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## Application of Artificial Neural Networks in Identification of Affinity Hydration Model Parameters

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### Abstract

Recent decades have witnessed rapid development in numerical modelling of structures as well as materials and the complexity of models increases rapidly together with their computational demands. Despite the growing performance of modern computers and clusters, a suitable approximation of an exhaustive simulation has still many applications in engineering problems. For example, the field of parameters identification may represent a large domain for very efficient applications. The layered neural networks are still considered as very general tools for approximation and they became popular especially for their simple implementation. This contribution presents different strategies for application of neural networks in calibration of affinity hydration model and discusses their possible advantages and drawbacks.

**Keywords:** artificial neural network, multi-layer perceptron, approximation, parameter identification, affinity hydration model, cement paste.

# **1** Introduction

Development in numerical modelling provides the possibility to describe a lot of complex phenomena in material or structural behaviour. The resulting models are, however, often highly nonlinear and defined by many parameters, which have to be estimated so as to properly describe the investigated system and its behaviour. The aim of the model calibration is thus to rediscover unknown parameters knowing the experimentally obtained response of a system to the given excitations. The principal difficulty of model calibration is related to the fact that while the numerical model of an experiment represents a well-defined mapping from input (model, material, structural, or other) parameters to output (structural response), there is no guarantee that the inverse relation even exists. The most broadly used approach to parameter identification is usually done by means of an error minimisation technique, where the distance between parameterised model predictions and observed data is minimised [22]. Since the inverse relation (mapping of model outputs to its inputs) is often ill-posed, the error minimisation technique leads to a difficult optimisation problem, which is highly nonlinear and multi-modal. Therefore, the choice of an appropriate identification strategy is not trivial.

Another approach intensively developed during the last decade is based on Bayesian updating of uncertainty in parameters' description [15, 14]. The uncertainty in observations is expressed by corresponding probability distribution and employed for estimation of the so-called posterior probabilistic description of identified parameters together with the prior expert knowledge about the parameter values [11, 23]. The unknown parameters are thus modelled as random variables originally endowed with prior expert-based probability density functions which are then updated using the observations to the posterior density functions. While the error minimisation techniques lead to a single point estimate of parameters' value, the result of Bayesian inference is a probability distribution that summarizes all available information about the parameters. Another very important advantage of Bayesian inference consists in treating the inverse problem as a well-posed problem in an expanded stochastic space.

Despite the progress in uncertainty quantification methods [16, 19], more information provided by Bayesian inference is generally related to more time-consuming computations. In many situations, the single point estimate approach remains the only feasible one and development of efficient tools suitable for this strategy is still an actual topic. Within the several last decades, a lot of attention was paid to the so-called intelligent methods of information processing and among them especially to soft computing methods such as artificial neural networks (ANNs), evolutionary algorithms or fuzzy systems [9]. A review of soft computing methods for parameter identification can be found e.g. in [13]. In this paper, we focus on applications of ANNs in the single point approach to parameter identification.

### 2 Aritificial neural network

Artificial neural networks (ANNs) [4, 5] are powerful computational systems consisting of many simple processing elements - so-called neurons - connected together to perform tasks analogously to biological brains. Their main feature is the ability to change their behaviour based on external information that flows through the ANN during the learning (training) phase.

A particular type of ANN is the so-called feedforward neural network, which consists of neurons organized into layers where outputs from one layer are used as inputs into the following layer, see Figure 1. There are no cycles or loops in the network, no feed-back connections. Most frequently used example is the multi-layer perceptron (MLP) with a sigmoid transfer function and a gradient descent method of training called the back-propagation learning algorithm. In practical usage, the MLPs are known for their ability to approximate non-linear relations and therefore, when speaking about an ANN, the MLP is considered in the following text.



Figure 1: Architecture of multi-layer perceptron

The input layer represents a vector of input parameters which are directly the outputs of the input layer. The outputs of one layer are multiplied by a vector of constants, the so-called synaptic weights, summarized and used as inputs into the following layer. Elements in the hidden and output layers - neurons - are defined by an activation function, which is applied on the input and produces the output value of the neuron. The synaptic weights are parameters of an ANN to be determined during the training process. The type of the activation function is usually chosen in accordance with the type of a function to be approximated. In the case of continuous problems, the sigmoid activation function is the most common choice.

One bias neuron is also added into the input and hidden layers. It does not contain an activation function, but only a constant value. Its role is to enable to shift the value of a sum over the outputs of his neighbouring neurons before this sum enters as the input into the neurons in the following layer. The value of biases is determined by training process together with the synaptic weights.

