

**METHODS USED FOR THE DEVELOPMENT OF NEURAL
NETWORKS FOR THE PREDICTION OF WATER RESOURCE
VARIABLES IN RIVER SYSTEMS: CURRENT STATUS AND FUTURE
DIRECTIONS**

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Abstract:

Over the past 15 years, artificial neural networks (ANNs) have been used increasingly for prediction and forecasting in water resources and environmental engineering. However, despite this high level of research activity, methods for developing ANN models are not yet well established. In this paper, the steps in the development of ANN models are outlined and taxonomies of approaches are introduced for each of these steps. In order to obtain a snapshot of current practice, ANN development methods are assessed based on these taxonomies for 210 journal papers that were published from 1999 to 2007 and focus on the prediction of water resources variables in river systems. The results obtained indicate that the vast majority of studies focus on flow prediction, with very few applications to water quality. Model inputs, appropriate data subsets and the best model structure are generally obtained in an *ad-hoc* fashion and require further attention. Although multi layer perceptrons are still the most popular model architecture, other model architectures are also used extensively. In relation to model calibration, gradient based methods are used almost exclusively. In conclusion, despite a significant amount of research activity on the use of ANNs for prediction and forecasting of water resources variables in river systems, little of this is focused on methodological issues. Consequently, there is still a need for the development of robust ANN model development approaches.

Keywords: Artificial neural networks, Water resources, River systems, Forecasting, Prediction, Modelling process, Model development, Review

1. Introduction

Over the last 15 years or so, the use of artificial neural networks (ANNs) for the prediction and forecasting of water resource variables has become a well-established research area. In the early years (1992 to 1998), ANNs were considered a novel modelling approach and, consequently, research efforts were directed primarily towards the application of ANNs to different types of problems and case studies in order to assess their utility as an alternative modelling approach. The large amount of research activity in this area led to a number of review papers in 2000 and 2001 (Maier and Dandy, 2000; ASCE, 2000; Dawson and Wilby, 2001), which not only confirmed the potential of ANNs for the prediction and forecasting of water resource variables, but also identified a number of challenges that needed to be addressed in order to ensure that ANNs become a mature modelling approach that can sit comfortably alongside other approaches in the toolkit of hydrological and water resource modelers.

In their review, Maier and Dandy (2000) suggested that there needed to be a shift in the focus of ANN research from the application of ANNs to various water resources case studies to addressing a number of methodological issues. Attention to good practice in model development is vitally important in all modelling efforts (Jakeman et al., 2006; Robson et al., 2008; Welsh, 2008), but is particularly important in the development of ANN models, as they are developed using available data and not based on underlying physical processes explicitly, thereby increasing the chances of developing a model that is not very meaningful. Consequently, the focus of this review paper is on the methodologies that are used in the development of ANN models for the prediction and forecasting of water quantity (e.g. flow,

level) and quality variables in river systems. The steps in the ANN model development process are outlined, taxonomies of the methods that are available at each of these steps are presented and the methods that have been utilized in 210 papers that have been published in well-known international journals from 1999 to 2007 are analysed in relation to these taxonomies. This provides a snapshot of the methods that are used at the various steps of the model development process during this time period. It should be noted that this paper does not evaluate the performance of ANN models relative to other water quantity and quality models, nor does it critically evaluate the latest advancements in ANN modelling. These should be the subject of other review papers. Throughout this paper, in-depth descriptions of the methodologies are not given, as readers are expected to be familiar with ANN modelling and the various methods employed therein. Information on the basic concepts of ANNs are given in many papers and textbooks (e.g. Flood and Kartam, 1994; Hassoun, 1995; Maren et al., 1990; Masters, 1993; Rojas, 1996; Bishop, 2004).

The remainder of this paper is organized as follows. In Section 2, details are given of how the database of papers was assembled, as well as an overview of the research activity in the use of ANNs for the prediction and forecasting of water quality and quantity variables in river systems from 1999 to 2007. This period was chosen as it follows on from the period time period covered in the review by Maier and Dandy (2000) (i.e. 1992 to 1998). In Section 3, a brief outline of the steps in the ANN model development process is provided, followed by the taxonomies of available options at the various steps in this process, against which the 210 papers are assessed in terms of the modeling approaches adopted. The final section provides a summary and conclusions of the findings of this paper.

2. Overview

The articles reviewed in this paper are taken from the following international refereed journals (the numbers in brackets are the journals' 2008 ISI impact factors): Advances in Water Resources (2.235), Civil Engineering and Environmental Systems (0.425), Environmental Modelling and Software (2.659), Environmetrics (0.719), Hydrological Processes (2.002), Hydrological Sciences Journal (1.216), Hydrology and Earth System Sciences (2.167), International Journal of Water Resources Development (0.738), Journal of Environmental Engineering (1.085), Journal of Hydroinformatics (0.681), Journal of Hydrologic Engineering (1.007), Journal of Hydrology (2.305), Journal of the American Water Resources Association (1.208), Journal of Water Resources Planning and Management (1.275), Nordic Hydrology (1.194), Stochastic Environmental Research and Risk Assessment (0.951), Water Resources Management (1.350), Water Resources Research (2.398), and Water SA (0.721). These journals were chosen because they are widely recognized international journals in the fields of hydrology and surface water resources. A keyword search of the ISI Web of Science was then conducted for these journals for the period 1999 to 2007 using the search term "Neural Networks", resulting in 516 articles. This list was refined manually to exclude papers focusing on rainfall, groundwater, lakes and reservoirs, parameter estimation etc., resulting in 210 selected papers focusing on the prediction and forecasting of water quantity and quality variables in river systems.

Details of the selected papers, including year of publication, authors, study location and variable predicted are given in Table 1. The distribution of papers by year of publication is given in Figure 1. As can be seen, there has been a strongly increasing trend in the number of papers published since 2001, with 46 papers published in 2007 alone.

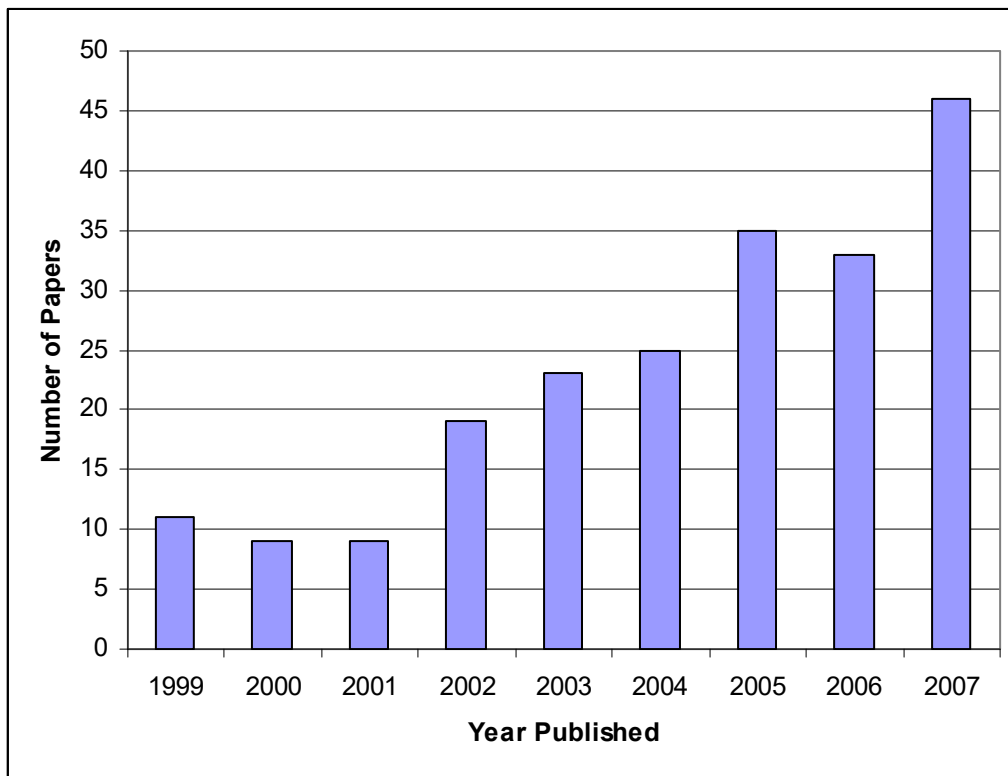


Figure 1: Distribution of Papers by Year of Publication

The number of papers in which water quantity and water quality variables were predicted is given in Figure 2. As can be seen, water quantity variables were predicted in more than 90% of the papers, of which flow was by far the most popular (see Table 1). Water quality variables were predicted in fewer than 10% of the papers.

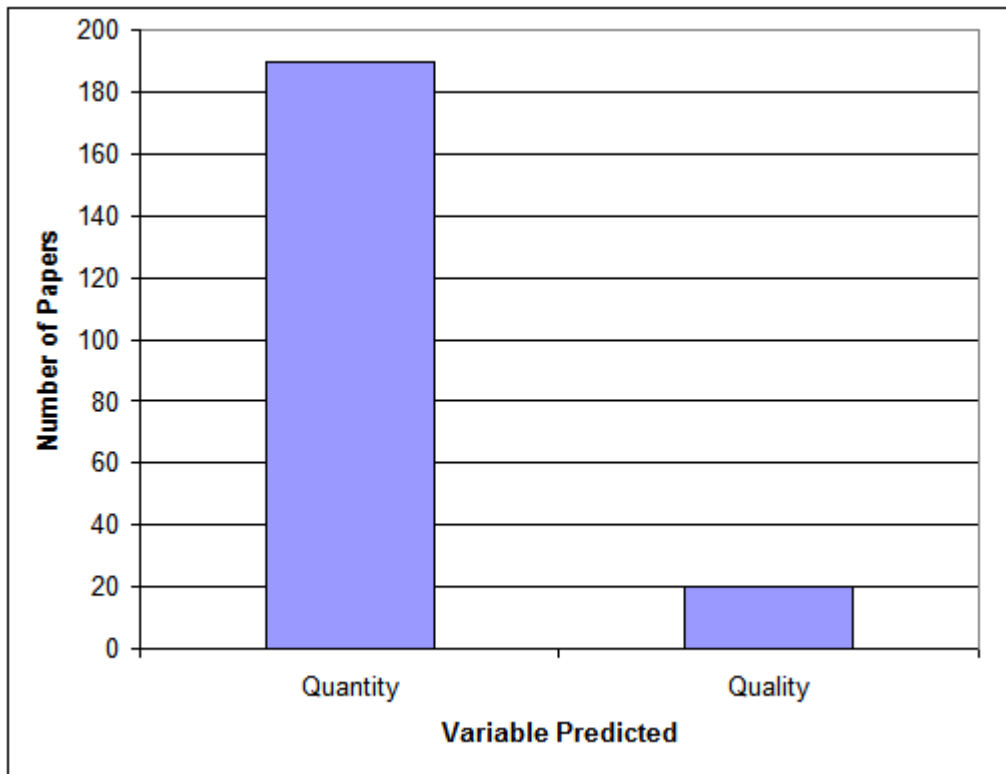


Figure 2: Number of Times Water Quantity and Water Quality Variables were Predicted

The distribution of time steps considered is given in Figure 3. As can be seen, a daily time step was used in 105 of the 210 papers reviewed, followed by hourly (49 papers) and monthly (34 papers) time steps. It should be noted that a number of different time steps were used in some of the papers reviewed

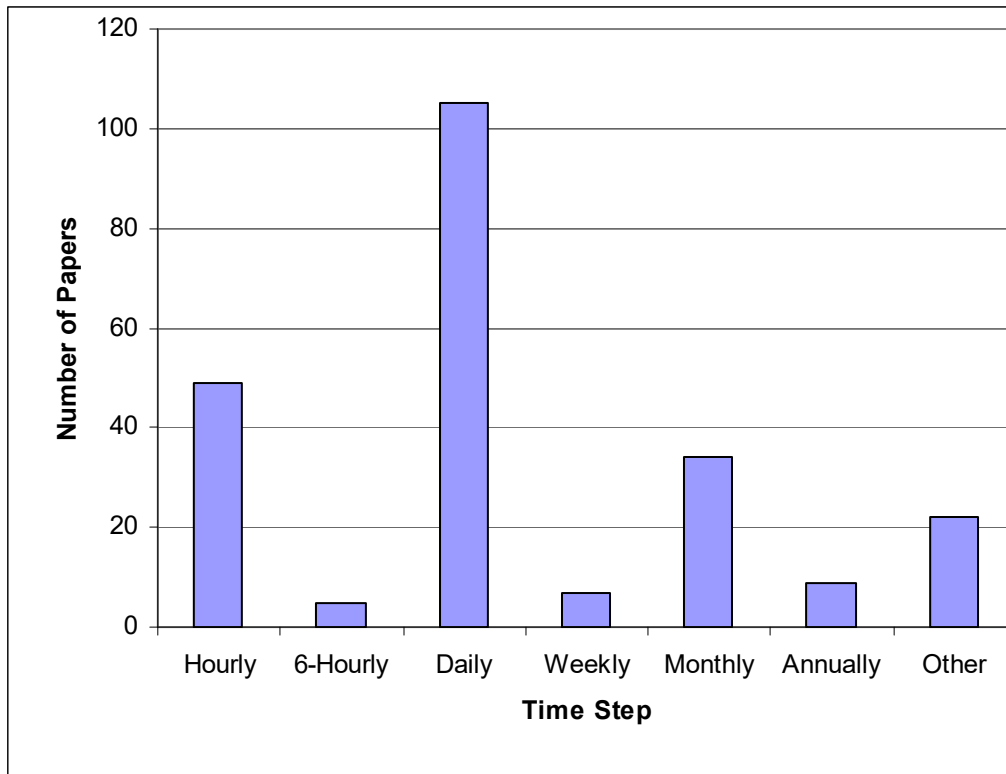


Figure 3: Number of Times Various Time Steps Have Been Used

Table 1: Details of Papers Reviewed

Year	Authors	River System(s)	Variable(s)
1999	Savic et al.	Kirkton River, Scotland	Flow
1999	Maier and Dandy	River Murray, Australia	Salinity
1999	Danh et al.	Da Nhim & La Nga Rivers, Vietnam	Flow
1999	See and Openshaw	Ouse River, England	Level
1999	Sajikumar and Thandaveswara	River Lee, UK; & Thuthapuzha River, India	Flow
1999	Zealand et al.	Winnipeg River, Canada	Flow
1999	Frakes and Yu	Susquehanna River, USA	Flow & Nitrate
1999	Jain et al.	Indravati River, India	Flow
1999	Campolo et al.	Tagliamento River, Italy	Level
1999	Campolo et al.	Arno River, Italy	Level
1999	Dawson and Wilby	River Mole, England	Flow
2000	Coulibaly et al.	Eight River Systems, Canada Little River & Reed Creek, USA, English	Flow
2000	Elshorbagy et al.	River, Canada	Flow
2000	Coulibaly et al.	Chute-du-Diable River, Canada	Flow
2000	Gautam et al.	River Tono, Japan	Flow
2000	Zhang and Govindaraju	Council Grove, El Dorado and Marion Rivers, USA	Flow

