

Modelling Lake Trophic State: A Random Forest Approach

Jeffrey W. Hollister^{*} ¹ W. Bryan Milstead¹ Betty J. Kreakie¹

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

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 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 R^2 of this model was 0.09 and 0.8, respectively. The second model uses universally available GIS data only. The mean squared error was 0.22 and the adjusted R^2 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 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

38 productivity (e.g. mesotrophic and eutrophic lakes) have greater nutrient loads, tend to be less clear,
39 have greater density of aquatic plants, and often support more diverse and abundant fish communities.
40 Higher primary productivity is not necessarily a predictor of poor ecological condition as it is natural
41 for lakes to shift from lower to higher trophic states but this is a slow process (Rodhe 1969). However,
42 at the highest productivity levels (hypereutrophic lakes) biological integrity is compromised (Hasler
43 1969, Smith et al. 1999, Schindler and Vallentyne 2008).

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

53 As trophic state and related indices can be best defined by a number of *in situ* water quality parameters
54 (modeled or measured), most models have used this information as predictors (Imboden and Gächter
55 1978, Salas and Martino 1991, Carvalho et al. 2011, Milstead et al. 2013). This leads to accurate models,
56 but also requires data that are often sparse and not always available, thus limiting the population of
57 lakes for which we can make predictions. A possible solution for this issue is to build models that use
58 widely available data that are correlated to many of the *in situ* variables. For instance, landscape metrics
59 of forests, agriculture, wetlands, and urban land in contributing watersheds have all been shown to
60 explain a significant proportion of the variation (ranging from 50-86%, depending on study) in nutrients
61 in receiving waters (Jones et al. 2001, 2004, Seilheimer et al. 2013). Building on these previously
62 identified associations might allow us to use only landscape and other universally available data to build
63 models. Identifying predictors using this type of ubiquitous data would allow for estimating trophic
64 state in both monitored and unmonitored lakes.

65 Many published models of nutrients and trophic state in freshwater systems are based on linear modelling

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

76 To build on past work, we have identified three areas in which this research contributes. First, we build,
 77 assess, and compare two random forest models of chlorophyll *a* 1) *in situ* and universally available GIS
 78 data and then 2) universally available GIS data only. Second, we convert the chlorophyll *a* estimates,
 79 for both models, to trophic state and assess the prediction accuracy and uncertainty. Third, we examine
 80 the important predictors for both models. Lastly, this paper, the code, and the data used in the models
 81 are made available as an R package from <https://github.com/USEPA/LakeTrophicModelling>.

82 2 Methods

83 2.1 Data and Study Area

84 We utilized three primary sources of data for this study, the National Lakes Assessment (NLA), the
 85 National Land Cover Dataset (NLCD), and lake morphometry modeled from the NHDPlus and
 86 National Elevation Data Set (Homer et al. 2004, USEPA 2009, Xian et al. 2009, Hollister and Milstead
 87 2010, Hollister et al. 2011, Hollister 2014). All datasets are national in extent and provide a unique
 88 snapshot view of the condition of lakes in the conterminous United States during the summer of 2007.

89 The NLA data were collected during the summer of 2007 and the final data were released in 2009 (USEPA
 90 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 various water quality measurements from the National Lakes Assessment (USEPA 2009).

Adding to the monitoring data collected via the NLA, we use the 2006 NLCD data to examine landscape-level 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 to characterize lake productivity, we 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.

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 to interpret, thus selecting the most important variables is an important first step. Several methods have been proposed to do this with random forest. For instance, this is a problem often faced in gene selection and in that field, a variable selection method based on random forest has been successfully applied and implemented in the R Language as the `varSelRF` package (Díaz-Uriarte and De Andres 2006), but this is limited to classification problems. Additionally, others have suggested alternative variable importance measures, but this is only needed with a large number of categorical variables which are selected against with traditional random forest approach (Strobl et al. 2007).

In our case, we are predicting a continuous variable, chlorophyll *a*, directly thus `varSelRF`, does not apply, and all of our variables are continuous so the approach suggested by Strobl (2007) is not necessary. Thus we developed an approach, similar to `varSelRF` but applied to random forest with regression trees. With this approach we fit a full random forest model that includes all variables and a large number of trees. We then rank the variables using the increase in mean square error, which has been shown to be a less biased metric of importance than the mean decrease in the gini coefficient (Strobl et al. 2007). Using this ranking, we then iterate through the variables and create a random forest with the top two variables and record mean square error and adjusted R^2 of the resultant random forest. We then repeat this process by adding the next most important variable in order of importance. With this information we identify both the top variables and the point at which adding variables does not improve the fit of the overall model. These variables are selected and used as the “reduced model.” With this method, a minimum set of variables that maximizes model accuracy is provided. This allows us to start with a full suite of predictor variables from which to select a minimum, easier to interpret set of variables.

2.3 Model Details

Using `randomForest` R package we ran models to predict chlorophyll *a* with two sets of predictors (Liaw and Wiener 2002). The first included *in situ* and universally available GIS predictors. We refer to this as the “All variables” model. Second, we use just the universally available data (i.e. no *in situ* information). This is referred to as the “GIS only” model. A list of the full suite of variables tested

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 among 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 ("All variables" and "GIS only").
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. Examine importance and partial dependence of the most important variables.

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 R^2 of the models. Second, we examine the accuracy of the model predictions when converted to trophic states classes (Table 1). We assess the classifications via a confusion matrix. A confusion matrix shows agreement and disagreement in a tabular form with predicted values forming the columns of the matrix and observed values, the rows. From this tabulated information we calculate the total accuracy (i.e. percent correctly predicted) and the kappa coefficient, which takes into account the error expected by chance alone (i.e. the off diagonal values of the matrix) (Cohen 1960, Hubert and Arabie 1985). The kappa coefficient can range from -1 to 1 with 0 equalling the agreement expected by chance alone. Values greater than 0 represent agreement greater than would be expected by chance, with values greater than 0.61 considered "substantial" agreement (Landis and Koch 1977). Negative values 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).

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 (Strobl et al. 2007), thus, we use percent increase in mean squared error to assess variable importance. Lastly, partial dependence plots provide a mechanism 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 for each the reduced models.

2.5 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 chlorophyll *a* models, we have 5,000 estimates of chlorophyll *a* for each lake. We convert these values to trophic states (Table 1) then count up total votes for each class and divide by total possible votes to get an estimate of 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 the “All variables” model were 95% for oligotrophic, 5% for mesotrophic, 0% for eutrophic, and 0% for hypereutrophic. The maximum probability provides the predicted class, in this case oligotrophic, and suggests little uncertainty in this prediction. We refer to this value as the “prediction probability.”

Further, we might expect higher total accuracy for lakes that have more certain predictions. This should be evident by looking at the total classification accuracy of lakes given their prediction probability is at or above a certain probability. To test this we use an approach similar to one outlined by Paul and MacDonald (2005) and implemented by Hollister et al. (2008). We utilize this approach and examine the change in total accuracy as a function of the prediction probability for both models.

3 Results

Our complete dataset included 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 used 1080 total observations, had a mean squared error of 0.09 and R^2 of 0.8. The accuracy of the four trophic states was 68.7% and the kappa coefficient was 0.57 (Table 2). The variable selection process identified 20 variables (Figure 2). The six most important variables were turbidity, total phosphorus, total nitrogen, elevation, total organic carbon, and N:P ratio (Figures 3). The role that each played in predicting chlorophyll *a* varied (Figure 4).

3.2 Models: GIS Only Variables

The GIS only model was built using 1138 total observations, had a mean squared error of 0.22 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 variable selection process for this model produced a reduced model with 15 variables (Figure 5). The six most important variables were ecoregion, percent cropland, elevation, latitude, percent evergreen forest, and mean lake depth (Figures 6 & 4).

3.3 Trophic State Probabilities

The “All variables” model provides more certain model predictions with a median prediction probability of 0.81 versus 0.72 for the “GIS only” model (Figure 8). Additionally, total accuracy of the predictions is a function of this uncertainty. Lakes with more certain predictions were more accurately classified (Figure 9). For both models, when prediction probabilities are approximately 0.8 or higher, the models had an accuracy of ~100%. This represents 55% of the lakes for the “All variables” model and 22% of

the lakes for the “GIS only” model. Lastly, as prediction probabilities increased, the difference in total accuracy between the two models decreased (Figure 9 & Table 4).

