A machine learning approach to water quality forecasts and sensor network expansion: Case study in the Wabash River Basin, USA

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Tyler Balson[1], Adam S. Ward[2,3]

1 - Luddy School of Informatics, Computing, and Engineering, Indiana University, Bloomington, IN, USA
2 - O'Neill School of Public and Environmental Affairs, Indiana University, Bloomington, IN, USA
3 - Biological & Ecological Engineering, Oregon State University, Corvallis, OR, USA

Abstract:
Midwestern cities require forecasts of surface nitrate loads to bring additional treatment processes online or activate alternative water supplies. Concurrently, networks of nitrate monitoring stations are being deployed in river basins, co-locating water quality observations with established stream gauges. However, tools to evaluate the future value of expanded networks to improve water quality forecasts remains challenging. Here, we construct a synthetic data set of stream discharge and nitrate for the Wabash River Basin - one of the U.S.'s most nutrient polluted basins - using the established Agro-IBIS and THMB models. Synthetic data enables rapid, unbiased, and low-cost assessment of potential sensor placements to support management objectives, such as near-term forecasting. Using the synthetic data, we established baseline 1-day forecasts for surface water nitrate at 12 cities in the basin using support vector machine regression (SVMR; RMSE 0.48-3.3 ppm). Next, we used the SVMRs to evaluate the improvement in forecast performance associated with deployment of additional nitrate sensors. We identified the optimal sensor placement to improve forecasts at each city, and the relative value of sensors at each candidate location. Finally, we assessed the co-benefit realized by other cities when a sensor is deployed to optimize a forecast at one city, finding significant positive externalities in all cases. Ultimately, our study explores the potential for machine learning to make near-term predictions and critically evaluate the improvement realized by expanding a monitoring network. While we use nitrate pollution in the Wabash River Basin as a case study, this approach could be readily applied to any problem where the future value of sensors and network design are being evaluated.

Keywords: water quality, forecast, machine learning, sensor network design, optimization

1. Introduction

Climate change will intensify the hydrologic cycle in the Midwestern U.S. (Cook et al., 2018; Ficklin et al., 2018; Le, 2011). Increased intensity and seasonality in precipitation (L. Wang et al., 2018) will exacerbate nonpoint source nutrient pollution (Loecke et al., 2017; Y. Wang et al., 2018). To cope with this pollution while meeting federal requirements, drinking water utilities are investing in infrastructure to either remove nitrogen pollution from source water or tap secondary sources to dilute below regulatory limits (e.g., Des Moines Water Works; EPA, 2009). Because these techniques are expensive to operate and take time to activate, near-term forecasting is essential to enable treatment processes to be brought online or pump stations to be activated when pollutants require these measures. At the same time, high temporal-resolution nutrient data that can be collected and assessed in near real-time are increasingly available. For example, Indiana has brought 8 nitrate monitoring stations online in the last 10 years while Iowa deployed a network of 68 stations in 2021. The degree to which existing discharge and nutrient monitoring networks can support near-term forecasting of in-stream nitrate remains unknown. Moreover, no tools nor strategies exist to identify the optimal places to invest in increased instrumentation to advance the accuracy of forecasting. Indeed, no clear approach exists to evaluate the value of future data collection to enable forecasting. Thus, our goals are to assess the potential for near-term stream nitrogen forecasting based on a currently deployed network, evaluate the relative value of each observation to forecasts, and identify locations to expand the network for the purpose of improved near-term forecasting.

The design and deployment of networks for water quality and quantity may take several forms. Some observational strategies can bring instrumentation online that provides complete spatial coverage. For example, the NEXRAD radar network and GRACE satellite each provide continuous spatial coverage and frequent repeat observations in time. Similarly, water quality in large rivers is measurable using remote sensing (Ross et al., 2019). However, limitations in resolution and the tree cover near headwaters means these approaches are limited in spatial coverage and still rely upon on-the-ground sensors to relate remotely sensed data to in-stream concentrations. Deployment of many point-scale observations create network-scale monitoring, but these are not necessarily optimized for forecasting. For example, the Iowa Water Quality Information System and Iowa Flood Information Systems Offer real-time water-related information and nutrient data from over 65 water quality sensors paired with stream stage sensors (IIHR—Hydroscience & Engineering, 2021). While comprehensive, the network was not designed with forecasting in mind. Other point-based strategies deploy sensors to meet a particular, localized goal. Often these strategies for sensor placement are to fill a data gap or to collect data for retrospective analysis for a single location or a collection of locations. Examples include bracketing a city with up- and downstream sensors to assess its contributions to runoff or nonpoint source pollution, or deployment at the outlet of a basin to assess the impact of changes in the watershed (Royer et al., 2006). As water utilities face never-before-seen combinations of land management and weather, their needs are shifting from retrospective analyses (e.g., post-hoc calculation of annual loads) to forecasts that enable real-time management of infrastructure (Dietze et al., 2018). As societal needs shift from monitoring to forecasting, scientists and resource managers require a basis to evaluate both present capabilities and the future value of investments in observational data and networks.

Near real-time water quality forecasts require three key elements: real-time data, a data assimilation and prediction scheme, and validation of model performance. First, real-time discharge data are relatively commonplace (e.g., the USGS gage network), but comparable nutrient data are in their infancy. Even with a growing network richness for nitrate, the relatively short time series - limited because sensors were only developed commercially within the last 15 years - mean that precious few data are available that span expected variation in weather (e.g., el Nino cycles). Relatively young sensor networks also include few examples of the extreme events that are known to drive nitrate dynamics in the midwestern US (Bernot et al., 2006; Royer et al., 2004, 2006; Vidon et al., 2008). Moreover, changes in land use and management during the period of record may confound the use of these records as a basis for purely empirical modeling from past data. Existing records are sparse in time, with sensors removed seasonally to avoid ice damage and incomplete data sets associated with growing pains of maintaining measurement quality for new technologies. In short, we lack the data required for near-term nutrient forecasts. Next, a scheme to assimilate data and make forecasts does not yet exist. Even with the data in-hand, existing computational models have not been deployed for operational forecasting. Instead, water quality forecasting is most often focused on longer-term, forward modeling of climate and/or land use scenarios (Andrade et al., 2021; Demaria et al., 2016; Paul et al., 2020; Quansah et al., 2021; Zhao & Wang, 2020). These models are highly parameterized and are too computationally intensive to implement for real-time forecasting (Dennis et al., 2017). Finally, the relatively short timescales for high resolution nutrient monitoring mean existing models are seldom validated at scales of individual storm events where drinking water utilities must respond to nutrient loads. Instead, existing models often rely upon monthly or irregular grab samples, which may not be appropriate for all responses of interest (Reynolds et al., 2016).

Given the limitations detailed above, one promising approach to advance near-term nutrient forecasting, particularly given the spatially sparse and temporally limited network of nutrient monitoring -- is machine learning (ML). Forecasts based on ML approaches have been shown to perform well with sparse datasets while producing computationally efficient and accurate results (Lim & Zohren, 2021; Masini et al., 2020). ML models have the ability to predict complex non-linear trends by learning from historical data. Indeed, applications of machine learning in time series forecasting are becoming increasingly common (e.g., (Ahmed et al., 2010; Deb et al., 2017; Lim & Zohren, 2021; Masini et al., 2020; Papacharalampous et al., 2018; Sit et al., 2020; Voyant et al., 2017)). In cases when sufficiently long or rich data sets are not available, such as the limited nutrient monitoring network in the midwestern U.S., ML models may be trained on synthetic data and still gain operational benefit, a strategy that has shown promise in ecological forecasts (Hittmeir et al., 2019). For nutrients in the Midwestern U.S., process based models have been a mainstay of research efforts and have proven capable of simulating existing observations (Kucharik, 2003; Kucharik et al., 2013; M. Motew et al., 2017). Thus, numerical simulations have potential as a basis to train ML models that could be subsequently operationalized for near-term forecasting using the existing sensor network.

