Machine learning for understanding inland water quantity, quality, and ecology

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Abstract

This chapter provides an overview of machine learning models and their applications to the science of inland waters. Such models serve a wide range of purposes for science and management: predicting water quality, quantity, or ecological dynamics across space, time, or hypothetical scenarios; vetting and distilling raw data for further modeling or analysis; generating and exploring hypotheses; estimating physically or biologically meaningful parameters for use in further modeling; and revealing patterns in complex, multidimensional data or model outputs. An important research frontier is the injection of limnological knowledge into machine-learning models, which has shown great promise for increasing such models' accuracy, trustworthiness, and interpretability. Here we describe a few of the most powerful machine learning tools, describe best practices for employing these tools and injecting knowledge guidance, and give examples of their applications to advance understanding of inland waters.

Keywords

machine learning; neural networks; deep learning; classification and regression trees; clustering; dimensionality reduction; data mining; artificial intelligence

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Glossary

black box: a model whose inner workings are not known to the user, whether because they are hidden or because they are too complex to readily grasp.

design: the use of human intelligence and knowledge to shape the structure, inputs, or algorithms of a model.

discovery: the use of algorithms to find values of model parameters, states, and/or equations that can suitably describe or reproduce observations.

distillation: reducing large volumes of information to smaller ones.

features: the variables used as inputs to a model; also sometimes called predictors, dependent variables, or drivers.

inference: discovering the model values - including parameters, equations, or internal states - that best fit the observations, with an interest in what the discovered values say about the real-world system and processes being modeled.

knowledge-guided: rooted in machine learning while also formally incorporating knowledge of real-world patterns or processes; also sometimes called process-guided, physics-guided, theory-guided, or process/physics/theory/knowledge-informed.

loss function: a function quantifying the success of a set of model predictions, usually by comparison to observations; also sometimes called objective function or cost function. The **loss** is the output of a loss function for a given set of training examples.

machine learning: the use of algorithms that learn about the world based on feedback rather than relying on a human-defined set of facts or equations; abbreviated ML.

prediction: estimating values of a dependent variable as a function of some inputs and a model; predictions may describe the past, present, or future at sampled or unsampled locations.

process-based: primarily containing equations and parameters that are human-interpretable representations of physical, chemical, or biological processes.

supervised: algorithms trained or calibrated to make predictions that closely match known outputs; contrast with unsupervised algorithms, which are trained to discover patterns in the data based on similarities among inputs.

training: the process by which machine learning models are iteratively modified until their performance minimizes the output of a loss function; roughly equivalent to model fitting or calibration for statistical or process-based models, respectively.

Introduction

Design and discovery

Limnology began with laborious field campaigns, from which observations were then used to develop empirical models to describe and explain patterns in aquatic ecosystems (e.g., Lindeman, 1942; Dillon and Rigler, 1974; Vollenweider, 1975). The advent of powerful new *in situ* and *ex situ* sensing techniques has given modern-day limnologists a much greater volume and variety of aquatic observations for testing theories and developing new models. At the same time, increases in computing power have opened the door to machine learning (ML) approaches that take advantage of this new wealth of data. A growing number of limnological studies now benefit from the strengths of ML models, which can include accurate predictions, short runtimes, and flexible equation structures that can capture non-linear relationships precisely (e.g., Hsu, Gupta and Sorooshian, 1995; Maier and Dandy, 1996; Fienen *et al.*, 2013; Pacheco *et al.*, 2017; Nolan *et al.*, 2018; Kratzert, Klotz, Shalev, *et al.*, 2019; Read *et al.*, 2019).

ML models and their alternatives - process-based, empirical, and statistical models - take a great variety of forms and can be distinguished by the degree to which they contain two elements: **design** is the extent to which humans have manually specified the structure or parameters of the model to reflect current understanding, and **discovery** is the extent to which algorithms ingest observations to learn useful values of the model parameters, equations, and states (Figure 1). For inland waters, design is guided by scientific knowledge of physical, chemical, biological, and ecological processes and patterns in aquatic systems; discovery is guided by data from *in situ* sensors, field samples and observations, remotely sensed images, etc. The strength of design is that it formalizes and enables tests of scientific theories, whereas discovery makes fuller use of the data and thus often yields the best predictions and may suggest new connections among variables. Both design and discovery can contribute substantially to our understanding of the natural world, especially when they are used in combination.

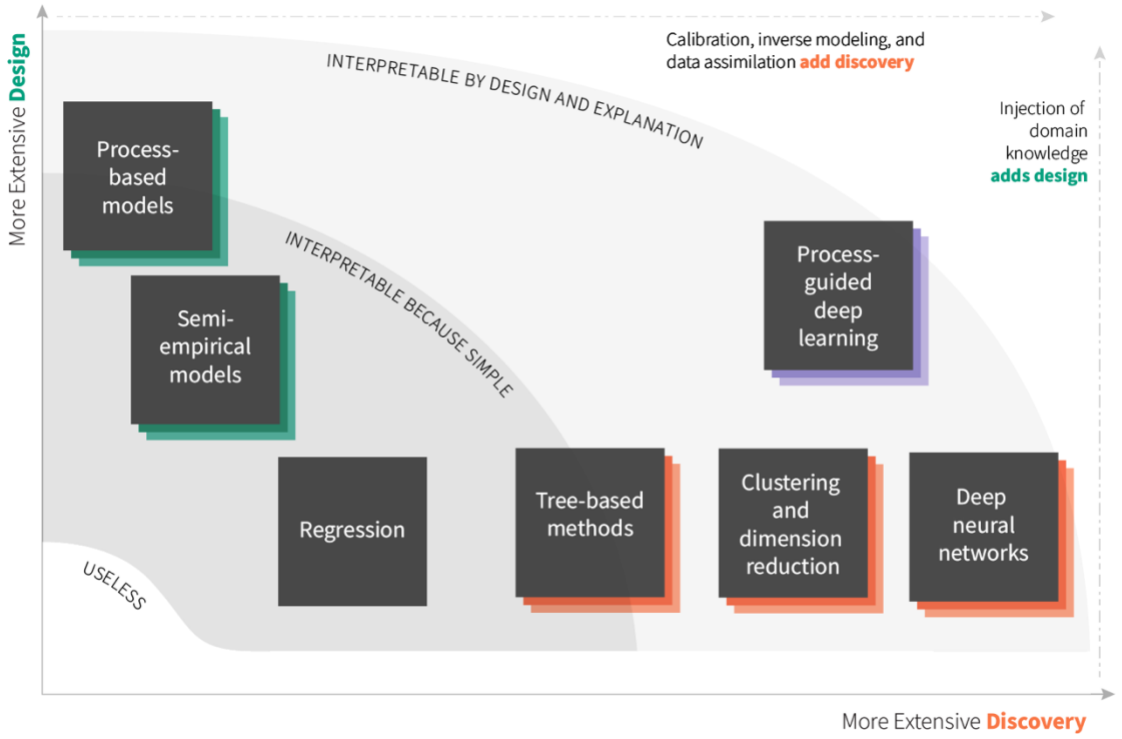

Figure 1. Model types positioned by their use of design and discovery. Machine learning models may be purely discovery-based (orange) or can include design (purple), and they are distinguished from other model types by their capability for substantial data-driven discovery of model parameters, equations, and/or states. As discussed in Section 7.4, the methods of interpretation by design and/or ML explanation have expanded rapidly in recent years such that it is now possible to derive some interpretive insights from nearly any model, and more for those discovery-based models that include some design.

ML models are distinguished from process-based and empirical models by their substantial use of discovery, which enables these models to benefit from large datasets. While substantial design is the distinguishing feature of process-based models, all models - from the simplest regressions to the most black-box-like ML models - contain some design in the form of expert-selected input variables and model structures that reflect expected relationships (Robson, 2014). ML models can be infused with additional limnological design elements in the numerous ways we will investigate throughout this chapter. Conversely, process-based and empirical models can be infused with discovery; this can be done by calibration, inverse modeling, or data assimilation, all topics that we leave to other texts.

Compared to non-ML models, ML models can offer greater prediction accuracy, faster training and execution times, and the flexibility to capture nonlinear relationships for which we lack good theory or direct observations (Solomatine, See and Abrahart, 2008; Shen, 2018; Reichstein *et al.*, 2019; Sun and Scanlon, 2019). Despite these many benefits, ML models have seen only moderate adoption in inland water sciences, perhaps because newcomers to ML often worry that ML is severely lacking in two areas: trustworthiness and contribution to scientific understanding. We argue that both of these areas deserve rigorous attention when applying ML and yet are poor reasons to shy away from ML, because (1) trust and understanding can be

earned by ML models, sometimes in ways that outshine non-ML alternatives; (2) trust and understanding are also challenges for non-ML models; and (3) the drawbacks of ML models are often outweighed by their benefits. We expand on these themes below and throughout the chapter.

Model trustworthiness

Models merit our trust when the outputs are accurate for all intended uses, often including application to new water bodies, time periods, aquatic communities, environmental conditions, or situations where data are sparse. Because we rarely have the right data to test a model for all intended uses, we often lean on a heuristic of process design: We tend to trust models whose equations and coefficients express processes as described in textbooks and the literature. However, this design heuristic is neither necessary nor sufficient. It is unnecessary because, as ML models have repeatedly demonstrated, transferable accuracy is achievable with black-box solutions and sufficient training data (DeWeber and Wagner, 2014; Kratzert, Klotz, Herrnegger, *et al.*, 2019). It is insufficient because models are always imperfect: In addition to the omnipresent lack of perfect input data about ecosystem properties and drivers, even our most "process-based" models are always semi-empirical simplifications of the true processes occurring at ecosystem scales (Simon, 1962). In fact, it can be argued that given enough data, ML models containing more parameters than a process-based model are capable of representing limnological processes more completely.

Instead of relying on a heuristic of textbook-like equations, the growth of ML pushes us to judge trustworthiness based on (1) consistent accuracy across a challenging range of test conditions and (2) model inspection to determine whether the model respects known physical and biological constraints and cause-effect relationships. Similarly, we *create* trustworthy models not by keeping them tied to hypothesized processes but by training on larger datasets, following known best practices for ML model development and testing, and - perhaps most importantly for limnology - by injecting design into ML models to encode well-understood processes, physical laws, and reliable patterns, while leaving less-understood phenomena to be discovered by the algorithms.

Limnological knowledge can be designed into ML models at many points in the model structure and in the model development process (Figure 2). All models permit - and in fact require - injection of knowledge-based design at the point of selecting and preparing input variables. Many ML models are capable of residual or hybrid modeling, i.e., ingesting residuals or outputs from other design-rich models and generating more accurate predictions of the same target variable. Some more advanced forms of design injection are limited to the more flexible model structures - for example, neural networks can be designed to assume temporal and/or spatial patterns in the inputs and outputs, and they can be trained or constrained to avoid violation of specific physical or biological rules. Specific modifications are discussed in detail in the Tools section of this chapter.

