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Suitability of Mechanics-Based and Optimized Machine Learning-Based Models in the Shear Strength Prediction of Slender Beams Without Stirrups

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Abstract: Accurate shear capacity estimation for reinforced concrete (RC) beams without stirrups is essential for reliable structural design. Traditional code-based methods, primarily empirical, exhibit variability in predicting shear strength for these beams. This paper assesses the effectiveness of mechanics-based and optimized machine learning (ML) models for predicting shear strength in stirrup-less, slender beams using a dataset of 784 tests. Seven ML models—artificial neural network (ANN), support vector machine (SVM), decision tree (DT), random forest (RF), AdaBoost, gradient boosting (GBR), and extreme gradient boosting (XGB)—were compared against three mechanics-based models: the Tran’s NLT Model (2020), the Multi-Action Shear Model (MASM), and the Compression Chord Capacity Model (CCC). Among the ML models, XGB and GBR demonstrated the highest predictive accuracy, with coefficients of determination (R^2) of 0.974 and 0.966, respectively, indicating strong correlation with experimental data. Performance metrics such as mean absolute error (MAE) and root mean squared error (RMSE) showed that XGB and GBR consistently outperformed other models, yielding lower error margins. Statistical analysis revealed minimal bias and variability in the predictions of XGB and GBR, with a coefficient of variation (CoV) of 14%, ensuring high reliability. The NLT model, the most accurate of the mechanical-based models, achieved a mean of 1.02 and a CoV of 16% for its model error, demonstrating reasonable prediction reliability but falling behind XGB and GBR in accuracy. With Shapley additive explanations (SHAPs), the beam width and depth were identified as primary predictors of shear strength, providing critical insights for enhancing design and construction practises.

Keywords: beams; shear strength; machine learning; model uncertainty; Shapley additive explanation method; XGBoost algorithm



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1. Introduction

Reinforced concrete beams are primarily subjected to bending since they are majorly flexural members. In addition to the predominant flexural force in a concrete beam, there are forces such as shear force (responsible for shear failure in beams), axial force, and torsion. Unlike the flexural resistance of beams without stirrups, which can be modelled and estimated with a generally and universally accepted method, “Euler–Bernoulli’s plane section theory” [1], the shear strength prediction of beams without stirrups is yet to receive a generally accepted design philosophy [2–4]. The combination of non-homogeneity, cracks, reinforcements, and nonlinearity in reinforced concrete contributes to the complex behaviour of reinforced concrete under shear [5]. Diagonal shear cracks occur when an RC structural element undergoes both shear and flexure, resulting in the development of

multi-axial stress states that occur in regions along a flexural beam that displays a particularly intricate response, hence, the actions of shear-resisting agents [6]. The activation and contribution of these shear transfer actions largely depend on the pattern or shape of the critical shear crack, the opening and sliding behaviour of the critical shear crack and its failure dynamics [7,8]. The mechanics of these shear-resisting actions differ considerably from each other and display a complicated relationship among themselves [9]. Subsequently, the development of a generally acknowledged formulation to represent shear forces has not been accomplished at this point, and it is important to take significant presumptions to determine approximate expressions.

Without controversy, these shearing mechanisms are well acknowledged in the research community as the dowel action v_d , interface shear transfer v_{ca} , residual tensile stress in concrete v_{cr} , uncracked compression zone v_{cc} , and stirrups v_s in the case of beams with web reinforcement [10–12]; yet, some shear mechanisms are still preferred as the governing shear transfer mechanisms based on various interpretations of the shear philosophy [8,13]. Bentz et al. [14], Yang [15], and Muttoni and Ruiz [16] identified the interface shear transfer (aggregate interlock) as the presiding shear transfer mechanism in beams without stirrups. Contrarily, Zararis [17], Tureyen and Frosch [18], and Park et al. [19] recognized the uncracked compression chord's shearing action as the key factor in the shear transfer mechanism.

According to Fenwick and Paulay [20] and Nakamura et al. [21], there are two classes of shear transfer mechanisms based on the ratio of shear span to effective depth (slenderness), namely arch action and beam–shear transfer action. The above-mentioned shear transfer mechanisms are purely beam–shear transfer actions. The beam action is initially responsible for carrying the total shear in a reinforced concrete beam without stirrups. After the failure of the beam action, a redistribution of shear stresses occurs, allowing the activation of the arch action [22,23]. When the arch action reaches its capacity, the shear failure of beams without stirrups becomes inevitable. Discussions and numerical analyses concerning the shearing mechanisms in beams without or with a small amount of shear reinforcement have been extensively examined in [24–30]; however, this research also provides a quick summary of the possible beam shear transfer actions.

Due to the lack of a uniform mechanical model, the shear capacity of an RC element without stirrups has long depended on empirical or semi-empirical equations [13] derived from the regression analysis of experimental data [31]. Shear design models in design specifications and standards are either empirically or semi-empirically derived. Empirical models do not, however, consider the influence of the shearing mechanisms, and are, without a doubt, only appropriate for the set of data from which they were derived [32,33]. The studies conducted in [34,35] revealed that empirical models are inherently associated with a considerable amount of uncertainty due to the difficulties of deriving an empirical model. As a result, concerns arise regarding the reliability of shear prediction using empirical and semi-empirical models.

The demand for new mechanics-based models is crucial since the quantity of experimental data affects the validity of an empirical model [33]. Furthermore, the adoption of mechanics-based models could potentially result in reduced safety factors and optimized design models [36].

Several mechanical models based on various mechanics concepts exist for estimating the shear capacity of RC beams without stirrups, including the critical shear crack theory [16], plasticity theory [37,38], compressive force path theory [39,40], truss model theory [41–43], splitting failure theory [44], modified compression field theory [45,46], and strain-based shear model [19,47]. Most of these theories slightly deviate from the principles upon which modern design is developed and continue to convey implicit presumptions that frequently conflict with the essential characteristics of concrete [48].

The purpose of this study was to determine the performance of new mechanical shear models based on the fracture mechanics theory by juxtaposing the predictions with machine learning (ML)-based shear models. The study conducted by Reinhardt [49] introduced the fracture mechanics concept to the research community to explain the size effect on shear

strength. Other researchers [50–59] have adapted the theory to define the shear transfer mechanism and developed respective shear estimation models. The study of fracture mechanics involves the mechanical analysis of structures to anticipate the propagation of cracks, which might be used to better understand shear failure processes and predict the conditions most likely to lead to failure. Research on fracture mechanics concerning the brittle failures in RC structures (such as diagonal shear, punching shear, and torsion) has emphasized the importance of incorporating fracture mechanics into design criteria. As a result, the cost-effectiveness and reliability following code-based shear models could be improved and allow for more uniform safety margins, especially for structures with varying geometrical configurations.

Research Significance

Design code provisions for shear capacity estimation must be based on theories that give a clearer understanding of the shear failure process with proper consideration of the shear transfer mechanisms and stress redistribution up until the failure point despite the desire for conservatism among practitioners as seen in empirical models. In this regard, this study contributes to the ongoing effort to support the adoption of mechanical-based shear models in design specifications by analyzing the accuracy of shear prediction in light of recent mechanical models.

Since ML shear models are demonstrated to be accurate in their predictions, this study validated the results of the mechanical-based shear models with ML-based shear models by juxtaposing the respective results to establish a similarity in performance. The investigation was carried out by statistically analyzing the respective predicted shear result of the considered mechanical shear methods and modelling the corresponding uncertainty with the framework of structural reliability. To characterize and quantify the model uncertainty, a subset of the ACI-DafStb shear experimental database on beams without stirrups, collected and collated in [60], was used in this work to deterministically determine the shear result of the relevant mechanical shear model. The same experimental dataset was categorized as input variables (model features) and output (target) to predict shear capacity by applying ML algorithms as defined in the sci-kit Learn and TensorFlow framework.

The examined models were categorized into fracture mechanics-based models (Tran [61] (NLT)), structural mechanics-based shear models (Cladera et al. [6] (MASM) and Cladera et al. [62] (CCC)), and ML-based models (including ANN, SVM, RF, DT, AB, GBR, and XGB). The contribution of each model feature (input) to the shear prediction (output) was determined following Shapely additive explanation (SHAP), which was further related to the shearing mechanism since the shearing mechanism also depends on parameters that impact shear strength (taken as the model features).

2. Shear Transfer Mechanism

2.1. Uncracked Compression Zone

About 20–40% of a reinforced flexural member's overall shear strength is supplied by the uncracked compression zone [63]. The contribution of this shear transfer mechanism is dependent on the depth of the uncracked compression zone [64] and the compressive strength of the member [23]. As a result, this mechanism significantly contributes to the overall shear strength in members with low slenderness ratios, such as deep beams. However, in slender beams, due to the fracture kinematics inside the compression zone, the uncracked compression chord's contribution to the overall shear capacity becomes inconsequential [27]. The neutral axis depth has a direct proportionality with the shear transferred by the uncracked concrete chord [65]. Cladera et al. [6] additionally stated that a high ratio of longitudinal reinforcement will have an impact on the neutral axis depth since the neutral axis depth relies on the longitudinal reinforcement ratio and the modular ratio. This increases the uncracked compression chord's ability to withstand shear.

