Harrmful Algal Bloom Prediction using Emprical Dynamic Modelling

Özlem Baydaroğlu

IIHR – Hydroscience & Engineering, University of Iowa, Iowa, USA

Abstract

Harmful Algal Blooms (HABs) can originate from a variety of reasons, including water pollution coming from agriculture, effluent from treatment plants, sewage system leaks, pH and light levels, and the consequences of climate change. In recent years, HAB events have become a serious environmental problem, paralleling population growth, agricultural development, increasing air temperatures, and declining precipitation. Hence, it is crucial to identify the mechanisms responsible for the formation of harmful algal blooms (HABs), accurately assess their short- and long-term impacts, and quantify their variations based on climate projections for developing accurate action plans and effectively managing resources. This present study utilizes empirical dynamic modeling (EDM) to predict chlorophyll-a (chl-a) concentration of Lake Erie. This method is characterized by its nonlinearity and nonparametric nature. EDM has a significant benefit in that it surpasses the constraints of conventional statistical modeling through the use of data-driven attractor reconstruction. Chl-a is a critical and commonly used parameter in the prediction of HAB events. Lake Erie is an inland water body that experiences frequent HAB phenomena as a result of its location. With a MAPE of 4.31%, an RMSE of 6.24, and a coefficient of determination of 0.98, the EDM showed exceptional performance. These findings suggest that the underlying dynamics of chl-a changes can be well captured by the EDM model.

Keywords: Prediction, Empirical dynamic modelling, Harmful algae, Chlorophyll-a, Lake Erie

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1. Introduction

Harmful algal blooms (HABs) originate from agricultural and industrial pollution, water temperature, and quality (Paerl and Paul, 2012; Graham et al., 2016). In addition to reducing the quality of drinking water, they also negatively impact the smell, taste, and aesthetics of lakes used for recreation and drinking. In their study, Dai et al. (2023) have investigated HABs from 2003 to 2020 by utilizing satellite data. It has been discovered that the extent of HABs expands by 13% and the occurrence of HABs escalates by 59% over this time frame. While there are variations in patterns across the globe, Europe and North America have been identified as the regions experiencing the highest number of HAB events.

In the past few years, there has been a sharp rise in HABs events due to environmental pollution, climate change (Baydaroğlu and Demir, 2024; Yeşilköy et al., 2023, 2024), the increasing number in global populations, the growth of agricultural production (Yeşilköy and Demir, 2024). HAB tracking (Greene et al., 2021), modeling (Baydaroğlu et al., 2024), and prediction (Yan et al., 2024) research have been expedited as a result of the increasing prevalence of HABs and their critical role in protecting public and environmental health.

Predicting HABs is challenging due to the scarcity and inconsistency of data (Kwon et al., 2023; Fung et al., 2023), the impact of several nonlinear environmental factors, and the complex nonlinear and seasonal patterns of HAB data. Notwithstanding these difficulties, there are quite a few efforts employing AI-based algorithms like random forest (Yan et al., 2024), support vector machines (Silva et al., 2023), neural network models (Chen et al., 2023), Bayesian modeling (Myer, 2020), logistic regression (Villanueva et al., 2023), long short-term memory (Busari et al., 2024), physically based models such as empirical dynamic modeling (Agarwal et al., 2023), and hybrid approaches including sparse identification of nonlinear dynamics (Baydaroğlu et al., 2024). These studies employ water quality indicators such as chl-a, microcystin, total inorganic nitrogen, total phosphorus, dissolved oxygen, and pH, as well as meteorological variables such as water and air temperatures, global solar radiation, wind speed, and physical parameters such as secchi disc depth and turbidity.

