Modelling Lake Trophic State: A Random Forest Approach

Jeffrey W. Hollister *
 1 W. Bryan Milstead 1 Betty J. Kreaki
e 1

¹US Environmental Protection Agency, Office of Research and Development, National Health and Environmental Effects Research Laboratory, Atlantic Ecology Division, 27 Tarzwell Drive Narragansett, RI, 02882, USA

* corresponding author: hollister.jeff@epa.gov

Abstract

2

13

15

17

21

22

Productivity of lentic ecosystems is well studied and it is widely accepted that as nutrient inputs increase, productivity increases and lakes transition from lower trophic state (e.g. oligotrophic) to higher trophic states (e.g. eutrophic). These broad trophic state classifications are good predictors of ecosystem condition, services, and disservices (e.g. recreation, aesthetics, and harmful algal blooms). While the relationship between nutrients and trophic state provides reliable predictions, it requires in situ water quality data in order to parameterize the model. This limits the application of these models to lakes with existing and, more importantly, available water quality data. To address this, we take advantage of the availability of a large national lakes water quality database (i.e. the National Lakes Assessment), land use/land cover data, lake morphometry data, other universally available data, and apply modern data mining approaches to predict trophic state. Using this data and random forests, we first model chlorophyll a, then classify the resultant predictions into trophic states. The full model estimates chlorophyll a with both in situ and universally available data. The mean squared error and adjusted R² of this model was 0.09 and 0.8, respectively. The second model (i.e. GIS only) uses universally available GIS data only. The mean squared error was 0.22 and the adjusted R² was 0.48. The accuracy of the trophic state classifications derived from the chlorophyll a predictions were 69% for the full model and 49% for the "GIS only" model. Random forests extend the usefulness of the class predictions by providing prediction probabilities for each lake. This allows us to make trophic state predictions and also indicate the level of uncertainty around those predictions. For the full model. these predicted class probabilities ranged from 0.42 to 1. For the GIS only model, they ranged from 0.33 to 0.96. It is our conclusion that in situ data are required for better predictions, yet GIS and universally available data provide trophic state predictions, with estimated uncertainty, that still have the potential for a broad array of applications. The source code and data for this manuscript are available from https://github.com/USEPA/LakeTrophicModelling.

1 Introduction

- Productivity in lentic systems is often categorized across a range of trophic states (e.g. the trophic
- continuum) from early successional (i.e. oligotrophic) to late successional lakes (i.e. hypereutrophic) with
- 136 lakes naturally occurring across this range (Carlson 1977). Oligotrophic lakes occur in nutrient poor
- areas or have a more recent geologic history, are often found in higher elevations, have clear water, and

are usually favored for drinking water or direct contact recreation (e.g. swimming). Lakes with higher productivity (e.g. mesotrophic and eutrophic lakes) have greater nutrient loads, tend to be less clear, have greater density of aquatic plants, and often support more diverse and abundant fish communities. Higher primary productivity is not necessarily a predictor of poor ecological condition as it is natural for lakes to shift from lower to higher trophic states but this is a slow process (Rodhe 1969). However, at the highest productivity levels (hypereutrophic lakes) biological integrity is compromised (Hasler 1969, Smith et al. 1999, Schindler and Vallentyne 2008).

Monitoring trophic state allows for rapid assessment of a lakes biological productivity and identification of lakes with unusually high productivity (e.g. hypereutrophic). These cases are indicative of lakes under greater anthropogenic nutrient loads, also known as cultural eutrophication, and are more likely to be at risk of fish kills, beach fouling, and harmful algal blooms (Smith 1998, Smith et al. 1999, 2006). Given the association between trophic state and many ecosystem services and disservices, being able to accurately model trophic state could provide a first cut at identifying lakes with the potential for harmful algal blooms (i.e. from cyanobacteria) or other problems associated with cultural eutrophication. This type of information could be used for setting priorities for management and allow for more efficient use of limited resources.

As trophic state and related indices can be best defined by a number of *in situ* water quality parameters (modeled or measured), most models have used this information as predictors (Imboden and Gächter 1978, Salas and Martino 1991, Carvalho et al. 2011, Milstead et al. 2013). This leads to accurate models, but also requires data that are often sparse and not always available, thus limiting the population of lakes for which we can make predictions. A possible solution for this issue is to build models that use widely available data that are correlated to many of the *in situ* variables. For instance, landscape metrics of forests, agriculture, wetlands, and urban land in contributing watersheds have all been shown to explain a significant proportion of the variation (ranging from 50-86%, depending on study) in nutrients in receiving waters (Jones et al. 2001, 2004, Seilheimer et al. 2013). Building on these previously identified associations might allow us to use only landscape and other universally available data to build models. Identifying predictors using this type of ubiquitous data would allow for estimating trophic state in both monitored and unmonitored lakes.

Many published models of nutrients and trophic state in freshwater systems are based on linear modelling
methods such as standard least squares regression or linear mixed models (Jones et al. 2001, 2004).
While these methods have proven to be reliable, they have limitations (e.g. independence and distribution
assumptions, and outlier sensitivity). Using data mining approaches, such as random forests, avoids
many of the limitations, may reduce bias and often provides better predictions (Breiman 2001, Cutler
et al. 2007, Peters et al. 2007, Fernández-Delgado et al. 2014). For instance, random forests are
non-parametric and thus the data do not need to come from a specific distribution (e.g. Gaussian)
and can contain collinear variables (Cutler et al. 2007). Second, random forests work well with very
large numbers of predictors (Cutler et al. 2007). Lastly, random forests can deal with model selection
uncertainty as predictions are based upon a consensus of many models and not just a single model
selected with some measure of goodness of fit.