4 Discussion

4.1 Trophic State Probabilities

Not surprisingly, lakes with more certain predictions (i.e. higher prediction probabilities) were more accurately predicted (Figure 9). The fact that the difference in accuracy between the two models decreased as certainty in the prediction increased suggests that models with lower overall accuracy, such as the “GIS only” model, may have acceptable accuracy for many individual cases (Table 4). Additionally, the prediction probabilities may be mapped for each of the four classes (Figure 10).

A map of this sort indicates several things. First, since low uncertainty is associated with high accuracy this map shows the broad spatial patterns of lake trophic state across the United States. The spatial patterns show little variability between the “All variables” and “GIS only” models, thus we only show the results from the more broadly applicable “GIS only” model (Figure 10). Hypereutrophic lakes are much more commonly predicted in the midwest and southeastern United States. Clear, oligotrophic lakes are in the northwestern United States, through the western mountains and in the northeastern United States. The middle trophic states are more evenly distributed across the country. Secondly, instead of mapping the probabilities for each trophic state separately, we can also map the prediction probabilities of the discrete predicted class. (Figure 11). This map shows where the model predicts well and where it is less certain. In general, the map shows most points with higher prediction probabilities than the midpoint of the range and the distribution of prediction probabilities is skewed left (Figure ??). While these patterns are not strong, they suggest that with slight improvements in the “GIS only” model we could skew the prediction probabilities further left and easily improve the overall accuracy of the model. This could be done using modeled, national estimates of nutrient loads (Moore et al. 2011, e.g. Milstead et al. 2013).

4.2 Partial dependencies of explanatory variables

In line with past predictive modelling of chlorophyll *a* concentrations the “All variables” model selected the water quality variables (turbidity, total organic carbon, total nitrogen, total phosphorus, and N:P ratios) as important variables (Downing et al. 2001). While there is variation in the response of chlorophyll *a* to changes in nutrient concentrations, the general pattern suggests that limiting nutrients have a predictable impacts. If we examine the partial dependencies of these variables we see a general linear increase in log chlorophyll *a* with nitrogen, phosphorus and organic carbon concentrations (Figure 4). This relationship holds until nutrient concentrations become saturated. The partial dependency plots (Figure 4) for the nitrogen:phosphorus ratio is more complicated, indicating that for ratios less than ~14 chlorophyll *a* increases but after ~14 there is marked decrease. The effect of the nitrogen phosphorus ratio on chlorophyll has been the subject of considerable research and our results are consistent with the majority of the findings suggesting that at low ratio values nitrogen is limiting. Conversely at higher ratios the phosphorus levels may be limiting. 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.

Turbidity was selected as the most important variable in the “All variables” model. The partial dependency analysis shows that, similar to the nutrients discussed above, log chlorophyll *a* increases with increased turbidity. At first this may seem counter intuitive since we might expect productivity to decrease as turbidity increases, and therefore light availability decreases. However, algal biomass can contribute heavily to measures of turbidity and we expect greater productivity to lead to increased turbidity. We interpret this pattern as indicating that as chlorophyll *a* concentrations increase we see a concomitant increase in turbidity.

Elevation was selected as an important predictive variable in both the all variables and the GIS only models; the partial dependencies (Figures 4 & 7) indicate a negative relationship between elevation and chlorophyll *a* concentration that is probably due to fact that the location of mountains in the United States is the spatial inverse of the distribution of agricultural and urban lands. As elevation increases we expect decreased loads due to smaller watershed contributing areas. In contrast lower elevation sites will have larger drainage areas and greater potential for increased nutrient loads from urban and agricultural sources.

The variables in the “GIS only” model captured the large scale spatial pattern of the trophic status gradient of lakes across the United States. In addition to elevation, mentioned above, the model was most sensitive to latitude and ecoregion. In general, chlorophyll *a* concentrations are highest in the Southern portions of the study area where temperatures can be higher (a known driver of productivity), elevations lower, and agricultural impacts more pronounced. Likewise ecoregion (see Figure ??) has a pronounced affect indicting continental scale effects of land use and geography. Agriculturally dominated landscapes such as the Temperate Plains, Southern Plains, and Coastal Plains show the highest levels of Chlorophyll *a*. Whereas high elevation zones (Western Mountains), arid lands (Xeric), Northern habitats (Upper Midwest) have lower concentrations.

Further evidence for the role of land use/land cover variables is shown by the selection of the percent cropland and percent evergreen forest variables. As indicated by the partial dependency plots (Figure 7), chlorophyll *a* increases with cropland and decreases with evergreen cover. It is not surprising that croplands were selected given the overwhelming impact of agriculture on the eutrophication process. The negative association of evergreens and chlorophyll *a* concentrations (Figure 7). As the percent of evergreens increases we are likely to see increased elevation and soil differences that limit agriculture.

Lastly, morphometry (e.g. depth) 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 such as in-lake nutrient processing and residence time.

5 Conclusions

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. The “All variables” model had an RMSE of 0.09 and an adjusted R^2 of 0.8 whereas, the GIS only models had an RMSE of 0.22 and the adjusted R^2 was 0.48. Our total accuracy in predicting chlorophyll *a* based trophic states was 69% for the “All variables” model and 49% for the “GIS only” model.

296 While the “GIS only” model showed lower prediction accuracies than the “All variables” model, the
 297 association between the uncertainty of prediction and total accuracy (Figure ?? and Table 4) suggest
 298 that the “GIS only” model will provide reasonable estimates of trophic state for many lakes across the
 299 United States. Furthermore, we can map the uncertainty of the predictions, thus, we know the spatial
 300 patterns and location of the lakes for which we are certain, or not, of their predicted trophic state.
 301 Given this and that these models may be applied to any lake in the United States we can recomend
 302 using this model. Future iterations of this modelling effort may be able to utilize modeled predictions
 303 of nutrients to improve accuracy and also maintain broad applicability (Milstead et al. 2013).

304 For the “All variables” model, the *in situ* water quality variables drove the predictions. This is not
 305 surprising. For the “GIS only” model, the results were more nuanced. Three broad categories were
 306 routinely being selected as important: broad scale spatial patterns in trophic state, land use/land cover
 307 controls of trophic state, and local, lake-scale control driven by lake morphometry.

308 A potentially useful benefit of models of trophic state and chlorophyll *a* are their use in assesing risk due
 309 to cyanobacteria. Cyanobacteria biomass should be closely associated with chlorophyll *a* and trophic
 310 state as cyanobacteria contribute to the chlorophyll concentration in a lake. If these associations are
 311 strong enough we may be able to expand models such as those reported here to also predict probability
 312 of cyanobacteria blooms and other indices realted to cyanobacteria (e.g. toxin presence). Others have
 313 seen these associations. For instance, Yuan et al. (2014) used the 2007 NLA to demonstrate that
 314 total nitrogen and chlorophyll *a* concentrations were good predictors of World Health Organization
 315 microcystin (a toxin produced by some cyanobacteria) criteria exceedences. Using this same data, we
 316 see a positive trend between cholorophyll *a* and cyanobacteria abundance (Figure 13). Both of these
 317 suggest that trophic state may be an acceptable proxy for cyanobacteria abundance or presence of
 318 microcystin.

319 Our results raise three important considerations related to managing eutrophication. First, the broad
 320 scale patterning, indicated by ecoregion as an important variable, suggests regional trends. This
 321 is noteworthy because it suggests that efforts to monitor, model and manage eutrophication and
 322 cyanobacteria should be undertaken at both national and regional levels. Second, while direct control
 323 of water quality in lakes would have a large impact, the land use/land cover drivers (i.e. non-point

sources) of water quality are also important, and better management of the spatial distribution of important classes such as forest and agriculture can provide some level of control on trophic state and amount of cyanobacteria present. Third, in-lake processes (i.e. residence time, nutrient cycling, etc.) are, as expected, important and need to be part of any management strategy. Building on these efforts through updated models, direct prediction of cyanobacteria, and additional information on the regional differences will help us get a better handle on the broad scale dynamics of productivity in lakes and the potential risk to human health from cyanobacteria blooms.

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.

