Spatially referenced Bayesian state-space model of total phosphorus in western Lake Erie

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Abstract. Collecting water quality data across large lakes is often done under regulatory mandate; however, it is difficult to connect nutrient concentration observations to sources of those nutrients and to quantify this relationship. This difficulty arises from the spatial and temporal separation between observations, the impact of hydrodynamic forces, and the cost involved in discrete samples collected aboard vessels. These challenges are typified in Lake Erie, where bi-national agreements regulate riverine loads of total phosphorus (TP) to address the impacts from annual harmful algal blooms (HABs). While it is known that the Maumee River supplies 50 % of the nutrient load to Lake Erie, the details of how the Maumee River TP load changes Lake Erie TP concentration have not been demonstrated. We developed a hierarchical spatially referenced Bayesian state-space model with an adjacency matrix defined by surface currents. This was applied to a 2 km-by-2 km grid of nodes, to which observed lake and river TP concentrations were joined. The model generated posterior samples describing the unobserved nodes and observed nodes on unobserved days. We quantified the impact plume of the Maumee River by experimentally changing concentration data and tracking the change in in-lake predictions. Our impact plume represents the spatial and temporal variation of how river concentrations correlate with lake concentrations. We used the impact plume to scale the Maumee River spring TP load to an effective Maumee River TP spring load for each node in the lake. By assigning an effective load to each node, the relationship between load and concentration is consistent throughout our sampling locations. A linear model of annual lake node mean TP concentration and effective Maumee River load estimated that, in the absence of the Maumee River load, lake concentrations at the sampled nodes would be 23.1 µg L⁻¹ (±1.75, 95 % CI, credible interval) and that for each 100 t of spring TP effective load delivered to Lake Erie, mean TP concentrations increase by 11 µg L⁻¹ (±1, 95 % CI). Our proposed modeling technique allowed us to establish these quantitative connections between Maumee TP load and Lake Erie TP concentrations which otherwise would be masked by the movement of water through space and time.

1 Introduction

In a collective response to the economic, human health, and environmental damage caused by pollution, assessing water quality is a regulatory mandate across many water bodies. In many aquatic ecosystems nutrient concentrations are a primary water quality analyte collected. Observed concentrations are driven by both point and non-point sources. For example, wastewater effluent and excessive nutrient export, primarily from agricultural watersheds, may lead to eutrophication and harmful algal blooms (HABs) and threatens drinking water contamination (Brooks et al., 2016; Mellios et al., 2020; Schneider and Bláha, 2020). Individual water bodies present data collection challenges, particularly large lakes. Even for those locations with well-funded sample collection schema, trying to describe the spatiotemporal heterogeneity in nutrients is difficult. Discernible trends are difficult to assess as samples represent discrete spatial data within a sys-
Bayesian inference can quantify uncertainty in the effect of et al., 2005), and fishery stocks (Meyer and Millar, 1999).

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The challenge is that nutrients in the lake move with the wa-
ter currents, resulting in a complex relationship of upstream

and downstream current dependence. Moreover, within-lake

phosphorus cycling is dynamic and impacted by biological

and physical processes (Li et al., 2021; Matisoff et al., 2016).

Additionally, the time between sampling events within this
time series and the size of the lake–river system where mod-
els need to be applied inherently adds uncertainty and re-
duces the predictive efficacy of transport models linked with
hydrodynamic models (Schwab et al., 2009).

Bayesian state-space models have been used in ecology to
incorporate temporal and spatial autocorrelation and quan-
tify observation error separate from the error attributable to
the modeled ecological process (Auger-Méthé et al., 2021;
Durbin and Koopman, 2012; Shumway and Stoffer, 2019).
State-space models are widely used in ecology to model an-
imal populations (Buckland et al., 2004), movement (Royer
et al., 2005), and fishery stocks (Meyer and Millar, 1999).
Bayesian inference can quantify uncertainty in the effect of

nutrient load on nutrient distribution within a dynamic sys-
tem such as Lake Erie. Non-stationary time-series models
have been used in the Great Lakes to model water levels (La-
mon and Stow, 2010; Sellinger et al., 2008) and to predict
polychlorinated biphenyl concentration in trout (Stow et al.,
2004). The goal of this study was to use a spatially depend-
time-series state-space model approach to define concen-
trations at unobserved locations and quantify the impact of
river nutrient delivery across western Lake Erie. While
spatial models have been used in the Great Lakes for predict-
ing HAB biomass, HAB extent, and nutrient transport (Fang
et al., 2019; Schwab et al., 2009), we proposed a Bayesian
framework for similar spatial data. We showed that phospho-
rus concentration, along with an informed uncertainty, can
be estimated by state-space models that incorporate concen-
tration data from within the lake, the rivers, and lake surface
currents. Although this approach is informed by the currents,
it is does not include all the explicit biogeochemical and
physical processes that are part of mechanistic models (Rowe
et al., 2019). Our contribution to the ecological state-space
model methodology is the incorporation of a surface-current-
derived adjacency matrix, combined disparate agency field
data, and inclusion of data from rivers as sources of infor-
mation in fitting estimated values within a system dominated
by missing values. Together our contribution will fit values
in the absence of observations and allow experimentation in
archival data previously not possible. Here, we quanti-
fied how well our model fits the data and generated predic-
tions of total phosphorus (TP) concentrations across western
Lake Erie. TP includes the dissolved and particulate forms
of phosphorus. Additionally, we experimentally manipulated
observed concentrations to estimate the spatial and tempo-
ral impact from the Maumee River plume. Using this delin-
eated Maumee River impact in time and space, we tested the
hypothesis that when water movement is incorporated, there
is a linear relationship between river load and western Lake
Erie water TP concentrations.

