Application of the Monte Carlo method to estimate the uncertainty in the compressive strength test of high-strength concrete modelled with a multilayer perceptron

Estimación de la incertidumbre de un perceptrón multicapa para la modelización del ensayo de resistencia a compresión del concreto de alta resistencia mediante la aplicación del método de Monte Carlo

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Abstract
The use of artificial neural networks as a modeling tool for the physic-mechanical properties of diverse materials has experienced great advances in the last ten years, mainly due to the increased in computing capacities of computers. This technique has been used in many different fields of science and its effectiveness is sufficiently proven. Its application in the particle board industry complies with the requirements of the test regulations for the use in production control, as an alternative method to normalized one. However, in spite of providing a result with a great approximation, they do not indicate anything about the uncertainty of the result. This last point is crucial when the results have to be compared with a product standard. There are internationally accepted deterministic techniques for obtaining the uncertainty of a test result, always starting from the knowledge of the function that relates the measure with the measurement parameters. However, these techniques are not entirely adequate for the case of excessively complex functions such as an artificial neural network. In these cases, the use of stochastic simulation methods such as the Monte Carlo method is more appropriate. In this article, an artificial neural network will be developed to obtain the compressive strength of high-strength concrete to later obtain the uncertainty by a Monte Carlo simulation.

Key words: Artificial neural network, compressive strength, high-strength concrete, uncertainty, Monte Carlo, GUM.

Resumen
La utilización de las redes neuronales artificiales como herramienta de modelización de las propiedades físico-mecánicas de muy diversos materiales ha experimentado un gran avance en los últimos diez años debido principalmente al incremento de las capacidades de cálculo de los ordenadores. Esta técnica ha sido empleada en muy diversos ámbitos de la ciencia y su efectividad está suficientemente acreditada. Su aplicación en la industria de tableros de partículas cumple con los requisitos de las normativas de ensayo para la utilización en el control de producción de métodos alternativos al normalizado. Sin embargo, pese a proporcionar un resultado con una gran aproximación, no indican nada sobre la incertidumbre de dicho resultado.

Y este último punto es crucial cuando se compara el resultado con la especificación del producto. Existen técnicas deterministas, aceptadas internacionalmente, para la obtención de la incertidumbre de un ensayo, siempre partiendo del conocimiento de la función que relaciona el mensurando con los parámetros de medida. Sin embargo estas técnicas no son del todo adecuadas para el caso de funciones excesivamente complejas como es el caso de una red neuronal artificial. En estos casos es más adecuado la utilización de métodos estocásticos de simulación como el método de Montecarlo. En este artículo se va a desarrollar una red neuronal artificial para la obtención de la resistencia a compresión del concreto para posteriormente obtener la incertidumbre mediante una simulación de Montecarlo.

Palabras clave: Red neuronal artificial, resistencia a compresión, concreto de alta resistencia, incertidumbre, Montecarlo, GUM.

Introduction

In recent years, the development of increasingly powerful computers has contributed to an increase in the use of modeling techniques using artificial neural networks in different areas of research. Various applications from home prices valuation (Nuñez Tabares, Rey Carmona & Caridad y Ocerín, 2013) to engineering (Çanakci, 2007) have benefited from these powerful modeling tools.

These tools provide a substantial improvement over any previously proposed model, regardless of its nature, with the added advantage that they do not need any prior assumption about the statistical structure of data (Khosravi, Nahavandi, Creigton & Atiya, 2011a).

Major advances have been made in industrial process control, mainly because they are capable of modeling complex relations and can adequately predict whether or not the product characteristics are in line with specifications (Sukthomya & Tannock, 2005). They have been widely used to characterize different materials such as cement (Baykasoğ, Delhi & Tanış, 2004), concrete (Bilim, Atiş, Tanyildizi & Karahan, 2009; Sandemir, 2009; Özcan, Atiş, Karahan, Uncuoğlu & Tanyildizi, 2009) and certain metals (Mukherjee, Schmauder & Rühle, 1995; Malinov, Sha & McKeown, 2001; Hassan, Alrashdan, Hayajneh & Mayyas, 2009; Ozerdem & Kolukisa, 2009).