In addition to their utility in forecasting, coupling ML models with process-based simulations may also have a role in sensor network design (Willard et al., 2020) . For example, process guided machine learning has been applied in ecology for producing Phosphorus budgets and studying streamflow and groundwater responses to ecological water replenishment (Hanson et al., 2020; Sun et al., 2021) . Coupling ML and physics-based models is a potential path to address the core challenge of designing a sensor network when the value of the data cannot be known a priori. In other words, a stream gage intended to improve flood forecasting may only prove its utility after a sufficient number of data have been collected spanning several rain events and antecedent conditions, compared to model results, and integrated into an operational forecasting scheme. How can the value of an observation be evaluated before the investment in the data is made? How many years of data or events are necessary to evaluate if the investment is providing measurable improvement? Any evaluation of a future network requires an unbiased way to relate the data from the added location to the quality of the forecasts being made. Machine learning provides one such way to screen potential gains of information and relate them directly to the improvement in forecasting. In fact ML is an exceptional candidate for this because of the efficient computation time allowing for the evaluation of benefits for a score of possible new data placements.

Our overarching objective in this study is to pilot an approach using ML models to inform sensor network design and gains in predictive power associated with expanding a sensor network, considering near-term nitrogen forecasts as a demonstration of the approach. Specifically we ask (1) How well can ML produce a 1-day future forecast for in-channel Nitrate based on an existing network for discharge and nitrate data?; (2) How much improvement can be gained at a single location by adding a single monitoring location to the current network?; and (3) How are benefits from additional data realized across a network of potential forecasting locations and beneficiaries? To answer these questions, we take one-day forecasting of in-stream nitrate concentrations in Wabash River Basin (WRB) in the Midwestern U.S. as a case study. The WRB is the epicenter of nutrient pollution in the US (Gammon, 1998; Minder & Pyron, 2018; Muenich et al., 2016; of Engineers), 2011; J. Tan et al., 2016) and includes a growing network of real-time nutrient monitoring that could be leveraged for operational forecasting. Illinois, Indiana and Ohio are actively expanding nutrient monitoring with real-time sensors in the basin and water quality impairments are increasingly concerning (J. Tan et al., 2016), making the WRB a relevant test case relvantent from management and practical standpoints. In this study, we use an agro-ecosystem model to generate a synthetic data set for in-stream nitrate and discharge, train ML models on synthetic data representing the existing monitoring network, and evaluate the locations where future data are most optimal to improve the forecasts. While this strategy is prototyped for nutrient monitoring and forecasting in the WRB, it serves as a proof-of-concept for the more generalized approach of coupling process-based and ML models to evaluate current capabilities and plan for future monitoring networks. Ultimately, we demonstrate the use of machine learning models to evaluate the value of future sensors for operational predictions, using the case study of one-day nitrogen forecasts in the Wabash River Basin as a case study to demonstrate an approach that could be readily applied to a host of different problems.

2. Methods

Evaluation of the design of a future monitoring system or sensor network and the forecasts it enables is a challenging proposition. Quantitative evaluation of a not-yet-deployed system is challenged by the lack of data to evaluate the value of a sensor a priori. While extensive networks may be pruned or optimized based on years of data and retrospective approaches, this is not possible for sparse networks with limited periods of record. In this section we outline the methods employed in our case study of one-day nitrate forecasts in the Wabash River Basin. These steps are intentionally organized in a manner that enables them to be generalized and implemented for other, similar applications (Fig. 1).

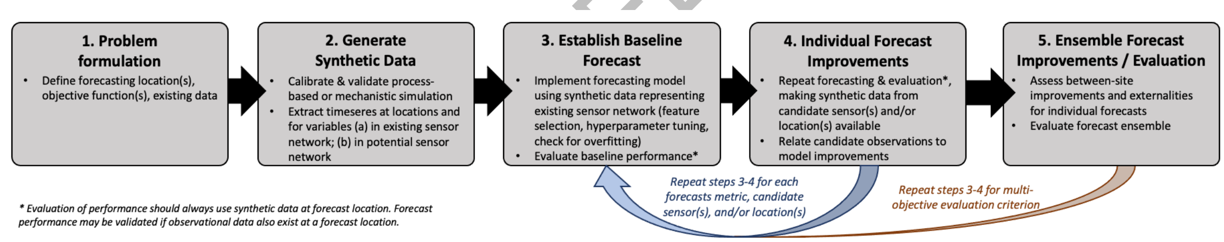

Fig. 1. Key steps in the approach implemented here to assess the value of future measurements for forecasts at individual sites and ensembles of sites. The numbers in each box correspond to the sub-sections in the study (e.g., manuscript section 2.1 with Box 1, text section 2.2 with Box 2, and so on).

2.1 Problem formulation

The Wabash River Basin (WRB) was selected as a test case as its land use is predominantly agricultural and its role as the single largest contributor of nitrogen pollution to the Mississippi River and ultimately the Gulf of Mexico. The WRB drains about 33,100 sq.mi. of Illinois, Indiana, and Ohio, with more than two-thirds of land in agricultural production, primarily in row-crop corn-soy. While a robust network of discharge gauges exist (329 USGS gages in the basin), comparable nutrient data are sparse in space and time (periods of record are less than 10 years at the network of 10 USGS gages with co-located data). A relatively young network of high resolution nitrate sensor has been deployed, but the periods of record are too short to enable robust forecasting. In this application, we take accurate one-day forecasting of in-stream nitrate concentrations as our objective. Forecasts will be evaluated in the rivers at the 12 largest cities, by population, in the WRB. This is a desirable forecast because near-term nitrate concentrations enable water utilities to proactively activate alternative water sources (e.g., blending surface and groundwaters to dilute stream concentrations) or bring additional treatment processes online to provide drinking water meeting US Safe Drinking Water Act requirements (nitrate concentrations below 10 ppm). In addition to baseline forecasts using existing data, we wish to evaluate the value (i.e., the improvement to the baseline forecast) associated with the addition of a single, additional nitrate sensor to the network and compare this value as a function of the forecast location (i.e., where the forecast is being made) as well as the added sensor location (i.e., the location where a new sensor would be installed).

For all forecasts described above, data are limited. We lack high temporal resolution nitrate data to calibrate and validate any forecasting approach at the network of 12 cities selected. Moreover, for evaluation of potential sites for future monitoring, data are - by definition - not yet in existence. Thus, we require a synthetic data set. We employ a mechanistic simulation that can accurately represent the system dynamics as a basis to generate a synthetic data set for evaluation. For predominantly agricultural systems in the Midwestern US, the combination of Agro-IBIS (Kucharik & Brye, 2003) and the Terrestrial Hydrology Model with Biochemistry (THMB; Coe, 1998) have proven successful in a host of comparable applications. The synthetic data set (detailed in the next section) enables answering questions about the value of future data to augment or supplement an existing network. Implicit in this approach are at least two important assumptions. First, this requires the assumption that the model used to generate the synthetic data set is capable of an accurate representation of the system processes and dynamics. If this assumption were not met, the synthetic data would be of little value. Broadly, this requirement can be satisfied by common post-hoc evaluation methods of models compared to existing data sets (see Section 2.2 of this study). Next, this approach requires the assumption that forecasting models trained on synthetic data (in the case of our study support vector machine regressions; Section 2.3 & 2.4) can also perform effectively using real-world data (as in Hittmeir et al., 2019). In the case of making forecasts and locations where data do not yet exists, such as the network of cities in our application, the second assumption cannot be explicitly tested, but remains an important caveat to consider.

