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THE ROLE OF BIG DATA AND MACHINE LEARNING IN HYDROLOGICAL PROCESSES

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Can machine learning accelerate process understanding and decision-relevant predictions of river water quality?

Charuleka Varadharajan[1] | Alison P. Appling[2] | Bhavna Arora[1] | Danielle S. Christianson[3] | Valerie C. Hendrix[3] | Vipin Kumar[4] | Aranildo R. Lima[5] | Juliane Müller[3] | Samantha Oliver[2] | Mohammed Ombadi[1] | Talita Perciano[3] | Jeffrey M Sadler[2] | Helen Weierbach[1] | Jared D. Willard[4] | Zexuan Xu[1] | Jacob Zwart[2]

[1]Earth and Environmental Sciences Area, Lawrence Berkeley National Laboratory, Berkeley, California, 94010, USA

[2]U.S. Geological Survey, Water Mission Area, Reston, Virginia, USA

[3]Computing Sciences Area, Lawrence Berkeley National Laboratory, Berkeley, California, 94720, USA

[4]Department of Computer Science and Engineering, University of Minnesota, Minneapolis, Minnesota, USA

[5]Aquatic Informatics, Vancouver, BC, V6E 4M3, Canada

Correspondence
Charuleka Varadharajan, 1 Cyclotron Road, Berkeley, CA-94720, USA.
Email: cvaradharajan@lbl.gov

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Abstract

The global decline of water quality in rivers and streams has resulted in a pressing need to design new watershed management strategies. Water quality can be affected by multiple stressors including population growth, land use change, global warming, and extreme events, with repercussions on human and ecosystem health. A scientific understanding of factors affecting riverine water quality and predictions at local to regional scales, and at sub-daily to decadal timescales are needed for optimal management of watersheds and river basins. Here, we discuss how machine learning (ML) can enable development of more accurate, computationally tractable, and scalable models for analysis and predictions of river water quality. We review relevant state-of-the art applications of ML for water quality models and discuss opportunities to improve the use of ML with emerging computational and mathematical methods for model selection, hyperparameter optimization, incorporating process knowledge into ML models, improving explainablity, uncertainty quantification, and model-data integration. We then present considerations for using ML to address water quality problems given their scale and complexity, available data and computational resources, and stakeholder needs. When combined with decades of process understanding, interdisciplinary advances in knowledge-guided ML, information theory, data integration, and analytics can help address fundamental science questions and enable decision-relevant predictions of riverine water quality.

KEYWORDS
analysis, machine learning, models, predictions, rivers, streams, water quality

1 | INTRODUCTION

Water quality refers to physical, chemical, and biological characteristics of water bodies. Water quality is an important aspect of our ability to use rivers and streams for drinking water, healthy aquatic ecosystems, farmland irrigation, and other beneficial purposes. River water quality has been declining globally over the past century due to population growth and increasing urbanization, industrialization, and

agriculture (Abbott et al., 2019). These stressors have led to salinization and alkalinization of rivers (Kaushal et al., 2013, 2021), nutrient runoff causing algal blooms and eutrophication (Hartmann et al., 2014; McDowell et al., 2020), and river contamination from persistent organic compounds, pesticides, and toxic metals (Schwarzenbach et al., 2010). Climate change and extreme events such as floods, droughts, and wildfires are projected to exacerbate problems of water quality by decreasing flows, changing biogeochemical cycles, and increasing contaminant concentrations (Lyubimova et al., 2016; Murdoch et al., 2000; Nilsson & Renofalt, 2008; Whitehead et al., 2009). The deterioration of river water quality has direct consequences for aquatic and human health. The costs of watershed management to comply with water quality regulatory criteria are significant, even when the benefits are uncertain (Keiser et al., 2019). Thus, water resource managers rely on monitoring and simulations of hydrological processes to make optimal decisions, and are helped by models that account for complex biogeochemical processes and their climactic, hydrological and human drivers.

Different classes of water quality models can be used for predictions depending on the relevant water quality variables, spatial scales (e.g., reach, watershed, regional), and complexity (Rode et al., 2010), some of which are described in recent reviews (Burigato Costa et al., 2019; Fu et al., 2020). High-fidelity mechanistic models can incorporate the tight coupling of physical and biogeochemical processes such as climatic variations, hydrologic fluxes, weathering, and biological interactions on solute transport and mixing at pore to subcatchment scales. For example, integrated surface-subsurface hydrologic models (e.g., Amanzi/ATS) coupled with reactive transport models (RTMs) can attain spatially explicit representations of critical zone components, and provide accurate estimates of geochemical exports to rivers at reach to hillslope scales (Arora, Spycher, et al., 2016; Dwivedi et al., 2018; Steefel et al., 2015; Xu et al., 2021). Despite the demonstrated success of these models, they face important challenges at larger spatial domains in part due to the computational expense from having highly resolved spatial grids and complex biogeochemical processes needed to represent heterogeneous watershed characteristics influencing water quality (Steefel, 2019). Capabilities for upscaling current RTMs and representation of geochemistry in larger scales are in their early stages of development (Arora et al., 2015; Jan et al., 2021; Li et al., 2021).

At watershed- to basin-scales, models such as the semi-empirical soil and water assessment tool (SWAT; Arnold et al., 1998) and hydrologic simulation program Fortran (e.g., HSPF; Bicknell et al., 1996) have been widely used for surface water quality modelling (Fu et al., 2019). The models contain elements called hydrologic response units (HRUs) that are non-continuous areas within a sub-basin grouped by similar properties such as land use, soil, or topography based on user-defined thresholds (Chen, Xu, et al., 2019; Her et al., 2015). This discretization approach makes the models computationally efficient but introduces limitations such as the lack of hydrologic connectivity between the HRUs and sensitivity of the models to the HRU definitions, although some of these limitations are addressed in newer versions of the code (e.g., SWAT+; Bieger et al., 2017; Her et al., 2015; Paul et al., 2019). The models also require watershed-specific calibration and validation, and the parameters can have substantial uncertainties due to equifinal solutions (Van Liew et al., 2003; White & Chaubey, 2007; Xie & Lian, 2013).

Most regional- to continental- scale process-based models that do capture geochemistry (e.g., WITCH; Roelandt et al., 2010) are zero-dimensional box-models, which are not adequate for representing complex flow and chemical transport dynamics (Li et al., 2017). Process-based models have been used to predict physical variables such as stream temperature (e.g., MOSART-heat, PRMS-SNTemp, VIC-RBM; Li et al., 2015; Sanders et al., 2017; van Vliet et al., 2012) at these spatial scales by incorporating thermodynamics and energy balance into terrestrial hydrology models. Alternatively, statistical models are also used for regional- to continental-scale predictions of water quality, although these have other significant limitations. For example, the SPARROW model (Schwarz et al., 2006) has been widely used for spatial water quality predictions at regional scales in the United States (U.S.) but assumes long-term steady-state behaviour, and efforts to incorporate temporal dynamics are nascent (Chanat & Yang, 2018). Multi-linear regression and auto-regressive integrated moving averages (ARIMA) are commonly used methods for temporal predictions of water quality variables but have limited applicability in complex systems with non-linear and non-stationary processes (Chen et al., 2020).

Apart from predictions, numerous studies have used statistical regression to analyse water quality trends and attribute drivers at local to continental scales (e.g., Guo et al., 2019; Kaushal et al., 2018; Monteith et al., 2007; Murphy, 2020; Murphy & Sprague, 2019). Generalized additive models that extend linear models are another statistical approach used to determine water quality trends (e.g., Morton & Henderson, 2008; Yang & Moyer, 2020) and can be adapted to large datasets (Wood et al., 2015). Another common statistical technique is correlation analysis between riverine chemical concentrations and discharge (typically referred to as C-Q relationships), which has been used for a variety of purposes such as examining constituent dynamics at short and long time-scales (e.g., Arora et al., 2020; Evans & Davies, 1998; Godsey et al., 2009; Moatar et al., 2017; Musolff et al., 2021), identifying sources and pathways of different solutes (see Musolff et al., 2021 and references therein), and analysing water quality monitoring data for watershed management (Bieroza et al., 2018; Pohle et al., 2021; Westphal et al., 2020). However, complex C-Q patterns, such as those resulting from variable lags between the hydrograph and chemograph, are difficult to interpret and attempts to link insights gained from C-Q analysis to models have been limited (Liu, Birgand, et al., 2021). Other statistical approaches such as Bayesian hierarchical models (Guo et al., 2019; Rode et al., 2010), wavelets (Arora, Dwivedi, et al., 2016; Parmar & Bhardwaj, 2013), and principal component analysis and non-negative matrix factorization (Liu, Zhang, et al., 2021; Shaughnessy et al., 2021) are used to identify key catchment attributes, sources, and ecosystem control points (Bernhardt et al., 2017) that influence stream water chemistry.

