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Challenges and opportunities of ML and explainable AI in hydrology

L. J. Slater[1], G. Blougouras[2,3], L. Deng[1,4], Q. Deng[1,5], E. Ford[1,6], A. Hoek van Dijke[7], F. Huang[2,3,8], S. Jiang[2,3], Y. Liu [1,9], S. Moulds[10], A. Schepen[11], J. Yin[4], B. Zhang[1]

[1]School of Geography and the Environment, University of Oxford, UK
[2]Department of Biogeochemical Integration, Max Planck Institute for Biogeochemistry, Germany
[3]ELLIS Unit Jena, Jena, Germany
[4]State Key Laboratory of Water Resources Engineering and Management, Wuhan University, Wuhan, China
[5]Department of Atmospheric Science, China University of Geosciences, Wuhan, China
[6]Department of Atmospheric Physics, University of Oxford, UK
[7]Louis Bolk Instituut, 3981 AJ Bunnik, NL
[8]School of Atmospheric Sciences, Sun Yat–Sen University, China
[9]Geography and Environment, Loughborough University, UK
[10]School of GeoSciences, University of Edinburgh, UK
[11]Commonwealth Scientific and Industrial Research Organisation, Dutton Park, Australia

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Author for correspondence:
Louise Slater
e-mail: louise.slater@ouce.ox.ac.uk

Machine learning (ML) is a powerful tool for hydrological modelling, forecasting, generation of new datasets, and process discovery. It is widely recognised for its ability to produce skillful predictions and generate insights about physical mechanisms through explainable AI (XAI). This manuscript outlines current progress in the use of ML in hydrology, new tools in XAI, and challenges in these areas. Continued areas of research for ML in hydrology include model interpretability, prediction in data-sparse regions, overcoming hydrology's 'cascade of uncertainty', multivariate prediction, and causality.

1. Foreword: strengths and weaknesses of ML in hydrology

Artificial Intelligence (AI) and Machine Learning (ML) are powerful tools for producing skillful predictions relative to traditional hydrological models (1; 2) and as a new approach to generate insights about physical driving mechanisms in hydrology (3; 4). Contrary to the widespread perception of ML models as 'black boxes', advances in explainable AI (XAI), a set of advanced techniques to interpret machine learning models, are now providing greater insight into the relationships between different variables and model predictions, particularly when combined with a large-sample approach. ML models extract insights directly from the underlying data, enabling them to uncover new processes and relationships if the model is well designed (5). However, ML models also face various challenges that may limit their adoption in the hydrological sciences. These challenges include data availability issues, such as the skewed over-representation of data from the global North, and particularly Europe and North America, which can lead to biased models. Additionally, model training problems can occur like shortcut learning (6), where models identify simpler patterns (shortcuts) in the training data that do not capture the true underlying relationships, leading to high performance on the original dataset but poor generalisation to new data.

This work does not seek to provide an exhaustive list of ML models, XAI tools, or taxonomies; the field is developing so rapidly that such efforts would quickly become outdated. Instead, we take a narrative approach, outlining the key successes of ML and interpretability within the hydrological sciences, and illustrating this progress through a few carefully-selected examples from the literature. We finish by outlining some key challenges of ML and XAI in hydrology.

2. ML for enhanced hydrological modelling, forecasting, and variable estimation

There exist already many reviews of ML in hydrology, including introductory overviews (e.g. 7; 8), in-depth reviews of the state-of-the-art deep learning and XAI implementations in hydrology (e.g. 9), and reviews of ML applications in specific areas such as water resources management (10). Here we focus on highlighting some of the main types of applications within hydrology, rather than listing techniques. These include simulation and forecasting of hydrological variables (streamflow, soil moisture, snow water equivalent, evapotranspiration), generation of new datasets (e.g. from remote sensing, digital elevation models, and in-situ measurements), and novel applications of differentiable or physics-informed hydrological models.

(a) ML for hydrological simulation

It is now well-established that Long Short-term Memory (LSTM) models trained on large samples of catchments systematically outperform traditional hydrological models (1; 2; 11) (Figure 1). LSTMs are a type of recurrent neural network (RNN) in deep learning designed to handle sequential data effectively by capturing long-term dependencies, which traditional RNNs struggle with. They achieve this by mitigating the vanishing gradient problem, where gradients become too small during training, hindering the model's ability to understand long-term dependencies in the data (12).

A robust model intercomparison in the Great Lakes region by Mai et al. found that an LSTM-lumped model significantly outperformed various types of basin-wise, subbasin-based, and gridded models with local to global calibration, not only in calibration but also in every validation scenario (1). While certain catchments remain difficult to model with LSTMs, such as those with spatially-variable human impacts, Lees et al. showed that LSTMs exhibit considerable promise for learning intermediate stores such as soil moisture (see section 3(c)), suggesting that during training the model implicitly learns certain hydrological processes that are explicitly defined in conceptual and physics-based models (2). Addressing a common misconception about ML

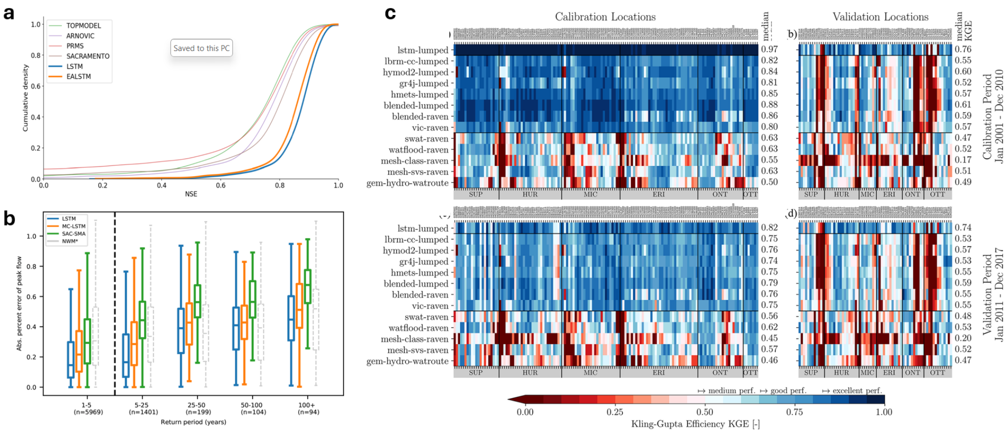

Figure 1. Benchmarking LSTMs against traditional hydrological models. (a) LSTMs are benchmarked against conceptual models in Great Britain (2); (b) LSTM, mass-conserving LSTM (MC-LSTM), Sacramento Soil Moisture Accounting model with SNOW-17 and a unit hydrograph routing function (SAC-SMA), and the National Oceanic and Atmospheric Administration National Water Model (NWM), compared in (11). (c) A suite of models including LSTM, basin-wise, subbbasin-based, and gridded models with local to global calibration from (1). In panel c, the performance is shown for each of the different models (y axis) across the calibration and validation locations (x axis).

models, Frame et al. showed that LSTMs are consistently better at predicting extreme events when compared to conceptual, process-based and physics-informed ML methods, even when comparable extreme events are not included in the training dataset (11).

Compared to traditional hydrological models, a key strength of deep learning methods for continuous streamflow prediction is their ability to leverage multiple data streams to improve simulation performance. One notable example of this is the synergistic use of meteorological drivers from different forcing products. For instance, Kratzert et al. found that an LSTM could dynamically extract information from three different meteorological forcing products over the continental United States, dynamically weighting the information from each forcing product depending on location and flow conditions (13).

Furthermore, recent progress has revealed the ability of DL models to integrate different types of spatial data for hydrological modelling (Figure 2). While existing DL models tended to use either Euclidean data, such as gridded meteorological forcing, or non-Euclidean data with irregular topological connectivity, such as information transfer between nodes along a river network, Deng et al. showed that the two types of information can be blended to systematically improve model performance (14). They integrated Convolutional Neural Networks (CNN) for regular spatial data and Graph Neural Networks (GNN) for handling irregular data, along with spatial attention mechanisms to focus on important features, and an LSTM to capture temporal dependencies. With this model structure they simulated streamflow multiple timesteps ahead, at multiple locations along a river network, showing superior performance compared to other deep learning model structures.

(b) ML for hydrological forecasting

The performance of ML models for dynamical streamflow prediction compared to traditional hydrological models means they are highly suitable for hydrological forecasting, where accuracy and reliability are primary concerns. In recent years, the Google Flood Forecasting team has built a suite of forecasting services based around LSTM neural networks to predict global flooding with up to 7 days lead time, demonstrating equal or better performance than GloFAS (15). In

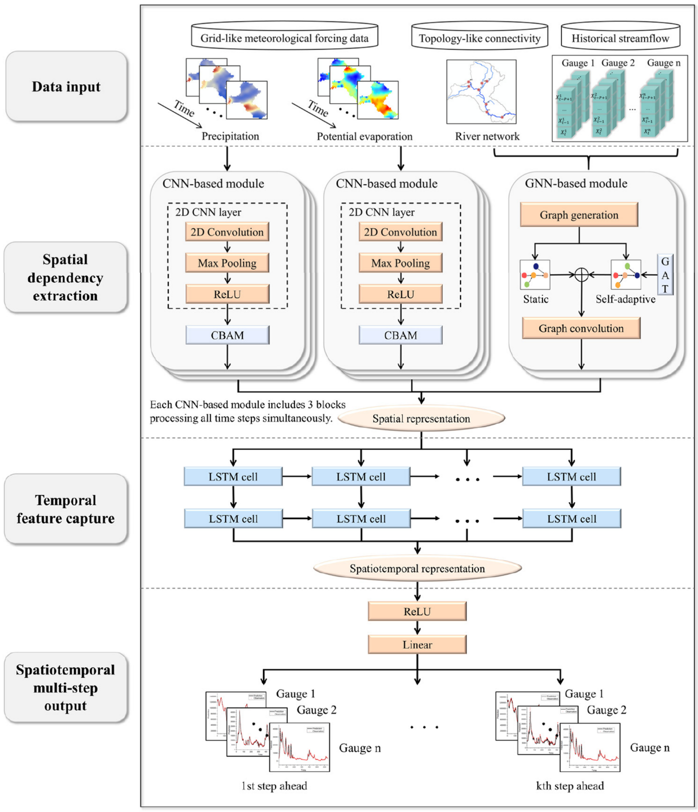

Figure 2. Spatiotemporal modelling. Figure reproduced from Deng et al. (14). The CNN-based modules and GNN-based modules in the spatial dependency extraction part are employed to recognize spatial information from Euclidean gridded meteorological forcings and non-Euclidean irregular topological connectivity respectively. The LSTM model in the temporal feature capture part is employed to extract temporal dependencies. The multi-step and multi-gauge streamflow simulations are output through the subsequent ReLU function and linear layers.

their approach, an encoder LSTM processes static geophysical data and 365 days of historical meteorological forcing data. The encoder's states are passed to a decoder LSTM, which runs over seven days of meteorological forecast data. The model outputs are time-step dependent parameters of an asymmetric Laplacian mixture distribution from which streamflow quantiles can be drawn. The advantages of this approach are that it allows streamflow forecasting directly from meteorological inputs, including in ungauged basins, and predicting the parameters characterises the uncertainty in the prediction.