2.2 Generation of a synthetic data set using agro-ecosystem simulations

The agro-ecosystem model Agro-IBIS (Kucharik & Brye, 2003) has been widely validated in the Midwestern U.S. and used to evaluate a host of management scenarios related to climate, energy crops, and crop rotation choices (Bagley et al., 2015; Bernacchi et al., 2013; Donner & Kucharik, 2008; Kucharik et al., 2013; M. M. Motew & Kucharik, 2013; Twine et al., 2013; VanLoocke et al., 2012, 2017; Walker et al., 2016). Agro-IBIS requires inputs including atmospheric forcing, on-farm management decisions (e.g., crop type, fertilizer application timing and rate, conservation practices), and intrinsic landscape properties (e.g., soil type, topography). These inputs are combined using mechanistic submodels to predict a host of state variables and fluxes related to carbon, nitrogen, water, and energy balances on the landscape. Notable model outputs for our study include overland and subsurface fluxes of water and nitrogen from the landscape to the stream network. Results from Agro-IBIS are subsequently routed using the THMB model (Coe, 1998), producing estimates of in-channel discharge and solute concentrations for the entire river network (Coe et al., 2008; Donner et al., 2002). THMB takes as inputs topography, water surface evaporation, precipitation, surface runoff, and subsurface drainage. These inputs are used to simulate the time-dependent flow and storage of the water and nutrients in rivers, lakes and wetlands.We implemented Agro-IBIS for the period 1948-2007 across the Mississippi River Basin, re-creating results from a previously published implementation of the model (M. M. Motew & Kucharik, 2013). Briefly, the implementation uses a 5-min x 5-min resolution, a spin-up procedure to build a stable soil carbon pool, observed atmospheric data for forcing from 1948-2007, soils based on the USDA State Soil GeographicDatabase (STATSGO) 1 km resolution data set, and land use based on the National Land Cover Database (2010). Results were routed using THMB (Coe et al., 2008), consistent with past implementations of the modeling approach (Chen et al., 2019; Donner & Kucharik, 2008; M. Motew et al., 2017). We confirmed the model was reasonably representing observations of discharge and nitrogen dynamics by comparing both daily and monthly averages for discharge and nitrate concentrations to 16 gages that are used by the USGS to estimate nutrient loads (Aulenbach et al., 2007; Goolsby et al., 1999). While our study only used data from the WRB for subsequent evaluation, the simulation spanning the same domain as past studies enables us to directly build upon their findings, and provides simulation data to be compared to the USGS network. We evaluated model goodness of fit using the coefficient of determination (Supplemental Fig 25, Supplemental Table 1). Timeseries of discharge and nitrate were extracted from THMB results that span the simulation period and exactly match the locations of the current monitoring network in the WRB. All subsequent forecasts and evaluations of data use results extracted from THMB locations corresponding to the existing USGS gage network.

2.3 Construction of baseline forecasts

With a synthetic data set generated (Section 2.2.), we next constructed predictive models for each of the 12 largest cities in the basin using support vector machine regressions (SVMRs). For the baseline model, we used synthetic data generated from THMB corresponding to the existing 329 discharge gages and 10 nitrate sensors in the WRB. This set of models produce forecasts based only on data from the existing network, representing the best forecasts this approach could make from existing data. While we selected SVMRs for their computational efficiency and known skill in time-series prediction (Jiake et al., 2013; Liu et al., 2013; G. Tan et al., 2012; Tay & Cao, 2001), we note here that in generalizing this approach a host of other tools could be used.

We implemented a forward feature selection scheme to construct parsimonious SVMRs for each forecast location using the baseline data as a model input (i.e., 10 sites with existing discharge and nitrate concentrations, 329 sites with discharge only). The radial basis function (rbf) was used as the kernel for all SVMR's. The term 'features' refers to the timeseries of discharge and nitrogen used as input to the SVMR to make a series of one-day forecasts at a particular city (i.e., a 'feature' is a timeseries of one variable from one site). This approach allows us to evaluate the existing data that are most valuable to nitrate forecasting at each city with respect to the selected objective function. For each city we used the default hyperparameters in Matlab and iteratively added features with the goal of minimizing RMSE between the SVMR forecast and synthetic nitrate timeseries at each city. Because use of the full 60-yr period was too computationally expensive, we performed the feature extraction scheme on the last ten years of data in the simulation, assuming they are most representative of modern climate and because they represent modern management regimes (e.g., fertilizer rates, crop variants). Features were added sequentially until adding a subsequent feature no longer reduced RMSE by more than 1%. The outcome of this step is a list of features that are added sequentially to minimize the RMSE between the SVMR prediction and the synthetic data. These features are taken as the best subset of the existing network to make baseline forecasts, and used in subsequent steps.

With the set of features established, we further tune our SVMR models by optimizing the model hyperparameters for each city. Briefly, hyperparameters function to restrict or broaden the flexibility of a model (put plainly, they are high-level controls on the assumptions internal to the SVMR approach) . For example, hyperparameters define when and where to assign penalties to values around the edges of the dividing hyperplanes in SVMRs. We optimized three hyperparameters for the existing monitoring network independently for each city by performing a grid search optimization for the box constraint, epsilon, and kernel scale hyperparameters. These three hyperparameters were optimized using the automatic hyperparameter optimization routine in MATLAB. The hyperparameters are determined by minimizing the five-fold cross-validation loss. The box constraint controls the penalty applied to the observations that violate the margin helping to prevent overfitting. Increasing values of the box constraint generally yields more flexible models, but can disproportionately increase the training computation time. As the box constraint controls the penalty imposed on observations, the epsilon value is the threshold for when a prediction error of a given observation is ignored (i.e. assigned a value of zero). In other words this means we are conceding that a prediction within a defined range is considered the correct result, which is why error is set to zero. Inverse to the box constraint, decreasing values of epsilon can yield more flexible models. The kernel scale sets a scale for the input in case there are large differences in the values of the features or feature values are large. Large values can lead to the inner-product dominating the computation of the kernel. Similar to epsilon, decreasing kernel scales leads to more flexible models(*Train Support Vector Machine (SVM) Classifier for One-Class and Binary Classification - MATLAB Fitcsvm*, n.d.). For all optimizations we standardized across the predictors which removes arbitrary dependence to the predictors scale, ensuring each predictor has a mean of 0 and standard deviation of 1. We performed thirty iterations for each city and selected the hyperparameters associated with the smallest estimated error. Models were also trained on the same training datasets, but default hyperparameter values were used to compare the effect of optimized versus un-optimized models in our system.