To build on past work, we have identified two areas in which this research contributes. First, we build, asses, and compare two random forest models of chlorophyll a 1) in situ and universally available GIS data and then 2) universally available GIS data only. Second, we examine the important predictors for both models. Lastly, this paper, the code, and the data used in the models is made available as an R package from https://github.com/USEPA/LakeTrophicModelling.

$_{ t 82}$ 2 Methods

$_{ ext{ iny 33}}$ 2.1 Data and Study Area

We utilized three primary sources of data for this study, the National Lakes Assessment (NLA), the
National Land Cover Dataset (NLCD), and lake morphometery modeled from the NHDPlus and
National Elevation Data Set (Homer et al. 2004, USEPA 2009, Xian et al. 2009, Hollister and Milstead
2010, Hollister et al. 2011, Hollister 2014). All datasets are national in extent and provide a unique
snapshot view of the condition of lakes in the conterminous United States during the summer of 2007.
The NLA data were collected during the summer of 2007 and the final data were released in 2009

90 (USEPA 2009 for detailed description of methods). With consistent methods and metrics collected

at over 1000 locations across the conterminous United States (Figure 1), the NLA provides a unique opportunity to examine broad scale patterns in lake productivity. The NLA collected data on biophysical measures of lake water quality and habitat as well as an assessment of the phytoplankton community. For this analysis, we only use the water quality measurements and total cyanobacteria abundance from the National Lakes Assessment (USEPA 2009).

Adding to the monitoring data collected via the NLA, we use the 2006 NLCD data to examine landscapelevel drivers of trophic status in lakes. The NLCD is a national land use/land cover dataset that also
provides estimates of impervious surface. We calculated total proportion of each NLCD land use land
cover class and total percent impervious surface within a 3 kilometer buffer surrounding each lake
(Homer et al. 2004, Xian et al. 2009). A three kilometer buffer was selected as an intermediate measure
of the adjacent neighborhood; the three kilometer buffer size is greater than the immediate parcel but
smaller than regional and whole-basin measures.

To account for unique aspects of each lake and characterize lake productivity, we also used measures of lake morphometry (i.e. depth, volume, fetch, etc.). As these data are difficult to obtain for large numbers of lakes over broad regions, we used modeled estimates of lake morphometry (Hollister and Milstead 2010, Hollister et al. 2011, Hollister 2014). These included: surface area, shoreline length, Shoreline Development, Maximum Depth, Mean Depth, Lake Volume, Maximum Lake Length, Mean Lake Width, Maximum Lake Width, and Fetch.

109 2.2 Predicting Trophic State with Random Forests

Random forest is a machine learning algorithm that aggregates numerous decision trees in order to obtain a consensus prediction of the response categories (Breiman 2001). Bootstrapped sample data are recursively partitioned according to a given random subset of predictor variables and a predetermined number of decision trees are developed. With each new tree, the sample data subset is randomly selected and with each new split, the subset of predictor variables are randomly selected. A detailed discussion of the benefits of a random forest approach is beyond the scope of this paper. To find out more see Breiman (2001) and Cutler et al. (2007).

Random forests are able to handle numerous correlated variables without a decrease in prediction accuracy; however, one possible shortcoming of this approach is that the resulting model may be difficult 118 to interpret, thus selecting the most important variables is an important first step. Several method 119 have been proposed to do this with random forest. For instance, this is a problem often faced in gene 120 selection and in that field, a variable selection method based on random forest has been successfully 121 applied and implemented in the R Language as the varSelRF package (Díaz-Uriarte and De Andres 122 2006), but this is limited to classification problems. Additionally, others have suggested alternative 123 variable importance measures, but this is only needed with a large number of categorical variables which 124 are selected against with traditional random forest approach (Strobl et al. 2007). 125

In our case, we are predicting a continuous variable, chlorophyll a, directly thus varSelRF, does not 126 apply, and all of our variables are continuous so the approach suggested by Strobl (2007) is not necessary. 127 Thus we developed an approach, similar to varSe1RF but applied to random forest with regression trees. 128 With this approach we fit a full random forest model that includes all variables and a large number of 129 trees. We then rank the variables using the increase in mean square error, which has been shown to be 130 a less biased metric of importance than the mean decrease in the gini coeffecient (Strobl et al. 2007). 131 Using this ranking, we then iterate through the variables and create a random forests with the top two 132 variables and record mean square error and adjusted R² of the resultant random forest. We then repeat 133 this process by adding the next most important variable in order of importance. With this information 134 we identify the top variables and the point at which adding variables does not improve the fit of the 135 overall model. These variables are selected and used as the "reduced model." With this method, a 136 minimum set of variables that maximizes model accuracy is provided. This allows us to start with a 137 full suite of predictor variables from which to select a minimum, easier to interpret set of variables. 138

139 2.3 Model Details

Using randomForest R package we ran models the predict chlorphyll a with two sets of predictors (Liaw and Wiener 2002); all precitors (in situ and universally available GIS predictors) and the GIS only variables (i.e. no in situ information). A listing of all considered variables is in Appendix 1. Our separation of predictors was chosen so that we could highlight the additional predictive performance

provided by adding the *in situ* water quality variables on top of the GIS only variables. Lastly, we used only complete cases (i.e. missing data were removed) so the total number of observations varied between models.

Our modelling work flow was as follows:

- 1. Identify a minimal set of variables that maximize accuracy of the random forest algorithm. This
 minimal set of variables, the reduced model, is calculated for each of the models.
- 2. Using R's randomForest package, we develop two random forest models.
- 3. Assess model performance for both the predicted chlorophyll *a* and for categorical trophic state classifications. Trophic state was defined using the NLA chlorophyll *a* trophic state cut offs (Table 1).