1.1 Study area and data curation

We limited the model spatial window to western Lake Erie
(bounded by the portion of the lake west of −83.1° W, Fig. 1),
which left ~ 600 km² to be defined. We gathered sur-
face concentrations of TP (µg L⁻¹) from publicly available
databases through Environment Climate Change Canada’s
Offshore Water Quality Survey, the US Environmental Pro-
tection Agency’s Great Lakes National Program Office, the
Canadian Ministry of the Environment, the Conservation
and Parks Great Lakes Intake program, the US National
Oceanographic and Atmospheric Administration (NOAA)
Great Lakes Environmental Research Laboratory (GLERL)
Ecosystem Dynamics Long-Term Research program, and
NOAA GLERL Western Lake Erie (WLE) Sampling (Ta-
ble A1). The data used here extended from 2008 to 2018.
For riverine TP concentrations from the Maumee River
Figure 1. Map showing the location of the study region in western Lake Erie. The inset map shows the tributaries and lake nodes that were included in the model. Our site boundary was defined by the western portions of Lake Erie. A grid of 2 km-by-2 km nodes was used to snap existing concentration data and define an adjacency matrix based on surface currents.

and Raisin River across the 2008–2018 interval, we downloaded data from the National Center for Water Quality Research (NCWQR) at Heidelberg University (Table A1). When multiple samples were collected from a node on a single day, the sample average was used.

1.2 Model description

We created a model where day \( t \) TP concentrations are predicted based on the concentrations “upstream” at day \( t - 1 \). The spatial adjacency of “upstream” relationships was defined by the direction and magnitude of surface currents.

To build our adjacency matrix, we first defined a hypothetical distance and direction that surface water moved based on surface currents. We used surface current data retrieved from the NOAA Great Lakes Coastal Forecasting System (GLCFS, Table A1) database. These data are defined by hourly eastward and northward water velocity (m s\(^{-1}\)) predicted across Lake Erie on a 2 km-by-2 km grid (Fig. 1). Hourly northward and eastward velocity (m d\(^{-1}\)) for each node for the years 2008 to 2018 defined surface current direction in radians (\( d_{\text{Lat}} \) and \( d_{\text{Lon}} \)) using the node latitude (\( \text{Lat}_0 \)) and longitude (\( \text{Lon}_0 \)), the Earth’s radius (\( R, 6378137 \) m), the northward velocity offset in meters (\( dN \)), and the eastward offset in meters (\( dE \)) (Eqs. 1 and 2). The direction the surface water travelled in radians was used to determine the latitude (\( \text{Lat}_1 \)) and longitude (\( \text{Lon}_1 \)) represented by each hourly movement (Eqs. 3 and 4) and was repeated for 24 h until the final position of the surface water movement from each node was determined (Fig. B1).

\[
d_{\text{Lat}} = \frac{dN}{R} \quad (1)
\]

\[
d_{\text{Lon}} = \frac{dE}{R \cdot \cos \left( \frac{\pi}{180} \cdot \text{Lat}_0 \right)} \quad (2)
\]

\[
\text{Lat}_t + 1 = \text{Lat}_t + d_{\text{Lat}} \cdot \left( \frac{180}{\pi} \right) \quad (3)
\]
Log-transformed TP concentration observations \((y_{model})\) variable \((x)\) of data \((y)\) where \(x\) for nodes in the lake, \(n\) for nodes in the river, \(t\) which transported TP to node \(k\) on day \(t\) with the node \(k\) on day \(t - 1\). The state-space model consists of two models, an observation model of data \((y)\) and a latent state \((x)\) process model.

\[
y_{n,t,y} \sim N \left( x_{n,t,y}, \sigma^2 \right) \tag{5}
\]

Log-transformed TP concentration observations \((y)\) at the \(r\)th node on the \(t\)th day of the \(y\)th year were estimated with a normal data model sampled from the unobserved latent state variable \((x)\) at the \(n\)th node on the \(t\)th day of the \(y\)th year with standard deviation \(\sigma\) (Eq. 5). The process model is a first-order Markov, only depending on the value of the node at time \(t - 1\) which transported TP to node \(n\) at time \(t\); that source node is denoted \(k\). For nodes in the river, \(k = n\), and for nodes in the lake, \(k\) is determined from the time \(t\) adjacency matrix.

\[
x_{n,t,y} \sim \text{truncated} \left( f \left( x_{n,t-1,y}, \tau^2 \right) I \left( a \leq x_{n,t,y} \leq b \right) \right), \tag{6}
\]

where

\[
f \left( x_{n,t-1,y} \right) = \begin{cases} 
    x_{k,t-1,y} \cdot \beta_{\text{mau}} & \text{if } n = \text{Maumee River node}, \\
    x_{k,t-1,y} \cdot \beta_{\text{rau}} & \text{if } n = \text{River Raisin node}, \\
    x_{k,t-1,y} \cdot \beta_{\text{self}} & \text{if } n = \text{same lake node}, \\
    x_{k,t-1,y} \cdot \beta_{\text{lake}} & \text{if } n = \text{different lake node}.
\end{cases} \tag{7}
\]

