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Impact of hidden weights choice on accuracy of MLP with randomly fixed hidden neurons for regression problems

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Abstract: Neural network is a well-known tool able to learn model from data with a good accuracy. However, this tool suffers from an important computational time which may be too expansive. One alternative is to fix the weights and biases connecting the input to the hidden layer. This approach has been denoted recently extreme learning machine (ELM) which is able to learn quickly a model. Multilayers perceptron and ELM have identical structure, the main difference is that only the parameters linking hidden to output layers are learned. The weights and biases which connect the input to the hidden layers are randomly chosen and they don't evolved during the learning. The impact of the choice of these random parameters on the model accuracy is not studied in the literature. This paper draws on extensive literature concerning the feedforward neural networks initialization problem. Different feedforward neural network initialisation algorithms are recalled, and used for the determination of ELM parameters connecting input to hidden layers. These algorithms are tested and compared on several regression benchmark problems.

1 INTRODUCTION

Since the backpropagation algorithm proposed by Rumelhart and McClelland (1986), neural networks have shown their abilities to solve a broad array of problem including regression, classification, clustering as examples. However, the design of a neural model needs a learning step which may be very computational time consuming. To overfit this drawback, Schmidt et al. (1992) have been the firsts to proposed to adapt only the weights and biases connecting the hidden to the output layers. Huang et al (2004) have formalised this approach and called it: Extreme Learning Machine (ELM). This tool has been the subject from many publications, including theoretical purpose (Lendasse et al. 2016) or application (Rajesh and Parkash 2011).

ELM structure is similar to structure of classical single hidden layer feedforward neural network. Multilayer perceptron (MLP) uses backpropagation algorithm in order to adapt all the parameters (weights and biases connecting the input to the hidden layers and those connecting the hidden to the output layers). Rather, in ELM, the weights and biases connecting the input to the hidden layers are

fixed and only those connecting the hidden to the output layers constitute the parameters set which are tuned by using one-pass algorithm. This fact leads to a great improvement of the learning computational time. Even if some authors claim that ELM preserves their habilités of universal approximator (Huang and Lai 2012, Javed et al. 2014), Li and Wang (2017) have proved that it was not true. However, ELM preserves their interest due to their good capabilities to deal with large data analysis, fast dynamic modelling and real-time data processing (Cui and Wang 2016).

The choice of the hidden nodes impacts the ELM accuracy (Huang and Lai 2012, Feng et al. 2009, Qu et al. 2016). To improve it, many researchers focus on the hidden nodes number determination by using genetic algorithm (Suresh et al. 2010), pruning procedure (Miche et al. 2010) or incremental learning approaches (Feng et al. 2009).

The random choice of the weights and biases connecting the input to the hidden layers is rarely discussed. We can cite Qu et al. (2016) which distinguish classification problems where orthogonal initialisation allows to improve accuracy, when better results are obtained if random initialisation is

used for regression problems. The great majority of works related to ELM include a simple random initialisation of these weights and biases (Huang et al. 2004, Huang et al. 2006). Some works proposed a more sophisticated initialisation procedure (Javed et al. 2014) including the use of evolutionary algorithms (Evolutionary-ELM) which may deteriorate the computational time (Zhu et al. 2005, Cao et al. 2012, Matias et al. 2014). At the oposite, other works do not say a word about this problem (Huang and Lai 2012, Yin et al. 2015).

On the contrary, in the MLP context, the problem of initialization of the weights and biases connecting the input to the hidden layers have been studied (Nguyen and Widrow 1990, Burel 1991, Drago and Ridella 1992, Thomas and Bloch 1997).

In this paper, the impact of the using of sophisticated MLP initialization algorithms for ELM model accuracy for regression purpose is investigated. Next section will present the structure and the learning algorithm of the considered ELM. The hidden nodes choice is also discussed. Section three recalls five MLP initialization algorithms. These algorithms are used for ELM models for three regression benchmarks in section four before to conclude.