4 2.4 Measures of Model Performance and Variable Importance

We assessed the performance of the random forest two ways. First we compare the root mean square error and the adjusted R² of the models. Second, we examine the accuracy of the model when converted 156 to trophic states classes (Table 1). We assess the classifications via a confusion matrix. A confusion 157 matrix shows agreement and disagreement in a tabular form with predicted values forming the columns 158 of the matrix and observed values, the rows. From this tabulated information we calculate the total 159 accuracy (i.e. percent correctly predicted) and the kappa coefficient, which takes into account the error 160 expected by chance alone (i.e. the off diagonal values of the matrix) (Cohen 1960, Hubert and Arabie 161 1985). The kappa coefficient can range from -1 to 1 with 0 equalling the agreement expected by chance 162 alone. Values greater than 0 represent agreement greater than would be expected by chance, with 163 values greater than 0.61 considered "substantial" agreement (Landis and Koch 1977). Negative values 164 are rare and would indicate no agreement between the predicted and observed values. Additionally, 165 random forest builds each tree on bootstrapped, random subsets of the original data, thus, a separate 166 independent validation dataset is not required and random forest error estimates are expected to be 167 unbiased (Breiman 2001). 168

69 The random forest algorithm explicitly measures variable importance with two metrics: mean decrease

in Gini and percent increase in mean squared error. For each of these they measure the impact on
the overall model when that particular variable is included and thus can be used to assess importance
(Breiman 2001). The Gini Index has been shown to have a bias that is less apparent than with percent
increase in mean squared error (Strobl et al. 2007), thus, we use this metric to asses variable importance.
Lastly, partial dependence plots provide a mecahnism to examine the partial relationship between
individual variables and the response variable (Jones and Linder 2015). We examine these plots for the
top variables as assigned by percent increase in mean squared error of for each the reduced models.

77 3 Results

Our complete dataset includes 1148 lakes; however 5 lakes did not have chlorophyll *a* data. Thus, the base dataset for our modelling was conducted on data for 1143 lakes. The lakes were well distributed both across the four trophic state categories (Table 1) and spatially throughout the United States (Figure 1).

3.1 Models: All Variables

The model built with all predictors had a mean squared error of 0.09 and and R² of 0.8. The accuracy of the four trophic states was 68.7% and the kappa coefficient was 0.57 (Table 2). The reduced, all variables model was built using 1080 total observations. The variable selection process identified 20 variables (Figure 2). The five most important variables were turbidity, total phosphorus, total nitrogen, elevation, and total organic carbon. (Figure 3).

188 [CREATE PARTIAL DEPENDENCE PLOTS AND ADD PARAGRAPH]

3.2 Models: GIS Only Variables

The GIS only model had a mean squared error of 0.22 and and R^2 0.48. Four trophic states were predicted with a total accuracy of 49% and had a kappa coefficient of 0.29 (Table 3). The gis only

variables model was built using 1138 total observations. The variable selection process for this model produced a reduced model with 15 variables (Figure 4). The five most important variables were ecoregion, percent cropland, elevation, latitude, and percent evegreen forest. (Figure 5).

195 [CREATE PARTIAL DEPENDENCE PLOTS AND ADD PARAGRAPH]

196 3.3 Per Lake Probability

The "All Variables" model provides more certain model prediction than the "GIS Only" model with a median prediction probability of 0.81 versus 0.72 (Figure 6). Additionally, total accuracy of the predictions is a function of this uncertainty. Lakes with more certain predictions are more accurately classified (Figure ??). For both models, when prediction probabilites are approximate 0.7 or higher, the models have an accuracy of 100%. This represents 81% of the lakes for the "All Variables" model and 60% of the lakes for the "GIS Only" model.

The trophic state predictions may be mapped discretely, yet this neglects to provide details on the 203 uncertainty of those predictions. It may be preferable to instead map the prediction probabilities for each 204 of the four classes and given the association between low uncertainty and high accuracy a map of this 205 sort shows the broad spatial patterns of lake trophic state across the United States. The spatial patterns 206 show little variability between the two models, thus we only show the reuslts from the more broadly 207 applicable "GIS only" model (Figure 7. Hypereutrophic lakes are much more commonly predicted in 208 the midwest and southeastern United States. Clear, oligotrophic lakes are in the northwestern united 209 states, throught the western mountains and in the northeastern united states. The middle trophic states 210 are more evenly distributed across the country. 211

$_{212}$ 4 Discussion

3 [JEFF START HERE]

214 4.1 Trophic State Probabilities

One of the powerful features of random forests is the ability to aggregate a very large number of competing models or trees. Each tree provides an independent prediction or vote for a pos-216 sible outcome. In the context of our trophic state models, we have 10,000 votes for each lake. 217 These values may be interpreted as the probability that a lake is in a given trophic state. For 218 instance, for a single lake (National Lake Assessment ID = NLA06608-0005), the vote prob-219 abilities for Model 1 were "r 100 round(lakeVotes[lakeVotes\$COMID==23491387,][,4],2)"% for 220 oligotrophic, "r 100 round(lakeVotes[lakeVotes\$COMID==23491387,][,5],2)"% for mesotrophic, "r 221 $100 round (lake Votes [lake Votes \$ COMID == 23491387,] [,6], 2) \text{ ``\% for eutrophic, and '`r 100 } \\ \text{round (lake Votes } \texttt{[lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and '`r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and '`r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and '`r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and '`r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and ''r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and ''r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and ''r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and ''r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and ''r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and ''r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and ''r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and ''r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and ''r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and ''r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and ''r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and ''r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and ''r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and ''r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and ''r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and ''r 100 } \\ \text{round (lake Votes \$ COMID == 23491387,] [,6], 2) $``\% for eutrophic, and ''\% for eutrophic,$ 222 for hypereutrophic. This suggests little uncertainty in the predicted oligotrophic state. 223