2000	Tingsanchali and Gautam	Pasak River & Nan River, Thailand	Flow
2000	Liong et al.	River systems in Bangladesh	Level
2000	Imrie et al.	Rivers Trent & Dove, UK	Flow
2000	Anmala et al.	Council Grove, El Dorado and Marion Rivers, USA	Flow
2001	Kim and Barros	Williamsburg, Raystown, Loyalsockville and Newport Rivers, USA	Flow
2001	Khalil et al.	English, Oslinka, Graham, Halfway and Nagagami Rivers, Canada	Flow
2001	Hu et al.	Hanjiang and Jingsh Rivers, China	Flow
2001	Elshorbagy et al.	Little River & Reed Creek, USA	Flow
2001	Coulibaly et al.	Chute-du-Diable River, Canada	Flow
2001	Chang and Chen	Da-cha River, Taiwan	Flow
2001	Coulibaly et al.	Chute-du-Diable River, Canada	Flow
2001	Chang et al.	Da-chia River, Taiwan	Flow
2001	Lischeid	Lehstenbach, Germany	SO4
2002	Xu and Li	Saikawa River, Japan	Flow
2002	Xiong and O'Connor	11 Rivers in China, Australia, Malaysia, Nepal, Bangladesh, Vietnam, Ireland, & Thailand	Flow
2002	Sivakumar et al.	Chao Phraya River, Thailand	Flow
2002	Sivakumar et al.	Coaracy Nunes/Araguari River, Brazil	Flow
2002	Shim et al.	Han River Basin, Korea	Flow
2002	Rajurkar et al.	Narmada River, India	Flow
2002	Ochoa-Rivera et al.	Tagus River, Spain	Flow
2002	Hsu et al.	Leaf River, USA	Flow
2002	Elshorbagy et al.	English River, Canada	Flow
2002	Elshorbagy et al.	English River, Canada	Flow
2002	Chang et al.	Da-Chia River, Taiwan	Flow
2002	Chang et al.	Lanyoung River, Taiwan	Flow
2002	Cannon and Whitfield	21 Rivers, Canada	Flow
2002	Cameron et al.	River South Tyne, England	Flow / Level
2002	Dawson et al.	River Yangtze, China	Flow
2002	Brath et al.	Sieve River, Italy	Flow
2002	Birikundavyi et al.	Mistassibi River, Canada	Flow
2002	Liong and Sivapragasam	Ganga, Jamuna, Brahmputra, Meghna Rivers, Bangladesh	Level
2002	Bowden et al.	River Murray, Australia	Salinity
2003	Zhang and Govindaraju	Back Creek and Indian–Kentuck Creek, USA	Flow
2003	Wilby et al.	Test River, England	Flow
2003	Suen and Eheart	Upper Sangamon River, USA	Nitrate
2003	Sudheer et al.	Baitarni River, India	Flow
2003	Solomatine and	Sieve River, Italy	Flow

	Dulal		
2003	Markus et al.	Sangamon River, USA	Nitrate
2003	Lischeid and Uhlenbrook	Brugga River, Germany	Flow & Silica
2003	Laio et al.	Tanaro River, Italy	Flow
2003	Kim and Valdes	Conchos River, Mexico	Palmer Drought Severity Index
2003	Huynh and Nguyen Deka and Chandramouli	Upper Red River, Vietnam	Level
2003		Brahamputra River, India	Flow
2003	Coulibaly	Chute-du-Diable River, Canada	Flow
2003	Cigizoglu	Goksu River, Turkey	Flow
2003	Cigizoglu	Göksu, Lamas and Ermenek Rivers, Turkey	Flow
2003	Chibanga et al.	Kafue River, Zambia	Flow
2003	Campolo et al.	River Arno, Italy	Level
2003	Anctil et al.	Serein River, France	Flow
2003	Abebe and Price	Sieve River, Italy	Flow
2003	Tayfur et al.	Laboratory Experiments (data from earlier work)	Sediment
2003	Khu and Werner	Bukit Timah River, Singapore	Flow
2003	Gaume and Gosset	Marne River, France	Flow
2003	Jain and Indurthy	Salado Creek, USA	Flow
2003	Phien and Kha	Red River, Vietnam	Level
2004	Wenrui et al.	Apalachicola River, USA	Flow
2004	Tomasino et al.	Po River, Italy	Flow
2004	Sudheer and Jain	Narmada River, India	Flow
2004	Shu and Burn	404 Catchments in UK	Flow
2004	Riad et al.	Ourika River Morocco	Flow
2004	Rajurkar et al.	Krishna & Narmada-India; Bird Creek-USA; Brosna-Ireland; Garrapatas-Columbia; Kizu-Japan; Pampanga-Phillipines	Flow
2004	Pan and Wang	Wu Tu River, Taiwan	Flow
2004	Nayak et al.	Baitarani River, India	Flow
2004	Moradkhani et al.	Salt River, USA	Flow
2004	Lin and Chen	Fei-Tsui River, Taiwan	Flow
2004	Kumar et al.	Hemavathi River, India	Flow
2004	Kisi	Tongue River, USA	Sediment
2004	Jain et al.	Kentucky River, USA	Flow
2004	Huang et al.	Apalachicola River, USA	Flow
2004	Cigizoglu	Schuylkill River, USA	Sediment
2004	Chiang et al.	Lan-Yang River, Taiwan	Flow
2004	Chang et al.	Da-Chia River, Taiwan	Flow
2004	Castellano-Mendez et al.	Xallas River, Spain	Flow
2004	Anctil and Lauzon	Kavi-Ivory Coast; Leaf & Salt Fork-USA; San Juan-Canada; Serein & Volpajola,	Flow

France			
2004	Anctil et al.	Serein River, France	Flow
2004	Anctil et al.	Serein River, France and Leaf River, USA	Flow
2004	Kisi	Go'ksudere River, Turkey	Flow
2004	Solomatine and Xue	Huai River, China	Flow
2004	Agarwal and Singh	Narmada River, India	Flow
2004	Jain and Srinivasulu	Kentucky River, USA	Flow
2005	Teegavarapu and Elshorbagy	Little River & Reed Creek, USA	Flow
2005	Sivapragasam and Muttill	Chehalis River, Morse Creek, & Bear Branch, USA	Flow
2005	Liong	Tryggevaelde River, Denmark	Flow
2005	Shrestha et al.	Neckar River, Germany	Flow
2005	Pan and Wang	Wu-Tu River, Taiwan	Flow
2005	Nayak et al.	Kolar River, India	Flow
2005	Kumar et al.	Malaprabha River, India	Flow
2005	Kisi	Quebrada Blanca & Rio Valenciano Stns., USA	Sediment
2005	Kingston et al.	River Murray, Australia	Salinity
2005	Khalil et al.	Sevier River, USA	Flow
2005	Jeong and Kim	Geum River, Korea	Flow
2005	Hu et al.	Seven Rivers in China	Flow
2005	Goswami et al.	Brosna River, Ireland	Flow
2005	Coulibaly and Baldwin	Saint-Lawrence River, Canada & Nile River, Egypt	Flow, Volume
2005	Coulibaly et al.	Kipawa & Matawin Rivers, Canada	Flow
2005	Cigizoglu	Seytan, Hayrabolu, and Ergene Rivers, Turkey	Flow
2005	Cigizoglu	Synthetic data	Flow
2005	Cigizoglu and Kisi	Filyos River, Turkey	Flow
2005	Chen and Ji	Yellow River, China	Flow
2005	Chang et al.	Lan-Yang River, Taiwan	Flow
2005	Chandramouli and Deka	Bharadhapuza River, India	Flow
2005	Bowden et al.	River Murray, Australia	Salinity
2005	Agarwal et al.	Vamsadhara River, India	Sediment
2005	Bruen and Yang	Citywest & Dargle Rivers, Ireland	Flow
2005	de Vos and Rientjes	Geer River, Belgium	Flow
2005	Kingston et al.	Boggy Creek, Australia	Flow
2005	Hettiarachchi et al.	Six rivers, England	Flow
2005	Anctil and Rat	47 rivers in France & USA	Flow
2005	Chau et al.	Yangtze River, China	Level
2005	Deka and Chandramouli	Brahmaputra River, India	Flow
2005	Sudheer	Narmada River, India	Flow

2005	Wu et al.	North Buffalo Creek, USA	Flow
	Schumann and		
2005	Lauener	Gornera River, Switzerland	Flow
	Giustolisi and		
2005	Laucelli	Luzzi and Liguori Rivers, Italy	Flow
		Wabash & Mississippi Rivers, USA and	
2005	Doan et al.	Rivers in Bangladesh	Flow, Level
2006	Wang et al.	Yellow River, China	Flow
2006	Srivastava et al.	West Branch Brandywine Creek, USA	Flow
			Flow, Turbidity, Specific Conductance, DO, pH, water temp.
2006	Sahoo et al.	Manoa and Palolo Streams, USA	Flow
2006	Sahoo and Ray	Waiakeakua and Manoa Streams, USA	Flow
	Pereira and dos		
2006	Santos	Tamanduatei River, Brazil	Flow, Level
2006	Panagoulia	Acheloos River, Greece	Flow
2006	Nilsson et al.	Bulken and Skarsvatn Rivers, Norway	Flow
2006	Melesse and Wang	Red River, USA	Flow
2006	Lin et al.	Lancang River, China	Flow
2006	Khan and Coulibaly	Serpent & Chute-du-Diable Rivers, Canada	Flow
2006	Keskin et al.	Dim Stream, Turkey	Flow
	Karunasinghe and	Mississippi & Wabash Rivers, USA and	
2006	Liong	Synthetic Data	Flow
2006	Kang et al.	Youngsan River, Korea	Flow
2006	Cigizoglu and Kisi	Schuykill River, USA	Sediment
2006	Chetan and Sudheer	Kolar River, India	Flow
2006	Chen et al.	Choshui River, Taiwan	Flow
2006	Chau	Shing Mun River, Hong Kong	Level
2006	Anctil et al.	Loire River, France	Flow
2006	Alvisi et al.	Reno River, Italy	Level
	Ahmad and		
2006	Simonovic	Red River, Canada	Flow
2006	Antar et al.	River Nile, Ethiopia and Sudan	Flow
2006	Lauzon et al.	Loire River, France	Flow
2006	Chen and Adams	Bei River, China	Flow
2006	Dawson et al.	850 catchments, UK	Flow
2006	Jain and Srinivasulu	Kentucky River, USA	Flow
2006	Jia and Culver	Buck Mountain Run River, USA	Flow
2006	Lohani et al.	Narmada River, India	Flow
2006	Chen and Adams	Bei River, China	Flow
2006	Garbrecht	Fort Cobb Watershed, USA	Flow
2006	Kim et al.	Geum River, Korea	Flow
2006	Raghuwanshi et al.	Siwane River, India	Flow, Sediment
2006	Tayfur and Guldal	Catchment in Tennessee Basin, USA	Sediment

2006	Parasuraman et al.	English River, Canada	Flow
2007	Toth and Brath	River Sieve and River Reno, Italy	Flow
2007	Piotrowski et al.	Murray Burn, Scotland	Concentration of tracer
2007	Chen and Yu	Lan-Yan River, Taiwan	Level
2007	Abraham and See	Hypothetical - Xianjiang Rainfall-Runoff model emulator	Flow
2007	Chau	Shing Mun River, Hong Kong	Level
2007	Gopakumar et al.	Achencoil River, India	Flow
2007	Alp and Cigizoglu	Juniata River, USA	Sediment
2007	Kisi and Cigizoglu	Filyos and Ergene Rivers, Turkey	Flow
2007	Kamp and Savenije	Alzette River Basin, Luxembourg	Runoff, River Discharge, Salinity and Secchi Depth
2007	Amenu et al.	Upper Sangamon River Basin, USA	Flow, Nitrate
2007	Nor et al.	Sungai Bekok and Sungai Ketil Catchments, Malaysia	Flow
2007	Parasuraman and Elshorbagy	Little River and Reed Creek, USA	Flow
2007	Ochoa-Rivera et al.	Jucar River, Spain	Flow
2007	Ahmed and Sarma	Pagladia River, India	Flow
2007	Nayak et al.	Narmada River, India & Kentucky River, USA	Flow
2007	Srivastav et al.	Kolar River, India	Flow
2007	Zou et al.	Synthetic data for the Loch Raven Reservoir, USA	DO, Chl a, total phosphorus and ammonia
2007	Shamseldin et al.	8 catchments from Nepal (1), China (3), Ireland (1), Vietnam (1), Malaysia (1) and Thailand (1)	Flow
2007	Yu and Liong	Tryggevælde catchment & Mississippi River at Vicksburg, USA	Flow
2007	de Vos and Rientjes	Greer River Basin, Belgium	Flow
2007	Tayfur et al.	upper Tiber, Italy	Flow
2007	Sivapragasam et al.	Periyar River, India	Flow
2007	Pulido-Calvo and Portela	Tua and Côa Rivers, Portugal	Flow
2007	Pang et al.	8 Watersheds in China	Flow
2007	Muluye and Coulibaly	Churchill Falls, Canada	Flow
2007	Mas and Ahlfeld	Gates Brook, MA USA	Faecal Coliform
2007	Lohani et al.	Narmada River, India	Sediment
2007	Kisi	North Platte River, USA	Flow
2007	Iliadis and Maris	70 Mountainous watersheds, Cyprus	Annual water supply
2007	Hu et al.	Darong River, China	Flow

