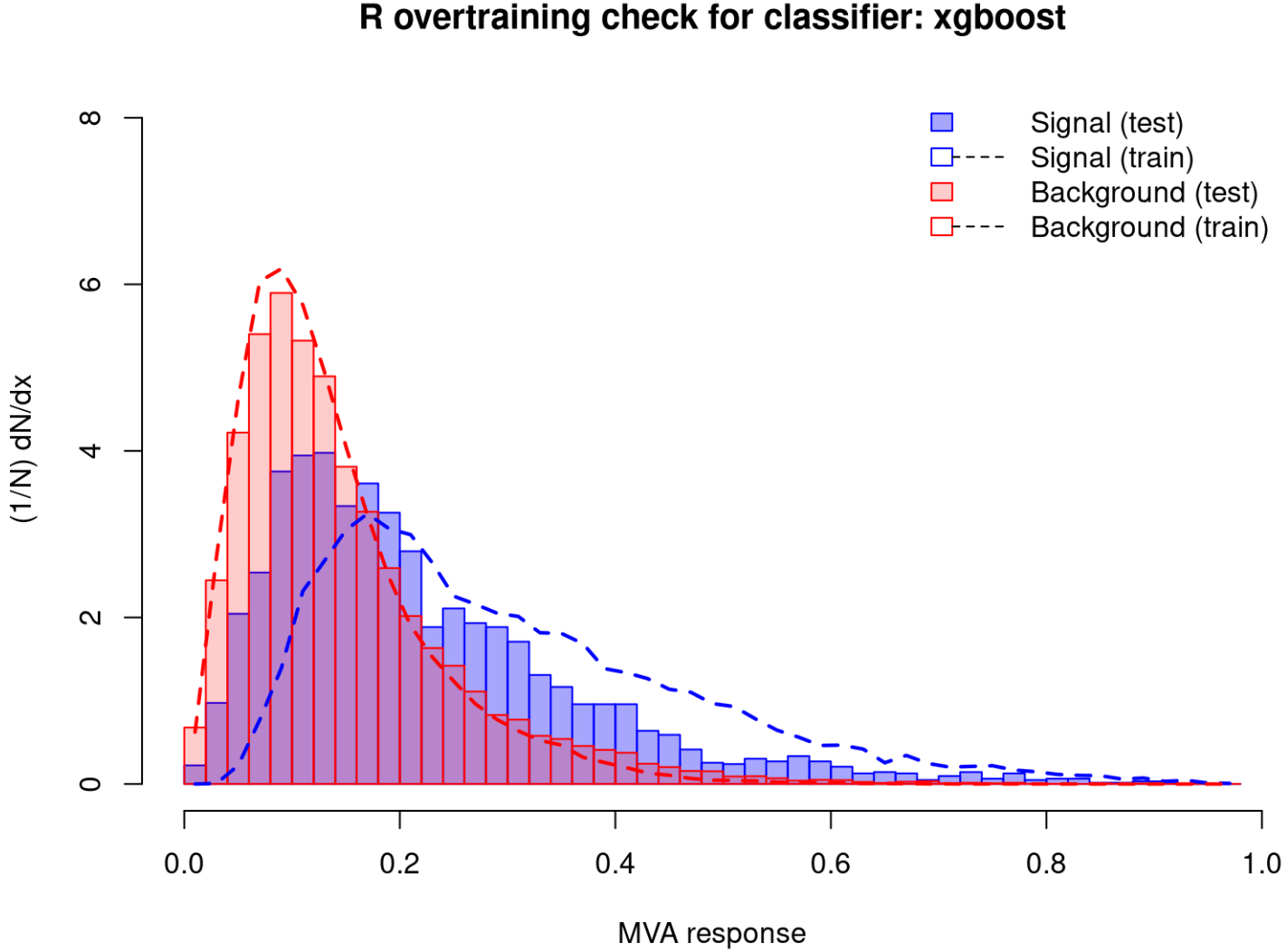

R overtraining check for classifier: glm
KS p-values (unweighted): S=0.974 B=0.999
Signal (test)
Signal (train)
Background (test)
Background (train)
(1/N) dN/dx
0
2
4
6
8
0.0
0.2
0.4
0.6
0.8
MVA response