339 **7 Figures**

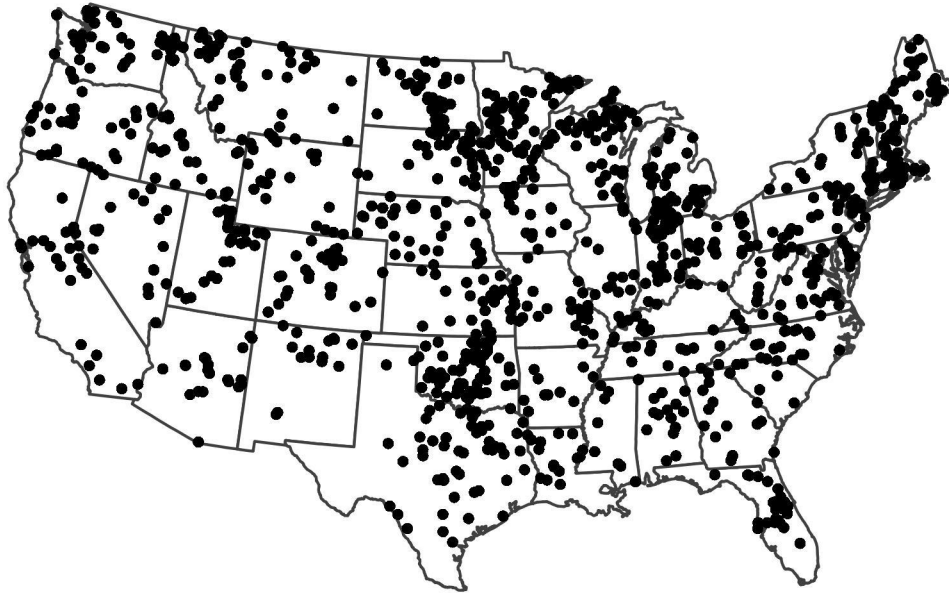


Figure 1: Map of the distribution of National Lakes Assessment Sampling locations

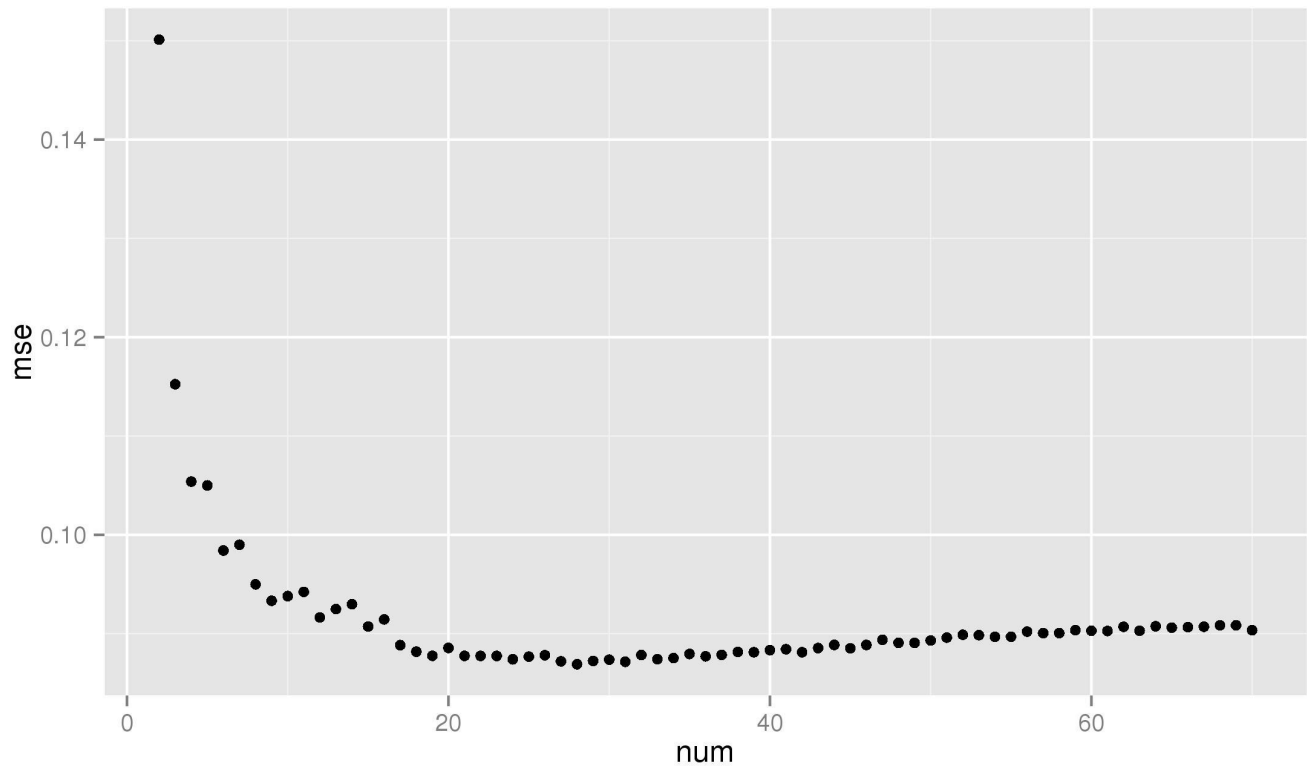


Figure 2: Variable selection plot for all variables. Shows percent increase in mean squared error as a function of the number of variables.

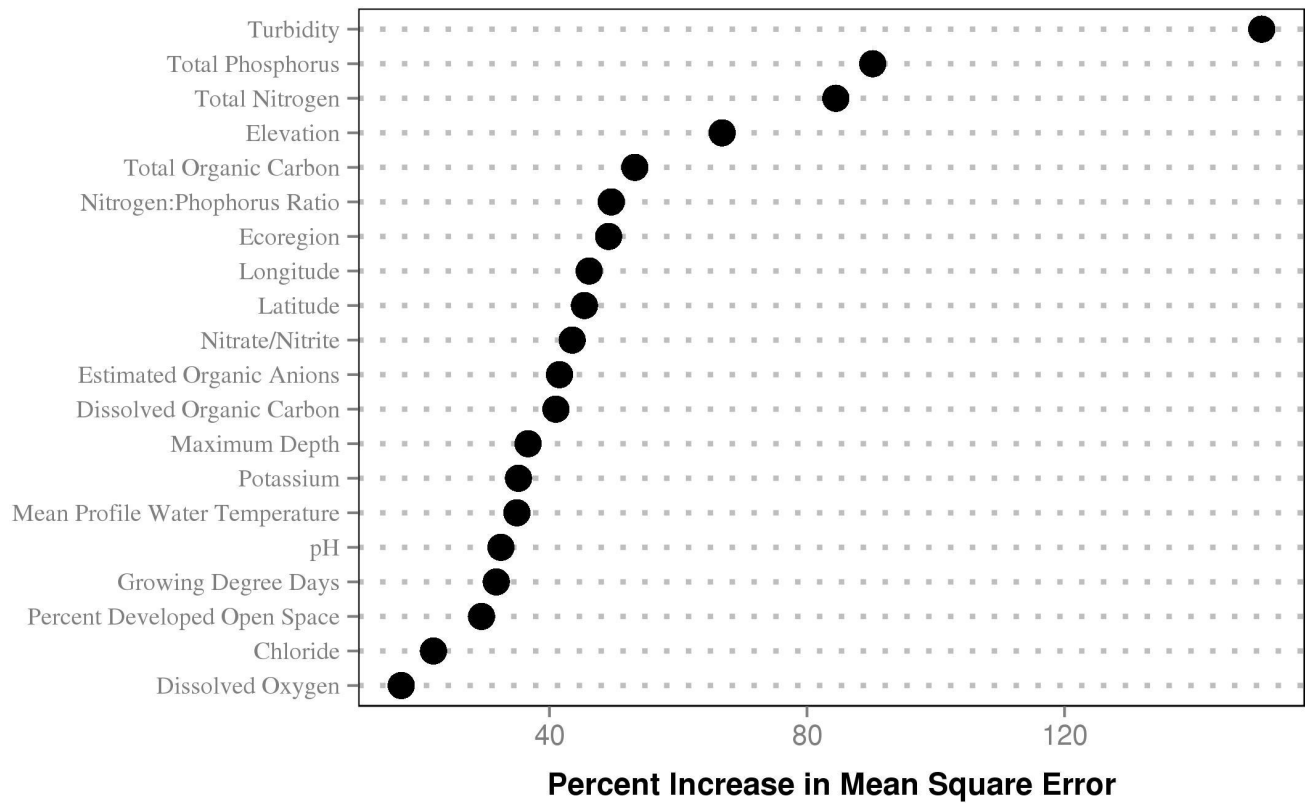


Figure 3: Importance plot for All Variables., shows percent increase in mean square error. Higher values of percent increase in mean squared error indicates higher importance.

