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Gulzar Mohammad

gm78691@gmail.com

CGC University

Wajahat Ali

Istanbul Beykent University

Nasser Alanazi

University of Ha'il

Article

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Explainable and Uncertainty-Aware Machine Learning for Compressive Strength Prediction of 3D-Printed Fiber-Reinforced Concrete

Gulzar Mohammad¹, Wajahat Ali² and Nasser Alanazi³

¹ Department of Applied Sciences, School of Engineering and Technology, CGC University, Mohali, India

² Department of Industrial Engineering, Istanbul Beykent University, Istanbul, 34398, Türkiye

³ Department of Civil Engineering, College of Engineering, University of Ha'il, Ha'il, 55474, Saudi Arabia.

Abstract

Accurate prediction of compressive strength is essential for the development and performance assessment of 3D-printed fiber-reinforced concrete (3DP-FRC), where mixture composition, fiber characteristics, curing age, and loading direction generate complex nonlinear relationships in strength response. This study develops an explainable machine-learning framework for predicting the compressive strength of 3DP-FRC using 299 experimental observations and 16 input variables. Four regression models, namely Support Vector Machine (SVM), Random Forest (RF), CatBoost, and Natural Gradient Boosting (NGBoost), were optimized and evaluated using repeated five-fold cross-validation and an independent 20% testing dataset. NGBoost achieved the highest testing R^2 of 0.9877 and the lowest RMSE of 4.9036 MPa, together with a maximum prediction error of 13.6904 MPa, whereas CatBoost produced the lowest testing MAE of 3.8031 MPa. SHAP, LIME, and partial dependence analysis identified the water-to-binder ratio, water content, silica fume, and superplasticizer as the most influential predictors, while loading direction and fiber volume fraction also contributed substantially to compressive-strength prediction. The explainability analyses revealed pronounced nonlinear relationships and interaction effects among mixture composition, fiber characteristics, and processing-related variables. NGBoost was subsequently integrated into an interactive graphical user interface to provide direct strength prediction, uncertainty estimation, and feature-contribution analysis. The proposed framework demonstrates the potential of explainable machine learning for reliable compressive-strength prediction and data-driven assessment of 3DP-FRC. The developed tool provides an accessible platform for model interpretation and preliminary strength assessment, while further independent experimental validation is required before its use in structural design applications.

Keywords: 3D-printed fiber-reinforced concrete; compressive strength; machine learning; explainable artificial intelligence; graphical user interface.

1. Introduction

Additive Manufacturing (AM) has been developing quickly in parallel with digitization, technological innovation and modernization since the start of the new millennium (Perrot et al., 2016). This revolutionary technology has encouraged automation processes, especially in the Construction Industry (CI), where 3D printing based on extrusion technology has become very popular. Rapid urbanization and industrialization have been hampered by persistent difficulties including lack of skilled manpower, limited resources and safety issues in the development of CI (Banihashemi et al., 2025; Hosseini et al., 2014). 3D printing (3DP) technology is a new method that has been introduced to the construction industry for researchers and engineers to deposit successive layers of printed material to form a three-dimensional structure. The goal of this is to drastically decrease the amount of solid waste generated in the CI and to decrease the construction costs and reliance on skilled labour (Panda et al., 2017). Recent studies show that the 3DP technology in the construction sector can reduce waste generation by 30-60 %, the need for labour by 50-80 % and production time by 50-70 %. Thus, the application of 3D printed concrete in civil engineering is a contemporary technique, and automation in construction is an inevitable and prominent trend in the future of the CI (Buswell et al., 2018).

Additive Manufacturing technology allows to create unique architectural elements and large building components by stacking layers, without the need for formwork. Furthermore, a number of 3D concrete printing methods have been developed to integrate the concepts of AM into the concrete construction process (Hou et al., 2021). The technologies can be grouped into two categories: powder based technologies (Emerging Objects, D-shape technique) and extrusion based technologies (Contour Crafting (CC), Concrete Printing, CONPrint3D) (Zareiyan & Khoshnevis, 2017; Sanjayan et al., 2018; Feng et al., 2015). The recently developed techniques are: rock printing, Fused Deposition Modeling (FDM), and MultiJet Fusion (Lowke et al., 2018; Lim et al., 2012). In the case of concrete and earthen architecture, the ability to build large-scale structures without formwork, although it is not the most productive, has proved to be of great importance in the design process, as it reduces material consumption and construction costs (Gomaa et al., 2022).

Since the technology is evolving towards 3D printing, it is necessary to obtain the desired material properties to meet the high efficiency requirements of the technology. The mechanical properties, workability and relationships between mechanical properties and workability of 3D-printed concrete have been investigated (Al-Qutaifi et al., 2018; Le et al., 2012; Liu et al., 2024; Panda et al., 2017). To date, however, an optimal mix proportion and a reliable way to

69 assess the printability of 3DPC has not been determined (Kazemian et al., 2017). In order to
70 achieve high performance 3DPC mixtures and conventional cement-based materials,
71 researchers have investigated different constituents, such as mineral powders (Buswell et al.,
72 2018) and geopolymer-based materials (Xia & Sanjayan, 2016).

73 While 3DPC infrastructure meets international dynamic requirements, many buildings have
74 been 3D printed with a few buildings being put into practice due to new safety concerns.
75 Eindhoven University of Technology in the Netherlands, for example, in 2015 printed the first
76 multistory building, fulfilling all the applicable standard requirements (Mechtcherine et al.,
77 2018). Likewise, in 2016, the local administration built the Dubai's first 3D-printed office
78 building that was comparable to a traditional building (Zhang et al., 2019). The D-shape
79 printing technique was used to print all eight components of the pedestrian bridge, which was
80 built by the Institute of Advanced Architecture of Catalonia (IAAC) and spans 40 ft. The next
81 year (Salet et al., 2018) printed and tested a prototype bridge in six sections without having to
82 overcome the span limitations of the printer. The structural strength and integrity were verified
83 with well-developed on-site testing procedures, even though there are no standard criteria for
84 testing printed structures. The 3DPC technology has great potential to develop, manufacture,
85 repair and restore complex structures that are difficult to form using traditional formwork
86 (Arunothayan et al., 2022). Although there are some disadvantages to 3DPC technology
87 (process complexity, lack of specifications, and economic feasibility) (Avrutis et al., 2019),
88 there is a great potential in 3DPC structures. This invention has the potential to be used in a
89 wide range of industries, and construction on Mars and the Moon could be more efficient. This
90 could thus allow for the potential acceleration of the plan of colonizing extraterrestrial areas
91 (Siddika et al., 2020). As 3DP technology continues to advance, its potential applications and
92 benefits are becoming increasingly evident.

93 Although the construction industry sees great potential in 3DPC, the conventional concrete is
94 brittle, and adding reinforcement is essential to meet critical construction requirements such as
95 elasticity and creep resistance, as well as durability (Marchment & Sanjayan, 2020; Liang et
96 al., 2022). Furthermore, 3DPC strength is typically lower than traditional cast concrete due to
97 various factors, including the lack of reinforcement, poor compaction of the concrete mix, and
98 potential non-uniformity during layer-by-layer deposition (Singh et al., 2022). Therefore,
99 structural elements made by 3DPC might have less performance than those made by
100 conventional construction technologies. Hence, it is crucial to reinforce 3DPC and enhance the
101 material properties to achieve the desired performance requirements (Bos et al., 2019). The
102 direct printing of steel reinforcement or steel tubes is an innovative way to concrete

reinforcement using 3DP technology (Ma et al., 2019). However, the use of the 3D-printed concrete with fiber reinforcement is still in its infancy. One effective approach to the reinforcement problem is to use short discontinuous fibers (Zhao et al., 2022). These fibres can be mainly carbon (Hambach et al., 2016), glass, basalt (Dong et al., 2022), polyethylene (PE) (Ding et al., 2020), polypropylene (PP) (Van Der Putten et al., 2021), polyvinyl alcohol (PVA) (Yu & Leung, 2018), and steel fibres (Arunothayan et al., 2021). However, there is an urgent need to develop the fiber-reinforced cement-based materials further to enable the widespread use of 3DP concrete in the construction of high-performance structures (Al Abadi et al., 2018; Melenka et al., 2016).

The sequential layer-by-layer deposition process of 3D printing concrete, however, is a challenge to integrate reinforcement. While a fully automated reinforcement system for 3D concrete printing has not yet been developed, many studies have been conducted on how to integrate reinforcement into 3DPC (Marchment & Sanjayan, 2021; Lim et al., 2018). A typical approach to strengthening structural elements fabricated with 3D printing is to pour concrete around hand-placed rebar (Wu et al., 2016). Another method is to embed steel cables into the extruded layers (Pham et al., 2020). Other reinforcement materials like fabrics, recycled glass and wire meshes have also been investigated to be incorporated into the extruded layers (Li et al., 2021). The reinforcement during the deposition of the layer needs to be done with the help of electromechanical equipment and other subsystems; however, it is important to develop and optimize automated procedures for these operations to ensure a continuous and uninterrupted construction process. Furthermore, the existing reinforcement methods may complicate the fabrication of 3DPC, which is one of the main benefits of automated construction provided by the 3D printing technology (Afroughsabet et al., 2016).

The active and passive techniques of curing can be effective in reducing the nano-scale deformation and cracking. Passive techniques are based on the use of well designed material mixtures with shrinkage control fibers, such as glass, polypropylene, polyethylene, basalt or steel fibers (Dong et al., 2022). They can also involve internal curing techniques such as the use of shrinkage-reducing agents (SRA) and the use of water-saturated fine aggregates (Lura et al., 2007; Bentz, 2006). Active methods try to reduce water loss from the surface of the concrete. Common techniques are to wet the concrete, apply anti-evaporation chemicals (membrane-forming waterproofing agents or protective foils) and to protect the concrete from direct exposure to the sun and wind. (Henkensiefken et al., 2010) The flexural capacity of 3DFRC is also found to be influenced favorably by the fiber diameter than fiber length, which can sometimes have a negative effect on CS. The observation indicates that the fiber aspect

ratio (in relation to nozzle diameter) should be taken into account in addition to a single geometric fiber parameter (Ye et al., 2021; Dulaj et al., 2022). The effect of water-to-binder ratios between 0.25 and 0.5 on 3D-printed graphene concrete was explored. As the silica fume content increased, the pore spheroid characteristics of 3DPFC became larger and the strength of the concrete remained similar (Liu et al., 2023).

To evaluate the mechanical performance of 3DP-FRC composites, compressive strength (CS) is widely considered an important mechanical property. Steel fiber-reinforced concrete (SFC) is the 3DP-FRC system with the highest reported CS (159 MPa) (Arunothayan et al., 2021). Variations in fiber content up to 1 % have shown the anisotropic behavior of 3DPFRC, which is seen at loading orientations of 90°, 45°, and 0° to the printing direction. Generally, the compressive strength in the printing direction is the highest, because more material is deposited in the longitudinal direction of the printing. Singh et al. (2022) studied the anisotropic properties of 3DPFRCs containing up to 1 % fiber content, and found that the CS values decreased by 3–14 % at 0° and 12–26 % at 90° compared to 45°. Printed mixes with PE fibers showed higher compressive strength than the molded mixes (Xiao et al., 2021). The strength of printed mixtures was significantly enhanced by adding 1 % glass fibers, which increased the strength by 108 % (Zhang & Aslani, 2021). However, to obtain the required porosity in the bulk slurry (Shakor et al., 2020), it is possible to induce an unfavorable orientation and entanglement of the fibers, which may lead to a decrease in strength (Liu et al., 2022). The compressive strength was decreased by 1.5 % by the use of PVA fibers, similar to the results obtained with glass and basalt fibers (Li et al., 2021). When subjected to axial compression, horizontally reinforced specimens tend to break along the weak interface, revealing the horizontal reinforcement. The addition of steel fiber up to 2 % in 3DPC resulted in a significant improvement in both CS and FS when compared with the conventional cast specimens (Arunothayan et al., 2021). The results showed that the addition of an adequate amount of fiber to the 3D concrete mixture can significantly improve the CS, especially when steel fibers are added, which is evident from their excellent performance (Arunothayan et al., 2021; Chu et al., 2021).

There are intrinsic and extrinsic factors that affect the compressive strength of 3DP-FRC. The mix proportions, raw material composition, and the type, dosage and geometry of the reinforcing fibers are intrinsic factors, whereas the curing age and loading direction are extrinsic factors, which are largely experimental. The lack of a universally accepted standard, testing protocol or mix-design procedure for 3DP-FRC is especially challenging in identifying an optimal mix formulation. It is very expensive and time consuming to experimentally

characterize the relationship between these many input parameters and the resulting mechanical performance. An alternative is to use data-driven methods that have the potential to be much more efficient, in that they can learn these complex, nonlinear relationships directly from existing experimental data, without the need for extensive physical testing.

