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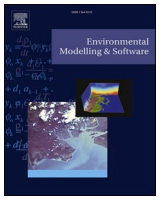

Position Paper

Deep learning, explained: Fundamentals, explainability, and bridgeability to process-based modelling

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A B S T R A C T

Recent breakthroughs in artificial intelligence (AI), and particularly in deep learning (DL), have created tremendous excitement and opportunities in the earth and environmental sciences communities. To leverage these new 'data-driven' technologies, however, one needs to understand the fundamental concepts that give rise to DL and how they differ from 'process-based', mechanistic modelling. This paper revisits those fundamentals and addresses 10 questions that might be posed by earth and environmental scientists, and with the aid of a real-world modelling experiment, it explains some critical, but often ignored, issues DL may face in practice. The overarching objective is to contribute to a future of AI-assisted earth and environmental sciences where AI models can (1) embrace the typically ignored knowledge base available, (2) function credibly in 'true' out-of-sample prediction, and (3) handle non-stationarity in earth and environmental systems. Comparing and contrasting earth and environmental problems with prominent AI applications, such as playing chess and trading in stock markets, provides critical insights for better directing future research in this field.

Plain language summary

The recent unprecedented performance of deep learning (DL) in image and language processing has accelerated applications in non-native areas such as earth and environmental sciences where knowledge-driven, process-based modelling has dominated to date. A major challenge, however, is DL and process-based modelling are rooted in different worldviews towards problem solving. This paper explains the 'whats' and 'whys' of DL from first principles and how they are different from those of process-based modelling. A hydrologic modelling experiment is presented to illustrate the fundamental differences between the two worldviews, and to shed light on some major issues DL has to deal with in the modelling of earth and environmental systems. These issues largely arise from the fact that such systems are complex, with behaviors that can change in ways that are physically explainable but not seen in the period of record, due to factors such as climate change and human interventions. Such issues must be addressed at the heart of the endeavor to extend DL techniques that embrace the knowledge base available, in anticipation of breakthroughs in an age of big data and computational power.

1. The rise of deep learning

The last decade has witnessed a tremendous rise in techniques called 'deep learning' (DL), under the umbrella of artificial intelligence (AI) and machine learning (ML), and their unprecedented performance in areas such as computer vision (Krizhevsky et al., 2012), natural language processing (Young et al., 2018), and gaming (Silver et al., 2018). These successes have motivated the application of DL across a wide range of disciplines, including medicine (Hosny et al., 2018), earth sciences (Reichstein et al., 2019), robotics (Torresen, 2018), engineering (Panchal et al., 2019), and finance (Lee et al., 2019). DL owes its exemplary success to the boom in computational power and the emergence of big data sources and associated data storage and sharing technologies.

Earth and environmental sciences appear to be positioned to benefit from DL, as big data sources on a range of in situ and remotely-sensed variables are becoming increasingly available with the advances in sensing technologies (Reichstein et al., 2019; Mao et al., 2020). The storage volume of remote sensing data for earth observations is already well beyond dozens of petabytes, with transmission rates exceeding hundreds of terabytes per day. Datasets based on model outputs are rising; for example, the climate assessment dataset provided by the

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Coupled Model Intercomparison Project Phase 6 may reach 40 petabytes (Eyring et al., 2016). Reanalysis climatic datasets have also grown; for example, NASA's Modern-Era Retrospective Analysis for Research and Applications version 2 (MERRA-2) is ~400 terabytes (Gelaro et al., 2017). In addition, datasets generated via tens of thousands of citizen science projects are providing large and rich sources of ground-based data.

This potential is shifting the attention of earth and environmental scientists and relevant funding agencies towards ML, as evidenced, for example, by the shift in research work presented at the American Geophysical Union (AGU)'s fall meetings, the largest assembly of earth and environmental scientists with more than 27,000 people in attendance and 25,000 presentations in 2019. The number of ML-related presentations has risen consistently—from 0.2% of total presentations in 2015 to 4.2% in 2020. In particular, this shift has been astonishing in the AGU's 'non-linear geophysics', 'earth and space science informatics', 'natural hazards', 'hydrology', and 'seismology' sections, where 28 (2.1), 18 (5.1), 9 (1.3), 7.5 (1.4), and 6.7% (0.9%) of total presentations, respectively, were related to ML in 2020 (2015).

Recent successful applications of DL techniques to earth and environmental sciences include weather nowcasting and forecasting (Shi et al., 2015, 2017), satellite precipitation bias reduction (Tao et al., 2016), rainfall-runoff modelling (Kratzert et al., 2018; Feng et al., 2020; Ma et al., 2021), rain and snow retrieval from spaceborne sensors (Tang et al., 2018), downscaling hydroclimatic variables (Ducournau and Fablet, 2016), precipitation estimation (Tao et al., 2018; Pan et al., 2019), and surrogate modelling (Gu et al., 2020; Yu et al., 2020). Unsuccessful applications, perhaps similar to many other areas, remain largely unreported in the peer-reviewed scientific literature but occasionally appear in other media (e.g., Wexler, 2017; Kolakowski, 2018; Rudin, 2019).

Notably, DL is a trendy term that refers to a specific class of artificial neural networks (ANNs), which have been around and widely applied in earth and environmental sciences since the early 1990s with the birth of domains such as Hydroinformatics (Abbott, 1991). These applications are documented in reviews by Gardner and Dorling (1998), Maier and Dandy (2000), Krasnopolsky (2007), Maier et al. (2010), Abrahart et al. (2012), Razavi et al. (2012), Shen (2018), Bergen et al. (2019), and Reichstein et al. (2019). Arguably, however, the uptake of ANNs, in general, to facilitate and advance earth and environmental sciences has not kept pace with data availability and computational power over the past three decades.

But why? The challenges impeding the widespread application of ANNs to earth and environmental problems to date may be rooted in the fact that convincingly casting those problems, for which an extensive knowledge base is usually available, within the ANN framework is often not straightforward. Moreover, the lack of interpretability and explainability of ANNs has been a major hindrance, as model developers need to be able to make sense of why a model functions the way it does, and to explain that to model users. These challenges can be further complicated in the absence of a solid understanding of the fundamentals of ANNs and how they differ from theory-driven, mechanistic modelling and prediction. Mechanistic modelling, also called process-based or knowledge-based modelling in this paper, has traditionally been the cornerstone of scientific advancement and policy support.

So why this paper? Motivated by the recent breakthroughs by DL in its original areas of application, namely computer vision and natural language processing, this paper aims to address the persistent challenges facing DL applications in non-native areas related to earth and environmental sciences. With this overarching aim, this paper addresses (but not necessarily answers) 10 questions regarding the fundamentals of DL and its explainability and bridgeability to earth and environmental systems modelling:

(1) What is DL and how did it evolve from ANNs?
(2) How can we interpret the internal functioning of DL?
(3) Does DL abandon Occam's razor or the principle of parsimony?
(4) Why is DL considered superior to other types of ML?
(5) How can DL account for memory and time dependency?
(6) How do DL and process-based models compare in calibration and validation and which one may be more trustworthy?
(7) What is the value of the often-ignored domain knowledge in DL and why may DL suffer from this ignorance?
(8) Why is DL essentially different from process-based modelling?
(9) What are the existing approaches to bridging DL and process-based modelling?
(10) What can we learn from prominent DL applications such as gaming and the stock market?

The structure of this paper is such that it best serves the reader when all sections are followed sequentially. However, an advanced reader could directly refer to a section that is more relevant to a question of interest. Sections 2 through 7 are about questions 1 through 6 and Sections 8.1 through 8.4 are about questions 7 through 10, respectively. A simple hydrological modelling problem and multiple synthetic functions are used to explain complex concepts via simple examples. The contents of this paper are intended to be accessible to a wide audience from various fields under the umbrella of earth and environmental sciences. However, the views presented mainly arise from the author's data- and theory-driven research background in hydrology and water resources.

This paper concludes in Section 9 by revisiting some ancient issues pertaining to modelling in general around the "mathematistry" trap, raised by the late prominent scientists George Box (1976) and Vit Klemeš (1986b). Those issues can be just as fresh today as they once were, particularly in the absence of a solid understanding of what DL can and cannot do in a project and in the presence of possible hype or over-excitement around it. Further, Section 10 is a postscript where the author reflects on some significant review comments received on this paper before its final publication.

2. Back to fundamentals

2.1. Why ML and DL?

ML, as a subclass of AI, is nowadays concerned with developing machines that improve their own performance in carrying out a given task over time by 'learning' from examples, with minimal human efforts to instruct the machines how to do so (Jordan and Mitchell, 2015). According to Goodfellow et al. (2016), however, the early efforts to generate AI were based on a knowledge-base paradigm to instruct machines with a formal set of step-by-step mathematical and if-then rules. Those efforts focused on carrying out tasks that were intellectually difficult for humans but straightforward for computers. Goodfellow et al. (2016) argue such efforts led to no major successes, and the AI of today is about enabling machines to perform tasks that humans perform intuitively and rather easily but have difficulty formally describing how they do so. Examples of such tasks include recognizing faces in a photo or comprehending spoken words.

Not only did state-of-the-art AI divorce from the knowledge base, but it also completely separated from classic data-driven modelling rooted in statistics such as regression. This separation was a response to the need for models that are not constrained by the many assumptions typical statistical models hold. For example, traditional statistical modelling requires a formalization of relationships between variables and assumptions about functional shapes, distributions of variables, and their inter-dependencies, which enables hypothesis testing and the generation of confidence bounds. Conversely, in the ML context the underlying relationships in data may have any complex form, which is typically unknown *a priori*, and the data used may have any size and distributional properties (see Dangeti, 2017, p. 10–11).

Because of these characteristics, ML is deemed suitable to pursue the

longstanding ambition to build machines that work with minimal or no human supervision and imposed assumptions. ML techniques nowadays, and in particular DL, provide such flexible tools that can adapt to a wide range of data and applications.

2.2. Evolution of DL and major milestones

It was 1957 when Frank Rosenblatt invented the first algorithm, termed 'perceptron' (Rosenblatt, 1957), which today forms the smallest computational unit of DL. A perceptron, alternatively termed a 'neuron' because of its resemblance to the basic working unit of the brain, is shown in Fig. 1a and formulated as:

$$y = f\left(\sum_{i=1}^{D} w_i x_i + b\right) \quad \text{(Eq. 1)}$$

where D is the dimension of input space, $\boldsymbol{x}$ is the input vector, $\boldsymbol{w}$ is a set of weights corresponding to the input vector, b is bias, and f is an 'activation' function. A perceptron has D+1 tunable parameters (i.e., D weights and one bias) and is basically nothing but a multiple linear regression augmented by an output function (f), which is non-linear. The form of the activation function was originally a step function, but now a range of monotonic functional forms, such as 'sigmoidal', are used.

The invention of perceptrons created significant excitement in the AI community and beyond. But, it soon became clear that a perceptron would not be able to map input spaces that are not linearly separable, such as the XOR problem (Minsky and Papert, 1969), rendering perceptrons of limited use in real-world applications. The reason for this inability is that the core of the perceptron is a linear regression.

Efforts to overcome this barrier could have followed two different avenues. Perhaps the most intuitive avenue was to employ non-linear regression, by allowing the terms inside the parentheses in Eq. (1) to be of other algebraic forms such as quadratic. However, this was not a viable option in part because the user then would need to specify the form of non-linearity which is not typically known *a priori*, requiring possibly extensive trial-and-error.

The second avenue that led to today's DL was to combine perceptrons both in parallel and in series to create so-called 'multi-layer perceptrons' (MLPs), as shown in Fig. 1b, with the hope this more complex system could overcome the barrier. An MLP would then have many more tunable parameters than the perceptron. The first layer of neurons, also called the first 'hidden' layer, would have $D.n_1$ weights and n_1 biases, where n_1 is the number of neurons in this layer. Similarly, the second hidden layer would have $n_1.n_2$. weights and n_2 biases, and the last layer, called the 'output' layer would have $n_{d-1}.n_d$ weights and n_d biases, where n_{d-1} and n_d are the numbers of neurons in the second-to-last and last layers, respectively, and d is the total number of layers. The total number of layers in an MLP and the number of neurons in each layer are 'hyper-parameters', to be specified by users. Also important is the choice of activation functions in each layer. Note that a linear activation function is typically only suitable for the last layer and, in general, any stack of linear layers is effectively equivalent to a single linear layer.

But, MLPs on their own did not go far and the field stagnated for many years because of the absence of an algorithm that could automatically derive from data the network weights and biases—a process referred to as 'training' in the AI community. It took until the mid-1980s when the first 'back-propagation' (BP) algorithm was invented to enable the training of MLPs with any network structure (Rumelhart et al., 1986). This invention marked the beginning of the 'second wave' of popularity of ANNs. BP is essentially an optimization algorithm, based on non-linear programing, that minimizes a loss function, F, representing the goodness-of-fit of predictions to observations, such as the 'sum of squared errors', as follows:

$$F = \sum_{k=1}^{M} \sum_{j=1}^{n_d} \left(T_j^k - y_j^k\right)^2 \quad \text{(Eq. 2)}$$

where y_j^k is the output of neuron j in the output layer when the network is forced with input data sample k and T_j^k is the respective desired target. Also, M is the size of training data, and n_d is the number of neurons in the output layer.

