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Compressive behavior of hybrid steel-polyvinyl alcohol fiber-reinforced concrete containing fly ash and slag powder: experiments and an artificial neural network model

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Data S1 Framework of the ANN model

1 ANN approach

An ANN consists of many artificial neurons. The neurons are connected to generate three main layers: input layer, hidden layer, and output layer. Fig. S1 shows the structure of the ANN approach used in this study, including one input layer, two hidden layers, and one output layer. The first hidden layer has 80 neurons and the second has 10. The architecture of the ANN model is optimized from different hidden layers (2 or 3), and different neurons in different hidden layers (20, 40, 60, and 80 neurons in the first hidden layer, and 10, 20, 30, and 40 neurons in the second hidden layer).

Assuming the input vector of neurons in one layer is $\boldsymbol{x}=[x_1, x_2, \ldots, x_m]$, the neurons in the next layer are calculated through two steps. First, $\boldsymbol{x}$ is transformed by a linear function; then the value of neurons z is evaluated using the activation function as follows:

$$
\begin{aligned}
&z = f(\boldsymbol{\omega}^{\mathrm{T}}\boldsymbol{x}+b) = f\left(\sum_{i=1}^{n}\omega_i x_i + b\right),\\
&\boldsymbol{x}\in R^{1\times m}, \boldsymbol{\omega}\in R^{1\times m}, z\in R,
\end{aligned}
\tag{S1}
$$

where $\boldsymbol{\omega}$ is the weight vector, b is the bias, and f is the activation function.

The activation function is critical to the neural network because it could increase the nonlinearity of the neural network. This study used the rectified linear unit (ReLU) function (Nair and Hinton, 2010) as the activation function, which is

$$f(x) = \max(0, x). \tag{S2}$$

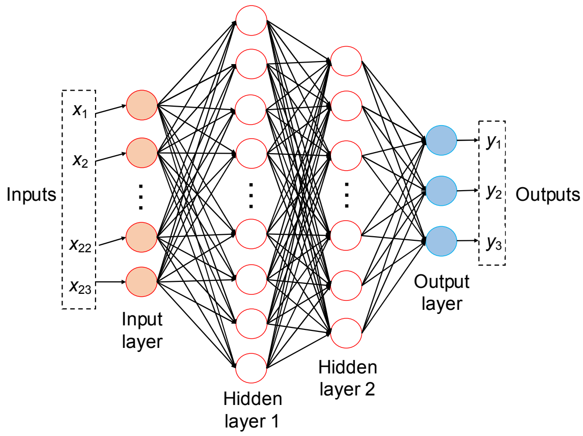

Fig. S1 Scheme of the ANN approach used in this study

2 Procedures of the ANN model

There are four main steps in the proposed ANN model of the compressive behavior of HFRC: dataset preprocessing, dataset splitting, ANN model training and evaluation, and prediction (Fig. S2).

1. Dataset preprocessing

The performance of the ANN model is strongly dependent on the quality of the database. To improve the complexity and diversity of the database, a series of compressive tests were carried out to obtain enough data on the compressive stress-strain curves of HFRC, in addition to relevant data collected from the literature (Zhou et al., 2019). The dataset was then selected as the input data and the output data for training the model.

As the size of datasets increase, their features should increase to prevent underfitting. Considering the components of HFRC and its compressive behavior, the input data in this study had a total of 23 features (Table S1). Besides these features, both the casting procedure and the orientation of fibers could also affect the mechanical behavior (Pujadas et al., 2014b; Pujadas et al., 2014c). However, considering the difficulty in defining these two features and the lack of available data, these two features were not considered in this work.

