## Modeling Lake Trophic State: A Random Forest Approach

Jeffrey W. Hollister \* 1 W. Bryan Milstead 1 Betty J. Kreakie 1

<sup>1</sup> US 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

16

17

19

20

23

24

25

26

27

Productivity of lentic ecosystems has been 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 and ecosystem services and disservices (e.g. recreation, aesthetics, fisheries, 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 expand our ability to predict trophic state in lakes without water quality data, 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 modern data mining approaches to build and assess models of lake trophic state that may be more universally applied. We use random forests and random forest variable selection to identify variables to be used for predicting trophic state and we compare the performance of two sets of models of trophic state (as determined by chlorophyll a concentration). The first set of models estimates three different trophic state classification with in situ as well as universally available data and the second set of models uses universally available GIS data only. Overall accuracy for models built from in situ and universal data ranged from 67% to 87%. For the universal data only models, overall accuracy ranged from 49% to 76%. Lastly, presence and abundance of cyanobacteria is often strongly associated with trophic state. To test this we examine the association between estimates of cyanobacteria abundance and measured chlorophyll a and find a positive relationship. These results suggest that predictive models of lake trophic state may be improved with additional information on the landscape surrounding lakes and that those models provide additional information on the presence of potentially harmful cyanobacteria taxa. Lastly, the source code and data for this manuscript are freely 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 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. 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 the identification of rapid shifts in trophic state or locating 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, 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 managment and allow for more effecient 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, e.g., 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 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, e.g., 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). 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 five areas in which our research contributes. First, we update trophic state modelling efforts with the use of random forests. Second, we assess the accuracy of predicted trophic state in lakes with the a) in situ and universally available GIS data and then b) with the universally available GIS data only. Third, we identify important variables for describing lake trophic state. Fourth, we explore associations between trophic state and cyanobacteria, a key taxa in harmful algal blooms, so that we may begin to understand how changes in trophic state may be linked to an important ecosystem disservice. Lastly, a key goal of this research is to provide full access to the data and code we used in this research. As such, this paper, the code, and the data used in the models is made available as an R package from https://github.com/USEPA/LakeTrophicModeling.

### $_{ iny 85}$ 2 Methods

#### 86 2.1 Data and Study Area

We utilize 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 scale 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 (USEPA 2009). With consistent methods and metrics collected at 1056 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 examined 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 100 cover class and total percent impervious surface within a 3 kilometer buffer surrounding each lake 101 (Homer et al. 2004, Xian et al. 2009). A three kilometer buffer was selected as an intermediate measure 102 of the adjacent neighborhood; the three kilometer buffer size is greater than the immediate parcel but

To account for unique aspects of each lake and characterize lake productivity, we also used measures 105 of lake morphometry (i.e. depth, volume, fetch, etc.). As these data are difficult to obtain for large 106 numbers of lakes over broad regions, we used modeled estimates of lake morphometry (Hollister and 107 Milstead 2010, Hollister et al. 2011, Hollister 2014). These included: surface area, shoreline length, 108 Shoreline Development, Maximum Depth, Mean Depth, Lake Volume, Maximum Lake Length, Mean 109 Lake Width, Maximum Lake Width, and Fetch. 110

#### 2.2Predicting Trophic State with Random Forests

smaller than regional and whole-basin measures.

103

104

Random forest is a machine learning algorithm that aggregates numerous decision trees in order to 112 obtain a consensus prediction of the response categories (Breiman 2001). Bootstrapped sample data are 113 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 115 and with each new split, the subset of predictor variables are randomly selected. A detailed discussion 116 of the benefits of a random forest approach is beyond the scope of this paper. To find out more see 117 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 downfall to this approach is that the resulting model may be difficult 120 to interpret. This is a problem often faced in gene selection and in that field, a variable selection 121 method based on random forest has been successfully applied and implemented in the R Language 122 as the varSelRF package (Díaz-Uriarte and De Andres 2006). With this method, a minimum set 123 of variables that maximizes model accuracy is provided. This allows us to start with a full suite of 124 predictor variables from which to select a minimum, easier to interpret set of variables. One issue with 125 the approach in varSelRF is that because of the randomization inherent in random forests it is possible 126 to get variation in the minimum selected set of variables. To account for this we repeated varSelRF 127 100 times. In our case, repeating the procedure 100 times quickly converged on a set of all possible 128 important variables. 129