2 EXTREME LEARNING MACHINE (ELM)

2.1 ELM structure and notations

The structure of an ELM is similar to the MLP structure and is given by:

$$z_k = \sum_{i=1}^{n_1} w_{ki} \cdot g \left(\sum_{h=1}^{n_0} v_{ih} \cdot x_h^0 \right) = \sum_{i=1}^{n_1} w_{ki} \cdot (V_i \cdot X) \quad (1)$$

$$= \sum_{i=1}^{n_1} w_{ki} \cdot H_i \quad \text{with } k = 1 \dots n_2$$

where, z_k are the n_2 outputs and x_h^0 are the n_0 inputs of the ELM ($x_{n_0}^0$ is a constant input equal to 1), v_{ih} are the weights connecting the input layer to the hidden layer, $g(\cdot)$ is the activation function of the hidden neurons, w_{ki} are the weights connecting the

hidden neurons to the output k , H_i is the output of the hidden neuron i (H_{n_1} is a constant input equal to 1). Equation 1 is written compactly as:

$$Z = W \cdot H \quad (2)$$

where Z is the estimated output matrix:

$$Z = \begin{bmatrix} z_1(1) & \cdots & z_{n_2}(1) \\ \vdots & & \vdots \\ z_1(N) & \cdots & z_{n_2}(N) \end{bmatrix} \quad (3)$$

H is the hidden layer output matrix:

$$H(V_1, \dots, V_{n_1}, X(1), \dots, X(N)) = \begin{bmatrix} g(V_1 \cdot X(1)) & \cdots & g(V_{n_1} \cdot X(1)) \\ \vdots & & \vdots \\ g(V_1 \cdot X(N)) & \cdots & g(V_{n_1} \cdot X(N)) \end{bmatrix} \quad (4)$$

and W the ELM parameters matrix:

$$W = \begin{bmatrix} W_1^T \\ \vdots \\ W_{n_2}^T \end{bmatrix} \quad (5)$$

Different activation functions have been proposed for the hidden nodes (Javed et al. 2014). In this paper, initialization algorithms are tested for ELM regression models. So the classical hyperbolic tangent is chosen.

2.2 ELM learning algorithm

Different learning algorithms have been proposed to determine the parameters of the model. The one used here is summarized as follow (Huang *et al.* 2006):

- The weights v_{ih} and biases b_i^1 connecting the input to the hidden layers are randomly selected.
- Calculate the hidden layer output matrix H by (4). Calculate the ELM parameters by using H^\dagger the Moore-Penrose generalized inverse of matrix H (Huang et al. 2006):

$$W = H^\dagger \cdot Y \quad (6)$$

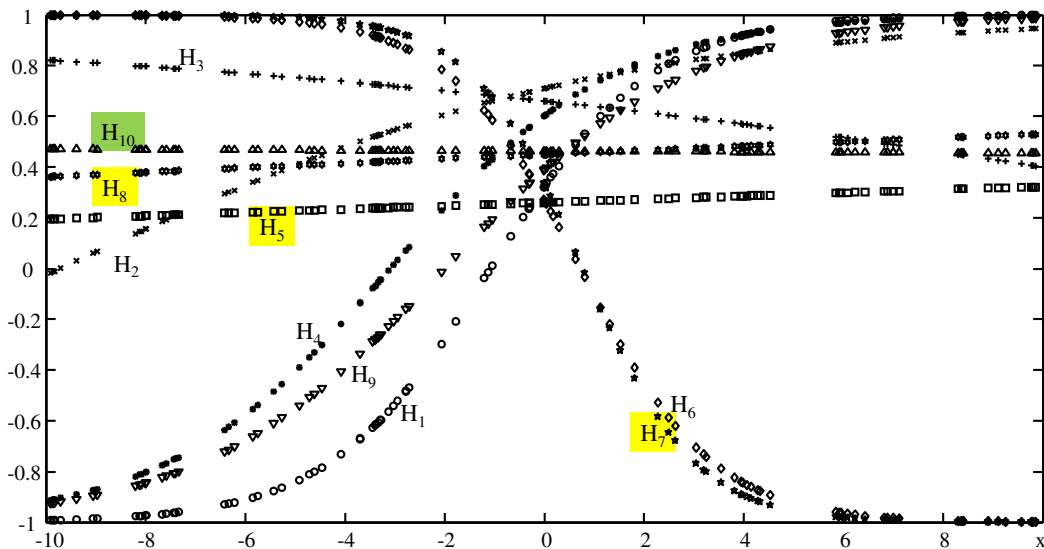


Figure 1: hidden neurons outputs for the “SinC” problem.

Many modification have been proposed to improve accuracy of such learning algorithms as robust ELM (Zhang and Luo 2015), regularized ELM (Deng et al. 2009), incremental (Huang et al. 2006), regularized incremental (Xu et al. 2016).

In this paper, the goal is to test MLP initialization algorithms. So the basic ELM algorithm (Huang et al. 2006) is sufficient here.

