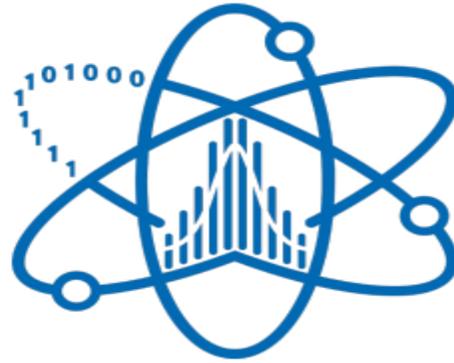




National Research
**Tomsk
State
University**



**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_1l_recalc_NOSYS,
bdt_delta_pT_1l_MET_recalc_NOSYS,
S,
bdt_delta_pT_1lb_MET_recalc_NOSYS,
YS,
bdt_eta_1lMetB_recalc_NOSYS,
bdt_m_11b_recalc_NOSYS,
bdt_m_12b_recalc_NOSYS,
bdt_pT_1lMetB_recalc_NOSYS,
bdt_pT_1lb_recalc_NOSYS,
bdt_sum_ET_recalc_NOSYS.

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

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

Background: $t\bar{t}$ (non-all-had)

•**Event weights:** auto-resolved to
 $\text{weight_mc_NOSYS} * \text{weight_pileup_NOSYS}$
 $* \text{globalTriggerEffSF_NOSYS}$.

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

Article's Report on BDT

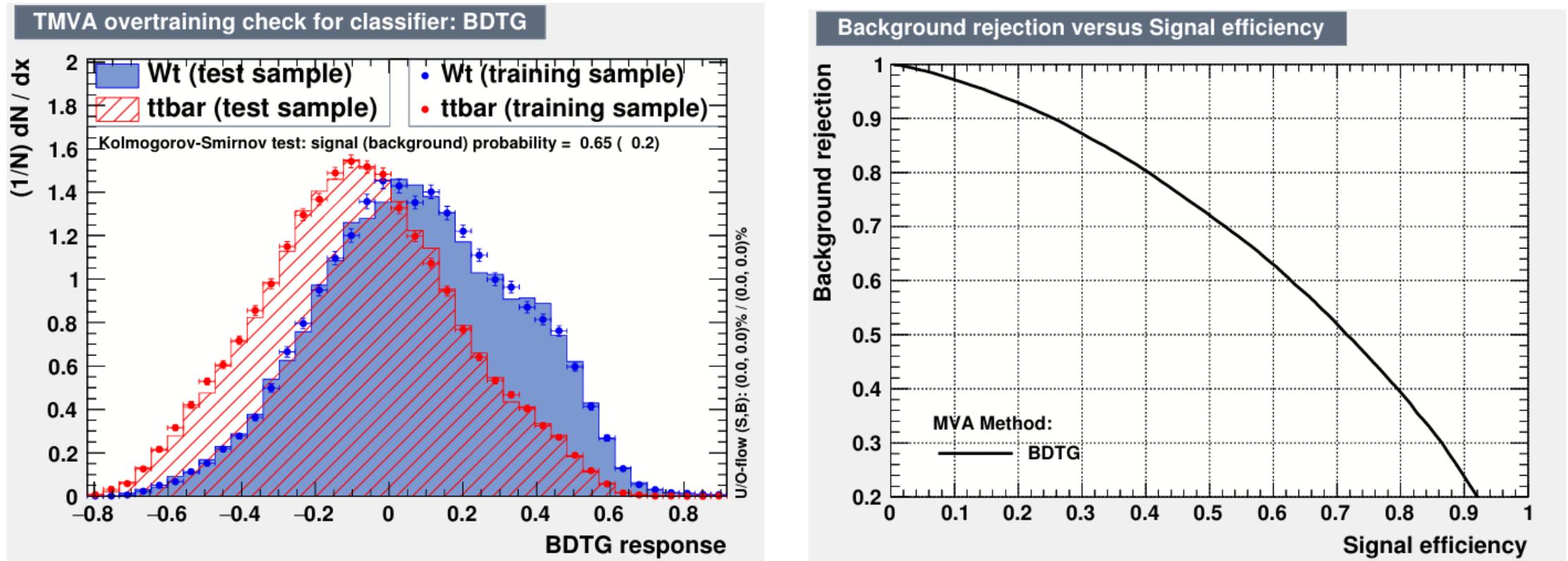


Figure 9: Comparison of test/training sample distributions and background rejection factor versus signal efficiency.

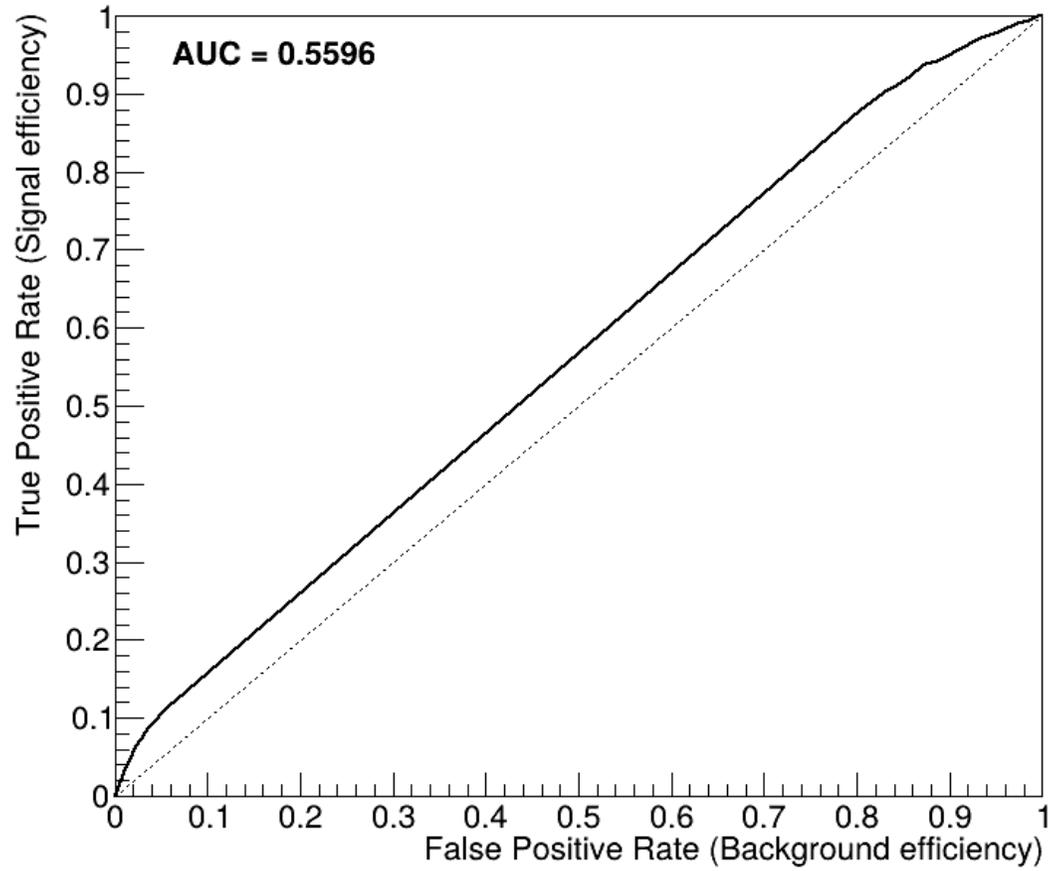
Results of Performance of ML Algorithms using K-fold on TMVA

27th January 2026

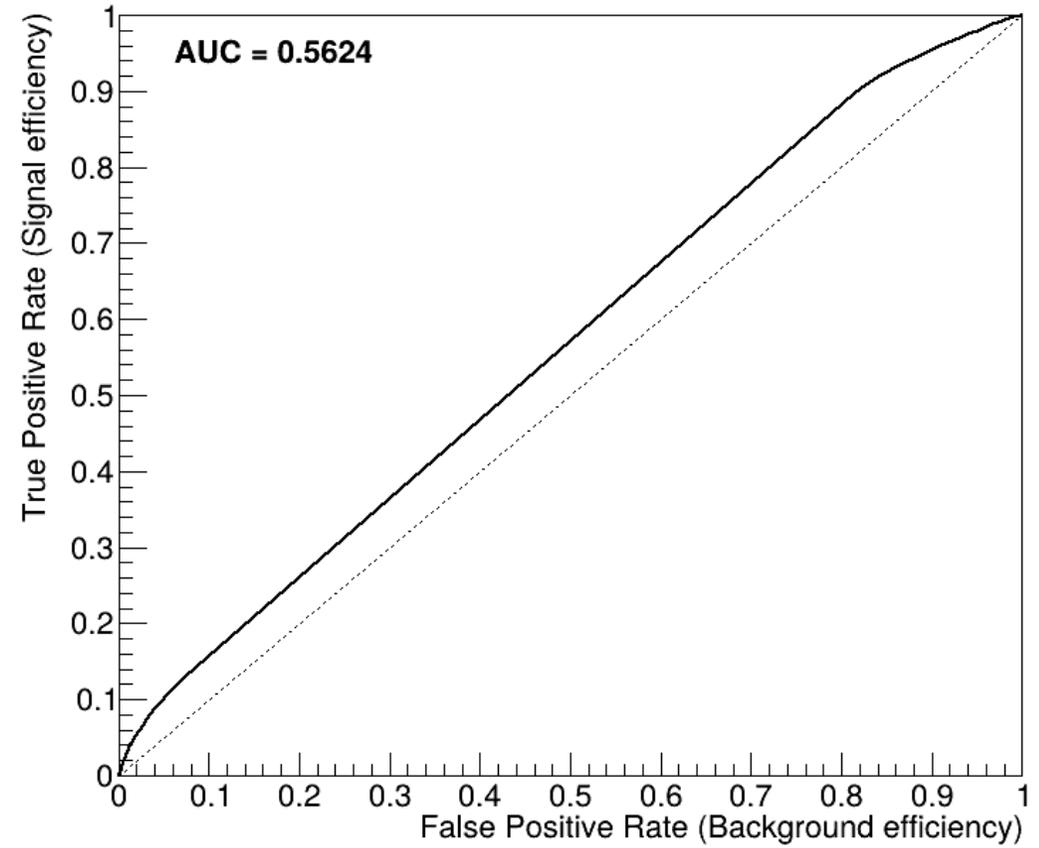
Algorithms	ROC_AUC_MEAN	ROC_AUC_STD	n_folds_used
BDTB	0.560854	0.003277	5
BDTG	0.55978	0.003049	5
Fisher	0.550102	0.00274	5
KNN	0.549632	0.003916	5
LD	0.547795	0.001821	5
Likelihood	0.523526	0.004158	5
MLP	0.561797	0.002013	5

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.

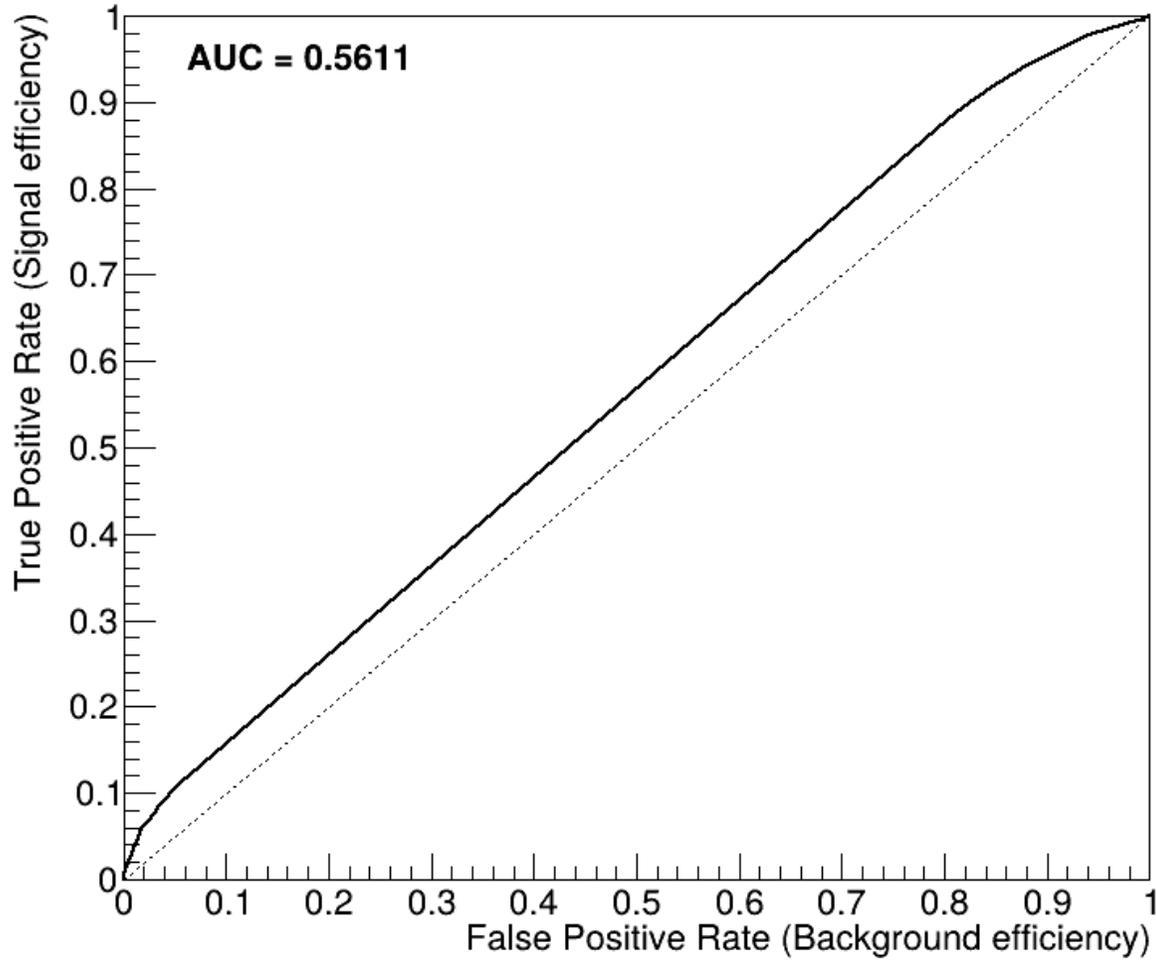
BDTG fold 3 ROC



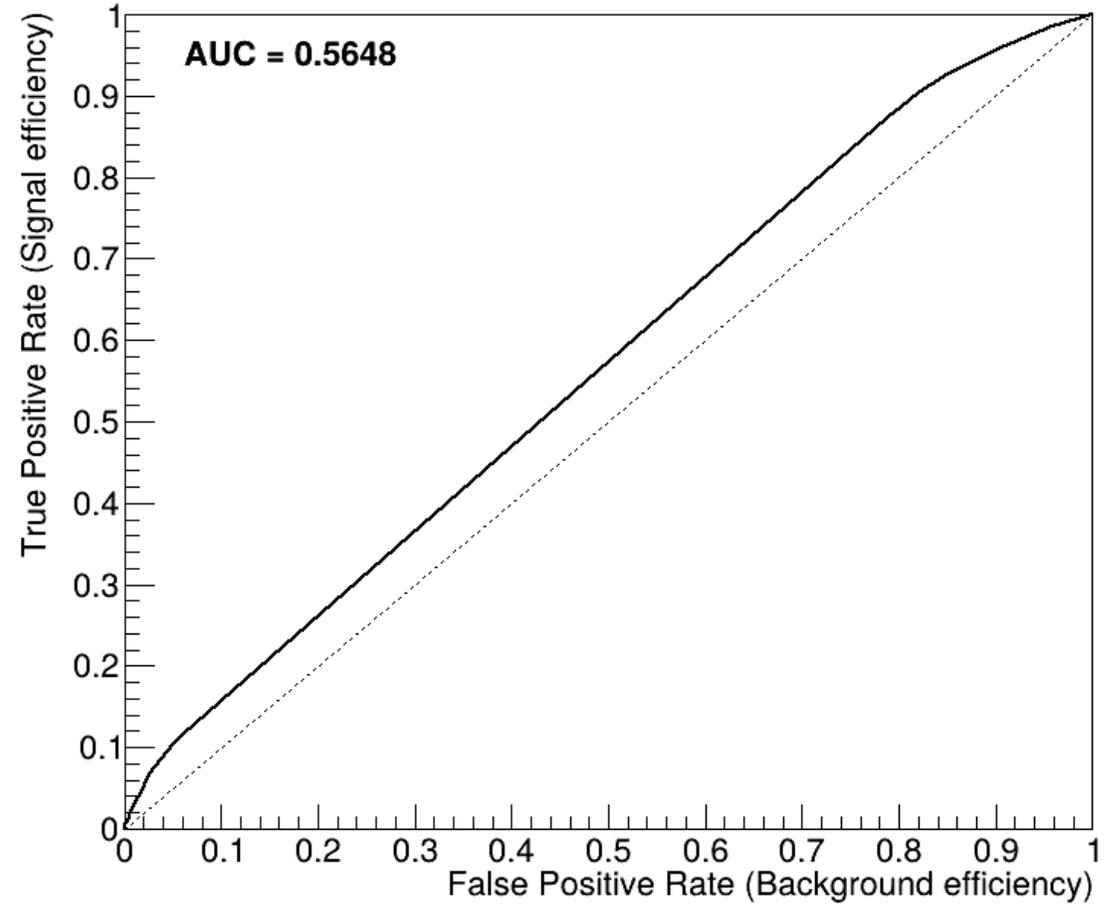
BDTG fold 5 ROC



MLP fold 3 ROC



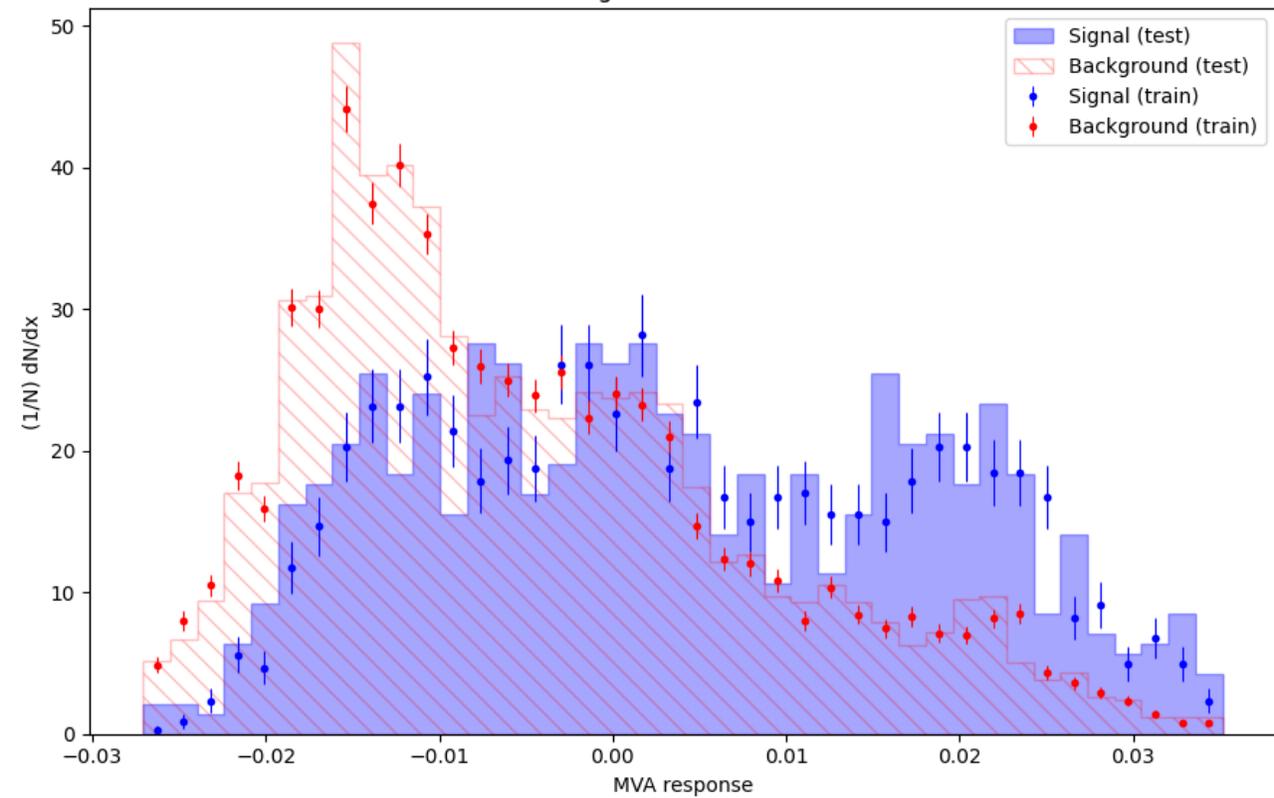
MLP fold 5 ROC



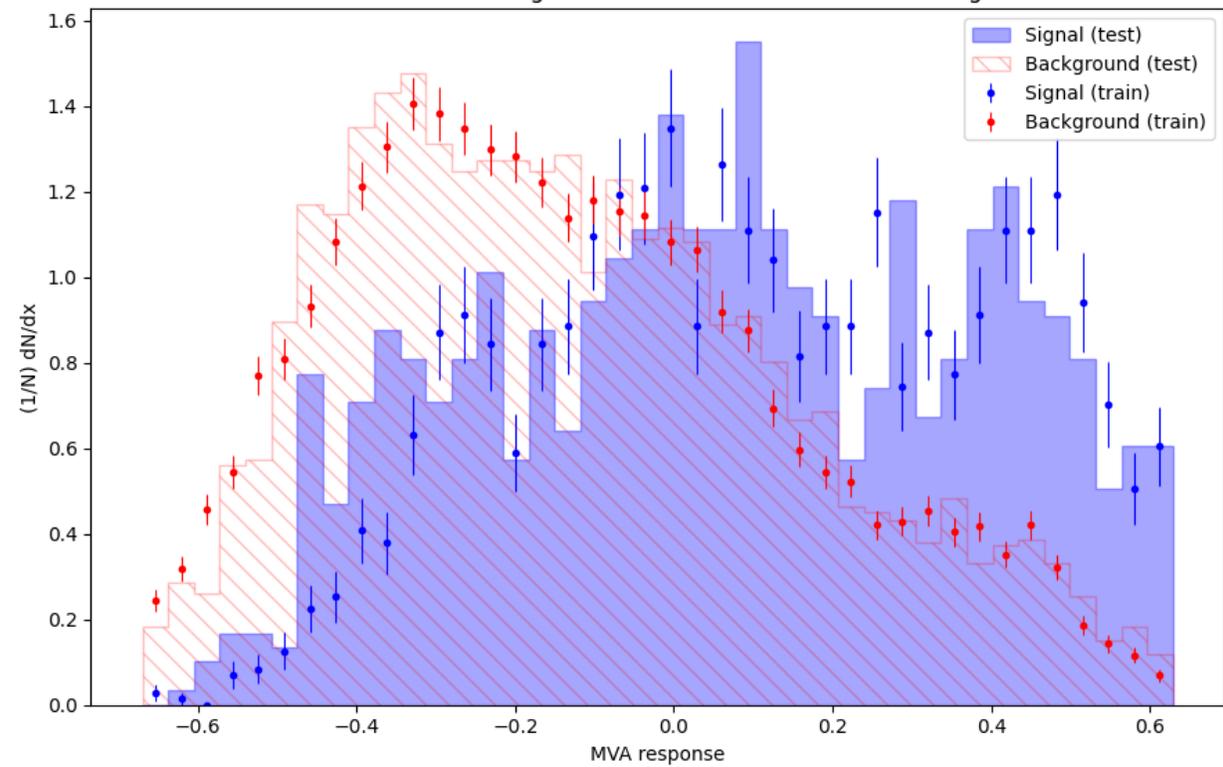
**Results of Performance of ML
Algorithms using K-fold on
Python Trial 3
27th January 2026**

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

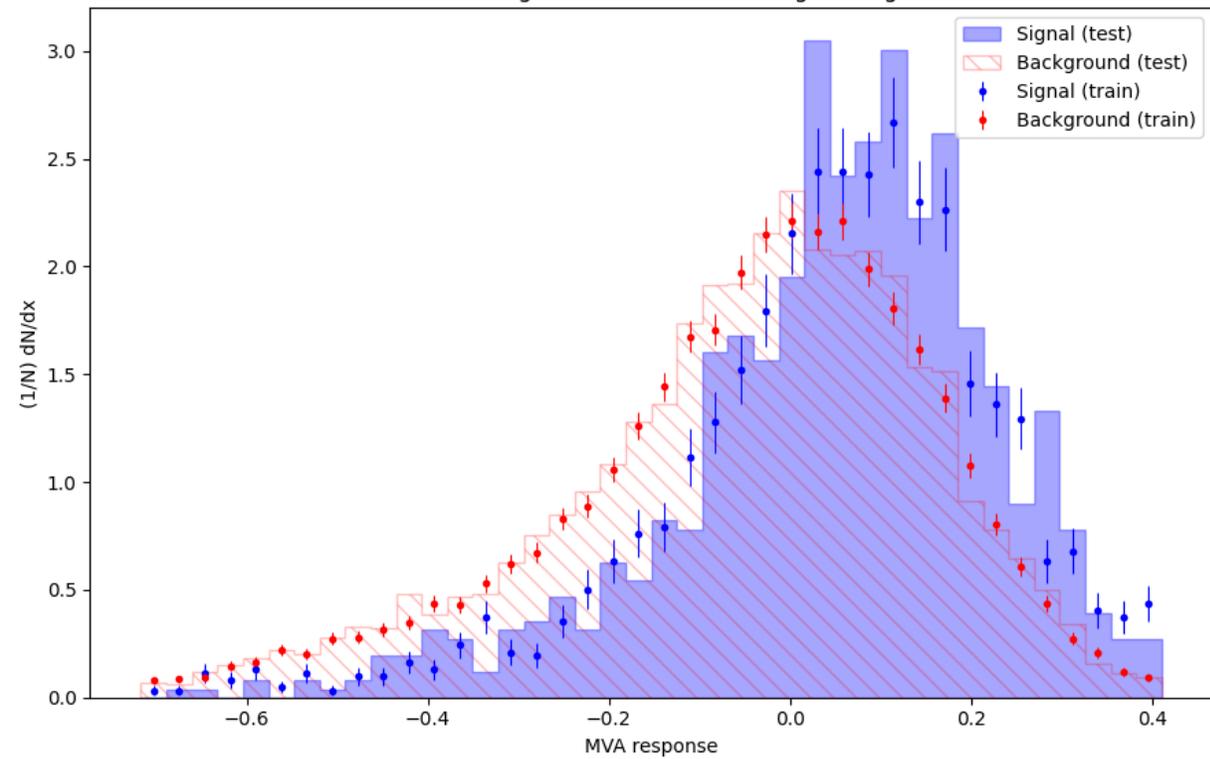
TMVA overtraining check for classifier: AdaBoost



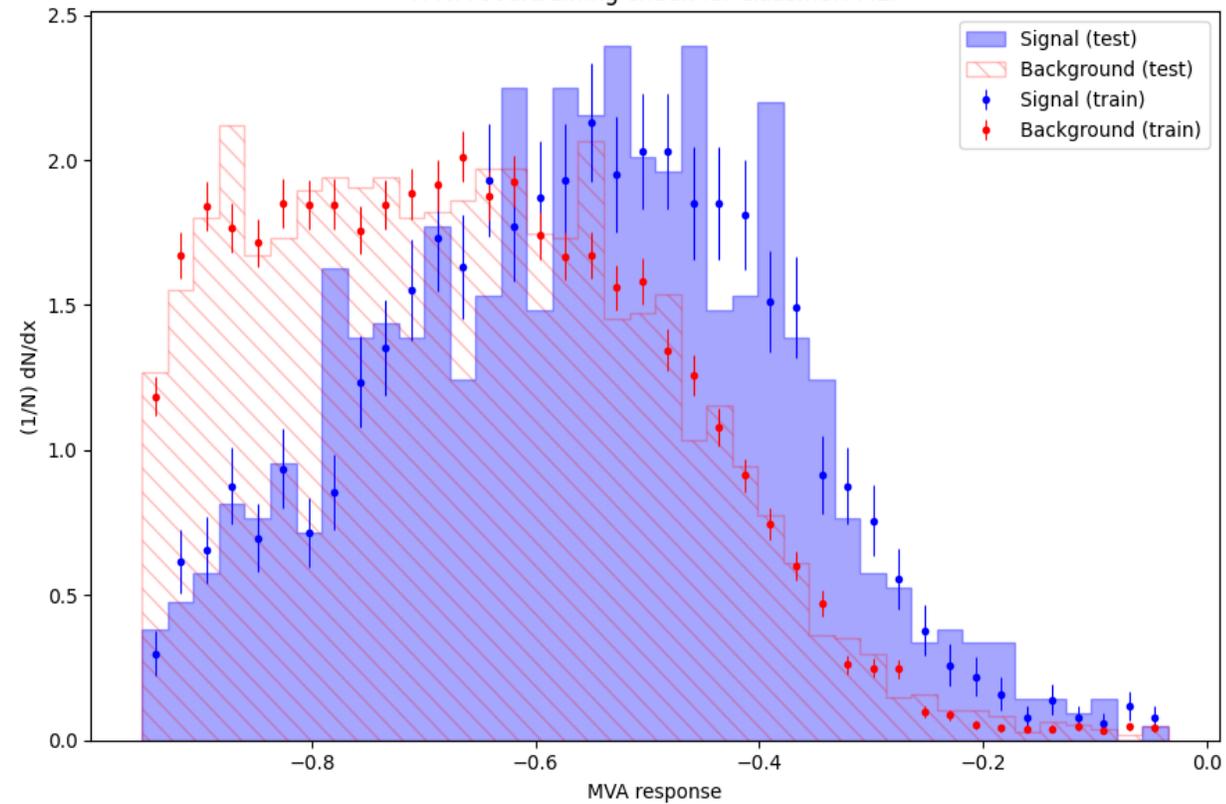
TMVA overtraining check for classifier: GradientBoosting