With the established hyperparameters and selected features we next trained our SVMR forecasts on the entire 60 year period from 1948-2007 to capture a broader suite of weather patterns and land management decisions, using the full data set to achieve a more robust model because this step is less computationally intensive than feature selection or hyperparameter optimization. We trained each SVMR by splitting the synthetic data into 80% training data and 20% testing data, inclusive of the full 1948-2007 simulation. After training the SVMRs, we established a baseline RMSE for each city using the last ten years of testing data to be consistent with the period used for hyperparameter optimization and feature selection. While models were optimized for minimizing RMSE, we also calculated Nash-Sutliffe efficiency to evaluate baseline model performance. The optimized SVMR represents the baseline condition for our study based on historically available data in the study basin (i.e., the best possible forecast using our ML scheme and data from the current discharge and nitrate monitoring network). Each baseline model was built using the same splitting of training and testing data to ensure the same days were being used for all model evaluations.

2.4 Evaluating the benefit of additional observations to a single forecast location

To estimate the value of an added sensor (i.e., the reduction in forecast error if additional data are made available), we used the synthetic data that were withheld from the baseline model development. We iterated through each potential location to add a nitrate sensor (the 329 USGS gages that do not currently have one), adding the synthetic nitrate data from that location to the feature set and re-training each SVMR. In total we trained an ensemble of 3,948 SVMRs to evaluate the value of each added sensor location for each forecasting location. For each combination of forecasting location and potential sensor location, we constructed an SVMR containing the previously selected features in addition to the added nitrate timeseries. We tabulated the improvement in RMSE and the Nash-Sutcliffe efficiency compared to the baseline model for each added nitrogen location, again calculated with the testing data from the last ten years. The key outcome of this step is a quantified improvement in model performance for each forecast and each location.

2.5 Evaluating the benefit of additional data to forecasting at network and subnetwork scales

The prior steps enable evaluation of a single added sensor site for a single forecast. However, the reality is that collaboration between cities may be desirable to operate as a collaborative network, from a state or federal agency seeking to manage the basin instead of the city, or simply to evaluate positive externalities of decisions (e.g., two potential sites may equally benefit the forecast of City A, but one site provides a substantial benefit to City B as well). To evaluate benefit beyond individual forecast locations, we implemented two approaches. First, for each potential new location for nutrient data, we calculated how many of the cities would realize a benefit of at least 1% by having access to that data (based on the same 1% threshold used when forward feature selection would stop for a city). Next, we calculated the total improvement in RMSE summed across all 12 cities associated with each of the 329 potential future nitrate monitoring locations, providing an overall measure of the value of each potential sensor location to the entire network of cities.

3. Results

3.1 Baseline models perform well and are parsimonious

For the twelve cities we tested, baseline model performance based on the testing data set ranged from 0.44 to 3.38 ppm RMSE (Table 1). All baseline models yielded acceptable fits during both baseflow periods and storm responses (Fig. 2A, Supplemental Figs. 1-12). As with any time-series simulation, some features will be over- or underpredicted. Thus, we use RMSE and NSE to evaluate performance quantitatively. Sequential feature extraction selected an average of about 17 features per model (Range 9-30; Fig. 2B) from the 339 possible features. Forecasts for each city included at least 5 discharge features and all cities except Columbus always included at least three nitrogen features. Notably, the baseline model for Columbus was only informed by discharge, selecting no nitrate features. Feature sets were unique for each city, indicating there is not a single set of dominant observations that is ubiquitously useful across the basin. No SVMR selected all available nitrate data, instead selecting 4 to 9 nitrate features. Co-located discharge and nitrate data were never both selected in baseline SVMRs.

Overall the hyperparameter optimization improved the baseline RMSE for all twelve cities by an average of 55% (range 3-86%; Table 1). The NSE for the baseline optimized models show generally satisfactory performance (range 0.15 to 0.52; Table 1) and show improvement with the addition of a nitrate sensor (range 0.75 to 0.94 for final models;Table 1). We tabulated the in-sample and out of sample errors (Table 1), finding that the RMSE's of the testing and training data sets were very similar, indicating that models are not overfit. Additionally, the response using the testing data does not have a noticeable reduction in performance as compared to the response using the training data (Table 1).While the final baseline models presented were evaluated only on the last 10-yr of synthetic data (optimized for RMSE; NSE also calculated post-hoc), we also tabulated the RMSE and NSE for final models for the full 60-yr simulation (Supplemental Table 2). Finally, the positive values for Nash-Sutcliffe Efficiency and the improvements provide an independent measure of model performance that serves as a check against overfitting and valides the utility of the SVMRs.

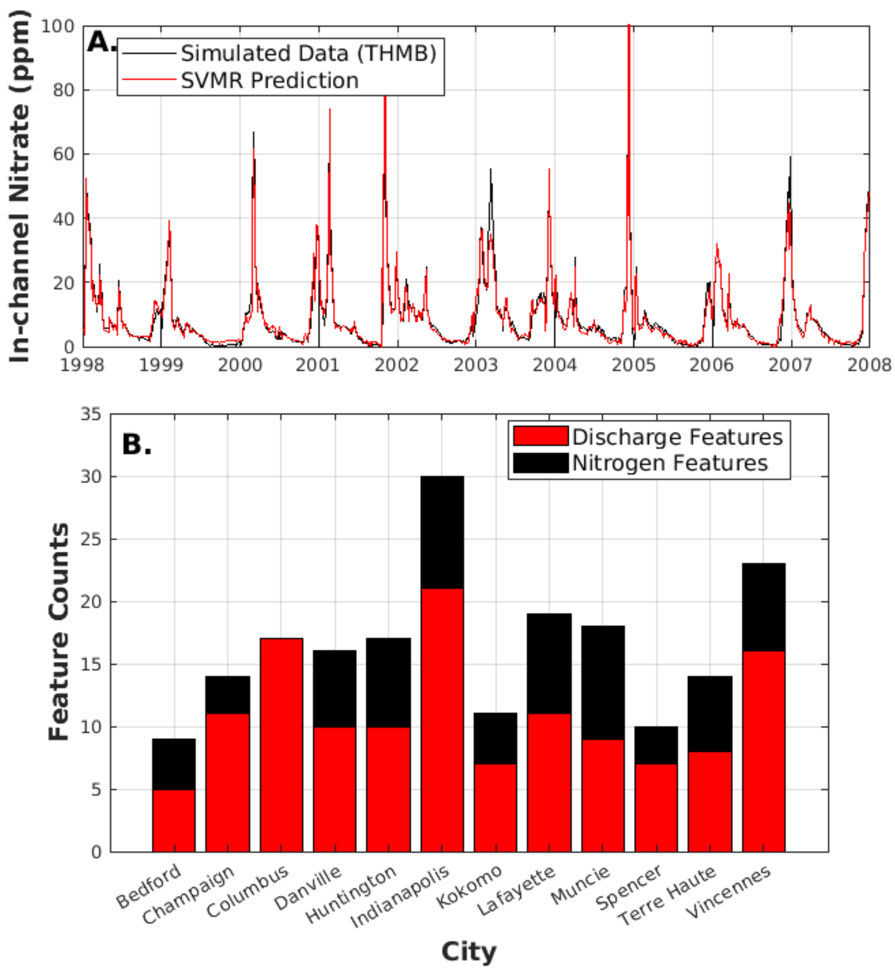

Fig. 2. (A) Representative example of Agro-IBIS and THMB simulated concentration timeseries (black) and baseline SVMR prediction (red) for Champaign, IL. The SVMR had an RMSE of 3.07 ppm. Supplemental Figs. 1-12 include comparable figures for all cities where forecasts were made, and Table 1 summarizes baseline model performance. (B) Stacked bars showing the number and type of features selected by the baseline SVMR for each city (i.e., the features used to construct the baseline SVMR for each city).