There are some HAB prediction endeavors using chl-a as a HAB indicator. Qui et al. (2023) employed shoreline, chl-a, algal bloom, wind direction, and dynamic indices to predict the HAB risks in areas with coastlines, creating a simulation model. To forecast HABs at 7-day and 14-day time frames, Li et al. (2014) used chl-a concentration, total inorganic nitrogen, orthophosphate, total phosphorous, water temperature, dissolved oxygen, secchi disc depth, global solar radiation, and wind speed. Agarwal et al. (2023) forecasts HABs on a sub-monthly level using empirical dynamical modeling. The results indicate that the forecasting of HABs is enhanced when the multivariate data is derived from measurable image characteristics. This enhancement is particularly apparent when time periods exceeding seven days are taken into account. The SINDy method was employed by Baydaroğlu et al. (2024) to simulate the alteration in microcystin, a toxin that algae produce. They utilized evaporation as a meteorological variable and dissolved oxygen as a water quality metric. Lee et al. (2022) created a model that predicts the concentration of chl-a by incorporating water quality factors (chl-a, electric conductivity, dissolved oxygen etc.) and meteorological variables (air temperature, wind speed and directions). The results show that chl-a either has no effect on electrical conductivity or performance is reduced in this regard. chl-a, ammonia nitrogen, nitrate/nitrite, shortwave solar radiation, pH, air and water temperature, total phosphorus, turbidity, land use, wind speed, dissolved oxygen, specific humidity, precipitation, agricultural land use were the variables used by Yan et al. (2024) to predict the levels of chl-a. According to the findings, forecasts made one month in advance are more accurate than those made for the current month.

The Great Lakes are the world's largest and most biodiverse freshwater reservoir, and its basin includes both manufacturing-oriented industrial facilities and agricultural areas (Tewari et al., 2022). Lake Erie is the Great Lakes' shallowest and smallest lake according to water capacity. Its geographical position has a substantial impact on nutritional overload (Tewari et al., 2022). Therefore, several studies on predicting HABs are conducted using water quality factors, physical characteristics, climatic variables, and teleconnections (Scavia et al., 2023; Manning et al., 2023).

Empirical dynamic modeling (EDM) is a technique rooted in dynamical system theory that does not rely on explicit dynamic equations (Sugihara and May, 1990; Ye et al., 2015; Chang et al., 2017). It is a potent technique for predicting and examining nonlinear dynamics (Johnson and Munch, 2022). EDM has been utilized in diverse research domains, such as wind turbine power forecasting (Ma et al., 2019), assessing the impact of climate on dysentery epidemics (Wu et al., 2020), identifying shared spatial patterns in air temperature, salinity, and ichthyoplankton diversity (Kuriyama et al., 2020), predicting water flow (Saberski et al., 2022), differentiating between abiotic and biotic factors influencing population fluctuations in sympatric fishes (Wasserman et al., 2022), forecasting coastal and riverine algal blooms (McGowan et al., 2017; Tian et al., 2024), and analyzing the causal relationship between crop yield and climate extremes (Simanjuntak et al., 2023; Baydaroğlu et al., 2024).

The global rise in HAB events poses a significant concern to public health, emphasizing the need for a comprehensive understanding of HAB formation mechanisms, accurate modeling, and informed decision-making about precautionary measures and rehabilitation efforts. Therefore, scientific studies in this field have gained momentum. EDM has proven to be highly effective in predicting ecological parameters (Sugihara et al., 2012; Wang et al., 2019, Tian et al, 2024). However, it has not yet been used to the prediction of chl-a. This study has utilized EDM to predict chl-a, a crucial indicator of HABs, and showed that EDM is a highly effective approach for predicting HABs.

For simplex projection, the study used the R package rEDM (Ye et al., 2016; Sugihara et al., 2019; Park et al., 2022; Sugihara et al., 2020). This paper is structured as follows: An explanation of the study area, the data, and the methodology is given in Section 2. Section 3 contains the findings and conclusion.