Nevertheless, a neural network itself does not provide any information on confidence intervals or results uncertainty (Khosravi et al., 2011a). This uncertainty is important not only as indicative of measurement process quality, but also provides a confidence interval on results (Solaguren-Beascoa Fernández, Alegre Calderón & Bravo Díez, 2009).

According to the international accepted definition, the uncertainty associated with a measurement can be defined as the square root of the variance of its probability density function. In this context, the Guide to the Expression of Uncertainty in Measurement (GUM) (BIMP, IEC, IFCC, ISO, IUPAC & OILM, 1995) indicates a method to obtain the uncertainty on a measurement from the input parameters values and their probability distributions. In most cases, the measurand is derived from a direct measurement, it is not difficult to assess its uncertainty. However, sometimes the measurand is defined as a function of the input values. In these cases, the uncertainty on the measurand can be obtained by the law of propagation of the variances (BIMP et. al, 1995).The use of this methodology implies a knowledge of the function relating the input parameters with the measurand. This is difficult when the model is derived through the numerical solution, for example, in case of models defined by differential equations (Esward, Ginestous, Harris & Hill, 2007) or when the model is excessively complex and nonlinear, i.e. in the case of an artificial neural network. In these cases, as well in the case of dominant contribution from a non-normal distribution function or when the distribution function of the measurand is asymmetric, an evaluation of the output uncertainty based on the law of propagation of uncertainty will provide values not entirely reliable (Esward et al., 2007).

To solve these problems, the Working Group 1 of the Joint Commitee for Guides in Metrology (JCGM) prepared a supplement to the GUM describing how to obtain the uncertainty on the measured through simulation by the Monte Carlo method (JGCM, 2008). This methodology is generally valid for a larger group of situations than the GUM (Müller et al., 2008).

This article develops a new methodology, based on the simulation by the Monte Carlo method as described in Supplement 1 of the GUM (JGCM, 2008), to evaluate the output uncertainty of a multilayer perceptron used to model the testing for compressive strength of high-strength concrete according to ASTM C 39 / C 39M (ASTM, 2001) with different curing times.

The multilayer perceptron is a type of network widely used to study the mechanical properties of different construction materials, not only cement (Sarıdemir, 2009; Özcan et al., 2009), but also basalt (Çanakci, 2007), various metals (Ozerdem & Kolukisa, 2009; Reddy, Krishnaiah, Hong & Lee, 2009) or wood-based panels (Cook & Chiu, 1997). In all cases, results indicate very good correlations between actual values and those simulated by the neural network. However, none of these studies provide any information on the uncertainty on the network output values.

High-strength concrete

This study used 1054 specimens of high-strength concrete made with different types and amounts of cement, sand, coarse aggregate and water. The specimens for compression testing were made according to ASTM standard C 192 / C 192M (ASTM, 2000). Compression tests were carried out according to ASTM standard C39 / C 39M (ASTM, 2001) after different curing times.

Axial compression tests were carried out on a Toni Technik machine with a 3000KN cell and a Tinius Olsen machine with a 1500KN cell (A). Following the results of similar studies (Torre, García, Moromi, Espinoza & Acuña, 2015; Acuña, Torre, Moromi & García, 2014), the explanatory variables chosen to model the compressive strength of concrete were: curing time; type, amount and percentage of additive; type, amount and percentage of microsilica; amounts of water, coarse aggregate, sand and cement; the nominal maximum coarse aggregate size; specific weights of sand and coarse aggregate; and the water-cement ratio.

The Table 1 shows the instruments used for testing, as well as their range of measurement and uncertainty.

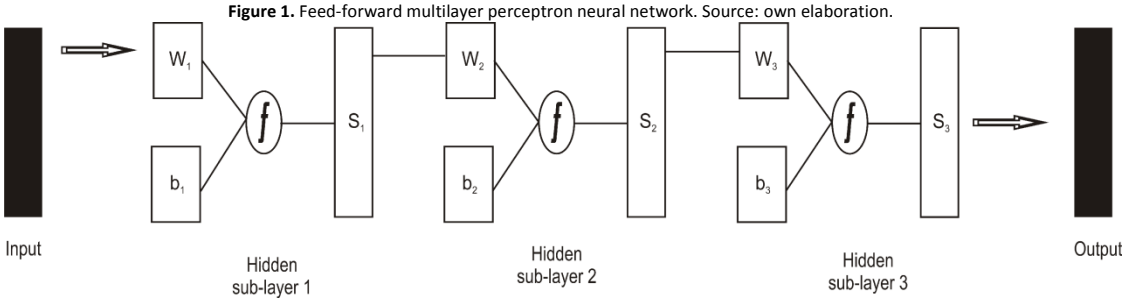
Table 1. Instruments used for variables measurements. Source: own elaboration.

