**Machine Learning Classification Algorithms for Predicting**

***Karenia brevis* Blooms on the West Florida Shelf**

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Abstract

The Clean Water Act of the United States requires states to establish water quality standards and criteria. For some types of waters, including coastal ocean waters experiencing harmful algal blooms (HABs), establishing criteria can be particularly challenging due to the complexity of factors related to the proliferation of these ecologically harmful events. From 2017 to early 2019, blooms of the toxic dinoflagellate *Karenia brevis* swept over the West Florida coast, resulting in thousands of tons of dead fish, deaths to many other marine organisms, numerous respiratory-related hospitalizations, and tens to hundreds of millions of dollars in economic damage. Four types of machine learning algorithms, including Support Vector Machine (SVM), Relevance Vector Machine (RVM), Naïve Bayes classifier (NB) and Artificial Neural Network (ANN), were developed and compared in their ability to predict *K. brevis* blooms. Comparing the 20-year monitoring data set of abundance of this dinoflagellate using all algorithms, the RVM and NB were found to have better skills in bloom prediction than the other two approaches according to *k-*fold and block cross-validation analyses. All models were comparable in how frequently false negatives were reported. Applying the RVM, the importance of upwelling-favorable northerly winds in increasing *K. brevis* probability, and of on-shore westerly winds in preventing blooms from dispersing offshore, were quantified. The SVM, RVM and NB models were also used to explore the importance of large river flows and the nutrients they supply with regard to bloom development. These relationships show the quantitative reductions in both N and P necessary to reduce blooms, and how reductions from multiple rivers may be more effective than reductions from a single river. These models provide new tools for predicting these devastating algal blooms and can be applied in exploring effective and scientifically defensible nutrient reduction strategies to mitigate water quality problems.

**Contribution to the field**

Four types of machine learning algorithms, including Support Vector Machine (SVM), Relevance Vector Machine (RVM), Naïve Bayes classifier (NB) and Artificial Neural Network (ANN), were developed and compared in their ability to predict blooms of the harmful marine dinoflagellate *Karenia brevis* in coastal waters of the West Florida Shelf. The State of Florida is working to establish water quality criteria and nutrient reduction targets to mitigate water quality problems. Incorporating outbreaks of harmful algal blooms (HABs) in criteria has been challenging. These events, through their biomass accumulation or toxicity, can cause severe ecological damage and human illness, but occur sporadically and many different sources of nutrients support the growth of bloom-forming species. Machine learning models were used to explore the importance of large river flows and the nutrients they supply with regard to bloom development. These relationships show the quantitative reductions in both nitrogen and phosphorus necessary to reduce blooms, and how reductions from multiple rivers may be more effective than reductions from a single river. These models provide new tools for predicting these devastating algal blooms and can be applied in exploring effective and scientifically defensible nutrient reduction strategies to mitigate these water quality problems.

# Introduction

The Clean Water Act of the United States requires states to establish water quality standards and criteria, and if waters do not meet criteria, total maximum daily loads (TMDLs) of each pollutant (including nutrients) must be developed (https://www.epa.gov/tmdl). In order to define criteria, states must first designate uses of the water body, for example as a water supply, an aquaculture site, or suitable for fishing and/or recreation. States must then establish the maximum pollutant load that can be sustained without degrading those uses. Criteria may be defined in a narrative form, but such a narrative description should then be translated to thresholds of water quality parameters that must not be exceeded and that can be quantitatively assessed.

The State of Florida, along with many other states and government entities around the world, has established, or is working to establish, nutrient reduction targets to mitigate water quality problems in their water bodies (Zhao et al., 2016; Herrero et al., 2019). Florida uses the following narrative criteria for defining degradation from nutrient loads: “In no case shall nutrient concentrations of a water body be altered so as to cause an imbalance in natural populations of aquatic flora or fauna” (Florida Department of Environmental Protection). While TMDLs have been adopted for many of Florida’s impaired waterways (Fig. 1A), there are many impaired waters for which water quality thresholds or TMDLs are still in the process of development (as of 2018). Even for those waters where TMDLs have been adopted, the process of implementation involves a re-evaluation of these values throughout the state on a 5-year basis. Continued monitoring and assessment methods will be essential, and improved approached for establishing criteria for additional waters and to manage water quality across greater regions will continue to be required.

For some types of waters, including coastal ocean waters, establishing criteria can be particularly challenging. Among these challenges is how to incorporate outbreaks of harmful algal blooms (HABs). These events, through their biomass accumulation or toxicity, can cause fish kills, deaths or illness to many higher consumers in the food web, including dolphins, manatees, turtles or birds, and though their accumulation can lead to hypoxia, and shading of submerged vegetation. Human health effects can be severe via exposure through contaminated seafood, drinking water or through aerosolized toxins (Glibert et al. 2018).

Coastal waters along the Florida southwestern coast are experiencing increasing frequencies of outbreaks of the toxic dinoflagellate *Karenia brevis*. While *K. brevis* is typically thought of as a coastal bloom species, blooms are actually initiated offshore in late summer or early fall, and then transported to coastal waters where they flourish and persist for months in nutrient-rich waters (Steidinger, 2009; Heil et al., 2014). Upwelling transports *K. brevis* cells to the coast (Weisberg and He, 2003; Liu and Weisberg, 2012; Mayer et al., 2017), but strong upwelling over the shelf break may actually suppress *K. brevis* blooms or favor competing taxa such as diatoms (Weisberg et al., 2014; Liu et al., 2016). Once inshore, multiple nutrient sources, including riverine input that brings wastewater effluent and agricultural runoff help to sustain blooms via multiple nutritional pathways (Hu et al., 2006; Vargo et al., 2008; Vargo, 2009; Lenes et al., 2008; Glibert et al., 2009; Heil et al., 2014; O’Neil and Heil, 2014).