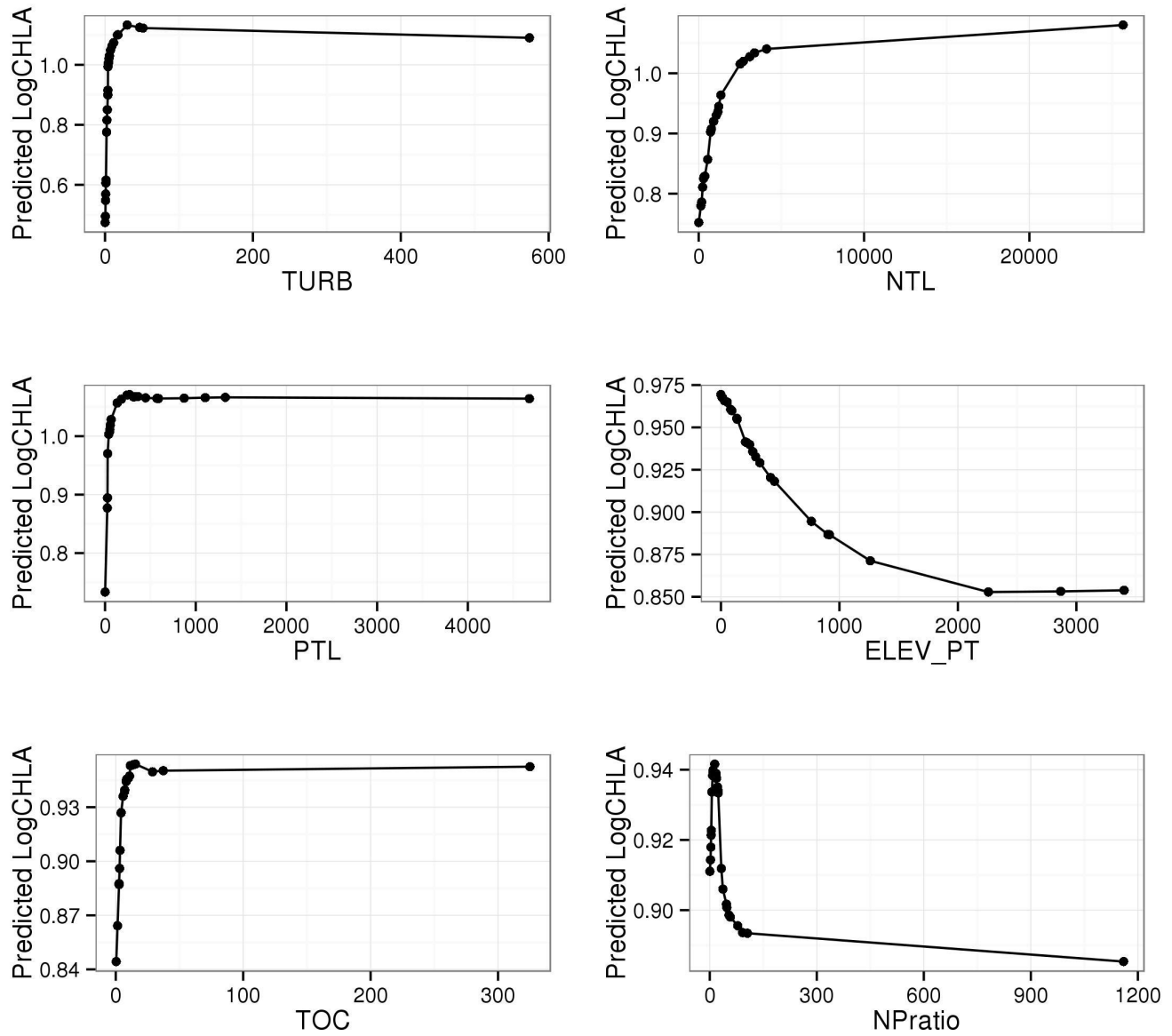


Figure 4: All Variables partial dependence plots for the top 5 most important variables.

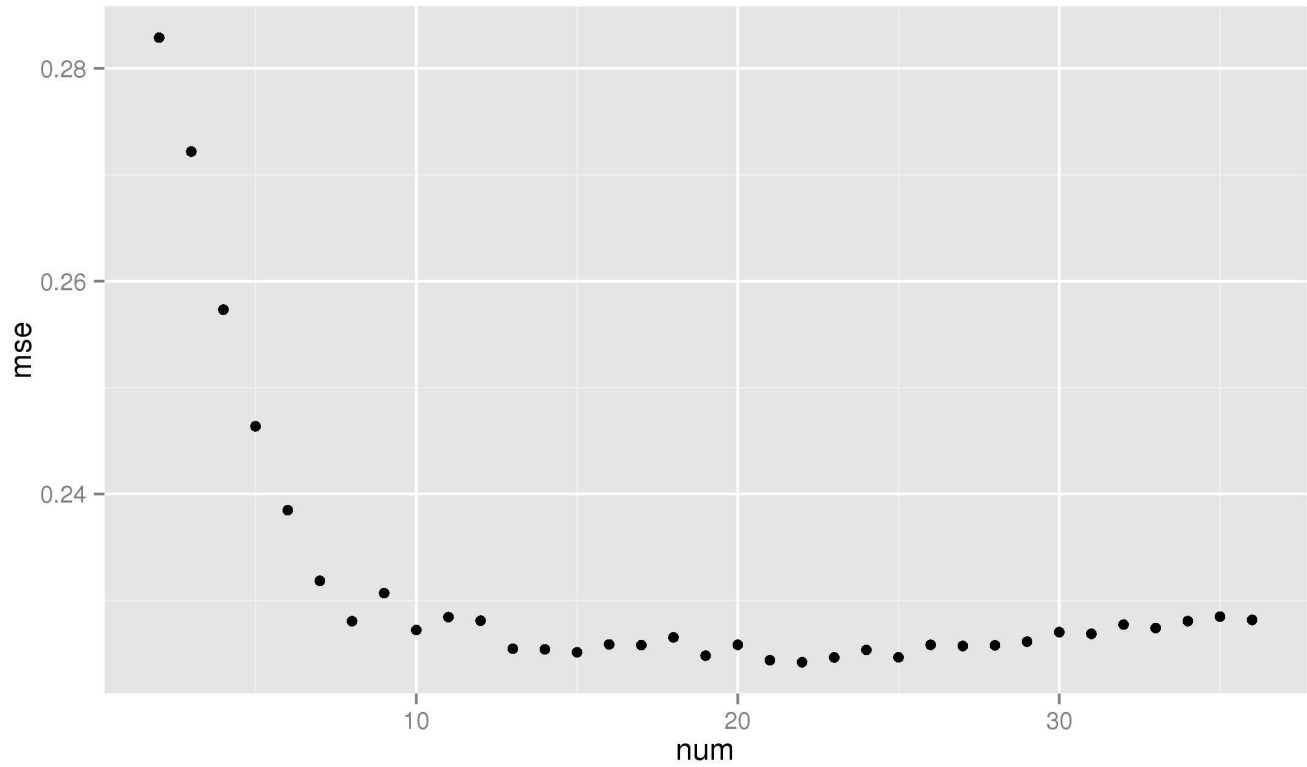


Figure 5: Variable selection plot for GIS only variables. Shows percent increase in mean squared error as a function of the number of variables.

