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Mechanical performance prediction of asphalt mixtures: a baseline study of linear and non-linear regression compared with neural network modeling

Przewidywanie właściwości mechanicznych mieszanek mineralno-asfaltowych: badanie modelowania sieciami neuronowymi w porównaniu z metodami referencyjnymi regresji liniowej i nieliniowej

Abstract: Accurate predictions of asphalt mixtures' mechanical performance are crucial to improve the conventional mix-design procedures and to optimize both pavements' performance and service life. This research explores this issue by means of a comparative analysis between different modeling approaches: conventional regressions, both linear and non-linear, and artificial neural networks. The former are widely used but may lack the flexibility to capture complex relationships between testing conditions and the corresponding mechanical behavior. The latter represent promising alternatives due to their capability to successfully model non-linear interactions between variables. This research compares the predictive accuracy of these different modeling approaches using experimental data resulting from 4-point bending tests carried out under several temperatures and loading frequencies. The outcomes suggest that neural networks outperform conventional regression models in capturing complex relationships, highlighting the strengths and limitations of each modeling approach and providing insights for selecting optimal models in road pavement engineering applications.

Keywords: artificial neural networks, asphalt mixtures, linear regression, machine learning; mechanical behaviour; non-linear regression.

Streszczenie: Dokładne przewidywanie właściwości mechanicznych mieszanek mineralno-asfaltowych jest kluczowe w doskonaleniu konwencjonalnych procedur projektowania mieszanek oraz optymalizacji ich właściwości i trwałości nawierzchni. Niniejsze badania dotyczą pogłębionej analizy tego zagadnienia z wykorzystaniem analizy porównawczej dwóch różnych podejść do modelowania: konwencjonalnymi metodami regresji liniowej i nieliniowej oraz metodą sztucznych sieci neuronowych. Pierwsze podejście z konwencjonalnymi metodami regresyjnymi jest szeroko stosowane, ale może mieć pewne ograniczenia co do zastosowania, szczególnie tam, gdzie należy uwzględnić złożone zależności między warunkami badania, a odpowiadającymi im wyjściowymi właściwościami mechanicznymi. Drugie podejście stanowi obiecującą alternatywę, ze względu na przydatność sztucznych sieci neuronowych w modelowaniu nieliniowych interakcji między zmiennymi. Niniejsze badania porównują dokładność przewidywania różnymi metodami predykcyjnymi właściwości mechanicznych mieszanek mineralno-asfaltowych, wykorzystując dane eksperymentalne uzyskane w badaniu cztero-punktowego zginania przeprowadzonych w różnych temperaturach i częstotliwościach obciążenia. Wyniki analiz wskazują na przewagę sieci neuronowych nad konwencjonalnymi metodami modeli regresyjnych ze względu na złożoność analizowanych zależności. Dodatkowymi efektami przeprowadzonych badań jest wskazanie mocnych i słabych strony każdego podejścia do modelowania oraz praktyczne rekomendacje dotyczące wyboru optymalnych modeli do zastosowania w praktyce inżynierskiej budownictwa drogowego.

Słowa kluczowe: sztuczne sieci neuronowe, mieszanka mineralno-asfaltowa, regresja liniowa, uczenie maszynowe, właściwości mechaniczne, regresja nieliniowa.

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1. INTRODUCTION

To determine if a designed asphalt mixture can be considered suitable for road pavement applications, its mechanical behavior needs to be evaluated in terms of some performance parameters [1, 2]. One of the most crucial is represented by the stiffness modulus, whose experimental determination involves the use of expensive laboratory facilities, quite complex investigations, and trained technicians capable of strictly following the required protocols [3, 4]. Recently, the academic community has tried to develop predictive models for the determination of such performance parameters, both with physically based constitutive equations and with non-physically based data-driven procedures. The former rely on materials mechanics equations, whereas the latter rely on soft-computing techniques that do not depend on the specific phenomena investigated [5-13]. According to the quality of the starting dataset, its variability, and the specific goal of the analysis, scientific literature provides many alternative soft-computing techniques to approach different phenomena [14-18]. Focusing in particular on pavement engineering, many studies can be found within scientific literature demonstrating the feasibility of accurately predicting physical-mechanical parameters of asphalt mixtures for road pavement purposes by means of data-driven methodologies [19-21].

