Harnessing Explainable AI for Multi-Step Forecasting of Water Quality with uncertainty quantification in Freshwater Reservoirs

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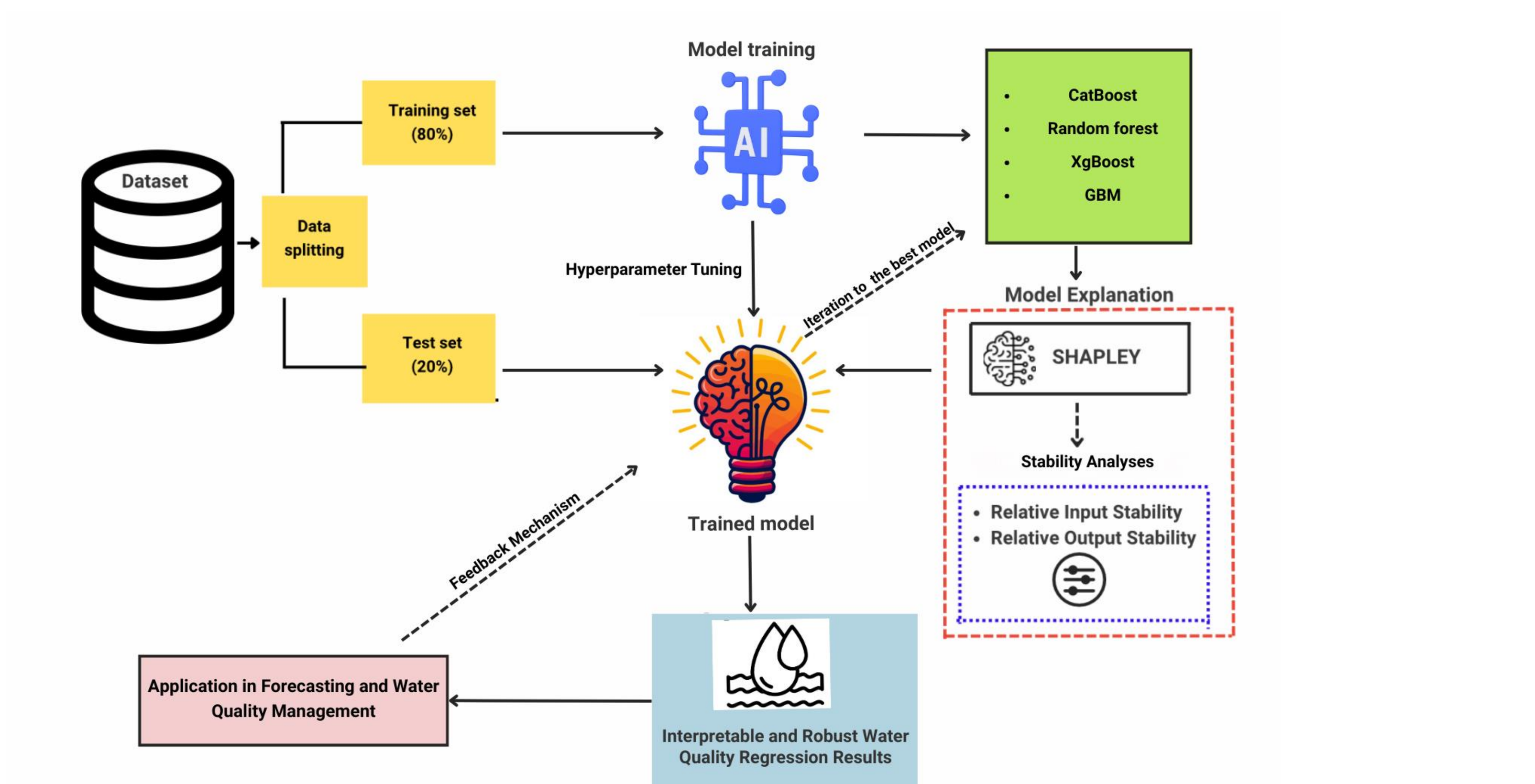
Research Motivation: Explore ensemble machine learning approaches to understand and forecast phytoplankton dynamics

