# **S1 Table. Performance statistics for the 12 ensemble models selected per endpoint.**

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
|  |  |  |  | Accuracy | Sensitivity | Specificity | BCR |
| Aggregation(e) | Max. Models Initial Population | Objective Function | Size | Train(a) | Sel. (b) | Ext. (c) | Train(a) | Sel. (b) | Ext. (c) | Train(a) | Sel. (b) | Ext. (c) | Train(a) | Sel. (b) | Ext. (c) | $\sqrt{Train\*Sel.}$(d) |
| **AGS** |
| MV | 5 | Error | 5 | 0.9791 | 0.8763 | 0.7803 | 0.9529 | 0.8780 | 0.7885 | 0.9962 | 0.8750 | 0.7750 | 0.9324 | 0.8739 | 0.7712 | 0.9027 |
| MV | 10 | Error | 7 | 0.9721 | 0.8660 | 0.7879 | 0.9412 | 0.8537 | 0.7885 | 0.9923 | 0.8750 | 0.7875 | 0.9173 | 0.8459 | 0.7872 | 0.8809 |
| MV | 15 | Error | 5 | 0.9791 | 0.9072 | 0.7803 | 0.9588 | 0.8780 | 0.7885 | 0.9923 | 0.9286 | 0.7750 | 0.9429 | 0.8577 | 0.7712 | 0.8993 |
| MV | 5 | AIC | 5 | 0.9698 | 0.8763 | 0.7955 | 0.9294 | 0.8537 | 0.7885 | 0.9962 | 0.8929 | 0.8000 | 0.8985 | 0.8390 | 0.7851 | 0.8683 |
| MV | 10 | AIC | 5 | 0.9791 | 0.8969 | 0.7803 | 0.9529 | 0.8780 | 0.7692 | 0.9962 | 0.9107 | 0.7875 | 0.9324 | 0.8652 | 0.7641 | 0.8982 |
| MV | 15 | AIC | 3 | 0.9837 | 0.8454 | 0.7727 | 0.9588 | 0.8293 | 0.7692 | 1.0000 | 0.8571 | 0.7750 | 0.9391 | 0.8197 | 0.7677 | 0.8774 |
| SV | 5 | Error | 4 | 0.9767 | 0.8660 | 0.7727 | 0.9529 | 0.8293 | 0.7692 | 0.9923 | 0.8929 | 0.7750 | 0.9343 | 0.8063 | 0.7677 | 0.8680 |
| SV | 10 | Error | 3 | 0.9884 | 0.8454 | 0.7727 | 0.9765 | 0.8293 | 0.7692 | 0.9962 | 0.8571 | 0.7750 | 0.9669 | 0.8197 | 0.7677 | 0.8903 |
| SV | 15 | Error | 3 | 0.9884 | 0.8351 | 0.7955 | 0.9706 | 0.8537 | 0.7885 | 1.0000 | 0.8214 | 0.8000 | 0.9563 | 0.8105 | 0.7851 | 0.8804 |
| SV | 5 | AIC | 5 | 0.9860 | 0.8660 | 0.7727 | 0.9765 | 0.8537 | 0.7692 | 0.9923 | 0.8750 | 0.7750 | 0.9688 | 0.8459 | 0.7677 | 0.9053 |
| SV | 10 | AIC | 2 | 0.9512 | 0.8144 | 0.7879 | 0.8882 | 0.8049 | 0.7885 | 0.9923 | 0.8214 | 0.7875 | 0.8424 | 0.7997 | 0.7872 | 0.8208 |
| SV | 15 | AIC | 5 | 0.9814 | 0.8454 | 0.7879 | 0.9529 | 0.8780 | 0.7885 | 1.0000 | 0.8214 | 0.7875 | 0.9305 | 0.8016 | 0.7872 | 0.8637 |
| Mean |  |  | 4.33 | 0.9779 | 0.8617 | 0.7822 | 0.9510 | 0.8516 | 0.7804 | 0.9955 | 0.8690 | 0.7833 | 0.9302 | 0.8321 | 0.7758 | 0.8796 |
| **NCI-N87** |
| MV | 5 | Error | 5 | 0.9912 | 0.8182 | 0.6471 | 1.0000 | 0.9091 | 0.6471 | 0.9825 | 0.7273 | 0.6471 | 0.9738 | 0.6694 | 0.6471 | 0.8074 |
| MV | 10 | Error | 19 | 0.9912 | 0.8182 | 0.7059 | 0.9825 | 0.8182 | 0.7059 | 1.0000 | 0.8182 | 0.7059 | 0.9738 | 0.8182 | 0.7059 | 0.8926 |
| MV | 15 | Error | 7 | 0.9912 | 0.8571 | 0.7059 | 1.0000 | 0.8182 | 0.7059 | 0.9825 | 0.8182 | 0.7059 | 0.9738 | 0.8182 | 0.7059 | 0.8926 |
| MV | 5 | AIC | 3 | 0.9825 | 0.7727 | 0.7059 | 0.9825 | 0.8182 | 0.7059 | 0.9825 | 0.7273 | 0.7059 | 0.9825 | 0.7025 | 0.7059 | 0.8308 |
| MV | 10 | AIC | 3 | 0.9649 | 0.8182 | 0.6471 | 1.0000 | 1.0000 | 0.6471 | 0.9298 | 0.6364 | 0.6471 | 0.8972 | 0.5207 | 0.6471 | 0.6835 |
| MV | 15 | AIC | 3 | 0.9912 | 0.7619 | 0.7353 | 0.9825 | 0.6364 | 0.7059 | 1.0000 | 0.8182 | 0.7647 | 0.9738 | 0.5950 | 0.6920 | 0.7612 |