Despite of ANN's popularity there are only few recommendations for the choice of ANN's architecture. The authors, e.g. in [8, 7], show that the ANN with any of a wide variety of continuous nonlinear hidden-layer activation functions and one hidden layer with an arbitrarily large number of units suffices for the "universal approximation" property. Therefore, we limit our numerical experiments to such case. The number of units in the input and the output layer is usually given by the studied problem itself, but there is no theory yet specifying the number of units in the hidden layer.

To overcome this problem, we use two sets of data for ANN's preparation: training data are used for calibration of the synaptic weights of the ANN with a chosen number of hidden units and the resulting ANN is then evaluated on independent validation data. Then, one hidden neuron is added to the existing ANN, which is again trained, evaluated on validation data and the ratio between the obtained error to the error obtained for the previous ANN is computed. We count the situations, where the ratio is

higher than 0.99. When these situations occur three times, the addition of hidden neurons is stopped. Then the ANN with the smallest error on validation data is employed for model calibration.

### **3** Strategies for model calibration

In overall, there are two main philosophies for application of ANN in identification problems. In a forward mode/direction, the ANN is applied to approximate the model response. The error minimisation technique then becomes a minimisation of distance between the ANN's predictions and experimental data. The efficiency of this strategy relies on the evaluation of the trained ANN to be significantly much faster than the full model simulation. The advantage of this strategy is that the ANN is used to approximate a known mapping which certainly exists and is well-posed. Computational costs of this strategy are separated in two parts of a similar size: (i) the ANN training - optimisation of synaptic weights and (ii) the minimisation of an error in ANN prediction for experimental data - optimisation of ANN inputs (i.e. determination of investigated model parameters). The latter part concerns optimisation of an error function which is often multi-modal, non-differentiable and some robust optimisation method has to be applied to solve this problem. An important shortcoming of this method is that this ill-posed optimisation problem needs to be solved repeatedly for any new experimental measurement. This way of ANN application to the parameter identification was presented e.g. in [1], where an ANN is used for predicting load-deflection curves and the conjugate directions algorithm is then applied for optimisation of ductile damage and fracture parameters. Authors in [18] train an ANN to approximate the results of FE simulations of jet-grouted columns and optimise the column radius and a cement content of the columns by a genetic algorithm. Principally same methods are used for identification of elasto-plastic parameters in [2].

The second philosophy, an inverse mode, assumes the existence of an inverse relationship between the outputs and the inputs of the calibrated model. If such a relationship exists at least on a specified domain of parameters' value, it can be approximated by an ANN. Then the retrieval of desired inputs is a matter of seconds and could be easily executed repeatedly for any new experiment and no other optimisation process is necessary. Here the ANN training represents the whole computational costs and a solution of the ill-posed problem. This way of ANN application to parameter identification was presented e.g. in [17] for identification of mechanical material parameters, in [25] for estimation of elastic modulus of the interface tissue on dental implants surfaces, in [26] for identification of interfacial heat transfer coefficient or in [12] for determination of geometrical parameters of circular arches.

Since the ANN training needs a preparation of a set of training data, it is also worthy to use these data for a sampling-based sensitivity analysis [6, 20] and obtain some information about importance of particular observations or significance of each parameter for a system behaviour. To achieve some reliable information from sensitivity analysis as well as a good approximation by ANN, one has to choose the training data carefully according to a suitable design of experiments, see e.g. [10] for a competitive comparison of several experimental designs.

### 4 Affinity hydration model

The affinity model provides a simple framework describing all stages of cement hydration. The rate of hydration can be expressed by the temperature-independent normalized chemical affinity  $\tilde{A}(\alpha)$  [3]

$$\frac{\mathrm{d}\alpha}{\mathrm{d}t} = \tilde{A}(\alpha) \exp\left(-\frac{E_a}{RT}\right) \,, \tag{1}$$

where  $\alpha$  stands for the degree of hydration, T is an arbitrary constant temperature of hydration, R is the universal gas constant (8.314 Jmol<sup>-1</sup>K<sup>-1</sup>) and  $E_{\alpha}$  is the apparent activation energy.

For the hydration heat prediction, an analytical form presented in [24] is used:

$$\tilde{A}(\alpha) = B_1 \left(\frac{B_2}{\alpha_{\infty}} + \alpha\right) (\alpha_{\infty} - \alpha) \exp\left(+\bar{\eta}\frac{\alpha}{\alpha_{\infty}}\right) , \qquad (2)$$

where  $B_1$  and  $B_2$  are coefficients related to chemical composition,  $\alpha_{\infty}$  is the ultimate hydration degree and  $\bar{\eta}$  represents microdiffusion of free water through formed hydrates. Then a curve of the degree of hydration development  $\alpha$  can be obtained by the numerical integration of equation (2).