2.2. Dowel Action

The relative vertical shear displacement between the crack surfaces at the level of the longitudinal reinforcement causes the dowel forces to be initiated [7]. The dowel forces contribute to the total shear resistance by preventing slippage that may be caused by shear displacement along the cracks in a concrete section [66]. The effectiveness of this mechanism can be attributed to the use of transverse reinforcement in RC members or concrete's inability to develop spalling cracks, as in the case of short-span beams. The effective area of the concrete in the region of the tensile reinforcement and its effective tensile strength determines the ability of the dowelling action to transmit shear [67]. However, in agreement with Jelic et al. [68], Muttoni et al. [16] stated that the significance of the contribution of the dowel action in RC beams without stirrups is inversely proportional to the slenderness ratio (a/d). The spacing of bending-related cracks, the positioning of lateral reinforcement, and the concrete cover all determine how the dowelling action affects shear strength [69].

2.3. Aggregate Interlock

The complexity of the shear transfer mechanism of the interface shear transfer action (aggregate interlock) can be attributed to the numerous mechanism that facilitates the interaction between the normal and shear stresses [70]. The aggregate particles moving over one another cause cracks to widen as they propagate [70] and, in the process, aggregate interlocking stresses (normal stresses (if reinforcements prevent the crack from widening) and shear stresses develop at the crack surface) [2,70]. When the cracks expand, the interface between the crack surfaces is disrupted, reducing the contribution of this shear mechanism to the overall shear strength. Therefore, the crack opening, relative crack sliding and the surface properties of concrete such as the aggregate and matrix strength and the surface roughness impose constraints on the shear strength that the transfer mechanism can supply [71,72].

2.4. Residual Tensile Stress

Even after cracking has occurred, the residual ability of concrete to transmit tensile stresses is still substantial if the crack width is within the acceptable range. According to Hordjick [73], a flexural element with a crack opening larger than 0.2 mm cannot continue to transfer tensile stresses. However, tensile stresses may still be transferred in cracked concrete up to crack widths of 0.05 to 0.15 mm [74]. The mode of residual tensile stress distribution in tensile concrete following crack formation, commonly known as the strain softening effect [30], has been thoroughly analyzed in [75]. The most significant contributing factor to the occurrence of flexural cracks is the strain softening of concrete in tension [76].

2.5. Stirrup Contribution

Stirrups do not fundamentally alter or modify the shear transfer mechanism in RC beams; rather, they improve the strength of the shear transfer actions both collectively and individually by carrying some of the shear [77–79], enhance the capacity of the dowel action by effectively supporting the flexural bars that are being crossed by flexural cracks, and constrain the opening or width of diagonal cracks within the elastic range [31] since shear reinforcement is unable to stop the formation of diagonal cracks. Hence, the inclusion of web reinforcement proves to be important to the behaviour of the shear action by the interface shear transfer (aggregate interlock). Stirrups provide confinement to the concrete when closely spaced, and as a result, the compressive strength of concrete is increased, and this helps in regions affected by the arching action. The web reinforcements also prevent bond failure when splitting cracks develop in the anchorage zones due to the dowel and anchorage forces.

3. Mechanics-Based Shear Models

The following is a summary of some of the recent mechanics-based shear models that are examined in this study.

3.1. Model Proposed by Tran [61] (NLT)

The shear capacity expression proposed by Tran [61] is considered to be the sum of the shear transfer mechanism in the tension zone (v_{ct}) and the compression zone (v_{cc}) accordingly, i.e., there are two explicit formulations combined into one. The first considers the shear transferred by the resisting mechanisms at the bottom of the concrete section, right before the neutral axis (the tension zone), and the second offers an estimate for the shear capacity of the uncracked compression zone, where the critical region is located. The shear parameters considered in the approach proposed by Tran [61] include tensile strength (f_{ct}), effective tensile strength ($f_{ct,ef}$), fracture energy (G_F), elastic modulus (E_c), crack width (w_{cr}), crack slip (s) and crack spacing (s_{cr}), and the expressions are as given below:

$$V_c = V_{ct} + V_{cc} \quad (1)$$

$$V_{cc} = \frac{2}{3} \tau_{max} \cdot b d k_x \quad (2)$$

$$V_{ct} = b d \frac{G_F}{w_{cr}} (1 - k_x) \quad (3)$$

$$V_c = \frac{2}{3} f_{ct,ef} \cdot b d \left[k_x + \frac{1.5 G_F}{f_{ct,ef} w_{cr}} (1 - k_x) \right], \quad (4)$$

where G_F , the fracture energy, is given as $0.03 f_c^{0.18} a_g^{0.32}$, with a_g = the maximum aggregate size and f_c as the compressive strength of concrete; and $f_{ct,ef}$, the effective tensile strength, $= f_{ct} \cdot \frac{1}{1+v} \approx 0.83 f_{ct}$.

The crack width w_{cr} is taken as

$$w_{cr} = s_{cr} (\varepsilon_{sm} - \varepsilon_{cm}) \quad (5)$$

where s_{cr} is the crack spacing, and $\varepsilon_{sm} - \varepsilon_{cm}$ is the difference between the mean strains of reinforcement and concrete, and can be determined as follows:

$$\varepsilon_{sm} - \varepsilon_{cm} = \frac{1}{E_s} \left[\sigma_s - \beta_t \frac{f_{ct}}{\rho_{s,ef}} (1 + n_e \rho_{s,ef}) \right] \geq (1 - \beta_t) \frac{\sigma_s}{E_s} \quad (6)$$

Here,

E_s = elastic modulus of steel;

E_c = elastic modulus of concrete;

σ_s = stress in longitudinal reinforcement;

β_t = coefficient to access the mean concrete strain over s_{cr} ;

$\rho_{s,ef}$ = effective reinforcement ratio in cracking calculation;

n_e = ratio of modulus of elasticity between steel and concrete.

Tran [61] presented a simplified approach (Equation (7)) with the same degree of precision to address the multiple computations of model parameters, as shown in Equations (4) and (6), allowing a quick evaluation of shear strength.

$$V_c = \frac{1}{3} f_{ct,ef} \cdot b d k_x \left[1 + \sqrt{1 + \frac{d_0}{d}} \right] \quad (7)$$

$$d_0 = 2 l_{ch} \cdot \frac{(3 - k_x)}{\lambda_s (1 - k_x)} \quad (8)$$

where λ_s = the effective shear span to depth ratio, and it is given as $M_E/V_E d$. l_{ch} is the characteristic length, and it is calculated as follows:

$$l_{ch} = \frac{E_c G_F}{f_{ct,ef}^2} \quad (9)$$

The relative depth of the compression = k_x , and it is given as

$$k_x = \left(\sqrt{1 + 2/(n_s p_s)} - 1 \right) n_e \rho_s \quad (10)$$

3.2. Model Proposed by Cladera et al. [62] (CCC)

By integrating the explicit expression of v_c , v_w , and v_l into v_c with average coefficients, Cladera et al. [62] simplified the resistance model proposed by Cladera et al. [6] and created a more concise formulation, naming the model the Compression Chord Capacity Model (CCC). The compression chord capacity model was founded on the assumption that the fundamental transfer action that resists or takes precedence in the failure state under consideration is the compression chord's shear transfer mechanism. The expression is given as

$$V_{cu} = 0.3 \zeta \frac{x}{d} f_{cd}^{2/3} b_{v,eff} d \not\leq v_{cu,min} \quad (11)$$

$$v_{cu,min} = 0.25 \left(\zeta \frac{x}{d} + \frac{20}{d_0} \right) f_{cd}^{2/3} b_w d \quad (12)$$

$$\frac{x}{d} = \alpha_e \rho_l \left(-1 + \sqrt{1 + \frac{2}{\alpha_e \rho_l}} \right) \approx 0.75 (\alpha_e \rho_l)^{\frac{1}{3}} \quad (13)$$

$$\zeta = \frac{2}{\sqrt{1 + \frac{d_0}{200}}} \left(\frac{d}{a} \right)^{0.2} \not\leq 0.45 \quad (14)$$

$b_{v,eff}$ = compression flange effective beam width. Note that for a rectangular beam, $b_{v,eff} = b_v = b$.

$$\text{When } x \leq h_f, b_{v,eff} = b_v = b_w + 2h_f \leq b \quad (15)$$

$$\text{When } x > h_f, b_{v,eff} = b_w + (b_v - b_w) \left(\frac{h_f}{x} \right)^{\frac{3}{2}} \quad (16)$$

Here, h_f is the height of the flange, x is the neutral axis depth, and b_w is width of the beam web. f_{ctm} is the mean concrete tensile strength ≤ 4.60 MPa, and E_{cm} is the secant modulus of elasticity ≤ 39 GPa. G_f is the concrete fracture energy, given as $G_f = 0.0028 f_{cm}^{0.18} d_g^{0.32}$, where f_{cm} is the mean value of the cylinder concrete compressive strength, and d_g is the maximum aggregate size.

d_0 = effective depth, $d \geq 100$ mm.