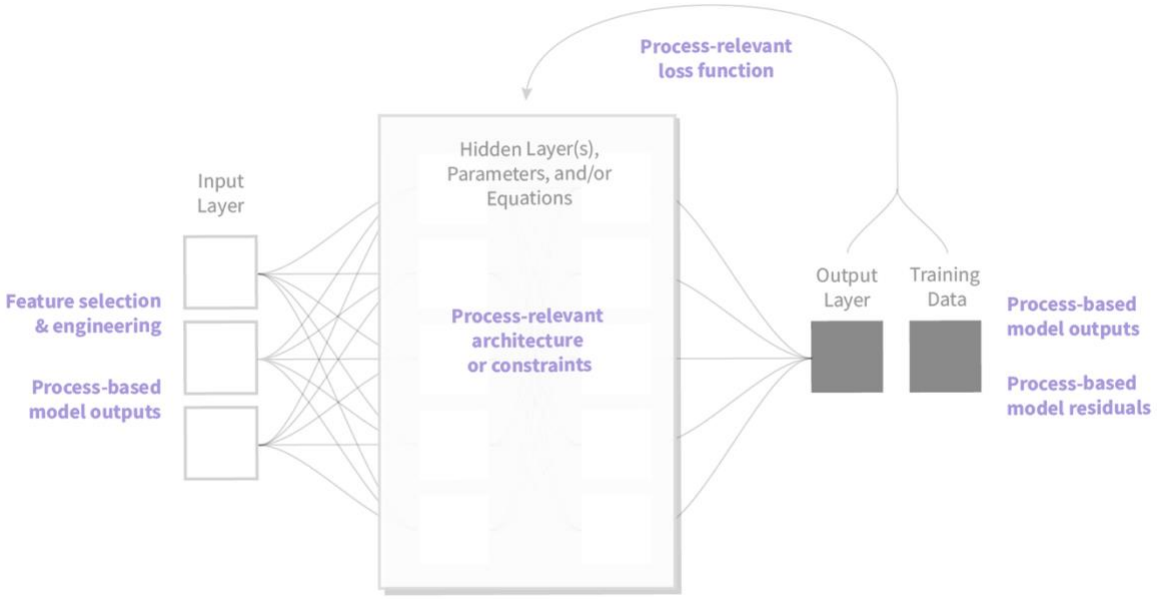

Figure 2. Injection of limnological design into machine learning models can occur at the points (purple text) of the model inputs, architecture, training data, and/or loss function.

Discovery-driven models have proven so powerful at prediction that Anderson (2008) questioned the value of continuing to develop new research theories at all. However, theory-based design is a powerful complement to discovery-based models, enhancing model trustworthiness and utility when the two are used together. Further, outside a modeling context, theory remains an important means to discuss, teach, and engage meaningfully with our world. So, it is fortuitous that even as theory-based design improves the realism and out-of-bounds accuracy of ML models, ML models of all kinds can be used to build understanding, including new and revised theories (Mazzocchi, 2015; Nearing *et al.*, 2020), as discussed in the next subsection. Theory and data will always be imperfect and incomplete, and the largest advances in limnological modeling will occur when flaws in either are identified and overcome by leveraging the other.

Pathways to understanding

Limnologists use models to improve understanding of inland waters - specifically, we seek the ability to concisely describe general aquatic patterns or processes via equations, natural language, or digestible images - i.e., we seek "intelligibility" (de Regt, 2017). Understanding of this form enables action: researchers can test hypotheses, develop new ones, and make predictions; environmental managers can choose and justify courses of action; and water users can appreciate and decide how to use water resources. Modeling typically supports understanding via pursuit of three major modeling pathways: **prediction**, **inference**, and **distillation** (Figure 3).

Prediction asks, “What does the current model say about the world?” The goal of prediction is to estimate values of a dependent variable as a function of a model and some inputs, where the dependent variable is usually a property of the world such as water quality, a nutrient transformation rate, or the size of a fish population. Although predictions are sometimes too detailed for immediate understanding, they provide the raw material from which patterns can be discovered, theories proposed or tested, and understandable summaries derived (Douglas, 2009). Predictions also support water resources decision-making directly, by precisely estimating aquatic ecosystem states and process rates for decision-relevant locations and time periods.

Inference asks, “What do the observations tell us about the underlying process being modeled?” Here we use “inference” in the statistical sense to mean discovering the model values (parameters, equations, and/or internal states) that best fit the observations, i.e., “answer[ing] questions about the model in the light of the data” (Cox, 2006). Fitted parameters, equations, and states often yield understanding directly or can be distilled to something even more understandable. Inference using discovery-driven tools is sometimes called “statistical learning” and distinguished from “machine learning” by the user’s objective (inference via statistics, prediction via ML; Bzdok, Altman and Krzywinski, 2018), but because the tools are almost always the same, we consider data-driven inference using ML to be within this chapter’s scope. We also expand the statistical definition slightly to include the use of one model to make inferences about another, where the second model may be data-driven, process-based, or even conceptual.

Distillation asks, “How can we say this more simply?” Distillation uses models to reduce large volumes of information to smaller ones. Distilled information may be directly useful to researchers or managers because it is more intelligible than the raw inputs, thus enhancing understanding of pattern or process. In addition, distilled information may be used as input to subsequent models, thereby reducing computation costs for those later models (because the distilled inputs are smaller and simpler) or improving their accuracy (because the distilled inputs contain less noise). While inference and prediction are commonly recognized as the core pathways trod by modelers (Sanders, 2019), distillation is an important third pathway because it bridges the gap between raw data or model outputs and truly useful information.

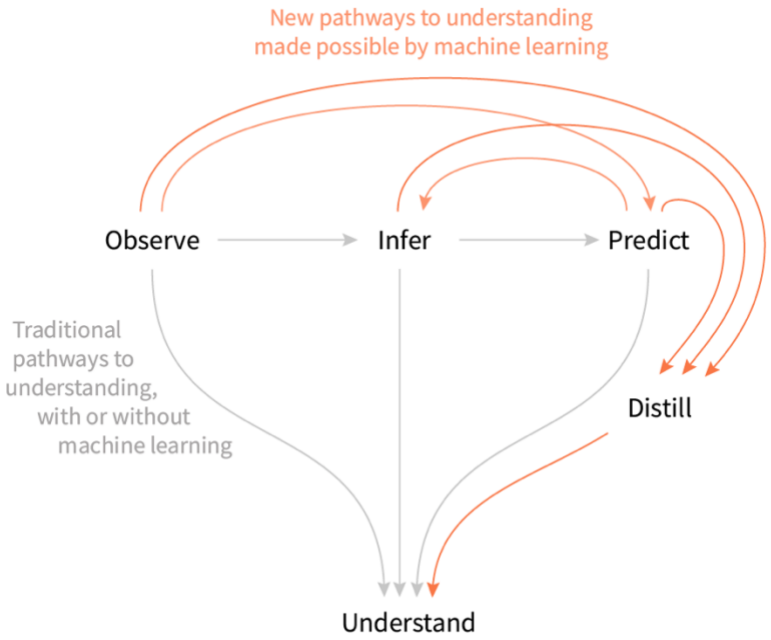

Figure 3. Pathways from data to understanding. Some data can be directly understood. Process-based, semi-empirical, and traditional statistical models enable inference, which can directly provide understanding or can lead to understanding via predictions (gray arrows). Machine learning (ML) models can yield understanding by the same pathways as non-ML models but also introduce additional pathways, including predictions that bypass inference, inferences that emerge from predictive models, and ML-enabled distillation of observations, inferences, and predictions (orange arrows).

Although ML models are sometimes criticized for failing to contribute to understanding, we argue that such criticism fails to recognize the several pathways by which modeling can inform understanding. We agree with the critics that little understanding would be gained by making inferences about ML equations and parameters that have little interpretable meaning (e.g., parameters in artificial neural networks or random forests). But ML models can support inference about meaningful limnological processes and states if we use ML differently - if we set the focal variables as the inputs or outputs of the model, or if we infuse certain parameters with meaning through strong doses of limnological design. And ML models are often *better* than non-ML models at prediction and distillation (Figure 3, Table 1). As we describe specific tools and applications throughout this chapter, we will elaborate on the diverse uses of ML to build understanding.

Table 1. Suitability of five major modeling approaches (columns) for three major modeling pathways (rows). Number of stars indicates level or frequency of suitability. Cells contain names of more specific methods for applying the approach to the pathway. Inference may also be addressed for all modeling approaches using model-agnostic interpretation techniques (see Section 7.4).

Objective	Process-based models	Statistical models	Neural networks	Tree-based models	Clustering and dimension reduction models
Prediction	** Simulation, out-of-bounds predictions	* Regression, additive models, time series models	*** Prediction, recurrence, convolution	*** Random forests, boosting	* Classification of new observations
Inference	*** Calibration, inversion	** Regression, hierarchical models	** Attention, prediction of parameters	* Decision trees	* Cluster and dimension characteristics
Distillation		** Regularization, model selection	** Autoencoders, regularization	** Pruning	*** Simplification of inputs

Chapter overview

In this chapter we present four classes of ML approaches - neural networks, classification and regression trees, clustering and dimensionality reduction methods, and model interpretation techniques. We chose these four classes because we see much application of them in the recent literature and great opportunity for fusion of discovery and limnological design, especially for neural networks. There are many other ML approaches and variants on these approaches (e.g., Support Vector Machines) that are not covered in detail here. To learn more about these other options, please refer to a primer on machine learning methods written for ecologists (Olden, Lawler and Poff, 2008) and a review of deep learning in the hydrologic sciences (Shen, 2018), and keep a watchful eye on new publications in this fast-growing field.

The main body of this chapter is divided into descriptions of these focal modeling approaches (Tools), guidelines for rigorous use of ML models (*Implementation*), and examples of how these approaches have been applied to meet goals for prediction, inference, or distillation for inland waters research and management needs (*Applications*). Recurrent themes throughout the chapter include gaining understanding of process or pattern, assessing model trustworthiness and prediction uncertainty, and injecting process design into model structures and the model-development process. We show that ML models, particularly when applied according to best practices and with heavy doses of both design and discovery, are powerful tools to support limnological investigation, understanding, and management.

Tools

Neural networks

Neural networks (NNs) are highly flexible black-box models that can mimic virtually any relationship between inputs and outputs, as long as the model and the training dataset are both sufficiently large (Goodfellow, Bengio and Courville, 2016). The flexibility of NNs makes them suitable for any of the three modeling pathways (prediction, inference, or distillation), although their prediction accuracy is most frequently touted. As computing power and datasets have grown to enable ever more complex NNs, the resulting growth in predictive accuracy has driven the explosive popularity of NNs, with a turning point at a series of high-profile modeling competitions on tasks such as speech recognition, image classification, and time series modeling (Lecun, Bengio and Hinton, 2015). Deep learning, which employs NNs with multiple layers, has also risen in popularity within limnology (see *Applications and Conclusion*).