Different variations of BP rooted in first- (e.g., gradient descent) or second-order (e.g., Newton's method) optimization, or a combination thereof, now exist; see e.g., the Levenberg-Marquardt algorithm as implemented by Hagan and Menhaj (1994). These algorithms are fundamentally the same as optimization algorithms used nowadays for calibration of process-based models. The only difference is that, in the case of ANNs, and unlike most process-based models, the partial derivatives of the loss function with respect to weights and biases are *analytically* available through the 'chain rule of differentiation'. In parallel, derivative-free and metaheuristic optimization algorithms have shown promise in training (e.g., Dengiz et al., 2009; Rakitianskaia and Engelbrecht, 2009; Razavi and Tolson, 2011), but have yet to become mainstream.

The training of ANNs is an iterative optimization process, where the network parameters are updated after each iteration (called an 'epoch' in the ANN context), to minimize the loss function. This process can be via 'batch training', where at each epoch the entire batch of training data (i.e., all M input-output sets) are used. Alternatively, each epoch can follow 'mini-batch training' based on a subset of training or

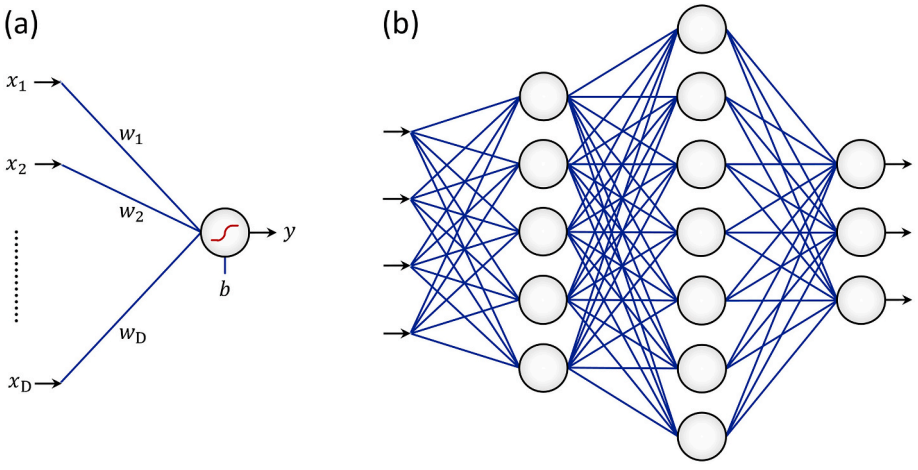

Fig. 1. (a) A perceptron and (b) a multi-layer perceptron with four inputs, two hidden layers, and three outputs.

'incremental/online training' based on a single training data sample, chosen randomly or otherwise (Hagan et al., 1996). These two approaches, also commonly referred to as 'stochastic gradient descent', are useful when the size of training data is large (Bottou, 1998, 2010).

In the late 1980s, after the invention of BP, MLPs were proven to be 'universal approximators' (Hornik et al., 1989). This proof indicated MLPs with only one hidden layer that possesses a sigmoidal activation function, and a linear output layer, would be able to approximate any function with any desired level of accuracy provided the number of hidden neurons is sufficient. Since then, the 'universal function approximation theorem' has been the fundamental driver of interest in MLPs across a variety of disciplines and applications.

MLPs gradually formed a prominent class of 'artificial neural networks', or simply 'neural networks', a name reflecting their perceived resemblance to biological neural networks. MLPs, which are also sometimes called 'feedforward neural networks' (FNNs), are the building blocks of a range of other ANNs developed later on, including 'autoencoders' (Bourlard and Kamp, 1988), 'recurrent neural networks' (RNNs; Elman, 1990) and its popular variation 'long short-term memory' (LSTM; Hochreiter and Schmidhuber, 1997), convolutional neural networks (CNNs; Lawrence et al., 1997), and generative adversarial networks (GANs; Goodfellow et al., 2014).

ANNs started receiving much attention in earth and environmental sciences in the early 1990s. The pioneering applications of ANNs include: Benediktsson et al. (1990), Badran et al. (1991), Stogryn et al. (1994), Bankert (1994), and Cabrera-Mercader and Staelin (1995) in the context of remote sensing of the environment; McCann (1992), Boznar et al. (1993), and Navone and Ceccatto (1994) in the context of atmospheric forecasting; and Kang et al. (1993), Hsu et al. (1995), and Minns and Hall (1996) in the context of hydrologic modelling. Perhaps the most prominent and widely used application of ANNs in these fields has been related to the development of PERSIANN, or 'Precipitation Estimation from Remotely Sensed Information using Artificial Neural Networks' (Hsu et al., 1997; Sorooshian et al., 2000; Ashouri et al., 2015), which has been maintained and updated for two decades (accessible at https://chrsdata.eng.uci.edu/).

Despite all of these advances, including the development of the now-highly-successful ANNs such as LSTM (Hochreiter and Schmidhuber, 1997) and CNN (Lawrence et al., 1997), investments in ANNs and therefore their popularity saw a decline in the AI community beginning in the mid-1990s. This was reportedly triggered by failures to fulfill overly ambitious or unrealistic promises by prominent AI scientists (Goodfellow et al., 2016) that brought about somewhat a negative reputation for ANNs (Duerr et al., 2020), as historically observed in 'AI winters' (Hendler, 2008). ANNs in earth and environmental sciences, however, remained fairly popular arguably until the mid-2000s. The focus of researchers in these fields was to find novel applications of ANNs across different earth and environmental problems.

It took until early 2010s before the third wave of popularity and interest in ANNs hit, when the field was revived and renamed 'deep learning'. 'Depth' is a recently popularized term and loosely refers to the number of hidden layers in ANNs. A related term is 'width', which loosely refers to the number of neurons in hidden layers. Now, a DL model typically refers to an ANN with more than a few hidden layers. The recent excitement around ANNs is despite the fact that the structure, formulation, and other properties of MLPs and some of their offsprings, such as LSTM that provides MLPs with a memory (see Section 6), have remained essentially unchanged since their inception, except for some minor modifications. So, one might ask: is DL merely a repackaging and rebranding of what existed before? The next section attempts to answer this question while reviewing the recent milestones.

2.3. Latest developments and rebranding the field

To better understand the recent developments in the field of ANNs, one first needs to know the history around the 'depth' concept. ANNs, since their inception, have been used with various numbers of hidden layers, that is with various depths. Most applications, however, remained limited to networks with only one hidden layer until very recently. For example, Razavi et al. (2012) surveyed ANN applications for surrogate modelling in water resources literature and reported that more than 90% of those had only one hidden layer. There was (and perhaps still is) no consensus about a proper network depth, because identifying the optimal network configuration for a given problem and dataset is challenging.

Historically, before the rise of DL, some researchers favored ANNs with more than one hidden layer, arguing that they require fewer hidden neurons to approximate the same function (see e.g., Tamura and Tateishi, 1997). On the other hand, others asserted that single-hidden-layer ANNs are superior to those with more than one hidden layer with the same level of complexity (see e.g., de Villiers and Barnard, 1993).

Three general reasons historically drove interests towards ANNs with a single hidden layer: (1) the universal function approximation theorem (Hornik et al., 1989), as it provided a compelling argument that such ANNs are fully capable of learning any function; (2) the principle of parsimony, as ANNs with fewer hidden layers are generally deemed less complex and more understandable; and (3) difficulty of training, as ANNs with more hidden layers are more complex to train (see e.g., de Villiers and Barnard, 1993).

So, what recently shifted the status quo towards ANNs with multiple (typically many) hidden layers? Goodfellow et al. (2016) attribute the beginning of this shift to the work of Hinton et al. (2006), where 'unsupervised learning' was used to pre-train 'deep' ANNs. They showed unsupervised learning could effectively initialize the network's parameters such that the subsequent training efforts through BP would become more successful. In AI, unsupervised learning refers to a process where a model learns from 'unlabeled' examples, which are technically inputs with no associated output. This is as opposed to 'supervised learning' where examples (i.e., data points) are 'labeled', meaning the output associated with each input is available; this process is called 'model calibration' in the context of process-based modelling.

Now, one might ask how unsupervised learning can be of any help in supervised learning. A common method for this purpose uses 'autoencoders', which are a class of ANNs historically used for dimensionality reduction and feature learning (Bourlard and Kamp, 1988). An autoencoder is an MLP, typically trained by BP, with one or more hidden layers that receives input and aims to produce the *same* input as its output. In a typical autoencoder, the middle layer has fewer neurons than the dimension of input, thereby acting as a bottleneck that encodes the input data in a lower dimensional space. The signals in the middle layer preserve the information contained in the inputs, which will be decoded back to the original space in the following layers. Autoencoders can pre-train some layers of a deep ANN such that the weights of those layers capture the main features in input data before passing them to the next layers. After the pre-training phase by unsupervised learning, the ANN needs to be further trained in the conventional supervised manner, using the actual output data and algorithms such as BP.

While the third wave of ANN popularity began by leveraging unsupervised learning to train deep ANNs, Goodfellow et al. (2016) argue the interest has gradually shifted back to the classic learning algorithms, such as BP, even for training deep ANNs. Those classic learning algorithms are now believed to work quite well in the DL context, perhaps due to the boom in computational power. In this regard, a game changer was the introduction of graphics processing units (GPUs) to the ANN community as a powerful tool to massively parallelize and thus expedite training algorithms (Raina et al., 2009). Such computational power has enabled the development of large ANNs, in terms of both depth and width. As such, ANNs with hundreds of millions (e.g., Devlin et al., 2018) or even a trillion parameters (e.g., Rajbhandari et al., 2019) are becoming common.

Such a tremendous revival of the field of ANNs might seem at first

surprising to those earth and environmental scientists who have known the field for a long time. This might be due, in part, to the fact that many ANN applications to earth and environmental problems nowadays are fundamentally similar to those performed in the 1990s and 2000s. More broadly, the basic forms of many ANNs used today have not changed much, other than becoming larger. Differences, if any in an application, are often in the details. For example, following Glorot et al. (2011), the tendency now is to use the rectified linear unit (ReLU), which is an unbounded function, instead of the standard 'sigmoidal' activation functions (see Eq. (1)).

This revival may be explained by the huge successes of some ANNs in their original areas of application, such as image processing (Krizhevsky et al., 2012) and speech recognition (Young et al., 2018), their commercial potential, and the resulting major investments by mega companies such as Google in this field. Perhaps recent rebranding of the field under the title of 'deep learning' might have been in part a marketing strategy (Duerr et al., 2020); while as cited in Schmidhuber (2015a), this term was first introduced by Dechter (1986) to ML and by Aizenberg et al. (2000) to ANNs.

3. Geometrical interpretation of DL

ANNs have always struggled with explainability and interpretability. Extensive research efforts have endeavored to peer inside the 'black box' of ANNs, via various heuristics rooted in sensitivity analysis of input-output mappings created by ANNs (e.g., Bach, 2015; Toms, 2020; or see Section 3.4 of Razavi et al. (2021) for a review) or techniques that attempt to explain the 'internals' of ANN models (e.g., Benítez et al., 1997; Tickle et al., 1998; Castro et al., 2002; Wilby et al., 2003; Xiang et al., 2005; See et al., 2008; Samek and Müller, 2019). Despite all these advances, the issues around explainability and interpretability of ANNs, and of many ML techniques in general, are as relevant today as ever (see Rudin, 2019).

This section utilizes a geometrical interpretation to illustrate the internal functioning of ANNs and explain why 'deeper' ANNs can be more powerful than 'shallower' ANNs in learning representations in data. This interpretation is adopted in part from the work of Razavi and Tolson (2011), in which they recast ANNs with respect to a new set of variables that are interpretable based on the network functional geometry.

3.1. A perceptron

An ANN is in principle made of a number of perceptrons (see Section 2.2). Consider a basic ANN with a single hidden layer with a sigmoidal activation function, as shown Fig. 2a. Each hidden neuron, e.g., the r^{th} neuron, is a perceptron whose output y_r^1 is multiplied by the weight $w_{1,r}^2$ before entering the output neuron. This hidden neuron, when only having one input x_1, forms a functional relationship such as that shown in Fig. 2b. This 'sigmoidal unit' can be characterized by three variables: 'slope', 'location', and 'height'. There is one-to-one mapping between these variables and the original network variables, $w_{r,1}^1$, b_r^1, and $w_{1,r}^2$, as shown in the figure. As such, one can directly control the shape of the sigmoidal unit through slope, location, and height, and where needed, map them onto the network's original variables. The benefit of doing so is that, unlike the original variables, the new variables are geometrically interpretable and therefore more intuitive.

