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Review

Machine Learning Methods without Tears: A Primer for Ecologists

Julian D. Olden*

School of Aquatic and Fishery Sciences, University of Washington Seattle, Washington 98195 USA

Corresponding author
Julian D. Olden
School of Aquatic and Fishery Sciences, University of Washington Seattle, Washington 98195 USA

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ABSTRACT

There is widespread agreement that machine learning methods—a collection of statistical approaches with AI roots—hold enormous potential to improve our capacity to comprehend and anticipate environmental occurrences. Ecological system modeling is a perfect fit for these modeling approaches because of their superior performance compared to more conventional methods (such as generalized linear models) and their adaptability to complicated situations involving several interacting parts. Literature reviews show that, in comparison to other fields, ecology makes very little use of these methods, despite their obvious benefits. The fact that machine learning methods do not fit cleanly into the category of statistical modeling tools that the majority of ecologists are acquainted with might be one reason for the lack of interest. This study introduces three machine learning methods that ecologists might utilize in their work: evolutionary computation, artificial neural networks, and classification and regression trees. We provide a concise overview of the technique, ecological examples of its use, details of model construction and execution, pros and cons, statistical software availability, and an example for each approac.

Keywords
Ecological informatics; Classification and regression trees; Artificial neural networks; Evolutionary algorithms; Genetic algorithms; GARP; Inductive modeling.

INTRODUCTION

A lot of people think that REDICTIVE ABILITY is the pinnacle of ecological science (Peters 1991). Because ecological forecasting is becoming more important in light of the growing dangers to biological variety posed by global environmental change, the significance of prediction in applied ecology has grown in recent decades (Clark et al. 2001). Ecosystems are notoriously difficult to study because of their multi-faceted nature, which includes factors such as past impacts, present interactions, time delays, nonlinearities, and spatially and temporally variable feedback loops (Levin 1998). Understanding and anticipating intricate ecological processes and patterns is therefore a significant problem for ecologists.

Current research and development in the field of ecological informatics is aimed at creating quantitative tools that may address environmental concerns such as global climate change, new illnesses, and biodiversity loss (Green et al. 2005). Regardless of the complexity of an ecosystem, ecological informatics (also known as eco-informatics) encourages the use of cutting-edge computing tools to uncover ecological processes and patterns (Recknagel 2003). Finding patterns in complicated, often nonlinear data and developing reliable prediction models are at the heart of machine learning (ML), a fast expanding subfield of eco-informatics. Big, high-resolution datasets covering previously inaccessible geographical and temporal extents are now within reach, thanks to recent advances in data gathering technologies like remote-sensing and data network centers and archives. Consequently, ecologists may use ML techniques to predict the intricate interactions present in these massive datasets, which is an interesting possibility. Practical Uses of ML Techniques

Ecology employs a wide variety of methods, from simulating species distributions for conservation and management planning to testing biogeographical, ecological, and evolutionary theories (e.g., Fielding 1999; Reckna-gel 2001, 2003; Cushing and Wilson 2005; Ferrier and Guisan 2006; Park and Chon 2007).

The goal of the modeling process might inform the taxonomy used to arrange ML algorithms. Ecologists have advocated for a variety of ML techniques as viable alternatives to more conventional modeling methods. Among these methods, there are supervised learn-

ing approaches that aim to simulate the connection between inputs and known outputs. These include artificial neural networks, cellular automata, classification and regression trees, fuzzy logic, genetic algorithms and programming, maximum entropy, support vector machines, and wavelet analysis. Also, ecological data may be analyzed using unsupervised learning methods such self-organizing maps and hop-field neural networks (Hopfield, 1982; Kohonen, 2001). According to several studies (Guisan and Zimmermann 2000; Peterson and Vieglais 2001; Olden and Jackson 2002a; Elith et al. 2006), these methods have been increasingly popular in recent years due to their capacity to model complex, nonlinear relationships in ecological data. This is in contrast to conventional, parametric approaches, which require users to meet restrictive assumptions. Consequently, ML methods are often more effective in describing and forecasting ecological phenomena. Ecological Informatics, a new scientific magazine, and the International Society for Ecological Informatics, both formed recently, proves that ML has progressed from a domain of theoretical demonstrations to one with substantial and practical use in ecology.