To provide some case studies as examples, Pattanaik et al. [22] introduced a ridge regression model for the prediction of the abrasion loss parameter in mixtures containing electric arc furnace steel slags; Tiwari et al. [23] similarly designed a predictive model based on decision tree architectures to predict several parameters related to the mechanical behavior of different asphalt mixtures for roadway applications; thereafter, Wang et al. [24] developed artificial neural networks and other machine learning algorithms aimed at predicting complex modulus and phase angle parameters to describe the viscoelastic behavior of asphalt mixtures.

Therefore, the main goal of the present study was to verify the feasibility of predicting the stiffness modulus of two different asphalt mixtures by means of different data-driven methodologies in order to characterize their mechanical behavior. In particular, conventional linear regression techniques, nonlinear polynomial regression techniques and the modern artificial neural network methodologies were investigated in order to identify the most suitable model to perform this task.

The dataset used to train, validate, and test the developed models is the result of a 4-point bending test laboratory investigation that was performed on two different asphalt mixtures prepared with spilite aggregate, limestone filler, and a traditional bitumen. These mixtures were tested for several combinations of temperatures and loading frequencies that were considered representative of both winter and summer conditions, along with both low- and fast-moving traffic.

The outcomes highlighted that all the designed data-driven machine learning methodologies proved to achieve satisfactory results, demonstrating their capability to successfully model the interactions between the considered variables. However, the artificial neural networks outperformed their competitor models, achieving the best parameters both in terms of the smallest error metrics and the highest correlation coefficients between the predicted and the experimentally observed values.

The structure of the paper is organized as follows: section 2 provides a detailed description of the experimental investigation, and the computational framework needed to develop the predictive models; section 3 describes the results obtained during modeling operations, comparing the performance achieved by each developed model; finally, the main conclusions are summarized in section 4, outlining interesting future developments.

2. MATERIALS AND METHODS

2.1. EXPERIMENTAL DATA

Two alternative asphalt mixtures are investigated within the present study. They were prepared with spilite aggregate having different nominal maximum aggregate size *NMAS*: one was designed for binder layer and had *NMAS* equal to 16 mm, whereas the other was designed for base layer and had *NMAS* equal to 22 mm. Both mixtures were prepared using limestone filler and a conventional bitumen that met the requirements provided by the EN 12591 [25] specifications. It was characterized by a penetration at 25°C equal to 59 mm/10, a softening point of 50.6°C, and a breaking point after Fraas of –11°C. After short-term ageing, the bitumen showed a remaining penetration of 41% and a softening point of 54.2°C.

Mix design was carried out following the specifications set within CSN 73 6121 [26], and the particle size curves along with their requirements have been described in Fig. 1. Both mixtures were also characterized from a volumetric point of view in terms of binder content, air voids, bulk density, moisture susceptibility, and IT-CY stiffness at 15°C: the results in terms of *NMAS* 16 and *NMAS* 22 mixtures resulted equal to 4.5% and 4.2%, to 5.2% and 5.3%, to 2.417 g/cm^3 and 2.421 g/cm^3, to 84% and 81%, and to 7537 MPa and 8257 MPa, respectively.

The Annex B of EN 12697-26 [27] provided all the detailed information about the apparatus and the methodology that were followed to carry out an extensive 4-point bending test experimental campaign.

Since regulations do not provide frequency or temperature values that need to be tested, stiffness modulus results were evaluated at conditions that were truly representative of the several conditions a road pavement is exposed to, i.e., winter and summer temperatures as well as low- and fast-moving traffic. As shown in Fig. 2, testing temperatures ranged from 0°C to 30°C, whereas loading frequences ranged from 0.1 Hz to 50 Hz, resulting in 99 observations of stiffness moduli that increased as loading frequency increased and decreased as testing temperature increased, ranging from 1222 MPa to 24133 MPa.