NNs are collections of connected variables, or *nodes*, where each node contains the weighted sum of its designated input nodes as transformed by an activation function such as a logistic curve (Figure 4). Nodes are typically organized into *layers* to represent discrete stages of information flow through the network, where successive layers build from preceding layers to extract increasingly complex features, compute interactions among features, and ultimately generate predictions. NN parameters are initialized to random values and then iteratively trained until the model performance minimizes the output of a **loss function**, a function that returns a designer-specified accuracy metric such as the root mean squared error of predictions relative to observations. Model training follows an iterative process in which a set of trial predictions is generated, then blame for the *loss* (the output of the loss function) is apportioned among the parameters, then the parameters are each slightly adjusted in proportion to their blame, and then the next iteration is begun. The efficiency of this training procedure is what makes it practical for NNs to be substantially more complex, and therefore more flexible, than other ML modeling structures.

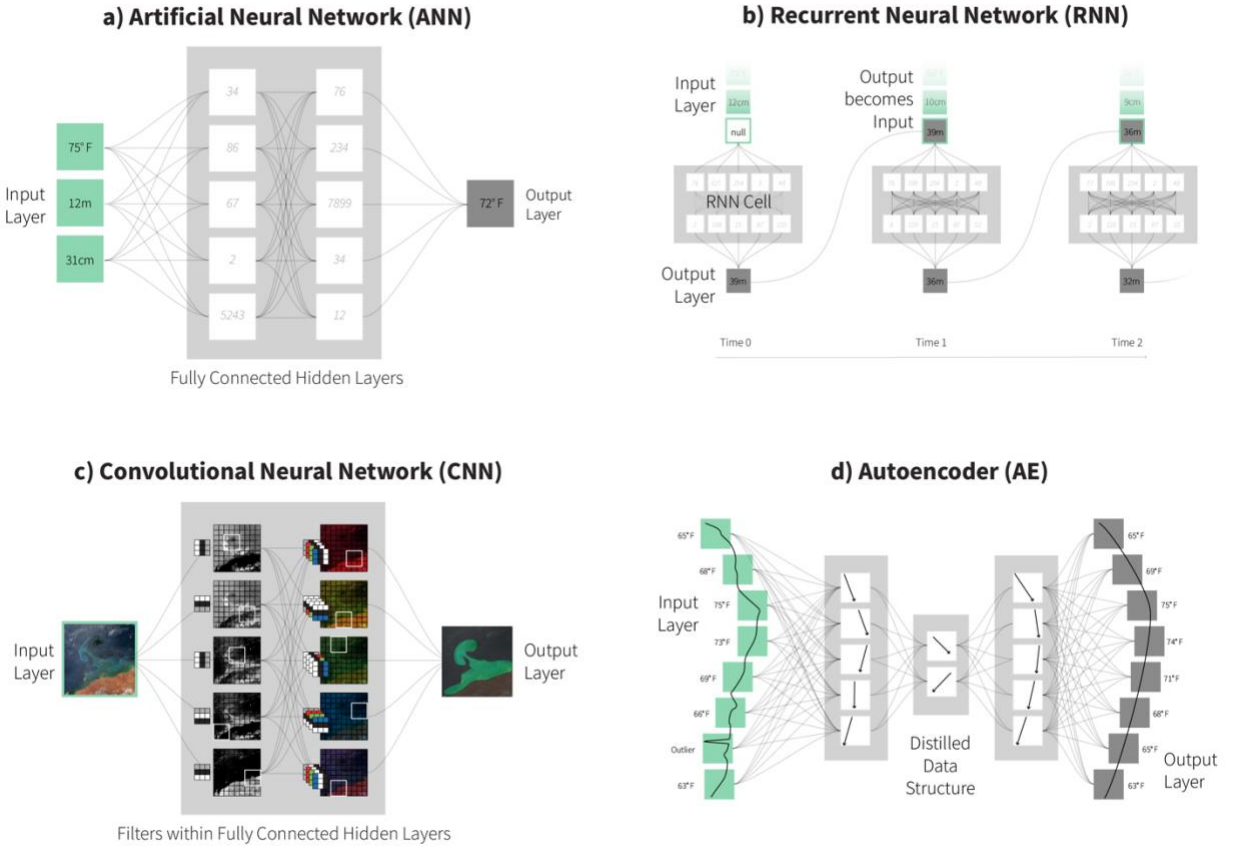

Figure 4. Structure of (a) a basic NN, with expansions useful for (b) temporally correlated data, (c) spatially structured data, and (d) compression or de-noising of complex inputs. Within each panel, information flows along the curved arrows. Where arrows meet, values are combined by a weighted sum, the addition of a constant (bias), and transformation by an activation function such as sigmoid or tanh. Light gray rectangles indicate the conceptual gathering of nodes into layers. Green, white, and dark gray boxes represent input, intermediate, and output nodes, respectively.

NNs can be a simple stack of fully connected layers (artificial neural networks, ANNs, Figure 4a), or they can have more complex structures that are suited to specific prediction problems. Recurrent neural networks (RNNs, Figure 4b) are useful for modeling time series of water chemistry (Li *et al.*, 2019), temperature (Rahmani *et al.*, 2020), quantity (Nagesh Kumar, Srinivasa Raju and Sathish, 2004), community composition (Chon *et al.*, 2001), etc. because they model whole sequences of inputs and outputs, using the same set of parameters for each transition between timesteps. RNN variants such as Long Short-term Memory (LSTM) and Gated Recurrent Units (GRU) transfer more detailed information among timesteps, enabling a memory of recent and more distant past events and cumulative ecosystem status (e.g., snowpack depth; Kratzert *et al.*, 2018). Raster-based convolutional neural networks (CNNs, Figure 4c) apply to spatially structured datasets such as remotely sensed images and 2D representations of water bodies (Syariz *et al.*, 2020). CNNs pass specialized parameter sets (kernels) over an input raster one spatially contiguous window at a time, extracting higher-level features from each window and representing those features in a new 2D layer that can itself be treated as a raster. Graph convolutional neural networks (GCNNs) allow spatial connections via

a graph rather than a grid, which may be preferable for modeling systems such as river networks or food webs (Jia *et al.*, 2021). Autoencoders (Figure 4d) are a means of information compression or smoothing; the network is trained to re-predict the original inputs after passing data through one or more constrained hidden layers, which typically have fewer nodes than the input layer. After training, these constrained layers concisely represent the essential information and may therefore support inference about properties of the aquatic system (Li *et al.*, 2020); alternatively, the modeler may be most interested in the final predictions for their smoothness or reduced noise relative to the original inputs. Other NN structures exist and continue to be invented, but ANNs, RNNs, CNNs, and autoencoders are readily and widely applicable for limnological modeling objectives.

Estimating Uncertainty: Many methods are available to quantify uncertainty in NN predictions (Kabir *et al.*, 2018). For example, some NNs are trained to directly predict two or more moments of the probability distribution of each prediction (e.g., the mean and variance; Nix and Weigend, 1994). Alternatively, Bayesian NNs represent each node as a distribution and thus can represent uncertainty throughout the network (e.g., Graves, 2011; Blundell *et al.*, 2015; Louizos and Welling, 2016; Pearce *et al.*, 2018). Ensemble methods are another option, where the ensemble prediction is the distribution of predictions from many different instances of the NN (Tibshirani, 1996). Variation among the ensemble members can be obtained by training each member separately, e.g., with different initial parameter values or resampled training data (Dietterich, 2000), or by dropout from a single trained model, where a random subset of the weight parameters are set to 0 at the time of prediction (Gal, 2016).

Integrating Design: NNs are highly amenable to the injection of limnological process knowledge, especially when the NN structure already represents temporal or spatial dimensions of an aquatic ecosystem. Beyond that structural decision, Willard *et al.* (2020) describe the following approaches to adding design: (1) Custom loss functions can encourage physically, chemically, or biologically realistic values of internal model states and final predictions (e.g., Beucler *et al.*, 2020; Jia, 2020). (2) The model architecture, i.e., the choice of layers and activation functions, can be designed to strictly enforce physical, chemical, or biological rules (e.g., Daw *et al.*, 2020). (3) Model weights can be initialized, or "pretrained," to emulate a process-based model by treating process-based model outputs as observations (Read *et al.*, 2019). (4) Models can be trained to predict the residuals between process-based model predictions and observations, rather than predicting the observations themselves. (5) NNs can be hybridized with process-based models, e.g., by passing the outputs from the process-based model as inputs to the NN (e.g., Karpatne *et al.*, 2017), or chaining outputs from the NN into the process-based model, or embedding one model as an intermediate component of the other model. Applications of such methods for Earth system sciences have been recently reviewed (Reichstein *et al.*, 2019).

Tree-based methods

Classification and regression trees (CART) algorithms (De'ath and Fabricius, 2000; Breiman *et al.*, 2017) can represent very complex, non-linear, multivariate relationships and are most

useful for building understanding via prediction (e.g., predicting groundwater pH from landscape features; Stackelberg *et al.*, 2021) or **supervised** distillation (e.g., identifying syndromes of lake properties and warming rates, O'Reilly *et al.*, 2015; or assigning phytoplankton species to functional groups, Kruk *et al.*, 2017). CART algorithms lack some flexibility relative to other methods described here, especially in their ability to simulate spatial and temporal relationships among states, provide unsupervised distillation, or accommodate designed structural components to integrate limnological knowledge. However, CART algorithms excel at ingesting and predicting categorical variables, are often competitive with basic NNs for prediction accuracy, and are highly interpretable at the level of individual decision trees, which can be drawn and visually inspected.

CART algorithms are like NNs in that they obtain their flexibility from many connected nodes that each perform a simple calculation. Whereas each NN node is a weighted, transformed sum of preceding nodes, CART nodes are decision points within a tree of if-else statements, each of which is a split on the axis of one input variable. Terminal nodes ("leaves") of classification trees predict class membership, while leaves of regression trees predict a continuous value as a simple average of the dependent variable from the training data for that node. Extensions of the regression tree include more complex functions at the leaves and sometimes the nodes, including using the last or all upstream predictors in a linear model to predict the continuous value (Quinlan, 1992).

Many popular CART algorithms use ensembles of trees, created largely by bootstrapping (bagging) or boosting methods. Bagging methods train many different trees and then report the average of the trees' predictions; for example, the random forest algorithm grows many trees by withholding random subsets of the inputs and randomly permuting a subset of features (Breiman, 2001). Boosting methods such as AdaBoost (Freund and Schapire, 1997) and Extreme Gradient Boosting (XGBoost; Chen and Guestrin, 2016) build an ensemble of trees whose predictions are added together, where each new tree is trained to predict the residuals of the sum of the previous trees' predictions. Ensemble CART methods perform well even for collinear predictors, high dimensionality data, and non-linear relationships between predictors and responses.

Estimating Uncertainty: Uncertainty in individual CART algorithm predictions can be estimated using method-specific algorithms, e.g., several methods for random forests (Meinshausen, 2006; Coulston *et al.*, 2016; Mentch and Hooker, 2016; Zhang *et al.*, 2020), ensembling for AdaBoost (Zhou *et al.*, 2017), and quantile regression for XGBoost (März, 2019). Many of these approaches leverage concepts from Bayesian statistics, from which they gain uncertainty estimates and also benefits to model robustness and accuracy (e.g., Quadrianto and Ghahramani, 2015). Bayesian Additive Regression Trees (BART) combine boosting and a Bayesian approach that generates predictions from a probability distribution rather than a point estimate (Chipman, George and McCulloch, 2012). New methods continue to be developed for uncertainty estimation, such as the probabilistic models implemented as NGBoost (Duan *et al.*, 2019).

