

Supplementary material

1. Experimental design

Table 4: Tuning the number of iterations for Boosting.

Number of iterations	Average accuracy
10	0.9126
20	0.9159
30	0.9171
40	0.9181
50	0.9195
60	0.9189
70	0.9181
80	0.9177
90	0.9165
100	0.9154

Table 5: Tuning the number of trees for Bagging.

Number of trees	Average accuracy
10	0.8926
20	0.8935
30	0.8942
40	0.8951
50	0.8949
60	0.8953
70	0.8968
80	0.8972
90	0.8977
100	0.8980

Table 6: Random subspace parameter tuning.

Number of iterations	Subspace sample size		
	0.25	0.5	0.75
10	0.8780	0.8526	0.8438
20	0.8731	0.8658	0.8341
30	0.8780	0.8682	0.8341
40	0.8804	0.8587	0.8365
50	0.9016	0.8574	0.8352
60	0.9001	0.8568	0.8349
70	0.8990	0.8557	0.8345
80	0.8878	0.8547	0.8345
90	0.8754	0.8539	0.8339
100	0.8750	0.8525	0.8324

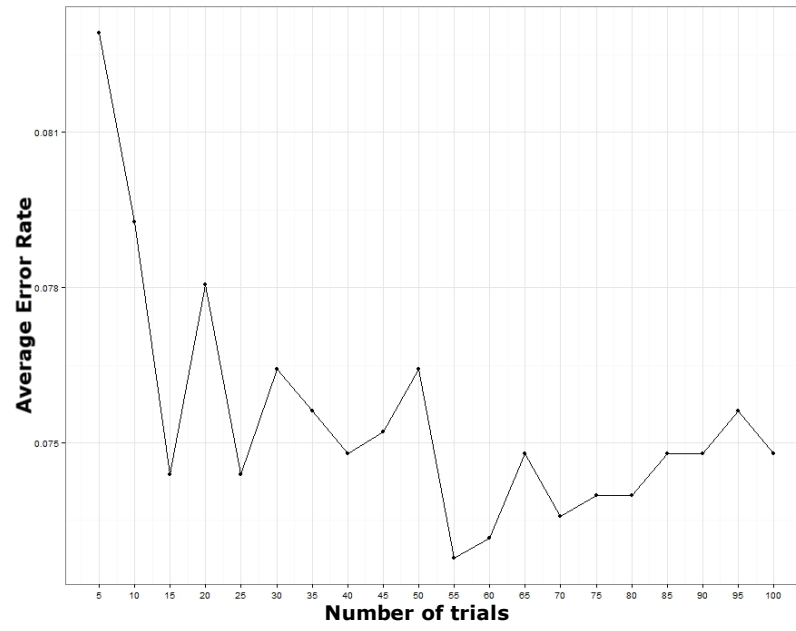


Figure 2: Number of trials optimization in C5.0.

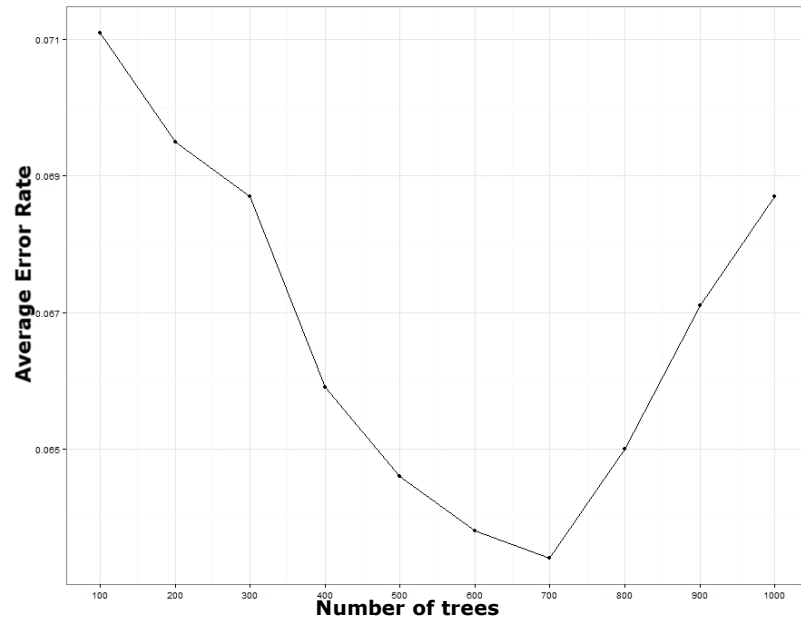


Figure 3: Number of trees optimization in Random forest.