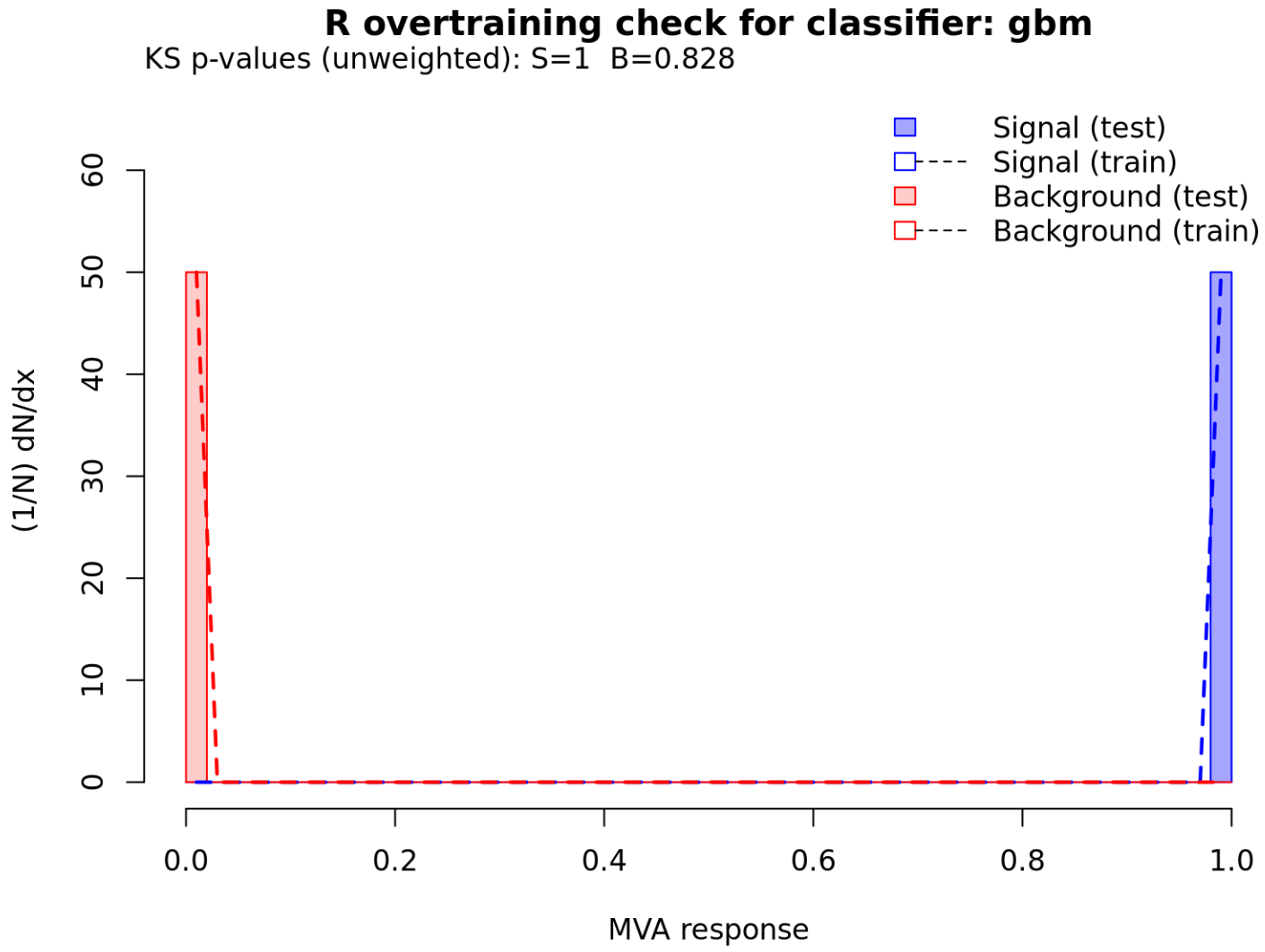

R overtraining check for classifier: mlp
Signal (test)
Signal (train)
Background (test)
Background (train)
(1/N) dN/dx
0
2
4
6
8
0.0
0.2
0.4
0.6
0.8
MVA response