Integrating Design: CART algorithms have a fairly rigid structure that limits the amount of knowledge-based design that can be injected. However, as with any model, modelers still use limnological knowledge when choosing which variables to input; knowledge-rich input variables may include derived variables that reflect important hydrologic or limnological properties. In addition, some algorithms and implementations offer opportunities to customize the training loss function (Chen and Guestrin, 2016) or constrain the output to be monotonic with respect to one or more input variables (Incer *et al.*, 2018), permitting limited but intriguing opportunities to design knowledge into these aspects of the model.

Clustering and dimensionality reduction methods

Clustering and dimensionality reduction techniques provide understanding via distillation, i.e., they condense large, complex datasets into more manageable, interpretable, or otherwise useful forms (Borcard, Gillet and Legendre, 2018). Unlike most other ML models, the techniques described here use unsupervised learning: rather than seeking to make predictions that match observable answers, they aim to reduce complexity while preserving the meaningful features of a dataset. Clustering methods classify similar observations into groups, which can yield insight about complex or high-dimensional data (e.g., quantifying changes in microbial community structure over time; Rubbens *et al.*, 2021), reveal previously unknown structure in the data (e.g., identifying distinct seasonal patterns in stream photosynthesis rates; Savoy *et al.*, 2019), or identify anomalies (e.g., detecting erroneous spikes and level shifts in water quality sensor data; Leigh *et al.*, 2019). Dimensionality reduction methods compress high-dimensional data to fewer dimensions, which can be useful for reduce noise in data (e.g., removing distortion from underwater images; Fabbri, Islam and Sattar, 2018), increase data-driven model performance by providing fewer and more meaningful predictor variables (e.g., simplifying hyperspectral imagery to a set of independent variables; Dierssen *et al.*, 2021), and aid in interpretation of results (e.g., describing effects of floodplain restoration on species richness of macroinvertebrates, macrophytes, and fish; Pander, Mueller and Geist, 2018).

Methods for clustering include k-means clustering, Gaussian mixture models (GMMs), and hierarchical clustering (Scrucca *et al.*, 2016; Bramer, 2020). In k-means clustering, data are grouped into k clusters by randomly selecting k data points to serve as the initial group centers, then iteratively adding nearby points to each group and computing the centers of the updated groups. K-means clustering performs best on groups that are spherical; GMMs overcome that limitation by describing each cluster with a different mean and standard deviation in each dimension, and allowing clusters to overlap, which allows clusters to take on complex shapes. Hierarchical clustering methods build trees by sequentially splitting or gathering data points into groups (divisive and agglomerative clustering, respectively). An important modeling decision for any clustering algorithm is the number of clusters to use (set directly for k-means clustering and GMMs or via tree depth for hierarchical clustering). This decision may be based on expert knowledge or by finding the value that minimizes within-group variance and/or maximizes between-group variance.

Dimensionality reduction techniques include time-honored linear transformation methods such as principal components analysis, linear discriminant analysis, and factor analysis; and non-linear methods such as isometric feature mapping, non-metric multidimensional scaling, locally linear embedding, t-distributed stochastic neighbor embedding, and uniform manifold approximation and projection. These methods have been joined by neural-network-based approaches such as autoencoder NNs (described above) and self-organizing maps (SOMs). SOMs are specially structured NNs that map multi-dimensional data points onto a 2-dimensional grid or honeycomb of nodes, simultaneously organizing similar data points spatially (a sort of "soft clustering") and reducing data dimensionality. Unlike most NNs, whose weights are adjusted based on their contribution to a loss function, the weights associated with each SOM node are iteratively updated until the map spans the full data space while preserving similarity among neighboring SOM nodes.

Estimating Uncertainty: Uncertainty in clustering and dimensionality reduction usually cannot be defined with respect to differences between predictions and observations because there is no "true" group membership or dimension definition to observe (autoencoders are a rare and partial exception). Instead, confidence in model output is assessed through goodness of fit, as described by measures of group distinctiveness or preserved distances among samples (see Model evaluation). Among clustering methods, GMMs shine with respect to uncertainty estimation because they naturally predict the probability that each data point belongs to its assigned cluster.

Integrating Design: Despite the data-driven, unsupervised nature of clustering and dimension reduction algorithms, design can be injected into these methods at the time of application. The researcher first chooses the variables to reduce, e.g., a set of potentially related biogeochemical measurements or gene abundances or a time series of model predictions across a set of sites that exhibit environmentally meaningful variation. For clustering algorithms, the researcher also selects meaningful measures of similarity, which may vary depending on the probability distribution, sparsity, or temporal or spatial structure of the data. Lastly, the researcher may apply expert judgement to the selection of model hyperparameters such as the number of clusters or dimensions to use, where the "right'' number is often a compromise that explains substantial variance and yet is still simple enough to yield scientific insight.

Interpretation techniques

Model interpretation is useful for assessing trustworthiness and extracting insight from ML models. It has sometimes been assumed that ML models sacrifice interpretability for the sake of accuracy, but the inevitability of that tradeoff is belied by recent progress in ML model design (Rudin, 2019) and ML explanation techniques (Samek *et al.*, 2019; Molnar, 2020) (Figure 1). Process-based components of ML models are intrinsically interpretable, another point in favor of integrating design into ML. Additionally, ML models may be structured so that they explain themselves, e.g., by making predictions based on similarity of the current inputs to prototypes encountered during training (Chen *et al.*, 2019). These structural approaches to

interpretability are largely new to limnology, but the field of model explanation for artificial intelligence (called "Explainable AI" or "XAI") offers a slightly better-trodden and complementary approach to model interpretation. Having already addressed process-guided designs in sections 7.1-7.3, here we provide a taste of the current options in XAI.

When inspecting predictions one at a time, intuition suggests that there should be some quantifiable contribution of each input feature such that the prediction is some fixed intercept plus the sum of all features' contributions. Shapley values are these quantifiable contributions (Shapley, 1951). For a simple linear regression with normalized features, Shapley values are equal to the fitted coefficients, but for more complicated models, the calculation of Shapley values must consider many possible combinations of feature values to isolate the effect of the feature of interest. SHapley Additive exPlanations (SHAP; Lundberg and Lee, 2017) further generalize the Shapley value idea from the effects of individual input features to the effects of feature combinations, e.g., all the pixels in a specific fish in an underwater image.

SHAP values can be inspected at multiple levels of detail (Lundberg and Lee, 2017). For a single prediction, the direction and magnitude of the contribution of each input feature can be visualized in a stacked bar plot. From there, stacked bar plots can be positioned side-by-side for many individual predictions, with predictions optionally grouped by the similarity of the input feature contributions to reveal clusters of conditions for which different sets of input features drive the predictions (note the use of a clustering algorithm to distill the SHAP results, already putting into action the tools described above). Effects of each feature can be summarized as a single value giving the mean absolute effect of that feature (one way to measure feature importance); as a density plot showing the distribution of effects of that feature over all training examples; or as a scatter plot with one point per training example showing the feature's effect (SHAP value) versus the feature's value.

Fast estimation algorithms have made SHAP a leading interpretation method in recent years; however, SHAP values are still computationally expensive to derive, are less informative when features are correlated with one another, and can't answer the question, "If I increase this feature by 5%, how will the prediction change?" An approach that does better with the first and third of these issues is Local Interpretable Model-agnostic Explanations (LIME; Ribeiro, Singh and Guestrin, 2016), in which a locally linear model is fit around a single input example to intelligibly describe the sensitivity of that prediction to small changes in the inputs (even for models that are globally nonlinear). There are also alternatives to SHAP for estimating feature importance (Breiman, 2001; Fisher, Rudin and Dominici, 2018) and partial dependence (Friedman, 2001) or variants that deal more elegantly with interactive effects (ICE; Goldstein *et al.*, 2015; ALE; Apley and Zhu, 2019).

While the above methods are model-agnostic or can be implemented for a variety of ML models, there are also interpretation methods specific to neural networks that offer additional forms of insight (Samek *et al.*, 2019; Toms, Barnes and Ebert-Uphoff, 2019). We will highlight two such methods here. Integrated Gradients (IG; Sundararajan, Taly and Yan, 2017) quantify the rate of change in the output with respect to change in an input feature, using a discrete

computation approach that reduces unwanted sensitivity of the interpretation to tiny variations in input values. Layerwise Relevance Propagation (LRP; Bach *et al.*, 2015) produces relevance scores that indicate the contribution of each model node to the nodes in the next NN layer, where the sum of the relevance scores in any one layer of an NN is equal to the predicted value. LRP can describe complex NN architectures including those with recurrence (RNNs; Arras *et al.*, 2019) and convolution (CNNs; Montavon *et al.*, 2019). As with model-agnostic approaches to ML interpretation, the subfield of NN-specific ML interpretation is evolving rapidly, and new techniques continue to emerge.

Implementation

Choosing a model

Various modeling challenges are best met with different models. To select a core model for a specific science challenge, first consider the degrees to which data availability enables reliable discovery and well-understood theory enables sound design. Next, bear in mind that many limnological questions may be best addressed with a combination of models that fill different roles; for example, ML models may make inferences about process-based model parameters or may make predictions that serve as inputs to a model of any other type. Thus, the best set of models to address an inland waters science question will depend on the extent of current understanding, the availability of data, and the pathway by which each subtask will be pursued (Figure 5).

- For **prediction**, discovery-rich models (e.g., tree ensembles and neural networks) of sufficient complexity can be very accurate in familiar conditions and are a clear best choice when theory is limited and data are abundant. Process-based, design-rich models may be less accurate in well-observed conditions but are often assumed to predict more reliably in new climates, geologies, etc. However, design and discovery need not be mutually exclusive: Process-guided neural networks have shown impressive accuracy in both familiar and new conditions, and both tree-based models and neural networks can be trained to emulate process-based models but with faster runtimes that make it feasible to explore predictions for many scenarios.
- For **inference**, very simple models or those whose design includes physically or biologically meaningful parameter values are the most rewarding, regardless of how much discovery is included. Simple decision trees and process-guided NNs are the ML models that best meet these criteria, while a wider variety of ML models can be used to make inferences about simpler statistical or process-based models. Lastly, model interpretation methods can be applied to any ML model to quantify the importance and effects of each input variable, describing relations between inputs and outputs that may yield insights into the limnological processes being modeled.
- For **distillation**, clustering and dimension-reduction models are good choices. Additionally, autoencoder neural networks, neural network regularization methods, and tree ensembles all provide built-in filtering or weighting of candidate predictors and constraints on model

complexity, such that these methods can implicitly or explicitly distill input data down to the most important information. In general, ML models are substantially more useful than process-based models for distillation, because ML models can discover rather than assert the structure of complex data.