#### so 2.3 Model Details

Using both the varSelRF and randomForest R packages we ran models for six sets of variables and 131 trophic state classifications (Liaw and Wiener 2002, Diaz-Uriarte 2010). These included three different 132 combinations of the chlorophyll a trophic states as the dependent variables and using all variables (in situ and GIS variables) or the GIS only variables (i.e. no in situ information) as the independent 134 variables in the random forest. A listing of all considered variables is in Appendix 1. Trophic state 135 was defined using the NLA chlorophyll a trophic state cut offs and the three combinations of trophic 136 state were used to highlight the possible error caused by misclassification of adjacent classes, such as 137 mesotrophic and eutrophic (Table 1). Our separation of predictors was chosen so that we could highlight 138 the additional predictive performance provided by adding the in situ water quality variables on top of 139 the GIS only variables. Lastly, we used only complete cases (i.e. missing data were removed) so the 140 total number of observations varied between models. 141

The six model combinations were:

145

- Model 1: Chlorophyll a trophic state (4 class) = All variables (in situ water quality, lake morphometry, and landscape)
  - Model 2: Chlorophyll a trophic state (3 class) = All variables (in situ water quality, lake

- morphometry, and landscape)
- Model 3: Chlorophyll a trophic state (2 class) = All variables (in situ water quality, lake morphometry, and landscape)
- **Model 4:** Chlorophyll *a* trophic state (4 class) = GIS Only variables (lake morphometry, and landscape)
- Model 5: Chlorophyll a trophic state (3 class) = GIS Only variables (lake morphometry, and landscape)
- Model 6: Chlorophyll a trophic state (2 class) = GIS Only variables (lake morphometry, and landscape)
- Our modelling work flow was as follows:

161

- 1. Use iterVarSelRF in the LakeTrophicModelling R package to identify a minimal set of variables
  that maximize accuracy of the random forest algorithm (Diaz-Uriarte 2010, Hollister et al. 2014).

  This subset of variables, the reduced model, is calculated for each of our 6 models.
- 2. Using R's randomForest package, we pass the reduced models selected with iterVarSelRF and assess model performance (Liaw and Wiener 2002).

#### 2.4 Measures of Model Performance and Variable Importance

We assessed the performance of the random forest models by comparing the total prediction accuracy and the kappa coefficient of the final confusion matrix. For each of the models, the final predictions 163 were compared to the original data via a confusion matrix. A confusion matrix shows agreement and 164 disagreement with predicted values forming the columns of the matrix and observed values, the rows. The total accuracy (i.e. percent correctly predicted) was calculated. Since some agreement can be 166 expected by chance alone, it is also useful to take this type of error into account. For this we calculated 167 the kappa coefficient from the confusion matrix for each model as well (Cohen 1960, Hubert and Arabie 168 1985). The kappa coefficient can range from -1 to 1 with 0 equalling the agreement expected by chance 169 alone. Values greater than 0 represent agreement greater than would be expected by chance, with 170 values greater than 0.61 considered "substantial" agreement (Landis and Koch 1977). Negative values 171

are rare and would indicate no agreement between the predicted and observed values. Additionally, random forest builds each tree on bootstrapped, random subsets of the original data, thus, a separate independent validation dataset is not required and random forest error estimates are expected to be unbiased (Breiman 2001).

Lastly, the random forest algorithm explicitly measures variable importance as mean decrease in Gini.

The Gini Index is a measure of how well the data are classified into homogeneous groups. For every node, the splitting variables are permuted and the change in actual Gini and permuted Gini is recorded. The mean decrease Gini is a summed and standardized value for each variable (Breiman 2001). Higher values of mean decrease Gini suggest a higher importance for that variable.

### 181 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. As chlorophyll a is used to create
the trophic state classifications, it was necessary to remove these data because no chlorophyll a trophic
state could be determined for these lakes. The lakes were well distributed both across the four trophic
state categories (Table 1) and spatially throughout the United States (Figure 1).

