Plot of Stacking model showing the contributions of each model for ganciclovir.

Une image contenant capture d’écran, texte, ligne, diagramme

Description générée automatiquement

Mlp: neural networks algorithm, boost\_tree: Xgboost algorithm

The penalty value associated with the smallest RMSE was 0.1.

The boosted tree and neural network models have the largest contributions to the ensemble.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| member | mtry | Min\_n | Tree\_depth | learn\_rate | sample\_size | coef | **hidden\_units** | **epochs** |
| tune\_xgb\_1\_09 | 6 | 5 | 6 | 0.00183 | 0.1426 | 5.47 |  |  |
| rand\_forest\_res\_1\_07 | 8 | 22 |  |  |  | 0.00233 |  |  |
| rand\_forest\_res\_1\_09 | 4 | 39 |  |  |  | 0.056822636 |  |  |
| nnet\_res\_1\_05 |  |  |  |  |  | 0.0157 | 6 | 961 |
| nnet\_res\_1\_07 |  |  |  |  |  | 4.975 | 1 | 70 |

Plot of Stacking model showing the contributions of each model for Valganciclovir.

Une image contenant texte, capture d’écran, Tracé, diagramme

Description générée automatiquement

Mlp: neural networks algorithm, boost\_tree: Xgboost algorithm, rand\_forest: Random Forest Algorithm

The penalty value associated with the smallest RMSE was 0.01.

The neural network and boosted tree models have the largest contributions to the ensemble.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| member | mtry | Min\_n | Tree\_depth | learn\_rate | sample\_size | coef | **hidden\_units** | **epochs** |
| tune\_xgb\_1\_04 | 5 | 10 | 4 | 0.04263 | 0.11053 | 0.1060 |  |  |
| tune\_xgb\_1\_05 | 6 | 2 | 10 | 0.06982 | 0.54676 | 0.0190 |  |  |
| tune\_xgb\_1\_10 | 6 | 39 | 2 | 0.00506 | 0.57713 | 0.0581 |  |  |
| rand\_forest\_res\_1\_07 | 4 | 22 |  |  |  | 0.19403 |  |  |
| nnet\_res\_1\_01 |  |  |  |  |  | 0.47555 | 3 | 23 |
| nnet\_res\_1\_04 |  |  |  |  |  | 0.01240 | 2 | 168 |
| nnet\_res\_1\_05 |  |  |  |  |  | 0.22842 | 7 | 346 |
| nnet\_res\_1\_06 |  |  |  |  |  | 0.80694 | 4 | 598 |
| nnet\_res\_1\_09 |  |  |  |  |  | 4.80588 | 3 | 227 |