The use of machine learning has been broadened to predict the mechanical properties of different fiber-reinforced concretes and other cementitious composites such as PVA-FRC, PP-FRC, PE-FRC, basalt FRC, steel FRC, FRP-strengthened composites, and self-compacting fiber-reinforced concrete, etc. These studies have shown that a variety of algorithms such as LightGBM, XGBoost, ANN, RF, SVM, AdaBoost, and ICA-XGBoost have been found to have strong predictive power, as shown in Table 1. In particular, tree-based ensemble and boosting techniques have shown to be superior to simpler regression-based methods in capturing the non-linear interactions between mix design variables and are thus widely used and improved upon in strength prediction applications for more advanced concrete systems.

However, the research on the prediction of compressive strength of 3DP-FRC based on ML is still limited. Previous research has focused on a limited number of algorithms, and has largely ignored the importance of model interpretability, with only a few studies reporting overall feature importance without systematically comparing multiple methods and their rationale for a model's prediction. Furthermore, very few of these studies convert their models into a form that can be immediately used by practicing engineers without programming skills. To tackle these challenges, four machine learning models, CatBoost, NGBoost, Random Forest (RF), and Support Vector Machine (SVM), are designed and comprehensively compared in the prediction of the compressive strength of 3DP-FRC. The novelty of this work is threefold: (1) the four algorithmically distinct models are benchmarked on the same dataset to determine which is the most reliable predictor of 3DP-FRC strength, (2) it interprets the model behavior from complementary global and local perspectives by combining SHAP, LIME, and Partial Dependence Plots (PDP) to reveal the overall influence of the features and the general trends of feature interactions, and LIME was used to explain individual instance-level predictions, providing a granular level of interpretability that has not been previously reported in 3DP-FRC strength models, and (3) it packages the best-performing model into an interactive Graphical User Interface (GUI) that enables practitioners and researchers to derive compressive strength predictions instantly by simply providing mix design and printing parameters, without requiring any coding or machine learning expertise. Overall, these contributions span the spectrum of predictive ability, model transparency, and applicability in the mix design of fiber-reinforced 3D printed concrete.

Table 1. Previous studies on predicting CS of different types of concrete

Concrete type	Dataset	Method	R ²	Ref.
HPC-GGBS	152	LightGBM	0.96	Zhao et al. (2022)
HSC	357	GEP	0.91	Hambach et al. (2016)
HPC-GGBS	152	LightGBM	0.96	Zhao et al. (2022)
PCM	154	XGBoost	0.96	Panda et al. (2017)
ECC	79	ANN	0.99	Uddin et al. (2022)
HPC	190	RF	0.98	Ding et al. (2020)
Normal concrete	15	SVM	0.95	Yu & Leung (2019)
RHAC	192	ANN	0.90	Van Der Putten et al. (2021)
UHPC	113	LightGBM	0.99	Uddin et al. (2022)
RAC	209	ICA-XGBoost	0.98	Duan et al. (2021)
FAC	270	SVM	0.98	Zhu et al. (2019)
Geopolymer concrete	35	RF	0.93	Arunothayan et al. (2021)
RAC	515	LightGBM	0.96	Li et al. (2022a)
Normal concrete	1030	AdaBoost	0.99	Liang et al. (2022)
UHPC	372	XGBoost	0.90	Li et al. (2022b)

2. Data collection

To develop reliable ML models for predicting the CS of 3DP-FRC, a total of 299 data points were collected from existing experimental studies (Feng et al., 2015; Al-Qutaifi et al., 2018; Liu et al., 2024; Panda et al., 2018; Panda et al., 2017; Soltan & Li, 2018; Ma et al., 2019; Ding et al., 2020; Van Der Putten et al., 2021; Yu & Leung, 2018; Arunothayan et al., 2021; Pham et al., 2020; Shehadeh et al., 2021; Lee et al., 2021; Duan et al., 2021; Pham et al., 2020; Alshboul et al., 2024). Sixteen parameters were taken as the input variables to study the factors affecting the overall CS prediction ML model. The parameters included were Ordinary Portland Cement (OPC), Sand (S), Water-to-Binder ratio (W/B), Fly Ash (FA), Ground Slag (GS), Silica Fume (SF), Super Plasticizer (SP), Hydroxypropyl Methylcellulose (HPMC), Water (W), Fiber Volume Fraction (VF), Curing Age (CA), Load Direction (LD), Fiber Diameter (DF), Fiber Length (LF), Aspect Ratio (AR), and Fiber Type (FT). The 3DP-FRC database includes five different fiber types with the codes 1, 2, 3, 4 and 5 for polyethylene (PE), steel, polyvinyl alcohol (PVA), polypropylene (PP), and basalt, respectively. The effect of loading angle on the compressive strength of 3D printed fiber-reinforced concrete has been shown in previous studies (Panda et al., 2017). For this reason, there are usually three loading

directions (X, Y, and Z) for compressive strength testing of 3DP-FRC. X and Y orientations are loading perpendicular and parallel to the printing direction of a single filament, respectively, and Z is loading in the vertical direction. In the database these loading orientations are assigned to the X direction (1), Y direction (2), and Z direction (3).

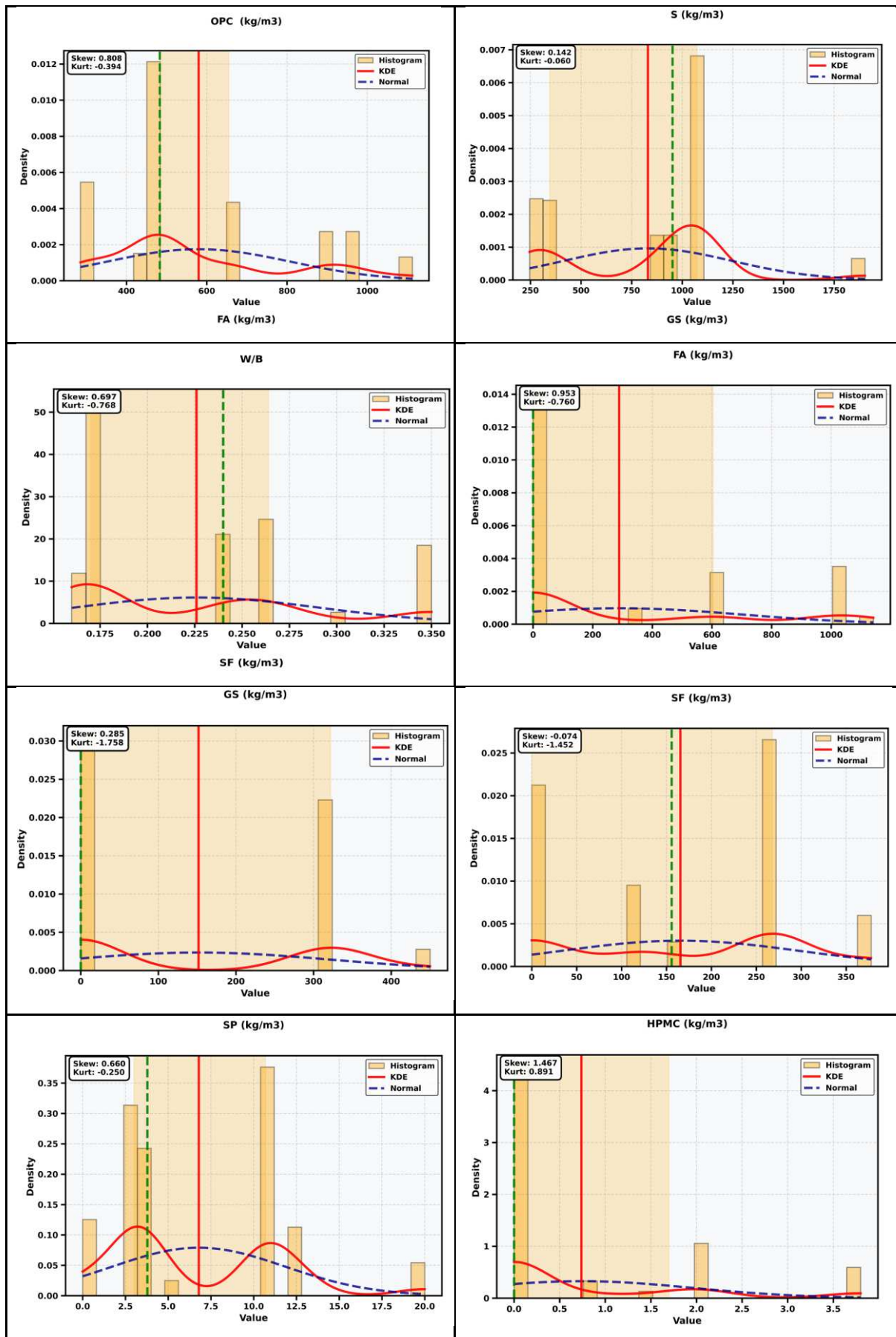
The statistical characteristics of the collected database, including measures of central tendency, dispersion, and distribution shape for both the training and testing subsets, are summarized in Table 2.

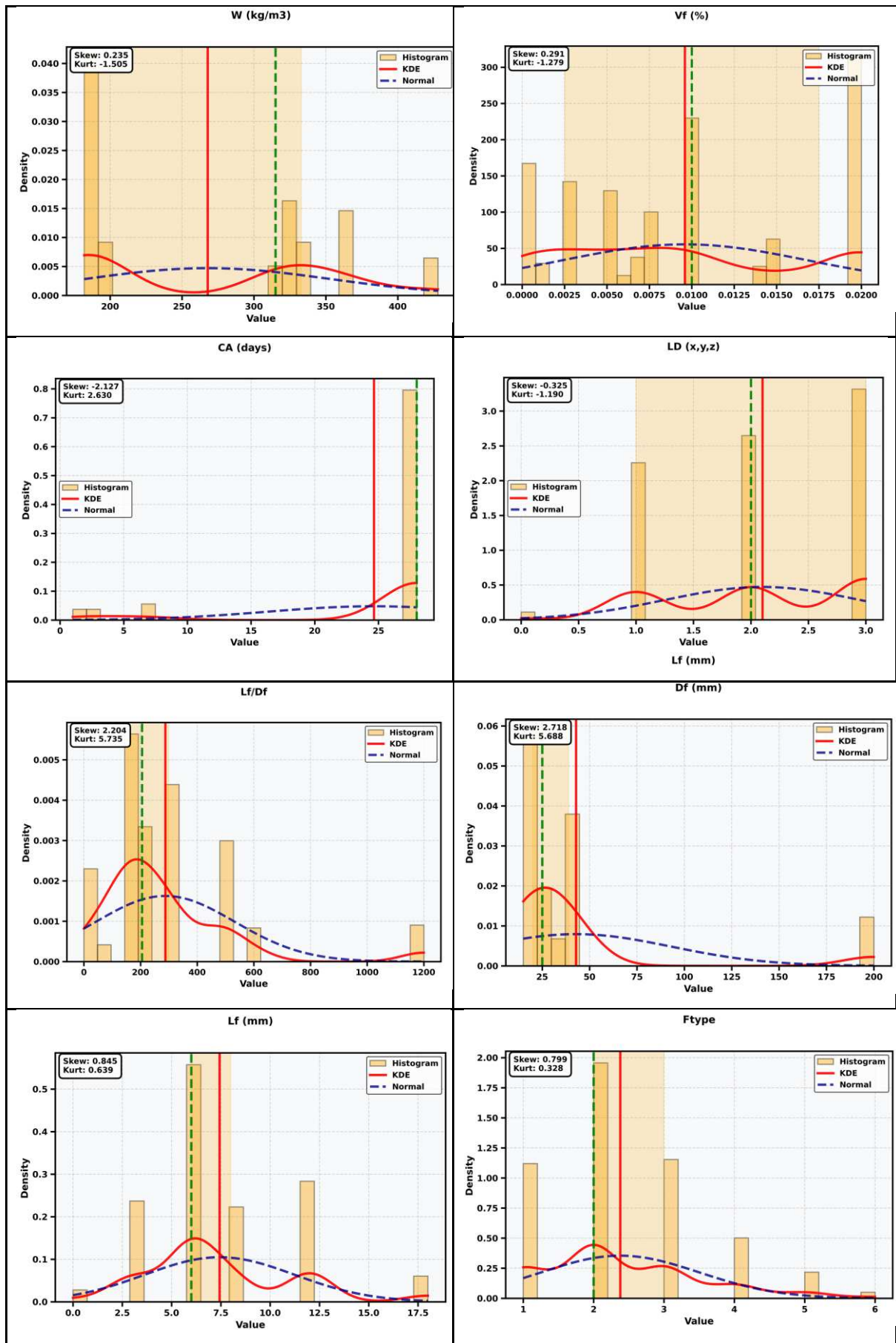
Table 2. Statistical characteristics of the input variables in the training and testing subsets