A growing body of work has shown the advantages of ML models trained on dynamical climate model forecasts to predict hydrological variability and extremes at subseasonal to seasonal and decadal lead times (16). Here, a key research area has been to define the necessary model complexity to achieve good predictions given uncertain climate forecasts. Hauswirth et al. (17) compared multilinear regression, lasso regression, random forests, and LSTM models trained on EFAS SEAS5 meteorological forecasts to make predictions of seasonal discharge and water levels in the Netherlands, and found only minor differences between the various approaches. This suggests that the degree of uncertainty in the seasonal climate forecasts diminished any advantage of more complex ML approaches (17). In the UK, a multi-catchment seasonal forecasting system was developed to predict monthly maximum daily streamflow up to four months ahead by training a quantile regresssion forest (QRF) model on dynamical seasonal forecasts of precipitation and temperature from a multi-model ensemble of C3S seasonal climate forecasts, allowing the ML model to implicitly perform bias-correction and downscaling. The multi-catchment ML model was marginally, but significantly, more skillful than a single-site approach (18), again suggesting that the advantage of a multi-site approach is reduced when the climate information is more uncertain.

Even though some studies have shown little difference in the performance of different ML methods, there may be other avenues which prove fruitful for more complex ML models. For example, coupling wavelets and CNNs to LSTMs produced more accurate predictions for monthly streamflow forecasting in China (19). Similarly, it was found that a combination of CNNs and gated-recurrent units (GRU) outperformed LASSO, XGBoost and standalone CNN or GRU, suggesting that combining spatial and temporal methods may yield the best results (20). A challenge to the ML community is to develop models that convey the uncertainty in forecasts through ensembles, for it remains common to employ deterministic ML or DL models (e.g. 21; 22). Hybrid approaches combining process-based models go some ways to addressing this problem (16; 17; 23), as does the Google approach of predicting distributional parameters.

(c) ML for generating hydrological datasets

ML is increasingly used for generating new datasets or predicting variables which are limited by record length or sparsely distributed in space. For instance, a ML-based reconstruction of global terrestrial water storage (GTWS-MLrec) was used to extend the record length of TWS data in time from 1940 to present (24), allowing a better understanding of multidecadal groundwater dynamics than permitted by GRACE/GRACE-FO data alone. ML has been used to develop static datasets of physical parameters that are important for hydrological modelling and analysis. For example, bankfull river discharge was predicted for millions of kilometers of streams and rivers globally using a random forest model trained on multiple static attributes (25). Other variables include the prediction of global river width (26) or river flood depth and extent (27). Such datasets can be interrogated to better understand global hydrological and morphological dynamics, or may be used to parameterize or validate process-based hydrological models. ML is also widely used to predict discrete hydrological variables such as streamflow signatures (e.g. 4; 28) and the characteristics of extreme events. Random forests are particularly suited to these applications because of their relative resistance to overfitting and ability to exploit nonlinear relationships between the features and the predicted variable through post-hoc explainable AI (XAI) tools (see section 3).

(d) Differentiable, physics-informed ML models for hydrology

Different approaches exist to combine ML with physical information, mainly through adding synthetic input data, imposing constraints on ML models, and blending ML models with process-based models. First, as ML models can sometimes perform poorly for predicting extreme events such as floods and droughts, synthetic atmospheric data can be included for ML models to learn the patterns of extreme events. Synthetic samples have been shown to effectively improve the ability of ML models to simulate extreme events and monotonic relationships (30). Second, ML models can ensure adherence to physical conservation principles, such as water and energy balance, by incorporating corresponding constraints into the loss functions as penalties. An example of lake temperature simulation after introducing energy conservation into the loss function proved to be physically consistent in the net thermodynamic fluxes into and out of the lake (31). In addition, constraints can also be imposed on the structure of ML models. In a physics-informed model, causal relationship constraints (CRCs) can be imposed on the layers of the model to force it to learn causal relationships. For instance, a causal physics-informed model developed for groundwater level modeling was used to explain future changes in groundwater levels based on the changes in vertical inflow and potential evapotranspiration under different climate scenarios (32). Third, hybrid methods that blend DL with conceptual hydrological models are increasingly popular to preserve specific process-based components such as the relationship

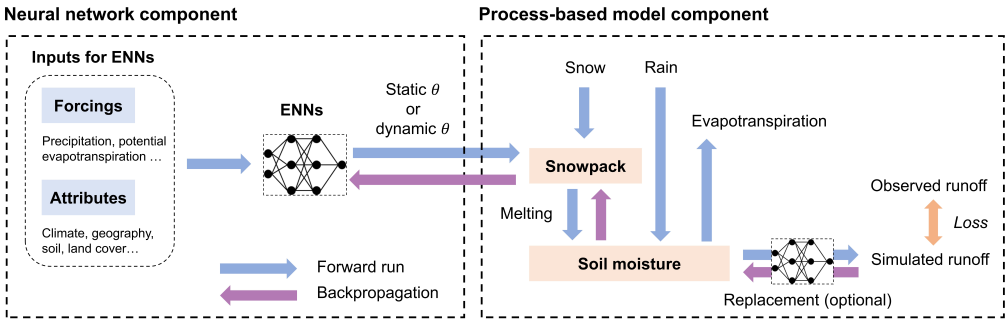

Figure 3. Structure of a differentiable hydrological model, modified from Shen et al. (29). A neural network receives dynamic inputs from meteorological forcings and static attributes across a large number of basins to provide regionalized parameterization for the process-based model. The hydrological parameters can be either static or dynamic.

between soil moisture and runoff generation. For instance, a conceptual hydrological model (GR4J) was blended with deep learning models to preserve the GR4J production storage processes and then route runoff based on net rainfall and runoff from the production storage (33). By incorporating DL, other time series such as temperature and antecedent streamflow could be included to improve predictive performance. The hybrid approach performed better than either the conceptual model or DL alone. Temporal dynamic models, often employed in the field of hydrology, can be inserted into an AI system as special recurrent neural layers to improve the representation of the physical system. This kind of physics-informed paradigm improves simulation accuracy, robust transferability and unobserved process inference (34).

As another genre of physical-informed hybrid model, differentiable models are generally composed of a process-based model (or a DL surrogate), which provides physical constraints, and embedded neural networks which can learn the model parameters or replace any internal modules of the physical model. For instance, a differentiable model based on the HBV conceptual hydrological model was used to develop a regionalized model parameterization (35), with the original soil moisture–runoff relationship replaced with an inserted neural network to learn the relationship between soil moisture, precipitation, and runoff (Figure 3). These models are called 'differentiable' because the gradients of the physical model outputs are tracked with respect to the inputs using differentiable programming and big data. This blending approach allows them to be framed either as ML models constrained by structural priors, or process-based models enhanced by learnable units (29). While their temporal performance approaches that of LSTMs, one of their strengths is that they can simultaneously respect mass conservation and output a suite of interpretable uncalibrated internal physical fluxes and state variables, such as evapotranspiration and soil moisture, which cannot be done with traditional DL such as LSTMs (29; 35). In addition, with the assistance of learnable units, differentiable models exhibit competitive or even better spatial generalization in predicting in ungauged basins and ungauged regions (36). These advantages are particularly relevant in predicting high flow trends in ungauged locations, where the model's treatment of hydrological extremes is grounded in physics. Explicit encoding of physical models in neural networks also allows data from multiple processes or subsystems to be assimilated in a physically consistent manner. For instance, integrating hydrological and dynamic vegetation modeling into differentiable models can significantly improve the spatio-temporal representation of evapotranspiration in catchments by accounting for the two-way interactions between vegetation and hydrology (37). Likewise, the explicit inclusion of river routing processes in the differentiable model allows for the effective use of streamflow observations from different gauges along a river network, thereby enabling hydrologically meaningful distributed modeling with ML (38; 39).

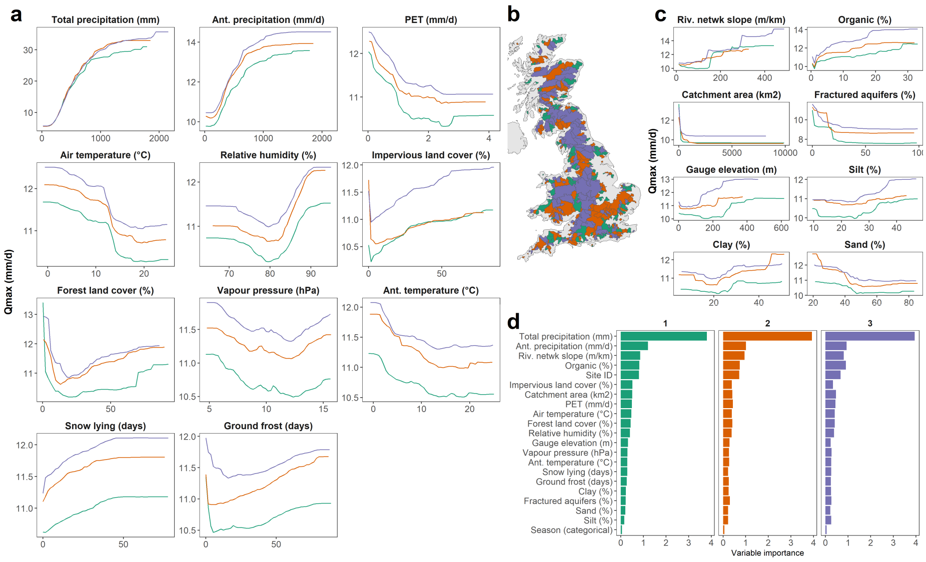

Figure 4. Partial dependence plots for a quantile regression forest (QRF) model with 1,268 gauges across Great Britain. Catchments are randomly split into three groups (3 colours) to assess consistency of partial dependence plots (panels a-c) and relative importance (panel d) across the three separate models. Features include time-series variables (a) and static catchment attributes (c). Reproduced from Slater et al. (4).