Table 1: Root mean squared error of the trained model on the training data set (in sample, the value used as our baseline RMSE) and on the testing data set (out of sample); the RMSE of optimized versus not optimized models; the Nash-Sutcliffe Efficiency (NSE) of the optimized baseline model; the NSE of the optimized model with optimal location added; and the number of Discharge and Nitrogen features selected for each city.

Cities	Out of Sample (Testing) Baseline RMSE	In Sample (Training) RMSE	Default Hyperparameters RMSE	Optimized Hyperparameters RMSE	Percent Difference (%)	NSE (Baseline)	NSE (Added N sensor)	No. of Discharge Features Selected	No. of Nitrate Features Selected	Total No. of Selected Features
Bedford	0.5	0.5	0.5	0.5	3.0	0.52	0.84	5	4	9
Champaign	3.4	2.8	6.0	3.1	65.2	0.51	0.94	11	3	14
Columbus	3.0	3.3	2.0	1.1	87.0	0.23	0.78	17	0	17
Danville	2.0	1.5	3.0	1.5	62.8	0.39	0.84	10	6	16
Huntington	2.0	1.5	2.7	1.5	56.6	0.37	0.82	10	7	17
Indianapolis	2.4	2.6	5.4	2.7	66.3	0.19	0.83	21	9	30
Kokomo	1.4	1.3	2.5	1.3	61.4	0.19	0.91	7	4	11
Lafayette	1.2	1.1	1.2	1.1	9.4	0.37	0.75	11	8	19
Muncie	1.6	1.2	2.3	1.2	63.2	0.40	0.83	9	9	18
Spencer	0.4	0.4	0.7	0.4	47.4	0.50	0.94	7	3	10
Terre Haute	0.9	0.8	1.8	0.8	77.6	0.15	0.88	8	6	14
Vincennes	2.6	3.1	8.3	3.3	86.3	0.27	0.83	16	7	23

3.2 Direct and indirect benefits from optimal sensor placement for individual cities

For each city there was one optimal future sensor location that maximized reduction in RMSE (e.g., the right-most bar in Fig. 3A for Bedford, IN). However, most candidate locations did provide at least modest performance improvements (Fig. 3A). Additionally, for each city there are a small number of locations that, when the SVMR is forced to include the additional nitrogen data, SVMR performance is ultimately worse than the baseline (i.e., negative values, Fig. 3A). In practice, building models with forward feature selection would simply not select features where the RMSE is reduced by less than 1%. Across the network of all 12 cities, the optimal sensor improved forecasts by an average of 31% (range 5-82%; diagonal in Fig. 4)

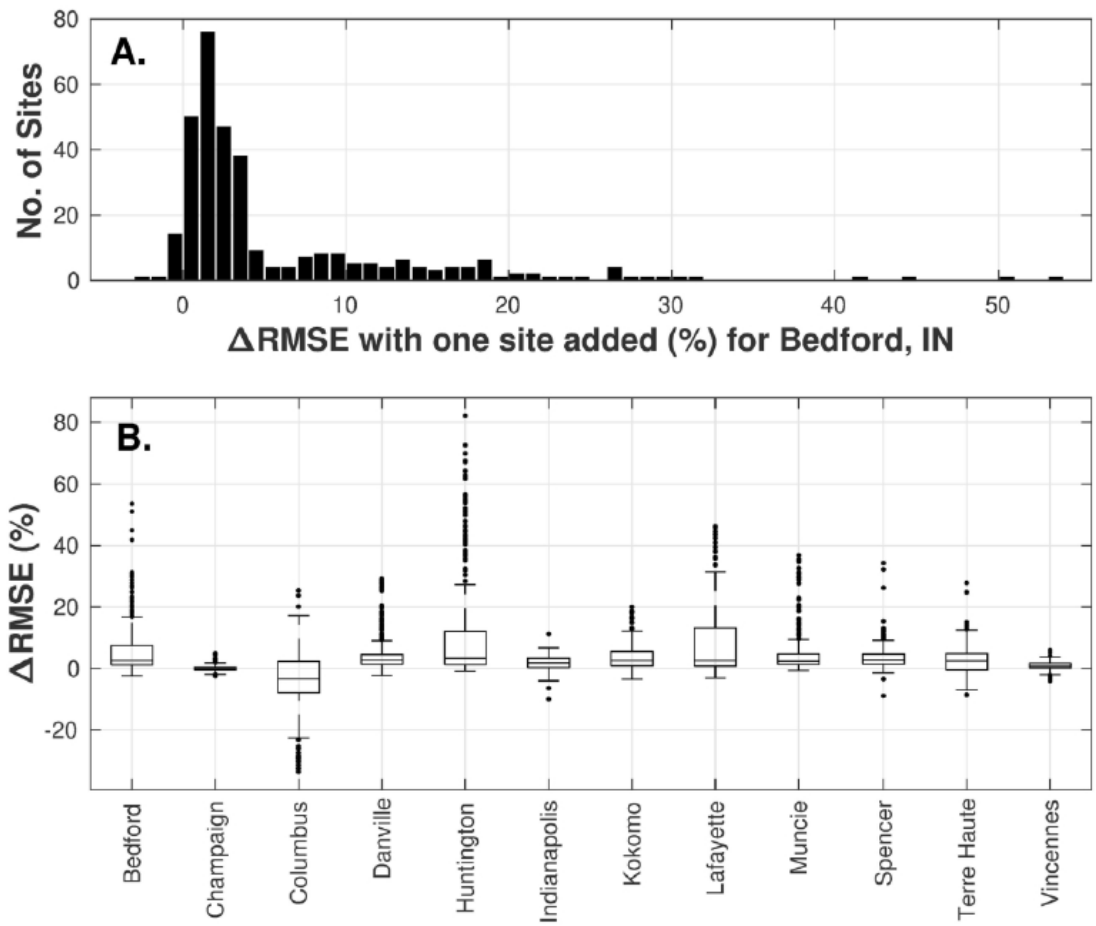

Fig. 3. (A) histogram of the changes to RMSE for the prediction at Bedford, IN when adding nitrogen data from each of the 329 possible locations considered to the forecast. (B) Boxplots of changes in RMSE for adding each of the 329 possible additional nitrogen sites to the forecast for each city. In both panels, values less than zero indicate decreasing model performance when the SVMR was forced to include the feature.

In addition to optimizing for each city, placement of an optimal sensor for each city yields a benefit of at least a 1% improvement in RMSE for the forecast in at least one other city in the network (off-diagonal cells in Fig. 3). These reductions in RMSE represent positive externalities, specifically the benefit that one city (columns in Fig. 4) would receive from the optimal sensor being installed for a different city (rows in Fig. 4). For two cities - Huntington and Lafayette - reductions in RMSE of more than 1% are realized from the optimal locations of eight other cities. In contrast, Champaign only benefits from the optimal placement for one other city. Importantly, relationships for mutual benefit are not always symmetrical. For example, while Champaign benefits from Kokomo’s optimal sensor location, Kokomo does not realize a comparable benefit from Champaign’s optimal sensor placement. For other cities, broad network benefit would be realized as a positive externality of their investment in a new monitoring location. For example, the optimal locations for Spencer, Muncie, Kokomo and Huntington generate improvement for all other locations (range 0.47-82.1% reduction in RMSE).