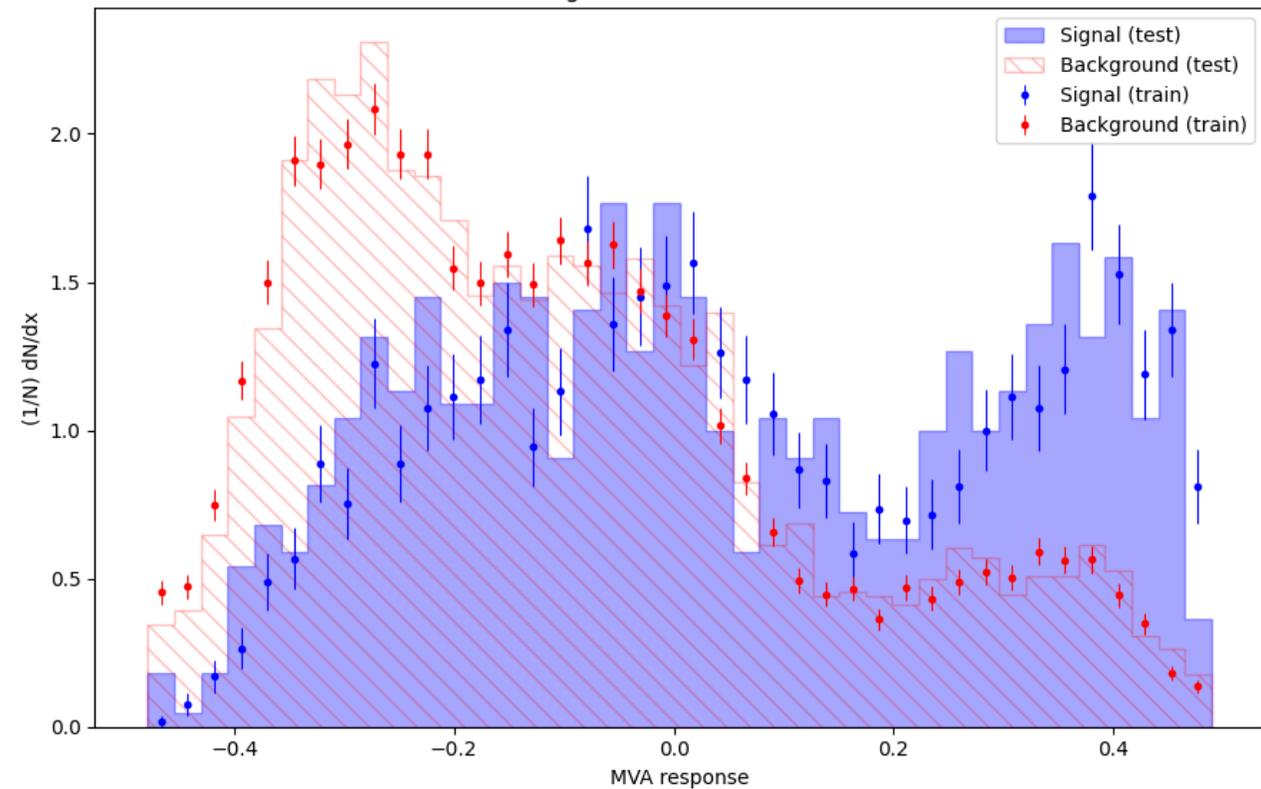
TMVA overtraining check for classifier: LogisticRegression



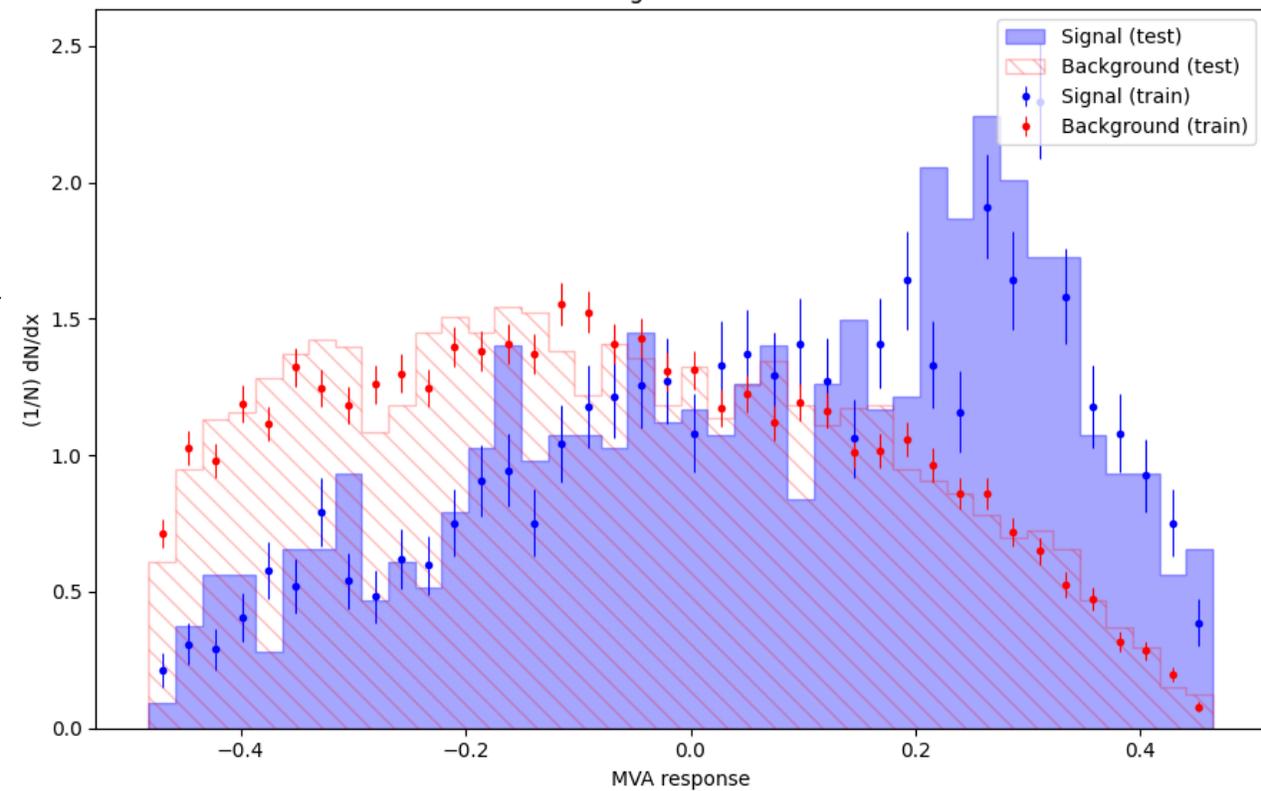
TMVA overtraining check for classifier: MLP



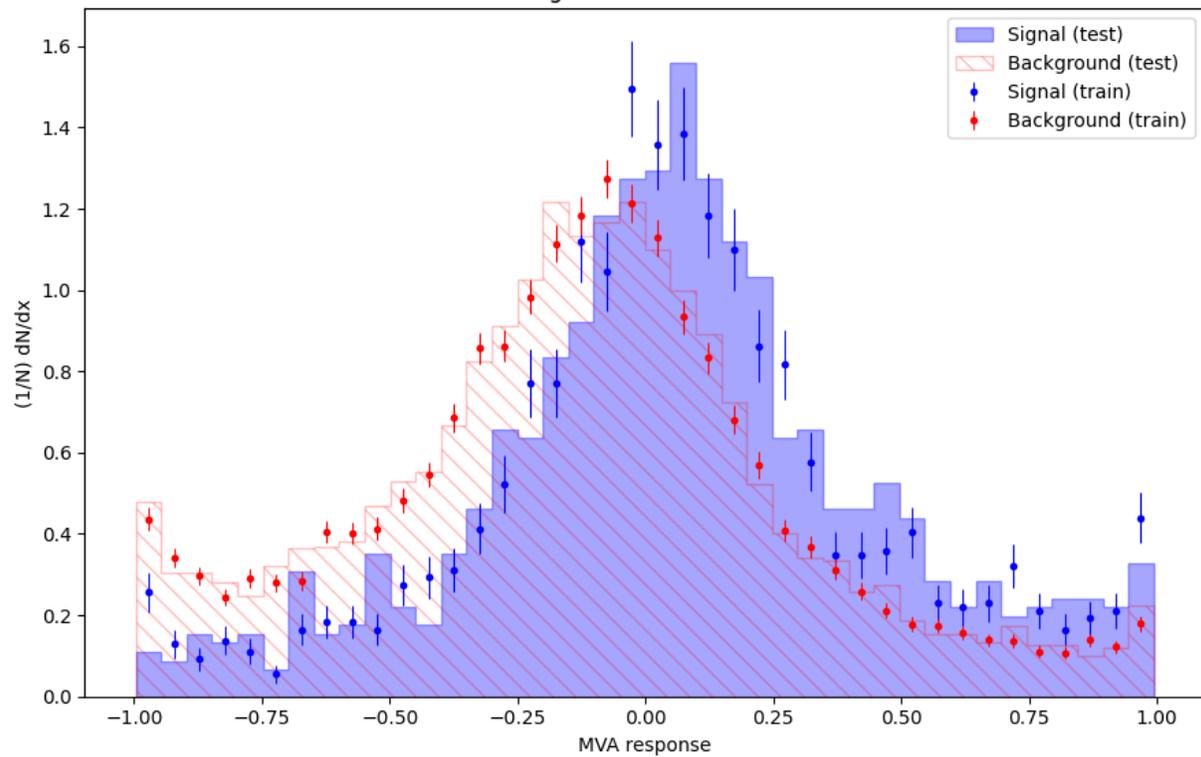
TMVA overtraining check for classifier: RandomForest



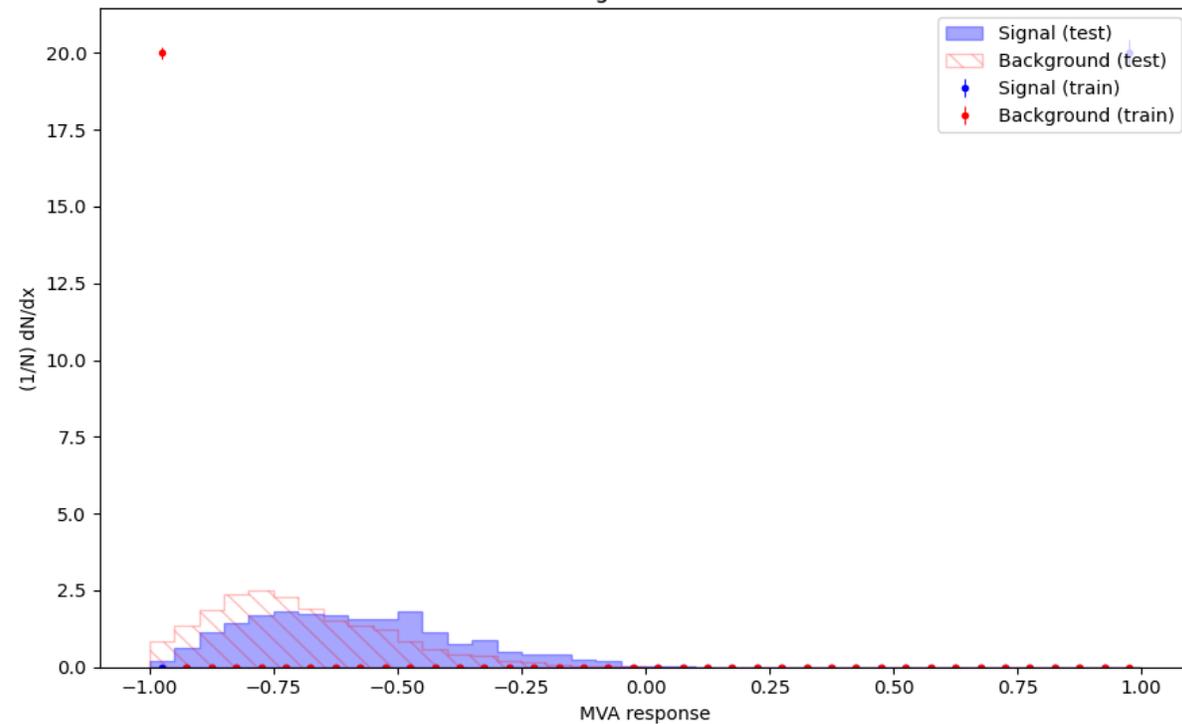
TMVA overtraining check for classifier: SVC



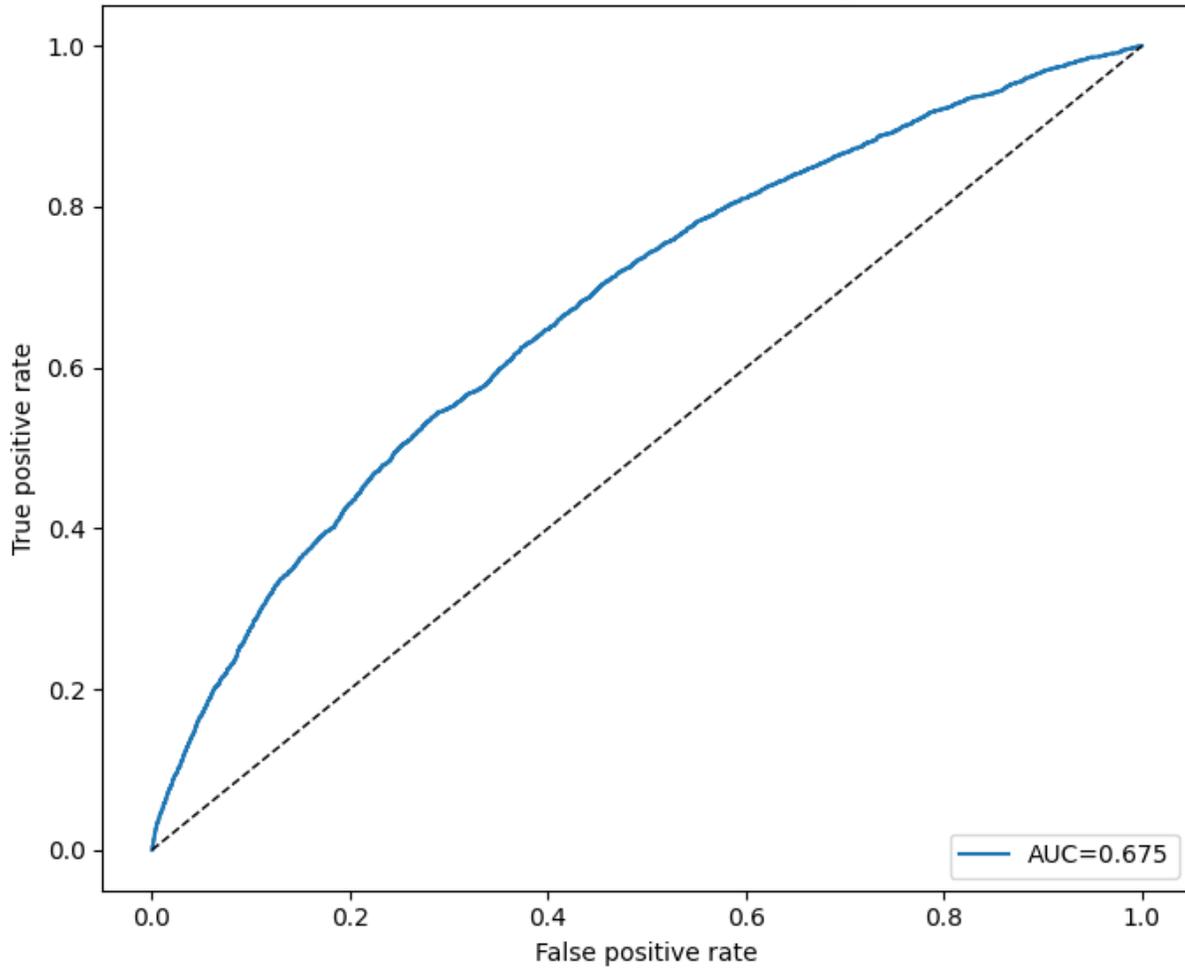
TMVA overtraining check for classifier: GaussianNB



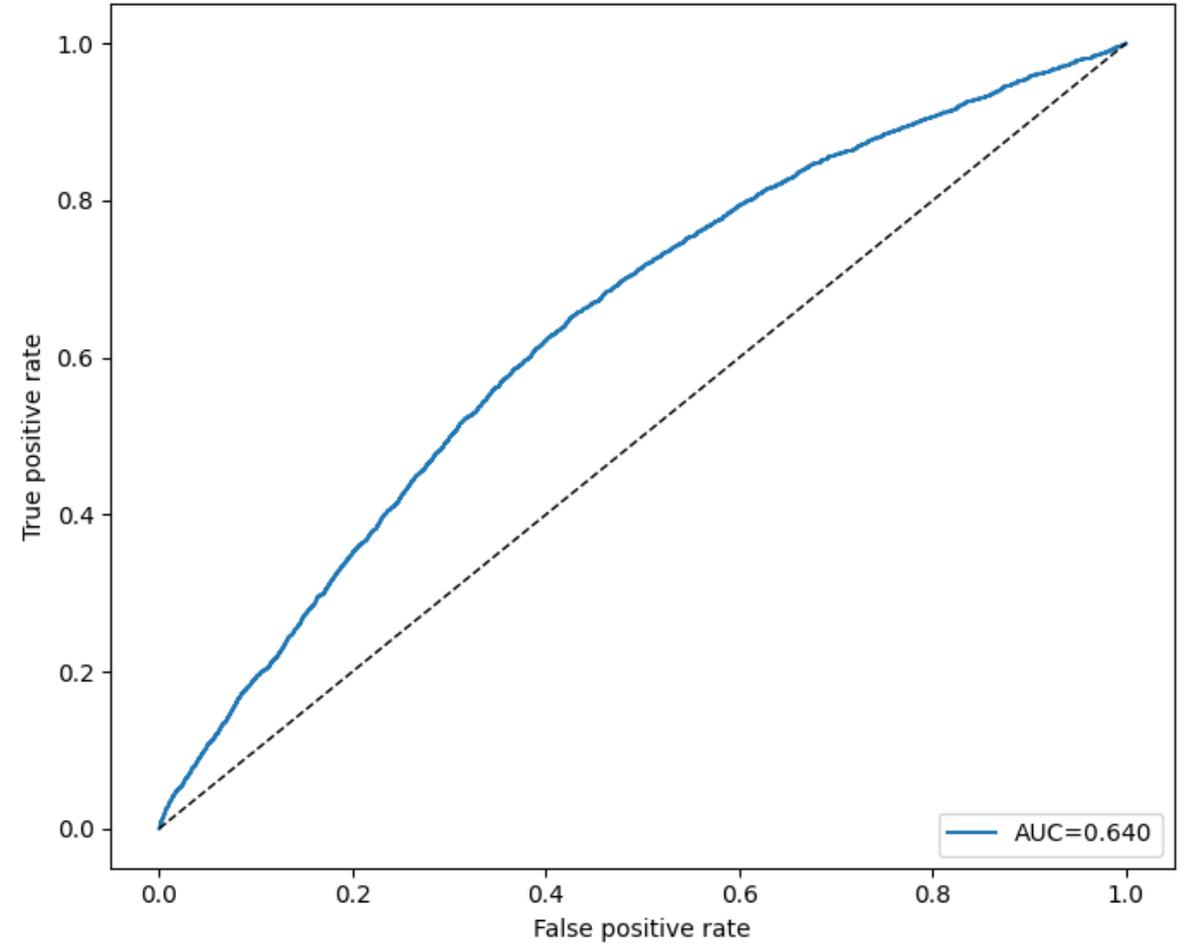
TMVA overtraining check for classifier: KNN