Blooms of *K. brevis* occur almost annually on the West Florida Shelf (WFS), and historical accounts show that they have occurred since at least the 16th century (Steidinger, 2009). However, recent analyses suggest that bloom events have increased 15-fold from the 1950s to 1990s (Brand and Compton, 2007) and further increases have been suggested since then. From 2017-2019, southwest Florida experienced an unusually prolonged (18 months) *K. brevis* bloom. At its maximum, this bloom covered more than 250 km of coastline, encompassing recreational beaches and numerous commercial and recreational shellfish beds causing both substantial ecological and economic harm (Fig. 1B; Glibert, 2019; Fears and Rozsa, 2018; Monuz, 2019). This *K. brevis* bloom resulted in hundreds of tons of dead fish, deaths of nearly 600 sea turtles, more than 200 manatees and about 150 bottlenose dolphins, along with unprecedented, massive stone crab mortalities (Glibert 2019). There were also numerous hospitalizations due to respiratory distress from aerosolized dinoflagellate toxin. Such blooms clearly cause an “imbalance in natural populations of aquatic flora and fauna”. However, the region encompassed by this particular bloom, and indeed encompassed by most *K. brevis* blooms, is part of the coastal waters for which TMDLs have yet to be established.

The massive bloom of 2017-2019, as well as another recent, large-scale bloom in 2005, which also resulted in large-scale ecological and human health problems, were likely a product of increased anthropogenic nutrient loading propelled by unusual events. Hu et al. (2006) suggested that nutrient inputs resulting from a series of hurricanes in southwest Florida in 2004 were linked with the severity of the 2005 bloom. Hurricanes can accelerate the yield of land-based nutrients from high riverine flow. Similarly, Hurricanes Irma (2017), Michael (2018) and Tropical Storm Gordon (2018) are suspected of contributing to the severity of the 2017-2019 *K. brevis* bloom (Glibert, 2019). Moreover, long periods of wet weather through 2018, combined with increased discharges from Lake Okeechobee and the Caloosahatchee River, added nutrients to coastal waters, sustaining large *K. brevis* blooms through early 2019.

There is a strong need to advance predictions of *K. brevis*, and other HABs more generally, to protect human health, fisheries and economies, but there are many challenges in modeling discrete HAB species (Glibert et al., 2010, in press; McGillicuddy et al., 2010; Anderson, 2014; Franks, 2018; Flynn and McGillicuddy, 2018). Several different types of models have been developed and are currently in operation for predicting *K. brevis* blooms (e.g., Steidinger, 2009; Stumpf et al., 2009, Weisberg et al., 2009). An operational forecasting modeling system, maintained by the National Oceanic and Atmospheric Administration, provides 3- to 5-day outlooks of *K. brevis* blooms, using satellite remote sensing of chlorophyll *a*, *in-situ* sampling of *K. brevis* cell density, and wind buoy data (Stumpf et al., 2003, 2009). The main goal of these forecasts is to inform managers and the public in coastal areas where public health may be compromised (Stumpf et al., 2009). Walsh et al. (2003), along with Weisberg and He (2003), used a three-dimensional (3D) biophysical-coupled model to hindcast bloom initiation and explore the impact of individual forcing functions (Walsh et al., 2006; Milroy et al., 2008, Lenes et al., 2012, 2013). However, these models utilize many biochemical and physiological parameters, some of which have not been well characterized either *in-situ* or in the laboratory. Weisberg et al. (2009) developed a high-resolution coastal ocean circulation model to track the movement of water particles associated with *K. brevis* populations. These 3D-coupled biophysical models are computationally expensive. These HAB events, forecasts and associated models have not been applied in either water quality criteria development in spite of the ecological harm caused when these events do occur.

Due to their powerful nonlinear modeling capability, machine learning methods are beginning to be used to predict HAB events. An artificial neural network (ANN) model was used to predict algal blooms in Hong Kong coastal waters (Lee et al., 2003) and to predict outbreaks of the dinoflagellate *Dinophysis acuminata* in southern Spain (Velo-Suarez and Gutierrez-Estrada, 2007). More recently, a neural network (NN) approach was used to predict the presence/absence and abundance of the dinoflagellate *Karlodinium* and the diatom *Pseudo-nitzschia* in Alfacs Bay in the northwest Mediterranean Sea (Guallar et al., 2016), and support vector machines (SVM) models were used to predict blooms in freshwater reservoirs (Xie et al., 2012).

Machine learning approaches have also been used in predicting HABs in the Gulf of Mexico, but with different objectives. Liu and Weisberg (2012) used such approaches to demonstrate the role of deep-ocean forcing on WFS in the major bloom occurrences. Weisberg et al. (2014) reported that the position of the Loop Current can affect blooms. When the Loop Current is in its southern position, it creates an upwelling of deep nutrients and fosters a diatom bloom that may outcompete any nascent *K. brevis* blooms. Liu et al. (2016) used Self-Organizing Maps to classify spatial patterns of the Sea Surface Height anomalies associated with the Loop Current and found no bloom developed when the Loop Current was in the southern position. That work focused exclusively on the potential effects of the Loop Current on *K. brevis* blooms and did not consider other factors such as river flows and riverine nutrient loading. Recently, Hill et al. (2019) used satellite remote sensing of chlorophyll *a* from 2003 to 2018, as well as sea surface temperature and bathymetry, as inputs to a convolutional NN (designed for spatial data) to detect the presence of *K. brevis* blooms on WFS, achieving a maximum detection accuracy of 91%. Such approaches have yet to be used to assess the effects of winds, river flows and river nutrient discharge on the likelihood of *K. brevis* blooms. Such approaches show promise for future application within the TMDL framework, especially in the development of TMDLs for complex coastal waters.