2. Results

Table 7: Average accuracy of single classifiers and ensemble methods across 30 runs in four GBS subtype classification. Ensemble methods are shown in bold.

Method	Average accuracy
Random forest	0.9366
C5.0	0.9272
kNN	0.9268
Boosting	0.9195
SVMLap	0.9163
SVMPoly	0.9142
SVMGaus	0.9126
C4.5	0.9114
SVMLin	0.9069
Random subspace	0.9016
Naive Bayes	0.9008
Bagging	0.8980
MLP	0.8915
RBF-DDA	0.8882
SLP	0.8850
JRip	0.8837
LDA	0.8825
MLR	0.8793
OneR	0.7972

Table 8: Impact analysis of the 16 relevant features in the diagnostic model using single classifiers. Highest values are shown in bold.

Single classifier	Using 16 relevant features	Using all features	Difference
Average Accuracy			
KNN	0.9268	0.8843	0.0425
SVMLap	0.9163	0.8878	0.0285
SVMPoly	0.9142	0.8692	0.0450
SVMGaus	0.9126	0.8932	0.0194
C4.5	0.9114	0.8826	0.0288
SVMLin	0.9069	0.8919	0.0150
Naive Bayes	0.9008	0.8607	0.0401
MLP	0.8915	0.7317	0.1598
RBF-DDA	0.8882	0.6731	0.2151
SLP	0.885	0.8207	0.0643
JRip	0.8837	0.8607	0.0230
LDA	0.8825	0.8268	0.0557
MLR	0.8793	0.7602	0.1191
OneR	0.7972	0.7606	0.0366

Table 9: Impact analysis of the 16 relevant features in the diagnostic model using ensemble methods. Highest values are shown in bold.

Ensemble method	Using 16 relevant features	Using all features	Difference
Average Accuracy			
Random forest	0.9366	0.9163	0.0203
C5.0	0.9272	0.9150	0.0122
Boosting	0.9195	0.9187	0.0008
Random subspace	0.9016	0.7163	0.1853
Bagging	0.8980	0.8979	0.0001

Table 10: Average results of ensemble methods across 30 runs in AIDP vs. ALL classification.

Method	Balanced Accuracy	Accuracy	Sensitivity	Specificity	Kappa	AUC
C5.0	0.8171	0.9048	0.6944	0.9398	0.6266	0.8171
	0.0976	0.0556	0.1861	0.0565	0.1806	0.0976
Boosting	0.8069	0.8992	0.6907	0.9231	0.6046	0.8069
	0.0827	0.0479	0.1750	0.0732	0.1670	0.0827
Random forest	0.7769	0.9270	0.5667	0.9870	0.6407	0.7769
	0.0888	0.0306	0.1836	0.0289	0.1645	0.0888
Bagging	0.7681	0.8960	0.6093	0.9269	0.5629	0.7681
	0.0818	0.0466	0.1829	0.1091	0.1682	0.0818
Random subspace	0.6815	0.9056	0.3666	0.9953	0.4661	0.6810
	0.1240	0.0351	0.2453	0.0129	0.2408	0.1218

Table 11: Balanced accuracy of single classifiers and ensemble methods across 30 runs in AIDP vs. ALL classification. Ensemble methods are shown in bold.