Fig. 2c shows the geometry of a perceptron with two inputs, x_1 and x_2. In this case, the resulting sigmoidal unit forms a *plane* that can be characterized by slope, location, and height, plus an additional variable called 'angle' that specifies the direction toward which the sigmoidal unit is facing. This geometry can be extended to perceptrons with three

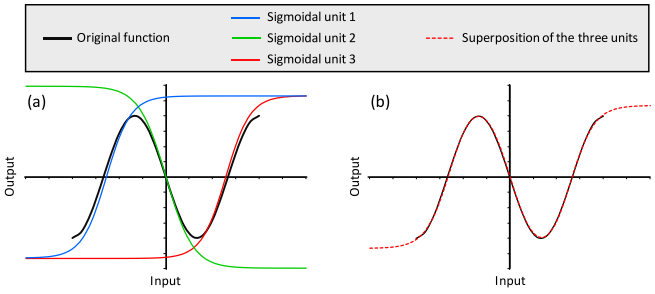

Fig. 3. (a) An original sine function and three sigmoidal units, each approximating a part of the sine function. (b) Output of the ANN that superposes the three sigmoidal units.

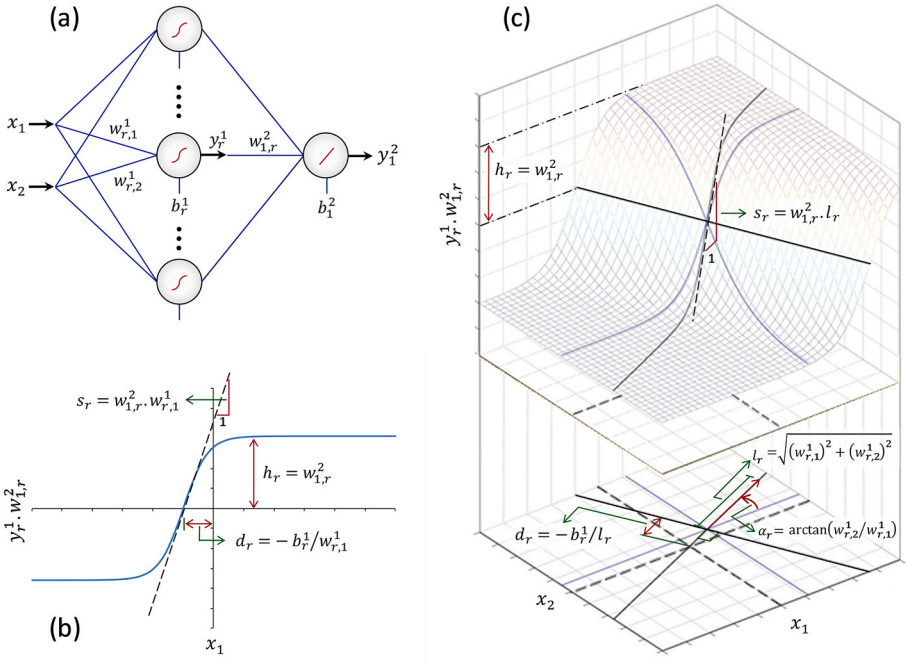

Fig. 2. (a) A basic ANN with a sigmoidal hidden layer and linear output layer. (b) The sigmoidal line formed by the r^{th} hidden neuron when the network has only one input, x_1. (c) The sigmoidal plane formed by the r^{th} hidden neuron when the network has two inputs, x_1 and x_2. A sigmoidal line can be defined by three variables that are related to the original weights and biases: h_r is the 'height' of the tails, s_r is the 'slope' of the tangent line at the inflection point, and d_r is the 'location' of the inflection point with respect to the origin. A sigmoidal plane can be defined based on those three variables as well as α_r, which is the 'angle' of the normal vector perpendicular to the plane. l_r is the length of this vector. This geometry can be extended to ANNs with any number of inputs (see Razavi and Tolson, 2011).

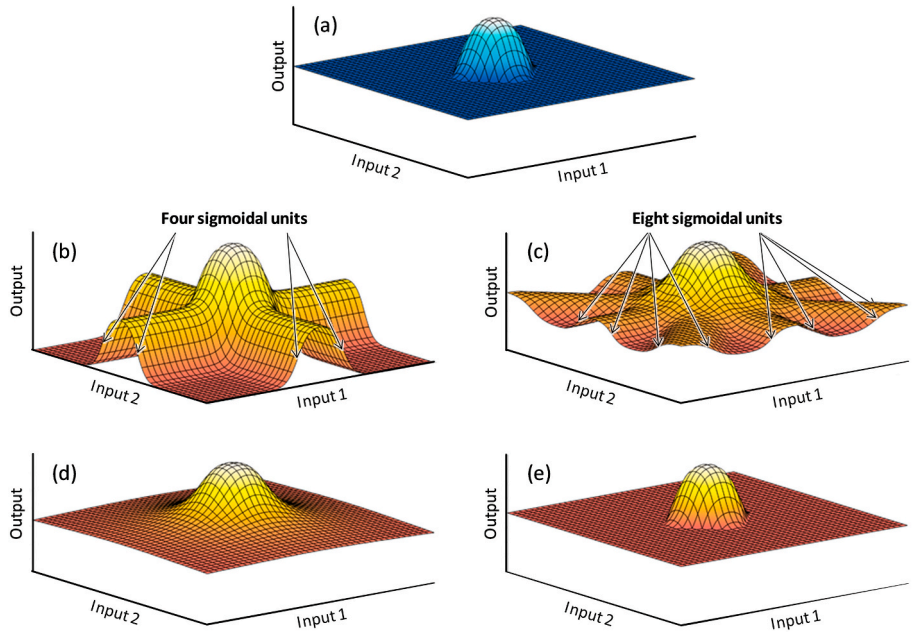

Fig. 4. (a) An illustrative dome-like function. Performance of an ANN in approximating the dome-like function when it has (b) four (c) eight, or (d) 40 sigmoidal hidden neurons and a linear output neuron. (e) Performance of an ANN with four sigmoidal hidden neurons and a sigmoidal output neuron.

or more (say D) inputs, where the sigmoidal unit becomes a *hyperplane*, characterized by a slope, location, and height and D-1 angles. Full details of this geometrical interpretation, and how it works in practice, are available in Razavi and Tolson (2011). Now let us see in the following how ANNs can approximate any function by putting together a large number of such sigmoidal units.

3.2. ANNs with one hidden layer

Single-hidden-layer ANNs are capable of approximating any function by combining, in parallel, as many sigmoidal units as required. For example, suppose the underlying function to approximate is the sine function shown in Fig. 3a. Three sigmoidal units, with almost equal heights, equal absolute slopes, and different locations, are required in parallel to represent the features of the function. These three units can be produced by the hidden layer of an ANN and fed into a linear output layer, where they are summed (superposed) to approximate the sine function, as shown in Fig. 3b.

For problems with two or more inputs, the function approximation is not as straightforward. For example, suppose the objective in a two-input problem is to approximate the dome-like feature shown in Fig. 4a. A single-hidden-layer ANN with four sigmoidal hidden neurons and one linear output neuron would be able to approximate the dome part of the space, as shown in Fig. 4b. This ANN would basically superpose four sigmoidal units with equal heights, equal slopes, equal locations, but different angles (90° apart). The performance of this ANN, however, is unacceptable, as it creates erroneous features on the tails.

But, can we rectify this issue by using more hidden neurons? Fig. 4c shows the performance of a network with eight sigmoidal units, all having the same heights, slopes, and locations, but different angles, 45° apart. With more sigmoidal units at work, the performance at the tails is improved, producing a smoother surface. Almost 40 hidden neurons are required, as shown in Fig. 4d, to generate almost completely smooth tails, similar to the original function shown in Fig. 4a. This example provides a geometrical proof for the universal function approximation theorem of Hornik et al. (1989) because, in principle, any complex function could be approximated by superposing a (large) number of such dome-like (i.e., basis) functions. The challenge, however, is that many (possibly an excessively large number of) hidden neurons may be required for a given problem to attain a desired level of approximation accuracy.

3.3. So, why more than one hidden layer?

As proven by Hornik et al. (1989), and geometrically shown in the example above, ANNs with a sigmoidal hidden layer and a linear output layer are capable of approximating any function with any desired level of accuracy. So, one may wonder about the need to have deeper ANNs. This section attempts to answer this question via an example.

Let us look back at the original function we aimed to approximate in Fig. 4a. Only four sigmoidal units were required, as seen in Fig. 4b, to reproduce the dome-like feature at the center. One might ask: Can we stick to these four sigmoidal units and somehow smooth the tails? Yes, all that is needed is a second layer with a *nonlinear* activation function (e.g., sigmoidal) to deactivate any feature that is under a threshold. In other words, in this process, the geometry formed by the sigmoidal units in the first layer filters through another sigmoidal unit that bounds that geometry. Fig. 4e shows how adding the second nonlinear layer enables the network to reproduce the original function, with only four neurons in the first hidden layer. Similar to single-hidden-layer ANNs, those with two hidden layers can approximate any function by putting a number of the dome-like functions side by side.

In general, and as shown in the example, deeper ANNs can provide more flexibility while they may require fewer hidden neurons across the network for representation learning. However, the training of deeper ANNs has been historically much more difficult because of the now well-known problem of 'vanishing and exploding' gradients. This problem relates to the fact that the partial derivatives of a loss function (Eq. (2)) with respect to weights and biases in first layers, obtained via the chain rule of differentiation, tend to become very small (i.e., close to zero) or very large (i.e., exponentially growing or fluctuating). Improved algorithms along with higher computational power have now eased that difficulty and made possible the training of very deep ANNs (Schmidhuber, 2015b).

Lastly, a related consideration about the proper number of hidden layers is about the fact that, in many problems, only a small part of the input space is active. In other words, some combinations of input variables might not occur in reality and therefore the accuracy of the ANN

might not matter much in the regions of input space containing those combinations. For example, consider a case similar to one shown in Fig. 4b, where the corners on the input space do not show up in the data available. A hydrological example is where snowfall and temperature are two inputs to ANNs. Because snowfall would never occur along with a high temperature, the respective part of the input space always remains inactive.

4. Relevance of Occam's razor and equifinality?

4.1. Issues with the complexity of ANNs

ANNs are known for their *hyper-flexibility* in fitting data, owing to their enormous degrees of freedom. For example, consider a problem with five inputs and one output. A single-hidden-layer ANN with 10 hidden neurons would have 71 tunable parameters (60 weights and 11 biases), and adding a second 10-neuron hidden layer would result in a network with 181 parameters (160 weights and 21 biases). Compare that with linear or quadratic regression models for the same problem, which would have six or 21 tunable parameters, respectively. Such large degrees of freedom, manifest in large numbers of parameters, encountered in the field of ANNs do not seem consistent with a basic principle in statistical modelling: *Occam's razor*.

Occam's razor, or principle of parsimony, indicates that simpler hypotheses or models should be preferred over more complex ones. In other words, those models that serve the purpose with as few parameters as possible should be chosen. However, many data-driven modellers, in particular in the field of ML, have arguably abandoned Occam's razor. For example, ANN users typically do not try simpler model types such as regression for the problem at hand. And, when using ANNs, they do not necessarily look for the most parsimonious network. Note that some literature proposes systematic approaches to choose a network structure based on growing, pruning, or other strategies (e.g., Reed, 1993; Teoh et al., 2006; Xu et al., 2006). In practice, however, such approaches have been of limited use and most ANN users choose the network structure on an *ad hoc* basis or by trial-and-error (see a survey by Wu et al., 2014). Recently, giant ANNs with hundreds of millions of parameters or more have become widespread (Devlin et al., 2018; Rajbhandari et al., 2019).

In addition, *equifinality*, a common and widely discussed issue in process-based modelling (Beven and Freer, 2001; Khatami et al., 2019), is not generally discussed or considered an issue in the context of ANNs. Equifinality concerns the fact that, in most cases, different model structures and parameter values can lead to similar modelling results. In other words, model structure and parameters are not uniquely identifiable from data (Guillaume et al., 2019). This is despite the fact that, loosely speaking, the level of equifinality of ANNs is much larger than other types of models because of their massively parallel nature in producing model outputs.

So, how does DL handle the above issues? The answer is 'indirectly', by trying to avoid their undesired implications, which are *overfitting* and *lack of generalizability*. The former refers to a situation where a model fits the noise in the data rather than the underlying function. The latter refers to a case where the model does poorly in 'out-of-sample prediction', that is predicting situations unseen in the data used for model training. Various techniques are available in the ANN literature to address these issues, as outlined in the following.

4.2. Leashing the hyper-flexibility of ANNs

Most techniques to control the hyper-flexibility of ANNs and to avoid overfitting fall under two general strategies, namely 'early stopping' and 'regularization'. Before reviewing these strategies in this section, let us revisit the common data-splitting approach for calibration and validation of models.

ANNs and traditional, mechanistic models have major differences in terms of calibration and validation. In traditional modelling practices, the available data are commonly divided into 'calibration' and 'validation' datasets. The former is used to identify the model structure and parameters, while the latter is used to test the model performance in out-of-sample prediction.