#### $_{187}$ 3.1 Models

Accuracy for the models built with all predictors ranged from 67% to 87% and the kappa coefficient had a minimum value of 0.55 and maximum of 0.73. The GIS only models had a total accuracy between 49% and 76% and kappa coefficient between 0.3 and 0.52. The importance of variables for the models including the *in situ* data were fairly stable while there was considerably more variation in variable importance for the three different GIS only models. Additionally, as each model contained a different subset of variables and since we removed observations with missing data, the total number of lakes varied across the models. Details for each model are discussed below.

5 Model 1: 4 Trophic States ~ All Variables

Total number of lakes for Model 1 was 1142 and the reduced model for Model 1 included turbidity, total phosphorus, total nitrogen, nitrogen:phosphorus ratio, total organic carbon, potassium, ecoregion, maximum depth, organic ions, and dissolved organic carbon. Of these, turbidity, total phosphorus, and total nitrogen were the three most important predictors of the four classes of trophic state (Figure 2).

Total accuracy for Model 1 was 67% and the Cohen's Kappa was 0.55 (Table 2).

#### 201 Model 2: 3 Trophic States ~ All Variables

For Model 2 there were 1130 observations and the reduced model included turbidity, total phosphorus, total nitrogen, total organic carbon, nitrogen:phosphorus, longitude, pH, estimated organic anions, elevation, maximum depth, dissolved organic carbon, potassium, latitude, ecoregion, chloride, ammonium and percent cropland (Figure 3). The top predictors for 3 trophic state classes were again turbidity, total phosphorus, and total nitrogen (Figure 3). Model 2 accuracy was 80% and the Cohen's Kappa was 0.61 (Table 3).

#### 208 Model 3: 2 Trophic States ~ All Variables

Model 3 was built with 1142 lakes and the reduced model was similar to Model 1 and Model 2. This model included turbidity, total phosphorus, total nitrogen, nitrogen:phosphorus, potassium, ecoregion, elevation, total organic carbon, growing degree days, longitude, sodium, maximum depth, estimated organic anions, latitude, and dissolved organic carbon (Figure 4). The top three predictors were the same as Models 1 and 2. (Figure 4). Total accuracy for Model 3 was 87% and the Cohen's Kappa was 0.73 (Table 4).

### 215 Model 4: 4 Trophic States ~ GIS Only Variables

Model 4 had a sample size of 1138. The selected variables for the Model 4 were longitude, latitude, elevation, estimated mean lake depth, percent evergreen forest, estimated maximum lake depth, percent cropland, and ecoregion (Figure 5). The three most important variables were longitude, latitude, and elevation (Figure 5); however, all variables except ecoregion were almost equally important. Total accuracy for Model 4 was 49% and the Cohen's Kappa was 0.3 (Table 5).

#### Model 5: 3 Trophic States ~ GIS Only Variables

A total of 1138 lakes were used for model 5 which included estimated mean lake depth, percent cropland, longitude, latitude, percent evergreen forest, elevation, estimated maximum lake depth, estimated lake volume, percent deciduous forest, percent developed open space, ecoregion, percent woody wetland, and percent shrub/scrub (Figure 6). The most important variables for model 5 were estimated mean lake depth, percent cropland, and longitude. (Figure 6). Total accuracy for Model 5 was 68% and the Cohen's Kappa was 0.35 (Table 6).

228 Model 6: 2 Trophic States ~ GIS Only Variables

Model 6 was built using 1138 total observations. The variable selection process for Model 6 produced a reduced model with ecoregion, growing degree days, percent evergreen forest, percent cropland, elevation, estimated mean lake depth, longitude, latitude, watershed area, estimated maximum lake depth, percent developed open space, percent deciduous forest, and estimated lake volume (Figure 7). The three most important variables were ecoregion, growing degree days, and percent evergreen. (Figure 7). Ecoregion had the highest importance with a slow decline in importance for the remainder of the variables. Total accuracy for Model 6 was 76% and the Cohen's Kappa was 0.52 (Table 7).

### 236 4 Discussion

#### 237 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 possible outcome. In the context of our trophic state models, we have 10,000 votes for each lake. These values may be interpreted as the probability that a lake is in a given trophic state. For instance, for a single lake (National Lake Assessment ID = NLA06608-0005), the vote probabilities for Model 1 were 81% for oligotrophic, 19% for mesotrophic, 0% for eutrophic, and 0% for hypereutrophic. This suggests little uncertainty in the predicted oligotrophic state.