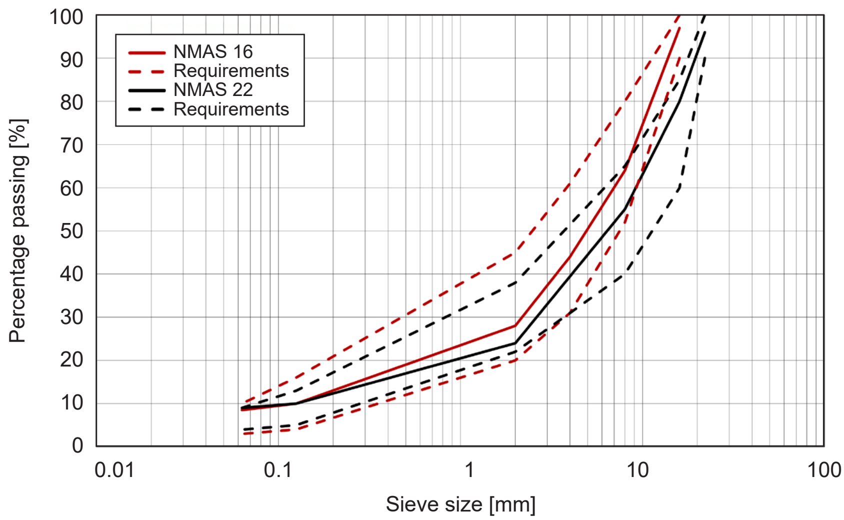

Fig. 1. Particle size curves of the two mixtures and CSN 73 6121 requirements

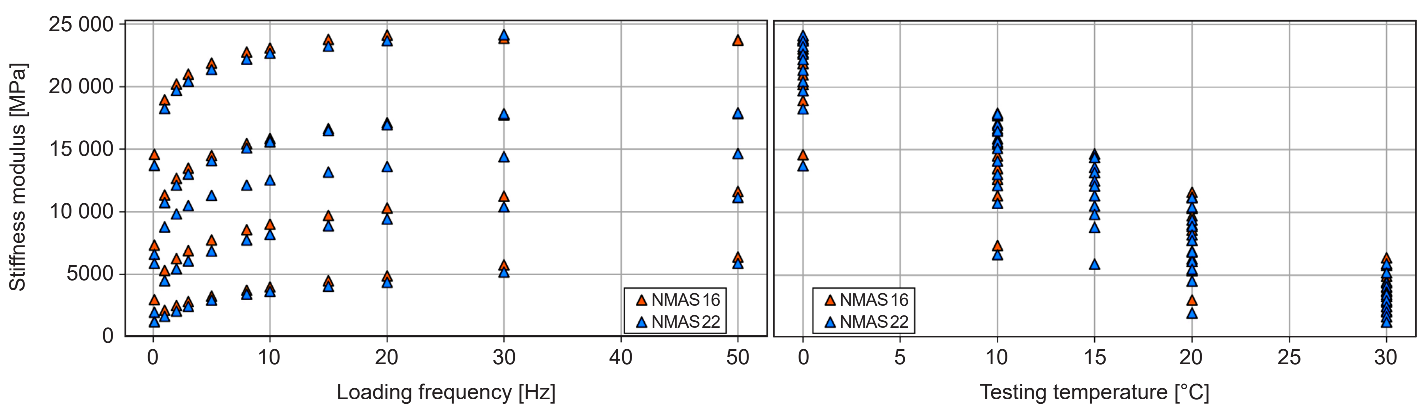

Fig. 2. Graphical representation of the observed stiffness modulus values

The following modeling operations will have as their main objective the development of accurate regression models capable of predicting the stiffness modulus dependent variable as a function of frequency and temperature independent variables, along with a categorical variable that was useful to distinguish between the two prepared mixtures. This approach could allow a comprehensive mechanical characterization of the two investigated mixtures, with the predicted stiffness values that could be easily integrated into conventional mix design operations.

2.2. COMPUTATIONAL FRAMEWORK

A statistical method conventionally used to model the relationship between a dependent variable and one or more independent variables is known as linear regression. In its simplest form, linear regression involves a predicted variable:

$$\hat{y} = \beta_0 + \beta_1 x \,, \tag{1}$$

where: $\hat{y}$ represents the predicted dependent variable, x is the independent variable, β_0 is the intercept, and β_1 is the slope coefficient. The difference between the observed (y) and the predicted $\hat{y}$ values is usually denoted as ε, and it represents the error. The main goal of a linear regression model is to find the best-fitting straight line by minimizing the sum of squared differences between observed and predicted values [28]. This method is known as Ordinary Least Squares (OLS), and it can be extended to multiple linear regression for multiple independent variables, whereas each variable contributes a coefficient indicating its individual impact on the target variable [29]:

$$\hat{y} = \beta_0 + \sum_{i=1}^{n} \beta_1 x_i \,. \tag{2}$$

Considering a dataset of m independent observations, the main goal of the multiple regression becomes the minimization of the so-called residual sum of squares RSS:

$$RSS = \sum_{j=1}^{m} (\beta_0 + \sum_{i=1}^{n} \beta_i x_{i,j} - y_i)^2 \,. \tag{3}$$

