- **Supplementary Materials**

# Prediction of South American Leaf Blight and Disease-Induced Photosynthetic Changes in Rubber Tree, Using Machine Learning Techniques on Leaf Hyperspectral Reflectance

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## Supplementary Tables

**Table S1.** Models features and parameter tuning for five machine learning algorithms

| Algorithm | Train model[a] | Tuning parameters | Predicted variable | Model' final hyperparameters |
|---|---|---|---|---|
| RF | rf | (i) 10-fold CV 5 times; (ii) number of randomly selected predictors (mtry) = seq(2, 20, by =2); (iii) number of trees =1000; (iv) tuneLength = 10; (v) importance = TRUE | Severity class | mtry = 8 |
| | | | *A* | mtry = 20 |
| | | | *E* | mtry = 20 |
| | | | *gs* | mtry = 10 |
| | | | *WUEe* | mtry = 10 |
| | | | *Fv/Fm* | mtry = 4 |
| | | | *Fv'/Fm'* | mtry = 2 |
| | | | NPQ | mtry = 18 |
| | | | ETR | mtry = 20 |
| | | | *qP* | mtry = 10 |
| BRT | gbm | (i) 10-fold CV 5 times; (ii) max tree depth (1, 3, 5 and 7); (iii) number of trees (100 to 1000, by 50); (iv) minimal terminal node size (10); shrinkage (0.01 and 0.1) | Severity class | number of trees = 100; shrinkage = 0.1; max tree depth = 1 |
| | | | *A* | number of trees = 1000; shrinkage = 0.1; max tree depth = 5 |
| | | | *E* | number of trees = 850; shrinkage = 0.1; max tree depth = 1 |
| | | | *gs* | number of trees = 450; shrinkage = 0.1; max tree depth = 7 |
| | | | *WUEe* | number of trees = 950; shrinkage = 0.1; max tree depth = 7 |
| | | | *Fv/Fm* | number of trees = 1000; shrinkage = 0.01; max tree depth = 1 |
| | | | *Fv'/Fm'* | number of trees = 300; shrinkage = 0.1; max tree depth = 5 |
| | | | NPQ | number of trees = 1000; shrinkage = 0.1; max tree depth = 1 |

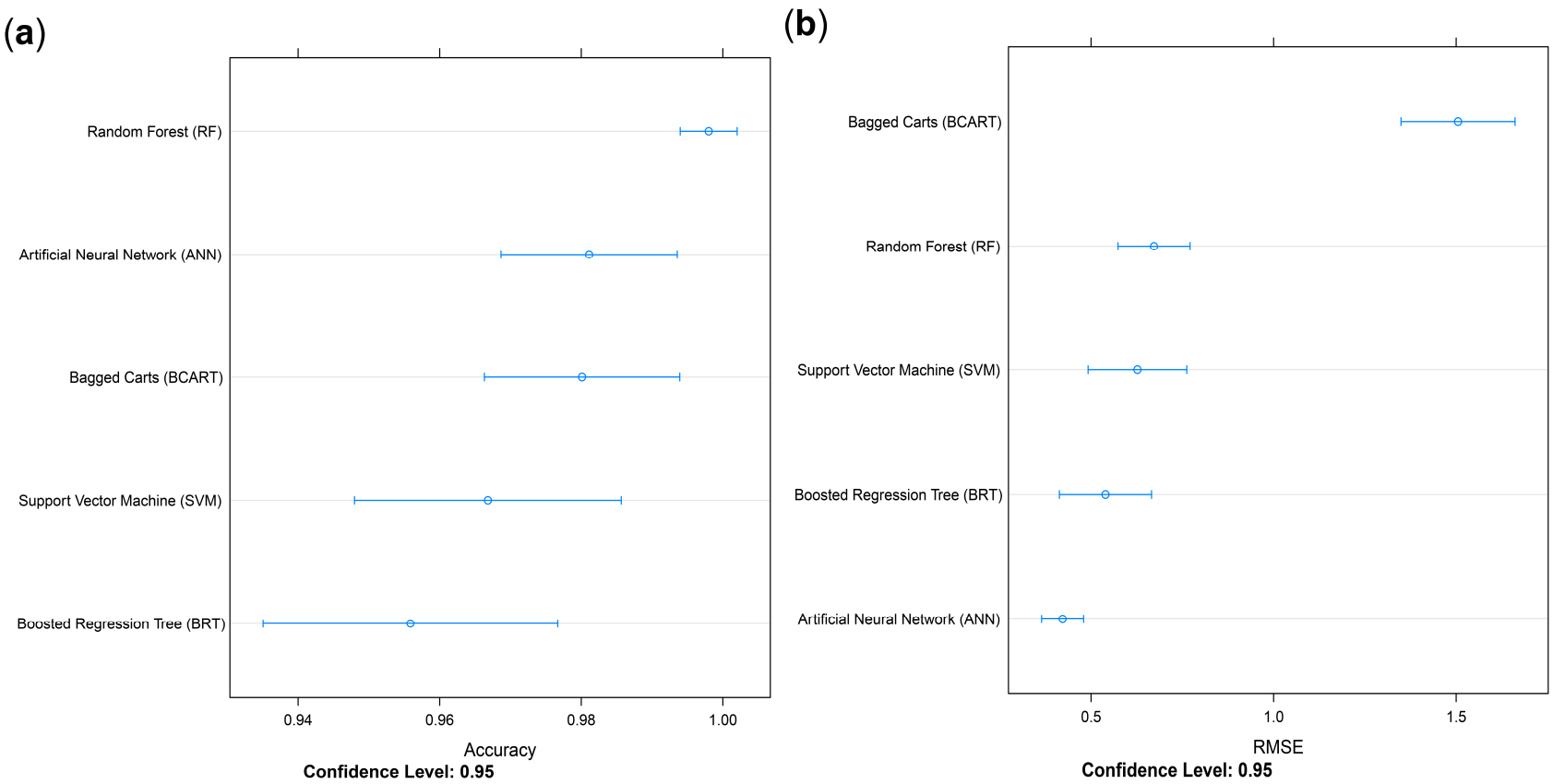
| | | | | |
|---|---|---|---|---|
| | | | ETR | number of trees = 950; shrinkage = 0.1; max tree depth = 7 |
| | | | *qP* | number of trees = 700; shrinkage = 0.01; max tree depth = 7 |
| BCART | treebag | (i) 10-fold CV 5 times; (ii) No other tuning parameters for this model | Severity class | - |
| | | | *A* | - |
| | | | *E* | - |
| | | | *gs* | - |
| | | | *WUEe* | - |
| | | | *Fv/Fm* | - |
| | | | *Fv′/Fm′* | - |
| | | | NPQ | - |
| | | | ETR | - |
| | | | *qP* | - |
| ANN | nnet | (i) 10-fold CV 5 times; (ii) size (1 to 9, by 2); (iii) decay (0.001, 0.01 and 0.1); (iv) preprocessing (center and scale); (v) maxit (1000); (vi) linout = TRUE; (vii) trace = FALSE | Severity class | size = 5; decay = 0.001 |
| | | | *A* | size = 3; decay = 0.01 |
| | | | *E* | size = 9; decay = 0.1 |
| | | | *gs* | size = 7; decay = 0.01 |
| | | | *WUEe* | size = 3; decay = 0.1 |
| | | | *Fv/Fm* | size = 7; decay = 0.001 |
| | | | *Fv′/Fm′* | size = 7; decay = 0.01 |
| | | | NPQ | size = 3; decay = 0.001 |
| | | | ETR | size = 1; decay = 0.1 |
| | | | *qP* | size = 3; decay = 0.1 |
| SVM | svmRadial | (i) 10-fold CV 5 times; (ii) sigma by default (i.e., sigma was held constant at a value of 0.1792956); (iii) cost (C) (2 to 500, by 2); (iv) tuneLength (15); (v) preprocessing (center and scale) | Severity class | C = 8 |
| | | | *A* | C = 32 |
| | | | *E* | C = 2 |
| | | | *gs* | C = 4 |
| | | | *WUEe* | C = 32 |
| | | | *Fv/Fm* | C = 2 |
| | | | *Fv′/Fm′* | C = 2 |
| | | | NPQ | C = 4 |
| | | | ETR | C = 256 |
| | | | *qP* | C = 4 |

