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Deep neural networks application in environmental and water resources simulations

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EXTENDED ABSTRACT

Traditionally, environmental and water resources simulations (EWRS) have relied on physics-based analytical and numerical models. These models employ parameters that characterize the environmental systems, system state variables, and external forces as input into mathematical equations to predict future conditions of environmental systems and water resources. The effectiveness of these models is frequently limited due to the considerable computational resources and lengthy simulation times required for large-scale or repetitive simulations, and the partial comprehension or flawed mathematical representation of the physical processes that result in a mismatch between the predicted outcomes of the models and real-world observations at the field scale (Rajabi et al., 2023).

To address these challenges, there has been a shift towards employing data-driven models that incorporate machine learning (ML) techniques. Compared to traditional physics-based models, ML models are typically faster, simpler to develop, and require less detail information. Historically, a range of ML tools have been applied to develop data-driven models for EWRS, including random forests, support vector machines, polynomial chaos expansion, and tree-based regression models. Nevertheless, conventional ML methods often face difficulties when encountering infrequent, black swan cases within the dataset, struggle to adapt to new scenarios not included in their training data, may not effectively manage large volumes of data, and fall short in identifying the deep relationships and complex patterns among the parameters that affect outcomes. Deep neural networks (DNNs), a newer segment of ML, provide more flexibility and have shown to offer higher accuracy in predictions, particularly with extensive datasets (Samek et al., 2021). Their advanced learning capacities make DNNs a highly researched tool for EWRS, demonstrating significant promise over classical ML techniques.

Neural networks are computational models inspired by the human brain's structure, consisting of layers of interconnected nodes that process information using weighted connections and activation functions. They refine and optimize their internal parameters through a technique called backpropagation. DNNs build upon this foundation by incorporating multiple hidden layers between the input and output, enabling the extraction of progressively more abstract features from the data (Shen, 2018). In the context of EWRS, DNNs have found applications across various areas, including but not limited to flood prediction (Kao et al., 2020), hydrological modeling (Li et al., 2023), sediment transport modeling, water quality forecasting (Liu et al., 2019), weather prediction (Ren et al., 2021), groundwater modeling (Wang et al., 2022), water demand projection (Gil-Gamboa et al., 2024), and modeling changes in land use and land cover (Stoian et al., 2019), among others. DNNs have become increasingly popular in tasks requiring iterative simulations, such as Monte Carlo-based uncertainty analysis

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and combined simulation-optimization, as well as near real-time forecasting.

DNNs come in various architectures, each optimized for specific data types and applications. Table 1 summarizes some prevalent DNN architectures along with their applications in EWRS. In recent years, the adoption of DNNs in EWRS has transitioned from primarily using deep feedforward neural networks to increasingly favoring convolutional neural networks (CNNs) and recurrent neural networks (RNNs), including long short-term memory (LSTM) networks, for their enhanced ability to model spatial and temporal patterns. Although graph neural networks (GNNs) and generative adversarial networks (GANs) are not as commonly employed, their adoption is on the rise. GNNs offer a valuable approach for analyzing unstructured data, whereas GANs are increasingly recognized for their ability to generate synthetic data. This progression underscores a wider movement towards adopting increasingly sophisticated DNN architectures to model the dynamics of EWRS. Concurrently, the utilization of DNNs in EWRS has undergone substantial development, transitioning from basic vector regression tasks to more sophisticated predictive modeling, including time series forecasting and both image-to-value and image-to-image regression. This advancement has been facilitated using CNNs and their combinations with RNNs, such as CNN-LSTMs, allowing for the efficient analysis of spatial and temporal data. More recently, attention has expanded to include processing point clouds collected via light detection and ranging (LiDAR) or similar technologies, employing advanced DNN architectures such as PointNet and various GNNs (Fang et al., 2024).

DNNs are commonly trained utilizing data obtained from physics-based simulations, positioning them not as replacements but as supplementary surrogates to conventional physics-based models (Rajabi et al., 2022). However, there is a gradual shift towards training DNNs with field data sourced from sensors or aerial imagery, expanding their applicability to phenomena that are inadequately understood and challenging to simulate using physics-based models. A relatively recent concept involves integrating residuals of physical equations into the loss function of DNNs. This approach, known as physics-informed or physics-constrained DNNs, utilizes physics-based losses either as a component of the objective function in backpropagation or as constraints. these physics-informed neural networks (PINNs) learn from both observational data and established physics principles, often creating a balance between the two to generate solutions that align with observations while remaining physically plausible. Compared to data-driven DNNs, PINNs also offer the advantage of requiring less data for training, as they leverage an additional source of information (Wang et al., 2022). The development of PINNs for EWRS represents an active area of research, as there is still much exploration to be done in various applications and issues such as convergence, computational efficiency, and determining the optimal balance between data-driven and physics-based components require further investigation.

Table 1
Examples of DNN architectures commonly used in environmental and water resources simulations

DNN architecture	Key features	Application examples
Feedforward neural networks (FFNNs)	Employs a straightforward architecture with layers connected in a feedforward manner. Commonly used for vector data.	Water demand forecasting (Gil-Gamboa et al., 2024).
Convolutional neural networks (CNNs)	Leverages convolutional layers for spatial hierarchy feature extraction. Go to option for image data and related tasks, such as image-to-image regression, image segmentation and image classification.	Forecasting contaminant and temperature distribution maps based on maps of material properties (Rajabi et al., 2022), Land cover prediction (Stoian et al., 2019).
Recurrent neural networks (RNNs)	Utilizes memory elements to process sequences and temporal dependencies.	Flood forecasting (Kao et al., 2020).
Hybrid CNN – Long- short-term memory (LSTM)	Developed for spatiotemporal data analysis.	Flowrate prediction in a watershed (Li et al., 2023).
Graph neural networks (GNNs)	Uses graph-based data representations for node and edge analysis. Compatible with point cloud and mesh-based data.	Groundwater level forecasting (Bai and Tahmasebi, 2023).
Generative adversarial networks (GANs)	Involves a dueling setup where one network generates data, and another evaluates it.	Generating synthetic weather data (Ji et al., 2024), Leak detection in water distribution networks (Rajabi et al., 2023).

Additional areas for future research encompass: (1) addressing the prevalent perception of DNNs as opaque black box tools by developing methodologies to improve their interpretability, thereby aiding stakeholders in understanding model predictions. (2) Developing DNNs capable of effectively capturing multi-scale interactions within environmental systems, enabling more comprehensive simulations of complex phenomena. (3) Addressing the scalability challenges associated with handling large-scale environmental datasets, including the exploration of scalable architectures and algorithms that can efficiently process and analyze vast amounts of data. (4) Investigating transfer learning approaches to leverage knowledge from related domains or datasets to enhance the performance of DNNs in environmental and water resource applications. (5) Exploring the integration of DNN-based predictive models into decision support systems for environmental management and planning, enabling stakeholders to make informed decisions based on the insights provided by DNNs.

Keywords: Data-driven models; Machine learning; Neural networks; Environmental simulations; Water resources modeling

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