In this research, 4 machine learning algorithms were used to predict *K. brevis* on the WFS over a 20-year period. Specifically, the ability of these different machine learning approaches was assessed with regard to the probability of change in *K. brevis* blooms with changing wind, discharge from different rivers, differing nutrient loads, as well as sea surface height. These models may provide new tools for defining scientifically defensible protective loads in future re-evaluations of Florida’s water quality criteria.

**2 Methods**

**2.1 The Data Set and Preparation of Explanatory and Dependent Variables**

To develop the machine learning models, *in-situ* data of *K. brevis* cell densities (cells L-1) over a 20-year period (1998-2018) on the WFS were obtained from the database available from the Florida Fish and Wildlife Conservation Commission (https://myfwc.com/). The data used herein were limited to water samples collected between latitudes of 25.85 degrees (Marco Island) and 29.14 degrees (Mouth of Suwanee River) and at most 9 km from the coast as most of the *K. brevis* blooms occurred within this area, and setting a fixed area for the data analysis ensured data consistency (Maze et al., 2015). These data represent water samples collected during regular monitoring along the Florida coast and during suspected or confirmed *K. brevis* events. Since the *K. brevis* measurements were largely collected if and when blooms were documented and not made on a continuous or regular basis, the data base has an under-sampling of *K. brevis* under low cell density conditions. In order to overcome the spatial and temporal inconsistency in the data, the 5 highest cell counts across the fixed area were averaged for each week to produce a weekly mean, following the approach used in previous studies (e.g. Liu et al., 2016). These cell numbers were discretized and weekly averages were combined into a binary variable, with a mean cell density greater than 105 cells L-1 counting as *K. brevis* events, consistent with the commonly used threshold for *K. brevis* blooms.

Streamflow data were obtained from United States Geological Survey (USGS) stations in the major rivers that discharge onto the WFS (<https://waterdata.usgs.gov/nwis>; Fig. 1B).The USGS stations included: Tampa Bay (USGS 2306647), Peace River (USGS 2296750), Lake Okeechobee (USGS 2274325), Suwanee River (USGS 2323500), Withlacoochee River (USGS 2319000), Hillsborough River (USGS 2303330), Little Manatee River (USGS 2300500), Myakka River (USGS 2298830), and Caloosahatchee Canal (USGS 2292000). Nutrient data from the major rivers, including total nitrogen (TN) and total phosphorus (TP) concentrations, were downloaded from the Tampa Bay and Charlotte Harbor Water Atlas (University of South Florida Water Institute, http://www.wateratlas.usf.edu). No comparable nutrient concentration data were available for the Suwanee River. Weekly averaged nutrient concentrations were multiplied by weekly averaged streamflow to estimate weekly TN and TP loads.

Hourly wind and temperature data were obtained from the National Data Buoy Center (NDBC) stations (<https://www.ndbc.noaa.gov/>; Fig. 1B) across the WFS. The hourly wind speeds were used to calculate weekly averages using a simple vector average. The hourly temperatures were used to calculate weekly averages. Satellite altimetry from the GLOBAL-REANALYSIS-PHY-001-030 reanalysis product, provided by the E.U. Copernicus Marine Service Monitoring Service (CMEMS; http://marine.copernicus.eu/), was used to calculate the difference in sea surface height at two locations to quantify the strength of the deep-sea coastal upwelling caused by the Loop Current, following Maze et al. (2015).

Data were aggregated into the following form; each row of the dataset is , where are the explanatory variables of river discharge , nutrient concentration, wind speed and direction, temperature, and sea surface height difference, with as the dependent variable of discretized *K. brevis* cell densities. Machine learning algorithms aim to map to.

The number of HAB events (318) over the 20-year period was less than half of the number of events without HABs (755), resulting in an imbalanced classification problem (Sun et al., 2009). Several approaches have been developed to address this issue. Two approaches were applied herein: (1) the minority class of the training data was randomly oversampled such that the sample size of events with and without HABs are roughly equal in the synthetic training dataset (Japkowicz and Holte, 2000); and (2) the minority class was oversampled by generating new synthetic data using a synthetic minority over-sampling technique (SMOTE) preprocessing algorithm (Chawla et al., 2002; Fernandez et al., 2018; Haibo and Garcia, 2009).

**2.2 Machine Learning Algorithms**

To predict *K. brevis* cell density and test the strength of various explanatory variables, the following machine learning algorithms were used: a) Support Vector Machine (SVM), b) Relevance Vector Machine (RVM, a modification of SVM), c) Naïve Bayes (NB), and d) Artificial NN (ANN). They represent a range of machine learning algorithms with different methodology and varying complexity. SVM belongs to a class of algorithms called kernel methods. RVM has an identical functional form to SVM but provides probabilistic classification. NB is a family of simple probabilistic classifiers. ANN is based on a system of connected nodes to mirror neurons in a biological brain.

