Theory-Guided Machine Learning Applied to Hydrogeology: State of the Art, Opportunities and Future Challenges – A review

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Abstract

Thanks to recent technological advances, hydrogeologists now have access to large amounts of data acquired in real time. Processing these data using traditional modelling tools is difficult and poses a number of challenges especially for tasks such as extracting useful features, uncertainty quantification or identifying links between various variables. Artificial Intelligence, and more specifically its subset Machine Learning, may represent a way of the future in hydrogeological research and applications. Unfortunately, several aspects of machine learning methods hamper its adoption as a complementary tool for hydrogeologists, namely the black-box nature of most models, an often-limited generalization ability, a hypothetical convergence, and uncertain transferability. Recently, an entirely novel paradigm in the field of machine learning has been identified: theory-guided machine learning, in which the models integrate some specific theoretical knowledge, laws or principles of the field of study. This review article set out to examine three theory-guided methods in their ability to overcome the limitations of machine learning for hydrogeological research and applications. These methods are, respectively, Theory-Guided Constrained Optimization (TGCO), Theory-Guided Refinement of Outputs (TGRO) and Theory-Guided Architecture (TGA). The analyses led to the following conclusions: the opacity of ML models can be reduced by any of the three theory-guided ML methods; convergence and generalizability can be enhanced by TGCO, TGA, or a combination of at least two of the theory-guided ML methods; no study conducted to date has made it possible to deduce the effectiveness of these methods on the transferability of ML models.

Keywords Theory-guided machine learning · Groundwater · Machine learning limitations · Statistical modelling

1. Introduction

Hydrogeological research and practices have evolved over the years with the challenges facing the world. Today, hydrogeology strives to find solutions to problems such as the sustainable supply of drinking water, geothermal energy production, environmental protection and the fight against climate change and its effects on groundwater. To provide a solution to these problems, Hydrogeologists systematically resort to modelling. To model simple hydrogeological problems, simplified models are usually used. For example, John and Das (2020) used a piezometric contour map to identify risk zone areas of declining piezometric levels, while Chesnaux et al. (2018) proposed analytical solutions obtained through idealized hypotheses, using groundwater travel time in Dupuit-Forchheimer aquifers, for assessing recharge. To address more complex problems, numerical models are employed to derive an approximate solution by iteratively solving a discrete form of the equation that governs the hydrogeological phenomenon under study (Feng et al. 2011, Raazia and Dar 2021).

Thanks to recent technological advances for data collection such as the Internet of Things (Su et al. 2020), hydrogeologists now have access to large amounts of data acquired in real time. Processing such amounts of data poses a challenge to traditional modelling tools for tasks such as extracting useful features, uncertainty quantification or identifying links between various variables (Tahmasebi et al. 2020). As a result, over the past two decades, the field of hydrogeology has viewed Machine Learning (ML) with increasing interest as a new complementary modelling paradigm. As a research subfield of Artificial Intelligence, the goal of ML is to design and implement parametric and non-parametric methods that are used to generate models to solve a specific problem. Besides semi-supervised learning and reinforcement learning, ML methods can be classified into two categories: supervised and unsupervised learning methods (Ayodele 2010).

In supervised learning, the goal is to allow the computer to learn to relate input and output variables using a set of data samples containing the data relating to the input variables and those associated with the output variable. For parametric methods for example, supervised learning consists in automatically adjusting the parameters of the ML method while minimizing a cost function which measures the gap between the outputs of the model and the corresponding true values. The adjustment stage is the first step in the model generation process by supervised learning. This adjustment stage is generally followed by a cross-validation stage which makes it possible to select the model with the best performance and finally, a test stage whose objective is to produce an unbiased evaluation of the model previously selected. Implementing different stages requires splitting the data into three subsets: a training set, a cross-validation set and a test set. Some popular examples of supervised learning methods are linear regression and artificial neural networks.

In unsupervised learning, the computer learns to identify hidden patterns in the data without any outside help. In particular, the computer learns to extract classes or groups of individuals having common characteristics. Principal component analysis is a well-known example of an unsupervised learning method.

In hydrogeology, supervised and unsupervised ML, including deep learning, have been used to address various issues such as the evaluation of groundwater quality (Khalil et al. 2005, Mohamed et al. 2019, Park et al. 2016, Wang et al. 2016), groundwater potential (Arabameri et al. 2019, Bahareh et al. 2019, Moghaddam et al. 2020, Naghibi et al. 2017), aquifer parameters (Tayfur et al. 2014, Tutmez et al. 2006), groundwater vulnerability (Afshar et al. 2007, Sajedi-Hosseini et al. 2018), water balance and recharge of aquifers (Gorgij et al. 2017, Pradhan et al. 2019) and groundwater level (Barzegar et al. 2017, Chang et al. 2016, Sahoo and Jha 2013, Tapoglou et al. 2014). For example, Tapoglou et al. (2014) used an artificial neural network, trained using an optimisation method called particle swarm, to generate a model to forecast groundwater levels on day *k* under climate change scenarios for a unique well. Rainfall at two meteorological stations, temperature and hydraulic head on day *k-1* were selected as input variables. To project the effects of climate scenarios, the meteorological time series were generated by a weather condition generator, the LARS-WG 5. The results indicated that the generated model is very accurate in representing the groundwater level dynamics and only the most severe climate change scenario results in a subsidence of groundwater levels. Chen et al. (2020a) performed a comparative study among ML and numerical models for simulating groundwater dynamics. Artificial neural networks and support vector machines have been used as ML methods, with time series of pumping rate, recharge rate, streamflow rate as input variables. The results have shown that in terms of accuracy, ML models produce better results the majority of time.

