Neuroemulation: definition and key benefits for water resources research

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Abstract Neuroemulation is the art and science of using a neural network model to replicate the external behaviour of some other model or component of a model. It is an independent activity that is distinct from neural network-based simulation. Neuroemulation has become a recognized and established sub-discipline in many spheres of study, but remains poorly defined in the field of water resources research. Its many potential benefits have not yet been adequately recognized or established. Lack of recognition can in part be attributed to difficulties involved in identifying, collating and synthesizing published studies on neuroemulation: query-based searching of a publications database fails to identify papers concerned with a field of study, for which no agreed conceptual and/or terminological framework as yet exists. Therefore, in this paper, we provide a first attempt at defining such a framework for use in water resources investigations. We identify eight key benefits offered by neuroemulation and exemplify current activities with relevant examples taken from published research in the field. The concluding section highlights a number of strategic research directions related to developing the identified potential of neuroemulator applications for water resources modelling.

Key words neural network; neuroemulation; metamodel; emulation; emulator

1 INTRODUCTION

Increasing awareness and adoption of emulators for performing water resources research, spurred on by associated developments in computer power and data-driven modelling, is causing a minor methodological revolution in the way things are modelled. In broad terms, emulation is the process of imitating an existing model of a system, or an internal component of a model, i.e. a sub-model. The emulation...
process produces a secondary model, which is designed to reproduce certain outputs of another model or component sub-model, but does not explicitly attempt to capture the internal state representations or underlying physical environment of the original model or system: an emulator only attempts to reproduce a source model’s external output(s). In a strict sense, model X is said to emulate another model, Y, if the external behaviour (response function) of X under similar conditions is approximately the same as that of Y, albeit that the mechanism which is being used to deliver a set of near-identical answers is different, i.e. the same input produces the same output but not necessarily for the same reason. Accordingly, an emulator model is not a full replica of the original source model being emulated. Thus, emulation differs from simulation, which occurs at a higher level, in several important respects, but the two can nevertheless sometimes be confused. In principle, the general focus of simulation is the imitation or the modelling of real-life systems in some meaningful way. Emulation might involve using similar source model inputs, to produce similar source model outputs, with the overall goal of predicting a particular system being a common factor in both simulation and emulation. Furthermore, simulation and emulation procedures might share common ground in their use of identical modelling tools, protocols and methodologies. For example, a black-box model can be used as a simulator as well as an emulator. This superficial overlap is the root of many potential misunderstandings.

Emulation is said to deliver numerous advantages (Friedman and Pressman 1988), which include: enhanced modelling efficiency; enhanced model elegance and simplification; opportunities for improved model exploration and interpretation; model generalization to other models of the same type; sensitivity analysis; model optimization; answering inverse questions and providing the researcher with a better understanding of the behaviour of both the system under study and the interrelationships among its variables.

Emulators can be developed for a number of different reasons. However, since their overall goal is to reproduce one or more outputs of some other model, it is theoretically possible to develop and implement:

- full emulation, using a complete set of original model inputs (i.e. identical drivers); or
- partial emulation, using a subset of original model inputs: by omitting certain predictors, for example, if standard input drivers are not immediately available, cannot be accessed, or for model reduction purposes; or
- augmented emulation, using a mixed combination of original and additional model inputs, such as “tangential” or “contextual” variables, i.e. information reflecting physical insight into a problem, or particulars relating to global properties of the original data set, e.g. parametric information describing some overall structural aspect or pertaining to certain specific features of a particular data set; or
- surrogated emulation, using a totally different set of model input drivers, to deliver identical and/or modified original model outputs.

Emulators can also be developed to fulfil the role of independent standalone applications and/or used as an integrated component as part of some larger system. The fundamental issue at stake is that the emulator must be reproducing some aspect of the original model.

Emulation commonly applies either a traditional/statistical black-box approach (e.g. Reichert et al. 2011), or, more recently, uses a neural network (NN) model. It has become an established element of modelling activities in many fields, such as industrial processing (e.g. Swingle 1996), where NN emulators are called “neuroemulators”; the art and science of constructing a neuroemulator is termed “neuroemulation”; and the established use of neuroemulator applications for modelling or controlling dynamic systems is widely acknowledged. Neuroemulation is also a recognized subset of neuro-hybrid modelling: for a discussion on other types of neuro-hybrid solution, see Van den Boogaard and Kruijssen (1996) and Abrahart et al. (2012). However, in water resources research, the establishment of neuroemulation as an activity distinct from NN-based simulation has not been so forthcoming. Indeed, hundreds of papers concerned with hydrological simulation using NNs can easily be identified using standard database searches (for example, Dawson et al. 2006, De Vos and Rientjes 2007, Anctil et al. 2008, Wu et al. 2009, Besaw et al. 2010). The same cannot be said for neuroemulation. This is because the framework of a clear conceptual definition and terminology that distinguishes neuroemulation from other NN modelling activities in water resources research is, as yet, not adequately established. This makes it extremely difficult to disentangle NN papers on emulation from the majority of publications that are primarily concerned with
Neuroemulation: definition and key benefits for water resources research

409

simulation. Each NN in the latter option is used to model real-world observed records, instead of modelling computer-predicted estimations of such items. It is not so much that hydrological neuroemulation is not being done, but that it is not being fully differentiated by those who are doing it, and this means that its specific benefits for water resource research are not being adequately recognized. Indeed, the challenge in establishing neuroemulation as a distinct hydrological sub-discipline, which is able to demonstrate its specific scientific and practical benefits to the water resources modeller, requires three core steps to be undertaken:

1. The conceptual and terminological definition of an emulation sub-discipline and its positioning within the context of broader water resources modelling activities so that it can be properly distinguished from them.
2. The identification of its benefits, as exemplified from existing studies in which emulation has been a central component.
3. The highlighting of research directions for which hydrological emulation offers clear potential, thereby encouraging others to pursue it and providing forward traction for future studies to further develop the emerging sub-discipline.