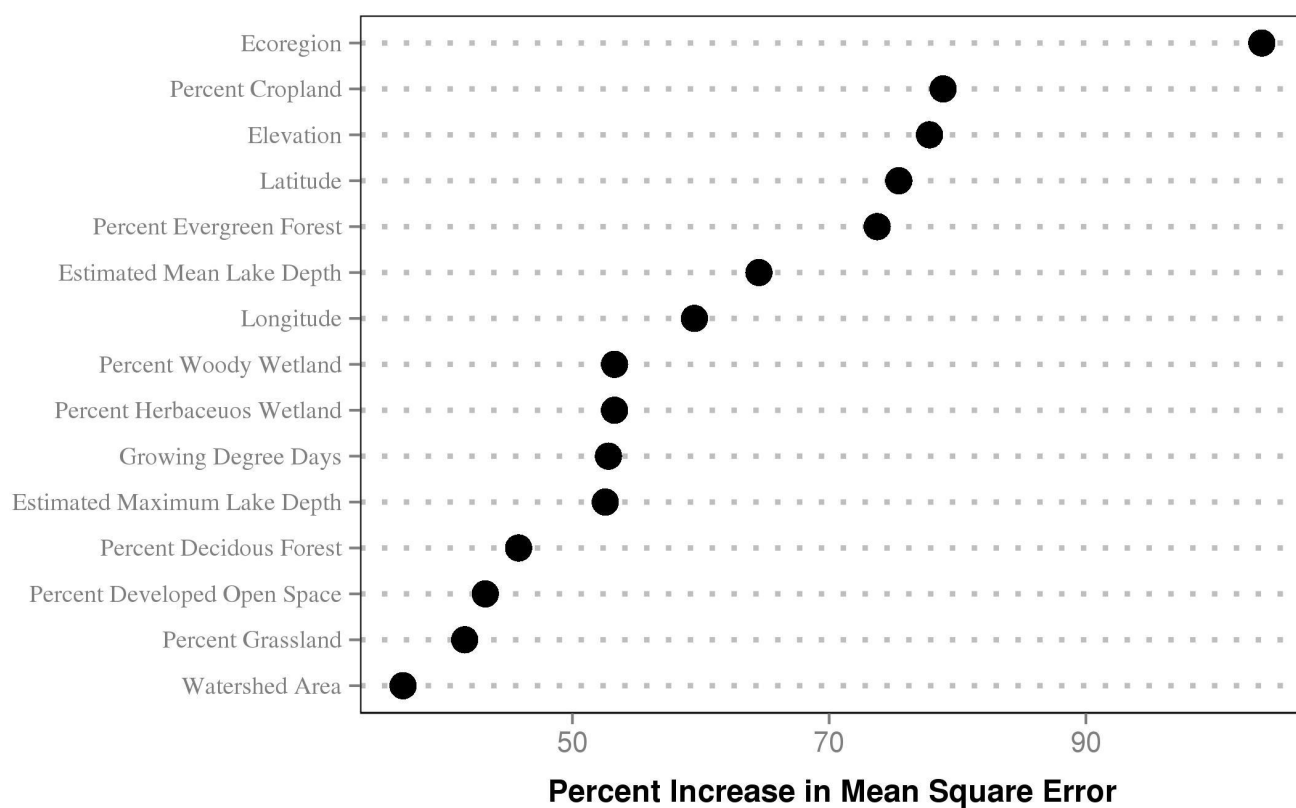


Figure 6: Importance plot for GIS Only Variables., shows percent increase in mean square error. Higher values of percent increase in mean squared error indicates higher importance.

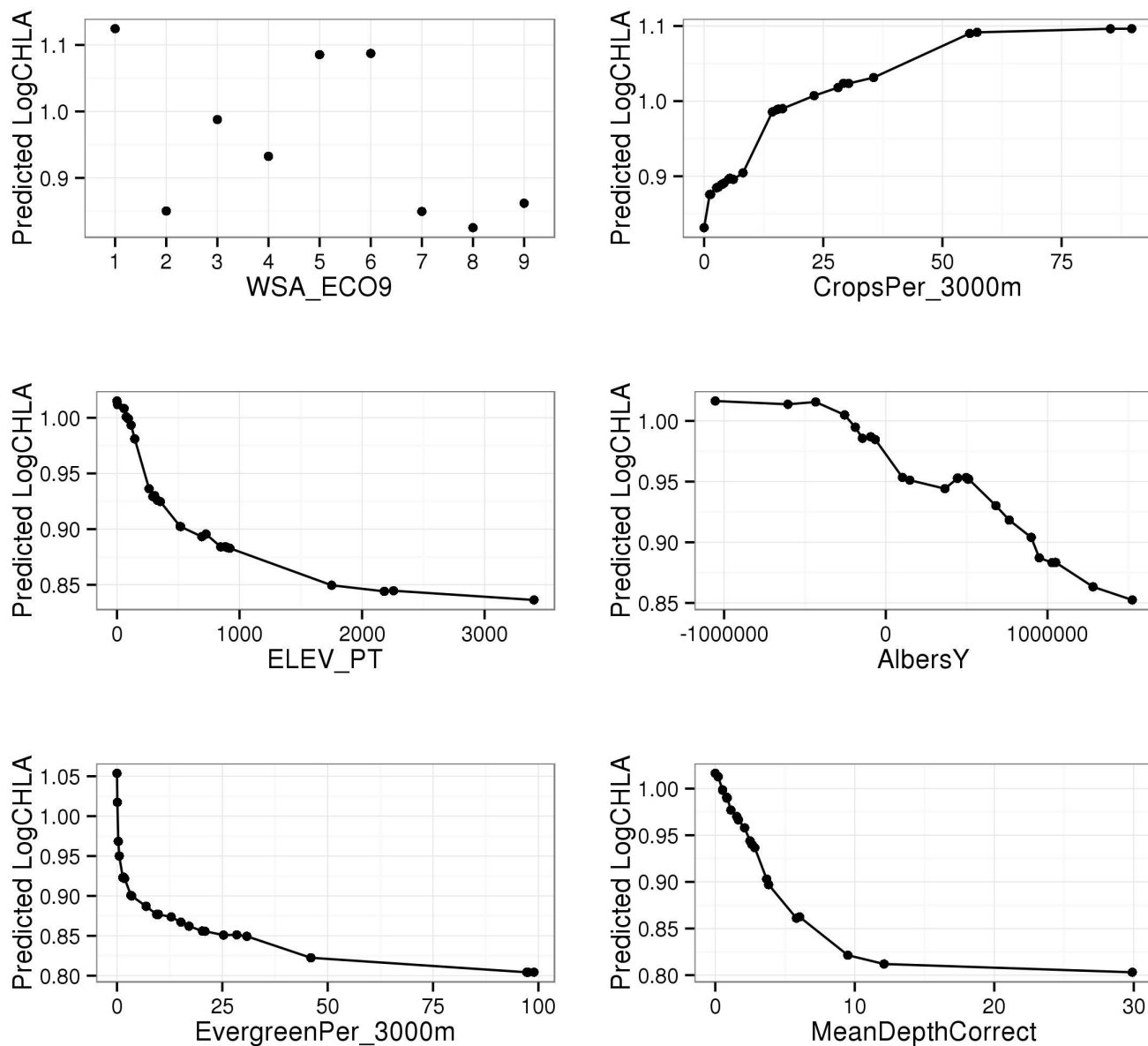


Figure 7: GIS Only Variables partial dependence plots for the top 5 most important variables.

