

Supplementary Materials

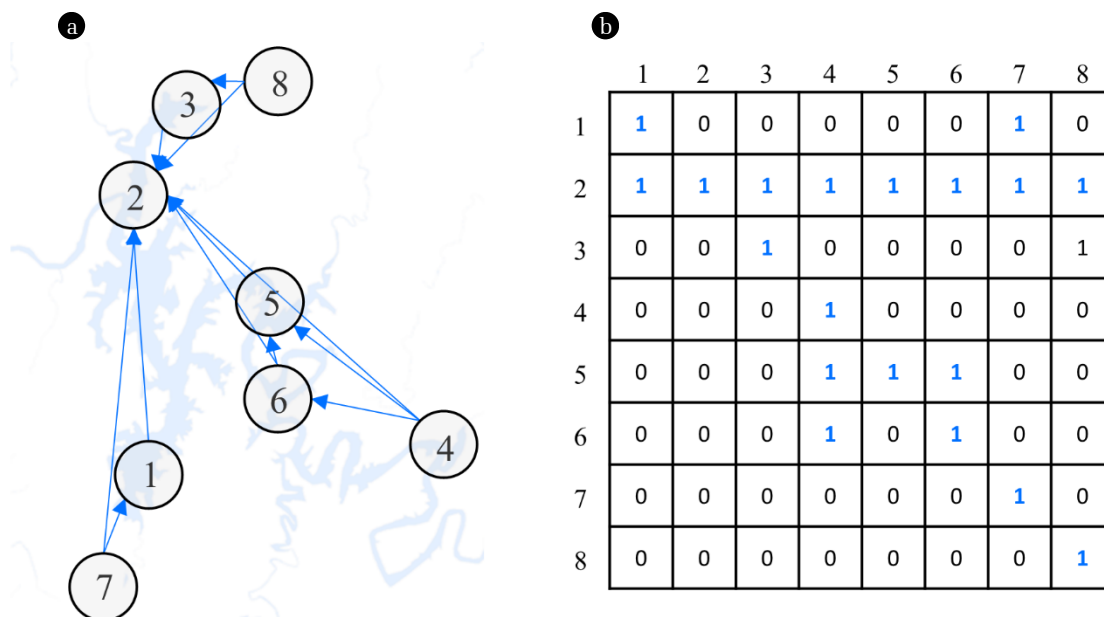


Fig. S1. A network graph of monitoring sites around Daecheong Reservoir was created (a), and an adjacency matrix was constructed based on the network graph (b). The black circles represent the monitoring sites, and the blue arrows indicate the influences between monitoring sites.

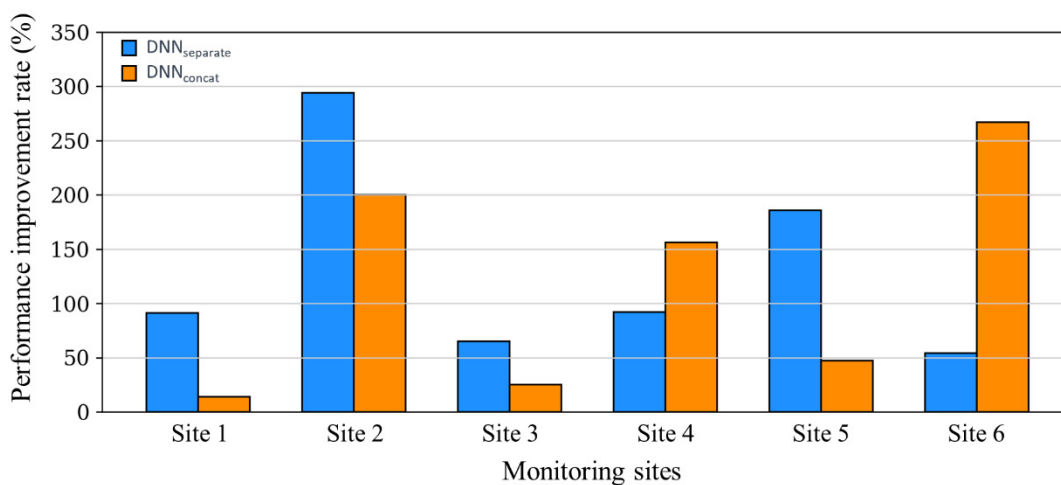


Fig. S2. Test performance improvement rates of GAT - DNN over the site-specific baseline models. The blue and orange bars are the improvements over DNN_{separate} and DNN_{concat}, respectively.

