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Prediction of Constituents of Concrete Mixtures Containing Fly Ash and Blast Furnace Slag Using Machine Learning Techniques

Mohammed Jaradat
Al-Zaytoonah University of Jordan

Mohammad Massoud
Al-Zaytoonah University of Jordan

Ahmad Manasrah
Al-Zaytoonah University of Jordan

Yousef Jaradat
Al-Zaytoonah University of Jordan

Abstract: The prediction of concrete mix proportions is of the utmost importance to civil engineers to complete the design process of structures. This process is usually done through a trial-and-error process which involves simple regression techniques and is usually done to achieve a specific strength at a specific age. The incorporation of supplementary cementitious materials into concrete mixtures for environmental purposes has deemed the prediction process more complex and created a need to come up with more advanced techniques. Furthermore, the ability to predict the constituents of concrete mixtures given multiple inputs is still limited. Hence, in this work several machine learning algorithms were utilized to make a prediction regarding mix proportions of concrete mixtures based on concrete compressive strength, concrete age, and density as inputs. Random forest, decision tree, and K-neighbors regressors were used to achieve this objective. Mean squared error as well as root squared error were used to measure the accuracy of the constructed models. Random Forest algorithm obtained the highest accuracy with 98.5%.

Keywords: Concrete, Compressive strength, Machine learning, Artificial intelligence, Supplementary cementitious materials.

Introduction

Concrete is a widely used construction material for infrastructure as it combines several beneficial characteristics such as strength, durability, and financial viability. The worldwide continuous growth in infrastructure means that concrete will remain in use for a long period of time. However, cement production, which is the main binder in concrete mixtures, is associated with negative impacts on the environment due to high carbon dioxide emissions (Lila et al., 2020; Schneider, 2019; Yang et al., 2015). This has led researchers to look for means to alleviate high CO_2 emissions through partially replacing cement with supplementary cementitious materials (SCMs) sourced from agricultural and industrial by-products (Abebaw et al., 2021; Berndt, 2009; Garcia-Lodeiro et al., 2016; Thomas et al., 2021). These materials are associated with pozzolanic activity which allows them to aid in the formation of CSH gel and, consequently, build-up compressive strength (Donatello et al., 2010). Therefore, this adds to the complexity of concrete mixtures which are usually made up of cement, water, aggregates, and admixtures. Thus, there is a continuous need to study this material to facilitate the design process and ensure its safety. One of the main performance indicators that is of great importance to design of infrastructure is the compressive strength of concrete. Therefore, the ability to predict mechanical

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properties of concrete is crucial to designers. However, it is a complicated task due to the heterogenous nature of this material which is increasingly becoming more complex with the addition of SCMs (Mohtasham- Moein et al., 2023). Therefore, the constituent materials of concrete can vary greatly from one mix to another in both types of material as well as the ratios of the materials used. The relationship between the constituent materials of concrete and its compressive strength development is most often a nonlinear one (Chou et al., 2011; Mohtasham- Moein et al., 2023). Furthermore, as the concrete ages, the strength development also varies. This time-dependent nature of concrete strength development is also nonlinear which adds to the complexity of compressive strength prediction.

Two main paradigms are typically followed by researchers to predict the compressive strength of concrete mixtures: empirical and computational (Li et al., 2022). The empirical models rely on linear and nonlinear regression models to predict concrete properties through the developed analytical models. These models depend on trial-and-error mixing and destructive testing of specimens at different ages of concrete to develop them. As a result, they are resources and time consuming to develop due to the trial-and-error nature of experiments (Ben Chaabene et al., 2020). Additionally, these models are considered sufficient for fairly simple concretes that are made up of cement, aggregates, and water. However, the rise in complexity of concrete materials necessitates the need for more practical and sophisticated models. Computational models, on the other hand, have been developed through using density-functional theory (DFT) and molecular dynamics simulations. These models require a deep understanding of the microstructural properties of the constituent materials of the concrete mixture. Moreover, the complex nature of cement hydration makes the generalization of models that can predict concrete properties a very challenging task. They are also computationally expensive and difficult to validate through experiments due to their small time and length scales (Li et al., 2022).