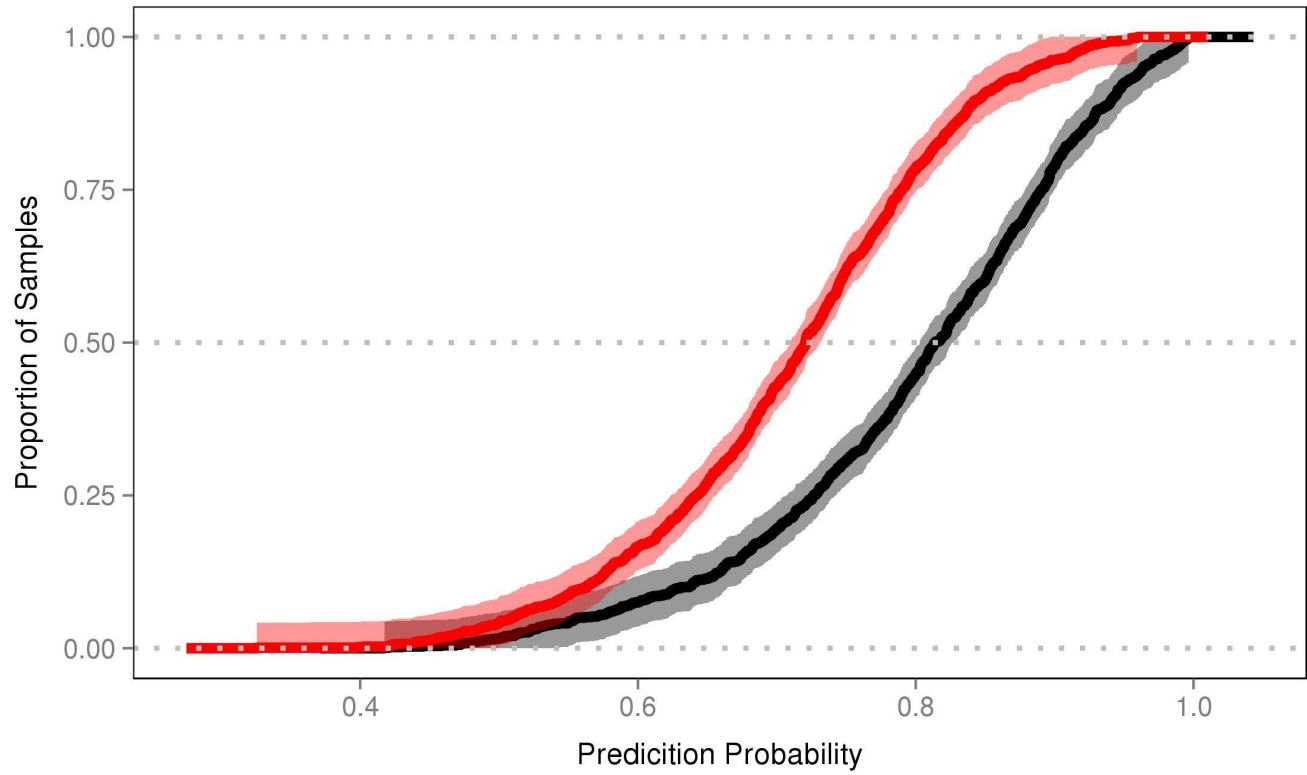


Figure 8: Prediction probabilities for the All Variables and GIS Only models.

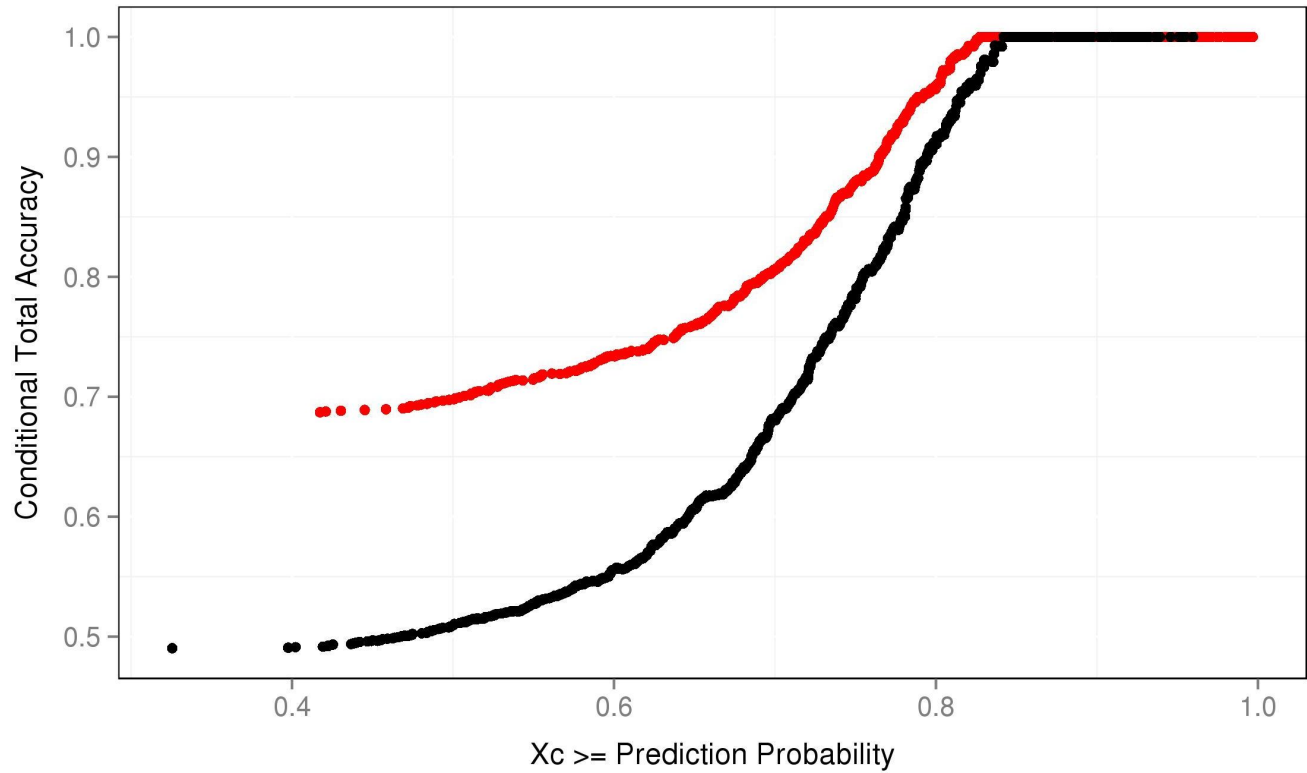


Figure 9: Accuracy of predictions as a function of lake prediction probability. The x-axis represents lakes with a prediction probability at a given level or higher.