ζ = size effect coefficient at critical shear crack failure.

$b_{v,eff}$ = effective beam width for compression flange. Note that for a rectangular beam, $b_{v,eff} = b_v = b$.

For more information on the parameters, the reader is referred to [62].

3.3. Model Proposed by Cladera et al. [6] (MASM)

The Multi-Action Shear Model (MASM) is an extension of a flexural shear model based on the concept of structural mechanics [6]. The model was initially created to assess the resistance of concrete flexural members longitudinally and/or transversally reinforced with fibre polymers. As the name implies, the shear model considers the shear strength as the sum of the various shear transfer actions, namely the uncracked compression chord (v_c), shear transferred along web cracks (v_w), shear contribution from the longitudinal

reinforcement (v_l), and contribution of the shear reinforcement (v_s). See Cladera et al.'s work [6] for an in-depth definition of model variables as given below:

$$V = (v_c + v_w + v_l) f_{ctm} \cdot b \cdot d + v_s \leq V_{max} \quad (17)$$

$$v_c = \zeta \left[\left(0.88 + \left(0.20 + 0.50 \frac{b}{b_w} \right) v_s \right) \frac{x}{d} + 0.02 \right] \frac{b_{v,eff}}{b} K_p \quad (18)$$

$$v_w = 167 \frac{f_{ctm}}{E_{cm}} \frac{b_w}{b} \left(1 + \frac{2G_F E_{cm}}{f_{ctm}^2 d_0} \right) \quad (19)$$

$$v_l = \frac{0.23 \frac{\alpha_e \rho_l}{1-x}}{d}, \text{ if } v_s > 0; v_l = 0, \text{ if } v_s = 0 \quad (20)$$

$$v_s = (d_s - x) \cot \theta \frac{A_{sw} \cdot f_{yw}}{s \cdot f_{ctm} \cdot b \cdot d} \approx \frac{0.85 d_s A_{sw} \cdot f_{yw}}{s \cdot f_{ctm} \cdot b \cdot d} \quad (21)$$

The symbols in Equations (18)–(21) are defined below. See [6] for more detailed definitions of the model parameters.

The neutral axis x is equivalent to the height of the uncracked compression zone, and it is given as

$$\frac{x}{d} = \alpha_e \rho_l \left(-1 + \sqrt{1 + \frac{2}{\alpha_e \rho_l}} \right) \approx 0.75 (\alpha_e \rho_l)^{\frac{1}{3}}$$

The above expression is valid for reinforced concrete members, where $\alpha_e = \frac{E_s}{E_c}$ is the modulus of elasticity ratio between steel and concrete, and ρ_l is the longitudinal reinforcement ratio.

f_{ctm} is the mean concrete tensile strength ≤ 4.60 MPa, and E_{cm} is the secant modulus of elasticity ≤ 39 GPa.

G_f is the concrete fracture energy, given as $G_f = 0.0028 f_{cm}^{0.18} d_g^{0.32}$, where f_{cm} is the mean value of the cylinder concrete compressive strength, and d_g is the maximum aggregate size. d_0 = effective depth, $d \geq 100$ mm.

ζ = size effect coefficient at critical shear crack failure, $\zeta = 1.2 - 0.2a \geq 0.65$, with a , the shear span, in m.

$b_{v,eff}$ = effective beam width for compression flange. Note that for a rectangular beam, $b_{v,eff} = b_v = b$.

K_p is a coefficient for considering the effect of the prestressing force in the cracking moment.

The existing literature has shown that the individual effect of the different shear-resisting actions, especially the dowel action, is limited and affected by the omission of stirrups [66]. Hence, v_s and v_l are disregarded in the estimation of the diagonal cracking shear strength for members without stirrups but included when considering a stirrup-based design.

4. Machine Learning (ML) Models

Machine learning, a subset of artificial intelligence, is being used as a tool to solve a variety of technical challenges, including the design improvement, stochastic simulation, reliability analysis, and performance assessment of structural systems of great complexities [80]. Due to the availability of shear experimental datasets, the accuracy of ML predictions, how the algorithm computerizes a type of dataset's innate knowledge to create an accurate input–output relationship [9], and its ability to express structural learning as a method in structural reliability analysis [81], ML is widely employed in research on the assessment of shear resistance. The use of conventional approaches, such as structural equation models for estimating shear resistance may require a lot of fine-tuning. Instead, this arduousness can be avoided using an ML method. Aldakheel et al. [82] agreed that data-driven models like ML, deep learning, and artificial neural network models can be utilized to simplify the complexity of conventional models. The research conducted in [83–91]

showed that ML models may be used to predict outcomes for problems involving shear strength, such as the shear strength prediction of steel fibre-reinforced concrete beams without stirrups, the shear strength prediction of reinforced concrete beams with and without stirrups, predicting the contribution of recycled aggregate concrete to the shear capacity of beams without stirrups, and the prediction of shear transfer strength of concrete joints.

4.1. Artificial Neural Networks (ANNs)

The term “artificial neural network” (ANN) refers to a mathematical representation of the human brain of which its underlying phenomena were inspired by the features and functions of the human brain. The neural network, or brain, is made up of around 10,000 connections between about 1011 neuronal cells that make up the brain. ANNs imitate the natural neural network found in the brain by connecting its artificial neurons in a similar manner [92]. The neural network is made up of three basic components, each of which has a special characteristic that supports the overall functionality of neural networks.

Given a real number input $w_i \in R$ with $i = 1, 2, \dots, n_x$, here, the number of input variables is n_x and $i \in N$ (set of integers). The neural network aims to apply a function to a linear combination of all inputs. Mathematical equations for the neural network algorithm are seen below.

$$z = w_1x_1 + w_2x_2 + \dots + w_{m_x}x_{m_x} + b \quad (22)$$

An output y will then be produced by applying a function f to z :

$$y(k) = f(z) = f\left(\sum_{i=0}^m w_i(k) \cdot x_i(k) + b\right) \quad (23)$$

where b is a modifiable value called bias;

$x_i(k)$ represents an input value in discrete time k , where i goes from 0 to m ;

$w_i(k)$ represents a weight value in discrete time k , where i goes from 0 to m ;

f is an activation function;

$y(k)$ is the predicted value in discrete time k .

The three basic components of the neural network include the input layer, the hidden layer, and the output layer.

Input layers are responsible for accepting training samples as a row vector $(x_1, x_2, x_3 \dots x_m)$ or a column vector $(x_1, x_2, x_3 \dots x_m)^T$. When computing a neural network, it is important to note that having too many input layers will considerably slow down the learning process, but the training accuracy will significantly increase. The input layer has a collection of synapses, or connecting links, each of which is distinguished by a weight.

The hidden layer is the second point of contact in the neural network architecture. It serves as an intermediary between the input layer and the output layer with the sole responsibility of applying weights to inputs and directing the product through an activation function. Overfitting will result from having too many hidden neurons, and the fundamental behaviour of the function will not be captured by having too few hidden layers [23]. Hence, cross-validation or a trial-and-error process may be used to determine the appropriate number of hidden layers and neurons to be included in a neural network. The results of the neural network computation are given by the output layer.

4.2. Support Vector Machine (SVM)

An SVM was extended to offer solutions to regression problems by predicting continuous variables as relevant to the problem scenario, although it was originally intended for predicting discrete values such as those in classification problems. Hence, the SVM is among those supervised ML algorithm that has dual applicability [93,94].

The basic concept underlying support vector regression is that the maximum margin is filled with data points, and the optimal data points inside the margin are utilized to create a line of best fit, much like in linear regression. In using the x -values (optimal data points)

that produced the line of best fit within the maximum margin, a corresponding y-value (prediction) is determined. This section provides a quick explanation of margin maximization based on the SVM method with the inclusion of a kernel trick and a slack variable.

Our aim in the support vector regressor is to derive the equation of hyperplane based on the best θ -coefficient, as in linear regression, that will maximize the margin with subjection to some constraints.

$$\text{Constraint 1 : given } (\theta_0, \theta_1, \theta_2, \dots, \theta_p), \text{ then } \sum_{j=1}^p \theta_j^2 = 1 \quad (24)$$

$$\text{Constraint 2 : given } (\xi_1, \xi_2, \xi_3, \dots, \xi_n), \xi_i > 0, \text{ then } \sum_{i=1}^n \xi_i \leq C \quad (25)$$

where C is a regularization parameter that controls the allowable degree of misclassification in the soft margin, and ξ is a slack variable that quantifies the margin violation of specific datapoints. The strength of regularization is inversely proportional to C , i.e., if the value of C is high, the strength of regularization is less and vice versa.