Further, the maximum probability for each lake can be used as a measure of how certain the random forest model was of the prediction. We would expect higher total accuracy for lakes that had more

certain predictions. Some lakes may have many votes for a single trophic state and few votes for other trophic states and these would thus have a large maximum probability and the random forest 248 predictions would be more certain. Alternatively, the 10,000 votes could have been spread more equally 249 across the trophic state classes for a lake and that lake would have a small maximum probability and 250 the final predictions would be less certain. This should be evident by looking at the total classification 251 accuracy of lakes given their maximum probability is above a certain point. To test this we can examine 252 the accuracy of trophic state predictions across the full range of trophic state probabilities, similar to an 253 approach outlined by Paul and MacDonald (2005) and implemented by Hollister et al. (2008). We utilize 254 this approach and examine the change in total accuracy as a function of the maximum probability for 255 each lake. As expected, lakes with higher maximum vote probabilities were more accurately predicted 256 (Figure 8). The increasing trend suggests that even for models with lower overall accuracy there can also be a large number of individual cases that are predicted with high accuracy.

#### 59 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 modeling 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 275 a portion of this trend. For instance, elevation and growing degree days both have obvious spatial 276 components, but may also be accounting for variation in temperature. 277

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 279 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 281 where as agricultural land shows a negative association. These more local scale relationships with land 282 use/land cover likely provide additional predictive power to the information in the broader scale data. 283 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 285 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.

#### Associating Trophic State and Cyanobacteria 4.3

278

286

287

Cyanobacteria biomass should be closely associated with trophic state as cyanobacteria contribute to the chlorophyll concentration in a lake. If these associations are strong enough we may be able to expand models such as those reported here to also predict probability of cyanobacteria blooms. To 291 test if trophic state can be used to differentiate cyanobacteria abundance, we examine distribution of 292 cyanobacteria abundance for each trophic state and also explored linear associations between chlorohyll a and cyanobacteria abundance. 294

The distribution of cyanobacteria abundance showed separation between all of the trophic state classifications (Figures 9, 10, and 11) and there was a significant linear relationship  $(r^2=0.33)$  between chlorophyll a and cyanobacteria abundance (Figure 12). Furthermore, Yuan et al. (2014) used the 297 2007 NLA to demonstrate that total nitrogen and chlorophyll a concentrations were good predictors of 298 World Health Organization microcystin (a toxin produced by some cyanobacteria) criteria exceedences.

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.

### 5 Conclusions

Our research goals were to explore the utility of a widely used data mining algorithm, random forests, in the modelling of 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 49% to 76%, and with the full suite of data our model accuracy had a minimum accuracy of 67% and maximum accuracy of 87%.

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 8). 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 316 in situ and GIS models, the in situ water quality variables drove the predictions. This is expected. For 317 the GIS only models, the results were more nuanced with three broad categories routinely being selected 318 as important: broad scale spatial patterns in trophic state, land use/land cover controls of trophic state, 319 and local, lake-scale control driven by lake morphometry. Lastly, associations between trophic state and 320 cyanobacteria showed that, at the broad scale of the 2007 NLA, there is a linear relationship between 321 chlorophyll a and cyanobacteria abundance and that using trophic state as a proxy for cyanobacteria 322 has potential. 323

These broad categories and the association between trophic state and total cyanobacteria abundance raise three important considerations related to managing eutrophication. First, the broad scale patterning

suggests regional trends. This is important because it suggests that efforts to monitor, model and manage eutrophication and cyanobacteria should be undertaken at both national and regional levels. 327 Second, while direct control of water quality in lakes would have a large impact, the land use/land 328 cover drivers (i.e. non-point sources) of water quality are also important, and better management of 329 the spatial distribution of important classes such as forest and agriculture can provide some level of 330 control on trophic state and amount of cyanobacteria present. Third, in-lake processes (i.e. residence 331 time, nutrient cycling, etc.) are, as expected, very important and need to be part of any management 332 strategy. Building on these efforts through updated models, direct prediction of cyanobacteria, and 333 additional information on the regional differences will help us get a better handle on the broad scale 334 dynamics of productivity in lakes and the potential risk to human health from cyanobacteria blooms. 335