This paper addresses these three core steps by formalizing the conceptual definition and terminology surrounding emulation, providing a classification of the benefits of neuroemulation in water resources modelling as evidenced and exemplified from published literature, and suggesting a range of future research directions that offer potential benefits.

1.1 Terminology

The conceptual definition and terminology surrounding emulation is clearly of importance, but can often be confusing or ambiguous. Terms such as emulator, metamodel, compact model, response surface, surrogate or proxy are often used in an interchangeable manner to mean the same thing. In certain cases, some penchant is expressed for one or other descriptor in a particular scientific discipline according to impulse or following an earlier precedent. The metamodel descriptor is of particular concern, since it is frequently used to represent a diverse set of fundamentally different scientific entities, spread across various modelling domains. For example:

- a categorization of theoretical models according to their quantitative or formal properties (Slobodkin 1958, cited in Chorley and Haggett 1967).
- a model of a numerical model (Blanning 1975, cited in Broad et al. 2005)
- a model of a physical laboratory model, such as a flume experiment (e.g. Kumar et al. 2010).
- a minimum information requirement lower-order model of the simplest structure that satisfies the modelling needs of some driving interest, whilst still ensuring that the model parameters retain their physical significance (e.g. Quinn 2004).
- a higher-level abstraction or description of an individual model highlighting certain specific properties of that original model, e.g. the explicit framework of rules, logic and reasoning which underpin it.

Consequently, a general tightening of meaning or so-called controlled vocabulary of terms for hydrological modelling emulator science is required, i.e. an explicitly enumerated and defined nomenclature must be established. This is essential for the existence of neuroemulation as a distinct hydrological sub-discipline and recognized field of research. All terms in a controlled vocabulary should have an unambiguous, non-redundant definition and, at a minimum, the following two rules should be enforced:

1. If the same term is commonly used to mean different concepts in different contexts, its name should be explicitly qualified to resolve this ambiguity.
2. If multiple terms are used to mean the same thing, one of the terms should be identified as the preferred term, and other terms listed as synonyms or aliases.

Figure 1 proposes a scheme for such a vocabulary based on a rationalization of existing modelling nomenclature used in water resources research. The emulator is situated in a basic hierarchy comprising real world, metamodel, functional model and emulator. Importantly, in our hierarchy a metamodel is a higher-order generalization of the real world. It documents a conceptual blueprint, to which some larger set of functional models will conform, in the same way that a computer program conforms to the grammar of the programming language in which it is written. In hydrology, a metamodel provides a conceptual framework for describing the catchment
response, detailing the various inter-links occurring between: drivers and processes affecting the hydrologic response; theories governing the operation of the hydrological process affecting the hydrologic response; and methodological approaches that are used to construct and test operational models of the hydrologic response, e.g. data-driven finite difference and finite element. This interpretation is consistent with other meta-prefix labellings in different subject domains and, as such, a metamodel abstraction is not a functional model. It cannot be used to deliver predicted output. Emulation is completely distinct from the metamodel and it functions at the lowest conceptual order. Emulators are substantially more removed from real-world physical processes, compared to a functional model simulator, and do not implicitly attempt to provide a degraded realization of some real-world “process”. They are not obliged to pay any genuine attention to the fundamental underlying physical or mechanical operations involved, although individual emulators may in fact be modelling a specific physical process on a one-to-one basis, or functioning as a sub-model to mimic a particular constituent part. Emulators are instead simply required to reproduce the original source model or sub-model output. In theory, each emulator should also be capable of predicting simulator output to an acceptable level of desired accuracy, and offer sufficient scope and flexibility to deliver a full set of probabilistic modelling opportunities.

1.2 Methodology

The identification of water resources papers in which neuroemulation features is particularly problematic. Standard contemporary approaches involving queries applied to a literature database can only ever uncover papers that have been indexed to an established and accepted taxonomy of disciplines and the sub-disciplines/activities that exist within them. At present, neuroemulation is an emerging field that has yet to be widely recognized as a distinct activity by the water resources research community. Thus, the terminology surrounding neuroemulation does not feature within the taxonomic structure to which these studies are indexed, and its explicit identification within the title, abstract and key words of papers is uncommon. Indeed, the present lack of a conceptual and terminological definition makes it difficult to identify the search terms best placed to identify neuroemulation papers in a database query of relevant literature on water resources research. The historical record of such activities is, as a result, very difficult to uncover, since papers that have deployed neuroemulators are hard to detect. This prohibits the production of a definitive list of all relevant neuroemulation papers in water resources research via standard searches.

For example, a systematic search for relevant papers on water resources issues was performed using the Thomson Reuters (formerly ISI)
Web of Knowledge research platform (http://www.webofknowledge.com) [19 July 2011]:

Topic=(emulator OR emulation OR neuroemulat∗ OR neuro-emulat∗ OR metamodel OR meta-model)
Refined by: Subject Areas=(WATER RESOURCES)
Timespan=1899-2010

This query returned only 38 papers, with a total citation count of 259, for the period 1992–2010 (Fig. 2). Metamodel was the most “popular” term. Neuroemulat∗/Neuro-emulat∗ did not identify any papers. Importantly, most papers that apply emulation and neuroemulation in water resources research, collected by the authors in an ad hoc manner over the course of several years of general research into the wider application of NN for hydroinformatics, were not identified.