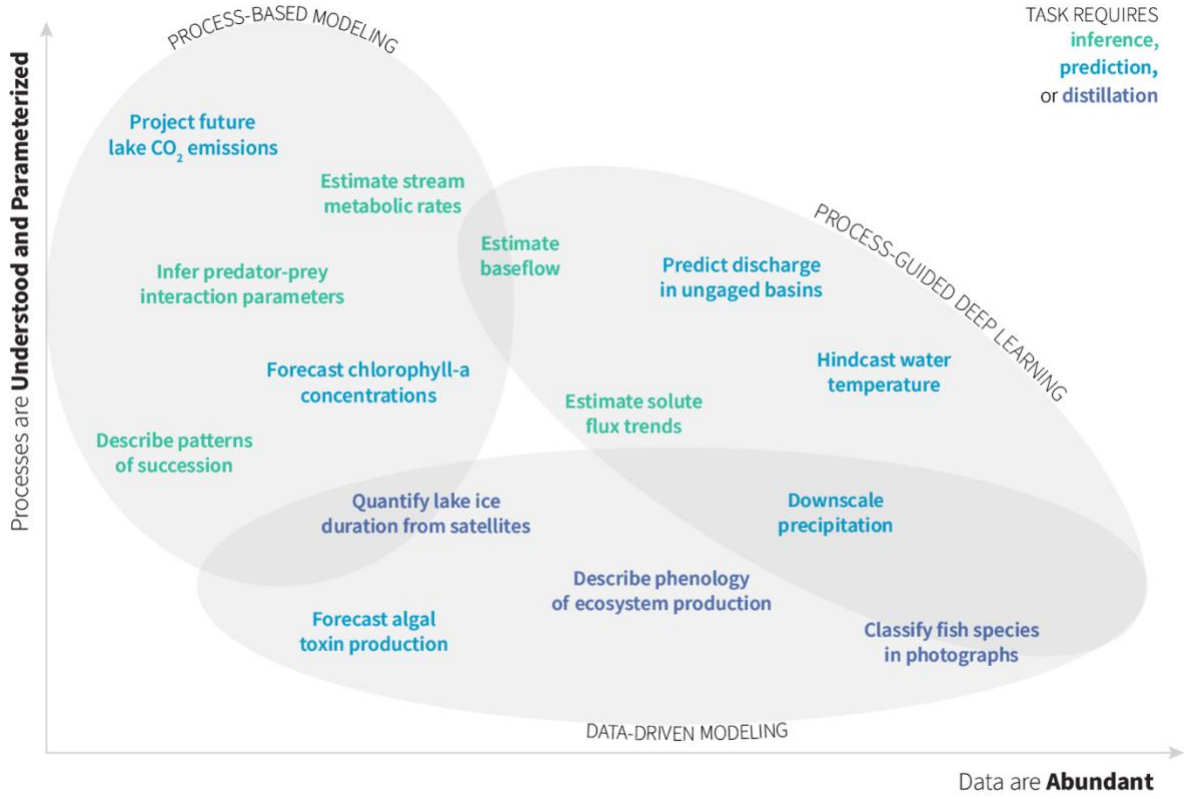

Figure 5. Limnological research tasks (words in colors) begin with differing amounts of data (x axis) and knowledge of the underlying processes and parameters (y axis). Where the modeler's task falls on this plot can help in selecting a modeling approach (labeled gray regions, roughly corresponding to position in Figure 1). The different tasks are colored according to whether the main goal of the task is to infer, predict, or distill, illustrating that each class of modeling approaches can serve several goals. Although the precise position of each research task can be debated, this figure illustrates the broad diversity of research tasks for inland waters with respect to theory, data, and beneficial approaches.

Ensuring reproducibility

Reproducibility ("re-performing the same analysis with the same code using a different analyst"; Patil, Peng and Leek, 2016) is essential to modern science, and applications of ML bring unique reproducibility challenges. One of the fundamental hurdles to clear is achieving reproducibility in the code scripts used to define and/or apply the ML models in a study. General guidelines for open and reproducible scientific computing are available elsewhere (Wilson *et al.*, 2014; Gil *et al.*, 2016), but a few guidelines are especially relevant to applying and experimenting with ML. First, if you are experimenting with variants in model structure, follow the Don't Repeat Yourself (DRY) rule: Write your code so that every variant can be run from the same code base, using concise arguments to specify which model variant is to be applied. When

publishing for reproducibility, publish an archive of every model training and prediction run. Include well-explained source code, information about the software and hardware environment, hyperparameter values, inputs, raw outputs (if not too large), and summary and evaluation metrics. Lastly, report how you selected the hyperparameters (see Hyperparameter Tuning below); this is an often undocumented but important step in the modeling process.

Arguably even more scientifically important than computational reproducibility is replicability ("re-performing the experiment and collecting new data"; Patil, Peng and Leek, 2016). The odds of replicability are higher if you avoid over-tuning your model to match the dataset in hand. Specifically, at the very beginning of your project, divide the available data into three partitions: a training set, a development ("dev" or "validation") set, and a test set. Use the training data to train your model, select hyperparameters based on model performance on the dev data, and withhold the test data until the very end of your project, after you have fully developed your model, to provide an honest assessment of model performance. If data are limited, use a variation on the basic train-dev-test partitioning to make fuller use of the available data while still ensuring that test data have no effect on the selection or refinement of the model - e.g., use cross-validation to do training and testing on several overlapping partitionings. Ideally, the dev and test sets will each provide some surprises relative to the training set, representative of the surprises that would occur when applying the fitted model to an entirely new dataset - to make surprises more likely, split time series data into temporally contiguous chunks so that whole sequences of events remain unseen during training, and split geospatial data in spatial chunks so that dev and testing data are less spatially autocorrelated with training data (Ploton *et al.*, 2020). To improve potential for both replicability and reproducibility, use the published model archive to identify which data were used for training, development, or testing, and document the rationale behind the selected data partitioning strategy.

Model evaluation

Rigorously evaluating model performance is the first step to building trust in an ML application. Model evaluation can be used to compare or choose among several candidate models, determine where each model fails, inform model refinements, and provide essential context for users of the model predictions. Post-hoc evaluation complements any uncertainty estimation method that may have been built into a model, allowing assessments of more diverse aspects of the model fit and providing a check on the uncertainty reported by the model.

For those models that predict observable states, prediction performance can be quantified with metrics such as root mean squared error, mean squared error, classification error, bias, or Nash-Sutcliffe efficiency. The accuracy of a model's uncertainty estimates can also be quantified, e.g., with the bracketing frequency metric. Alternatively, accuracy might be most usefully assessed with respect to values that are computed from the model predictions before being used by the target audience - for example, fisheries managers may be most interested in values computed from daily predictions, such as growing degree days, annual nutrient loads, or the probability of an algal toxin exceedance in a given week. Accuracy in predicting threshold exceedances may be assessed with Receiver Operating Characteristic (ROC) curves and/or

Heidke Skill Scores (HSS), with the ROC curves providing a more nuanced view of event prediction by evaluating model sensitivity (false positive rate) against model specificity (false negative rate) for a range of thresholds (Shin *et al.*, 2020). Continuous Ranked Probability Scores (CRPS) can also be used to evaluate probabilistic predictions and are analogous to mean absolute error (Gneiting *et al.*, 2005; Thomas *et al.*, 2020).

At the community level, accuracy of predictions (or of values computed from those predictions) on common datasets is a valuable means of comparing multiple models to one another. The inland waters community has made recent gains in data sharing through the publication of large, model-ready datasets such as GAGES-II (Falcone, 2011), LAGOS (Soranno *et al.*, 2015; Cheruvelil *et al.*, 2021), CAMELS (Addor *et al.*, 2017), AquaSat (Ross *et al.*, 2019), and DeepFish (Saleh *et al.*, 2020). Development of more such datasets, and widespread use of them for model testing and reporting, would substantially improve our ability to identify top-performing models for limnological prediction.

For unsupervised ML models (e.g., those that provide clustering or dimension reduction), truth is often unmeasurable, and thus prediction accuracy cannot be directly assessed. Instead, clustering models are typically assessed by measures of distinctiveness such as the amount of variance within each group relative to the total variance of the data. Dimension reduction methods can be evaluated by their success in preserving the relative distances among the data points. Bootstrapping methods can also be used to compute the frequency with which a cluster appears over many resamplings of the data or to assess the robustness of conclusions drawn from dimensionality reduction.

Model refinement

Most ML models are defined by (1) a structure and training algorithm and (2) hyperparameters that specify variations within that general framework (James *et al.*, 2021). Examples of hyperparameters (also called “tuning parameters” or “parameters”) include the learning rate in neural networks, the number of candidate features per tree in a random forest, the possible shapes of the relationships among features in a Gaussian mixture model, and the map size of a self-organizing map. Although a sense of effective hyperparameter values can sometimes be pulled from published model applications or software defaults, optimal hyperparameter values are usually discovered by trial and error for each specific application. Data partitioning into training and development sets enables this trial-and-error exploration: Models are trained with a variety of hyperparameter values and then assessed on the development set to identify the most successful combination of hyperparameter values, where success is evaluated by a metric of the modeler’s choice (e.g., root mean squared error). Because the number of possible hyperparameter value combinations is usually infinite, modelers explore a finite number of combinations and then accept the best of those options. This exploration can be done manually, with brute-force search algorithms such as random sampling or grid-based sampling of possible hyperparameter combinations, or using an additional layer of modeling (“surrogate modeling”) to iteratively predict and explore promising regions of hyperparameter space (Feurer and Hutter, 2019).

Perhaps the most important consideration when tuning hyperparameters is the balance between underfitting (unnecessarily limiting the complexity of a model) and overfitting (excessively tailoring a model to the sample in hand). The flexibility of ML models makes them especially vulnerable to overfitting; fortunately, principled train-dev-test data partitioning and hyperparameter tuning are precisely the tools needed to find the right balance. Hyperparameters that affect underfitting and overfitting typically relate to model complexity and include the number of nodes and training iterations in neural networks, the depth and pruning methods for tree-based models, and the number of clusters or dimensions in distillation-focused methods. The values that best balance overfitting with underfitting are those for which accuracy is high for training predictions and yet only modestly worse for development predictions. Underfitting manifests as inaccurate training predictions, which can be addressed by adding model complexity or (if possible) providing additional input features. Overfitting manifests as substantially worse development predictions, which can be addressed by reducing or constraining model complexity, or (if possible) collecting more training data.

Model complexity is most obviously a function of the number of parameters in the model (neural network nodes, k-means clusters, etc.), but model complexity can also be reduced by constraining the range of values that each parameter can take on. Process-agnostic versions of this approach are known as regularization; a common example is to include a penalty term for the sum of all parameter values in the loss function used for model training, such that the model learns to achieve reasonable prediction accuracy with smaller and/or fewer parameters. Physical or limnological knowledge can also be used to guide parameter values toward a subset of the mathematically possible options; for example, a gradient boosting regression might be constrained to predict photosynthesis rates that increase monotonically relative to light intensity, and a neural network might be encouraged, via a loss function term, to predict changes in nutrient flux that conserve mass balance. Although neither of these process guidance examples constrains or penalizes parameter complexity directly, both indirectly limit the range of parameter values that the trained model is likely to include.