Training Phase 239							
Feature	Mean	Median	Std	Variance	Maximum	Skewness	Kurtosis
OPC (kg/m3)	578.951	483.000	228.529	52225.276	1112.300	0.838	-0.312
S (kg/m3)	829.054	951.500	421.198	177407.389	1902.000	0.170	-0.072
W/B	0.229	0.240	0.066	0.004	0.350	0.636	-0.861
FA (kg/m3)	292.829	0.000	411.476	169312.764	1141.100	0.935	-0.783
GS (kg/m3)	153.004	0.000	171.330	29353.945	450.000	0.296	-1.751
SF (kg/m3)	160.380	155.700	130.992	17158.776	377.800	-0.031	-1.466
SP (kg/m3)	6.902	3.780	5.001	25.015	20.000	0.703	-0.131
HPMC (kg/m3)	0.703	0.000	1.177	1.385	3.800	1.540	1.221
W (kg/m3)	270.827	315.000	85.109	7243.477	427.900	0.173	-1.526
Vf (%)	0.009	0.008	0.007	0.000	0.020	0.323	-1.265
CA (days)	24.577	28.000	8.476	71.842	28.000	-2.115	2.592
LD (x,y,z)	2.088	2.000	0.848	0.719	3.000	-0.294	-1.239
Lf/Df	298.024	205.128	249.322	62161.384	1200.000	2.139	5.426
Df (mm)	40.640	25.000	47.655	2270.962	200.000	2.964	7.220
Lf (mm)	7.536	6.000	3.886	15.099	18.000	0.790	0.488
Ftype	2.356	2.000	1.132	1.281	6.000	0.810	0.288
Testing Phase 60							
OPC (kg/m3)	583.387	483.000	229.440	52642.834	1112.300	0.723	-0.590
S (kg/m3)	834.677	951.500	391.465	153245.230	1902.000	0.013	0.191
W/B	0.215	0.170	0.061	0.004	0.350	1.001	-0.102
FA (kg/m3)	271.238	0.000	415.311	172483.199	1141.100	1.081	-0.560
GS (kg/m3)	147.033	0.000	164.737	27138.236	450.000	0.244	-1.930
SF (kg/m3)	185.463	268.000	136.011	18498.997	377.800	-0.273	-1.381
SP (kg/m3)	6.340	3.500	5.276	27.833	20.000	0.571	-0.557
HPMC (kg/m3)	0.879	0.000	1.378	1.898	3.800	1.251	0.083
W (kg/m3)	255.805	201.500	83.034	6894.612	427.900	0.507	-1.357
Vf (%)	0.010	0.010	0.007	0.000	0.020	0.182	-1.319
CA (days)	24.933	28.000	7.944	63.114	28.000	-2.284	3.480
LD (x,y,z)	2.150	2.000	0.840	0.706	3.000	-0.471	-0.941
Lf/Df	245.379	162.637	225.402	50806.040	1200.000	2.700	9.348
Df (mm)	51.633	37.000	59.311	3517.829	200.000	2.119	2.761
Lf (mm)	7.033	6.000	3.479	12.101	18.000	1.131	1.908
Ftype	2.467	2.000	1.112	1.236	6.000	0.814	0.829

The mean compressive strength values of the mix constituents in the training subset ($n = 239$) and testing subset ($n = 60$) are closer to each other, as summarized in Table 2, which confirms that there is no systematic bias between the two subsets due to the random partitioning of the database, and that the testing set is statistically representative of the training set. There are several variables with significant non-normality, such as the fly ash (FA) and ground slag (GS), which have medians of zero and positive skewnesses (0.94 and 0.30 in the training set, respectively), indicating that these ingredients are not present in many of the mixes and are only added in certain formulations, and hydroxypropyl methylcellulose (HPMC), which has a median of zero and a skewness of 1.54 in the training set, indicating that it is present in very few of the mixes. Both subsets have the highest skewness (2.14-2.96) and kurtosis (5.4-9.3) values for the fiber geometry parameters L_f/D_f , D_f , and L_f , meaning that there are a few mixes with very high L_f/D_f , D_f , or L_f values, respectively, compared to the rest of the database. The curing age is highly left skewed (-2.12 to -2.28) with the majority of the specimens being tested at the standard 28 day age and a minority being tested at an earlier age. These properties justify the application of ensemble and probabilistic machine learning models, which, in general, are more robust to non-Gaussian and skewed feature distributions than classical linear regression models.

The probability density distributions of the sixteen input variables and compressive strength (CS) are shown in Fig. 1, which displays a histogram, a kernel density estimate (KDE, red curve), and a fitted normal distribution (blue dashed curve) for each variable, with solid red and dashed green vertical lines indicating the mean and median, respectively. The distributions of several cementitious constituents (OPC, W/B, FA, SP, HPMC) are right-skewed and multimodal, and deviate significantly from normality, reflecting the categorical nature of many mix designs of the underlying experimental studies, with only a few discrete dosages tested. The fiber geometry descriptors (L_f/D_f , D_f , L_f) exhibit the highest positive skewness and leptokurtic (sharply peaked) behavior, with a group of low-aspect-ratio fibers and a few long, slender fibers. The age at curing (CA) is highly skewed, with most of the specimens being at 28 days. The output variable compressive strength (CS, panel q) is relatively closer to a bimodal distribution centered around 30 MPa and 90 MPa, which is in line with the fact that relatively weak fiber-reinforced mixes and high strength, densely packed mixes (such as mixes with steel fibres) co-exist in the database. This lack of uniformity in the feature and target distribution is another reason why tree-based and kernel-based machine learning algorithms are well suited for this task, as they do not require normally distributed inputs, as does classical parametric regression techniques.





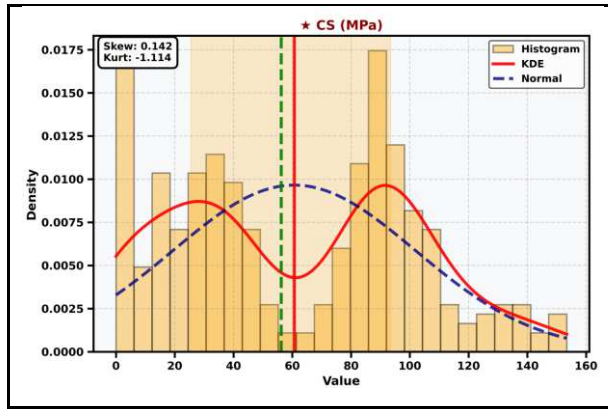


Fig. 1. Probability density distributions of the model variables

The sixteen input parameters and the output compressive strength (CS) are plotted in a lower triangular Pearson correlation matrix in Fig. 2, which shows the pairwise linear relationships. The water content (W) is the variable most strongly negatively correlated with r ($r = -0.82$), as expected given that the strength of 3D printed cementitious composites is conventionally related to water content. Silica fume (SF) exhibits the strongest positive correlation with r ($r = 0.94$), consistent with its well-established pozzolanic and pore-refining effect on the microstructure of 3D printed cementitious composites. The water-binder ratio (W/B) and the amount of fly ash (FA) are also negatively correlated with CS ($r = -0.84$ and -0.59 , respectively). The mix design variables are also correlated with each other, with several values above 0.70, suggesting that these variables are not independent of one another, but are adjusted together in the experimental mix designs compiled from the literature - most notably between fiber length and fiber diameter (Lf-Df, $r = 0.86$), fiber diameter and HPMC dosage ($r = 0.85$), and W/B with SF ($r = -0.86$). The correlation between CA and CS is weak to moderate ($r = 0.43$) indicating that hydration effects are secondary to the effects of mix proportioning within the range of 1-28 days of curing age. There are comparatively weak linear correlations between Ftype and LD and CS ($r = -0.14$ and -0.12 , respectively), suggesting that they may have more of a nonlinear or conditional effect on strength, further supporting the use of a multivariate, nonlinear machine learning approach used in this study.

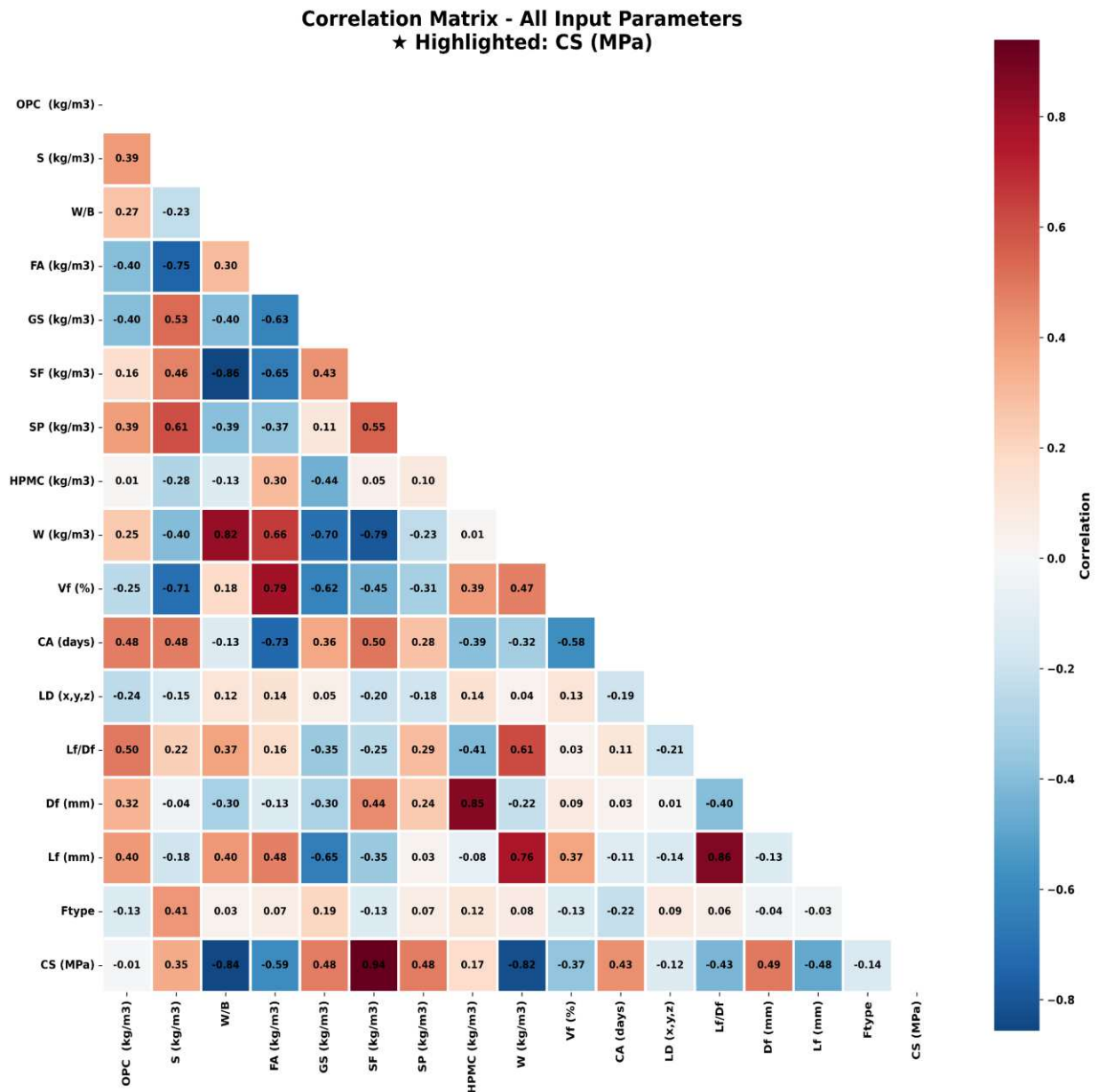


Fig. 2. Lower-triangular Pearson correlation matrix

3. Methodology

In this study, four machine learning models with different learning paradigms were chosen for the prediction of compressive strength of 3DP-FRC: CatBoost, NGBoost, Random Forest (RF), and Support Vector Machine (SVM). CatBoost uses ordered boosting with symmetric decision trees, which helps to minimize overfitting and prediction shift and works with categorical features like fiber type and loading direction natively. NGBoost is an extension of conventional boosting that models the expected compressive strength and its uncertainty of prediction using a probabilistic distribution, with the help of natural-gradient optimization. Ensemble methods like RF are based on bagging, which involves creating multiple decision trees on random samples of the data, using random feature subsets for each split, and averaging. In SVM, the

mix design and printing parameters are projected into a higher dimensional space using kernel functions, which are able to capture the relationship between the variables in a non-linear manner, compressing the compressive strength. These four models cover gradient boosting, probabilistic boosting, bagging ensembles and kernel-based regression, which allows a thorough comparison of predictive mechanisms under a common preprocessing, hyperparameter optimization, and validation framework, and facilitates the reliable identification of the best performing model for 3DP-FRC strength prediction.