The latent state \((x_{n,t,y}, \text{Eq. 6})\) is sampled from a normal distribution of a predicted latent state \((f(x_{n,t-1,y}, \text{Eq. 7}))\) and standard deviation \(\tau\). \(x_{n,t,y}\) was truncated by the detection limit of TP laboratory analysis \((5 \mu g L^{-1}, a, \text{Eq. 6})\) and the maximum value observed in each year \((y)\) within the Maumee River \((b, \text{Eq. 6})\). The maximum observed Maumee River concentration was used as the upper truncating value because no observation in the lake will exceed this value. Priors were uninformative and defined as

\[
\begin{align*}
\sigma, \tau & \sim \text{Gamma} (0.001, 0.001), \\
\beta_{\text{self}}, \beta_{\text{lake}} & \sim \text{Normal} (0, 10000), \\
\beta' & \sim \text{Normal} (0, 10000), \\
\tau_{\text{mau}}, \tau_{\text{rau}} & \sim \text{Gamma} (0.001, 0.001), \\
\beta_{\text{mau}} & \sim \text{Normal} \left( \beta', \tau_{\text{mau}}^2 \right), \\
\beta_{\text{rau}} & \sim \text{Normal} \left( \beta', \tau_{\text{rau}}^2 \right).
\end{align*}
\]

River model coefficients \((\beta_{\text{mau}} \text{ and } \beta_{\text{rau}})\) were fit hierarchically \((N(\beta', \tau^2))\) because the ecological and anthropogenic processes enacted on these watersheds are similar, if at different scales. The two lake models were fit with two independent \(\beta\) coefficients depending on whether the nearest adjacent node \(k\) is the same as the estimated node \(n\) \((\beta_{\text{self}})\) or whether a different node \(k\) is nearest \((\beta_{\text{lake}})\). Separate independent in-lake models were used to capture different potential drivers of TP concentration through time depending on whether each node was subject to little surface water movement \((\beta_{\text{self}})\) or active surface water movement \((\beta_{\text{lake}})\). In 2012 there were no Raisin River observations, and so the model in 2012 treats the Raisin River node as a lake node. The model was run in R (version 4.0.2) and JAGS (version 4.3.0) (Eddelbuettel, 2017; Microsoft Corporation and Weston, 2020; Plummer, 2019). Each year’s model iteration count was 50 000 with a thin of 10, representing 5000 effective samples along three independent Markov chains. The chain convergence was monitored by Gelman and Rubin’s convergence diagnostic. Scale factors less than 1.1 were used to define when chains had converged (Plummer, 2019). Initial conditions for the latent state \((x_{n,t=1,y})\) were defined as the mean and variance of the previous year’s first 20 d. The first year’s \((y)\text{ year 2008})\) initial conditions were estimated as \(N(12, 5)\) (Rockwell et al., 2005). The goodness of fit of the models was described via posterior predictive \(p\) values (Gelman, 2013) and Bayesian \(R^2\) (Gelman et al., 2019), while the performance between years and across nodes was assessed with \(K\)-fold cross-validation (CV) utility (Geisser and Eddy, 1979; Piironen and Vehtari, 2017) (Eq. 8).

\[1.2.2 \text{ Fitting the SSM and diagnostics}\]

Posterior predictive \(p\) values were calculated by model year with test statistic mean TP concentration to compare means

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of observations to the means of the model outputs. For each year, a posterior p-value distribution was described by 15,000 bootstraps of 100 resamples from the observed node posteriors. Bayesian $R^2$ defined as the fitted variance ($\text{var}_{\text{fit}}$) divided by the sum of $\text{var}_{\text{fit}}$ and the residual variance ($\text{var}_{\text{res}}$) was calculated for each model year. Model $\text{var}_{\text{res}}$ was the variance of the modeled predictive mean, while $\text{var}_{\text{res}}$ is estimated by squared standard deviation of the errors (Gelman et al., 2019).

$K$-fold CV utility compared model predictive performance across years and across nodes. The cross-validation via leave one node out was used to evaluate model predictions where observations are not available. This estimate of model performance is needed as our data set has far fewer observations than the product of nodes and time points, and estimates of $R^2$ report how well the model does while given all the available data. Additionally, the cross-validation estimates aggregated by unobserved node (space) or by year (time) define how well the model estimates TP values irrespective of the node’s proximity to the TP river sources or the number and location of annual in-lake observations. The cross-validated utility was applied by removing all $d$ observations from a randomly selected node $k$ with at least 10 observations collected during the model year. $K$-fold CV was calculated three times per year; for years that had fewer than three nodes with at least 10 observations, all nodes that satisfied the 10-observation cut-off were used. $K$-fold CV, the mean leave-one-node-out log-predictive density from posterior samples of the omitted $d$ observation $\hat{y}_{k,t,y}$ at node $k$, day $t$, and year $y$, were compared to observed concentrations at $y_{k,t,y}$ (Piironen and Vehtari, 2017) (Eq. 8).

$$K\text{-fold CV}_{n,y} = \frac{1}{d} \sum_{d=1}^{D} \log p\left(\hat{y}_{k,t,y} | y_{k,t,y}\right)$$  \hspace{1cm} (8)

Using a model that describes posterior predictive distributions of mean $K$-fold CV across years and nodes, we examined whether our state-space approach preferentially generated predictions for certain years or certain nodes that contain the observed values (Eqs. 9 and 10); 95% credible differences between group means (for nodes $\mu_n$ or for years $\mu_y$) that do not contain 0 were used to determine whether groups were different (e.g., if the 95% credible difference from $\mu_{2018}$ to $\mu_{2017}$ contains 0, these means are not considered different).

$$K\text{-fold CV}_{n} \sim N\left(\mu_{on} + \frac{1}{n} \sum_{n} \mu_n, \sigma_{\mu_n}^2\right)$$  \hspace{1cm} (9)

$$K\text{-fold CV}_{y} \sim N\left(\mu_{oy} + \frac{1}{y} \sum_{y} \mu_y, \sigma_{\mu_y}^2\right)$$  \hspace{1cm} (10)

$\mu_{on}$ and $\mu_{oy}$ were fit with normal priors ($N(0,1,\sigma_{\mu}^2)$) and $\sigma_{\mu}$, which functions as the within-group variance has a gamma prior with rate and shape estimated from the mode and standard deviation of the $K$-fold CVs (Kruschke, 2015, p. 560). Finally, $\sigma_n$ and $\sigma_y$, which represent the between-group variance, were fit with a uniform prior (uniform(100–1, $\sigma_{KFCV}$, 10·$\sigma_{KFCV}$)). $\sum \mu_n$ and $\sum \mu_y$ were constrained to 0 when fitting $\mu_{on}$ and $\mu_{oy}$.