2. Materials and Methods

2.1 Study Area

The region encircling the Great Lakes, the world's largest and most biologically diverse freshwater system, is characterized by a combination of industrial and agricultural land use. Lake Erie is distinguished from its interconnected counterparts by virtue of its relatively shallow depth and lesser volume. Its geographic position renders it particularly susceptible to nutrient pollution (Tewari et al., 2022). Since 2002, Lake Erie has grappled with HABs, with their severity escalating dramatically in recent years (Ai et al., 2023, Badshah et al., 2024).

Figure 1 shows the region to the west of Lake Erie where the HAB events are mostly taking place, along with the specific locations of the monitoring stations.

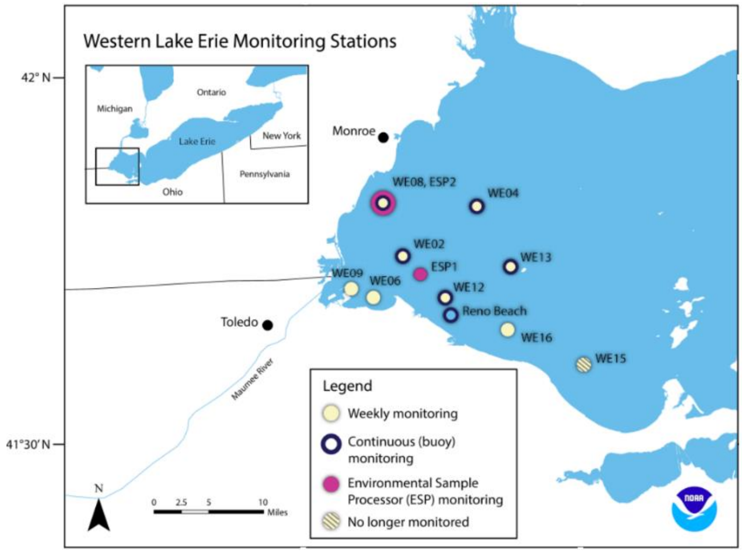

Figure 1. Western Lake Erie monitoring stations of NOAA's Great Lakes Environmental Research Laboratory (Retrieved from https://www.glerl.noaa.gov/res/HABs_and_Hypoxia/ rtMonSQL.php).

2.2 Data

As is known, HAB formations occur in the spring and summer months. The study has utilized Chl-a data collected from May to October between the years 2012 and 2022. The sampling processes for the analysis of water quality parameters in lakes and oceans are quite irregular, particularly when the data from previous years is analyzed.

For instance, sampling intervals may vary from one week to eleven days or fourteen days in certain months. There is even data from different hours of the same day.

All chl-a data from all stations illustrated in Figure 1 have been pooled due to the need for a substantial quantity of data for dynamical modeling. These datasets have been obtained from National Oceanic and Atmospheric Administration (NOAA) - National Centers for Environmental Information (NCEI) Granule Geoportal.

Figure 2 illustrates the mean values of all station data per year. The data from Figure 2 clearly shows a noticeable increase in chl- a level in the years 2013, 2015, 2017, 2019, and 2022.

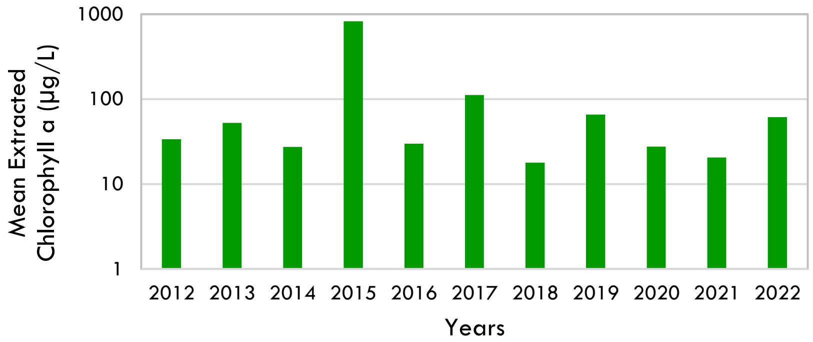

Figure 2. Mean chl-a values Of Lake Erie per year.