Despite the variety of statistical and modelling approaches available, it is still challenging to make accurate and timely water quality predictions, particularly at large spatial scales, due to the variability of

water quality with space, time, and disturbance (natural or human), and the effect of local characteristics and complex processes on solute transport. There is consensus that water quality modelling has plateaued, with recent studies focusing on incremental improvements to existing models and case study demonstrations for individual basins rather than transformational advances that address the challenges involved (Fu et al., 2020). The field is fragmented, with the choice of model varying substantially depending on the spatial scale and parameters being modelled, as well as access to computation and modelling expertise (Fu et al., 2020), limiting our ability to make decision-relevant predictions.

Recent advances in machine learning (ML) and artificial intelligence (AI) spurred by the increasing availability of public datasets, development of software frameworks, and cloud computing resources have the potential to stimulate a new class of water quality models that can be run at decision-relevant scales, resolutions, and lead times. Artificial intelligence encompasses technologies that can understand inputs from the environment, reason and take actions to meet a performance objective, while ML (the focus of this paper) is a subset of AI that focuses on learning patterns from complex data (Russell & Norvig, 2020). Thus ML is useful for problems that require predictions, deriving insights from data, and decision making (Jordan & Mitchell, 2015). ML applications for geosciences broadly span modelling, automation tasks and data-driven discovery, and include approaches such as classification, spatial or temporal regression, and anomaly detection (Bergen et al., 2019; Reichstein et al., 2019). ML methods include supervised learning, wherein known observations are used to train a model to learn patterns or make predictions on a target variable; unsupervised learning, wherein the algorithm learns patterns or structures in the data heuristically without apriori knowledge of the target; and reinforcement learning, wherein the model learns to make decisions under uncertainty through trial and error interactions with its environment to maximize a reward (see Shen, 2018; Bergen et al., 2019; Xu & Liang, 2021 and references therein for an overview of ML in hydrology and geosciences). Traditional ML methods (also referred to as classical or conventional ML) include support vector machines (SVM), decision trees such as random forests (RF) and gradient boosted trees, and simple artificial neural networks (ANN; e.g., feed forward ANN, extreme learning machines, multi-layer perceptron). Deep learning (DL) models are neural networks (NN) with multiple processing layers that make it possible to learn complex patterns from large datasets and have high predictive skill. Common DL architectures include the convolutional neural network (CNN), recurrent neural networks (RNN) of which the long short term memory (LSTM) network is a popular choice, deep belief networks (DBN) that are composed of restricted Boltzmann machines (RBM), and sparse autoencoders (LeCun et al., 2015; Shen, 2018; Shrestha & Mahmood, 2019). In this paper, we use the term "machine learning" to refer to both traditional ML and DL models.

Over the past decade, there has been a large increase in the use of ML for hydrological predictions (Xu & Liang, 2021) to the point where its adoption in future physical hydrology models seems inevitable (Nearing, Kratzert, et al., 2021). A wide variety of ML approaches have been explored for water quality modelling in rivers across the world, and collectively indicate their potential to extract scientific knowledge and enable optimal management of water quality (Section 2). Yet the rapidly increasing use of ML raises several questions. First, given the diversity of modelling approaches, what are the situations where ML can add value and what are its limitations? What are the primary considerations for model and feature selection? How do we compare performance and evaluate whether models have been constructed and parameterized appropriately? How can ML approaches complement process-based models to improve our prediction capabilities? And most importantly, how can we trust and use models that make predictions based on machine-derived information that is beyond human comprehension?

In this paper, we discuss the potential for using ML in water quality modelling for decision-relevant predictions. We first provide a brief review of ML methods used for several water quality applications that demonstrate its value for modelling and knowledge discovery (Section 2). We then present opportunities for advancement of ML model architectures, transferability, and interpretability, which includes the integration of process knowledge into model design (Section 3). We finally present considerations for the choice of model based on the scale and complexity of the problem being addressed, and availability of data and computational power (Section 4). We posit that the time is ripe for *judiciously* incorporating ML into riverine water quality models for the purposes of improving predictive capabilities and deciphering the complex, diverse human-natural processes that affect water quality. Throughout, we use the term "models" to refer to codes that both generate predictions and analyse data to extract information.

2 | STATE-OF-THE-ART MACHINE LEARNING IN RIVER WATER QUALITY MODELS

Machine learning models have been used for predictions of many water quality variables using various approaches from simple models to hybrid methods combining ML with process-based models (Table 1). Stream temperature is a widely measured physical water quality variable and has been successfully predicted using different ML methods. For example, classical ML methods have been used for monthly to daily predictions of stream temperatures in catchments with different characteristics, and include support vector regression (SVR; Rehana, 2019; Weierbach et al., 2022); decision tree-based regression models such as RF, XGBoost, and their variations (Feigl et al., 2021; Lu & Ma, 2020; Weierbach et al., 2022); and simple ANNs (Feigl et al., 2021; Zhu & Piotrowski, 2020). Among DL models, the LSTM deep neural network has become an increasingly popular choice for regional-scale hydrological predictions due to its ability to encode prior system states in the cell memory (e.g., Kratzert et al., 2018). For example, Rahmani, Lawson, et al. (2021) originally used an LSTM network to predict daily stream temperatures for 118 pristine catchments in the continental U.S. and in a subsequent study extended the LSTM approach to make predictions in data-sparse, unmonitored and dammed catchments (Rahmani, Shen, et al., 2021). Approaches that

TABLE 1 Examples of water quality applications where machine learning has been applied

Application	Stream water quality variables	Classical ML (single or ensemble)	Deep learning	Hybrid process + ML	Unsupervised learning
Time-series predictions	Temperature, DO, conductivity, nutrients, pH, turbidity, cations, anions, dissolved organic matter, BOD, COD, chlorophyll-a	SVR; decision trees, ANN, GP, fuzzy logic, ensembles (Chen et al., 2020; Feigl et al., 2021; Khullar & Singh, 2020; Rajaee et al., 2020; Rehana, 2019; Weierbach et al., 2022; Zhu & Piotrowski, 2020)	LSTM (Rahmani, Lawson, et al., 2021; Zhi et al., 2021); LSTM+CNN (Baek et al., 2020), DBN (Solanki et al., 2015; Yan et al., 2020)	LSTM and graph RNN combined with stream temperature process model (Jia, Zwart, et al., 2021); ANN + salinity process model (Hunter et al., 2018)	
Predictions in ungaged basins	Temperature	XGBoost, SVR (Weierbach et al., 2022)	LSTM (Rahmani, Shen, et al., 2021)		
Short-term predictions, surrogates for monitoring and detection	Temperature, DO, pH, conductivity, turbidity, nutrients, water quality indices	SVM, RF, ANN, ensembles (Bui et al., 2020; Green et al., 2021; Harrison et al., 2021; Lu & Ma, 2020; Paepae et al., 2021)	LSTM (Liu et al., 2019)		Dynamic time warping clustering (Lee et al., 2020)
Event dynamics and classification	Suspended sediments	Restricted Boltzman machines, Bayesian belief networks (Hamshaw et al., 2018, 2019; Murray et al., 2012)	CNN (Hamshaw et al., 2019)		Multivariate event time series clustering (Javed et al., 2021)
Process understanding and knowledge discovery	Temperature, pH, TDS, conductivity cations, anions, nutrients, *Escherichia coli*	Decision trees, NN (Álvarez-Cabria et al., 2016; Mirzaei et al., 2020; Povak et al., 2014; Wang et al., 2021)			
Remote sensing estimates	Suspended and other sediments, turbidity, DO, metals, nutrients, chlorophyll-a, organic matter, blue-green algae	ANN, SVM, GP, decision trees (Topp et al., 2020)	Progressively deep NN (Peterson et al., 2020)		
Decision support and management scenarios	Conductivity, pH, DO, nutrients, suspended sediments, anions, chlorophyll	Bayesian networks/ probabilistic graph models (Forio et al., 2015; Mount & Stott, 2008; Phan et al., 2019)			

Note: See references for further details on techniques used for specific water quality variables.

combine process-based models with DL have also been used for basin-scale stream temperature predictions, particularly in regions with sparse data (e.g., Jia, Zwart et al., 2021, Section 3.2). In all cases, the ML approaches were able to improve prediction accuracies compared to base statistical and process-based models.