3.1 Brief overview of Models

The four selected models represent different parts of the non-linear relationships between the sixteen-mix design and printing parameters and compressive strength: CatBoost and NGBoost are boosting models, RF is a randomized decision tree ensemble, and SVM is a kernel based non-linear mapping. All models were trained and tested in the same framework to make a fair comparison on the predictive performance and generalization capability of all models. Then SHAP, LIME and Partial Dependence Plots (PDP) were applied to quantify feature contributions and characterize the global and instance-level effects of each feature on predicted compressive strength further elucidating the relationships learned by the best-performing model. Below are described the principles underlying each model briefly.

3.1.1 CatBoost Model

CatBoost is a modern gradient boosting system developed by (Prokhorenkova et al., 2018; Dorogush et al., 2018) that is able to work with categorical data and reduce information loss. It has proven to be very predictive in structured tabular data, especially in problems with non-linear relationships between the input variables. The CatBoost has been widely used in the field of data-driven prediction tasks in different engineering fields thanks to its powerful boosting structure, anti-overfitting, and good generalization ability. CatBoost was chosen as one of the benchmark machine-learning models for the present study because it is well suited for nonlinear regression and has shown to be reliable on the mixed engineering datasets. Note that the categorical information in the compiled database was fed into the modeling process by preprocessing prior to the training of the model (Diao et al., 2019; Fan et al., 2020; Xia et al., 2020). The application of CatBoost with optimization methods and SHAP-based interpretation to predict the mechanical response of reinforced concrete members has been recently integrated in order to make it as an accurate and interpretable model for structured engineering datasets (Zhang et al., 2026). In recent years, some methods have included synthetic data generation and stacking ensemble methods to enhance data diversity, and fuse the prediction power of various models (Liu et al., 2026). These techniques were not adopted in the current research,

but they give directions for future improvement of the proposed framework. In this study, CatBoost was therefore mainly evaluated as an algorithm for structured prediction that can be used to efficiently handle categorical features.

3.1.2 Random Forest Model

Random Forest (RF) is a powerful, non-parametric ensemble learning algorithm which is commonly employed for regression and classification tasks. During training, the algorithm builds many decision trees that make independent predictions, and then averages the results of these predictions to get the final prediction. This ensemble approach not only enhances the predictive power but also mitigates the high variance and overfitting that are common in single decision tree models (Shoar et al., 2022). RF builds multiple decision trees with randomly selected subsets of the training data and feature space. The trees are trained separately and their predictions are then combined to get the final prediction (Liu et al., 2021; Hussien et al., 2023). This inherent randomness enables the model to capture complex patterns while reducing the risk of overfitting commonly observed in single decision trees. For a new input sample x , the final aggregated prediction $\hat{y}_{RF}$ is obtained by calculating the arithmetic mean of the predictions generated by all BB trees (Kim et al., 2024).

$$\hat{y}_{RF} = \frac{1}{B} \sum_{b=1}^B T_b(x) \quad 1$$

This ensemble approach enables RF to effectively capture complex and nonlinear patterns. It can handle various types of data, and it is also interpretable due to its intrinsic ranking feature importance, which makes it valuable for applications like materials design and optimization.

3.1.3 Support Vector Machine Model

Supervised machine-learning algorithm, called Support Vector Machine (SVM), is widely used for classification and regression. The basic idea behind SVM is to find an optimal hyperplane which maximizes the separation between the different classes in the feature space. It uses the kernel trick to map nonlinear feature spaces into higher dimensional linear spaces, thus increasing the computational efficiency (Wang, 2022). SVM aims to find a decision boundary which is well-generalizable for unseen data.

$$\min_{w,b} \frac{1}{2} \|w\|^2 + C \sum_{i=1}^n \xi_i \quad 2$$

Here, (w) represents the weight vector, (b) denotes the bias term, ξ_i is the slack variable accounting for misclassification, and (C) represents the regularization parameter.

3.1.4 Natural Gradient Boosting Model

In real-world applications, uncertainty in machine-learning predictions is a key factor. In addition to the correct prediction, users need the reliable estimate of the uncertainty of each prediction. This is in contrast to gradient boosting which provides only a point estimate, and in this context NGBost is a combination of generic probabilistic prediction with gradient boosting that gives a robust uncertainty quantification, an efficient way to estimate the predictive uncertainty by generating a complete probability distribution over the outcome space (Duan et al., 2020). The objective of NGBost is to estimate the parameters of a conditional probability distribution $P_\theta(y | x)$ as functions of x using boosting techniques, where $\theta \in \mathbb{R}^p$ denotes the parameter vector of the distribution. NGBost comprises three abstract and modular components: (i) the base learners f , (ii) the parametric probability distribution P_θ , and (iii) the scoring rule $\mathcal{S}$.

For probabilistic forecasting using NGBost, the forecast $y | x$ for a new input x is represented by the conditional probability distribution (P_θ). Here, the parameters θ are obtained by combining the outputs of M base learners with the initial parameter $\theta^{(0)}$. Given a dataset $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$ ($x_i \in \mathbb{R}^D, y_i \in \mathbb{R}$), the parameters of the probability distribution are first initialized as follows:

$$\theta^{(0)} = \operatorname{argmin}_{\theta} \sum_{i=1}^n \mathcal{S}(\theta, y_i) \quad 3$$

where n denotes the total number of training samples. Subsequently, the parameters are updated sequentially over M iterations. At each iteration, for every sample (x_i, y_i) , the natural gradient $g_i^{(m)}$ of the scoring rule $\mathcal{S}$ is computed with respect to the current conditional probability distribution $P_{\theta^{(m-1)}}(y_i | x_i)$.

$$g_i^{(m)} = \mathcal{J}_{\mathcal{S}}(\theta_i^{(m-1)})^{-1} \nabla_{\theta} \mathcal{S}(\theta_i^{(m-1)}, y_i) \quad 4$$

where $\mathcal{J}_{\mathcal{S}}(\theta_i^{(m-1)})$ denotes the Riemannian metric of the statistical manifold at θ , while $\nabla_{\theta} \mathcal{S}(\theta_i^{(m-1)}, y_i)$ represents the ordinary gradient. The estimated natural gradients $g_i^{(m)}$ are then

used to train the base learner $f^{(m)}$ at iteration m using the corresponding input vectors x_i . Subsequently, the stage-specific scaling factor $\rho^{(m)}$ is estimated as:

$$\rho^{(m)} = \operatorname{argmin}_{\rho} \sum_{i=1}^n \mathcal{S}(\theta_i^{(m-1)} - \rho \cdot f^{(m)}(x_i), y_i) \quad 4$$

Finally, using $\rho^{(m)}$ and the common learning rate η , the parameters for each sample are updated as follows:

$$\theta_i^{(m)} = \theta_i^{(m-1)} - \eta \left(\rho^{(m)} \cdot f^{(m)}(x_i) \right) \quad 5$$

3.1.5 Partial dependence plot (PDP)

Partial dependence plot (PDP) analysis is a useful approach to explain the individual or joint impact of selected features on the prediction made by a machine learning model (Zhang et al., 2020). Partial dependence plots can show if the mapping between the output parameter and input variables is relatively simple or complex (Tran et al., 2022). The PDP function is the average prediction of a value of a variable when the parameter values are held constant for the dataset while the value of the variable changes. Important, PDPs are produced without changing the other features, allowing for a focused evaluation of the average impact of a specific feature on model predictions (Li et al., 2022)]. PDPs are computed by either fixing the value of all the other input variables and varying one input variable (1D-PDP) or fixing the values of all the other input variables and varying two input variables (2D-PDP) to determine the effect of each input variable on the output accurately (Zhang et al., 2020).

3.1.6 Shapley additive explanations (SHAP)

SHAP is a framework designed to explain the predictions made by machine learning models by assigning a "SHAP value" to each feature in the model. SHAP values are based on the principles of cooperative game theory and offer a holistic framework for understanding the results of machine learning models (Zheng et al., 2023). These values measure the contribution of individual parameters to the predictions accounting for the interaction among the parameters and all combinations of features (Ekanayake et al., 2022). Thus, SHAP serves as a valuable tool for evaluating and understanding the importance of features in predictive models, highlighting which parameters are most significant for a particular prediction and how much each parameter contributes to the result (Haque et al., 2023).

3.1.7 Local interpretable model-agnostic explanations (LIME)

LIME is a unique interpretable AI framework that explains predictions on an individual-instance basis, focusing on the preservation of local fidelity by a model, regardless of its architecture. Local fidelity allows the properties of the property to be explored in the context of the particular prediction, assuring the correctness of the representation of the model. But perfect correspondence with the model may not always be possible; sometimes local fidelity may explain the process by which a prediction is generated. To explain a prediction and to determine whether the local neighborhood of that prediction is reliable, LIME looks at the neighboring instances, and may highlight features that are influential in that local neighborhood, exploring the neighborhood surrounding the prediction to provide insight into the algorithm's reasoning. This is especially true when the outcome is correct, but the factors that generate the outcome are not included in the general modeling framework (Ribeiro et al., 2016).

3.2 Hyperparameter tuning

The hyperparameters of each model were optimized by systematically searching over a set of predefined hyperparameter ranges and selecting the best performing model based on cross-validation on the training subset, to reduce the risk of overfitting and to maximize predictive performance. The number of iterations, tree depth, learning rate, subsampling ratio and L2 leaf regularization were optimized for CatBoost for the trade-off between model complexity and generalization. To achieve a stable natural-gradient boosting process with good uncertainty estimates, NGBoost was tuned by varying the number of estimators, learning rate, and minibatch fraction. The parameters of the number of trees, maximum depth, feature subsampling ratio and minimum split/leaf sample constraints were tuned to control variance without excessive pruning of tree growth for RF. The SVM kernel type, penalty parameter (C), gamma, and epsilon were optimized to capture the non-linear relationship between mix design and printing parameters and compressive strength, without overfitting the training data, for SVM. To guarantee repeatability, a fixed random seed was used in all models. The best hyperparameter settings found for each model are shown in Table 3.

447 **Table 3.** Optimal hyperparameter configurations obtained for each regression model

Model	Hyperparameters
CatBoost	iterations = 700, depth = 5, learning rate = 0.07, subsample = 0.9, l2_leaf_reg = 1, border_count = 32, loss/eval metric = RMSE, random seed = 42
NGBoost	n_estimators = 700, learning rate = 0.07, minibatch_frac = 0.7, col_sample = 1.0, natural_gradient = True, tol = 1×10^{-5} , random state = 42
SVM	kernel = RBF, C = 1000, gamma = auto, epsilon = 0.05, degree = 5, tol = 1×10^{-4} , max_iter = 50 000
Random Forest	n_estimators = 500, max_depth = 12, max_features = 0.5, min_samples_split = 2, min_samples_leaf = 1, min_impurity_decrease = 5×10^{-4} , ccp_alpha = 5×10^{-4} , random state = 42

448

449 **3.3 Cross-Validation and Generalization Testing**

450 The cross-validated mean squared error (MSE) computed during randomized hyperparameter
451 search was computed on the same partition of training data that was used for hyperparameter
452 search and internal evaluation of the model; therefore it is not indicative of the predictive
453 stability of the finalized model, but rather the performance of the model-selection procedure.
454 For each optimized model, hyperparameter optimization was then repeated with the same
455 models evaluated again with repeated 5-fold cross validation (RepeatedKFold) to separate
456 hyperparameter optimization from model evaluation, resulting in 25-fold-wise evaluations per
457 model. For each split the model was retrained with the finalized hyperparameters and the
458 coefficient of determination (R^2), root mean squared error (RMSE), and mean absolute error
459 (MAE) were calculated for the held-out fold. These were presented as mean $\pm$ SD for the 25
460 splits, reflecting the variation in performance as a result of the training/validation split.
461 This repeated cross-validation was also independent of the final generalization assessment,
462 performed on a 20% unseen test set that was not used in the development of the models. The
463 test-set predictions were resampled with replacement (1000–2000 times) to estimate percentile-
464 based confidence intervals for R^2 , RMSE and MAE. Thus, repeated cross validation gives an
465 idea of the sensitivity of model performance to data partitioning, while the bootstrap confidence
466 intervals give an idea of the uncertainty of the final test-set performance estimates. The two
467 complementary evaluation stages together offer strong evidence for the stability of the model
468 and for its generalization ability, which is well known, as a single train–test split may give an
469 overly optimistic, or unstable, estimate of predictive performance.