**2.2.a. Support Vector Machine**

The SVM model is a supervised machine learning algorithm that seeks the hyperplane that best separates two labeled classes from each other (Fig. 2A),

 (1)

where  represents the vector for the explanatory variables,  is the hyperplane that separates the two classes,  is the slope of the hyperplane, *b* is the intercept, and f()is the classifier output which takes the value of either 1 or -1. SVM seeks a solution for the hyperplane by maximizing the width of the gap between the two data clouds, represented by the cost function (CF, Eq. 2, Fig. 2A),

 (2)

Sometimes the SVM cannot achieve a perfect separation. The soft-margin loss formulation allows some data points to lie within the margin of tolerance but penalizes them in the cost function (Cortes and Vapnik, 1995) as follows (Eq. 3),

 (3)

where in the slack variables, , is either 1 or -1, and is a hyperparameter which determines the trade-off between maximizing the margin width and minimizing the associated error (Fig. 2A). This new cost function is then optimized, yielding the linear support vector expansion for the classifier (Eq. 4):



 (4)

where are the Lagrangian multipliers and is rewritten as a linear combination of the training patterns (Nello and Shawe-Taylor, 2000). The constant *b* can be found with the Karush-Kuhn-Tucker Conditions (Basak et al., 2007; Vapnik, 1995).

The linear support vector expansion cannot be used to describe nonlinear relationships between the explanatory and dependent variables. To describe nonlinear datasets, kernel functions are used to map the data to higher dimensions where they exhibit linear patterns and the linear model can be applied in that feature space (Boser et al., 1992; Scholkopf and Smola, 2002). The Gaussian radial basis function was chosen as the kernel function because of its computational efficiency (Eq. 5),

(5)

where is the kernel parameter controlling the sensitivity of the kernel function.

SVM has two hyperparameters that cannot be determined from optimization: C and Both were determined with a grid search method on the training data.

**2.2.b. Relevance Vector Machine**

The RVM model has an identical functional form to SVM but uses a Bayesian probabilistic framework to estimate the parameters (Tipping, 2001; Camps-Valls et al., 2006). To obtain the maximum likelihood estimate of , and to avoid overfitting, the Bayesian approach is taken to constrain the parameters by defining an explicit prior probability distribution over them. The prior probability distribution is chosen to be a Gaussian distribution, and RVM introduces a vector to enforce a preference for smoothness. Then, the posterior estimate of the unknown parameters given the data is obtained using Bayes’ rule. Since the posterior probability can be evaluated exactly, RVM seeks to maximize the marginal likelihood with respect to the hyperparameters. RVM typically uses much fewer basis functions than SVM. RVM was applied herein using the radial basis function as the kernel function.

**2.2.c. Naïve Bayes**

The NB classifier is a simple probabilistic classifier based on the Bayes’ Rule and requires strong “naïve” independence between the features (Maron, 1961; Hand and Yu, 2001). Given a new observation **x**, it finds the class that maximizes the conditional probability , the likelihood of a class given the observation. Uses Bayes’ theorem, the conditional probability can be calculated as follows (Eq. 6),

(6)

where is the prior probability of observing a class , is the likelihood of observing **x** given , and is the probability of observing **x**. Assuming strong naïve independence, the probabilistic chain rule can be used to transform the likelihood of **x** into the probabilities of each of the features of **x** given a class (Eq. 7),

(7)

This study used the Gaussian NB in which the Gaussian distribution (Eq. 8),

(8)

is assumed to underlie the sample distribution. To train the NB classifier, the data were segmented by the classes, and the mean and standard deviation of each of the features for each of the classes were calculated, giving a probability distribution for each of the classes.

**2.2.d. Artificial Neural Network**

The ANN is based on the feedforward multilayer perceptron architecture, consisting of an input layer, one or more sets of hidden layers, and one output layer 5 (Hassoun, 1995; Schmidhuber, 2015). ANN can be turned into a classifier by discretizing the network’s output. The basic substructure of ANN is a perceptron (Fig. 2B). Each perceptron has an input (the outputs of the previous layer), a series of weights, a transfer function, and an output. A transfer function is applied to the dot product of the inputs and weights for each perceptron, giving an output for the next layer. The output for node j in layer l is as follows (Eq. 9),

 (9)

where **x** are the input variables,  is the output at layer (l-1), wji are the synaptic weights, and  is the activation function.

Initially, random numbers are assigned to the synaptic weights. The weights are adjusted with the training data. There are two main steps to the training of the ANN: forward computation and back propagation. In forward propagation, input signals are propagated through the network, layer by layer. In back propagation, the error for the entire network is calculated (Werbos, 1990). Then, the errors are computed for each neuron, and then the local gradients for the synaptic weights of the network are calculated. Gradient descent is then used to adjust the synaptic weights. These steps are repeated until the error reaches below a desired threshold. Herein, two hidden layers with 20 and 10 neurons were used in the ANN model.

To implement these machine learning algorithms, open source R packages were used: raster 3.0-7 (Hijmans, 2017), doParallel 1.0.15 (Calaway, 2017), Kernlab 0.9-29 (Karatzoglou et al., 2004), DMwR 0.4.1 (Torgo, 2010), PBSmapping 2.72.1 (Schnute et al., 2017), e1071 1.7-2 (Meyer et al., 2019), neuralnet 1.44.2 (Fritsch et al., 2019), R 3.6.1 (R Core Team, 2017).