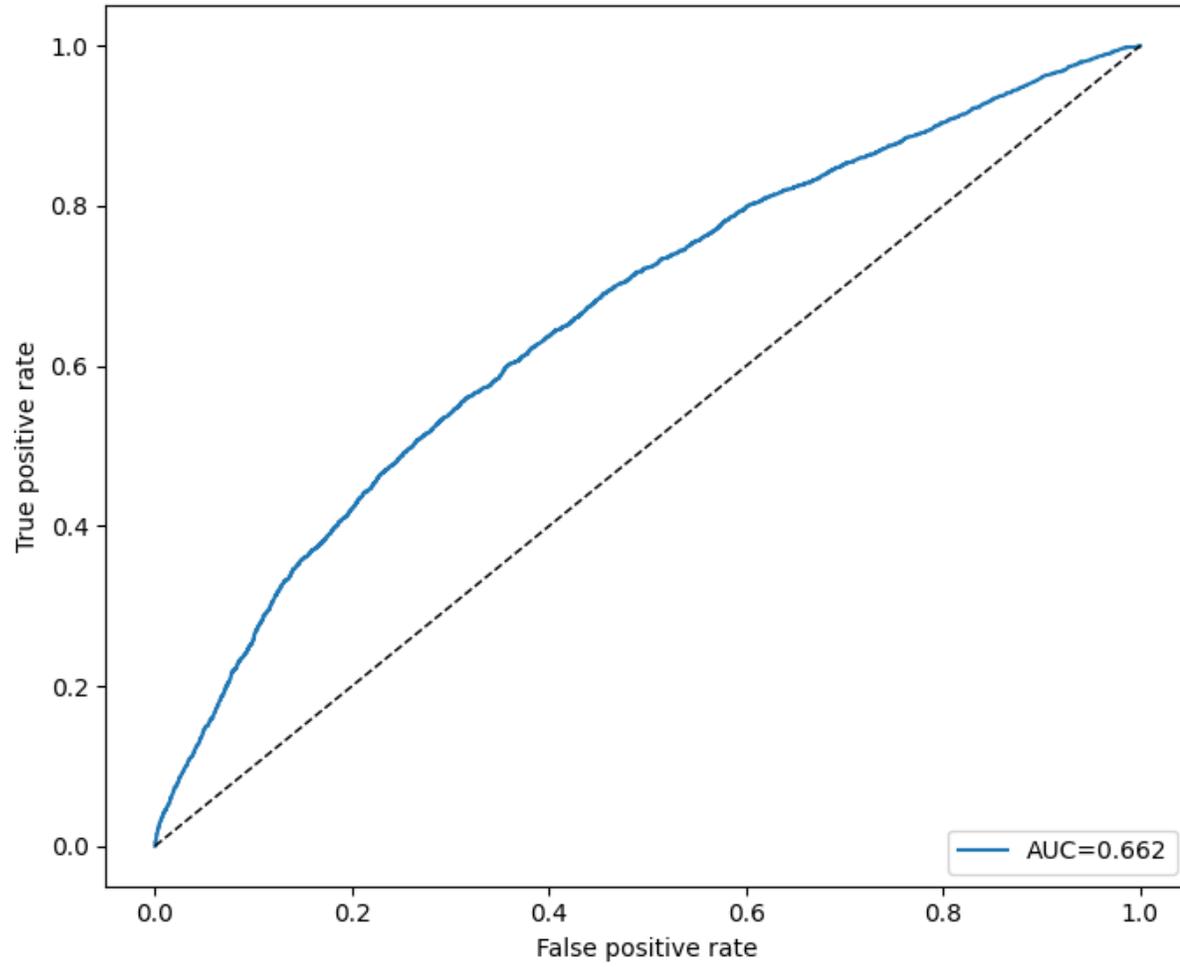
OOF ROC - GradientBoosting



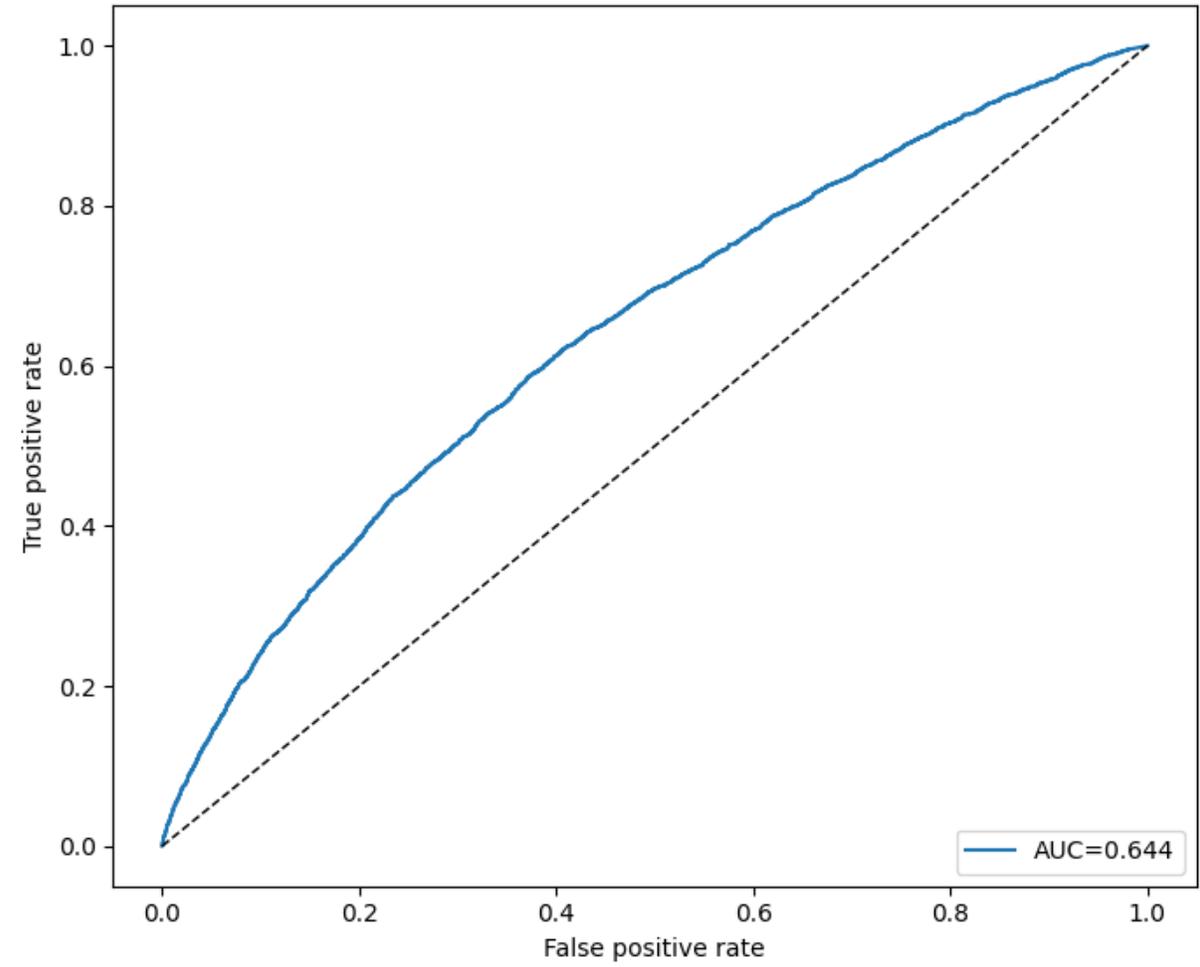
OOF ROC - GaussianNB



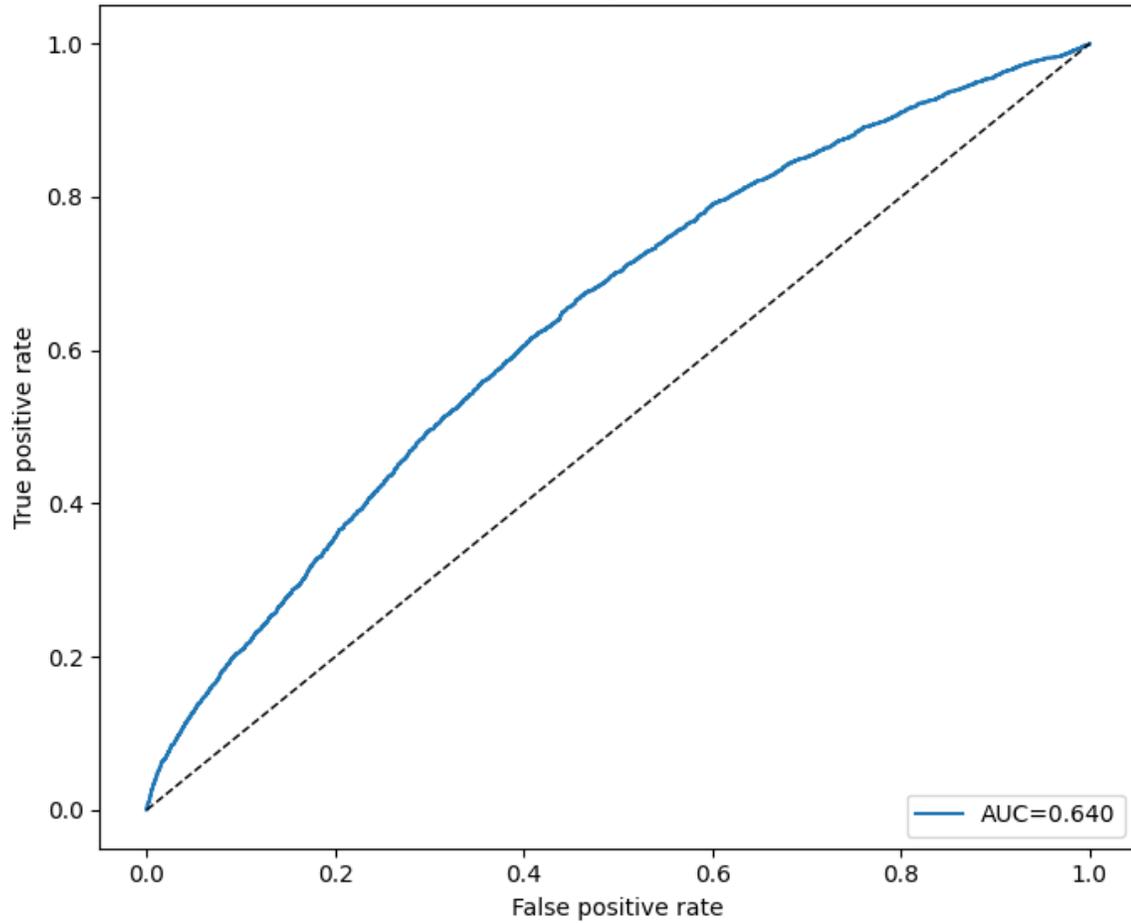
OOF ROC - AdaBoost



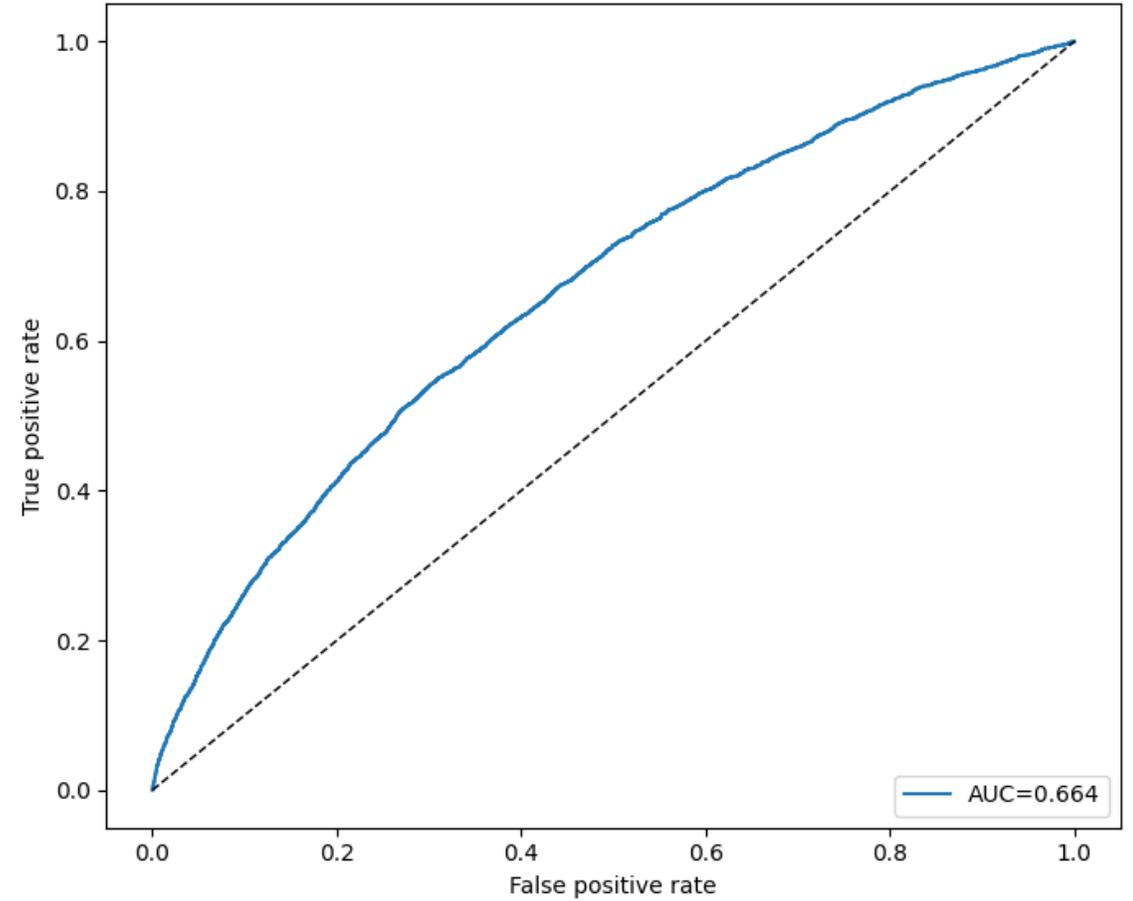
OOF ROC - KNN



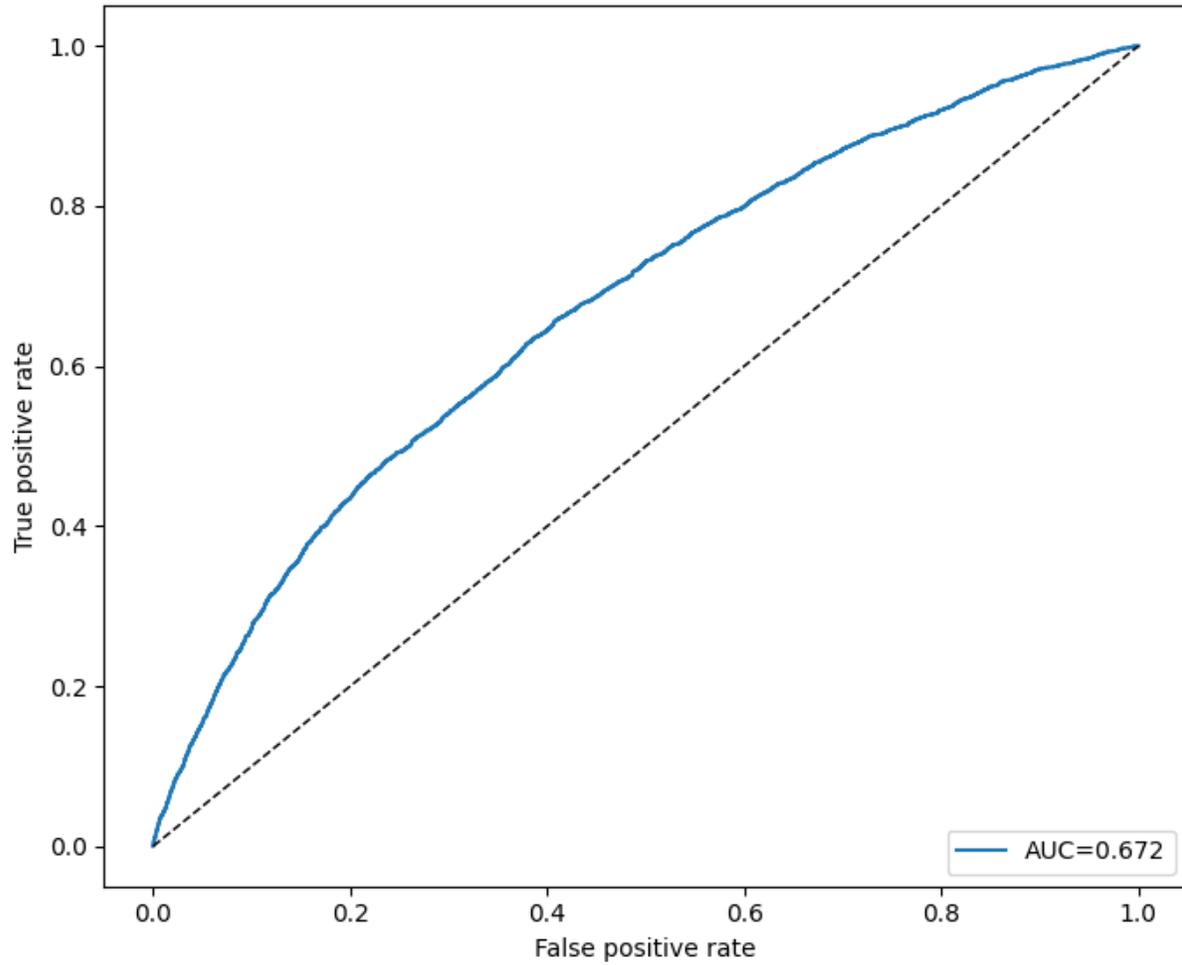
OOF ROC - LogisticRegression



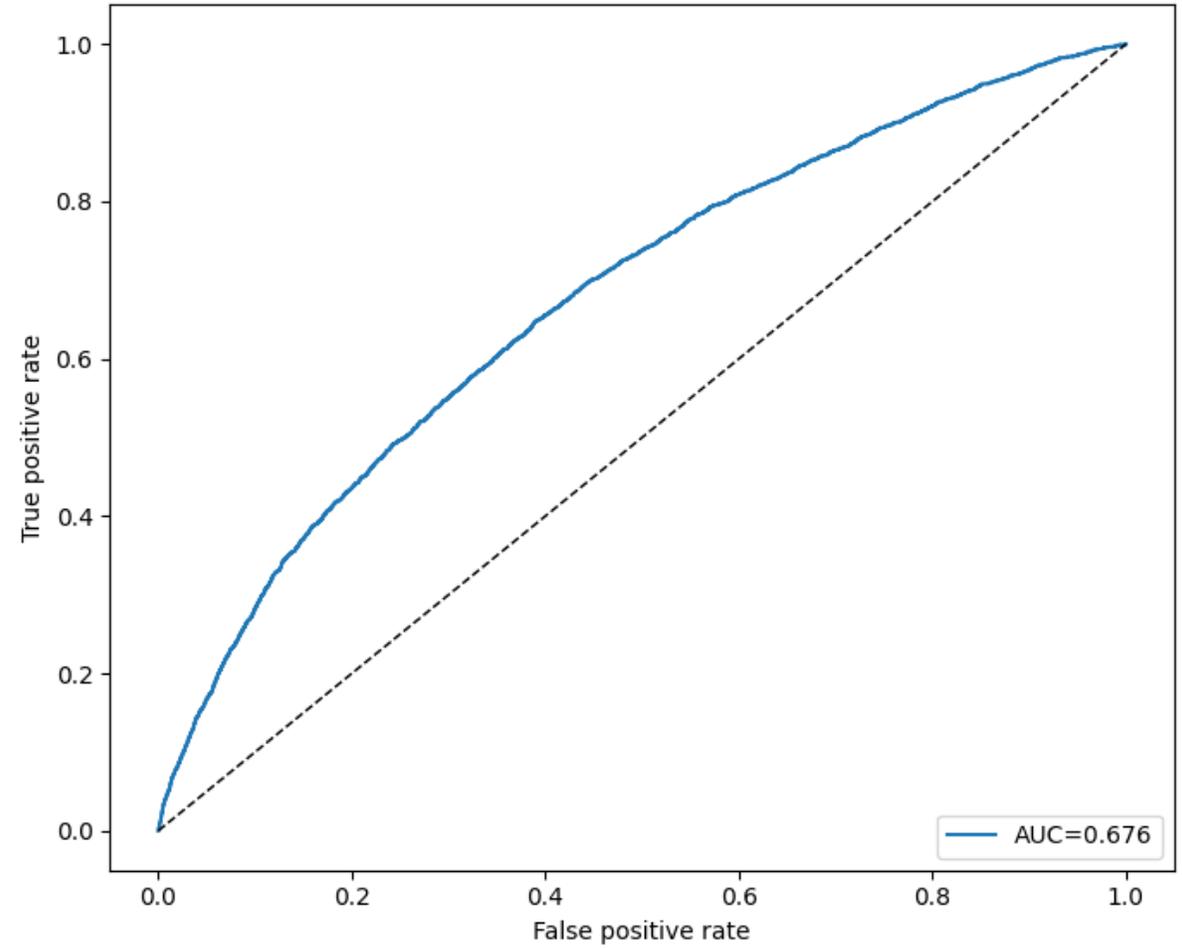
OOF ROC - MLP



OOF ROC - RandomForest



OOF ROC - SVC



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

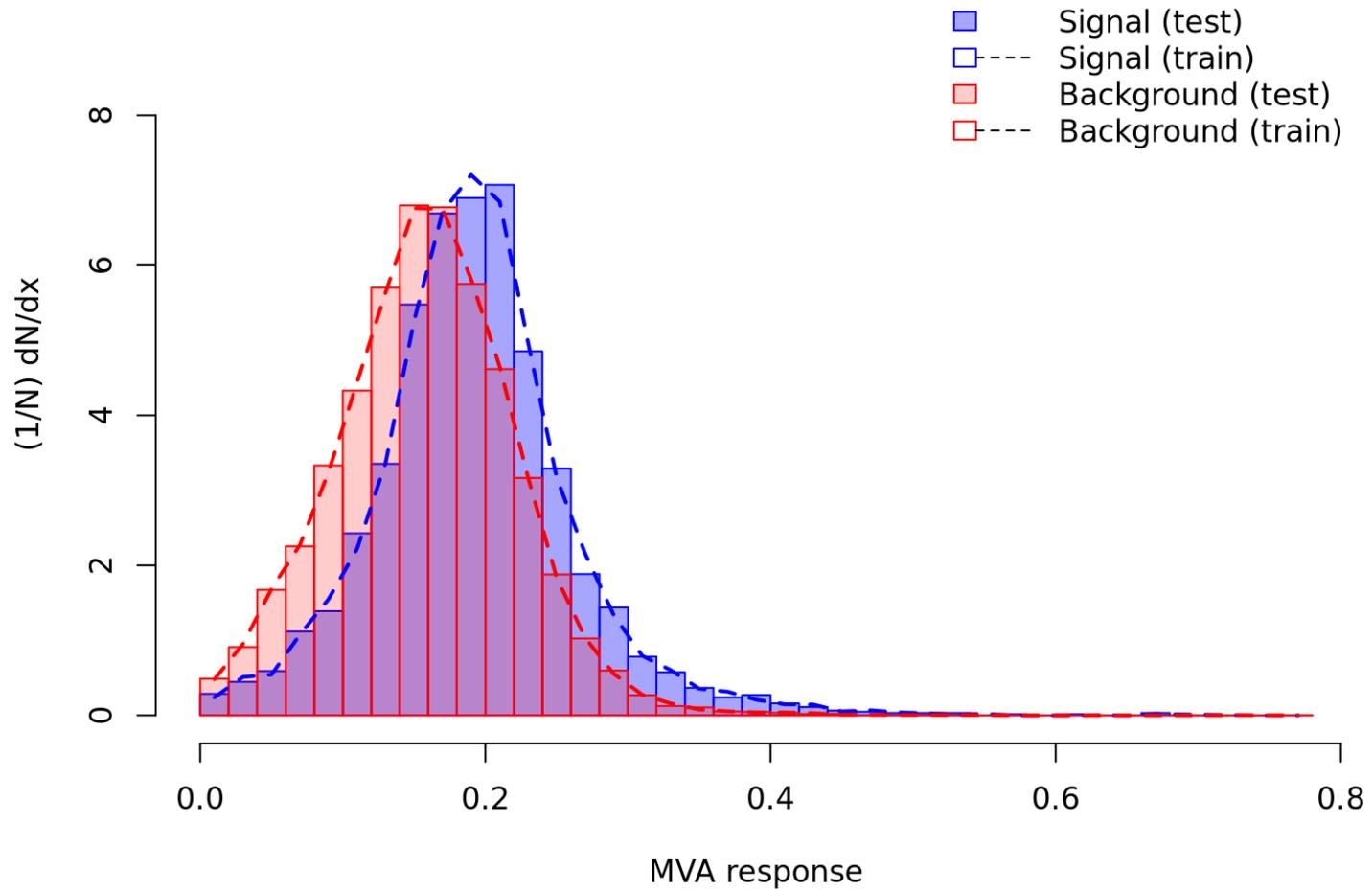
Methods: GLM, RF, GBM, XGBOOST, SVM,
KNN, NB, MLP

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

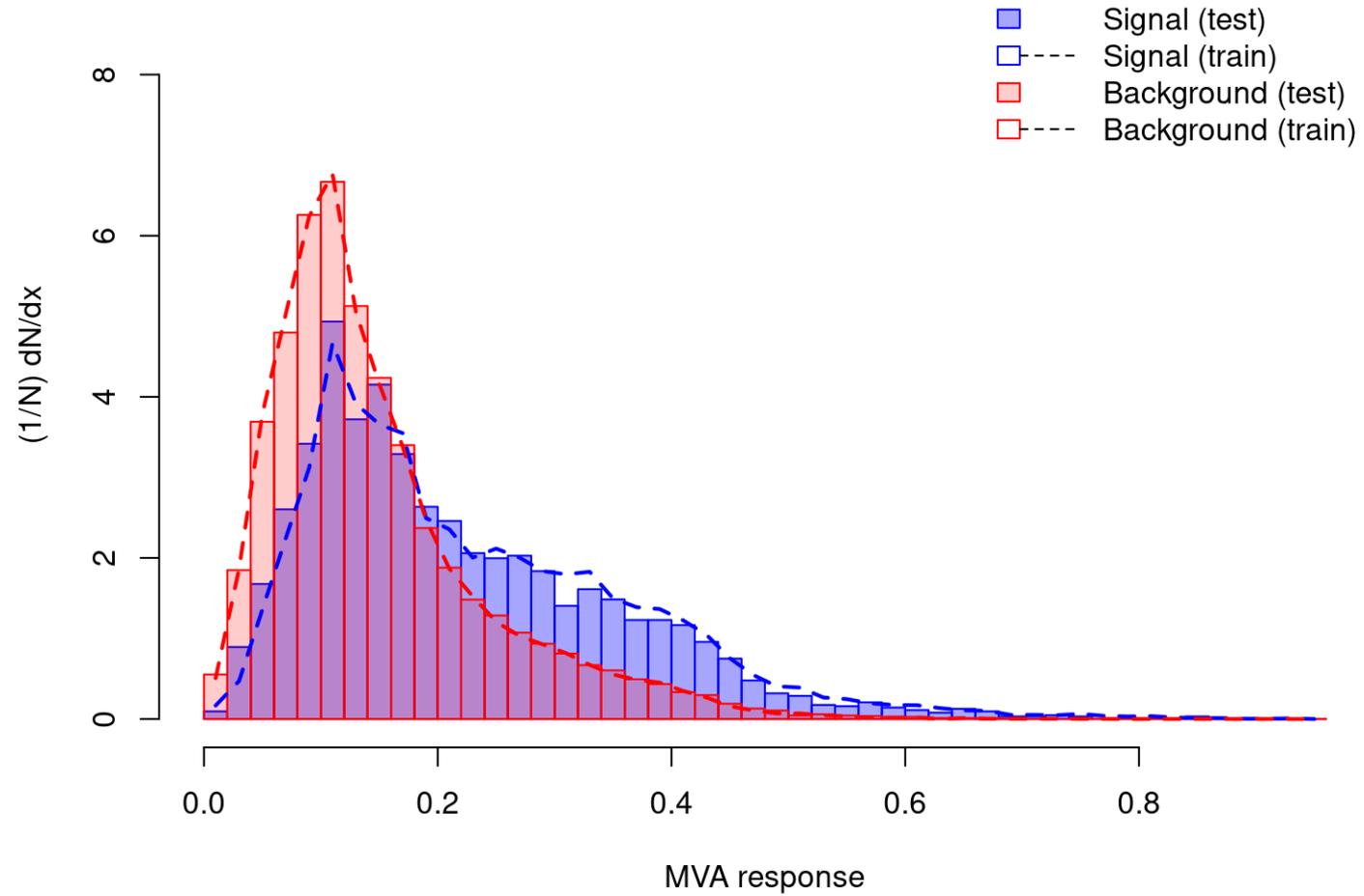
<i>Algorithm (R)</i>	<i>auc_oof_weighted</i>	<i>acc_oof_weighted</i>
GBM	1	1
MLP	0.660152	0.836995
XGBOOST	0.659179	0.835844
RF	0.656103	0.835792
GLM	0.643484	0.836315
NB	0.640344	0.813926
SVM	0.590384	0.836263

R overtraining check for classifier: glm

KS p-values (unweighted): S=0.974 B=0.999

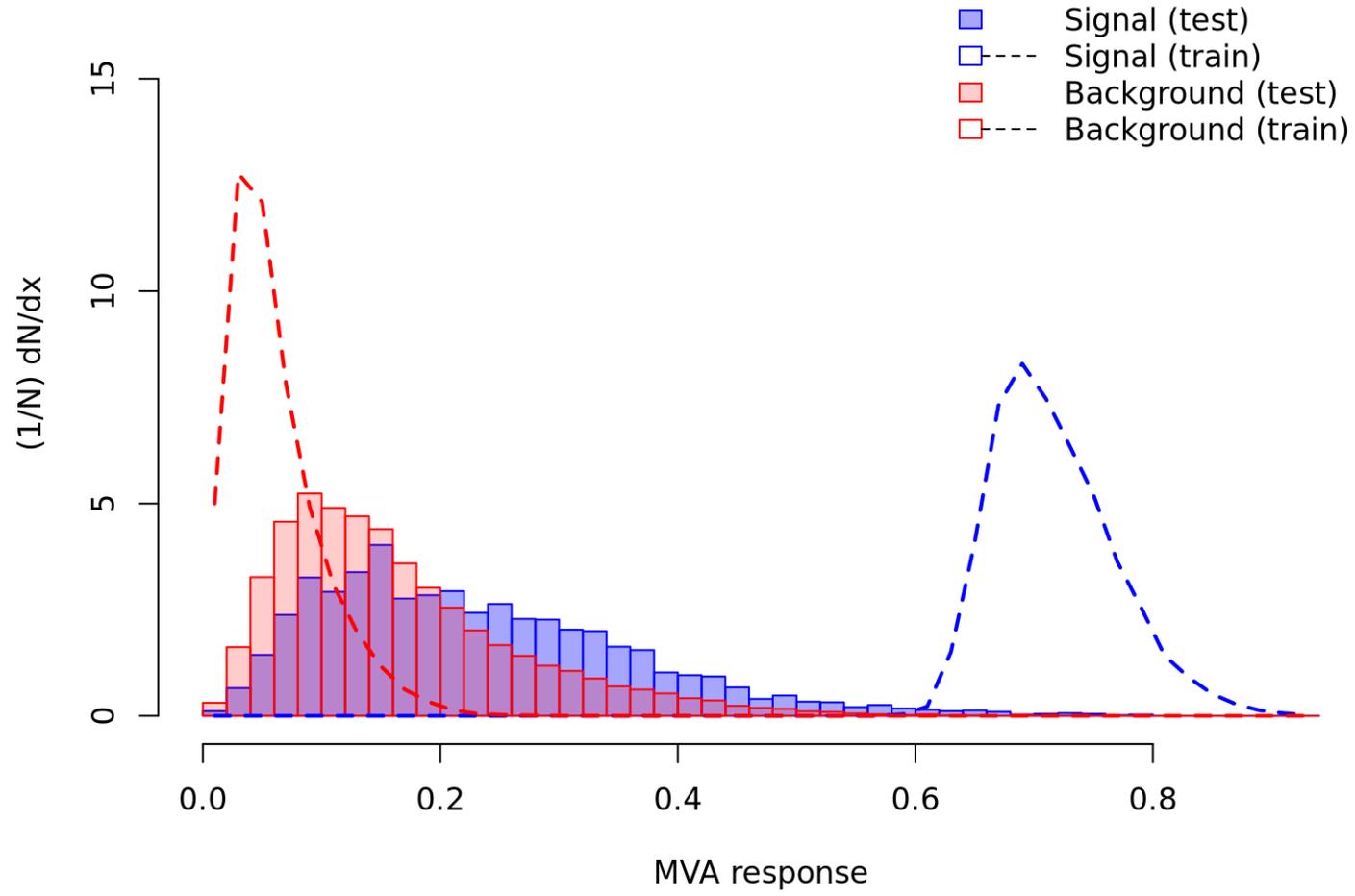


R overtraining check for classifier: mlp

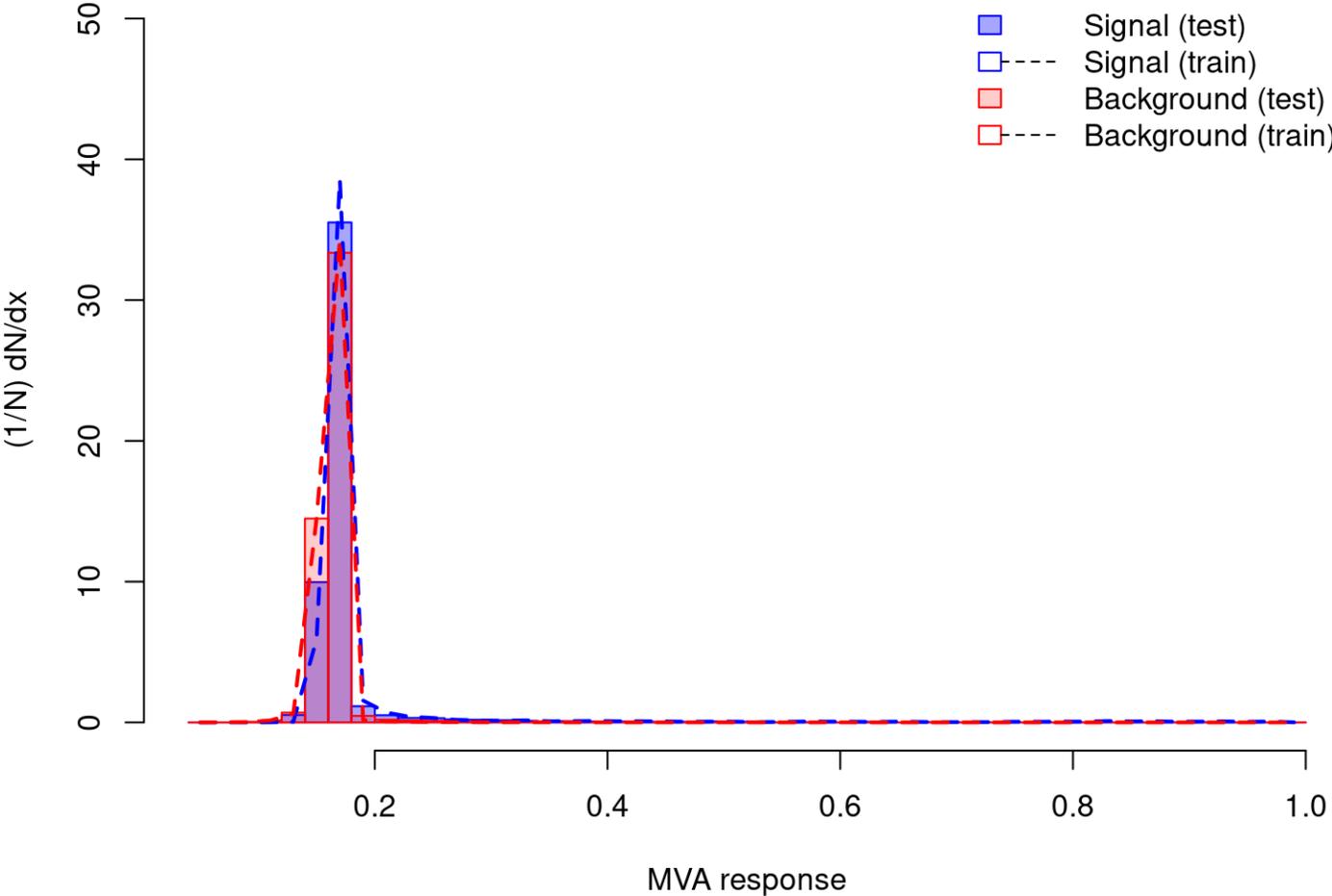


R overtraining check for classifier: rf

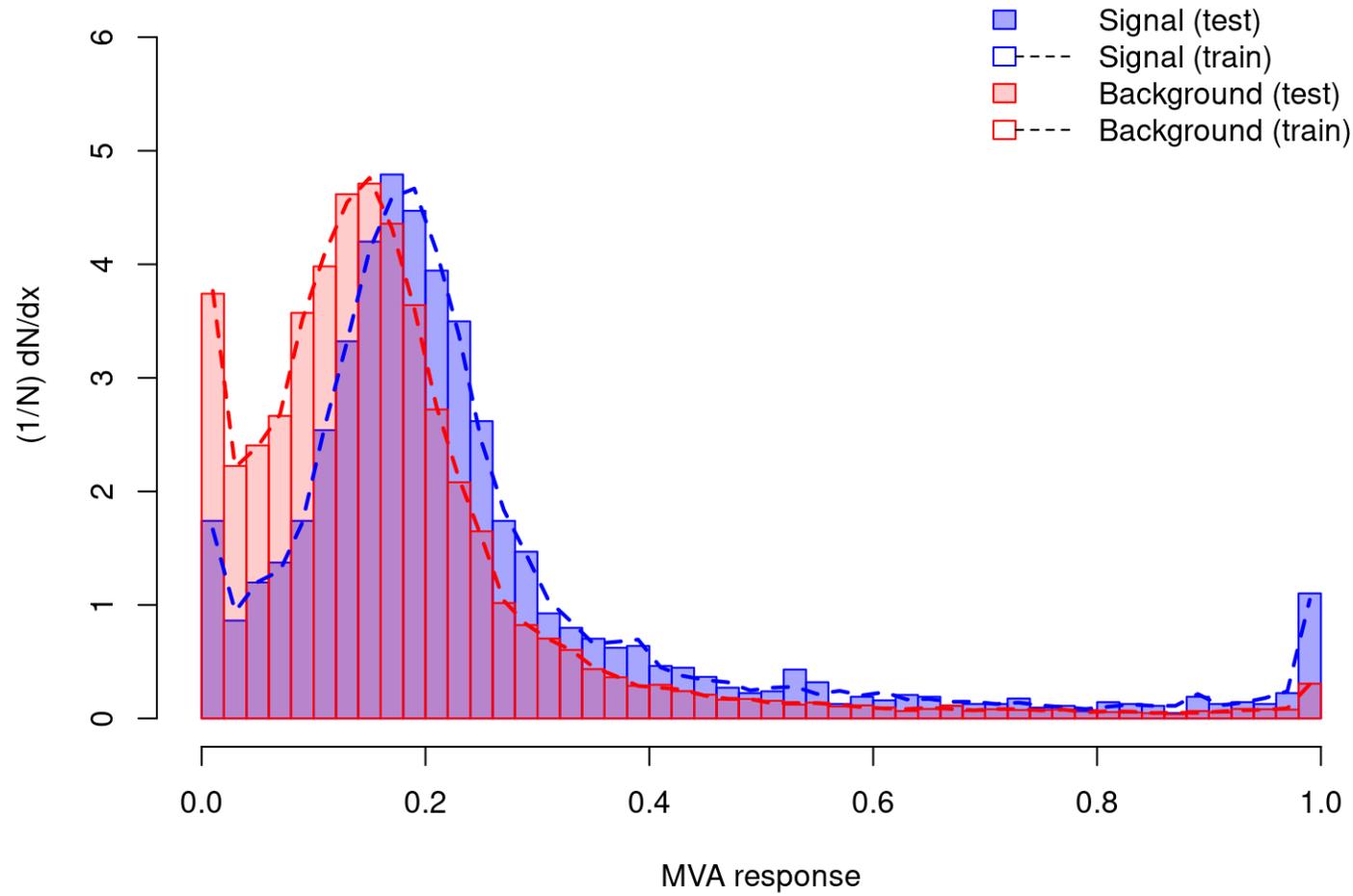
KS p-values (unweighted): S=0 B=0



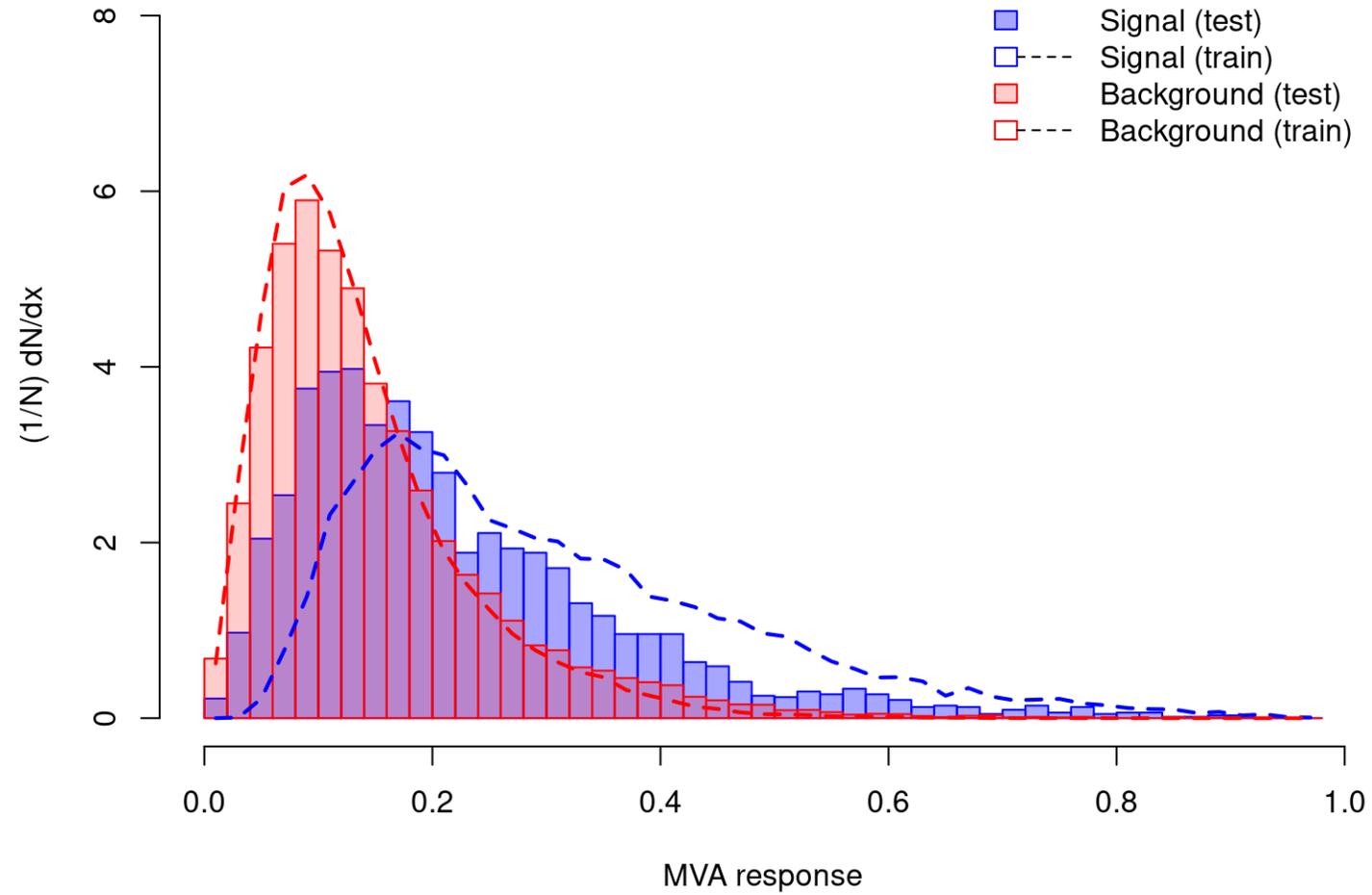
R overtraining check for classifier: svm