The alternative to database searching is the adoption of a more traditional approach to uncovering relevant literature that places the emphasis on the ability of those seeking the literature to adequately synthesize and collate it. Indeed, in seeking to define new or emerging areas of study, the use of researchers’ experience and contextual knowledge of a wide body of potentially-relevant literature is arguably an appropriate way to proceed. This approach allows for a flexible re-interpretation of the conceptual underpinnings, semantics and terminology detailed in each study to a new framework defining the emergent sub-discipline or field. This is an essentially qualitative process founded on a high-level abstraction and it cannot be duplicated by simple Boolean search operations in a standard publications database such as Scopus (http://www.scopus.com) or Web of Knowledge. The method used to identify papers for inclusion in our analysis follows this approach, and draws upon the authors’ own collections of several hundred papers, spanning the last two decades, in which data-driven modelling in general, and NN modelling in particular, are applied in water resource studies. The case studies are selected by the authors primarily for their illustrative value as exemplars of particular modelling opportunities/benefits. Further, in most sections, the selected papers also represent the first recorded pioneering application(s) on a particular topic or issue of interest. It is, however, accepted that the discovery of additional neuroemulation publications may shed more light on the issues that are discussed in this manuscript, and potentially suggest new or amended categories of neuroemulator applications.

The remaining sections of this paper are devoted to delivering an overview of potential applications of neuroemulation for different aspects of water resources research. The material is organized according to a structured categorization of eight key benefits, developed iteratively. Each category includes example...
2 NEUROEMULATION APPLICATIONS IN WATER RESOURCE RESEARCH

The use of emulators in water resources research has traditionally comprised a response to objectives situated on a continuum ranging between operational and scientific. If the emphasis is placed on operational deliverables, the objective is to develop models that are more efficient in terms of computational speed and/or data requirements. For example, Bond et al. (1979) developed a simple parametric input–output emulator to predict the simulated output response obtained using a complex physically-based catchment model. More recently, Reichert et al. (2011) approximated the dynamics of an original hydrological model as a function of both model inputs and model parameters using a simplified linear state model emulator. If the emphasis is placed on scientific deliverables, the objective is to support knowledge acquisition, such as an improved understanding about the functioning of a particular model and its ability to adequately replicate processes in the domain of interest. For example, Rosso (1984), Chuta and Dooge (1990) and Shamseldin and Nash (1998) emulated a complex geomorphologically-based network of linear reservoirs using the Gamma Distribution Instantaneous Unit Hydrograph Model (Nash 1958).

Similarly, the scope and purpose of neuroemulator applications can be mapped against such a continuum. In Fig. 3, we position our iteratively-developed categories along this continuum according to the extent to which the reported objectives of each type of study is considered to be either more or less scientific. This ordering then forms the basis for a structural organization of our eight subsequent sections.

2.1 Supporting proof of concept

Neuroemulation can be used to support NN activities by demonstrating proof-of-concept modelling capabilities in a simplified and regulated virtual experimental test bed environment. Novel methods and approaches are put on trial under controlled conditions provided by the original model. The sole purpose of the original model in such cases is to deliver comprehensive data sets of an exact relationship that are easier to model, i.e. containing smooth, free-of-noise, self-consistent relationships. The end product will nevertheless deliver inflated levels of performance during the modelling of equation-generated outputs, in contrast to estimating observed records, with the latter anticipated to yield a substantially weaker solution and greater errors (Moreno et al. 2010). This category is illustrated by means of specially selected case studies, which soundly demonstrate the potential merit of neuroemulation for proof-of-concept explorations. The neuroemulators in such cases aimed to reproduce predicted model outputs...
obtained from a set of complex mathematical procedures, but used substantially different input drivers from those which the original modelling mechanisms required.

French et al. (1992) neuroemulated predicted spatial and temporal rainfall outputs originating from a mathematical simulator. Their approach was considered advantageous, since it is not subject to data quality and observational error issues, and an essentially unlimited set of records could be generated. The stochastic rainfall model, developed by Rodriguez-Iturbe and Eagleson (1987) and modified by Krajewski and Rodriguez-Iturbe (1990), was utilized to construct simulated rainfall patterns which served as “target output”. This model conceptualizes rainfall as a spatially-random Poisson process, in which summed contributions of “rainfall cells” over spatial and temporal domains produce realistic-looking rainfall fields. The cells are characterized by their attributes, e.g. time of birth, location of birth, rainfall intensity at the centre, velocity. The model, although an obvious simplification of reality, was considered sufficiently complex to provide a sound case study. The simulation domain was 100 km × 100 km at a resolution of 4 km, yielding a regular grid of 25 × 25 points (625 points). The NN inputs comprised spatially-distributed rainfall intensity records: output was forecast intensity valid 1 hour ahead over the same region. The simulation model was used to generate 75 statistically independent events, using identical parameters, such that the statistical characteristics of any sample of events were expected to be preserved. NN performance was compared against persistence and nowcasting approaches. The NN was found to be capable of learning the complex relationship describing the space–time evolution of rainfall, such as that inherent in a complex rainfall simulation model.

Minns and Hall (1996) neuroemulated predicted discharge outputs originating from a well-established conceptual model: RunOff Routing B (RORB: Mein et al. 1974). Their experiments were designed to assess the extent to which NN modelling approaches could capture the rainfall and runoff relationship; thereby assessing the learning capability of a NN. Theoretical catchments were used to investigate a range of different hydrological behaviours, varying from linear to highly nonlinear, all other factors being regarded as equal. Important controls are difficult to isolate and/or assess on real data sets since: (i) it would require prior classification of river regimes according to differing degrees of linearity or nonlinearity; and (ii) influential catchment characteristics will never be exactly equal. RORB is a general runoff and streamflow routing program. It is used to calculate flood hydrographs, by subtracting losses from rainfall, to produce rainfall-excess and routing that result through catchment storage to deliver its output. The program settings for their hypothetical catchment equated to a rural drainage area of about 30 km² in southern England. For simplicity, no losses were separated and the catchment was considered to have no impervious area. Monte Carlo methods, involving parametric assumptions, were used to construct six storm sequences. Events of varying duration, total depth and profile, occurring at irregular intervals, produced corresponding streamflow outputs. For simplicity, these rainfalls were treated as areal averages. NNs were found to be capable of identifying usable relationships between discharge and antecedent rainfall. It was also suggested that great caution should be applied in studies involving extreme flood events.

