SUPPORTING INFORMATION

Water Quality Inversion of a Typical Rural Small River in South-eastern China Based on UAV Multispectral Imagery: A Comparison of Multiple Machine Learning Algorithms

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Figure legends

Table contents

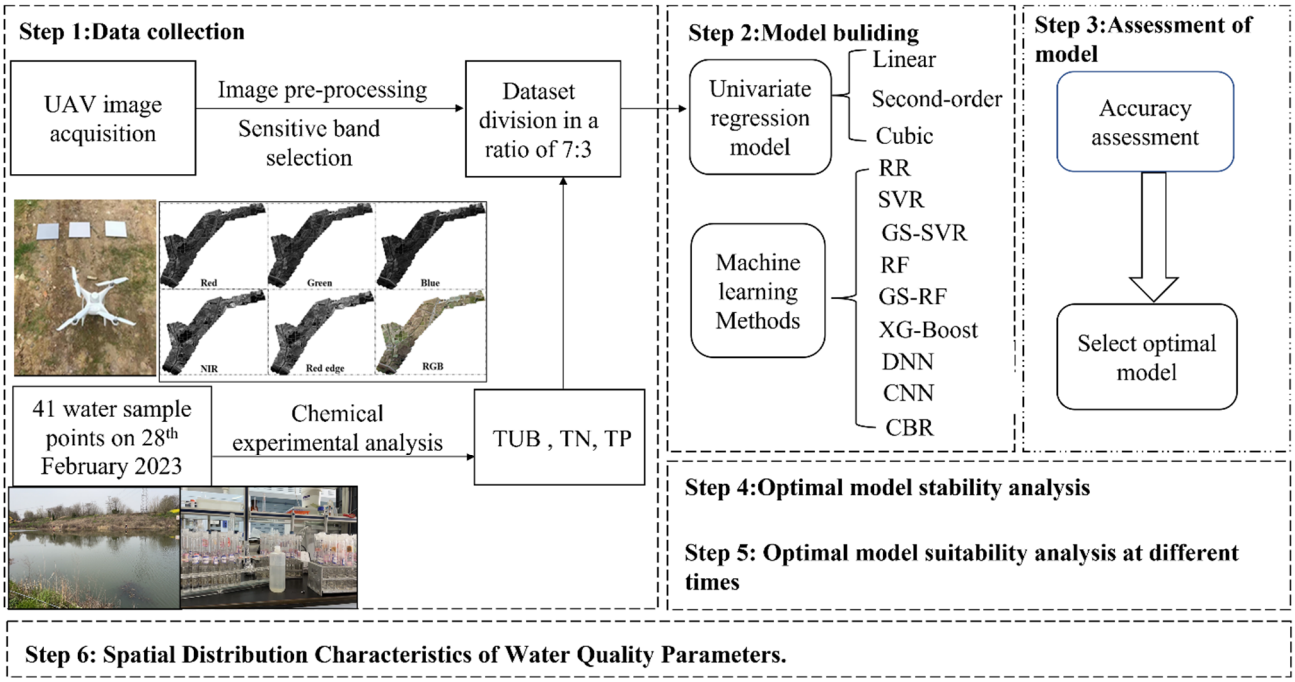

Figure S1. Research schematic diagram of this study.

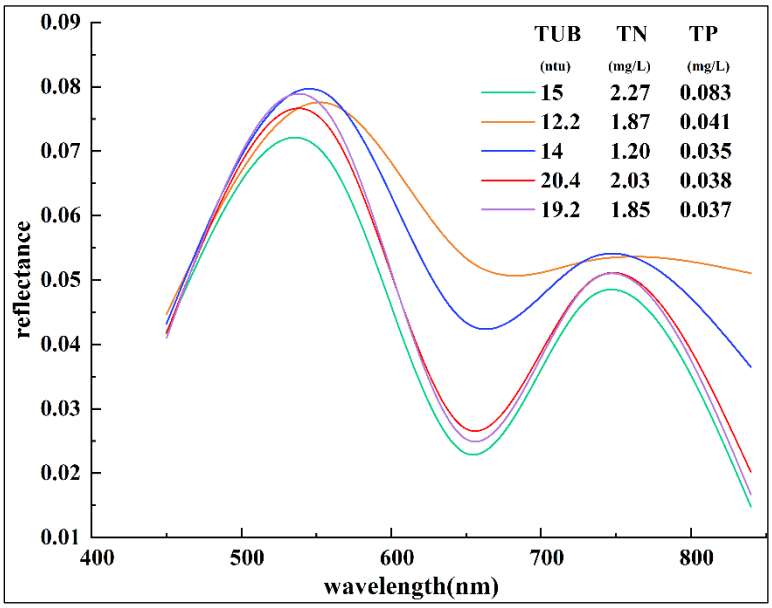

Figure S2. Spectral curves of water sampling.

Table S1. Calculation of the selected band combinations.