ML models have also been used for predictions of other water quality variables and indices such as dissolved oxygen (DO), electrical conductivity, total dissolved solids (TDS), pH, nutrients, suspended sediments and turbidity, cations, anions, biological oxygen demand (BOD), chemical oxygen demand (COD), and chlorophyll. Recent

reviews identify popular classical ML methods for time-series predictions including ANN, decision trees, SVM, genetic programming (GP), fuzzy logic, and hybrid approaches such as genetic algorithm-NN, adaptive neuro-fuzzy inference systems, and wavelet-NN (Chen et al., 2020; Khullar & Singh, 2020; Rajaee et al., 2020). Hybrid models with ensembles of standalone ML models using methods such as bagging and random subspace (Melesse et al., 2020) or combining ML with process-based models (Hunter et al., 2018) have been used to predict salinity at river basin- to reach-scales in Iran and Australia. Examples of recent efforts to incorporate DL approaches for these predictions include the use of an LSTM to predict DO concentrations in 506 pristine U.S. catchments achieving moderate accuracy (Zhi et al., 2021), and an LSTM paired with a CNN (that generated streamflow estimates) to predict total nitrogen, phosphorus, and organic carbon in a major Korean river basin (Baek et al., 2020). LSTM, RF, and hybrid ML models have also been used for short-term predictions of a suite of water quality variables (e.g., DO, pH, conductivity, turbidity, nutrients, water quality indices) with high-frequency monitoring; in some cases classical ML surrogate models are used as soft sensors to make predictions of variables that are difficult or laborious to measure directly such as those that require laboratory sample analysis (Bui et al., 2020; Green et al., 2021; Harrison et al., 2021; Liu et al., 2019; Lu & Ma, 2020; Paepae et al., 2021).

In addition to predictions, ML approaches are used to discover understanding about the dynamics of water quality and underlying sources, drivers, and mechanisms. A common use of ML is to detect events of interest from high-frequency data obtained from sensor networks. For example, insights into episodic sediment dynamics from hundreds of storm events were derived using RBMs and CNNs to automate analysis of C-Q plots (Hamshaw et al., 2018, 2019). Classification and clustering pattern recognition techniques have been used to identify similarities between monitoring stations (Lee et al., 2020), hydrological events (Javed et al., 2021), and contaminant sources (Vesselinov et al., 2018). Classical ML methods such as decision tress, NN, and self-organizing maps have been used to identify landscape attributes and human factors that affect stream water quality (Álvarez-Cabria et al., 2016; Mirzaei et al., 2020; Wang et al., 2021), and characterize relevant processes such as cation weathering rates (Povak et al., 2014).

Another application area is the use of ML for analysis and estimation of inland water quality parameters obtained from remote sensing imagery. The estimates are most commonly derived using classical ML approaches, but are limited to larger rivers and a few variables due to the spatial resolution of land surface sensors (~10–30 m), and broad spectral bands (Hassan & Woo, 2021; Hestir et al., 2015; Topp et al., 2020). Peterson et al. (2020) demonstrated that a progressively deep NN model outperformed SVR, extreme learning machine, and multi-linear regression in estimating water quality parameters such as blue-green algae, chlorophyll-a, fluorescent dissolved organic matter (FDOM), DO, conductance, and turbidity in the Upper Mississippi River using data from Landsat-8 and Sentinel-2. A harmful algal bloom (HAB) detection system HABNet (Hill et al., 2020) for coastal waters used a CNN combined with an LSTM, SVM, or RF applied on data from moderate resolution imaging spectroradiometer (MODIS) data. Remote sensing datasets relevant to river water quality are likely to grow in the future with newer high-resolution satellites, instruments with hyperspectral bands, and increasing use of unmanned autonomous vehicles (UAV) to acquire water quality data (Sibanda et al., 2021; Topp et al., 2020), and can potentially address data gaps for water quality ML (Section 4.4).

Finally, probabilistic graph models such as Bayesian networks have been used extensively for decision support in water management (Phan et al., 2019). Bayesian networks can integrate both quantitative data (e.g., time-series of measured concentrations and discharge), and qualitative data (e.g., expert knowledge and stakeholder beliefs), and can generate probabilistic predictions for different management and climate scenarios. For example, Bayesian networks were used to design rules for trading transferable pollutant discharge permits in rivers (Mesbah et al., 2009), for real-time monitoring and contaminant warning systems (Murray et al., 2012), and to predict water quality in different types of catchments (Forio et al., 2015; Mount & Stott, 2008).

These examples illustrate the value of using ML for a variety of global river water quality modelling and monitoring applications. The use of DL and hybrid models combining ML and process-based codes is still nascent and is expected to grow in the near future. In the next two sections, we describe how the appropriate use of ML for different water quality applications can best incorporate recent computational and mathematical developments due to the large number of variables of interest, heterogeneity of human and natural processes that influence water quality, and scarcity of available data.

3 | OPPORTUNITIES FOR ADVANCEMENT OF WATER QUALITY ML

ML methods have advanced rapidly over the past decade, and diverse approaches can be used to improve model performance, efficiency, and robustness. Here we highlight particularly promising techniques, many of which have been used in hydrological applications, to address questions raised in Section 1 related to the use of ML for water quality modelling (also see Varadharajan et al., 2021).

3.1 | How do we select and design optimal model architectures?

ML model selection and architectures (e.g., number of layers, batch size, nodes for neural networks) can affect model performance and computational costs. The choice of the best performing model (ML, statistical, or process-based) will depend on the metrics considered including model accuracy, variance, robustness, bias, and computational speed (Belitz & Stackelberg, 2021; Kratzert, Klotz, Shalev, et al., 2019). A common approach for model selection in many of the studies cited above (Section 2) is to train different model types, and choose the model with the greatest predictive skill. Another approach

to model selection is to *not* choose, i.e., to create model ensembles that exploit the diversity of predictive skill from different models. Model ensemble approaches are common in hydrology (Fleming et al., 2021). Specifically, ML ensembles have shown promise in improving predictions (e.g., flood forecasting), quantifying uncertainty (Fleming et al., 2015; Jiang et al., 2014; Zounemat-Kermani et al., 2021), and are now being incorporated into operational models (Fleming et al., 2015, 2021). Ensembles can be formulated in many ways, from traditional methods such as bagging, boosting, dagging, model averaging, and stacking to more sophisticated combinations such as running simulations on different classes of models or pre-training ML models on different process models (e.g., Section 4.2). Ensemble combinations of multiple models can be even more beneficial when the errors of individuals models are not correlated (Hsieh, 2009).

Besides model selection, other important choices in the application of ML are selection of optimal input features, model training, and architecture design. In regression and classification, a best practice is to use k-fold cross-validation that partitions available data into k-sets and iteratively trains the model using data from each set for testing, which leads to better model generalizability (Bergmeir & Benítez, 2012). Common pitfalls in model design are including excess irrelevant or redundant variables as inputs, variable selection bias (i.e., using the same data for training and inputs), resubstitution validation (i.e., testing the model with training data), use of inconsistent cross-validation and resampling procedures across model architectures being implemented, and data leakage (e.g., using testing data for model training or hyperparameter optimization, or pre-processing the entire dataset prior to splitting the data into cross-validation folds), which can lead to overfitting (Gharib & Davies, 2021; Zhang, 2007). These pitfalls can be avoided by understanding the details and limitations of the models being implemented, following best practices, and using robust ML workflows (Gharib & Davies, 2021; Zhang, 2007).