3. Generating novel hydrological insights through explainability and attribution of ML models

One of the key challenges for hydrologists is using ML to derive new knowledge and findings. Hydrology generally seeks to quantify relationships within the data, identify influential variables, and understand the nature of their influence (linear, non-linear, or conditional). XAI plays a key role in equipping hydrologists with tools to measure these relationships. Specifically, XAI methods allow for the analysis of the relationships learned by complex ML models, evaluating model components or sensitivities, and thereby helping to generate new hypotheses about the underlying mechanisms (5). Multiple approaches exist for evaluating the relative importance or contribution of feature variables within an ML model, but the explanation obtained can vary depending on the technique used. It is thus essential to understand exactly how each technique works. Some methods are specific to certain models (i.e. intrinsic) while others can be applied to different ML model types (i.e. post-hoc). We focus principally on post-hoc approaches which can be applied to different types of ML models. Many XAI methods rely on a perturbation-based approach, whether implicitly through post-hoc interpretability methods such as relative importance, Partial Dependence Plots (PDPs), Individual Conditional Expectations (ICEs), Accumulated Local Effects (ALEs), or SHAP, discussed in section 3(a), or more explicitly through hypothesis testing and sensitivity testing, discussed in section 3(d).

(a) Model-agnostic post-hoc explainability methods

In this section we provide an overview of some key, model-agnostic XAI techniques, and we discuss issues and challenges which may arise from their use. The different methods described below all provide a form of relative feature (i.e. predictor) importance. Some techniques describe the magnitude of that effect (e.g. relative importance; Figure 4), while others describe the direction of the association between a predictor and the target variable - i.e. PDPs, ICEs, and ALEs (Figure

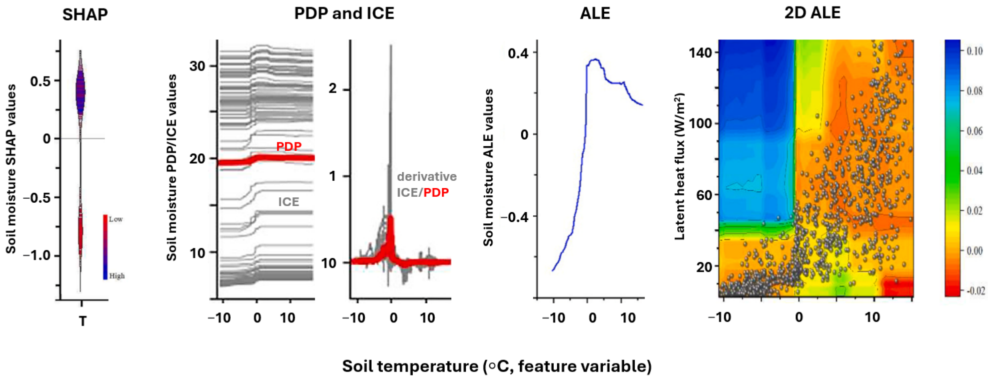

Figure 5. Four XAI metrics showing the effect of soil temperature (℃, feature variable) on the predicted soil moisture (target variable). The four sets of plots indicate (1) Distribution of SHAP values, with red colours indicating low feature values (low soil temperature) and blue colours high values (high soil temperature); (2) Partial dependence plot (PDP, red line) and Individual conditional expectations (ICE, grey lines) on same plot, along with derivative PDP and ICE; (3) Accumulated Local Effects (ALE); and (4) two-dimensional ALE plot, with soil temperature on the x-axis, latent heat flux on the y-axis, and soil moisture as colour bar. Modified from Huang et al. (3).

5). It remains important to remember that XAI methods do not explain the physical reality but the ML model's representation of the physical reality.

(i) Relative importance

Relative importance describes the contribution or influence of each feature in the model's predictions, helping to understand which of the features are more influential in predicting the target variable (e.g. Figure 4). Permutation importance is the most simple to implement and understand; it provides an intuitive measure of feature importance by observing the effect of randomly shuffling the features. This also provides insights for feature engineering decisions, as features with low importance can be removed in cases where the model needs to be simplified. However, permutation importance can be computationally expensive with large datasets, can provide misleading importance in the presence of correlated features, and can be unstable if the model is not robust. In contrast, feature importance from tree-based models (such as Gini importance) is derived directly from the model training process, making it more computationally efficient. However, it can give more importance to predictors with more categories, and can also be misleading in the presence of correlated features. Another point worth noting is that relative importance approaches provide a global summary of feature importance (i.e. in the full model), ignoring potentially important local variability. Moreover, feature importance techniques only provide information on the importance of a given variable and not the direction of a relationship between a feature and the outcome. It is thus valuable to combine relative importance with other interpretation methods for greater insight.

(ii) Partial dependence, ICE and ALE

Three techniques are listed here which provide information on the nature of the relationship between a feature variable and the predicted outcome. Outside of these ML techniques, such relationships can also be described with statistical summary tools such as elasticity curves, which depict, for instance, streamflow sensitivity to precipitation across the entire flow distribution (40).

Partial Dependence Plots (PDPs) provide an intuitive visualisation of the relationship between an input feature and the target prediction within a ML model. They show the marginal effect of the feature on the predicted outcome of the model (i.e. how a change in the feature affects the prediction, while averaging out the effect of all other features). For instance, in Figure 4a, increases in precipitation are associated with increases in flood magnitude (4). PDPs can also show the effect of pairs of features on the target variable while keeping all other features fixed. One of the key limitations of PDPs is that they assume each feature of interest is independent of the other features, an assumption which may lead to potentially misleading interpretations when features are correlated. It is therefore worth assessing how the PDPs change when a correlated variable is removed from the model. Additionally, they only show the average effect of the feature in the model, rather than the full range.

Individual Conditional Expectation plots (ICEs), which visualize how changes in a particular feature influence the model's prediction for individual instances, can thus provide greater insight than the PDP (41). ICEs help detect heterogeneity in the model's predictions, help identify outliers and extreme cases, reveal interactions between features, and enhance overall model interpretability. In Figure 5, the grey lines show the ICEs of individual instances within the data while the red line shows the PDP, which displays the average effect across all features.

Accumulated Local Effects (ALE) are also used to assess a feature's marginal effect on the predicted outcome. ALEs are considered more robust than PDP because they do not assume feature independence. Figure 5 shows that temperature is one of the key features affecting the predicted soil moisture using various interpretability techniques. When the temperature reaches 0◦C, the thawing rate increases and the snowmelt leaches into the soil, significantly increasing the soil moisture. The derivative ICE of temperature shows a surge around 0◦C in accordance with the ICE and ALE. The two-dimensional ALE of temperature and latent heat flux shows the distribution of instances as dots. As the temperature increases above 0◦C (x-axis), the soil moisture decreases (colour bar), while latent heat flux rises. This can be explained by the joint effect of latent heat flux and temperature, both of which have a negative impact on soil moisture above freezing (3).

(iii) SHAP: the additive explanations approach

SHapley Additive exPlanations (SHAP) is an additive variable attribution method used to make models interpretable (see Figure 5). In contrast with the methods described above, SHAP provides additive explanations, meaning the prediction can be expressed as the sum of the feature contributions. For instance, if the prediction is streamflow, the SHAP value for each predictor represents the contribution of that predictor to the deviation of the streamflow prediction from the average streamflow. In other words, the sum of SHAP values equals the model's output difference from the baseline prediction.

SHAP is considered more robust than other relative importance measures due to its fair handling of feature contributions. Derived from game theory, SHAP values are calculated based on each feature's contribution to the prediction across all possible combinations of feature subsets, ensuring consistent and fair explanations. Correlated features are handled more robustly by distributing contributions among features based on their marginal contributions. SHAP allows for the interpretation of both the direction and the magnitude of the impact of each feature on target variable prediction, and provides insights at the global level (overall model behaviour; SHAP summary plots) and the local level (individual predictions; SHAP dependence plots).

For example, De Meester and Willems (42) used SHAP summary plots to assess four drought metrics, including drought intensity, drought severity, number of dry days, and summer volume, to reveal that the proportion of irrigation in the catchment was one of the leading contributing factors of drought intensity and summer flow volumes in Flanders, Belgium. It is also possible to explicitly compute the interaction effects between features, to assess their combined effects after accounting for individual contributions, through SHAP interaction values (43). These values are represented as a matrix for each sample with dimensions $M \times M$, where M is the number of features. Jiang et al. (44), for instance, used the variability of SHAP interaction values across different flood sizes to assess the complexity of flood generation processes in individual

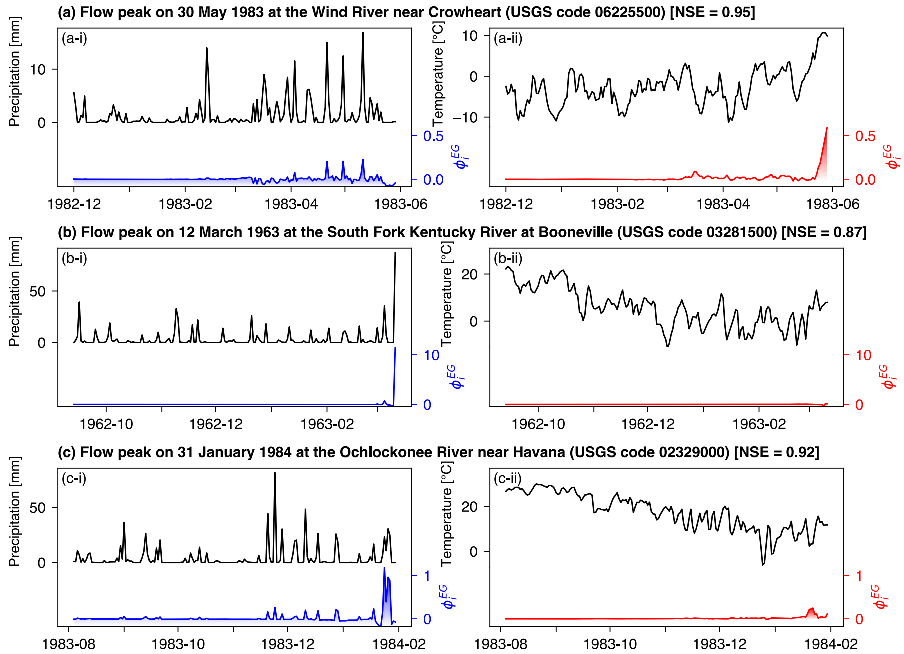

Figure 6. Observations (black lines) and feature importance scores (i.e., expected gradients; colour lines) of precipitation and temperature for three representative discharge peaks from three U.S. catchments. Each panel indicates the average NSE value of the target catchment during the test period in square brackets. Reproduced from Jiang et al. (46).

catchments, noting that this complexity is likely to undermine the reliability of traditional flood frequency analyses.