The simplicity and the interpretability of Linear Regression make this method widely applicable, although few improvements have been developed over the years, namely ridge and lasso regularization techniques [30]. Both methods add a penalty term to the standard linear regression's loss function, helping to prevent overfitting and improving model's generalization capabilities on new data. In particular, ridge regression (RR) introduces an L2 penalty term to the loss function, representing the sum of the squared coefficients:

$$\text{Loss function}_{\text{RR}} + \alpha \sum_{j=1}^{m} \beta_j^2 \,. \tag{4}$$

This term forces the model to reduce the regression coefficients toward zero, and the regularization strength is determined by a hyperparameter α that controls the trade-off between model complexity and training data fitting [30]. On the other hand, lasso regression (LR) introduces an L1 penalty term to the loss function, representing the sum of the absolute values of the coefficients:

$$\text{Loss function}_{\text{LR}} = RSS + \alpha \sum_{j=1}^{m} \left| \beta_j \right| \,. \tag{5}$$

This regularization allows some coefficients to become exactly zero, thus effectively performing a feature selection if needed [30]. Also in this case, the regularization strength is determined by the hyperparameter α.

An alternative approach suitable to capture the nonlinear interactions between data consists of multi-nonlinear polynomial regression [31], frequently used to model complex relationships between a dependent variable and multiple independent variables by fitting a polynomial equation of varying degrees. The predicted target variable can be represented as follows:

$$\hat{y} = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{12} x_1 x_2 + \beta_{22} x_2^2 + \ldots + \beta_n x_n^k \,, \tag{6}$$

where: $\hat{y}$ is the target variable, $x_1, x_2, \ldots, x_n$ are the independent variables, $\beta_0, \beta_1, \ldots, \beta_n$ are the model coefficients, and k represents the polynomial degree. This approach provides a higher flexibility in accurately fitting complex datasets by adjusting the polynomial degree and introducing interaction terms [31].

The recent introduction of the artificial neuron notion and the subsequent neural networks provided a different approach to address regression problems on the basis of data-driven machine learning algorithms [32]. Unlike conventional regression methodologies that rely on the described mathematical equations, artificial neural networks (ANN) employ input, hidden, and output layers of interconnected neurons to model complex relationships between inputs and outputs. This functioning is inspired by that of the biological human brain and allows complex patterns to be learnt as a result of a training process that consists of iterative adjustments of connection weights to minimize the predictive error [33]. The capability to capture even nonlinear interactions within the data makes the ANN an accurate and flexible tool: however, this flexibility requires a careful tuning of hyperparameters (e.g. the learning rate, the training algorithm, the number of hidden neurons and their activation function) in order to avoid overfitting issues [34]. Iteration by iteration, the outcome of the neural model computations is determined based on the following equation:

$$f(X) = W_2[f_a(W_1X)]. \tag{7}$$

Input variables are represented by $X = \{x_1, x_2, \ldots, x_n\}$, whereas f_a represents the activation function the hidden layer is equipped with. W_1 and W_2 represent the weights and biases matrices that link the input layer to the hidden one and the hidden layer to the output one, respectively. They are iteratively updated according to the corrections made by the implemented training algorithm: the most robust algorithms, as well as the most frequently used activation functions, are well-documented within the relevant scientific literature [35-37]. To mitigate the risk of overfitting, an overfitting detection algorithm was employed allowing the early stopping procedure to be followed. During the learning process, if the validation scores stopped to show significant improvements (defined as a standard threshold equal to 10^{-4}) over several consecutive iterations, the training process was terminated. The maximum number of such consecutive iterations was set equal to 20, following the recommendations of the relevant literature [38].

A Pearson correlation matrix has been reported in Fig. 3 in order to evaluate the existing correlations between the considered variables. No significant correlation could be observed between loading frequency, testing temperature and the encoded categorical variable: these considerations allowed these three variables to be suitable for the following modeling operations. Conversely, stiffness modulus showed Pearson correlation coefficients equal to –0.04, 0.28 and –0.92 with the encoded categorical variable, loading frequency and testing temperature, respectively.

