Supplementary

Supplementary Figures



Supplementary Figure 1. Spatial distribution of simulated species richness, predicted species richness by random forest and boosted regression model (with 64,620 samples), and the associated prediction errors (residuals), showing spatial random error distributions (little or no spatial bias).



Supplementary Figure 2. Retrieved PDP and ALE curves (with the existence of V1 and V2) and the original functional relationship in the simulation dataset using one single 5,500 bootstrap of the dataset.



Supplementary Figure 3. Retrieved PDP and ALE curves (V1 and V2 omitted) and the original functional relationship in the simulation dataset for one single bootstrap with 5,500 samples.

Supplementary Table 1. Summary of packages and functions of interpretation methods for machine learning models in R.

Interpretation method	R Package	Function	Machine learning model	Measure confidence level
Variable importance	randomForest	varImpPlot	Random forest	
	rfPermute	rp.importance	Random forest	p value
	vita	compVarImp	Random forest	
	party	varimp	Random forest and bagging ensemble	conditional=True
	ranger	importance_pvalues	Random forest	p value

	interpretR	variableImportance	Random forest	
	caret	varImp	Any ML model	
	pdp	vip	Any ML model	
	iml	FeatureImp	Any ML model	Importance 0.95
Partial dependence plot	randomForest	partialPlot	Random forest	
	Mvtboost	Plot	Tree Boosting	
	gbm	plot.gbm	Generalized Boosted Regression Models	
	interpretR	parDepPlot	Random forest	Predictions at quantiles
	pdp	partial, plotPartial	Any ML model	
	DALEX	<pre>single_variable (type="pdp"); variable_response(type="pdp")</pre>	Any ML model	
	iml	FeatureEffect (method="pdp")	Any ML model	
	h2o	partialPlot	Any ML model	Standard error
Accumulated Local Effects	DALEX	Single_variable (type="ale"); variable_response (type="ale")	Any ML model	
	iml	FeatureEffect (method="ale")	Any ML model	
	ALEPlot	ALEPlot	Any ML model	
3-D loess plane	car	scatter3d	Any ML model	