(b) Gradient-based interpretability methods

Various other methods besides the the post-hoc model-agnostic XAI methods described above can be used to interpret ML models. Gradient-based methods quantify the sensitivity of model predictions to small changes to the input features. They embed core explainability principles of sensitivity (features that have the most influence on model predictions are assigned greater importance) and completeness (the total contribution of all features explains the model's output), ensuring they generate accurate and meaningful explanations (45). They are popular methods for interpreting neural networks because the gradients can be retrieved through a backward pass after training.

Integrated and expected gradients are two approaches used for interpreting DL models. In integrated gradients (IG), the prediction of the DL model is attributed to its input features by computing the integral of gradients of the model's prediction with respect to the input along a straight path from a baseline (often zero) to the input (47). This results in an attribution score for each input feature. Expected gradients (EG) are a variant of IG, where the attribution is averaged over multiple samples across a distribution of inputs, reducing the sensitivity to any single baseline in complex models or when dealing with noisy or diverse data distributions to provide a more robust attribution (48).

Gradient-based methods have been used, for instance, to interpret LSTM models that predict streamflow based on meteorological drivers, revealing temporal feature importance scores for precipitation and temperature in relation to annual maximum discharges (46; 49). Figure 6 exemplifies three distinct temporal patterns of these feature importance scores (colored lines) for flood events from different U.S. catchments. In the first pattern (Figure 6a), precipitation (blue line) slightly influences the peak discharge over an extended period, while temperature (red line) is more influential near the peak. The second pattern (Figure 6b) shows minimal temperature impact and significant precipitation influence only near the peak. In the third pattern (Figure 6c), precipitation has a sustained impact before the peak, suggesting historical precipitation may contribute significantly to peak flow. These patterns are consistent with three known flooding mechanisms—snowmelt, recent precipitation, and antecedent precipitation (also known as excessive soil moisture). This approach innovatively identifies flood mechanisms that emerge from complex interactions among flood drivers, without the (often subjective) classification criteria previously required, and supports further analysis of how climate and land surface shape these mechanisms and how they may change under global warming.

There are several other types of gradient-based methods that have been applied to CNN-based models. These include saliency maps (50), guided backpropagation (51), gradient $\times$ input (52), smooth gradients (53) and layer-wise relevance propagation (LRP) (54). Given gridded input features, these methods can relate the model output back to each pixel of an input feature. This generates a saliency map or heatmap that allows for the identification of the input regions that are most crucial for the model's output, which is particularly well-suited for physical inference in the geosciences.

(c) Using latent variables to assess learnt processes

Latent variables offer an alternative approach to understand what a DL model has learned during training. They represent hidden factors or underlying structures in the data that the model has inferred but not observed directly. By analyzing these latent variables it is possible to gain insights into the model's internal representations and how it processes and interprets the data. For instance, Lees et al. designed an experiment to assess whether the learned relationships of an LSTM for streamflow simulation could be related to specific hydrological processes (55). By extracting the tensors (i.e. the learned relationship), they assessed the hypothesis that the LSTM had learnt a real world process. The cell-state vector, which represents the memory of the LSTM, was mapped to soil moisture and snow. The high correlation between the probe outputs and soil moisture/snow showed that the LSTM had learned the governing hydrological processes (see Figure 7). Similar results were found by Jiang et al., who trained a physics-informed ML model on streamflow observations but could still accurately infer catchment-wide snow dynamics through one of the recurrent NN's intermediate cell-states (34).

(d) Perturbation-based methods: hypothesis testing and sensitivity testing

One intuitive approach for analysing ML models is through model perturbation, where input features are systematically removed or replaced with permuted or randomly subsampled values to see how the outcome changes. Such approaches have been used to test the role of different driving mechanisms. For example, Hoek van Dijke et al. (56) used a DL-based approach to derive insights about driving mechanisms via hypothesis testing. They evaluated whether streamflow typically increased or decreased across different catchments of the globe in the years following a major drought, i.e. producing a "drought legacy effect" on streamflow. They formulated two hypotheses: (1) that streamflow would increase following a drought in cases where drought-induced vegetation mortality decreased catchment evaporation, and (2) that streamflow would decrease following a drought in cases where the groundwater was depleted. To assess these hypotheses, they first trained an LSTM model to predict streamflow from multiple variables, omitting the drought legacy years from the training data (following (57)). They then calculated the drought legacy effect based on the positive/negative model error in the drought legacy year (see Figure 8). They found that in catchments with widespread vegetation mortality following a drought the inclusion of Normalized Difference Vegetation Index (NDVI) data in the LSTM model decreased the occurrence of model underestimation compared to the model without NDVI, suggesting that the observed increases in streamflow were caused by reductions in evaporation

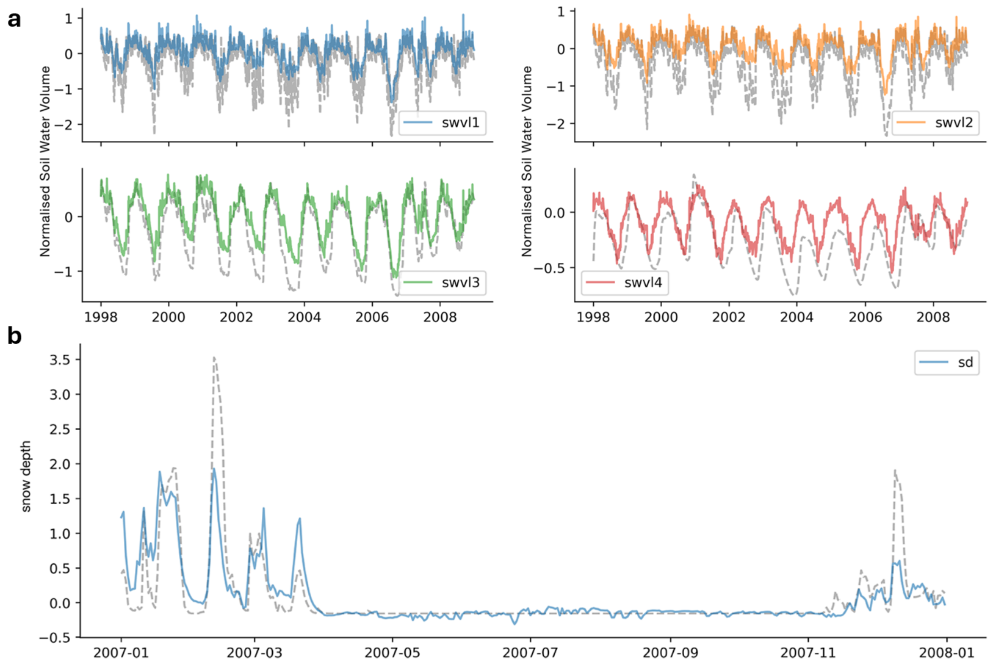

Figure 7. Using probes to explore hydrological variables learned by an LSTM model during training. (a) shows probe prediction time series (as coloured lines) alongside the target variables (as grey dotted lines) for the Read Brook catchment at Hookagate, for four soil moisture levels. The probe correctly captures the temporal dynamics of the soil moisture signals, despite some systematic bias. Zero defines the mean soil moisture across Great Britain. Panel (b) shows probe predictions for the snow depth target variable at one site located in the Cairngorm Mountains. Reproduced from Lees et al. (55).

from vegetation mortality. Likewise in catchments with depleted groundwater resources, they found that the inclusion of terrestrial water storage (TWS) in the model decreased the occurrence of model overestimation compared to relative to the model without TWS, suggesting that the decreases in streamflow following droughts were largely due to groundwater depletion (56).

Aside from hypothesis testing, another approach to understand the model predictions is model sensitivity testing. This is a form of perturbation analysis. For instance, Slater et al. developed a quantile regression forest model across 1268 UK NRFA catchments and used this model to quantify the sensitivity of flood magnitude to a 10% increase in precipitation, a 1°C rise in air temperature, or a 10 percentage point increase in urban or forest land cover (4). The results of the sensitivity testing showed which catchments were more sensitive to changes in climate and land cover, revealing that increases in precipitation and urbanization tended to amplify flood magnitudes more in catchments that had high baseflow contribution, while rising air temperature and afforestation decreased flood magnitudes more in the catchments with low baseflow index.