Before processing the data, the observations underwent a min-max normalization procedure: features were scaled to the range between 0 and +1, and this helped ensuring that all the developed models performed optimally by addressing the issues related to scale differences [39]. The dataset was then partitioned by randomly allocating roughly 75% of the observations to the training set and the remaining 25% to the test set. The training set was further partitioned into training and validation based on a *k*-fold cross-validation with *k* equal to 5. This ensured a balanced evaluation of training and validation results, allowing hyperparameters to be optimized by means of a grid search approach whose hyperparameters and search ranges are outlined in Table 1.

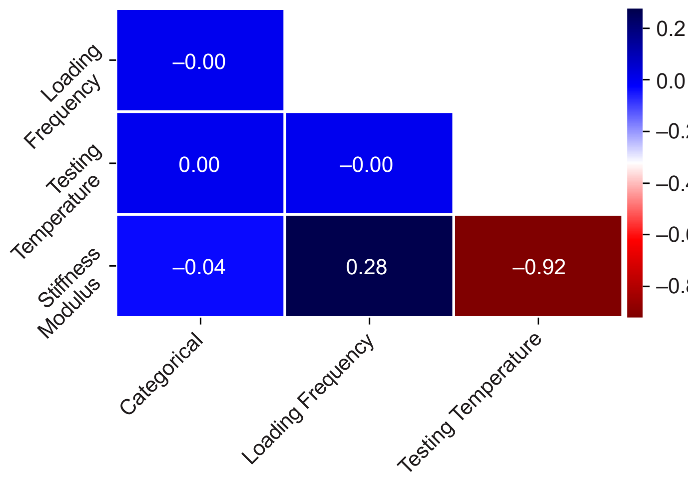

Fig. 3. Pearson correlation matrix

Table 1. Hyperparameters grid search

Model	Hyperparameter	Search range	Selected value
RR	α	$10^{-4} \div 10^{5}$	10^{-1}
LR	α	$10^{-4} \div 10^{5}$	10^{-3}
NLR	Polynomial degree	2, 3, 4	2
ANN	Hidden layer size	1 ÷ 50	30
	Activation function	Identity, Logistic, TanH	TanH
	Training algorithm	LBFGS [35], SGD [36], Adam [37]	LBFGS
	Maximum iterations	500, 1000, 5000	500

The entire methodology described in this study, from experimental data reading to the design of the different machine learning models, was implemented using a Python programming language, in its 3.9.12 version.

3. RESULTS

3.1. MODELS PERFORMANCE

A full set of goodness-of-fit parameters was used to evaluate the performance of linear regressions, nonlinear regression and artificial neural network models. Specifically, mean absolute error *MAE* and mean absolute percentage error *MAPE* were used to provide insights into the average magnitude of errors in both absolute and percentage terms, mean square error *MSE* and root mean square error *RMSE* were used to further penalize larger errors, Pearson correlation coefficient R and the coefficient of determination R^2 were used to respectively assess the linear correlation between actual and predicted values and the percentage of target variable variance explained by the model. Together, these metrics provided a solid evaluation framework, facilitating a more detailed comparison between the predictive accuracy and the generalization capabilities of each investigated model [40].

3.2. MODELS COMPARISON

During models' fine-tuning procedures, temperature and frequency conditions, jointly with a label-encoded categorical variable that distinguished the two *NMAS* values, were used as input features, whereas the stiffness modulus was returned as output. In order to fairly compare the performance of each regression approach, all the developed models were trained and validated using the same observations that underwent the same normalization and cross-validation procedures. This allowed the most suitable modeling methodology to be selected based on consistent goodness-of-fit metrics that were obtained during the testing phase and summarized in Table 2. It can be observed that all the developed models showed successful results, characterized by *MAE* between 692.75 MPa and 1829.35 MPa, *MAPE* between 8.77% and 26.46%, R between 0.9458 and 0.9942, and R^2 between 0.8917 and 0.9849. RR and LR approaches achieved nearly comparable performance, both in terms of error metrics and correlation coefficients. However, a significant improvement in overall metrics was obtained by using a NLR model, which was still outperformed by the ANN model that improved all the investigated goodness-of-fit metrics by roughly an order of magnitude. A graphical representation of the just discussed considerations can be observed in Fig. 4. Here the absolute values of the experimental observations and the predictions made by the different ML models were graphically represented by means of a histogram diagram. In particular, the black histograms represented the experimentally determined values that built the test set, whereas the gray, cyan, red and green histograms represented the corresponding values predicted by the ANN, NLR, LR and RR models, respectively. It can be observed that the gray histograms tended to be the closest to the black ones, accounting for a higher reliability of the predictions made by the ANN model. Then the accuracy gradually decreased from the ANN model to the NLR one to the simplest LR and RR models. This justified the choice of the ANN model as the best-performing approach that outperformed the conventional linear and non-linear regression ones.