470 **3.4 Computational Environment**

471 The machine learning models were built using Python programming language in the Jupyter
472 Notebook environment. The models were developed, data were preprocessed using the Scikit-

learn library, and hyperparameter optimization was done using RandomizedSearchCV. Hyperparameter search was done using RandomizedSearchCV, and cross-validation was done using KFold/RepeatedKFold, while NGBoost was implemented using the dedicated ngboost library. Data handling, statistical computations were performed using NumPy, Pandas and SciPy, and visualizations were made using Matplotlib and Seaborn. The interpretability of the models was evaluated with SHAP for feature attribution at the global and local level, LIME for explanation at the instance level and with PDP to characterize the relationships between the features and the response, while taking into account the correlations between the features; the trained models were serialized using Joblib to ensure the models' reproducibility. The interactive prediction interface was created with the Tkinter library in Python, as described in Section 3.5. All calculations were carried out on a workstation with Intel Core i5 (10th generation) processor and 16 GB of RAM memory running the Windows operating system.

3.5 Performance Evaluation Metrics

Model performance was measured by five complementary measures because no single measure can measure the accuracy of prediction, magnitude of error, and practical reliability. The proportion of variance in the experimental compressive strength explained by each model was quantified by R^2 , while RMSE, MSE and MAE were used to measure the magnitude of the prediction error, with RMSE and MSE being formulated in terms of squared prediction errors. R^2 was used to quantify the proportion of variance in the experimental compressive strength explained by each model, while RMSE, MSE and MAE were used to assess the magnitude of the prediction error, with RMSE and MSE being formulated in terms of squared prediction errors. The maximum error was also reported to accentuate the largest individual error, especially when considering the safety concerns when underpredicting concrete compressive strength. All metrics were calculated independently for the training set and the test set in order to differentiate between model fit and model generalisation. The mathematical expressions and typical ranges of interpretation of these metrics are summarized in Table 4.

Table 4. Mathematical expressions and standard ranges of the evaluation metrics

Name of Criteria	Expression	Standard Range
Root Mean Squared Error (RMSE)	$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2}$	≥ 0 (0 indicates smallest error)

Coefficient of Determination
(R^2)

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$$

0–1 (1 indicates
strongest
agreement)

Mean Absolute Percentage
Error (MAPE)

$$MAPE = \frac{100}{n} \sum_{i=1}^n \left| \frac{y_i - \hat{y}_i}{y_i} \right|$$

≥ 0 (0 indicates
smallest error)

Mean Squared Error (MSE)

$$MSE = \frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

≥ 0 (0 indicates
smallest error)

Mean Absolute Error (MAE)

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i|$$

≥ 0 (0 indicates
smallest error)

Note: n represents the number of samples. y_i represents the experimental compressive strength, $\hat{y}_i$ represents the predicted compressive strength, $\bar{y}$ represents the mean experimental value, and N represents the number of predictions within the defined error threshold.

4. Results and Discussion

The section introduces and analyzes the predictive performance, error characteristics, statistical evaluation, interpretability, practical application and engineering implications of the four machine-learning models created to predict compressive-strength of 3D-printed fibre-reinforced concrete. The results are presented in a progressive way, starting from direct predictive performance and error analysis, and then to the interpretation of the relationships learned by the models and their application. In Sections 4.1–4.3, the predictive performance of the Support Vector Machine (SVM), Random Forest (RF), CatBoost and the Natural Gradient Boosting (NGBoost) models is assessed by comparing the experimental measurements with the predictions of these models, residual-error analysis, and Taylor-diagram analysis. In Sections 4.4–4.6, the learned prediction behaviour is explored through the lens of three methods: learned influential variables, local and global contributions, and characterising the nonlinear response patterns. The practical application of the NGBoost model is explained in Section 4.7 using an interactive graphical user interface (GUI) for prediction, uncertainty estimation, and interpretation using SHAP. The findings from the predictive and diagnostic, interpretability, and deployment are combined into an overall interpretation in Section 4.8. The practical application of the developed framework to assess and plan 3DP-FRC mixtures for preliminary experiments is discussed in Section 4.9, and the shortcomings of the present study are outlined and directions for future research are identified in Section 4.10.

4.1 Predictive performance: experimentally measured–predicted scatter plots

The observed-predicted relationships of the compressive strength are shown in panels (a)–(d) of Figure 3 for the support vector machine (SVM), Random Forest, CatBoost and NGBost models, respectively. In each of the four models, the values predicted within the full testing range are tightly clustered around the 1:1 reference line, which demonstrates that the learned mappings are able to capture the experimentally measured compressive-strength trend for both low- and high-strength mixtures. Importantly this agreement is not restricted to a narrow zone in the middle of the response, a property which is especially significant for a database with a significant variation in binder composition, water availability, fibre content, fibre geometry, curing age and loading direction. The algorithm that performs best in the middle of the distribution would be of limited use for a data set like this that is heterogeneous and multi-factorial, and the results shown in Figure 5 suggest that this is not a significant drawback for any of the four algorithms.

As shown in Figure 3a, SVM has a good agreement between experimental and predicted results with a testing RMSE of 6.663 MPa and MAE of 4.693 MPa. Random Forest (Figure 3b) yields a much more compact distribution and a testing R^2 of 0.9858 and RMSE of 5.287 MPa. CatBoost (Figure 3c) also shows a very close relationship with 1:1, and has the lowest testing MAE (3.803 MPa), with the smallest mean absolute error of the experimentally measured strengths. NGBost (Figure 3d) has the highest testing R^2 (0.9877), lowest testing RMSE (4.904 MPa) and the lowest maximum error (13.690 MPa). The four models show consistently good predictive performance and the error profiles vary in ways that can only be fully resolved by considering several complementary measures of performance together and not any one measure alone. The detailed training and testing performance metrics of all four models are presented in Table 5.

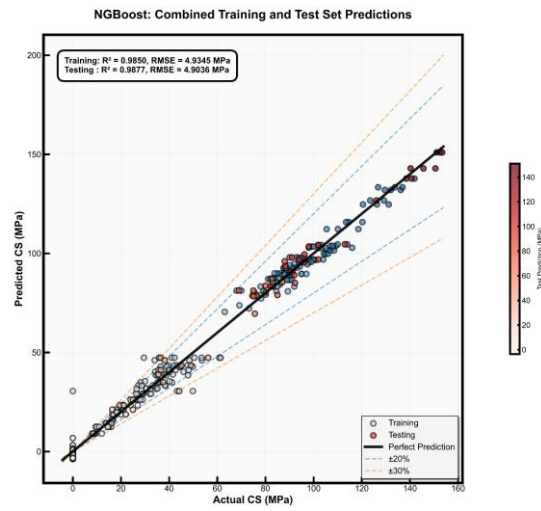
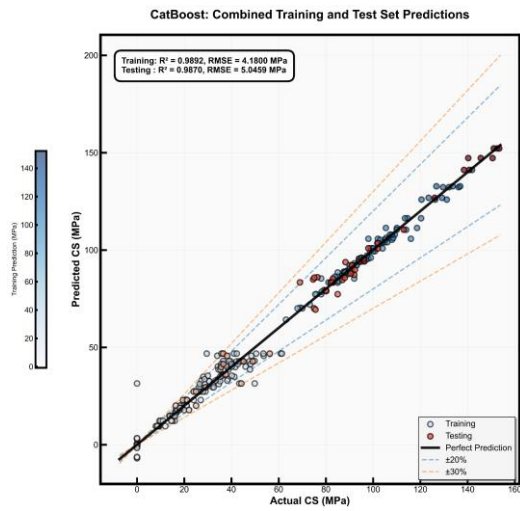
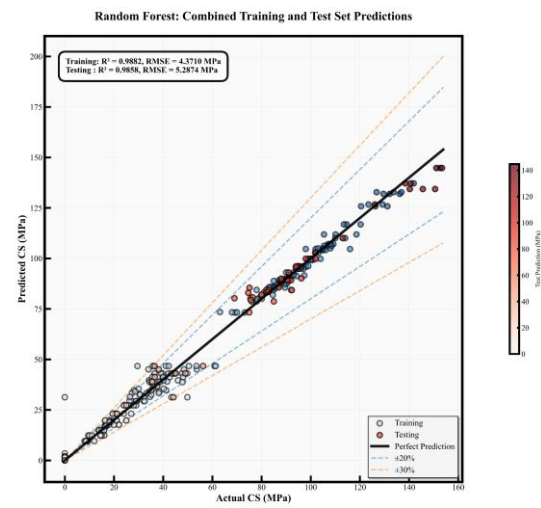
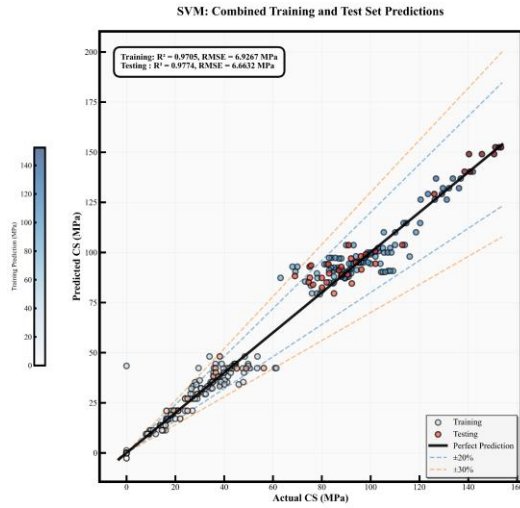


Fig. 3. Experimentally measured versus model-predicted compressive strength for (a) SVM, (b) Random Forest, (c) CatBoost and (d) NGBoost.

Table 5. Performance comparison of the machine learning models on the training and test datasets

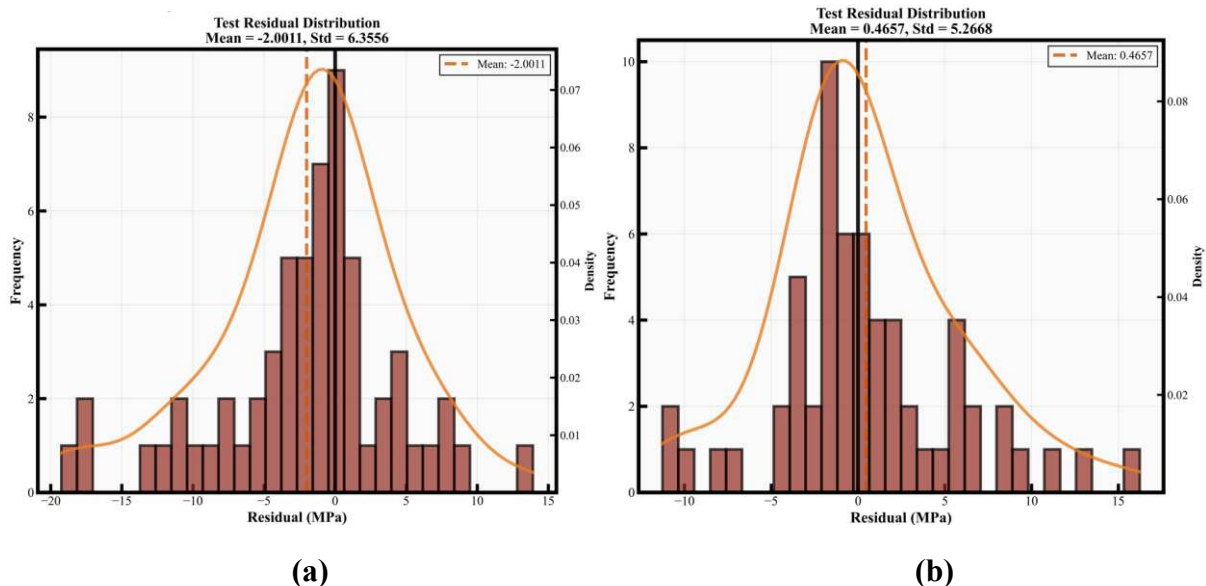
Model	Training set			Test set			
	MAE	RMSE	R^2	MAE	RMSE	R^2	Max error
SVM	3.951	6.927	0.971	4.693	6.663	0.977	19.256
Random Forest	2.592	4.371	0.988	3.837	5.287	0.986	16.231
CatBoost	2.335	4.180	0.989	3.803	5.046	0.987	14.378
NGBoost	3.407	4.935	0.985	3.839	4.904	0.988	13.690

MAE, mean absolute error; RMSE, root mean squared error; R^2 , coefficient of determination. Bold values indicate the best result in each column.