2.3 Empirical Dynamical Modeling (EDM)

EDM is a chaos theory-based, equation-free method for analyzing dynamical systems (Sugihara and May, 1990; Ye et al., 2015; Wang et al., 2019). It can be applied to predict single or multivariable as well as determine the causality or nonlinearity of a system. The effectiveness of EDM that includes simplex projection, s-map and cross convergent mapping in dealing with complex and nonlinear systems has been convincingly proven (Sugihara et al., 2012; Ushio and Kawatsu, 2020; Agarwal et al., 2023; Tian et al, 2024). This study utilizes a single variable for the purpose of making predictions.

2.3.1 Phase Space Reconstruction

Since EDM is stochasticity-sensitive, it needs to be used in systems that exhibit deterministic dynamics (Cummins et al., 2015; Nova et al., 2019). In order to assess low-dimensional deterministic dynamics, it can be conducted univariable phase space reconstruction (PSR) for attractor generation for each variable and employ simplex projection to verify that the predictive ability diminishes over time.

The trajectories in the phase space can depict the time evolution of a phenomena. Each point in a phase space represents a specific state of the system, while each trajectory illustrates the system's time evolution under different initial conditions. In a phase space, clusters of points have a distinct form that draws trajectories towards it, known as attractors (Baydaroğlu and Koçak, 2014). The embedding theorem (Takens, 2006) allows for the construction of a phase space from a one-dimensional time series. For a time series $x_t \in \mathbb{R}, t = 1,2, \ldots, N$, reconstruction equation is as follows:

$$X_t = \left(x_t, x_{t-\tau}, \ldots, x_{t-(E-1)\tau}\right) \quad (1)$$

where X_t are E dimensional vectors and τ is a time delay.

2.3.2 Simplex Projection & Sequential Locally Weighted Global Linear Map

By calculating a weighted average of the trajectories of the nearest neighbors of the new state, simplex projection calculates the trajectory of that state (Ye et al., 2015). It uses embedding dimension-lagged coordinates to forecast future values (Sugihara and May, 1990; Hsieh et al., 2005; Steele, 2023).

To determine the nearest neighbors of a new state $\boldsymbol{x}_s$, it is initially determined the m nearest neighbors ($m = E + 1$): The neighbors are represented by the vectors $\boldsymbol{x}_n(s,i)$, where $n(s,i)$ is the time index of the ith nearest neighbor to $\boldsymbol{x}_s$. The neighbors are subsequently forward-evolved, and a weighted average of the forward evolutions is computed for estimating $\boldsymbol{x}_{s+h}$:

$$\hat{\boldsymbol{x}}_{s+h} = \left(\sum_{i=1}^{m} w_i(s)\boldsymbol{x}_{n(s,i)+h}\right) / \sum_{i=1}^{m} w_i(s) \quad (2)$$

where $w_i(s)$ are weights. $w_i(s)$ are determined by the distance between $\boldsymbol{x}_s$ and its ith neighbor, $\boldsymbol{x}_n(s,i)$, which is scaled to the distance to the nearest neighbor:

$$w_i(s) = \exp\left(-d(\boldsymbol{x}_s, \boldsymbol{x}_{n(s,i)}) / d\left(\boldsymbol{x}_s, \boldsymbol{x}_{n(s,1)}\right)\right) \quad (3)$$

where $d(\boldsymbol{x}_s, \boldsymbol{x}_t)$ is the Euclidean distance between $\boldsymbol{x}_s$ and $\boldsymbol{x}_t$ (Ye et al., 2015).

Moreover, the S-map (sequential locally weighted global linear map) test for nonlinearity (Sugihara 1994) can be employed to assess the presence of nonlinear state dependency in a variable. (Sugihara and May, 1990; Nova et al., 2019). S-map combines E-lagged coordinates and a weighting parameter θ to predict future values in a nonlinear manner (Sugihara, 1994; Steele, 2023).