Different hyperparameter optimization (HPO) methods have been developed to find the best-performing ML model architectures (Yu & Zhu, 2020). In many applications such as those cited above, the hyperparameters are either not chosen (i.e., default hyperparameters selected), hand-tuned (trial and error of different architectures), or selected using a grid or random search approach (Bergstra et al., 2011). In a few models (e.g., RF), default hyperparameters can work well (Probst et al., 2019); however, in general HPO is expected to improve model performance. Although random search has been shown to outperform grid search (Bergstra & Bengio, 2012), both approaches require a time-consuming approach of training each architecture, which can be computationally expensive, result in inferior performance, and limit the number of architectures that can realistically be explored. Instead, efficient solution methods using Bayesian optimization methods such as the Tree-of-Parzen-Estimators in the Python package Hyperopt can be applied (Bergstra et al., 2013). Müller et al. (2020) demonstrate another derivative-free Bayesian optimization method using surrogate models, such as Gaussian process or radial basis functions, to map the architecture search space to its performance and allows efficient exploration of the space by adaptive sampling approaches. Near-optimal hyperparameters for different NN including DL architectures can be found with relatively few evaluations using this approach (e.g., Figure 1).

Automated machine learning (AutoML) frameworks that use concepts of ensembles and automatic HPO are emerging as a promising approach for reducing the barrier to adoption of ML, and have shown improvements in the efficiency and robustness of ML algorithms (Feurer et al., 2015; Hutter et al., 2019). A forward-looking automated ML approach for model design is "neural architecture search" (Ren et al., 2021) where algorithms automatically design model architecture. This approach has been successfully applied to algal classification using CNNs (Park et al., 2019) and spatiotemporal predictions (Li et al., 2020), and is even being considered for physics-based learning models (Ba et al., 2019).

3.2 | How do we incorporate scientific knowledge into ML models?

Traditional ML models can produce physically inconsistent results (Karpatne et al., 2017; Kashinath et al., 2021) as they only look for statistical relationships in the training data and are unable to extrapolate outside of the training dataset used for building the ML model. The sparseness of water quality and related environmental datasets, and projected changes in climate and land use make it challenging to use ML models per se for predictions in unmonitored regions or for long-term projections because they can only be trained, validated, and evaluated on past data (Duan et al., 2020; Kratzert, Klotz, Brandstetter, et al., 2019; Xu & Liang, 2021).

The scientific community has been converging on the use of knowledge-guided ML (KGML; see Figure 2 as an example) to make physically consistent and generalizable predictions (including out-of-bounds estimates) and decrease training times (Kashinath et al., 2021). KGML approaches have been used to incorporate scientific knowledge into ML model training and predictions in several ways (Willard et al., 2022) that include (i) modification of loss functions to penalize the model when violating known physical laws and relationships (Jia et al., 2019; Karpatne et al., 2018), (ii) training or pre-training ML models on process-based model output (Konapala et al., 2020; Read et al., 2017), (iii) incorporating differential equations in ML models (Chen, Rubanova, et al., 2019; He et al., 2020; Rackauckas et al., 2020), (iv) multi-task learning for multi-objective optimization (Sadler et al., 2022), (v) modifying ML model architecture to impose symmetry or better represent the system being modelled (Daw et al., 2020; Khandelwal et al., 2020; Kunin et al., 2021; Ling et al., 2016), and (vi) most commonly surrogate (or reduced-order) models that emulate process model behaviour with considerably less computational expense (Xu & Liang, 2021). Hybrid KGML methods have also been used for hypothesis generation and establishing causal relationships between system drivers and responses (Tsai et al., 2020).

Numerous combinations of LSTM models and their variants with different process models have been shown to improve predictive

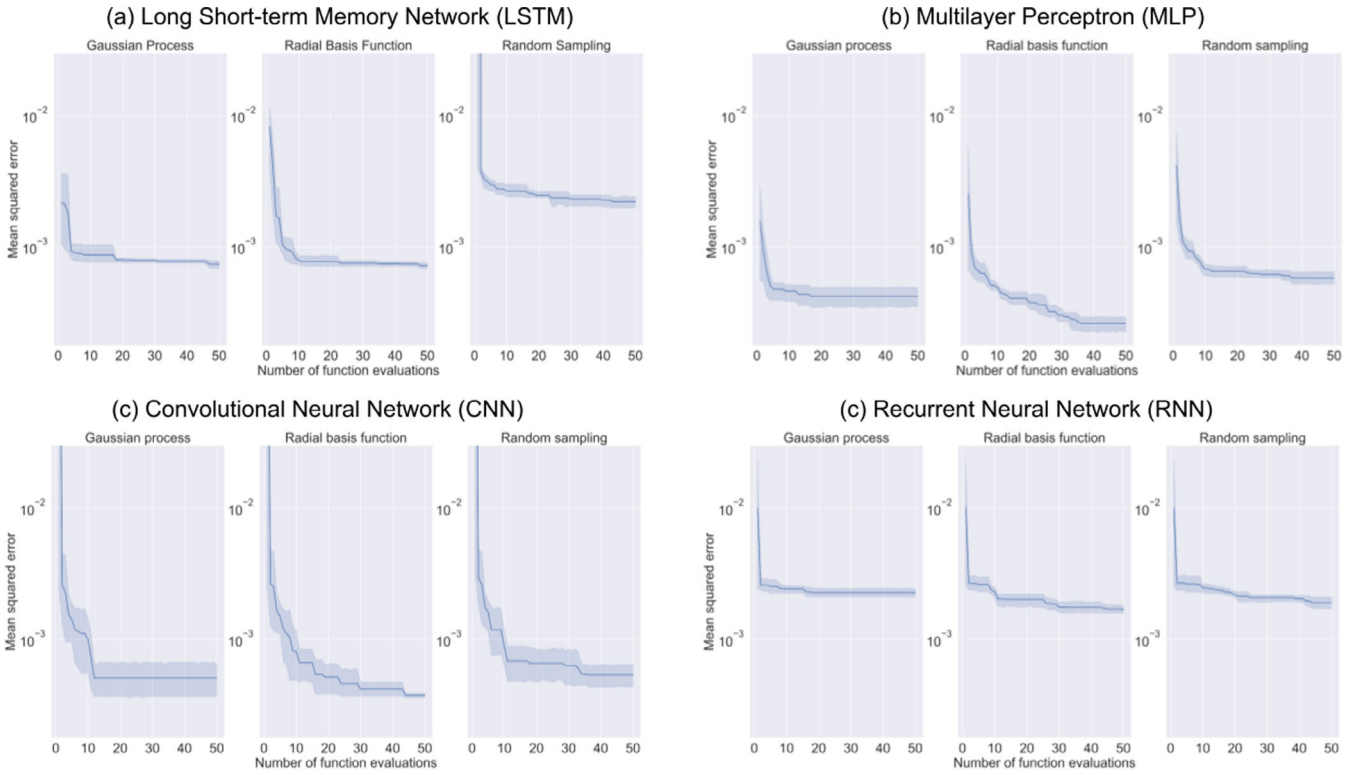

FIGURE 1 Bayesian optimization approaches using surrogate models such as Gaussian process and radial basis functions enable faster convergence to the optimal set of hyperparameters for deep learning models used to predict groundwater levels (figure modified from Müller et al., 2020)