R overtraining check for classifier: nb

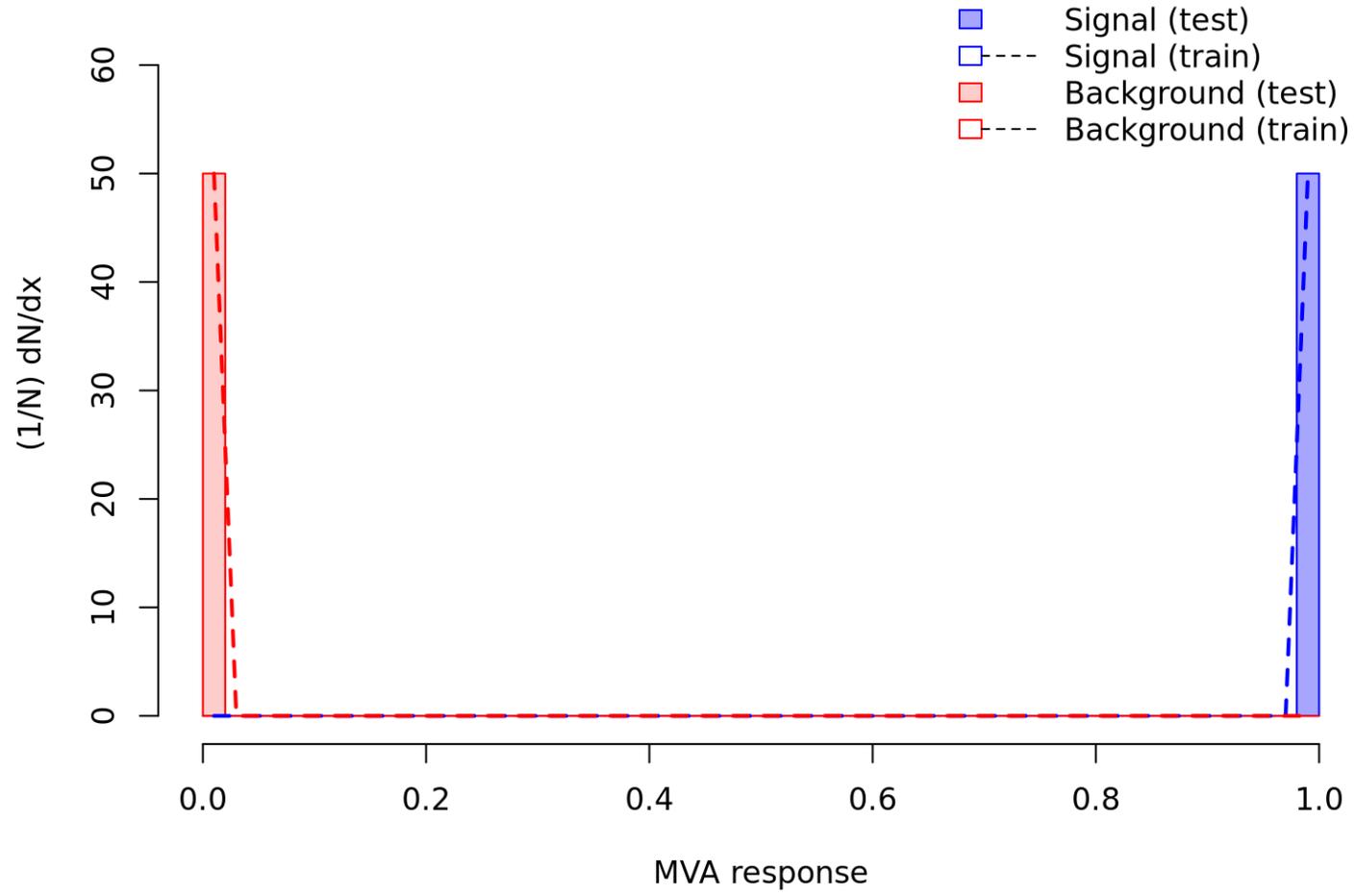


R overtraining check for classifier: xgboost

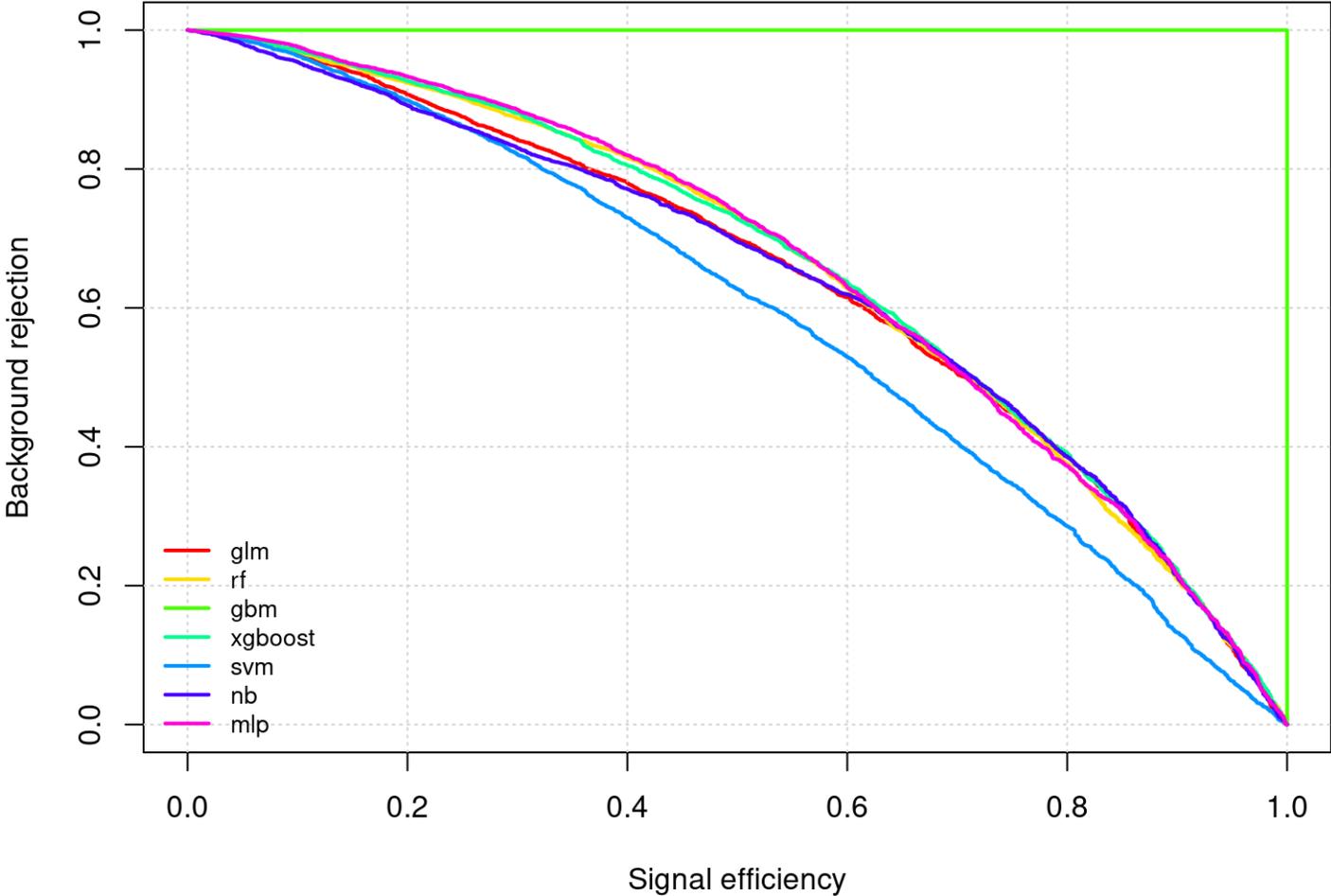


R overtraining check for classifier: gbm

KS p-values (unweighted): S=1 B=0.828



ROC curves (TMVA style): all methods



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

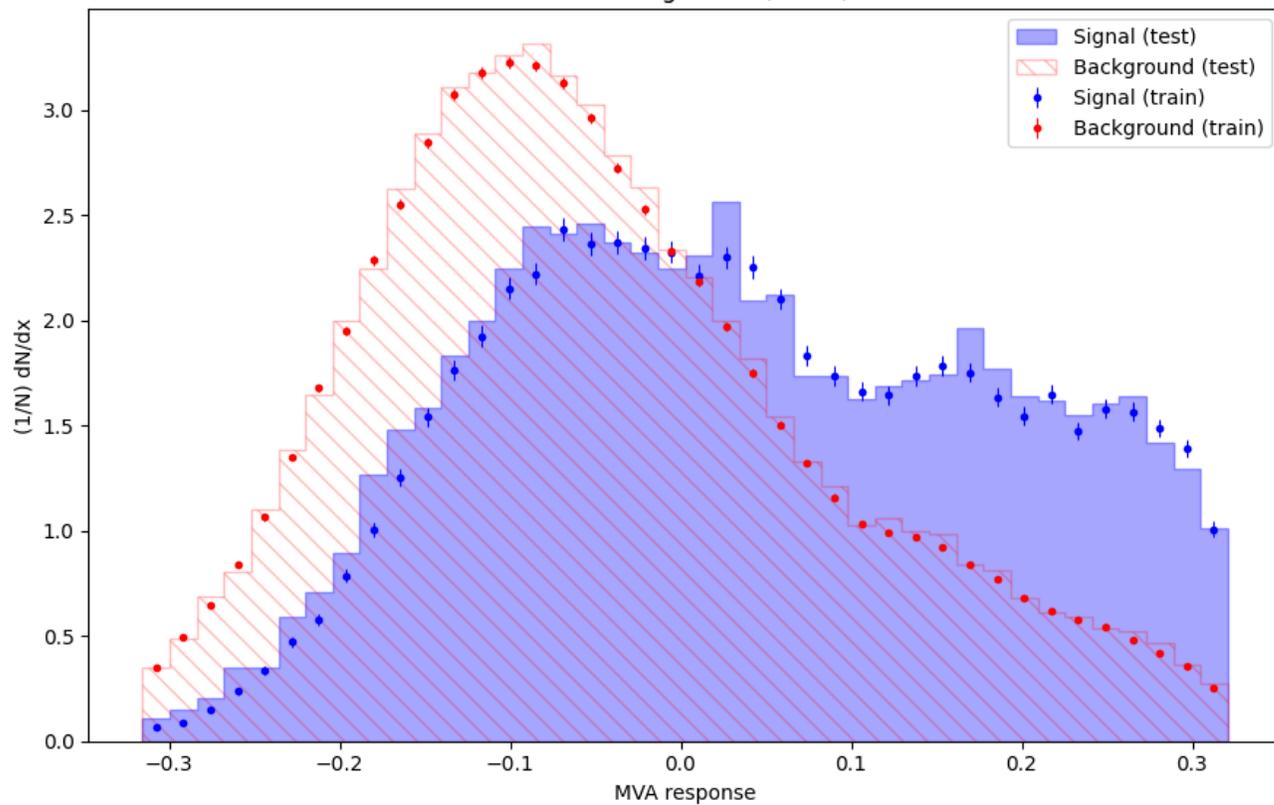
Results of Performance of ML Algorithms using K-fold on TMVA

10th February 2026

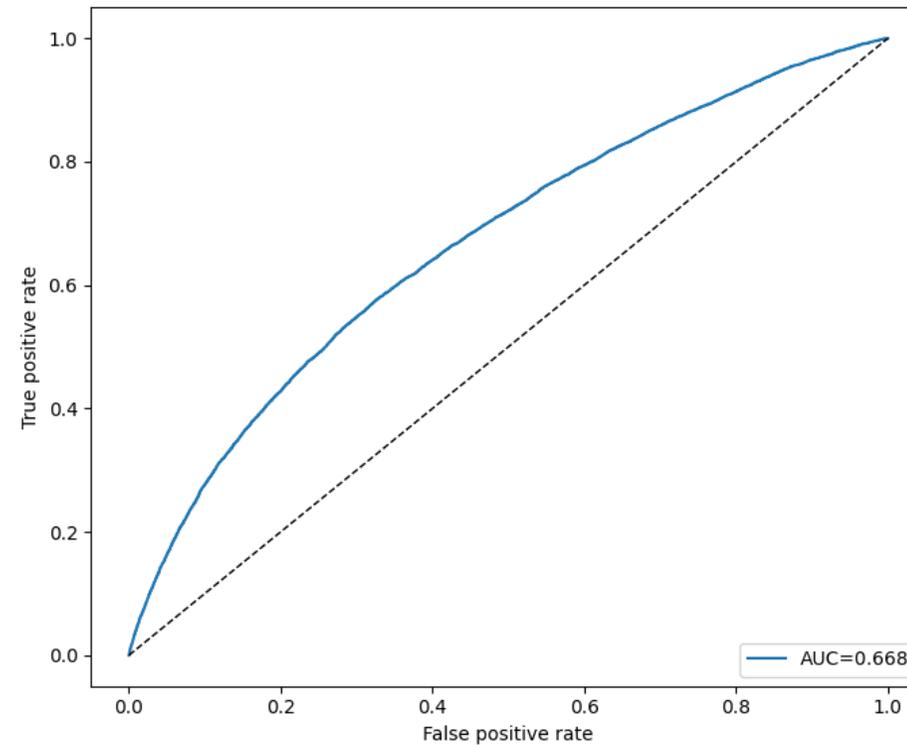
TMVA (k-fold) Results on New Data

Algorithm (TMVA)	kfold	n_trials	best_mean_auc
BDT	5	20	0.668182
BDTG	5	20	0.670094
Fisher	5	20	0.637319
kNN	5	20	0.651456
Likelihood	5	20	0.650749
MLP	5	20	0.668192

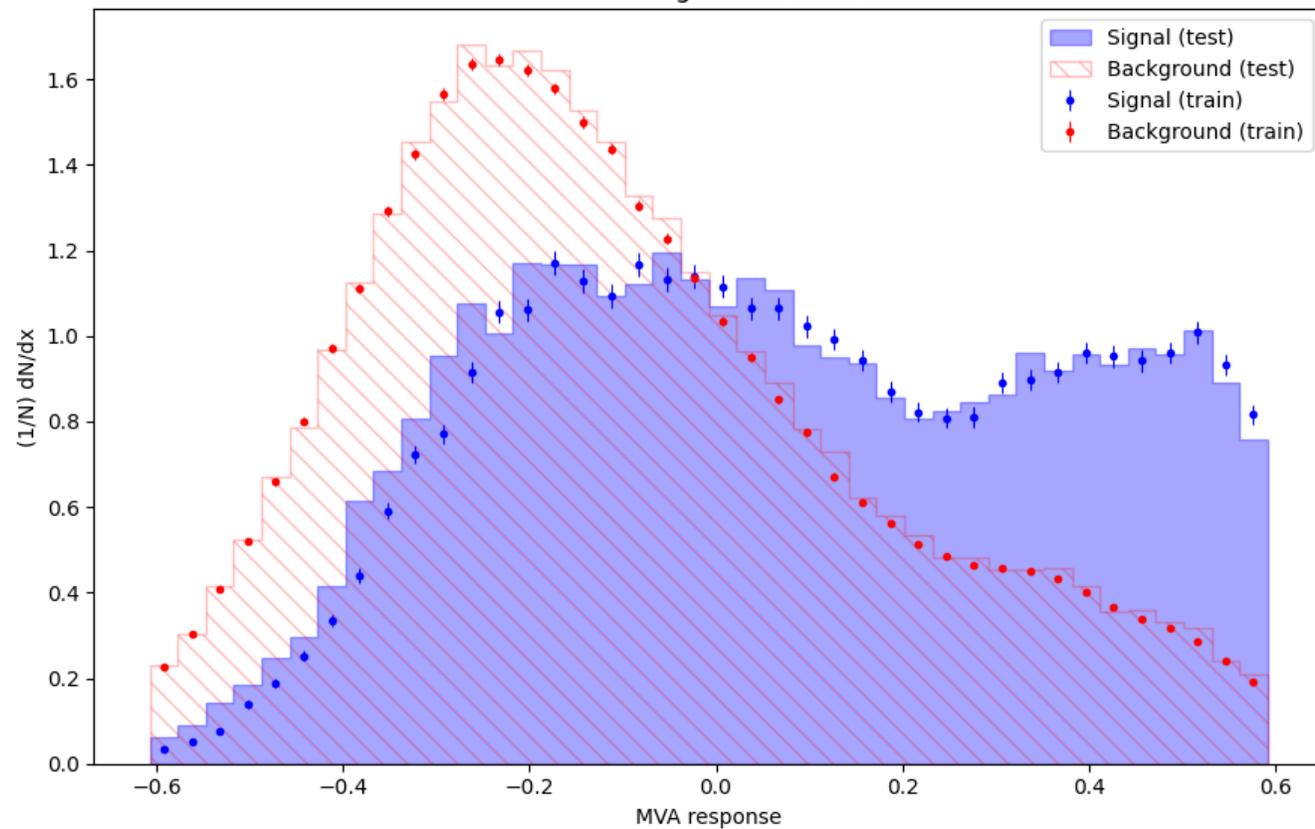
TMVA overtraining check (k-fold): BDT



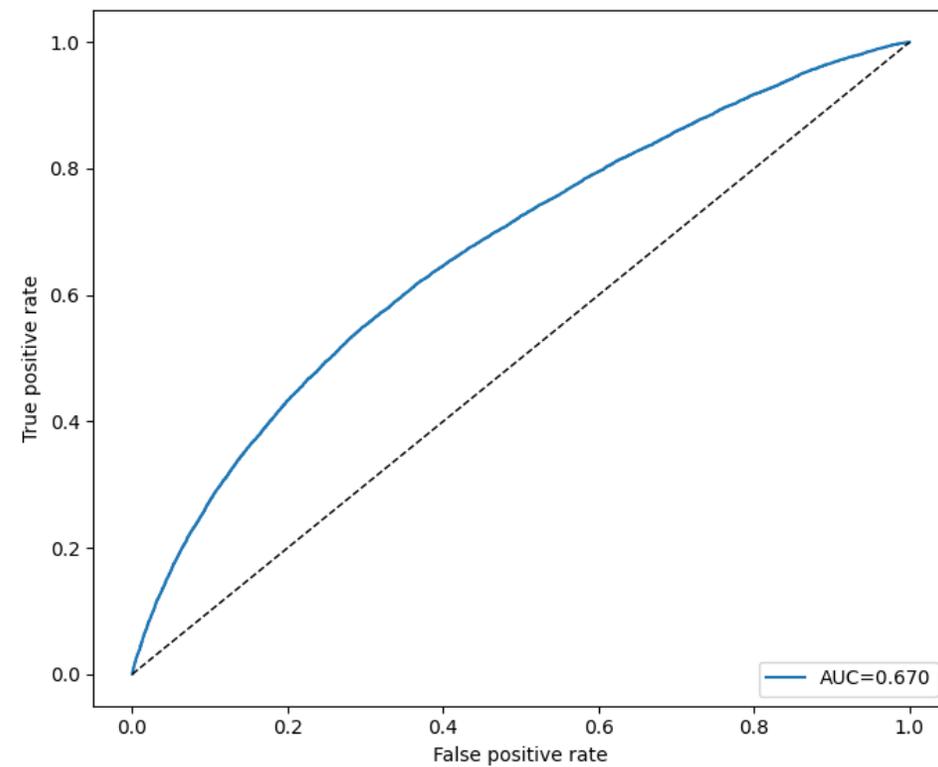
TMVA k-fold ROC - BDT



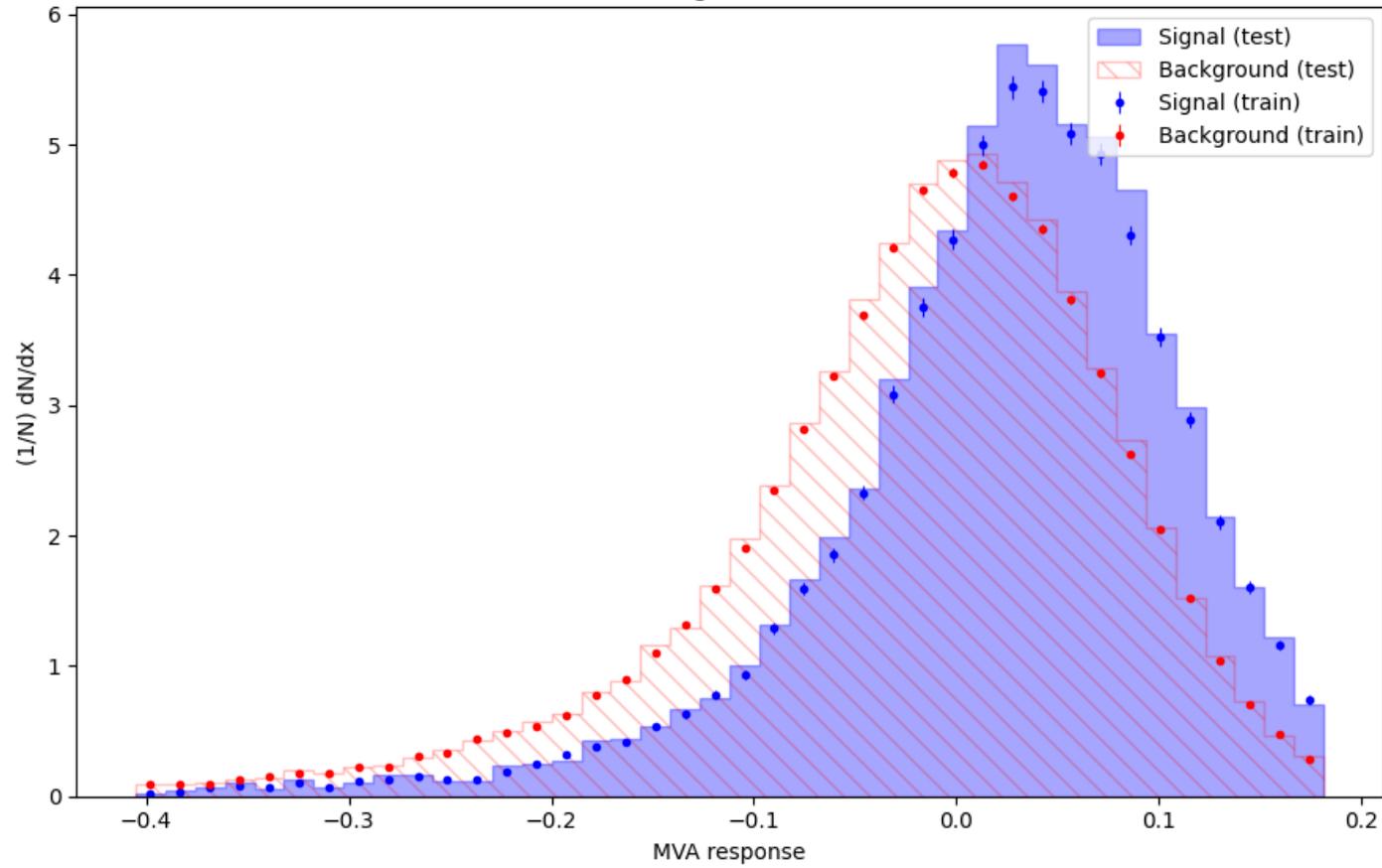
TMVA overtraining check (k-fold): BDTG



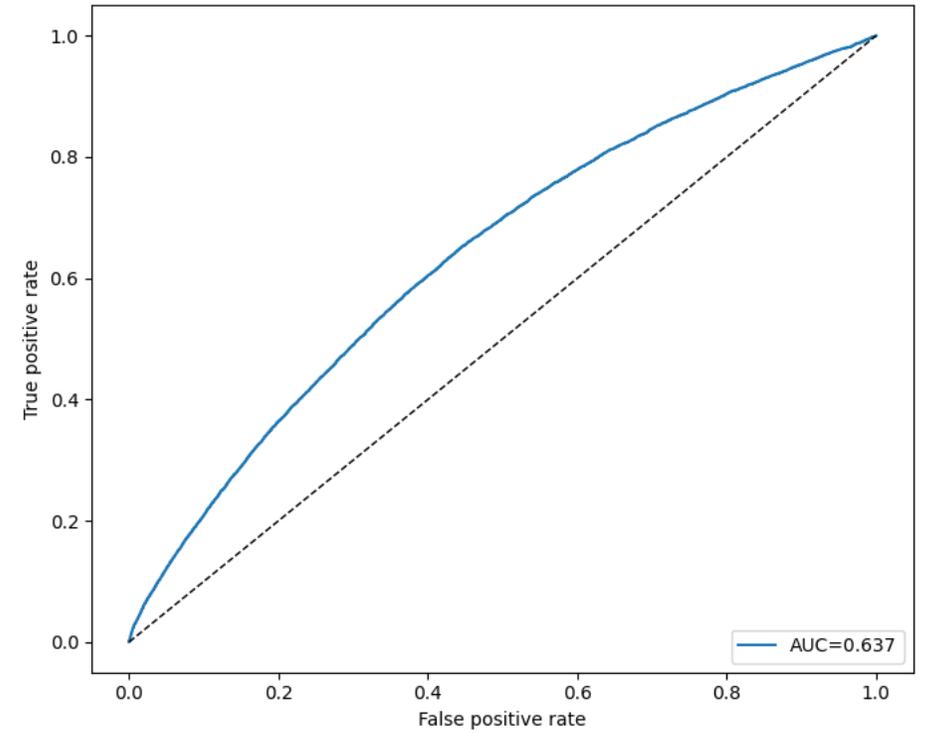
TMVA k-fold ROC - BDTG



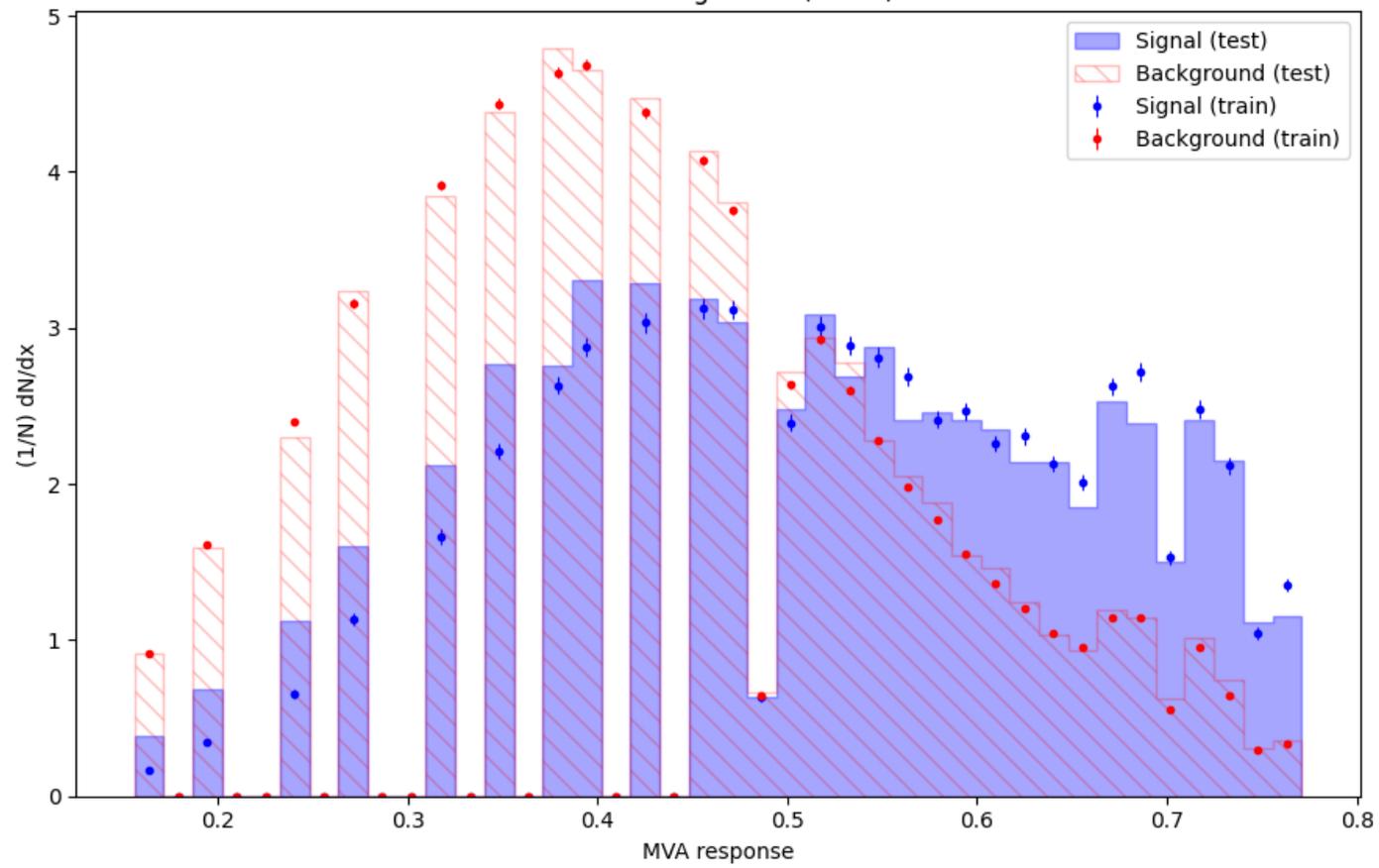
TMVA overtraining check (k-fold): Fisher