2.3 Impact of hidden nodes choice

The classical “SinC” example is used to illustrate the impact of hidden nodes choice:

$$y(x) = \begin{cases} \sin(x)/x & x \neq 0 \\ 1 & x = 0 \end{cases} \quad (7)$$

Two datasets including 1000 pairs (x_n, y_n) each, are built for the learning and the validation. The x_n are uniformly randomly distributed between -10 and 10 and the learning dataset is polluted by a random noise uniformly distributed between -0.2 and 0.2. The ELM includes 10 hidden neurons (plus one hidden node constant and equal to 1). The parameters of these hidden nodes are randomly uniformly distributed between -1 and 1.

Figure 1 presents the output H_i of the 10 hidden nodes for the validation datasets. Five of them require a particular attention: H_5 , H_8 and H_{10} on the one hand, and H_6 and H_7 on the other hand.

First, it appears that H_5 , H_8 and H_{10} are near to be constant on the considered input domain and are not significantly different to the bias node H_{11} . Second,

the outputs H_6 and H_7 seems very similar. So, a cross correlation test is performed on these two outputs and presented figure 2. This correlation test confirms that these two hidden neuron outputs are closely correlated. So, only one of them gives information.

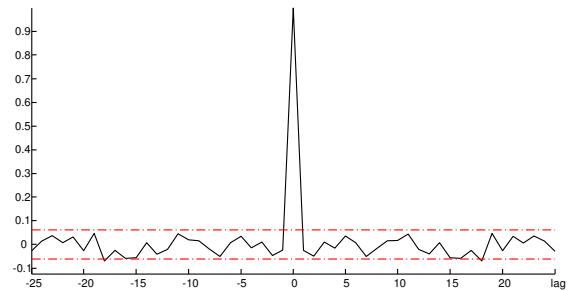


Figure 2: Cross correlation between H_6 and H_7 .

So despite the fact that we include ten hidden nodes in the model, only six of them are really useful. To confirm this fact, the accuracy of two models is compared on the validation dataset. The first ELM model includes all the hidden nodes and the resulting sum squared errors (SSE) is equal to $1.51 \cdot 10^{-4}$. The second ELM model includes only six hidden nodes (H_5 , H_6 , H_8 and H_{10} are discarded). The SSE obtained for this model is $2.23 \cdot 10^{-4}$. The difference between the results obtained is not statistically significant.

This experience shows that even if the parameters are randomly chosen, a lack of diversity may lead to the fact that some of the hidden nodes are useless. To make an analogy with classifiers

ensembles, the accuracy of the ELM depends on the diversity of its individual components (hidden nodes) (Kuncheva and Whitaker 2003). That's why ELM needs a good initialization algorithm in order to improve diversity between the hidden nodes.

3 MLP INITIALISATION ALGORITHMS

Many algorithms have been proposed in the past in order to initialize MLP.

3.1 Random initialization (Ra)

Random initialization has been the first approach to initialize parameters since the pioneering work of Rumelhart and McClelland (1986). This approach is mainly used in ELM approach since the work of Huang *et al.* (2004). This approach consist to uniformly randomly initiate the parameters between $-r$ and r . Initially, nothing is said about the value of r . In this paper, r is tuned to 1 in accordance with settings encountered in the literature (Norgaard 1995, Zhu and Huang 2004). This algorithm will be denoted "Ra" in the sequel.

3.2 Burel initialization (Bu) (Burel 1991)

The arbitrarily setting of r has been discussed in the past and researchers have exploited some information to tune it. Within this philosophy, Burel (1991) searches to give an equivalent influence for each hidden neuron on the model accuracy. To do that, the weights and biases connecting the input to the hidden layers must be tuned such that:

$$\begin{cases} (C1) & E(V_i \cdot X(n)) = 0 & i = 1, \dots, n_1 \\ (C2) & \text{var}(V_i \cdot X(n)) = \sigma_z^2 & i = 1, \dots, n_1 \end{cases} \quad (8)$$

Satisfy the requirement C1 allows to use the full variation of the activation range. C2 serves to control the variation amplitude range. C1 is validated if the two bounds r and $-r$ are symmetrical. To respect C2, r must be tuned to:

$$r = \frac{\sqrt{3\sigma_z^2}}{\sqrt{\sum_{h=1}^{n_0} E((x_h)^2)}} = \frac{0.87}{\sqrt{\sum_{h=1}^{n_0} E((x_h)^2)}} \quad (9)$$

σ_z is tuned to 0.5 because the hyperbolic tangent is nearly linear between -0.5 and 0.5. This

tuning of r implies that this initialisation algorithm requires a complete dataset. This initialization algorithm will be denoted "Bu".