The prediction skill in both simplex projection and s-map is measured using the Pearson correlation coefficient. lyapExp in MatLab and libraries of nonlinearTseries and tseriesChaos of R have been employed to estimate the maximum Lyapunov exponent. Besides, the rEDM library of R has been used for simplex projection.

3. Results and Discussion

As stated before, the main difficulty in predicting HAB-related parameters such as Chl-a is that the available data are limited, sparse, and have irregular sampling intervals. For instance, the quantity of data points may be insufficient in certain years, while it may be adequate in others. Or there may be weeks in which no data is collected, while others may have three to four daily data points due to the fact that multiple measurements are obtained. Due to this limitation, the chl-a amounts have been calculated on an annual basis rather than looking at monthly or yearly fluctuations (see Fig. 2). As a result of this situation, it is challenging to establish a precise prediction interval and accurately represent the presence of nonlinearity. In light of this scenario, Lyapunov exponents (λs) have been computed as a metric for quantifying the degree of nonlinearity exhibited by the data. Lyapunov exponents have been demonstrated to be the most valuable tool for analyzing the dynamics of chaotic systems. They are the mean exponential rates at which neighboring trajectories in phase space either diverge or converge. Due to the exponential divergence of close trajectories, systems with initially equivalent states will quickly exhibit significant variances, leading to a rapid loss of predictive capability. A system that possesses at least one positive Lyapunov exponent is classified as chaotic (Wolf et al., 1985).

The chl-a data has been determined to have a positive maximum Lyapunov exponent. Given that the highest Lyapunov exponent is positive, it can be inferred that the data exhibits chaos or nonlinearity (Grassberger et al., 1991; Kantz, 1994). Moreover, the nonlinearity of chlorophyll-a (chl-a) has been ascertained using S-map (see Figure 3). If the nonlinear parameter (θ) has a value of zero at the time where the prediction skill achieves its maximum level, then the model is classified as linear. Nevertheless, if the value exceeds zero, the model is categorized as nonlinear (Sugihara, 1994). Based on Figure 3, the chl-a data can be considered nonlinear due to its nonlinear parameter value of 7.

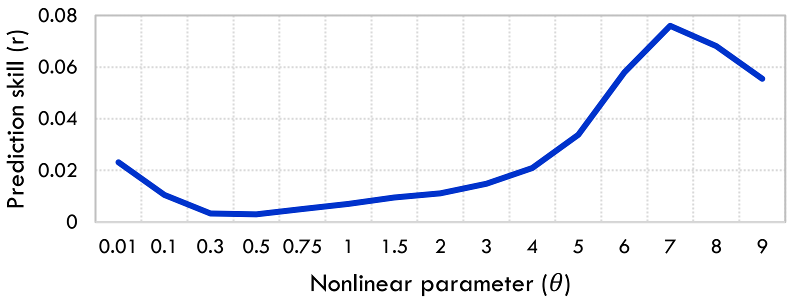

Figure 3. Ch-l a data first differences S-map prediction skill as a function of S-map nonlinear parameter.

As seen in Figure 4, the optimal embedding dimension has been determined to be 2 using simplex projection. The maximum resolution for embedding is achieved by employing a time delay of 1 in simplex projection (Javier et al., 2022; Bonotto et al., 2022; Tian et al., 2024). Therefore, the time delay has been set to 1 to ensure the highest possible temporal resolution, as the chl-a data is not collected on a daily basis.

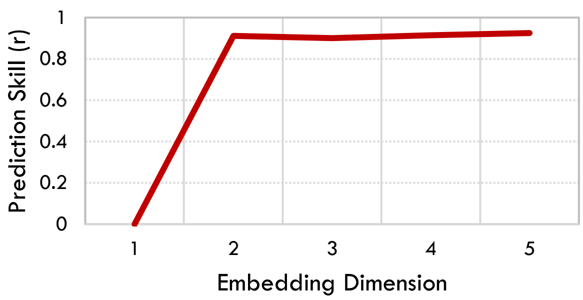

Figure 4. Simplex projection prediction skill based on embedding dimensions.