Constraint 3: the sum of the orthogonal or perpendicular distance must not be less than $M(1 - \xi_i)$.

$$y_i \left(\theta_0 + \sum_{j=1}^p \theta_{ji} x_{ij} + \sum_{j=1}^p \theta_{j2} x_{ij}^k \right) \geq M(1 - \xi_i) \quad (26)$$

where θ s are model coefficients, x s are model features, and M = Maximum margin.

The power k denotes that the original input space has been projected into a higher dimensional space. The support vector algorithm becomes more complex when projecting into a higher-dimension space, which might result in an overfitting issue. The kernel function and trick are used to address this problem.

By applying the kernel trick, we try to calculate the dot product of the training observations in a linear support vector classifier.

$$F(x) = \theta_0 + \sum_{i=1}^n \alpha_i \langle x, x_i \rangle \quad (27)$$

The dot product of all training observations or data points is given as

$$\alpha_1 x_1 + \alpha_2 x_2 + \alpha_3 x_3 + \dots + \alpha_n x_n \quad (28)$$

α_i refers to the Lagrange multiplier associated with each datapoints, and it selects or controls the non-zero support vectors. The idea of the kernel trick is to only select the non-zero support vectors and not all data points to save on computation time and reduce the complexity of the algorithm.

To complete the kernel trick transformation, the kernel function is introduced into the dot product equation to completely decrease the algorithm complexity in a higher-dimensional feature space. The specialty of the kernel function is to quantify the similarity between the original feature space and the enlarged feature, providing the equivalence of the data in each feature space regardless of the dimension in which the data were originally defined.

The SVM equation then becomes

$$F(x) = \theta_0 + \sum_{i=1}^n \alpha_i K \langle x, x'_i \rangle \quad (29)$$

The term ' $K \langle x, x'_i \rangle$ ' is the kernel function that performs the kernel transformation and controls the complexity of the algorithm with the dot product concept.

For a polynomial kernel function, $K \langle x, x'_i \rangle$ is given as

$$K \langle x, x'_i \rangle = \left(1 + \sum_{i=1}^p x_{ij} x'_{ij} \right)^d \quad (30)$$

The equation of the SVM with a polynomial kernel function becomes

$$F(x) = \theta_0 + \sum \alpha_i \left(1 + \sum_{i=1}^p x_{ij} x'_{ij} \right)^d \quad (31)$$

4.3. Decision Tree (DT)

A DT is an algorithm based on the information theory concept developed by Shannon [95]. The tree-based method solely focuses on measuring information purity only. A statistical DT is used in ML to model choices and results based on certain criteria. Breiman et al.'s [96] CART algorithm serves as the foundation for the decision tree regressor. However, decision trees now use a modified version of Quinlan's C4.5 algorithm [97].

A leaf node and an internal/decision node, which includes a root node, make up a DT [98]. A root node is first initialized, after which it is divided into sub-trees. According to the splitting criteria, such as information gain, Gini impurity, and entropy for classification tasks, or mean squared error (MSE) and Poisson regression for regression tasks, the optimal split is established. Based on the terminating requirements, the splits are categorized as either terminal/leaf nodes or decision/internal nodes. Each internal node is then processed independently until there are no internal nodes to separate, and this procedure continues. In general, the algorithm performs well with missing data, but it can suffer from overfitting, which can be avoided by limiting the tree depth and maximum features [99]. The Scikit learn ML library includes some other splitting criteria for regression tasks such as the Friedman MSE and absolute error. The main goal of the DT in regression is to minimize all the error metrics.

4.4. Random Forest (RF)

Breiman [100], who was motivated by the previous work of Amit and Geman [101], developed the random forests algorithm. RF was created as an alternative to boosting, and it is an extension of Breiman's bagging concept [102]. RF is an extension of the DT model; researchers developed the RF algorithm to improve the performance of the decision tree model. The decision tree limitation that inspired the creation of the RF model was that it does not learn using all of the characteristics in a dataset and could generalize poorly due to its vulnerability to overfitting, but the RF approach does learn across all dataset features, and it is not prone to overfitting.

RF is an ensemble learner. Ensemble means that the combination of multiple algorithms are compounded as one. When referring to RFs, it would be the fusion of several decision trees constructed using various characteristics chosen at random. It is significant to emphasize that the decision tree model's parameters and guiding principles also apply to the RF model, but the improvement requires some new concepts to be introduced into the model.

The idea behind RF was to create multiple trees from randomly selected subsets of a dataset. By doing this, we explore and include the entire feature space, and this results in an ensemble of various decision trees.

Bootstrapping is a random sampling method used in RF to reduce correlation and multi-collinearity in generated trees, resulting in more diverse configurations of decision trees. In RF, all features are considered to build a tree, unlike in decision trees where only a single feature is selected based on information metrics. Bagging combines bootstrapping and aggregating to derive a single outcome from the averaged results of every tree's leaf node. N-estimators, max features, and OOB-score are other features introduced in the RF model. RF models with bootstrapping generalize better and generate strong learners.

4.5. Adaptive Boosting

AdaBoost was originally proposed by Freund et al. [103] and was later extended to solve regression problems by Friedman [104]. By aggregating several weak learners (stump), AdaBoost creates a strong ensemble learner. AdaBoost regression is a modification of the AdaBoost classification algorithm in which regression models are used in place of

weak learners. Using the same dataset, the algorithm iteratively trains regression models, assigning greater weight to samples with larger errors. The goal of AdaBoost is to improve the performance of weak learners that have been previously trained, by adapting their learning to minimize the prediction error for the current model. Several regression models are combined in the final model, which is weighted according to the accuracy of each model.

The mathematical formula for Adaboost regression can be expressed as follows:

Let $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ be the training dataset and x_i , a feature vector used as input, and y_i be the output to be predicted by a function $F(x)$ such that

$$F_T(x) = \sum_{t=1}^T f_t(x) \quad (32)$$

where t = the number of ML models in the ensemble, $f_t(x)$ = an individual learner, and $F_T(x)$ = the overall boosting function.

$$f_t(x) = \alpha_t [h_t(x)] \quad (33)$$

where $h_t(x)$ = the hypothesis function (output from an individual ML model), and α_t = the weight of an individual/weak learner.

The weight of each sample feature in the prediction is initialized such that $w_i = \frac{1}{n}$; $i = 1, 2, \dots, n$.

An error rate (e_t) of each hypothesis function ($h_t(x)$) is determined following each training iteration of a weak learner.

$$e_t = \sum_{i=1}^n w_{t,i} e_{t,i} \quad (34)$$

$e_{t,i}$ is the error for each sample in the training data, given as

$$e_{t,i} = \frac{|y_i - h_t(x_i)|}{E_t} \quad (35)$$

E_t is the total weighted error at iteration t , given as

$$E_t = \sum_{i=1}^n w_{t,i} |y_i - h_t(x_i)|, \quad i = 1, 2, \dots, n$$

y_i is the actual value for the target variable.

The weight of each weak learner (α_t) is computed as

$$\alpha_t = \frac{1 - e_t}{e_t} \quad (36)$$

The weights of the training samples are updated after each iteration such that

$$w_{i+1} = w_i * \exp(\alpha_t * |h_t(x_i) - y_i|) \quad (37)$$

The weights are normalized such that their total equals 1: $\sum w_{i+1} = 1$.

4.6. Gradient Boosting Regression Trees (GBR)

GBR was first presented by Friedman [105], and it entails creating a series of models, each trained on the residuals of the previous model to obtain high accuracy in regression tasks by progressively lowering residual errors. One advantage of GBRT is its capacity to manage intricate and nonlinear interactions between features and the target variable. Decision trees are employed here as weak learners because they can capture nonlinear relationships between features. Although gradient boosting is a strong algorithm, it has certain flaws. For big datasets in particular, it can be computationally costly and sensitive to hyperparameter optimization [98]. Nonetheless, in many real-world situations, it may produce extremely accurate forecasts with proper parameter selection and optimization.

Suppose that $(x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ are feature vectors and their corresponding target value from a training set of n observations. To successfully forecast y_i for new input features (x_i) , we must learn a function $f(x)$.