**2.3 Model Evaluation and Metrics**

The predictive skill of the machine learning algorithms was evaluated using two approaches. First, a *k*-fold cross-validation approach that has been widely used in machine learning classification (Anguita et al., 2009; Cawley and Talbot, 2004) was applied. In this approach, the data are randomly subdivided into *k* disjointed subsets of equal size. Then, for each different combination of *k*-1 of the *k* subsets, one of the *k* models is trained, and the test statistic for that model is evaluated on the remaining subset (Stone, 1974; Geisser, 1975). The mean of the test statistics over all *k* models is the cross-validation estimate. In this study, *k*=10 so that each subset spanned 2-years of data. The data are assumed to be independent during the *k*-fold cross-validation. However, this assumption might be inappropriate for time series which may be auto-correlated. Thus, the data herein were further validated by block cross-validation (Bergmeir and Benitex, 2012; Roberts, 2017; Burman et al., 1994; Racine, 2000). To do this, the data were divided by chronological order into 10 subsets of 2-years each: 1998-1999, 2000-2001… 2017-2018. In one iteration of the cross-validation procedure, the models were trained on the data from 1998-2016 and then tested on data from 2017-2018. This procedure was repeated for all the 2-year blocks.

Four metrics were used to evaluate the performance of the machine learning classifiers in predicting *K. brevis* blooms (Sun et al., 2009; Powers, 2011). Accuracy measures the overall accuracy of the prediction (Eq. 10),

(10)

where TrPos is the number of weeks with blooms predicted correctly (true positives), FNeg is the number of weeks with blooms predicted to be non-HAB weeks (false negatives), TrNeg is the number of non-HAB weeks predicted correctly (true negatives), and FPos is the number of non-HAB weeks predicted to be weeks with HABs (false positives). *A* is the measure of all the correctly identified cases. Recall is the ratio of the correctly-predicted HAB weeks to the total number of the observed HAB weeks (Eq. 11),

. (11)

Precision is the ratio of the correctly-predicted HAB weeks to the total number of the predicted HAB weeks (Eq. 12),

. (12)

F1 measures the balance between precision and recall (Eq. 13),

. (13)

While *A* is most often used when there are similar amounts of each class, *F1* score is a better metric where there are imbalanced classes. The testing metrics were averaged for both the *k-*fold or block validation procedures. To further test the models’ predictions, a time series of the cross-validation predictions was created.

In addition to the four metrics, the robustness of each model such as sparsity was examined. The mean number of support vectors (SVs) / relevance vectors (RVs) was calculated for the SVM and RVM, and the Akaike Information Criterion (AIC) was determined for the ANN.

**2.4 Sensitivity Analysis**

In order to determine how environmental factors affect the probability of *K. brevis*, Platt scaling (Platt, 1999) was applied. This uses a logistic transformation to convert classifier predictions into probability distributions over the classes. First, each machine learning algorithm was trained on the entire dataset. Platt scaling was then applied to calculate the probability of *K. brevis* blooms (Eq. 14),

(14)

where is a sample, is one of the classes, is the classifier output, and A and B are scalar constants (Lin et al., 2007). To assess the impact of environmental variables, each explanatory variable was varied by 1-2 standard deviations around its mean while the other variables were set to their respective annual mean values. Since the *K. brevis* blooms most frequently occurred between September and the following January, the sensitivity analysis was not conducted using deviations from the annual mean temperature. The probability of a HAB as a function of explanatory variables was explored by varying one or two explanatory variables at a time.

**3. Results**

**3.1 Overall Model Performance**

The predictability of *K. brevis* blooms over the 20-year time series (1998-2018) was tested relative to the observed *K. brevis* cell concentrations along the WFS using all 4 machine learning approaches. All models captured the general time series of *K. brevis* events, encompassing both prolonged blooms with high cell counts as well as periods of only a short duration with relatively low cell counts (Fig. 3,4).

Results from the random oversampling and SMOTE sampling method were similar for all 4 approaches (Table 1). According to block cross-validation, SVM and ANN achieved significantly higher prediction accuracy (0.62 and 0.61, respectively, from random oversampling) than RVM and NB (0.55 and 0.47). In contrast, when comparing the recall values using the same block cross-validation with random oversampling, NB had the highest value (0.72), and RVM the next highest value (0.58), implying that these models correctly predicted 72% and 58% of the prior *K. brevis* blooms, while SVM and ANN had much lower recall values (0.27 and 0.33). All models predicted a similar number of false positives, as shown by their precision values ranging between 0.32 and 0.35. The F1 score, the balance between recall and precision, was highest for RVM and NB, 0.43 and 0.45.

For every metric, values were lower when block cross-validation was applied than when *k*-fold validation was applied. SVM had good recall and precision values in the *k*-fold cross-validation but much lower values in the block cross-validation (Table 1). ANN also showed similar skill deterioration between the *k*-fold and block cross-validation. The deterioration of recall and precision was less with RVM and NB models when the different cross-validation techniques were compared. Thus, the RVM was the most robust model overall.

**3.2 Role of Wind**

Using RVM, the probability of *K. brevis* blooms as a function of wind speed components was examined in the north-south direction (negative for northerly wind) and the east-west direction (negative for easterly wind). Bloom probability was much higher under northerly winds than under southerly winds (Fig. 5A). Bloom probability reached a maximum of 0.57 under northerly wind, while strong southerly wind reduced bloom probability to <0.3. Northerly winds drive coastal upwelling, thereby transporting *K. brevis* from the offshore waters to coastal waters. Additionally, coastal upwelling delivers inorganic nutrients from the ocean that can help fuel the blooms. Strong, compared to weak, westerly winds increased bloom probability by 0.18, from a low of 0.36 to a high of 0.53 (Fig. 5B). Once *K. brevis* reaches nearshore locations, westerly winds help hold *K. brevis* blooms against the shore where they can access nutrient sources from land and rivers.