2007	Han et al.	Bird Creek, Oklahoma, USA	Flow
2007	Goswami and O'Connor	Bronsa, Ireland; Le Guindy à Plouguiel, France	Flow
2007	El-Shafie et al.	Nile River (inflow to Aswan High Dam), Egypt	Flow
2007	Elgaali and Garcia	Arkansas River, USA	Water available for diversion 6 WQ Params for Axios (nitrates, specific conductivity, DO, Na, Mg, Ca) and 3 for Strymon (nitrates, spec cond, DO)
2007	Diamantopoulou et al.	Axios & Strymon Rivers, Greece	
2007	Corzo and Solomatine	Bagmati basin, Nepal; Sieve basin, Italy; Brue basin, UK	Flow
2007	Chiang et al.	Wu-Tu River, Taiwan	Flow
2007	Chen and Yu	Lang-Yang River, Taiwan	Level (flood stage)
2007	Chang et al.	Chen-Eu-Lan River, Taiwan	Debris Flow
2007	Chang et al.	Da-Chia River, Taiwan	Flow
2007	Chang et al.	Upstream sections of both Da-Chia and Kee-Lung river basins, Taiwan	Flow
2007	Bae et al.	Songgyang Dam, North Han River, South Korea	Dam inflow
2007	Aqil et al.	Cilalawi River, Indonesia	Flow
2007	Aqil et al.	Cilalawi River, Indonesia	Flow
2007	Alp and Cigizoglu	Juniata River, Pennsylvania, USA	Sediment
2007	Abrahart et al.	River Ouse, England	Flow

3. Methods Used for ANN Model Development

3.1 Introduction

The main steps in the development of ANN prediction models, as well as the way the data flow through, and the outcomes achieved at, different steps, are given in Figure 4. It should be noted that the model development steps covered here represent a subset of the ten steps presented by Jakeman et al. (2006), which cover the full scientific process, including

formulating a hypothesis, collecting appropriate observations and data and a review of the hypothesis.

The first step in the model development process presented here is the choice of appropriate model output(s) (i.e. the variable(s) to be predicted) and a set of potential model input variables from the available data. Although ANNs are data-driven models, it is up to the modeller to choose which input variables should be *considered* as part of the model development process. This can be done based on *a priori* knowledge and/or the availability of data. The resulting data set constitutes the “Selected Data (Unprocessed)” (Figure 4). It should be noted that once the model outputs have been chosen, the number of nodes in the output layer has also been determined (Figure 4). Next, the unprocessed data, which consist of measured values of the *potential* model input variables, as well as the model output variable(s), have to be processed (e.g. scaled, lagged) so that they are in a suitable form for the subsequent steps of the model development process. Once the processed database of potential model inputs and outputs has been assembled (“Selected Data (Processed)”), the actual model can be developed.

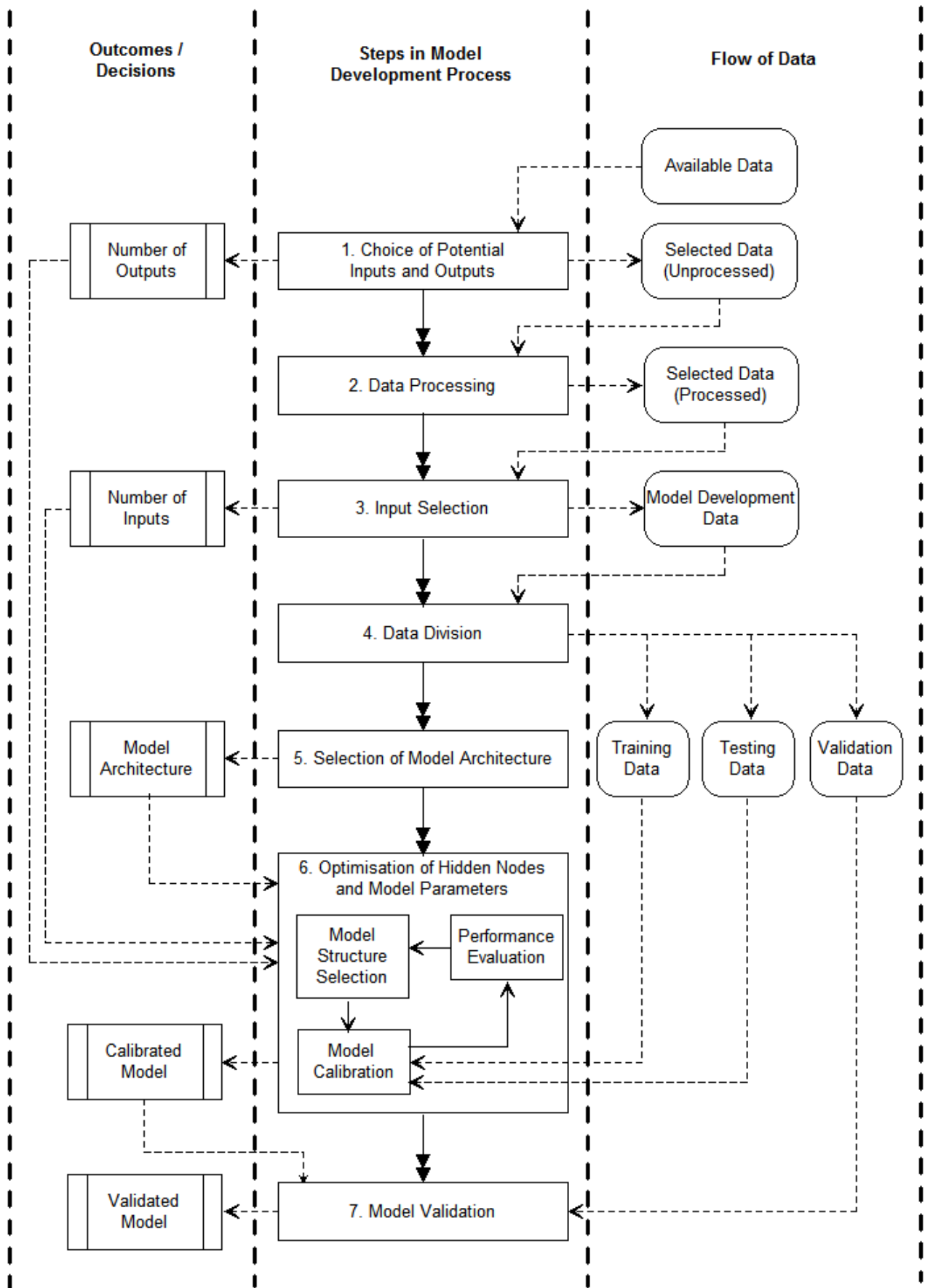


Figure 4: Steps in ANN Model Development Process

All ANN prediction models take the following form:

$$Y = f(X, W) + \varepsilon \quad (1)$$

Where:

Y = Vector of model outputs

X = Vector of model inputs

W = Vector of model parameters (connection weights)

f(•) = Functional relationship between model outputs, inputs and parameters

ε = Vector of model errors

Consequently, in order to develop an ANN model, the vector of model inputs (X), the form of the functional relationship (f(•)), which is governed by the network architecture (e.g. multi-layer perceptron) and geometry (e.g. the number of hidden layers and nodes, type of transfer function) and the vector of model parameters (W), which includes the connection and bias weights, need to be defined.

The vector of appropriate model inputs is determined during the “Input Selection” step (Figure 4). This can be achieved either by using a model-free approach, which uses statistical measures of significance, or a model-based approach, as part of which appropriate inputs are selected based on the performance of models with different sets of inputs. In the latter case, steps 5 and 6 in Figure 4 have to be repeated for each set of model inputs tried. Once the vector of model inputs has been selected, the number of model inputs, and hence the number of nodes in the input layer of the ANN model, are known (Figure 4).

The resulting “Model Development Data” are usually divided into calibration and validation subsets. The calibration data are used to estimate the unknown model parameters (connection weights) and the validation data are used to validate the performance of the calibrated model on an independent data set. If cross-validation is used as the stopping criterion, the calibration data are divided into training and testing subsets (Figure 4).

Next, the functional form of the model, $f(\bullet)$, needs to be selected, which depends on the model architecture (e.g. multi layer perceptron, radial basis function), as well as an appropriate number of hidden nodes and how they are arranged (e.g. single layer, two layers). It should be noted that while the selection of an appropriate model structure is required for most ANN architectures, it is superfluous for some, such as Generalised Regression Neural Networks (GRNN), which have a fixed structure.

While the choice of an appropriate model architecture is a function of modeler preference, the optimal model structure generally needs to be determined using an iterative process. This involves selecting a network with a certain structure (e.g. number of hidden nodes, transfer functions), calibrating (training) the selected ANN model, as part of which an estimate of the vector of model parameters (W) is obtained, evaluating its performance and then repeating the Calibration and Evaluation steps for different network configurations (Figure 4). Once the network configuration that performs best on the calibration data is identified, the calibrated model needs to be validated using an independent data set. As ANNs are prone to overfitting the calibration data, cross-validation is generally used, as part of which the calibration data are divided into training and testing subsets, which enables the performance of models with different network configurations to be validated during the model calibration phase to ensure overfitting of the training data has not occurred.

In the subsequent sections, the input selection, data division, model architecture selection, model structure selection, model calibration (training) and model evaluation stages of the ANN model development process are considered in more detail. In each sub-section, the purpose and importance of the particular step in the ANN model development process considered are introduced, followed by a taxonomy of the main options available to modelers. Next, the options selected in the 210 papers considered are reviewed in light of these taxonomies, thereby presenting a snapshot of the ANN model development approaches used from 1999 to 2007. It should be noted that this information is presented in terms of the number of times a particular method has been used in the papers reviewed. This is because some papers used multiple methods and details about some of the methods addressed were not provided in some of the papers. Consequently, the total number of times a particular method has been used in the papers reviewed can be more or fewer than the number of papers reviewed (i.e. 210).

3.2 Input Selection

3.2.1 Introduction

One of the most important steps in the ANN model development process is the determination of an appropriate set of inputs (X). However, this task is generally given little attention in ANN modelling and most inputs are determined on an ad-hoc basis or using *a priori* system knowledge (Maier and Dandy, 2000). This can result in the inclusion of too few or too many model inputs, both of which are undesirable.

The consequence of excluding one or more significant inputs is that the resulting model is not able to develop the best possible input-output relationship, given the available data. The omission of important model inputs is more likely to occur in time series applications, where the potential model inputs consist of not only different input variables, but also their lagged values (unless recurrent neural network architectures are used). This increases the number of potential model inputs (as distinct from input variables) considerably, and in many previous studies, lags have been chosen on an ad-hoc basis (Maier and Dandy, 2000), with the associated danger that important system dynamics have not been captured.

The inclusion of too many inputs is usually caused by input redundancy, where some of the selected inputs provide significant information, but are related to each other and therefore provide redundant information. This can cause a number of problems. Firstly, redundant inputs increase the likelihood of overfitting (overtraining). This is because a larger number of inputs generally increases network size, and hence the number of connection weights (i.e. model parameters) that need to be calibrated. As the number of training samples is generally fixed, the addition of redundant model inputs increases the ratio of the number of connection weights to the number of training samples, thus increasing the likelihood of overfitting, while not providing any additional information to the model. Secondly, the inclusion of redundant model inputs introduces additional local minima in the error surface in weight space. For example, if two model inputs (x_1 and x_2) are highly correlated, and thus essentially represent the same input information, there are likely to be many combinations of weights that will result in identical model performance. If the underlying relationship is $y = x_1$, then a unique relationship exists if either x_1 ($y = x_1$) or x_2 ($y = x_2$) are included as model inputs. However, if both inputs are included ($y = w_1x_1 + w_2x_2$), the same model output is obtained for a large number of combinations of weights (e.g. $w_1=1$ & $w_2=0$, $w_1=0$ & $w_2=1$, $w_1=0.5$ & $w_2=0.5$,

$w_1=0.3$ & $w_2=0.7$ etc.). The presence of local minima in weight space makes it more difficult to find an optimal set of weights, as well as resulting in input-output relationships that are not unique, making it more difficult to extract physical meaning from calibrated models.

3.2.2 Taxonomy

A number of techniques are available for assessing the significance of the relationship between potential model inputs and output(s), as shown in Figure 5. The primary distinction is between Model Free and Model Based approaches. Model Based approaches rely on the development (structure selection, calibration and evaluation) of a number of ANN models with different inputs to determine which of the candidate inputs should be included. The primary disadvantage of this approach is that it is time consuming, as a number of ANNs have to be developed. In addition, it has the potential for masking the effect different model inputs have on model performance, as the latter is also a function of network structure (e.g. number of hidden nodes), which ideally should be optimized for each input set investigated, and the quality of the calibration process, which is a function of a number of user-defined parameters (e.g. learning rate and momentum if the back-propagation algorithm is used), which should also be optimized for each candidate input set. Consequently, it is difficult to isolate the impact of different model inputs on model performance.

