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Impact Statement: Deep learning may assist hydrological inference through its increased capacities to interpolate, classify and hierarchically model databases.

Introduction

Decision making relative to groundwater resources requires the characterization, modeling and prediction of complex and dynamical systems with many degrees of freedom. Nonetheless, these systems have large-scale structure that emerges from hierarchical properties based on conservation principles applied to fundamental physical quantities (e.g. mass, momentum, energy). Difficulties arise as hydrologic systems are inherently heterogeneous and sometimes chaotic. This is not specific to hydrology, it is generic to natural or man-made complex systems. Two approaches have been proposed to handle these complex systems. Whether they are called model-driven or data-driven, explicit or implicit, they differ widely by methodology. In the explicit model-driven approach, processes are physically modeled at each characteristic scale and progressively scaled up. Patterns, equivalent properties and effective laws emerge progressively through upscaling. This has been done extensively in stochastic hydrology to derive equivalent permeability and in percolation theory to identify universal scaling laws (Stauffer and Aharony 1992). Large-scale observations are integrated by adapting the model parameters through the classic, but generally ill-posed, inverse problem (Zimmerman et al. 1998). In the implicit data-driven approach, minimal assumptions are made on the structure of the models developed (Hastie et al. 2003; Montgomery 2006). Rather, this approach relies on generic data-driven analysis based on statistics and artificial intelligence. Among numerous methods, supervised-learning algorithms and, especially, artificial neural networks became popular in the 90s in hydrology. One well-cited example is their use for prediction and understanding of rainfall runoff processes (Hsu et al. 1995; Hsu et al. 2002).

Implicit data-driven methods have been less active for the past decade (a period called the Artificial Intelligence Winter). But, there is renewed interest in machine learning methods due to the recent successes of deep neural networks in several Artificial Intelligence benchmarks including the first-time computer win at the game of Go (Silver et al. 2016). In general, deep network successes have been attributed to their ability to provide efficient high-dimensional interpolators that cope with multiple scales and heterogeneous information (LeCun et al. 2015; Mallat 2016). This suggests a natural opportunity for the use of deep networks for hydrological sciences. We discuss these possibilities with particular focus on their complementary and combined use with well-established model-driven approaches.

Generalization, classification and hierarchical combination abilities in deep learning

Deep learning is a new class of machine learning algorithms that recognizes high level abstractions in data. They are called deep because they are made up of some tens of hierarchically arranged layers, compared to classic neural networks that had only very few. Abstraction is achieved through the processing of the data by the internal layers to automatically identify patterns of increasing complexity. We review three essential properties for their potential interest in hydrological sciences.

Deep learning can be used for calibration. Classic neural networks have been shown to be universal estimators (Hornik et al. 1989). Deep learning can significantly improve their efficiency and accuracy (Bengio and Delalleau 2011; Mhaskar and Poggio 2016).

Deep learning can find robust invariants from large, high dimensional datasets, leading to improved interpolation and generalization (Hinton and Salakhutdinov 2006). For example, a deep convolutional generative adversarial network (Goodfellow et al. 2014) was able to generate new bedroom images having all the same elements (bed, lamp, bedside table…) as the bedroom pictures used for training (Radford et al. 2015).

Deep learning successes might indicate fundamental capacities to replicate multiscale modeling of physical principles. Generalization properties of deep convolutional networks have been related to the locality and upscaling principles of wavelets (Mallat 2016). The multilayer convolutive structure of deep networks is well adapted to let hierarchical patterns emerge through the combination of smaller scale elements. Potential consistency with physical processes may be further linked to the compositional nature of some physical processes, which might be derived from advanced combinations of symmetry, locality and compositional principles (Lin and Tegmark 2016). As an illustration, deep networks have prospectively been used to infer quantum energy of complex molecules, reaching state of the art quality of evaluation alternatively derived from Schrödinger equations (Hirn et al. 2016). This inherent upscaling opens new opportunities to apply deep learning to real physical systems (Baldi et al. 2014; Denil et al. 2016).