### 1.3 Model experimentation

Our state-space models were used to test the hypothesis that western Lake Erie TP concentrations are a linear function of Maumee River TP load when surface water movement is incorporated. We incorporate water movement into our linear model by first estimating the spatial impact of the Maumee River. The Maumee River impact plume was estimated by artificially reducing the Maumee River TP concentrations by 50% ($\hat{y}_{\text{Maumee},t,y}$); each year’s model was then refit (Eqs. 5–7). The model output for each node was examined, and the position of each node’s concentration ($\hat{y}_{n,t,y}$) 95% PI (predictive interval) was compared to the original model ($y_{n,t,y}$). The change from the original 95% PI of $y_{n,t,y}$, which we call the deflection, was interpreted as evidence that the Maumee River node was, at some time step, influencing node $n$. The annual mean root-squared sum of the $\hat{y}_{n,t,y}$, 95% PI change compared to the $y_{n,t,y}$ was then normalized by the largest value for that model year (y); this normalized estimate of PI change ($d_{n,y}$) across the 254 nodes within our spatial window was used to define effective Maumee River spring TP impact within Lake Erie. We estimated Maumee River spring load estimates ($l_y$, tons TP) by multiplying NCWQR daily flow and TP concentration data (Table A1) from 1 March to 31 July annually. Finally, we multiplied $d_{n,y}$ and $l_y$ to represent a spatially explicit effective Maumee River spring TP load at each node ($\hat{l}_{n,y}$).

A linear model of mean TP concentration ($\bar{y}_{n,y}$) per year per node ($n$, where node $n$ had at least one observation) as a function of effective spring Maumee River TP load ($\hat{l}_{n,y}$) was used to test for a linear relationship between Maumee River and Lake Erie surface water TP concentrations. The model was fit in a Bayesian framework, which allowed us to fit the heteroscedastic relationship of concentration and effective load by fitting a positive linear relationship to model variance and effective load (Eq. 11). $\beta_{1,2}$ were given non-informative normal priors ($N(0,1,\frac{1}{0.001^2})$), while $\alpha_{1,2}$ were given non-informative log-normal priors ($\log N (0,1,\frac{1}{0.001^2})$) because they must be positive random variables.

$$\bar{y}_{n,y} \sim N\left(\beta_1 + \beta_2 \cdot \hat{l}_{n,y}, (\alpha_1 + \alpha_2 \cdot \hat{l}_{n,y})^2\right)$$  \hspace{1cm} (11)

### 2 Results

The annual data sets defined by TP concentration observations and riverine TP data on our 2 km-by-2 km grid in
western Lake Erie contained an average of 99.1 % missing values. The number of nodes that contained observations ranged from 14 to 40 among years. The mean number of samples available at each observed lake node during the model year ranged from 2 to 9. Within the 252 Lake Erie nodes across the available 11 years, a total of 1218 observations were collected; our hierarchical spatially referenced Bayesian state-space model was then able to provide estimates for the 375 774 unobserved TP concentrations. Between the Maumee River and Raisin River, a total of 2258 observations were available in the data set, and the missing 734 values were also described by posterior distributions. The mean values of the observed TP concentrations within the Maumee River, Raisin River, and western Lake Erie were 170 µg L$^{-1}$ (95 % interval, 3.5 to 438 µg L$^{-1}$), 80 µg L$^{-1}$ (95 %, 40 to 215 µg L$^{-1}$), and 38 µg L$^{-1}$ (95 %, 10 to 203 µg L$^{-1}$), respectively.

### 2.1 State-space model fit

To assess the goodness of fit of the model, we determined annual Bayesian $R^2$, posterior predictive $p$ values, and $k$-fold CV utility. The 11 years of models had mean Bayesian $R^2$ values from 0.84 to ~1 and mean posterior predictive $p$ values from 0.42 to 0.59 (Table 1). Posterior predictive $p$ values of 0.5 indicate a good fit between model output and observations, and the 95 % CI of all our yearly posterior $p$-value distributions contains 0.5. Finally, the results of the $k$-fold cross-validation utility 95 % credible difference showed no difference across all pairwise comparisons of mean $K$-fold CV by year or node.