Phytoplankton blooms in freshwater systems, driven by eutrophication and climate change, threaten ecosystems, human health, and economies. Traditional process-based models are constrained by computational demands, parameterization uncertainties, and limited predictive accuracy in capturing the nonlinear dynamics of phytoplankton. Machine learning (ML) offers promise but is limited by its inherent "black-box" nature and sensitivity to input data and output predictions; consequently, applications of machine learning for water quality forecasting have been limited to date. In this analysis, we explore ML approaches to answer: **How can a ML framework enhance phytoplankton bloom forecasting, and Explainable AI (XAI) quantify the dynamic, horizon-dependent influence of environmental drivers**?

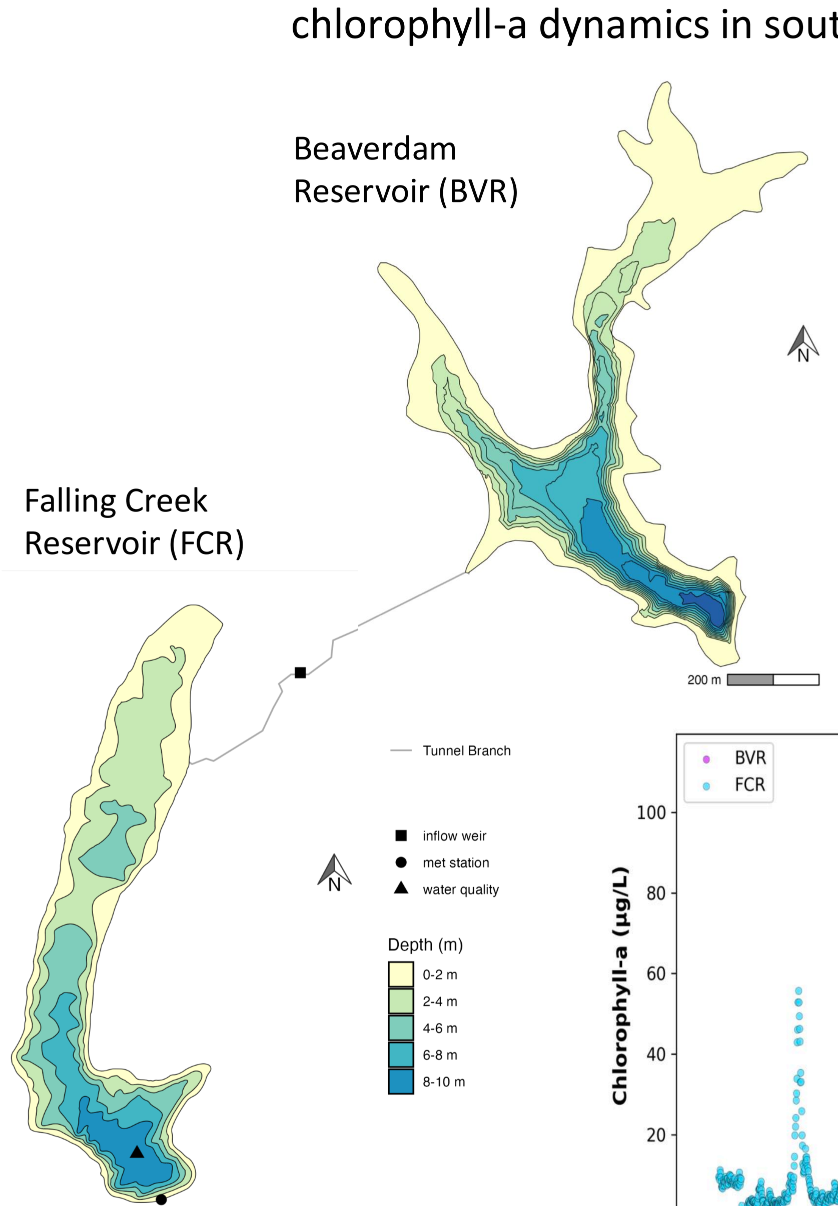
Integrating ML-XAI into Forecasting Workflow