2.2 Enabling structural diagnostics

Neuroemulation, by definition, is intended to replicate the external behaviour of selected models. However, from a scientific viewpoint, it is also instructive to compare and contrast the internal structures and/or processing mechanisms arising, with potential counterparts located inside the source model. The modeller could thereby establish the extent of functional similarities and differences and in so doing ascertain if the emulator is: (i) modelling throughput in a comparable manner for the purposes of providing additional credibility to the emulator; or, conversely, (ii) providing alternative answers, which could be suggestive of conceptual improvements that might be applied to the original functional model or higher-level metamodel. Moreover, by means of such extended investigation and reporting, it should be possible to obtain a better understanding of internal neuroemulator dynamics which will in turn assist the neuroemulation community in developing improved solutions.

Wilby et al. (2003) neuroemulated predicted discharge outputs originating from a parsimonious Conceptual Water Balance Model (CWBM: Greenfield 1984, Wilby et al. 1994) of the Test River Basin, in Hampshire, UK. Their diagnostic experiments were designed to move away from the concept of using individual NN connection weights as a basis for analysis, and instead consider hidden units
et al. Xinanjiang Rainfall–Runoff Model (XRRM: Zhao et al. 1980, Zhao 1992). Their diagnostic experiments were designed to identify the nonlinear nature of different functional response surfaces being captured by the NN. The analysis spanned a modest range of rainfall events and catchment conditions, using a constrained random sampling methodology. XRRM was originally intended for use in humid and semi-humid regions. It has a small number of parameters, its structure and components have strong physically plausible meaning, and these factors in combination make it a popular tool for hydrological modelling purposes. The model in the reported paper was formulated as a single equation containing four variables (three inputs and one parameter) and no temporal component. The use of random inputs, possessing a uniform distribution, meant that certain unlikely combinations could occur. Full emulations were initially developed using the original model inputs and one of two different outputs: original computed discharge and a calculated runoff coefficient. Partial emulations were also developed on a smaller number of input variables, using omission and conflation of the original inputs, to reveal the changing nature of particular response surfaces which the authors considered to be of hydrological interest. The use of different input combinations also enabled the competencies of neural solutions developed on a reduced number of variables to be assessed. Their visual depictions provided indisputable evidence of reliable nonlinear input–output mappings being performed, confirming that given a respectable data set, neural computing can deliver what is required.

2.3 Performing sensitivity and uncertainty analysis

Neuroemulation can be used to examine internal sensitivity and uncertainty in the source model. This can be achieved by means of performing a great number of repeat runs, each based on a series of modified inputs or different parameter sets. The results of such explorations are subsequently used for generating statistical population distributions and in setting confidence limits on the original model. This method of analysis is identical to that used for traditional modelling applications, albeit that the neuroemulator is very much quicker. It is also possible, however, to build a NN model of error surface parameters derived from the source model. NN flexibility and adaptability with regard to inputs and outputs can be employed to deliver sound estimations of several different error quantiles and, by analogy, the shape of probability distributions at each individual point in a forecast.

Shrestha et al. (2009) neuroemulated parameter uncertainty bounds originating from a simplified version of the daily lumped conceptual rainfall–runoff Hydrologiska Byråns Vattenbalansavdelning model (HBV: Bergström and Forsman 1973, Lindström et al. 1997). Instead of building a NN model of the error in process model output, as in standard error updating, a predictive model of parameters describing an error distribution was developed. This is a useful activity, since direct estimation of model uncertainty bounds could remove the need to perform a Monte Carlo simulation on real-time applications. It would be especially advantageous if a large number of model runs was not practical, for example in the case of applying complex physically-based hydrological models, or if the forecast lead time was very short. Testing was performed on the Brue catchment in southwest England. Nine parameters were involved: using ranges based on calibrations derived from other model applications and/or hydrological descriptions of the catchment, extended as necessary, if potential solutions occurred
near a border. Monte Carlo simulation was performed on random parameterizations, sampled from nine uniform distributions. HBV is run on each set and a likelihood rejection filter applied. The remainder are used to produce a distribution of potential realizations at each time step: such that calculated upper and lower quantiles can be used to provide an output predictand in the form of either an upper or a lower prediction interval, i.e. “synthetic uncertainty descriptors”. The inputs were standard NN inputs: comprising selected lagged or differenced discharge and effective rainfall records. This method can be extended to predict several different quantiles and, by analogy, the shape of probability distributions.

2.4 Facilitating scenario analysis and decision making

Neuroemulation is often used to substantially increase the processing speed of an existing application; but, commensurate with such improvements, the very nature and scale of what can actually be achieved within an acceptable waiting period is also changed. High-speed modelling and faster completion times will permit more demanding types of problem to be addressed over realistic periods of computer calculation: (i) by reducing the computational burden involved in resolving convoluted multifaceted planning and design issues arising from scenario analysis; (ii) by enabling “number crunching” to be replaced with “model crunching”; and (iii) by supporting the implementation of extended runs on large data sets over very long periods of time, e.g. commensurate with our need to understand the surface impact of global warming. The net gain is twofold: greater end-user empowerment; and a more exciting field of thought-provoking opportunities for model builders.

Neuroemulation has been employed on numerous occasions to produce a quicker groundwater emulator solution, delivering processing speeds that can be up to two orders of magnitude faster. Each solution is subsequently coupled to a genetic algorithm and used to produce an optimal groundwater remediation strategy. The simulated aquifer contained a dissolved contaminant plume and different pump-and-treat abstraction and/or injection options are evaluated to discover the optimum number, location and pumping rates for remediation wells.