Options for selecting which input combinations to try as part of Model Based approaches include an ad-hoc approach, where the model developer selects which combinations of model inputs should be tried, a stepwise approach, where inputs are systematically added (constructive) or removed (pruning), or a global approach, where a global optimization algorithm, such as a genetic algorithm, is used to select the combination of inputs that maximizes model performance. Another approach is to develop an ANN model with a

relatively large number of inputs and to use sensitivity analysis to determine which inputs should be excluded.

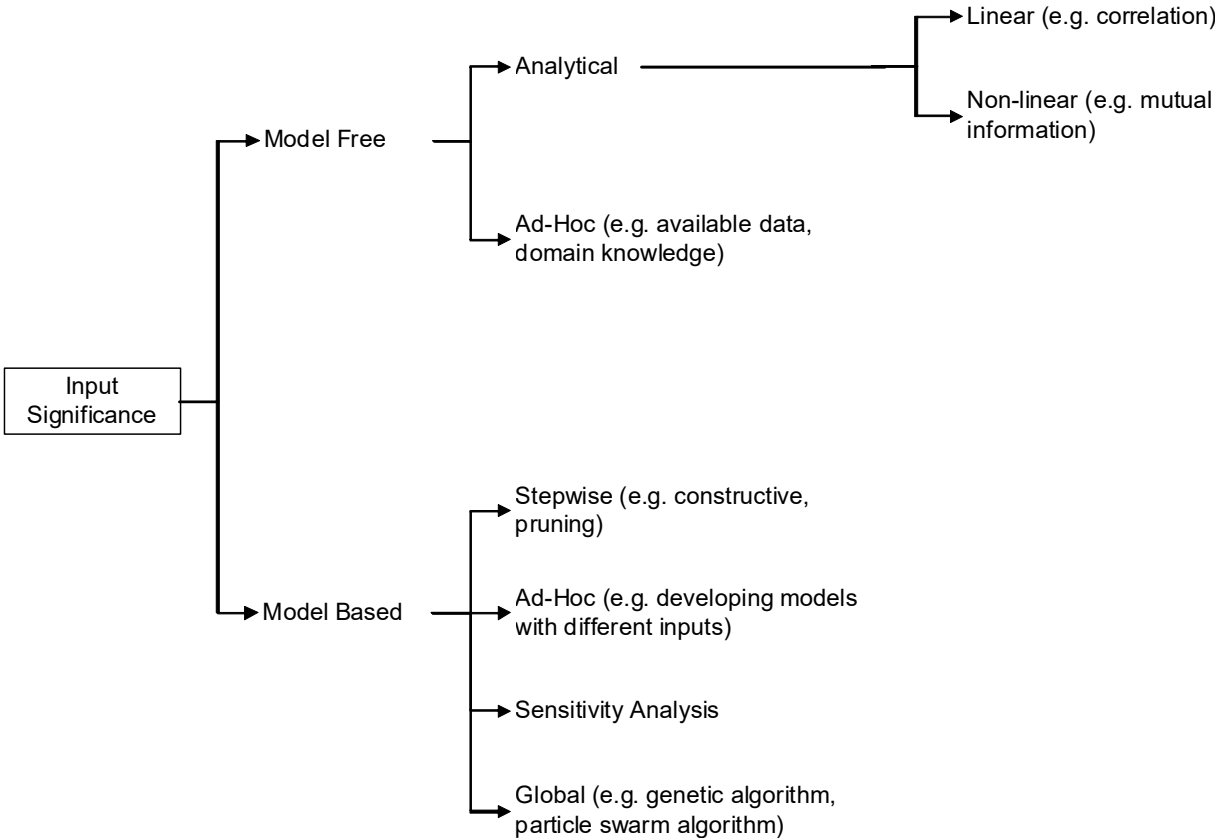


Figure 5: Taxonomy of Approaches to Determining Input Significance

In contrast to Model Based approaches, Model Free approaches to input selection do not rely on the performance of trained ANN models for the selection of appropriate inputs. As shown in Figure 5, model free approaches can be divided into two categories: ad-hoc and analytical. As part of ad-hoc model free approaches, inputs are selected by the model developer on an arbitrary basis or based on domain knowledge, for example. When an analytical model free approach to input selection is used, a statistical measure of significance is generally used to assess the strength of the relationship between potential model inputs and outputs. The most commonly used measure of statistical dependence for input selection is correlation, which has

the disadvantage of only measuring linear dependence between variables. This is particularly relevant in the context of developing ANN models, as ANNs are generally used in preference to linear modelling approaches, such as linear regression, in cases where input-output relationships are suspected to be highly non-linear, which is often the case in water resources problems. Consequently, the use of non-linear statistical dependence measures, such as mutual information, is more appropriate for determining inputs to ANN models.

In order to overcome the problem of redundant inputs discussed earlier, Input Independence needs to be considered in addition to Input Significance. As can be seen in Figure 6, there are two main approaches to accounting for input independence, namely dimensionality reduction and filtering. The aim of the former is to reduce the dimensionality of the input space by eliminating correlated candidate inputs. There are two main approaches to achieving this, including rotation of the input vectors, as is the case in principal component analysis, or clustering of the input space and choosing representative inputs from each cluster for further consideration. Dimensionality reduction generally forms the first part of a two step process, the second of which is to select the inputs that have the most significant relationship with the model output(s) using one of the methods in Figure 5.

The second approach to account for input independence in the input selection process is filtering. The most prominent example of this is the constructive stepwise model-building process, as part of which the candidate input that has the most significant relationship with the model output(s) is selected first, followed by the candidate input that has the next biggest *additional* impact and so on. Classic examples of this are the partial correlation and partial mutual information input variable selection algorithms (see May et al., 2008a, 2008b), which combine a stepwise partial modelling approach that caters for input independence

(redundancy) with an analytical measure of statistical dependence that caters for input significance. The stepwise, constructive model based approach achieves a similar aim, although the criteria used to decide when to stop adding candidate inputs are less well defined. Other model based input selection approaches, such as global optimization and stepwise pruning approaches cannot be combined with filtering approaches and have to rely on dimensionality reduction approaches to cater for input independence (redundancy).

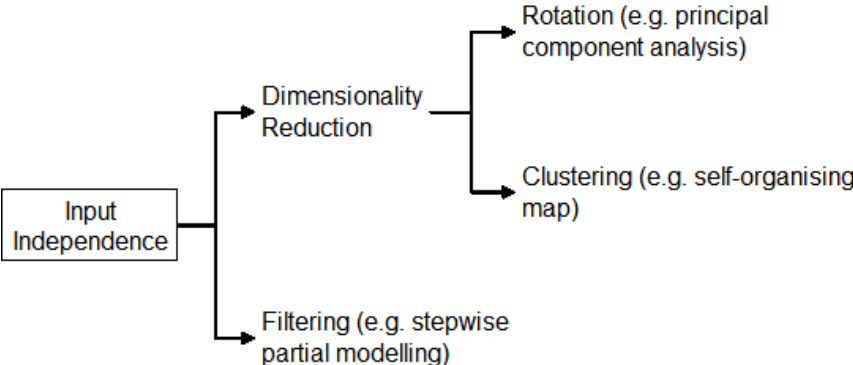


Figure 6: Taxonomy of Approaches to Accounting for Input Independence

3.2.3 Results

As illustrated in Figure 7, a model free input selection approach was used 146 times, compared with 72 occasions on which a model based approach was used. Of the model free approaches, ad-hoc methods were most popular with applications in 79 papers, followed by linear analytical approaches, such as correlation, which were used on 60 occasions. A non-linear analytical method was only used 7 times, which seems inconsistent with the non-linear premise that underpins all ANN models.

In 37 of the 72 instances where a model based input selection approach was used, this was done in an ad-hoc fashion. A stepwise model building approach was used 14 times, followed by sensitivity analysis of trained models (7 times) and use of a global search procedure (5 times).

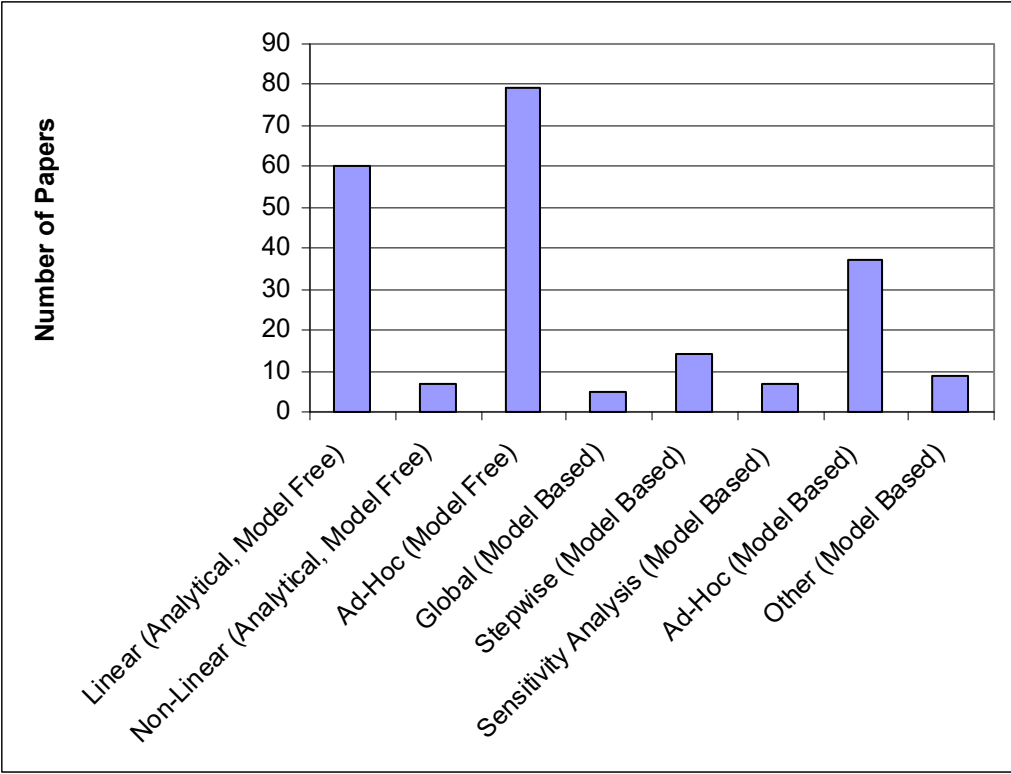


Figure 7: Number of Times Various Methods of Determining Input Significance Have Been Used

Input independence was only considered in 18 of the 210 papers reviewed (Figure 8). Filtering was the most commonly used approach, with 10 applications, followed by clustering and rotation, which were applied 6 and 2 times, respectively.

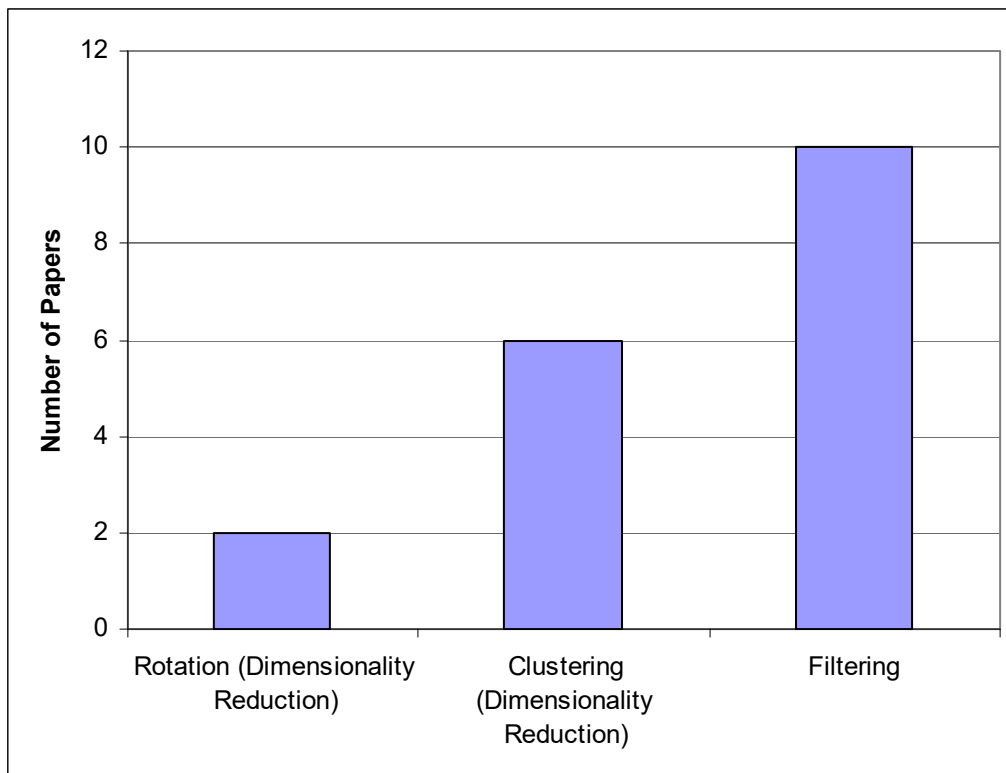


Figure 8: Number of Times Various Methods of Determining Input Independence Have Been Used

3.2.4 Conclusion

The results of the review reveal that there is a need to pay greater attention to the input selection step in the development of ANN models. The inputs selected can have a significant impact on model performance, yet ad hoc approaches to input selection (either model based or model free) were used in the majority of papers surveyed. While analytical model free approaches were also popular, almost all of these used a linear method for determining input significance, which is counter to the premise of using a non-linear model, such as an ANN, as the actual model. Consequently, there is a need to make greater use of non-linear analytical approaches to input selection.