Reducing overfitting by collecting more observational training data is only sometimes an option in limnological modeling, despite major data-compilation initiatives (e.g., Soranno *et al.*, 2017) and the continual expansion of public monitoring and remote-sensing datasets (e.g., Read *et al.*, 2017; Topp *et al.*, 2020). Fortunately, limnological expertise can be used to sensibly augment the training dataset, making up with quantity what is lacking in quality in the augmenting information. For example, when remote-sensing-based estimates of a variable can be used to complement *in situ* measurements, these two data sources can be assigned different weights, reflecting their known information quality, in the loss function that guides model training. Another effective approach is to embed information from the lower-quality, higher-volume data into a pretrained model, which can then be finetuned (i.e., trained further) with the high-quality data. For example, Kaya *et al.* (2019) finetuned a generic neural network image classification model, which had been pretrained on images of all kinds, to classify plant species. Synthetic data are also sometimes an option for pretraining or training a useful model; for example, synthetic images with realistic features and background can be used, or a model of

depth to groundwater might be trained on synthetic observations of depth=0 at the margins of streams and lakes. Similarly, Read *et al.* (2019) first pretrained a neural network on process-based model predictions of lake temperatures, then finetuned the model on *in situ* temperature observations. A distinct advantage of pretraining on process-based model outputs is that the ML model can learn from predictions for input conditions that have never yet been observed, allowing the ML model to learn from the process-based model about how to extrapolate to those new conditions in limnologically realistic ways.

Applications

Quality control

Raw data inevitably contain measurement error, whether due to human mistakes, sensor malfunctions, or environmental interference. Previously, human inspection was used to flag errant data, but today's larger and always-growing datasets can only feasibly be processed with automation. A major challenge in quality control (QC) is in distinguishing between errant measurements (e.g., biofouling of a sensor; sun flecks interfering with a remote sensing measurement) and surprising realities (e.g., an extreme algal bloom or sediment transport event), a task that ML models can perform either with no human intervention (for easier problems) or by directing human attention to the ambiguous cases (for harder ones). The line between "easy" and "hard" continues to shift as ML techniques improve, training datasets grow, and theory develops to guide QC targets.

ML methods for detecting data abnormalities primarily follow prediction or distillation pathways and can use a wide variety of model architectures. Supervised prediction methods can be used to predict ("reconstruct") clean datasets with fewer errant measurements. Both random forests and neural networks have been used for this purpose. Autoencoder neural networks are especially suitable because observational outliers are relatively incompressible and are thus greatly altered when the autoencoder compresses and then re-predicts the inputs (Zhou and Paffenroth, 2017). Generative adversarial networks can be used for the same purpose (e.g., for removing distortion from underwater images: Fabbri, Islam and Sattar, 2018) (Figure 6). As an alternative to prediction of clean data, categorical classification and clustering methods can classify data into regimes to enable algorithmic correction for some regimes and targeted expert intervention for others: Supervised classification can group data into modeler-determined regimes such as "clean," "common error pattern," and "needs inspection," while unsupervised clustering can assign data to algorithm-determined groups that the modeler can triage afterward. Both ML and non-ML approaches have been widely used to detect data abnormalities; see Pimentel *et al.* (2014) for a broad review and Kiran, Thomas and Parakkal (2018) for tools specific to video and imagery.

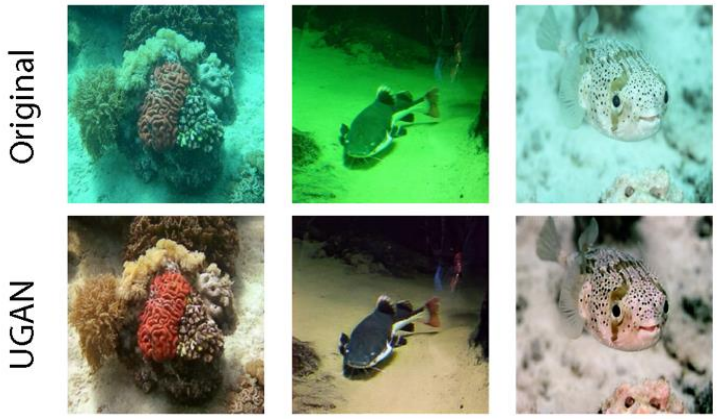

Figure 6. Original distorted underwater images (top row) and images corrected with an underwater generative adversarial network (UGAN, bottom row). Modified from Fabbri, Islam and Sattar (2018).

Preprocessing data for further modeling

Modern limnological models often ingest complex datasets: imagery from satellites, drones, cameras, or underwater videos, high-frequency observations from mobile or stationary sensors, and multidimensional inputs from rich public databases. Although ML promises a reduced need to simplify the features before building the model (because many ML models can filter the features themselves), this promise is not made for process-based or most statistical models, and in practice even ML models often show improved performance when given inputs that are already distilled to their most informative elements. Fortunately, specialized ML models for preprocessing can provide the link between complex raw datasets and data designed to be used by other models for inputs, training, or testing.

Preprocessor ML models can make use of prediction, inference, and/or distillation to extract information from raw data, reduce dataset complexity, and combine multiple datasets. For example, convolutional neural networks (CNNs) can learn to emulate human interpretations of images, enabling automation of labor-intensive tasks such as identifying fish species from underwater photographs (dos Santos and Gonçalves, 2019), classifying phytoplankton in flow cytometry images (Dunker *et al.*, 2018) (Figure 7), or estimating flood heights from social media images (Chaudhary *et al.*, 2019). Alternatively, ML models can generate their own rules for data distillation, reducing an extensive time series to a smaller set of information-rich features (CNNs for soil moisture prediction: Feng, Fang and Shen, 2020) or identifying smaller, and thus more interpretable, sets of predictors (self-organizing maps for river salinity predictors: Bowden, Maier and Dandy, 2005; feature selection for groundwater nitrate predictors: Rodriguez-Galiano *et al.*, 2018). Some distillation activities make rare use of inference on ML models, learning values of ML parameters that have no a-priori meaning to humans but are identified as important by the distilling ML model and can be used effectively by subsequent ML models; for example, Peleato, Legge and Andrews (2018) used the values in the most-compressed layer of an autoencoder as the distillation of results of a multivariate water quality assay. Yet another approach to preprocessing combines multiple datasets in space, either interpolating from observed to unobserved locations (with random forest prediction: Mital *et*

al., 2020) or combining spatial datasets of varying resolution to downscale a coarse data layer to finer resolution for subsequent modeling (with CNNs: Baño-Medina, Manzanas and Gutierrez, 2020).

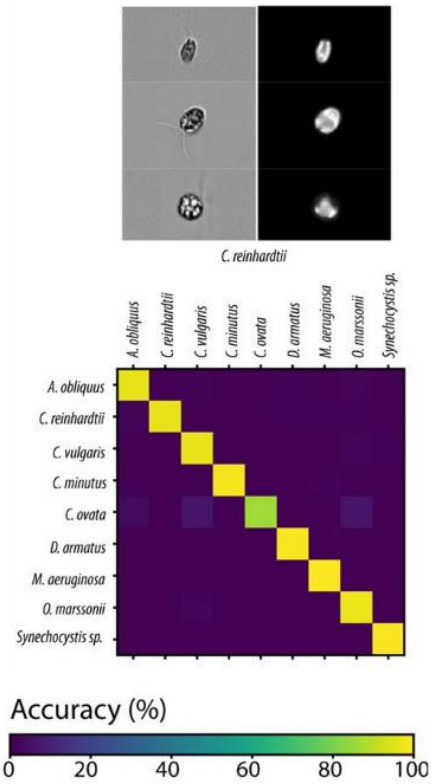

Figure 7. CNN classifiers can be used to identify phytoplankton species from flow-cytometry images (examples in top panel). In the confusion matrix plot (bottom panel), rows give the true species, columns give the predicted species, and color indicates the percentage of images in each row that the model assigned to that column, such that a fully yellow diagonal and purple background would indicate perfect accuracy. Modified from Dunker et al. (2018).

As with other applications, ML models for preprocessing can benefit from injection of limnological design. For example, fish species identification was more accurate when a CNN was trained to predict fish family and order as well as species (dos Santos and Gonçalves, 2019), and distinguishing between land and water pixels in a remote sensing image was more accurate when the classification was tied to estimated bathymetry such that deeper pixels were labeled "water" before shallower pixels (Khandelwal, Mithal and Kumar, 2016).

Exploring hypotheses

One common modeling goal is to gain insight about the drivers and processes underlying an observed pattern or prediction. With ML models, such insight is often obtained by post-hoc model interpretation techniques, although the use of ML to estimate parameters (next section) can be a complementary way to learn about drivers. ML models are well suited to explore

poorly understood relationships between input features and predictions because they are typically robust to high dimensionality and redundant features, and they can capture feature-prediction relationships of any shape. ML interpretation techniques are valuable for generating hypotheses and confronting them with the available data (sometimes even employing formal causal reasoning, e.g., Nauta, Bucur and Seifert, 2019), thus nudging the field toward understanding of the many complex and hard-to-measure processes in inland waters. Hypotheses generated with ML may even be treated as prior beliefs to be merged quantitatively with the results of other experiments with data or process-based models (Tsai, Fang, *et al.*, 2020).

Feature interpretation methods are often used to quantify the importance and effect shapes of features for a wide range of limnological response variables. For example, Worland, Farmer and Kiang (2018) used feature importance (FI) to identify primary drivers of annual low stream flows, then used partial dependence plots (PDPs) to visualize the shapes of the effects of each primary driver. Similar approaches have been used to assess the relationships between newly proposed hydrologic metrics and depth to water table (Belitz *et al.*, 2019); regional-to-local lake properties and water quality (Read *et al.*, 2015); and potential drivers of groundwater nitrate concentrations (Ransom *et al.*, 2017), fish reproductive success (Buston and Elith, 2011), and fish species richness (Franceschini *et al.*, 2019). The shapes of relationships in PDPs have also been used to suggest thresholds in stream and watershed disturbance that trigger regime shifts in stream temperatures (Hill, Hawkins and Carlisle, 2013).

Neural-network-specific interpretation methods are not yet widely used in studies of water quality or ecology but have been recently embraced in the physical geosciences. Kratzert, Herrnegger, *et al.* (2019) discovered memory nodes in a recurrent neural network whose states correlated over time with water storage states from a process-based hydrologic model; they then used Integrated Gradients to confirm that a node correlated with snow water equivalent was influenced by precipitation and minimum air temperature in early winter, a finding consistent with theory. Barnes *et al.* (2020) used Layerwise Relevance Propagation to identify those regions of global temperature and precipitation maps that were used by a neural network to predict the year of the maps, i.e., those regions that distinguished the climate in that year from other years (Figure 8). Identifying the variables, times, and locations that a neural network is relying on for a prediction allows researchers to check for consistency with theory, explain errors, and examine the identified information for additional insights.