Further, the maximum probability for each lake can be used as a measure of how certain the random 224 forest model was of the prediction. We would expect higher total accuracy for lakes that had more 225 certain predictions. Some lakes may have many votes for a single trophic state and few votes for 226 other trophic states and these would thus have a large maximum probability and the random forest 227 predictions would be more certain. Alternatively, the 10,000 votes could have been spread more equally 228 across the trophic state classes for a lake and that lake would have a small maximum probability and 229 the final predictions would be less certain. This should be evident by looking at the total classification 230 accuracy of lakes given their maximum probability is above a certain point. To test this we can examine 231 the accuracy of trophic state predictions across the full range of trophic state probabilities, similar to an 232 approach outlined by Paul and MacDonald (2005) and implemented by Hollister et al. (2008). We utilize 233 this approach and examine the change in total accuracy as a function of the maximum probability for 234 each lake. As expected, lakes with higher maximum vote probabilities were more accurately predicted (Figure ??). The increasing trend suggests that even for models with lower overall accuracy there can 236 also be a large number of individual cases that are predicted with high accuracy. 237

²³⁸ 4.2 Variable Selection and Importance

There was a great deal of agreement on the important variables for each set of models. In line with past predictive modelling of cyanobacteria abundance and not surprisingly, the *in situ* models consistently select the water quality variables (turbidity, total nitrogen, total phosphorus, and N:P ratios) as important variables (Downing et al. 2001). While there is variation in the response of cyanobacteria to changes in relative nutrient concentrations, the general pattern suggests that limiting nutrients have considerable impact once amounts increase beyond expected levels.

The mechanistic role of turbidity on lake trophic state is more complex. Light availability in turbid waters is lower than in clear waters. This would suggest a negative relationship between turbidity and chlorophyll a. Second, chlorophyll a can also be a component of turbidity and lakes with higher chlorophyll a concentrations will also be more turbid. Last, chlorophyll a is not the only component of of turbidity and turbid waters can be caused by, for example, increased sediment loads or tannin. This would be a cause for concern with linear models; however, linearity is not an assumption of tree-based modelling approaches such as random forest.

Our models with the GIS-only variables captured the large scale spatial pattern of the trophic status gradient of lakes across the United States. We reliably saw latitude and longitude and ecoregion selected as important variables. It is also possible that other variables selected as important are also capturing a portion of this trend. For instance, elevation and growing degree days both have obvious spatial components, but may also be accounting for variation in temperature.

The land use/land cover variables were also important in describing trophic state patterns. Like elevation and growing degree days, broad scale spatial patterns are inherent in the data. For instance, the relative continental position of mountains in the United States is the spatial inverse of the distribution of agricultural lands. However, it is known that forests are positively associated with lower nutrient loads where as agricultural land shows a negative association. These more local scale relationships with land use/land cover likely provide additional predictive power to the information in the broader scale data.

Lastly, morphometry (e.g. depth and volume) also proved to be important in the prediction of lake trophic state. As morphometry shows little to no broad scale spatial pattern and is unique to a given

lake, these data are likely illuminating the local, lake scale drivers of trophic state. As only depth and volume were selected, this likely shows the importance of in-lake nutrient processing and residence time.

Cyanobacteria biomass should be closely associated with trophic state as cyanobacteria contribute to

4.3 Associating Trophic State and Cyanobacteria

the chlorophyll concentration in a lake. If these associations are strong enough we may be able to 269 expand models such as those reported here to also predict probability of cyanobacteria blooms. To 270 test if trophic state can be used to differentiate cyanobacteria abundance, we examine distribution of 271 cyanobacteria abundance for each trophic state and also explored linear associations between chlorohyll 272 a and cyanobacteria abundance. The distribution of cyanobacteria abundance showed separation between all of the trophic state 274 classifications (Figures ??, ??, and ??) and there was a significant linear relationship (r²=0.33) between 275 chlorophyll a and cyanobacteria abundance (Figure ??). Furthermore, Yuan et al. (2014) used the 276 2007 NLA to demonstrate that total nitrogen and chlorophyll a concentrations were good predictors of 277 World Health Organization microcystin (a toxin produced by some cyanobacteria) criteria exceedences. 278 These results suggest that trophic state is indeed an acceptable proxy for cyanobacteria abundance and

that in lakes with higher trophic state it is also reasonable to expect higher cyanobacteria.

$_{281}$ 5 Conclusions

280

Our research goals were to explore the utility of a widely used data mining algorithm, random forests, in the modelling of chlorophyll a and lake trophic state. Further, we hoped to examine the utility of these models when built with only ubiquitous GIS data, which allows estimation of trophic state for all lakes in the United States. We were able to successfully predict a variety of trophic state classes. With the GIS only models our total accuracy ranged from , and with the full suite of data our model accuracy had a minimum accuracy of %.

While some of the models (i.e. Model 4) showed relatively low prediction accuracies, another feature of

the random forest, votes, can provide additional information. In addition to providing a single estimate of trophic state for each lake, our models also indicated the probability that a lake was classified in any of the categories. These probabilities may be mapped directly to show the uncertainty of a given predicted class. Furthermore, as the certainty of prediction increases, so does overall trophic state classification accuracy (Figure ??). These results suggest that our models will provide reasonable estimates of trophic state across the United States.

There was great deal of agreement on the important variables for each set of models. For the combined in situ and GIS models, the in situ water quality variables drove the predictions. This is expected. For the GIS only models, the results were more nuanced with three broad categories routinely being selected as important: broad scale spatial patterns in trophic state, land use/land cover controls of trophic state, and local, lake-scale control driven by lake morphometry. Lastly, associations between trophic state and cyanobacteria showed that, at the broad scale of the 2007 NLA, there is a linear relationship between chlorophyll a and cyanobacteria abundance and that using trophic state as a proxy for cyanobacteria has potential.