There has been very little adoption of ML methods outside of the ecologists' specialized computational subfield, which is not unexpected. Why haven't ecologists embraced ML approaches more? Ecologists may not have the foundational knowledge to fully grasp and use these strategies, and they might not know which approaches would work best for their specific situation. Researchers in ecological informatics, however, are pushing for more advanced ML algorithms, claiming that larger ecological data sets will become more widely available and that faster computers would propel them into the mainstream. While ML technology continues to advance, most people still need a fundamental understanding of when, when, why, and how to use these methods, which makes these techniques inaccessible to them.

We contend that the ecological literature lacks several case studies that showcase the potential of ML approaches and inspire their investigation and use. This paper will address this concern by offering a thorough evaluation of three machine learning (ML) methods that have lately become popular among ecologists: classification and regression trees, artificial neural networks, and evolutionary computation (genetic algorithms and programming). Nevertheless, we acknowledge that other statistical approaches, such as multivariate adaptive regression splines and generalized additive models, have also shown usefulness in ecology (e.g., Austin 2007; Elith and Leathwick 2007). For each technique, we will offer a quick overview, show some examples of how it has been used in ecology, explain how to build and implement a model, go over its pros and cons, and look at the statistical tools that are available. So that the fundamentals of the ML methodology may be better shown, gies, we will model species richness (the dependent variable) as a function of environmental characteristics (the independent variables) and apply each technique to this common ecological challenge. Our review is not an attempt to supplant other works on ML (such as Fielding 1999 or Lek and Gue'gan 2000), but rather an attempt to make ML approaches more approachable to a wider audience of ecologists by providing a more accessible introduction. To do this, we eliminate the statistical jargon that makes ML techniques difficult to understand for ecologists and instead rely on textual explanations rather than mathematical formulae. In a nutshell, we're crossing our fingers that this study will spark more interest in and use of ML methods in environmental research.

Methods for Machine Learning Illustrated

We will utilize 8236 north-temperate lakes in Ontario, Canada, to demonstrate ML techniques and the relationship between fish species richness and environmental characteristics. Because environmental variables can interact in non-linear ways to impact the number of species at any given location, identifying patterns and causes of species richness has long been an issue in ecology. We are not attempting to compare methods here; rather, we are illustrating a typical statistical issue when researchers want to describe a single dependent variable as a function of several independent factors. For the sake of clarity, we opted for this easy-to-understand ecological topic and dataset. Even if ML techniques work well with apparently basic issues, they may also be used to far more complicated situations, bringing their benefits with them.

Based on what is known about the habitat needs of temperate fish species in the Ontario region, we have chosen eight whole-lake descriptions (Minns 1989). Temperatures measured in degrees Celsius, or the mean monthly air temperature, were used to depict the regional climate. and monthly precipitation (in centimeters) for every lake, from 1960 to 1989, according to data gathered by the Atmospheric Environment Service of Environment Canada from 1836 monitoring stations (Vander Zanden et al. 2004). The following habitat metrics were measured across the whole lake: pH, secchi disc depth (SDD), maximum depth (MAXD), total shoreline perimeter (SHP, km), elevation (ELEV, m), and lake surface area (AREA, km2). Data about fish distribution was mostly culled from the Ontario Ministry of Natural Resources' Fish Species Distribution Data System. Using 10-fold cross-validation, we evaluated the models' prediction abilities. The first step of this process is to partition the original data into 10 subsamples, with each subsample having n/10 observations. One subsample is kept as validation data to test the model, while the other 9 subsamples are utilized for training. After that, the subsamples are utilized exactly once as validation data in the cross-validation procedure, which is then repeated ten times (hence, folds). A single set of predictions for all n observations is generated by combining the 10 results. We direct readers to Fielding and Bell (1997) for more general information on subjects beyond the scope of our work, such as model selection, model validation, and the evaluation of predicted performance.