**3.3 Role of river flow and associated nutrients**

For all rivers, and across all discharge levels examined, the probability of *K. brevis* blooms increased with river flow (Figs. 6A-E). For all rivers, bloom probability predicted by the NB was always greater than that predicted by the RVM, which was always larger than that predicted by the SVM. The NB model had the highest recall value; the RVM ranked second; the SVM had the lowest value (Table 1). The ANN was excluded from the sensitivity analysis because the ANN yields probability predictions that are either very close to 0 (<0.01) or 1 (>0.99), making it difficult to fit the logistic function (Eq. 14) in Platt’s scaling.

As discharge changed, using RVM as the example, the slope in bloom probability was highest with the Hillsborough River, with low discharge yielding a 0.20 probability in blooms, increasing to 0.55 with high discharge. Increases in discharge from the Peace and Suwanee Rivers also increased bloom probability substantially, from 0.33-0.52 and 0.23-0.54 respectively, across the range of typical flows. Changes in discharge from the Myakka River yielded probabilities that changed from 0.34-0.55. Across all discharge levels, bloom probability was consistently higher (0.49-0.51) with increased Caloosahatchee River discharge than for the other rivers examined, and it increased linearly as river discharge increased. The Caloosahatchee River has the highest discharge of the rivers examined, and it transports the highest amount of nutrients.

The composition of the nutrients discharged by the different rivers also varied and accordingly the probability of blooms varied for their different nutrient loads (Figs. 6F-M). Applying the 3 models, SVM, RVM and NB, with increasing TN, the largest increase in bloom probability was found for the Myakka River, whereas smaller increases were found for the Peace and Caloosahatchee Rivers. For the Hillsborough river, *K. brevis* probability as a function of the TN loads resembles a parabolic function. For TP, increases in probability were seen for the Peace and Caloosahatchee Rivers, but a parabolic relationship was noted for the Hillsborough and Myakka Rivers. As nutrient loads increase, it is possible that *K. brevis* may be either outcompeted by a different species or and/or become limited by a different growth factor. However, there were some differences among the three models. For example, the bloom probability versus the Peace River TP load had a slope that was less steep in the NB model than in the RVM and SVM. While the probability increased slightly with TN in the Caloosahatchee River in the NB and SVM, it decreased in the SVM.

**3.4 Role of Sea Surface Height**

Sea surface height difference was chosen as one of the explanatory variables in our machine learning algorithms as previous studies (e.g., Maze et al., 2015) have related this variable to position of the Loop Current. Results for the RVM model were nearly identical with or without this explanatory variable (not shown) and given this outcome, this factor was not tested with the other models. Nevertheless, for 1998, 2002, 2009, 2010, and 2013, when the Loop Current was in its southern position, the RVM model generally had a much lower precision value (0.36, 0.42, 0.00, 0.00, 0.25, and an average of 0.21) versus 0.35 for all years. This suggests other factors not considered in the explanatory variables may be needed to improve bloom prediction for those years.

**4 Discussion**

Models, however imperfect, can be useful for testing the strength of particular factors or variables on outcomes. Models may be biased, yielding either false positives (indicating blooms or conditions for blooms when they do not occur) or false negatives (indicating no bloom when in fact they do occur). Both can be problematic in terms of protecting human health and economies. False positives may be preferable if the goal is to protect human health– better “safe than sorry”, but false positives can also be more expensive economically (Flynn and McGillicuddy, 2018). For example, a fishery may be closed when it was not necessary to do so. False negatives are not protective of human or ecological health. Running *in silico* experiments in which nutrient sources are turned on or off, or climate variables altered, give clear clues as to the importance of such factors both for present and future conditions (Glibert et al., 2010, in press). In this study, different machine learning classifiers were used to predict the likelihood of *K. brevis* blooms between 1998 and 2019.

Comparing the 20-year monitoring data set of abundance of this dinoflagellate using all algorithms, the RVM and NB were found to have better skills in bloom prediction than the two other approaches. All models were comparable in how frequently false negatives were reported. Since the number of weeks with blooms was about 42% of the number of non-bloom weeks, it required the classifiers to learn from an imbalanced dataset. This challenge was resolved by two different methods that oversample the minority class: random oversampling and generation of synthetic data using SMOTE. The predictive skills were very similar between the two data sampling methods, further lending evidence for the robustness of model predictions (Table 1). This result is perhaps not surprising because the ratio of the samples in the minority to the samples in the majority class was only 1:2.4, in comparison to models in which the imbalanced class classifications ranged as high as 1:10 to 1:100 (Sun et al., 2009).

Both *k*-fold and block cross-validation methods were used to evaluate the predictive skills of the machine learning classifiers. Although the SVM achieved good scores (recall=0.63, precision=0.64, and F1=0.64 using random oversampling) during the *k*-fold cross-validation, its performance deteriorated significantly during the block cross-validation (recall=0.27, precision=0.32, and F1=0.29) (Table 1). A similar deterioration was seen in the ANN between *k*-fold and block cross-validation methods. When trained using the random oversampling approach and tested with the *k*-fold cross-validation procedure, the SVM used 533 number of support vectors and the ANN had a high Akaike Information Criterion score of 1,814. It is possible that these two algorithms overfitted the training data and their predictive skills deteriorated when tested on completely independent data as done in the block cross-validation analysis. In contrast, the RVM only had 19 number of relevance vectors, and NB was a simple probabilistic classifier, thus producing more robust algorithms. The accuracy, recall, precision and F1 scores remained higher, regardless of the cross-validation methods.