#### **5** Sensitivity analysis

Since the bounds for model parameters vary in orders, one can employ the expert knowledge about the parameter meanings and before preparation of training data transform them into standardised parameters  $p_i \in [0; 1]$ . The bounds for affinity model parameters together with relations to the standardised parameters  $p_i$  are given in Table 1.

Parameter	Minimum	Maximum	Relation
$B_1$	$10^{6}$	$10^{7}$	$p_1 = \log B_1 - 6$
$B_2$	$10^{-6}$	$10^{-3}$	$p_2 = (\log B_2 + 6)/3$
$ar\eta$	-12	-2	$p_3 = (-\bar{\eta} - 2)/10$
$\alpha_{\infty}$	0.7	1.0	$p_4 = (\alpha_{\infty} - 0.7)/0.3$

Table 1: Bounds for affinity model parameters.

In the space of standardised parameters we prepare a design of experiments having 100 samples based on Latin Hypercube Sampling optimised with respect to modified

 $L_2$  discrepancy. In [10] it is shown that such an experimental design has a good spacefilling property and is nearly orthogonal. For each design point we perform a model simulation to obtain a bundle of 100 curves for the degree of hydration  $\alpha(t)$ , see Figure 2.



Figure 2: Bundle of degree of hydration curves obtained for design points.

Since the model response is represented by the degree of hydration being a function of the time, the time domain is discretised into 199 steps uniformly distributed with the logarithm of the time. Hence, the model input vector consists of 4 parameters and the output vector consists of 199 components. For each input-output pair with 100 simulations we evaluate the Spearman's rank correlation coefficient  $\rho$  in order to compute the sensitivity of output to input parameters [6]. The results of such a sampling-based sensitivity analysis are plotted in Figure 3.



Figure 3: Sensitivity analysis for input-output pairs.

## 6 Neural network training

Results of the described 100 simulations are also used as training data for ANNs. Then, the last preparatory step concerns the generation of validation data for evaluation of particular ANN's architecture (i.e. the number of hidden nodes) and testing data for final assessment of resulting ANNs. For each of these data sets we run 50 simulations for randomly generated sets of input parameters.

In forward mode, the aim was to approximate the curve of hydration degree discretised in 199 time steps. Instead of developing an ANN with 199 outputs we add the value of the time as an additional input of ANN which then have only one output corresponding to the degree of hydration at a given time step. With such a configuration of ANN inputs, the set of 100 training curves discretised into 199 time steps turns into  $100 \times 199$  training samples. Evaluate so many samples at every iteration of ANN training process is however time-consuming and hence the  $\alpha$  values only in every 10th time step (i.e. at  $t_1, t_{11}, \ldots, t_{191}$ ) were included for ANN training. Similar selection was performed on validation and testing data, but for shifted time steps  $t_6, t_{16}, \ldots, t_{196}$ .

Also in the inverse mode, only selected  $\alpha$  values can be employed as ANN inputs so as to keep the ANN complexity reasonable. A particular choice should take into account not only the results of sensitivity analysis, but also a possible measurement error in experimental data as well as any other expert knowledge. Figure 3 shows that each part of the  $\alpha$  curve is strongly sensitive to one of the model parameters, which suggests that the inputs should uniformly cover whole curve. However, Figure 2 reveals extremely small dispersion of  $\alpha$  at early stage, which is actually smaller than realistic measurement error, as it is shown later in Section 7. Hence to reduce the impact of experimental error, we choose the ANN inputs from regions with high dispersion of training data. In particular, eight values of  $\alpha$  are selected corresponding to time steps  $t_{38+20i}$  with  $i = 0, \ldots, 7$ , where early stage is excluded. The particular choice of ANN inputs, outputs and the number of hidden neurons achieving best results on validation data are presented in Table 2.

ANN	Input	Hidden	Output	$\varepsilon_{\rm train}[\%]$	$\varepsilon_{\text{valid}}[\%]$	$\varepsilon_{\text{test}}[\%]$
Forward	$p_1, p_2, p_3, p_4, t$	6	$\alpha$	2.34	2.37	2.24
Inverse	8 values of $\alpha$ at $t_{38}, t_{58}, \ldots, t_{178}$	5	$p_1$	0.87	1.40	1.26
	8 values of $\alpha$ at $t_{38}, t_{58}, \ldots, t_{178}$	6	$p_2$	1.47	1.09	2.63
	8 values of $\alpha$ at $t_{38}, t_{58}, \ldots, t_{178}$	8	$p_3$	2.02	2.90	2.72
	8 values of $\alpha$ at $t_{38}, t_{58}, \ldots, t_{178}$	3	$p_4$	0.12	0.10	0.16

Table 2: Architecture of particular ANNs and their errors on training, validation and testing data.