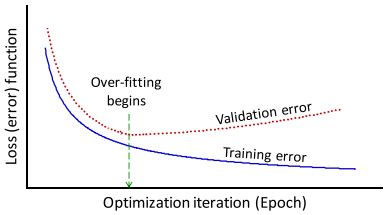

Fig. 5. Illustration of the need for 'early stopping'. The loss function on the 'training' dataset generally decreases with more epochs, whereas the loss function on the 'validation' dataset decreases early on but begins to increase at some point, marking the commencement of overfitting.

In ANN practices, however, the available data are typically divided into three sets, commonly referred to as 'training', 'validation', and 'testing' datasets. Any data chosen for 'training' and 'testing' in the ANN context are respectively treated like 'calibration' and 'validation' datasets in the traditional modelling context. The third, 'validation' dataset in the ANN context is needed to leash the hyper-flexibility of the network while training. The simultaneous use of 'training' and 'validation' datasets during ANN training may be best described with the early-stopping strategy, as follows.

In the early-stopping strategy, the quality of fit to the validation dataset is evaluated after each epoch, that is an optimization iteration trying to minimize the loss function on the training data (see Section 2.2). Empirically speaking, as the training error decreases over time, the validation error decreases as well for a while. However, at some particular epoch, the validation error may begin to increase while the training error may keep decreasing (see Fig. 5). This epoch is deemed to mark the beginning of overfitting; thus, the user stops the training process. This strategy is therefore called early stopping in the sense that the training stops early, before it can further improve the fit to the training dataset (for a review, see Prechelt, 1998). When the training process stops, the generalizability of the trained network is assessed via out-of-sample prediction on the testing dataset.

Regularization is another commonly used strategy to put a leash on the hyper-flexibility of ANNs. Unlike early stopping, this strategy tries to minimize a 'regularization function' during training, to control the ANN flexibility and tailor it to the problem at hand. This strategy has roots in the theory of 'Tikhonov regularization' and typically views a more regularized model as one with a smoother response surface (Tikhonov and Arsenin, 1977; Johansen, 1997). A traditional regularization function in the ANN context is the sum of the square of all network parameters (Krogh and Hertz, 1991), based on the notion that, in general, the smaller the parameters of a neuron, the less activated it is. For example, in an extreme case where all parameters of a neuron are zero, that neuron becomes fully inactive and does not contribute a feature to the overall network response. Razavi and Tolson (2011) provide a more efficient regularization function, based on the geometry presented in Section 3, where the regularization function is the sum of squares of all of the slopes. This regularization function only targets and removes the unnecessary features, which are unsupported by data, from the overall network response.

But how can one balance the goodness of fit and smoothness of the network response? In practice, this is a bi-objective optimization problem, where one objective is to minimize the error function and the other is to minimize the regularization function. These two objective functions are commonly integrated into one loss function via weighting schemes. Fig. 6 shows how the two objectives compete in a real example. Ideally, one may wish to achieve a performance such as that shown in Fig. 6e. Doing so is not trivial, however, because in practice the underlying

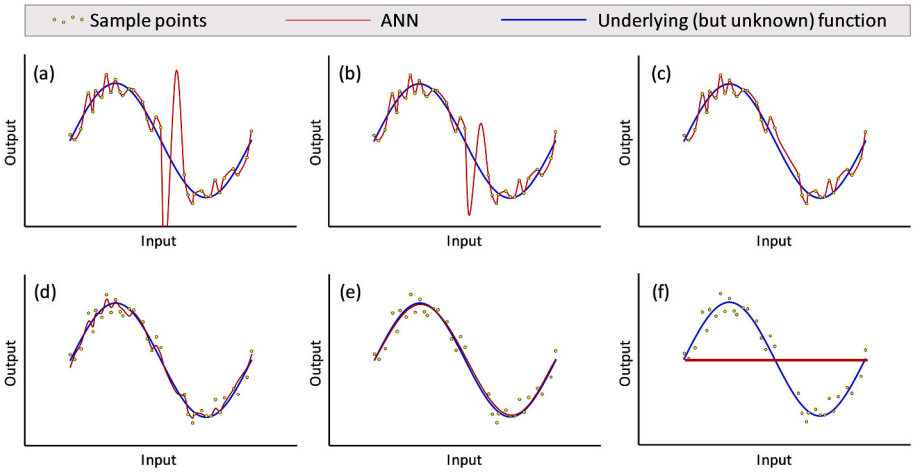

Fig. 6. An illustrative example of how regularization works to leash the hyper-flexibility of ANNs. Plot (a) shows an extreme case with no regularization where the ANN overfits data. Plot (b) shows a case where the regularization function is added to the loss function but marginally weighted. Plots (c) through (e) show cases with incremental increases in the weight of the regularization function. Plot (f) shows the other extreme case where the regularization function is dominantly weighted, making the ANN effectively inactive. These plots are based on a real experiment, where the data sample was taken from the underlying sine function shown and polluted with random noise.

function is unknown, available data are limited, and response surfaces are multi-dimensional and cannot be easily visualized. The Bayesian regulation method developed by MacKay (1992) and extended by Foresee and Hagan (1997) has proven useful to adaptively assign the weights associated with each function during training.

A more advanced and recently developed regularization strategy is called 'dropout' (Hinton et al., 2012; Srivastava et al., 2014). Dropout is a heuristic, particularly designed for deep ANNs, that randomly deactivates and then activates different neurons or groups of neurons at each epoch in the course of training. When a part of an ANN is inactivated in this process, the resulting network is called a 'thinned' network. The ultimate prediction after training with dropout is viewed as an approximation of the ensemble average of predictions by many independent ANNs. Basically, the many different thinned networks created throughout the process are assumed to represent ANNs with different configurations and parameters. This heuristic discourages neurons to co-adapt too much and, as such, is believed to avoid overfitting. One may find parallels between the ensemble-average philosophy of dropout and that of the more traditional 'bagging' strategy in ML, originally developed by Breiman (1996), that bootstraps available data to develop an ensemble of models and average their outputs.

5. Fundamental differences from other ML methods

5.1. Local versus distributed representations

Most ML methods, such as those based on kernel functions, are based on 'local representations'. These methods, while forming *connectionist* networks like ANNs, represent each entity (e.g., a training sample point in the input space) via an independent processing unit. For example, radial basis functions (Broomhead and Lowe, 1988), Gaussian emulator machines (Kennedy and O'Hagan, 2000), and support vector machines (Vapnik, 1998; Cherkassky and Ma, 2004) may use as many kernels as the number of training samples. Each kernel typically has a limited radius of influence in the input space, and therefore only responds to inputs located in their local neighborhood. Kernel-based methods may face major difficulties when training data include identical or similar samples.

Conversely, a unique feature of ANNs is their ability to learn through 'distributed representations' (Hinton et al., 1986). They typically represent an entity via collective efforts distributed among multiple processing units (e.g., sigmoidal units). Unlike kernel functions, the sigmoidal units typically have large regions of influence (see e.g., Fig. 2c) that overlap each other in the input space (see e.g., Fig. 4b). The former figure shows that a sigmoidal unit influences the entire input space, by dividing it into three zones: lower tail, upper tail, and slope. The latter figure shows how the influences of four such sigmoidal units are superposed to generate the network response.

5.2. Implications for users

The use of distributed representations has several practical implications. To the author's knowledge, these include:

- ***Transparency***: The internal functioning of methods based on local representations is more transparent. Local representations are the most straightforward and easy-to-interpret way of learning, whereas distributed representations can be complex, often leading to emergent properties that cannot be easily explained by local representations (Hinton et al., 1986).
- ***Learning difficulty***: Distributed representations are more difficult and time-consuming to learn. In local representations, the role of each processing unit may be assigned independently of the other units, but in distributed representations, many processing units may be configured together in complex ways to represent a feature in the data.
- ***Network size***: Distributed representations often need much smaller network sizes. In general, the size of the networks based on local representations is directly proportional to the size of the dataset, in most cases with a proportionality constant of one; that is, the number of processing units mirrors the number of training data samples. The size of networks based on distributed representations, however, depends on the complexity of features in the dataset, not its size. This ability enables ANNs to scale relatively easily to big data sizes, whereas many kernel-based methods can become computationally intractable in the presence of large data sets; for example, Ratto et al. (2007) report a limit of only 400 sample points for the use with Gaussian emulator machines.
- ***Inexact interpolation or emulation***: Networks based on distributed representations are generally 'inexact emulators'. This means they do not exactly fit the training samples to represent the features and patterns in the data. This is unlike some other ML methods, such as radial basis functions (Broomhead and Lowe, 1988) and Gaussian emulator machines (Kennedy and O'Hagan, 2000), that are 'exact emulators', perfectly interpolating the training samples. Other inexact emulators include support vector machines (Vapnik, 1998; Cherkassky and Ma, 2004) and multivariate adaptive regression splines (MARS; Friedman, 1991).

In addition, ANNs are essentially multi-output models because they can have as many output neurons as required for a given problem. This means a single ANN can simultaneously predict different variables while

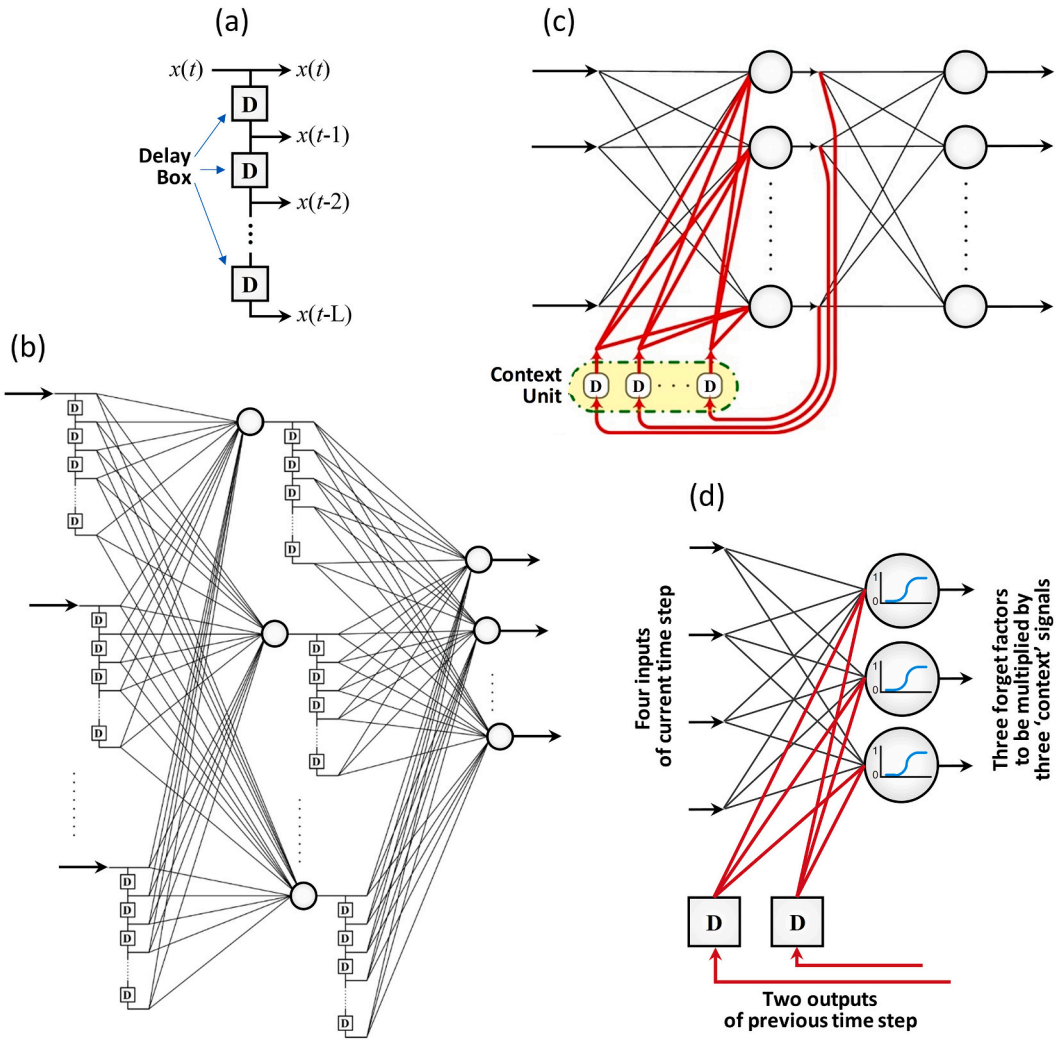

Fig. 7. (a) A tapped delay line (TDL), receiving the scalar $x(t)$ at each time step t and outputting the vector $[x(t), \ldots, x(t\text{-L})]$, where L is the length of the TDL. (b) A time delay neural network (TDNN) with one hidden layer and TDLs installed on the input and hidden layers. (c) A recurrent neural network (RNN) with one hidden layer and recurrent connections from the hidden neurons to themselves. In the case of long short-term memory (LSTM) networks, the context unit is controlled by gate layers that adjust the properties of the network's memory. (d) A sample 'forget gate' layer to be assembled on an LSTM model which has four inputs, two outputs, and three context signals that evolve through time steps.

accounting for their possible cross-correlations. Many other ML methods are single-output models. For example, in the case of support vector machines, one needs to develop two independent models to be able to predict two variables in the same system.