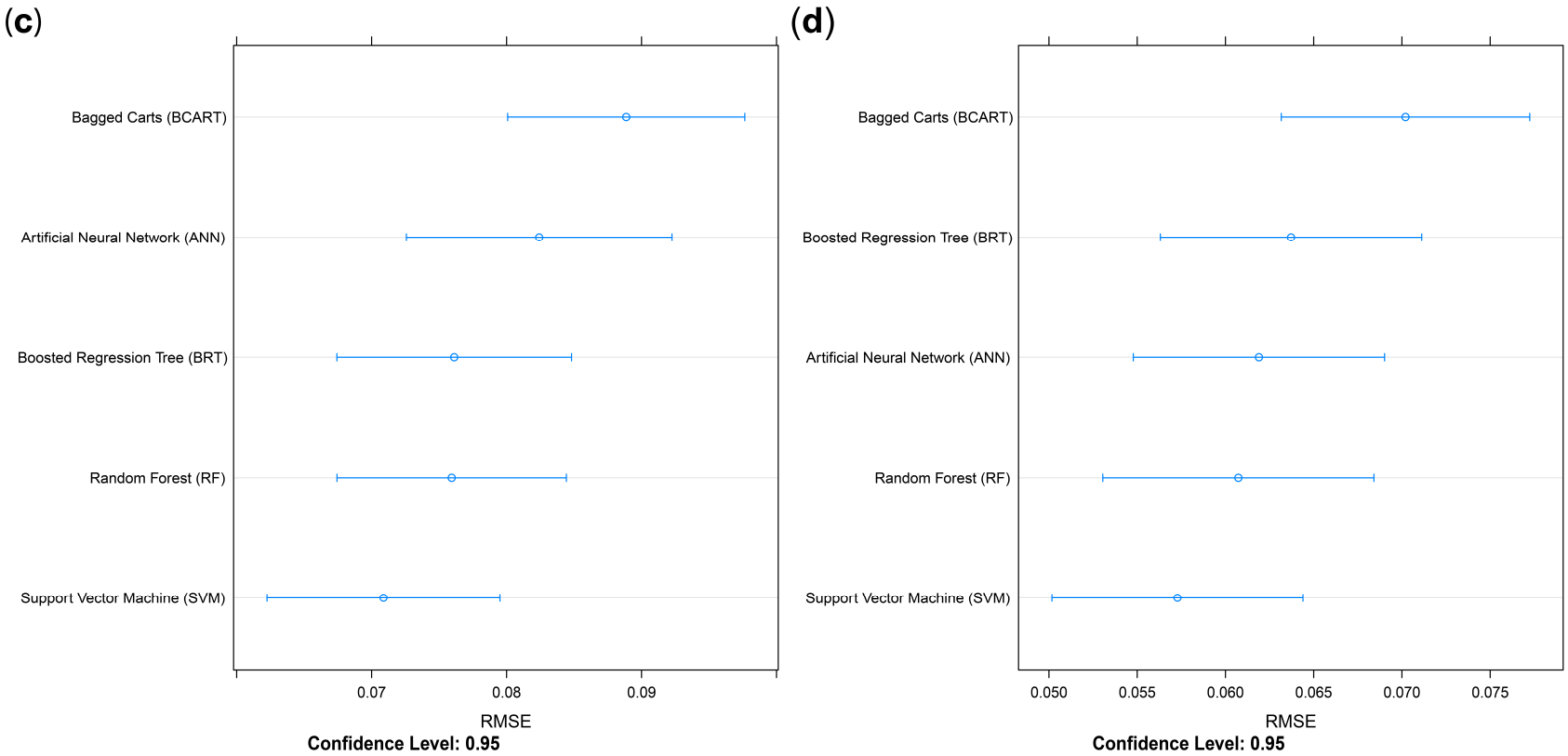
[a]Train model from R Package caret

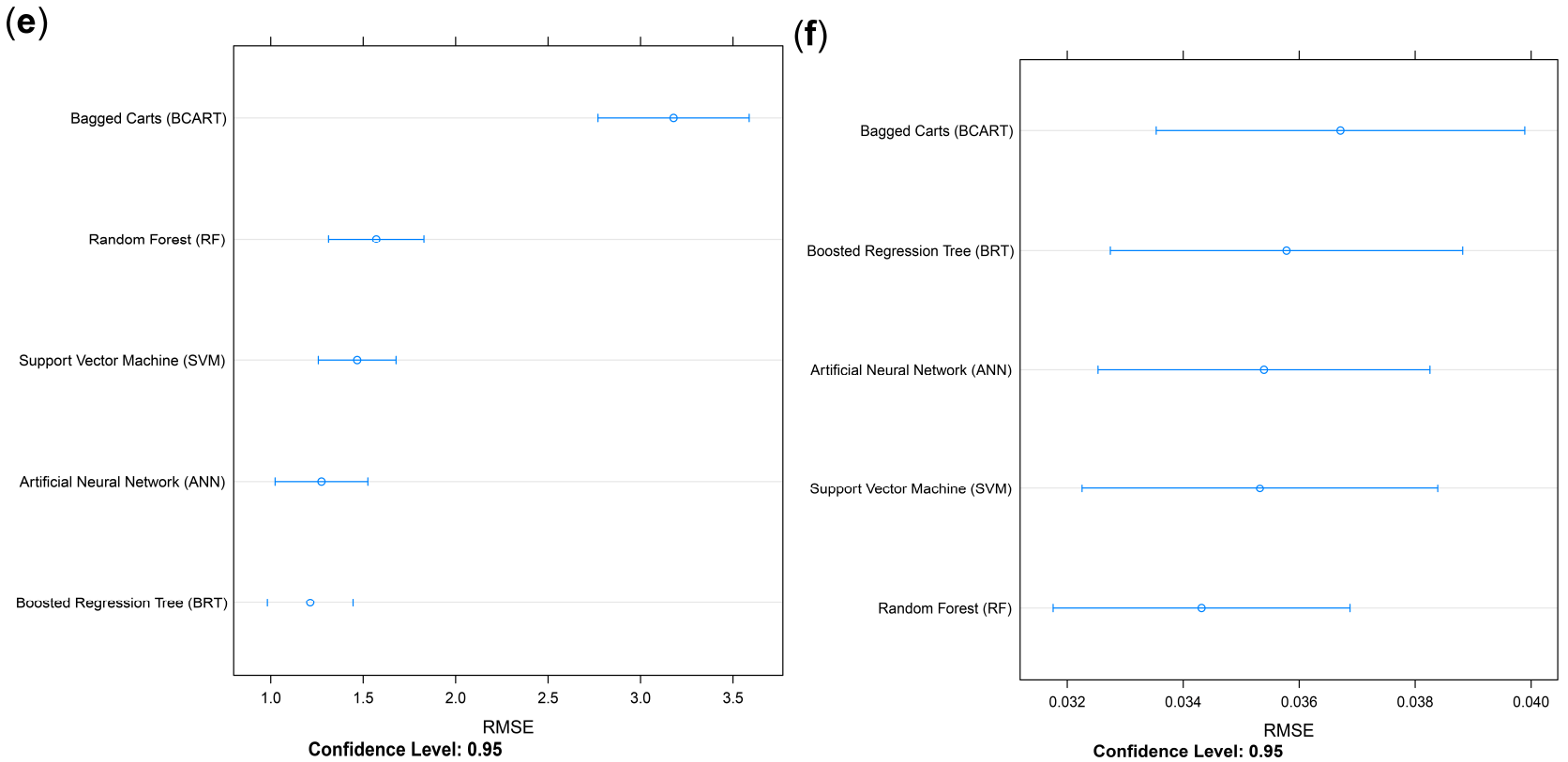
- No appply

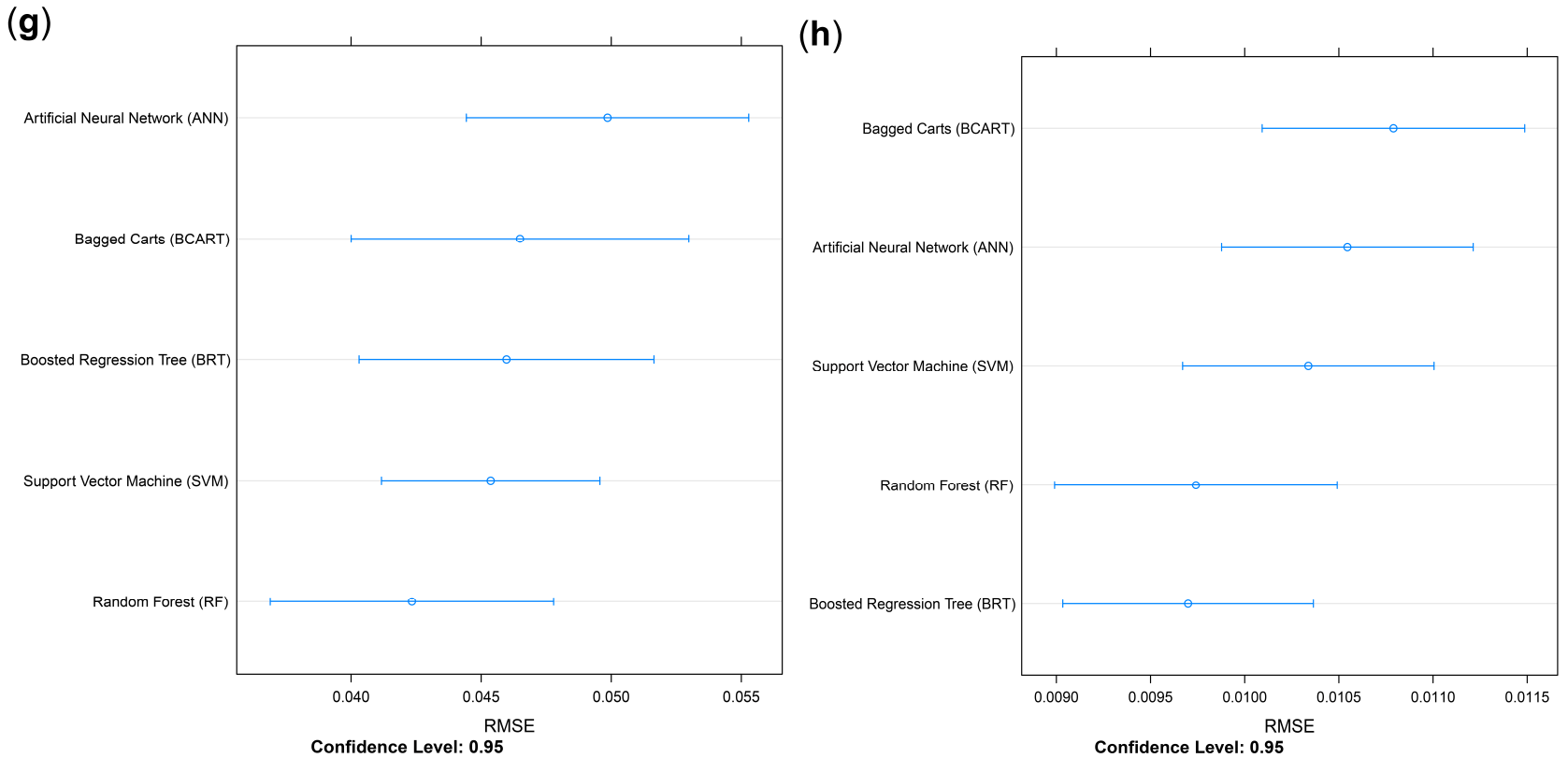
Random Forest (RF), Boosted Regression Tree (BRT), Bagged Classification and Regression Tree (BCART), Artificial Neural Network (ANN), Support Vector Machine (SVM), Net $CO_2$ assimilation rate (*A*) (μmol $CO_2$ $m^{-2}$ $s^{-1}$), transpiration rate (*E*) (mmol $H_2O$ $m^{-2}$ $s^{-1}$), stomatal conductance to water vapor ($g_s$) (mol $H_2O$ $m^{-2}$ $s^{-1}$), water use efficiency extrinsic ($WUE_e$) (μmol $CO_2$ mmol $H_2O^{-1}$), maximum quantum yield of photosystem II (PSII) ($F_v/F_m$), efficiency of excitation energy capture by open PSII reaction centers ($F_v'/F_m'$), non-photochemical quenching coefficient (NPQ), electron transport rate (ETR), and photochemical quenching coefficient (*qP*).