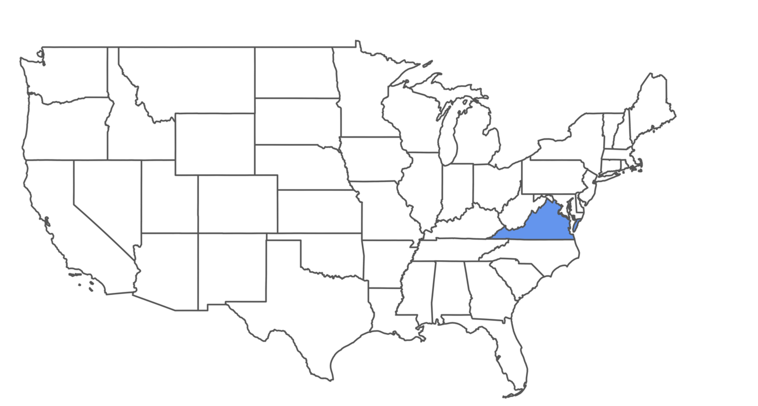


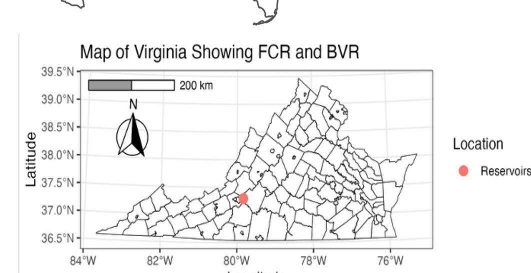
1. *Leveraging explainable AI (XAI) for improving model interpretability.*
2. ***To integrate a define-by-run API based multi-objective hyperparameter tuning, creating an automated system for real-time optimization.***
3. ***Applying ML models for multi-step Chlorophyll-a forecasting and feature importance analysis across different forecast horizons.***
4. ***Bootstrapped based ensemble ML models for uncertainty quantification***.

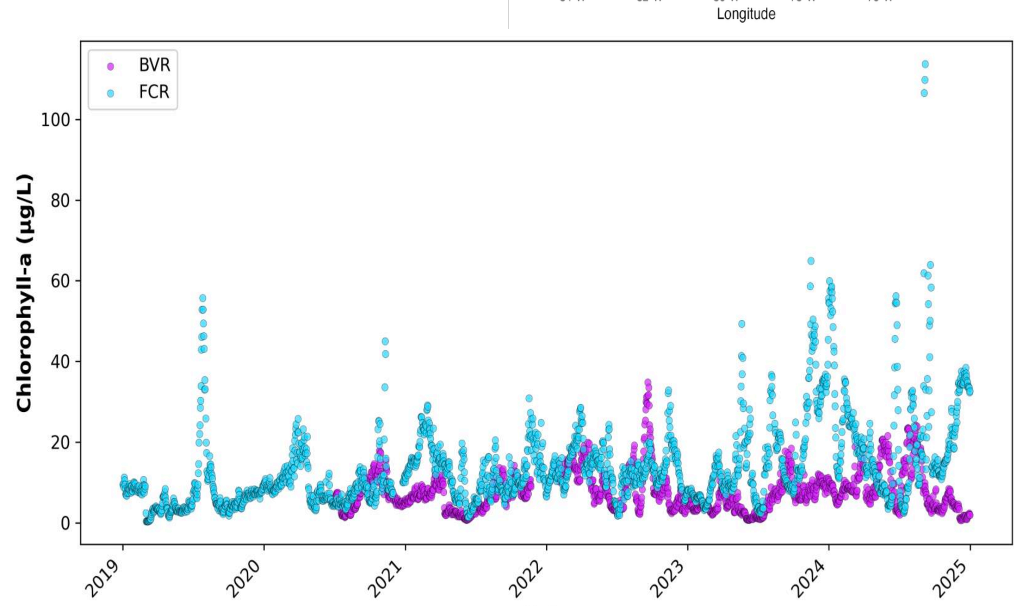
Domain: Two drinking water reservoirs, Virginia, USA