(a) Rogers and Dowla (1994) tested different remediation strategies for multiple contaminant plumes using a hypothetical heterogeneous aquifer. Their work followed the advection–dispersion method for solute transport modelling. Modelling adopted a discrete set of pumping rates, i.e. maximum permitted pumping or not pumping. Training examples were obtained from numerous simulation scenarios using two-dimensional hybrid finite difference/finite element flow and transport code (Voss 1984).

(b) Rao and Jamieson (1997) performed similar investigations on a simplified but representative approximation to a real aquifer contaminated with chlorinated solvents. The aquifer was assumed to be confined, homogenous and isotropic. Emulation again involved two discrete representations of pumping rates and examples developed using a vertically-averaged two-dimensional representation of coupled partial differential equations describing fluid flow, velocity and solute transport (Bear 1972).

(c) Aly and Peralta (1999) modelled observed records for a real single-layer aquifer contaminated with trichloroethylene, but did not opt to develop their own physical process source code, preferring instead to use a combination of two well-established and internationally recognized mathematical software products: Modular Three-Dimensional Finite-Difference Groundwater Flow Model (MODFLOW: McDonald and Harbaugh 1983, 1988) and Model Transport in Three Dimensions (MT3D: Zheng 1990). The former is a three-dimensional finite-difference groundwater flow model; the latter is a three-dimensional solute transport model that simulates advection, dispersion and chemical reactions of dissolved constituents in groundwater systems.

Parkin and associates (Parkin et al. 2007, Birkinshaw et al. 2008) neuroemulated predicted river-aquifer “interactions” originating from the complex process-based distributed integrated catchment modelling tool Système Hydrologique Européen TRANSPORT (SHETRAN: Ewen et al. 2000). Their motivation was to provide a means for rapidly assessing the impact of groundwater abstractions on river flow. Modelling sought to capture different controlling factors by means of a generic model for different types of river-aquifer system in England and Wales. Hypothetical case studies were used to develop a neuroemulator. SHETRAN required information on recharge and groundwater abstractions plus parameter values for different hydrogeological settings.
The simulations were also transient and involved time-varying recharge. The original model delivered 74 self-consistent outputs comprising: time series for flow depletion at the catchment outlet, spatial patterns of flow depletions along a river channel and water table drawdowns at various points around the abstraction well. To reduce that number, a generalized family of well-behaved curves were fitted to certain outputs, shape parameters being used to represent four curves, in which individual points formed part of a continuous response from SHETRAN. The generic emulator proved to be an efficient tool for representing the impact of groundwater abstractions across a wide range of conditions. It was also successfully tested on a field data set for a chalk aquifer, the Winterbourne Stream (Lambourn Catchment, Thames Basin, UK). Their reported method swiftly reproduced detailed process-based evaluations but it also highlighted the potential for developing generic emulators, which are not tied to a specific data set, and/or for adopting non-physical outputs in a NN.

2.5 Providing model calibration response surfaces

Neuroemulation is primarily focused on delivering faster and/or more efficient equivalents, but it can also be used to support traditional modelling operations. For example, a substantial speed-up in calibration (parameter estimation) and model assessment procedures can be invoked by means of an emulator. The development of an input–output response surface can also be quicker and better for other reasons, since the initial number of complex mathematical realizations required to produce an acceptable outcome can be much lower: small gaps can be in-filled; hydraulic insight can be applied in selecting strategic/tactical records, especially for large and complex field sites, supporting further acceleration and perhaps a better overall result. Field-scale applications, demanding the use of complex physical models—containing hundreds of parameters—that require slow and complicated numerical optimization procedures, would clearly benefit.

Liong and Chan (1993) neuroemulated predicted storm-event runoff outputs originating from the widely-used Storm Water Management Model (SWMM: Huber et al. 1982). The motivation behind their experiment was to develop a functional response surface that related model calibration parameters to final model output—similar to the full second-order polynomial procedure of Ibrahim and Liong (1992)—from which optimum settings could thereafter be identified. SWMM is a dynamic, physically-based, deterministic rainfall–runoff model that is used to perform single-event or long-term (continuous) simulations of runoff quantity and quality from primarily urban areas. SWMM was used to deliver simulated runoff volumes for the urbanized Upper Bukit Timah catchment in Singapore. Ten single-burst storm-event records were considered. Three representative storms were used to provide a modelling data set: their selected storms portraying upper, intermediate and lower magnitude scenarios of the available rainfall record. The other storms were reserved for out-of-sample testing. For each individual storm, 273 different realizations of eight physical modelling parameter values were implemented. Bounded parameter search was performed, within a physically meaningful range, by means of random sampling from a uniform distribution. The required response surface could thereafter be constructed. The nine neuroemulator inputs comprised eight calibration parameters plus rainfall volume: predicted output was runoff volume. The simulation period required for response surface development was reduced from seven hours for the equivalent mathematical procedure to about one minute or less for the neuroemulator. The neuroemulator also yielded relatively low prediction error: ranging from 2% to 5% on their testing data sets.

Khu et al. (2004) neuroemulated predicted discharge outputs originating from the MIKE-11 NAM model (Nedbor Afstromning Modele: Nielsen and Hansen 1973). Like Liong and Chan (1993), they sought to develop a functional response surface that related model parameters to final model output. Their hybrid solution was intended to reduce the number of simulation runs required, improving the feasibility of automatic calibration, by addressing the challenges of modelling a “changing landscape”, i.e. as more cases are gathered, the neuroemulator will require adjustment, such that greater efficiencies might be gained from performing search and update in a dynamic manner. NAM is a general-purpose lumped conceptual hydrological rainfall–runoff model, in which four interrelated storages are used to represent different physical elements of a catchment. The nine most important parameters of the model were to be determined by calibration (see Madsen 2000). First, a genetic algorithm is used to search for an initial population of preferred solutions in much the same way as any other optimization routine might be performed. This information is used in a neuroemulator
to construct an initial response surface, which is thereafter applied in a second genetic algorithm loop, as a rapid initial selection or rejection filter of candidate solutions, prior to implementing best-individual-based updating of the neuroemulator with NAM. The proposed method was tested on daily data sets for the Treggevaede catchment in Denmark. The results were comparable to that of a standard genetic algorithm, but the number of mathematical model runs required was reduced by 60%.