![Image](image-url)

**Table 1.** Bayesian model assessment via $p$ value (posterior predictive $p$ values of 0.5 are indicative of a good fit and 95 % CI (credible interval) of our yearly results, each containing 0.5), and $R^2$ (each year > 0.8) showed the model-generated posterior samples similar in structure to the observations.

| Year | Posterior predictive $p$ values | $R^2$ |
|------|-------------------------------|-------|
|      | 95 % CI | 95 % CI |
| 2008 | 0.4 | 0.6 | 0.987 | 0.999 |
| 2009 | 0.49 | 0.68 | 0.965 | 0.978 |
| 2010 | 0.4 | 0.59 | 0.838 | 0.882 |
| 2011 | 0.37 | 0.56 | 0.995 | 1 |
| 2012 | 0.4 | 0.6 | 0.994 | 1 |
| 2013 | 0.32 | 0.51 | 0.914 | 0.974 |
| 2014 | 0.4 | 0.59 | 0.936 | 0.974 |
| 2015 | 0.37 | 0.57 | 0.931 | 0.969 |
| 2016 | 0.41 | 0.6 | 0.925 | 0.962 |
| 2017 | 0.41 | 0.61 | 0.993 | 1 |
| 2018 | 0.39 | 0.59 | 0.995 | 1 |

### 2.2 State-space model outputs

Posterior distributions for each node on each day provide estimates for TP concentrations where observations are present and in the absence of observations (2018 in Fig. 2, 2008–2017 in Appendix D). Mean and 95 % PI model posterior samples of each node at every day defined our predicted concentration. By example, the Maumee River node in 2018 shows the model following the data and widening PIs where observations are missing (Fig. 2a). For Lake Erie nodes that contained observations, the posterior samples follow the broad trend in the observed data (Fig. 2b). Nodes without any observations also follow the trend in downstream observed nodes, and while the uncertainty is larger at unobserved nodes, the PIs stay within expected values (Fig. 2c).

### 2.3 Model experimentation

After artificially reducing the Maumee River concentrations by 50 %, the nodes where TP concentration PIs were altered were defined as being within the Maumee River area of impact. The mean square root of each node’s summed squared deflection annually normalized by the largest mean value ($d_{n,y}$) in general was highest near the mouth of the Maumee. The impacted area spread south and east along the state of Ohio’s coast most years, but some years were subject to larger plumes distributed further north (Fig. 3, Video Supplement 1).

The normalized annual mean Maumee impact estimates ($d_{n,y}$) generated per node were used to adjust spring load to an effective spring load ($l_{n,y}$) at each node where samples were collected. Lake Erie TP concentration was linearly correlated with the effective Maumee River TP spring load (mean node concentration = 23.1 (±1.75, 95 % CI) + 0.11 (±0.01, 95 % CI) × effective spring load (tons TP); Fig. 4). The heteroscedastic error in the mean concentration ($\gamma_{n,y}$) and effective load ($l_{n,y}$) relationship was defined by a linear function ($\alpha_1 + \alpha_2 \cdot l_{n,y}$). $\alpha_1$ was estimated to be 2.9 (±1.4, 95 % CI), and $\alpha_2$ was 0.04 (±0.008, 95 % CI).

### 3 Discussion

#### 3.1 State-space model fit

By combining the western Lake Erie TP observations with riverine data and surface currents within a Bayesian model framework, we were able to generate estimates of TP across time and space. The models consistently generated plausible posterior samples for mean TP concentration as each 95 % CI of annual posterior predictive $p$ values included 0.5, and annual Bayesian $R^2$ 95 % CI values ranged from 0.84 to 0.99 (Table 1). Annual posterior predictive $p$ values indicate that our model framework is performing well in predicting water quality within large water bodies, even with sparse observations within the data. While our high Bayesian $R^2$
Figure 2. For 2018 the total phosphorus concentrations (µg L$^{-1}$) at observed and unobserved nodes were estimated from the model posterior samples. Mean (solid black line) and 95 % PI (dashed blue line) for the model posterior samples of each node at every day for (a) the Maumee River, (b, c, e, f) western Lake Erie nodes, and (d) the Raisin River.
values appear to support the use of our model, it is likely that they represent an inappropriate model metric. The state-space framework forces the model to pass through the observed data, and the daily observations in the river data sets (Fig. 2a and d) are likely driving Bayesian $R^2$ values higher with their constrained predictive intervals. Because of these elevated Bayesian $R^2$ estimates, the $k$-fold CVs are important checks on the applicability of this state-space approach. The $k$-fold CV results generated by removing all the observations of a randomly selected lake node with at least 10 observations showed that model predictions were equally accurate across years and by node. Predicting equally well across the nodes and within any year provides strong support for this framework as being a useful application of Bayesian methods in water quality modeling.

TP is a conservative water quality constituent. TP observations are insensitive to biogeochemical transformations of phosphorus form because these data represent both the organic and inorganic forms of phosphorus occurring in the water column. $\beta_{\text{Mau}}, \beta_{\text{Ras}}, \beta_{\text{Lake}},$ and $\beta_{\text{Self}}$ fit in our models had 95% predictive intervals encompassing a value of 1. Coefficients were close to 1 because, on our daily time step, the TP concentrations do not widely vary (e.g., the concentration today is similar to the concentration yesterday). The uncertainty in the process and data models allows the model predictions to trend toward the observations where available and be constrained where previous time steps passed through observations. Were these coefficients to exceed 1, this would be evidence of other inputs of $P$ or less that 1 would indicate some internal loss such as settling or dilution. TP is conservative to processes within the water column because it accounts for the dissolved and particulate $P$; if our model was applied only to dissolved $P$, which is subject to strong assimilation pressure by phytoplankton, the model coefficients would likely be negative. While dilution, settling, and internal loading of TP are happening within our modeled extent in western Lake Erie, our model lacks the specificity to capture dilution, settling, and internal loading, and therefore their effect is being accumulated in our error terms. However, this state-space framework could be defined with a mechanistic process model that did capture these effects. Additionally, while our framework could be implemented with the coefficients ($\beta_{\text{Mau}}, \beta_{\text{Ras}}, \beta_{\text{Lake}},$ and $\beta_{\text{Self}}$) fit hierarchically by year potentially defining the overall effect of dilution, set-
The lack of coefficients (Auger-Méthé et al., 2021) (Fig. C1a and b). By visually determining whether priors dominated the fit of spatial and temporal models, it could be effective. To prevent accurate outputs estimating TP concentrations at observed nodes yet model uncertainties are within the range of TP concentrations expected for western Lake Erie. Nodes along the eastern perimeter of the spatial window of our model have additional uncertainty inherent in their position. Occasionally, they will not be associated with the proper “down-gradient” node because the extent removes those nodes. Within our system there is little practical effect as these nodes are far from the Maumee River and are dominated by low concentrations. This is a potential problem in other systems and may necessitate wider spatial windows to eliminate.