## Supplementary Figures




(c)
Bagged Carts (BCART)
Artificial Neural Network (ANN)
Boosted Regression Tree (BRT)
Random Forest (RF)
Support Vector Machine (SVM)
0.07
0.08
0.09
RMSE
Confidence Level: 0.95
(d)
Bagged Carts (BCART)
Boosted Regression Tree (BRT)
Artificial Neural Network (ANN)
Random Forest (RF)
Support Vector Machine (SVM)
0.050
0.055
0.060
0.065
0.070
0.075
RMSE
Confidence Level: 0.95


(e)
Bagged Carts (BCART)
Random Forest (RF)
Support Vector Machine (SVM)
Artificial Neural Network (ANN)
Boosted Regression Tree (BRT)
1.0
1.5
2.0
2.5
3.0
3.5
RMSE
Confidence Level: 0.95
(f)
Bagged Carts (BCART)
Boosted Regression Tree (BRT)
Artificial Neural Network (ANN)
Support Vector Machine (SVM)
Random Forest (RF)
0.032
0.034
0.036
0.038
0.040
RMSE
Confidence Level: 0.95


(g)
Artificial Neural Network (ANN)
Bagged Carts (BCART)
Boosted Regression Tree (BRT)
Support Vector Machine (SVM)
Random Forest (RF)
0.040
0.045
0.050
0.055
RMSE
Confidence Level: 0.95
(h)
Bagged Carts (BCART)
Artificial Neural Network (ANN)
Support Vector Machine (SVM)
Random Forest (RF)
Boosted Regression Tree (BRT)
0.0090
0.0095
0.0100
0.0105
0.0110
0.0115
RMSE
Confidence Level: 0.95