### 2.6 Supplying surrogate parts for system optimization

Neuroemulation can be used to deliver independent standalone applications, but it could also be used to develop smaller replacement modular components, which subsequently act as an integrated part of some larger system. The act of partitioning a larger problem into a set of smaller modelling challenges is expected to result in the production of superior internal components and an improved overall model. If one or more slow(er) components inside a complex system are replaced by emulators, the original mechanism will run much faster, whilst, from an overall conceptual position, everything else remains largely unaltered. Neuroemulation also offers a greater degree of independence from structures and methods related to the original model or program; something that might be very important in the case of a dedicated software product. It will, moreover, support “ease of extension”, since to encompass alternative inputs and/or mechanisms and implement different objective functions is a straightforward matter.

Solomatine and associates (Solomatine and Avila Torres 1996, Dibike et al. 1999) neuroemulated predicted downstream water-level outputs originating from MIKE-11: an industry standard hydrodynamic modelling system (Havnø et al. 1995). Two MIKE-11 computational modules were involved: (i) a lumped conceptual rainfall–runoff component (NAM, described earlier); and (ii) its core one-dimensional HydroDynamic (HD) component. Their primary goal was one of multi-criterial decision making for a three-reservoir system in the Apure River basin of Venezuela in which operational demands required water releases (turbine throughput and bottom outlet) for power generation, and operational constraints included minimal water releases for navigational, industrial, ecological and drinking purposes. The overall river control process was to be optimized by means of dynamic programming, requiring a hydrodynamic model of the river system to be incorporated into a standard optimization loop. MIKE-11 was used to perform the required downstream water level simulations, using observed data sets, but: (i) it is menu driven, i.e. modules could not be run unattended or controlled from an external program; and (ii) the time needed to perform an optimization loop would have been prohibitively long. Instead, neuroemulators were used to predict downstream depth at points of interest, receiving as input upstream sub-catchment discharges, releases from reservoirs, plus initial water level. The output was final water level. Each neural solution was converted into source code and compiled to provide a small compact executable, that was fast to run, and could be incorporated in the reservoir operation optimization loop as a direct replacement for MIKE-11. Different objective functions and/or optimization procedures could also thereafter be applied in a straightforward manner.

Wang and Jamieson (2002) neuroemulated predicted downstream biological oxygen demand outputs originating from TOMCAT (Temporal/Overall Model for CATchments: Bowden and Brown 1984, Cox 2003): a process-based river water quality simulation model developed by Thames Water (UK). TOMCAT was used to predict downstream consequences arising from treated effluent discharged into a river for different combinations of either: (i) a fixed-emission standard, enabling site selection; or (ii) individual standards for different plants so as to meet in-stream water quality requirements, enabling simultaneous site selection/waste load allocation. Their primary goal was cost reduction in which modelling sought to minimize the total (capital and operating) cost of treatment under different regulatory scenarios for works situated in the Upper Thames basin of southern England. The overall process was optimized by means of a genetic algorithm. TOMCAT is a complex mathematical “cause and effect” model. It is designed to account for assimilative capacity such as in-stream dilution, dispersion and natural purification (re-oxygenation), but is computationally demanding and not easily incorporated into a standard optimization loop. Neuroemulation delivered a simpler and faster mechanism, supporting rapid, near-optimal convergence, under different combinations of plants, standards and hydrological conditions. However, increased processing speed was supported by other massive computational savings. The number of TOMCAT model runs needed was substantially reduced: for a single river quality objective, from a
full search necessitating in excess of 5000 to only 500. This was considered sufficient to produce an appropriate spread of input–output pairings for building a NN.

Muleta and Nicklow (2004) neuroemulated predicted sediment yield and agricultural profit, at the level of a hydrologic response unit, originating from the Soil and Water Assessment Tool (SWAT: Arnold et al. 1998, American Society of Civil Engineers 1999). SWAT is a physically-based distributed river basin-scale public domain model that was developed to quantify the impact of land management practices in large, complex watersheds. The primary goal was speed-up: so as to improve the practical utility of an operational decision support tool for a typical user. This involved installing a neuroemulator replacement for the SWAT hydrological simulation component contained inside a previously developed multi-objective decision-support system. That particular routine formed part of a larger hybrid-coupling that was designed to aid in reducing the impact(s) of erosion while considering social and economic dynamics of a watershed. The overall process was optimized by means of a “Strength Pareto Evolutionary Algorithm” which searched for optimal or near-optimal watershed landscapes. These were defined as that combination of land use and farm management practices, at the spatial scale of a farm field, which simultaneously minimizes sediment yield and maximizes net agricultural profit over a specified period (Muleta and Nicklow 2002, Muleta 2003). The original watershed decision support model took 2.5 central processing unit days to process Big Creek: a 130 km² watershed in southern Illinois, USA. Neuroemulation reduced the computational period required to identify preferred landscapes and generate watershed management policies by some 75% (including data set creation and model development): run-time processing dropped from 63.25 hours to 4.5 minutes.

2.7 Streamlining of individual and modular solutions

Neuroemulation can deliver less complicated modelling solutions in the form of interpreted or compiled products that can be much easier to work with, i.e. a tool that is less difficult, convoluted, inconsistent, problematic or demanding. This statement might appear contradictory, given that each NN is a complex parallel processing mechanism, comprising an assemblage of numerous simple components, but not being simple in itself. However, their ability to acceptably perform full, partial, augmented or surrogated modelling will support the rapid production of simpler and less demanding mechanisms. From a practical, operational and managerial viewpoint, such products would be substantially easier to install, administer and resource. Their flexibility and adaptability with regard to inputs and outputs could also be used to deliver sound multi-model couplings. The simplicity of neuroemulators can provide an open ended “bridging mechanism” that relays diverse information from different models as part of a cascading series.