These broad categories and the association between trophic state and total cyanobacteria abundance raise 303 three important considerations related to managing eutrophication. First, the broad scale patterning 304 suggests regional trends. This is important because it suggests that efforts to monitor, model and 305 manage eutrophication and cyanobacteria should be undertaken at both national and regional levels. 306 Second, while direct control of water quality in lakes would have a large impact, the land use/land 307 cover drivers (i.e. non-point sources) of water quality are also important, and better management of 308 the spatial distribution of important classes such as forest and agriculture can provide some level of 309 control on trophic state and amount of cyanobacteria present. Third, in-lake processes (i.e. residence 310 time, nutrient cycling, etc.) are, as expected, very important and need to be part of any management 311 strategy. Building on these efforts through updated models, direct prediction of cyanobacteria, and 312 additional information on the regional differences will help us get a better handle on the broad scale 313 dynamics of productivity in lakes and the potential risk to human health from cyanobacteria blooms. 314

315 6 Acknowledgements

We would like to thank Farnaz Nojavan, Nathan Schmucker, John Kiddon, Joe LiVolsi, Tim Gleason, and Wayne Munns for constructive reviews of this paper. This paper has not been subjected to Agency review. Therefore, it does not necessary reflect the views of the Agency. Mention of trade names or commercial products does not constitute endorsement or recommendation for use. This contribution is identified by the tracking number ORD-011075 of the Atlantic Ecology Division, Office of Research and Development, National Health and Environmental Effects Research Laboratory, US Environmental Protection Agency.

7 Figures

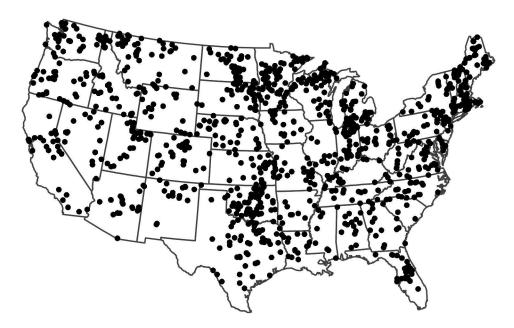


Figure 1: Map of the distribution of National Lakes Assesment Sampling locations

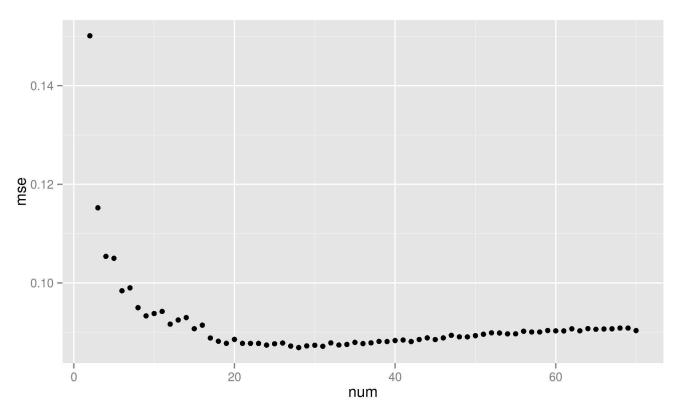


Figure 2: Variable selection plot for all variables. Shows percent increase in mean squared error as a function of the number of variables.

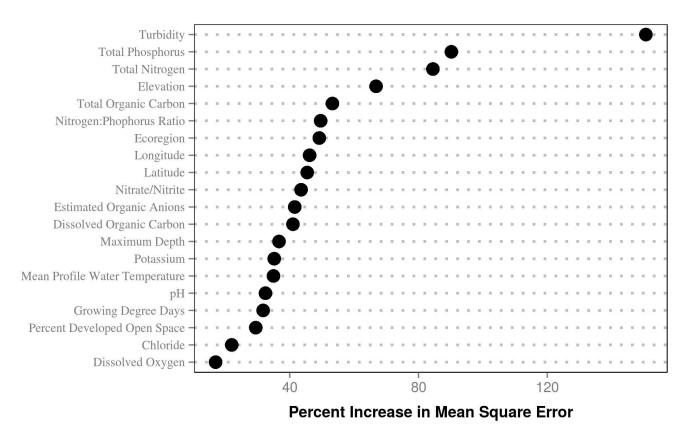


Figure 3: Importance plot for All Variables., shows percent increase in mean square error. Higher values of percent increase in mean squared error indicates higher importance.

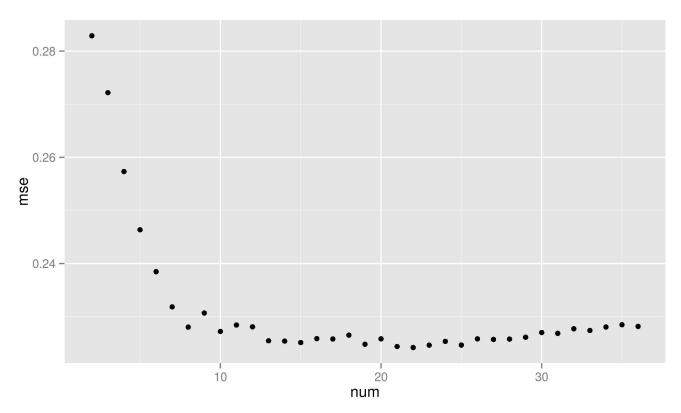


Figure 4: Variable selection plot for GIS only variables. Shows percent increase in mean squared error as a function of the number of variables.