Deep learning prospects for hydrological inference

Among the different interests of deep learning for hydrology, the first is its potential contribution to calibration, following the use of artificial neural networks in the 90s. Deep networks are especially designed for handling large data sets. They might be considered for prediction issues (Figure 1, blue arrows), provided that the following conditions are met. Hydrological data are highly diverse and would require some extensive pre-processing to produce uniform training sets for deep networks. Basic prerequisite of deep learning methods should also be checked in terms of the density and nature of the training information. Nevertheless, deep neural networks have already been used for predicting precipitation from satellite clouds images and reduce significantly the bias compared to traditional neural networks (Tao et al. 2016).

Second, deep networks may contribute to the initial choice of the structure of a physical model, which strongly conditions eventual predictions. For geological storage of high-level nuclear wastes, this issue has been handled by requesting independent models (models ensemble) from different research groups (Zimmerman et al. 1998; Bodin et al. 2012). Such benchmarks are, however, possible only for highly sensitive applications with significant costs. On the other hand, modeling as well as computational capacities have critically progressed to the point such that it is feasible to simulate a broad range of model configurations (Kumar 2015). Models also become more faithful to the point where synthetic catchments, synthetic aquifers and virtual observatories no longer seem out of reach (Thomas et al. 2016; Yu et al. 2016). The limiting factor increasingly comes from the exploration and analysis of the resulting simulations (Hermans 2017). Deep networks might contribute to more systematic interpretation through interpolation and category classification. They could be considered for interpolating explicit models as has been done in surrogate modeling (Figure 1, green arrows) (Razavi et al. 2012; Asher et al. 2015). They could also be trained on extensive databases of model realizations that support uncertainty analyses (de Pasquale 2017). The advantage of deep networks over other interpolators is their ability to cope with many simulations while inherently complying with different levels of organization of the hydrological systems (Sposito 1998). Practically, this will require careful consideration of methods to execute many models, manage errors, systematize formatting of inputs and outputs, and ensure easy access to simulation results.

Using deep networks as a possible high-dimensional interpolator is motivated by some reduction in computational costs through the use of existing simulations. But, current interest is also directed to model reduction, category classification and uncertainty quantification through the constitution of extensive databases of simulations (Figure 1, green arrows) (Clark et al. 2015). Model reduction is an active field of research in applied mathematics and computational science (Schilders 2008) designed to retain only the key structural parameters of the models for the phenomena or predictions of interest (Castelletti et al. 2012). While the first target would be to refine our understanding of hydrological processes, several other issues could be handled. For example, the ability to identify model classes would help to address the question of the model structural adequacy beyond the identification of optimal parametrization (Gupta et al. 2012; Guthke 2017). It might also contribute to identify classes of acceptable models at the core of null-space identification (Gallagher and Doherty 2007), equifinality analysis (Beven 2006), and, more generally, uncertainty quantification. Even more prospectively, we might investigate its potentialities in proposing alternative model structural assumptions, especially for investigating the likelihood of diverse hydrological scenarios of critical importance for stakeholders (Ferre 2017; Marshall 2017) and in assisting the design of hydrological experiments (Kikuchi et al. 2015) (Figure 1). Deep networks might be used to assess expert knowledge in a more systematic way (Seibert and McDonnell 2002; Hrachowitz et al. 2014). The real strength of deep networks, and implicit data-driven models in general, is that emergent system properties can be identified that cannot be uncovered by explicit models that are imposed on an analysis (Figure 1, orange arrows). This may automatically adapt our models to conform to natural processes and to the data available (Kirchner 2006; Troch et al. 2009), while exploring model space more completely.