CLASSIFICATION AND RegReSSION TReeS (CARTS)
BACKgROUND AND eCOLOgICAL APPLICATIONS

Classification and Regression Trees (CARTs), collectively called decision trees, date from the pioneering work of Morgan and Sonquist (1963) in the social sciences, and their use in statistical literature was re- kindled by the seminal monograph of Breiman et al. (1984). Since this time, deci- sion trees have been widely used in a number of applied sciences including medicine, com- puter science, and psychology (Ripley 1996). Recent years have seen CARTs emerge as powerful statistical tools for analyzing com- plex ecological datasets

because they offer a useful alternative when modeling nonlinear data containing independent variables that are suspected of interacting in a hierarchical fashion (De'ath and Fabricius 2000).

There have been numerous ecological applications of CARTs across a wide range of topics. Decision trees have been used to develop habitat models for threatened birds (O'Connor et al. 1996), tortoise spe- cies (Anderson et al. 2000), and endan- gered crayfishes (Usio 2007). Iverson and Prasad (1998) forecasted potential shifts in tree species distributions resulting from cli- matic warming, Rollins et al. (2004) quan- tified the relationship between the fre- quency and severity of forest fires and landscape structure, and Mercado-Silva et al. (2006) predicted patterns of fish species invasions in the Laurentian Great Lakes. Other applications have involved modeling patterns of variability in PCB concentra- tions of salmonid species (Lamon and Stow 1999), predicting days postpartum from fatty acids measured in harbor seal milk (Smith et al. 1997), delineating geo- graphic patterns of bottlenose dolphin ecotypes (Torres et al. 2003), and develop- ing models that assessed the vulnerability of the landscape to tsunami damage (Iver- son and Prasad 2007).

MeTHODOLOgY

CART analysis is a form of binary recur- sive partitioning where classification and regression trees refer to the modeling of categorical and continuous response vari- ables, respectively (Bell 1999). The general anatomy of a decision tree is presented in Figure 1. The term "binary" implies that each group of observations, represented by a node in a decision tree, is split into two child nodes, a process through which the original node becomes a parent node. The term "recursive" refers to the fact that the binary partitioning process can be applied repetitively. Thus, each parent node can give rise to two child nodes and, in turn, each of these child nodes may themselves be split, forming additional children. The term "partitioning" refers to the fact that the dataset is split into sections or parti- tioned. Although there are many different versions of binary recursive partitioning available, each with its own unique details, CART analysis consists of three basic steps. The first step involves tree building, during which a decision tree is built by repeatedly partitioning the data set into a nested series of mutually exclusive groups, each of them as homogeneous as possible with respect to the response variable. Tree building begins at the root node with the entire dataset, and the algorithm formu- lates split-defining conditions for each possible value of all the independent variables to create candidate— or surrogate—splits. Other splitting criteria are also available. Next, the algorithm selects the best candi- date split that minimizes the average "im- purity" of the two child nodes. Impurity is based on a goodness of fit measure, such as the information (entropy) index and the Gini index for classification trees and sums of squares about group means for regression trees (De'ath and Fabricius 2000). The algorithm continues recursively with each of the new children nodes until tree building is stopped.

Classification and regression trees (CARTs), artificial neural networks (ANNs), and evolutionary algorithms (EAs) are compared to the family of generalized linear models (GLMs) that are traditionally used in ecology. Comparisons are generalized to include both classification and prediction problems. Values are based on Hastie et al. (2001), peer-reviewed literature, and the personal experiences of the authors.

learning sample values can lead to signifi- cant changes in the variables used in the splits. As a result, overall variable impor- tance cannot be determined by only exam- ining the final tree; it also requires the examination of all possible surrogate splits. Fifth, perhaps the greatest weakness of CARTs is that the final decision tree is not guaranteed to be the optimal tree. At each splitting decision in the tree growing pro- cess, the selected split is the one that results immediately in reduced impurity (for classification) or variation (for regression). One might expect that some other split, which would appear suboptimal at the time, could produce more effective future splits (Sutton 2005). A variety of approaches have been developed to address the latter two problems, including the application of bagging and boosting techniques and the creation of an ensemble tree based on random forests of multiple trees. We refer the reader to De'ath (2007) and Cutler et al. (2007) for an ecological treatment of these topics.