Despite the growing interest in ML in hydrogeology and the very high level of accuracy it can offer, at least four factors still hamper the adoption of ML models as an effective complementary tool to traditional models such as numerical models. The first limiting factor is that most ML models have a black-box nature (Rudin 2019). Black-box models establish a relationship between some inputs and outputs of a system, without any knowledge of the laws that govern its functioning or the causal relationships existing between the related variables. Unlike the parameters of hydrogeological variables such as hydraulic conductivity, storativity, parameters of ML black-box models have no physical significance (Zhang 2010). Therefore, the use of ML black-box models does not allow hydrogeologists to explain or justify model outputs, whether it be to gain understanding of the modelled phenomenon or to attain confidence levels sufficient for supporting high-stakes decision-making. Groundwater exploitation activities most often present major issues related to the water supply in regard to populations or their health risks. An erroneous forecast made by a black-box model can therefore have significant socio-economic consequences.

The second limiting factor is that, even if ML models applied to hydrogeology offer an adequate level of simulation accuracy, the same is not always the case for their generalization ability. Several studies have pointed out that ML models are generally subject to poor generalization ability (Adamowski and Chan 2011, Ch and Mathur 2012, Huang et al. 2019). The generalization ability is poor when the model provides fair simulations but struggles to make predictions for data that it did not encounter during training (Urolagin et al. 2011) . Formally, the generalization ability can be represented as the ratio between the prediction error and the training error (Chen et al. 2020a). When the ratio is higher than 1, the model is said to poorly generalize. A poor generalization ability may be due either to the use of a training dataset that is too small, less representative or that contains too much noise, or it may be due to the trade-off that is made between the desired accuracy and the assumptions on the complexity of the problem to be solved (Ying 2019). Fundamentally, ML models with relatively low generalization ability cannot be used with confidence to study the future behaviour of a hydrogeological system with respect to a given phenomenon.

The third limiting factor is that, ML models may not converge (Zobeiry et al. 2020b). ML models being analogous to a classical discretization scheme used to solve a problem involving differential equations (Bar-Sinai et al. 2019) as is the case for the modelling of groundwater flow, the convergence of ML models is governed by two components namely physical consistency and stability (Arnold 2015). Consistency is a quantity which evaluates to what extent the outputs of ML models satisfy the theory and more specifically, in the context of groundwater modelling, the differential equation governing water dynamics. The physical consistency is evaluated by calculating the average residue of the PDE governing the functioning of the system. The more the mean residual tends towards zero, the more consistent the model. As for stability, it describes the robustness of ML models facing a minor disruption applied to the data (Shaham et al. 2018). Stability can be evaluated by calculating the relative error, given by the ratio between the error associated with the disrupted solution (outputs of the model) and that associated with the disrupted data (e.g., inputs of the model). The model is stable if the relative error is bounded. A ML model converges if it is both consistent and stable. Convergence is essential to provide reliable prediction (Bakshi et al. 2016).

And finally, the fourth limiting factor is that ML models are not automatically extensible to adapt to the occurrence of a new event in the modelled system. The ability of a ML model to adapt to new tasks is generally referred to as transferability. This can be illustrated by taking the example of an unconfined aquifer whose groundwater levels are influenced only by precipitation and temperature and for which a ML model must be implemented. Intuitively, precipitation and temperature will be chosen as the model input to represent the groundwater levels. Suppose that shortly after implementing the model, a pumping well is installed in the aquifer. It is very likely that the model is not able to represent the influence of the well on the groundwater levels. To handle this new event, a new model must be built. In other words, a ML model that was built based on a certain hydrogeological configuration cannot be used for a different configuration. In various studies such as Sahoo and Jha (2013), Shiri et al. (2013) and Sahoo et al. (2017), perhaps due to a lack of data, ML is used to relate complex hydrogeological variables such as hydraulic head or contaminant concentration with a set of input variables chosen without necessarily considering domain knowledge and theory. To some extent, these studies limit the modelled problem to a representation of reality that does not represent its true complexity. Therefore, the model transferability is reduced by default.

To alleviate some of the limiting factors of ML in the physical sciences, various authors have proposed different methods. To solve poor generalization ability problems, some authors propose to add a data processing operation aimed at reducing noise (Clark and Niblett 1989, Pazzani and Brunk 1991). Others propose to either acquire more data or manipulate the existing data to generate some new data (Sun et al. 2014, Yip and Gerstein 2009). Still others propose to limit the effect of non-relevant input variables by means of regularization methods (Srivastava et al. 2014, Warde-Farley et al. 2013) or to use validation data to prevent a poor generalization ability (Brodeur et al. 2020). To mitigate the black-box nature of some ML models, methods of a subfield of artificial intelligence, eXplainable Artificial Intelligence (XAI), have been used by several authors such as Nguyen et al. (2020b) and Nguyen et al. (2020c) in the field of hydrogeology or Kavvas et al. (2020) in the field of genetics. XAI aims to design and implement methods that make it possible to understand what is happening in the black box.

Recently, a new paradigm of ML has started to emerge in geosciences. Theory-guided machine learning (Karpatne et al. 2017), sometimes also referred to as Physics-informed machine learning (Raissi et al. 2019), consists of integrating theoretical knowledge into the learning process of ML models. The learning process is made to include, for example, the advection-dispersion equation, the diffusion equation or the applicable physical constraints, so that the ML model not only learns the patterns contained in the data but is also given the knowledge allowing it to avoid violating the known theory about the phenomenon studied. This approach seems likely to present the combined advantages of ML models and numerical models. These include rapid model implementation, e.g. in few days (Chen et al. 2020a), high simulation accuracy, modelling at any scale easily, low computational costs for ML and a better understanding of hydrogeological processes, good generalization ability and a possible transferability under certain conditions for numerical models. Theory-guided machine learning models have shown promising results in various scientific disciplines (Liu et al. 2013, Piccione et al. 2020, Zobeiry et al. 2020a). However, in hydrogeology, the application of Theory-guided machine learning is quite new. Consequently, few studies exist.