The GBR algorithm starts by fitting an initial model $f_0(x)$ to the training data. We then iteratively improve this model by adding new models to the ensemble. With each n th iteration, we fit a new model $h_m(x)$ to the residuals of the previous model $(r_{i,m})$, which are as follows:

$$r_{i,m} = y_i - f_{m-1}(x_i); i = 1, \dots, n \quad (38)$$

The new model $h_m(x)$ is then added to the ensemble with a weight w_m , which is determined by minimizing the loss function L between the predictions of the current ensemble and the true target values:

$$w_m = \operatorname{argmin}_w L(y, f_{(m-1)}(x) + wh_m(x)) \quad (39)$$

Generally, a mean squared error is employed as the loss function.

$$L(y, f_{(m-1)}(x) + wh_m(x)) = \frac{1}{n} \left(\sum_{i=1}^n (y_i - f_{(m-1)}(x_i) - wh_m(x_i))^2 \right) \quad (40)$$

For iteration m , the new ensemble model is provided by

$$f_m(x) = f_{(m-1)}(x) + wh_m(x) \quad (41)$$

where w = the weight for the current model, and $h_m(x)$ = the new model added to the ensemble.

The algorithm terminates after m iterations or when a set of stopping requirements is satisfied. The ending conditions often include a maximum number of iterations or when the improvement in the loss function is below a certain level.

4.7. Extreme Gradient Boosting

XGBoost/XGB, a scalable and accurate algorithm, was introduced by Chen and Guestrin [106] as a variant of the gradient boosting ML model, which improves the performance of weak models by iteratively adding new models to an ensemble. XGBoost has several advantages over traditional base models, including being able to handle large datasets with high-dimensional feature spaces, handling missing values, and an integrated regularization method to prevent overfitting [106]. In XGBoost, a gradient optimization technique is applied to a loss function to build an ensemble of decision trees. The algorithm uses regularization and line search techniques to prevent overfitting and to find the best weights and base models to add to the ensemble.

Given a dataset $D = (x_i, y_i) : i = 1, \dots, n$ for $x_i \in \mathbb{R}^m$, $y_i \in \mathbb{R}$, n observations with m characteristics each and an associated variable y are collected for which a function that predicts $\hat{y}$ is required to be learnt.

The algorithm starts by initializing a constant prediction $f_0(x)$ for all examples:

$$f_0(x) = \operatorname{argmin}_c \sum_{i=1}^n L(y_i, c) \quad (42)$$

where L is a loss function expressed as a mean squared error (MSE) or log loss.

With the addition of new models to the ensemble, the model is improved iteratively. Hence, a new model, $h_m(x)$, is fitted to the negative gradients of the loss function in relation to the existing predictions at each iteration m .

$$g_{im} = -\frac{dL}{dy_i} \left(y = y_{(m-1)}(x_i) \right) \text{ for } i = 1, \dots, n \quad (43)$$

$$h_m(x) = \operatorname{argmin}_h \sum_{i=1}^n [g_{im} - h(x_i)]^2 + \lambda * \Omega \quad (44)$$

where Ω is a regularization term used to prevent overfitting, and λ is a regularization hyperparameter that controls the trade-off between fitting the data and the complexity of the model.

$h_m(x)$ is then added to the ensemble with a weight w_m , which is determined by a line search that minimizes the loss function between the predictions of the current ensemble and the true target values:

$$w_m = \operatorname{argmin}_w \sum_{i=1}^n L(y_i, f_{(m-1)}(x_i) + w * h_m(x_i) + \gamma * \Omega) \quad (45)$$

where γ is a regularization parameter for the weights.

Lastly, we provide the updated ensemble model at iteration m .

$$f_m(x) = f_{(m-1)}(x) + \eta * w_m * h_m(x) \quad (46)$$

where η is the learning rate that controls the step size of the update.

5. Dataset

Experimental studies [10–19] focusing on the shear behaviour of reinforced concrete beams without stirrups have shown that parameters including b_w , d , f_{ck} , a/d , and ρ_l are considered significant in the prediction of the shear capacity of RC beams without stirrups. Hence, these parameters are designated as the input parameters for ML. In total, 784 experimental data points for the shear experiment (see Table 1) collected in [62] were utilized to build all ML models and perform a deterministic analysis. The collected dataset was split in a ratio of 75:25 for training and testing. The heatmap showing the correlation matrix of the dataset depicted in Figure 1 shows that no multicollinearity was involved in the modelling since the correlations between input parameters are insignificant. The range and mode of the input parameters are shown in Figure 2, and the relationship between each input parameter and the target shear is shown in Figure 3.

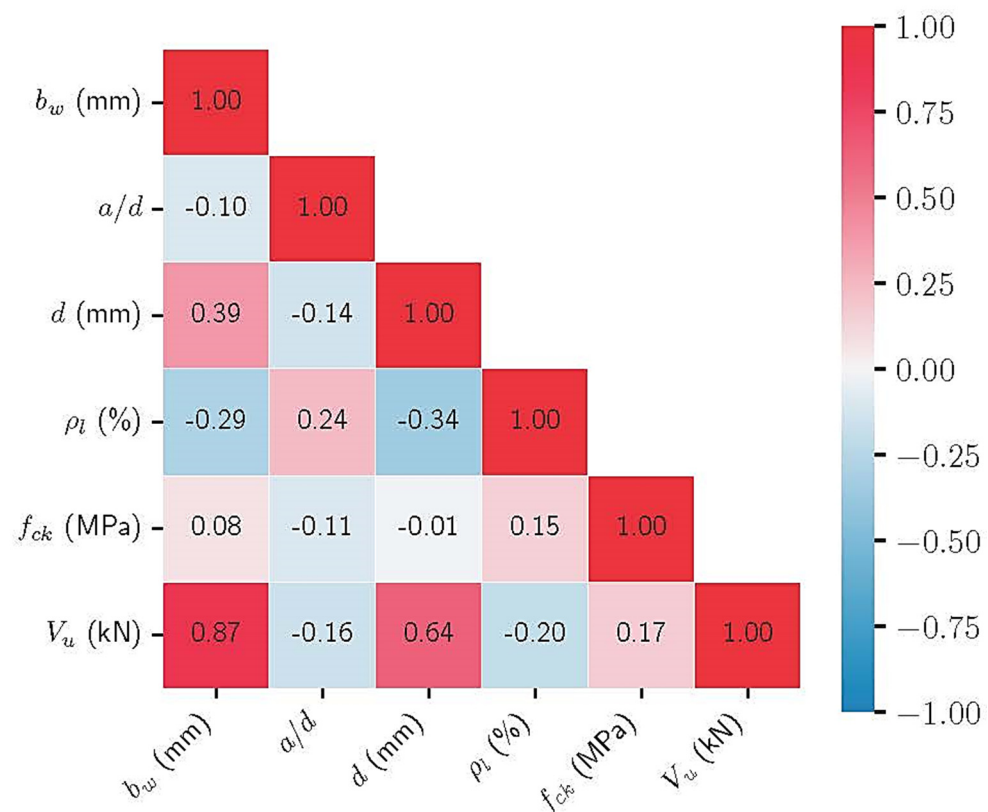
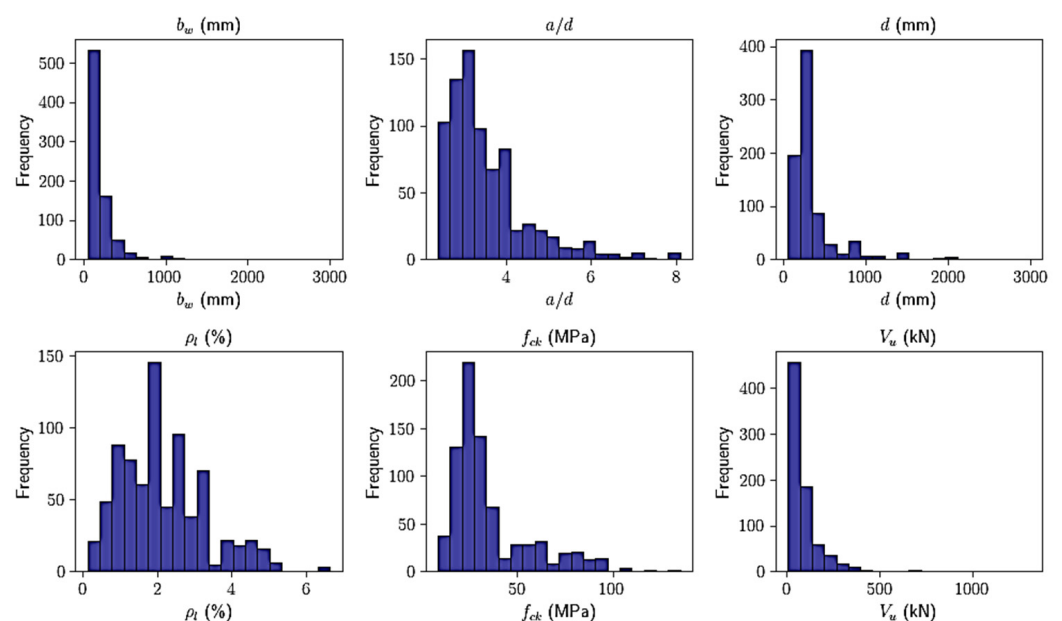


Figure 1. Heatmap with annotated correlation matrix.