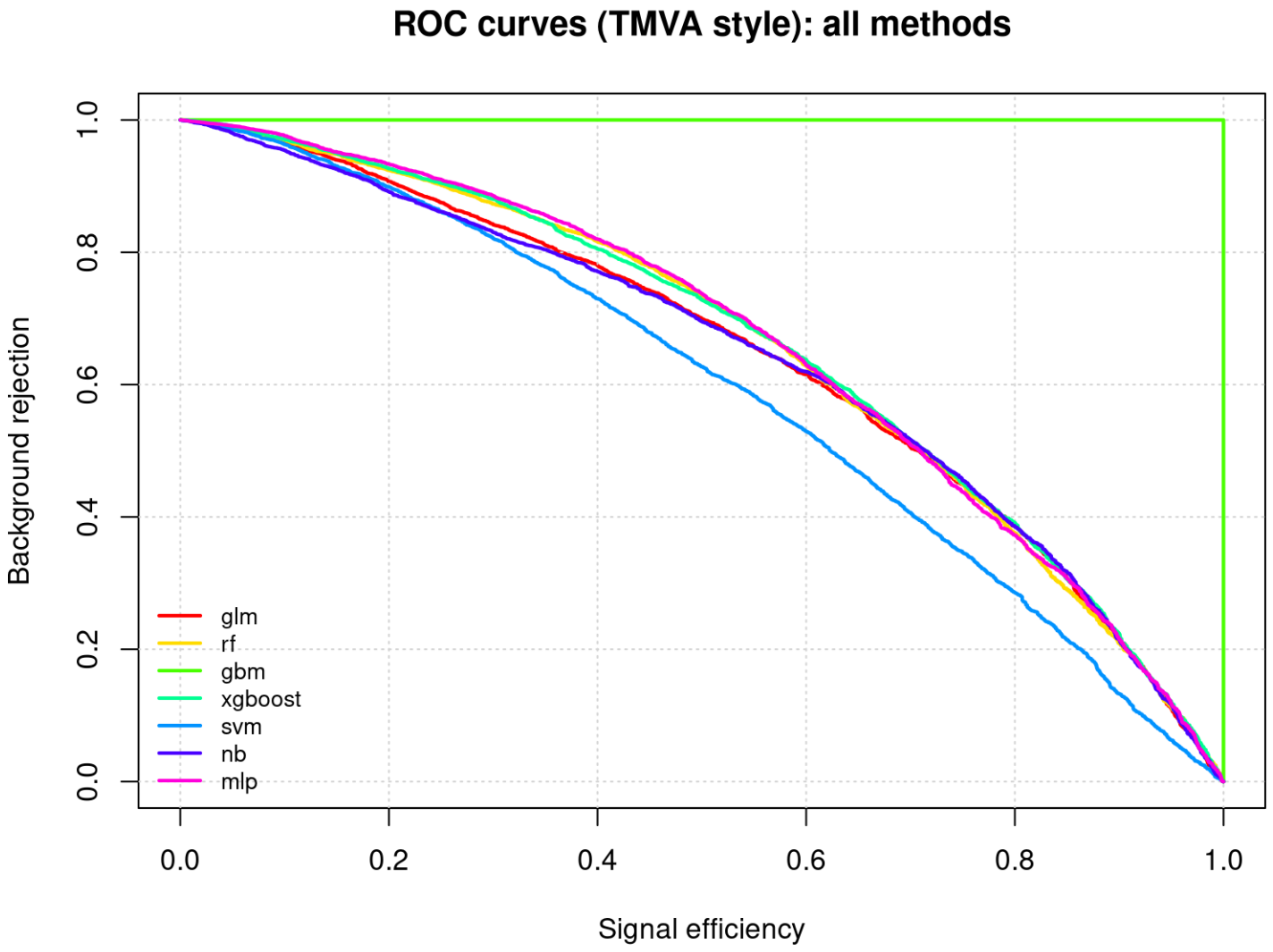

R overtraining check for classifier: rf
KS p-values (unweighted): S=0 B=0
Signal (test)
Signal (train)
Background (test)
Background (train)
(1/N) dN/dx
0
5
10
15
0.0
0.2
0.4
0.6
0.8
MVA response


R overtraining check for classifier: svm
Signal (test)
Signal (train)
Background (test)
Background (train)
(1/N) dN/dx
0
10
20
30
40
50
0.2
0.4
0.6
0.8
1.0
MVA response


R overtraining check for classifier: nb
Signal (test)
Signal (train)
Background (test)
Background (train)
(1/N) dN/dx
0
1
2
3
4
5
6
0.0
0.2
0.4
0.6
0.8
1.0
MVA response


R overtraining check for classifier: xgboost
Signal (test)
Signal (train)
Background (test)
Background (train)
(1/N) dN/dx
0
2
4
6
8
0.0
0.2
0.4
0.6
0.8
1.0
MVA response