The purpose of this article is to review mainly the existing hydrogeological literature on the topic of Theory-guided Machine Learning as well as that of other scientific domain and assess the extent to which Theory-guided Machine Learning can help overcome the stated limiting factors of ML in hydrogeological research and applications. As a reminder, the limiting factors concern the black-box nature of most ML models, an often-limited generalization ability, hypothetical convergence, and uncertain transferability. In view of the current literature, no review on the topic still exists in hydrogeology. This paper is organized as follows: Section 2 describes the state of the art of the methods of Theory-guided machine learning used in hydrogeology, including an analysis of the literature to highlight the ability of Theory-guided methods to overcome or not the limiting factors mentioned above. Section 3 identifies and discusses some of the remaining challenges, as well as future avenues.

2. Theory-guided ML vs ML limiting factors in Hydrogeology

Although theory-guided machine learning has been used as a paradigm in the physical sciences for a long time, only recently has a taxonomy of its characteristics been proposed by Karpatne et al. (2017). Theory-guided machine learning consists in incorporating theoretical knowledge, such as governing equations, prior domain knowledge or causal relations into the learning process of ML models. The use of theory-guided learning is supposed to allow the model to agree with both observations and theory. In the existing hydrogeological literature on theory-guided machine learning, there are three approaches for integrating fundamental knowledge of hydrogeology into the models. The first, designated as Theory-Guided Constrained Optimization, consists in integrating the theory into the cost function (Tartakovsky et al. 2020, Wang et al. 2020a, Xu et al. 2020). The second, called Theory-Guided Refinement of Outputs, consists in postprocessing the outputs of the model to make theme conform to the theory as accurately as possible (Chen et al. 2020b, Hautier et al. 2010, Khandelwal et al. 2015). The third, designated as Theory-Guided Architecture, consists in using what is known theoretically about the phenomenon under study to design the architecture of the ML model (Daw et al. 2020, Tartakovsky et al. 2020, Udrescu and Tegmark 2020) . In the following section, these three approaches are presented and their ability to overcome the limiting factors of ML models is analysed. It is important to note that other approaches of Theory-guided ML exist in the literature and are well described from a general point of view by various other review articles such as that of Karpatne et al. (2017) or that of Willard et al. (2020).

2.1. Theory-Guided Constrained Optimisation

To introduce the basic idea behind Theory-Guided Constrained Optimisation (TGCO), consider a 2D subsurface flow in saturated homogeneous and isotropic porous medium as in Wang et al. (2020a). This subsurface flow satisfies the following governing equation:

$$K\left(\frac{\partial^2 h}{\partial x^2}+\frac{\partial^2 h}{\partial y^2}\right)=S_s\frac{\partial h}{\partial t} \tag{1}$$

Where h is the hydraulic head (m); K is the hydraulic conductivity (m/s); S_s is the specific yield (-); x, y are the horizontal space variables (m); t is the time (s). The initial condition can be expressed as follows:

$$h(t_{IC})=h_{IC} \tag{2}$$

The Dirichlet and Neumann boundary conditions can be expressed respectively as follows:

$$h(x_D, y_D)=h_D \tag{3}$$

$$K\frac{\partial h}{\partial n}=q \tag{4}$$

Where h_{IC}, represents the initial hydraulic head (m), h_D, the specified hydraulic head (Dirichlet boundary condition) (m), and q, the constant flux related to Neumann boundary condition (m/s). t_{IC} is the initial time (s) and x_D, y_D are the spatial coordinates of the points located on the Dirichlet boundary (m). Also, denote by $\hat{h}$ the hydraulic head simulated by the ML model to train (m), and the observed value by h (m). Generally, a standard cost function for a ML model is defined as follows:

$$\mathcal{L}_{std}=\frac{1}{2}\left(\hat{h}-h\right)^2 \tag{5}$$

Since the training consists in adjusting the ML model parameters using the cost function as a guide, the adjusted parameters of the ML model that will have led to a low value of the cost function will be closer to the optimal values. However, nothing guarantees that the simulation will not violate the governing equation. Thus, in TGCO, it is considered important to re-constrain the hydraulic head simulations by adding other terms in the cost function representing the residual of the governing equation and the residual of initial, Dirichlet and Neuman boundary conditions defined respectively as follows:

$$\mathcal{R}_{eq}=K\left(\frac{\partial^2 \hat{h}}{\partial x^2}+\frac{\partial^2 \hat{h}}{\partial y^2}\right)-S_s\frac{\partial \hat{h}}{\partial t} \tag{6}$$

$$\mathcal{R}_{IC}=\hat{h}-h_{IC} \tag{7}$$

$$\mathcal{R}_D=\hat{h}-h_D \tag{8}$$

$$\mathcal{R}_N = K\frac{\partial \hat{h}}{\partial n} - q \tag{9}$$

To compute the residual $\mathcal{R}_{eq}$ of the governing equation and the residual $\mathcal{R}_N$ of the Neumann boundary condition, Wang et al. (2020a) applied the chain rule through automatic differentiation, but the residuals can also be approximated by discretization methods such as finite element method or finite difference method as in Chen et al. (2020b). Finally, the cost function according to the TGCO method can be defined as follows:

$$\mathcal{L} = \lambda_1\mathcal{L}_{std} + \lambda_2\mathcal{R}_{eq}^2 + \lambda_3\mathcal{R}_{IC}^2 + \lambda_4\mathcal{R}_D^2 + \lambda_5\mathcal{R}_N^2 \tag{10}$$

Where $\lambda_{i=1\ldots5}$ is a coefficient making it possible to weight the importance of the corresponding term in the cost function. Other constraints can be added according to additional knowledges or observations regarding the aquifer. For example, it could have been observed that the hydraulic head at a point of interest never falls below a certain value. So, it could be useful to impose this constraint during the model training. Fig. 1 locates the part of the ML process modified by the TGCO method, that is, the cost function. Such an intervention is meant to allow the generated ML model to correspond as accurately as possible to the theory.