| SV | 5 | Error | 11 | 1.0000 | 0.8182 | 0.7059 | 1.0000 | 0.8182 | 0.7059 | 1.0000 | 0.8182 | 0.7059 | 1.0000 | 0.8182 | 0.7059 | 0.9045 |
| SV | 10 | Error | 8 | 1.0000 | 0.9091 | 0.7059 | 1.0000 | 0.9091 | 0.7059 | 1.0000 | 0.9091 | 0.7059 | 1.0000 | 0.9091 | 0.7059 | 0.9535 |
| SV | 15 | Error | 6 | 1.0000 | 0.8636 | 0.7647 | 1.0000 | 0.9091 | 0.7647 | 1.0000 | 0.8182 | 0.7647 | 1.0000 | 0.7851 | 0.7647 | 0.8861 |
| SV | 5 | AIC | 2 | 0.9912 | 0.7727 | 0.7941 | 0.9825 | 0.9091 | 0.8235 | 1.0000 | 0.6364 | 0.7647 | 0.9738 | 0.5620 | 0.7474 | 0.7398 |
| SV | 10 | AIC | 2 | 0.9912 | 0.8182 | 0.7059 | 1.0000 | 0.9091 | 0.7059 | 0.9825 | 0.7273 | 0.7059 | 0.9738 | 0.6694 | 0.7059 | 0.8074 |
| SV | 15 | AIC | 1 | 1.0000 | 0.6818 | 0.6471 | 1.0000 | 0.7273 | 0.6471 | 1.0000 | 0.6364 | 0.6471 | 1.0000 | 0.6198 | 0.6471 | 0.7873 |
| Mean |  |  | 5.83 | 0.9912 | 0.8092 | 0.7059 | 0.9942 | 0.8485 | 0.7059 | 0.9883 | 0.7576 | 0.7059 | 0.9769 | 0.7073 | 0.6984 | 0.8289 |
| **SNU-1** |
| MV | 5 | Error | 7 | 0.9877 | 1.0000 | 0.6296 | 0.9697 | 1.0000 | 0.6364 | 1.0000 | 1.0000 | 0.6250 | 0.9550 | 1.0000 | 0.6235 | 0.9772 |
| MV | 10 | Error | 7 | 0.9877 | 0.8846 | 0.6296 | 0.9697 | 1.0000 | 0.6364 | 1.0000 | 0.8125 | 0.6250 | 0.9550 | 0.7363 | 0.6235 | 0.8386 |
| MV | 15 | Error | 9 | 0.9877 | 0.9231 | 0.6667 | 0.9697 | 0.9000 | 0.6364 | 1.0000 | 0.9375 | 0.6875 | 0.9550 | 0.8843 | 0.6281 | 0.9190 |
| MV | 5 | AIC | 7 | 0.9383 | 0.8462 | 0.6923 | 0.8485 | 0.7000 | 0.6364 | 1.0000 | 0.9375 | 0.6875 | 0.7842 | 0.6243 | 0.6281 | 0.6997 |
| MV | 10 | AIC | 5 | 0.9877 | 0.8462 | 0.7407 | 0.9697 | 0.7000 | 0.7273 | 1.0000 | 0.9375 | 0.7500 | 0.9550 | 0.6243 | 0.7218 | 0.7721 |
| MV | 15 | AIC | 7 | 0.9877 | 0.9231 | 0.7407 | 0.9697 | 0.8000 | 0.7273 | 1.0000 | 1.0000 | 0.7500 | 0.9550 | 0.7200 | 0.7218 | 0.8292 |
| SV | 5 | Error | 3 | 0.9877 | 0.6538 | 0.6667 | 0.9697 | 0.4000 | 0.6364 | 1.0000 | 0.8125 | 0.6875 | 0.9550 | 0.3562 | 0.6281 | 0.5832 |
| SV | 10 | Error | 10 | 0.9877 | 0.8077 | 0.5556 | 0.9697 | 0.9000 | 0.5455 | 1.0000 | 0.7500 | 0.5625 | 0.9550 | 0.7013 | 0.5445 | 0.8184 |
| SV | 15 | Error | 8 | 0.9877 | 0.9231 | 0.6667 | 0.9697 | 1.0000 | 0.6364 | 1.0000 | 0.8750 | 0.6875 | 0.9550 | 0.8203 | 0.6281 | 0.8851 |
| SV | 5 | AIC | 5 | 0.9877 | 0.9615 | 0.5556 | 0.9697 | 0.9000 | 0.5455 | 1.0000 | 1.0000 | 0.5625 | 0.9550 | 0.8550 | 0.5445 | 0.9036 |
| SV | 10 | AIC | 3 | 0.9877 | 0.6154 | 0.5926 | 0.9697 | 0.5000 | 0.6364 | 1.0000 | 0.6875 | 0.5625 | 0.9550 | 0.4824 | 0.5552 | 0.6788 |
| SV | 15 | AIC | 4 | 0.9877 | 0.8077 | 0.5556 | 0.9697 | 0.8000 | 0.5455 | 1.0000 | 0.8125 | 0.5625 | 0.9550 | 0.7962 | 0.5445 | 0.8720 |
| Mean |  |  | 6.25 | 0.9835 | 0.8494 | 0.6410 | 0.9596 | 0.8000 | 0.6288 | 1.0000 | 0.8802 | 0.6458 | 0.9408 | 0.7167 | 0.6160 | 0.8147 |
| (a) Training data set. (b) Selection data set. (c) External data set. (d) Geometric mean of the BCR metric across training and selection sets(e) Aggregation algorithm. MV: Majority Vote, SV: Scores Vote. The best performing model per endpoint is highlighted gray |