The issue of input independence was ignored in almost all of the papers reviewed, which can have significant negative impacts on model performance and the ability to extract any meaningful information about underlying physical processes from trained ANN models. Consequently, this issue requires increased attention.

3.3 Data Division

3.3.1 Introduction

As part of the ANN model development process, the available data are generally divided into training, testing and validation subsets. The training set is used to estimate the unknown connection weights, the testing set is used to decide when to stop training in order to avoid overfitting and/or which network structure is optimal, and the validation set is used to assess the generalisation ability of the trained model. As ANNs, like all empirical models, perform best when they are not used to extrapolate beyond the range of the training data, all patterns that are contained in the available data need to be included in the training set. Similarly, since the test set is used to determine when to stop training and/or which network geometry is optimal, it needs to be representative of the training set and should therefore also contain all of the patterns that are present in the available data. If all of the available patterns are used to calibrate the model, then the most challenging evaluation of the generalisation ability of the model is if all of the patterns are also part of the validation set. Consequently, the training, testing and validation sets should have the same statistical properties in order to develop the best possible model, *given* the available data.

3.3.2 Taxonomy

The methods for dividing the available data into appropriate subsets can be divided into supervised and unsupervised approaches (Figure 9). Unsupervised approaches do not take the statistical properties of the data subsets into account explicitly and only stratified unsupervised approaches attempt to ensure that the statistical properties of the subsets are similar. For example, a self-organising map (SOM) (see Kalteh et al., 2008) can be used to cluster the available data and to allocate data samples from each cluster to the training, testing and validation subset, thereby ensuring that patterns from different regions of the multivariate input-output space are represented in each subset. In the random unsupervised approach, the data are divided into their respective subsets on a random basis. In the physics based approach, the data are divided into various classes based on knowledge about the underlying physical processes or domain knowledge. In the ad-hoc approach, data might be divided such that the first XX observations are allocated to the training set, the next YY observations are allocated to the testing set and the final ZZ observations are allocated to the validation set. However, this does not take any account of the statistical properties of the data subsets, making it difficult to know whether the best possible model, given the available data, has been developed or whether model performance based on the validation set is representative of model performance under a range of conditions. For example, the patterns in the validation set might only be representative of average conditions, thereby inflating model performance on the validation data. Alternatively, the validation data might contain rare events not used during training (calibration), thereby diminishing the apparent capability of the model to capture the relationship contained in the available data.

The explicit goal of supervised data division methods is to ensure that the statistical properties of the various subsets are similar. This can be achieved by using a trial-and-error approach, as part of which manual adjustments are made to the composition of the various subsets until an arbitrarily satisfactory level of agreement between the statistical properties of the various data subsets has been reached, or by using a formal optimization approach to minimize a measure of difference between the statistical properties of the data subsets.

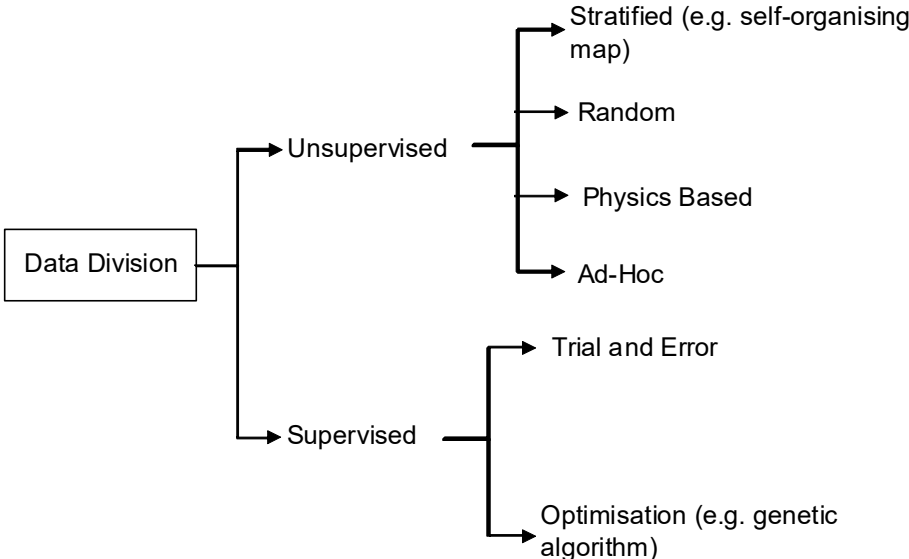


Figure 9: Taxonomy of Approaches to Data Division

3.3.3 Results

In the papers reviewed, unsupervised data division methods were used 177 times (Figure 10). Among these, ad-hoc data division was the predominant method used. Only a small number of papers used the more sophisticated stratified and physics based approaches. An equally small number used a random data division approach.

Supervised data division methods were only used on 24 occasions, with an approximately equal split between trial and error and optimization based approaches for achieving similar statistical properties between the various data subsets. It should be noted that data division was not discussed in some of the papers reviewed.

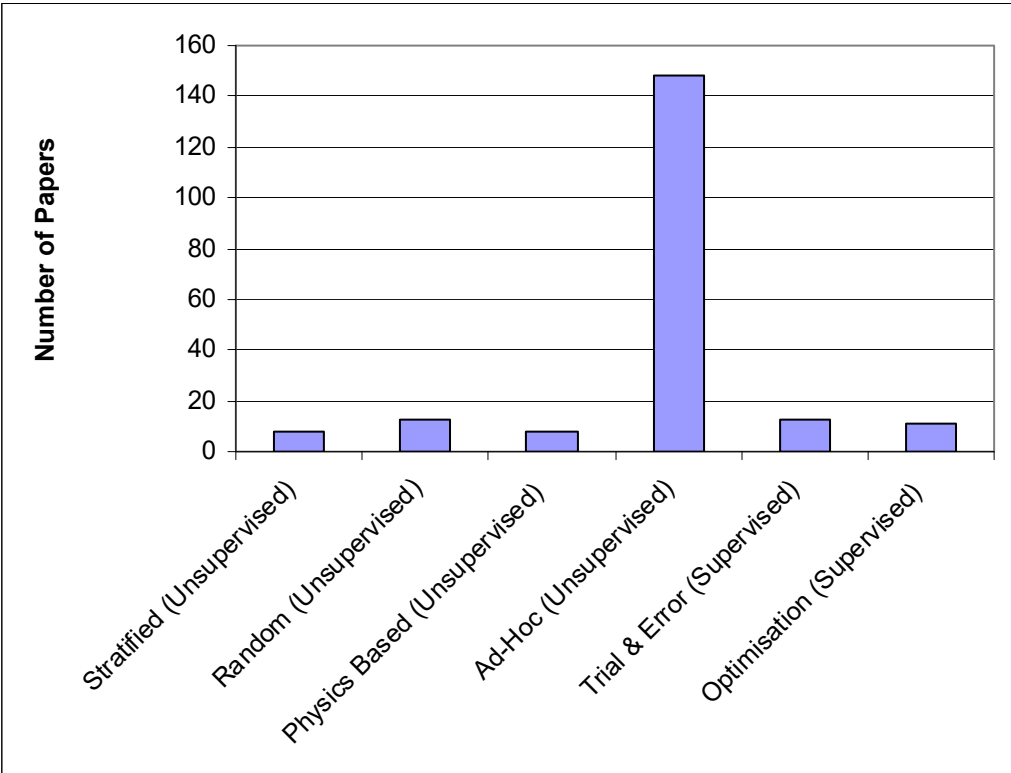


Figure 10: Number of Times Various Methods of Data Division Have Been Used

3.3.4 Conclusion

Even though the way the data are divided can have a significant impact on model performance, and the validity of the results presented, data division was conducted in an ad-hoc fashion on almost 150 occasions. Consequently, there is a need to pay increased attention to data division in the ANN model development process.

3.4 Model Architecture Selection

3.4.1 Introduction

Model (network) architecture determines the overall structure and information flow in ANN models. Consequently, it has a significant impact on the functional form of the relationship between model inputs and output(s), $f(\bullet)$.

3.4.2 Taxonomy

Traditionally, ANN architectures have been divided into feed-forward and recurrent networks (Figure 11). In feed-forward networks, the information propagation is only in one direction i.e. from input layer to the output layer. Multilayer Perceptrons (MLPs) are the most common form of feed-forward model architecture. Other feed-forward network architectures in use include Generalised Regression Neural Networks (GRNNs), Radial Basis Function (RBF) networks, Neurofuzzy networks and Support Vector Machines (SVMs).

A MLP uses three or more layers of artificial neurons with linear aggregation functions and linear and/or non-linear activation functions. The input layer neurons simply pass on the weighted inputs to the subsequent layer neurons. The possibility of using non-linear activation functions at the hidden and output layers of a MLP provide the capability of capturing the complexity and non-linearity inherent in the systems being modeled. A GRNN is capable of approximating any function using input and output data like an MLP but differs

in its structure, which consists of four layers, an input layer, a pattern layer, a summation layer, and an output layer. Unlike MLPs, GRNNs do not rely on iterative procedures for their training and are based on a standard statistical technique called kernel regression. RBF networks are motivated by locally tuned biological neurons, whose response characteristics are bounded in a small range of the input stimuli. The structure of RBF networks is similar to that of the feedforward MLPs and consists of three layers, an input layer, a hidden layer, and an output layer. The major difference is that the hidden layer neurons are specified by radial basis functions and the output layer neurons necessarily use linear activation functions. The training of an RBF network is usually a two stage process in which the basis functions are established at the hidden layer in the first stage and the weights connecting hidden layer and output layer neurons are directly determined in the second stage. Neurofuzzy networks are based on an integration of neural networks and fuzzy logic. The learning capability of neural networks is exploited to design the complex fuzzy system (or generation of IF THEN rules) in a Neurofuzzy model. Neurofuzzy models offer the advantages of both fields and have provided more accurate results than a simple ANN model in many hydrological applications. Recently, SVMs have attracted the attention of some researchers. SVMs are machine learning algorithms in which the ‘empirical risk’ in terms of prediction error and structural risk associated with the model structure are minimized simultaneously.

While feed-forward architectures are the most popular architectures among researchers, recurrent neural networks have also received some attention. In recurrent networks, information may propagate not only in the forward direction but also in the backward direction through feedback loops. The output layer neurons may feed back the output to input and/or hidden layer neurons. The existence of a feedback mechanism in recurrent networks makes it simpler for a neural network to model highly dynamic systems with time delays.

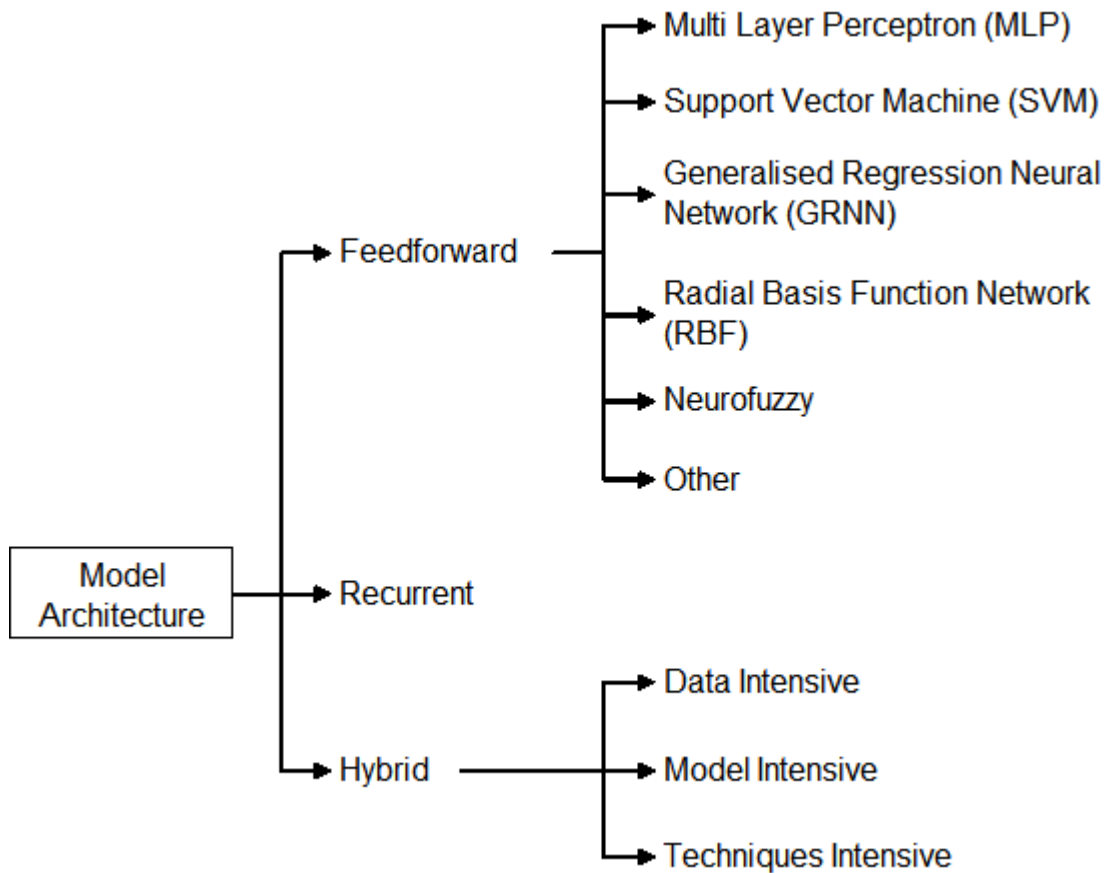


Figure 11: Taxonomy of Model Architectures

Environmental and hydrological systems are extremely complex, non-linear, and dynamic in nature, involving a wide variety of physical variables that exhibit significant spatio-temporal variation and are often inter-related and uncertain in nature, thereby posing major challenges to the scientific community involved in modeling such systems. A single technique may not be able to capture the complex nature of environmental and hydrological systems. Consequently, a number of hybrid modelling approaches have been developed to exploit the advantages of the available modeling paradigms in order to capture the complexities involved in such systems (Figure 11).