### 336 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

#### 345 ## Loading required package: grid

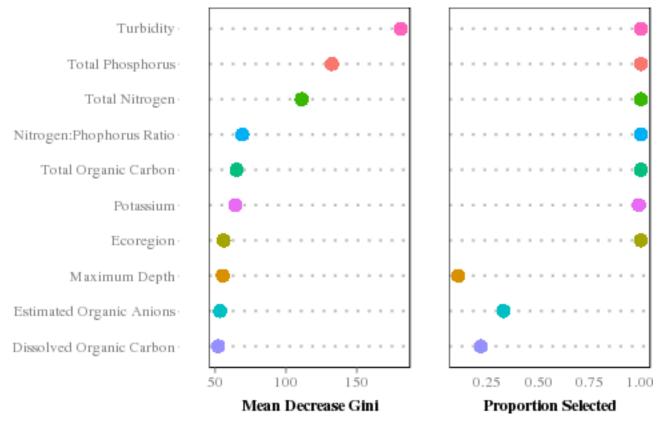


Figure 2: Importance plot for Model 1, shows mean descrease gini and proportion of times a variable was selected for inclusion in the model. Higher values of mean decrease gini indicate higher importance.

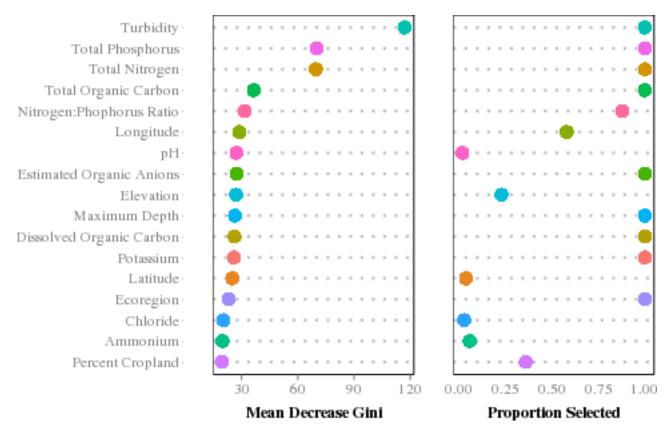


Figure 3: Importance plot for Model 2, shows mean descrease gini and proportion of times a variable was selected for inclusion in the model. Higher values of mean decrease gini indicate higher importance.

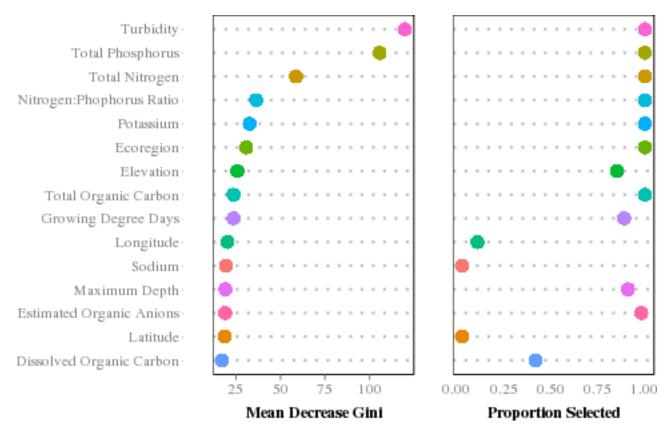


Figure 4: Importance plot for Model 3, shows mean descrease gini and proportion of times a variable was selected for inclusion in the model. Higher values of mean decrease gini indicate higher importance.

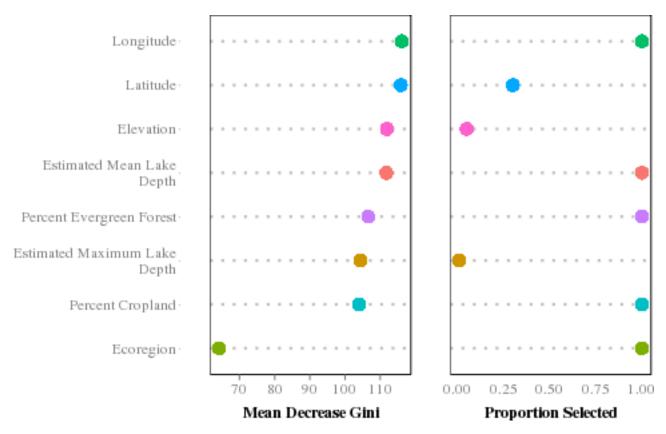


Figure 5: Importance plot for Model 4, shows mean descrease gini and proportion of times a variable was selected for inclusion in the model. Higher values of mean decrease gini indicate higher importance.

