

Supplementary Material

A transferable explainable and uncertainty-aware machine learning framework for water quality classification in data-scarce regions

Overview

This supplementary file provides additional tables and figures supporting the reproducibility and interpretation of the proposed framework. It includes extended model selection outputs, Water Potability feature-engineering results, explainability summaries, strict uncertainty diagnostics and complementary figures.

Table 1: Supplementary Table S1. Final selected models and predictive performance.

Task	Dataset	Model	Accuracy	Balanced accuracy	F1-macro
Binary potability	Water Potability	random forest	0.6890	0.6627	0.6655
Groundwater quality	Telangana 2018	hist gradient boosting	1.0000	1.0000	1.0000
Groundwater quality	Telangana 2019	hist gradient boosting	1.0000	1.0000	1.0000
WQI rule-recovery	Water Quality Testing	extra trees	1.0000	1.0000	1.0000
WQI rule-recovery	Water Quality Data	lightgbm	0.9894	0.9792	0.9861

Table 2: Supplementary Table S2. Best feature-engineered Water Potability model configurations.

Rank	Configuration	Prototype	Features	Accuracy	F1-macro
1	base only; quantile normal; smote; random forest	Yes	9	0.6890	0.6655
2	base missing; quantile normal; borderline smote; random forest	Yes	18	0.6753	0.6522
3	ratio interaction; quantile normal; none; hist gradient boosting	No	42	0.6707	0.6515
4	base missing; standard; smote; extra trees	Yes	18	0.6753	0.6498
5	base missing; robust; none; extra trees	No	18	0.6951	0.6489
6	base missing; standard; none; extra trees	No	18	0.6951	0.6489
7	ratio interaction; quantile normal; none; mlp	Yes	42	0.6768	0.6486
8	base missing; robust; smote; mlp	Yes	18	0.6860	0.6445

Table 3: Supplementary Table S3. Feature-engineering inventory for the Water Potability task.

Feature set	Features	Description
base only	9	Original physicochemical variables only
base missing	18	Original variables with missingness indicators
base nonlinear	45	Original variables with nonlinear transformations
domain reference	55	Distance and exceedance descriptors relative to reference values
ratio interaction	42	Physicochemical ratios, interactions and differences
engineered all	106	Feature-engineering group
base safe wqi	13	Feature-engineering group
engineered all safe wqi	110	Feature-engineering group

Table 4: Supplementary Table S4. Explainability summary across task families.

Task	Dataset	Model	Dominant variables
Binary potability	Water Potability	random forest	sulfate, ph, solids, chloramines, hardness
Binary potability	Water Potability	extra trees	ph, sulfate, solids, chloramines, hardness
Groundwater quality	Telangana 2018	hist gradient boosting	electrical conductivity, sar, sodium, total hardness, bicarbonate
Groundwater quality	Telangana 2019	hist gradient boosting	electrical conductivity, potassium, sodium, groundwater level, rsc
WQI rule-recovery	Water Quality Testing	extra trees	dissolved oxygen, conductivity, ph, temperature, turbidity
WQI rule-recovery	Water Quality Data	lightgbm	ph, dissolved oxygen, salinity, water depth, temperature

Table 5: Supplementary Table S5. Strict uncertainty and reliability synthesis.

Task	Dataset	Model	Accuracy	Review rate	Reliable rate	Reliable accuracy
Binary potability	Water Potability	random forest	0.6585	0.6311	0.0625	0.8780
Binary potability	Water Potability	extra trees	0.6418	0.5747	0.0991	0.8462
Groundwater quality	Telangana 2018	hist gradient boosting	1.0000	0.0000	1.0000	1.0000
Groundwater quality	Telangana 2019	hist gradient boosting	0.9863	0.0137	0.9863	1.0000
WQI rule-recovery	Water Quality Testing	extra trees	1.0000	0.0100	0.9900	1.0000
WQI rule-recovery	Water Quality Data	lightgbm	0.9810	0.0000	0.9979	0.9831

Table 6: Supplementary Table S6. Cross-task uncertainty comparison and calibration indicators.

Task	Dataset	Model	ECE uncal.	ECE cal.	Threshold	Caution rate
Binary potability	Water Potability	random forest	0.0393	0.0292	0.67	0.3064
Binary potability	Water Potability	extra trees	0.0746	0.0367	0.66	0.3262
Groundwater quality	Telangana 2018	hist gradient boosting	0.0100	0.0847	0.50	0.0000
Groundwater quality	Telangana 2019	hist gradient boosting	0.0163	0.0895	0.50	0.0000
WQI rule-recovery	Water Quality Testing	extra trees	0.0129	0.0206	0.50	0.0000
WQI rule-recovery	Water Quality Data	lightgbm	0.0139	0.0296	0.50	0.0021

Table 7: Supplementary Table S7. Strict uncertainty selected models.