Table 1. Descriptive statistics of the dataset.

	b_w (mm)	a/d	d (mm)	ρ_l (%)	f_{ck} (MPa)	V (kN)
Counts	784	784	784	784	784	784
Mean	218.54	3.50	345.50	2.2	35.32	98.10
SD	207.10	1.00	303.30	1.1	21.09	124.00
CoV	0.95	0.29	0.88	0.5	0.60	1.26
Min	50.00	2.40	57.20	0.1	8.90	7.20
25%	150.00	2.90	204.60	1.2	22.23	41.22
50%	153.00	3.20	268.20	1.9	28.00	61.05
75%	203.00	4.00	336.00	2.7	39.42	106.15
Max	3005.00	8.10	3000.0	6.6	135.00	1308.40

**Figure 2.** Frequency distribution of input parameters.

The correlation indices in Figure 1 provide valuable insights into the relationship between shear strength and the input parameters. Beam width (b_w) shows the strongest positive correlation with shear strength (0.87) (see Figure 3a), indicating that as the width increases, the shear strength increases significantly. The beam depth (d) also exhibits a moderately strong positive correlation (0.64) (see Figure 3c), suggesting that deeper beams contribute to greater shear strength, likely because of their increased resistance to shear forces through geometry. This is contrary to the size effect phenomenon because the shear strength should decrease as the beam depth increases; however, a closer examination revealed a corresponding increase in the beam width as the depth increases.

In contrast, the a/d ratio shows a weak negative correlation (-0.16), implying a slight tendency for shear strength to decrease as a/d decreases (see Figure 3b). Similarly, the percentage of longitudinal reinforcement (ρ_l) has a weak negative correlation (-0.20), which indicates that the shear strength slightly decreases as ρ_l increases (see Figure 3d). Compressive strength (f_{ck}) shows a weak positive correlation (0.17), suggesting that while higher concrete strength slightly improves shear strength, its effect is minimal compared to geometric factors.

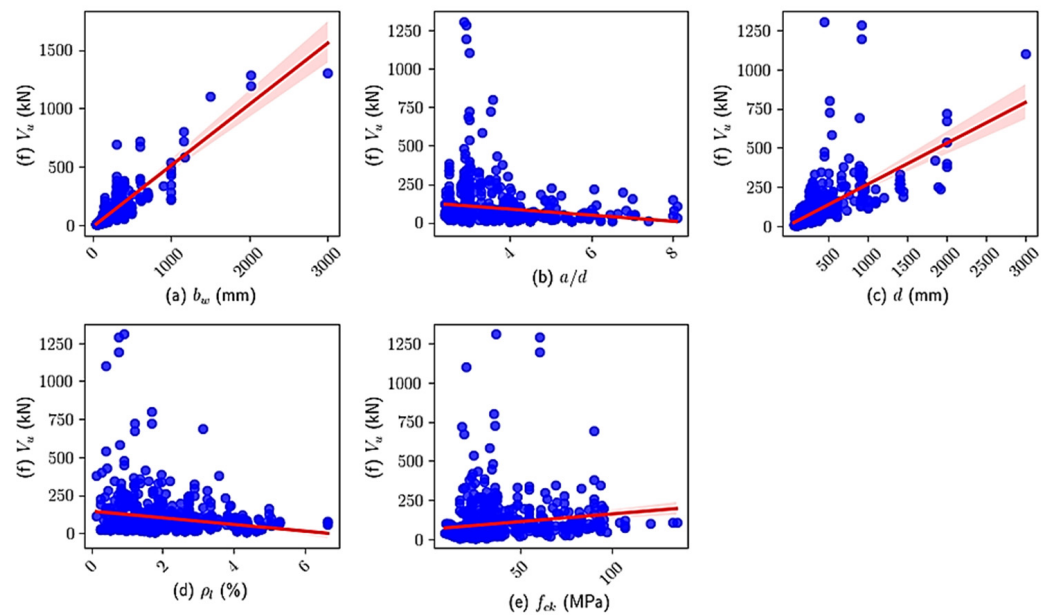


Figure 3. Relationship between input parameters and target variable.

6. Methodology

The mechanical models considered in this study were subjected to a mean value deterministic analysis with the exclusion of partial safety factors or reduction factors together with the use of mean values of concrete properties instead of characteristic values. Shear values derived from the mean value deterministic analysis and the predictions of the ML-based shear models were used as inputs in determining the uncertainty of the models with respect to the experimental shear values. The principles for uncertainty quantification provided in [107,108] were used to estimate the model uncertainty/factor associated with the considered models and their related statistical and parametric assessment. The ML-based shear models were optimized by adjusting their respective parameters for improved prediction capabilities following a 5-fold grid search cross-validation. The accuracy of the ML models was assessed by employing four parametric-based performance evaluators (see Table 2). Additionally, an explainable AI library (SHAP) was used to determine the most important feature in shear prediction. This was further related to the shear transfer mechanism with the aim of determining the governing shearing mechanism upon which future fracture mechanics-based models can be based.

Table 2. Parametric-based performance evaluation metrics.

Performance Metric	Formula
Root mean square	$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^n (y - x)^2}$
Mean absolute percentage error	$MAPE = \frac{100}{n} \sum_{i=1}^n \left \frac{y - x}{y} \right $
Coefficient of determination	$R^2 = \left[\frac{\sum_{i=1}^n (x - x') (y - y')}{\sqrt{\sum_{i=1}^n (x - x')^2 \sum_{i=1}^n (y - y')^2}} \right]^2$
Mean absolute error	$MAE = \frac{1}{n} \sum_{i=1}^n y - x $

Here, n is the number of observations, y is the experimental shear strength, x is the predicted shear strength from ML models, and y' and x' are the mean values of y and x .

Each error metric was carefully chosen to provide a robust assessment of the ML predictive capacity across different aspects. For example, RMSE is more sensitive to larger errors due to its squaring of the differences, making it a useful metric when we are concerned with penalizing larger deviations more heavily. This is important in our

study where large errors in shear strength predictions could have significant implications for structural safety. MAE, on the other hand, provides a linear measure of error without disproportionately penalizing large discrepancies. This allows for a clearer understanding of the average magnitude of the errors, which is useful for assessing the overall predictive performance of the models.

7. Results and Discussion

Figure 4 presents the comparison between the predicted shear values of ML models and experimental results. The results indicate that the extreme gradient boosting and gradient boosting models demonstrate the best agreement with experimental values, as evidenced by the low scatter around the trendlines and a high coefficient of determination (R^2) of 0.974, as seen in Figure 5. The RF and GBR models also provide comparable shear predictions to the XGB model, albeit with slightly lower R^2 values of 0.954 and 0.966, respectively. The artificial neural network (ANN) and Adaptive boosting (AdaBoost) models yielded intermediate shear results compared to the ML models, while the decision tree and SVM models performed moderately relative to the other ML-based shear models.

7.1. Performance Evaluation of ML Shear Results

Figure 5 shows the performance of the ML models according to various performance metrics. The models were evaluated using four different metrics, namely, mean absolute error (MAE), mean absolute percentage error (MAPE), root mean squared error (RMSE), and coefficient of determination (R^2). Overall, RF, XGB, and GBR performed the best based on most of the metrics. They all had lower values of MAE, MAPE, and RMSE, indicating that their predictions were closest to the actual values. Additionally, they had high R^2 values, indicating a good fit to the data. ANN also performed well, with a high R^2 value, but its MAE and RMSE were higher than those of GBR and XGB. SVM, DT, and AdaBoost had higher MAE, MAPE, and RMSE values and lower R^2 values compared to GBR, XGB, and RF.

7.2. Optimal Hyperparameter of ML Models Selected via Cross-Validation

The grid search cross-validation in the model selection sub-library of the sci-kit learn ML library package was used to perform a five-fold cross-validation with a specified parameter grid that contains the most important combination of parameters required for an optimal model tuning. After the hyperparameter tuning, the grid search CV selected the best parameters upon which the architecture of the ML models was built (see Table A1 in Appendix A).

All of the performance evaluators and reliability methods employed in this study to identify the most appropriate ML-based model in predicting the shear strength of beams without stirrups presented the boosting models (XGB and GBR) as the best predictors of shear strength. The artificial neural network also provided good remarks in its evaluation score, making it the next possible choice after the gradient boosting models.

The more complex algorithms used in this study, such as XGB, GBR, and Adaboost, demand substantial computational resources for training, primarily due to their iterative processes and the need for hyperparameter fine-tuning, which often involves evaluating numerous model configurations. Although these models, excluding Adaboost, excel in predictive accuracy as evidenced by high R^2 values and low error metrics, their training involves numerous iterations and cross-validation, leading to extended processing times compared to simpler models.