Recently, artificial intelligence (AI), machine learning (ML), and deep learning methods have been adopted to produce predictive models of concrete compressive strength. These models can make up for what the conventional regression models and the sophisticated computational models lack through their special algorithms. They can accommodate large amounts of data and learn from them to predict the mechanical properties of concrete. Researchers have utilized artificial neural networks (ANN), support vector machine (SVM), random forest (RF), and decision tree (DT) algorithms (Khambra & Shukla, 2023) among others, in concrete science for various reasons. The unique characteristics of machine learning aided researchers in not only predicting various properties of concrete, but also finding the influencing factors of these properties. Gucluer et al. (2021) developed a machine learning model using input data from nondestructive testing (NDT) techniques as well as physical properties of the hardened concrete to predict its compressive strength. Several ML algorithms were used; however, DT algorithm was able to provide the least amount of error. Sun et al. (2023) combined the use of machine learning algorithms with analytical hierarchy process (AHP) to optimize the design of ultra-high performance concrete (UHPC) mixtures. The optimized design was set to meet low carbon and low-cost requirements. Several machine learning algorithms were included in their work but XGBoost provided the best prediction performance in terms of compressive strength. Researchers have also worked on providing a machine learning based model to predict the compressive strength of concrete containing recycled aggregates. Shang et al. (2022). Found that AdaBoost regressor provides higher values of R^2 as opposed to decision tree algorithm. On the other hand, Salimbahrami et al. (2021) utilized multiple linear regression (MLR) as well as ANN and SVM. The results indicated the superiority of machine learning methods over MLR and concluded that SVM was able to provide a model with higher prediction accuracy than ANN. On the other hand, Deng et al. (2018). Proposed a predictive model based on convolutional neural network (CNN) and then the results were compared with a traditional neural network model. It was shown that CNN provides higher precision and efficiency as well as better generalization ability when compared to ANN. ML predictive models of the compressive strength of nano-modified concrete were also developed Nazar et al. (2022). The input variables were different nanomaterials in addition to the components on conventional concrete. The results showed that RF had a better performance than both DT and gene expression programming models.

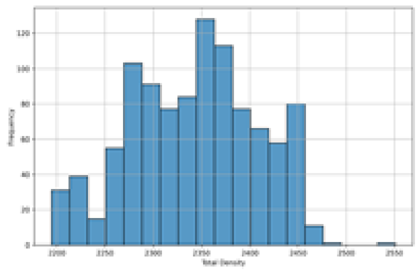
Researchers have utilized various ML methods in their quest to develop a predictive model to estimate the compressive strength of concrete containing SCMs. For instance, Khursheed et al (2021) utilized several machine learning techniques to predict the 28-day compressive strength of concrete mixtures that contain fly ash. It was concluded that minimum probability machine regression (MPMR) provides the most accurate prediction. Moreover, Song et al. (2021) applied machine learning techniques to experimental data to predict the compressive strength of concrete mixtures with fly ash as an admixture. The bagging algorithm showed higher prediction accuracy than other machine learning techniques. Ahmad et al (2021) employed several supervised ML techniques such as bagging, AdaBoost, gene expression programming, and decision tree to predict the compressive strength of concrete containing fly ash and blast furnace slag. The input variables were the constituents of a concrete mix in addition to its age. The authors found that bagging algorithms were more effective in their prediction prowess than the other algorithms used. Furthermore, Qi et. al. (2022) proposed ML-based model that can estimate the compressive strength of concrete that contains BFS, FA, and superplasticizer (SP). RF algorithm was used in conjunction with principal component analysis (PCA) and particle swarm optimization to estimate the strength of concrete. It was concluded that RF algorithm can provide an excellent prediction of the compressive strength, however, PCA processing negatively impacts its predictive capability. Kocamaz et al. (2021) used the tree model M5P to predict both the compressive strength and ultrasonic pulse velocity of concrete that contains SF, FA, and BFS. The results of the study support the use of this tree model for concrete containing mineral admixtures. Jiang et al. (2022) proposed four machine learning algorithms to predict the compressive strength of fly ash containing concrete. Eight input variables, all pertaining to the concrete mix ratios and age, were used as inputs. The study showed that the use of a hybrid model that incorporates support vector regression and grid search optimization algorithm was the most successful. It was able to capture the correlations between the input variables as well as an accurate prediction of the compressive strength. In this work, the constituents of concrete mixtures containing fly ash and blast furnace slag, which are widely used industrial by-products with good pozzolanic activity, are predicted using several machine learning algorithms.