Method	Balanced Accuracy
kNN	0.8227
C5.0	0.8171
Boosting	0.8069
C4.5	0.8042
MLP	0.8014
SVMLap	0.8009
Random forest	0.7769
Bagging	0.7681
RBF-DDA	0.7648
SLP	0.7551
SVMLin	0.7542
LDA	0.7537
SVMGaus	0.7491
JRip	0.7407
SVMPoly	0.7389
Naive Bayes	0.7231
BLR	0.7181
Random subspace	0.6815
OneR	0.6222

Table 12: Average results of ensemble methods across 30 runs in AMAN vs. ALL classification.

Method	Balanced Accuracy	Accuracy	Sensitivity	Specificity	Kappa	AUC
Boosting	0.9214	0.9341	0.8989	0.9439	0.8384	0.9214
	0.0599	0.0441	0.1045	0.0591	0.1098	0.0599
Random subspace	0.9138	0.9143	0.9112	0.9155	0.7992	0.9133
	0.0449	0.0418	0.0788	0.0545	0.0926	0.0442
C5.0	0.9136	0.9302	0.8750	0.9522	0.8290	0.9136
	0.0487	0.0385	0.0948	0.0461	0.0911	0.0487
Random forest	0.9033	0.9214	0.8611	0.9456	0.8069	0.9033
	0.0550	0.0406	0.1057	0.0424	0.1006	0.0550
Bagging	0.8542	0.8952	0.7872	0.9211	0.7303	0.8542
	0.0727	0.0462	0.1624	0.0929	0.1313	0.0727

Table 13: Balanced accuracy of single classifiers and ensemble methods across 30 runs in AMAN vs. ALL classification. Ensemble methods are shown in bold.

Method	Balanced Accuracy
kNN	0.9356
SVMGaus	0.9256
Boosting	0.9214
SVMPoly	0.9203
SVMLap	0.9181
Random subspace	0.9138
C5.0	0.9136
C4.5	0.9067
Random forest	0.9033
MLP	0.8978
SVMLin	0.8969
SLP	0.8778
Naive Bayes	0.8700
RBF-DDA	0.8689
LDA	0.8594
Bagging	0.8542
JRip	0.8472
BLR	0.8214
OneR	0.6336

Table 14: Average results of ensemble methods across 30 runs in AMSAN vs. ALL classification.

Method	Balanced Accuracy	Accuracy	Sensitivity	Specificity	Kappa	AUC
Random forest	0.8924	0.8960	0.8544	0.9304	0.7889	0.8924
	0.0429	0.0417	0.0814	0.0621	0.0849	0.0429
Boosting	0.8786	0.8810	0.8671	0.8902	0.7591	0.8786
	0.0386	0.0375	0.0663	0.0796	0.0762	0.0386
C5.0	0.8782	0.8810	0.8491	0.9072	0.7588	0.8782
	0.0494	0.0480	0.0779	0.0532	0.0978	0.0494
Random subspace	0.8688	0.8722	0.8617	0.8798	0.7425	0.8708
	0.0410	0.0440	0.0550	0.0664	0.0878	0.0416
Bagging	0.8555	0.8587	0.8365	0.8744	0.7137	0.8555
	0.0526	0.0515	0.0960	0.1012	0.1047	0.0526

Table 15: Balanced accuracy of single classifiers and ensemble methods across 30 runs in AMSAN vs. ALL classification. Ensemble methods are shown in bold.

Method	Balanced accuracy
<i>k</i> NN	0.8953
Random forest	0.8924
C4.5	0.8852
Boosting	0.8786
C5.0	0.8782
SVMLap	0.8756
RBF-DDA	0.8695
Random subspace	0.8688
SLP	0.8644
Bagging	0.8555
SVMPoly	0.8504
SVMGaus	0.8492
MLP	0.8490
JRip	0.8449
OneR	0.8219
Naive Bayes	0.8166
SVMLin	0.8101
LDA	0.8072
BLR	0.7971

Table 16: Average results of ensemble methods across 30 train-test runs in MF vs. ALL classification.