6. How to introduce order, time-dependency, and memory

Basic ANNs provide *static* mapping from inputs to outputs. However, many applications require mappings with a formal representation of time evolution and memory. To enable ANNs to do so, different approaches have been developed in the literature using operators such as delay boxes, recurrent connections, and information gates, as explained in the following.

6.1. Tapped delay lines

A tapped delay line (TDL) consists of a certain number of time delay operators arranged in an incremental order (Fig. 7a). TDLs can be installed on any parts of ANNs to represent time explicitly. The resulting ANN shown in Fig. 7b, commonly referred to as a 'time delay neural network' (TDNN; Waibel et al., 1989), has been widely used in a range of time-series processing applications. As such, TDNNs possess a *static memory with an adjustable length*. The length of a TDL can be viewed as a hyper-parameter to be tuned during training, along with network structural properties such as the numbers of layers and neurons in each layer.

Adding TDLs to an ANN significantly increases the number of tunable parameters. For example, a standard ANN with three inputs and 10 neurons in the first hidden layer would have 30 weights in that layer, while adding TDLs with a length of five to the inputs would result in an additional 150 weights (180 in total) to be trained.

6.2. Recurrent connections

TDLs, as described in Section 6.1, explicitly represent time with memory units of limited length. Unlike TDLs, recurrent connections, first introduced by Jordan (1986), enable ANNs to account for time evolution based on an *implicit* memory concept, which is theoretically of unlimited length and is highly context dependent (Elman, 1990). Recurrent connections receive the outputs of a layer at every time step and feed them back to the same or some other layer in the next time step. Technically, they do so via a 'context unit' that stores those outputs in a

set of delay boxes (Fig. 7c). Recurrent connections can be installed on one or more layers (e.g., Jordan, 1986; Elman, 1990) or locally on some select neurons (e.g., Frasconi et al., 1992).

An ANN enabled with recurrent connections is commonly called a 'recurrent neural network' (RNN). An RNN can possess many more tunable parameters compared to a standard ANN with the same number of layers and neurons. Using the example given in Section 6.1, an ANN with three inputs and 10 neurons in the first hidden layer would have 30 weights in that layer, whereas adding recurrent connections to that layer (similar to Fig. 7c) would add 100 more weights (130 in total) to that layer.

Unlike TDNNs that possess only a short-term memory, RNNs in theory can represent long-term dependencies as well. In practice, however, the implicit memory created by recurrent connections can easily be dominated by short-term dependencies. In other words, even very small features arising from short-term dependencies tend to mask features arising from long-term dependencies. In addition, RNNs are prone to the problem of exploding and vanishing gradients in their training, explained in Section 3.3 (Bengio et al., 1994). This is because RNNs, even with a single hidden layer, are in principle deep networks implicitly possessing an infinite number of recursive layers.

6.3. Gate layers to preserve or forget information over time

To balance and explicitly account for both short- and long-term dependencies, Hochreiter and Schmidhuber (1997) introduced a new type of RNNs, called 'long short-term memory' (LSTM). They extended and further parametrized the context unit (also called 'cell') such that the network can more explicitly control what information to hold over time and what to forget. The LSTM's context unit modulates not only the outputs in the previous time step but also the inputs to the network in the current time step. It typically does so via three new, independent layers of neurons arranged in the so-called 'forget gate', 'input gate', and 'output gate' layers. The neurons of each gate layer receive recurrent connections as well as the new input to the network, and generate their response between *zero* and *one* via using a logistic function (see e.g.,

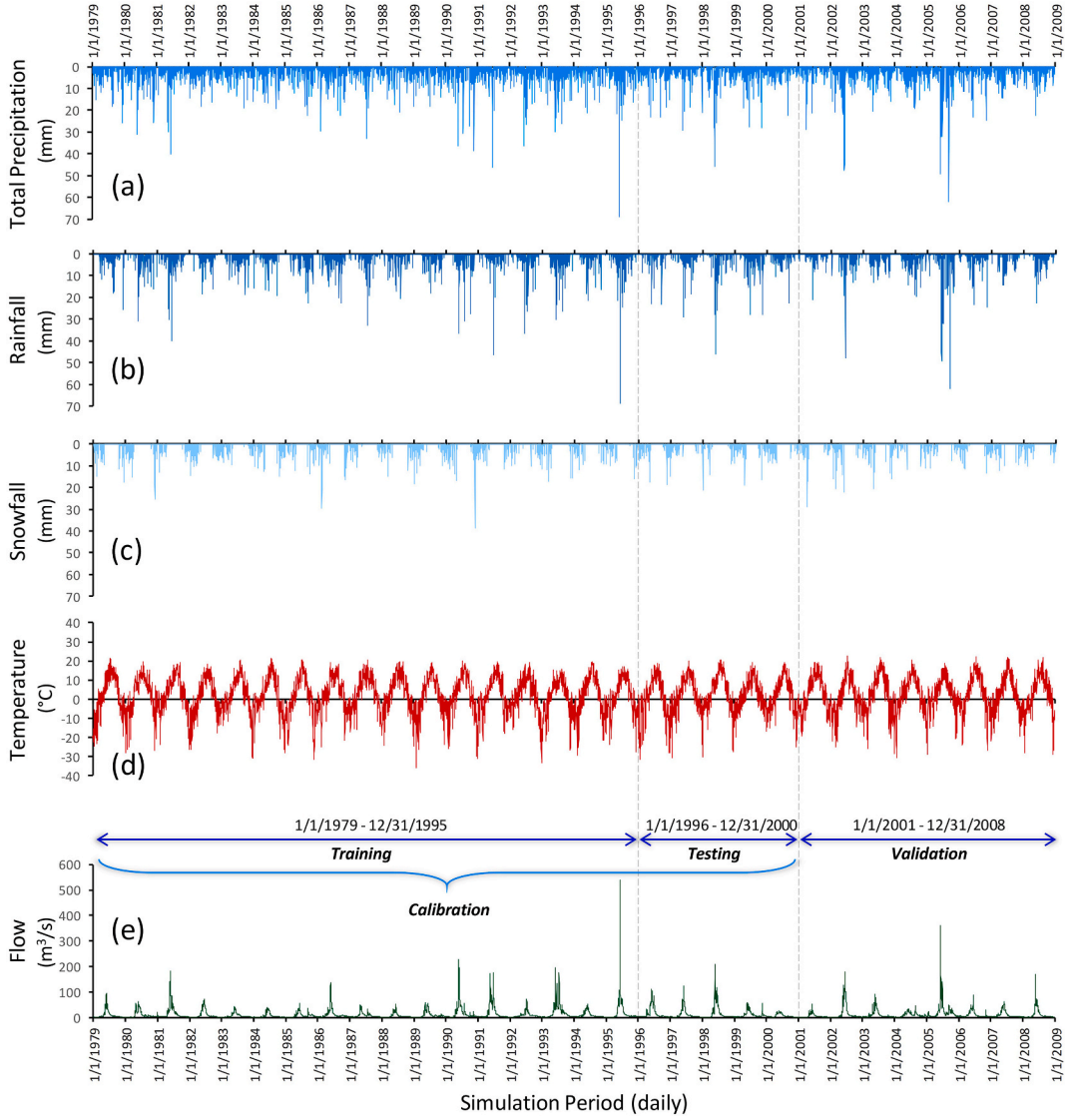

Fig. 8. The dataset used for the comparative modelling experiment with LSTM and HBV. (a) Measured precipitation time series (rainfall + snowfall). (b) Estimated rainfall time series (precipitation when daily temperature ≥ 0 °C). (c) Estimated snowfall time series (precipitation when daily temperature < 0 °C). (d) Measured temperature time series. (e) Measured river flow time series. The training period was used for LSTM training, while the testing period was used for early stopping. The calibration (training + testing) period was used for HBV calibration. The validation period was used to evaluate the performance of both LSTM and HBV in out-of-sample prediction. Note the naming convention in the ANN literature for the 'validation' and 'testing' periods is often the other way around.

Fig. 7d). These responses are then multiplied by their respective signals flowing through the context, which means a value of zero would kill a signal whereas a value of one would fully preserve it. Due to the additional weights and biases in the gate layers, an LSTM typically has many more tunable parameters than a conventional RNN.

LSTMs are now perhaps the most popular and widely used type of ANNs with memory. However, LSTMs took a long time (more than a decade) to become known and mainstream, particularly beyond their core computer science community. Their widespread application nowadays owes in part to recently developed software tools such as those in Python's *TensorFlow* that efficiently implement variations of LSTMs for a range of problems.

6.4. Training considerations when the order of data matters

The training of memory-enabled ANNs, such as TDNNs, RNNs, and LSTMs is different from that of standard ANNs in terms of the way time-ordered data are presented to the network. To train standard ANNs, the data entries can be presented in any order even randomly, for example through stochastic gradient descent (Bottou, 2010). In memory-enabled ANNs, however, the data entries should be presented in order of occurrence so that the structure of the time dependency is preserved. While this point might seem trivial, it requires careful attention in practical applications.

Another point to consider in the training of memory-enabled ANNs is that all data entries are typically viewed to have equal importance, regardless of their location in the sequence. When used in an online operational forecast, however, the 'forgetting factor' approach can be used to discount older samples. This approach allows the network to adapt to non-stationary environments, where more recent data are more representative of the underlying processes than older data (Razavi and Araghinejad, 2009).

Lastly, the above operators can be combined in a variety of ways. A well-known combination is 'time-delay recurrent neural networks' developed by Kim (1998) and used in various applications such as long-term precipitation forecasting in Karamouz et al. (2008). While such combinations may show improved modelling power compared to other ML or statistical methods, the attribution of memory gains to the different elements can arguably be challenging, if possible at all.

7. ML versus process-based modelling – an experiment

ML has been extensively used to model systems for which process-based models are also available. Process-based models are based on the physics governing the underlying processes and are therefore typically evaluated based on both their physical realism and goodness of fit to data. ML, however, does not do much, if anything, with the underlying physics while reportedly doing a superior job in fitting data, even in out-of-sample prediction. A fairly large body of literature benchmarks ML techniques, particularly ANNs, against process-based models. Examples of such comparisons (directly or indirectly) in the context of hydrologic modelling include Hsu et al. (1995), Tokar and Markus (2000), Wilby et al. (2003), Kratzert et al. (2018), Kratzert et al. (2019), Feng et al. (2020), and Ma et al. (2021). Some studies, such as Wilby et al. (2003), also detected correlations between the weights of an ANN and state variables of a process-based hydrologic model as a way to verify that their ANN can capture the underlying processes in a hydrologic system.

This section provides an experiment that runs and compares an ANN and a process-based model for the same problem and walks the reader through all of the steps involved. In particular, the processes around calibration and validation, role of physics, and interpretations of out-of-sample prediction are discussed. This experiment is performed in the context of hydrologic modelling, which has seen tremendous progress over the years with respect to both ML and process-based modelling.

7.1. Data and models

The case study used aims to model the hydrologic system of the Oldman River watershed in Alberta, Canada. This watershed has an area of 1434.73 km^2 at Waldron's Corner with a long-term average temperature of 2.2 °C. On average, this watershed receives 611 mm of precipitation (rainfall + snowfall) annually and generates 11.7 m^3/s of river flow. Fig. 8 shows the 30-year long daily time series data used. The first 22 years were used for model 'calibration' (i.e., the 'seen' data in model development) and the last eight years for model 'validation' (i.e., the 'unseen' data in model development). The first three months of the calibration period were used for model spin-up. For the ANN training, the calibration period was further broken into 'training' (17 years) and 'testing' (5 years) periods, the latter for early stopping of the training process to avoid overfitting. Note that, as explained in Section 4.2, the naming convention in the ANN context for the 'validation' and 'testing' periods is often the other way around.