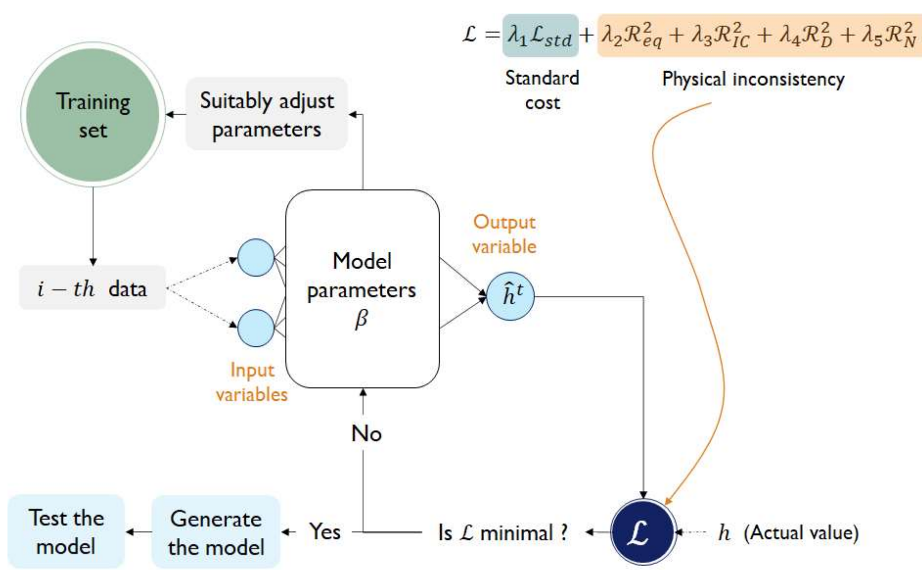

Fig. 1 Part of the ML process modified by the TGCO method, that is, at the level of cost function (*solid blue circle*)

The TGCO method is one of the most developed methods in the field of physical sciences in general and in hydrogeology in particular for tasks such as solving partial differential equations (Karimpouli and Tahmasebi 2020, Meng et al. 2020), building surrogate models and uncertainty quantification (Wang et al. 2021), inverse modelling (Kadeethum et al. 2020, Kahana et al. 2020, Sun 2018), or data generation (Zobeiry and Humfeld 2021).

Karimpouli and Tahmasebi (2020) compared the performance of two ML methods to solve a time-dependent 1D seismic wave equation, namely a Gaussian process and a TGCO neural network. The results showed that the TGCO neural network is more accurate for velocity (P and S waves) and density inversion. Zobeiry and Humfeld (2021) compared the performances of standard neural network and TGCO neural network with feature engineering in modelling the conductive heat transfer. The models built were validated by comparing their results with those of a numerical finite element model (FE). The results showed that although the standard neural network and the TGCO match the FE results in the training zone, only the TGCO with feature engineering can capture the physics of the problem to produce accurate predictions beyond the training stage. This result demonstrates that TGCO models are physically consistent and stable when properly tuned and correctly constructed. Consistent and stable TGCO models can be used to generate data for other applications, as might be done with a classical numerical model. Kahana et al. (2020) integrated a cost function term associated with the physical consistency of the temporal dynamics of waves to model the inverse problem of identifying the location of an underwater obstacle from acoustic measurements using a deep learning framework. The results showed that the use of TGCO led to a better accuracy and robustness of the model relative to its generalization. Meng et al. (2020) developed a parareal TGCO neural network by decomposing a long-time problem into many independent short-time problems supervised by an inexpensive solver designed to provide approximate predictions of the solution at discrete times, while initiating many fine TGCO neural networks simultaneously to correct the solution iteratively. The goal of this approach is to allow a significant acceleration of the resolution of partial differential equations (PDEs) on large spatio-temporal domains provided that the solver is fast and can provide reasonable predictions. Applied to solve the Burgers equation and a two-dimensional nonlinear diffusion-reaction equation, the results demonstrated that a parareal TGCO neural network model converges in a couple of iterations with significant speed-ups proportional to the number of time-subdomains employed. Kadeethum et al. (2020) proposed to study the influence of batch size on the TGCO neural network accuracy to approximate the parameters of PDEs in the context of inverse modelling. Applying this study to Biot's equation, they showed that training with small batch sizes provides better approximations of physical parameters than using large batches but at the expense of longer training time.

In hydrogeology, Wang et al. (2020a) used the TGCO method to simulate the dynamics of groundwater levels in different hydrogeological configurations ranging from the simplest to more complex configurations including external variables such as pumping rate and noise in the data or even outliers. The results in Wang et al. (2020a) indicate that, with low noise data, the theory-guided model prediction errors are reduced by a factor of 4 to 11 compared to the model trained in the standard way. The TGCO method is therefore likely to improve the model's performance. Despite using data containing up to 20% noise, the predictions of the theory-guided model are hardly affected by noise. ML models generated using the TGCO method seem to be robust despite more or less minimal changes in the data. Xu et al. (2020) used a so-called weak form of the governing equation of groundwater flow to reduce computational cost and to capture local discontinuities. The results show an improvement of the model accuracy as well as its robustness in the presence of noise compared to a strong form of the governing equation as used by Wang et al. (2020a). Guo et al. (2020) demonstrated that under certain conditions, the model trained using the TGCO method could converge. Wang et al. (2021) used a TGCO fully connected neural network surrogate model coupled with the Monte Carlo method (MC) for uncertainty quantification for dynamic subsurface flow. The results showed that the TGCO neural network based surrogate can significantly improve the efficiency of uncertainty quantification tasks compared to the simulation-based implementation. Indeed, for any stochastic input sample, the output can be easily obtained from the surrogate TGCO neural network without having to solve the partial differential equation an umpteenth time. Therefore, the TGCO neural network surrogate can speed up the uncertainty quantification tasks.