3.3 Drago and Ridella initialization (DR) (Drago and Ridella 1992)

Within the same philosophy as Burel (1991), Drago and Ridella (1992) search to find a good tuning of r .

They tried to control the proportion of samples in the dataset leading to the saturation of the activation function. They defined the "Paralyzed Neuron Percentage" (PNP) which represent the proportion of samples leading to obtain paralyzed neuron(s). They found a relation between this parameter and r :

$$r = \frac{\sqrt{3}}{\text{erf}^{-1}\left(\frac{1}{2} - \frac{\beta}{2} \cdot \text{PNP}\right)} \quad (10)$$

where $1/\beta$ represents the probability that at least one output of the network is incorrect:

$$\frac{1}{\beta} = \left(1 - \frac{1}{2^{N_o}}\right) \quad (11)$$

The goal of this algorithm is to maintain the PNP to a small value. So PNP is tuned to 5% in (10). This initialisation algorithm needs a complete dataset. It will be denoted "DR" in the sequel.

3.4 Nguyen and Widrow initialization (NW) (Nguyen and Widrow 1990)

Nguyen and Widrow (1990) algorithm can be view as a slice linearization. Its goal is to determine parameters such that all hidden nodes represents a linear function on a small interval of the input space.

To do that, the size of the intervals and their localisation in the input space must be determined. The size is controlled by the amplitude of the weights vectors $|V_i| = \left[[v_{i1} \dots v_{in_0-1}] \right]$, $i=1, n_1-1$ (not including biases v_{in_0}) when the localisation is controlled by the biases v_{in_0} of the hidden neurons.

In order to break the symmetry in the network, all the weights and biases are randomly uniformly distributed between -1 and 1. In a second step, the amplitude of the weights vectors $|V_i|$ are adjusted in function of the number of inputs and hidden units:

$$|V_i| = 0.7 * n_1^{1/n_0} \quad (12)$$

Multiplying by 0.7 gives a slight overlapping of the intervals. The localisation of the intervals in the input space is determined by the tuning of the biases of the hidden neurons v_{i_0} . They are uniformly randomly chosen in the range $[-|V_i|, |V_i|]$.

Initially, this algorithm has been designed in order to work with normalised inputs between -1 and 1. In order to work with no normalized inputs, Demuth and Beale (1994) have implemented an improvement of this algorithm in matlab®. To do that, each weight v_{ih} , $i=1, \dots, n_1-1$, and $h = 1, \dots, n_0-1$, are divided by the amplitude of the input h :

$$\alpha_h = \frac{\max(x_h) - \min(x_h)}{2} \quad (13)$$

The centres of the intervals are repositioned in the input space by adding to the biases of the hidden neurons v_{i_0} :

$$\beta_i = \sum_{h=1}^{n_0} v_{hi} \frac{\min(x_h) + \max(x_h)}{2} \quad (14)$$

This algorithm requires to know the amplitude of each input. It will be denoted "NW" in the sequel.

3.5 Chen and Nutter initialization (CN) (Chen and Nutter 1991)

Chen and Nutter (1991) proposed a totally different approach. They tried to estimate the initial parameters of each layers sequentially. The main problem is that the outputs of the hidden neurons are unknown. So Chen and Nutter proposed to initialize the parameters in different stages. First all the parameters are randomly uniformly distributed between -1 and 1. Second, parameters which connect the hidden to the output layers are estimated:

$$W = (H^T \cdot H)^{-1} \cdot H^T \cdot T \quad (15)$$

Third, the desired output T is retro propagated to the hidden neurons:

$$\bar{H} = \begin{cases} T \cdot (W^{-1})^T & \text{if } \text{rank} \left(\begin{bmatrix} W^T & T^T \end{bmatrix} \right) = \\ & \text{rank}(W) = N_h \\ T \cdot (W^T \cdot W)^{-1} \cdot W^T & \text{if } \text{rank} \left(\begin{bmatrix} W^T & T^T \end{bmatrix} \right) = \\ & \text{rank}(W) < N_h \\ T \cdot W^T \cdot (W \cdot W^T)^{-1} & \text{if } \text{rank} \left(\begin{bmatrix} W^T & T^T \end{bmatrix} \right) \neq \\ & \text{rank}(W) \end{cases} \quad (16)$$

The estimated outputs of the hidden neurons are finally obtained by mixing information given by output and by inputs:

$$\hat{H} = H + \lambda \cdot \bar{H} \quad (17)$$

with λ , a parameter chosen randomly between 0 and 1. This estimation of the hidden neurons outputs may lead to values outside the bounds -1, 1. These value must be truncated between -1 and 1.