To model this system, an LSTM configuration was chosen here as a state-of-the art model that accounts for time dependency and memory. The inputs to the LSTM model are daily precipitation and temperature (Fig. 8a and d) and the output is the concurrent daily flow (Fig. 8e). The LSTM structure was rather arbitrarily chosen to have one hidden layer with five neurons, resulting in 166 calibration parameters. For benchmarking purposes, a classic hydrologic model called HBV (Lindström et al., 1997), as implemented in HBV-SASK (Razavi et al., 2019), was used with the same data. HBV-SASK is based on a conceptualization of physical principles governing the water movement in a watershed using 12 calibration parameters. Each of these parameters has a physical interpretation and a physically justified feasible range (see Fig. 9 and Table 2 of Razavi et al., 2019). Full detail (including data) of this

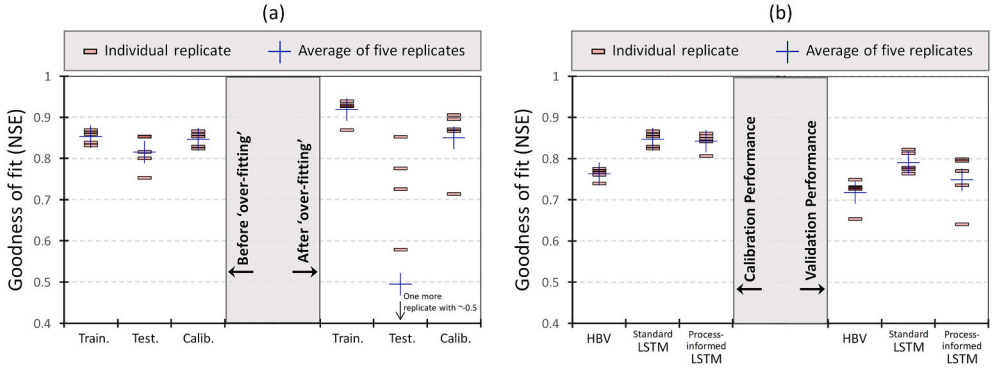

Fig. 9. (a) The performance of LSTM in training, testing, and calibration (training + testing) periods before and after 'over-fitting'. Training of each replicate was stopped once overfitting began - at epoch numbers ranging from 30 to 110 (left panel). Then, each replicate continued to complete 250 epochs in total to merely evaluate the impact of overfitting (right panel). (b) A comparison of LSTM and HBV in out-of-sample prediction. Standard LSTM and process-informed LSTM are discussed in Sections 7.4 and 7.5, respectively.

Oldman River watershed case study, which has been developed for educational purposes, is available with the source code.

7.2. Model performance in calibration

The model calibration problem was cast as an optimization problem that tries to maximize the goodness of fit to data by tuning the model parameters, with the Nash-Sutcliffe efficiency (NSE; Nash and Sutcliffe, 1970) as the objective function. NSE is essentially a normalized version of mean squared errors computed as 1-[VAR(errors)/VAR(observations)]. As such, an NSE of one indicates a perfect fit, and an NSE of zero indicates the model prediction is not any better than the average of observations. As a rule of thumb, hydrologists often call an NSE of 0.7 and higher an acceptable fit.

The LSTM model was calibrated using BP with the early-stopping strategy. In each epoch, the training period data were used to update the network parameters, while the testing period data were used to detect possible overfitting. Five independent replicates of LSTM calibration (with different initial random seeds) were conducted to account for possible variability of model performance. Fig. 9a shows the training results of the five replicates compared to a case where the training would not have stopped. As expected, the LSTM performance keeps improving in training, whereas in testing it begins to degrade at some point. The objective function in training came very close to one after many more epochs but with very poor performance in testing (not shown).

The HBV model was calibrated by a multi-start Newton-type optimization algorithm. Similar to LSTM, five independent replicates of HBV calibration were run. Fig. 9b compares the performance of HBV with that of LSTM in calibration. At this point, only check the performance of the 'standard' LSTM model in calibration. The figure shows all five replicates of LSTM outperform those of HBV. Note that the calibration performance of HBV shown herein is almost the best the author has achieved so far for this watershed. Based on these results, the superiority of LSTM over HBV in calibration is quite significant in regards to the goodness-of-fit to streamflow. The performance of the two models in validation is discussed in Section 7.4, but before that the next section discusses what information the two contained prior to calibration.

7.3. What about a priori information encoded in the models?

At this point, let us step back and investigate what we have achieved in terms of learning from data for both the LSTM and HBV models. The development of the LSTM model was not based on any *a priori* knowledge of how a watershed system works and the governing physical principles. As such, the model learned everything from scratch merely using examples from data. Basically, the model started with a fully randomized internal configuration controlled by a large number (i.e., 166) of parameters and then tuned those parameters to adapt the internal functioning of LSTM to the underlying real-world system represented in the data. Fig. 10a shows the LSTM performance of arbitrarily chosen replicates before and after calibration. The model response to inputs before calibration seems to be completely random but, after calibration, the model response has learned to closely follow the underlying system response.

Unlike LSTM, HBV encodes the expert knowledge available in the field of hydrology. This model is a collection of conservation of mass equations and process parametrizations that represent how hydrologists conceptualize the way a watershed works. This 'physically-based' modelling structure is presumably able to emulate the behavior of any watershed by tuning only 12 parameters. Fig. 10b shows how the HBV model performs before calibration, with parameter values chosen to be at the midpoint of their ranges, and after calibration. The figure shows the 'uncalibrated' model responds reasonably to the inputs; it generally captures the timing of flows and emulates the low flow segments well but is overly responsive to large precipitation events, generating spurious spikes in flows. Calibration, either manual by expert knowledge or automatic as done here via optimization, can fix the discrepancies and fit the model output to observations.

So, a fundamental difference between the two approaches is now clearer: using a process-based model is about directly using the expert knowledge available in a scientific field and tuning it to the case study of interest, while using ANNs is about learning everything from scratch directly from data. This difference is manifest in the number of parameters that need to be tuned to achieve a reasonable performance. Notably, the LSTM model achieved a better performance in emulating observations after calibration, as evident in a comparison of Fig. 10a and b. However, in any modelling exercise, one needs to ensure the model gives the right answer for the right reasons (Kirchner, 2006). That is why proper model evaluation in out-of-sample prediction is critically important, as discussed in the next section.

7.4. Model validation: standard versus true out-of-sample prediction

In general, validation and verification of mathematical models are very challenging in some scientific disciplines, if possible at all (Oreskes et al., 1994). The standard practice, however, is to test the performance

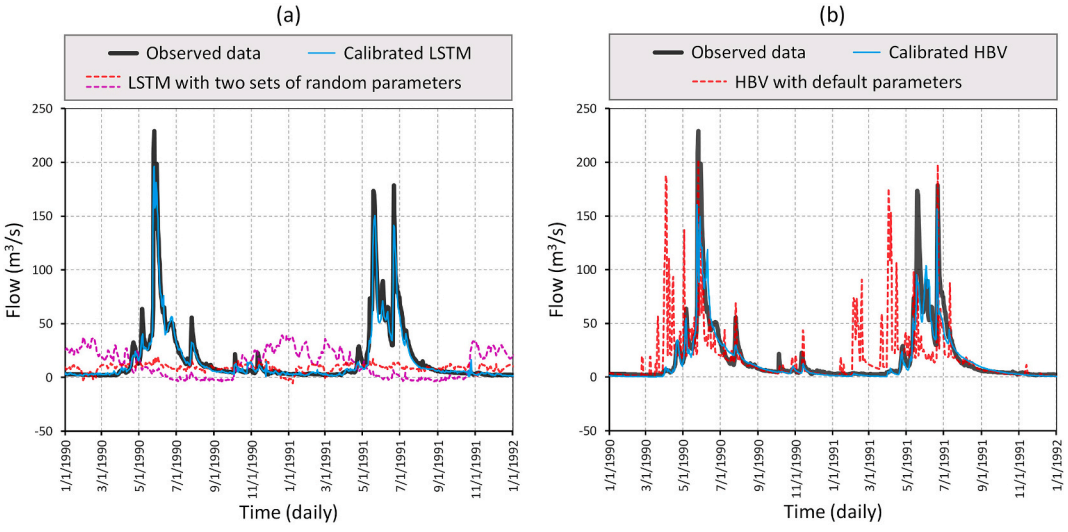

Fig. 10. What does a model learn through calibration? Performance samples of (a) LSTM and (b) HBV before and after calibration for a select two-year period.

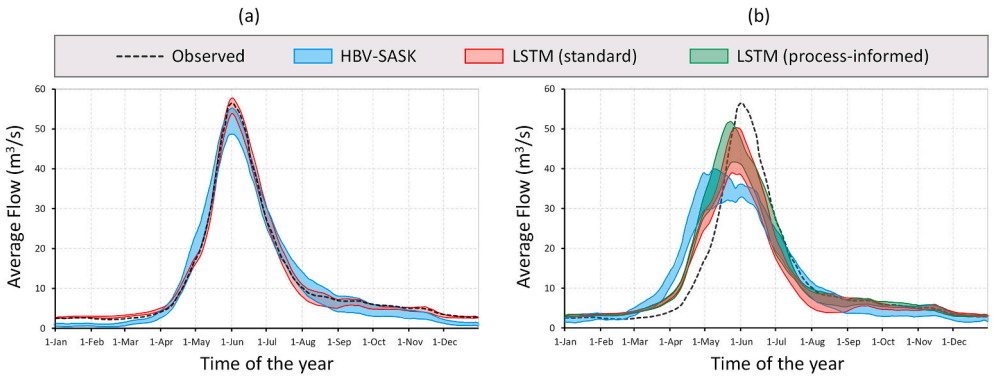

Fig. 11. Long-term average of daily flows throughout the year under the (a) historical and (b) hypothetical conditions. The envelopes represent the ranges of daily flows obtained by the five replicates of each model. The curves were smoothed by a 20-year moving average filter.

of the model under investigation in terms of reproducing some historical record not seen during model calibration (Klemeš, 1986a), a process called 'out-of-sample prediction' in this paper. Fig. 9b shows the results of such practice in the validation period set in Fig. 8. In this case, both LSTM (standard) and HBV models do reasonably well in regards to goodness-of-fit to streamflow, with LSTM outperforming HBV across all replicates. In addition, and as expected, both models produced slightly lower NSE values in validation compared to those in calibration.

A point is, as Oreskes et al. (1994) articulated, the above so-called 'model validation' is inherently partial. While the performance of LSTM appears to be better than that of HBV in a 'relative' sense, one needs to take extra care before making such a conclusion. As argued by Klemeš (1986a) more than three decades ago, a strong assumption in this type of validation is that the conditions under which the model will be used will be similar to the conditions under which the model has been developed and calibrated. It is now well-recognized that such an assumption may not hold, as many natural systems are essentially non-stationary (Milly et al., 2008). Despite such recognition, this standard model validation practice has arguably remained unchanged (Humphrey et al., 2017; Beven, 2018).

Here, let us take a stress-test approach via a *what-if scenario* question to test and compare the performance of both models in a 'true' out-of-sample prediction, basically under conditions that have not truly been seen in the process of model development and calibration. The question is how the system would behave if the average temperature warmed by 2 °C while everything else remained the same. To assess this hypothetical scenario, both calibrated models were fed a new temperature time series obtained by adding 2 °C to all daily temperature values of Fig. 8d. These new 'synthetic' inputs roughly provide a picture of what might happen in this watershed under global warming. The modelling results under such scenarios are typically used to inform policy making for climate change adaptation.

Now let us use the two different models to evaluate the possible changes in the watershed behavior in response to a 2 °C warming. Here, instead of looking at individual simulated time series, the possible change in the average seasonality of flows is of interest. First, look at Fig. 11a to check the consistency of simulated flows for the historical period. Both models generally follow the observed seasonality, but the range provided by the LSTM model is generally narrower and better encapsulates observations in both low and high flows.

Under the new conditions, however, the two models show the two distinct behaviors shown in Fig. 11b. According to LSTM, peak summer flows would decline by about 25% on average and the time of the peak would shift backward by about a week, from the beginning of June to a time in the fourth week of May. According to HBV, however, the changes would be more pronounced. The peak flows would decline by about 35% on average and the flows might show two modes: the higher one at the beginning of May and the other at the beginning of June, at about the same time as the peak in the historical observations. Are such differences not sufficiently large so as to make the user skeptical about the modelling process?

7.5. Injecting some physics into ML

At this point, one may wonder about the possibility of ensuring that LSTM results be physically consistent, particularly under new conditions. Let us give it a try by recasting the modelling problem based on some understanding of the governing physics in hydrology. For example, physics tells us that the freezing point of water is around 0 °C and, therefore, this threshold could be used as an approximation to differentiate rainfall from snowfall on a daily basis, i.e., if the temperature on a day is above/below 0 °C, the precipitation on that day, if any, is considered to be rainfall/snowfall (see Fig. 8b and c). This differentiation is actually a part of process parameterization in HBV, similar to many other hydrologic models, via a parameter called 'temperature threshold' (TT) for freezing/thawing and separating rain and snow, with a feasible range from −4 to +4 °C. The warming of a watershed would naturally change the rainfall to snowfall ratio, and so integrating this domain knowledge with the LSTM model makes sense.

Perhaps the most straightforward way of introducing the TT concept to LSTM is via pre-processing of the inputs. Therefore, a new LSTM model was developed and calibrated, called 'process-informed LSTM' in this paper, with three inputs: rainfall, snowfall, and temperature as shown in Fig. 8b, c, and d. Similar to the original, the new LSTM model has one hidden layer with five neurons, resulting in 186 calibration parameters. The procedure for the calibration and validation of the process-informed LSTM was the same as for the 'standard LSTM', already explained in Sections 7.2 and 7.4. Fig. 9b compares the performance of the process-informed LSTM with HBV and the standard LSTM. The figure shows the two LSTM models perform comparably well. Process-informed LSTM results in a slightly lower average NSE in validation but, with only five replicates, this small difference should be interpreted with caution.