Instrument	Uncertainty
Sieve3/4"	0.05 mm
Sieve1”	0.04 mm
Scale 0-100 kg	0.02 kg
Scale 0-21000 g	2.5 g
Vernier0-300 mm	$5 \cdot 10^{-3}$ mm

Multilayer perceptron

The multilayer perceptron (Figure 1) could be defined as a computing system that imitates the computational capabilities of biological systems by using a large number of interconnected elements. Its characteristics as a universal approach function (Hornik, 1989) allows the modeling of complex nonlinear relationships.

Figure 1. Feed-forward multilayer perceptron neural network. Source: own elaboration.



To design a multilayer perceptron is a slow and complex process. There are no fixed rules to establish the internal structure of the network. However, there are a number of recommendations available regarding its design, based on the quantity of available data (Sha, 2007), or on the most desirable type of configuration (Vanstone & Finnie, 2009). There are as well a number of conditions that must be met to ensure that the network will perform properly, especially concerning the avoidance of overfitting (Bishop, 1995).

To avoid overfitting and to evaluate the reliability of the network, the initial dataset was randomly divided into three subsets: the training, validation and testing subsets. The first two were used for the training phase and for the prevention of overfitting, respectively. The third subset was used to assess the level of reliability of the network (Bishop, 1995).

The sigmoid hyperbolic tangent (Eq. 1) was used as a transfer function; it is mathematically equivalent to the hyperbolic tangent, but improves the network performance (Demuth, Beale & Hagan, 2002).

$$f(x) = \frac{2}{1 + e^{(-2x)}} - 1 \quad (1)$$

where:
f(x): neuron output value.
x: neuron input value.
The values of all variables, both dependent and independent, were normalized to avoid large values of x, for which the derivative of f(x) is close to zero. This permits a higher effectiveness of the transfer function (Eq. 2) (Demuth, Beale & Hagan, 2002).

$$X' = \frac{X - X_{min}}{X_{max} - X_{min}} \quad (2)$$

where:
X':value after normalization of vector X.
X_{min} y X_{max}: maximum and minimum values of vector X.

The training algorithm used was the resilient backpropagation, which greatly improves the results with sigmoidal transfer functions (Demuth, Beale & Hagan, 2002).

Modeling with artificial neural networks can provide output values which closely approximate to the experimental values obtained in laboratory, but it cannot provide an estimation of the uncertainty associated with the output value. This uncertainty is the result, on one hand, of the simplification of the phenomenon by modeling mathematically; and on the other hand, of the variability and noise which are inherent in the input values (Mazloumi, Rose, Currie & Moridpour, 2011).

Various studies have been undertaken to obtain confidence intervals, but always in particular cases, such as perceptrons with only one hidden layer, with normal distributions of the input variables, or with the assumption of normality of the output errors (Khosravi et, al, 2011a; Papadopoulos, Edwards & Murray, 2001; Chryssolouris, 1996). These particular cases do not cover the whole field of development of neural networks since they do not consider cases for which the perceptron has more hidden layers (Figure 1) or another type of network.

Calculation of test uncertainty

The GUM (BIMP et al., 1995) includes a series of international recognized recommendations to evaluate the uncertainty on measurement results. It introduces in particular the law of propagation of uncertainty to obtain the uncertainty on a measurement from the uncertainties of variables involved in the process:

If $y = f(x_1, x_2, \ldots x_n)$ is the function that determines the final value of the measurement result and x_i $(i = 1, \ldots, p)$ are all variables that influence the measurement result, the law of propagation of uncertainty specifies that the combined uncertainty (u^2_y) of the final value of the result is defined by (Eq. 3):

$$u_y^2 = \left(\frac{\partial y}{\partial x_1}\right)^2 u_{x_1}^2 + \left(\frac{\partial y}{\partial x_2}\right)^2 \cdot u_{x_2}^2 + \ldots\ldots + \left(\frac{\partial y}{\partial x_j}\right)^2 \cdot u_{x_j}^2 + \left(\frac{\partial y}{\partial x_p}\right)^2 \cdot u_{x_p}^2 + \ldots\ldots$$
$$+ 2 \cdot \left(\frac{\partial y}{\partial x_1}\right) \cdot \left(\frac{\partial y}{\partial x_2}\right) \cdot u_{x_1} \cdot u_{x_2} \cdot \gamma(x_1, x_2) + \ldots\ldots + 2 \cdot \left(\frac{\partial y}{\partial x_i}\right) \cdot \left(\frac{\partial y}{\partial x_j}\right) \cdot u_{x_i} \cdot u_{x_j} \cdot \gamma(x_i, x_j) + \ldots\ldots \quad (3)$$
$$+ 2 \cdot \left(\frac{\partial y}{\partial x_{p-1}}\right) \cdot \left(\frac{\partial y}{\partial x_p}\right) \cdot u_{x_{p-1}} \cdot u_{x_p} \cdot \gamma(x_{p-1}, x_p)$$

where:
u^2_y: combined test uncertainty
x_i: variables influencing the measurement
u_{xi}: measurement uncertainty of variable x_i.

y=f(x): function relating the measurements with the measurand
$\gamma(x_i, x_j)$: correlation coefficients between variables.

Correlation coefficients between the different variables involved in the process, $\gamma(x_i, x_j)$, represent the possible influence that may have one measurement with one instrument, over another measurement performed later with the same instrument or a different one.

The adaptive Monte Carlo method

The GUM (BIMP et al., 1995) attempts to cover a variety of different situations that can occur during the measurement process. However, in many cases, such as the non-normality of a key input variable, or the complexity of the function relating input and output variables, or the lack of normality of the output errors, using the law of propagation of uncertainty can provide unreliable results (Esward et al., 2007).

The Supplement 1 to the GUM (JGCM, 2008) describes a numerical method based on Monte Carlo simulation to calculate this uncertainty. The number of simulations will depend on the degree of confidence desired for the results. As general rule, 10^6 simulations are usually required to obtain 95% confidence intervals (JGCM, 2008).

However several factors, such as the nature and type of distribution of the input data, the model function, or the nature itself of output values *Y*, can influence the required number of simulations.

The adaptive Monte Carlo method described in section 7.9 of Supplement 1 (JGCM, 2008) solves this problem by determining the number of simulations through an iterative method based on the desired level of precision for the uncertainty and the required confidence interval:

Let δ be the acceptance factor, function of the required accuracy (Eq. 4):

$$\delta = \frac{10^{-n}}{2} \quad (4)$$

where:
n: required number of significant digits.
δ: numerical tolerance factor.

Let *M* be the number of data for each simulation, function of the required coverage factor (Eq. 5):

$$M = Max\ (10^4,\ J) \quad (5)$$

where:
J: rounding down of 100/(1-q).
q: coverage probability required.
M: number of Monte Carlo trials.

1. Let the parameter *h = 1* be the number of times to repeat the process till the numerical tolerance factor is reached.
2. Randomly the set $X\ (x_1, x_2 \ldots x_m)$ of *M* data is generated, to obtain a matrix of dimension (p x M), where *p* is the dimension of the input vector (number of input variables) and *M* the parameter is calculated above. (A)
3. The simulation sequence *h* of the model is carried out for the M data (Eq. 6).

$$Y = f(X) \quad \Rightarrow \quad y_i = f(x_i) \quad (6)$$

where:
Y: output vector.
X: input vector.
f: model function.

4. Starting from $y_i(i=1\ldots M)$, compute for each simulation sequence *h*:

a. Mean $y^{(h)}$ (Eq. 7).

$$y^{(h)} = \frac{1}{M}\sum_{1}^{M} y_i \tag{7}$$

where:
M: number of Monte Carlo trials.
$y^{(h)}$: mean of each simulation.

b. Uncertainty $u(y^{(h)})$, computed like the standard deviation (Eq. 8).

$$u(y^{(h)}) = \sqrt{\frac{1}{M-1}\sum_{1}^{M} (y_i - y^{(h)})} \tag{8}$$

where:
M: number of Monte Carlo trials.
$y^{(h)}$: mean of each simulation.
$u(y^{(h)})$: uncertainty associated with each $y^{(h)}$.