Fourth, the parameters connecting the input to the hidden layers are estimated:

$$V = \begin{cases} (X^{-1})^T \cdot g_h^{-1}(\hat{H}) & \text{if } \text{rank} \left(\begin{bmatrix} X & g_h^{-1}(\hat{H}) \end{bmatrix} \right) \\ & = \text{rank}(X) = N_i \\ X^T \cdot (X \cdot X^T)^{-1} \cdot g_h^{-1}(\hat{H}) & \text{if } \text{rank} \left(\begin{bmatrix} X & g_h^{-1}(\hat{H}) \end{bmatrix} \right) \\ & = \text{rank}(X) < N_i \\ (X^T \cdot X)^{-1} \cdot X^T \cdot g_h^{-1}(\hat{H}) & \text{if } \text{rank} \left(\begin{bmatrix} X & g_h^{-1}(\hat{H}) \end{bmatrix} \right) \\ & \neq \text{rank}(X) \end{cases} \quad (18)$$

This algorithm needs a complete dataset. It will be denoted "CN".

4 EXPERIMENTAL RESULTS

The five MLP initialisation algorithms are tested in order to initialize ELM model on three regression benchmarks. For each initialization algorithm and for each benchmark, twenty initial parameters sets are built. For each benchmark, the number of hidden neurons is fixed according to the studies of Huang et al. (2006).

4.1 Comparison criterion

The selection criterion used to compare the results obtained is the classical Root Mean Square Error (RMSE):

$$RMSE = \sqrt{\frac{1}{N} \sum_{n=1}^N (t(n) - z(n))^2} \quad (19)$$

However, two values of RMSE may be sufficiently close such that the difference is statistically insignificant. So to compare two ELM models, their residuals populations P_0 and P of mean 0 and of variance σ_0^2 and σ^2 respectively must be compared by using a two tailed hypothesis test in order to determine if σ^2 is statistically different of

σ_0^2 . The null hypothesis \mathcal{H}_0 (the two variance are statistically equal) and its alternative \mathcal{H}_1 are:

$$\begin{cases} \mathcal{H}_0: \sigma^2 = \sigma_0^2 \\ \mathcal{H}_1: \sigma^2 > \sigma_0^2 \\ \sigma^2 < \sigma_0^2 \end{cases} \quad (20)$$

\mathcal{H}_0 is rejected with a risk level of 5% if:

$$\begin{cases} \Gamma = \frac{(N-1) \cdot \sigma^2}{\sigma_0^2} < \Gamma_{c_1} = \chi^2\left(v, \frac{\alpha}{2}\right) \\ \Gamma = \frac{(N-1) \cdot \sigma^2}{\sigma_0^2} > \Gamma_{c_2} = \chi^2\left(v, 1 - \frac{\alpha}{2}\right) \end{cases} \quad (21)$$

where v is the number of degree of freedom, and α is the confidence level.

4.2 Abalone dataset

This abalone dataset is a collection of 4177 samples and the goal is to predict the age (output) of these shells considering eight physical measurements (inputs) (Waugh 1995, UCI 2017). From these 4177 samples, 2000 are used for the learning and 2177 for the validation. The output is normalised between -1 and 1. No normalisation is performed on the inputs.

Table 1 presents the results obtained for all the ELM models.

The first row of table 1 presents the mean computational time for each algorithm. Four of them presents a very short and similar computational time (Bu, DR, NW and Ra). These four algorithms are very simple, when CN performs least square calculus twice.

The six succeeding rows give respectively the min, mean and max values of RMSE on the learning and the validation datasets. The best RMSE value on the learning and validation datasets is given by Bu. For the validation dataset, Ra gives the same optimum. So, Bu and, to a lesser extent Ra, give the best results concerning the RMSE value.

However, it is likely that some of the other results are statistically equal to the best one. The two bounds Γ_{c_1} and Γ_{c_2} of the statistical test (21) are equal to 2050 and 2308 respectively for this example. The last row of table 1 presents the proportion of ELM models which gives a RMSE statistically equivalent to the best one on the validation data set (here best Bu model).

Only three initialisation algorithms (Bu, NW and Ra) are able to give results statistically equivalent to the best one. Among them, NW is the one which maximizes this proportion (30%).