Blooms of *K. brevis* occur almost annually in the eastern Gulf of Mexico, typically initiating in early fall, but varying in intensity and duration (Heil et al. 2014). The bloom of 2017-2019 was among the largest and most expensive in recent history. It caused the deaths of hundreds of tons of fish, hundreds of manatees, dolphins, and sea turtles, as well as many reports of hospitalization visits due to respiratory distress (e.g., Munoz, 2019). Fisheries closures, as well as revenue lost by local businesses, also had economic impacts in the tens to hundreds of millions of dollars (Glibert, 2019). Understanding the links between physical controls (upwelling, river flow), nutrient inputs and extreme weather events has been a high priority in order to make long-term predictions to protect environmental as well as human health. The results reported herein confirm that wind direction, river flow and nutrient load are important explanatory variables with regard to *K. brevis* probabilities. Although sea surface height (as a proxy for the Loop Current) did not contribute to improved probabilities, the increase in false positives for select years (lower precision values) suggests that the height values alone do not capture the effect of this current adequately.

Using a convolutional NN approach, Hill et al. (2019) was able to achieve high accuracy in detecting blooms of *K. brevis*. There are several differences between the methodology applied herein and the Hill et al. (2019) analysis. The Hill et al. (2019) study used satellite remote sensing of chlorophyll *a* as a proxy to detect *K. brevis*, whereas direct cell counts were used here. Also, they did not explore the role of wind speed, river flow or nutrient loads. These approaches are all complementary and show the promise of machine learning approaches not only in modeling various aspects of *K. brevis* blooms, but HAB events more generally.

Although there have been debates about the extent to which anthropogenic nutrients fuel *K. brevis* blooms (e.g., Brand and Compton, 2007; Heil et al., 2014 and references therein), there is no doubt that Florida’s continuing population growth has accelerated eutrophication. With Florida’s continuing population growth and its coastal development and dependence on tourism, more people are exposed to *K. brevis* and its toxins than in decades past, and the prolonged duration of recent blooms is also increasing the period of exposure when blooms do occur (Heil et al., 2014). Both nutrient pollution and climate change are now recognized to play important roles in this expansion (Heisler et al., 2008; Fu et al., 2012; Wells et al., 2015; Glibert and Burford, 2017; Glibert, 2020). Thus, HABs in Florida, like those elsewhere in the world have been increasing, often lasting longer and having a wide range of environmental impacts and toxicities (e.g., Anderson, 1989; Hallegraeff, 1993; Glibert and Burkholder, 2018, Phlips et al., 2020).

The approach for nutrient criteria development in Florida is basin-by-basin, with highest priority for those waters where the most straightforward restoration strategies, such as wastewater treatment plant upgrades, are available (e.g. Lapointe et al. 2015). This has left large areas of Florida’s waters, including the region typically impacted by *K. brevis* blooms, impaired but without criteria. Florida has placed priority on those waters for which restoration strategies will result in water quality improvements. By comparing TN and TP discharge from different rivers, it can be seen that large reductions in both nutrients are needed to have a substantial impact on reducing the frequency of *K. brevis* blooms (Fig. 7), based on the results from the RVM. These comparisons, based on variations of 1-2 standard deviations from the mean (and setting other features to the mean), illustrate the magnitude of reductions necessary to reduce the probability of blooms from >0.6 to <0.2. While these examples are meant to highlight interactions between nutrient discharge from different rivers, these models can be used to explore multiple different types of scenarios. Changes in flow, such as that due to hurricanes or intensive wet weather, bring new nutrients that can help to support blooms. The statistical analysis by Maze et al. (2015) indicates that there are significant differences in the Peace and Caloosahatchee River flows between periods of large blooms and periods without blooms. The machine learning algorithms used here illustrated strong relationships between river flow and blooms. New approaches outlined here may not only be helpful in future criteria evaluation, but also meet the scientifically defensible requirement.

Air temperatures over the Eastern North America (including Florida) are expected to increase ~1.5 oC by 2050 and 3-4 oC by 2100 (relative to 2000), according to recent climate projections (IPCC, 2014). Additionally, rainfall over Florida is projected to decrease by 20-30% during the summer but to increase by 10-20% during the fall-winter, which is the season during which *K. brevis* blooms typically occur. This work underscores the important interactive roles of nutrient pollution and river flow in the increased frequency of *K. brevis* blooms in Florida. With climate change and the predicted increase in extreme precipitation events in a warming climate (Sillman et al., 2013a,b; Russo et al., 2014), it is expected that will likely be more frequent HABs in the future, in Florida and elsewhere, unless substantial reductions in TN and TP land-based use and loading in the major rivers is accomplished.

From local to global scales, environmental conditions supporting HABs are changing, leading to increasing challenges for understanding–and modeling–the habitats that support and stimulate them. Herein, 4 new machine learning models were developed for the WFS and explored with regard to wind direction, temperature, river flow, nutrient load and sea surface height as explanatory variables in predicting *K. brevis* blooms. The models had different strengths, due to the differing degrees of complexity of the models, and they responded differently to the cross-validation procedures used. Overall, the RVM and NB models performed the best in predicting past events. By manipulating the range of explanatory variables, insight into the strength of their impact on blooms was obtained. These findings highlight that not only are reductions in both N and P necessary to reduce blooms, but reductions from multiple rivers are more effective than reductions from a single river. These models can be helpful in exploring the most effective combinations of nutrient reductions and in future implementation of watershed nutrient TMDLs. Since river drainage basins are large, a 10-20% increase in fall-winter rainfall will translate into increases in discharges of multiple rivers with their combined higher nutrient loads during the *K. brevis* bloom period. This implies that to control blooms through nutrient reductions, greater reductions will be required.

# Conflict of Interest

*The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest*.