5. If $h=1$, increase it by 1 and return to step 4.

6. After each simulation sequence, calculate:
a. Mean and standard deviation of $y^{(h)}$(Eq. 9).

$$\hat{y} = \frac{1}{h}\sum_{1}^{h} y^{(i)}$$
$$s_{\hat{y}} = \sqrt{\frac{1}{h\cdot(h-1)}\sum_{1}^{h} (y^{(i)} - \hat{y})^2} \tag{9}$$

where:
h: number of simulation trials.
$y^{(i)}$: mean of each simulation trial.
$\hat{y}$: mean of all the simulation trials.
$S_{\hat{y}}$: standard deviation of the simulation trials.

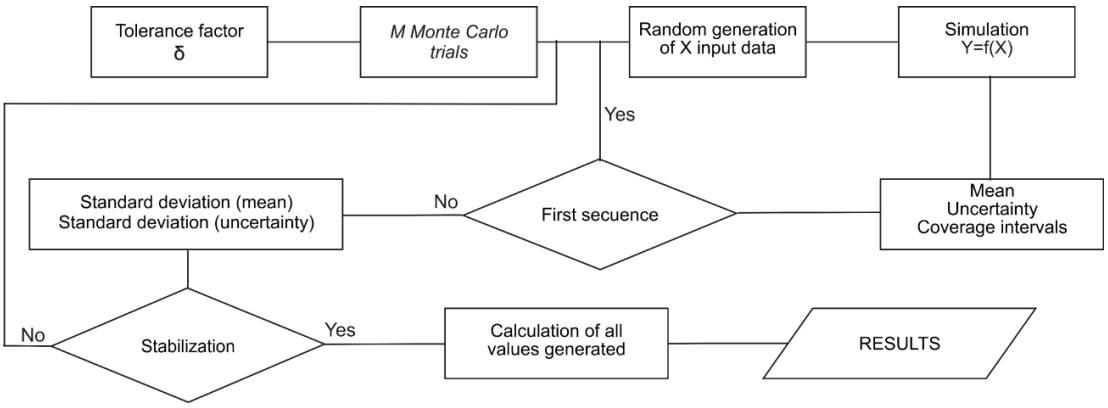
b. Mean and standard deviation of $u(y^{(h)})$(Eq. 10).

$$\hat{u}(y) = \frac{1}{h}\sum_{1}^{h} u(y^{(i)})$$
$$s_{u(y)} = \sqrt{\frac{1}{h\cdot(h-1)}\sum_{1}^{h} (u(y^{(i)}) - \hat{u}(y))^2} \tag{10}$$

where:
h: number of simulation trials.
$y^{(i)}$: mean of each simulation trial.
$u(y^{(i)})$: uncertainty associated with each simulation $y^{(i)}$.
$\hat{u}(y)$: meanof the uncertainties associated witheachsimulation.
$s_{\hat{u}(y)}$: standard deviation of the uncertainties associated with each simulation.

7. If any of the values of $2\cdot S_{\hat{y}}$ or $2\cdot S_{u(\hat{y})}$ is larger than δ, increase h by 1 and return to step 4.
The following graph (Figure 2) describes the entire process for estimating the uncertainty of the output data in a multilayer perceptron.

Figure 2. Flowchart for the adaptive Monte Carlo method. Source: own elaboration



The evaluation of the confidence intervals quality is done with the prediction intervals coverage probability (PICP) (Khosravi et. al, 2011a; Khosravi et al. 2011a; Mazloumi et al., 2011) (Eq. 11) which measures the number of experimental data included within the confidence interval. This measure is a good indicator of the quality of the obtained confidence intervals (Khosravi et al., 2011b).

$$PICP\ (\%) = 100 \cdot \frac{1}{n_{test}} \sum_{1}^{n_{test}} c_i$$

$$c_i = \begin{cases} 1 & t_i \in [L_i, U_i] \\ 0 & t_i \notin (L_i, U_i) \end{cases} \qquad (11)$$

where:
n_{test}: number of experimental data.
L_i y U_i: lower and upper limits of the confidence intervals of the i-th value.
t_i:i-thexperimental value.
According to (Mazloumi et al., 2011) and (Khosravi et al., 2010), the PICP is expected to exceed 95%.
All calculations were done with a specific computer program developed in MATLAB.