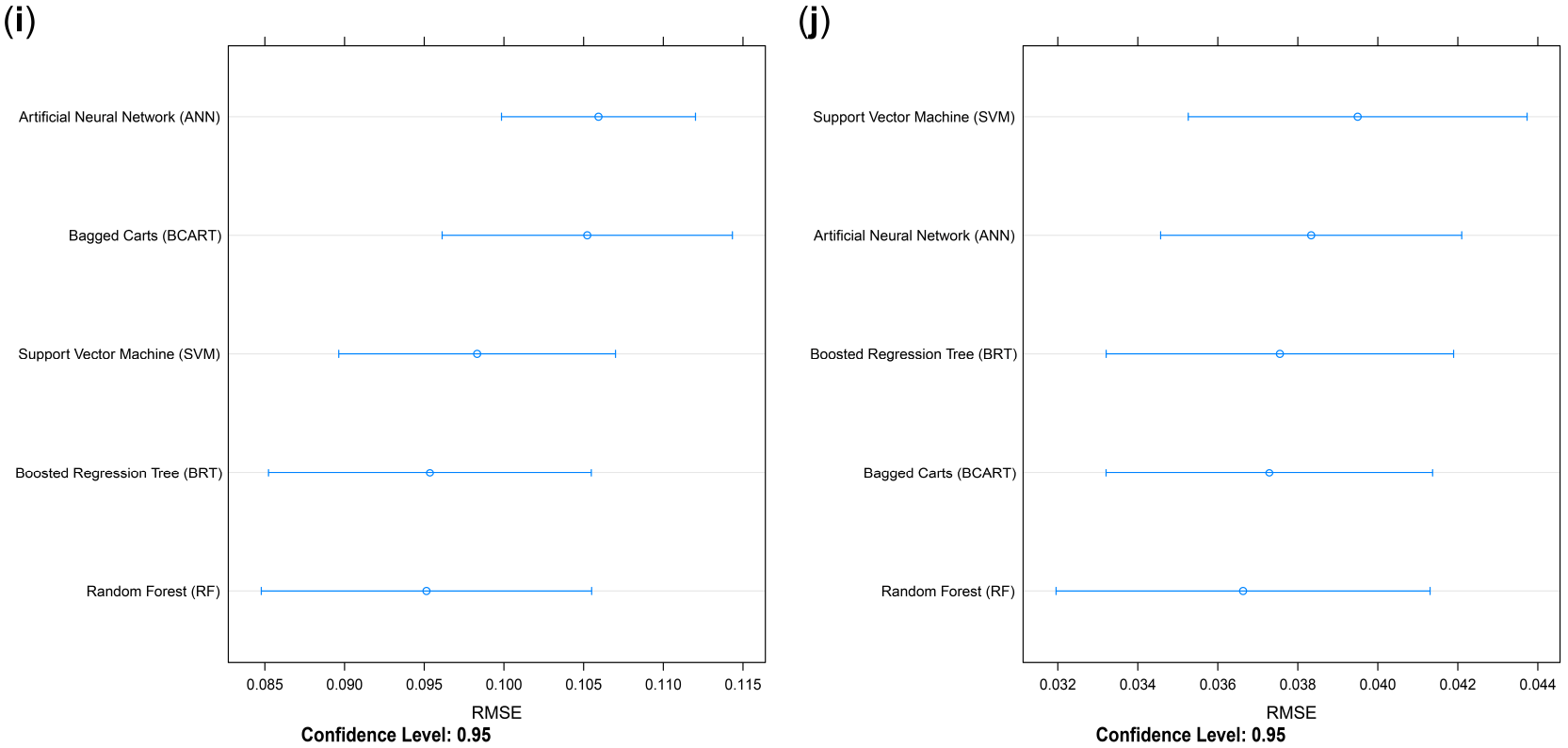
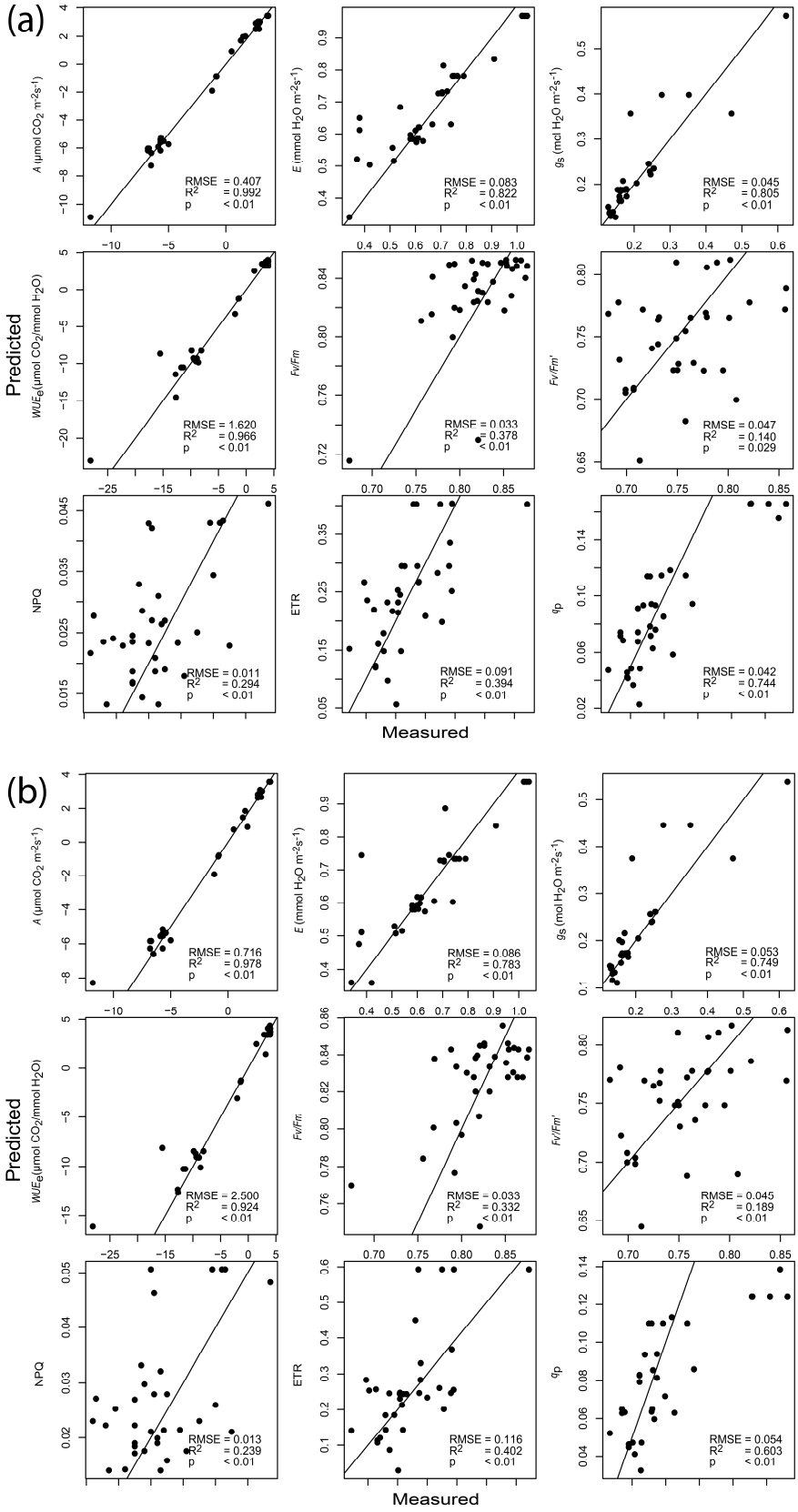