4.2 Residual-error distribution

To determine if the high predictive accuracy seen in the measured–predicted comparisons were due to systematic bias or too much error dispersion, residual analysis was conducted, an analysis that is critical to ensure that the high R^2 was not the result of the model being well-calibrated but biased or that errors were simply correlated with the response. As can be seen in Fig. 4, the testing residuals of all four models are centred around zero, but the spread of the testing residuals appreciably varies. SVM has the largest residual spread with a mean residual of -2.001 MPa and a standard deviation of 6.356 MPa. Random Forest gives a small positive mean residual of 0.466 MPa, whereas CatBoost and NGBoost give mean residuals of -0.323 and -0.362 MPa, respectively.

The size of the signed residual is small for Random Forest, CatBoost and NGBoost, suggesting that on average these models do not have strong over/under prediction tendencies in their testing predictions, while the four models do not show evidence of strong over/under prediction tendencies. Additionally, NGBoost has the smallest residual standard deviation (4.890 MPa), and CatBoost has a similar small distribution of the residuals, with Random Forest having a slightly larger spread. Together with Section 4.1, the residual distributions suggest that the high R^2 values are not merely due to a good central trend that would otherwise obscure systematic deviations in the tails of the distributions, but rather due to controlled prediction errors. The detailed testing residual statistics for the four investigated models are presented in Table 6.



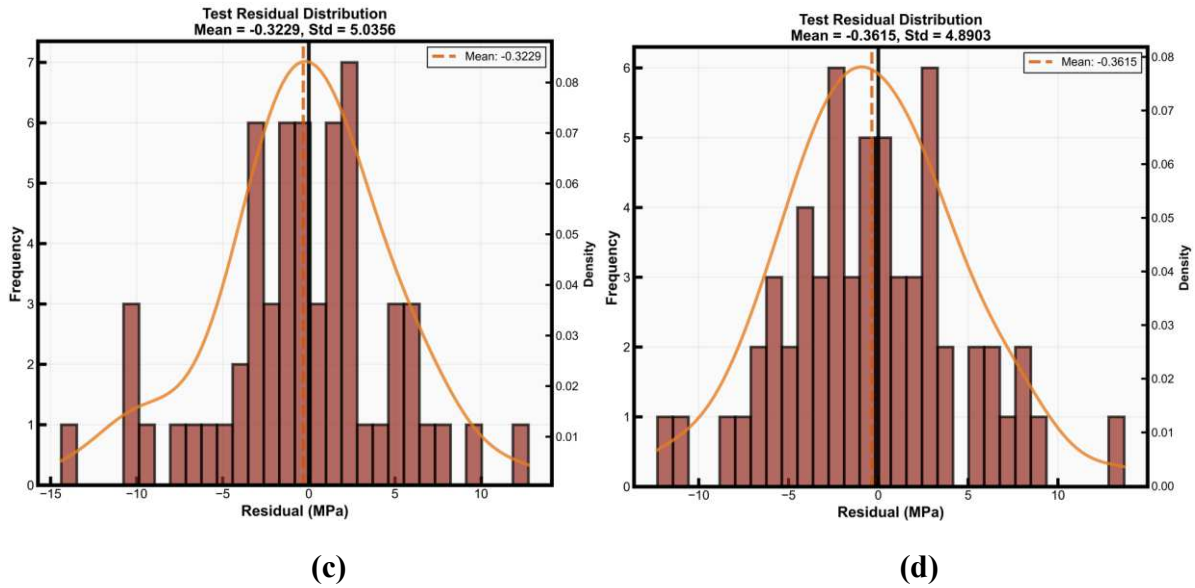


Fig. 4. Testing residual-error distributions for (a) SVM, (b) Random Forest, (c) CatBoost and (d) NGBost

Table 6. Mean and standard deviation of prediction residuals for the machine learning models on the test set

Model	Mean residual (MPa)	Residual SD (MPa)
SVM	-2.001	6.356
Random Forest	0.466	5.267
CatBoost	-0.323	5.036
NGBost	-0.362	4.890

Residual = experimental – predicted (MPa). Bold values indicate the mean residual closest to zero and the lowest residual standard deviation.

4.3 Taylor-diagram assessment of training and testing performance

The Taylor diagrams in Fig. 5 are used to complement the statistical evaluation of the model predictions, as they show the correlation, the standard deviation and the centred root-mean-square difference in a single polar representation. It is useful, because the three statistics can be considered together and not in turn, and because it shows departures from the reference experimental distribution graphically. The training diagram (Fig. 5a) shows that all models result in a response that has a high correlation with the principal statistical structure of the training response. The R^2 values of the training data for the CatBoost and Random Forest models are 0.9892 and 0.9882, respectively, which is why they are closest to the reference experimental distribution. NGBost also retains a relatively small deviation from the reference state while SVM has a relatively large deviation in its statistical representation of the response.

The high-correlation behaviour is maintained for experimental records which are not used in the model fitting process, as shown in the independent testing diagram of Fig. 6b, which is a more stringent and practically relevant test of generalisation. The ensemble models are not far from the reference standard-deviation and low-error region, while NGBoost has the highest correlation with the lowest testing RMSE. The similarity of the training and testing representations suggests that the dominant statistical structure that is learned during model development is preserved under independent evaluation, thus offering converging evidence (along with the scatter and residual analyses of Sections 4.1 and 4.2) that the reported performance is a true indication of a generalisable predictive relationship, and not simply a product of memorising the training set.

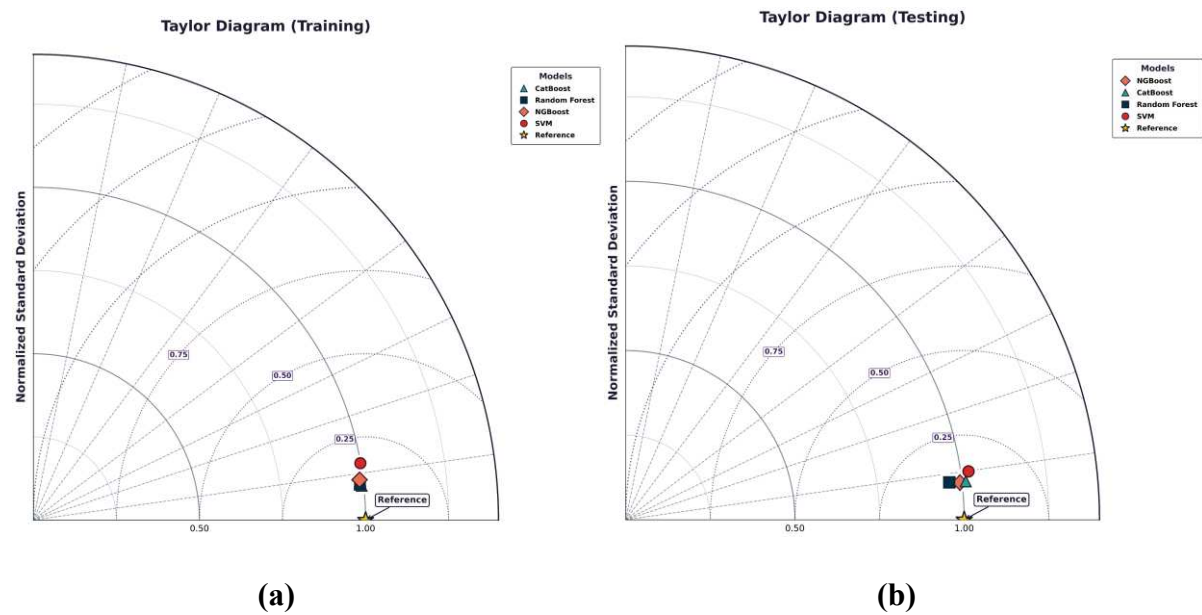
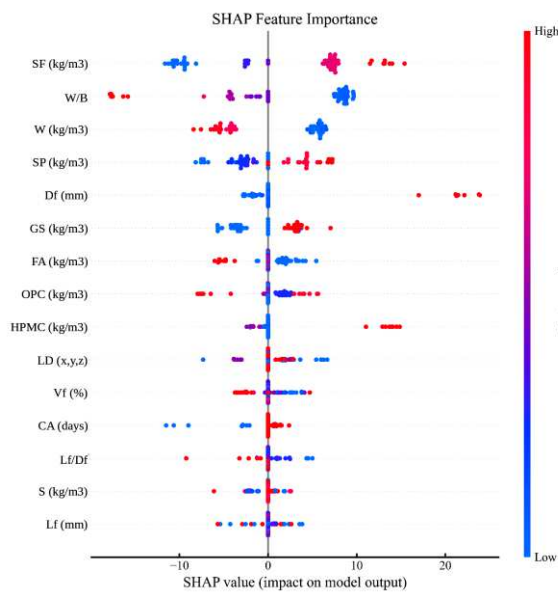


Fig. 5. Taylor-diagram comparison of model performance for (a) the training subset and (b) the independent testing subset

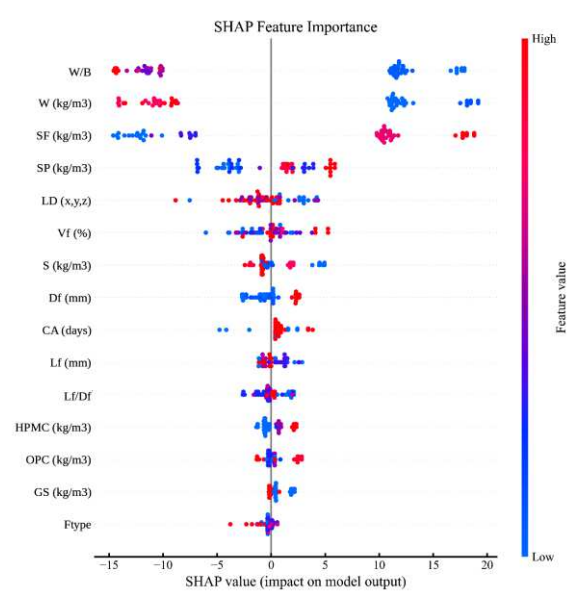
4.4 SHAP-based global interpretation

To quantify the contribution of individual input variables to the model predictions, and to compare feature-attribution patterns across the four algorithms, SHapley Additive exPlanations (SHAP) analysis was used. The water-to-binder ratio (W/B), water content (W), silica fume (SF), superplasticizer (SP), loading direction (LD) and fibre volume fraction (Vf) are repeatedly found among the most influential variables as shown in figure 6. These variables are common to four structurally different algorithms (a kernel-based method, a bagged tree ensemble, and two boosted tree ensembles) suggesting that the principal predictive signal arises from a property of the mixture–process–property relationship, not an artefact of the learning algorithm and inductive bias.

The water-to-binder ratio (W/B and W) makes particularly strong contributions across the models, highlighting the significance of water availability and the concentration of the binders within the predictive relationships learnt, in line with the established primary role of the water-to-binder ratio as a determinant of the formation of hydration products and capillary porosity in cementitious systems. The influence of pore refinement and rheological workability during the extrusion process is also largely represented by SF and SP, while the influence of printing related anisotropy and fibre reinforcement are captured by LD and Vf, respectively. The other variables, such as fibre diameter, fibre length, aspect ratio, fibre type, hydroxypropyl methylcellulose (HPMC), curing age and aggregate-related variables, have lower relative contributions but can also be relevant through nonlinear effects and interactions. It is therefore legitimate to interpret the SHAP results as a multi-factor result, with compressive strength being related to the combined effect of mixture chemistry, mixture rheology, fibre architecture, curing and loading orientation, instead of one of these factors being the dominant cause.