Compared model results between two co-located reservoirs with different chlorophyll-a dynamics in southwestern Virginia, USA









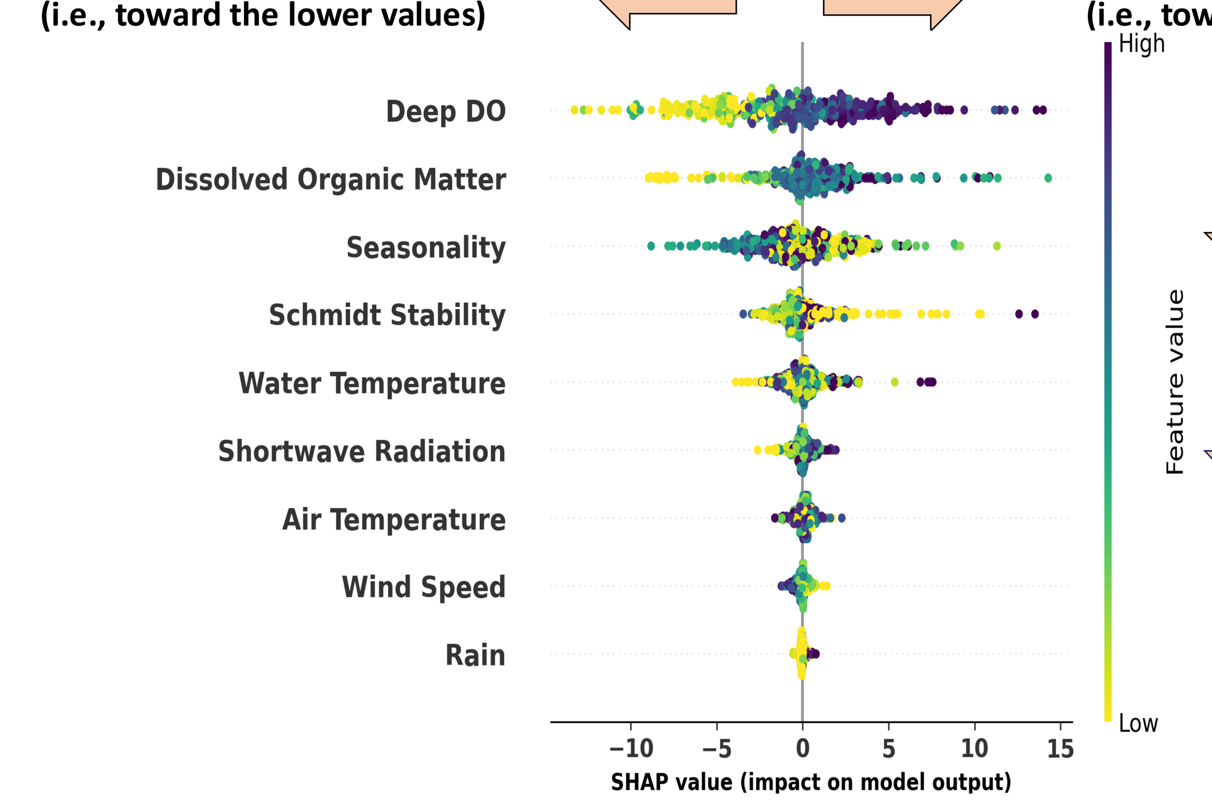
XAI revelations to reservoir phytoplankton dynamics

In addition to physio-chemical drivers, seasonality is included in the model to capture cyclical seasonal patterns using sinusoidal function