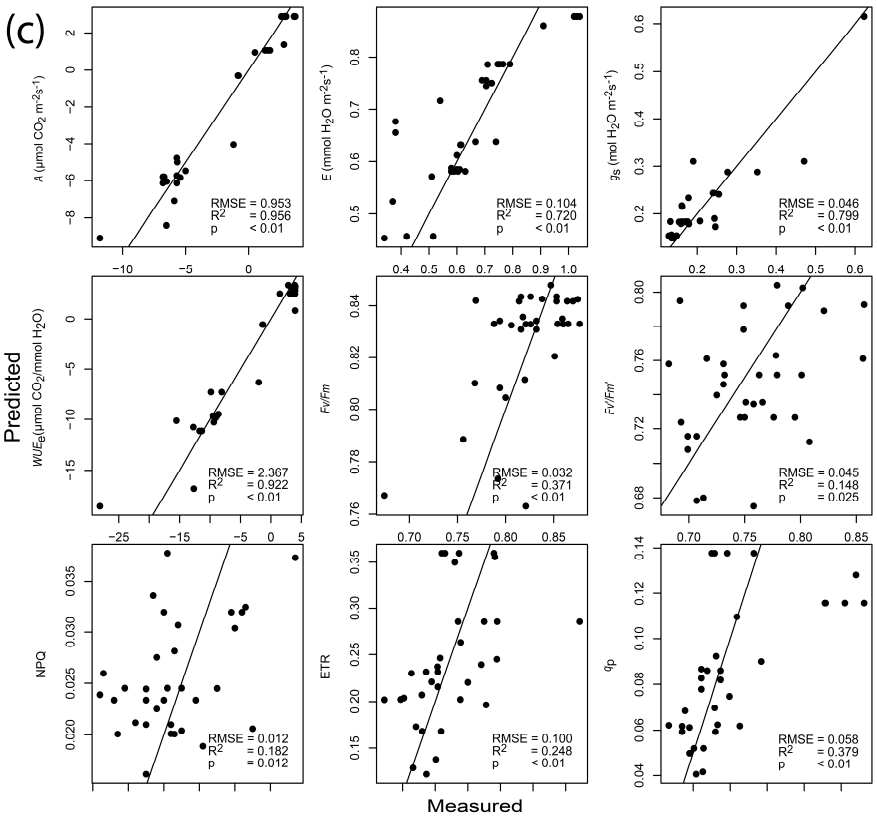
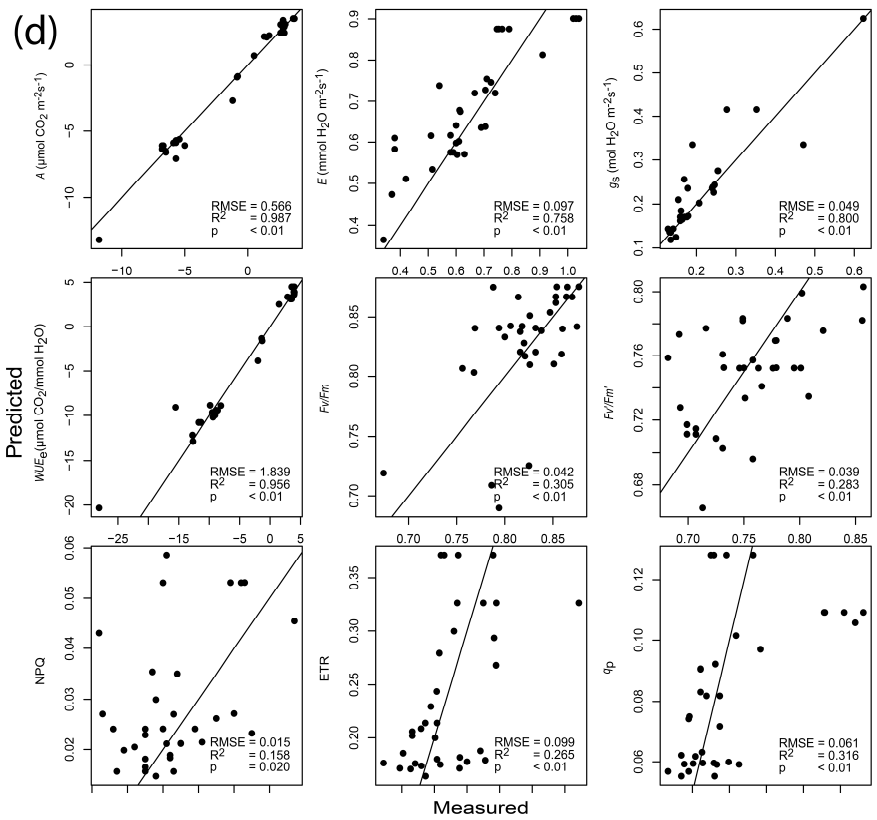