From the off diagonals of the (Fig. 4), it is clear that some cities will derive benefit from several potential nitrogen data locations in the network (consistent with Fig. 3A). For example, the optimal sensor location for Danville results in a 29.2% reduction in RMSE compared to the baseline. However, 15 other potential sensor locations would each result in 10% reduction in RMSE for that city, and more than 100 candidate sensor locations result in more than 1% reduction in RMSE at Danville (Fig-2A; see supplemental figures 13-24 for other cities). Thus, while there is a single, optimal location to benefit each city, there is also a larger network of locations that provide some benefit to each city (i.e., positive externalities of the decision made), some of which will have benefit for multiple cities.

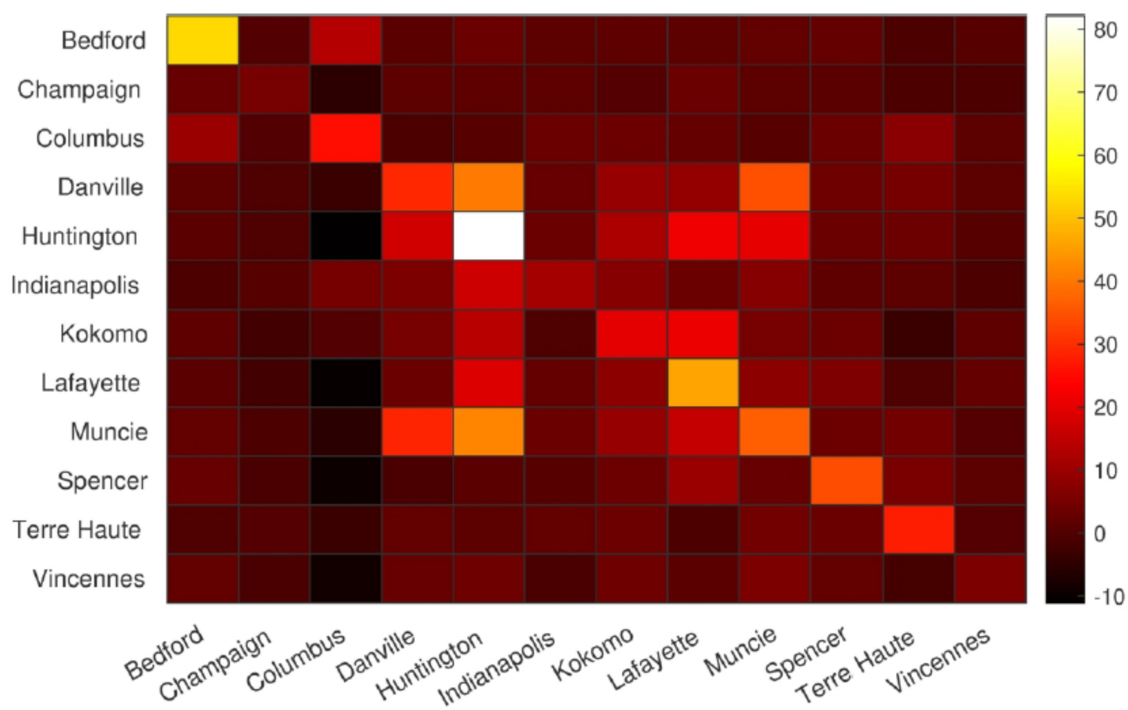

Fig. 4. Pairwise consideration of how the optimal sensor for one city (rows) changes the RMSE in each other city (columns). The diagonal represents the improvement at a city for the optimal added sensor location for that city, while off-diagonals represent benefit by one city from an optimal sensor for another city. Negative values indicate performance in the column is degraded from its baseline if forced to include a sensor placed for a different city (row).

3.3 Indirect benefits from sensor placement for the network of cities

While sensors can be optimized for a single city and some benefit is realized by a subset of other cities, could a network be designed to maximize benefit to all cities taken as a network? Summed improvements to RMSE for all the cities provide a simple indicator of total benefit to the network. The average RMSE improvement realized across s the entire network of 12 forecasting locations by adding one sensor is 41% (range -17 to 156%; Fig. 5A). However, these benefits are not equally distributed. Some sensor placements yield substantial improvements at one location while others will provide modest benefit at several locations (Fig. 5C). Useful solutions might be considered along the front that maximizes both number of cities benefiting and total benefit (i.e., the upper right portion of Fig. 5B). There is one location that improves RMSE for ten cities by at least 1% each (top point in the right-most column of Fig. 5), and one location that only benefits a single city (left-most point on Fig 4). Most locations for future data benefit multiple cities (a median of 8 cities benefit from adding nitrate data at one of the 329 candidate locations). Still, even these locations vary widely in the reductions in RMSE realized by the populations of cities they benefit (i.e., there is a wide vertical range in Fig. 5 for a given x-coordinate). However, even when the total benefit to the network is large, it is not ubiquitous. For example, Champaign has a degradation to its RMSE when the location that maximized RMSE reduction summed across the entire network is used.

