

Table S1. Complete AGB model evaluations including tuned hyperparameters.

Train/eval structure	Feature set	Algorithm	Parameters	Parameter values	Train R ²	Train RMSE	Test R ²	Test RMSE
nested CV: outer random 10-fold, inner random 5-fold	Spectral bands + indices	SVR	C, gamma	1931, 0.07	0.87	465	0.72	679
		RF	max_depth, min_samples_leaf, min_samples_split, n_estimators	90, 1, 2, 100	1.00	73	0.71	683
		PCA	n_components	13	0.68	717	0.63	769
		PLSR	n_components	11	0.68	716	0.64	760
		XGB	learning_rate, max_depth, min_child_weight, n_estimators	0.05, 3, 10, 800	1.00	58	0.69	704
		LASSO	mean alpha	2.3	0.68	715	0.65	759
nested CV: outer LOGO by plot, inner 5-fold group by plot	Spectral bands + indices	SVR	C, gamma	10000, 0.07	0.90	405	0.73	656
		RF	max_depth, min_samples_leaf, min_samples_split, n_estimators	30, 1, 2, 400	1.00	56	0.69	710
		PCA	n_components	13	0.68	718	0.63	776
		PLSR	n_components	9	0.68	717	0.63	774
		XGB	learning_rate, max_depth, min_child_weight, n_estimators	0.2, 3, 1, 100	0.99	92	0.66	746
		LASSO	mean alpha	2.6	0.68	718	0.64	769
nested CV: outer LOGO by date, inner 5-fold group by date	Spectral bands + indices	SVR	C, gamma	10000, 0.003	0.68	723	0.45	941
		RF	max_depth, min_samples_leaf, min_samples_split, n_estimators	90, 2, 5, 100	0.99	109	0.48	916
		PCA	n_components	13	0.67	727	0.60	800
		PLSR	n_components	8	0.68	724	0.59	811
		XGB	learning_rate, max_depth, min_child_weight, n_estimators	0.05, 3, 1, 100	0.98	188	0.49	914
		LASSO	mean alpha	2.4	0.68	716	0.58	825

holdout set: Train BRU 3-fold CV by plot, Test NFREC	Spectral bands	SVR	C, gamma	1931, 0.07	0.75	680	0.25	937
		RF	max_depth, min_samples_leaf, min_samples_split, n_estimators	30, 1, 2, 200	1.00	0	0.05	1050
		PCA	n_components	7	0.63	820	0.28	915
		PLSR	n_components	6	0.65	799	0.31	900
		XGB	learning_rate, max_depth, min_child_weight, n_estimators	0.05, 3, 10, 100	0.89	449	0.02	1069
		LASSO	mean alpha	1.5	0.66	791	0.27	923

Table S2. Complete %N model evaluations including tuned hyperparameters.

Train/eval structure	Feature set	Algorithm	Parameters	Parameter values	Train R ²	Train RMSE	Test R ²	Test RMSE
nested CV: NFREC only - outer random 5-fold, inner random 3-fold	Spectral bands + indices	SVR	C, gamma	14, 0.014	0.80	0.25	0.65	0.34
		RF	max_depth, min_samples_leaf, min_samples_split, n_estimators	30, 1, 2, 100	0.99	0.05	0.57	0.37
		PCA	n_components	10	0.74	0.29	0.66	0.33
		PLSR	n_components	12	0.75	0.29	0.64	0.34
		XGB	learning_rate, max_depth, min_child_weight, n_estimators	0.05, 6, 10, 100	0.97	0.1	0.50	0.40
		LASSO	mean alpha	0.001	0.75	0.29	0.65	0.34
		SVR	C, gamma	72, 0.014	0.82	0.24	0.70	0.31

nested CV: NFREC only - outer LOGO by plot, inner 3- fold group by plot	Spectral bands + indices	RF	max_depth, min_samples_leaf, min_samples_split, n_estimators	30, 1, 2, 200	1.00	0.04	0.55	0.38
		PCA	n_components	11	0.74	0.29	0.65	0.34
		PLSR	n_components	9	0.75	0.29	0.66	0.33
		XGB	learning_rate, max_depth, min_child_weight, n_estimators	0.05, 6, 1, 800	1.00	0.01	0.52	0.40
		LASSO	mean alpha	0.0005	0.75	0.29	0.66	0.33
nested CV: NFREC only - outer LOGO by date, inner 3-fold group by date	Spectral bands	SVR	C, gamma	10000, 0.0001	0.72	0.30	0.55	0.38
		RF	max_depth, min_samples_leaf, min_samples_split, n_estimators	70, 1, 2, 100	0.99	0.05	0.20	0.51
		PCA	n_components	8	0.69	0.31	0.53	0.39
		PLSR	n_components	7	0.72	0.30	0.55	0.38
		XGB	learning_rate, max_depth, min_child_weight, n_estimators	0.05, 3, 1, 400	0.97	0.10	0.25	0.49
		LASSO	mean alpha	0.001	0.72	0.30	0.60	0.36
nested CV: NFREC only - outer LOGO by year, inner 3- fold group by plot	Spectral bands	SVR	C, gamma	373, 0.003	0.78	0.27	0.27	0.49
		RF	max_depth, min_samples_leaf, min_samples_split, n_estimators	30, 1, 2, 200	0.99	0.04	-0.41	0.68
		PCA	n_components	6	0.75	0.29	0.28	0.48

		PLSR	n_components	5	0.74	0.29	0.21	0.51
		XGB	learning_rate, max_depth, min_child_weight, n_estimators	0.05, 3, 1, 100	0.95	0.13	-0.41	0.68
		LASSO	mean alpha	0.0013	0.74	0.29	0.36	0.46

Table S3. Parameter ranges for all algorithms

Algorithm	Parameters	Ranges
SVR	C	0.1, 0.51794747, 2.6826958, 13.89495494, 71.9685673, 372.75937203, 1930.69772888, 10000
	gamma	0.0001, 0.00051795, 0.0026827, 0.01389495, 0.07196857, 0.37275937, 1.93069773, 10
RF	max_depth	30, 70, 90
	min_samples_leaf	1, 2
	min_samples_split	2, 5
	n_estimators	100, 200, 400, 800
PCA	n_components	Length of features (10 or 20 if indices included)
PLSR	n_components	Length of features (10 or 20 if indices included)
XGB	learning_rate	0.05, 0.1, 0.2
	max_depth	3, 6, 9
	min_child_weight	1, 10, 100
	n_estimators	100, 400, 800
LASSO	alpha	100-n sequence determined by LassoCV function in scikit-learn library