Falling Creek Reservoir (FCR)
Surface chlorophyll-a is strongly related to bottom water oxygen and dissolved organic matter

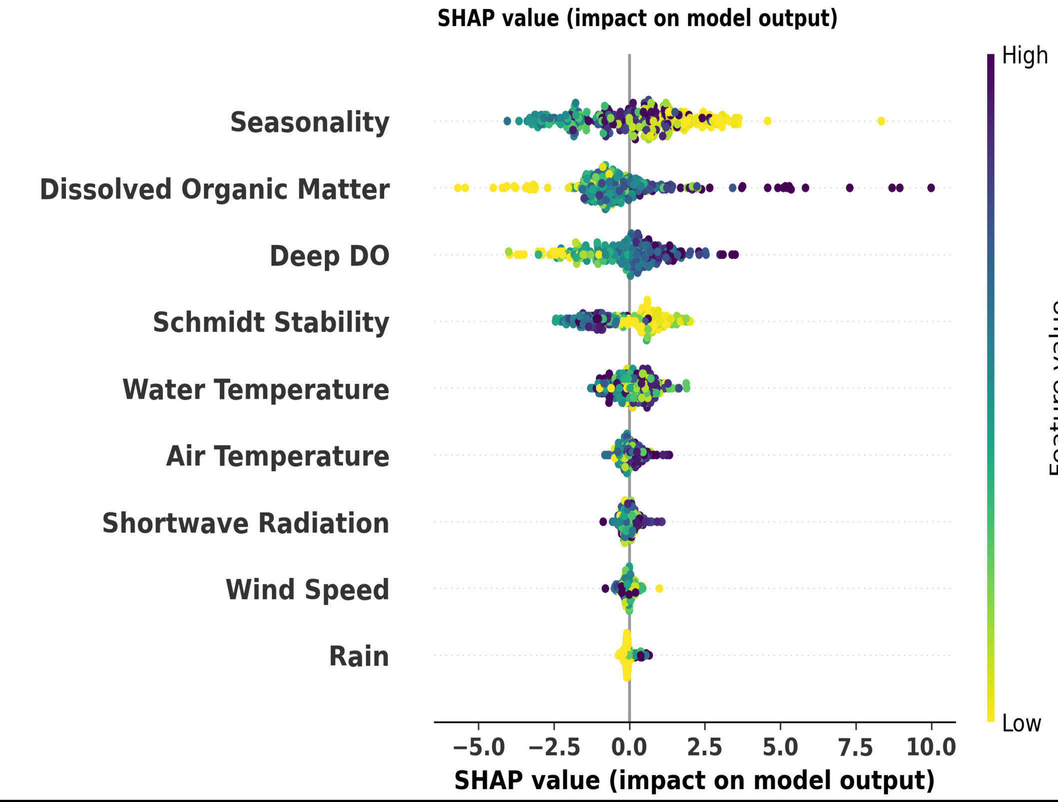
Feature pushes prediction down (i.e., toward the lower values)

Feature pushes prediction up (i.e., toward the higher values).