These studies lead to conclude that the TGCO method improves the convergence of ML models and their ability to generalize. Theoretical models make it possible to represent, understand and explain the functioning of a phenomenon. Therefore, incorporating theory into the training process help to reduce the opacity of ML models to some extent. The cost function, in which the theory is integrated, plays a role only during the training stage. The appropriate choice of model inputs and a better design of the model architecture are therefore necessary to ensure that the model has the capacity to adapt to the occurrence of new events in the system under study. Finally, the use of the TGCO method for solving PDEs may not be fruitful in some real-life applications, in particular when the parameters of PDEs are uncertain or even unknown. Indeed, the resolution of PDEs for the study of the dynamics of a system requires a calibration of the parameters of these PDEs which cannot be possible if these parameters are unknown. The use of the TGCO method must be well supervised. In particular, the TGCO method must serve primarily to ensure the physical consistency of ML models in contexts where the physical parameters of PDEs are available.

2.2. Theory-Guided Architecture

Theory-Guided Architecture (TGA) consists in using the architectural properties of ML methods to integrate the properties and the laws of physics to ensure that the resulting models are consistent with the physics related to the problem being treated. The TGA method implicitly leads to reducing the opacity of ML models and promoting their interpretation and the understanding of their functioning. The TGA method can be used for inverse modelling (Tartakovsky et al. 2020), uncertainty quantification (Daw et al. 2020) or even the discovery of symbolic governing equations (Udrescu and Tegmark 2020). The applicable theory can be integrated into the architecture of ML models in several ways, namely the explicit incorporation of physically relevant variables, the decomposition of a problem into theoretically related sub-problems or the implementation of basic physical principles common to several dynamic physical systems such as invariance or monotonicity (Karpatne et al. 2017, Willard et al. 2020). For example, Muralidhar et al. (2020) proposed a convolutional neural network model using the TGA method for modelling the drag forces acting on each particle in a Computational Fluid Dynamics-Discrete Element Method. The drag force on a particle can be easily determined by knowing two intermediate variables namely the pressure field and the velocity field around the surface of the particle. Knowing that the pressure field directly affects the pressure component of the drag force, and the velocity field directly affects the shear component of the drag force, they built their model architecture to express physically meaningful intermediate variables such as the pressure field, velocity field, pressure component, and shear component in the neural pathway from the input features to the drag force. In short, this architecture is a succession of layers of neural networks linked together according to the understanding provided by the theory applicable to the problem being studied. The model was compared to several ML models and the results showed that the model achieved a significant performance improvement of 8.46% on average. A similar method was used in hydrogeology by Tartakovsky et al. (2020). Their study consisted in solving an inverse problem: determining the hydraulic conductivity at any point of the field of study by assuming access to either the observations of the hydraulic conductivity and the hydraulic head or only to the observations of the hydraulic head. Since the hydraulic conductivity can depend on the hydraulic head (e.g., to determine groundwater flow in an unsaturated zone), the authors proposed to model the hydraulic conductivity by adopting an architecture in the form of a two-step process: on the one hand, a model that learns the hydraulic conductivity, and on the other hand, another model which uses the simulations of the previous model to ensure that these simulations better represent the observations of the hydraulic head. Daw et al. (2020) proposed a Long Short-Term Memory model (LSTM), a Deep Learning neural network, using the TGA method in the context of lake temperature modelling. The architecture admits three components, the first of which makes it possible to extract temporal features from the input data. These features were used in the second component to generate an intermediate variable, that is, the density whose monotonicity is ensured (the density of water increases with depth). The third component uses the densities from the second component as well as the input data to predict the lake's temperature. The resulting model, associated with the Monte Carlo approach, is used to quantify the uncertainty. The results demonstrated the effectiveness of the approach in ensuring better generalization as well as physical consistency.

It is possible to implement physically consistent ML models by building their architecture in such a way as to integrate the properties of invariance and symmetry (Oberlack 2002, Willard et al. 2020). Wang et al. (2020b) proposed deep learning models to model physical dynamics by incorporating symmetries into the prediction model. The idea is that the integration of a certain symmetry in the architecture of the model can increase the likelihood of conserving the associated quantity, therefore rendering the prediction of the model more physically accurate. The results showed that the generalization ability of their proposed models was greatly improved. Ling et al. (2016) proposed a TGA neural network which embedded Galilean invariance in order to learn a model for the Reynolds stress anisotropy tensor. The results demonstrated that the TGA neural network made it possible to improve prediction accuracy compared with a standard neural network architecture. Udrescu and Tegmark (2020) combined a neural network with some physics-inspired techniques to help find a symbolic expression that matches the data of an unknown function. They built the architecture of neural networks in such a way that the resulting models were able to discover a hidden simplicity such as symmetry or data separability, which allows more difficult problems to be broken down recursively into simpler problems with fewer variables. Applied to 100 equations from the Feynman Lectures on Physics, the proposed algorithm was able to uncover them all, improving the peak success rate from 15 to 90% of existing methods.

Studies that have used the TGA method have shown that this method reduces the opacity of ML models. Indeed, the TGA method makes it possible to materialize the physical relationships between input and output variables or to forcibly integrate the laws of conservation into the structure of ML models. This has the advantage of improving the physical consistency of the resulting models and of promoting their convergence. It may further be stated that appropriate construction of the architecture of the model can promote its transferability to other hydrogeological configurations. However, there are currently no studies supporting this latter hypothesis. Fig. 2 illustrates a theory-guided design of architecture by means of decomposition of a problem into theoretically related sub-problems in modelling groundwater flow.