**Figure S1**. Dot plots for the Accuracy (classification) and RMSE (numerical prediction) metrics using the 10-fold cross-validation repeated 5 times method for five machine learning models. Each line represents the mean and 95% confidence interval. (**a**) Severity class, (**b**) net $CO_2$ assimilation rate ($A$) (μmol $CO_2$ $m^{-2}$ $s^{-1}$), (**c**) transpiration rate ($E$) (mmol $H_2O$ $m^{-2}$ $s^{-1}$), (**d**) stomatal conductance to water vapor ($g_s$) (mol $H_2O$ $m^{-2}$ $s^{-1}$), (**e**) water use efficiency extrinsic ($WUE_e$), (**f**) maximum quantum yield of photosystem II (PSII) ($F_v/F_m$), (**g**) efficiency of excitation energy capture by open PSII reaction centers ($F_v'/F_m'$), (**h**) non-photochemical quenching coefficient (NPQ), (**i**) electron transport rate (ETR), and (**j**) photochemical quenching coefficient ($qP$)


(a)
A (μmol CO2 m-2s-1)
RMSE = 0.407
R2 = 0.992
p < 0.01
E (mmol H2O m-2s-1)
RMSE = 0.083
R2 = 0.822
p < 0.01
gs (mol H2O m-2s-1)
RMSE = 0.045
R2 = 0.805
p < 0.01
WUEe (μmol CO2/mmol H2O)
RMSE = 1.620
R2 = 0.966
p < 0.01
Fv/Fm
RMSE = 0.033
R2 = 0.378
p < 0.01
Fv'/Fm'
RMSE = 0.047
R2 = 0.140
p = 0.029
NPQ
RMSE = 0.011
R2 = 0.294
p < 0.01
ETR
RMSE = 0.091
R2 = 0.394
p < 0.01
qp
RMSE = 0.042
R2 = 0.744
p < 0.01
Predicted
Measured
(b)
A (μmol CO2 m-2s-1)
RMSE = 0.716
R2 = 0.978
p < 0.01
E (mmol H2O m-2s-1)
RMSE = 0.086
R2 = 0.783
p < 0.01
gs (mol H2O m-2s-1)
RMSE = 0.053
R2 = 0.749
p < 0.01
WUEe (μmol CO2/mmol H2O)
RMSE = 2.500
R2 = 0.924
p < 0.01
Fv/Fm
RMSE = 0.033
R2 = 0.332
p < 0.01
Fv'/Fm'
RMSE = 0.045
R2 = 0.189
p < 0.01
NPQ
RMSE = 0.013
R2 = 0.239
p < 0.01
ETR
RMSE = 0.116
R2 = 0.402
p < 0.01
qp
RMSE = 0.054
R2 = 0.603
p < 0.01
Predicted
Measured