Table 1: Results for the Abalone dataset.

			Bu	CN	DR	NW	Ra
	computational time (s)		0.0016	0.0055	0.0016	0.0016	0.0016
identification	RMSE	min	0.0757	0.0868	0.0791	0.0765	0.0765
		mean	0.0796	0.0906	0.0863	0.0791	0.0801
		max	0.0862	0.0915	0.0926	0.0844	0.0908
validation	RMSE	min	0.0723	0.0833	0.0775	0.0731	0.0723
		mean	0.0769	0.0865	0.084	0.0782	0.0773
		max	0.0829	0.0875	0.0951	0.0936	0.0857
	% Γ		15%	0%	0%	30%	15%

Table 2: Results for the Auto Price dataset.

			Bu	CN	DR	NW	Ra
	computational time (s)		0.0047	0.0039	0.001	0.0023	0.001
identification	RMSE	min	0.07	0.1315	0.0687	0.0773	0.1123
		mean	0.0898	0.1799	0.0827	0.0976	0.1549
		max	0.1228	0.1821	0.1072	0.1211	0.1821
validation	RMSE	min	0.0663	0.1178	0.071	0.0614	0.1
		mean	0.083	0.1494	0.0803	0.0891	0.1499
		max	0.1073	0.1508	0.0964	0.1058	0.1508
	% Γ		10%	0%	15%	20%	0%

Table 3: Results for the CPU dataset.

			Bu	CN	DR	NW	Ra
computational time (s)			0.0008	0.0031	0.008	0.0008	0.0008
identification	RMSE	min	0.0223	0.1058	0.0494	0.0207	0.0944
		mean	0.0272	0.1076	0.0701	0.0263	0.1047
		max	0.0442	0.1077	0.0884	0.0413	0.1071
validation	RMSE	min	0.0494	0.1617	0.081	0.0549	0.1537
		mean	0.1293	0.1643	0.1185	0.0837	0.1622
		max	0.4022	0.1645	0.142	0.1468	0.1774
% Γ			15%	0%	0%	20%	0%

4.3 Auto price dataset

This dataset regroups the price of cars (output) and fifteen of their characteristics (inputs) (Kibler et al. 1989, UCI 2017). The missing values are discarding leading to a dataset comprising 159 samples randomly divided into 80 samples for the learning and 79 for the validation. The output is normalized and all ELM models include five hidden neurons. The results of all the ELM models are presented table 2.

The mean computational time for all algorithms are quite similar.

The best RMSE on the learning dataset is given by DR algorithm. But, for the validation dataset, it is NW which gives the best one.

For the statistical test (21) the two bounds Γ_{c_1} and Γ_{c_2} are equal to 56.3 and 105.5 respectively. The last row presents the proportion of model which give results statistically equivalent to the best one (here best NW model).

This time, the three initialisation algorithm which gives results statistically equivalent to the best one are (Bu, DR and NW). NW is again the one which maximizes chances to find good model (20%).

4.4 CPU dataset

The Computer Hardware dataset problem is to predict the estimated relative performance from the original article (Kibler and Aha 1988, UCI 2017). It comprises 209 samples randomly divided into learning dataset (100 samples) and validation one (109 samples). There are six inputs, and the output is normalized. Each ELM model includes ten hidden neurons.

Table 3 presents the results obtained with the five initialisation algorithms. The computational time for BU, DR NW and Ra are quite similar when the one for CN is greater.

The best RMSE value is given by NW on the learning dataset and by Bu on validation one. Considering the statistical test (21) ($\Gamma_{c_1} = 82$ and $\Gamma_{c_2} = 140$), these two algorithms are the only ones which are able to gives results statistically equivalent to the best one.

5 CONCLUSIONS

This paper presents a study about the impact of hidden nodes choice on the ELM model accuracy. This initialisation problem has been investigated in the MLP context in the past and five initialisation algorithms are recalled before to be tested and compared for the ELM initialisation on three regression benchmarks.

The results obtained shown that two algorithms (Bu and NW) outperform the others in terms of chances to obtain satisfactory results. However, even these algorithms give acceptable results in less than 30% of the cases. This fact implies that performing the learning of ELM model needs to be done on several different initialisation parameters sets.

Our future works will focus on how to improve this initialization step by combining different initialization algorithms, particularly Bu and NW.

Another question concerns the impact of inputs selection on the ELM accuracy. In all the benchmarks used in this study, all the inputs are linked with the output. When it is not the case, the impact of these spurious inputs on the ELM model accuracy must be studied.

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