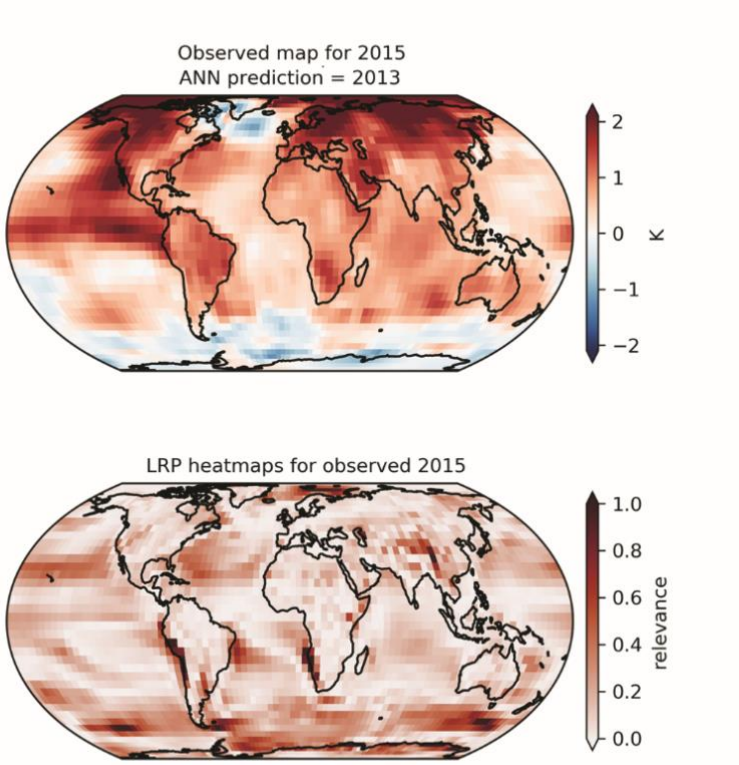

Figure 8. Layerwise Relevance Propagation (LRP) can be used to propose regions of the globe where air temperature signals are most indicative of the year of an air temperature map. Top: temperature anomalies in 2015 relative to 1979-2099. Bottom: LRP heatmaps show the relevance of each input grid cell to the model's prediction that the map is from 2013, permitting exploration of features that are similar between 2013 and 2015 and different from other years. Modified from Barnes et al. (2020), Fig. 10.

Estimating parameters and states

As a way of developing process understanding, modelers often work to refine qualitative descriptions of patterns into process-based or semi-empirical equations that describe relationships among inputs, outputs, and internally represented states. Further process understanding then takes the form of estimated values of the parameters or states used in those equations. ML models can assist in this estimation of parameters and states (collectively termed "variables" in this subsection). However, in contrast to the designed variables of process-based models, ML variables typically lack connection to known process equations, such that ML modelers have turned to creative techniques, either estimating the variables of process-based models or developing process-guided ML models that contain some interpretable variables.

One approach to the use of ML for parameter estimation is to train an ML model to emulate a process-based model, leveraging the quick prediction times of ML models to explore parameter space more rapidly. For example, Gong *et al.* (2015) experimented with random forests and neural networks as surrogates for a computationally expensive land surface model. They then used the surrogates in a parameter optimization algorithm to find suitable values of soil porosity and other parameters.

As an alternative to emulating a process model, an ML model can also be used to directly predict the values of variables within the process model. For example, Sun (2018) trained a generative adversarial network to predict a map of groundwater hydraulic heads from a map of aquifer hydraulic conductivities or vice versa, where hydraulic heads are more often observed (albeit sparsely) and hydraulic conductivities have historically been solved by inversion of a process-based model, i.e., running that model repeatedly with different conductivities until the predicted hydraulic heads match observations (Figure 9). ML can also be used to develop transfer functions, i.e., functions that ingest widely measurable predictor variables and output parameter estimates. For mapping river basin characteristics (e.g., soil properties) to hydrologic model parameters (e.g., infiltration curve parameters), Feigl *et al.* (2020) used a text-generating autoencoder to discover the equation forms and coefficient values of transfer functions, and Tsai, Pan, *et al.* (2020) trained a recurrent neural network to itself act as a transfer function.

Lastly, although the approach is not yet common, ML training strategies and structures can be designed to encourage meaning in otherwise "black-box" states or parameters. For example, Jia *et al.* (2021) pretrained intermediate states of a neural network on the predictions of streamflow and water temperature from a process-based model, such that the final ML state predictions encoded estimates of these process-relevant state variables.

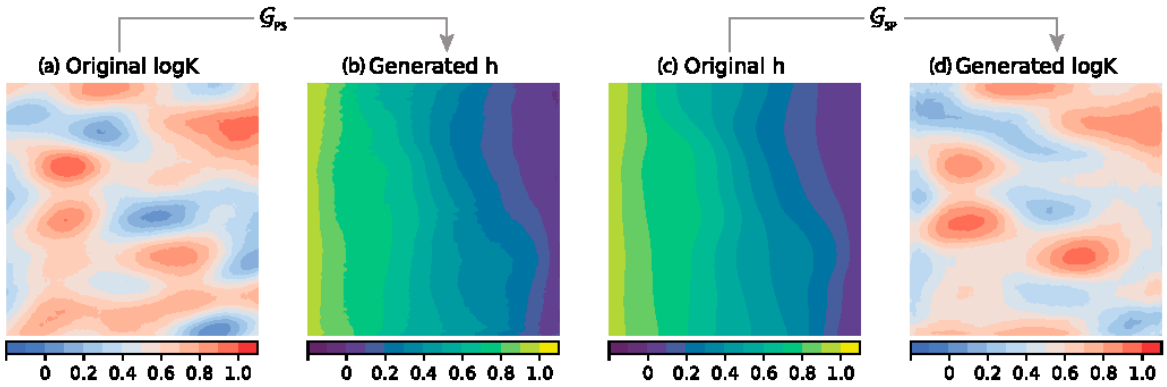

Figure 9. Example of a generative adversarial network used to predict model parameters and states. There are two competing models in this example: one to predict groundwater hydraulic head states (b) from a set of hydraulic conductivity parameters (a), and one to do the opposite (c and d). Modified from Sun (2018) Figure 2.

Predicting, forecasting, and projecting

ML models are capable of highly accurate predictions and thus have been applied extensively to prediction challenges for inland waters (Maier and Dandy, 2000; Maier *et al.*, 2010). Accurate predictions can fill knowledge gaps in space or time, facilitate scientific hypothesis generation, and support water resources decision-making. An example need for spatial gap filling is that lake water temperature models must usually be trained on a lake-by-lake basis using local observations but would ideally be leveraged for unobserved lakes. Willard *et al.* (2021) developed a gradient boosting regression model that uses lake features to select a trained lake model to use in predicting temperatures in a new, unobserved lake. For filling gaps in time,

Toth & Brath (2007) and Kratzert, Klotz, *et al.* (2019) have shown that NNs can predict streamflow with comparable or better accuracy than calibrated process-based models. ML models also excel at capturing nonlinear dynamics, which can be useful in identifying threshold responses; Hansen *et al.* (2017) fit random forest models of fish abundance and used the resulting nonlinear partial dependence plots to project how fish habitat would change under future climate scenarios (Figure 10).

In addition to their accuracy, trained ML models also offer relatively fast prediction runtimes, making them efficient choices for generating predictions over large spatial or temporal extents or in real time, for robust uncertainty estimation via large ensembles of predictions, or for decision support applications that explore many potential scenarios. For example, Nolan *et al.* (2012) used an ML model to emulate a process-based model of the unsaturated zone to predict nitrate losses from agricultural fields throughout a large region of the United States. Fienen *et al.* (2013) used a Bayesian network model to emulate a large-scale groundwater model for adaptive management on an island threatened by sea level rise. The faster emulator allowed for uncertainty estimation and scenario testing for predicting depth to water table, a metric related to plover foraging habitat and access to freshwater for wild horses.

One concern for prediction using ML models is that they are data hungry and may not generalize well to new inputs such as climate scenarios that have never existed in the past. Incorporation of limnological knowledge can improve prediction accuracy and help ML models earn trust. For example, Franceschini *et al.* (2019) used knowledge of fish species interactions to develop an NN model that more accurately predicted the occurrence probabilities of a target fish species by including two meaningful intermediate variables, the occurrence probabilities of two secondary fish species. Noori, Kalin and Isik (2020) passed outputs from a process-based water quality model into an ANN to achieve more accurate predictions of riverine nutrient loads in and around Atlanta, Georgia. Read *et al.* (2019) showed that lake temperature models pretrained with a process-based model, and incorporating physical laws in the loss function, significantly improved performance of an RNN even under sparse data conditions. Recent work has explored real-time data integration into ML models to overcome data sparsity and noise issues and improve near-term forecasts of water resources such as streamflow (Feng, Fang and Shen, 2020).

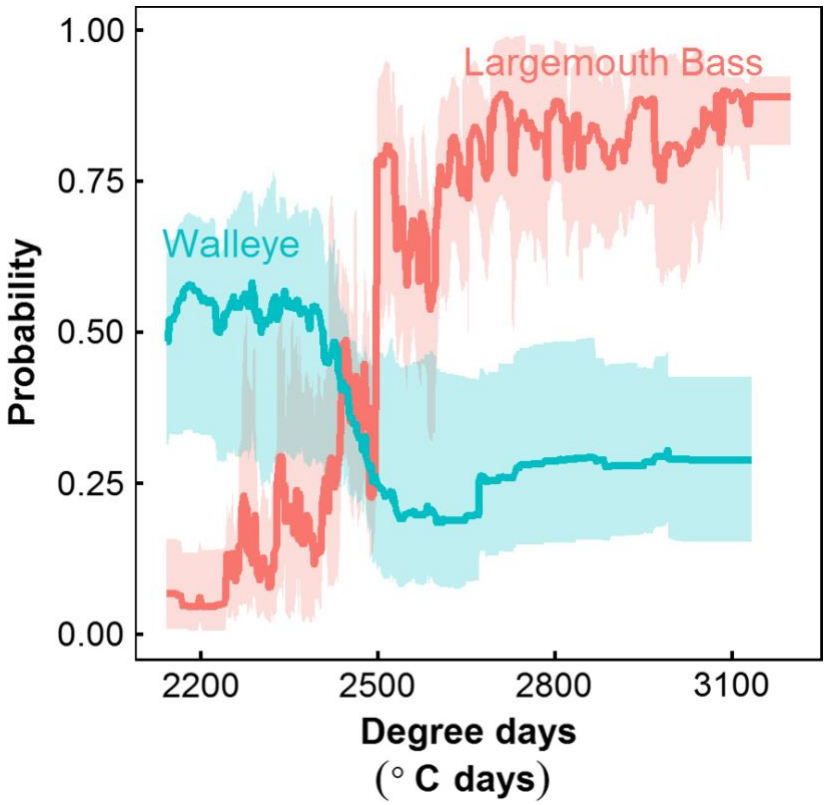

Figure 10. Random-forest-based partial dependence plot showing the nonlinear relationships between mean lake temperature degree days (horizontal axis) and the probability of walleye (Sander vitreus) recruitment or high largemouth bass (Micropterus salmoides) abundance (vertical axis). In this plot, solid lines are median responses and ribbons are 25th-75th percentile responses to the degree day value across all possible combinations of the other predictors (lake area, conductivity, and shoreline complexity for walleye; lake order and Secchi depth for largemouth bass). From Hansen et al. (2017) Figure 1.