Choosing a small embedding dimension may result in overlapping points in the phase space, while selecting a large embedding dimension may cause the points to be far separated from each other (Lang et al., 2022; Agarwal et al., 2023). Consequently, the prediction accuracy has been evaluated by increasing the embedding dimension and observing the resulting change in accuracy. Figure 5 illustrates the variations in performance metrics based on the embedding dimension. The embedding dimension value that yielded the lowest prediction error and the maximum prediction accuracy has once again been determined to be 2.

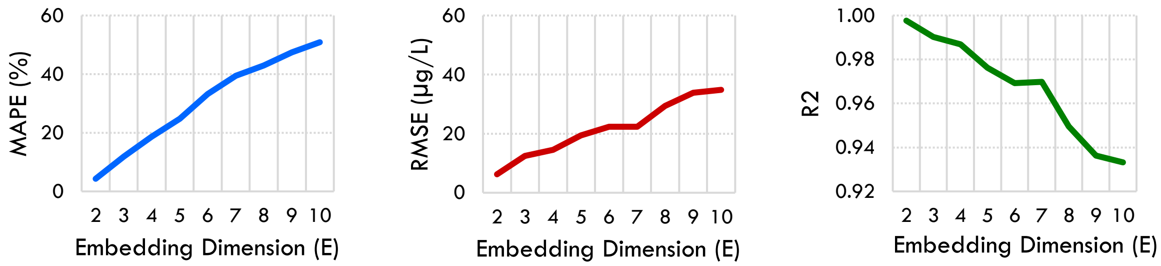

Figure 5. Change of performance criteria based on embedding dimensions.

The chl-a data 3d attractor is illustrated in Figure 6. x, y, and z are defined as $x(t)$, $x(t-\tau)$, and $x(t-2\tau)$, respectively.

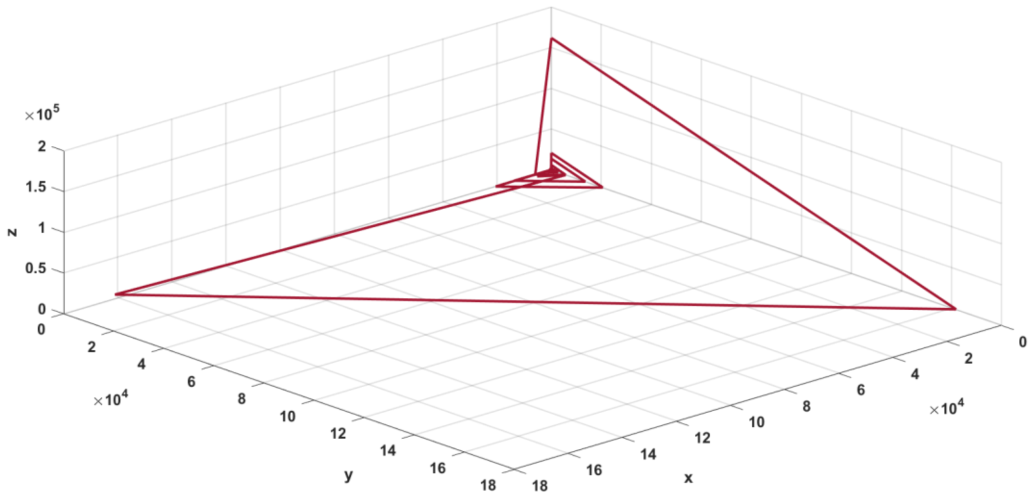

Figure 6. The attractor of chl-a data.

Based on Figure 6, it can be concluded that the chl-a data exhibits chaotic behavior. This is because the limit cycles ($\lambda = 0$) appear to be diverging from each other ($\lambda > 0$), suggesting that small perturbations in the system could grow over time, leading to chaotic behavior.