In this paper, hybrid modelling frameworks that include ANN models have been divided into the following three classes (Figure 11):

(a) Data Intensive: A data intensive approach is one that attempts to classify the data in accordance with different dynamics and separate models are then developed for the separate classes. The data classification can be either soft or hard depending on the methods employed. As part of soft classification, unsupervised learning methods can be used (e.g. Kohonen's self organizing map (SOM)) to identify the input output patterns belonging to a particular class. Alternatively, hard approaches, such as domain knowledge about the physical system, can be used for data classification. Once the data have been classified using either soft or hard approaches, each category of data can be modeled separately using neural networks or process based approaches. Such a data intensive approach offers the advantage of being able to model clustered data generated by different dynamics.

(b) Model Intensive: A model intensive approach is one that employs different models for different sub-components of the overall physical system and then aggregates various responses calculated from different models. On the other hand, it is possible to model the same process using two different types of models and then combine the outputs from two or more models to obtain the desired output.

(c) Technique Intensive: A technique intensive approach is the one in which a neural network is combined with a different technique (e.g. regression, time series, or conceptual) with the objective of developing a hybrid modeling framework that is capable of exploiting the advantages offered by different techniques. For example, a neural network / time series

hybrid model offers the advantage of first removing the deterministic trends from the data, enabling any nonlinear relationships that remain to be modeled using neural networks. Similarly, it is possible to combine conceptual and/or regression techniques with neural networks to develop hybrid models in order to achieve superior model performance.

3.4.3 Results

The results obtained indicated that there has been a significant amount of activity on the development and evaluation of alternative network architectures in order to improve model performance between 1999 and 2007. While multilayer perceptrons (MLPs), which have been used traditionally in applications in hydrology and water resources (Maier and Dandy, 2000), were still by far the most popular network architecture, MLP performance was compared with that of alternative feedforward network architectures, recurrent architectures and a variety of hybrid architectures in a large number of studies (Figure 12). The number of studies in which alternative architectures were applied was reasonably uniform, varying between 5 and 20, compared with 178 instances where MLPs were used.

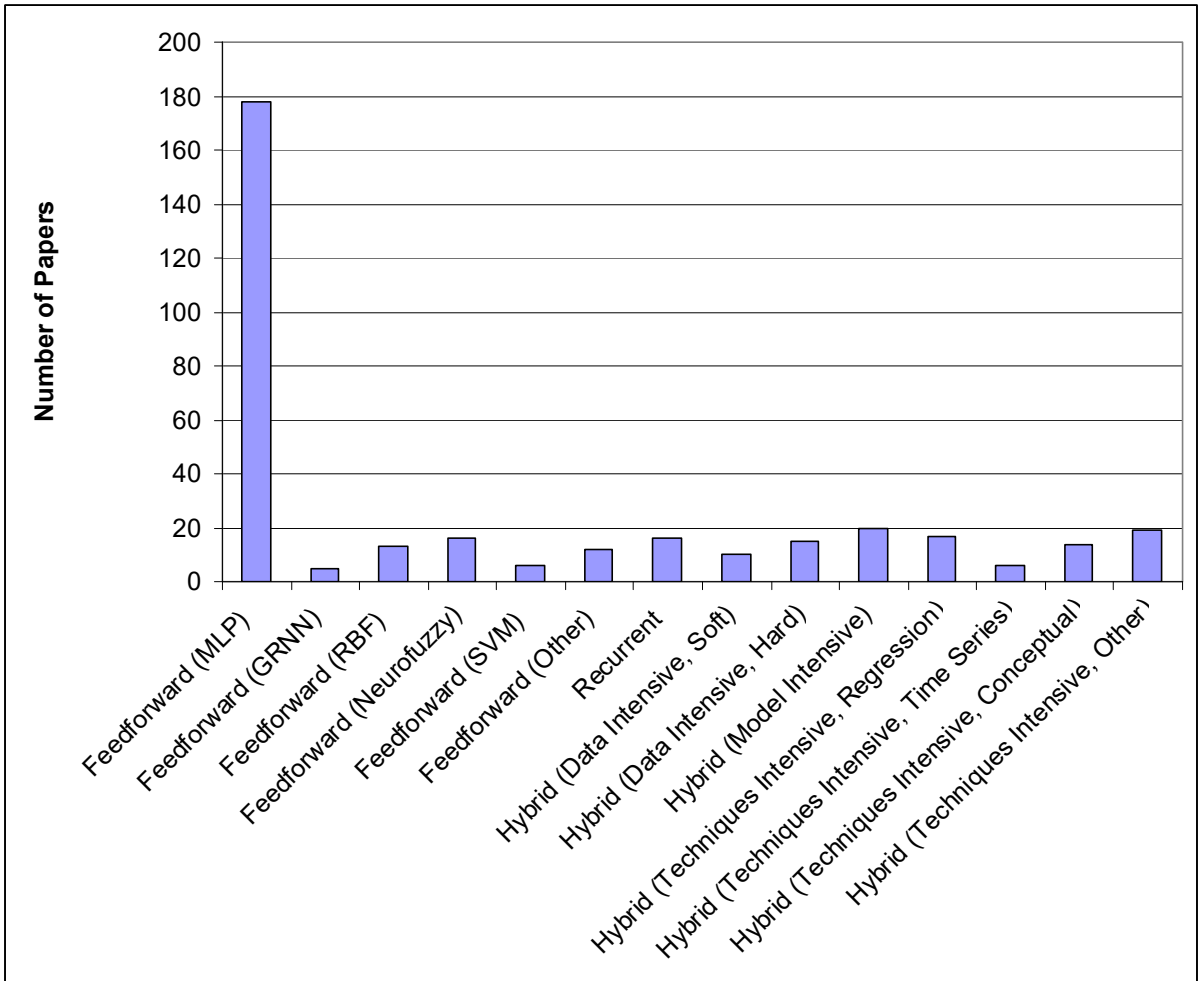


Figure 12: Number of Times Various Model Architectures Have Been Used

3.4.4 Conclusion

Much effort has been directed towards the evaluation of existing ANN architectures and the development of and evaluation of new ANN architectures. The latter has been primarily in the form of hybrid ANN architectures that aim to exploit the strengths and eliminate the weaknesses of different modelling approaches. However, given the wide variety of hybrid modelling approaches and range of applications to which they have been applied, it is not possible to draw any conclusions as to which model architecture should be used in a particular circumstance. This should be the focus of future research efforts.

3.5 Model Structure Selection

3.5.1 Introduction

Model (network) structure, together with model (network) architecture, defines the functional form of the relationship between model inputs and output(s), $f(\bullet)$. Determination of an appropriate network structure involves the selection of a suitable number of hidden nodes, how they are arranged (e.g. number of layers, number of nodes per layer) and how they process incoming signals (e.g. type of transfer function etc.). The optimal network structure generally strikes a balance between generalisation ability and network complexity (e.g. network size and the number of free parameters). If network complexity is too low or an inappropriate functional form is selected, the network might be unable to capture the desired relationship. However, if network complexity is too high, the network might have decreased generalisation ability and processing speed, could be more difficult to calibrate and might be less transparent.

3.5.2 Taxonomy

The taxonomy of methods for determining the optimal ANN structure is shown in Figure 13. The methods can be classified into three types, global, stepwise, or ad-hoc. In the first method, the structure of an ANN model in terms of hidden layers and/or hidden neurons is arrived at using global methods based on competitive evolution found in nature e.g. genetic algorithm, particle swarm optimization, simulated annealing, etc. Using this approach, it is possible to simultaneously optimize network parameters (e.g. network weights) and structure (e.g. the number of hidden layer nodes). If used appropriately, global methods are likely to result in the best ANN structure and/or parameters; however, they are computationally expensive.

Alternatively, a stepwise trial and error procedure can be used (Figure 13), in which a basic ANN structure is first assumed, which is modified with each trial with the objective of achieving a structure that is neither too complex nor too simple. The stepwise methods can further be divided into two categories, one based on pruning algorithms and the second based on constructive approaches. A pruning algorithm starts with a sufficiently complex ANN structure that is assumed to be capable of capturing the complexities involved in the physical system being modeled. Then, the connection weights and associated neurons (based on a rating system of their magnitude) are successively removed, one at a time, until model performance deteriorates significantly. On the other hand, in a constructive algorithm, one starts with the simplest ANN structure, which is successively made more complex by adding hidden neurons/layers one at a time and calibrating the resulting model. This process is repeated until there is no significant improvement in model performance. Pruning and constructive algorithms can also be computationally intensive, as ANN models with many different structures generally need to be trained, and manually examined before arriving at the optimal structure.

Other approaches to determining an appropriate network structure, such as using a trial-and-error approach to determining the optimal number of hidden nodes, rather than a strict constructive or pruning approach, or selecting a network structure based on experience and/or intuition, have been classified as ad-hoc.

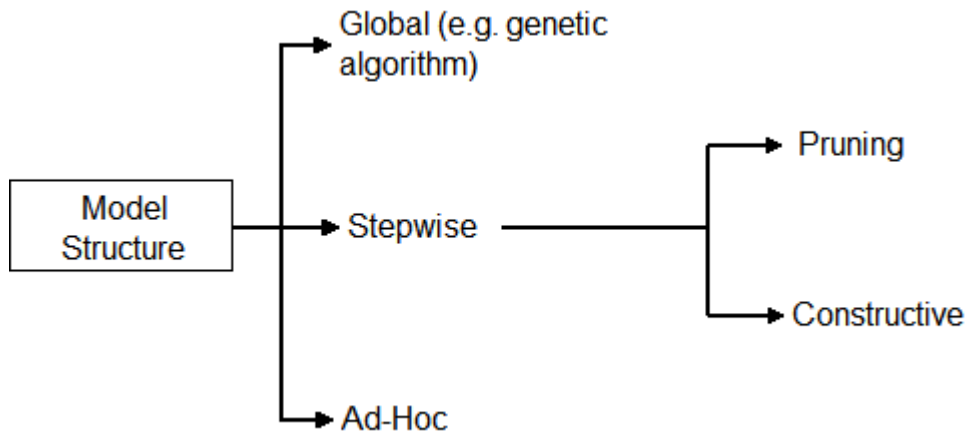


Figure 13: Taxonomy of Methods for Optimising Model Structure

3.5.3 Results

As can be seen in Figure 14, an ad-hoc approach to determining the structure of ANN models was by far the most popular, with 115 applications. Of the structured approaches, constructive stepwise approaches were used 52 times, whereas pruning and global approaches were only used on a small number of occasions (7 and 11, respectively).

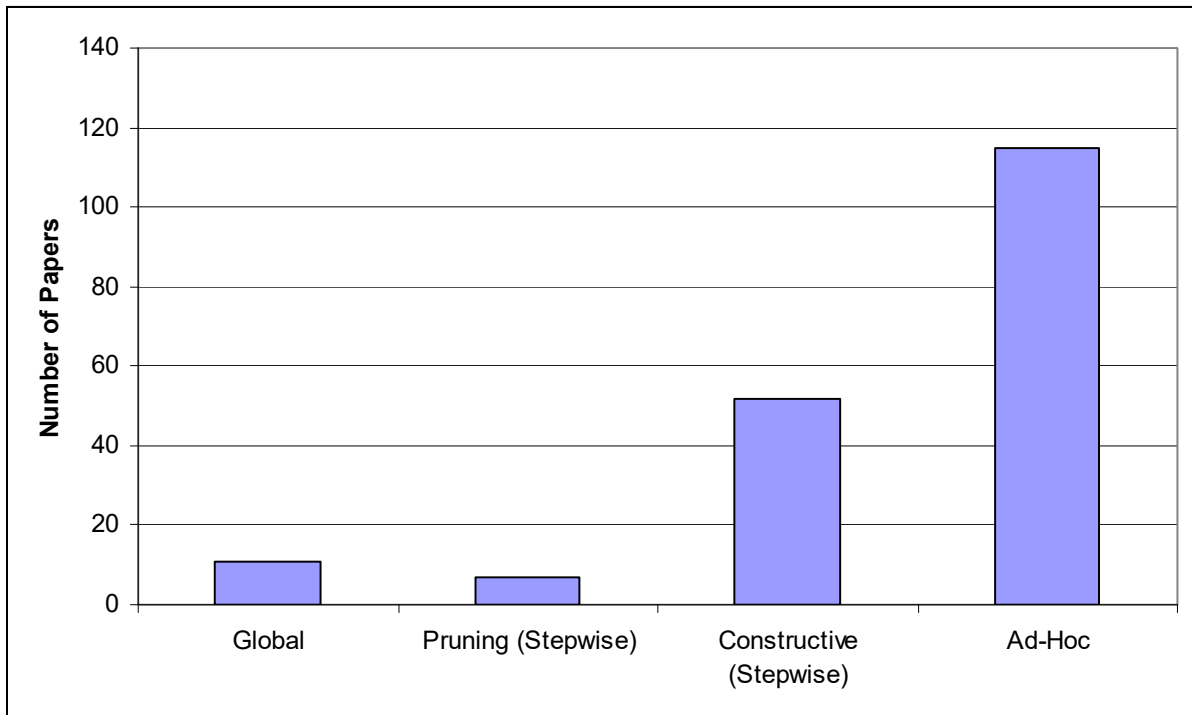


Figure 14: Number of Times Various Model Structure Determination Methods Have Been Used

3.5.4 Conclusion

Despite the important role network structure plays in determining the desired relationship between model inputs and outputs, little effort has been directed into this area of the ANN model development process, with most studies adopting an ad-hoc approach to determining an appropriate network structure. There has been reasonable adoption of constructive, stepwise model building approaches, but the use of global optimization methods has received little attention. In order to ensure that the best possible ANN models are being developed, this step in the model development process requires further attention.