(a)



(b)

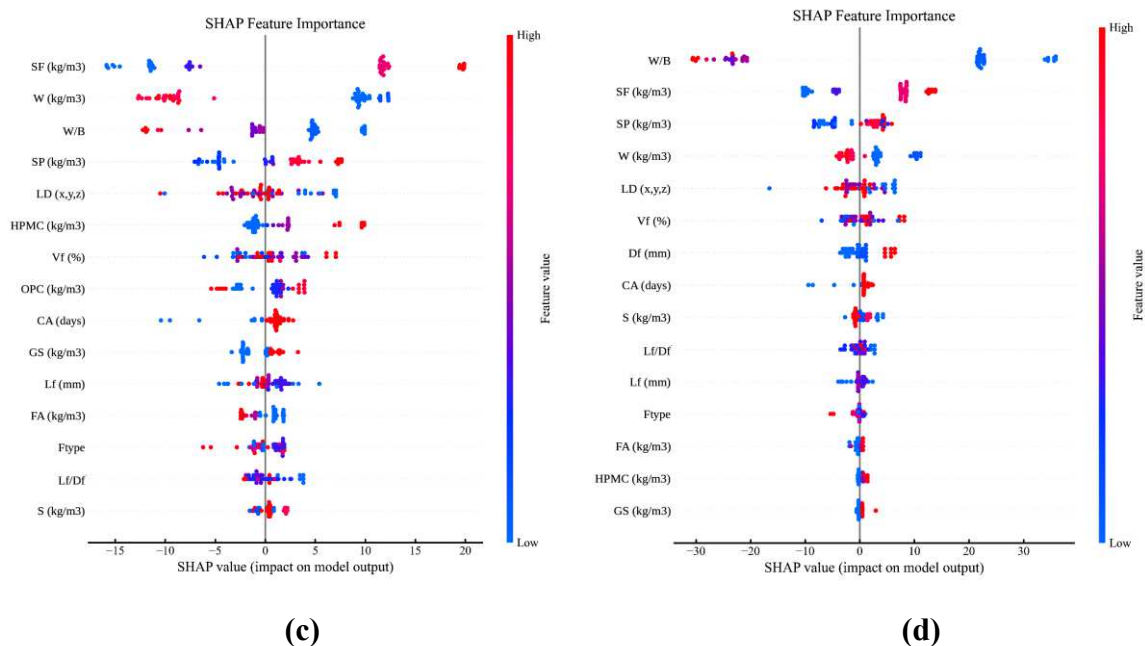


Fig. 6. SHAP feature-attribution patterns for (a) SVM, (b) Random Forest, (c) CatBoost and (d) NGBoost

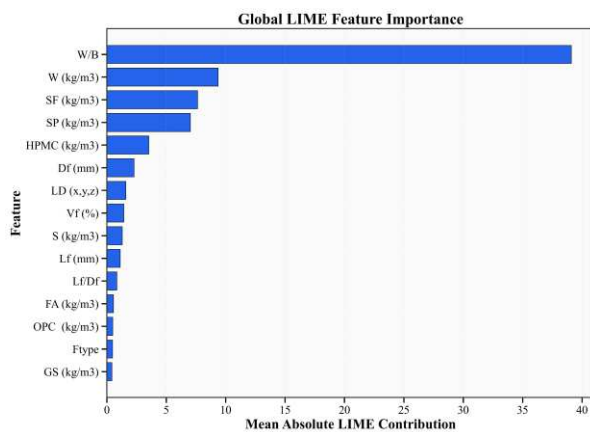
4.5 LIME-based local interpretation and stability

To complement the global SHAP analysis, local Interpretable Model-agnostic Explanations (LIME) were employed to explore local feature contributions and stability of the explanations generated per prediction. The importance pattern of the global variables (Figure 7a) is dominated by W/B, followed by W, SF and SP. This ordering is in line with the SHAP analysis and offers an independent, local-surrogate view of the key drivers, enhancing confidence that the identified variables are indeed drivers and not a methodological artifact of either ordering method.

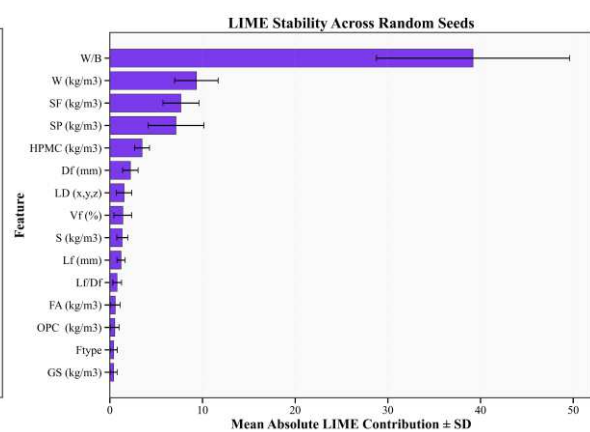
As seen in the stability analysis (Fig. 7b), W/B, W, SF and SP are still the most prominent variables in repeated local explanations, while lower-ranked variables have a higher relative variation. The local-error analyses also indicate that the sign and the size of a feature contribution can be different for different experimental records: for example, the local sign of W/B is case dependent, and it has a strong contribution overall. Therefore, the importance of a particular feature should not be seen as a universal monotonic relationship for all mixtures, but rather the contribution of the variable to the model is dependent on the local interaction with the other input variables, which is the motivation for the partial-dependence analysis discussed in Section 4.6.

The local explanations for the maximum-error and median-error cases are shown in Figs. 7c and 7d, respectively. In both records, W/B makes by far the largest positive contribution

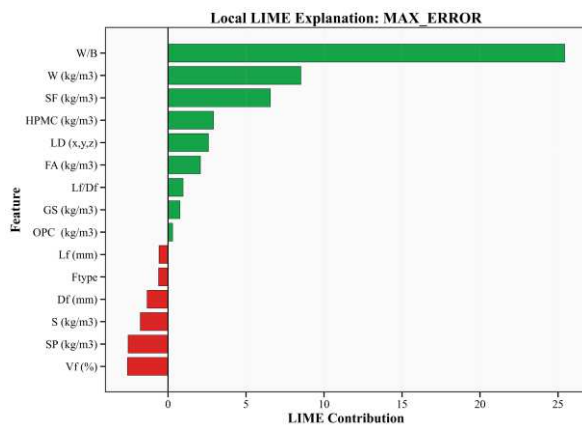
(approximately 25 on the LIME contribution scale), which is consistent with its dominant global rank in Fig. 7a. Beyond W/B, however, the ranking and even the sign of several variables differ between the two records. For the maximum-error case (Fig. 7c), W (about 8.5) and SF (about 6.6) are the next largest positive contributors, followed by smaller positive contributions from HPMC, LD and FA, whereas Vf, SP, S and Df contribute negatively. For the median-error case (Fig. 7d), SP (about 11), W (about 10) and SF (about 9) all contribute strongly and positively, and HPMC becomes the largest negative contributor (about -4), followed by Df, Vf and Lf. SP and HPMC therefore reverse their local sign between the two records, which supports the observation that the influence of a variable depends on the local mixture context and not on a fixed monotonic trend. The fibre-related variables (Vf, Df and Lf) act negatively in both records but with comparatively small magnitudes, while LD remains a small positive contributor in both. These local contributions describe how the surrogate model attributes each individual prediction and should not be interpreted as the physical cause of the prediction error in either case.



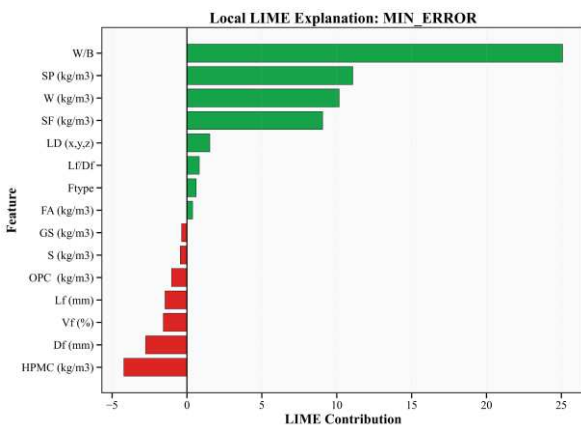
(a)



(b)



(c)



(d)

Fig. 7. LIME interpretation showing (a) global feature importance, (b) explanation stability, (c) local contributions for maximum-error cases and (d) local contributions for median-error cases.

4.6 Partial-dependence analysis of nonlinear response behaviour

Partial-dependence plots (PDPs) were created to see how the model-estimated compressive-strength response varies as each input variable is changed over the range of values in the experimental dataset, while the other variables are held constant. From the relationships learned, it is clear that most of them are nonlinear, with several variables showing threshold-like transitions, plateau and non-monotonic responses (see Figure 8). The overall decrease in the predicted response of W/B is consistent with its known physical role in controlling capillary porosity, while W has a distinct drop in response following a high response region. The dosage effect of SF is clearly indicated by the marked increase followed by a higher plateau, whereas that of SP is indicated by an increase followed by a gradual approach to a stable region, which corresponds to a saturation-type dosage effect.

The other variables also illustrate the nonlinear structure that is captured by the models. The segmented changes and plateaus in HPMC, a non-monotonic predicted response with a trade-off between reinforcement efficiency and workability at higher fibre dosages, and the increase in predicted strength with curing age followed by a plateau in Vf, reflecting the well documented deceleration of strength gain with curing age due to hydration, are all characteristic of the strength development of these material systems. The loading direction gives rise to different predicted responses as expected from the anisotropy of extrusion-based fibre-reinforced concrete, and the preferential fibre and interlayer orientation during printing. The fibre geometry also contributes to the model-estimated response via coupled effects rather than simply linear effects, as shown by the transition regions in fibre aspect ratio, diameter and length. The PDPs for ordinary Portland cement (OPC), sand, fly ash and ground slag show minor, but still non-linear, marginal changes.

The PDP results, together with the results from the feature-attribution analysis presented in Sections 4.4 and 4.5, offer an interpretation in terms of the response shape. SHAP and LIME provide information on which variables are important for model predictions, while the PDPs provide information on how the model estimated response varies across the input domain represented by the experimental data. The overall evidence suggests that the compressive-strength response is not fully captured by the linear individual effect of the mixture, processing and fibre descriptors, and therefore machine-learning techniques which are able to capture

interactions between mixture, processing and fibre descriptors over classical linear regression techniques are recommended.

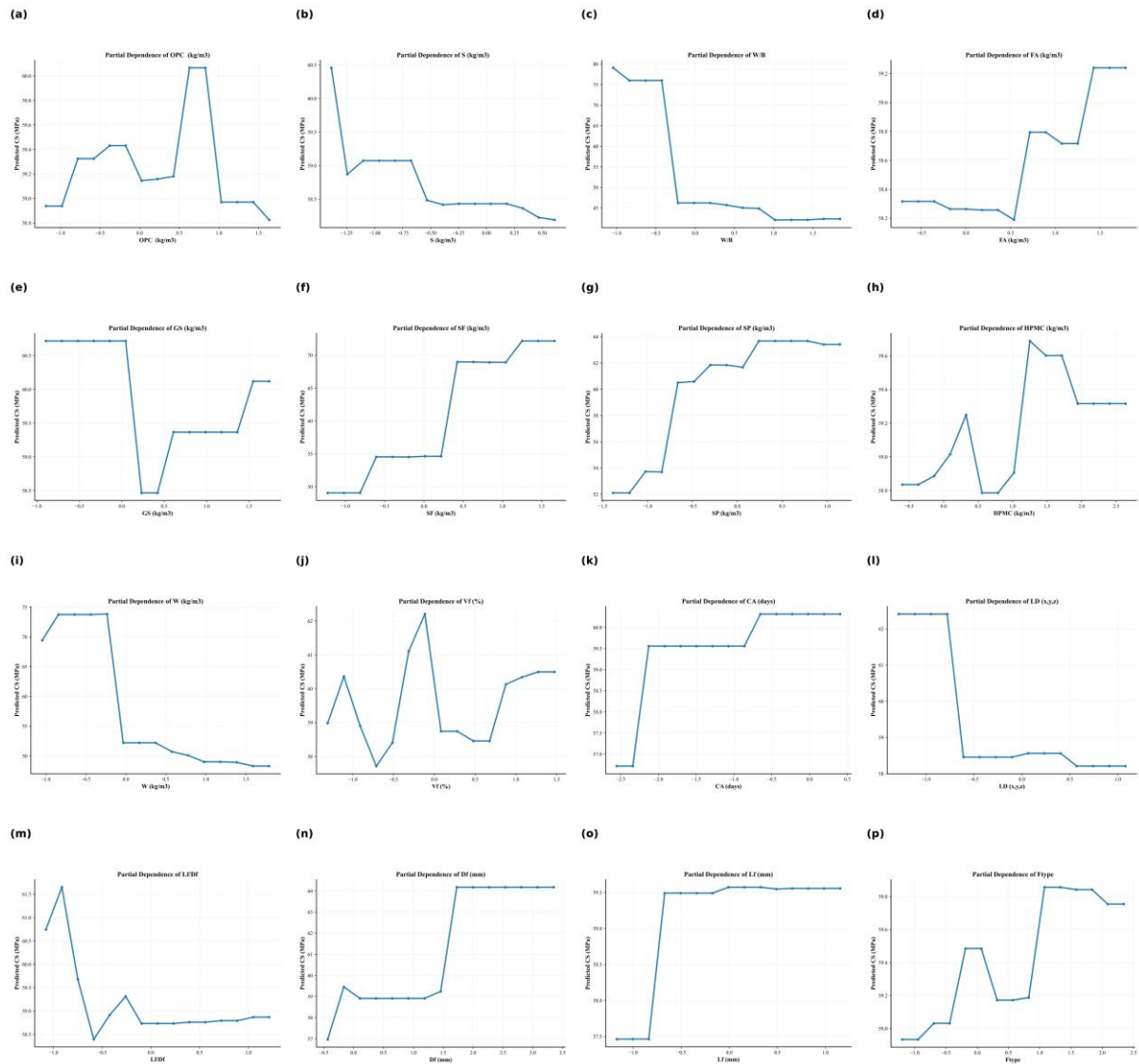


Fig. 8. Partial-dependence plots for the sixteen input variables used for compressive-strength prediction