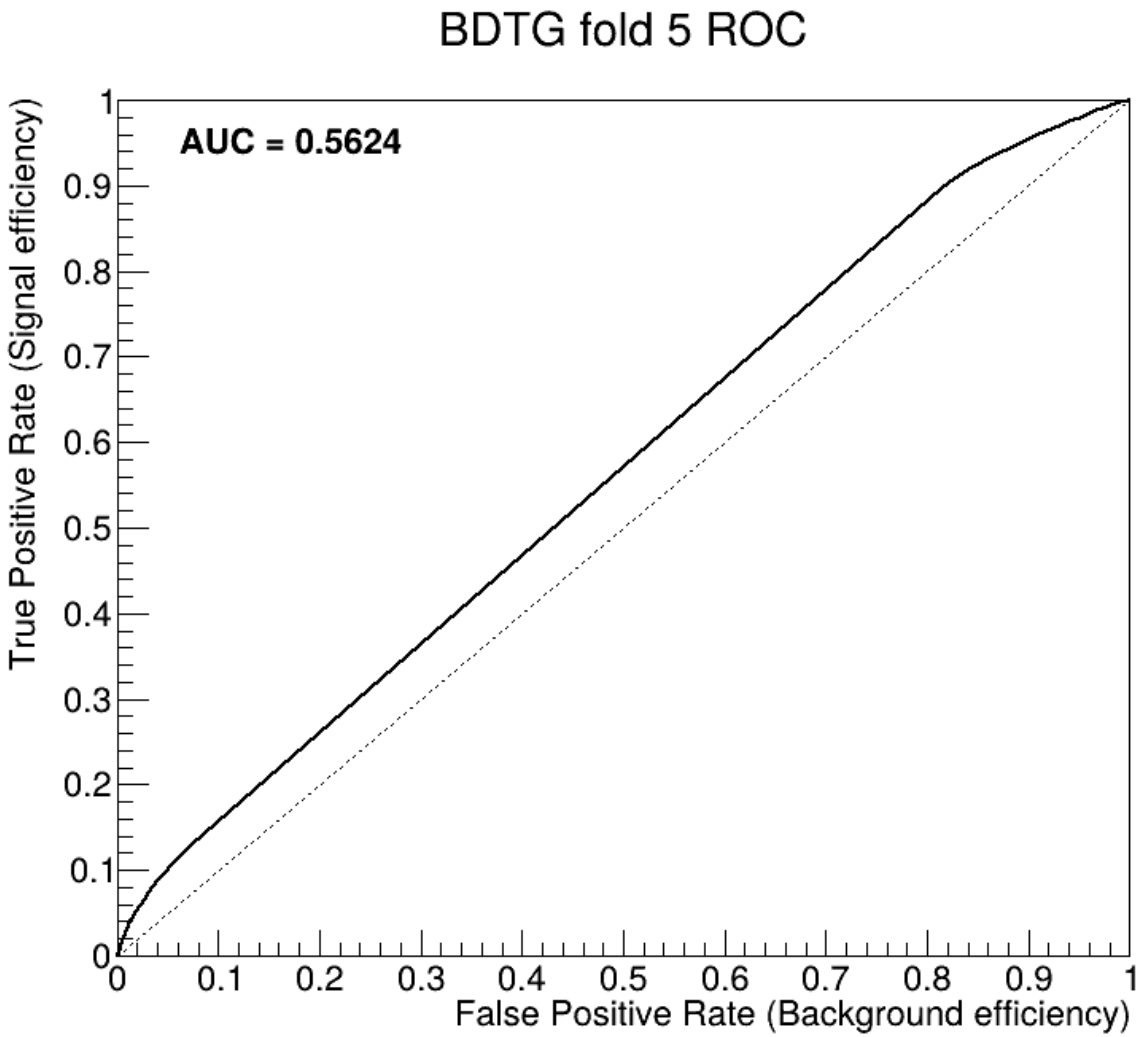

R overtraining check for classifier: gbm
KS p-values (unweighted): S=1 B=0.828
Signal (test)
Signal (train)
Background (test)
Background (train)
(1/N) dN/dx
0
10
20
30
40
50
60
0.0
0.2
0.4
0.6
0.8
1.0
MVA response


ROC curves (TMVA style): all methods
Background rejection
Signal efficiency
0.0
0.2
0.4
0.6
0.8
1.0
glm
rf
gbm
xgboost
svm
nb
mlp

Comparison of Results from Python and R (k-fold)

Model	R AUC (oof_weighted)	Python mean_fold_auc	Python overall_oof_auc	Δ AUC (R − Py overall)
Gradient Boosting (gbm)	**1.000000**	0.675134	0.674820	**+0.325180**
MLP (mlp)	0.661500	0.665761	0.664427	−0.002927
Random Forest (rf)	0.656103	0.672187	0.671608	−0.015505
Logistic Regression (glm)	0.643484	0.639506	0.639507	+0.003977
Naive Bayes (nb)	0.640344	0.640700	0.639867	+0.000477
SVM / SVC (svm)	0.590934	0.676572	0.676277	−0.085343

TMVA BDTG did not change, Working on it to improvise



National Research
Tomsk
State
University

Лаборатория
анализа данных
физики высоких энергий
Томского
государственного
университета

Thank you for your attention!!!