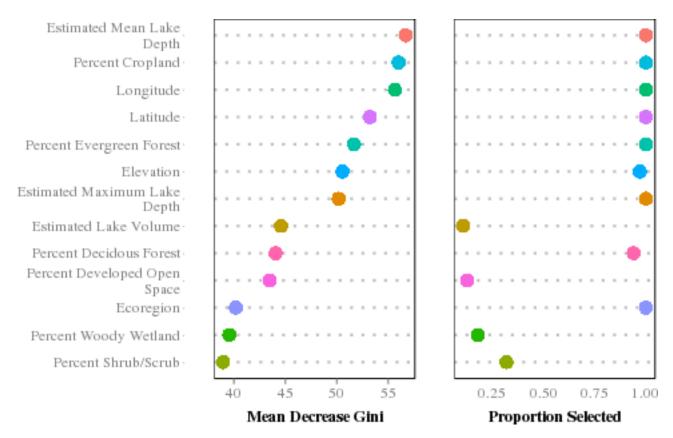


Figure 6: Importance plot for Model 5, shows mean descrease gini and proportion of times a variable was selected for inclusion in the model. Higher values of mean decrease gini indicate higher importance.

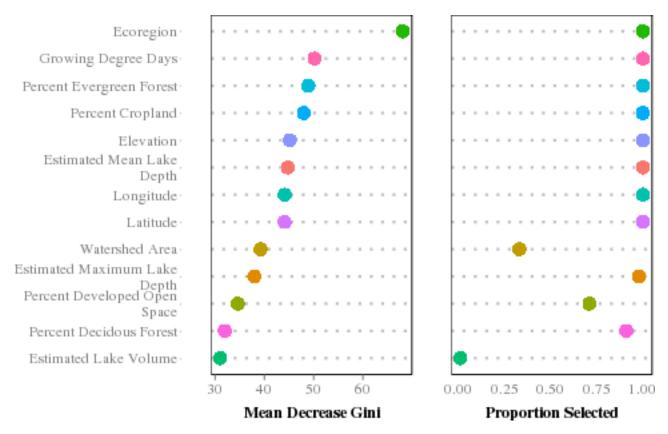


Figure 7: Importance plot for Model 6, shows mean descrease gini and proportion of times a variable was selected for inclusion in the model. Higher values of mean decrease gini indicate higher importance.

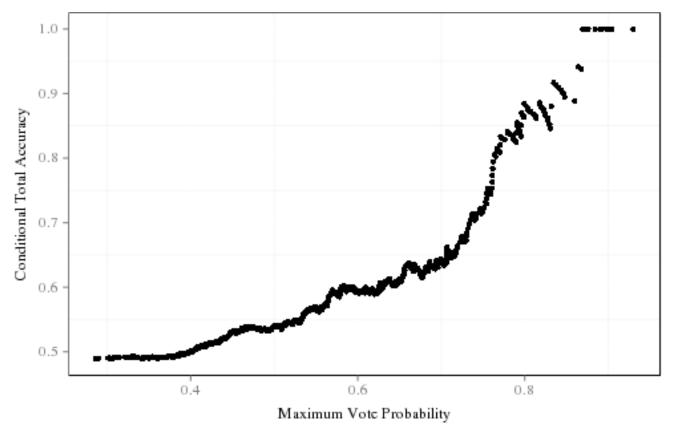


Figure 8: Comparison of certainity of trophic state prediction and total accuracy

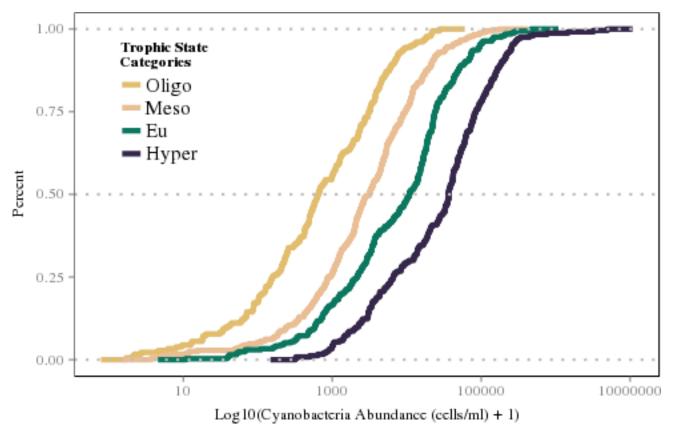


Figure 9: Cumulative distribution function of cyanobacetria abundance for 4 trophic state classes