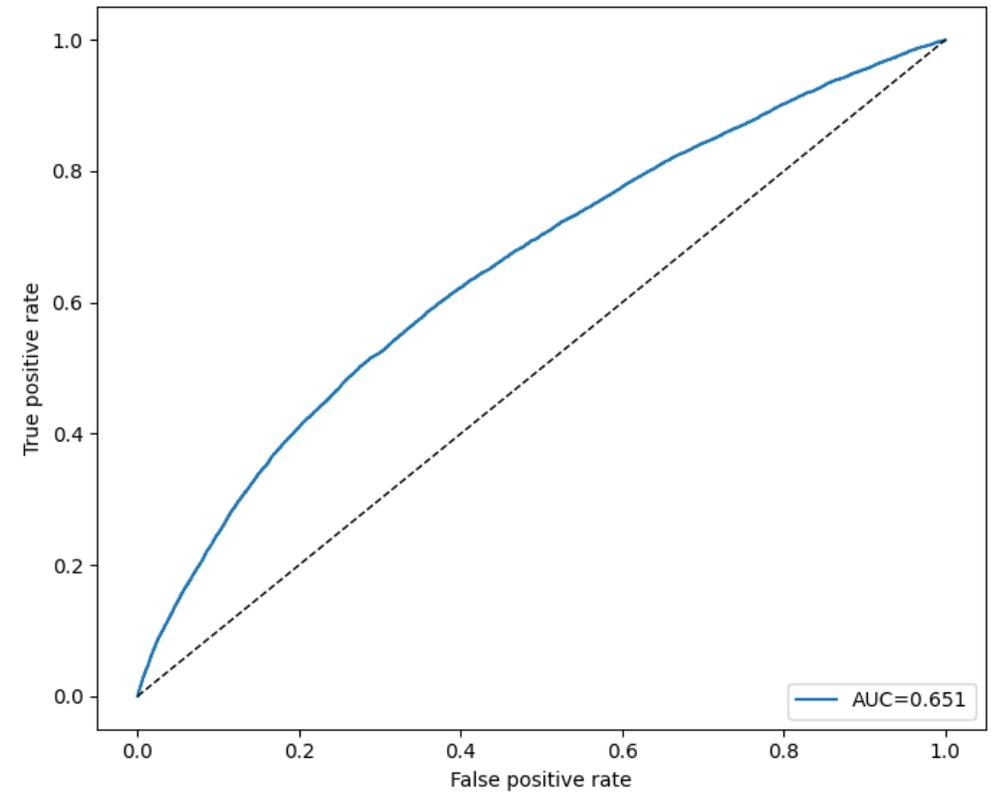
TMVA k-fold ROC - Fisher



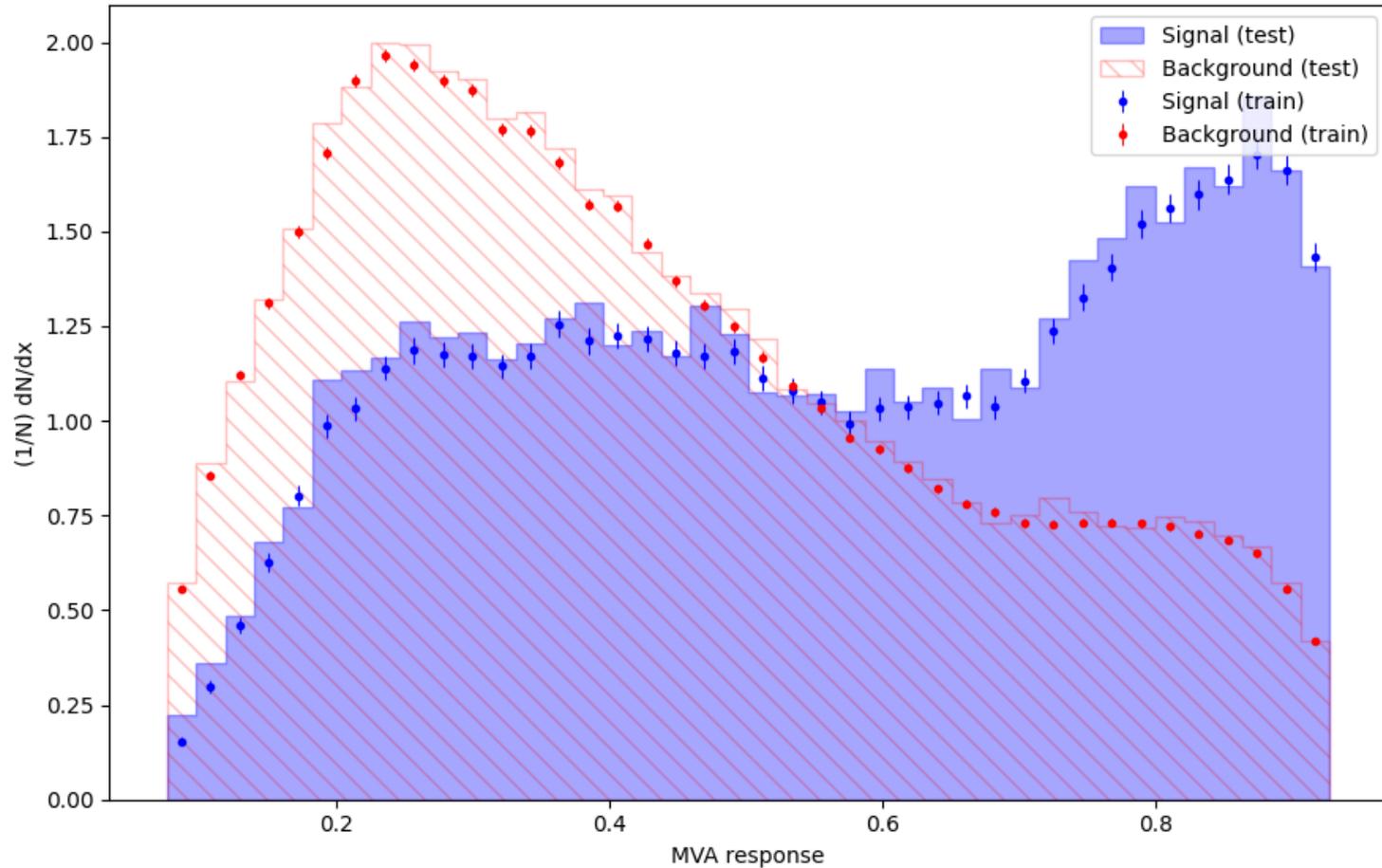
TMVA overtraining check (k-fold): kNN



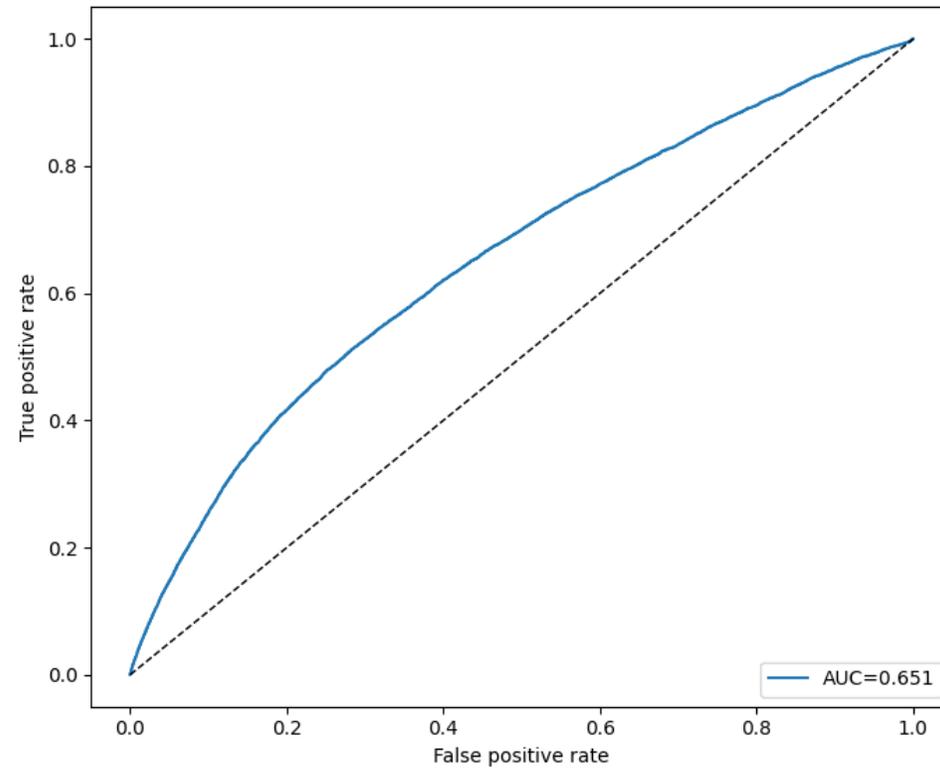
TMVA k-fold ROC - kNN



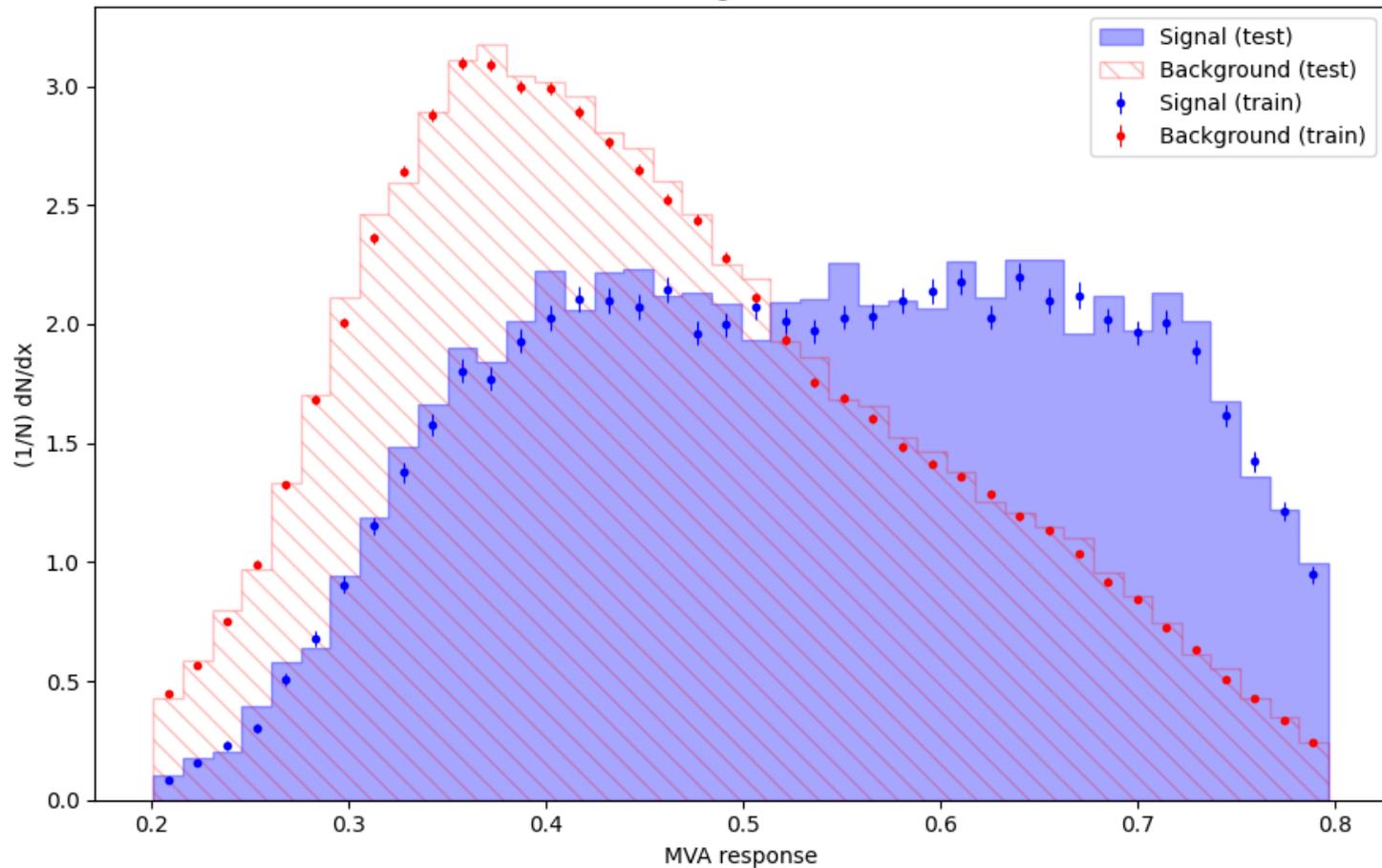
TMVA overtraining check (k-fold): Likelihood



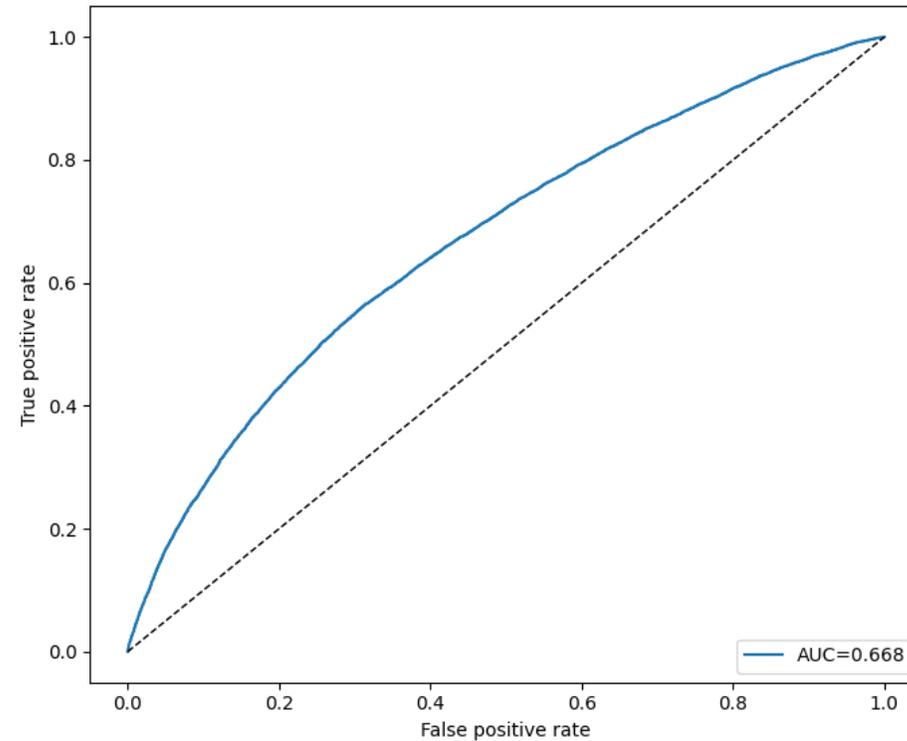
TMVA k-fold ROC - Likelihood



TMVA overtraining check (k-fold): MLP



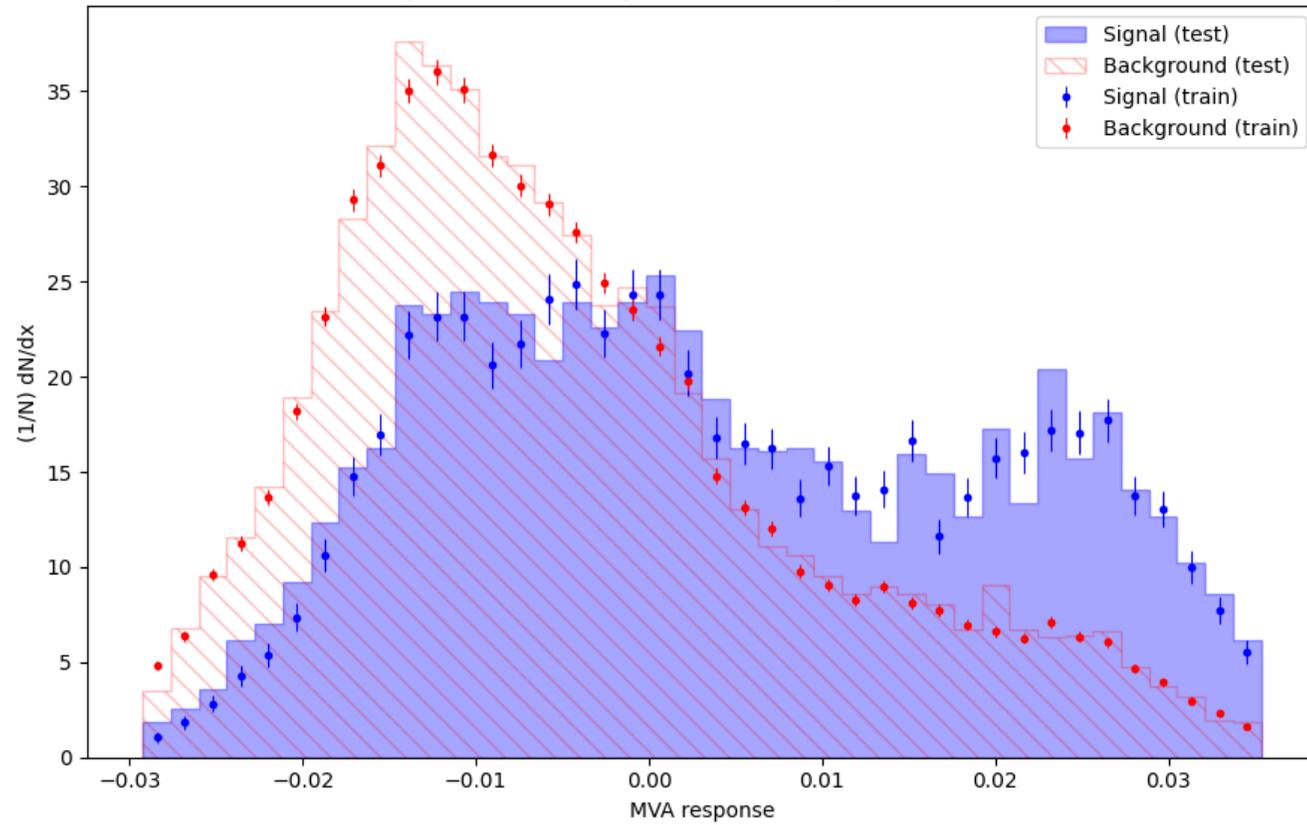
TMVA k-fold ROC - MLP



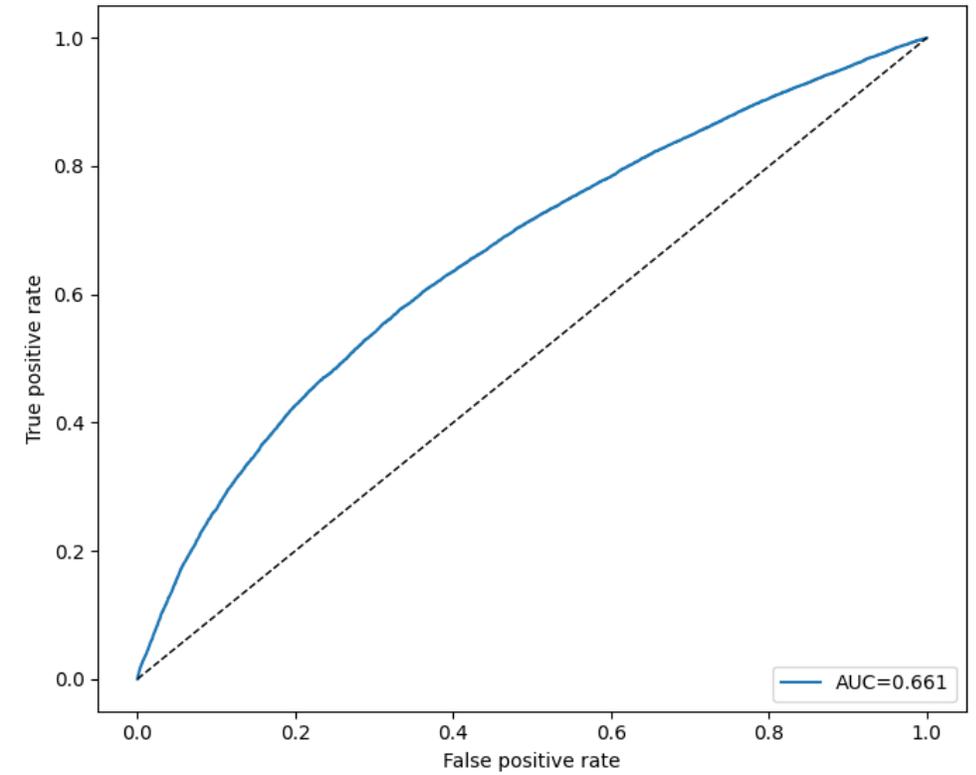
**Results of Performance of ML
Algorithms using K-fold on
Python 4th Trial More
algorithms added
10th February 2026**

Algorithm (Python)	outer_k	inner_k	n_iter	mean_fold_auc	std_fold_auc	overall_oof_auc	mean_fold_wacc	std_fold_wacc	overall_oof_wacc
AdaBoost	5	3	25	0.663612	0.006768	0.660667	0.62078	0.004724	0.62078
Bagging	5	3	25	0.647918	0.007531	0.647809	0.502429	0.000625	0.502429
ExtraTrees	5	3	25	0.667711	0.006485	0.667169	0.622879	0.005654	0.622879
GaussianNB	5	3	25	0.636746	0.008755	0.636637	0.59563	0.004879	0.59563
GradientBoosting	5	3	25	0.670242	0.007283	0.670033	0.625561	0.006146	0.62556
HistGradientBoosting	5	3	25	0.668588	0.006794	0.668074	0.624038	0.005583	0.624038
KNN	5	3	25	0.649829	0.006528	0.649802	0.500247	0.000234	0.500247
LDA	5	3	25	0.633161	0.009455	0.632984	0.500227	4.95E-05	0.500227
LinearSVC	5	3	25	0.638989	0.00895	0.638861	0.602301	0.008101	0.6023
LogisticRegression	5	3	25	0.641267	0.008797	0.641124	0.604398	0.007429	0.604398
MLP	5	3	25	0.66697	0.007911	0.666548	0.50295	0.00077	0.50295
QDA	5	3	25	0.645348	0.007435	0.645249	0.51138	0.002164	0.511379
RandomForest	5	3	25	0.667747	0.006265	0.667129	0.620657	0.006323	0.620657
SGDClassifier	5	3	25	0.652858	0.006399	0.652702	0.570652	0.004155	0.570652
SVC	5	3	12	0.668126	0.006504	0.667912	0.62335	0.00485	0.62335

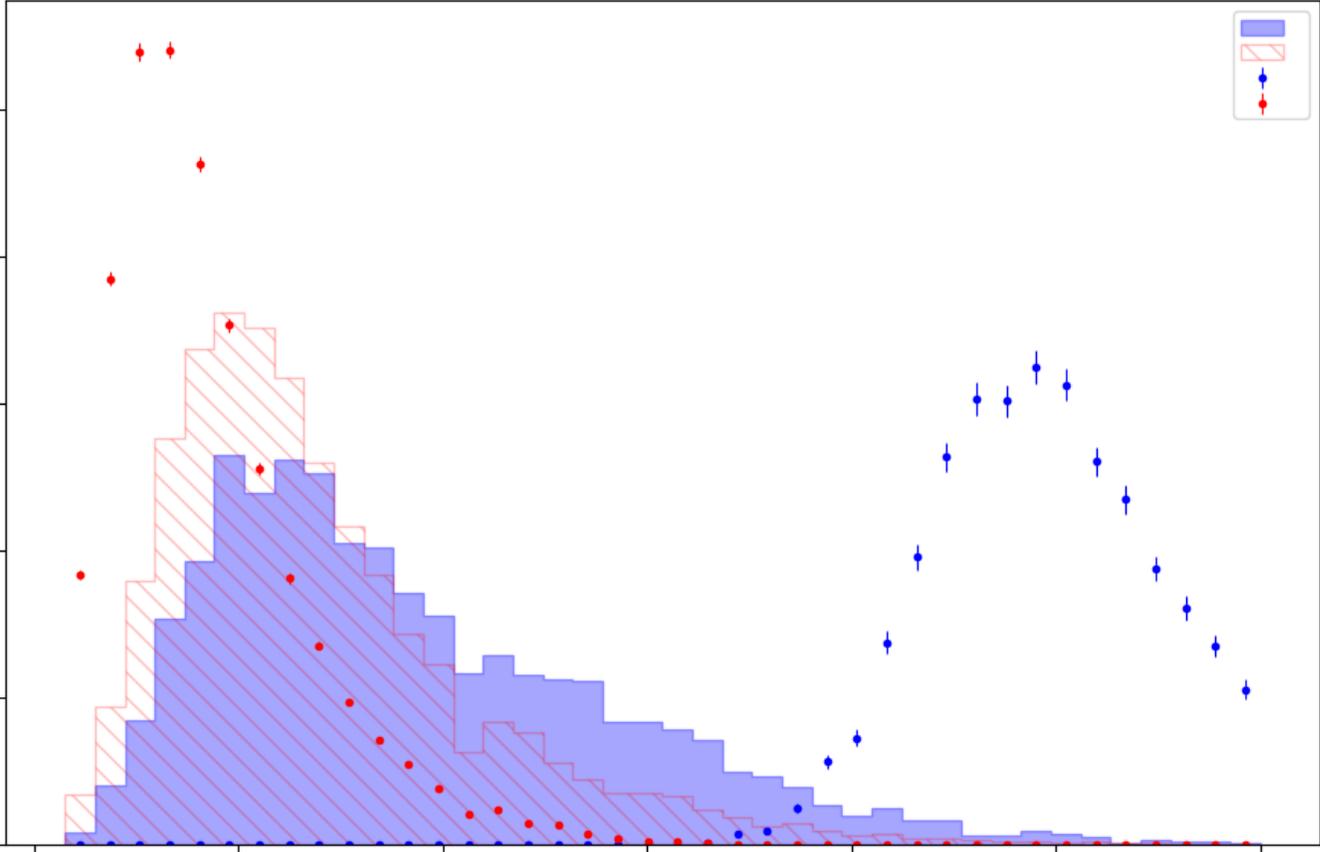
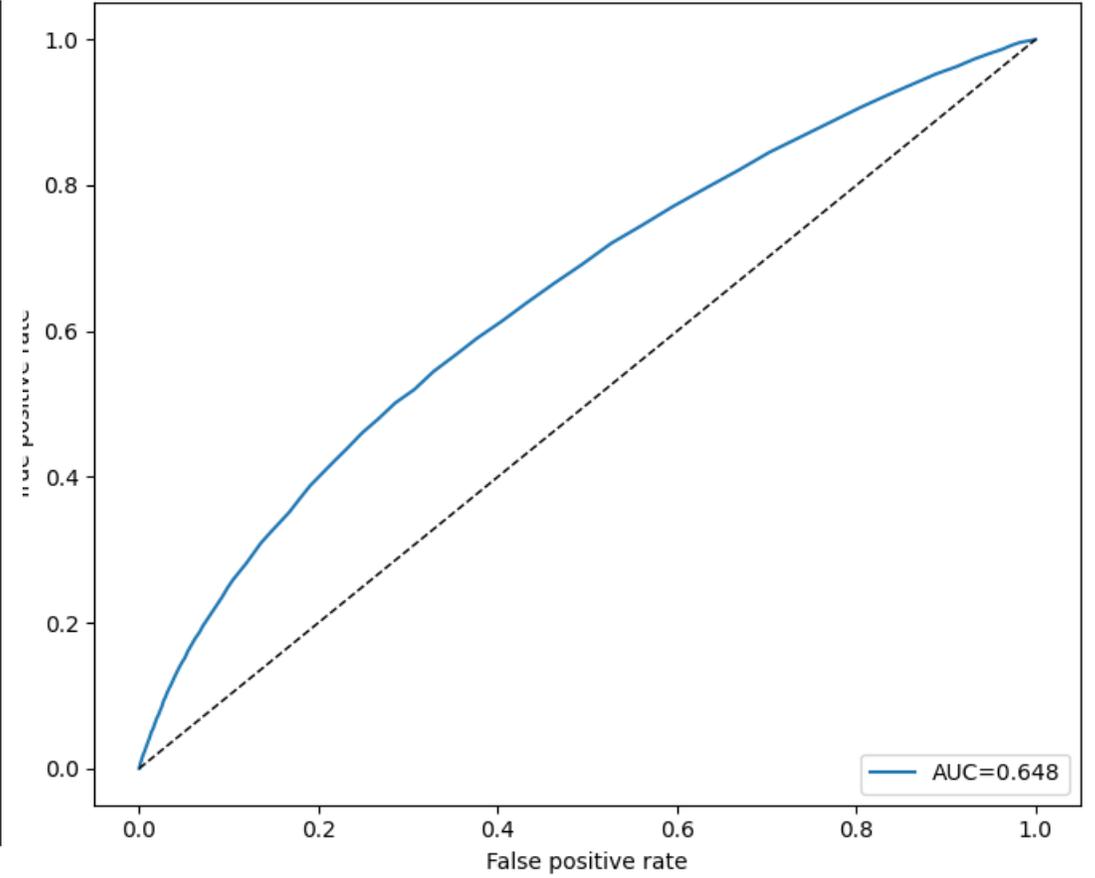
Python overtraining check (TMVA-style): AdaBoost