Method

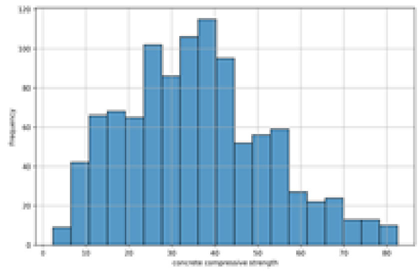
To construct a machine learning model, a dataset is required to train and test the model. The dataset found in I-Cheng Yeh (1998) consists of nine different columns. The description of these columns is shown in Table 1

Table 1. Description of dataset

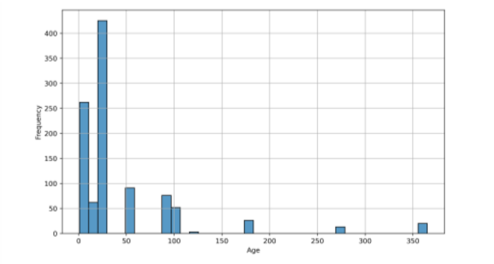
Material	Units	Description
Cement (C)	Kg/m^3	Output
Blast Furnace Slag (BFS)	Kg/m^3	Output
Fly Ash (F)	Kg/m^3	Output
Water (W)	Kg/m^3	Output
Superplasticizer (SP)	Kg/m^3	Output
Coarse Aggregate (CA)	Kg/m^3	Output
Fine Aggregate (FA)	Kg/m^3	Output
Density	Kg/m^3	Feature
Age	Days (1-365)	Feature
Compressive Strength (f'_c)	MPa	Feature



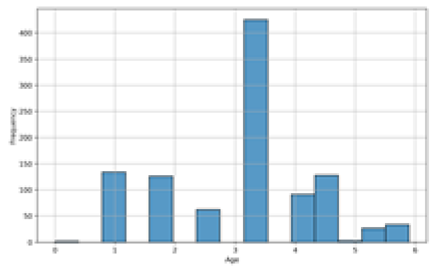
(a)



(b)



(c)



(d)

Figure 1. Histogram statistics for feature variables: (a) total density, (b) compressive strength, (c) age, and (d) semi-normally distributed age

A new column has been added to the dataset, which is the total density. This column is the sum of the first seven columns. Unlike the models that have been trained in the related works, the proposed model predicts the components of the mixture and not its strength. This means that the strength, age and the total density are the input features of the proposed model, and the output results are the seven components of the mixtures. The dataset is 1030x10. Seven output columns and three features.The total density and the strength features are normally distributed as shown in Figures 1a and 1b, however, the age is not. Logarithmic transformation has been utilized to transfer these features into semi-normally distributed as shown in Figures 1c and 1d, respectively.

Figure 2 shows the correlation heatmap of the dataset. We can observe that the output columns have positive correlation with at least one of the input features utilized in the model. Finally, the dataset has been normalized to make all the values in the interval {-1, 1} by subtracting the mean and divide by the max value of each feature. The final dataset has been divided into 70% training, 15% for testing and 15% for validation.