The conjugate gradient-based method [21] was employed as a training algorithm for the ANNs. The synaptic weights optimisation process was stopped either when the number of iterations achieved 5000 or if the ratio of the average error on training data during last 100 iterations to the error obtained for previous 100 iterations was higher than 0.999.

In order to evaluate the quality of particular ANNs, the relative errors  $\varepsilon$  are computed for training, validation and testing data according to

$$\varepsilon = \frac{\sum_{i=1}^{I} |O_i - T_i|}{I(T_{\max} - T_{\min})},\tag{3}$$

where  $O_i$  are the ANN outputs,  $T_i$  are the target values (i.e.  $\alpha$  in case of the forward mode and  $p_i$  in case of inverse mode), I is the number of samples in a given data set (training, validation or testing) and  $T_{\text{max}}$ ,  $T_{\text{min}}$  are the maximal and minimal target values in training data set, respectively. The resulting errors on training, validation and testing data for all the created ANNs are listed in Table 2.

#### 6.1 Verification of model calibration

The errors in Table 2 represent the quality of constructed ANNs. Next we have to compare the quality of identification procedures. While in the inverse mode the ANNs predict directly the values of model parameters, in the forward mode we have to perform an optimisation of the parameters minimising the distance between the ANN prediction and target model response:

$$\sum_{m=1}^{M} (O(t_m) - \alpha(t_m))^2,$$
(4)

where M = 199 is the number of model response components. The optimisation process is governed by the GRADE evolutionary algorithm, see [13] for details about this method<sup>1</sup>.

The optimisation process was performed for all training, validation and testing data and the relative errors  $\varepsilon$  according to equation (3) for parameter predictions were then computed for both the identification modes. The obtained results are listed in Table 3.

	$p_1$		$p_2$		$p_3$		$p_4$		α						
	train	valid	test	train	valid	test	train	valid	test	train	valid	test	train	valid	test
Forward	8.93	7.70	7.39	15.81	11.56	14.83	3.92	4.52	3.61	1.79	1.88	1.86	0.56	0.60	0.52
Inverse	0.87	1.40	1.26	1.47	1.09	2.63	2.02	2.90	2.72	0.12	0.10	0.16	0.28	0.39	0.35

Table 3: Results of identification procedure in relative errors  $\varepsilon$  [%].

To assess the quality of identification procedure in terms of model response, the model simulations were performed for all sets of identified parameters and the relative error  $\varepsilon$  was computed between the obtained responses and the original target responses. These results are also written in Table 3.

<sup>&</sup>lt;sup>1</sup>The parameters of GRADE algorithm were set to pool\_rate = 4, radioactivity = 0.33 and cross\_limit = 0.1. The algorithm was stopped after 10000 cost function evaluations.

One can see that while the parameter  $p_2$  is correlated mainly to early stage of hydration which was excluded from training data for inverse mode of identification, the errors in  $p_2$  predictions are quite small, especially in comparison with forward mode of identification where all of the data were employed. In overall, the inverse mode of identification resulted in better estimation in terms of parameters as well as the model response, but results of both methods can be assumed as very good.

### 7 Validation of model calibration

The previous section was focused on mutual comparison of the presented identification strategies on simulated data. However, a complete comparison has to include their validation on experimental data. To that purpose we used the curve of hydration degree obtained by isothermal calorimetry for cement "Mokra" CEM I 42.5 R taken directly from Heidelberg cement group's kiln in Mokrá, Czech Republic [24].

In general, validation does not allow for a comparison in terms of parameters value, because these are not known a priori. Nevertheless, the simplicity and the fast simulation of affinity hydration model permit a direct optimisation of model parameters without any incorporated approximation and the resulting optimal parameter values can be compared with the results obtained using the ANN approximations.

In direct optimisation, we have to formulate the cost function specifying how good the model prediction is. In our numerical study, we decided to test two widely used cost functions:

$$F_{1} = \sum_{\substack{m=1 \ M}}^{M} (\alpha(t_{m}) - \alpha^{\text{Mokra}}(t_{m}))^{2}, \qquad (5)$$

$$F_2 = \sum_{m=1}^{M} |\alpha(t_m) - \alpha^{\text{Mokra}}(t_m)|, \qquad (6)$$

where M = 199 stands again for the number of discretised values of hydration degree,  $\alpha(t_m)$  is the model response and  $\alpha^{\text{Mokra}}(t_m)$  are the interpolated experimental data. We applied again the GRADE algorithm with the same setting as in the previous section to minimise the both cost functions (5) and (6). The obtained parameter and cost functions values are written in Table 4 and the resulting degree of hydration curves can be compared with experimental data in Figure 4a.