3.6 Model Calibration

3.6.1 Introduction

The aim of model calibration (ANN training) is to find a set of model parameters (e.g. connection weights) that enables a model with a given functional form to best represent the desired input / output relationship. If overfitting is not considered to be a problem and the training data are representative of the modelling domain, this is achieved when a suitable error measure between actual and predicted training outputs is minimised. If overfitting is a possibility, optimal generalisation ability is achieved when a suitable error measure between actual and predicted outputs in the test set is minimised, provided that training and testing data are representative of the modelling domain.

Determination of the combination of model parameter values (i.e. weights) that minimises the training or testing error is not a simple problem. As each combination of parameter values generally results in a different model error, an error surface exists in parameter (i.e. weight) space. This is illustrated for a model with a single parameter in Figure 15, where different values of the model parameter generally result in different model errors. It can be seen that the degree of difficulty in finding the parameter value or combination of parameter values that results in the smallest model error is affected by the “ruggedness” of the error surface. Ruggedness is a measure of the number, spacing and steepness of the craters and valleys in the error surface. As can be seen in Figures 15 (a), if the error surface is smooth, there are fewer local minima, and the global optimum can be found more easily. In contrast, as illustrated in Figure 15 (b), if the error surface is more rugged, it generally has more local

minima, and the global optimum is more difficult to find. The degree of ruggedness of an error surface is usually problem dependent and is affected by the number of model parameters, among other things. As the number of model parameters increases, so does the size of the search space and, generally, the number of local optima. In addition, a larger number of parameters makes it more difficult to interpret the model and increases the risk of allowing spurious modes of model behaviour and fitting bad data, such as outliers and other anomalies. Consequently, it is important to find the model with the smallest number of inputs and parameters that is able to describe the underlying relationship in the data, as discussed previously.

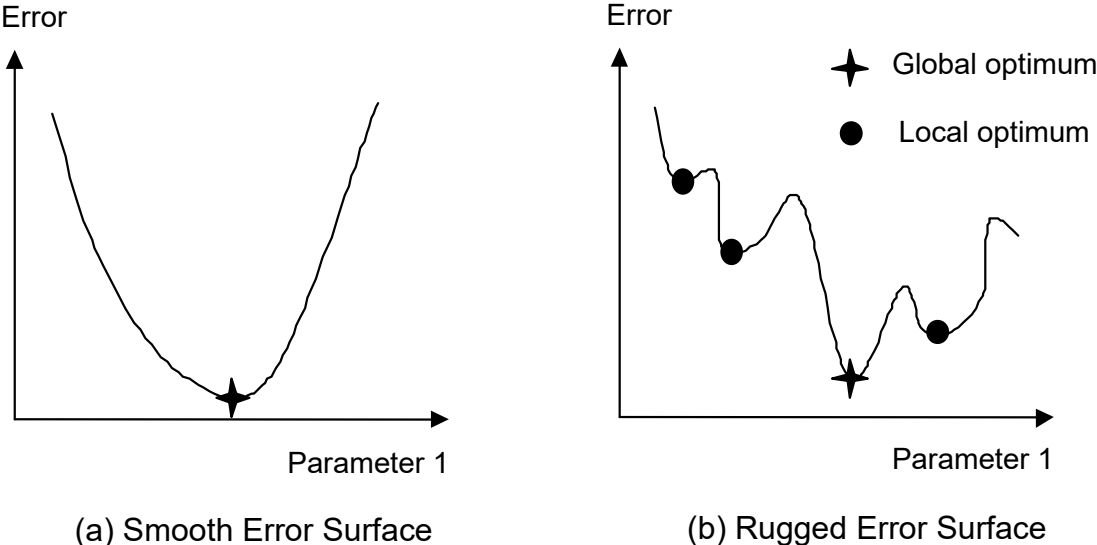


Figure 15: Error Surface with Different Degrees of Ruggedness for a Model with One Parameter

3.6.2 Taxonomy

Due to the difficulty of the ANN calibration problem outlined above, ANN calibration is generally conducted using a suitable optimization algorithm. The vast majority of these approaches are deterministic, in the sense that they attempt to identify a single parameter vector that minimizes an error measure between predicted model outputs and their corresponding measured values for the training set. These methods generally belong to either local or global optimization approaches (Figure 16). Local methods usually work on gradient information, and are therefore prone to becoming trapped in local optima if the error surface is reasonably rugged. However, these methods are generally computationally efficient. Gradient methods can be further sub-divided into first-order methods (e.g. back-propagation) or second-order methods (e.g. Newton's method). Global optimization methods, such as genetic algorithms, have an increased ability to find global optima in the error surface, although this is generally at the expense of computational efficiency.

In order to account for parameter uncertainty during the calibration process, stochastic calibration methods can be used. These approaches can be used to obtain distributions of the model parameters, rather than finding a single parameter vector. This has the advantage that prediction limits can be obtained. In order to achieve this, Bayesian methods are commonly used.

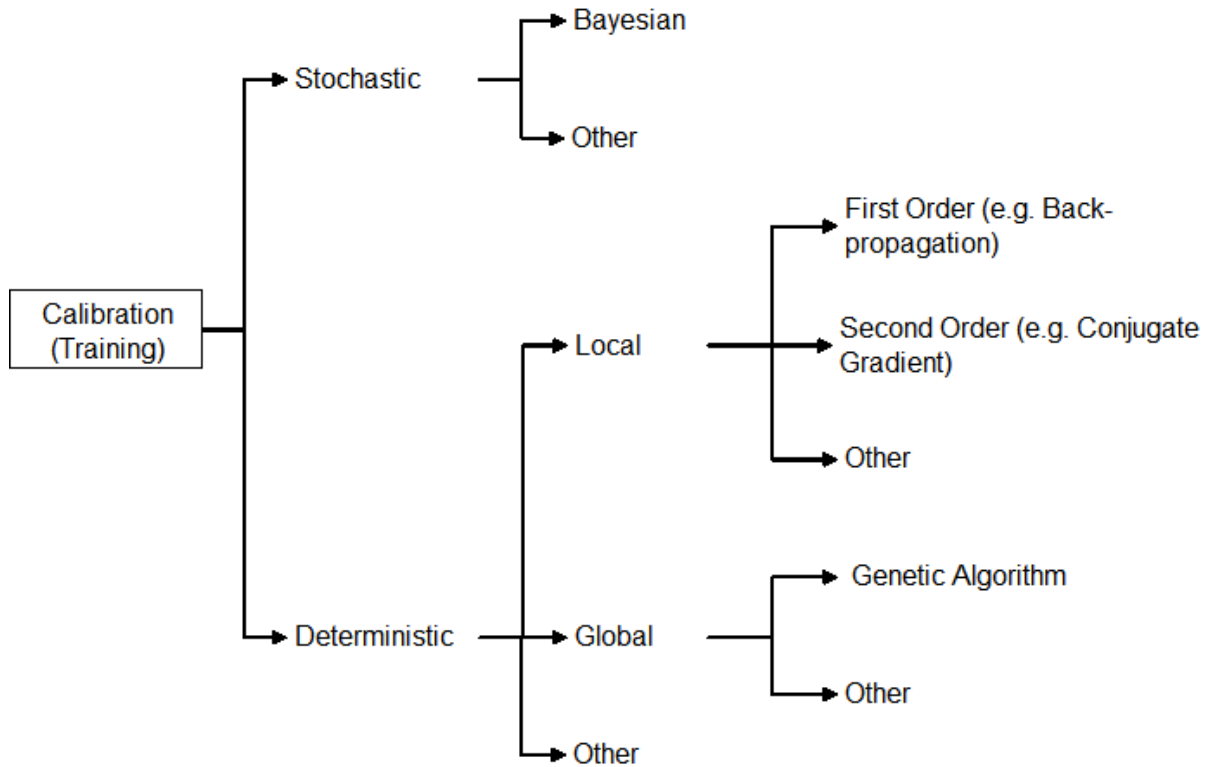


Figure 16: Taxonomy of Calibration (Training) Methods

3.6.3 Results

The results in Figure 17 illustrate that deterministic calibration methods were used predominantly (193 times), although there were 17 studies that embraced Bayesian and other stochastic approaches in order to account for parameter uncertainty. Of the deterministic calibration methods, first-order approaches, such as the backpropagation algorithm, were used most frequently, with 103 applications. However, second order methods, such as the Levenberg Marquardt algorithm, were been used extensively, with 64 applications. Use of other local and global optimization algorithms was limited.

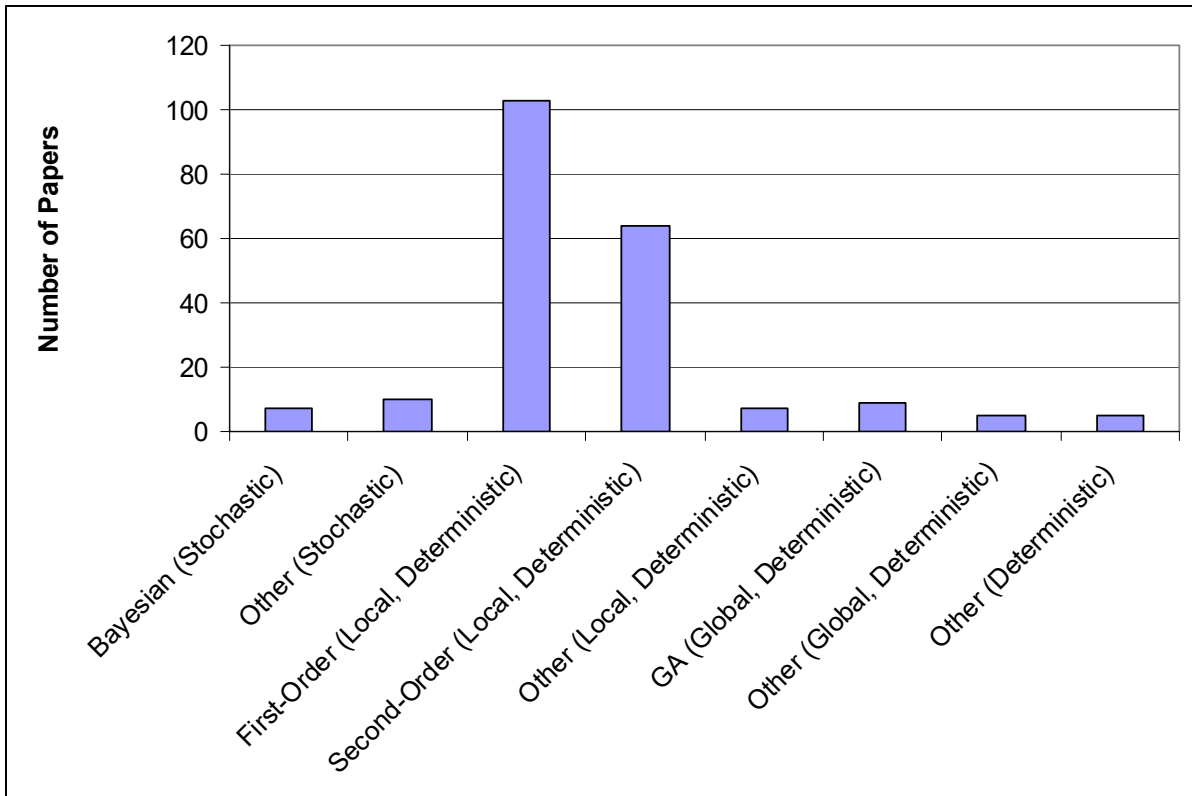


Figure 17: Number of Times Various Calibration Methods Have Been Used

3.6.4 Conclusion

In the majority of studies, first-order local search procedures, such as the backpropagation algorithm, were used, although second order methods were also used extensively in order to improve the computational efficiency of ANN calibration. However, there was little work on investigating the potential benefits of using global optimization techniques in terms of improving the predictive ability of ANN models, which is an area worthy of further exploration. In addition, although some work was done on the incorporation of parameter uncertainty into ANN model calibration, this also presents an area of future research.

3.7 Model Evaluation

3.7.1 Introduction

In order to determine which network structure is optimal, the performance of a calibrated model is evaluated against one or more criteria. This also applies to determining the optimal set of model inputs, if a model based input selection approach is used. As discussed previously, if overfitting is not considered to be a problem, model performance is assessed using the training data, whereas the test data are used for this purpose if overfitting is a concern.

3.7.2 Taxonomy

ANN model performance is usually assessed using a quantitative error metric. A taxonomy of the commonly used metrics is given in Figure 18. Squared errors are based on the squares of the differences between actual and modeled output values. Commonly employed metrics belonging to this category include the sum of squared errors (SSE), root mean square error (RMSE) and the Nash Sutcliffe efficiency (E). A feature of squared error metrics is that they tend to be dominated by errors with high magnitudes. Alternatively, absolute errors can be used, which are based on the absolute differences between actual and modeled outputs and include measures such as the total sum of absolute deviations (TSAD) and the mean sum of absolute deviations (MSAD). While absolute errors provide information on the magnitude of the error, they do not provide information on the performance of the model in terms of overall under- or over-prediction. This problem can be overcome by considering the total or mean

sum of the differences without taking absolute values, resulting in total bias (TBIAS) and mean bias (MBIAS) statistics. In order to allow the performance of models with outputs of different magnitudes to be compared more easily, relative error metrics, such as the average absolute relative error (AARE), the normalized root mean square error (NRMSE) and the normalized mean bias error (NMBE) can be used. Finally, a measure of the empirical error between actual and modeled outputs can be obtained by using product difference moment error statistics, of which the Pearson correlation coefficient is the most well-known.