Method	Balanced Accuracy	Accuracy	Sensitivity	Specificity	Kappa	AUC
Random subspace	0.8471	0.9333	0.7500	0.9525	0.6413	0.8513
	0.1067	0.0296	0.2274	0.0349	0.1509	0.1074
Bagging	0.8342	0.9024	0.7675	0.9009	0.5498	0.8342
	0.1298	0.0513	0.2460	0.1297	0.2213	0.1298
C5.0	0.8048	0.9167	0.6667	0.9430	0.5601	0.8048
	0.1329	0.0487	0.2653	0.0484	0.2145	0.1329
Boosting	0.7572	0.9183	0.5697	0.9447	0.5022	0.7572
	0.1346	0.0323	0.2802	0.0881	0.2085	0.1346
Random forest	0.7463	0.9254	0.5250	0.9675	0.4973	0.7463
	0.1519	0.0311	0.3104	0.0246	0.2599	0.1519

Table 17: Balanced accuracy of single classifiers and ensemble methods across 30 train-test runs in MF vs. ALL classification. Ensemble methods are shown in bold.

Method	Balanced Accuracy
Naive Bayes	0.8939
Random subspace	0.8471
Bagging	0.8342
C5.0	0.8048
LDA	0.7818
C4.5	0.7691
Boosting	0.7572
JRip	0.7678
SVMGaus	0.7581
Random forest	0.7463
BLR	0.7316
SVMLin	0.7221
MLP	0.7193
SVMPoly	0.7086
SLP	0.6875
OneR	0.6853
SVMLap	0.6664
kNN	0.6539
RBF-DDA	0.5042

Table 18: Average results of ensemble methods across 30 runs in AIDP vs. AMAN classification. Standard deviation of each metric is shown in normal font.

Method	Balanced Accuracy	Accuracy	Sensitivity	Specificity	Kappa	AUC
Bagging	0.9597 0.0458	0.9630 0.0395	0.9472 0.0861	0.9722 0.0551	0.9171 0.0882	0.9597 0.0458
C5.0	0.9597 0.0530	0.9611 0.0487	0.9556 0.0868	0.9639 0.0566	0.9139 0.1078	0.9597 0.0530
Boosting	0.9486 0.0473	0.9556 0.0397	0.9278 0.0895	0.9694 0.0599	0.8997 0.0889	0.9486 0.0473
Random subspace	0.9325 0.0887	0.9444 0.0652	0.8833 0.1703	0.9751 0.0445	0.8683 0.1589	0.9292 0.0890
Random forest	0.9097 0.0805	0.9315 0.0540	0.8444 0.1747	0.9750 0.0497	0.8368 0.1348	0.9097 0.0805

Table 19: Balanced accuracy of single classifiers and ensemble methods across 30 runs in AIDP vs. AMAN classification. Ensemble methods are shown in bold.

Method	Balanced Accuracy
JRip	0.9639
Bagging	0.9597
C5.0	0.9597
OneR	0.9583
Boosting	0.9486
C4.5	0.9458
SVMLin	0.9347
SLP	0.9333
MLP	0.9333
Random subspace	0.9325
Naive Bayes	0.9278
SVMLap	0.9125
Random forest	0.9097
SVMGaus	0.9014
RBF-DDA	0.8958
SVMPoly	0.8722
kNN	0.8639
BLR	0.8542
LDA	0.8389

Table 20: Average results of ensemble methods across 30 runs in AIDP vs. AMSAN classification. Standard deviation of each metric is shown in normal font.

Method	Balanced Accuracy	Balanced Accuracy	Sensitivity	Specificity	Kappa	AUC
Random forest	0.9102	0.9387	0.8556	0.9649	0.8312	0.9102
	0.0588	0.0430	0.1136	0.0485	0.1137	0.0588
Boosting	0.8972	0.9160	0.8532	0.9412	0.7797	0.8972
	0.0609	0.0539	0.1032	0.0623	0.1308	0.0609
Bagging	0.8854	0.9067	0.8480	0.9228	0.7565	0.8854
	0.0774	0.0675	0.1211	0.0798	0.1635	0.0774
C5.0	0.8683	0.8893	0.8278	0.9088	0.7095	0.8683
	0.0755	0.0563	0.1348	0.0569	0.1434	0.0755
Random subspace	0.8674	0.9093	0.7834	0.9491	0.7459	0.8662
	0.0755	0.0481	0.1524	0.0544	0.1324	0.0744

Table 21: Balanced accuracy of single classifiers and ensemble methods across 30 runs in AIDP vs. AMSAN classification. Ensemble methods are shown in bold.