Despite the potential contributions of deep learning, we do not suggest that they should replace classic approaches in hydrology. Rather, they are attractive as a complementary tool having, at least conceptually, some properties highly relevant to hydrological systems like their built-in hierarchical combination. This could similarly benefit ongoing automated model-building efforts that also require some definition of the range of model structures to consider and the ways in which they should be combined (Clark et al. 2015). In addition to these enhanced capacities, deep networks will find particular use in integrating larger data sets and explicit model results produced by rapid technological progress in automated and remote sensing. In this sense, we see deep learning as a loose coupling between growing data-driven and model-driven approaches (Figure 1). It is not designed as an effective calibration technique applied on explicit physical models (Certes and de Marsily 1991; Doherty 2003), but rather as an implicit data-driven approach to correct errors from explicit physical based models (Szidarovszky et al. 2007; Demissie et al. 2009; Gusyev et al. 2013). Prospective testing and interactions are needed with the deep learning community to understand how information content between synthetic models and field data should be balanced in the training sequence (Nearing and Gupta 2015).

A roadmap to investigate the relevance of deep learning to hydrology

We propose three steps toward integrating deep learning into hydrologic science: testing on data; testing on benchmarks; and collaboration with the wider deep learning community.

Testing on hydrological numerical data will require the collection and organization of systematic and well-organized databases. Availability of such database has been one of the main reasons for the success of deep learning techniques (Krizhevsky et al. 2012). This could include measured data, but should also rely heavily on synthetic data sets. Such synthetic hydrological databases are achievable, for example by building extensive stochastic simulations performed on heterogeneous media (Pirot 2017). Constitution of systematic and standardized field databases is also under way following the dynamics of critical zone observatories, open international normalization initiatives (Ames et al. 2012) and regulatory incentives.

Testing on hydrological benchmarks can begin with target synthetic benchmarks described above. More complicated benchmarks can be developed according to their consistency with existing deep learning benchmarks, i.e. based on images or succession of images to describe processes (Mathieu et al. 2015). Hydrologic insight will be necessary to ensure that the benchmarks are relevant to important hydrological complexities, especially those related to the multi-scale nature of the hydrologic systems.

Cross-disciplinary discussions with the deep learning community will be required to take full advantage of deep learning methods and to introduce hydrology as a topic of interest to that community. Data heterogeneity, in terms of quantities measured and scales, have already been mentioned and are critical to improve our ability to integrate diverse information sources. Hydrology offers an opportunity for the deep learning community to expand their interest beyond controlled and deterministic systems like the double pendulum (Schmidt and Lipson 2009) to natural systems that are characterized by epistemic or aleatory uncertainties. The heterogeneous and sometimes chaotic nature of the hydrologic system makes it difficult to directly transpose existing results obtained on deterministic experiments but is an opportunity to assess deep learning potentialities.