Information criteria, such as the Akaike information criterion (AIC) and Bayesian information criterion (BIC) consider model complexity in addition to model error. Consequently, they have the potential to result in more parsimonious models.

In addition to the metrics mentioned above, there are a number of other statistics than can be used in order to evaluate model performance. An example of this are threshold statistics (TS), which are capable of providing the distribution of the number of data points predicted from an ANN model having various levels of absolute relative error (ARE). In addition, the performance of ANN models can also be based on the accuracy of predicting particular time series (e.g. hydrograph) characteristics, such as errors in estimating peak flow, timing of the peak and total volume.

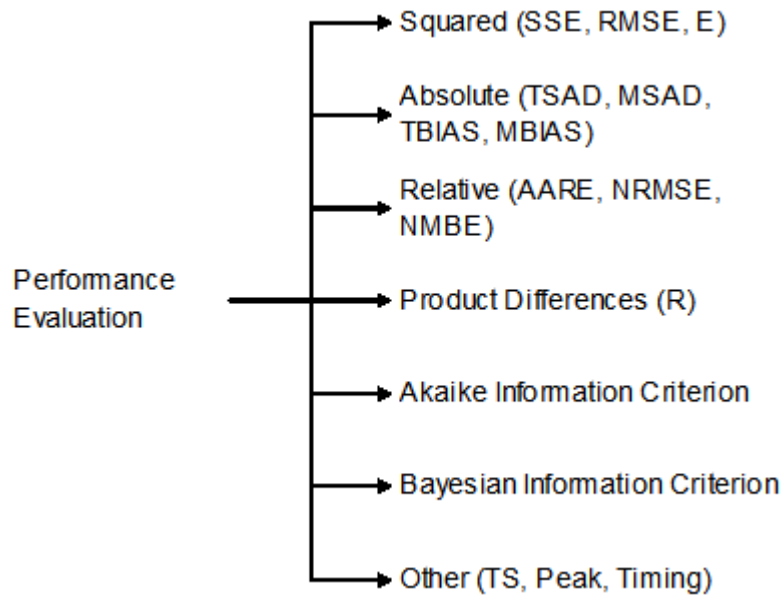


Figure 18: Taxonomy of Performance Evaluation

3.6.3 Results

The results obtained indicate that a range of performance criteria were used in most studies (Figure 19). This is considered good practice, as different criteria capture different performance characteristics, as discussed previously. While squared error metrics were most widely used (170 times), measures based on absolute and relative errors, as well as correlation, were also used extensively. As can be seen from Figure 19, “other” non-standard, problem specific evaluation criteria were used relatively frequently. However, the use of information criteria was restricted to a small number of studies.

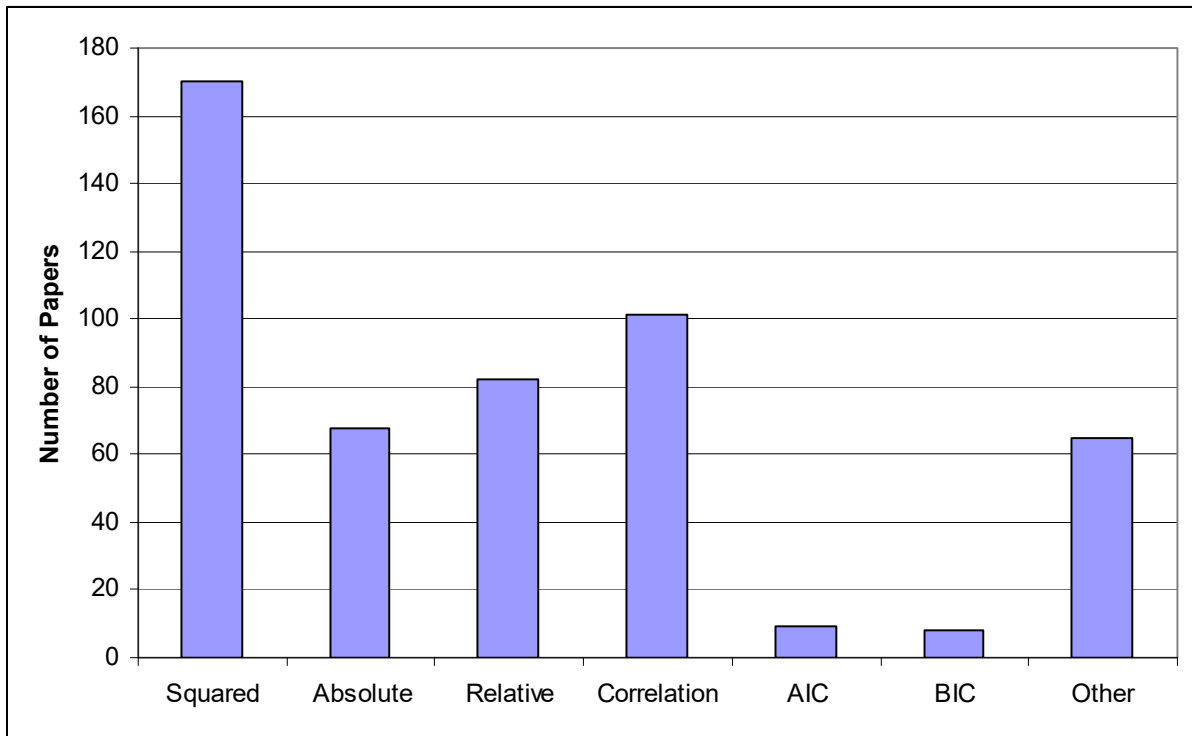


Figure 19: Number of Times Various Performance Evaluation Criteria Have Been Used

3.6.4 Conclusion

Review of the 210 papers has indicated that a range of performance criteria were used in most of the studies. This increases confidence in the evaluation of the performance of the models developed, as different performance criteria generally emphasize different aspects of predictive performance. However, increased use of information criteria, such as the AIC and BIC, could be beneficial in an effort to balance predictive performance with model parsimony.

4. Summary and Conclusions

Since the period 1992 to 1998, which is the subject of the review paper by Maier and Dandy (2000), research activity in the field of forecasting and prediction and water quantity and quality variables in rivers using ANNs has increased dramatically. From 1992 to 1998, the average number of journal papers published was 6.1 per year. This has increased to an average of 23.3 papers per year for the period of this review paper (1999 to 2007). This is despite the fact that a restricted journal list was considered for this paper and that the review was restricted to prediction in rivers, meaning that prediction of a number of water resource variables, such as rainfall, was excluded. Even within the period covered by this paper, there has been a marked increase in the number of papers published in the later years, with an average of 38 papers per year from 2005 to 2007.

As was the case from 1992 to 1998, the primary application area has been flow forecasting and prediction. Very few papers have focused on other water quantity variables and even fewer have considered water quality. If anything, the emphasis on flow modelling has increased in recent years, rather than diminished. Consequently, there is a need to broaden the application area of ANN models to focus on other predictive variables, especially those concerned with water quality. Given the universal function approximation capability of ANNs, they would seem to be ideally suited to modelling the complex relationships that are a feature of water quality processes. However, one factor limiting the application of ANNs in the water quality modelling arena might be the lack of good quality, long term data.

The adoption of appropriate input determination approaches was an area identified as deficient by Maier and Dandy (2000) and based on the findings of this study, not much has

changed in the subsequent 9 years. In the vast majority of studies reviewed in this paper, inputs were determined using an ad-hoc approach, either model based or model free. While it is pleasing to see that analytical, model free approaches were used 67 times, non-linear approaches were only used in 7 of these. Using a linear approach to identify which of the potential input variables have a significant relationship with the model output is not appropriate for the development of ANN models, as ANN models are generally used because of their ability to represent non-linear relationships between input and output data. Consequently, there is a need to adopt non-linear model input selection approaches (e.g. May et al., 2008a, 2008b).

Another aspect of input selection that has received even less attention is the issue of input independence. While models with redundant inputs might perform well from the perspective of being able to obtain a good match to the calibration data, they increase model complexity and parameter uncertainty. As a result, this issue needs to receive increased attention in order to reduce the uncertainty surrounding ANN model outputs and to enable research into knowledge extraction from ANNs to proceed with increased confidence.

Maier and Dandy (2000) concluded that data division was not carried out adequately in most of the 43 papers reviewed in their study. Unfortunately, the same still applies today. In the 210 papers that were the subject of this review, attempts to ensure that the statistics of the various data subsets were similar were only made on 24 occasions, whereas ad-hoc data division methods were used 148 times. This can cast serious doubts on the quality and repeatability of the results obtained, as different data splits are likely to result in different calibrated models and different model performance on the validation data. Consequently, there is a need to consider well established data sampling approaches for the division of the

available data into the requisite model development and evaluation subsets (e.g. May et al., 2010).

In relation to model architecture, there was a significant amount of research activity in the nine years covered by this review. Maier and Dandy (2000) found that feedforward networks were used almost exclusively from 1992 to 1998, most of which were MLPs. While MLPs were still found to be the dominant ANN architecture in this paper, they were used as a benchmark against which to compare alternative architectures in many of the papers reviewed. There was a significant amount of experimentation with other types of feedforward architectures, such as generalized regression neural networks, radial basis function networks, neurofuzzy models and support vector machines, recurrent networks and, most importantly, different types of hybrid network architectures. The development of hybrid ANN model architectures is an important advance, as it emphasizes that ANNs have a role to play not only as an alternative to traditional modelling approaches, but as a complementary modelling tool that can be used to improve the performance of existing approaches. The acknowledgement that ANNs should be used in circumstances that exploit their strengths, rather than as a panacea for the shortcomings of more traditional modelling approaches, is part of the evolution of ANNs towards a mature modelling approach that can sit comfortably alongside more traditional approaches in the toolkit of hydrological modelers.

The way in which optimal model structures are obtained is an area that has received little attention in the papers that form part of this review. As was the case in the findings of Maier and Dandy (2000), optimal network geometries were generally obtained using ad-hoc approaches, primarily using trial and error. While there was some increase in the use of systematic approaches to determining the optimal number of hidden nodes during this review

period compared with the previous one, the development and application of methods for determining the optimal model structure remains an area of ongoing work.

There was also little activity in relation to model calibration during the time period considered for this paper. As was the case from 1992 to 1998, first order local optimization methods were by far the most common, although an increasing number of second order local methods were used in the papers published between 1999 to 2007. However, surprisingly, there was little adoption of global optimization methods, which have been found to outperform more traditional methods when used in conjunction with other water resource modelling approaches in recent years. It was good to see that some effort was devoted towards the development of Bayesian and other stochastic approaches to model calibration in order to enable parameter uncertainty to be taken into account and to enable confidence limits on predictions to be obtained, but there is a need to expand this work into the future.

In the majority of papers reviewed, different methods were used to evaluate model performance, which is considered good practice. However, there is scope for improving the way models are evaluated by applying the various measures in a consistent and informed manner (see Dawson et al., 2007). In addition, in order to enable better comparison of ANN development methods across studies, the use of open access data sets should be encouraged.

5. Recommendations for Future Research

Based on the review of 210 papers on the prediction and forecasting of water quantity and quality variables in rivers conducted in this paper, the following recommendations for future work are made:

1. More work needs to be undertaken on the prediction of water quality variables (e.g. May and Sivakumar, 2009, Dellana and West, 2009) in order to further test the utility of ANN models as a predictive tool in hydrology and water resources. Even though there are fewer water quality data than rainfall-runoff data, there are still sufficient water quality data available to develop ANN models. The fact that ANNs are data-driven, and are thus able to make best use of existing data, should give them an advantage over process-driven water quality models, which require data on all variables, which are often more difficult to obtain.
2. Work should continue on the development and evaluation of hybrid model architectures that attempt to draw on the strengths of alternative modelling approaches (e.g. Lin et al., 2008). Given the amount of work that has already been done in this area, a review of this emerging field of research would seem timely.
3. Greater attention should be paid to the input variable selection and data division steps of the ANN model development process. Currently adopted ad-hoc methods in both of these areas have the potential to significantly degrade model performance and therefore need to be replaced with state-of-the art approaches. In relation to input variable selection, non-linear approaches that are able to account for input independence should be used (e.g. May et al., 2008a, 2008b; Fernando et al., 2009; May et al., 2009). As far as data division is concerned, appropriate sampling

techniques should be used to ensure that the data in all subsets are representative of each other (see May et al., 2009; May et al., 2010).

4. There has been increasing adoption of second order local methods for model calibration, but the use of global optimization methods is still limited. Consequently, there is scope for comparative studies investigating the relative performance of various global and local optimization algorithms in the context of ANN model calibration (training).
5. Research into the best way to incorporate uncertainty into ANN models should be continued. Current work on the incorporation of parameter uncertainty via Bayesian and other stochastic calibration methods should be extended to include other types of uncertainty (e.g. Kingston et al., 2005a).
6. Appropriate methods for determining the optimal ANN model structure remain elusive. Although some work has been done on this recently (e.g. Kingston et al., 2008), this is an area that requires further research. Increased utilization of ANN architectures that have a fixed structure, such as generalized regression neural networks, might also be worthy of consideration.

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