Task	Dataset	Model	Augmentation	F1-macro	Ranking metric
Binary potability	Water Potability	random forest	smote	–	0.6655
Binary potability	Water Potability	extra trees	borderline smote	–	0.6482
Groundwater quality	Telangana 2018	hist gradient boosting	random oversampling	1.0000	1.0000
Groundwater quality	Telangana 2019	hist gradient boosting	borderline smote	1.0000	1.0000
WQI rule-recovery	Water Quality Testing	extra trees	none	1.0000	1.0000
WQI rule-recovery	Water Quality Data	lightgbm	none	0.9861	0.9861

Supplementary figures

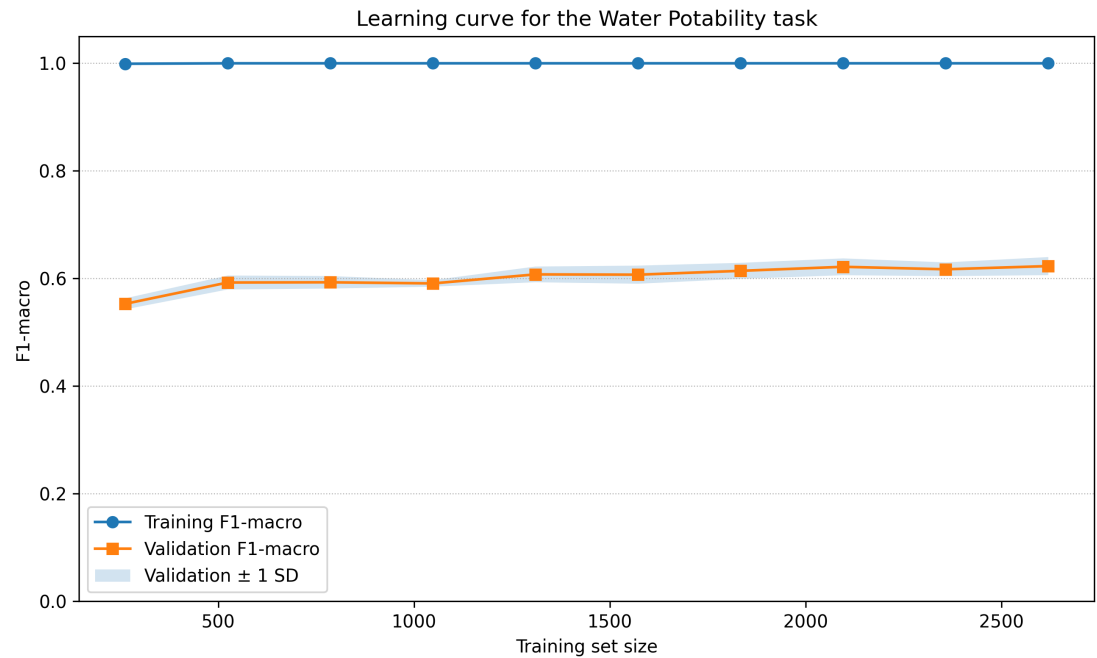


Figure 1: Supplementary Figure S1. Learning curve for the Water Potability task using F1-macro as the evaluation metric.

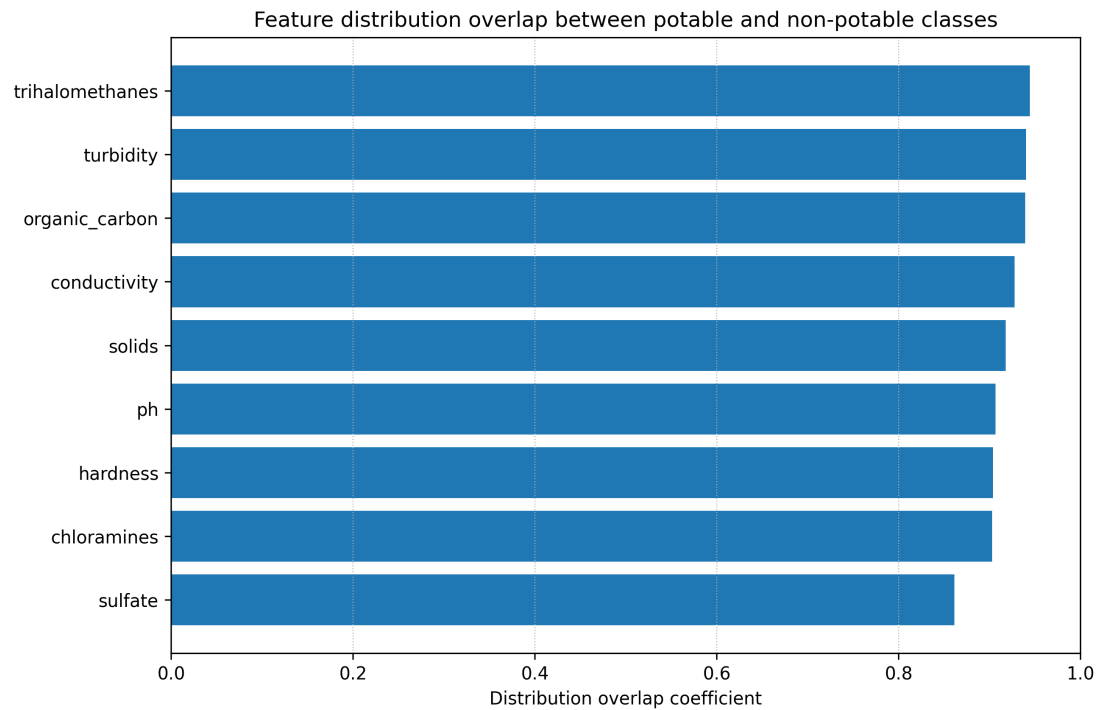


Figure 2: Supplementary Figure S2. Feature-overlap analysis between potable and non-potable samples. Higher overlap values indicate stronger similarity of feature distributions across the two classes.

Repository note

The processed tables, Python scripts and extended result files may be deposited in an online repository. The repository link or DOI should be added here when available.