**Chapter 1: Successful production of near-term, iterative forecasts of phytoplankton blooms using autoregressive linear models**

**Near-term iterative forecasts of algal dynamics informed by modeling at multiple time scales**

* Intro
  + Ecosystem services provided by lentic freshwater systems are crucial to society, and yet lakes and reservoirs are increasingly threatened by eutrophication.
    - Services include cultural and aesthetic value, food production, drinking water, etc.
    - Broad examples of the pattern of increasing water quality degradation in drinking water sources (citations, look to Inland Waters paper)
      * Increases in eutrophication and cyanobacterial blooms are one particularly harmful water quality problem that needs to be addressed in order to continue providing water quality needs to communities at large.
  + Algal dynamics are governed by highly variable processes that exhibit both fast and slow responses to changing environmental conditions (CITATIONS). Baseline algal densities may fluctuate at small scales on a daily to weekly basis, but quickly ramp up to exponential growth and decay during the development or senescence of large blooms. While HABS are ephemeral, short-term events that are uncharacteristic of the preceding, underlying algal conditions, HABs have large economic and ecological impacts, making them critical to anticipate.
    - **This paragraph should dive into HABs ecology and modeling, making the case for both daily and weekly monitoring needs as a result of multiple timescales of phytoplankton growth responses**
      * Kara et al 2012: short-term phyto dynamics difficult to reproduce, Rigossi 2013
    - As the degradation mentioned in paragraph 1 continues to increase, it has become more important than ever to not only respond to eutrophication events but to be able to anticipate them before they occur.
  + One tool that may provide managers with the ability to adapt or prevent HABs is through the use of forecasts. Forecasting has been instrumental to society through the development of successful forecasts in multiple fields, including meteorology, economics, agricultural science, and epidemiology (citations from prospectus). Forecasting of ecological variables is in its relative infancy (Dietze, 2017) but has shown promise in many sub-disciplines of ecology (citations? Thomas et al 2019? Carey et al. 2020 😊) to improve management of freshwater ecosystems
    - Citations for other HABs modeling approaches in freshwater and marine systems
      * Discuss the different methods currently being used for forecasting HABs
  + However, because algal dynamics exhibit distinct bimodal?? patterns of growth (i.e., baseline conditions vs. bloom development and senescence), it is unclear as to what timestep can best model both of either of these processes.
    - Long-term monitoring of lakes and reservoirs typically takes place on a weekly scale, from which historical time series models can easily be built but because of the large timestep may miss important dynamics as a result of ‘fast processes’.
    - However, use of high-frequency sensors has allowed researchers to build time series models at a much finer time-resolution.
    - These high-frequency measurements also increase the skill of a null model
  + Another utility of forecasts as decision support tools is in the ability to represent uncertainty in forecast estimate.
    - Crucial to the application of forecast products in order to properly inform management decisions
    - Often unconsidered or at least unreported
    - Can add to basic and applied scientific value by informing ways to improve forecasts, as well as in management of drinking water
  + To further assess the success of empirical models in forecasting HABs, we developed near-term (2 week), iterative forecasts using several types of autoregressive (AR) linear models. We aimed to answer FIVE? main questions:
    - 1. How well can we forecast near-term (two-week horizon) chlorophyll-a (a proxy for HABs) over a one-year time period using a daily and a weekly model?
    - 2. How well does a daily and weekly model forecast under different conditions (e.g., bloom and nonbloom conditions)?
    - 3. How does forecast skill change with time horizon in both daily and weekly models?
    - 4. What are the major contributions of uncertainty over time in our forecasts?
    - 5. How does uncertainty change between the daily and weekly model?
* Methods
  + Study site
    - Falling Creek Reservoir is a small (0.119 km2), eutrophic drinking water reservoir serving the town on Vinton, VA. It is owned and operated by the Western Virginia Water Authority and has been monitored regularly by Virginia Tech since 2013.
    - **Figure 1. Map of study site**
  + Historical Weekly Dataset and Model Development
    - The weekly training dataset covered four years (2013-2016) and was developed from weekly measurements of chlorophyll-a, meteorological variables, as well as discharge at the major inflow to the reservoir. These were all chosen as covariates because they are either available as forecasts from National Oceanic and Atmospheric Administration (NOAA) or able to be forecasted using simple linear regression models (e.g., discharge). Chlorophyll-a was estimated by taking weekly profiles using a CTD (SeaBird SERIAL NUMBER). We measured discharge using a pressure transducer at a weir installed at the major inflow to FCR. Flow was measured every 15 minutes, and discharge to the reservoir was calculated, as described in Gerling et al. (2014). A meteorological station measuring X, Y, Z collected data every ten minutes using THESE INSTRUMENTS (serial numbers) from YYYY-present. Any weeks were data was missing (n=XX) were linearly interpolated. Variables that did not follow a normal distribution were transformed to meet the assumptions of a linear model. An autoregressive lag of chlorophyll-a was chosen at one timestep (i.e. one week) and was determined using the package ‘asta’ in R (some citation).
    - The weekly training dataset was limited to May to October, as this is when sampling consistently occurred on a weekly basis. Using the training dataset described above (number of datapoints = XX), we fit multiple linear regression models using the function ‘dredge’ in the package ‘MuMIn’, and selected the best and most parsimonious model using AICc. Our weekly autoregressive model is as follows