Results

Uncertainties on the input variables

Uncertainties on the input and output variables were obtained from the test data calculated according to the propagation of uncertainty Theorem (Eq. 3).

The values obtained for each one of the input parameters and their uncertainties are shown in the following Tables 2 and 3. Those uncertainties are obtained from the calibration certificates of the instruments (Table 1) combined with the heterogeneity uncertainty from the variability of variables.

Table 2. Input variables for the neural networl model. Source: own elaboration.

Variable	Mean	Standard deviation	Minimum	Maximum	Uncertainty
Curing time (days)	43.2	30.3	7	91	0.04
Additive (%)	2.0	0.35	1.6	2.5	$1.2 \cdot 10^{-2}$
Additive (kg/m^3)	12.7	3.8	8.5	18.6	0.7
Microsilica (%)	7.5	2.0	5.0	10.0	$6.6 \cdot 10^{-2}$
Microsilica (kg/m^3)	48.1	15.0	26.6	74.6	0.8
Water / cement ratio (A)	0.3	0.04	0.25	0.35	$1.5 \cdot 10^{-3}$
Cement (kg/m^3)	586.7	80.0	479.3	708.3	2.6
Nominal maximum Aggregate size (“)	1	0.06	0.75	1	$2.2 \cdot 10^{-3}$
Sand (kg/m^3)	423.7	93.3	282.5	546.9	2.9

Table 3. Input constants for the neural networl model. Source: own elaboration.

Parameter	Value	Uncertainty
Water (L/m^3)	186.4	0.7

Specific weight of sand (Ton/m^3)	2.7	$8.1 \cdot 10^{-4}$
Coarse aggregate (kg/m^3)	1006.2	0.7
Specific weight of coarse aggregate (Ton/m^3)	2.7	$8.1 \cdot 10^{-4}$

Artificial neural network

The optimal architecture for a multilayer perceptron consists of an input layer of 15 variables, two hidden layers with 6 and 1 neuron each and an output of one variable. The results of the training, validation and testing processes can be seen in the Table 4.

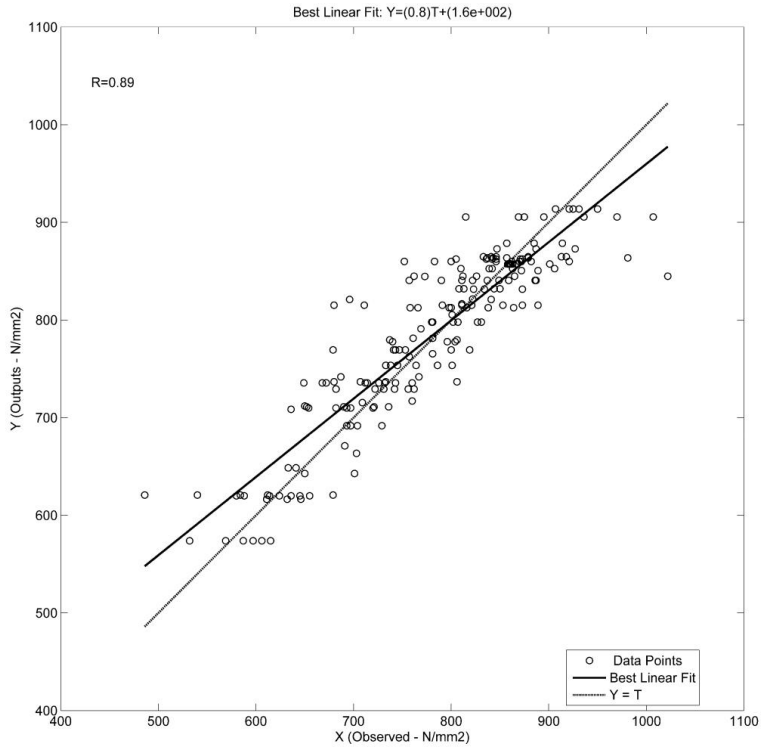
T**able 4.** Result of the artificial neural network design. Source: own elaboration.