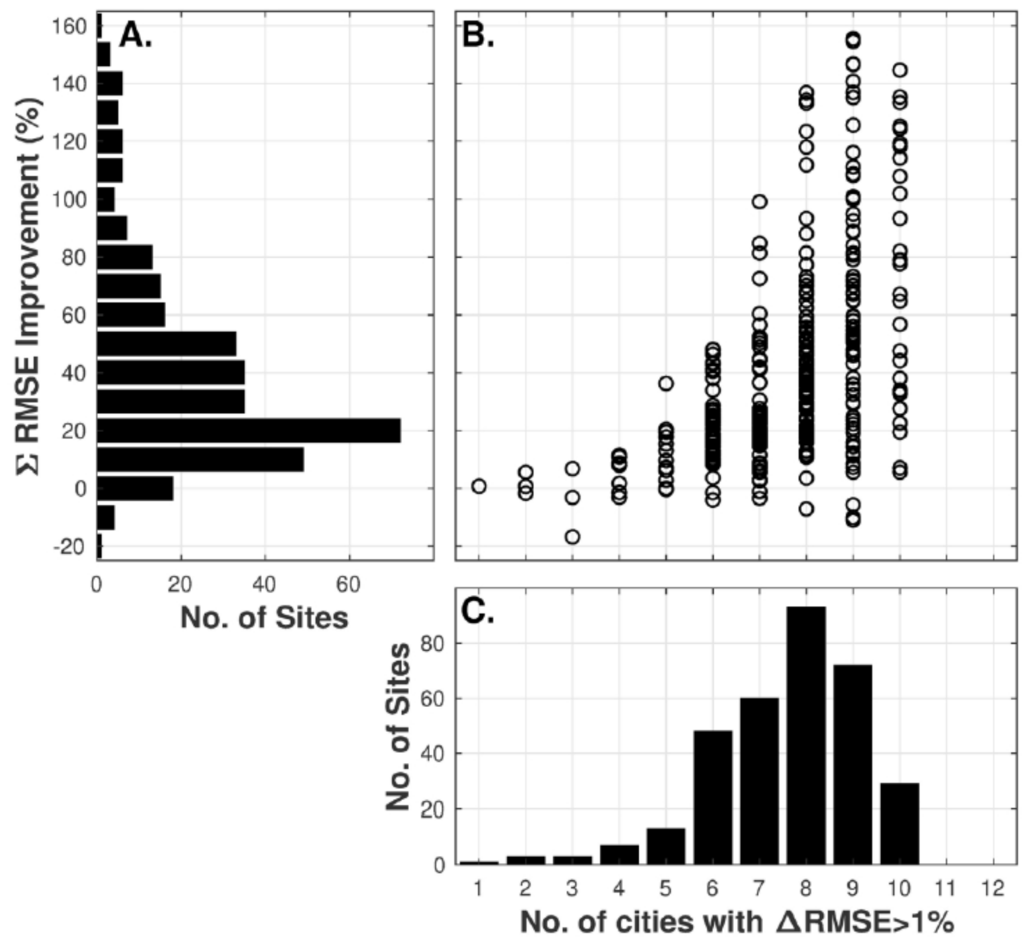

Fig. 5. (A) histogram of RMSE summed across all 12 forecast locations (i.e., cities) for each of the 329 possible additional nitrogen sensor locations. (B) scatter plot of summed RMSE improvement vs. number of cities whose RMSE improved by at least 1% with the site added. (C) Histogram of the number of cities where RMSE improved by at least 1% by adding each of the 329 potential additional nitrogen sensor locations.

Table 2. Percent improvement realized by each city and its optimal location for one added nitrate sensor; the total summed network benefit from the other 11 cities at each optimal location; the USGS gage number of the optimal location and the USGS site name associated with the gage.

City	Percent Improvement for City	Overall Network Improvement	USGS Gage No. w/ greatest improvement	USGS Gage Name for Location w/ Greatest Improvement
Bedford	53.6	81.4	3344250	RAS RIVER TRIBUTARY NEAR GREE
Champaign	4.9	13.1	3337000	BONEYARD CREEK AT URBANA, IL
Columbus	25.3	57.6	3361890	GILMORE CR NR BARGERSVILLE, IND.
Danville	29.1	133.4	3325500	SISSINEWA RIVER NEAR RIDGEVILLE
Huntington	82.1	154.6	3324350	BROOK CR TRIB NR WARREN, IND.
Indianapolis	11.2	59.4	3339230	WOODS DITCH NR FRANKFORT, IN
Kokomo	20.0	67.3	3333700	WILDCAT CREEK AT KOKOMO, IN
Lafayette	46.2	84.0	3329720	)BINSON BRANCH NR DELPHI, INDIA
Muncie	36.8	140.7	3347000	WHITE RIVER AT MUNCIE, IN
Spencer	34.2	51.4	3356780	LIMESTONE CR TRIB NR GOSPORT, IND.
Terre Haute	27.8	41.2	3341500	WABASH RIVER AT TERRE HAUTE, IN
Vincennes	6.0	15.3	3378900	TLE WABASH RIVER AT LOUISVILLE,
Network	-	155.5	3326070	LICK CREEK NEAR HARTFORD CITY

4. Discussion

4.1 What is the expected value of an additional nitrogen monitoring location?

An optimal sensor location to improve forecasts exists for each individual city. Every baseline model could be improved if more data were available from a new sensor location (Table 1). Moreover, every city can benefit from many potential stations (Fig. 3B). Most cities derive at least some benefit from most sensor locations, suggesting overall that forecasts will benefit to some degree regardless of where a sensor is placed. However, this does not guarantee that any data are useful for any goal, as sensors can be functionally useless to a given forecast (i.e., values below 0 in Fig. 2). More data is not universally better for a forecast, and there is a wide separation between marginally useful and optimally useful stations for a forecast of interest. Put another way, sensor deployment and data collection unto itself is not guaranteed to be useful in forecasting. As current approaches to sensor deployment may be random, or at least not include a robust evaluation of network design, knowing these locations when planning of deployment could yield benefits as cities and state agencies expand and invest in real-time networks in support of forecasting.

The optimal location to add a nitrate sensor for each individual city generates benefit for at least one other city (off-diagonals in Fig 3). The benefit derived from City A from the optimal placement of a sensor for City B is a positive externality of City A's decision to act in its own self interest. Optimal sensor placement for four cities (Huntington, Kokomo, Muncie and Spencer) each generate positive externalities for all other cities (i.e., average reduction of 103.5% RMSE summed across all 12 sites). Conversely, the optimal locations for Champaign and Columbus reduce RMSE at that city by 5% and 25% respectively, and generate small positive externalities for some cities and large negative externalities for other cities (i.e., average reduction is negative for both -0.14% and -1.1% RMSE). While it is simple to consider the benefit to the network as the summed reduction in RMSE (e.g, Fig 4A), this obscures the distribution of positive externalities. For example, Spencer's RMSE is reduced by 34% by adding its optimal sensor to the network. The total benefit summed across all sites is 51% reduction in RMSE, meaning the 11 other cities benefit by only about 17% in total (1.4% average). Even when cities act in their own self interest, their optimal location generates indirect benefits to at least one other city, but those benefits may be non-uniform across other locations. Again, while more data are generally better, these disparities and the non-reciprocal nature of co-benefit suggest that partnering on water quality networks could require careful planning to ensure mutual and equal benefit for the participants.

As an alternative approach to individual cities acting in their own self interest, the network could be designed and managed to maximize benefit across multiple cities. For example, a watershed management group or state agency may seek to maximize benefit across the network of cities rather than at one individual location. We considered the simple case of equally weighting benefit to all cities, yielding the summed RMSE reductions across the network as an evaluation criterion (Fig. 5C). From our analysis, there are groups of 6-8 cities that derive a meaningful benefit from a small number of shared sensor placements (highest y-axis points in Fig. 5B). While no locations provide large benefit to the entire network, this may not be an operational necessity. Indeed, baseline models for some cities are already strong, so a state agency may focus on improvements where error is largest. Thus, our approach also provides important insight about what is possible with existing networks that may guide evaluation of how to deploy limited resources to achieve a goal (in this case, adding one sensor to reduce error in one-day nitrate forecasts). In this scenario, managers considering the entire network must understand the baseline capabilities of models and the distribution of potential gains from investments in sensors. For our network of cities, this might include a consideration of the baseline model performance (e.g., no new sensors needed when baseline performance is strong) and the potential benefit across multiple cities (e.g., place one sensor to generate improvement at a maximum number of cities even if it is not optimal for other cities).

As a tangible example, consider forecasts at Bedford, IN. The current network informed a baseline SVMR for Bedford using 9 features (5 discharge, 4 nItrogen) and achieved a baseline RMSE of 0.46 ppm, relatively strong model performance. If Bedford acts in its own self interest it can see an improvement to the RMSE of about 57%, reducing forecast error by about 0.26 ppm. Moreover, Bedford does not receive much benefit from other locations within the network (Table 2; Fig. 2). From Bedford's perspective, a strong baseline and lack of benefit from other locations may guilde local decision making to opt-out of a consortium approach. However, a manager at the state level may use this knowledge to prioritize benefit in other cities given that Bedford (1) has a strong baseline model, and (2) is unlikely to derive significant benefit (as total reduction in ppm). In contrast, cities like Danville, Huntington, Lafayette and Muncie derive benefits from many other locations (Fig. 4), so a state-level evaluation may then target a high-error location (e.g., Vincennes, IN), recognizing that solutions there are likely to help moderate-error cities. While these are idealized hypotheticals, they demonstrate the potential application of this approach to understanding what is presently possible and how future investments in monitoring data could be optimized as a function of which goals are being prioritized. Moreover, this approach provides an objective way to screen potential sites for their expected benefits to forecasts, enabling a proactive, science-based, unbiased evaluation of alternative scenarios. Contrast this with present activities, where simple logic might say 'City X benefits from a sensor upstream of that City' without any basis for knowing this to be true.