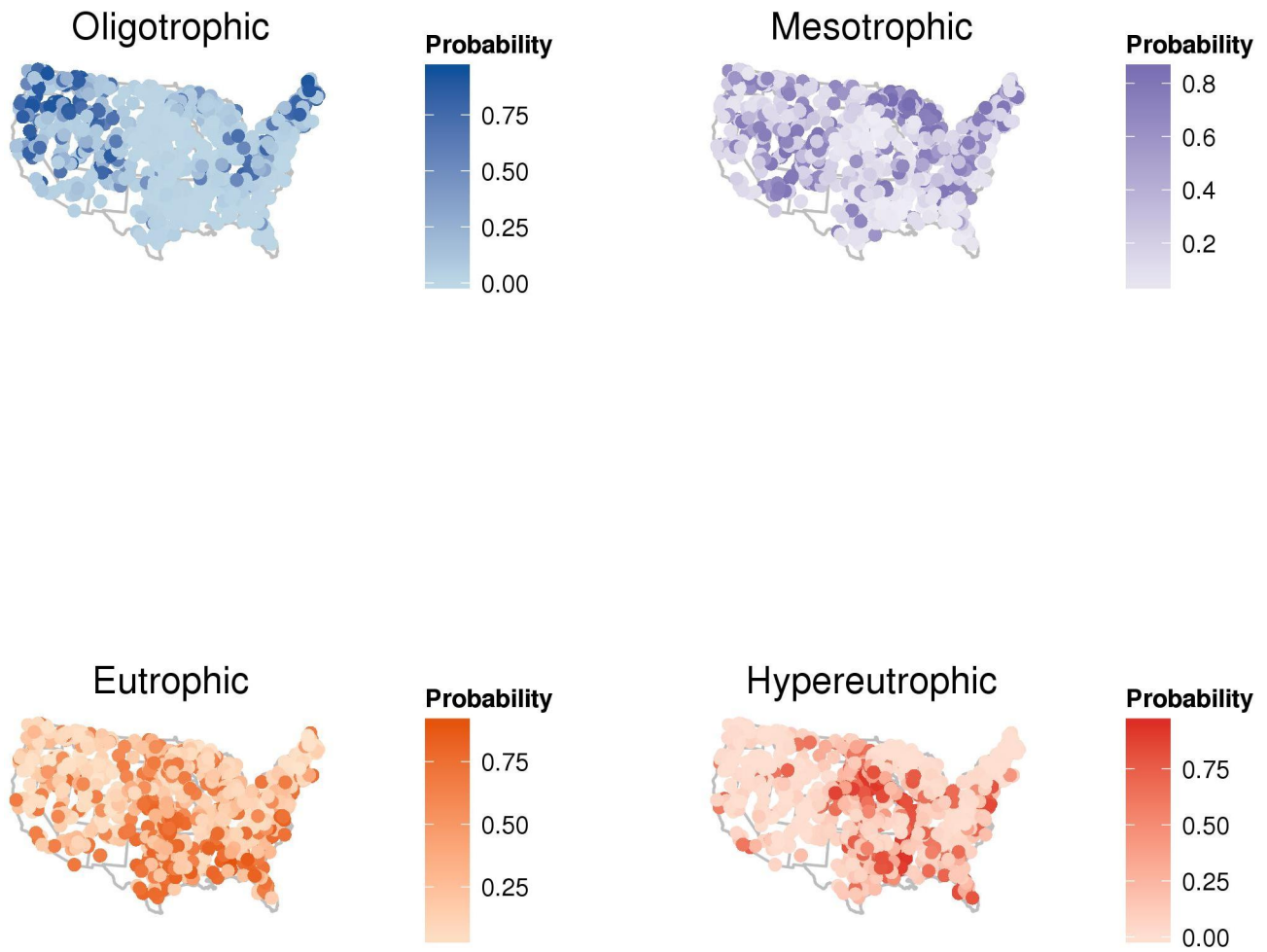


Figure 10: Maps of prediction probabilities for each of the four chlorophyll *a* trophic states

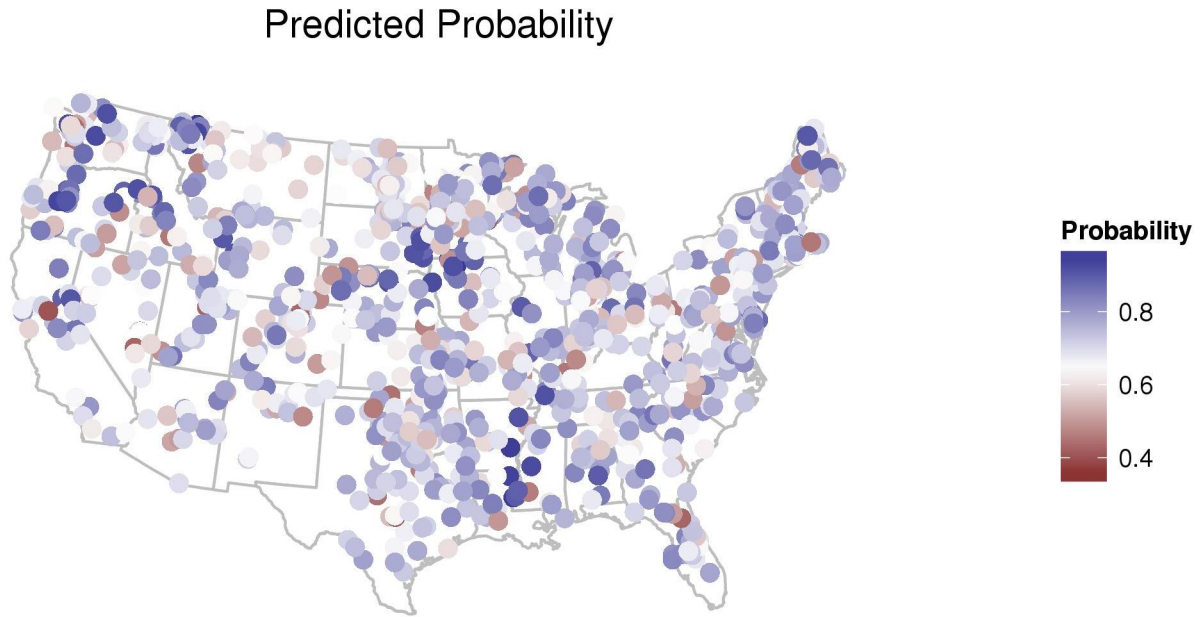


Figure 11: Maps of prediction probabilities for the discrete, predicted chlorophyll *a* trophic state. Shows spatial patterns of prediction uncertainty.

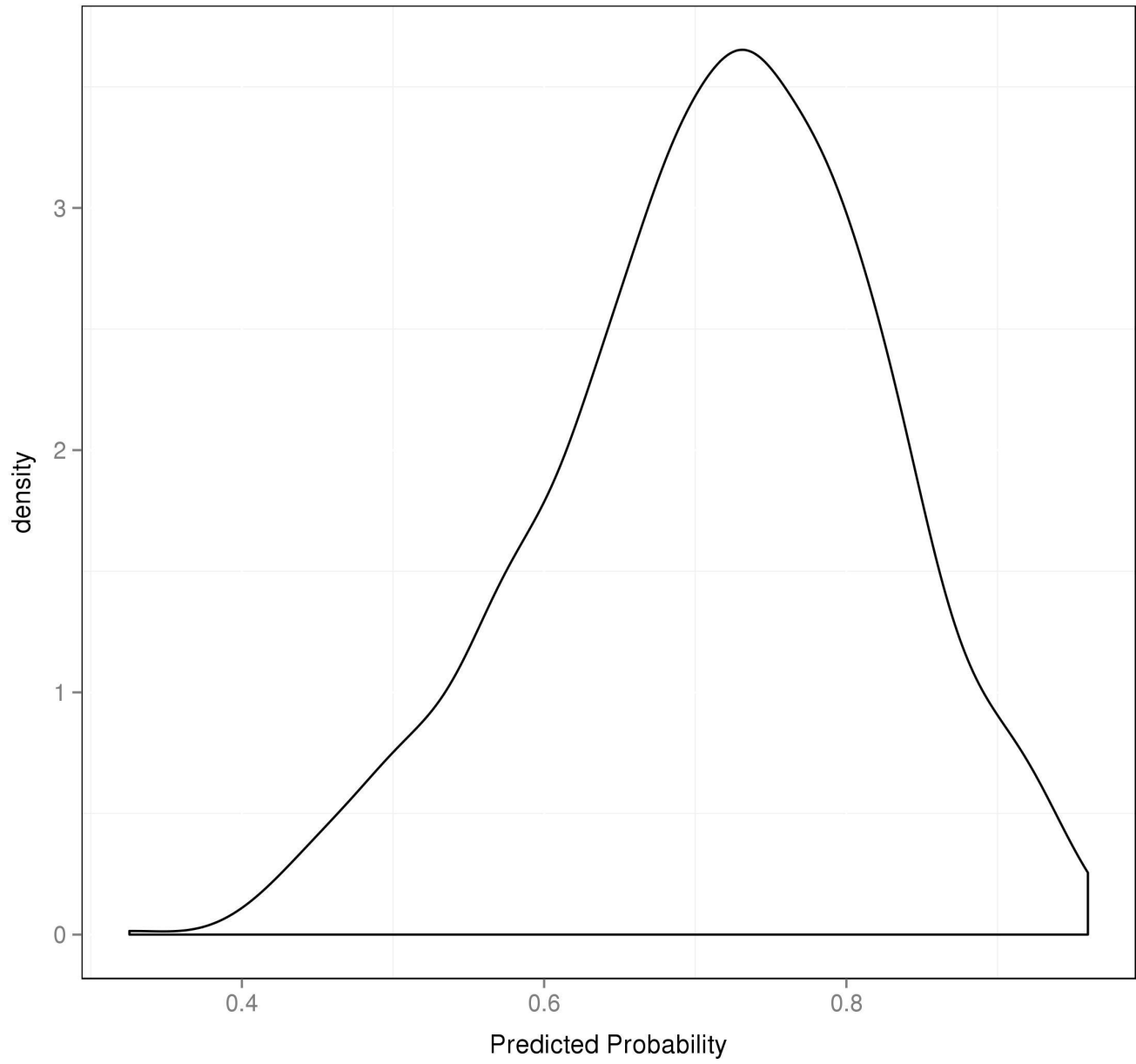


Figure 12: Distribution of predicted probabilities.