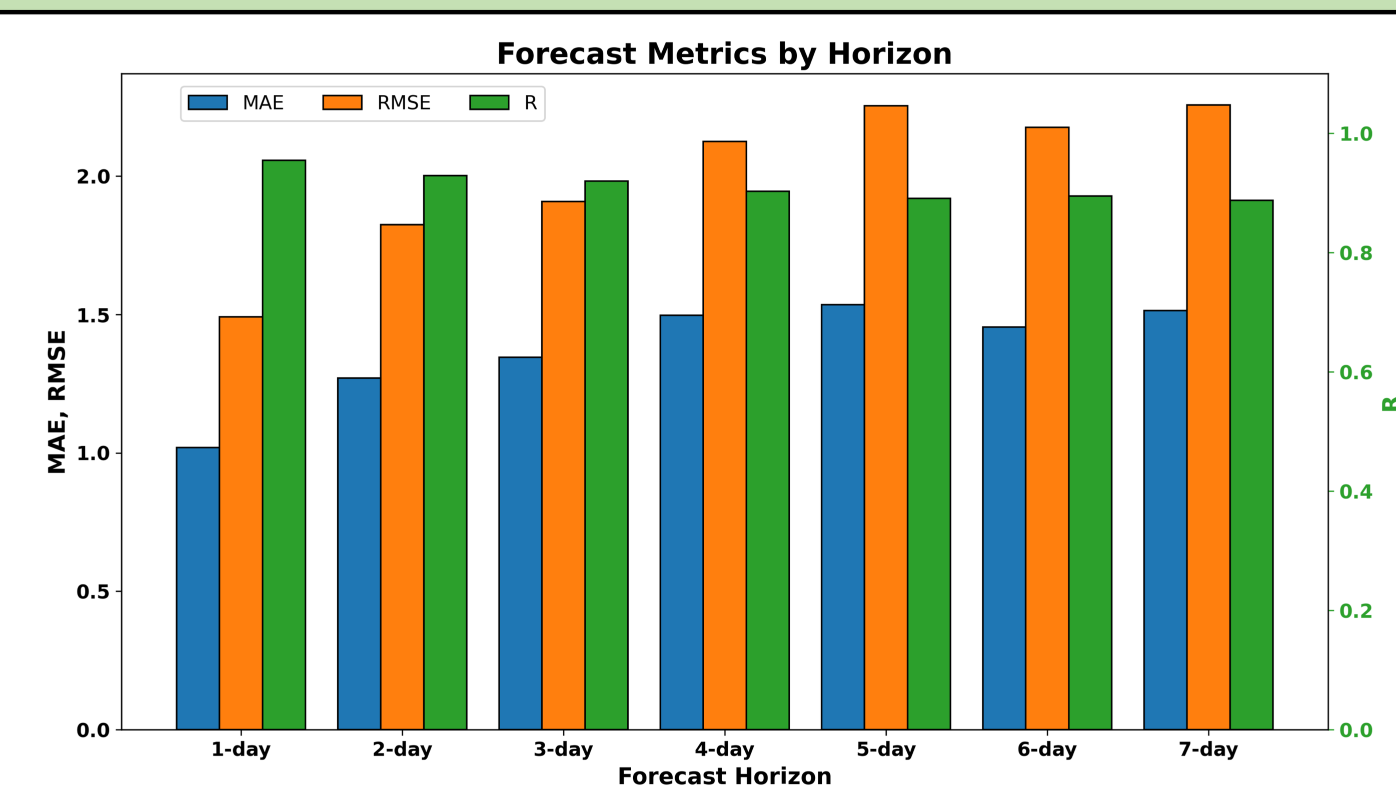
Features in descending order of overall importance.

Color (feature value) Gradient (e.g. purple →yellow) shows the feature value (high to low).