Our objective function throughout this study was minimizing RMSE in nitrate forecasts. Treating the network problem as a whole as an optimization problem allows for the swap out of any objective function or model. We are using SVMR's becasue they perform well for forecasting and we selected to minimize RMSE between the simulated THMB data and the SVMR prediction because the mechanistic model generating the synthetic data is well documented and performs strongly in the region. Arguments for any objective function and model can be made depending on the application. As an independent confirmation that building SVMRs to minimize RMSE was producing quality models we calculated the Nash-utcliffe efficiency for each location's baseline model and the improved model with a new nitrogen feature (Table 2). Some of the baseline NSE values are low (Indianapolis, Kokomo, Terre Haute), however all cities improved their NSE value with the additional nitrogen feature (Table 1). Importantly, while minimization of RMSE was selected here, an alternative objective function could be readily formulated to focus on improved prediction of the timing and/or magnitude of nitrate responses to storm events.

4.2 A generalizable approach for design and evaluation of sensor networks in data poor systems

This study pioneers the use of synthetic data (generated from process-based forward models) as a basis to evaluate the value of potential sensor placement on ML forecast skill. Critically, this approach is predicated on the process-based model being trustworthy (i.e., representing the system processes and their dynamics germane to the forecast desired). In this case, the widespread application and validation of Agro-IBIS and THMB for simulations of agro-ecosystem dynamics in the midwestern US provides such a basis (Bagley et al., 2015; Donner & Kucharik, 2008; Kucharik et al., 2013; M. M. Motew & Kucharik, 2013; Twine et al., 2013; Vanloocke et al., 2010; VanLoocke et al., 2012, 2017). While this exact model may not be appropriate for all outcomes, scales, or forecasts of interest, the underlying concept of using machine learning to assess baseline performance and evaluate potential future locations for sensor data is an exciting path toward a proactive, forecast-oriented future. This is in contrast to present deployments of some water quality monitoring and stream gages, which are primarily recording data for post-hoc or retrospective analysis. Indeed, this approach could be applied in any situation where it is too expensive or difficult to prototype and evaluate a sensor layout at scale. We contend this approach (ML based on synthetic data) is a useful exercise to at least screen potential monitoring locations, particularly when the alternative is to deploy and maintain a network for a sufficiently long period to enable post-hoc evaluation of the network. Our approach enables evaluation of model skill using existing infrastructure and supports proactive planning for network expansion in service of a given forecast. While we focused on a relatively simple objective - minimization of RMSE for one-day forecasts at individual cities - our workflow could be readily applied to networks designed around different targets (e.g., 7-day forecasts) or more complex objective functions (e.g., improvement of only the timing of concentrations in excess of regulatory limits). Other formulations might consider targets like projected total nutrient loads during the spring which drive Gulf of Mexico dead zone size (Wendel, 2015), or classified forecasting of low-moderate-high probability of exceeding 10 ppm. Still more advanced applications could include forward modeling of future scenarios (e.g., changing climate, land use change, implementation of a best management practice) to assess the robustness of current and proposed networks to the dynamics that will be important in the future or optimized for change-detection.

Network expansion is inevitable. In an age where sensor costs are plummeting and connectivity is increasing, water utilities must prepare to harness the ‘data deluge’ to address increasingly frequent contamination of source waters. This is evident in the USGS’s Integrated Water Prediction Program and the Next Generation Water Observing System, an active program seeking to develop forecasts and models across all facets of the water cycle(Eberts et al., 2019; Miller et al., 2020, 2021). Finding a balance of design outcomes and optimal locations for those outcomes would provide managers with the necessary power to make informed decisions about their networks. This approach provides a way toward evaluating future locations and future networks without having to deploy a new sensor or prototype an entire network. Thus making this approach an essential tool for the design of new networks and additions to existing networks.

We prototyped a single objective optimization approach to determine where within an existing network adding a single new data stream would reduce the overall RMSE (objective function). In water resources, especially basin level management, there are scores of parameters that need to be evaluated and considered. Extending our approach to a multi-objective optimization scheme would allow managers to evaluate the parameters that are most important to their system. We concede that forecasting may not be the top priority of a basin manager, however with the recent philosophical shifts across agencies to support forecasting (Bateman, 2020) there is a demand for approaches to evaluate the value of additional data to forecasts. Implementations of multi-objective optimizations for water quality sensor placement have already been used within drinking water distribution networks to monitor system performance (e.g., chlorine residuals and contaminant detection in distribution lines)(Eliades & Polycarpou, 2007; Haxton T. et al., 2011; He et al., 2018; Huang Jinhui Jeanne et al., 2008; Marques et al., 2015; Ohar & Ostfeld, 2014; Preis et al., 2011). Early work was based on the Maximal Covering Location Problem (Xu et al., 2010). Later, Genetic algorithms were used to determine sensor placement for water quality monitoring (Brentan et al., 2021; Preis et al., 2009; Yoo et al., 2015). Optimizing sensor placement for precipitation monitoring (K. Wang et al., 2020) addresses similar geographical scales as river basins, but this work is based around monitoring as opposed to operational forecasting. Extending this work to incorporate forecasts has been hindered by the lack of data needed to validate forecasts. This framework gives basin managers a way to incorporate forecasts in their analysis of trade-offs for various management decisions.

5. Conclusions

The need for near term forecasting of water quality is increasing as resource managers are having to make real time decisions about water treatment in the face of increasingly frequent extreme weather events and the nutrients they mobilize. With the availability of low-cost sensors and desire for forecasts, resource managers must decide where to invest resources to collect data, a challenging prospect given the inability to evaluate the value of future data. Here, we address this challenge by training ML models on synthetic data from process-based simulations. We used these synthetic data to systematically evaluate baseline model conditions (i.e., what is possible with present data), finding that parsimonious, reasonably accurate forecasts (RMSE ranging from 0.44 to 3.38 ppm) could be constructed immediately. We found forecast error at 12 locations could be reduced by 5-82% by adding a single optimal sensor for each site, but that sites each realized some benefit from many potential locations (Fig. 3). Additionally, the NSE improves with optimal sensor placement (Table 1). We documented linkages between actions for one city and benefits to another (Fig. 4), noting that relationships are not always symmetrical in their benefit. Finally, we assessed the benefit considering the network as a whole instead of on the basis of individual cities, identifying locations to maximize both the number of cities benefiting and the total reduction in RMSE across the predictive network.

Overall, design of sensor networks to enable or improve forecasts is a challenging problem because the true value of a new observation cannot be realized until a retrospective analysis is performed. However, we demonstrate one approach to combine process-based models and ML approaches to estimate the value of sensor data in a way that is unbiased and quantitative, which may serve as one input to decision-making. While our approach was limited to adding a single sensor to improve a single objective function, this approach could be readily generalized to multi-objective optimization and for a host of different problems or applications. Ultimately, our approach demonstrates one way that current networks can be evaluated for their value in forecasting, and potential sites can be screened to estimate the benefit of future data before investing in a sensor deployment.

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