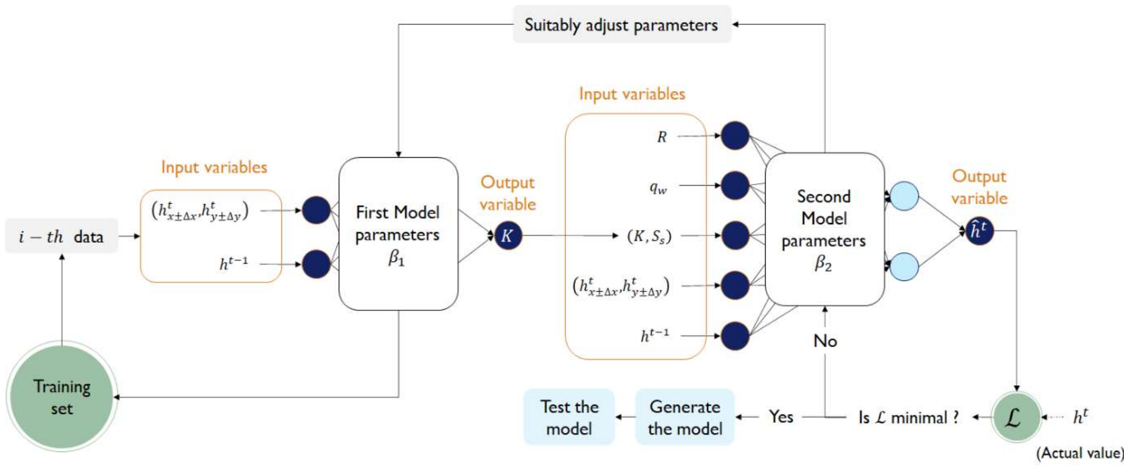

Fig. 2 Example of theory-guided design of architecture by means of decomposition of a problem into theoretically related sub-problems in modelling groundwater flow. R, q_w, K, S_s, $(h^t_{x\pm\Delta x}, h^t_{y\pm\Delta y})$, h^{t-1}, h^t, $\hat{h}^t$ represent respectively the recharge rate, pumping rate, hydraulic conductivity, storativity, hydraulic head in the neighbourhood of the point of interest, previous, current, and estimated hydraulic head at the point of interest.

2.3. Theory-Guided Refinement of Outputs

The principle of Theory-Guided Refinement of Outputs (TGRO) is to apply a transformation to the outputs of the ML models so that these outputs are consistent with governing equations. In the hydrogeological literature, this method has mainly been used by Chen et al. (2020b). To understand how the TGRO method works, the example employed by Chen et al. (2020b) will be shown here. The example consists in describing a 2D subsurface flow in a saturated porous medium without source or sink terms, whose governing equation is given as:

$$S_s \frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(K(x,y)\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K(x,y)\frac{\partial h}{\partial y}\right) \tag{11}$$

The TGRO method consists in applying a transformation function ϕ to the hydraulic head $\hat{h}$ simulated by the ML model to provide a new value $\hat{h}_r$ intended to be much closer to observed value h and to not violate the governing equation. Function ϕ approximates the governing equation while considering the initial and boundary conditions. All the means making it possible to approximate the governing equation and to bring $\hat{h}$ as close as possible to the observed value can be used. Chen et al. (2020b) proposed to use a projection method. First, they discretize Eqn (11) by means of a second order centre difference scheme along the x and y dimensions and a first-order backward Euler scheme along the t dimension:

$$0 = -S_s \frac{h^t - h^{t-\Delta t}}{\Delta t} + \left(\frac{K_{x-\frac{\Delta x}{2}}}{\Delta x^2} h^t_{x-\Delta x} + \frac{K_{x+\frac{\Delta x}{2}}}{\Delta x^2} h^t_{x+\Delta x} - \frac{K_{x-\frac{\Delta x}{2}} + K_{x+\frac{\Delta x}{2}}}{\Delta x^2} h^t \right) + \left(\frac{K_{y-\frac{\Delta y}{2}}}{\Delta y^2} h^t_{y-\Delta y} + \frac{K_{y+\frac{\Delta y}{2}}}{\Delta y^2} h^t_{y+\Delta y} - \frac{K_{y-\frac{\Delta y}{2}} + K_{y+\frac{\Delta y}{2}}}{\Delta y^2} h^t \right) \tag{12}$$

Second, they rearrange Eqn (12) for projection purposes, as follows:

$$0 = \frac{S_s}{\Delta t} h^{t-\Delta t} + \left(-\frac{S_s}{\Delta t} - \frac{K_{x-\Delta x/2} + K_{x+\Delta x/2}}{\Delta x^2} - \frac{K_{y-\Delta y/2} + K_{y+\Delta y/2}}{\Delta y^2} \right) h^t + \frac{K_{x-\Delta x/2}}{\Delta x^2} h^t_{x-\Delta x} + \frac{K_{x+\Delta x/2}}{\Delta x^2} h^t_{x+\Delta x} + \frac{K_{y-\Delta y/2}}{\Delta y^2} h^t_{y-\Delta y} + \frac{K_{y+\Delta y/2}}{\Delta y^2} h^t_{y+\Delta y} \tag{13}$$

Third, a matrix decomposition that divides the discretized equation into a prediction matrix $\widehat{\boldsymbol{H}}$ and a constraint matrix $\boldsymbol{C}$ is realised. The prediction matrix collects all the hydraulic head variables of Eqn (13) and the constraint matrix gathers all the other parameters. In other words, Eqn (13) is equal to the product of matrix $\widehat{\boldsymbol{H}}$ by matrix $\boldsymbol{C}$.

$$\widehat{\boldsymbol{H}} = \left[\hat{h}^{t-\Delta t}, \hat{h}^t, \hat{h}^t_{x-\Delta x}, \hat{h}^t_{x+\Delta x}, \hat{h}^t_{y-\Delta y}, \hat{h}^t_{y+\Delta y} \right]^T \tag{14}$$

$$\boldsymbol{C} = \left[\frac{S_s}{\Delta t}, -\frac{S_s}{\Delta t} - \frac{K_{x-\frac{\Delta x}{2}} + K_{x+\frac{\Delta x}{2}}}{\Delta x^2} - \frac{K_{y-\frac{\Delta y}{2}} + K_{y+\frac{\Delta y}{2}}}{\Delta y^2}, \frac{K_{x-\frac{\Delta x}{2}}}{\Delta x^2}, \frac{K_{x+\frac{\Delta x}{2}}}{\Delta x^2}, \frac{K_{y-\frac{\Delta y}{2}}}{\Delta y^2}, \frac{K_{y+\frac{\Delta y}{2}}}{\Delta y^2} \right] \tag{15}$$