Subsequently, the forward and both inverse modes of identification were applied to the experimental data using the prepared ANNs. The identified parameters are again written in Table 4 and corresponding simulated degrees of hydration are plotted in Figure 4b.

The results show that the forward mode of identification leads to a significant error on experimental data. The reason is probably that ANNs are good in approximation and interpolation, but very bad in extrapolation. Due to this, the ANN-based approach is very sensitive to the noise and measurement errors in experimental data. Measurement errors can easily lead to ANN's input values which are out of the convex hull

Method	$p_1$	$p_2$	$p_3$	$p_4$	$F_1$	$F_2$
Direct1	0.856	1.000	0.208	0.053	0.002	0.336
Direct2	0.858	1.000	0.208	0.050	0.002	0.271
Forward	0.922	0.911	0.339	0.051	0.135	2.333
Inverse	0.736	1.100	0.124	0.051	0.023	0.854

Table 4: Parameter values identified on experimental data obtained for "Mokra" cement together with the corresponding values of cost functions. The methods Direct1 and Direct2 correspond to the optimisation of cost functions  $F_1$  and  $F_2$ , respectively.



Figure 4: Comparison of experimentally obtained degree of hydration for "Mokra" cement with simulations for directly optimised model parameters (a) and for identified parameters using ANN approximations (b).

constructed on the training examples and the ANN is then forced to extrapolate. This situation happened here, because the experimental curve is out of the bundle of training curves in the early stages, see Figure 5a. At the start of hydration, the measured values of  $\alpha$  are equal to zero and the curve is under the training bundle. After this starting constant period, the experimental degree of hydration starts to grow very quickly and very soon exceeds the values of all the training simulations. The direct optimisations also lead to a limit value of  $p_2$  parameter, which was not exceeded, because the optimisation was constrained. The explanation of the phenomenon can be either the imperfection of a model or measurement error not only in hydration values but also in the estimation of the hydration start so as to experimental curve does not exceed the training data by moving whole curve by five time steps assuming that the hydration started 2.7846 minutes later, see Figure 5b.

After the described correction of experimental data, the direct optimisations as well as both identification procedures were performed again and the resulted parameter predictions and error estimates for the degree of hydration are given in Table 5. Finally, the curves of the hydration degree obtained by direct optimisation are plotted in Figu-



Figure 5: Detailed comparison of experimentally obtained degree of hydration for "Mokra" cement with training simulations at early stages (a) and in whole time span (b).

Method	$p_1$	$p_2$	$p_3$	$p_4$	$F_1$	$F_2$
Direct1	0.647	1.000	0.208	0.053	0.002	0.332
Direct2	0.650	1.000	0.207	0.050	0.002	0.268
Forward	0.718	0.958	0.255	0.038	0.017	1.114
Inverse	0.571	1.098	0.186	0.050	0.005	0.423

Table 5: Parameter values identified on **corrected** experimental data obtained for "Mokra" cement together with the corresponding values of cost functions. The methods Direct1 and Direct2 correspond to the optimisation of cost functions  $F_1$  and  $F_2$ , respectively.

re 6a and curves obtained by ANN-based identification procedures are plotted in Figure 6b.

### 8 Conclusions

This paper reviews possible applications of artificial neural networks for the calibration of numerical models. The basic identification modes are described in detail: the forward and the inverse. Their advantages and drawbacks are illustrated on the calibration of the affinity hydration model. Verification of the procedures is performed using 50 independent testing data obtained from numerical simulations and experimental data obtained for cement "Mokra" CEM I 42.5 R are subsequently employed for the validation of the presented methods. The main advantage of the inverse approach is an easy application to new measurements. The computationally consuming and difficult part concerns the ANN development which has to be done only once. An important shortcoming of this procedure is that this inverse relationship between



Figure 6: Comparison of experimentally obtained degree of hydration for "Mokra" cement with simulations for directly optimised model parameters (a) and for identified parameters using ANN approximations (b).

model outputs and model inputs does not need to exist. Nevertheless, if it does exist as in the case presented here, its application is very easy and simpler than application of forward identification, which includes an optimisation process which may not be trivial. Another weak point of ANN usage is related to its sensitivity to experimental noise, measurement error or data lying far from the training simulations. Then some expert's knowledge has to be involved to make the model calibration successful. Hence, our future works will be aimed on development some techniques to make the ANN implementation more robust.

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