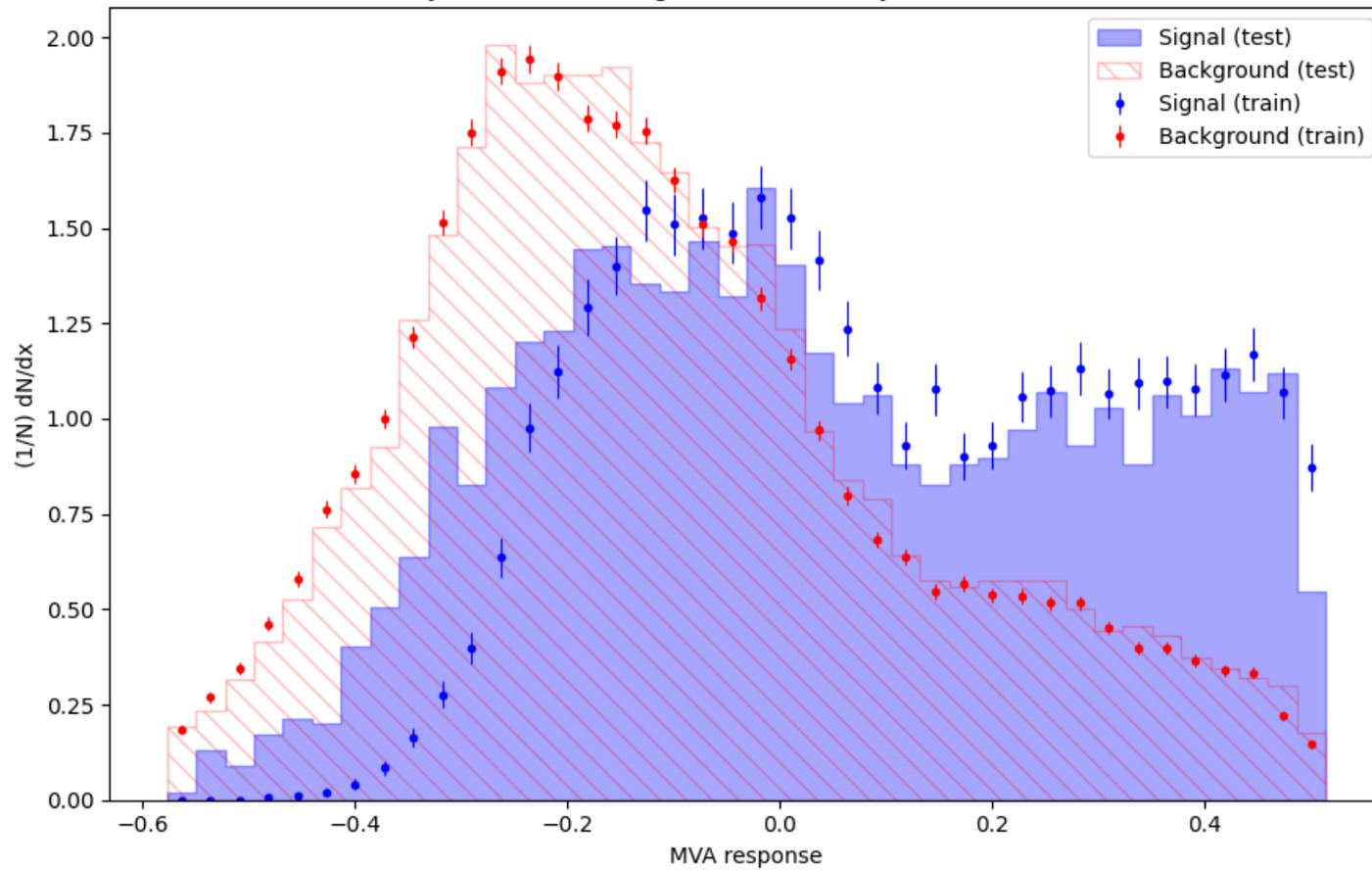
OOF ROC - AdaBoost



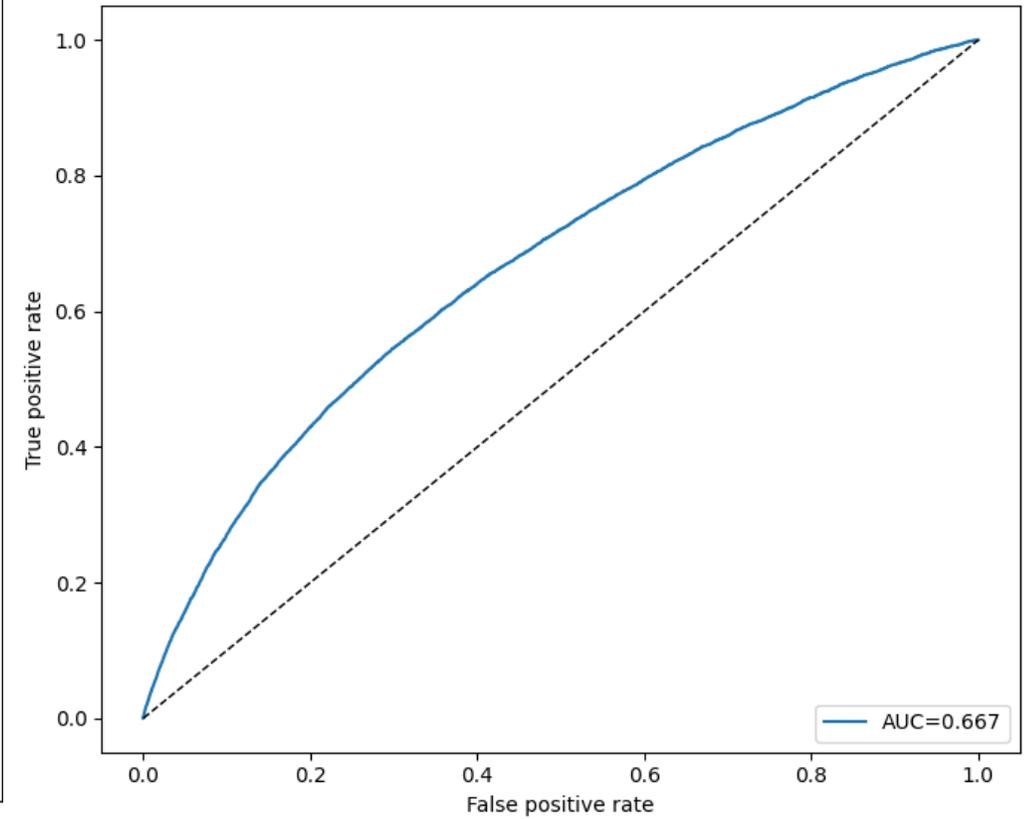
OOF ROC - Bagging



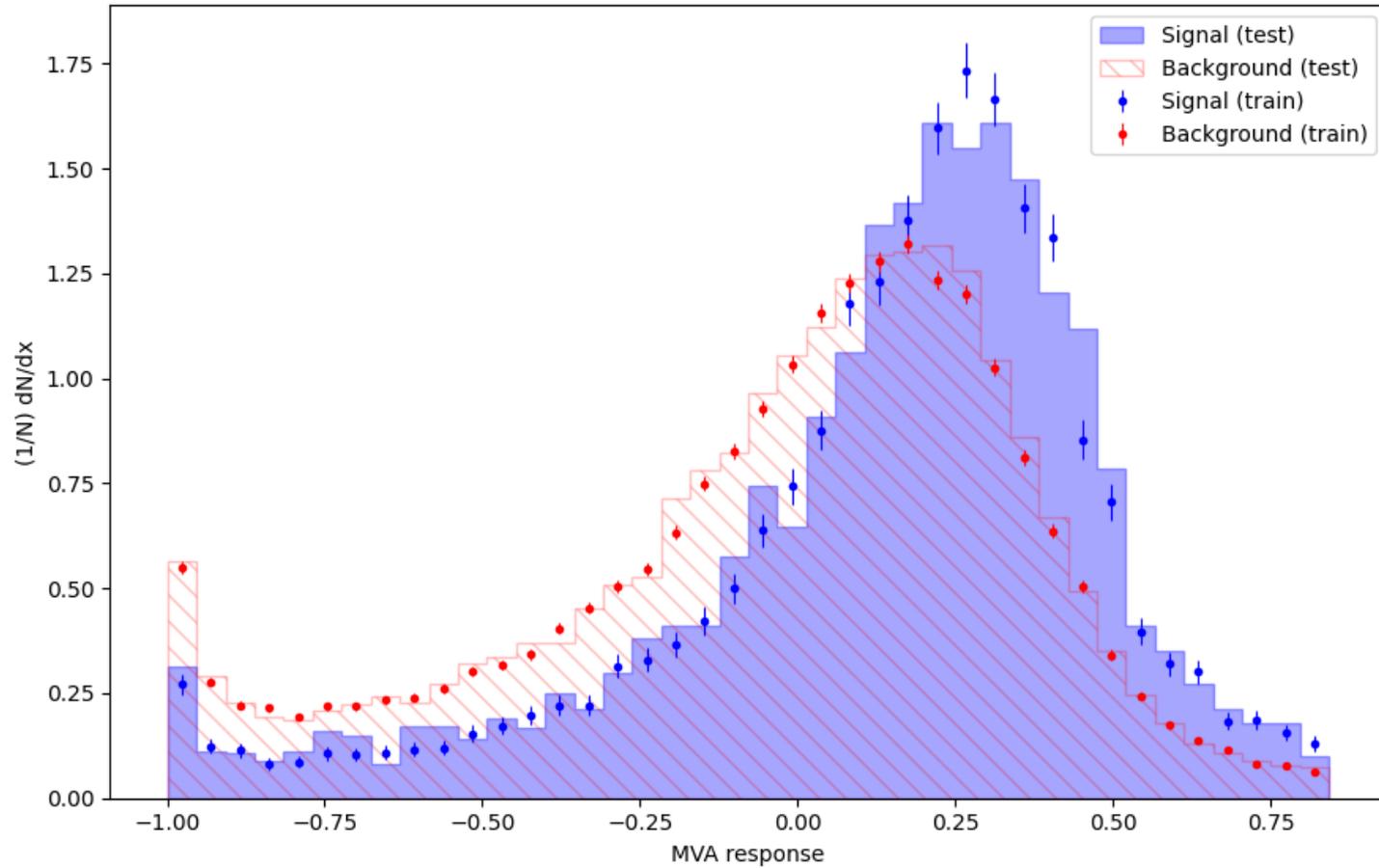
Python overtraining check (TMVA-style): ExtraTrees



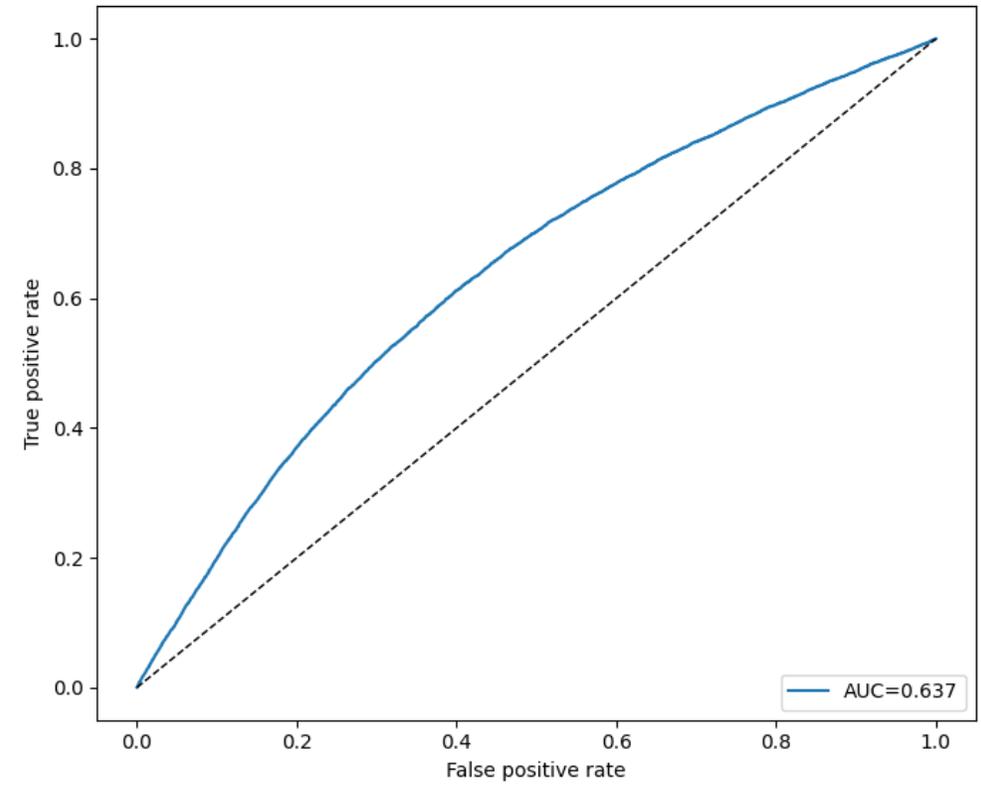
OOF ROC - ExtraTrees



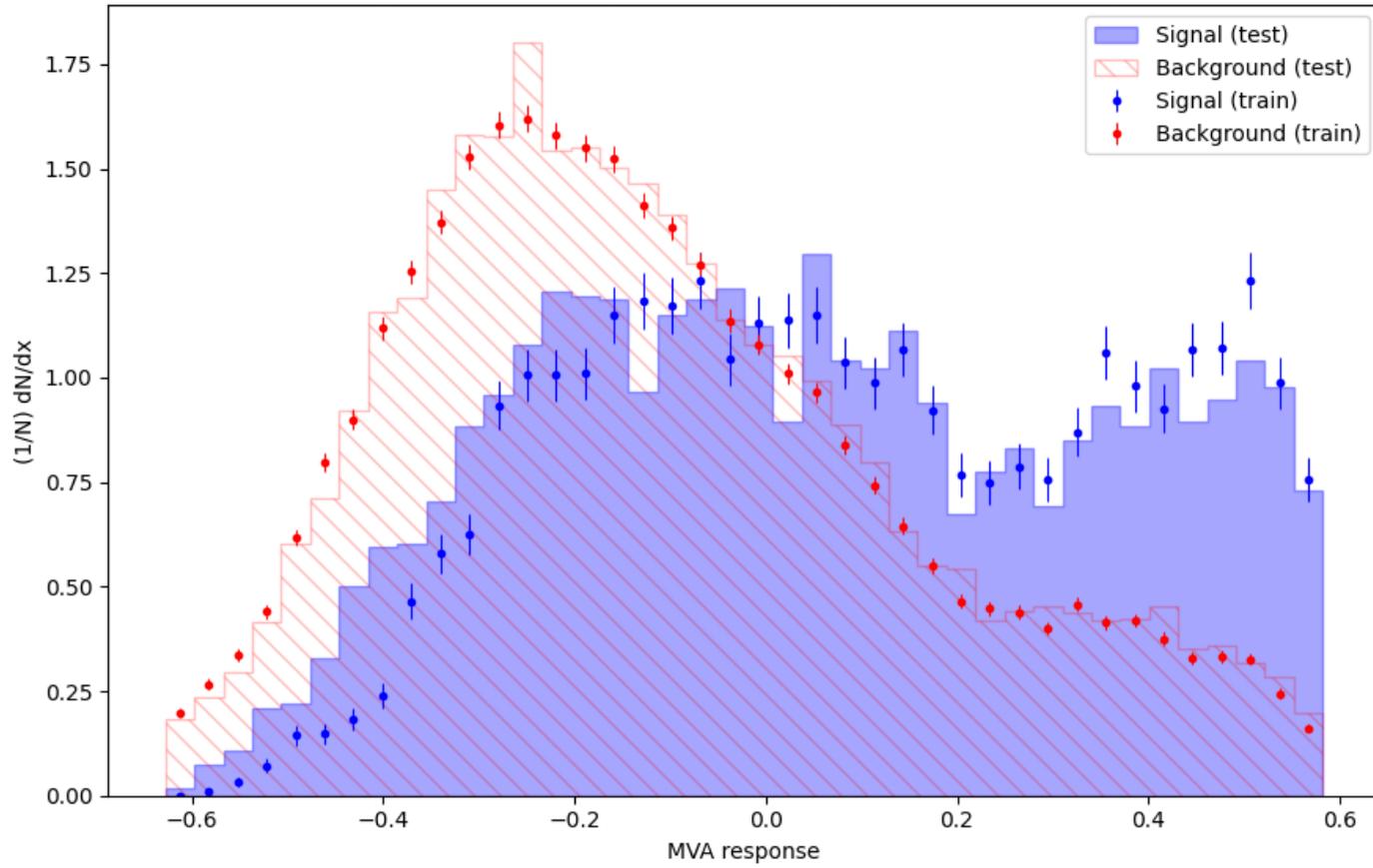
Python overtraining check (TMVA-style): GaussianNB



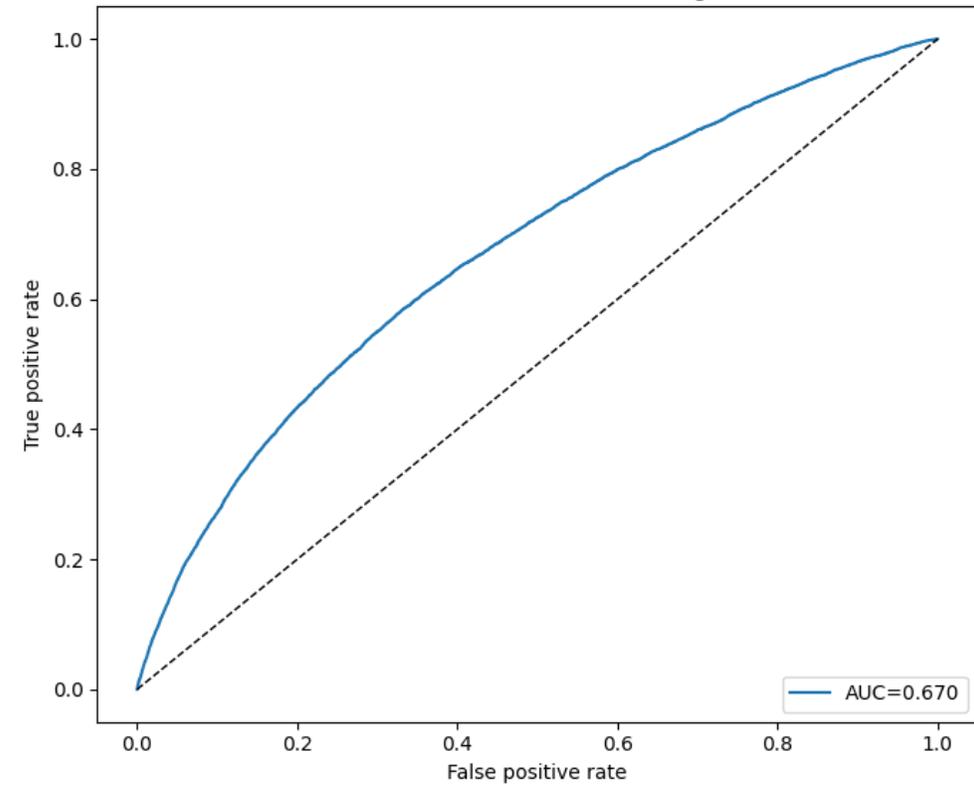
OOF ROC - GaussianNB



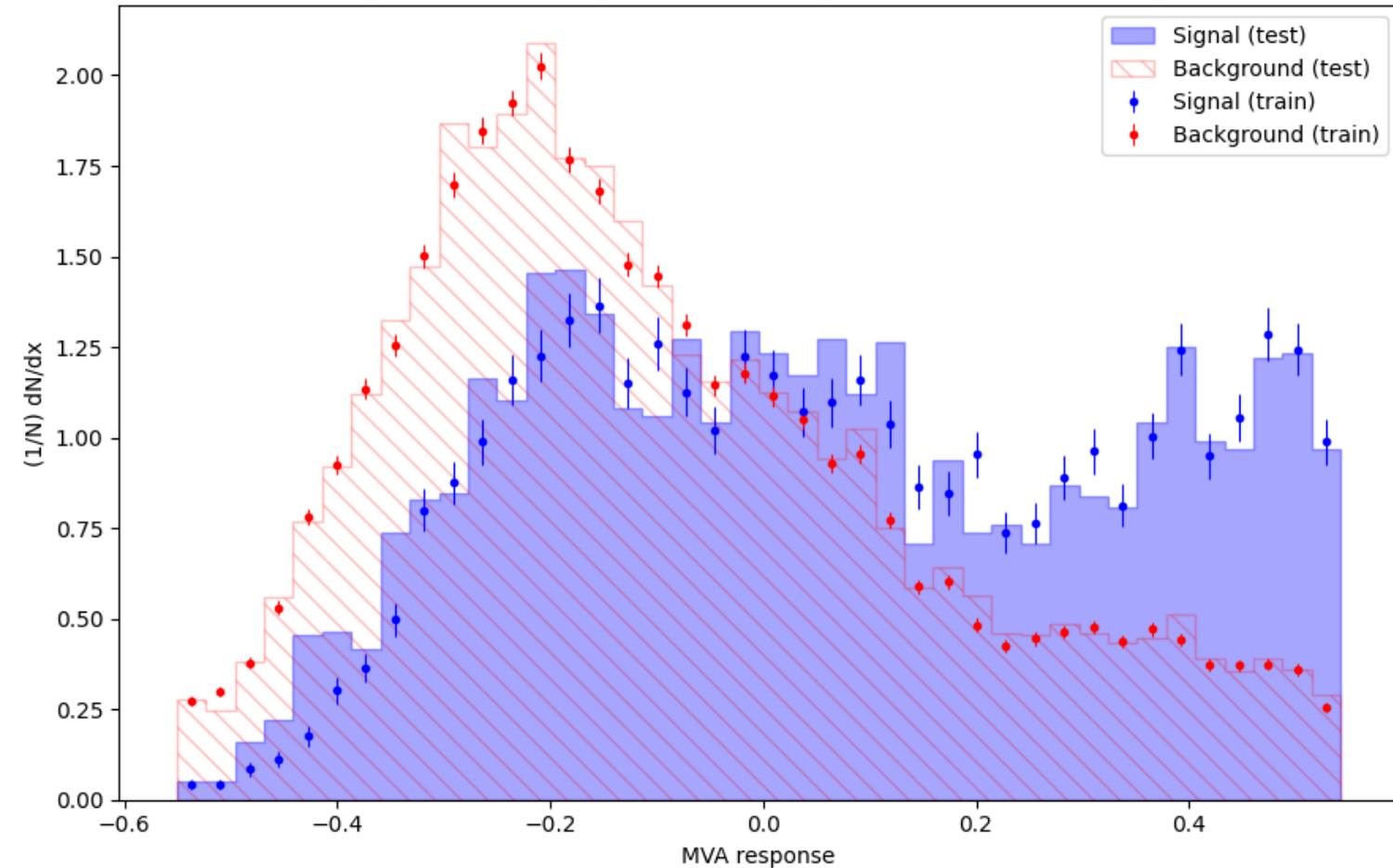
Python overtraining check (TMVA-style): GradientBoosting



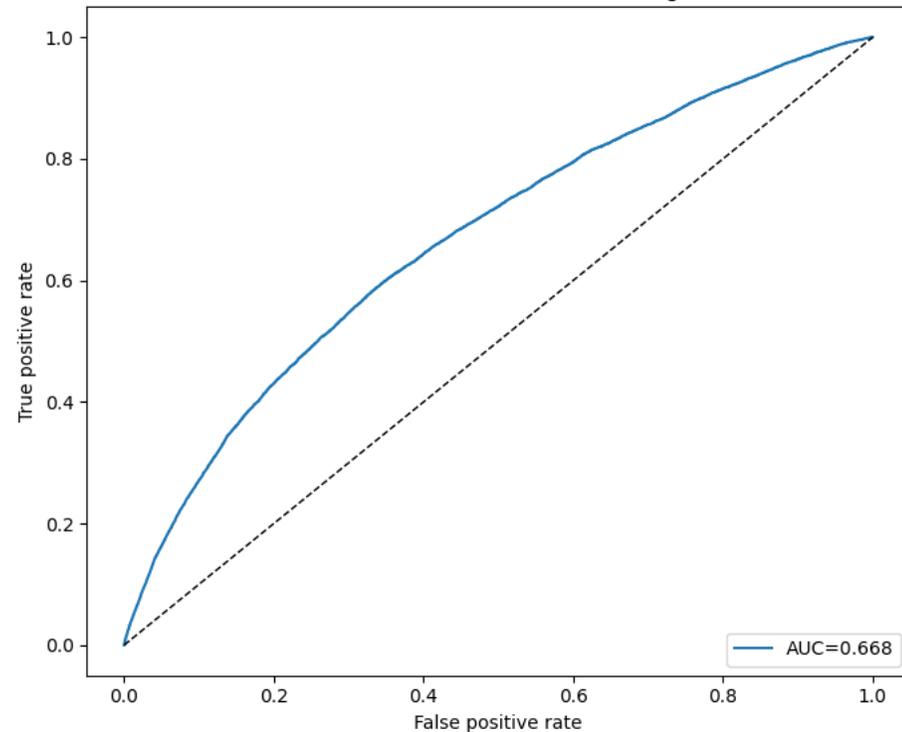
OOF ROC - GradientBoosting



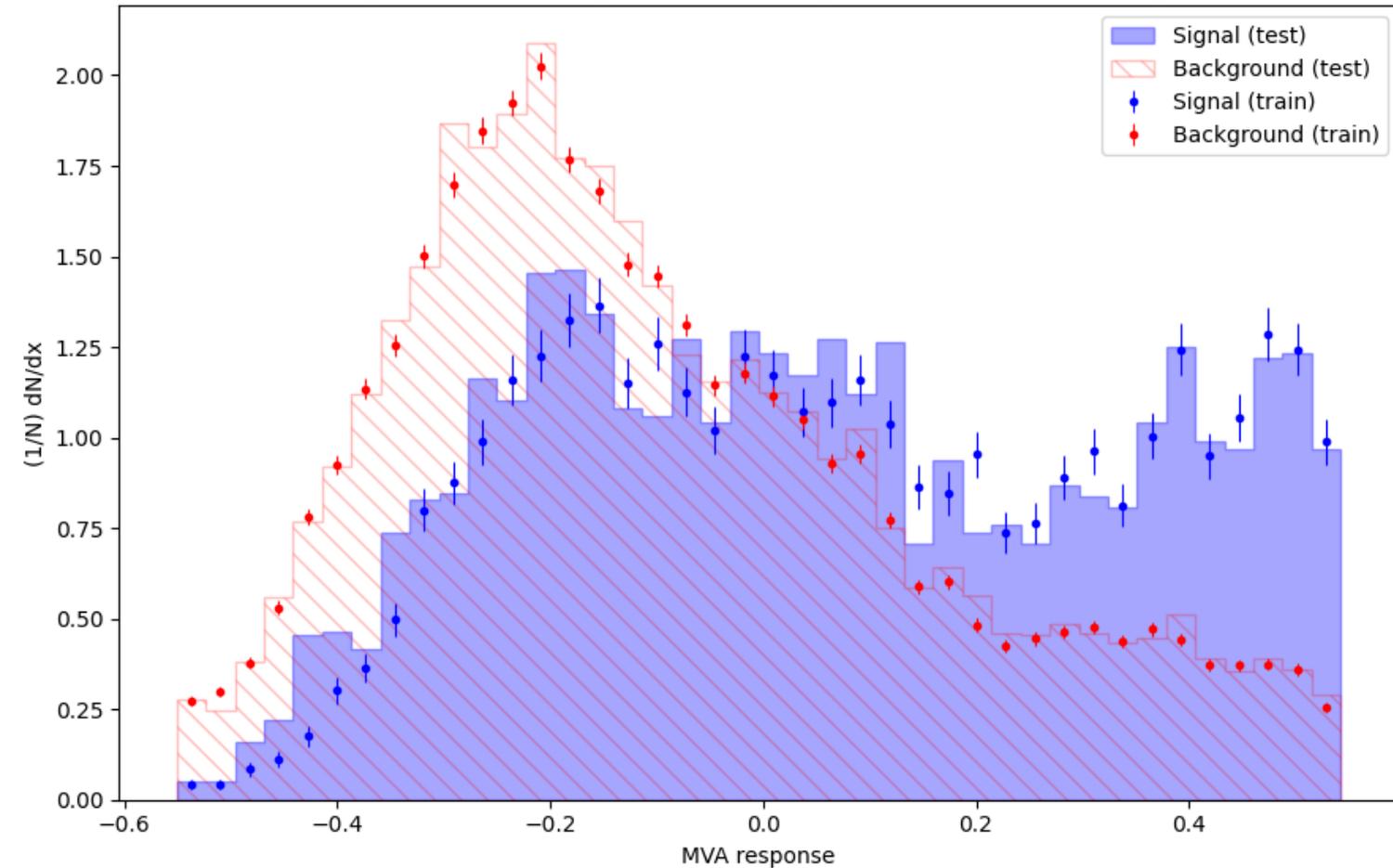
Python overtraining check (TMVA-style): HistGradientBoosting