(c)
A (μmol CO2 m-2s-1)
RMSE = 0.953
R2 = 0.956
p < 0.01
E (mmol H2O m-2s-1)
RMSE = 0.104
R2 = 0.720
p < 0.01
gs (mol H2O m-2s-1)
RMSE = 0.046
R2 = 0.799
p < 0.01
WUEB(μmol CO2/mmol H2O)
RMSE = 2.367
R2 = 0.922
p < 0.01
Fv/Fm
RMSE = 0.032
R2 = 0.371
p < 0.01
Fv'/Fm'
RMSE = 0.045
R2 = 0.148
p = 0.025
NPQ
RMSE = 0.012
R2 = 0.182
p = 0.012
ETR
RMSE = 0.100
R2 = 0.248
p < 0.01
qp
RMSE = 0.058
R2 = 0.379
p < 0.01
Predicted
Measured


(d)
A (μmol CO2 m-2s-1)
RMSE = 0.566
R2 = 0.987
p < 0.01
E (mmol H2O m-2s-1)
RMSE = 0.097
R2 = 0.758
p < 0.01
gs (mol H2O m-2s-1)
RMSE = 0.049
R2 = 0.800
p < 0.01
WUEB(μmol CO2/mmol H2O)
RMSE = 1.839
R2 = 0.956
p < 0.01
Fv/Fm
RMSE = 0.042
R2 = 0.305
p < 0.01
Fv'/Fm'
RMSE = 0.039
R2 = 0.283
p < 0.01
NPQ
RMSE = 0.015
R2 = 0.158
p = 0.020
ETR
RMSE = 0.099
R2 = 0.265
p < 0.01
qp
RMSE = 0.061
R2 = 0.316
p < 0.01
Predicted
Measured

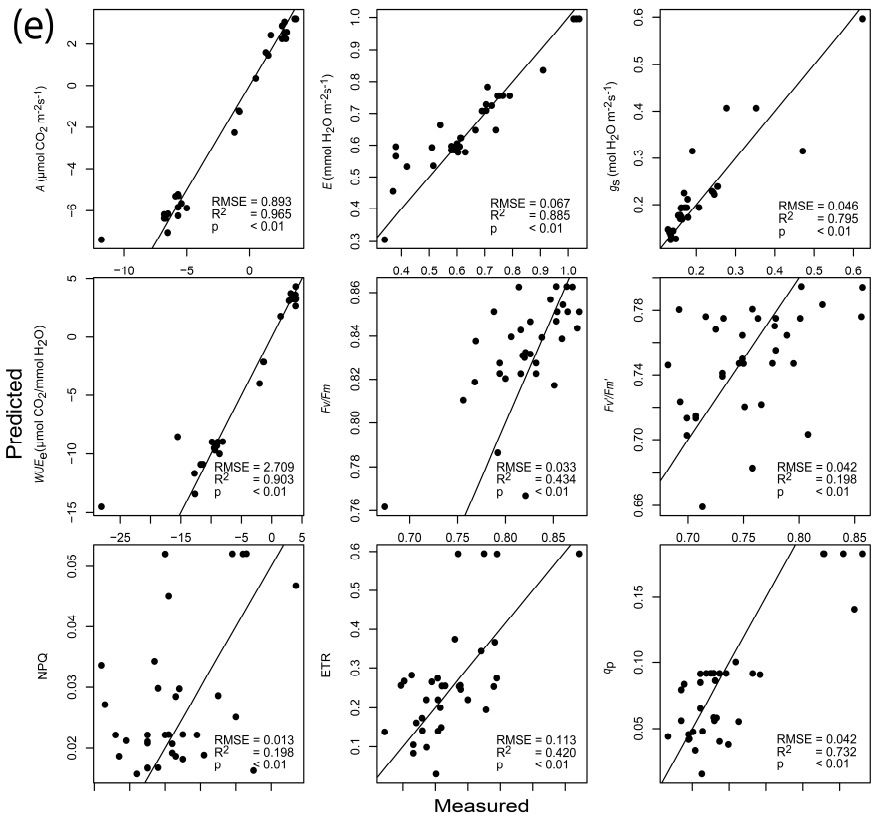



**Figure S2**. Predicted vs. measured values plots of the testing datasets results for five machine learning models used to predict nine photosynthetic traits: net $CO_2$ assimilation rate ($A$) (μmol $CO_2$ $m^{-2}$ $s^{-1}$), transpiration rate ($E$) (mmol $H_2O$ $m^{-2}$ $s^{-1}$), stomatal conductance to water vapor ($g_s$) (mol $H_2O$ $m^{-2}$ $s^{-1}$), water use efficiency extrinsic ($WUE_e$) (μmol $CO_2$ mmol $H_2O^{-1}$), maximum quantum yield of photosystem II (PSII) ($F_v/F_m$), efficiency of excitation energy capture by open PSII reaction centers ($F_v'/F_m'$), non-photochemical quenching coefficient (NPQ), electron transport rate (ETR), and photochemical quenching coefficient ($qP$). (**a**) Random Forest (RF), (**b**) Boosted Regression Tree (BRT), (**c**) Bagged Classification and Regression Tree (BCART), (**d**) Artificial Neural Network (ANN), and (**e**) Support Vector Machine (SVM)