Index	Formula	Index	Formula	Index	Formula	Index	Formula
V1	B1	V13	B3+B4	V25	B4-B5	V37	B3/B5
V2	B2	V14	B3+B5	V26	B1/B2	V38	B4/B5
V3	B3	V15	B4+B5	V27	B1/B3	V39	(B1+B2)/(B1-B2)
V4	B4	V16	B1-B2	V28	B1/B4	V40	(B1+B3)/(B1-B3)
V5	B5	V17	B1-B3	V29	B1/B5	V41	(B1+B4)/(B1-B4)
V6	B1+B2	V18	B1-B4	V30	B2/B1	V42	(B1+B5)/(B1-B5)
V7	B1+B3	V19	B1-B5	V31	B2/B3	V43	(B2+B3)/(B2-B3)
V8	B1+B4	V20	B2-B3	V32	B2/B4	V44	(B2+B4)/(B2-B4)
V9	B1+B5	V21	B2-B4	V33	B2/B5	V45	(B2+B5)/(B2-B5)
V10	B2+B3	V22	B2-B5	V34	B3/B1	V46	(B3+B4)/(B3-B4)
V11	B2+B4	V23	B3-B4	V35	B3/B2	V47	(B3+B5)/(B3-B5)
V12	B2+B5	V24	B3-B5	V36	B3/B4	V48	(B4+B5)/(B4-B5)

Note: labels V1-V48 represent the number of each index.

Table S2. Hyperparameter settings for each model of the three water quality indicators.

Indicators	Models	Optimal Values of Hyperparameters
TUB	RR	*λ=3,* max iter =50
	SVR	C=100, gamma=0.2
	GS-SVR	grid search with C = {50, 100,500, 1000, 1500, 2000} gamma = {0.001, 0.01, 0.05, 0.1,0.2} obtained the optimal parameters as C = 50 and gamma=0.05.
	RF	estimators =500, max feature=4
	GS-RF	grid search with estimators = {100, 400, 800, 1200, 1600, 2000} max feature = {1, 2, 3, 4, 5} obtained the optimal parameters as estimators = 100 and max feature = 2.
	XGBoost	max depth=2, learning rate=0.05, estimators=100, gamma=0.3
	DNN	three hidden layers are set up, the number of neurons is 100, 168, and 80; learning rate=0.05
	CNN	two hidden layers are set, the number of convolution kernels is 36,12; the size of the convolutional kernel=3*3, the learning rate is 0.01, and the number of iterations is 200.
	CBR	interations=100, learning rate=0.1, depth= 4
TN	RR	λ=7, max iter =20
	SVR	C=100, gamma=0.02
	GS-SVR	grid search with C = {10,20,30,40,50,60,70} gamma = {0.001, 0.01, 0.05, 0.08,0.1} obtained the optimal parameters as estimator = 10 and gamma=0.08.
	RF	estimators =500, max feature=4
	GS-RF	grid search with estimators = {400, 800, 1200, 1600, 2000} max feature = {1, 2, 3, 4, 5} obtained the optimal parameters as estimator = 1600 and max feature = 3.
	XGBoost	max depth=3, learning rate=0.05, estimators=80, gamma=0.05
	DNN	three hidden layers are set up, the number of neurons is 100, 168, and 80; learning rate=0.05
	CNN	two hidden layers are set, the number of convolution kernels is 54,108; the size of the convolutional kernel is 3*3, the learning rate is 0.01, and the number of iterations is 100.
	CBR	interations=100, learning rate=0.1, depth=4
TP	RR	*λ=4,* max iter =10
	SVR	C=100, gamma=0.01
	GS-SVR	grid search with C = {50, 100,500, 1000, 1500, 2000} gamma = {0.001, 0.01, 0.05, 0.1} obtained the optimal parameters as estimator = 50 and gamma=0.01.
	RF	estimators =200, max feature=4
	GS-RF	grid search with estimators = {100, 400, 800, 1200, 1600, 2000} max feature = {1, 2, 3, 4, 5} obtained the optimal parameters as estimator =100 and max feature =4.
	XGBoost	max depth=3, learning rate=0.1, estimators=600, gamma=0.01
	DNN	three hidden layers are set up, the number of neurons is 100, 168, and 80; learning rate=0.01
	CNN	two hidden layers are set, the number of convolution kernels is 48, 108, the size of the convolutional kernel is 3*3, the learning rate is 0.01, and the number of iterations is 200.
	CBR	interations=100, learning rate=0.1, depth=3

Table S3. Single-variable regression results of water quality parameters.

Parameter	Index	Correlation coefficient	Method	Training set	Test Set			
				R^2	R^2	*RMSE*	*MAE*	*RPD*
TUB	V3	0.89	Linear	7.36×10^-1	0.69	3.16	2.28	1.79
			Second-order	0.74	0.78	2.69	1.93	2.11
			Cubic	0.74	0.79	2.59	1.83	2.19
TN	V3	-0.66	Linear	5.52×10^-1	0.17	0.31	0.24	1.10
			Second-order	5.52×10^-1	0.16	0.29	0.24	1.09
			Cubic	5.53×10^-1	0.14	0.29	0.24	1.08
TP	V10	0.42	Linear	0.44	-	0.053	0.04	-
			Second-order	0.51	-	0.23	0.10	-
			Cubic	0.52	0.36	0.02	0.02	1.25

Note: "-" represents the presence of negative values of the spectral index, and thus the second and cubic polynomial models of TP could not be fitted.