$\widehat{\boldsymbol{H}}$ and $\boldsymbol{C}$ are a collection in matrix form of the realizations of Eqn (13) at each of the points located in the vicinity of the point of interest according to the collocation point method that the authors used in their study. From there, the prediction matrix is projected onto the hyperplane determined by the constraint matrix. This results in a new matrix called the projected prediction matrix which collects the values of the hydraulic head at the point of interest and at the adjacent points; these values are believed to be closer to the observed value. The projected prediction matrix is expressed as follows:

$$\widehat{\boldsymbol{H}}_{\boldsymbol{r}} = \phi(\widehat{\boldsymbol{H}}) = \left(\boldsymbol{I} - \widehat{\boldsymbol{H}}^{\boldsymbol{T}} \left(\widehat{\boldsymbol{H}} \widehat{\boldsymbol{H}}^{\boldsymbol{T}} \right)^{-1} \widehat{\boldsymbol{H}} \right) \boldsymbol{C} \tag{16}$$

Where I is the identity matrix, $\boldsymbol{C}\widehat{\boldsymbol{H}}_{\boldsymbol{r}} = \boldsymbol{0}$ and,

$$\widehat{\boldsymbol{H}}_{\boldsymbol{r}} = \left[\hat{h}_r^{t-\Delta t}, \hat{h}_r^t, \hat{h}^t_{r,x-\Delta x}, \hat{h}^t_{r,x+\Delta x}, \hat{h}^t_{r,y-\Delta y}, \hat{h}^t_{r,y+\Delta y} \right]^T \tag{17}$$

If the point of interest is a boundary point, it is sufficient to impose values of hydraulic conductivity or hydraulic head corresponding to the boundary condition. For example, for a no-flow boundary point, a zero value of hydraulic conductivity would be appropriate. With the TGRO method, the cost function can remain equal to the standard cost function $\mathcal{L}_{std}$ as presented in section 2.1, or the standard cost function can be combined with the cost related to the violation of the physics of groundwater flow. Fig. 3 illustrates the TGRO method.

Beyond hydrogeology, the TGRO method has been applied for the mapping of water bodies or the discovery of new materials. For example, Khandelwal et al. (2015) proposed a new method for refining post classification labels in the context of water body mapping. The goal was to use relevant information such as elevation to eliminate classifications that are theoretically inconsistent. The methodology consisted of producing a first map of the extension of a water body from a remote sensing image and to constrain this map with the elevation data to produce a physically consistent map. Hautier et al. (2010) used a combination of machine learning techniques and high throughput ab initio computations to find new compounds and their crystal structures. From a training database of materials of known structure and properties, they were able to train a model capable of finding materials whose properties and structure were previously unknown. To eliminate theoretically inconsistent materials, model outputs were refined using expensive ab initio calculations. This study made it possible to discover 209 new compounds with a limited calculation budget.

The TGCO and TGRO methods are basically the same, except that TGCO incorporates the theory into the cost function, whereas the TGRO method post-processes the model outputs to conform as accurately as possible to the theory. Because of this similarity, the conclusions drawn from the analysis of studies using TGCO can very likely be transposed to studies using the TGRO method. However, a very small number of studies have been published on the topic, so this cannot be confirmed with certainty. One advantage offered by TGRO is that the post-processing operator (e.g.: the transformation function for systems described by partial differential equations) remains present even after the training stage and, therefore, it may always be possible to adapt the model when a new event occurs. Again, a limited number of studies have been published on this topic and at this time, it is not possible to confirm or refute the transferability of ML models generated via the TGRO method.

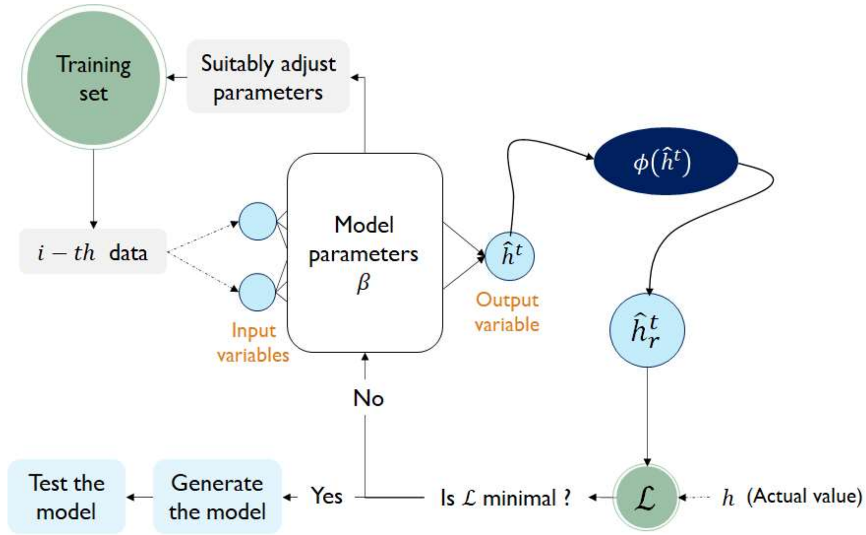

Fig. 3 Part of the ML process modified by the TGRO method, that is, at the level of model outputs (*solid blue oval circle*)

Table 1 shows some situations in which each of the theory-guided ML methods presented in this study can be applied. Table 2 presents a summary of the discussions concerning the ability of theory-guided ML methods to overcome the mentioned limitations of ML for hydrogeological applications. Question marks indicate a lack of available factual evidence to support the theory-guided method's ability to overcome the identified limitations.

Table 1 Some situations in which the theory-guided ML methods presented in this study may be applied. A dash indicates the absence of a supporting published study.

Tasks	TGCO	TGA	TGRO
Uncertainty quantification	✓	-	-
PDE resolution	✓	-	-
Discovery of symbolic governing equation	-	✓	-
Data generation	✓	-	-
Prediction improvement	✓	✓	✓
Inverse modelling	✓	✓	-
Surrogate modelling	✓	-	-

Table 2 Comparison of efficiency of the different methods of theory-guided machine learning with respect to ML limiting factors. Question marks indicate an absence of available factual evidence.