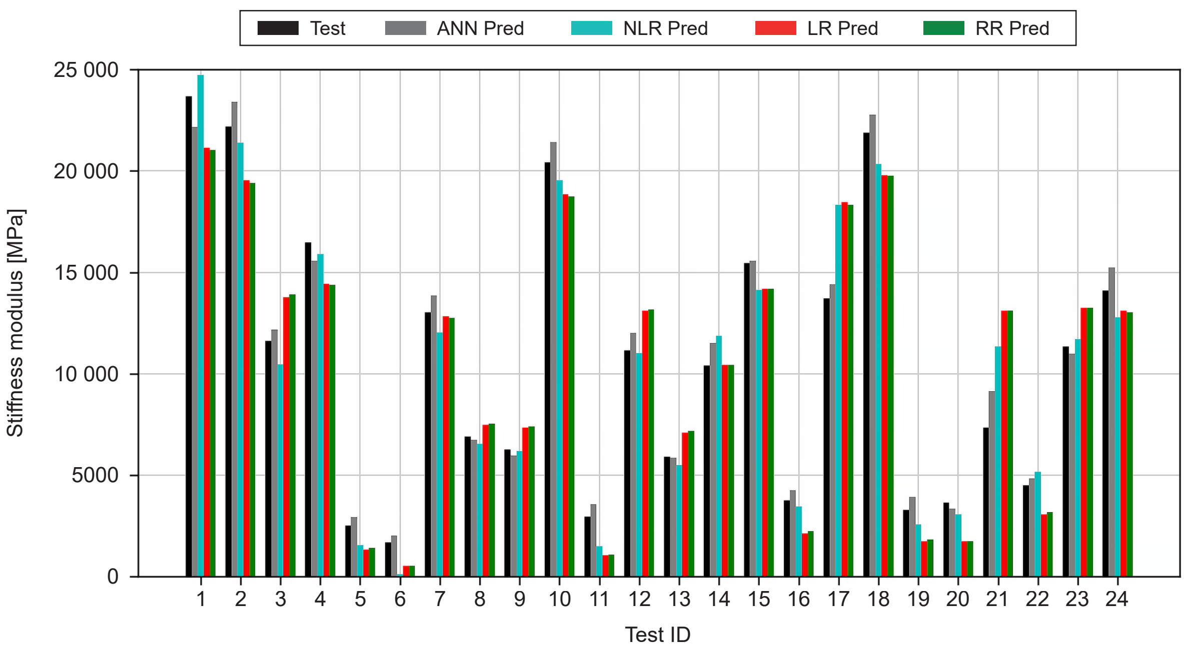

Fig. 4. Measured and predicted values of the stiffness modulus

Table 2. Performance parameters of each ML model evaluated on the test set.

Performance parameter	ML model			
	RR	LR	NLR	ANN
MAE [MPa]	1829.35	1811.79	1143.40	692.75
MAPE [%]	26.21	26.46	17.76	8.77
MSE [MPa^2]	4.83×10^6	4.80×10^6	2.42×10^6	6.71×10^5
RMSE [MPa]	2198.33	2190.26	1554.98	819.48
R	0.9458	0.9466	0.9744	0.9942
R^2	0.8917	0.8925	0.9458	0.9849