Chl-a(t) = β1 + β2Chl-a(t-1) + β3SW mean(t) + β4mean flow(t) + Ɛ (Eq. 1)

* + - Where the response, Chl-a(t), is the chlorophyll-a concentration at the forecasted timestep, t. Chl-a(t-1) is the autoregressive term or chlorophyll-a at the previous timestep, 1 week earlier. SW mean(t) is the mean shortwave on the forecasted timestep. Mean flow(t) is the mean discharge on the forecasted timestep. β1 , β2, β3, and β4 are parameters and Ɛ is an error term.
    - **Table 2. Summary of historical and sensor datasets, including data measured and length of dataset**
  + Daily Dataset and Model development
    - Beginning in August, 2018, an EXO sonde (serial numbers) was installed at the deepest site at FCR, measuring chlorophyll-a fluorescence at 15-minute intervals. Using the same potential covariates as listed above for the weekly model (i.e., meteorological and discharge variables), and following the same model selection protocol, we developed all possible combinations of autoregressive linear models. Because the weekly model was limited to XX number of datapoints in its training dataset, we trained our daily model on the same number of datapoints, which results in a training dataset from August 15, 2018 to December 15, 2018. Our best selected daily model is as follows

Chl-a(t) = β1 + β2Chl-a(t-1) + β3RelHum mean(t) + Ɛ (Eq. 1)