4. Challenges associated with ML and XAI in hydrology

(a) Causality in ML models

Most supervised ML models are built to leverage patterns in the data rather than to specifically identify causal relationships. In general, predictive models based on supervised ML focus on estimating the observational probability by predicting the likely values of Y when X is takes on a

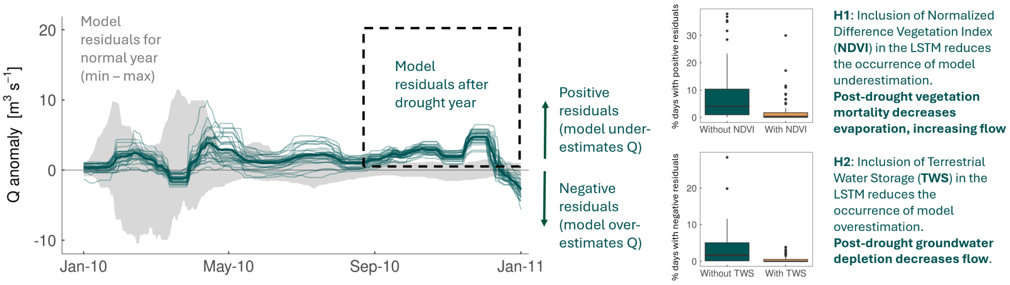

Figure 8. Hypothesis testing the causal mechanisms of post-drought streamflow legacy effects using a DL model. Grey shading shows model residuals in normal years; green lines indicate model residuals in drought years. Positive model residuals here (green lines enclosed in dashed black rectangle outline) show cases of the model underestimating streamflow in post-drought years. Top boxplots show that the inclusion of NDVI in post-drought years decreases the magnitude of residuals, reflecting the reduction in evaporation caused by vegetation mortality. Bottom boxplots show that the inclusion of TWS in post-drought years also decreases the magnitude of residuals, reflecting the decrease in streamflow from groundwater depletion. Example modified from Hoek van Dijke et al. (56).

certain value. In contrast, causal tasks aim to determine the interventional probabilities, to assess the impact of changes or interventions in X (e.g., setting X to a specific value) on Y (58). A critical requirement for a predictive model to estimate causal effects is that confounding variables-those affecting both the predictor and the target-are properly accounted for. If these confounders are not controlled, the interpretations derived from the model lack clarity regarding whether a given variable is a cause, an effect, or unrelated to the target variable (59).

Several promising methods are emerging to attempt to assess causality in ML models, but they are not yet widely applied in hydrology. Causal ML methods which formalize the data-generation process through structural causal models (SCMs) have surged in recent years in other disciplines (60). The causal random forests approach (61) can be implemented to estimate quantile treatment effects nonparametrically based on the generalized random forests method, along with a measure of variable importance. Counterfactual approaches, i.e. hypothetical retrospective interventions to explain an outcome, are also increasingly popular in the causal ML literature. Some causal ML approaches applied to soil moisture–precipitation coupling include a causal inference approach by Li et al. who combined Granger causality analysis and ML (62) and a new methodology proposed by Tesch et al., who trained a DL model to reflect causality using prior knowledge on additional variables that might affect the causal relationship (63). The authors also suggested two additional approaches to assess whether the detected causality was more than a spurious outcome.

Although causal explanations remain the holy grail, there is still no existing approach for uncovering process mechanisms with certitude. Causal inference methods are not specific to ML and have various challenges such as contemporaneous causation, hidden confounding, and nonlinearity - especially in the context of time series modelling (64). Challenges in causal ML include the loss of generalization performance when the data distribution shifts (60). In hydrology, this may occur when the hydrological models are trained on observations, but the forecasts use predictor variables with a different distribution, such as climate model outputs. Another key challenge when using XAI to uncover causality lies in the fact that ML models capture correlations and patterns in the data (such as non-linear relationships between the target variable and predictors), but these relationships do not necessarily represent true causal relationships. Thus, while XAI tools can help interpret some of these patterns, providing insights into model behaviour and decision-making processes, they often struggle to distinguish between correlation and causality. More rigorous causal inference techniques are required to reliably separate spurious correlations from genuine causal effects.

(b) Prediction in ungauged catchments/regions

Prediction in ungauged basins remains a longstanding problem in hydrology. Early applications of ML to address this challenge involved techniques for parameter regionalisation (e.g. (65)), but the use of LSTMs delivered a major step forward. For example, Kratzert et al. (66) showed that an LSTM outperformed a conceptual model calibrated to a specific catchment, even when that catchment was left out of the data used to train the LSTM. In the Great Lakes Intercomparison Project (1), LSTM models systematically outperformed conceptual and physics-based models on the same test datasets (Figure 1). Apart from LSTM models, random forest and differentiable models have also shown good performance and stability in data-scarce regions (e.g. 36).

The performance of ML models in ungauged basins varies depending on the composition of the training dataset in relation to the ungauged basins. For instance, Fang et al. (67) showed that the highest predictive performance was achieved when the training dataset was representative and heterogeneous – a notion they termed 'data synergy'. Kratzert et al. (68) observe that, in order to train as accurate as possible rainfall-runoff LSTM models, hydrologically diverse data from at least hundreds of basins should be employed, even if the geographical area of interest is limited. This contrasts with conventional hydrological modelling approaches where models are tailored to specific regions or regimes of interest. The implication is that hydrological predictions tend to improve in ungauged locations as the diversity of training data is increased.

Many applications of AI to hydrology rely on pre-compiled datasets with static attributes (such as the "CAMELS" datasets). The performance of AI models in ungauged locations is typically assessed by evaluating the model on a subset of test basins that were left out during training. However, there are significant gaps in global coverage of these datasets, especially in Africa and Asia. Numerous efforts are underway to address this data gap, including the deployment of low-cost sensor networks and the use of satellite altimetry aboard missions such as SWOT. Nevertheless, the question of how best to combine these novel data sources with AI to improve the accuracy and coverage of streamflow estimates worldwide remains an open question.

(c) Uncertainty quantification in hydrological ML models

Probabilistic methods have been slowly emerging in machine learning for hydrology (69; 70), with entire families of ML regression algorithms designed to provide probabilistic predictions, as summarised in Figure 9 from (69). These families include: (i) Quantile regression algorithms that can support conditional quantile estimation (including quantile regression LSTMs, XGBoost, and more). Most of these algorithms are based on the idea of using a 'pinball loss' function, rather than typical (mean) regression algorithms. (ii) Expectile regression algorithms are similar to quantile regression algorithms, except they focus on conditional expectiles rather than quantiles, and are still unexplored in hydrology. (iii) Distributional regression algorithms (i.e. parametric algorithms) are expected to exhibit better skill than the first two types when sufficient information about the required predictive probability distribution is available. Papacharalampous and Tyralis highlight that the relative performance of these algorithms depends largely on the real-world problem that needs to be solved, as well as their degree of interpretability and flexibility.

In neural networks, different approaches have also been suggested to quantify uncertainty. Approaches include the running of Monte Carlo simulations, bootstrapped training samples, Bayesian approximations, or modifying the dropout scheme during inference (71). The dropout technique (72) can be used during testing to generate an ensemble of predictions. By dropping units, 'thinned' networks can be trained. Compared to multiparameter ensembles, dropout ensembles offer more reliable (but less sharp) coverage of prediction intervals, and only require a single calibration run, thus no additional computational cost (71).

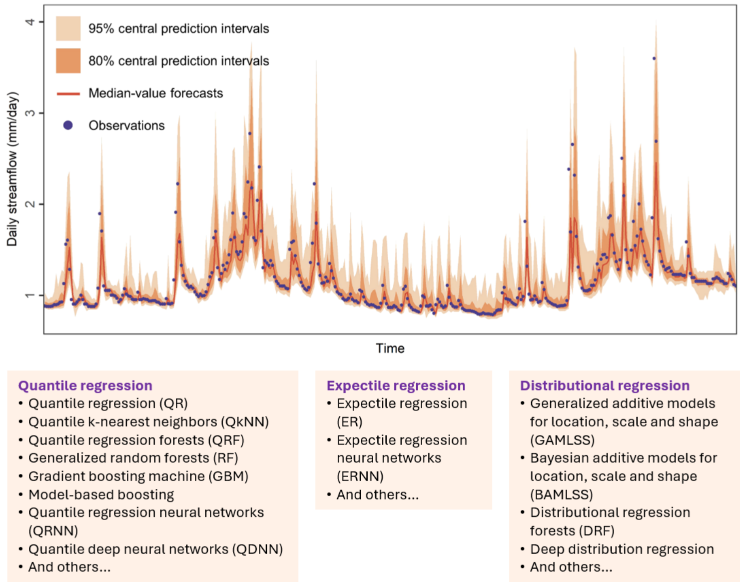

Figure 9. Probabilistic daily one-day ahead machine-learning streamflow forecasts. Median value is indicated in red, 80% (95%) central prediction intervals as dark (light) orange ribbon, and observations as purple circles. Modified from Papacharalampous and Tyralis (69).

(d) Uncertainty of XAI methods for model interpretability

The use of post-hoc XAI methods on ML models for process understanding can lead to misinterpretations (e.g., 73; 74) partly because there is no clear consensus on what constitutes a valid explanation. As such, many have argued that we should favour models that are interpretable to begin with, rather than post-hoc interpretations (73). However, intrinsic models sometimes fail to match the predictive performance of more complex ML models, in part because these complex models have access to a larger solution space. For this reason, post-hoc XAI methods are often used to give the model posterior interpretability, balancing the need for high performance with the desire for interpretability.

The interpretation of different features in a machine learning model can be highly variable depending on the choice of data sources (and their uncertainties), the type of ML model used, the choices made in the model structure and training, and the choice of XAI methods, including specific assumptions and computations inherent in each XAI method (e.g., 5). Often, the application of different XAI methods to a single model (75), or even the repeated application of the same XAI method to the same model and input instance (76), can lead to interpretation results that differ to varying degrees. One question is thus whether researchers should combine insights from all interpretation techniques and 'average' results to reach a reliable conclusion, or favour specific techniques over others. This domain is highly unregulated, and many researchers use different combinations of techniques, or just one.