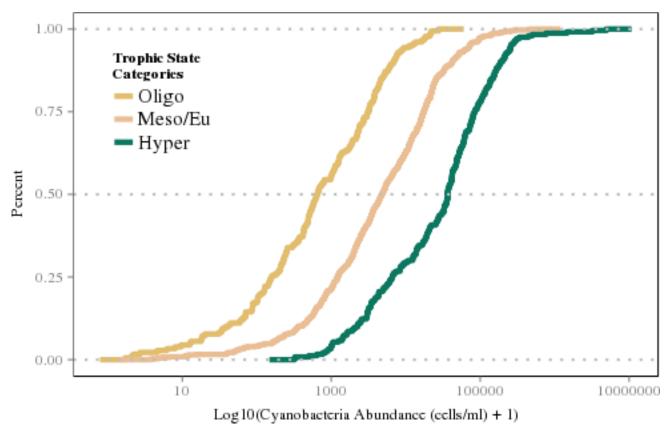


Figure 10: Cumulative distribution function of cyanobacetria abundance for 3 trophic state classes

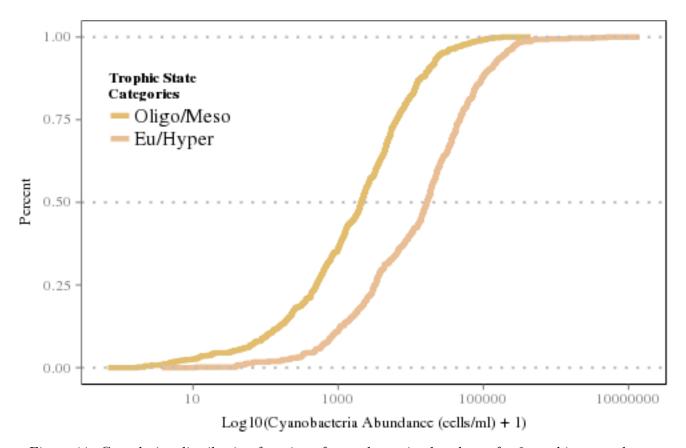


Figure 11: Cumulative distribution function of cyanobacetria abundance for 2 trophic state classes

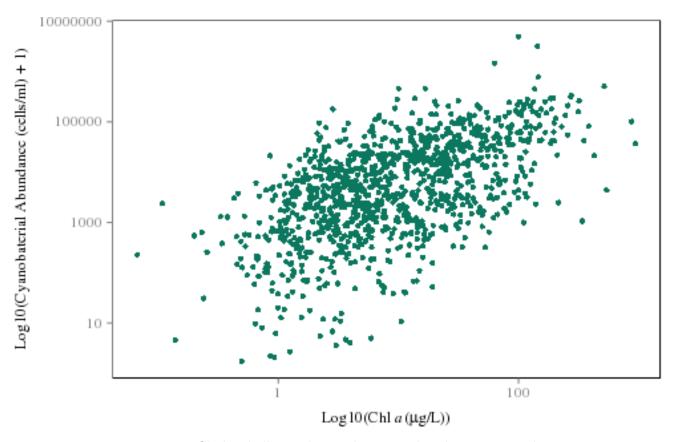


Figure 12: Cholorphyll a and cyanobacteria abundance scatterplot

# 346 8 Tables

Table 1: Chlorophyll a based trophic state cut-offs with total number of possible observations.