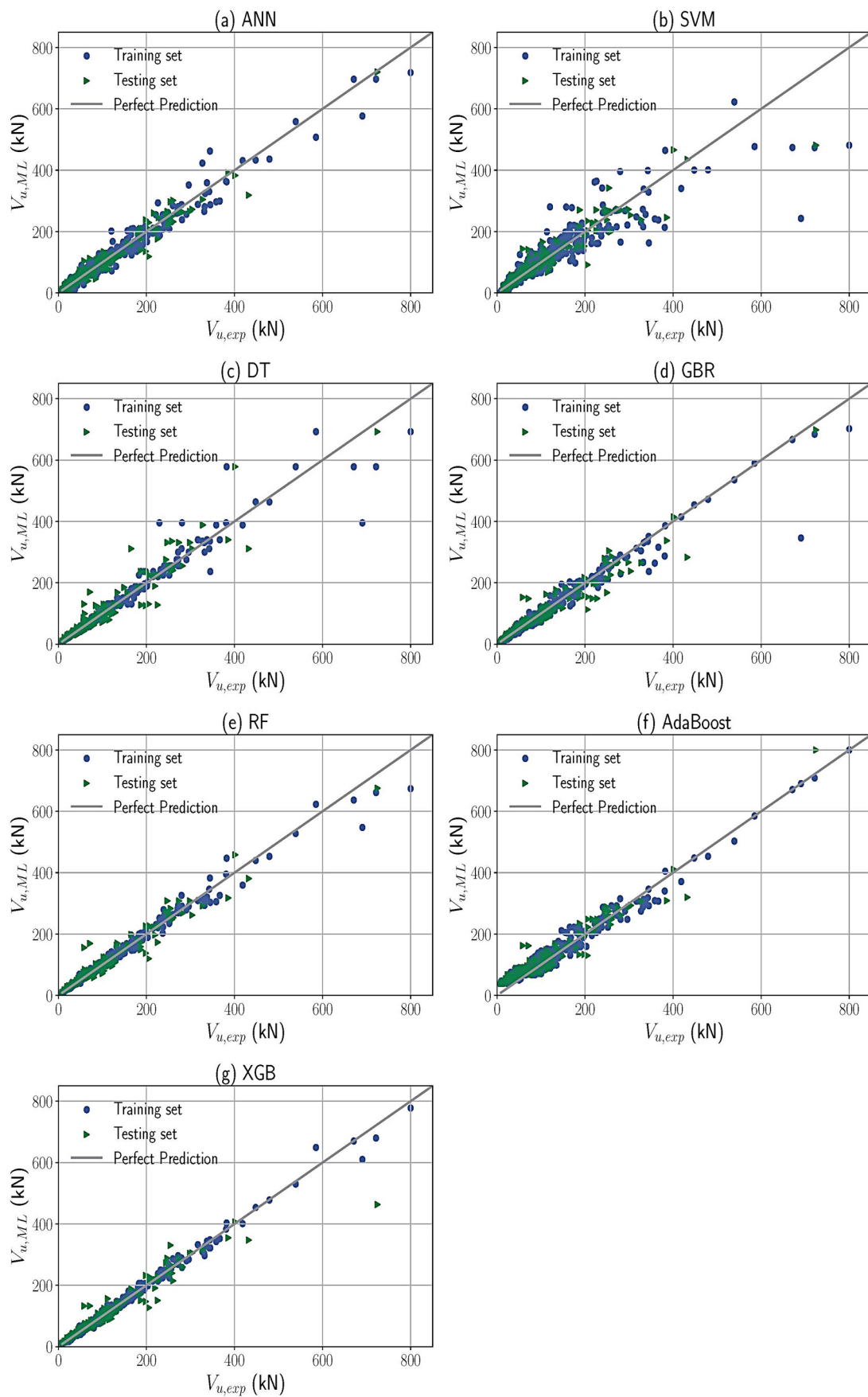


Figure 4. Comparison of experimental shear strength ($V_{u,exp}$) to ML-predicted shear strength ($V_{u,ML}$).

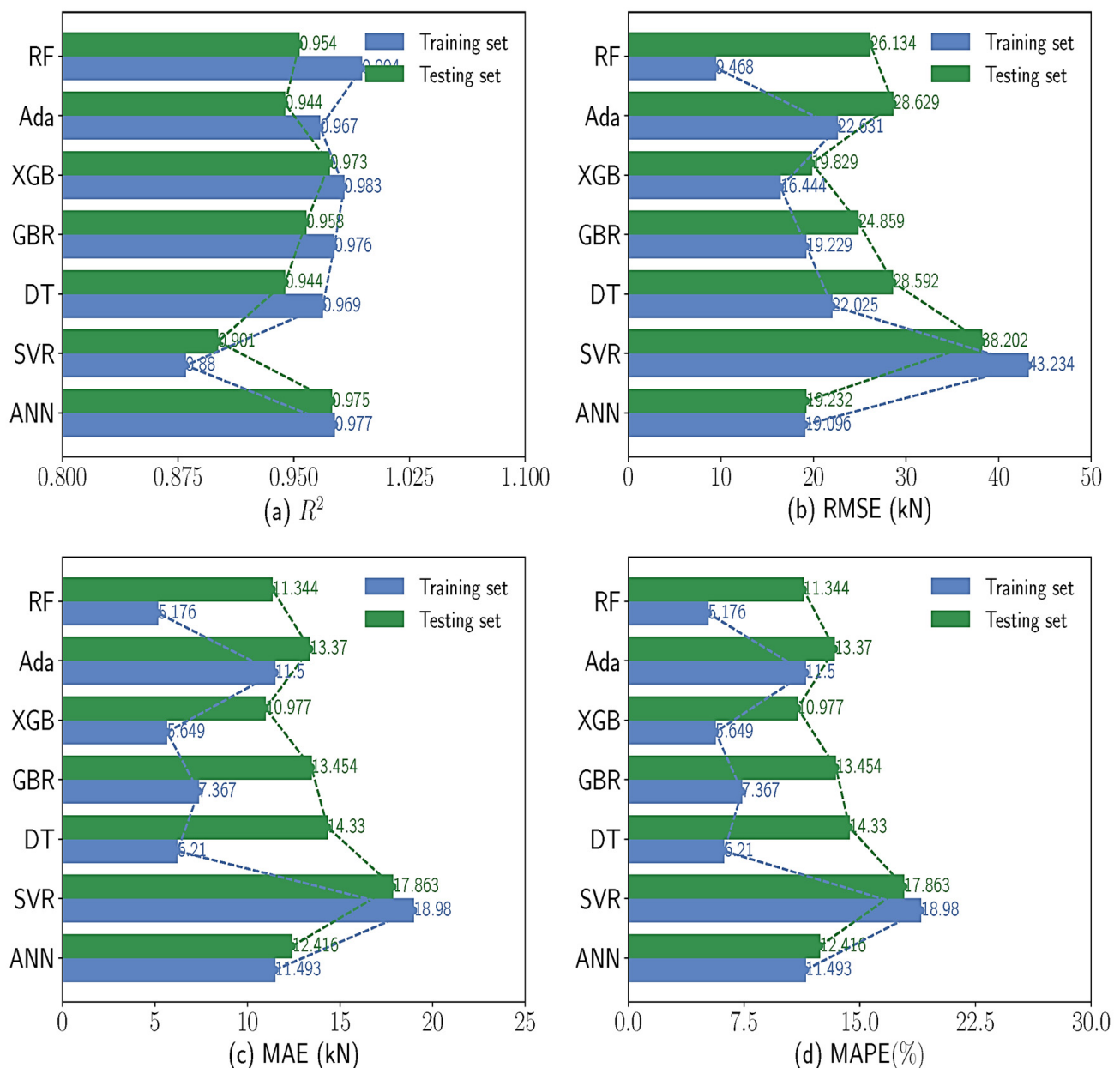


Figure 5. Bar charts displaying the metrics score of ML models' shear results.

ANNs also exhibits higher computational demands than simpler models like DT, RF, or SVM, due to its iterative procedure (epochs) in propagating residual errors. Factors such as the number of layers and neurons, as well as the choice of activation functions and optimization methods, contribute to the increased training burden due to increased complexity of model architecture. Despite achieving commendable predictive accuracy, ANN trains slower than tree-based models like XGB and GBR, which are better optimized for large-scale data.