Phase	Structure	R^2	R	Error (%)
Training		0.81	0.90	4.3
Validation	[15 6 1 1]	0.81	0.90	4.2
Testing		0.80	0.89	4.2

R and R^2 are de correlation coefficients between experimental data (targets) and simulated data by the neural network (outputs).

Figure 3 shows the correlations between the experimental data and the network results for the testing phase.

Figure 3. Correlation between observed and predicted values for the testing set. Source: own elaboration.



The coefficient of determination of the testing set (Table 4) is 0.80, indicating that the model is able to explain 80% of the samples variability.

The Table 5 reflects the study of the differences between the experimental values and those obtained by the network for the testing set.

Table 5. ANOVA table comparing experimental results with those obtained by the artificial neural network for the testing set. Source: own elaboration.

Source	SS	d.f.	MS	F	P-value
Columns	1267.2	1	1267.2	0.14	0.7
Error	3445489.8	394	8744.9		
Total	3446756.0	395			

SS: sums of squares, d.f.: degrees of freedom, MS: mean squares (SS/d.f.), F: Fisher statistic, P-value: p-value for F.

Since p-value is greater than 0.05, there are no significant differences between the experimental values and those obtained by the artificial neural network, at 95% significance level.

Simulation of the uncertainty through Monte Carlo simulation

Uncertainty results obtained through the Monte Carlo simulation on the training, validation and testing data sets are shown in the Table 6.

Table 6. PICP for all the data sets. Source: own elaboration.

Set	PICP (%)
Training	98.3
Validation	98.2
Testing	97.8

Discussion

The results obtained with the neural network are within the range of values obtained in other studies of modeling concrete properties. The results obtained with correlation coefficients between 0.90 and 0.91 are consistent with those obtained by other authors (Lee, 2003; Oztas, Pala, Ozbay, Kanka, Caglar & Bhatti, 2006; Ukrainczyk & Ukrainczyk, 2008; Ozerdem & Kolukisa, 2009; Prasad, Eskandari & Reddy, 2009; Yaprak, Karaci & Demir, 2013), who obtained correlation coefficients between 0.81 and 0.98.

Similarly, the determination coefficients (R^2 = 0.80 and R^2 = 0.81) are higher than those reported by Yeh (1998) and similar to those by Ozturan, Kutlu & Ozturan (2008), who obtained maximum coefficients of 0.78.

The values obtained for PICP are about 98% (Table 6) indicating that nearly all the experimental data are included within the confidence interval. These values for the PICP are above 95% level indicated by Mazloumi et al. (2011) and are within ranges obtained by Mazloumi et al. (2011), Khosravi et al. (2011a) or Khosravi et al. (2011b), who obtained confidence intervals between 75% and 100%, depending on the method used for the simulation.

Our result obtained is better than the result reported in a study of confidence intervals for the forecasts in energy markets (Khosravi et al., 2010), where PICP between 92.6% and 94.1% were obtained.

The result is also superior to the one obtained by Shrivastava & Panigrahi (2013) on a study of confidence intervals for the demand prediction in the electricity market, which obtained a PICP between 50% and 100%.

It is also higher than results reported by Wan et al. (2014), with 95% of coverage factor, obtained a PICP between 89.6% and 99.6%, depending on the modeling method. And it is consistent with the results of Khosravi & Nahavandi (2014), with obtained PICP values over 95% with more than 50 simulations.

Conclusions

An artificial neural network has been obtained with a confidence level such that could be used as an alternative to the standard method to predict results of compressive strength of high-strength concrete.

Monte Carlo method has been used to obtain the uncertainty on the output values of an artificial neural network, resulting in confidence level similar to those of other studies.

Therefore, these results have proven the validity of using the Monte Carlo method to simulate the uncertainty in compressive strength values obtained with an artificial neural network.

The possibility of using artificial neural networks is opened for in-factory control of compressive strength, since the uncertainty associated with the test permits the evaluation of the degree of compliance / non-compliance with a specification when the results are close to the specification limits.

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