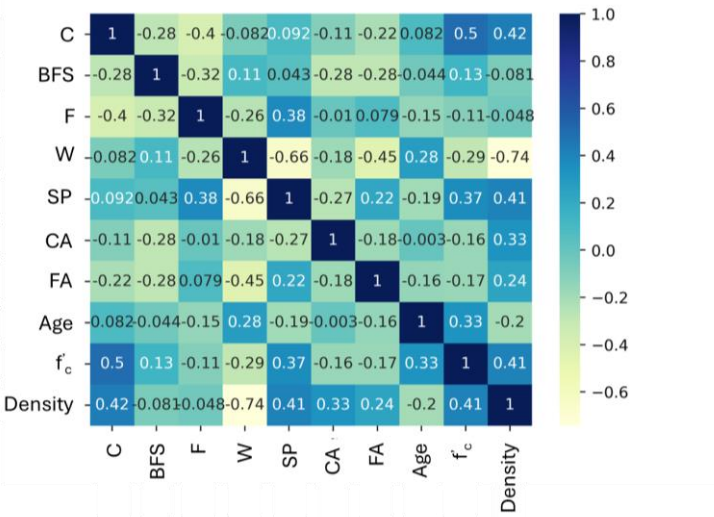
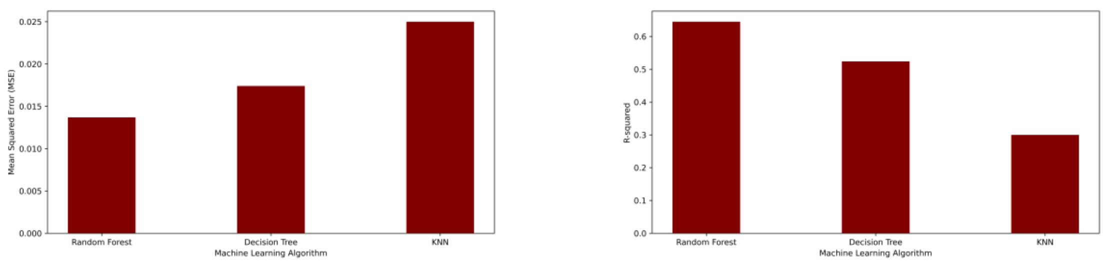


Figure 2. Correlation heatmap

Three different machine learning algorithms have been utilized in this work; random forest, decision tree and Knn. The regression version of these models have been leveraged since the prediction problem is continuous or a regression problem. Python has been used to train these models and to test their accuracy. Mean square error (MSE) and R^2 have been used to validate the accuracy of these models. The training process of the models have been repeated 30 times and the average accuracy of these iterations have been recorded.

Results and Discussion

Figure 3a shows the MSE value of the three models. We can observe that the random forest has the highest accuracy compared with the KNN and decision tree. However, we can observe that the accuracy of the three models is more than 97%. It is worth mentioning that KNN has the highest accuracy value before the logarithm conversion of the age feature and the decision tree has the lowest with 97.2% for KNN and 96.1% for decision tree. Figure 3b shows the R^2 value of these models. We can observe that the random forest model has the highest R^2 value among these models.



(a) (b)

Figure 3. Performance measures using (a) MSE and (b) R^2

Conclusion

This study showcases the exciting potential of machine learning to revolutionize concrete mix design—a crucial task for civil engineers. Moreover, this work addresses the growing need for sustainable construction practices by emphasizing on the incorporation of supplementary cementitious materials into concrete mixtures. By moving away from the traditional trial-and-error methods, we used various algorithms, with the Random Forest model standing out, achieving an impressive accuracy of 98.5%. This success highlights how machine learning models can simplify the complexities of predicting concrete mix proportions based on factors like compressive strength, concrete age, and density. Nevertheless, rheological factors such as workability were not considered in this work which limits the applicability of the developed predictive models. Furthermore, the size of the data set can be increased and include more supplementary cementitious materials to enhance the predictive accuracy of the developed models. Hence, there's a lot of potential for further exploration. We can adapt these machine learning techniques to different concrete scenarios and conditions, making them even more useful for the industry.

Scientific Ethics Declaration

The authors declare that the scientific ethical and legal responsibility of this article published in EPSTEM Journal belongs to the authors.

Acknowledgements or Notes

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Author Information

Mohammed Jaradat
Al-Zaytoonah University of Jordan
Amman 11733, Jordan
Contact e-mail: *m.jaradat@zuj.edu.jo*

Mohammad Massoud
Al-Zaytoonah University of Jordan
Amman 11733, Jordan

Ahmad Manasrah
Al-Zaytoonah University of Jordan
Amman 11733, Jordan

Yousef Jaradat
Al-Zaytoonah University of Jordan
Amman 11733, Jordan

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