Huang et al. (77), for example, compared the instance-level variable importance in a ML model and a deep learning model. They predicted the land atmosphere coupling (LAC) strength, which has been increasing over the last four decades in South America, using both a machine learning (Random Forest, RF) and deep learning (ConvLSTM) model, and then compared the performance of XAI metrics on both models (77). For the RF model they considered random forest importance (RFI), SHAP and perturbation importance (PI), and for the DL model the perturbation importance (PI) and integrated gradient (IG). They found the prediction of both models was comparable; DL had slightly less bias but also exhibited 'smoothed' predictions. The

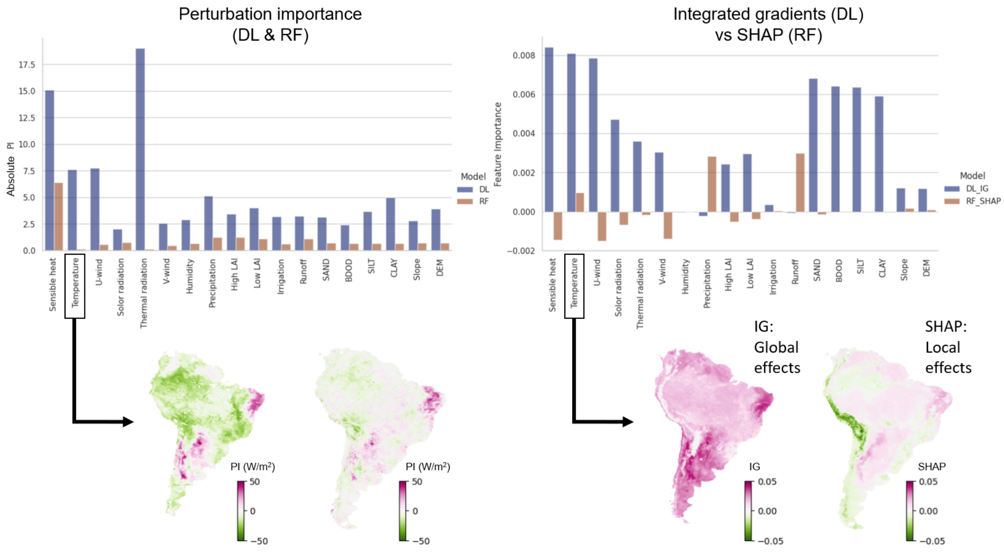

Figure 10. Comparison of instance-level variable importance in a deep learning (ConvLSTM) and a machine learning (Random forest) model. Both models predict land-atmosphere coupling. Modified from Huang et al. (77).

DL model's integrated gradients provide global information about model behaviour, while the RF model's importance metric provides local information. In Figure 10, the left panel shows the inconsistency between DL and RF. The permutation importance is higher in the DL model, showing greater sensitivity to perturbation. In the right panel, the SHAP values emphasize the local effects of precipitation and runoff in the ML model, while the IG values emphasize the global effects of meteorological and static variables in the DL model. Overall, this example highlights the importance of understanding and justifying the choice of specific XAI approaches selected for any given task in hydrology.

Ahmed et al. (10) highlight the importance of model interpretability and understanding ML models, so that there is transparency in any conclusions which may impact policy decisions. Moreover, the question of whether XAI results should be interpreted through the lens of pre-existing domain knowledge is a challenge in itself. Promptly disregarding methods where the results are not fully aligned with pre-existing knowledge can limit the potential of hydrological XAI, reinforcing established theories, rather than recognising the potential of ML as an exciting new approach to reveal novel and possibly counter-intuitive patterns directly from data (5).

5. Conclusion: ML and XAI limitations and future recommendations

Based on the current state of the art in ML and XAI in the field of hydrology, we believe some of the principle limitations and remaining challenges are as follows.

(1) Hydrologists should be mindful of inconsistencies in ML model interpretability. Different ML models and XAI approaches can produce conflicting interpretability results, and as such can lead to different interpretations (e.g. 75; 77; 78). Rather than considering specific methods to be wrong, and others 'right', users need to be aware of the inherent strengths and limitations of each ML model or XAI method. We have attempted to outline some of the strengths and weaknesses of ML/DL models and XAI tools herein. For instance, PDPs can be highly sensitive to variable multicollinearity, and should be assessed alongside potentially more robust approaches such as ALE. Our discussion of these different XAI/interpretability methods aims to provide some guidelines on their respective utility and trustworthiness. In practice, it is recommended that the XAI analysis be repeated by resampling the data, using different subsets of data, varying initial seeds in ML models, or using multiple XAI methods in different runs (79). This strategy can potentially prevent the finding from being the product of a specific data set, ML model, or XAI method, and also allows for estimation of the variability and confidence intervals of the interpretation results.

(2) Hydrological prediction in data-sparse and human-modified regions remains a challenge. Despite considerable progress in the field of hydrological prediction in ungauged basins and regions, with many papers showing the strengths of ML compared to traditional hydrological models, we believe there remain areas for further research and improvement. Understanding to what extent ML can generate reliable predictions in highly data-sparse regions, or in heavily modified or regulated catchments, remains an open question. Additionally, we believe there is room for further research on the ability of DL to learn different anthropogenic impacts on hydrological variables. Ultimately, increasing data collection is needed to address regional gaps in global hydrological observations (80).

(3) Multivariate prediction remains a long-term goal of hydrological ML. Predicting multiple dependent variables (outcomes) simultaneously is particularly useful in terms of accuracy and insights. One of the strengths of differentiable modelling is the ability to consider multiple hydrological variables simultaneously. However, an equivalent data-driven approach for handling multivariate hydrological outputs remains an area for further research. Recently, there have been explorations in multi-task learning that incorporate basic hydrological principles, such as water balance, to constrain the relationships between variables computed by ML models (e.g., 37; 38; 81). These studies show great promise for multi-variable constraints compared to focusing only on streamflow or a single variable, which may not sufficiently constrain the internal processes in the hydrologic system.

(4) ML presents an opportunity to rethink hydrology's "cascade of uncertainty". The traditional hydroclimatic modelling framework includes multiple sources of uncertainty arising from the climate models and other data inputs through to the hydrological models and post-processing. In contrast, ML models can implicitly handle steps such as downscaling and bias correction of climate forcing data by developing direct relationships between good quality data sources (e.g. 16; 82). This is evident in that the higher resolution of meteorological inputs obtained through downscaling and bias correction does not necessarily lead to better hydrological ML model performance (e.g. 14). We argue that in some cases there is scope for prediction methods that combine ML with dynamical climate model outputs to shorten the hydrological modelling chain, or to 'skip the hydrologist' altogether (82).

(5) Causality remains an ongoing challenge. Hydrologists, ourselves included, are often at risk of implying causality when discussing the drivers of hydrological processes, and still need to be careful not to claim causality too quickly. High predictive accuracy does not guarantee valid causal inference. The challenge of 'equifinality', in which different models can produce a similar result, exists also in ML. Within this context, XAI offers hydrologists a powerful tool to interrogate ML models and assess which one offers the most faithful representation of reality. However, results should always be interpreted with caution, as XAI only reveals the internal mechanics of the ML model, which should not be mistaken for the real world. Although XAI alone does not confirm causality, the correlations and patterns it uncovers can nevertheless provide valuable insights. For example, XAI may reveal that certain predictors thought to be unimportant exert a significant influence on predictions, or that the importance of variables changes unexpectedly in different environmental contexts (5). Such revelations may prompt hydrologists to reevaluate their assumptions, leading to further testing and targeted studies. Therefore, in most cases where causality is still a challenge, it is preferable to consider XAI findings as hypotheses rather than definitive causal conclusions.

(6) As ML and XAI methods grow in hydrology, we should actively seek to learn from and share our failures. Most papers present only the successes of their ML modeling attempts and the promises of their model architectures, with some briefly mentioned drawbacks in the Discussion sections. However, when it comes to new ML and XAI methods in hydrology, where best-practices are still not well established, it would be highly beneficial to share our ML and XAI difficulties. Sharing our model failures and shortcomings would significantly speed up scientific advancements, both in terms of methods and results. Such efforts are considerably enhanced by making code and data freely available to the research community (83).

Taking these limitations and recommendations into account, we remain highly optimistic on the future of ML and XAI in hydrology. There is considerable potential to drive future progress in the field, to enhance early warning systems, and discover new processes which diverge from our traditional understanding. Here, we are not suggesting a move away from process-based modeling; rather, we highlight the complementary advantages that ML and XAI offer for tackling challenges that traditional methods may struggle with. Looking ahead, we foresee hydrologists widely embracing the nonlinear insights provided by ML, leveraging it as a powerful analytical tool in this data-rich era. We also expect increased cross-disciplinary collaborations, where hydrologists, data scientists, and machine learning experts work together to develop and fine-tune ML and XAI tools specifically designed to meet the diverse needs of different sub-disciplines of hydrology. Overall, we think AI/ML has clear potential for better water resources management in a rapidly changing world.

References

1 Mai J, Shen H, Tolson BA, Gaborit É, Arsenault R, Craig JR, Fortin V, Fry LM, Gauch M, Klotz D et al.. 2022 The great lakes runoff intercomparison project phase 4: the great lakes (GRIP-GL). *Hydrology and Earth System Sciences* **26**, 3537–3572. (10.5194/hess-26-3537-2022)

2 Lees T, Buechel M, Anderson B, Slater L, Reece S, Coxon G, Dadson SJ. 2021 Benchmarking data-driven rainfall–runoff models in Great Britain: a comparison of long short-term memory (LSTM)-based models with four lumped conceptual models. *Hydrology and Earth System Sciences* **25**, 5517–5534. (10.5194/hess-25-5517-2021)

3 Huang F, Shangguan W, Li Q, Li L, Zhang Y. 2023 Beyond prediction: An integrated post-hoc approach to interpret complex model in hydrometeorology. *Environmental Modelling & Software* **167**, 105762. (10.1016/j.envsoft.2023.105762)

4 Slater L, Coxon G, Brunner M, McMillan H, Yu L, Zheng Y, Khouakhi A, Moulds S, Berghuijs W. 2024 Spatial sensitivity of river flooding to changes in climate and land cover through explainable AI. *Earth's Future* **12**, e2023EF004035. (10.1029/2023EF004035)

5 Jiang S, Sweet Lb, Blougouras G, Brenning A, Li W, Reichstein M, Denzler J, Shangguan W, Yu G, Huang F et al.. 2024 How Interpretable Machine Learning Can Benefit Process Understanding in the Geosciences. *Earth's Future* **12**, e2024EF004540. (10.1029/2024EF004540)