Table S1. Number and proportion of missing values for all input features

Category	Variable	Total data	Number of missing values	Percentage of missing values
Hydrological	Precipitation	1321	0	0
	Total discharge	1321	31	2
Meteorological	Water level	1321	31	2
Water quality	TOC	1321	528	40
	Water temperature	1321	528	40
	TN	1321	528	40
	TP	1321	528	40
	SS	1321	528	40
	Chlorophyll-a	1321	0	0

Table S2. Hyperparameter search space for GAT-DNN, DNN_{separate}, DNN_{concat}

Hyperparameter	GAT-DNN		DNN _{separate}		DNN _{concat}	
	Range	Interval	Range	Interval	Range	Interval
Learning_rate	$10^{-6} - 10^{-3}$	10^{-6}	$10^{-6} - 10^{-3}$	10^{-6}	$10^{-6} - 10^{-3}$	10^{-6}
Weight_decay	$10^{-5} - 10^{-4}$	10^{-5}	$10^{-5} - 10^{-4}$	10^{-5}	$10^{-5} - 10^{-4}$	10^{-5}
Batch_size	9, 18, 24, 36, 48, 60, 72		9, 18, 24, 36, 48, 60, 72		18, 24, 36, 48, 60, 72	
Epsilon	$10^{-6} - 10^{-4}$	10^{-6}	$10^{-6} - 10^{-4}$	10^{-6}	$10^{-6} - 10^{-4}$	10^{-6}
GAT_dropout	0 - 1	0.1	-	-	-	-
DNN_dropout	0 - 1	0.1	0 - 1	0.1	0 - 1	0.1
DNN_hidden units1	110 - 250	20	70 - 210	20	110 - 250	20
DNN_hidden units2	110 - 250	20	70 - 210	20	110 - 250	20

Table S3. Sets of optimal hyperparameters for forecasting the chlorophyll-a concentrations using GAT - DNN and the baseline models (DNN_{separate} and DNN_{concat})

Optimized hyperparameter	GAT-DNN	DNN _{concat}	DNN _{separate}					
	Site 1-6	Site 1-6	Site 1	Site 2	Site 3	Site 4	Site 5	Site 6
Learning_rate	9.23×10^{-4}	8.49×10^{-4}	5.17×10^{-4}	3.33×10^{-4}	7.2×10^{-4}	9.95×10^{-4}	9.89×10^{-4}	3.95×10^{-4}
Weight_decay	8×10^{-5}	8×10^{-5}	5×10^{-5}	2×10^{-5}	9×10^{-5}	7×10^{-5}	10^{-5}	9×10^{-5}
Batch_size	60	48	24	24	60	36	18	72
Epsilon	6×10^{-5}	2.3×10^{-5}	6.7×10^{-5}	3.6×10^{-5}	8.9×10^{-5}	6.7×10^{-5}	2.1×10^{-5}	3.4×10^{-5}
GAT_dropout	0.0	-	-	-	-	-	-	-
DNN_dropout	0.1	0.7	0.6	0.9	0.5	0.9	0.6	0.9
DNN_hidden units1	130	110	190	110	190	190	110	70
DNN_hidden units2	250	190	110	130	110	110	190	170

Table S4. Test performances of forecasting chlorophyll-a concentration at each study site using the GAT - DNN, DNN_{separate}, and DNN_{concat}

Site	GAT-DNN		DNN _{separate}		DNN _{concat}	
	R ²	RMSE	R ²	RMSE	R ²	RMSE
Site1	0.67	0.08	0.35	0.47	0.59	0.31
Site2	0.63	0.06	0.16	0.69	0.21	0.53
Site3	0.76	0.07	0.46	0.60	0.61	0.44
Site4	0.69	0.08	0.36	0.47	0.27	0.63
Site5	0.63	0.08	0.22	0.42	0.43	0.46
Site6	0.77	0.08	0.50	0.39	0.21	0.75

Table S5. Performance of GAT-DNN across various forecast horizons.

Site	t = 1		t = 2		t = 3		t = 4		t = 5		t = 6	
	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE	R ²	RMSE
Site 1	0.67	0.08	0.55	0.10	0.57	0.10	0.51	0.11	0.54	0.09	0.53	0.10
Site 2	0.63	0.06	0.52	0.10	0.54	0.11	0.67	0.07	0.15	0.10	0.51	0.10
Site 3	0.76	0.07	0.61	0.09	0.45	0.11	0.52	0.11	0.41	0.11	0.47	0.10
Site 4	0.69	0.06	0.47	0.12	0.45	0.10	0.60	0.17	0.40	0.12	0.71	0.10
Site 5	0.63	0.08	0.62	0.08	0.44	0.09	0.30	0.12	0.35	0.10	0.29	0.10
Site 6	0.77	0.08	0.67	0.11	0.58	0.09	0.57	0.12	0.76	0.12	0.59	0.12
Range	0.61 – 0.75	0.06 – 0.08	0.50 – 0.64	0.09 – 0.11	0.44 – 0.58	0.09 – 0.11	0.40 – 0.66	0.09 – 0.15	0.24 – 0.64	0.10 – 0.12	0.38 – 0.66	0.09 – 0.11
(Mean)	(0.69)	(0.07)	(0.57)	(0.10)	(0.51)	(0.10)	(0.53)	(0.12)	(0.44)	(0.11)	(0.51)	(0.10)