SOFTWARe

Many commercial packages are available to implement CART. This software varies from requiring a fair amount of user design and programming to Windows-based programs to powerful and user-friendly Graphical User Interfaces. Windows-based programs include CART (www.salford-systems.com), DTREG (www.dtreg.com), KnowledgeSEEKER (www.angoss.com), QUEST (www.stat.wisc.edu/~loh), PolyAnalyst (www.megaputer.com), Random Forests (www.stat.berkeley.edu/ users/breiman), Shih Data Miner (www.shih.be), See5/C5.0 (www.rulequest.com), and XpertRule Miner (www.attar.com). Modules and libraries for statistical software packages include AnswerTree for SPSS (www.spss.com/answertree), Multivariate Exploratory Techniques (Classification Trees) for Statistica (www.statsoft.com), Enterprise Miner for SAS (www.sas.com), Tree library for S-Plus (http://lib.stat.cmu.edu/S), and Rpart for the R-package (http://cran.r-project.org).

ARTIFICIAL NeURAL NeTWORKS (ANNS) BACKgROUND AND eCOLOgICAL APPLICATIONS

An artificial neural network (ANN), or, more generally, a multilayer perception, is a modeling approach inspired by the way biological nervous systems process complex information. The key element of the ANN is the novel structure of the information processing system, which is composed of a large number of highly interconnected elements called neurons, working in unity to solve specific problems. The concept of ANNs was first introduced in the 1940s (McCulloch and Pitts 1943); however, it was not popular- ized until the development of the back- propagation training algorithm by Rumelhart et al. (1986). The flexibility of this modeling technique has led to its wide- spread use in many disciplines such as physics, economics, and biomedicine.

Researchers in ecology have also recog- nized the potential mathematical utility of neural network algorithms for addressing an array of problems. Previous applications include the modeling of species distribu- tions (Mastrorillo et al. 1997; O¨ zesmi and O¨ zesmi 1999), species diversity (Gue´gan et al. 1998; Brosse et al. 2001; Olden et

al. 2006b), community composition (Olden et al. 2006a), and aquatic primary and sec- ondary production (Scardi and Harding

Results from the regression tree for predicting fish species richness as a function of environmental charac- teristics for 8236 north-temperate lakes in Ontario, Canada. (A) 10-fold cross-validation (solid circles) and resubstitution (empty circles) relative error for the regression tree. The dashed line represents + 1-SE of the relative error for the minimum regression tree (i.e., 15 nodes), and the selected tree under the 1-SE rule is indicated by the arrow. (B) Relative importance of the environmental variables for predicting fish species richness (note that values do not sum to 100). Variables include mean monthly air temperature (TEMP) and precipitation (PPT), lake surface area (AREA), total shoreline perimeter (SHP), maximum depth (MAXD), elevation (ELEV), secchi disc depth (SDD), and pH. (C) The final regression tree relating fish species richness to lake environmental characteristics. Node precision is indicated by Root-Mean-Squared-Error.1999; McKenna 2005). Cornuet et al. (1996) used a neural network to assign individuals to appropriate taxonomic groups using mul- tilocus genotypes. Spitz and Lek (1999) modeled wildlife damage to farmlands, and Thuiller (2003) assessed the potential im- pacts of climate change on the distribution of tree species in Europe. Other applications have occurred in the fields of water resource management (Maier and Dandy 2000), inva- sive species biology (Vander Zanden et al. 2004), and pest management (Worner and Gevrey 2006). A collection of ANN appli- cations in ecology is presented in Lek and Gue´gan (2000), Recknagel (2003), and O¨ zesmi et al. (2006), as well as in special issues of Ecological Modelling and Ecological Informatics (e.g., Recknagel 2001; Park and Chon 2007).

MeTHODOLOgY

There are many types of supervised and unsupervised learning methods for ANNs (Bishop 1995). Here we describe the most frequently used method in ecology: the one hidden-layer, supervised, feedforward neural network trained by the back- propagation algorithm. These neural net- works are popular in the ecological literature because they are considered to be universal approximators of any continuous function (Hornik et al. 1989). In this sec- tion, we will discuss neural network archi- tecture and the back-propagation algo- rithm used to parameterize the network, and we will describe the various methods available to quantify variable importance.