* + - Where the response, Chl-a(t), is the chlorophyll-a concentration at the forecasted timestep, t. Chl-a(t-1) is the autoregressive term or chlorophyll-a at the previous timestep, ‘n’ days earlier. RelHum mean(t) is the mean relative humidity on the forecasted timestep. β1 , β2, and β3 are parameters and Ɛ is an error term.
  + Forecasting framework (FLARE)
    - Using the linear autoregressive model described above (Eq. 1), the model was adapted to produce forecasts with uncertainty using the Forecasting Lake and Reservoir Ecosystems (FLARE) forecasting framework (Thomas et al. 2020?). Using FLARE, real-time sensor data is automatically uploaded to a data repository (GitHub, link?). Sensor data includes a suite of physical, chemical, and biological data, including chlorophyll-a fluorescence measured using an EXO sonde (serial numbers and company), meteorological variables (At FCR, weather data arewere collected on the minute resolution from a meteorological station (with sensors measuring air temperature, wind speed, relative humidity, shortwave and longwave radiation, and precipitation; see Carey et al. 2019x) and discharge at the major inflow to the reservoir.
    - Something about the Bayesian framework
    - Number of ensembles
    - **Figure 2. FLARE Workflow**
  + Weekly forecasts
    - Using the weekly model developed above, weekly forecasts, providing 1-week ahead and 2-week ahead forecasts, were produced every day from January 01, 2019 to December 22, 2019. The time period from August 15, 2018 to December 15, 2018 (number of datapoints = K) when the driver data was available on a daily basis was used as a spin-up period. While in forecasting mode, new driver data was assimilated weekly on Monday (in order to follow the weekly timestep), and the model was re-fit at each time step under a Bayesian framework to allow the parameter values to evolve over time. All ensemble members (n=420) and parameter values were saved for archiving at each timestep.
  + Daily forecasts
    - Using the daily model developed above, daily forecasts, from 1- to 16-days ahead, were produced from January 01, 2019 to December 22, 2019. To allow a spinup period similar to the weekly model, forecasts from December 15, 2018 to January 01, 2019 were used as a spinup period and not included in final forecast analyses. While in forecasting model, new driver data was assimilated daily when available, and the model was re-fit at each time step under a Bayesian framework to allow the parameter values and model fit to evolve over time. All ensemble members (n=420) and parameter values were saved for archiving at each timestep.
  + Forecast assessment
    - Assessing skill under different conditions
      * Because phytoplankton exhibit different growth responses to ecological conditions at different times, we analyzed our forecasts under three time period: 1) the entire year period where forecasts were produced, 2) under nonbloom conditions, defined as X days before and after the peak observed chlorophyll-a value, and 3) under bloom conditions
    - Null-persistence model
      * We developed a null-persistence model in order to test the robustness of our forecasts. Our null model assumes that the chlorophyll-a concentration at the next timestep will be unchanged from the current timestep, with process error from the Bayesian model added. We calculated an ensemble of null models in order to compare to our ensemble forecasts by sampling 420 times (the number of ensembles) from the distribution of the process error term from the Bayesian model output at each timestep and adding this value to the observed chlorophyll-a concentration (e.g., for the 8-day forecast, the observed chlorophyll-a concentration from 8 days prior is the null model, plus the process error from the model fit, sampled for each model ensemble).
    - Forecasts and null models were assessed using RMSE, R2 (?), and CRPS.
  + Uncertainty analysis
    - We partitioned five types of uncertainty for our weekly model and four for the daily model which contribute to the variance in our forecasts
      * Process
      * Initial conditions
      * Discharge driver (weekly model only)
      * Meteorological driver
      * Parameter
    - Relative contributions of uncertainty were quantified by isolating each type of uncertainty and allowing that uncertainty vary while holding all others constant
* Results
  + Forecasts over a one-year period
    - Both daily and weekly forecasts over one year generally capture observed chlorophyll-a dynamics (Fig. 3).
    - However, the daily forecasts were not better than a null persistence model at any timestep (Fig 4a).
    - For both the daily and weekly model, forecasts do slightly worse than the null model at 7 days (i.e., one week) ahead, but at two weeks ahead, the weekly forecast is significantly better than the null model.
      * **Figure 3. Muti-panel figure with daily and weekly models at various timesteps and observed chl** 
        1. Day 1 forecast, daily model
        2. Day 7 forecast, daily model
        3. Day 7 (i.e. week 1) forecast, weekly model
        4. Day 14 forecast, daily model?
        5. Day 14 forecast, weekly model?
  + Forecasts during nonbloom conditions
    - Under nonbloom conditions, the daily forecast is slightly better than the null until 9 days into the future (Fig 4b). However, the weekly forecast is better than the null at both 1-week and 2-week forecasts, with the forecast being much better than the null at 2-weeks ahead (Fig 4b). Interestingly, the 14-day ahead forecast of the daily model is substantially worse than the null (Fig 4b).
  + Forecasts during bloom conditions—TBD
    - **Figure 4. RMSE of forecasts at all timesteps**
    1. **RMSE over forecast horizon for daily and weekly models over whole year**
    2. **RMSE for daily and weekly models over nonbloom period only**
    3. **RMSE for daily and weekly models over bloom period only**
  + Uncertainty analysis
    - Process error dominant source when averaged over the entire time period
    - Uncertainty sources not constant over time series
    - In weekly model, during bloom, parameter uncertainty increased dramatically, indicating that parameters were not properly fitted to capture bloom dynamics
    - **Figure 5. Relative proportion of uncertainty over entire time series**
      1. **Weekly model**
      2. **Daily model**
* Discussion
  + We successfully developed a near-term, iterative forecast of chl-a that produced both daily and weekly forecasts up to 16 days ahead.
  + While daily forecasts were not an improvement over a null model over the entire time period, we did find that under nonbloom conditions the daily forecasts did slightly better than the null persistence model. Additionally, the weekly forecasts did substantially better than the null at both 1 and 2-week time horizons under nonbloom conditions. This is not surprising given than the model was calibrated to model weekly patterns which are clearly not well captured by the null model.
  + Interestingly, contrary to commonly upheld forecasting theory (Dietze 2017) we found with our weekly model that the forecastability did not decrease with forecast horizon. This pattern holds true especially under nonbloom conditions, but is also seen over the entire year period.
  + Our dominant source of uncertainty was process error, indicating that our model was missing key processes that control dynamics in phytoplankton abundance. This is not surprising given that due to the data latency constraints of a forecasting system, we were limited to driver variables which were also forecastable (i.e., nutrients or predator abundance are not reasonable covariates in a forecasting framework)
  + Relative contributions of uncertainty were not static throughout the year.
    - Driver uncertainty, particularly discharge driver uncertainty, increased in relative importance at various time throughout the year, especially during periods of high precipitation (e.g., fall hurricane season and spring rainfall).
      * Must have confidence in forecasts of covariates
    - Further, parameter uncertainty increased dramatically during the bloom in weekly forecasts.
  + Model I missed large bloom events in 2019
    - Do some analysis similar to the % likelihood of turnover to analyze how far ahead the model needed to recognize the bloom (because it eventually recognizes high concentrations or something about how long it took to get back into the CI of the forecast
    - Not uncharacteristic of AR models
  + Copper sulfate events
    - The model was unable to immediately anticipate this event, but does readjust after a short period of time.
  + Discussion of utility of developing other types of models
    - Other empirical models (GAM, ANN, process-based, etc.)
    - Modeling averaging/ensembles
    - Would process-based approaches do better at predicting blooms?
  + Applications/uses of HABs forecasts
    - What is a useful forecast?
      * What time step
        + Why are weekly chl forecasts still useful?
      * What level of accuracy (# of ug/L?) is needed for management?
      * What level of uncertainty
      * How to deliver information to stakeholder
        + Uncertainty visualization
  + Scaling AR forecasts to other water bodies
    - GLEON
    - Using simplistic AR models helps move us toward implementation of forecasts in a diverse set of lakes and reservoirs

Figure and table list