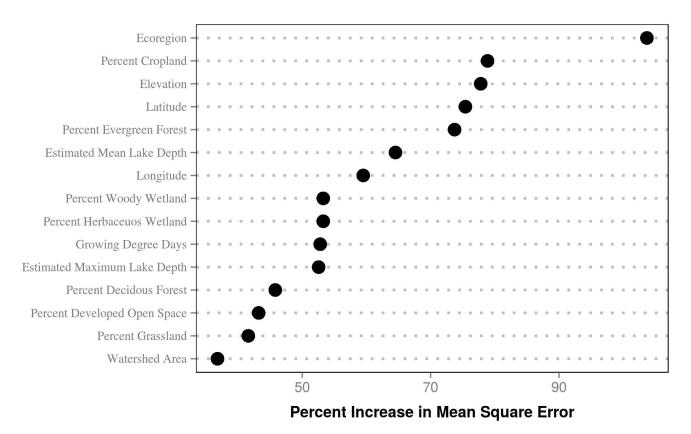


Figure 5: Importance plot for GIS Only Variables., shows percent increase in mean square error. Higher values of percent increase in mean squared error indicates higher importance.

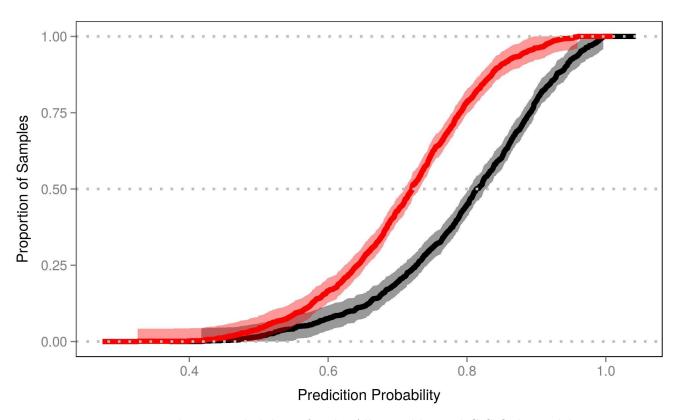
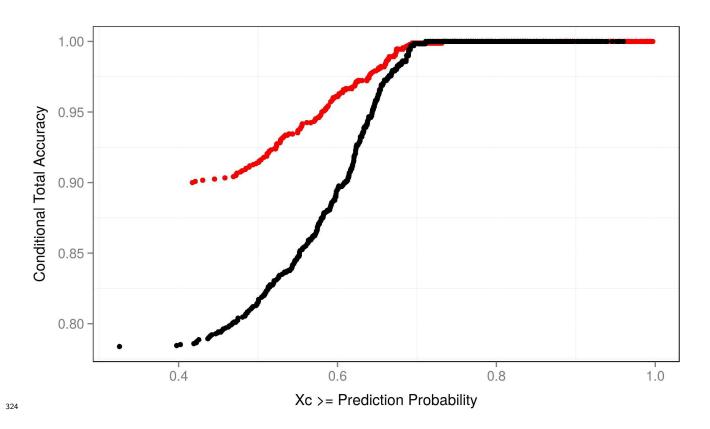


Figure 6: Prediction probabilities for the All Variables and GIS Only models.



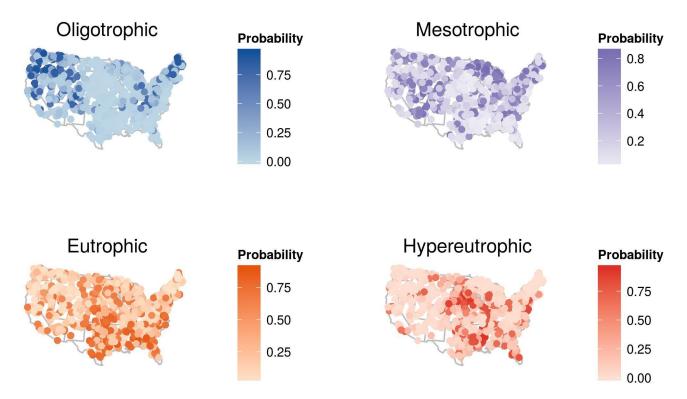


Figure 7: Maps of prediction probabilities for each of the four chlorophyll a trophic states

325 8 Tables

Table 1: Chlorophyll a based trophic state cut-offs.

| Trophic State (4 class) | Trophic State (2 class) | Concentration Cut-off |
|-------------------------|--------------------------|-----------------------|
| oligotrophic | oligotrophic/mesotrophic | <= 2 |
| mesotrophic | oligotrophic/mesotrophic | >2-7 |
| eutrophic | eutrophic/hypereutrophic | >7-30 |
| hypereutrophic | eutrophic/hypereutrophic | >30 |

Table 2: Random Forest confusion matrix for All Variables model converted to 4 trophic states. Columns show predicted values and rows show observed values. Agreement indicated on diagonal and accuracy for each trophic state indicated in 'Class Accuracy' column.

| | oligo | meso | eu | hyper | Class Accuracy (%) |
|-------|-------|------|-----|-------|--------------------|
| oligo | 115 | 31 | 0 | 0 | 78.77 |
| meso | 67 | 251 | 63 | 0 | 65.88 |
| eu | 7 | 61 | 217 | 75 | 60.28 |
| hyper | 0 | 5 | 29 | 159 | 82.38 |

Table 3: Random Forest confusion matrix for GIS Only model converted to 4 tropic states. Columns show predicted values and rows show observed values. Agreement indicated on diagonal and accuracy for each trophic state indicated in 'Class Accuracy' column.

| | oligo | meso | eu | hyper | Class Accuracy (%) |
|-------|-------|------|-----|-------|--------------------|
| oligo | 65 | 14 | 6 | 0 | 76.47 |
| meso | 101 | 213 | 98 | 18 | 49.53 |
| eu | 29 | 126 | 193 | 141 | 39.47 |
| hyper | 1 | 8 | 38 | 87 | 64.93 |