Network architecture refers to the num- ber and organization of the neurons in the network (see Figure 3 for the general anat- omy of a neural network). In the feedfor- ward network, neurons are organized in an input layer, a hidden layer, and an output layer, with each layer containing one or more neurons. Each neuron is connected to all neurons in adjacent layers with an axon; however, neurons within each layer and in nonadjacent layers are not con- nected. The input layer typically contains p neurons, one neuron representing each of the independent variables x1 through xp. The number of neurons in the hidden layer can be selected arbitrarily or deter- mined empirically by the investigator to minimize the trade-off between bias and variance (Geman et al. 1992). The addi- tion of hidden neurons increases the abil- ity of a network to approximate any under- lying relationship among the variables, i.e., resulting in reduced bias, but also in- creases the variance of predictions due to overfitting the data. Although mathemati- cal derivations exist for selecting an opti- mal design (see Bishop 1995), in practice it is common to train networks with different numbers of hidden neurons and to use the performance on a test data set to choose the network that performs the best. For continuous and binary response variables, the output layer commonly contains one neuron, but the number of output neu- rons can be greater than one if there is more than one response variable or if the response variable is categorical (i.e., a sep- arate neuron for classifying observations into each category). Additional bias neu- rons with a constant output are also added to the hidden and output layers, although this is not mandatory, as these neurons play a similar role to the intercept term in general linear regression.

Each neuron in the network has an "ac- tivity level" that is defined by the value of the incoming signals received from the other neurons connected to it. In turn, each

axon in a network is assigned a "con- nection weight" that reflects the overall in- tensity of the signal it transmits (i.e., input to hidden or hidden to output). The activ- ity levels of the input neurons are defined by the values of the predictor variables (Figure 3). The state of each hidden neu- ron is evaluated locally by calculating the weighted sum of the incoming signals from the neurons of the input layer, which is then subjected to an activation function, i.e., a differentiable function of the neu- ron's total incoming signal from all input neurons. The same procedure described above is repeated for the axon signals from the hidden layer to the output layer.

CONCLUSION

In the field of ecology, machine learning techniques may help with both understanding and predicting future outcomes. By demonstrating the use of CART, ANN, and EC to tackle difficult issues, this paper aims to expose ecologists to ML. Our goal in doing so was to provide ecologists with some good alternatives to the standard statistical methods now used in the field. Although ML techniques have had some uptake in ecology in recent years, it's still early days compared to other fields, and many are skeptical of its usefulness for quantitative analyses. Many ecologists may be reluctant to devote their time to learning comprehensive programming syntax and language since they do not have the computational background necessary to run the software that implements these techniques (Fielding 1999). More user-friendly software is being produced at a quick pace due to the rising popularity of these techniques. This study provides examples of such software, which will raise ecologists' understanding of ML, encourage its use, and ultimately lead to the improvement of these analytical tools.

Our capacity to model ecological systems will be greatly improved by the use of machine learning technologies, which are potent instruments for explanation and prediction. You can't expect them to fix every problem with ecological modeling, however. Both ML methods and more conventional statistical techniques have their limitations, and no one method is going to be able to solve every issue. Although ML approaches are sometimes more adaptable when it comes to modeling complicated relationships and unstructured datasets, the models they generate aren't always easy to compare, and the modeling process isn't always visible either.

While machine learning does improve our capacity to simulate ecological phenomena, it is equally essential that we learn more about

the underlying brain processes that cause these phenomena. While some claim that ML algorithms try to do away with ecological intuition in data analysis, we couldn't be more disagreed. Due to the analyst's need to define the data representation and the search algorithms to characterize the problem, human intuition cannot be fully removed. According to Olden et al. (2006b), ML is not meant to replace human modelers but rather to automate certain tasks within the modeling process. We anticipate that more ecologists will be able to incorporate machine learning techniques into their quantitative toolbox as a result of our review, and that they will be better equipped to make informed decisions regarding the use of machine learning vs more conventional statistical methods in their future modeling projects.

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