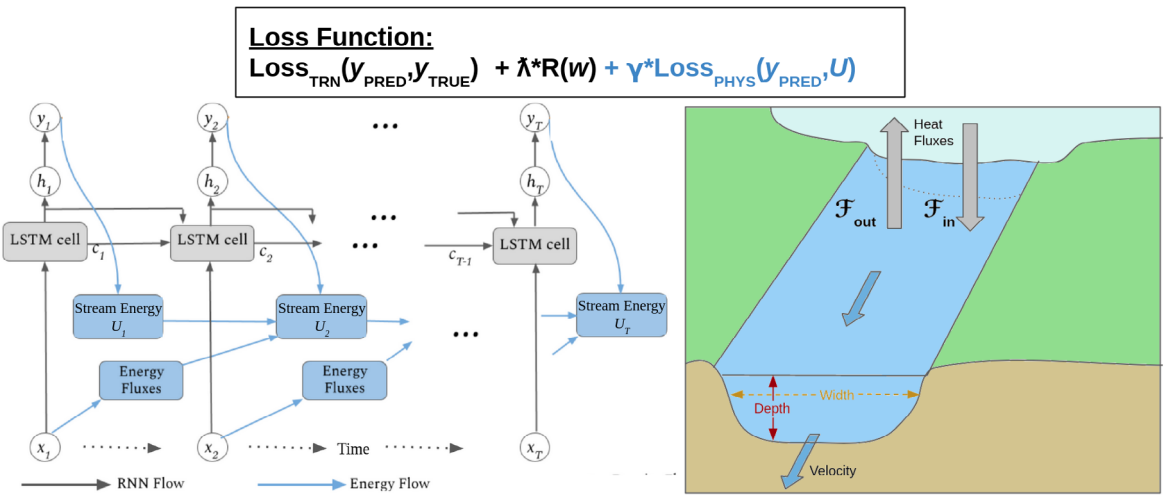

FIGURE 2 Overview of knowledge-guided machine learning (ML) approaches incorporating physical constraints into the loss function of a long-short term memory (LSTM) network used to model stream temperatures. The loss function penalizes the ML model for errors in predicting stream temperature (yPRED = model-predicted stream temperature; yTRUE = observed stream temperature) and stream thermal energy (*U*), the latter of which cannot be created or destroyed from one time step to the next according to thermodynamics. Energy fluxes can be transformed or transported into (fin) or out of (Fout) the stream system according to equations in the process-based model. *R*(*W*) represents a standard complexity regularization on the model parameters weighted by λ, and Loss_{PHY} aims to ensure consistency with physics by balancing the energy fluxes and is weighted by γ. Figure modified from Willard et al. (2022) and https://www.usgs.gov/media/images/diagram-channel-cross-section-subsections

performance for streamflow and river and lake water quality including out-of-bounds predictions in comparison to base process or LSTM models (Frame et al., 2021; Hanson et al., 2020; Jia, Zwart, et al., 2021; Konapala et al., 2020; Read et al., 2017). For example, Jia et al. (2021) used a modified graph-based LSTM that included representations of the river network hydrography, pre-trained with output

from a process-based model PRMS-SNTemp (Sanders et al., 2017) to predict daily stream temperatures across the Delaware River Basin. This study demonstrated that the hybrid model was able to outperform base LSTM models in terms of prediction accuracies and the ability to extrapolate when data were sparse (Figure 3).

Other KGML approaches include variations of GP, a supervised ML technique that mimics biological evolution. The advantages of GP include its ability to produce explicit mathematical relationships between input and output variables, add constraints based on physical realistic possibilities, and generate interpretable results. Genetic programming has been used extensively in hydrology to build interpretable rainfall-runoff, groundwater, and water quality models; estimate evapotranspiration; and extract information about reservoir operations (Danandeh Mehr et al., 2018; Fallah-Mehdipour & Haddad, 2015; Herath et al., 2021). KGML versions of GP models include a tree-adjoining grammer (TAG) formalism for representing dynamic processes that has been demonstrated for predictions of phytoplankton biomass in rivers (Park et al., 2021).

3.3 | How can ML be used to make generalizable predictions with sparse data?

Water quality data tend to be sparse (Section 4.4), and there is a need to transfer models from data-rich, small-scale monitored sites to other regions in a manner that accounts for the spatial heterogeneity of watershed characteristics. Recent studies have demonstrated the use of LSTM and ensemble XGBoost models for predictions of streamflow and stream temperature in unmonitored basins (Kratzert, Klotz, Herrnegger, et al., 2019; Rahmani, Shen, et al., 2021). Another ML approach to generalize models is Transfer Learning (Weiss et al., 2016), which translates models built on highly observed locations to other sites that are data-sparse or unmonitored, although the challenge lies in choosing which models to transfer to a given site. Recently, meta transfer learning (MTL) has been proposed as a means to address this problem, wherein multiple base models (ML or site-specific process model) can be trained or calibrated for different tasks such as prediction at a given location, and then a meta-learning model (de Oliviera, 2019;

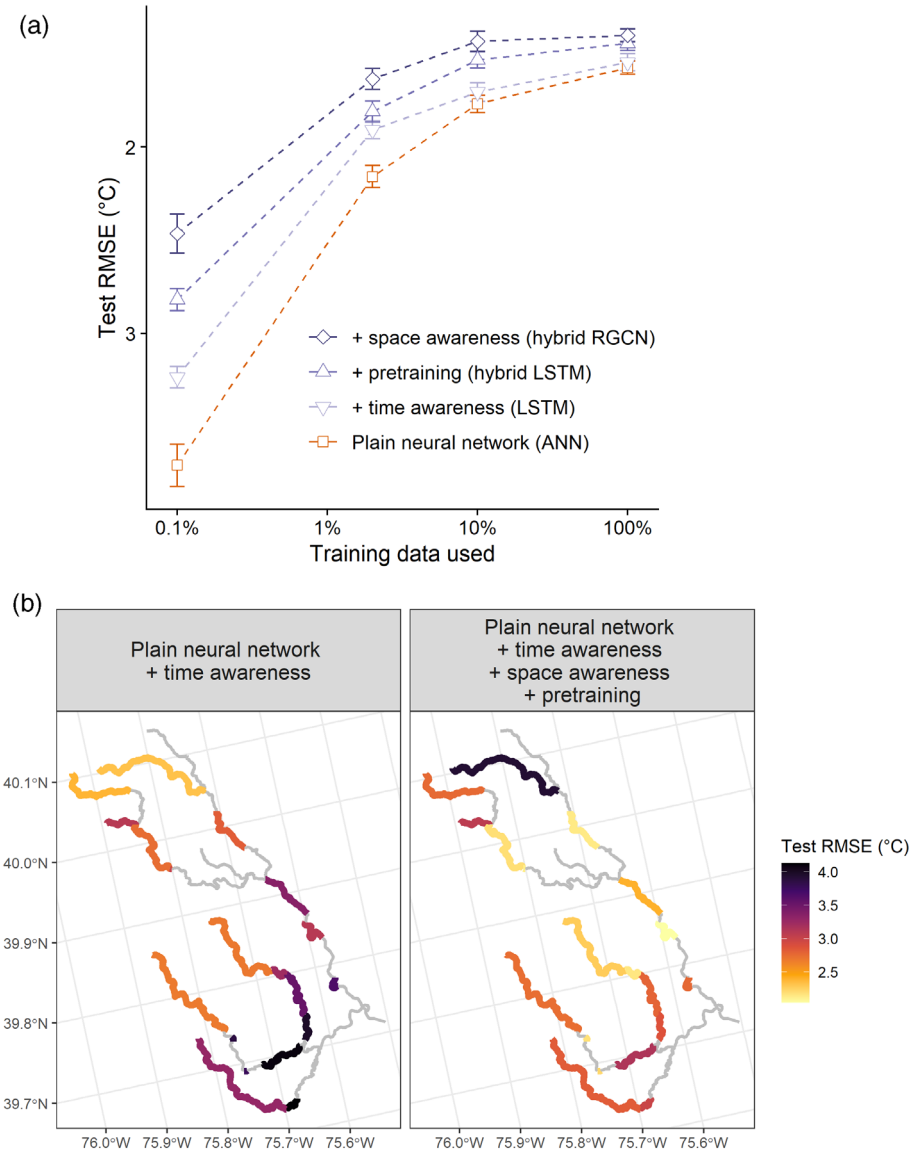

FIGURE 3 (a) Comparison of pure machine learning (ML) approaches using artificial neural networks (ANN) to various process inclusions (time and space awareness, pre-training with a process model) for predicting stream temperature in the Delaware River basin (data from Jia et al., 2021). The error bars in panel a represent the standard deviation of test root mean squared error (RMSE) across five model runs. Panel (b) shows model performance comparison between a neural network with time awareness (i.e., long short-term memory network; long short term memory (LSTM); left) and a hybrid graph neural network (recurrent graph convolutional network; RGCN; right) with time and space awareness in addition to being pre-trained with a process model. Models shown in panel (b) were trained using 0.1% of available data during the training period and only segments with more than five observations during the test period are shown (data from Jia et al., 2021)

Vanschoren, 2019) predicts which base model to transfer based on past performance metrics and location-specific attributes (Willard, Read, et al., 2020). For example, Willard, Read et al. (2020) used MTL for predictions of lake temperature in 305 artificially defined "unmonitored" lakes (targets) by transferring process-based and hybrid KGML models calibrated for 145 data-rich lakes (sources) using past performance metrics of the source models along with features such as lake attributes (e.g., surface area, maximum depth), meteorological statistics, and source lake temperature statistics. MTL flexibly allows the use of any type of model built on well-observed locations making it a noteworthy candidate for increased regional scaling.