Trophic State (4 class)	Trophic State (3 class)	Trophic State (2 class)	Concentration Cut-off
oligotrophic	oligotrophic	oligotrophic/mesotrophic	<= 0.2
mesotrophic	mesotrophic/eutrophic	oligotrophic/mesotrophic	>2-7
eutrophic	mesotrophic/eutrophic	eutrophic/hypereutrophic	>7-30
hypereutrophic	hypereutrophic	eutrophic/hypereutrophic	>30

Table 2: Random Forest confusion matrix for Model 1. 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	135	58	4	1	68%
Meso	42	233	77	10	64%
Eu	2	66	222	46	66%
Hyper	0	3	69	174	71%

Table 3: Random Forest confusion matrix for Model 2. 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	122	74	0	62%
Meso/Eu	43	604	42	88%
Hyper	0	72	173	71%

Table 4: Random Forest confusion matrix for Model 3. 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/Meso	485	75	87%
Eu/Hyper	77	505	87%

Table 5: Random Forest confusion matrix for Model 4. 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	94	72	28	2	48%
Meso	50	201	80	30	56%
Eu	21	110	131	73	39%
Hyper	1	34	80	131	53%

Table 6: Random Forest confusion matrix for Model 5. 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	80	115	1	41%
Meso/Eu	50	585	61	84%
Hyper	0	142	104	42%

Table 7: Random forest confusion matrix for Model 6. 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/Meso	428	129	77%
Eu/Hyper	147	434	75%

# <sup>347</sup> 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
${\rm DevOpenPer\_3000m}$	Percent Developed Open Space	GIS
DevLowPer_3000m	Percent Low Intensity Development	GIS
${\rm DevMedPer\_3000m}$	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	рН	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
$\operatorname{CL}$	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.
- <sup>350</sup> 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.
- <sup>352</sup> Cyanobacterial blooms: Statistical models describing risk factors for national-scale lake assessment and
- lake management. Science of The Total Environment 409:5353–5358.
- <sup>354</sup> COHEN, J. 1960. A coefficient of agreement for nominal scales. Educational and Psychological
- 355 Measurement 20:37–46.
- 356 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.
- DIAZ-URIARTE, R. 2010. VarSelRF: Variable selection using random forests. R package version 0.7-3.
- http://CRAN.R-project.org/package=varSelRF.
- <sup>360</sup> 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.
- 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 B. J. KREAKIE. 2014. LakeTrophicModelling: Package to
- reproduce Hollister et al. (2014) Modeling lake trophic state: A data mining approach.
- HOLLISTER, J. W., W. B. MILSTEAD, AND M. A. URRUTIA. 2011. Predicting maximum lake depth
- 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
- <sup>376</sup> land-cover database for the united states. Photogrammetric Engineering & Remote Sensing 70:829–840.
- Hubert, L., and P. Arabie. 1985. Comparing partitions. Journal of classification 2:193–218.
- <sup>378</sup> IMBODEN, D., AND R. GÄCHTER. 1978. A dynamic lake model for trophic state prediction. Ecological
- 379 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
- 382 61:1503–1512.
- Jones, K. B., A. C. Neale, M. S. Nash, R. D. Van Remortel, J. D. Wickham, K. H. Riitters,
- <sup>384</sup> 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
- 386 16:301–312.
- LANDIS, J. R., AND G. G. KOCH. 1977. The measurement of observer agreement for categorical data.
- 388 biometrics 33:159–174.
- LIAW, A., AND M. WIENER. 2002. Classification and regression by randomForest. R News 2:18–22.
- 390 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
- $_{392}$  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.
- 396 HUYBRECHTS. 2007. Random forests as a tool for ecohydrological distribution modelling. Ecological
- <sup>397</sup> Modelling 207:304–318.
- SALAS, H. J., AND P. MARTINO. 1991. A simplified phosphorus trophic state model for warm-water
- tropical lakes. Water research 25:341–350.
- 400 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.
- 402 SEILHEIMER, T. S., P. L. ZIMMERMAN, K. M. STUEVE, AND C. H. PERRY. 2013. Landscape-scale
- 403 modeling of water quality in lake superior and lake michigan watersheds: How useful are forest-based
- 404 indicators? Journal of Great Lakes Research 39:211–223.
- 405 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.
- 409 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.
- 411 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,
- 413 DC.
- 414 XIAN, G., C. HOMER, AND J. FRY. 2009. Updating the 2001 national land cover database land
- cover classification to 2006 by using landsat imagery change detection methods. Remote Sensing of
- 416 Environment 113:1133-1147.
- 417 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
- 419 Biology 59:1970–1981.