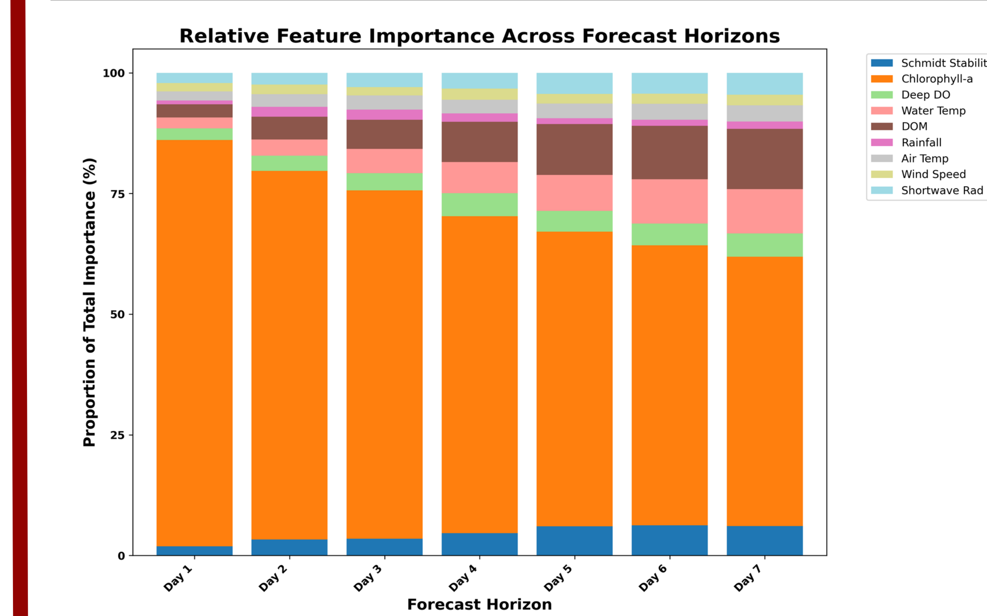


Beaverdam Reservoir (BVR) Surface chlorophyll-a is strongly related to seasonality and dissolved organic matter

XGBoost model performance Analyses

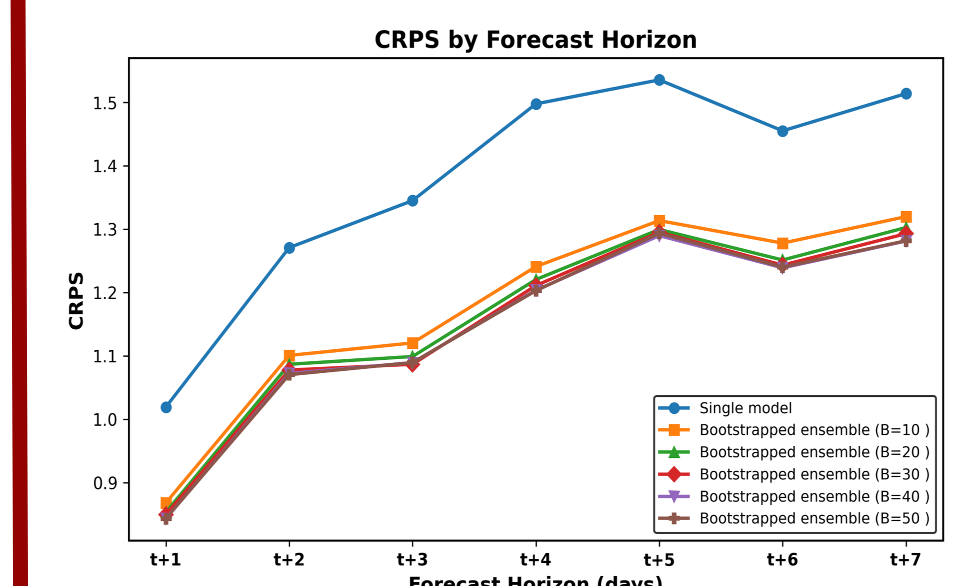


Results



- **Dominance of persistence in Short-Term Forecasts:**
  - For immediate predictions (Day 1-3), the model is dominated by the previous day's chlorophyll-a concentration.
- **Increasing Environmental Influence with Extended Horizons:**
  - As the forecast horizon lengthens (Day 4-7), the model's reliance on environmental drivers like Water Temperature and Dissolved organic matter steadily increases.

Figure 5: Relative feature importance for the daily phytoplankton forecast model across a 7-day horizon, generated using Explainable AI (XAI). Each stacked bar illustrates the proportional contribution (%) of environmental variables and the initial Chl-a to the model's prediction for a specific day's forecast.



- The bootstrapped ensemble models consistently outperform the single model, showing significantly better forecast skill (lower error) at all lead times.
- All the models become less accurate as the forecast horizon extends to 7 days, the ensembles provided a more reliable prediction.
- Increasing the number of ensemble members from 10 to 50 offered only a marginal improvement.

