Predicting tetrodotoxin contamination in bivalve mollusks using explainable AI

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Introduction

- Tetrodotoxin (TTX) can contaminate seafoods from Europe
  - Such as from the Netherlands, England, and Greece
- TTX originates from a variety of marine bacteria
  - Exact cause of TTX in the Netherlands remains unknown
- TTX is both a food safety and economical problem
  - Contaminated production areas are temporally closed
- TTX builds up over time, differentiating between locations
  - Influencing factors are shallow habitats, seasonality, and climate
- Temporal aspect for TTX contamination was not assessed before

Objectives

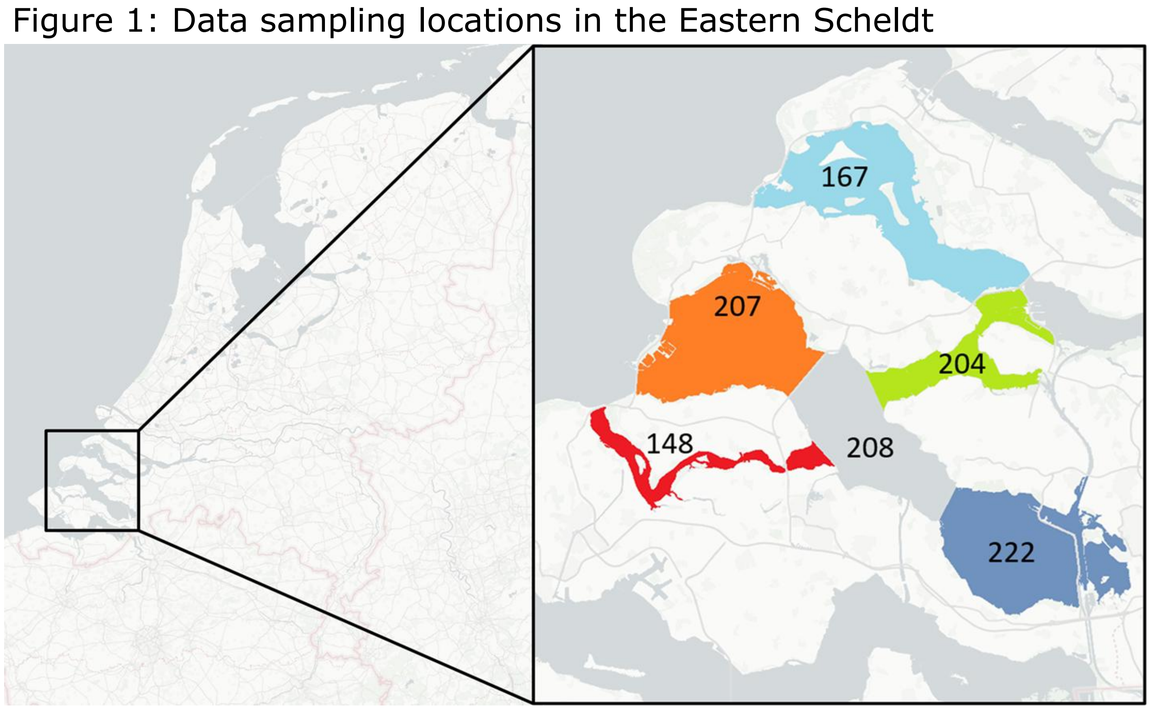
1. Predict TTX contamination in bivalve mollusks using AI

2. Interpret predictions with post-hoc eXplainable AI (XAI)

Methods

- **Analytical results** from the Netherlands between 2016-2023
  - Bivalve mollusks from the Eastern Scheldt
  - TTX quantified by LC-MS/MS
  - 1,156 results, 75 (6.4%) above Action Limit (22 µg TTX/kg)
- **Temporal deep learning model** (Long Short-Term Memory, LSTM)
- Input features: **weather** (KMNI[1]) and **water** (RWS[2]) data
- Output: **presence** or **absence** of TTX contamination
  - Classification threshold: Action Limit
- Model validation
  - **Area Under the Curve** (AUC), sensitivity, and specificity
  - Sensitivity analysis: bootstrapping the validation set
- **Explainable AI** (XAI): Shapley Additive exPlanations (SHAP)