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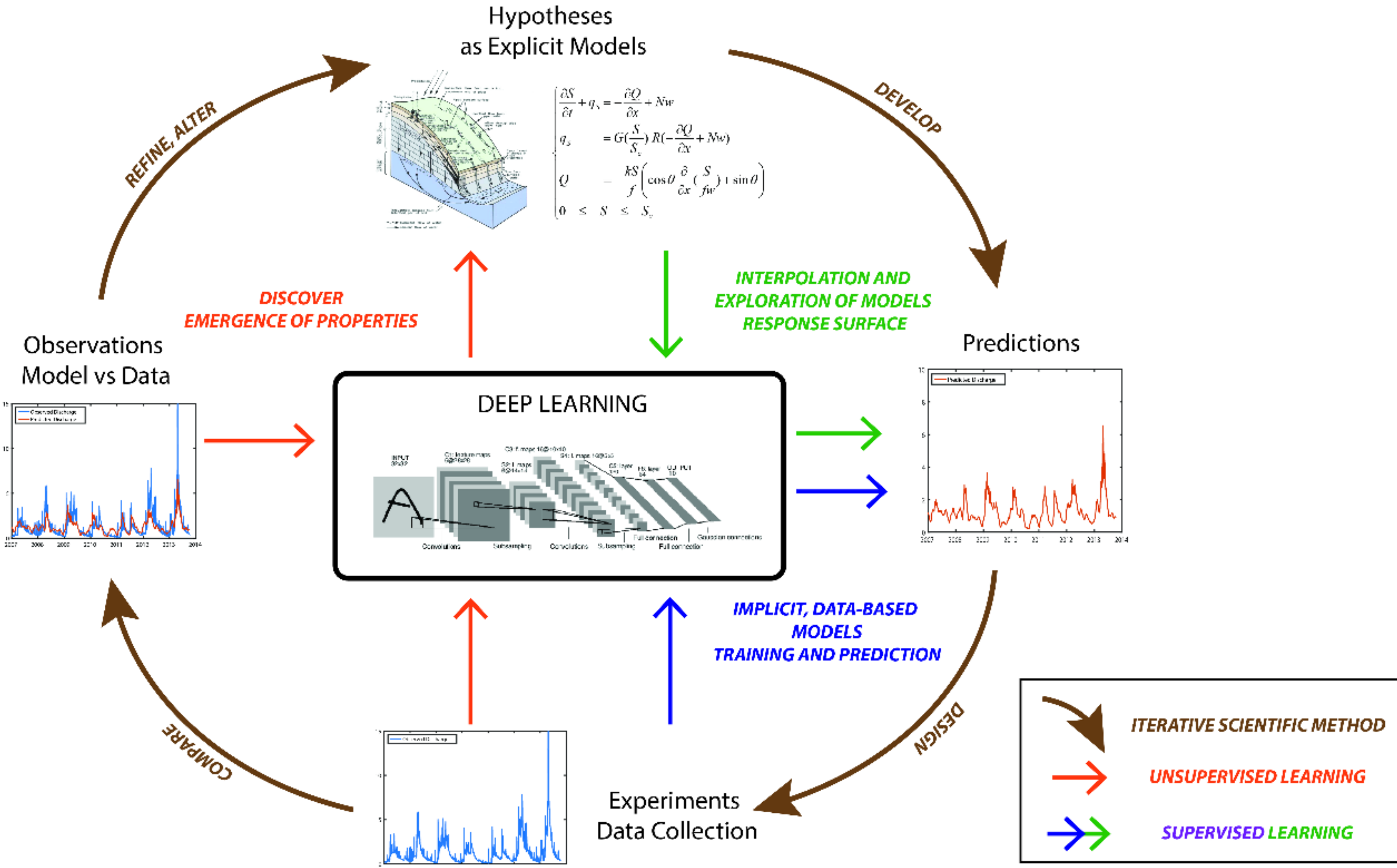
Figure

Figure 1: Deep learning seen as a complementary tool to assist iterative hydrological inference. Brown arrows show the classic methodology for understanding processes (here rainfall/runoff processes) by confronting hypotheses (explicit, process-based models) formulated as predictions to experiments and data. Deep learning could be used as implicit, data-based models trained (calibrated) on real datasets to perform predictions (blue arrows). It could provide a tool to explore and interpolate model simulations, or even model ensembles (green arrows). More prospectively, it might be applied to discover patterns in data, find trends in synthetic versus real data misfits to assist hydrologists in formulating testable hypotheses (orange arrows). This last possibility is seen as an unsupervised learning task as opposed to supervised learning for the other ones with real or synthetic datasets.



Hypotheses
as Explicit Models
DEVELOP
REFINE, ALTER
DISCOVER
EMERGENCE OF PROPERTIES
INTERPOLATION AND
EXPLORATION OF MODELS
RESPONSE SURFACE
Observations
Model vs Data
Predictions
DEEP LEARNING
IMPLICIT, DATA-BASED
MODELS
TRAINING AND PREDICTION
COMPARE
DESIGN
Experiments
Data Collection
ITERATIVE SCIENTIFIC METHOD
UNSUPERVISED LEARNING
SUPERVISED LEARNING