Method	Balanced Accuracy
Random forest	0.9102
SVMLap	0.9061
SVMPoly	0.8990
Boosting	0.8972
MLP	0.8949
SVMGaus	0.8931
SVMLin	0.8928
kNN	0.8899
Bagging	0.8854
SLP	0.8841
Naive Bayes	0.8728
C4.5	0.8692
C5.0	0.8683
Random subspace	0.8674
JRip	0.8588
BLR	0.8423
RBFD	0.8339
OneR	0.8316
LDA	0.7836

Table 22: Average results of ensemble methods across 30 runs in AIDP vs. MF classification. Standard deviation of each metric is shown in normal font.

Method	Balanced Accuracy	Accuracy	Sensitivity	Specificity	Kappa	AUC
Random subspace	0.8951 0.0673	0.8733 0.0785	0.7944 0.1288	0.9917 0.0456	0.7527 0.1494	0.8930 0.0671
Bagging	0.8750 0.1089	0.8533 0.1167	0.8333 0.1578	0.9167 0.1681	0.7158 0.2223	0.8806 0.0867
Random forest	0.8306 0.0847	0.8267 0.0785	0.8111 0.1366	0.8500 0.1925	0.6460 0.1626	0.8306 0.0847
C5.0	0.8014 0.1167	0.7967 0.0999	0.7778 0.1337	0.8250 0.2555	0.5820 0.2221	0.8014 0.1167
Adaboost	0.7694 0.1275	0.7767 0.1165	0.7167 0.2037	0.8222 0.2303	0.5333 0.2337	0.7806 0.0996

Table 23: Balanced accuracy of single classifiers and ensemble methods across 30 runs in AIDP vs. MF classification. Ensemble methods are shown in bold.

Method	Balanced Accuracy
Random subspace	0.8951
Bagging	0.8750
OneR	0.8667
JRip	0.8528
kNN	0.8417
MLP	0.8347
Naive Bayes	0.8319
Random forest	0.8306
C4.5	0.8236
SVMGaus	0.8222
SVMPoly	0.8069
SVMLap	0.8028
C5.0	0.8014
SLP	0.7708
Boosting	0.7694
SVMLin	0.7542
RBF-DDA	0.7042
LDA	0.6250
BLR	0.6111

Table 24: Average results of ensemble methods across 30 runs in AMAN vs. AMSAN classification. Standard deviation of each metric is shown in normal font.

Method	Balanced Accuracy	Accuracy	Sensitivity	Specificity	Kappa	AUC
Random forest	0.9474	0.9505	0.9333	0.9614	0.8950	0.9474
	0.0415	0.0347	0.0859	0.0389	0.0752	0.0415
Random subspace	0.9390	0.9473	0.9057	0.9736	0.8872	0.9396
	0.0420	0.0344	0.0840	0.0359	0.0752	0.0414
Boosting	0.9284	0.9355	0.9216	0.9352	0.8625	0.9284
	0.0464	0.0397	0.0689	0.0960	0.0865	0.0464
C5.0	0.9242	0.9290	0.9028	0.9456	0.8505	0.9242
	0.0651	0.0625	0.0981	0.0725	0.1293	0.0651
Bagging	0.8940	0.8989	0.8877	0.9003	0.7879	0.8940
	0.0648	0.0632	0.0768	0.1065	0.1327	0.0648

Table 25: Balanced accuracy of single classifiers and ensemble methods across 30 runs in AMAN vs. AMSAN classification. Ensemble methods are shown in bold.