Hsu et al. (2003) neuroemulated predicted suspended sediment concentration outputs originating from the popular Hydrologic Simulation Program Fortran (HSPF: Bicknell et al. 1997). The motivation behind their experiment was to develop: (i) a less complicated surrogate that demanded fewer, easier/cheaper to acquire inputs; and (ii) a tool that could be operated by non-professional staff, i.e. model reduction/simplification. HSPF was considered difficult to support due to its heavy demands for numerous data sets and experienced personnel. This river basin modelling program is used to assess the effects of land-use change, reservoir operations, point or nonpoint source treatment alternatives, flow diversions, etc. It requires continuous temporal records of rainfall, temperature and solar radiation; surface characteristics such as land-use patterns; and information on land management practices in order to simulate the processes that occur in a watershed. Flow, sediment, nutrient and pesticide concentrations are all predicted. HSPF was applied to the Chi-Cha-Wan watershed in Central Taiwan. It was used to model Typhoon Seth (calibration) and Typhoon Tim (verification) in 1994. Ten other rainfall records for different typhoon events were thereafter passed through HSPF and its model outputs used to develop a neuroemulator. The NN inputs comprised a simple sequence of past rainfall and current discharge records, which were straightforward to collect, meaning that it could be applied in numerous situations where the demands of their original complex model could not be resourced. Their two models provided similar results, but the neuroemulator was quicker to implement and easier to run. Execution times are not reported.

Kamp and Savenije (2007) neuroemulated four different physical models: a daily lumped conceptual rainfall–runoff model (HBV, defined earlier); a 30-min one-dimensional hydraulic river channel routing model (Duflow: http://www.duflow.nl/); a 30-min estuarine salt intrusion model (Savenije 1989, 1993, 2005); and a 30-min ecological water quality
underwater light model (Secchi-depth Model: Blom 1992). Each model formed part of a larger loose-coupled “modular solution” in which outputs from the rainfall–runoff model were fed into the hydraulic model, and so on cascading down through the system in a serial manner. The main issue of interest was not emulation per se but to encourage simpler and sounder model coupling in which NNs deliver a “bridging mechanism”. The authors recognized an increasing need for different models to be coupled, but also understood that such activities were frequently handicapped by: (i) a requirement to run individual models in particular software packages; (ii) incompatibility issues related to dissimilar data formats and scales; and (iii) an inability to directly modify source code—a problem related to intellectual property rights. Four individual neuroemulators were developed for the Alzette Basin in Luxembourg. Three of the four solutions performed reasonably well, but their salt intrusion model struggled to represent both short-term (tidal) and long-term (hydrological) processes. The intermediate channel routing NN could nevertheless be used to connect two physical models. However, running four neuroemulators in series suffered from accumulated error build-up, mainly stemming from the rainfall–runoff and salinity NNs.

2.8 Delivering faster time-critical processing

Neuroemulation can deliver sound modelling solutions, possessing run speeds that are orders of magnitude faster. Speed-up offers clear benefits for both operational and non-operational applications. Neuroemulators can be used in operational systems where real-time demand places important deadlines, or perhaps mission-critical constraints on the activities and deliverables that must occur between “event” and “response”. The replacement of traditional mathematical products with neuroemulators could, for instance, deliver major improvements in processing speed for decision making and operational control in a dynamic water environment. However, productivity per time unit is also important in other ways, for example by delivering practical benefits for laboratory modelling even if a fast response time, or high performance operation is not essential.

Jamieson and associates (Jamieson et al. 2007, Rao and Alvarruiz 2007, Salomons et al. 2007, Martinez et al. 2007) neuroemulated predicted hydraulic and water-quality behaviour in pressurized pipe networks originating from a complex simulation model: EPANET (Rossman 2000). EPANET is public-domain water distribution system modelling software developed by the United States Environmental Protection Agency. It performs extended-period simulation of pipeline distribution systems and was developed to help water utility companies maintain and improve their delivery of water to consumers. To estimate the physical consequences of different pump and value settings for fluctuating spatial and temporal patterns of demand necessitates a process-based hydraulic simulation model. The computational demands of such approaches are nevertheless substantial. They require greater processing efficiencies to be acquired, so that real-time, near-optimal control of larger distribution networks and their frequently adjusted operational apparatus can be supported. Neuroemulators were used to capture the complex domain knowledge base of this hydraulic simulation model in an accurate and robust manner under different test conditions. The reported gains in computational speed-up to predict the consequences of different control settings were \( \times 10 \) for a hypothetical 41-pipe 19-node “Any Town” network (Walski et al. 1987). Higher gains were reported using larger emulators coupled to a genetic algorithm optimization procedure. This matched control settings to operating costs and water demand forecasts: \( \times 25 \) for a 112-node 126-pipe Haifa-A network (a sub-set of the water distribution network for Haifa in northern Israel); \( \times 94 \) for a 725-node 772-pipe city-scale network of Valencia in Spain.