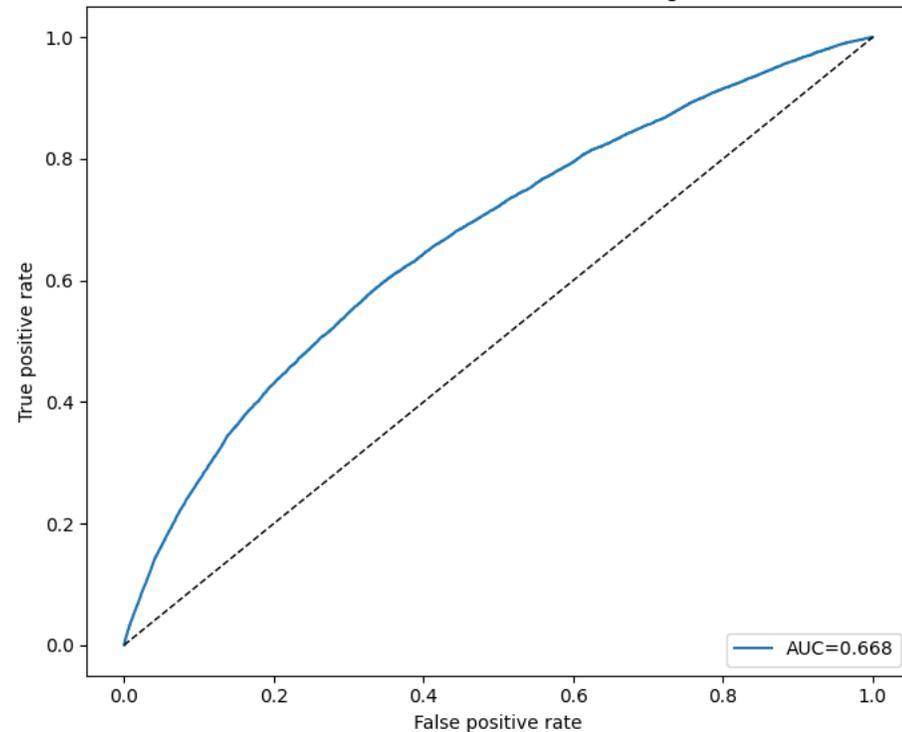
OOF ROC - HistGradientBoosting



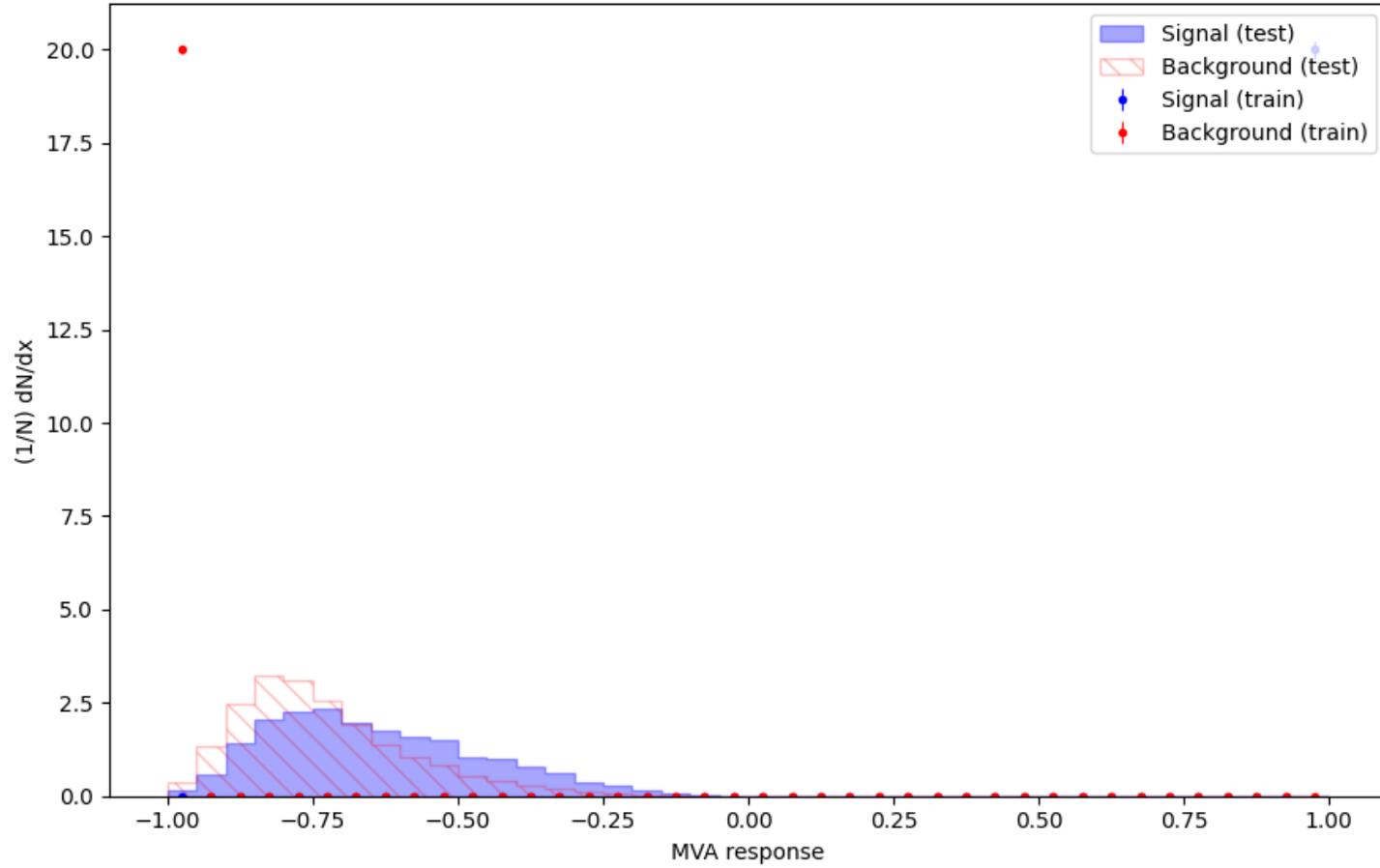
Python overtraining check (TMVA-style): HistGradientBoosting



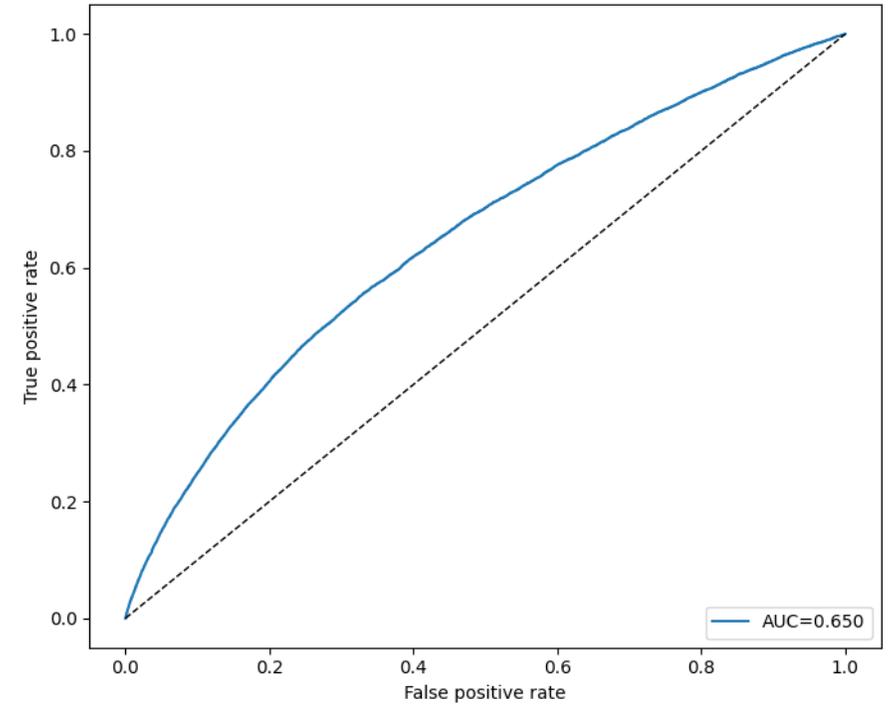
OOF ROC - HistGradientBoosting



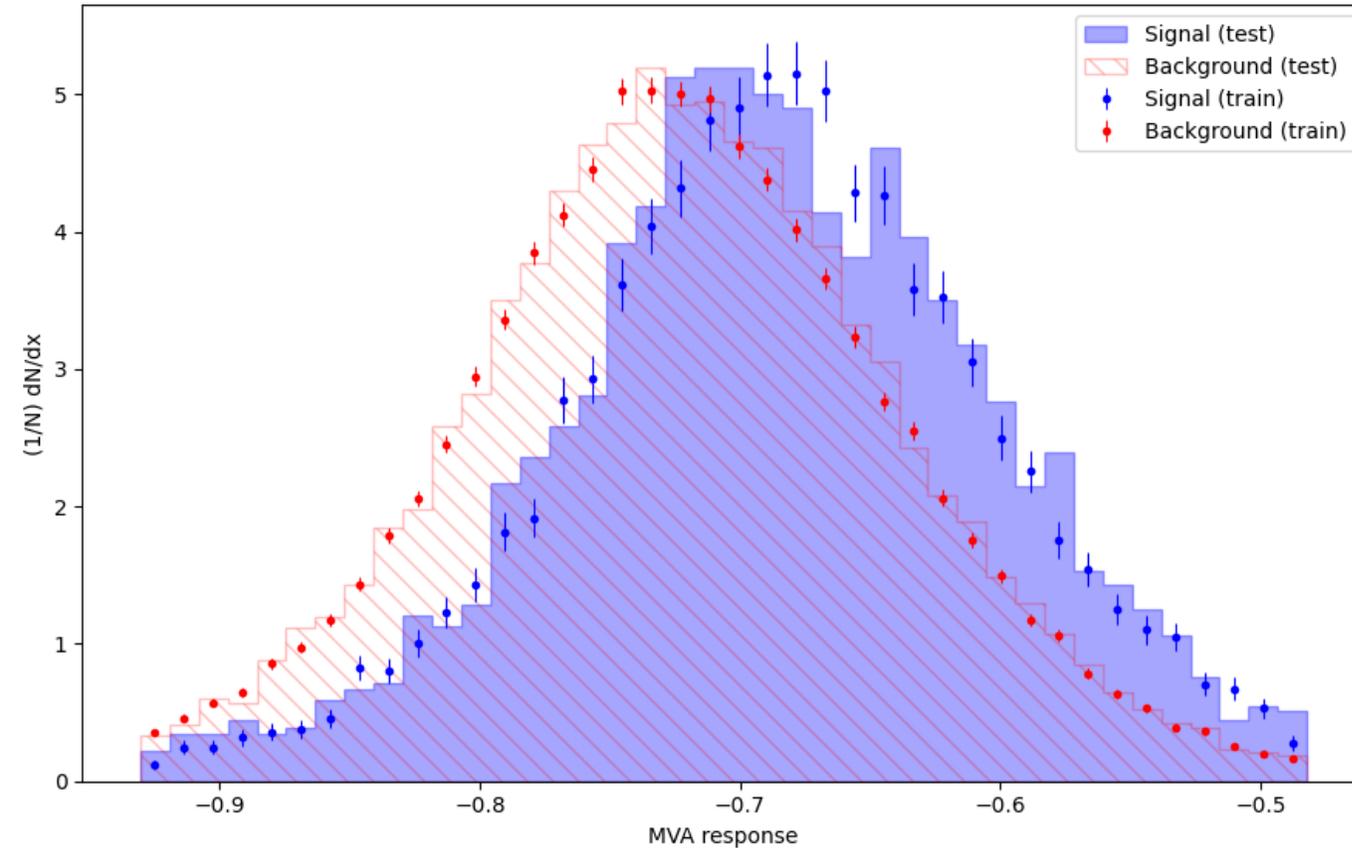
Python overtraining check (TMVA-style): KNN



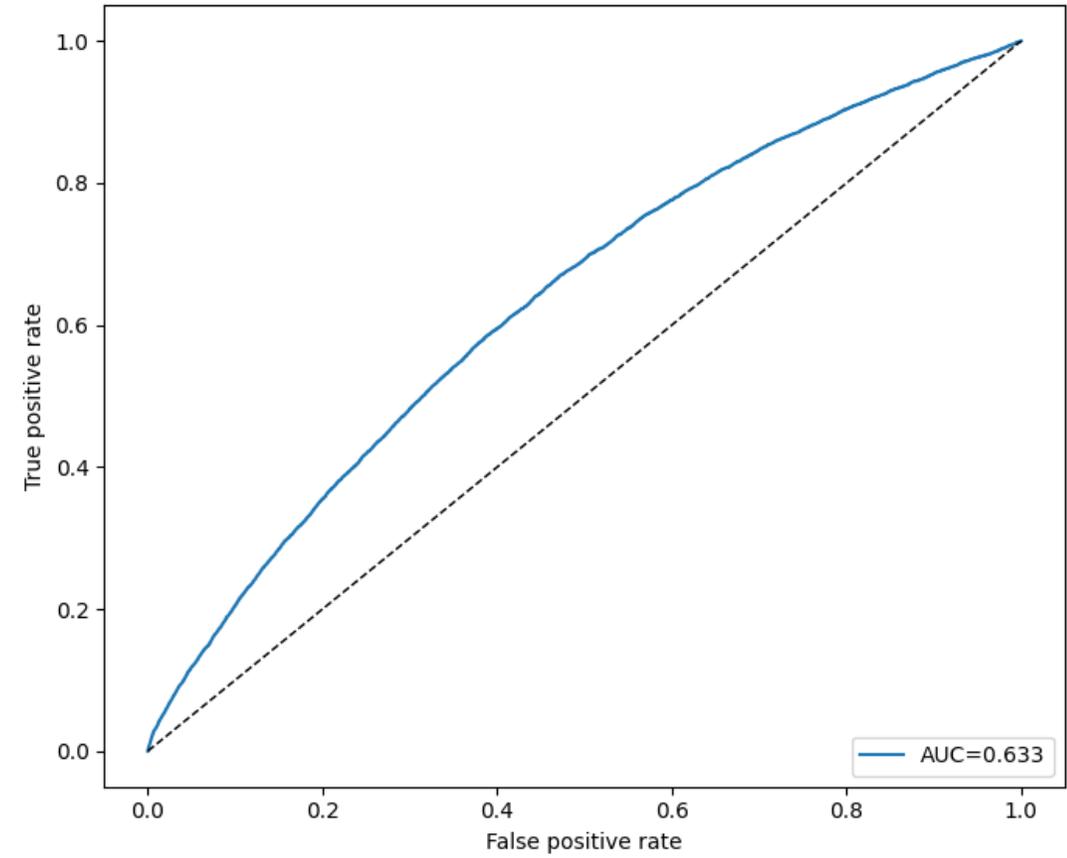
OOF ROC - KNN



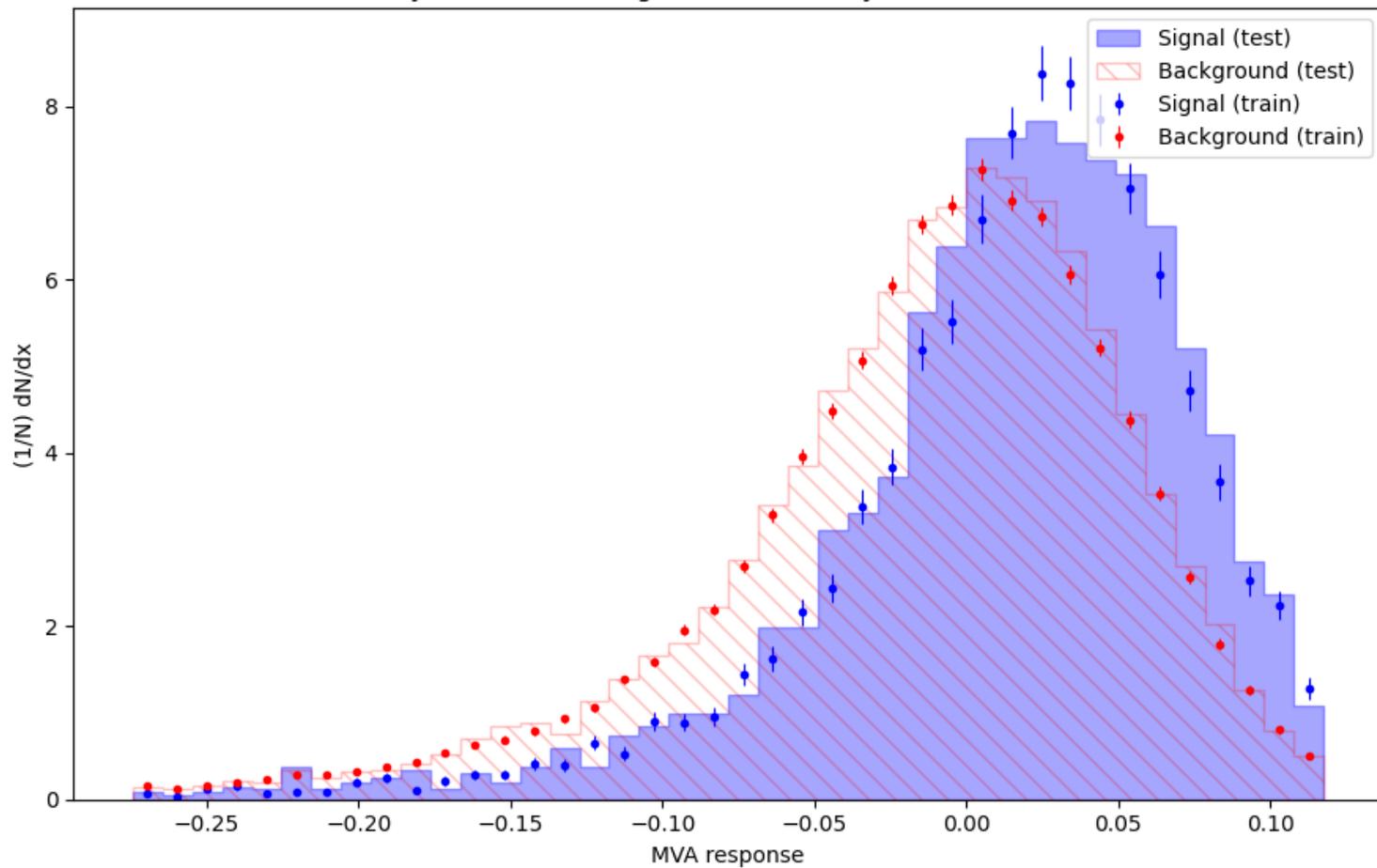
Python overtraining check (TMVA-style): LDA



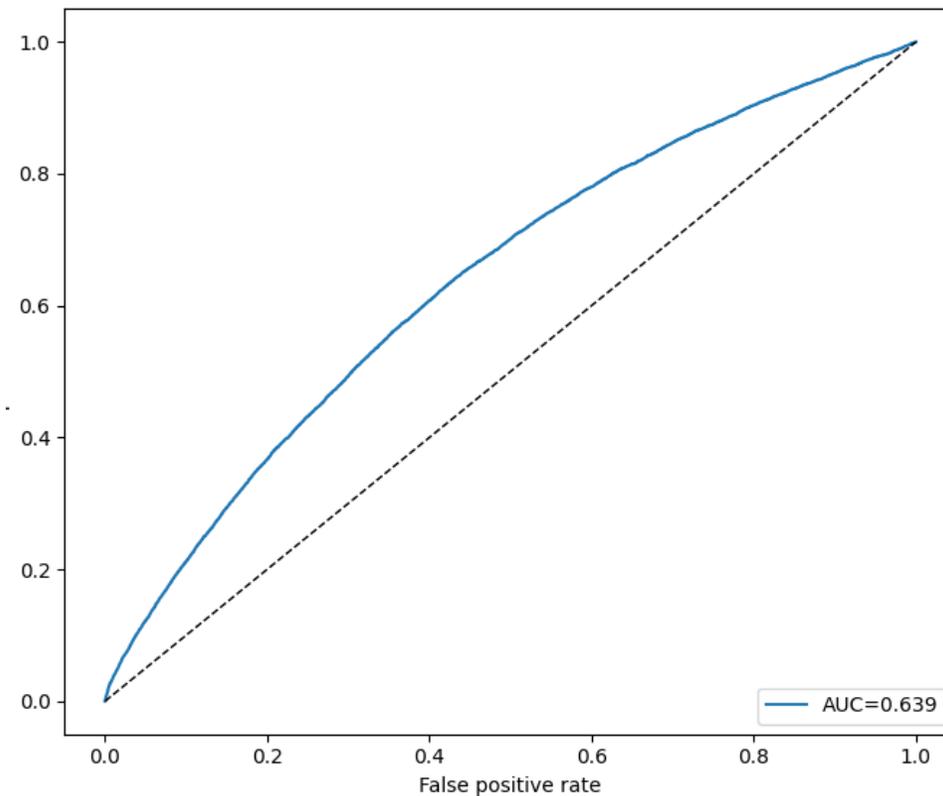
OOF ROC - LDA



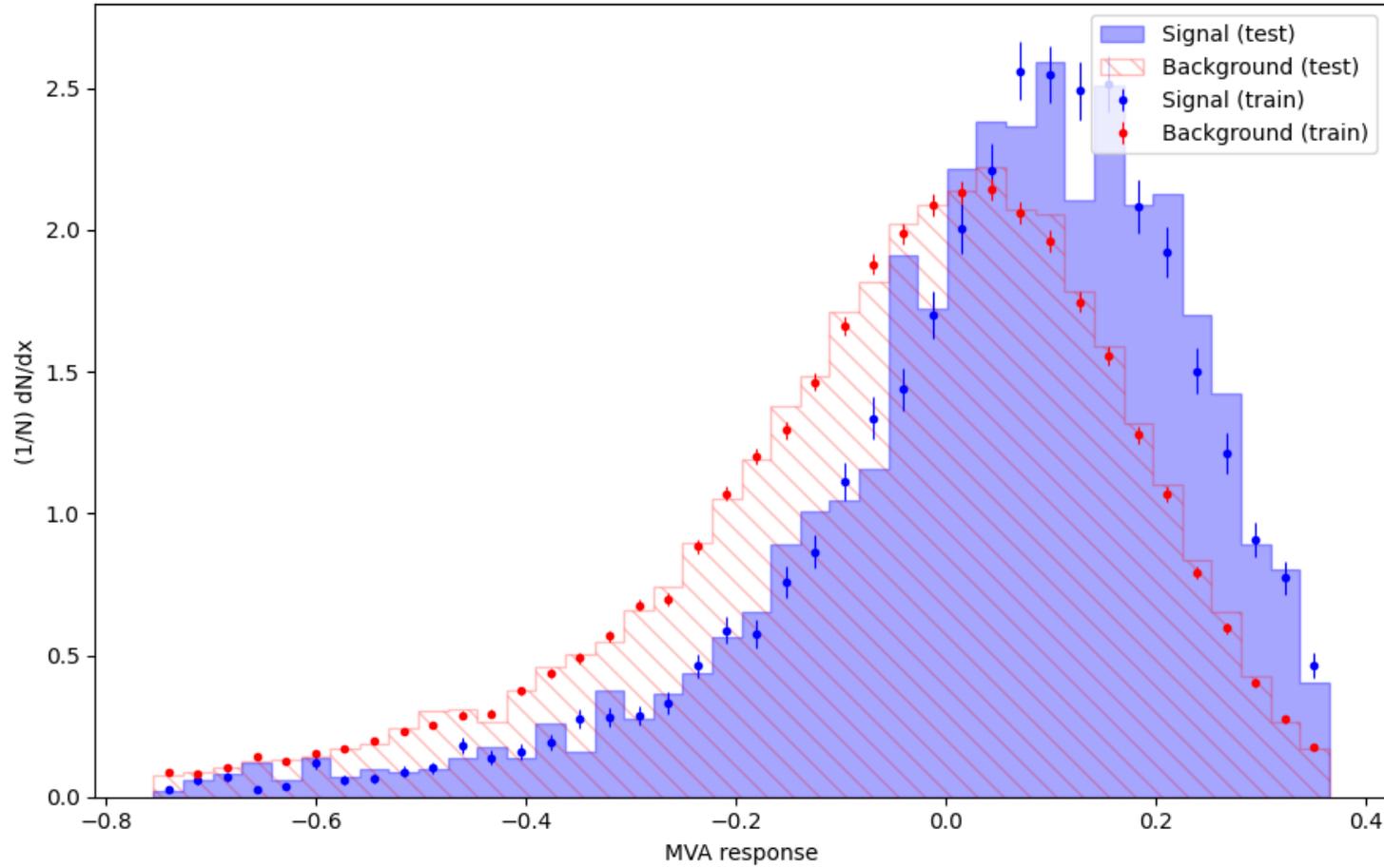
Python overtraining check (TMVA-style): LinearSVC



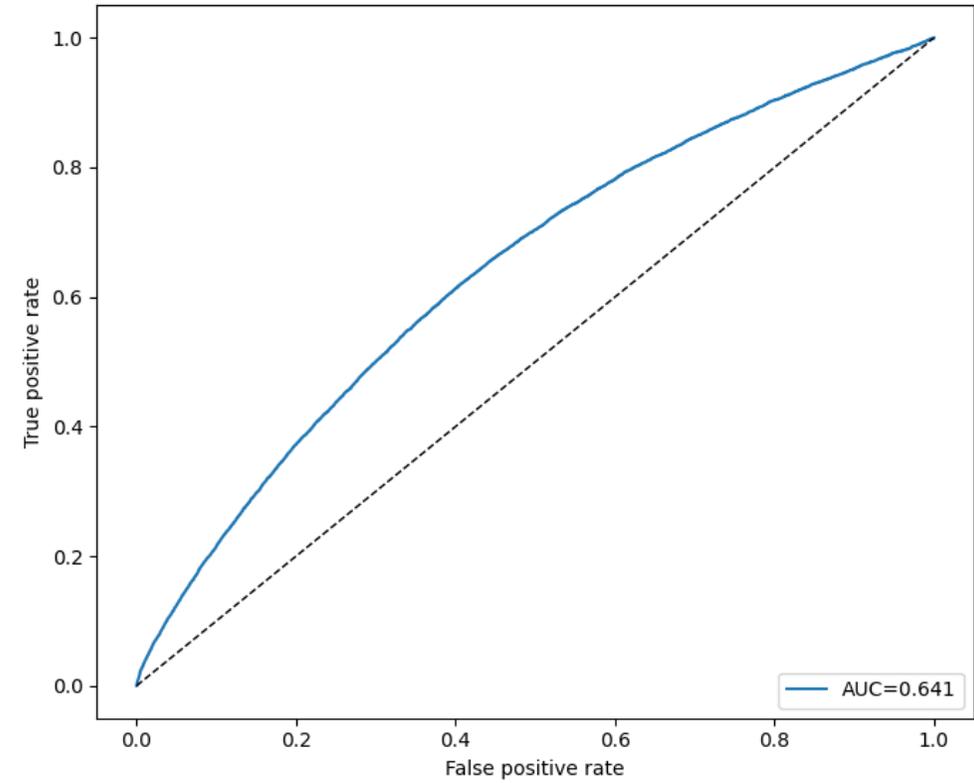
OOF ROC - LinearSVC



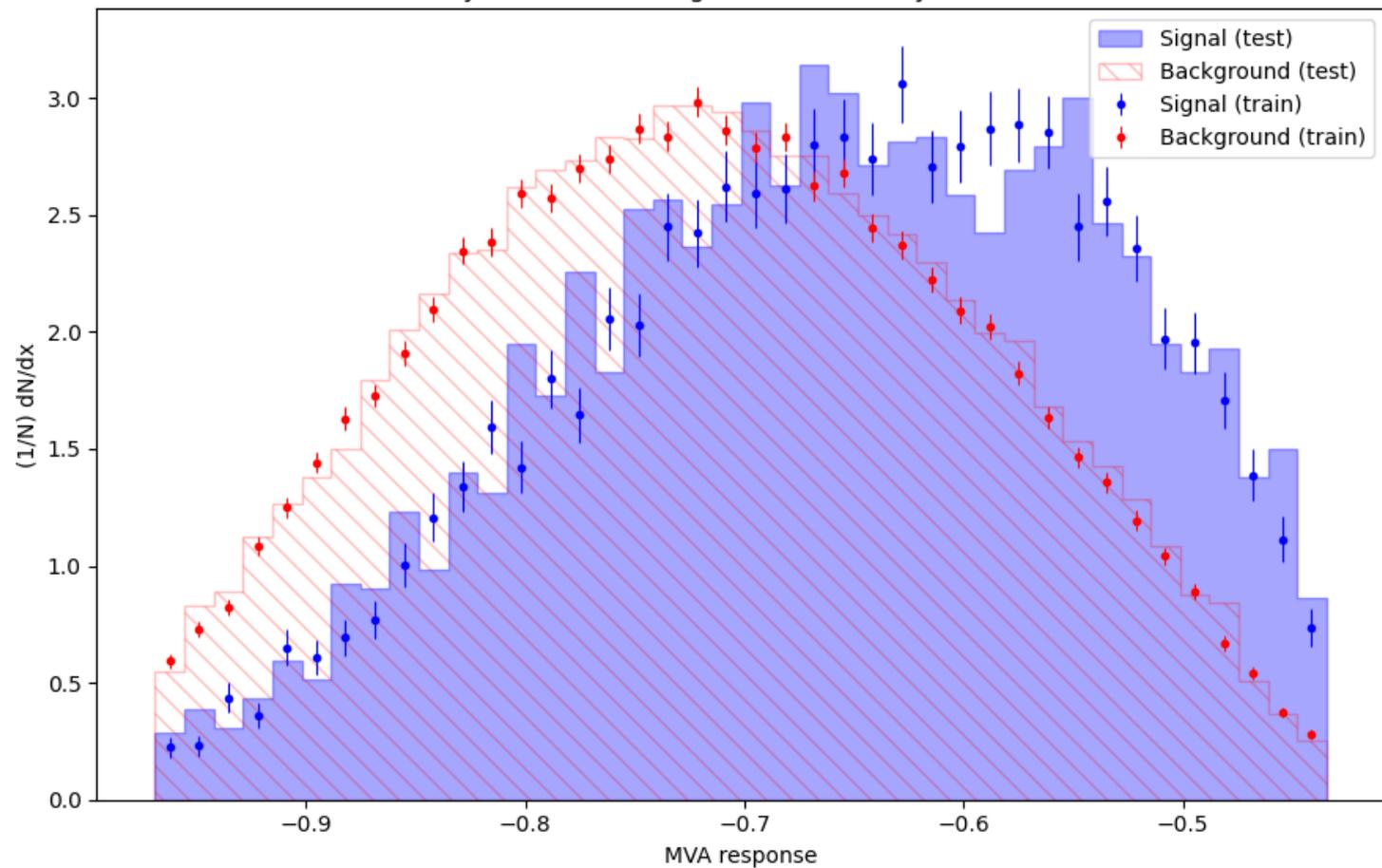
Python overtraining check (TMVA-style): LogisticRegression