Our model framework allows information from discrete grab samples to be shared across any water body where the movement pattern of water is available. Additionally, this model can generate estimates at unobserved nodes or at unobserved time steps of observed nodes without requiring defined biogeochemical processes of a mechanistic model. For our application, the 2 km-by-2 km grid was chosen to match the surface current data set. While we did not experiment with other grid distances, any applicable configuration will work. Defining a reasonable grid distance could be based on the spatial distribution of the available data and the user’s willingness to extrapolate or average surface current direction and magnitude. Similarly, our temporal time step was daily, but this could also be applied to monthly data in data-sparse systems or hourly data in data-rich applications. This spatial and temporal flexibility or using state-space frameworks gives users the capacity to tune the computational runtime and resolution of models to fit the hypothesis tested.

Within Lake Erie, having estimates for unobserved nodes and nodes that are infrequently sampled allows a connection between discrete point data collected by boat and data layers which cover large sections of a lake surface. The spatial distance and temporal disconnect between the data generated by multiple actors on the same water body often preclude the combined use of data from multiple projects. However, state-space models which explicitly incorporate time as well as space via water movement could harness more of the available data to make predictions beyond the spatial bounds of the original projects. For example, remotely sensed data layers would be especially useful in this model structure, both as predictor variables and as the response variables. Connecting estimates of TP concentrations to chlorophyll-a concentrations would enhance existing predictive models of cyanobacteria distribution and biomass (Fang et al., 2019).

The agencies and organizations collecting grab samples within Lake Erie would also be able to use the state-space model output to select sample locations specific to hypotheses. The model can be used to predict the movement of high nutrient water masses which investigators could target. Additionally, projects examining the impact of the Maumee River

![Figure 4. Mean concentration at the observed nodes for each year was modeled as a function of the relative Maumee River spring TP load (mean concentration = 23.1 (±1.75, 95 % CI) + 0.11 (±0.01, 95 % CI) × effective load), where variance in concentration increased linearly with effective load. Effective load was defined by multiplying the normalized river impact generated by experimentally tracing the Maumee River’s impact on Lake Erie nodes annually; 95 % predictive intervals of the data (green dotted lines) and 95 % credible intervals of the linear relationship (blue solid lines) were generated from the model output.](https://doi.org/10.5194/hess-26-1993-2022)
could sample in and out of the Maumee River impact plume. Beyond the impact on fieldwork, this modeling approach can also be used in model selection. Since this modeling approach is based entirely on observations in the absence of independent explanatory variables, it should be used as a benchmark model for future mechanistic or more complex models to be tested against.

3.3 Model experimentation

Having demonstrated the functional capacity of our hierarchical spatially referenced Bayesian state-space model predicting TP concentrations, our hypothesis was that a linear relationship exists between spring Maumee River load and observed Lake Erie concentrations. By experimentally reducing the concentrations for the Maumee River and rerunning the model, we were able to track the “downstream” repercussions for the lake-node-predicted values and to infer the Maumee River impact plume. Tracking a plume of TP impact using the grab samples was not previously possible because of the distances between sampling locations and the fact that the number of unobserved days outnumbers the observed days. Distance and direction across our model extent are wrapped up in the change observed in predictive intervals through time. In our framework distance and whether the water mass from the Maumee River physically moves toward a node combine. There are several days in which even the nodes closest to the Maumee River are bypassed because the currents take Maumee River water in a different direction. The dual complications of distance and movement have complicated previous attempts at defining a single relationship between Maumee River load and observed in-lake concentrations, which we overcome here.

The plume extent in general follows the southern coast (Fig. 3), which would be expected because of the movement associated with the Coriolis effect. Importantly, this is not a plume that displays a high concentration of TP; rather, this is the impact plume of the Maumee River. Concentrations outside the impact plume are not influenced, or are weakly influenced, by the Maumee River, and thus load reductions within the Maumee River would not impact lake concentrations in those areas. Our linear model (Eq. 11) estimated that when the effective load of the Maumee River was 0, the mean annual concentration in the area where samples were collected would be 23.1 µg L$^{-1}$ ± 1.75, 95 % CI.

Each year the Maumee River TP impact plume dimension and intensity changed. Rowland et al. (2019) demonstrated how a linear model of Lake Erie TP observations as a function of Maumee River spring loads defined positive relationships at the closest nodes. Here, we were able to fit parameters that define the load-to-concentration relationship across all of western Lake Erie. Much of the regulatory attention in addressing Lake Erie HABs has focused on Maumee River spring export, and providing this quantitative connection is important in furthering watershed TP reduction efforts. Our model estimated that for each 100 t of spring TP effective load delivered to Lake Erie, TP concentrations in the lake increase by 11 µg L$^{-1}$ (±1, 95 % CI). We could use our defined linear relationship for hindcasting expected concentration reductions in western Lake Erie based on Maumee spring TP loads which were reduced by 40 % for all our model years. Additionally, given a mean concentration maximum, we could predict the load reductions required in previous years to meet that target. Using our linear relationship between lake concentration and spring load to make forecasts for future years is harder. The size and shape of the Maumee River impact ($d_{n,y}$) change each year (Video Supplement 1), and our method defines the river impact from observations. Without being provided an estimate of $d_{n,y}$, a forecast of mean western Lake Erie TP concentrations based on a proposed spring TP load is not achievable. An achievable next step for this modeling framework could be to link the size of the Maumee River plume and Lake Erie TP concentrations to HABs biomass and toxin production; the spatial aspect of such a model could explain why the relationship between bloom biomass and Maumee TP export is not linear (Obenour et al., 2014).