Cullmann and associates (Schmitz and Cullmann 2008, Cullmann et al. 2009) neuroemulated predicted discharge outputs originating from two coupled public-domain products: (i) the detailed grid- and physically-based distributed rainfall–runoff hydrologic Water Flow and Balance Simulation Model (WaSiM-ETH: Gurtz et al. 2000); and (ii) optionally, to cover extended flooding or significant backwater effects at confluences, the Hydrologic Engineering Center River Analysis System (HEC-RAS: Brunner 2002). Their hydrodynamic model was parameterized for the Freiberger Mulde catchment in the Ore Mountains of Germany. The precipitation record was thereafter enhanced by including synthetic scenarios derived from a stochastic rainstorm generator. This mirrored typical meteorological catchment behaviour so as to represent all possible “constellations of flood formation”. The generator settings were based on meteorological analysis, and operating the hydrodynamic model on their revised data set enabled certain particulars to be considered as “state feature
Robert J. Abrahart et al.

vectors”. This resulted in a database of input/output vectors, which was thereafter completed by generally available hydrological and meteorological data for characterizing catchment conditions prior to each storm event. Their solution was considered sound. It was also able to reproduce the dynamics of a real flood. The reported gains in computational speed-up exceeded \( \times 100 \). Such rapidity is important in delivering flash-flood warnings, where every minute counts. It would permit real-time analysis and management of different structural defence scenarios, if such items were to be included. Their methodology was also applied to an ensemble of temporal and spatial rainfall scenarios containing 200 members, facilitating a straightforward evaluation of meteorological forecast uncertainty.

3 SUMMARY AND CONCLUSIONS

This paper provides a dedicated introduction to the subject of neuroemulation for water resources modelling and offers a structured categorization of on-going developments in an expanding field of uncharted research activity. The authors recognize that the methodology employed in synthesizing and collating relevant literature is counter to contemporary norms by which many appraisals are now being conducted (i.e. extensive database searching). However, we argue that, in exemplifying the benefits of the newly-emerging sub-discipline of neuroemulation, for which a standard terminology is as yet unrecognized in water resources research, the reported adoption of a qualitative analysis of relevant literature based on expert knowledge is an appropriate starting point. There is a possibility that more sophisticated and more comprehensive full-text search methodologies may identify additional relevant studies that can build on those presented here, particularly if soft or fuzzy search schema are employed. Indeed, conducting such an investigation represents a future study that is worthy of deeper consideration and appropriate funding.

It is argued that neuroemulation activities have not been awarded sufficient recognition, nor given due past credit in the water resources domain. In part, this may be attributed to the need for a consistent and coherent vocabulary surrounding emulation activities, which makes important applications hard to identify in the research literature. If the field is to become better established, some meaningful agreement that delivers stronger recognition and appropriate and consistent language is required. However, one could also speculate that this lack of a developed nomenclature is simply symptomatic of a more general lack of recognition of the importance of emulation by researchers. Indeed, the process of using one model to represent another model is sometimes considered to be less scientific or less elegant than resolving other, more pressing, or more controversial, modelling challenges.

The literature presented here challenges recent concerns that further investigation into the use of NN tools for water resources modelling might prove to be an academic cul-de-sac (Wilby et al. 2003, p.164) by highlighting their potential implementation as emulators. Indeed, when NNs are used to perform emulation, particularly in situations where out-of-sample testing is paramount and no physical hydrological considerations are involved, arguments about the lack of transparency or hydrological knowledge in NN solutions become less important. Indeed, in this context, the potential value of NN research is more evident. The following caveats should nevertheless be noted:

- the time and effort needed to construct a NN solution must be offset against potential gains;
- emulator performance will depend on the performance of the parent model; and
- emulator performance could deteriorate if it is applied beyond the range of conditions used in development.

To conclude, three potential avenues for further research emerge from the literature presented in this review:

1. **Neuroemulator choice and evaluation** Most reported experiments involved a single individual neuroemulator. No comparison of different types of emulator or different emulation strategies was provided. Thus, two key questions remain unanswered: (i) how should the form and function of a neuroemulator to be determined; and (ii) how is the preferred neuroemulator mechanism for a particular situation to be decided?

Several major models have been emulated to good effect but no comprehensive evaluation was reported. Indeed, neuroemulator mechanisms were only tested for accuracy. Following Jin et al. (2000), it is our belief that various factors contribute to the success of a given emulator, including nonlinearity of model behaviour, dimensionality and data sampling, and internal parameter selection.
settings for the method under test. They contended that multiple metrics should be considered for comparison, including accuracy, efficiency, robustness, model transparency and simplicity. Knowledge of performance and of the impact of contributing factors to its success is of utmost importance to designers when trying to choose an appropriate method for emulating a particular application. The development of neuroemulators in most reported instances equated to a straightforward mundane operation, but experiments performed on perfect data sets, which were designed to provide a good fit to the simulator, might deliver a different product to a solution trained on real-world observations that contained random noise or systematic error in inputs and/or outputs. The adoption or inclusion of modified and disrupted input–output pairings should, in consequence, be tested.

2. Methods for constraining neuroemulators In choosing and evaluating a neuroemulator, the satisfaction of constraints will be an important factor, since a neuroemulator cannot take specific advantage of the original model structure, making it vulnerable to the production of inappropriate solutions and/or outputs. Indeed, a neuroemulator must not only provide an accurate representation throughout the full operational range of its parent simulation model, it should also recognize and account for physical modelling controls in the original source model such that pertinent limiting factors are not compromised. This requirement not only applies in the vicinity of the global optimum, but it is also vital that an appropriate numerical representation is provided at the margins of the model development process. If the neuroemulator wrongly indicates that a particular solution is feasible and/or the output is correct, the search process could be directed into an undesirable region of the solution space, resulting in the capture of local sub-optimum relationships as opposed to the production of a global optimum representation in the final model.

3. Methods for efficient neuroemulator development Most studies that were reviewed involved the production of massive data sets, a tedious and time-consuming business. The reported neuroemulators were developed on a random sampling of the solution space, but more efficient and effective methods could be used. These might include the adoption of non-uniform sampling strategies, as reported in other subjects, e.g. performing a local search around optimal solutions using the original simulation model. Similarly, the use of neuroemulators is of particular interest in the case of large models possessing numerous inputs and outputs. However, for really massive simulators requiring hundreds of inputs and parameters to be incorporated, some sort of “screening” or “input/parameter reduction” procedure would be very useful. The different potential methodologies that might be adopted could be explored.

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