3.4 | Can ML methods be adapted to predict extreme values?

Typical ML methods have inbuilt assumptions (e.g., the random variables follow a Gaussian distribution), which can lead to poor estimates when they do not apply for some datasets. In particular, the choice of a loss functions can directly affect the results (Bishop, 2006). For example, a squared loss (L2 norm) is more sensitive to outliers than absolute value loss (L1 norm; Breiman & Friedman, 1985; Hastie et al., 2009; Zhang, 2007). When outliers are equally important as in the case of extreme events, it is not uncommon to utilize the probability distribution within the loss function (Cawley et al., 2007; Hsieh, 2009) or choose alternate loss functions such as the relative entropy loss that computes the distance between two distributions (Qi & Majda, 2020).

Many studies in hydrology have attempted to improve predictions of extremes such as floods (Mosavi et al., 2018) using multiple techniques that include using different criteria for model selection (Coulibaly et al., 2001), conditional density estimation networks (Cannon, 2012), training exclusively on extreme events such as historical high-flow data (Fleming et al., 2015), adjustment of ML prediction bias to improve performance on the tails of the distribution (Belitz & Stackelberg, 2021), and using KGML models, for example by training an ML model on simulation data containing extremes that might not exist in the observation data (Read et al., 2017; Xie et al., 2021). However, in some cases KGML models may perform worse than traditional DL models; for example, Frame et al. (2021) found that an LSTM constrained to conserve mass was not able to predict peak flows as well as the base LSTM, although both models had lower errors than the process-based model used for comparison. Although these examples show the potential for using ML for predictions of extreme values, data scarcity for rare events warrants consideration in model choice and design, and alternate ML methods may need to be used (or modified) to handle extreme values (Cannon, 2010).

3.5 | How do we represent complex, hierarchical data in ML models?

The heterogeneity and multi-scale nature of water quality processes and their drivers requires representation of high-dimensional complex data in ML models, but this can be challenging to do in a computationally tractable manner. One approach that has been used is to modify ML models to embed complex spatial information for time-series predictions. For example, Kratzert et al., (2019) developed an entity aware-LSTM to include information on static catchment attributes into the input gate of an LSTM to improve streamflow predictions across 531 pristine basins. Jia et al. (2021) used a recurrent graph convolution network to include spatial information on river segments into the predictions, and in a subsequent study developed a real-time active learning approach that used spatial and temporal information to select representative samples for optimizing model training (Jia, Lin, et al., 2021). Creating advanced multi-scale graph-based data representations that represent river network structure and carry a diverse set of node and edge attributes can enable embedding multimodal, multi-scale, and multi-temporal information, and correlate structures across different scales and time-steps.

Probabilistic graph models (PGMs), which are data structures for encoding probability distributions, can also be used to include such structural information (Koller & Friedman, 2009). In a PGM, the nodes of the graph represent random variables, and the edges represent dependencies between variables. An optimization process using a PGM involves defining an energy function, which can embed contextual information about the data, i.e., relationships among data points at different resolutions, scales, or time steps (prior knowledge). PGMs can be optimized by targeting the maximization of the joint probability (or the minimization of the energy function) of the graph (Laude et al., 2018), which would result in specific river network predictions. Although classes of PGMs (e.g., Bayesian network models) have been used for water quality applications (Section 2), newer models that integrate PGM with DL such as DBN have been used for water quality predictions (Solanki et al., 2015; Yan et al., 2020).

3.6 | How do we build trustworthy and interpretable ML models?

Domain experts often are hesitant to replace process-based models with ML on the grounds that the explainability, interpretability, and trustworthiness of ML frameworks are questionable even if predictions are more accurate (Rudin, 2019). Model transparency and interpretability is especially important for water management decisions that have important societal implications and that have to consider future unknown scenarios.

Recent advances in explainable AI such as local interpretable model-agnostic explanation (LIME; Ribeiro et al., 2016) or Shapley additive explanations based on occlusion analysis (SHAP; Lundberg & Lee, 2017) can explain individual predictions by many ML models (Samek et al., 2021). Both methods have been successfully implemented for explaining predictions in rainfall-runoff modelling (Althoff et al., 2021; Yang & Chui, 2021), and are applicable for water quality applications as well (Wang et al., 2021). Also in the rainfall-runoff domain, Kratzert et al. (2019) used integrated gradients (Sundararajan et al., 2017) to confirm a theory-consistent influence of precipitation and air temperature on a NN state that correlated with

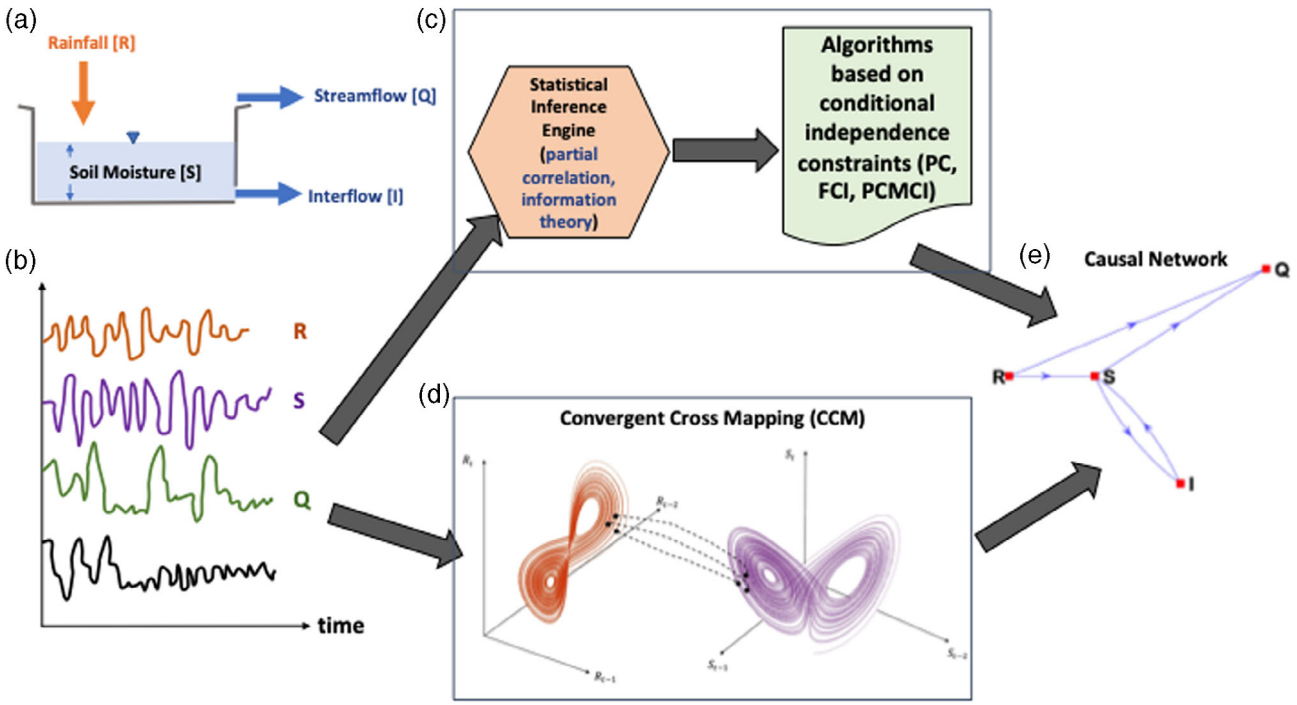

FIGURE 4 Graphical illustration of the use of causal inference methods (highlighted in boxes) for hydrological applications: (a) conceptual understanding of a physical system (i.e., rainfall-runoff process; hydrologic bucket model), (b) observational time series of the four system variables in panel a, (c) a broad class of causal inference algorithms are based on conditional independence constraints such as Granger (Granger, 1969), transfer entropy (Schreiber, 2000), PC algorithm (Spirtes & Glymour, 1991), fast causal inference; FCI (Spirtes & Glymour, 2000), and PCMCI (Runge et al., 2019). Conditional independence is performed using a statistical inference engine (e.g., partial correlation or information theory), (d) an alternative paradigm of causal inference are methods based on time-delay embedding whereby pairwise-bivariate timeseries (e.g., R and S) are used to construct attractors from which causal relations can be assessed (Sugihara et al., 2012), (e) the causal network obtained from causal inference algorithms where nodes represent variables and edges represent causal relations. The obtained causal inference network can be compared and contrasted to the conceptual a priori understanding of the system shown in panel a

snow water equivalent, building trust in the ability of such models to capture known physical processes. More recent work on the same subject used probes (e.g., linear regression models or stacked multilayer perceptrons) to connect LSTM cell states to the output for tracking the evolution of the LSTM during the training process and verifying whether the LSTM learned physically realistic mappings from inputs to outputs (Lees et al., 2021).