Figure 1: Data sampling locations in the Eastern Scheldt



Results

Figure 2: Model validation:

- AUC in test set: 0.93
- Test sensitivity: 93%
- Test specificity: 81%

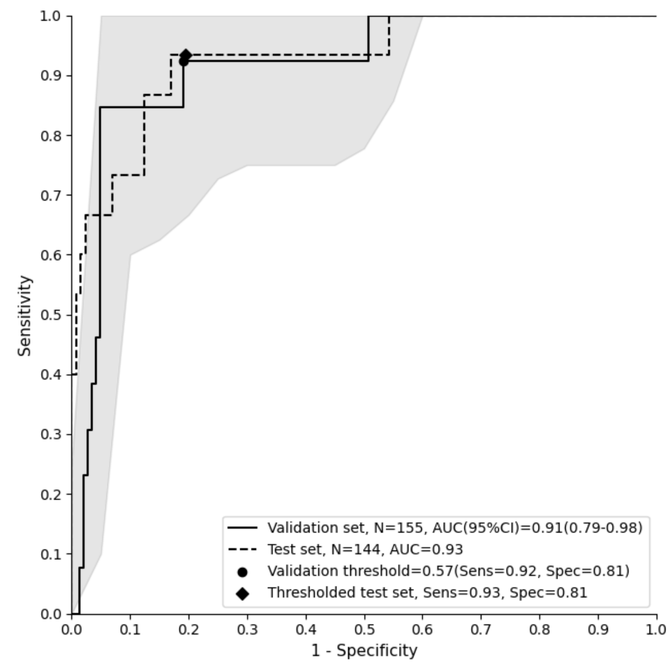


Figure 3: Most important factors for TTX identified with XAI

- Day length, global radiation, diluted chloride, and water temperature

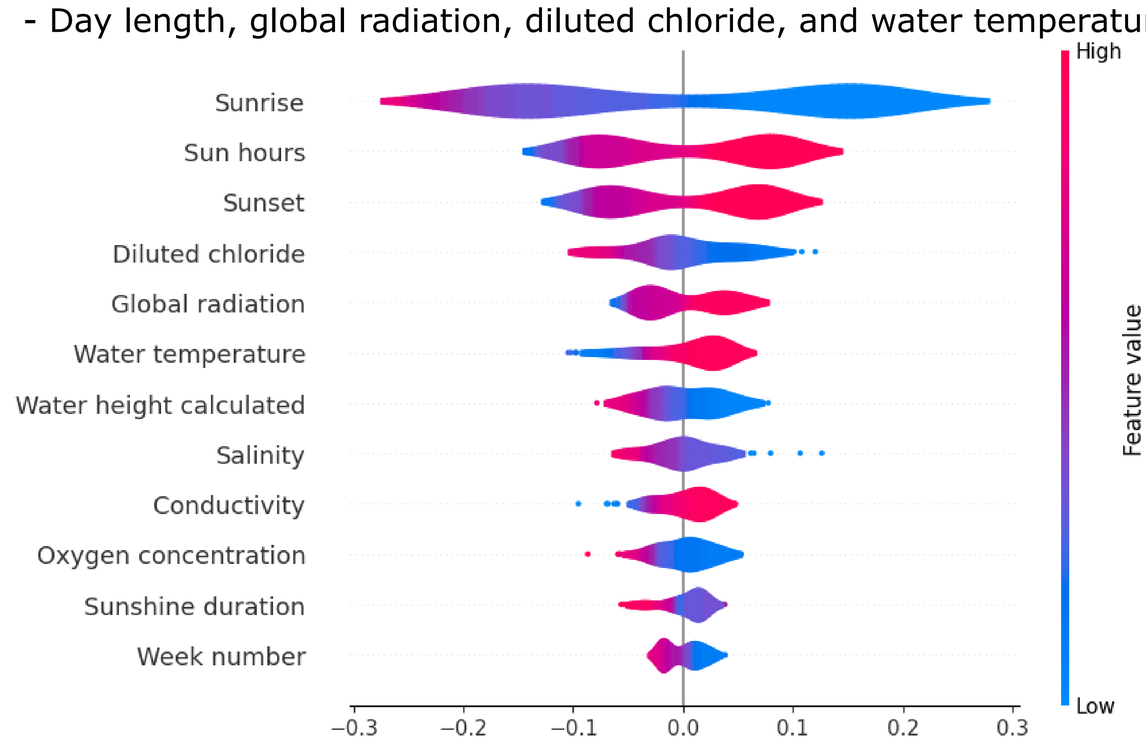
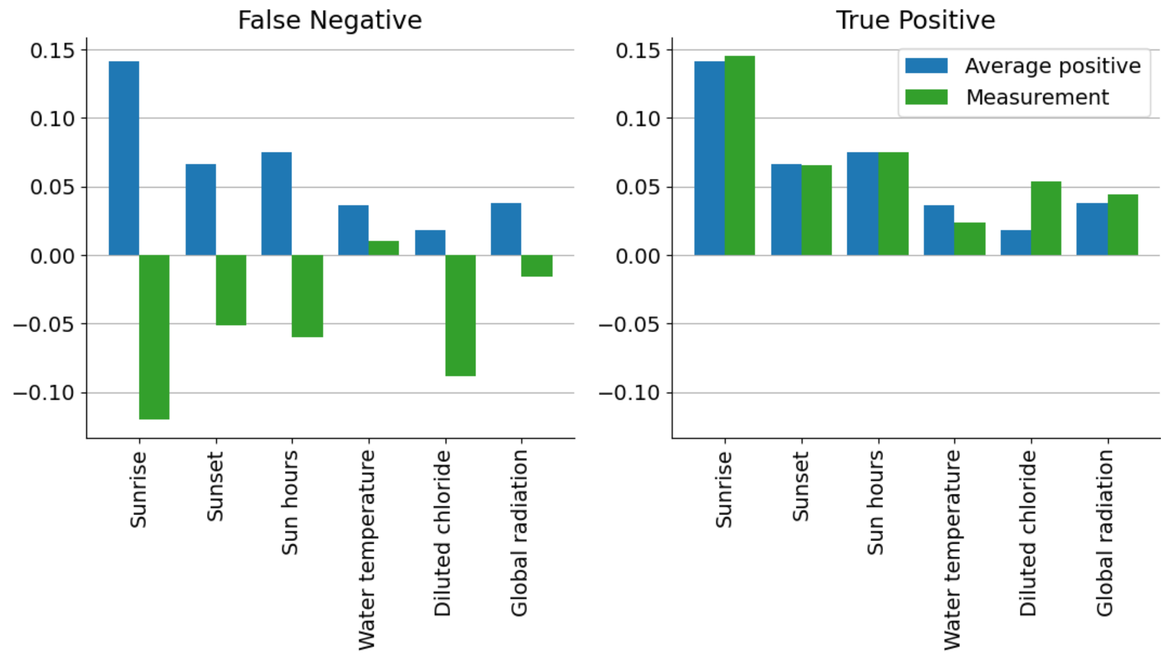


Figure 4: Local explanations provide insight into faulty predictions



Conclusions

- AI could accurately predict tetrodotoxin (TTX) contamination in bivalve mollusks
- XAI helps understanding individual predictions and false negatives
- XAI identified seasonality, temperature, and diluted chloride concentrations to drive TTX accumulation in bivalve mollusks

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1. KNMI: https://www.knmi.nl/nederland-nu/klimatologie/daggegevens
2. RWS: https://waterinfo.rws.nl/