³²⁶ 9 Appendix 1. Variable Definitions

| variable_names | description | type |
|--------------------------------|--------------------------------------|---------------|
| PercentImperv_3000m | Percent Impervious | GIS |
| $WaterPer_3000m$ | Percent Water | GIS |
| $IceSnowPer_3000m$ | Percent Ice/Snow | GIS |
| DevOpenPer_3000m | Percent Developed Open Space | GIS |
| DevLowPer_3000m | Percent Low Intensity Development | GIS |
| ${\rm DevMedPer}_3000{\rm m}$ | Percent Medium Intensity Development | GIS |
| $DevHighPer_3000m$ | Percent High Intensity Development | GIS |
| BarrenPer_3000m | Percent Barren | GIS |
| DeciduousPer_3000m | Percent Decidous Forest | GIS |
| EvergreenPer_3000m | Percent Evergreen Forest | GIS |
| ${\it MixedForPer_3000m}$ | Percent Mixed Forest | GIS |
| $ShrubPer_3000m$ | Percent Shrub/Scrub | GIS |
| $GrassPer_3000m$ | Percent Grassland | GIS |
| PasturePer_3000m | Percent Pasture | GIS |
| $CropsPer_3000m$ | Percent Cropland | GIS |
| WoodyWetPer_3000m | Percent Woody Wetland | GIS |
| $HerbWetPer_3000m$ | Percent Herbaceuos Wetland | GIS |
| AlbersX | Longitude | GIS |
| AlbersY | Latitude | GIS |
| LakeArea | Lake Surface Area | GIS |
| LakePerim | Lake Perimeter | GIS |
| ShoreDevel | Shoreline Development Index | GIS |
| DATE_COL | Date Samples Collected | Water Quality |
| WSA_ECO9 | Ecoregion | GIS |
| BASINAREA | Watershed Area | GIS |
| DEPTHMAX | Maximum Depth | Water Quality |

| variable_names | description | type |
|---------------------|----------------------------|---------------|
| ELEV_PT | Elevation | GIS |
| DO2_2M | Dissolved Oxygen | Water Quality |
| PH_FIELD | pH | Water Quality |
| COND | Conductivity | Water Quality |
| ANC | Acid Neutralizing Capacity | Water Quality |
| TURB | Turbidity | Water Quality |
| TOC | Total Organic Carbon | Water Quality |
| DOC | Dissolved Organic Carbon | Water Quality |
| NH4 | Ammonium | Water Quality |
| NO3_NO2 | Nitrate/Nitrite | Water Quality |
| NTL | Total Nitrogen | Water Quality |
| PTL | Total Phosphorus | Water Quality |
| CL | Chloride | Water Quality |
| NO3 | Nitrate | Water Quality |
| SO4 | Sulfate | Water Quality |
| CA | Calcium | Water Quality |
| MG | Magnesium | Water Quality |
| Na | Sodium | Water Quality |
| K | Potassium | Water Quality |
| COLOR | Color | Water Quality |
| SIO2 | Silica | Water Quality |
| Н | Hydrogen Ions | Water Quality |
| ОН | Hydroxide | Water Quality |
| NH4ION | Calculate Ammonium | Water Quality |
| CATSUM | Cation Sum | Water Quality |
| ANSUM2 | Anion Sum | Water Quality |
| ANDEF2 | Anion Deficit | Water Quality |
| SOBC | Base Cation Sum | Water Quality |

| variable_names | description | type |
|------------------|--------------------------------|---------------|
| BALANCE2 | Ion Balance | Water Quality |
| ORGION | Estimated Organic Anions | Water Quality |
| CONCAL2 | Calculated Conductivity | Water Quality |
| CONDHO2 | D-H-O Calculated Conductivity | Water Quality |
| TmeanW | Mean Profile Water Temperature | Water Quality |
| DDs45 | Growing Degree Days | GIS |
| MaxLength | Maximum Lake Length | GIS |
| MaxWidth | Maximum Lake Width | GIS |
| MeanWidth | Mean Lake Width | GIS |
| FetchN | Fetch from North | GIS |
| FetchNE | Fetch form Northeast | GIS |
| FetchE | Fetch from East | GIS |
| FetchSE | Fetch from Southeast | GIS |
| MaxDepthCorrect | Estimated Maximum Lake Depth | GIS |
| VolumeCorrect | Estimated Lake Volume | GIS |
| MeanDepthCorrect | Estimated Mean Lake Depth | GIS |
| NPratio | Nitrogen:Phophorus Ratio | Water Quality |

References

- Breiman, L. 2001. Random forests. Machine learning 45:5–32.
- 329 CARLSON, R. E. 1977. A trophic state index for lakes. Limnology and oceanography 22:361–369.
- CARVALHO, L., C. A. MILLER, E. M. SCOTT, G. A. CODD, P. S. DAVIES, AND A. N. TYLER. 2011.
- 331 Cyanobacterial blooms: Statistical models describing risk factors for national-scale lake assessment and
- lake management. Science of The Total Environment 409:5353–5358.
- ³³³ COHEN, J. 1960. A coefficient of agreement for nominal scales. Educational and Psychological
- 334 Measurement 20:37–46.
- Cutler, D. R., T. C. Edwards Jr, K. H. Beard, A. Cutler, K. T. Hess, J. Gibson, and J. J.
- LAWLER. 2007. Random forests for classification in ecology. Ecology 88:2783–2792.
- DÍAZ-URIARTE, R., AND S. A. DE ANDRES. 2006. Gene selection and classification of microarray
- data using random forest. BMC bioinformatics 7:3.
- DOWNING, J. A., S. B. WATSON, AND E. McCauley. 2001. Predicting cyanobacteria dominance in
- lakes. Canadian journal of fisheries and aquatic sciences 58:1905–1908.
- Fernández-Delgado, M., E. Cernadas, S. Barro, and D. Amorim. 2014. Do we need
- hundreds of classifiers to solve real world classification problems? Journal of Machine Learning Research
- 343 15:3133–3181.
- HASLER, A. D. 1969. Cultural eutrophication is reversible. BioScience 19:425–431.
- HOLLISTER, J. W. 2014. Lakemorpho: Lake morphometry in R. R package version 1.0. http://CRAN.R-
- project.org/package=lakemorpho.
- HOLLISTER, J. W., W. B. MILSTEAD, AND M. A. URRUTIA. 2011. Predicting maximum lake depth
- 348 from surrounding topography. PLoS ONE 6:e25764.
- HOLLISTER, J. W., H. A. WALKER, AND J. F. PAUL. 2008. CProb: A computational tool for