Fig. 11b demonstrates the performance of the process-informed LSTM model in the 'true' out-of-sample prediction. According to this model, the summer peak flows would decline by 20% on average and the time of peak would appear about two weeks earlier than in the historical record, in the third week of May. In general, accounting for some known physics shifted the timing of the LSTM's rising limb to the left, to become more consistent with that of HBV. Such a shift is expected because now the model accounts for the new conditions under which there would be more rain and less snow, and rain tends to run off more quickly, whereas snow is stored in the mountain for longer times before it melts and appears in streamflows downstream. Incorporating any further physical knowledge to the LSTM will likely further shift the rising limb to the left. For example, one may attempt to inform the model about the known

direct relationship between temperature and snowmelt rate and the thawing/freezing threshold. Doing so, however, is less straightforward than the basic approach implemented above and requires modifying the 'internals' of the model. A review and discussion on more advanced strategies to incorporate the knowledge available into ANNs come later in the paper in Section 7.3.

7.6. So, what model should we trust: the ML or process-based model?

Now the question is which one of the three models produced the most credible picture of possible watershed behavior under the new conditions. In practice, this question is very difficult to answer, if possible at all. In general, the prediction of such changes can be debated and might vary from one study to another, depending on the models and data used and disciplinary views. Perhaps, a definite answer would need to wait until the future has come and shown such possible changes. And, from a bigger-picture point of view, models of natural systems cannot be verified or validated in true out-of-sample prediction, because those systems are never closed and not everything can be represented in a model, as argued by Oreskes et al. (1994) nearly three decades ago.

But, as scientists, we have our own perceptions and intuitions. These might be biased but still useful to provide a ground for building confidence in the credibility of a model. In the context of the case study given, previous research on the Canadian Rocky Mountains has indicated that warming *alone* will result in a considerable reduction in flows and earlier peaks in watersheds similar to the Oldman River watershed. A synthesis of research efforts under the Changing Cold Regions Network (CCRN; DeBeer et al., 2021) on the cold interior of western Canada indicates a shift in timing of the spring hydrograph rise and peak flows of nearly two weeks earlier by mid-21st century, and as much as one month by the late 21st-century. These projections, which themselves are based on rigorous atmosphere-landsurface modelling, are consistent with the modelling results presented in the previous sections but cannot pinpoint the most accurate model.

What is worrisome is the large divergence in behavior of models in response to expected, but yet to be seen perturbations, whereas those models produce comparable results in standard out-of-sample prediction. Broadly speaking, one might say any known consistency of a model with the known underlying physics can improve model's explainability and interpretability, thereby helping us better explain the model behavior in response to such perturbations. Explainability and interpretability are fundamental assets in building trust in a model, and of course, physically-based models are advantaged in that respect.

Related to the notion of explainability and interpretability, one way to boost confidence in a model is to go beyond checking only for the intended predictand (streamflow in this example) and to analyze or even constrain the model performance in terms of other fluxes such as evapotranspiration (e.g., Vervoort et al., 2014) or state variables such as soil moisture (e.g., Yassin et al., 2017). ML models, however, are typicality not developed to allow such analyses, while doing so is relatively straightforward in the case of process-based models. Enabling ML to do so requires an in-depth understanding and appreciation of the value of domain knowledge, as discussed in the next section.

8. Discussion

8.1. What is the typically ignored value of domain knowledge in DL?

True out-of-sample prediction is nothing but 'extrapolation' beyond the observed data and behaviors used in model development and calibration. Extrapolation is a reality that many predictive models nowadays must face because of 'non-stationarity' in climate and the environment (Milly et al., 2008). Any purely regression-type model, including those arising from DL, would be disadvantaged in extrapolation as, by definition, extrapolating would require working in parts of the problem space for which they have not received any information. Conversely, mechanistic models may be salvaged in extrapolation by the domain knowledge encoded within them.

But what does domain knowledge offer when it comes to extrapolation? The answer is a set of principles modulated via conservation laws (e.g., mass, energy, and momentum) and process parametrizations, which represent our perceptions of how two or more variables might be related (Gupta et al., 2012). Such principles have been developed and evolved over time based on extensive observation and research by scientists and practitioners. The *limits of validity* of such principles are typically known. In the following, the importance of taking advantage of those principles in modelling and prediction is discussed with respect to three aspects: conservation laws, monotonicity and rates, and feedback mechanisms.

Conservation laws: In physics, a conservation law states that a specific measurable property does not change within an isolated system with time. Such a law is usually expressed as a 'continuity equation'; that is, a differential equation equates the rate of change in storage within a control volume with the difference between what comes in and what goes out of the control volume. In land-surface modelling, for example, conservation laws are built into mechanistic models to ensure water and energy balance is preserved in simulations over time. ML models, however, do not automatically account for such laws and, as a result, water or energy can be *falsely* introduced or lost in the course of simulation.

Monotonicity and rates: The knowledge base includes the general characteristics of some causal relationships between various physical variables. For example, we know from basic thermodynamics that the relationship between melt rate and available heat is *monotonic*; that is, more heat causes a higher melt rate. Furthermore, we have some rough estimate of the feasible range of the *rate* of change in one with respect to the other. Similarly, from basic hydrology we know the causal relationships governing the way a hillslope stores and releases water are generally such that a positive correlation exists between water available in the soil and its contribution to flows; more water means more flows due to gravitational forces.

Mechanistic models directly account for such knowledge on causal relationships. This knowledge is encoded in process parametrizations typically in the form of deterministic, monotonic functions, or rarely in hysteretic forms, with a limited number of parameters to be calibrated to the specific case study in hand (Gupta et al., 2012). However, in the case of hyper-flexible models such as ANNs, such functions need to be entirely derived from data, all from scratch, and ignoring the knowledge base related to those monotonic relationships. Therefore, extrapolation runs the risk that such relationships become non-monotonic and/or have unrealistic rates, producing erroneous behaviors. This risk is exacerbated by the fact that identifying and diagnosing such errors are very difficult, if possible at all.

Feedback mechanisms: A real-world physical system is a combination of variables that interact over time, typically via a range of feedback mechanisms. Such feedback mechanisms control the internal dynamics of the system and are key to its evolution over time. For example, consider a coupled water-vegetation system in which precipitation, available soil moisture, and plant biomass interact in complex time-dependent ways, even at times creating positive feedbacks that destabilize the system's behavior (Rodriguez- Iturbe et al., 1991; Scheffer et al., 2001). The knowledge base available about these feedback mechanisms is often built into mechanistic models, using differential equations (ordinary or partial) to describe the system dynamics. The representation of such dynamics in the making of models is important, particularly for long-term predictions and over long time scales.

DL models are often unable to account explicitly for such long-term dynamics. If a particular dynamical behavior is present in training data, then DL can capture that behavior in its mapping from input onto output. DL however has no explicit mechanism to represent that dynamic under perturbed conditions beyond what has been recorded in the training data.

Is mechanistic modelling immune to issues with extrapolation? Certainly not. While a discussion on the limitations and prospects of mechanistic modelling is beyond this paper, one solution to improve extrapolability of mechanistic modelling over time, which is also relevant to ML, is 'space-for-time substitution'. Assuming spatial and temporal variations are equivalent, this strategy is to investigate multiple or many sites simultaneously, instead of one, to infer a temporal trend for a site based on information from other sites that have different properties and/or experienced different conditions. For example, refer to Pickett (1989) and Blois et al. (2013) in the context of ecology and Singh et al. (2011) in the context of hydrology. In the era of big data, ML can benefit explicitly or implicitly from such strategies when spatio-temporal data across large domains are available. For example, Kratzert et al. (2019), Feng et al. (2020), and Ma et al. (2021) utilize the CAMELS dataset, which includes catchment attributes and hydrometeorological data across many different sites (Newman et al., 2014; Addor et al., 2017), to improve the performance of DL in hydrological modelling applications.

In addition, both modelling paradigms, ML and mechanistic modelling, can benefit from knowledge-based patterns and behaviors derived from data around a real-world system. For example, the notions of limits of acceptability (Beven, 2006), hydrological signatures (Gupta et al., 2008), and pattern-oriented modeling (Grimm et al., 2005; Grimm and Railsback, 2012) can potentially inform the process of developing and validating models of any type. Such knowledge may be directly incorporated into the loss functions used to train DL models, as described in Section 8.3.

The bottom line is that mechanistic models are generally expected to be less prone to generating spurious behaviors in true out-of-sample prediction. Therefore, many domain experts may be inclined to trust physically-based models as their behavior is constrained by physical laws that are perceived as unchanging with time. The points made in this section will become clearer in the next section, where the essential differences between DL and mechanistic modelling are discussed.

8.2. Why is DL essentially different from process-based modelling?

In the author's view, the first principles of ANNs are rooted in *connectionism, hyper-flexibility,* and *vigorous optimization*. These characteristics are fundamentally different from the guiding principles of developing and calibrating mechanistic models, as described in the following.

Connectionism is an approach that orchestrates a set of simple algebraic operations in a massively parallel manner to create a model that is able to carry out complicated tasks. Following this approach, ANNs represent the response of a system under consideration to an input by summing the collective efforts of many neurons, whose roles cannot be easily attributed to individual processes involved in that system. This is unlike mechanistic modelling where each part of a model is designed to be responsible for a specific process.

Hyper-flexibility is a characteristic of a model with excessive degrees of freedom, which can literally fit any dataset, and is not constrained by the many assumptions held by typical statistical models. ANNs are known to be hyper-flexible. Mechanistic models, however, have limited degrees of freedom depending on the knowledge base available about the processes being modelled. Ideally, mechanistic models tend to have just as many degrees of freedom as can be supported and constrained by available knowledge and data.

Vigorous optimization here refers to the practice of manipulating model parameters at any cost to maximize the goodness-of-fit to calibration data. The training of ANNs is all about minimizing an error function; that is, among two competing ANNs, the one producing smaller errors in calibration and validation is the winner. Optimization is also often an essential part of mechanistic modelling to calibrate model parameters. However, in mechanistic modelling, minimizing the errors is not the goal but a means to improve the realism of the model. In other words, unlike the case of ANNs, physical feasibility of a parameter, its identifiability, and equifinality are typical considerations in mechanistic modelling.

The recognition of these fundamental differences is critically important when one aims to choose the right modelling paradigm for a purpose, compare the two paradigms in a case study, or attempt to bridge the two paradigms, possibly for improved modelling performance. The following section outlines the status quo for bridging the two paradigms and some emerging trends.

8.3. How can we bridge DL and process-based modelling?

The history of research on reconciling and bridging ANNs with mechanistic modelling in earth and environmental sciences dates back to the early 2000s or perhaps earlier. These efforts have generally had the objective of simultaneously leveraging the strengths of the two modelling paradigms to further our knowledge and predictive ability. Abrahart et al. (2012) reviewed such research in the context of hydrology and refer to it as 'hybridization'. They introduced three possible approaches for this purpose, which herein are referred to as 'surrogate modelling', 'one-way coupling', and 'modular coupling'. Seven years later, Reichstein et al. (2019) in an influential article in Nature re-introduced the notion of 'hybrid modelling' and the above three approaches as the next steps in earth science. In the following, these three approaches are explained, and then more modern existing approaches arising from research fields beyond earth and environmental sciences are discussed.

Surrogate modelling, alternatively called metamodelling or model emulation, refers to the process of developing and applying a simpler, cheap-to-run model in lieu of a more complex, computationally intensive model. In this process, a data-driven surrogate, such as an ANN, is trained on samples of a limited number of original model runs to approximate the model response surface. The developed surrogate model can then be used in different frameworks in conjunction with the original model in multi-query applications such as optimization and uncertainty quantification. Example applications of ANNs as surrogates of mechanistic models include Johnson and Rogers (2000), Broad et al. (2005), Behzadian et al. (2009), and Vali et al. (2021). The reader may refer to a review by Asher et al. (2015) for a range of approaches used for surrogate modelling.

One-way coupling refers to the process combining a mechanistic model with an ML model such that the output of the former feeds into the latter as input. A general rationale for such a combination is that a mechanistic model may not be able to fully explain the observed data and, therefore, an ML model could be of help in extracting any information left in the residuals of the mechanistic model. For example, consider a case where a mechanistic hydrologic model is used for streamflow forecasting and, as expected, some errors in model outputs are present. An ANN can be used to model such errors over a historical period to provide some predictive ability on the distribution of errors for a time step into the future. Then, running these two models in sequence may provide higher forecasting skills. Example applications of such one-way coupling include Shamseldin and O'Connor (2001), Anctil et al. (2003), Solomatine and Shrestha (2009), Wani et al. (2017) and Li et al. (in review).

Modular coupling refers to cases where an ML model is used as a module/sub-model of a larger mechanistic model or *vice versa*. The rationale for this type of coupling may be that a particular model might have proven skills in representing a particular process and is therefore preferred, while other processes are better represented by another model. Modular coupling is intrinsically an *ad hoc* process which can be done in a variety of ways, depending on the problem at hand and models and data available. For example, Chen and Adams (2006) and Corzo et al. (2009) used ANNs as the routing module within a distributed hydrological model. Chua and Wong (2010) developed an ANN-based hydrologic model using the output of a kinematic wave model as one of its inputs. Mekonnen et al. (2015) developed and coupled a

process-based model and an ANN model for simulating hydrology in contributing and non-contributing areas of prairie regions, respectively. Humphrey et al. (2016) developed an ANN model of monthly streamflow prediction that receives simulated soil moisture as an input from a process-based hydrologic model. Hunter et al. (2018) coupled a process-based in-stream salt transport model, an ANN-based saline groundwater accession model, and linear regression models of floodplain storage. Bennett and Nijssen (2021) developed an ANN model for the simulation of turbulent heat fluxes and built it into a process-based hydrologic model.