Figure 6: Evaluation of forecast skill using the Continuous Ranked Probability Score (CRPS) to quantify uncertainty. Forecasts were evaluated across a 7-day forecast horizon , where lower CRPS values indicate a more skillful probabilistic forecast.

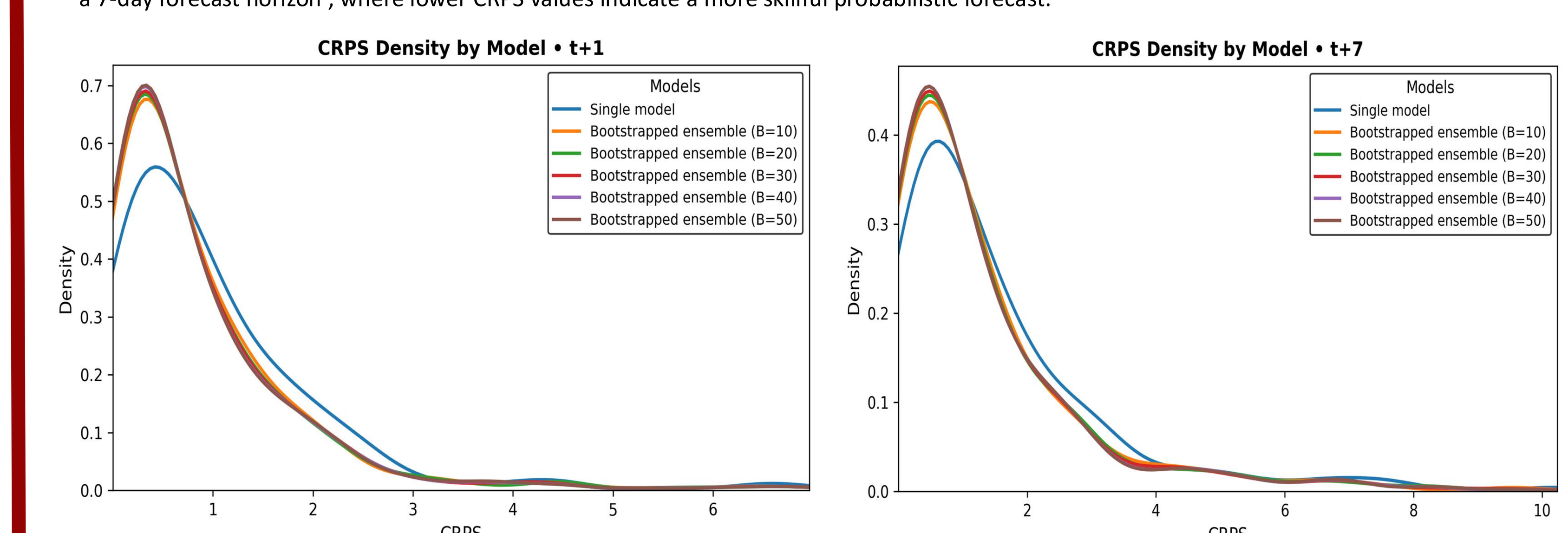


Figure 7: Density distributions of the CRPS for the 1-day (t+1) and 7-day (t+7) forecast horizons. A peak that is higher and shifted to the left for the ensemble models shows a more skillful and reliable forecast. Overall skill score decreased as the forecast horizon advanced from 1 to 7 days.

Conclusions

- **Reservoir-Specific Driver Signatures** : Adjacent sites exhibit distinct drivers of phytoplankton dynamics, necessitating ecosystem-specific modeling approaches.
- **Ensemble Models Provide Superior Skill and Reliability**: Bootstrapped ensemble models reduced the uncertainty in the forecasting framework.
- **This dynamic, horizon-dependent strategy**: The framework Identifies how forecast drivers change with the horizon, providing resource managers with the actionable insights needed for proactive ecosystem management.

Acknowledgments

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