6 Geirhos R, Jacobsen JH, Michaelis C, Zemel R, Brendel W, Bethge M, Wichmann FA. 2020 Shortcut learning in deep neural networks. *Nature Machine Intelligence* **2**, 665–673. (10.1038/s42256-020-00257-z)

7 Xu T, Liang F. 2021 Machine learning for hydrologic sciences: An introductory overview. *Wiley Interdisciplinary Reviews: Water* **8**, e1533. (10.1002/wat2.1533)

8 Lange H, Sippel S. 2020 Machine learning applications in hydrology. *Forest-water interactions* pp. 233–257. (10.1007/978-3-030-26086-$6_1$0)

9 Tripathy KP, Mishra AK. 2023 Deep learning in hydrology and water resources disciplines: Concepts, methods, applications, and research directions. *Journal of Hydrology* p. 130458. (10.1016/j.jhydrol.2023.130458)

10 Ahmed AA, Sayed S, Abdoulhalik A, Moutari S, Oyedele L. 2024 Applications of machine learning to water resources management: A review of present status and future opportunities. *Journal of Cleaner Production* p. 140715. (10.1016/j.jclepro.2024.140715)

11 Frame JM, Kratzert F, Klotz D, Gauch M, Shalev G, Gilon O, Qualls LM, Gupta HV, Nearing GS. 2022 Deep learning rainfall–runoff predictions of extreme events. *Hydrology and Earth System Sciences* **26**, 3377–3392. (10.5194/hess-26-3377-2022)

12 Hochreiter S. 1997 Long Short-term Memory. *Neural Computation MIT-Press*. (10.1162/neco.1997.9.8.1735)
13 Kratzert F, Klotz D, Hochreiter S, Nearing GS. 2021 A note on leveraging synergy in multiple meteorological data sets with deep learning for rainfall–runoff modeling. *Hydrology and Earth System Sciences* **25**, 2685–2703. (10.5194/hess-25-2685-2021)
14 Deng L, Zhang X, Slater LJ, Liu H, Tao S. 2024 Integrating Euclidean and non-Euclidean spatial information for deep learning-based spatiotemporal hydrological simulation. *Journal of Hydrology* **638**, 131438. (10.1016/j.jhydrol.2024.131438)
15 Nearing G, Cohen D, Dube V, Gauch M, Gilon O, Harrigan S, Hassidim A, Klotz D, Kratzert F, Metzger A et al.. 2024 Global prediction of extreme floods in ungauged watersheds. *Nature* **627**, 559–563. (10.1038/s41586-024-07145-1)
16 Slater LJ, Arnal L, Boucher MA, Chang AYY, Moulds S, Murphy C, Nearing G, Shalev G, Shen C, Speight L et al.. 2023 Hybrid forecasting: blending climate predictions with AI models. *Hydrology and earth system sciences* **27**, 1865–1889. (10.5194/hess-27-1865-2023)
17 Hauswirth SM, Bierkens MF, Beijk V, Wanders N. 2023 The suitability of a seasonal ensemble hybrid framework including data-driven approaches for hydrological forecasting. *Hydrology and Earth System Sciences* **27**, 501–517. (10.5194/hess-27-501-2023)
18 Moulds S, Slater L, Arnal L, Wood A. 2024 Skilful probabilistic predictions of UK floods months ahead using machine learning models trained on multimodel ensemble climate forecasts. (10.31223/X5X405)
19 Ni L, Wang D, Singh VP, Wu J, Wang Y, Tao Y, Zhang J. 2020 Streamflow and rainfall forecasting by two long short-term memory-based models. *Journal of Hydrology* **583**, 124296. (10.1016/j.jhydrol.2019.124296)
20 Xu W, Chen J, Corzo G, Xu CY, Zhang XJ, Xiong L, Liu D, Xia J. 2024 Coupling Deep Learning and Physically Based Hydrological Models for Monthly Streamflow Predictions. *Water Resources Research* **60**, e2023WR035618. e2023WR035618 2023WR035618 (10.1029/2023WR035618)
21 Di Nunno F, de Marinis G, Granata F. 2023 Short-term forecasts of streamflow in the UK based on a novel hybrid artificial intelligence algorithm. *Scientific Reports* **13**, 13456. (10.1038/s41598-023-34316-3)
22 Granata F, Di Nunno F. 2024 Forecasting short- and medium-term streamflow using stacked ensemble models and different meta-learners. *Stochastic Environmental Research and Risk Assessment*. (10.1007/s00477-024-02760-w)
23 Moulds S, Slater LJ, Dunstone NJ, Smith DM. 2023 Skillful Decadal Flood Prediction. *Geophysical Research Letters* **49**, e2022GL100650. (10.1029/2022GL100650)
24 Yin J, Slater LJ, Khouakhi A, Yu L, Liu P, Li F, Pokhrel Y, Gentine P. 2023 GTWS-MLrec: global terrestrial water storage reconstruction by machine learning from 1940 to present. *Earth System Science Data* **15**, 5597–5615. (10.5194/essd-15-5597-2023)
25 Liu Y, Wortmann M, Slater L, Hawker L, Neal J, Yin J, Boothroyd R, Gebrechorkos S, Leyland J, Darby S, Griffith H, Cloke H, Vahidi E, Nicholas A, Delorme P, McLelland S. 2024 First global estimation of bankfull river discharge. Technical report. (10.5194/egusphere-egu24-19997)
26 Lin P, Pan M, Allen GH, de Frasson RP, Zeng Z, Yamazaki D, Wood EF. 2020 Global estimates of reach-level bankfull river width leveraging big data geospatial analysis. *Geophysical Research Letters* **47**, e2019GL086405. (10.1029/2019GL086405)
27 Hosseiny H. 2021 A deep learning model for predicting river flood depth and extent. *Environmental Modelling & Software* **145**, 105186. (10.1016/j.envsoft.2021.105186)
28 Coxon G, McMillan H, Bloomfield JP, Bolotin L, Dean JF, Kelleher C, Slater L, Zheng Y. 2024 Wastewater discharges and urban land cover dominate urban hydrology signals across England and Wales. *Environmental Research Letters* **19**, 084016. (10.1088/1748-9326/ad5bf2)
29 Shen C, Appling AP, Gentine P, Bandai T, Gupta H, Tartakovsky A, Baity-Jesi M, Fenicia F, Kifer D, Li L et al.. 2023 Differentiable modelling to unify machine learning and physical models for geosciences. *Nature Reviews Earth & Environment* **4**, 552–567. (10.1038/s43017-023-00450-9)
30 Xie K, Liu P, Zhang J, Han D, Wang G, Shen C. 2021 Physics-guided deep learning for rainfall-runoff modeling by considering extreme events and monotonic relationships. *Journal of Hydrology* **603**, 127043. (10.1016/j.jhydrol.2021.127043)

31 Jia X, Willard J, Karpatne A, Read J, Zwart J, Steinbach M, Kumar V. 2019 Physics guided RNNs for modeling dynamical systems: A case study in simulating lake temperature profiles. In *Proceedings of the 2019 SIAM international conference on data mining* pp. 558–566. SIAM. (10.1137/1.9781611975673.63)
32 Adombi AVDP, Chesnaux R, Boucher MA, Braun M, Lavoie J. 2024 A causal physics-informed deep learning formulation for groundwater flow modeling and climate change effect analysis. *Journal of Hydrology* p. 131370. (10.1016/j.jhydrol.2024.131370)
33 Kapoor A, Pathiraja S, Marshall L, Chandra R. 2023 DeepGR4J: A deep learning hybridization approach for conceptual rainfall-runoff modelling. *Environmental Modelling & Software* **169**, 105831. (10.1016/j.envsoft.2023.105831)
34 Jiang S, Zheng Y, Solomatine D. 2020 Improving AI system awareness of geoscience knowledge: Symbiotic integration of physical approaches and deep learning. *Geophysical Research Letters* **47**, e2020GL088229. (10.1029/2020GL088229)
35 Feng D, Liu J, Lawson K, Shen C. 2022a Differentiable, learnable, regionalized process-based models with multiphysical outputs can approach state-of-the-art hydrologic prediction accuracy. *Water Resources Research* **58**, e2022WR032404. (/10.1029/2022WR032404)
36 Feng D, Beck H, Lawson K, Shen C. 2022b The suitability of differentiable, learnable hydrologic models for ungauged regions and climate change impact assessment. *Hydrology and Earth System Sciences Discussions* **2022**, 1–28. (10.5194/hess-27-2357-2023)
37 Zhong L, Lei H, Li Z, Jiang S. 2024 (under review) Advancing streamflow prediction in data-scarce regions through vegetation-constrained distributed hybrid ecohydrological models. *Journal of Hydrology*.
38 Wang C, Jiang S, Zheng Y, Han F, Kumar R, Rakovec O, Li S. 2024 Distributed hydrological modeling with physics-encoded deep learning: A general framework and its application in the Amazon. *Water Resources Research* **60**, e2023WR036170. (10.1029/2023WR036170)
39 Zhong L, Lei H, Yang J. 2024 Development of a distributed physics-informed deep learning hydrological model for data-scarce regions. *Water Resources Research* **60**, e2023WR036333. (10.1029/2023WR036333)
40 Anderson BJ, Brunner MI, Slater LJ, Dadson SJ. 2024 Elasticity curves describe streamflow sensitivity to precipitation across the entire flow distribution. *Hydrology and Earth System Sciences* **28**, 1567–1583. (10.5194/hess-28-1567-2024)
41 Goldstein A, Kapelner A, Bleich J, Pitkin E. 2015 Peeking inside the black box: Visualizing statistical learning with plots of individual conditional expectation. *journal of Computational and Graphical Statistics* **24**, 44–65. (10.1080/10618600.2014.907095)
42 De Meester J, Willems P. 2024 Analysing spatial variability in drought sensitivity of rivers using explainable artificial intelligence. *Science of The Total Environment* **931**, 172685. (10.1016/j.scitotenv.2024.172685)
43 Lundberg SM, Erion G, Chen H, DeGrave A, Prutkin JM, Nair B, Katz R, Himmelfarb J, Bansal N, Lee SI. 2020 From local explanations to global understanding with explainable AI for trees. *Nature machine intelligence* **2**, 56–67. (10.1038/s42256-019-0138-9)
44 Jiang S, Tarasova L, Yu G, Zscheischler J. 2024 Compounding effects in flood drivers challenge estimates of extreme river floods. *Science Advances* **10**, eadl4005. (10.1126/sciadv.adl4005)
45 Wang Y, Zhang T, Guo X, Shen Z. 2024 Gradient based Feature Attribution in Explainable AI: A Technical Review. (https://doi.org/10.48550/arXiv.2403.10415)
46 Jiang S, Zheng Y, Wang C, Babovic V. 2022 Uncovering flooding mechanisms across the contiguous United States through interpretive deep learning on representative catchments. *Water Resources Research* **58**, e2021WR030185. (10.1029/2021WR030185)
47 Sundararajan M, Taly A, Yan Q. 2017 Axiomatic attribution for deep networks. In *International conference on machine learning* pp. 3319–3328. PMLR. (10.5555/3305890.3306024)
48 Sturmfels P, Lundberg S, Lee SI. 2020 Visualizing the impact of feature attribution baselines. *Distill* **5**, e22. (10.23915/distill.00022)
49 Jiang S, Bevacqua E, Zscheischler J. 2022 River flooding mechanisms and their changes in Europe revealed by explainable machine learning. *Hydrology and Earth System Sciences* **26**, 6339–6359. (10.5194/hess-26-6339-2022)