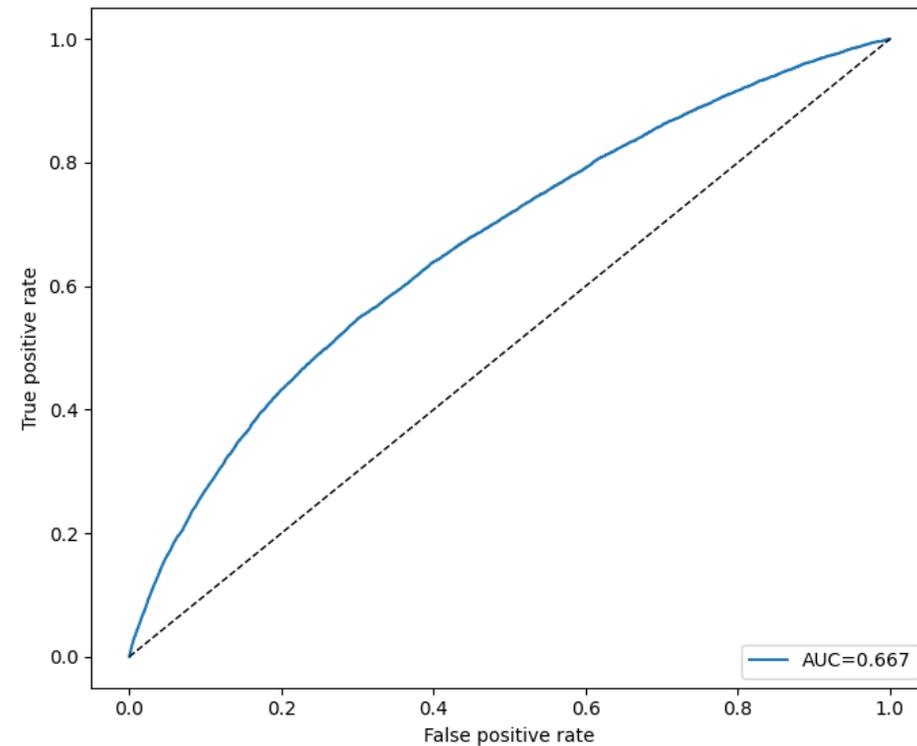
OOF ROC - LogisticRegression



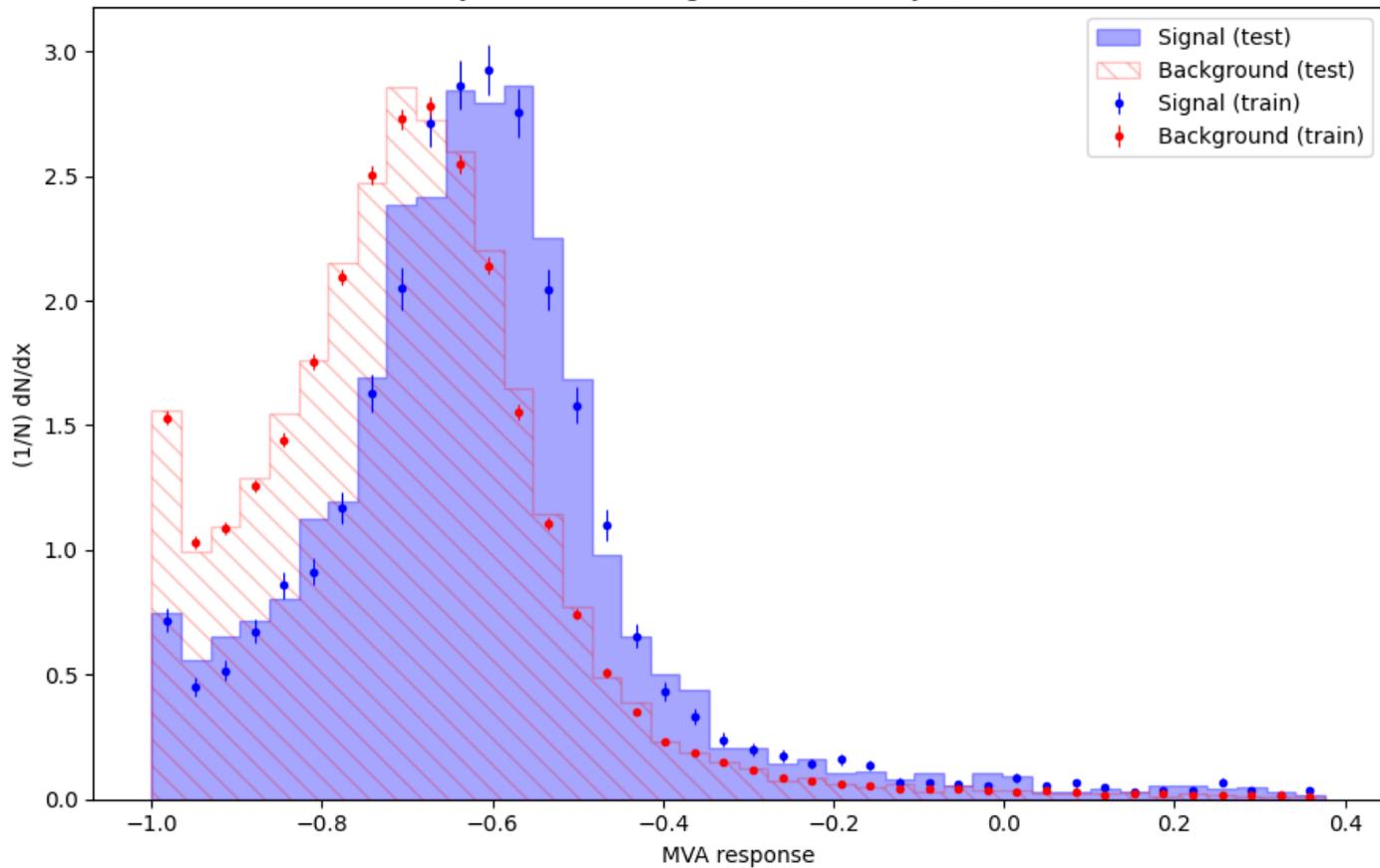
Python overtraining check (TMVA-style): MLP



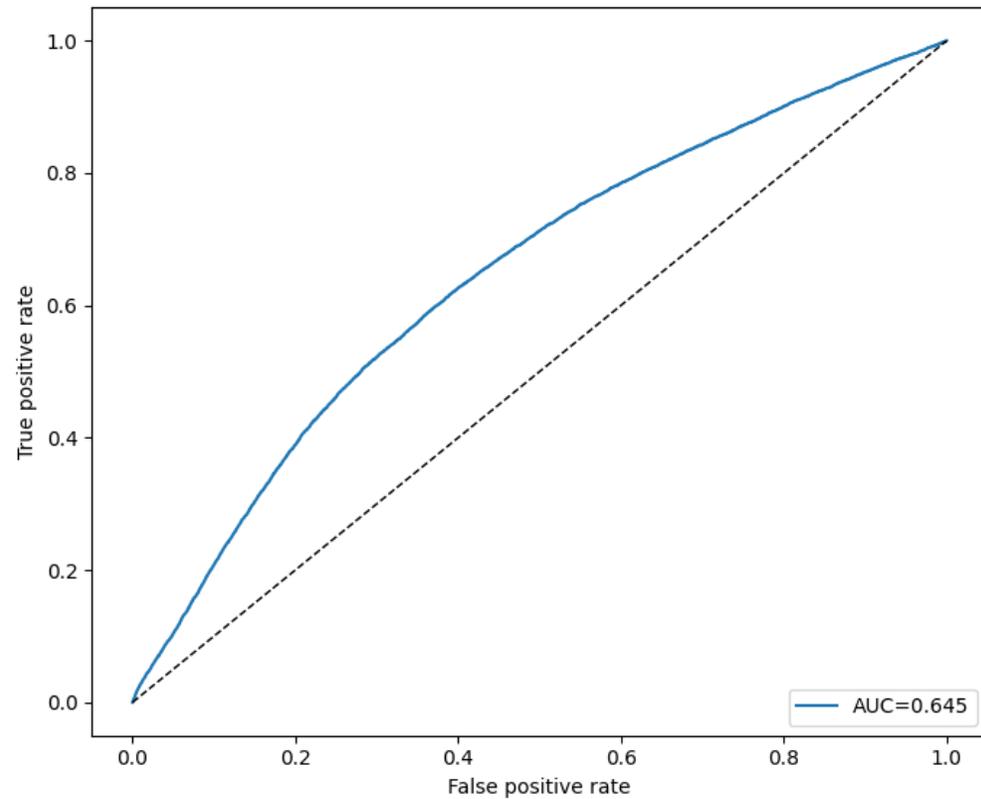
OOF ROC - MLP



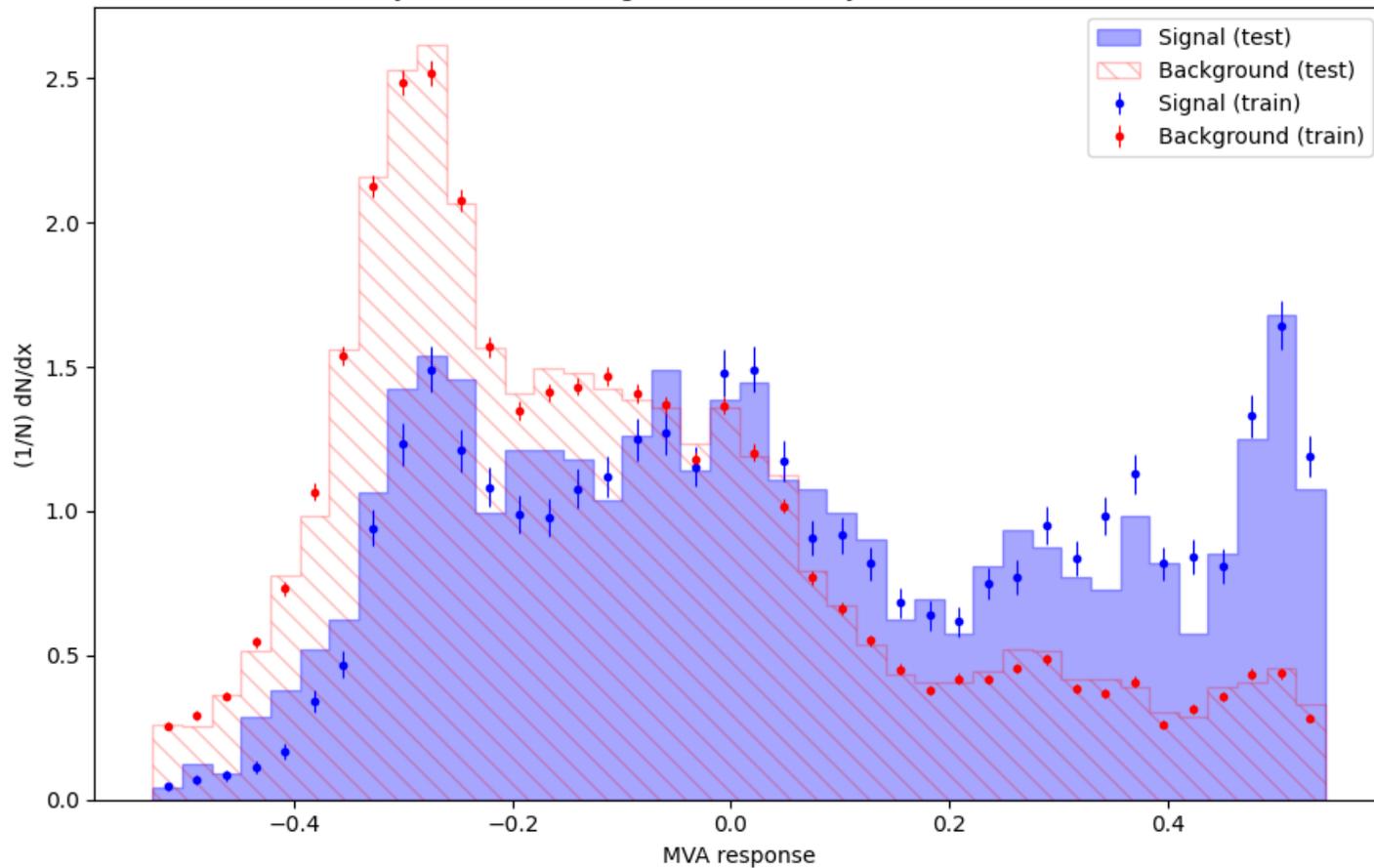
Python overtraining check (TMVA-style): QDA



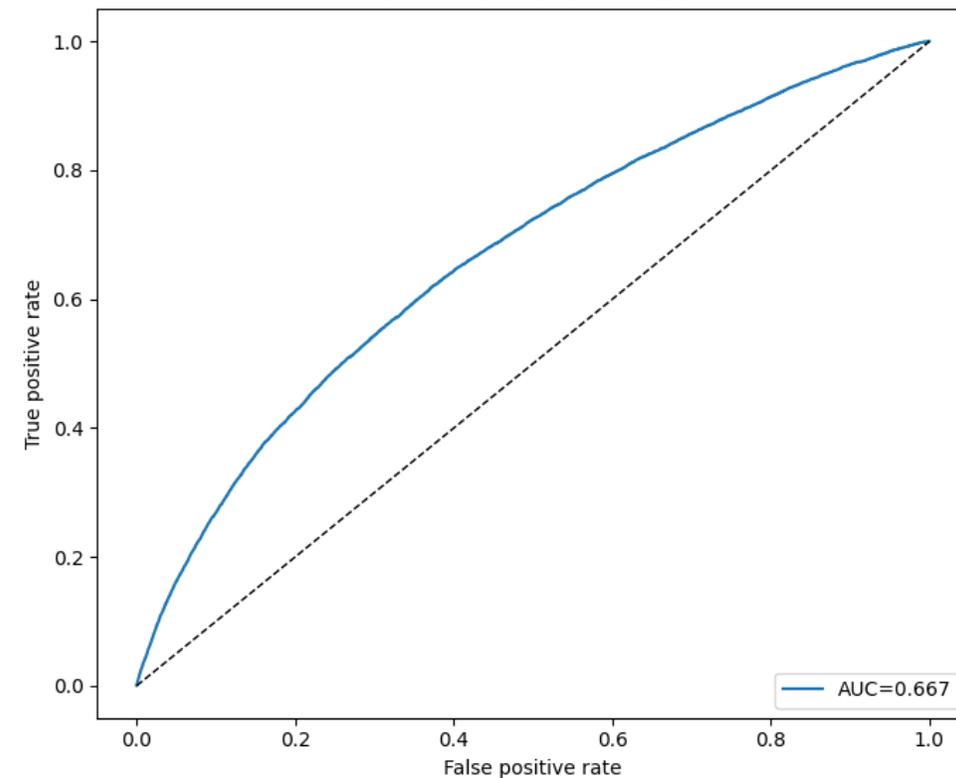
OOF ROC - QDA



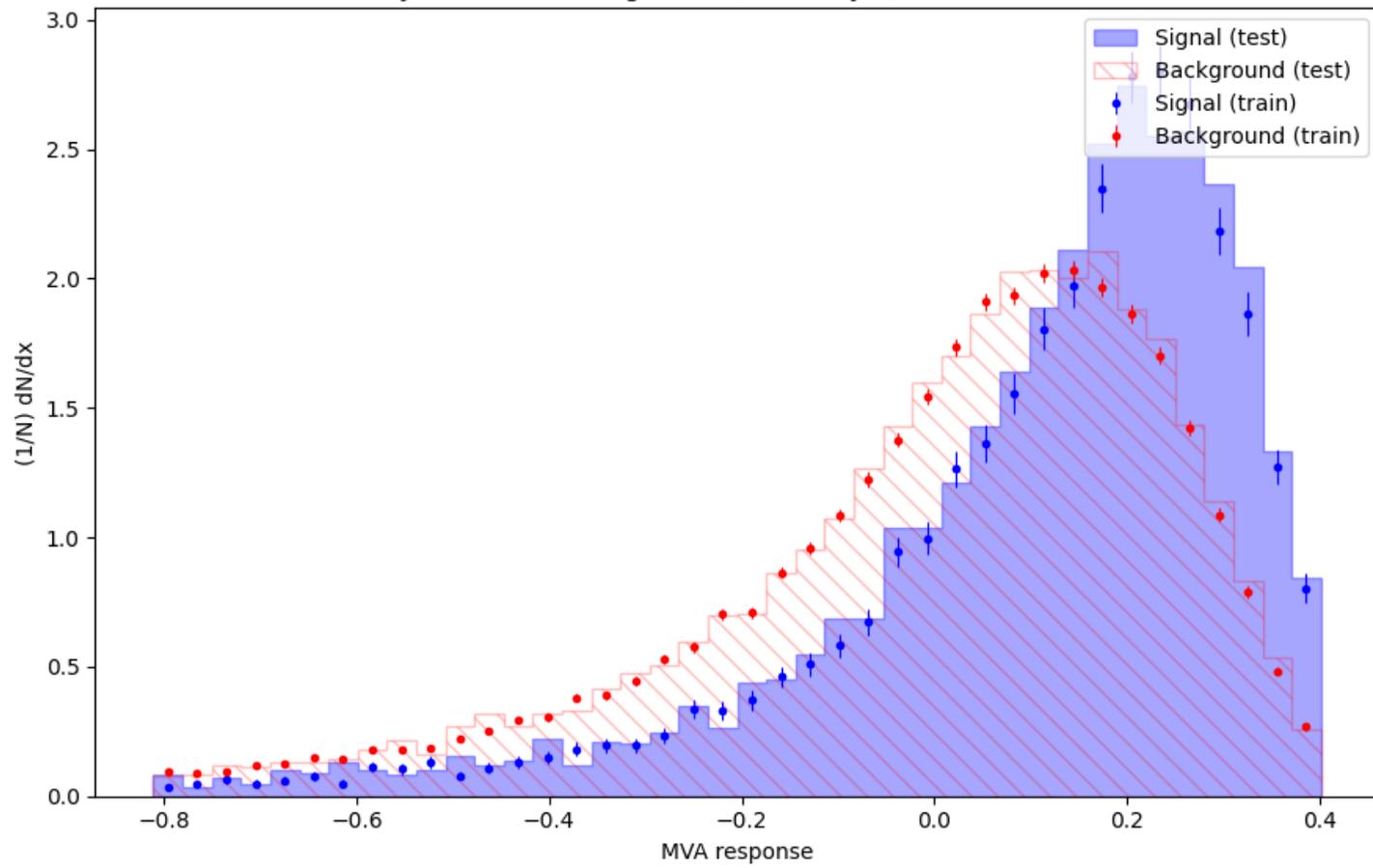
Python overtraining check (TMVA-style): RandomForest



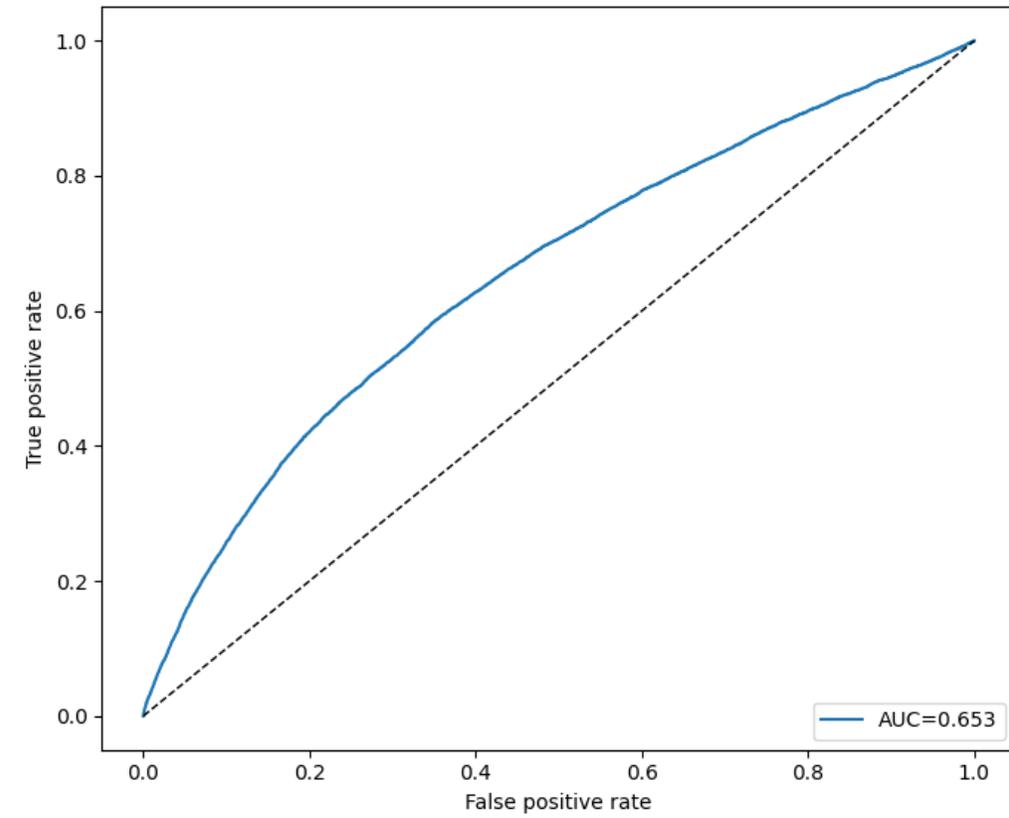
OOF ROC - RandomForest



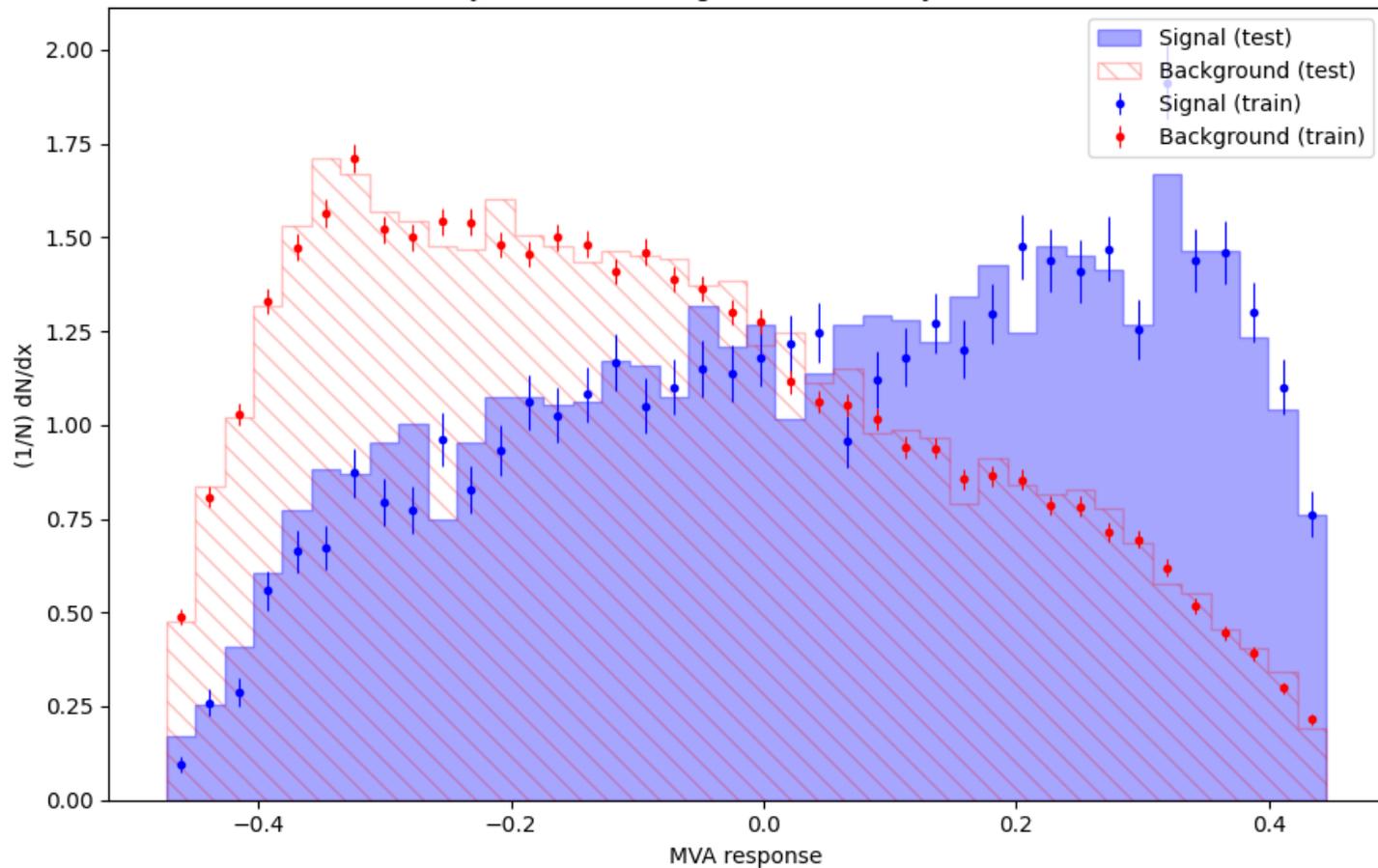
Python overtraining check (TMVA-style): SGDClassifier



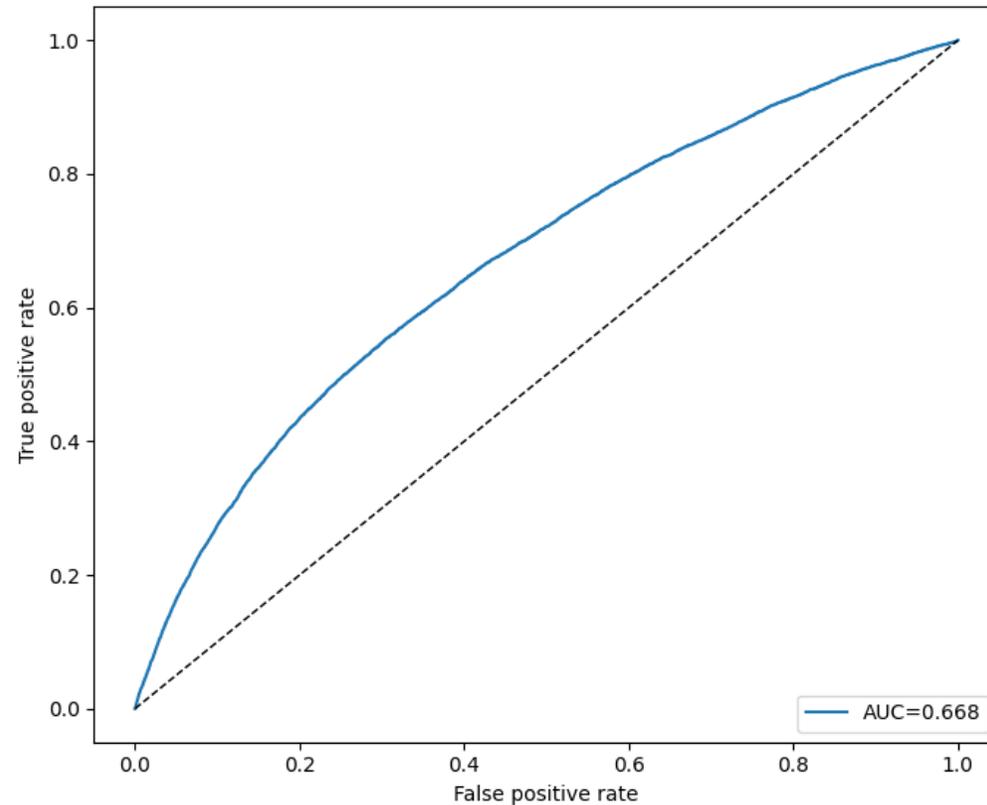
OOF ROC - SGDClassifier



Python overtraining check (TMVA-style): SVC



OOF ROC - SVC



Comparison Table of all platforms with kfold=5

Model family (common name)	TMVA algorithm (if available)	TMVA best_mean_auc	R AUC (oof_weighted)	Python mean_fold_auc	Python overall_oof_auc	Δ AUC (R – Py overall)	Δ AUC (TMVA – Py overall)
Gradient Boosting (GBM)	BDTG	0.670094	1.000000	0.675134	0.674820	+0.325180	–0.004726
MLP	MLP	0.668192	0.661500	0.665761	0.664427	–0.002927	+0.003765
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 (SVM/SVC)	—	—	0.590934	0.676572	0.676277	–0.085343	—

Best Performnace across each platform

TMVA, Python and R

with k-fold=5

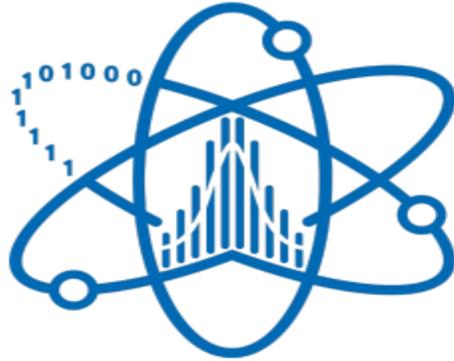
Platform	Best algorithm	Best score (AUC)	Score type (as reported)
TMVA	BDTG	0.670094	best_mean_auc (k-fold)
Python	GradientBoosting	0.670033	overall_oof_auc (out-of-fold)
R	MLP	0.660152	auc_oof_weighted (out-of-fold, weighted)

**1. Could not work on Caret package this week
(Since there was no response from Eduard yet
on installation. He said it is taking long time on
his side too.)**

**2. And working on preparing script for
transformers and see how it goes this week**



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**Лаборатория
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Thank you for your attention!!!