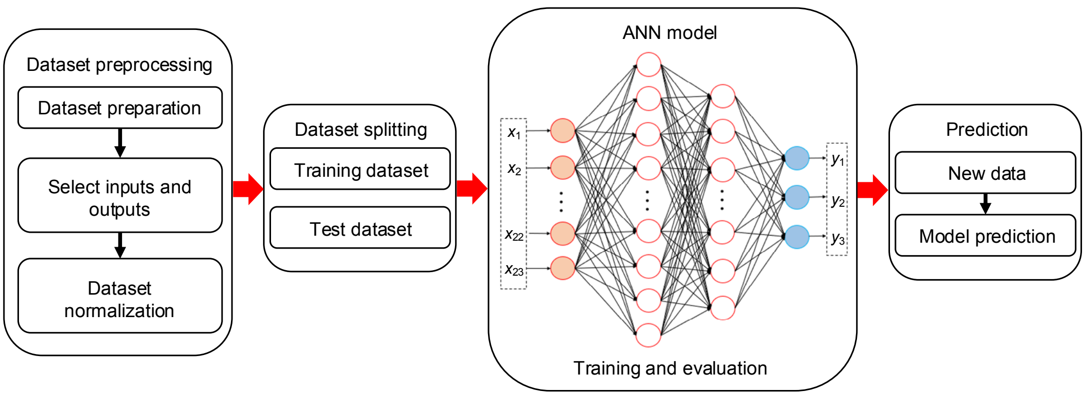

Fig. S2 Framework of the ANN model developed in this study

Table S1 Features of the input data

Part	Feature
Strain	Strain
Steel fiber	Fiber volume
	Weight
	Length
	Diameter
	Aspect ratio
	Reinforcement index
PVA fiber	Fiber volume
	Weight
	Length
	Diameter
	Aspect ratio
	Reinforcement index
Mechanical properties of plain concrete	Elastic modulus
	Compressive strength
	Strain corresponding to compressive strength
Components of HFRC	Weight of the cement
	Weight of fly ash
	Weight of slag powder
	Weight of water
	Weight of coarse aggregate
	Weight of fine aggregate
	Water binder ratio

To predict the compressive stress-strain curve and evaluate the compressive behavior of HFRC, the output data included the stress, the compressive strength of HFRC, and the strain corresponding to compressive strength of HFRC.

All the above data needs preprocessing because the amplitude and range of different input features vary greatly. For example, the strain of HFRC changes from 0 to 0.03 and had at least 3000 data points for each HFRC specimen, but there were only 3 options for the length of the steel fiber and its maximal value was up to 50 mm. The different amplitudes and ranges of input features could worsen the performance of the model and make it difficult to train the model. Therefore, Min-Max normalization was used to process the data and eliminate these variations. Min-Max normalization can normalize the data to a range from 0 to 1 by using the following equation,

$$x_{j,\text{scaled}}^{(i)} = \frac{x_j^{(i)} - x_{\min}^{(i)}}{x_{\max}^{(i)} - x_{\min}^{(i)}}, \tag{S3}$$

where i=1, 2, …, m (m is the number of features), j=1, 2, …, n (n is the number of data samples); and $x_{\max}^{(i)}$ and $x_{\min}^{(i)}$ are the maximal and minimal values of the ith feature, respectively; $x_j^{(i)}$ is the original jth data sample of the ith feature, and $x_{j,\text{scaled}}^{(i)}$ is the scaled jth data sample of the ith feature. Different features of the input data are scaled independently. Min-Max normalization is achieved using the preprocessing module of scikit-learn (Pedregosa et al., 2011).

2. Dataset splitting

To train and evaluate the ANN model, the dataset needs to be divided into two subsets: the training dataset and the test dataset. The training dataset is used to train the ANN model and the test dataset is used to evaluate it. This step is completed by the model selection module of scikit-learn (Pedregosa, et al., 2011). The whole dataset is first shuffled, then 70% of the dataset is recognized as the training dataset and the remainder as the test dataset.

3. ANN model training and evaluation

The ANN model (Fig. S1) is formulated on the open-source framework Pytorch (Pedregosa, et al., 2011). The loss function adopts the mean square error (MSE) function, which is usually used in regression problems. The optimizer used is the adaptive moment estimation (Adam), which is an optimization algorithm for first-order gradient-based optimization of stochastic objective functions (Kingma and Ba, 2014). The batch size of the dataset is 128. There are 1000 epochs to run the model. During each epoch, the model is first trained by the training dataset and then evaluated by the test dataset. The loss of the training dataset and the test dataset is then compared to avoid underfitting or overfitting the ANN model.

The learning rate is a tuning parameter that determines how fast the loss function moves towards the minimum at each iteration. In this study, the initial learning rate is 0.01 and the learning rate decay is used to speed up the convergence of the ANN model. This means the learning rate will decrease after a certain epoch, such as becoming one tenth of the old learning rate after 480 epochs.

4. Prediction

After training, the new input dataset is fed into the ANN model to predict the stress, compressive strength, and strain corresponding to compressive strength. Each datapoint input has its own three outputs. The predicted stress can be combined with the input strain to plot the predicted compressive stress-strain curve. The mean predicted compressive strength and strain corresponding to compressive strength of each HFRC sample would be recognized as these two final predicted items.