50 Simonyan K, Vedaldi A, Zisserman A. 2014 Deep Inside Convolutional Networks: Visualising Image Classification Models and Saliency Maps. (10.48550/arXiv.1312.6034)
51 Springenberg JT, Dosovitskiy A, Brox T, Riedmiller M. 2015 Striving for Simplicity: The All Convolutional Net. (10.48550/arXiv.1412.6806)
52 Shrikumar A, Greenside P, Kundaje A. 2019 Learning Important Features Through Propagating Activation Differences. (10.48550/arXiv.1704.02685)
53 Smilkov D, Thorat N, Kim B, Viégas F, Wattenberg M. 2017 SmoothGrad: removing noise by adding noise. (10.48550/arXiv.1706.03825)
54 Bach S, Binder A, Montavon G, Klauschen F, Müller KR, Samek W. 2015 On Pixel-Wise Explanations for Non-Linear Classifier Decisions by Layer-Wise Relevance Propagation. *PLOS ONE* **10**, 1–46. (10.1371/journal.pone.0130140)
55 Lees T, Reece S, Kratzert F, Klotz D, Gauch M, De Bruijn J, Kumar Sahu R, Greve P, Slater L, Dadson S. 2021 Hydrological concept formation inside long short-term memory (LSTM) networks. *Hydrology and Earth System Sciences Discussions* **2021**, 1–37. (10.5194/hess-26-3079-2022)
56 van Dijke AH, Oh S, Yu X, Orth R. 2024 Analyzing drought legacy effects on streamflow with machine learning. Technical report EGU General Assembly 2024, Vienna, Austria, 14–19 Apr 2024. (10.5194/egusphere-egu24-13019)
57 Yu X, Orth R, Reichstein M, Bahn M, Klosterhalfen A, Knohl A, Koebsch F, Migliavacca M, Mund M, Nelson JA et al.. 2022 Contrasting drought legacy effects on gross primary productivity in a mixed versus pure beech forest. *Biogeosciences Discussions* **2022**, 1–27. (10.5194/bg-19-4315-2022)
58 Pearl J, Mackenzie D. 2018 *The book of why: the new science of cause and effect*. Basic books.
59 Molnar C, König G, Herbinger J, Freiesleben T, Dandl S, Scholbeck CA, Casalicchio G, Grosse-Wentrup M, Bischl B. 2020 General pitfalls of model-agnostic interpretation methods for machine learning models. In *International Workshop on Extending Explainable AI Beyond Deep Models and Classifiers* pp. 39–68. Springer. (10.1007/978-3-031-04083-2_4)
60 Kaddour J, Lynch A, Liu Q, Kusner MJ, Silva R. 2022 Causal machine learning: A survey and open problems. *arXiv preprint arXiv:2206.15475*. (10.48550/arXiv.2206.15475)
61 Chen Je, Hsiang CW. 2019 Causal random forests model using instrumental variable quantile regression. *Econometrics* **7**, 49. (10.3390/econometrics7040049)
62 Li L, Shangguan W, Deng Y, Mao J, Pan J, Wei N, Yuan H, Zhang S, Zhang Y, Dai Y. 2020 A causal inference model based on random forests to identify the effect of soil moisture on precipitation. *Journal of Hydrometeorology* **21**, 1115–1131. (10.1175/JHM-D-19-0209.1)
63 Tesch T, Kollet S, Garcke J. 2023 Causal deep learning models for studying the Earth system. *Geoscientific Model Development* **16**, 2149–2166. (10.5194/gmd-16-2149-2023)
64 Runge J, Gerhardus A, Varando G, Eyring V, Camps-Valls G. 2023 Causal inference for time series. *Nature Reviews Earth & Environment* **4**, 487–505. (10.1038/s43017-023-00431-y)
65 Ragettli S, Zhou J, Wang H, Liu C, Guo L. 2017 Modeling flash floods in ungauged mountain catchments of China: A decision tree learning approach for parameter regionalization. *Journal of Hydrology* **555**, 330–346. (10.1016/j.jhydrol.2017.10.031)
66 Kratzert F, Klotz D, Shalev G, Klambauer G, Hochreiter S, Nearing G. 2019 Towards learning universal, regional, and local hydrological behaviors via machine learning applied to large-sample datasets. *Hydrology and Earth System Sciences* **23**, 5089–5110. (10.5194/hess-23-5089-2019)
67 Fang K, Kifer D, Lawson K, Feng D, Shen C. 2022 The Data Synergy Effects of Time-Series Deep Learning Models in Hydrology. *Water Resources Research* **58**, e2021WR029583. e2021WR029583 2021WR029583 (10.1029/2021WR029583)
68 Kratzert F, Gauch M, Klotz D, Nearing G. 2024 HESS Opinions: Never train an LSTM on a single basin. *Hydrology and Earth System Sciences Discussions* **2024**, 1–19. (10.5194/hess-2023-275)
69 Papacharalampous G, Tyralis H. 2022 A review of machine learning concepts and methods for addressing challenges in probabilistic hydrological post-processing and forecasting. *Frontiers in Water* **4**, 961954. (10.3389/frwa.2022.961954)

70 Tyralis H, Papacharalampous G. 2024 A review of predictive uncertainty estimation with machine learning. *Artificial Intelligence Review* **57**, 94. (10.1007/s10462-023-10698-8)

71 Althoff D, Rodrigues LN, Bazame HC. 2021 Uncertainty quantification for hydrological models based on neural networks: the dropout ensemble. *Stochastic Environmental Research and Risk Assessment* **35**, 1051–1067. (10.1007/s00477-021-01980-8)

72 Srivastava N, Hinton G, Krizhevsky A, Sutskever I, Salakhutdinov R. 2014 Dropout: a simple way to prevent neural networks from overfitting. *Journal of machine learning research* **15**, 1929–1958.

73 Rudin C. 2019 Stop explaining black box machine learning models for high stakes decisions and use interpretable models instead. *Nature machine intelligence* **1**, 206–215. (10.1038/s42256-019-0048-x)

74 Arif S, MacNeil MA. 2022 Predictive models aren't for causal inference. *Ecology Letters* **25**, 1741–1745. (10.1111/ele.14033)

75 Mamalakis A, Barnes EA, Ebert-Uphoff I. 2022 Investigating the fidelity of explainable artificial intelligence methods for applications of convolutional neural networks in geoscience. *Artificial Intelligence for the Earth Systems* **1**, e220012. (10.1175/AIES-D-22-0012.1)

76 Müller S, Toborek V, Beckh K, Jakobs M, Bauckhage C, Welke P. 2023 An empirical evaluation of the Rashomon effect in explainable machine learning. In *Joint European Conference on Machine Learning and Knowledge Discovery in Databases* pp. 462–478. Springer. (10.1007/978-3-031-43418-1_2)

77 Huang F, Shangguan W, Jiang S. 2024 Identifying potential drivers of land-atmosphere coupling variation under climate change by explainable artificial intelligence. Technical report EGU General Assembly 2024, Vienna, Austria, 14–19 Apr 2024. (10.5194/egusphere-egu24-7202)

78 Schmidt L, Heße F, Attinger S, Kumar R. 2020 Challenges in applying machine learning models for hydrological inference: A case study for flooding events across Germany. *Water resources research* **56**, e2019WR025924. (10.1029/2019WR025924)

79 Li W, Migliavacca M, Forkel M, Denissen JM, Reichstein M, Yang H, Duveiller G, Weber U, Orth R. 2022 Widespread increasing vegetation sensitivity to soil moisture. *Nature Communications* **13**, 3959. (10.1038/s41467-022-31667-9)

80 Krabbenhoft CA, Allen GH, Lin P, Godsey SE, Allen DC, Burrows RM, DelVecchia AG, Fritz KM, Shanafield M, Burgin AJ et al.. 2022 Assessing placement bias of the global river gauge network. *Nature Sustainability* **5**, 586–592. (https://doi.org/10.1038/s41893-022-00873-0)

81 Kraft B, Jung M, Körner M, Koirala S, Reichstein M. 2021 Towards hybrid modeling of the global hydrological cycle. *Hydrology and Earth System Sciences Discussions* **2021**, 1–40. (10.5194/hess-26-1579-2022)

82 Nearing GS, Kratzert F, Sampson AK, Pelissier CS, Klotz D, Frame JM, Prieto C, Gupta HV. 2021 What role does hydrological science play in the age of machine learning?. *Water Resources Research* **57**, e2020WR028091. (10.1029/2020WR028091)

83 Kratzert F, Nearing G, Addor N, Erickson T, Gauch M, Gilon O, Gudmundsson L, Hassidim A, Klotz D, Nevo S et al.. 2023 Caravan-A global community dataset for large-sample hydrology. *Scientific Data* **10**, 61. (https://doi.org/10.1038/s41597-023-01975-w)

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