4 Conclusions

Our state-space model framework was shown to fit the data well, generated reasonable estimates of concentration at observed and unobserved locations, was modified experimentally to estimate a river impact plume, and used the experimentally derived plume to test a regulatory relevant hypothesis. Adequately characterizing water quality in a large water body is difficult. Sampling and laboratory analysis are expensive and excessively time-consuming for feasibly covering even a portion of Lake Erie with high temporal and spatial resolution. However, we demonstrate that a Bayesian state-space framework informed by an adjacency matrix defined by surface currents can generate daily TP concentrations which are constrained by uncertainties appropriate for lake conditions. By combining the data from two rivers entering the lake, our model (Eqs. 5–7) enables the rivers to inform the observed and unobserved lake nodes, the observed lake nodes inform the unobserved lake nodes, and unobserved lake nodes also inform unobserved and observed nodes. This information sharing across time and space empowers this model to connect sparse data across large distances. By experimenting with the model, we were able to estimate a plume of impact from the Maumee River and to apply the experimental results to hypothesis testing. The model is amenable to using remote sensing data and can effectively connect lake-wide data sets with discrete grab samples. The application here used TP, but any analyte could be modeled in this same structure to generate estimates through time and space, test hypotheses, or build baseline models to test process-based models against.
Table A1. The data sources for total phosphorus concentrations and surface currents were all retrieved from publicly available online repositories.

| Agency | Link | Data type | n (2008 to 2018) |
|--------|------|-----------|------------------|
| Environment Climate Change Canada’s Offshore Water quality Survey | Digital object identifier: https://doi.org/10.18164/495eb10d-d423-432a-980f-264ef287d45b | Total phosphorus concentration (µg L\(^{-1}\)) | 121 |
| US Environmental Protection Agency’s Great Lakes National Program Office | https://cdx.epa.gov/ (last access: June 2021) | Total phosphorus concentration (µg L\(^{-1}\)) | 149 |
| Ministry of the Environment, Conservation and Parks Great Lakes Intake Program | http://files.ontario.ca/moe_mapping/downloads/2Water/GLIP/All_Lakes_GLIP.csv (last access: June 2021) | Total Phosphorus concentration (µg L\(^{-1}\)) | 637 |
| National Oceanographic and Atmospheric Administration (NOAA) Great Lakes Environmental Research Laboratory (GLERL) Ecosystem Dynamics Long-Term Research program | Digital object identifier: https://doi.org/10.25921/11da-3x54 | Total Phosphorus concentration (µg L\(^{-1}\)) | 111 |
| NOAA GLERL Western Lake Erie Sampling | Digital object identifier: https://doi.org/10.25921/11da-3x54 | Total Phosphorus concentration (µg L\(^{-1}\)) | 1145 |
| National Center for Water Quality Research at Heidelberg University | https://ncwqr-data.org/ (last access: June 2021) | Total phosphorus concentration (µg L\(^{-1}\)) | 2258 |
| NOAA Great Lakes Coastal Forecasting System | https://www.glerl.noaa.gov/res/glcfs/ (last access: June 2021) | Surface currents (meters north, meters east) | 1 020 318 |
Appendix B

Figure B1. Surface current data were available hourly within western Lake Erie. These 24 h data were used to track the daily movement of water from each node.

Appendix C

Figure C1. Non-informative priors were used to fit the state-space coefficients of the Maumee River ($\beta_{mau}$, all values represented as red polygons), Raisin River ($\beta_{ras}$), the western Lake Erie nodes subject to movement ($\beta_{lake}$, b red polygons), and those Lake Erie nodes which did not encounter sufficient water movement to associate with an “upstream” node ($\beta_{self}$). The fitted values for every year (a and b, all values represented as black polygons) do not appear to be overly influenced by the uninformed priors. The log data model and process model uncertainty (c) for every year were also well identified (the uncertainty $\sigma$ was logged to aid in visually comparing prior and fitted values).
Table C1. State-space models in western Lake Erie fit coefficients predicting TP concentrations from the previous time step within the Maumee River, the Raisin River, Lake Erie, and lake locations where the current time step is informed by the same location, $\beta_{\text{mau}}$, $\beta_{\text{rai}}$, $\beta_{\text{lake}}$, and $\beta_{\text{self}}$, respectively. The 95% PI (predictive interval) for each year and coefficient was examined. The same models fit the annual process model and data model precision.