- conducting conditional probability analysis. Journal of environmental quality 37:2392–2396.
- HOLLISTER, J., AND W. B. MILSTEAD. 2010. Using gIS to estimate lake volume from limited data.
- Lake and Reservoir Management 26:194–199.
- Homer, C., C. Huang, L. Yang, B. Wylie, and M. Coan. 2004. Development of a 2001 national
- land-cover database for the united states. Photogrammetric Engineering & Remote Sensing 70:829–840.
- 355 Hubert, L., and P. Arabie. 1985. Comparing partitions. Journal of classification 2:193–218.
- ³⁵⁶ IMBODEN, D., AND R. GÄCHTER. 1978. A dynamic lake model for trophic state prediction. Ecological
- 357 modelling 4:77–98.
- Jones, J., M. Knowlton, D. Obrecht, and E. Cook. 2004. Importance of landscape variables
- and morphology on nutrients in missouri reservoirs. Canadian Journal of Fisheries and Aquatic Sciences
- 360 61:1503—1512.
- Jones, K. B., A. C. Neale, M. S. Nash, R. D. Van Remortel, J. D. Wickham, K. H. Riitters,
- 362 AND R. V. O'NEILL. 2001. Predicting nutrient and sediment loadings to streams from landscape
- metrics: A multiple watershed study from the united states mid-atlantic region. Landscape Ecology
- 364 16:301-312.
- Jones, Z., and F. Linder. 2015. Exploratory data analysis using random forests. in The 73rd annual
- mPSA conference. MPSA.
- LANDIS, J. R., AND G. G. KOCH. 1977. The measurement of observer agreement for categorical data.
- 368 biometrics 33:159–174.
- LIAW, A., AND M. WIENER. 2002. Classification and regression by randomForest. R News 2:18–22.
- MILSTEAD, W. B., J. W. HOLLISTER, R. B. MOORE, AND H. A. WALKER. 2013. Estimating summer
- nutrient concentrations in northeastern lakes from sPARROW load predictions and modeled lake depth
- and volume. PloS one 8:e81457.
- PAUL, J. F., AND M. E. McDonald. 2005. Development of empirical, geographically specific water

- quality criteria: A conditional probability analysis approach 41:1211–1223.
- Peters, J., B. D. Baets, N. E. Verhoest, R. Samson, S. Degroeve, P. D. Becker, and W.
- 376 HUYBRECHTS. 2007. Random forests as a tool for ecohydrological distribution modelling. Ecological
- 377 Modelling 207:304–318.
- Rodhe, W. 1969. Crystallization of eutrophication concepts in northern europe.
- SALAS, H. J., AND P. MARTINO. 1991. A simplified phosphorus trophic state model for warm-water
- tropical lakes. Water research 25:341–350.
- 381 SCHINDLER, D. W., AND J. R. VALLENTYNE. 2008. The algal bowl: Overfertilization of the world's
- freshwaters and estuaries. Page 334. University of Alberta Press Edmonton.
- SEILHEIMER, T. S., P. L. ZIMMERMAN, K. M. STUEVE, AND C. H. PERRY. 2013. Landscape-scale
- modeling of water quality in lake superior and lake michigan watersheds: How useful are forest-based
- indicators? Journal of Great Lakes Research 39:211–223.
- SMITH, V. H. 1998. Cultural eutrophication of inland, estuarine, and coastal waters. Pages 7–49 in
- Successes, limitations, and frontiers in ecosystem science. Springer.
- SMITH, V. H., S. B. JOYE, R. W. HOWARTH, AND OTHERS. 2006. Eutrophication of freshwater and
- marine ecosystems. Limnology and Oceanography 51:351–355.
- SMITH, V. H., G. D. TILMAN, AND J. C. NEKOLA. 1999. Eutrophication: Impacts of excess nutrient
- inputs on freshwater, marine, and terrestrial ecosystems. Environmental pollution 100:179–196.
- 392 STROBL, C., A.-L. BOULESTEIX, A. ZEILEIS, AND T. HOTHORN. 2007. Bias in random forest variable
- importance measures: Illustrations, sources and a solution. BMC bioinformatics 8:25.
- USEPA. 2009. National lakes assessment: A collaborative survey of the nation's lakes. ePA 841-r-09-001.
- Office of Water; Office of Research; Development, US Environmental Protection Agency Washington,
- 396 DC.
- 397 XIAN, G., C. HOMER, AND J. FRY. 2009. Updating the 2001 national land cover database land

- ³⁹⁸ cover classification to 2006 by using landsat imagery change detection methods. Remote Sensing of
- 399 Environment 113:1133–1147.
- 400 Yuan, L. L., A. I. Pollard, S. Pather, J. L. Oliver, and L. D'Anglada. 2014. Managing
- microcystin: Identifying national-scale thresholds for total nitrogen and chlorophyll a. Freshwater
- 402 Biology 59:1970–1981.