Causal inference is another approach to extract information on complex water quality processes and infer the effect of one variable on other system responses (Pearl, 2009; Sugihara et al., 2012). Causal inference methods can be grouped into three categories: (1) algorithms based on conditional independence constraints such as Granger causality (Granger, 1969), transfer entropy (Schreiber, 2000), PC algorithm (Spirtes & Glymour, 1991), fast causal inference (FCI; Spirtes et al., 2001), PC mutual condition information (PCMCI; Runge et al., 2019), (2) methods based on time-delay embedding and chaos theories such as convergent cross mapping (CCM) (Hannart et al., 2016; Sugihara et al., 2012), and (3) approaches based on counterfactual causal theory and structural causal models (Hoyer et al., 2009; Pearl, 2009; Peters et al., 2017). These methods have been adopted in climate and hydrologic sciences (Arora et al., 2019; Hannart et al., 2016; Ombadi et al., 2020; Runge et al., 2019) to extract relationships among system variables and disentangle governing parameters to inform process-based or ML models (e.g., Figure 4).

3.7 | How do we quantify the uncertainties in model predictions?

An important aspect of modelling is uncertainty quantification (UQ), which in ML models includes uncertainties in the data, selection of input features, and model design (Abdar et al., 2021). A common approach to test the robustness of models to inputs is to perform variable feature selection and calculate model errors resulting from choosing different combinations of inputs. Other UQ approaches include Bayesian methods such as Markov chain Monte Carlo, Bayesian active learning, and variational auto encoders and ensemble methods, which can be computationally expensive (Abdar et al., 2021).

Additional UQ challenges to be addressed are the variability of model performance from tuning hyperparameters due to stochastic optimizers used for training (model uncertainty) and use of noisy measurement data (measurement uncertainty). An approach to address

model uncertainty is to use Monte Carlo dropout in model training, wherein each node has a certain probability of being dropped out (dropout rate) and not contributing to the model (Gal & Ghahramani, 2016). Measurement noise should ideally be propagated through the model, but computing required probability densities analytically is possible only for specific types of activation functions (Gast & Roth, 2018; Loquercio et al., 2020). Uncertainty quantification methods that exploit and extend such approaches to obtain confidence intervals for predictions are needed (Dumont et al., 2021).

3.8 | How do we integrate and assimilate relevant datasets into ML models?

Water quality models rely on having access to high-quality, publicly accessible data, and on software tools that enable data integration and assimilation. Many ML studies use readily available off-the-shelf products such as the catchment attributes and meteorology for large-sample studies (CAMELS; Addor et al., 2017), which may impair their extensibility to practical, realistic applications where such data may not be available. Assimilation of new data into models using methods such as ensemble Kalman filters and autoregression (Brajard et al., 2020; Nearing, Klotz, et al., 2021; Zwart et al., 2021), and the use of integrated datasets tailored for the problem can improve prediction outcomes. Software that synthesize data for on-demand queries such as brokering-based tools (Horsburgh et al., 2016; Varadharajan et al., 2022), and methods to streamline quality control and outlier detection, gap-fill, downscale observations, and determine parameters for process models (Bennett & Nijssen, 2021; Campbell et al., 2013; Hill & Minsker, 2010; Leigh et al., 2019; Mital et al., 2020; Russo et al., 2020) would ideally be integrated into ML workflows in parallel with advances in modelling approaches.

4 | CONSIDERATIONS FOR THE USE OF ML IN WATER QUALITY MODELS

Water quality modelling poses several challenges regardless of whether the approach involves ML, statistical, or process-based codes. While each approach has its strengths and limitations, the ultimate model choice, structure, inputs, and parameters would need to take into account the following considerations.

4.1 | Process complexity

River water quality involves a wide range of physical (e.g., temperature, turbidity, conductance), chemical (inorganic and organic), and biological (e.g., bacteria, phytoplankton) parameters. Each parameter can be affected by many natural and anthropogenic factors including solute transport through runoff, groundwater exchange, instream biogeochemical processes, and land use (Lintern, Webb, Ryu, Liu, Bende-Michl, et al., 2018). For example, water temperature is strongly driven by climate but can also be influenced by snowmelt, groundwater influx, and reservoir and power plant operations (Caissie, 2006). Biogeochemical transformations such as redox reactions, uptake of nitrogen, or respiration of dissolved organic carbon add process complexity for non-conservative constituents. Even relatively conserved species such as salts can be affected by processes such as road salt runoff, surface-groundwater interactions, and tidal influence in coastal zones (Kaushal et al., 2018). Disturbances can modify the extent to which different drivers control water quality – e.g., drought increases groundwater influences on salinity and instream biotic influences on nutrient transformation rates (Mosley, 2015). The need for explicit representation of different processes and their feedbacks in mechanistic models has resulted in increasingly complex model structures, and larger parameter spaces that are more difficult to constrain (Rode et al., 2010). ML approaches present an alternative to process models for complex systems where the dynamics are not fully understood, if sufficient data are available through direct or proxy measurements. However, ML and especially DL models with large sets of hyperparameters can also be complex depending on many factors such as model design, optimization process, and data dimensionality (Hu et al., 2021). An important aspect of choosing a model is determining the right level of model complexity required for the decisions to be made. Adding model complexity does not necessarily improve performance, and will increase computational and data requirements (Orth et al., 2015; Rode et al., 2010). Ideally, the choice of a more complex model (e.g., a DL-based architecture) is justified by comparing performance against some baseline lower-complexity ML, statistical, or process models (e.g., multi-linear regression or persistence models).

4.2 | Scale, heterogeneity, and generalizability

The factors influencing riverine water quality can differ in space and time ranging from local-scale surface groundwater fluxes and hyporheic exchange (Sear et al., 1999), reach-scale habitat and riparian vegetation (Newcomer et al., 2021), watershed-scale geomorphology and geology (Burns et al., 2020; Varanka et al., 2015), to regional-scale climate and land use patterns (Guo et al., 2019; Lintern, Webb, Ryu, Liu, Waters, et al., 2018). Building models that translate across spatiotemporal scales and incorporate process understanding of heterogeneous drivers is a significant challenge. Typically models have tried to capture catchment heterogeneity using characterizations of representative field sites from intense, multidisciplinary field investigations (Brantley et al., 2017) or other (e.g., remote sensing) datasets. However, upscaling mechanistic understanding from data-rich small-scale testbeds to other regions has been challenging, in part due to the spatial heterogeneity of watershed characteristics and the need to have computationally tractable models (Tang et al., 2019). Although parameter regionalization and classification of process-based models by catchment have attempted regional scaling with mixed results (Archfield et al., 2015), new approaches to bridge scales for key water quality variables using ML are needed. Although ML models are

typically scale-invariant, their implementation for predictions of a particular spatial and temporal scale may require different model architectures and inputs depending on the processes involved at each scale. Recent hydrological studies explored the use of ML across spatial scales (Gauch et al., 2021; Kratzert, Klotz, Herrnegger, et al., 2019), and approaches such as transfer learning (Section 3.3) can also be used to address this challenge. Finally, the effects of human activity or natural disturbances can persist over long timescales (sometimes decades) requiring some models to include the lagged effects of drivers. For systems where memory effects are significant, ML models that use lagged variables or architectures that support prior states (e.g., LSTM or other sequence models) are warranted.

4.3 | Desired accuracy and computational complexity

A key consideration for model choice is the extent of accuracy and robustness needed to meet the stakeholder objectives (Section 4.5). For example, daily reservoir operations have a much lower tolerance for errors in streamflow and temperature predictions in comparison to longer-term planning for climate change (Culhane et al., 1987). There are tradeoffs to be made between model accuracy, complexity, and computational costs. For example, classical ML models can be trained with substantially lower computational expense and smaller datasets (Hu et al., 2021), and are more interpretable (Rudin, 2019). Deep NN can have lower prediction errors, but have many more parameters than classical ML models thus requiring larger datasets and more computational resources to train, and are more difficult to interpret (Hu et al., 2021; Reichstein et al., 2019).