Once it was verified that the approach based on artificial neural networks was the most suitable one to perform the investigated regression task, further analysis was carried out to gain a deeper understanding of how accurate the model was. A regression plot was diagrammed, where stiffness modulus values predicted by the ANN during training, validation, and test phases were cross plotted against the corresponding experimental values that were observed during the laboratory investigation. The black solid line represented the line-of-equality (LOE) that identified the 100% accuracy condition, whereas red, green, and blue markers referred to training, validation, and test phases, respectively. Pearson correlation coefficient reported at the top of the diagram is referred to the test phase, as can be also read in Table 2. In Fig. 5, it can be observed that all the markers are close to the LOE, highlighting the outstanding performance of the ANN model. During the training and validation phases, *R* values of 0.9968 and 0.9959 were achieved, respectively. Similarly, also the R^2 values obtained during training and validation (0.9937 and 0.9908) resulted slightly better than the value achieved during the test phase (0.9849). This further confirmed that the model had properly understood the relationship between the considered variables and achieved excellent results during all the modeling stages. However, it is important to note that all the outcomes discussed in this study pertain to the laboratory investigation considered and the subsequent modeling procedures. Consequently, data coming from different experimental campaigns may require new identification of the best hyperparameters and new considerations regarding the performance achieved.

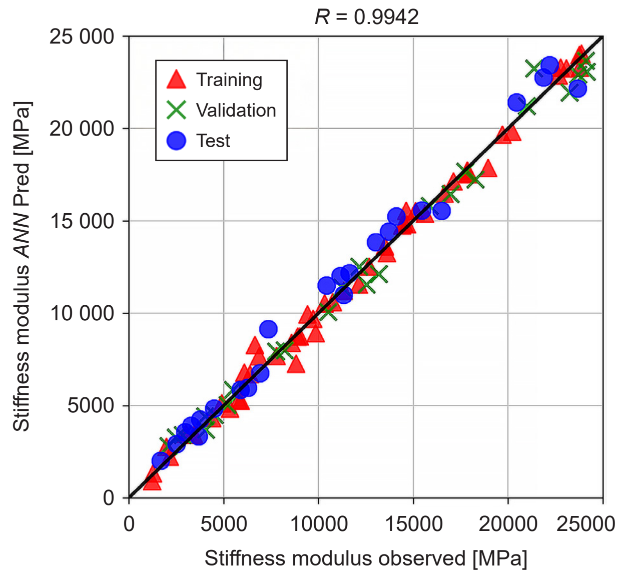

Fig. 5. *ANN* predicted values against measured stiffness modulus values

4. CONCLUSIONS

Stiffness modulus accounts for a key parameter when dealing with asphalt mixtures for road pavements. For this reason, its careful evaluation is essential even if it typically requires the use of expensive laboratory equipment and time-intensive experimental procedures. In this respect, methodologies based on regression techniques can provide a viable alternative that can significantly reduce the laboratory workload. Data-driven procedures are indeed capable of providing very reliable predictions if properly tuned and optimized, and the goal of this study was to verify whether conventional linear or nonlinear regression techniques or the modern and advanced artificial neural networks represented robust techniques to model the stiffness modulus of the investigated mixtures. These tools could therefore support conventional mix design procedures traditionally employed in professional practice, assisting the pavement engineers involved in managing data analysis operations. Based on the described and discussed outcomes, the following findings can be concluded:

1. Within the framework of the two investigated asphalt mixtures identified by means of a categorical variable, the stiffness modulus could be successfully predicted based on temperature and frequency conditions using either linear regression techniques, nonlinear regression techniques, or artificial neural networks, with different reliability and accuracy performance.

2. Data normalization procedure and *k*-fold cross-validation, coupled with the hyperparameters optimization, allowed the best performance to be identified in terms of each investigated approach.
3. Although all the developed models achieved satisfactory performance, the ANN obtained the best goodness-of-fit metrics during the test phase, represented by *MAE*, *MAPE*, and R^2 equal to 692.75 MPa, 8.77%, and 0.9849, respectively.
4. The achievement of successful ANN modeling was further evidenced by the excellent performance metrics obtained also during training and validation phases, which were slightly better than those obtained during the test phase.

The promising results obtained within the present study represent the feasibility of a predictive tool that could reliably predict the stiffness modulus of the two investigated mixtures based on the test conditions related to temperature and loading frequency. However, there are many aspects that can be further investigated in future developments. By way of example, it will be interesting to expand the experimental database by considering additional mixtures and verifying the goodness-of-fit and the generalization capabilities of the developed predictive models; different strategies for hyperparameter optimization could be further explored in order to find an architecture that could lead to even better performance; and finally, different performance parameters related to the mechanical behavior of these mixtures could be considered as outputs to improve the mechanical characterization allowed by these machine learning models.

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