# Author Contributions

MJL developed the models and wrote the paper. PMG advised the project and edited the manuscript.

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# Data Availability Statement

All the data and code are publicly available and accessible online. The data and code can be found at: <https://github.com/lim09749/WFS_ML/>.

**Table 1.** Comparison of the four machine learning approaches applied herein (Support Vector Machine, SVM; Relevance Vector Machine, RVM; Naïve Bayes, NB; and Artificial Neural Network, ANN), as validated using *k*-fold cross-validation and block cross-validation. See text for equations applied.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | | *k***-fold**  **cross-validation**  **(random oversampling)** | *k***-fold**  **cross-validation**  **(SMOTE)** | **Block cross-validation**  **(random oversampling)** | **Block cross-validation**  **(SMOTE)** |
| **SVM** | **Accuracy** | 0.79 | 0.79 | 0.62 | 0.62 |
| **Recall** | 0.63 | 0.63 | 0.27 | 0.26 |
| **Precision** | 0.64 | 0.65 | 0.32 | 0.32 |
| **F1** | 0.64 | 0.64 | 0.29 | 0.29 |
| **RVM** | **Accuracy** | 0.62 | 0.76 | 0.55 | 0.59 |
| **Recall** | 0.73 | 0.72 | 0.58 | 0.47 |
| **Precision** | 0.42 | 0.58 | 0.35 | 0.35 |
| **F1** | 0.53 | 0.64 | 0.43 | 0.40 |
| **NB** | **Accuracy** | 0.52 | 0.54 | 0.47 | 0.47 |
| **Recall** | 0.85 | 0.78 | 0.72 | 0.73 |
| **Precision** | 0.37 | 0.37 | 0.33 | 0.32 |
| **F1** | 0.52 | 0.50 | 0.45 | 0.45 |
| **ANN** | **Accuracy** | 0.74 | 0.71 | 0.61 | 0.60 |
| **Recall** | 0.57 | 0.56 | 0.33 | 0.40 |
| **Precision** | 0.55 | 0.51 | 0.34 | 0.34 |
| **F1** | 0.56 | 0.53 | 0.34 | 0.37 |

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**Figure Legends**

**Fig. 1 (A)** Map of Florida indicating regions where total maximum daily load (TMDL) values have been adopted, where they are being developed, and waters not attaining standards. **(B)** Map of Florida and the West Florida Shelf (WFS) showing the region in red where *Karenia brevis* blooms are most frequently observed. The major rivers that discharge onto the WFS and/or for which nutrient (total nitrogen and total phosphorus) data were used herein are indicated. Red dots mark the United States Geological Survey (USGS) stations and green dots mark the National Data Buoy Center stations from which wind and temperature data were acquired. Note that the red tide region overlaps with the coastal waters regions not attaining water quality standards. Figure A modified from https://fdep.maps.arcgis.com/home/webmap/print.html.

**Fig. 2.** (A) Schematic diagram of the Support Vector Machine (SVM) classifier. The SVM model is a supervised machine learning algorithm that seeks a hyperplane that best separates two labeled classes from each other. The SVM maximizes the width of the gap between the two data clouds. In some cases, not all of the data points can be fitted into the two data clouds outside the shaded gap region. In the soft margin formulation of the SVM, points are allowed inside the gap but penalized in the cost function. (B) Schematic diagram of the Artificial Neural Network (ANN) model. The ANN is based on the feedforward multilayer perceptron architecture, consisting of an input layer, one or more sets of hidden layers, and one output layer. The ANN can be turned into a classifier by discretizing the network’s output. The basic substructure of the ANN is perceptron. For all but the input layer, the perceptron has an input (the outputs of the previous layer). The vectors of inputs and the neuron’s weights are multiplied by a dot product. Then, a transfer function is applied to the sum, giving an output for the next layer of perceptrons.

**Fig. 3.** Comparison of Relevance Vector Machine (RVM) output and observational data of *Karenia brevis.* (A) Time series of the observed (black line) and predicted (green dots) area-averaged *K. brevis* concentrations from 1998-2018. (B) Snapshots of the observed *K. brevis* distribution in selected months. The twenty-year timespan includes many years with blooms (2002, 2005, 2012, 2018) and without blooms (1998, 2010). The horizontal line delineates 5000 cell L-1, the value typically taken to define blooms.

**Fig. 4.** Time series of the observed (black line) and predicted (green dots) area-averaged *K. brevis* concentrations from 1998-2018 for (A) Support Vector Machine (SVM), B) Naïve Bayes classifier (NB), and (C) Artificial Neural Network (ANN) model outputs. The horizontal line in each panel delineates 5000 cell L-1, the value typically taken to define blooms.

**Fig. 5.** Probability of *Karenia brevis* as a function of wind speed and direction, obtained from the sensitivity analysis using the RVM. Northerly wind generates the coastal upwelling that transports *K. brevis* from offshore regions to coastal waters, producing favorable conditions for growth. Once *K. brevis* reaches coastal waters, westerly wind keeps populations near the coast and prevents them from dispersing offshore.

**Fig. 6.** Probability of *K. brevis* blooms as a function of riverine discharge (panels A-E), total nitrogen loading (TN; panels F-I) and total phosphorous loading (TP; panels J-M), obtained from three machine learning models: RVM (thick green lines); NB (dotted blue lines); SVM (dashed red lines).

**Fig. 7.** Contour plots of *K. brevis* probability as a function of combinations of riverine nutrient loads, obtained from the sensitivity analysis using the RVM. (A) Hillsborough and Peace River total nitrogen (TN). (B) Hillsborough and Caloosahatchee total phosphorus (TP).