Method	Balanced accuracy
k NN	0.9588
Random forest	0.9474
SVMLap	0.9406
Random subspace	0.9390
MLP	0.9344
Boosting	0.9284
RBF-DDA	0.9265
C5.0	0.9242
SVMGaus	0.9236
SLP	0.9202
SVMPoly	0.9189
C4.5	0.9138
SVMLin	0.9125
Naive Bayes	0.9091
Bagging	0.8940
LDA	0.8838
JRip	0.8827
BLR	0.8559
OneR	0.8437

Table 26: Average results of ensemble methods across 30 runs in AMAN vs. MF classification. Standard deviation of each metric is shown in normal font.

Method	Balanced Accuracy	Accuracy	Sensitivity	Specificity	Kappa	AUC
Random forest	0.9333	0.9625	0.9917	0.8750	0.8908	0.9333
	0.0838	0.0452	0.0335	0.1706	0.1346	0.0838
Bagging	0.9181	0.9313	0.9611	0.8750	0.8214	0.9181
	0.0705	0.0502	0.0811	0.1431	0.1271	0.0705
Boosting	0.9167	0.9417	0.9639	0.8694	0.8449	0.9201
	0.0922	0.0655	0.0779	0.1662	0.1888	0.0967
C5.0	0.9069	0.9313	0.9556	0.8583	0.8201	0.9069
	0.0802	0.0664	0.0750	0.1421	0.1619	0.0802
Random subspace	0.7543	0.8708	0.9917	0.5083	0.5749	0.7500
	0.1227	0.0567	0.0253	0.2583	0.2123	0.1228

Table 27: Balanced accuracy of single classifiers and ensemble methods across 30 in AMAN vs. MF classification. Ensemble methods are shown in bold.

Method	Balanced Accuracy
SVMGaus	0.9542
SVMLap	0.9542
RBF-DDA	0.9528
Naive Bayes	0.9486
SVMLin	0.9431
kNN	0.9417
SVMPoly	0.9375
Random forest	0.9333
Bagging	0.9181
Boosting	0.9167
MLP	0.9125
C5.0	0.9069
SLP	0.9056
LDA	0.9056
C4.5	0.8889
BLR	0.8833
oneR	0.8806
JRip	0.8792
Random subspace	0.7543

Table 28: Average results of ensemble methods across 30 runs in AMSAN vs. MF classification. Standard deviation of each metric is shown in normal font.

Method	Balanced Accuracy	Balanced Accuracy	Sensitivity	Specificity	Kappa	AUC
Random subspace	0.8879	0.8928	0.8964	0.8750	0.6786	0.8857
	0.0862	0.0556	0.0561	0.1574	0.1590	0.0855
C5.0	0.8651	0.9130	0.9386	0.7917	0.7032	0.8651
	0.0898	0.0379	0.0480	0.1979	0.1272	0.0898
Bagging	0.8645	0.8957	0.8961	0.8329	0.7195	0.8978
	0.1789	0.1749	0.1869	0.2177	0.2482	0.0757
Random forest	0.8539	0.9217	0.9579	0.7500	0.7113	0.8539
	0.1061	0.0418	0.0350	0.2177	0.1727	0.1061
Boosting	0.8246	0.9058	0.9364	0.7127	0.6519	0.8246
	0.1155	0.0458	0.0717	0.2463	0.1888	0.1155

Table 29: Balanced accuracy of single classifiers and ensemble methods across 30 runs in AMSAN vs. MF classification. Ensemble methods are shown in bold.

Method	Balanced Accuracy
Naive Bayes	0.8980
Random subspace	0.8879
LDA	0.8656
C5.0	0.8651
Bagging	0.8645
MLP	0.8588
Random forest	0.8539
SLP	0.8493
SVMGaus	0.8480
SVMLap	0.8316
JRip	0.8248
Boosting	0.8246
k NN	0.8099
BLR	0.8042
C4.5	0.8026
SVMLin	0.8013
SVMPoly	0.7974
OneR	0.7811
RBF-DDA	0.6757