For this study, 80% of the data is allocated for the library, while the remaining 20% is set aside for prediction. The predicted and observed chl-a data are shown in Figure 7. The x-axis of the graph displays a time interval that corresponds to 20% of total data due to the irregularity in HAB data collecting. This figure clearly demonstrates that EDM is highly effective in making accurate predictions, particularly in accurately capturing the dynamics of the nonlinear chl-a data.

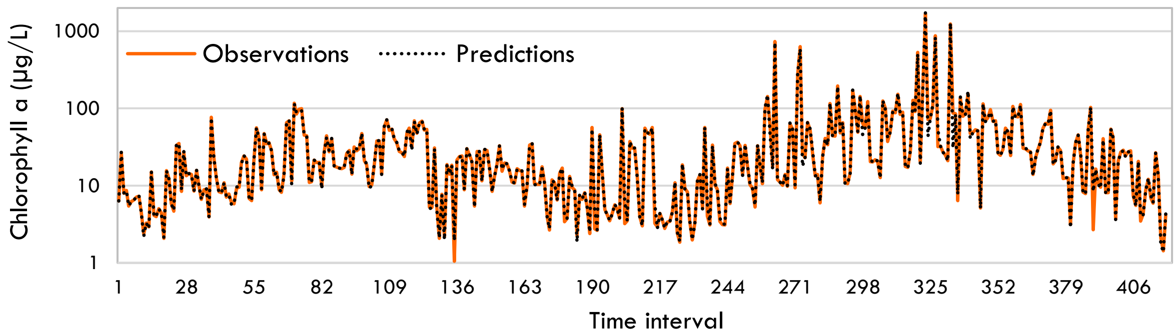

Figure 7. The observed and the predicted chl-a data based on time interval.

Table 1 shows the chl-a prediction model performance results. Mean absolute percentage error (MAPE), root mean square error (RMSE) and coefficient of determination (R2) are used as performance indicators. Chl-a prediction using EDM has been evaluated using a comprehensive set of performance metrics, including MAPE, RMSE, and R^2. As presented in Table 1, the model demonstrated outstanding performance, achieving a MAPE of 4.31%, RMSE of 6.24, and an R^2 of 0.98. These results indicate that the EDM model can accurately capture the underlying dynamics of chlorophyll-a variations.

Table 1. Performance criteria of chl-a prediction using EDM.

Performance criteria	
MAPE (%)	4.31
RMSE (μg/L)	6.24
Coefficient of determination (R^2)	0.98

4. Conclusion

To address the HAB problem, exacerbated by the impacts of climate change on public and environmental health, it is imperative to accurately identify the problem and make future predictions. Based on this perspective, an important indicator of HABs, known as chl-a, has been predicted via EDM.

As mentioned before, the key obstacle in HAB prediction research is the lack of data and intermittency. The reason for the intermittency is that HABs occur during the summer months (May to October). Another factor that complicates prediction research is the lagged impacts of climate on HABs. Furthermore, it may be asserted that the challenges associated with manual, long-term water monitoring and disruptions in water analysis also have a significant impact on prediction studies. Despite several challenges, it is evident that EDM effectively simulates chaotic data, such as chl-a. In this study, the model's ability to predict both short-term and long-term trends in chl-a concentrations suggests its potential for operational applications in water quality management.

Utilizing water quality metrics, meteorological factors, and physical features such as distances to agricultural and industrial fields may enhance the efficacy of models in predicting and modeling harmful algal bloom (HAB) indicators like chl-a. Furthermore, employing physics-based machine learning techniques (Baydaroğlu et al., 2024) instead of relying solely on machine learning models or traditional approaches can yield more accurate prediction results.

Data Availability

Chl-a data: https://www.ncei.noaa.gov/metadata/granule/geoportal/#searchPanel

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