Beyond the earth and environmental sciences community, the notion of bridging the knowledge base and ML has a long history (e.g., see the 'knowledge-based artificial neural networks' by Towell and Shavlik (1994)), but it has received significantly more attention recently. Different approaches mostly arising from mathematics and computer science have been proposed under titles such as 'theory-guided data science' (Karpatne et al., 2017a), 'informed machine learning' (von Rueden et al., 2019), and 'physics-informed neural networks' (Raissi et al., 2019), to name a few. Providing a full coverage of such approaches is beyond the scope of this paper, and many of them have been developed for specific application areas with limited relevance to earth and environmental problems. In the following, three relevant approaches are explained.

Regularizing ANNs via knowledge-based loss terms: A new regularization function can be developed based on the available knowledge surrounding a given problem and be added to the loss function used in training. For example, any violation of the conservation laws or monotonicity of relationships, as described in Section 8.1, can be quantified and penalized during training. Refer to Stewart and Ermon (2017) and Karpatne et al. (2017b) to see how this approach can work in two different application areas, the former in image processing and the latter in lake temperature modeling.

Using mechanistic model runs to augment ANN training data: A mechanistic model can be used to simulate the system under investigation under a range of conditions to generate 'synthetic data' to augment the available training data. This approach may be particularly useful in guiding ANNs in extrapolation beyond conditions seen in the original training data (see the discussion in Section 8.1). This approach is based on the assumption that the mechanistic model used is sufficiently accurate—an assumption that needs to be treated with caution. For an example of this approach in the field of systems biology, see Deist et al. (2019).

Integrating differential equations into ANNs: This approach is a very recent and perhaps the most mathematically elaborate in terms of integrating the knowledge base into ANNs, primarily developed by Raissi et al. (2019). It parametrizes the known differential equations describing a system and integrates them into the body of ANNs. The integrated model is then trained to the available data, simultaneously inferring the parameters of the differential equations and network weights. One could view this approach as an extension to the knowledge-based loss terms described above where the new loss term penalizes the network for deviations from those known differential equations. This approach still seems embryonic but perhaps with great potential for scientific breakthroughs.

8.4. What can we learn from prominent ML applications?

ML has already been used across a wide range of disciplines and applications but with varying degrees of success. Here, and for context, consider two special and well-known applications: playing chess and predicting the stock market. ML has achieved incredible, superhuman-level performance in chess and similar games (Silver et al., 2018), while its performance in stock market prediction has been criticized despite its widespread application (e.g., Pearlstein, 2018). These opposing outcomes may be explained by the following reasons:

- Chess does not possess any properties of 'complex systems' (Bar-Yam, 1997), whereas financial systems are essentially *complex*, with a wide range of agents interacting at a wide range of scales, giving rise to emergent behaviors and even black swans. Any AI-based financial services themselves would also be agents influencing the stock market, even possibly inducing vicious cycles.
- Chess can be viewed as a *closed* system, as no exogenous factors influence any properties or dynamics of the board and players, whereas stock markets are open systems and, for any analyses, the assumed boundary conditions depend on the analyst's judgement.
- Chess is a *fully observable* system, as the entire board, pieces, rules, and moves are seen by the players, but stock markets are only *partially observable* and some controlling elements in the market might be hidden to the analysts.
- Chess is *stationary*, as the properties and governing rules of the game remain constant over time, whereas stock markets are *non-stationary* and their long-term dynamics and behaviors may change in unpredictable ways driven by political, social, economic, or natural events.

So what? Earth and environmental systems arguably fall somewhere in between these two specific applications with respect to their four fundamental and inter-related characteristics: such systems are *complex, open*, *partially observable*, and *non-stationary*. Loosely speaking, understanding and predicting earth and environmental systems face similar challenges to those of the stock markets in terms of those four characteristics. However, unlike stock market systems that are conceived to be partially predictable at best (Fama, 1970; Malkiel, 2003), the behaviors of earth and environmental systems are generally believed to be predictable, with limits of predictability that have been improving as more knowledge and data become available.

The comparisons above try to convey two points. First, the revolutionary success of DL in one field of application cannot necessarily be extended directly to another field of application. The context matters, and success depends on the characteristics of the problem at hand. Second, different disciplines may cross-fertilize DL applications and learn from one another. However, cross-fertilization is non-trivial and requires more direct communications between experts in different disciplines about existing methods, common issues, and ways forward.

9. Concluding remarks

DL has perhaps by now served every researcher and practitioner in earth and environmental sciences communities in tasks such as image and language processing, at least through their smart phones. Such astonishing and within-reach technologies have boosted interest in DL, and in AI in general, within these communities, evidenced by the significant growth in the number of their research papers on DL. Many, including the author of this paper, believe the combination of AI with unprecedented data sources and increased computational power will offer exciting new opportunities for expanding our knowledge about various earth and environmental systems. Unsurprisingly, similar to many other innovations, AI and particularly DL techniques are facing different and sometimes contrasting views towards their future; for example in the hydrology context, Nearing et al. (2020) suggest a divorce from the current hydrological theories while Beven (2020) advocates for the fundamental role of knowledge base in DL interpretation.

It is certainly an exciting time for earth and environmental sciences to benefit from DL tools. Shen et al. (2018) picture a bright future but articulate some important technical and cultural challenges to overcome in the years to come, by more targeted educational and organizational efforts. We need also to be mindful of any possible risk of hype and over-excitement around these new tools. Arguably, still many applications of DL in earth and environmental sciences have primarily focused on off-the-shelf applications of methods largely developed by mathematicians and computer scientists to problems in a new domain with no or limited considerations of the available domain's knowledge base. The

immediate risk of such practices is that the popularity of AI tools in earth and environmental sciences would then follow the ups and downs of those tools in the areas from which they originate. There is also a greater risk, in the author's view, as follows.

Let us flash back to more than three decades ago, when the prominent statistician George Box (1976, p. 797–798) warned about the "mathematistry" trap, "characterized by development of theory for theory's sake, which since it seldom touches down with practice, has a tendency to redefine the problem rather than solve it". He argued that "there is unhappy evidence that mathematistry is not harmless. In such areas as sociology, psychology, education, and even, I sadly say, engineering, investigators who are not themselves statisticians sometimes take mathematistry seriously. Overawed by what they do not understand, they mistakenly distrust their own common sense and adopt inappropriate procedures devised by mathematicians with no scientific experience." This sentiment was then echoed by the prominent hydrologist Vit Klemeš (1986b, p. 177 and p. 185), who said "The danger increases with the proliferation of computerized "hydrologic" models whose cheaply arranged ability to fit data is presented as proof of their soundness and as a justification for using them for user-attractive but hydrologically indefensible extrapolations." He continued, "The danger to hydrology from extrapolations based on mathematistry is that they lead it on the path of bad science."

The point here is that the risk of mathematistry seems to be just as fresh as it must have been back then, particularly when it comes to the application of AI tools in earth and environmental sciences. Due to the very nature of such tools, this risk may even well extend to their original areas of application, party because of their lack of explainability and interpretability, to a point that such practice has been referred to as a form of modern "alchemy"; see Rahimi and Recht (2017) for the sentiment, LeCun (2017) for a rebuttal, and Hutson (2018) for a summary. At a more fundamental level, Rudin (2019) argues that "trying to explain black box models, rather than creating models that are interpretable in the first place, is likely to perpetuate bad practice and can potentially cause great harm to society." This point is not to undermine the benefits of AI technology, particularly for earth and environmental applications. Instead, it calls for improved rigor and better appreciation of possible issues. After all, it has been long known even in environmental sciences that complex models can be made to produce virtually any desired behavior (fallaciously) given their large degrees of freedom, as articulated by Hornberger and Spear (1981) three decades ago.

Having such risks in mind, the new potential afforded by AI for earth and environmental sciences is great. To realize this potential, we need to reconcile data-driven AI techniques and the theory-driven knowledge base. The knowledge base is at the heart of 'traditional programming', which is still a major building block of process-based, mechanistic modelling in earth and environmental sciences. Clearly, the traditional, knowledge-based programming and AI are made up of two fundamentally different worldviews for problem solving and, therefore, their reconciliation will not be straightforward. This paper tried to address some critical questions in this regard and provide some perspective for this important endeavor, in anticipation of new breakthroughs in earth and environmental sciences in an age of big data and computational power.

10. Postscript

I had the privilege to receive relatively extensive feedback after this paper was posted on an open-access venue until the formal peer-review process was completed. I attribute this interest (and sometimes perhaps disinterest) in the paper to the extensive excitement that currently exists around AI and ML in earth and environmental sciences community. Among the review comments that I received, there were two extreme but contrasting views on the message and sentiments of this paper. One reviewer believed that this work is an attempt to ignore or minimize the benefits of the recent developments in DL for environmental modelling, which are essentially the applications of deeper ANNs that have been made possible by the growth in computational power and data availability. Conversely, another reviewer believed that this paper exaggerates such benefits and that the classic, shallower ANNs, that have been subject to extensive research in the past three decades, can work at least equally well in environmental modelling. I was intrigued by these two contrasting views and thought I would reflect on them in this postscript section.

This paper was not intended to support any of these contrasting views. Instead, the intention was to provide a rather balanced overview of how far we have come and the long-standing challenges, in an attempt to better inform and shape future AI-initiates in our community, away from any possible hype or over-excitement, one way or the other. My take is that either of those contrasting views may be subject to personal biases arising from factors such as research background and career stage. The former view seems to resonate primarily with the newer generation of researchers who are currently championing DL in earth and environmental sciences. The latter view, however, seems to be shared by more senior colleagues whose research portfolios include a long history of work on ANNs. My personal communications suggest that this group often feels frustrated by the recent avalanche of papers branded under "deep learning", many of which might be considered by the group as "reinventing the wheel", ignoring similar previous successful work in the field of environmental modelling and beyond. Being mindful of this fact, the present paper included numerous 'older' papers with ideas that still seem fresh today.

With respect to branding, I would like to include a quote from a recent book by Duerr et al. (2020) that:

> "In the earlier days of machine learning (ML), neural networks (NNs) were already around, but it was technically impossible to train deep NNs with many layers, mainly because of a lack of computer power and training data. […] Why do we talk about DL instead of artificial NNs? DL sells better than artificial NNs. This might sound disrespectful, but such rebranding was probably a smart move, especially because NNs haven't delivered what was promised during the last decades and, therefore, gained a somewhat bad reputation."

and a quote from the famous book by Goodfellow et al. (2016) that:

> "At this point [the authors refer to the early 2000s], deep networks were generally believed to be very difficult to train. We now know that algorithms that have existed since the 1980s work quite well, but this was not apparent circa 2006. The issue is perhaps simply that these algorithms were too computationally costly to allow much experimentation with the hardware available at the time."

Any interpretation of the above statements should of course consider their context, which is computer science, and areas of applications, which primarily are computer vision and natural language processing. Also, deep ANNs in those applications typically have thousands of layers, while in earth and environmental modelling, deep ANNs may have significantly fewer layers, perhaps in the order of tens or less. However, the above statements suggest that our community might need to be more careful in branding recent projects and initiatives around DL, with stronger connection with earlier similar work performed in our fields.

A reviewer asked for a direct comparison of deep versus shallow ANNs, wondering if deeper ones have really any superiority for environmental modelling. I think running such comparisons would require extensive numerical experiments across several case studies and may not be straightforward. Instead, this paper tried to explain an old theorem in simple language: how ANNs, either shallow or deep, are universal function approximators and can basically approximate any function if set up properly. Therefore, for typical environmental modelling, I am of the mind that one can make either one work, but the modelers need to be aware of nuanced issues as described in this paper.

Beyond any debate around deep versus shallow ANNs, a primary motivation of writing this paper was to address a long-standing issue that there is some mistrust in ML in part of our community, particularly among process hydrologists and theory-driven modellers. I have extensively dealt with that issue over the years as a researcher who started his research career with ML and ANNs in hydrology, back in 2003, but gradually delved into process-based modelling. My observations suggest that ML and process-based modelling have largely evolved in isolated research camps, among which the co-creation or exchange of knowledge has been limited.

The present paper might serve in bringing the two worldviews together and promote the dialogue between the champions of process-based modelling and those of ML. This dialogue might be much needed at this time of excitement and increased funding around ML in earth and environmental communities. Such dialogues can help us ensure proper training of the current students so they retain curiosity about physical understanding and expand our knowledge base while being equipped with the emerging data-science technologies and the ever-growing computational power.

Declaration of competing interest

The author declares that he has no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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