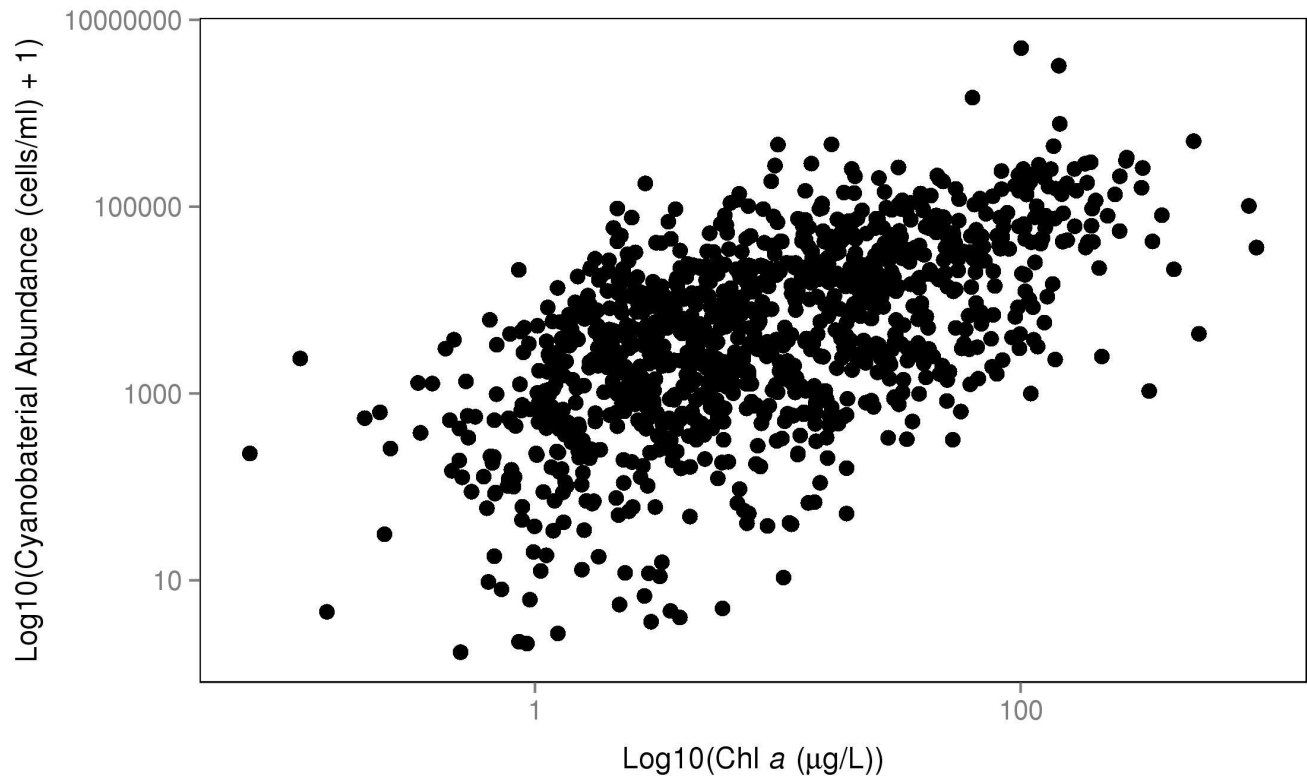


Figure 13: Cholorphyll *a* and cyanobacteria abundance scatterplot

340 **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 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	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

Table 4: Summary of relationship between prediction probabilities, total accuracy, and number of lakes.

	“All Var.”	“All Var.”	“All Var.”	“GIS Only”	“GIS Only”	“GIS Only”
Prediction	Total	Percent of	Number of	Total	Percent of	Number of
Prob.	Accuracy	Sample	Samples	Accuracy	Sample	Samples
All	69	100	846	49	100	878
0.50	70	98	829	51	95	834
0.60	73	91	770	56	81	711
0.70	81	77	654	68	56	490
0.80	96	51	434	91	24	212
0.90	100	20	173	100	5	41

341 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
DevMedPer_3000m	Percent Medium Intensity Development	GIS
DevHighPer_3000m	Percent High Intensity Development	GIS
BarrenPer_3000m	Percent Barren	GIS
DeciduousPer_3000m	Percent Deciduous Forest	GIS
EvergreenPer_3000m	Percent Evergreen Forest	GIS
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 Herbaceous 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
H	Hydrogen Ions	Water Quality
OH	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 from 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:Phosphorus Ratio	Water Quality

References

- BREIMAN, L. 2001. Random forests. *Machine learning* 45:5–32.
- 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. Cyanobacterial blooms: Statistical models describing risk factors for national-scale lake assessment and lake management. *Science of The Total Environment* 409:5353–5358.
- COHEN, J. 1960. A coefficient of agreement for nominal scales. *Educational and Psychological 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* 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 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.
- HUBERT, L., AND P. ARABIE. 1985. Comparing partitions. *Journal of classification* 2:193–218.
- IMBODEN, D., AND R. GÄCHTER. 1978. A dynamic lake model for trophic state prediction. *Ecological 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* 61:1503–1512.
- JONES, K. B., A. C. NEALE, M. S. NASH, R. D. VAN REMORTEL, J. D. WICKHAM, K. H. RIITTERS, 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* 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. *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.
- MOORE, R. B., C. M. JOHNSTON, R. A. SMITH, AND B. MILSTEAD. 2011. Source and delivery of

389 nutrients to receiving waters in the northeastern and mid-atlantic regions of the united states. JAWRA
 390 Journal of the American Water Resources Association 47:965–990.

391 PAUL, J. F., AND M. E. McDONALD. 2005. Development of empirical, geographically specific water
 392 quality criteria: A conditional probability analysis approach 41:1211–1223.

393 PETERS, J., B. D. BAETS, N. E. VERHOEST, R. SAMSON, S. DEGROEVE, P. D. BECKER, AND W.
 394 HUYBRECHTS. 2007. Random forests as a tool for ecohydrological distribution modelling. Ecological
 395 Modelling 207:304–318.

396 RODHE, W. 1969. Crystallization of eutrophication concepts in northern europe.

397 SALAS, H. J., AND P. MARTINO. 1991. A simplified phosphorus trophic state model for warm-water
 398 tropical lakes. Water research 25:341–350.

399 SCHINDLER, D. W., AND J. R. VALLENTYNE. 2008. The algal bowl: Overfertilization of the world’s
 400 freshwaters and estuaries. Page 334. University of Alberta Press Edmonton.

401 SEILHEIMER, T. S., P. L. ZIMMERMAN, K. M. STUEVE, AND C. H. PERRY. 2013. Landscape-scale
 402 modeling of water quality in lake superior and lake michigan watersheds: How useful are forest-based
 403 indicators? Journal of Great Lakes Research 39:211–223.

404 SMITH, V. H. 1998. Cultural eutrophication of inland, estuarine, and coastal waters. Pages 7–49 *in*
 405 Successes, limitations, and frontiers in ecosystem science. Springer.

406 SMITH, V. H., S. B. JOYE, R. W. HOWARTH, AND OTHERS. 2006. Eutrophication of freshwater and
 407 marine ecosystems. Limnology and Oceanography 51:351–355.

408 SMITH, V. H., G. D. TILMAN, AND J. C. NEKOLA. 1999. Eutrophication: Impacts of excess nutrient
 409 inputs on freshwater, marine, and terrestrial ecosystems. Environmental pollution 100:179–196.

410 STROBL, C., A.-L. BOULESTEIX, A. ZEILEIS, AND T. HOTHORN. 2007. Bias in random forest variable
 411 importance measures: Illustrations, sources and a solution. BMC bioinformatics 8:25.

412 USEPA. 2009. National lakes assessment: A collaborative survey of the nation’s lakes. ePA 841-r-09-001.

413 Office of Water; Office of Research; Development, US Environmental Protection Agency Washington,
414 DC.

415 XIAN, G., C. HOMER, AND J. FRY. 2009. Updating the 2001 national land cover database land
416 cover classification to 2006 by using landsat imagery change detection methods. *Remote Sensing of*
417 *Environment* 113:1133–1147.

418 YUAN, L. L., A. I. POLLARD, S. PATHER, J. L. OLIVER, AND L. D’ANGLADA. 2014. Managing
419 microcystin: Identifying national-scale thresholds for total nitrogen and chlorophyll a. *Freshwater*
420 *Biology* 59:1970–1981.