4.4 | Data availability, integration, processing and representation in models

Riverine water quality modelling typically requires the use of highly diverse multi-scale, multimodal data (e.g., time-series data of flow and solute concentrations, geospatial data such as soil layers and hydrography, remote sensing data, or products of land cover and land use) for parameterization and validation. Model data requirements depend on the complexity, desired scale and resolution, and can be specific to the management question at hand. The amount of data available needs to be considered in choosing the ML model, with classical ML approaches needing less data than DL models. Hybrid KGML models (Section 3.2) and MTL (Section 3.3) can also be better suited for situations with sparse data.

A challenge for water quality modelling is that data are typically sparse because many relevant parameters are measured infrequently using laboratory characterization of manually collected samples, and can be biased due to sampling network design, flow conditions, and time of day when the samples were collected (Smith et al., 1997; Zhang et al., 2019). In-situ sensor technologies that collect high-resolution data only span a limited range of physical and chemical variables (Kruse, 2018), although soft sensor surrogate modelling approaches can be used to generate estimates of variables that are not measured (Section 2). While spatially dense remote sensing observations can be difficult to obtain at sufficiently fine resolutions, there are opportunities to bridge spatial scales by integrating limited point measurements from monitoring networks with remote sensing estimates of water quality (Ross et al., 2019; Topp et al., 2020). Autonomous observations from instruments such as aquatic drones guided by ML (Castellini et al., 2019, 2020) is a future direction that could enable data collection at larger scales.

Discovering, integrating, and processing data for models is also challenging. Typically data of interest are spread across a myriad of sources in different formats, and do not have sufficient metadata, quality, or provenance information to support integration (Larsen et al., 2016). Often co-located datasets on water quality and its drivers are either not available or not easily discoverable. Data also may need to be gap-filled and quality checked prior to use in a model. In particular, water bodies with strong human influence are extremely difficult to model and upscale because predictor datasets on activities such as point source discharge, water withdrawals, and reservoir releases are limited or not easily reusable. Thus many observations are underutilized for ML despite large-scale consolidation efforts such as the Water Quality Portal and GLORICH databases (Hartmann et al., 2014; Read et al., 2017), because it is labor-intensive to harmonize and process data (Shaughnessy et al., 2019; Sprague et al., 2017). Recent efforts to make water data more broadly available and usable such as the U.S. Open Water Data Initiative and the California open water data system are essential for effective management and decision making (Blodgett et al., 2015; Cantor et al., 2021; Larsen et al., 2016). Because data preparation is one of the most time-consuming aspects of model development, the development of benchmark datasets following FAIR (Findable, Accessible, Reusable, Interoperable) principles (Wilkinson et al., 2016), and the use of automated tools that make it easier to discover, synthesize, and assimilate data (e.g., Section 3.8) can accelerate adoption of ML approaches.

4.5 | Data-driven decisions considering stakeholder objectives

Data-driven decision making refers to the concept of making decisions based on data analysis or modelling, and the use of ML for making optimal decisions has been proposed for numerous applications such as business intelligence, healthcare, network optimization, and precision agriculture (Chen, Liu, & Peng, 2019; Liakos et al., 2018; Ma et al., 2020; Provost & Fawcett, 2013). Water management is a complex endeavour, and managers are tasked with making decisions at local (e.g., temperature and salinity control in a reach) to regional (e.g., integrated river basin management) spatial scales. The lead times needed for different decisions can be very different (DeFlorio et al., 2021; Sene, 2016) ranging from months to years for long-term planning (e.g., capital investments, climate adaptation), weeks to

months for seasonal water supply management (e.g., drought and snowmelt forecasting), and hours to weeks for tactical operations and emergency response (e.g., daily reservoir operations, spill mitigation). Water quality management can be especially challenging given the range of variables that are typically regulated (e.g., temperature, salts, oxygen, nutrients, metals, organics) and the diffuse nature of their sources and sinks. Models used for water quality management serve exploratory, planning, or regulatory purposes, which have different requirements for acceptable accuracies, uncertainties, and biases (Harmel et al., 2014).

Ultimately, it is important to consider stakeholder needs and available resources in deciding the appropriate complexity, scale, and resolution of the models. For example, many ML models have been developed for operational decisions that have short lead times (e.g., near-term forecasting), and are typically focused on predictions of a single variable although multitask learning approaches are being explored (e.g., Sadler et al., 2022; Zhu & Piotrowski, 2020; Zwart et al., 2021). ML models can also be run with substantially less computational expense than process models, and thus can be used to explore different scenarios for decision-making. Early stakeholder engagement can help determine desired objectives, accuracies, and lead times (Castilla-Rho, 2017; White, 2017), which could be enabled through collaborations between hydrological/water quality experts and data scientists with stakeholders such as watershed managers, regulators, and the public (Sun & Scanlon, 2019). Additionally, incorporating explainable AI approaches into decision frameworks will be important to increase transparency and build stakeholder trust in model projections. Finally, there are ethical considerations regarding the use of ML for decision-making, which include examining algorithmic assumptions, data bias and quality, and human-derived decision rules (Lo Piano, 2020).

In summary, ML paired with other emerging technologies such as cloud and exascale computing, 5G networks, and big data tools has the potential to significantly advance data-driven decisions and knowledge discovery for watershed and water quality management (Hubbard et al., 2020; Sun & Scanlon, 2019). The field of ML, and more broadly AI, has had a long history of developing other relevant technologies that are not discussed here including intelligent agents, decision theory, and reinforcement learning, which warrant further consideration in data-driven decision support systems for watershed management (Russell & Norvig, 2020). The potential for improving water quality models using ML can be realized by making deliberate choices for model selection, design, and evaluation based on the above considerations and incorporating the latest computational and mathematical advances.

5 | CONCLUSIONS

Improving water quality models for timely, decision-relevant predictions would be beneficial in the face of climate and land use change, growing populations, and a greater likelihood of extreme events. Water quality modelling poses many challenges due to the diversity of parameters and processes involved, the need for scaling, and data availability. The rapid growth in use of the state-of-the-art ML and DL models in hydrology, and recent computational and mathematical advances have demonstrated the potential for using ML for water quality modelling. Models can be improved using new approaches for model selection, hyperparameter optimization, knowledge-guided ML, transfer learning, new representations for complex data, explicit treatment for extremes, UQ, and explainable AI methods. At the same time, development of tools to integrate and process observational datasets, and methods for data assimilation would enhance the use of ML for water quality modelling. For decision-relevant predictions, consideration of stakeholder needs in model selection and evaluation of trade-offs between desired accuracy, complexity, timeliness, and available data and computational resources are important. With thoughtful implementation, ML models have the potential to accelerate decision-relevant predictions and process understanding of river water quality.

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DATA AVAILABILITY STATEMENT

Data sharing is not applicable to this article as no datasets were generated or analysed for this study.

ORCID

Charuleka Varadharajan https://orcid.org/0000-0002-4142-3224
Alison P. Appling https://orcid.org/0000-0003-3638-8572
Bhavna Arora https://orcid.org/0000-0001-7841-886X
Danielle S. Christianson https://orcid.org/0000-0002-8663-7701
Valerie C. Hendrix https://orcid.org/0000-0001-9061-8952
Vipin Kumar https://orcid.org/0000-0002-9040-2665
Aranildo R. Lima https://orcid.org/0000-0003-2514-891X
Juliane Müller https://orcid.org/0000-0001-8627-1992
Samantha Oliver https://orcid.org/0000-0001-5668-1165
Mohammed Ombadi https://orcid.org/0000-0001-7793-9137
Talita Perciano https://orcid.org/0000-0002-2388-1803
Jeffrey M Sadler https://orcid.org/0000-0001-8776-4844
Helen Weierbach https://orcid.org/0000-0001-6348-9120
Jared D. Willard https://orcid.org/0000-0003-4434-051X
Zexuan Xu https://orcid.org/0000-0001-9534-7370
Jacob Zwart https://orcid.org/0000-0002-3870-405X

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