Summarizing research results

In this age of sensors and powerful computers, it is common for observations and even model outputs to be too detailed for direct human interpretation. ML models can be used to impartially reduce a multidimensional result to two dimensions that can be visualized on a screen or printed page. Autoencoder neural networks are a potentially powerful tool for this application, as evidenced by their usefulness in distilling multivariate or timeseries data during preprocessing (see above), although we have yet to find examples of their use in interpreting water resources research results. Self-organizing maps have been used to summarize the multidimensional relationship between particle size and fluorescence properties in river water feeding to the largest freshwater lake in China (Yan *et al.*, 2018) and to compress aquatic insect (chironomid) community data to a two-dimensional map that enabled (1) further clustering into three general community types and (2) comparison with concentrations of chemical stressors (Milošević *et al.*, 2018).

We have long organized our understanding into categories such as biomes, aquifer types, aquatic trophic classes, and lake stratification regimes, but the use of discovery rather than design to identify such states has the potential to hasten the development of new intuitions about how to make sense of inland waters and their drivers. For example, Pacheco *et al.* (2017)

used a self-organizing map followed by U-matrix clustering to reduce continuous values in seven water quality dimensions down to six categorical clusters of water quality regimes observed along the Paraíba do Sul River in Brazil, which they then were able to tie to geographic location and local land use (Figure 11). Savoy *et al.* (2019) used dynamic time warping to quantify the similarity between pairs of time series of photosynthesis rates in 47 rivers and then used hierarchical agglomerative clustering to identify four common patterns in the annual onset, peak, and decline of photosynthesis. Labels such as "Spring Peak River" or even just "Cluster 6" enable conceptual discussions that would otherwise be mired in numbers.

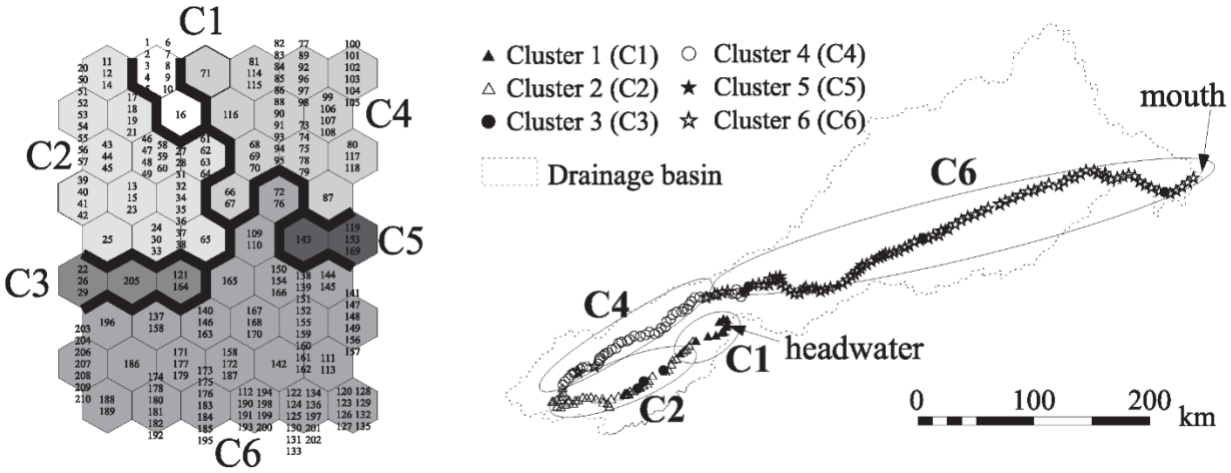

Figure 11. Example of using a self-organizing map (SOM) to reduce seven continuous water quality parameters to six categorical water quality regimes. Left: Codes in the SOM honeycomb correspond to sampling sites where the number 1 represents the river source, and 210 the river mouth. Right: Map of the catchment and main river channel show the six clusters of the 210 sampling sites. Modified from Pacheco et al. (2017) Figure 2a,c.

Conclusion

Water quantity and quality models are central to an increasing number of policy and regulatory decisions, and deliberate selection of the best available ML, process-based, or statistical modeling approaches will be critical to address environmental problems and advance scientific understanding. As described in this chapter, shortcomings of ML models exist but are often overstated and similar to limitations of other approaches. Recognition of ML's value is reflected in the growing proportion of inland waters publications that mention one or more of the tools described in this chapter, although that proportion is still small and indicates room for continued growth (Figure 12, left panel). Additionally, new research to inject limnological design into ML models is improving predictions and uncovering insights with fewer drawbacks, leading to the rapid recent growth in design-infused ML applications in inland waters and many other domains (Figure 12, right panels).

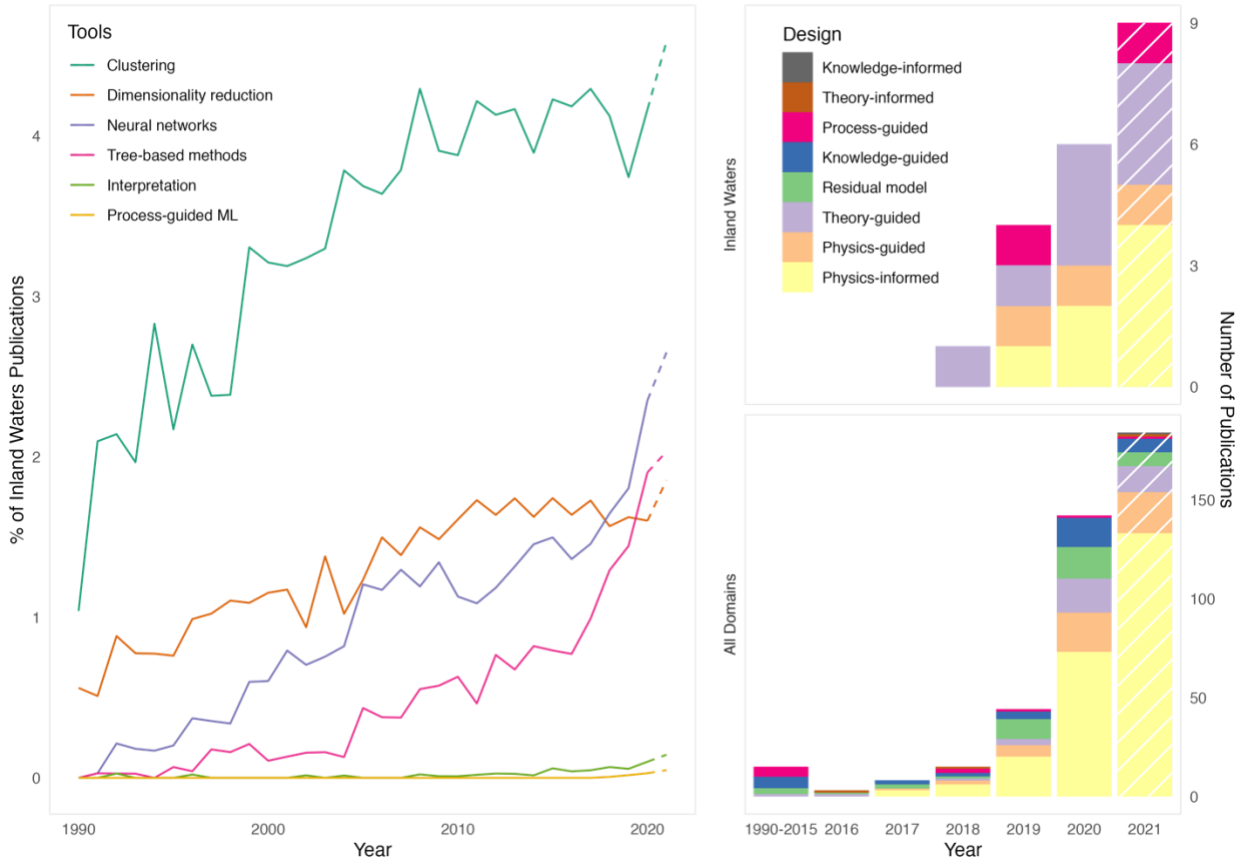

Figure 12. Publication counts from Web of Science queries for inland waters publications mentioning one of the major tools described in this chapter (left panel) and machine learning (ML) with knowledge-guided design (right panels) for inland waters (top) or all domains (bottom). All major ML tools described in this chapter have become more popular over time, with neural networks, tree-based methods, interpretation, and knowledge-guided machine learning showing the most rapid recent growth. 2021 counts (dotted lines and striped bars) were queried September 5, 2021; counts were multiplied by 365/248 to project the 2021 totals in the left panel and left unmodified in the right panels. Methods in the keys are ordered vertically in the same order as they appear in the figure panels. Exact search terms included many specific approaches within each Tools category (left panel) and required some mention of ML or neural networks along with the text in the Design legend (right panels). Researchers have not yet settled on a consistent term for designed machine learning, hence the diversity of terms in the right panels; "hybrid" yielded many query results but was excluded because it ambiguously describes several methodological and biological concepts. Data from Web of Science, provided by Clarivate. © Copyright Clarivate 2021. All rights reserved.

The undeniable benefits of ML are creating opportunities for innovation in new dimensions of the aquatic sciences, including assembly and publication of datasets for benchmarking and training, versioned release of model codes for extension and reuse, and model development via interdisciplinary collaborations with computer scientists and technologists. There are also opportunities at the institutional level, where research incentives and resources could be better aligned with the pursuit of machine learning applications and innovation. Given the complementary nature of process-based, statistical, and machine learning modeling, the aquatic sciences are sure to gain by embracing ML models as one set of valuable tools for prediction, inference, and distillation.

Knowledge gaps

- Additional core aquatic datasets and baseline performance metrics would support development and comparison of different model architectures, including process-based, statistical, and ML.
- The limnology community would benefit from a general understanding of the conditions under which ML models and process-based models are reliable for extrapolation.
- Establishing common patterns or practices for extracting interpretive insights from ML models would improve model trust and contribute to greater understanding of inland waters.
- Methods to integrate different data types (e.g., single-point data, continuous data, multi-dimensional data, and remotely sensed data) into ML models could improve accuracy and utility.
- Infusion of process knowledge into ML models is a concept in its research infancy, with much left to discover about techniques, potential and limitations, and best practices.
- The limnology community would benefit from a taxonomy by which researchers can communicate the mechanisms and extent to which approaches integrate limnological theory into ML models.
- In contrast to physical processes, biogeochemical and ecological processes can seldom be described with exact equations, such that new techniques may be needed to integrate empirical knowledge about those processes into ML models.

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