Methods	Mitigation of black-box nature	Improvement of generalization ability	Improvement of convergence	Transferability
TGCO	✓	✓	✓	?
TGA	✓	✓	✓	?
TGRO	✓	?	?	?
TGRO + TGCO	✓	✓	✓	?
TGCO + TGA	✓	✓	✓	?
TGRO + TGA	✓	✓	✓	?
TGCO + TGRO + TGA	✓	✓	✓	?

The TGCO method, by itself or combined with one of the two other methods makes it possible to reduce the opacity of ML models, to improve their generalization ability and to promote their convergence. However, there is no evidence supporting the transferability of ML models. The TGA method, by itself or combined with at least one of the two other also makes it possible to overcome all the limitations of ML models, with the exception of transferability for which there are no supporting studies. Finally, concerning the TGRO method, the only certainty is its ability to reduce the black-box nature of ML models.

3. Challenges of Theory-Guided Machine Learning Methods

Theory-guided machine learning has been identified as a promising paradigm that may make it possible to give ML models the ability to agree with hydrogeological knowledge. The purpose of this article was to assess to what extent theory-guided methods would be able to overcome the various limitations of ML, namely the black-box nature of most models, an often-limited generalization ability, a hypothetical convergence, and uncertain transferability. Three approaches were evaluated as to their capability of satisfying this objective, at least in part. These methods are Theory-Guided Constrained Optimization (TGCO), Theory-Guided Refinement of Outputs (TGRO) and Theory-Guided Architecture (TGA). Table 2 presents a comparison of the different methods of theory-guided machine learning commonly used in hydrogeology with respect to their ability to overcome ML limiting factors. The table indicates that the opacity of ML models can be reduced by any of the three theory-guided ML methods presented. Convergence and generalizability can be enhanced by TGCO, TGA, or a combination of at least two of the three theory-guided ML methods. To date, there is no study making it possible to deduce the effectiveness of these methods on the transferability of ML models. The first challenge would be to conduct more studies to fill the remaining knowledge gaps on the effectiveness of the presented methods to overcome ML limitations for hydrogeological applications.

In most of the studies analysed in this review, the application of theory-guided methods was performed on idealized configurations. Although these methods are convincing from a theoretical point of view, it is not possible to assess to what extent their use can be generalized in practical applications. It would therefore be interesting to be able to show or prove the transferability of these methods to real hydrogeological applications.

There does exist a way to quantify the generalization ability and the convergence of ML models. For example, the generalization ability can be defined as the ratio of the mean squared error between the model results and the observations during the test and training stages. When this ratio is close to 1, it is possible to conclude that the model shows a good generalization ability. However, it is not yet possible to measure the degree of attenuation of the black-box nature of ML models as well as the degree of improvement of their transferability in regression tasks through theory-guided methods. This remains an open research subject which could lead to the formulation of related metrics. The notion of mitigating the black box-nature of ML models is subjective in that it depends on the audience questioning the model (e.g., hydrogeologist, stakeholders, …). The first step in defining a metric to assess the degree of attenuation of the black box nature of theory-guided models would be to provide a mathematical definition, which currently does not exist. To assess the transferability of theory-guided models to new hydrogeological configurations for a given aquifer, it would be interesting to evaluate how well the occurrence of an entirely new event in that aquifer is considered by these models. This could involve evaluating the performance of the model both in the absence of, and in the presence of, the new event. Stable performances would probably indicate a model well suited to new events. In other words, the metric used to assess the generalization ability could be adapted to assess the model's transferability. It should have the merit of being tested. Also, it could be interesting to adapt the metric implemented by Nguyen et al. (2020a), the Log Expected Empirical Prediction (LEEP), to measure the transferability of classifiers, to regression contexts.

In the TGRO method, model outputs need to be transformed to guarantee physical consistency. The transformation function used to refine model output data must be well constructed. But in what manner? This also remains an open research field and a great challenge for hydrogeologists. Possible ways of constructing transformation functions that can be explored are the use of Laplace transforms on the equations governing groundwater flows or an adaptation of the collocation point method.

Finally, given the increasing availability of globally accessible data and satellite data, it would be interesting to conduct studies as well as large-scale comparison campaigns to better document the application of theory-guided machine learning in hydrogeology and obtain more general conclusions.

4. Conclusion

In this article, three theory-guided machine learning methods that have been used in hydrogeology are assessed for their ability to address four identified ML limiting factors in hydrogeological research and applications, namely the black-box nature of most models, an often-limited generalization ability, a hypothetical convergence, and uncertain transferability. The three methods are Theory-Guided Constrained Optimization (TGCO), Theory-Guided Refinement of Outputs (TGRO) and Theory-Guided Architecture (TGA). The analysis of these three methods through the hydrogeological literature led to the following conclusions: the opacity of ML models can be reduced by any of the three theory-guided ML methods presented; convergence and the generalizability can be enhanced by TGCO, TGA, or a combination of at least two of the three theory-guided ML methods; to date, there is no study making it possible to deduce the effectiveness of these methods on the transferability of ML models. It was concluded that more studies are needed to fill the remaining knowledge gaps regarding the effectiveness of Theory-guided ML methods in overcoming the limitations of ML. Also, given that Theory-guided ML methods have only been applied to idealized configurations and systems, it would be useful to carry out additional studies on real configurations in order to assess to what extent these methods can be generalized. There is a need for methods allowing the development of transformation functions that are consistent with theory to achieve full use of the TGRO method in hydrogeology. This review also identifies the need to define metrics to quantify the extent to which the black-box nature as well as the transferability of ML models could be overcome by theory-guided methods. Finally, it is hoped that this article will enable and encourage hydrogeologists to use ML in a way that benefits research and practical applications in hydrogeology.

Declaration of Competing Interest

On behalf of all authors, the corresponding author states that there is no conflict of interest.

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