| Year | $\beta_{\text{mau}}$ | $\beta_{\text{rai}}$ | $\beta_{\text{lake}}$ | $\beta_{\text{self}}$ | Process $\sigma$ | Data $\sigma$ |
|------|----------------------|----------------------|-----------------------|----------------------|----------------|----------------|
|      | 95% PI               | 95% PI               | 95% PI                | 95% PI               | 95% PI        | 95% PI        |
| 2008 | 0.989 1.008          | 0.985 1.013          | 0.986 0.999           | 0.963 1.012          | 0.263 0.331   | 0.02 0.098    |
| 2009 | 0.993 1.005          | 0.992 1.007          | 0.991 1.000           | 0.984 1.002          | 0.168 0.193   | 0.125 0.165   |
| 2010 | 0.994 1.003          | 0.993 1.006          | 0.988 0.994           | 0.992 1.001          | 0.13 0.183    | 0.326 0.404   |
| 2011 | 0.993 1.006          | 0.99 1.008           | 0.991 1.006           | 0.985 1.007          | 0.174 0.209   | 0.017 0.061   |
| 2012 | 0.993 1.007          | 0.804 1.186          | 0.997 1.008           | 0.983 1.005          | 0.177 0.218   | 0.017 0.062   |
| 2013 | 0.993 1.007          | 0.992 1.008          | 0.992 1.003           | 0.978 1.008          | 0.181 0.277   | 0.135 0.25    |
| 2014 | 0.992 1.005          | 0.99 1.006           | 0.991 1.001           | 0.991 1.018          | 0.173 0.235   | 0.145 0.232   |
| 2015 | 0.992 1.006          | 0.989 1.007          | 0.992 1.003           | 0.982 1.003          | 0.212 0.264   | 0.156 0.238   |
| 2016 | 0.993 1.005          | 0.991 1.005          | 0.996 1.004           | 0.983 1.001          | 0.161 0.2     | 0.146 0.214   |
| 2017 | 0.993 1.006          | 0.991 1.008          | 0.995 1.003           | 0.978 0.998          | 0.197 0.24    | 0.019 0.079   |
| 2018 | 0.992 1.007          | 0.99 1.008           | 0.983 0.991           | 0.966 0.997          | 0.221 0.26    | 0.018 0.065   |

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Figure D1. For 2008 the total phosphorus concentrations (µg L$^{-1}$) at observed and unobserved nodes were estimated from the model posterior samples. Mean (solid black line) and 95% PI (dashed blue line) for the model posterior samples of each node at every day for (a) the Maumee River, (b, c, e, f) western Lake Erie nodes, and (d) the Raisin River.
For 2009 the total phosphorus concentrations (µg L$^{-1}$) at observed and unobserved nodes were estimated from the model posterior samples. Mean (solid black line) and 95% PI (dashed blue line) for the model posterior samples of each node at every day for (a) the Maumee River, (b, c, e, f) western Lake Erie nodes, and (d) the Raisin River.
For 2010 the total phosphorus concentrations ($\mu g L^{-1}$) at observed and unobserved nodes were estimated from the model posterior samples. Mean (solid black line) and 95% PI (dashed blue line) for the model posterior samples of each node at every day for (a) the Maumee River, (b, c, e, f) western Lake Erie nodes, and (d) the Raisin River.
Figure D4. For 2011 the total phosphorus concentrations (µg L$^{-1}$) at observed and unobserved nodes were estimated from the model posterior samples. Mean (solid black line) and 95% PI (dashed blue line) for the model posterior samples of each node at every day for (a) the Maumee River, (b, c, e, f) western Lake Erie nodes, and (d) the Raisin River.
Figure D5. For 2012 the total phosphorus concentrations (µg L$^{-1}$) at observed and unobserved nodes were estimated from the model posterior samples. Mean (solid black line) and 95% PI (dashed blue line) for the model posterior samples of each node at every day for (a) the Maumee River, (b, c, e, f) western Lake Erie nodes, and (d) the Raisin River.
For 2013 the total phosphorus concentrations (µg L\(^{-1}\)) at observed and unobserved nodes were estimated from the model posterior samples. Mean (solid black line) and 95% PI (dashed blue line) for the model posterior samples of each node at every day for (a) the Maumee River, (b, c, e, f) western Lake Erie nodes, and (d) the Raisin River.
For 2014 the total phosphorus concentrations ($\mu$g L$^{-1}$) at observed and unobserved nodes were estimated from the model posterior samples. Mean (solid black line) and 95% PI (dashed blue line) for the model posterior samples of each node at every day for (a) the Maumee River, (b, c, e, f) western Lake Erie nodes, and (d) the Raisin River.
Figure D8. For 2015 the total phosphorus concentrations (µg L$^{-1}$) at observed and unobserved nodes were estimated from the model posterior samples. Mean (solid black line) and 95% PI (dashed blue line) for the model posterior samples of each node at every day for (a) the Maumee River, (b, c, e, f) western Lake Erie nodes, and (d) the Raisin River.
Figure D9. For 2016 the total phosphorus concentrations (µg L$^{-1}$) at observed and unobserved nodes were estimated from the model posterior samples. Mean (solid black line) and 95 % PI (dashed blue line) for the model posterior samples of each node at every day for (a) the Maumee River, (b, c, e, f) western Lake Erie nodes, and (d) the Raisin River.
Figure D10. For 2017 the total phosphorus concentrations (µg L$^{-1}$) at observed and unobserved nodes were estimated from the model posterior samples. Mean (solid black line) and 95 % PI (dashed blue line) for the model posterior samples of each node at every day for (a) the Maumee River, (b, c, e, f) western Lake Erie nodes, and (d) the Raisin River.
Code and data availability. Template code for reproducing our model is available publicly on Zenodo at https://doi.org/10.5281/zenodo.5570508 (Maguire et al., 2021a). All the data used here were from publicly available sources which we provide in Appendix A. On the Zenodo site we made our curated data for 2018 available.

Video supplement. A supplemental video of Maumee River impact plume through time is available through https://doi.org/10.5446/53429 (Maguire et al., 2021b).

Author contributions. TJM, CAS, and CMG designed the models, the model fitting quality control, and the model experiments. TJM developed the model code and performed the simulations. TJM prepared the manuscript with contributions from CAS and CMG.

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