4.7 Practical deployment through the developed GUI

The predictive framework was then translated into an interactive graphical user interface (GUI) using the NGBoost model that was chosen for its best test R^2 , RMSE and maximum-error performance (Section 4.1) and its native probabilistic output. The interface enables the user to input the material, fibre, curing and loading parameters in the modelling framework and to receive an instant prediction of the compressive strength modeled. It also provides an approximate 95% prediction interval and the NGBoost native predictive standard deviation,

preserving the probabilistic information that the selected model provides, instead of just presenting a single deterministic point estimate.

The GUI incorporates SHAP-based contribution information so that the user can view the variables for a specific contribution to a single model prediction, and thus connect the interpretability analyses of Sections 4.4–4.6 directly to a practical tool for decision support. It also offers reference functions based on the dataset, such as the minimum and maximum values recorded in the experiment and sample-based checking to identify inputs that are outside the range of the dataset. The relative strength category shown in the interface is based on the experimental data in the underlying database and should therefore be used as a screening aid, and not as an independent structural design classification. This distinction is of special importance if the tool is used on a mixture outside the area spanned by the training data, and will be discussed again in Section 4.9 when discussing limitations.

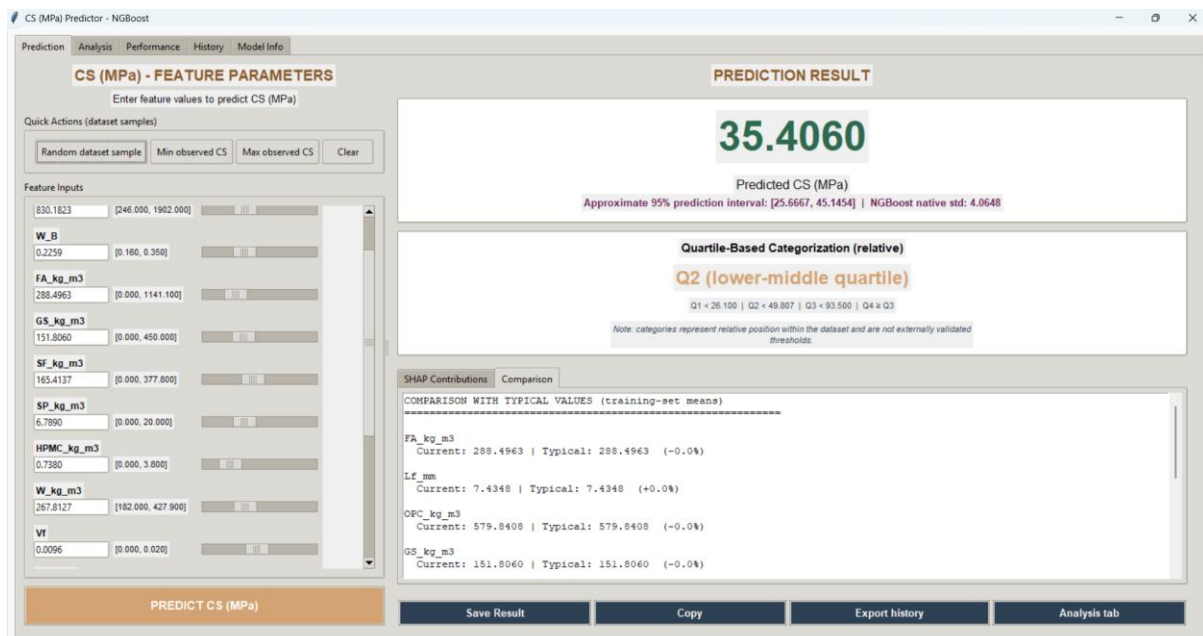


Fig. 10. Developed GUI for interactive NGBoost-based compressive-strength prediction and interpretation

4.8 Integrated discussion of predictive performance and interpretability

The outcomes provide a logical sequence from predictive performance and error diagnosis to statistical validation, model interpretation and finally to practical deployment. The comparisons between experimental and model-predicted strengths, along with the Taylor diagrams, indicate good agreement between the predictions and the experimental response, and the residual distributions indicate relatively small signed errors for the ensemble models. NGBoost offers the best testing R^2 , and the smallest testing RMSE and maximum error, while CatBoost offers the smallest testing MAE. These differences between the metrics show that the

ranking of models should not be based on a single summary measure of predictive error, because the ranking can vary depending on which part of the predictive error is the most important for the specific application.

The interpretability analyses yield a consistent and plausible set of influential descriptors. W/B, W, SF and SP are consistently the most significant variables, whereas LD, Vf, fibre geometry and curing age are significant with nonlinear and in some instances non-monotonic response patterns. These three, methodologically independent, interpretability techniques (SHAP, LIME, PDPs) have a common set of dominant variables, and the convergence on a common set of dominant variables gives a stronger evidentiary basis than any of the three techniques alone. Lastly, the GUI converts these analytical components into a usable prediction and interpretation space that non-machine learning practitioners can use. The analyses are grouped together to establish a relationship between predictive performance and interpretable material and process relationships for the compressive-strength assessment of 3D-printed fibre-reinforced concrete, as well as to provide a workflow of prediction, validation, interpretation and deployment which can be transferred to other performance properties and other additive-manufacturing material systems. A consolidated overview of the predictive performance, interpretability findings and deployment outcomes is presented in Table 7.

Table 7. Summary of the main findings from the predictive, error, interpretability and application analyses.

Analysis	Evidence	Main finding
Predictive agreement	Scatter plots and Taylor diagrams	Strong agreement across all four models; NGBoost testing $R^2 = 0.9877$.
Error behaviour	Residual distributions	NGBoost has the smallest residual SD (4.890 MPa); CatBoost has the lowest test MAE (3.803 MPa).
Global importance	SHAP	W/B, W, SF, SP, LD and Vf repeatedly appear among the influential descriptors.
Local explanation	LIME	Dominant variables remain stable, while local contribution direction can vary with the observation.
Response shape	PDP	Several variables show nonlinear, threshold-like, plateau or non-monotonic behaviour.
Practical use	GUI	Interactive prediction, approximate 95% interval, native SD and SHAP-based interpretation are integrated.

W/B, water-to-binder ratio; W, water content; SF, silica fume; SP, superplasticizer; LD, loading direction; Vf, fibre volume fraction; SHAP, SHapley Additive exPlanations; LIME, local interpretable model-agnostic explanations; PDP, partial dependence plots; GUI, graphical user interface; SD, standard deviation.

4.9 Practical Implications

The proposed machine-learning framework is a practical solution for the preliminary prediction of the compressive strength of 3D-printed fiber-reinforced concrete (3DP-FRC). The framework can be used to provide a preliminary evaluation of the performance of various 3DP-FRC mixtures, and decrease the number of trial mixtures requiring experimental testing, by incorporating mixture composition, fiber characteristics, curing age and loading direction. The predictions can then be used to help determine which combinations of mixtures are likely to be of interest to the detailed laboratory testing.

The explainability analyses are also useful for practical purposes as they show which variables are most strongly associated with the model predictions. Specifically, water-to-binder ratio, water content, silica fume, and superplasticizer were consistently found to be significant variables and the fiber characteristics, curing age, and loading direction also had an impact on the predicted strength. These results can help researchers and engineers determine which parameters should be more focused on when developing the mixture and planning experiments. The developed NGBoost-based framework also gives probabilistic prediction information, which can be used to consider the predicted compressive strength along with its uncertainty. This is more informative than using only one of the predicted values, especially if the model is used for the initial engineering assessment. The developed GUI further enhances the practical accessibility by enabling the user to enter the required input parameters and get the predicted compressive strength as well as prediction and explainability information without having to implement the machine-learning code.

The overall framework can be used as a screening and decision support tool for 3DP-FRC mixture development. It can help you to compare candidate mixtures, to understand what variables are important, and to design future experiments. The model predictions should however be experimentally verified before final choice of material or structural design.

4.10 Limitations and Future Research

The proposed machine-learning framework is a practical solution for the preliminary prediction of the compressive strength of 3D-printed fiber-reinforced concrete (3DP-FRC). The framework can be used to provide a preliminary evaluation of the performance of various 3DP-FRC mixtures, and decrease the number of trial mixtures requiring experimental testing, by incorporating mixture composition, fiber characteristics, curing age and loading direction. The predictions can then be used to help determine which combinations of mixtures are likely to be of interest to the detailed laboratory testing.

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5. Conclusions

1. A machine-learning framework was developed to predict the compressive strength of 3D-printed fiber-reinforced concrete using 299 experimental observations and 16 input variables covering mixture composition, fiber characteristics, curing age, and loading direction.
2. Four machine-learning models—CatBoost, NGBoost, Random Forest, and SVM—were tested with hyperparameter optimization, repeated cross validation, and an independent test set. The predictive ability of all models was good over the dataset investigated.
3. NGBoost achieved the highest testing R^2 of 0.9877 and the lowest testing RMSE of 4.9036 MPa, while CatBoost achieved the lowest testing MAE of 3.8031 MPa. NGBoost was therefore selected for the practical GUI implementation because of its strong predictive performance and probabilistic prediction capability.
4. The explainability analysis identified water-to-binder ratio, water content, silica fume, and superplasticizer as important predictors, while fiber characteristics, curing age, and loading direction also contributed to the model predictions.

5. SHAP, LIME, and partial dependence analyses provided complementary interpretation of the model, demonstrating that the relationship between the input variables and compressive strength is nonlinear and varies across the investigated parameter ranges.
6. The inclusion of fiber-related parameters and loading direction provides a more comprehensive representation of 3DP-FRC than approaches based solely on conventional mixture proportions, particularly for accounting for differences associated with fiber characteristics and directional loading.
7. The developed GUI provides a practical implementation of the proposed framework, enabling users to obtain compressive-strength predictions together with prediction uncertainty and feature-contribution information.
8. The proposed framework can support preliminary mixture screening, experimental planning, and interpretation of 3DP-FRC strength behavior, while experimental testing remains necessary for final validation and engineering application.
9. Future validation using larger, independent, and study-wise datasets is required to further establish the generalizability of the framework and its applicability to a wider range of 3D-printing materials and processing conditions.

6. Statements and Declarations

Author Contributions: The authors confirm their contribution to the paper as follows: **Gulzar Mohammad:** Software Development, Machine Learning Model Development, Data Preprocessing, Model Training and Validation, Methodology, Writing – Review & Editing. **Wajahat Ali:** Model Validation, Formal Analysis, Writing – Review & Editing. **Nasser Alanazi:** Conceptualisation, Methodology, Formal Analysis, Visualization, Writing – Original Draft Preparation.

Corresponding Author: Correspondence concerning this article should be addressed to the corresponding author at: gm78691@gmail.com

Data Availability: The dataset was compiled from previously published studies, with sources cited in manuscript. The complete dataset is available from the corresponding author upon reasonable request.

GUI Code: The graphical user interface developed in this study is openly available in the public GitHub repository: <https://github.com/gm78691-web/GUI>

Ethics Approval: The authors confirm that this manuscript is original, has not been published previously, and is not currently under consideration for publication elsewhere.

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Consent for Publication: All authors have reviewed and approved the final manuscript and consent to its publication.

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