While optimizing the ML algorithms through hyperparameter tuning is expedient for achieving high accuracy and preventing overfitting, it is equally important to consider the complexity of the dataset itself. Specifically, reducing the Kolmogorov complexity of the dataset as detailed in [109,110], which denotes the length of the shortest algorithm that can generate the dataset, can significantly enhance model performance. A dataset with lower Kolmogorov complexity can be achieved by eliminating noise, redundancy, or irrelevant features. This enables the model to focus on meaningful patterns and relationships, thereby improving predictive accuracy. This process not only minimizes the risk of overfitting but

also enhances computational efficiency during training. Therefore, apart from refining the model through parameter optimization, efforts to simplify the dataset structure by leveraging techniques such as feature selection based on the problem domain has been employed in this study to maximize the effectiveness of machine learning models in predicting shear strength.

7.3. Statistical Comparative Analysis of Model Factor (MF) of ML Models

From Table 3, MF_{XGB} , MF_{GB} , and MF_{RF} all have a mean value of 1 and 1.01, respectively; this indicates that there is no form of bias in the shear prediction from these AI-based shear models. Moreover, the measure of the dispersion of MF_{XGB} and MF_{GB} , which is closer to zero (0.14) compared to MF_{ANN} , and MF_{RF} (0.18 and 0.19), presents the realization of both MF_{XGB} and MF_{GB} to be more accurate. The coefficient of variation (Ω) also infers a nominal variability in the realization of both MF_{XGB} and MF_{GB} with values of $\Omega_{MF(XGB)} = 14\%$ and $\Omega_{MF(GB)} = 14\%$. The low degree of variability in the model factor realization buttresses the certainty in the shear predictions of MF_{XGB} and MF_{GB} although the COV% is marginally higher than the 10% threshold recommended value given in [111]. Positive results are presented by the statistics of MF_{ANN} and MF_{RF} in comparison to MF_{XGB} , and MF_{GB} .

Table 3. Statistical parameters of model factors for ML-based shear models for testing data.

	MF_{ANN}	MF_{SVM}	MF_{RF}	MF_{DT}	MF_{Ada}	MF_{GB}	MF_{XGB}
Counts	196	196	196	196	196	196	196
Mean	0.95	1.07	1.01	1.04	0.80	1.00	1.00
Std	0.18	0.32	0.19	0.38	0.20	0.14	0.14
CoV	19%	30%	19%	37%	24%	14%	14%
Max	1.99	2.58	1.60	1.78	1.58	1.82	1.72
Q1	0.89	0.88	0.92	0.91	0.60	0.93	0.91
Q2	0.98	1.00	1.00	0.99	0.80	1.03	1.00
Q3	1.09	1.18	1.08	1.09	0.97	1.14	1.06
Min	0.56	0.41	0.44	0.42	0.22	0.39	0.38

MF_{SVM} has a mean value of 1.07, which is indicative of a small bias, and 7% conservatism, while MF_{DT} is just 4% conservative with a mean value of 1.04. Although the small bias indicates that the shear models built on the architecture of SVM and decision trees are somewhat accurate in shear prediction, the wide dispersion of the realized model factors around the mean brings to light the uncertainty in the performance of DT and SVM models in shear prediction with $\sigma_{MF(SVM)} = 0.32$ and $\sigma_{MF(DT)} = 0.38$. Also, the coefficient of variation seen in Table 3 suggests that a significant degree of variation in their model factor realization is considerably greater than the recommended extent of variation for shear models [109].

7.4. Outlier Identification

Figure 6 presents a box plot of the model error/factor for the respective ML models in the prediction of shear strength. Shear prediction following the SVR ML model shows significant variability as indicated by the prediction points outside of the $\mu \pm 3\sigma$ range across both training and testing sets. While the ANN model exhibits some notable outliers beyond the maximum, all other models, excluding AdaBoost and DT, have fewer outliers on either side of the whiskers. Overall, XGB, RF, and GBR provide a less variable prediction of shear strength, as evidenced by fewer outlier points in Figure 6.

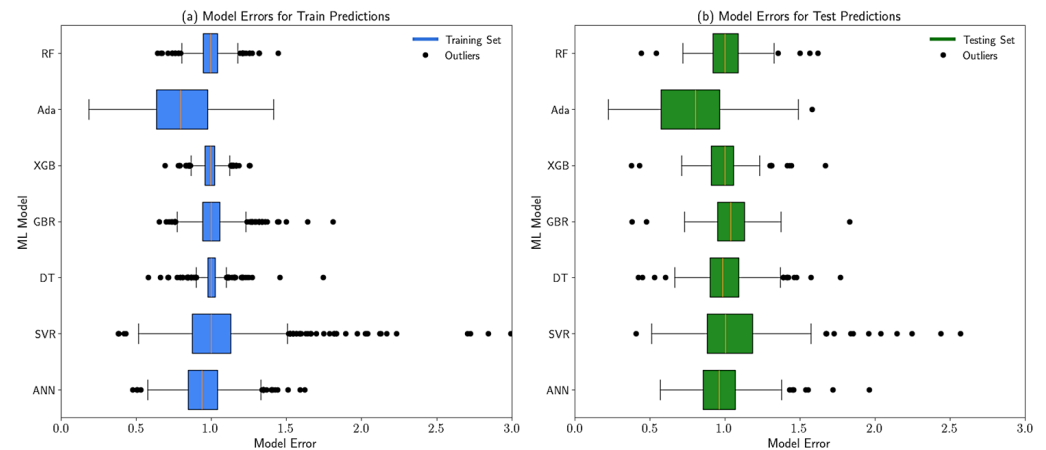


Figure 6. Box plots showing (a) model errors for training prediction and (b) model errors for test predictions.

7.5. Correlation Analysis of Model Factor Against Input Parameters

As seen in Table 4, the correlation analysis indicates that MF_{DT} and MF_{RF} exhibit the highest number of correlations with the input variables, with r values of $b_w = 0.2$, $\rho_l = 0.27$, and $f_{ck} = 0.25$ for MF_{DT} and $a/d = -0.29$, $\rho_l = 0.2$, and $f_{ck} = 0.21$ for MF_{RF} , respectively. These results suggest that the input variables have a relatively weak linear association with the shear capacity predicted with MF_{DT} and MF_{RF} . MF_{AB} also demonstrates a mild correlation with some input variables, with r values of -0.3 , and 0.32 for a/d and f_{ck} , respectively. The correlation between the input variables and MF_{AB} 's predictions imply that the model is sensitive to changes in the input variables.

Table 4. Pearson correlation index of ML model factors with shear parameters.

	Pearson Correlation Coefficient (r)				
	b_w (mm)	a/d	d (mm)	ρ_l (%)	f_{ck} (MPa)
MF_{ANN}	0.023	−0.18	−0.14	0.036	0.24
MF_{SVM}	0.018	−0.071	−0.11	0.0033	−0.021
MF_{RF}	0.025	−0.29	0.0012	0.2	0.21
MF_{DT}	0.2	−0.18	0.052	0.27	0.25
MF_{AB}	0.19	−0.3	0.14	0.18	0.32
MF_{GB}	−0.082	−0.16	−0.059	0.083	0.17
MF_{XGB}	−0.082	−0.13	−0.17	0.15	0.13

In contrast, MF_{GB} and MF_{XGB} exhibit very weak correlations with the input variables, with r values ranging from -0.082 to 0.17 and from -0.082 to 0.13 , respectively. These results suggest that the input variables have no significant linear association with model factor realizations of the GB and XGB shear models and that the predictions from these models are more reliable than those from the other models. Likewise, the correlation index of MF_{SVM} with the input variables illustrates the absence of any form of linear association, while the model factor of the ANN shear model is seen to have a weak correlation with the concrete strength only.

7.6. Shapely Additive Explanation (Explainable AI) for Shear Model

Shapley values represent a concept derived from cooperative game theory that measure the average contribution of each feature, akin to a player, in ML predictions. The features' relative significance for the model predictions is evaluated by comparing their absolute average Shapley values, with larger values indicating greater importance. It is

important to acknowledge that the SHAP method assesses the effect of features on the trained model, rather than on the dataset used for training. Consequently, if the model is not accurate, the SHAP feature importance and dependence estimates will also be flawed. In this study, SHAP values were obtained from the XGB model, which exhibited the highest accuracy level. Thus, evaluating the SHAP feature importance and dependence for the optimized models can offer insight into the genuine effects of independent variables in the database on shear resistance in slender beams without shear reinforcement.

Figure 7 displays the SHAP summary plot for the XGB model, where each dataset sample's Shapley value is represented by a point. The point's colour signifies the feature value range, ranging from low (blue) to high (red). Points with identical Shapley values for each feature are plotted vertically to display their distribution, with feature importance ranking from top to bottom. Based on the SHAP summary plot shown in Figure 4, the explainable AI model identifies the beam width (b_w) and effective depth (d) as the most important factors for predicting shear strength in slender beams without stirrups. This indicates that these two features contribute the most to the model's predictions, and any changes made to them may have a significant impact on the predicted shear resistance of the beam. In contrast, the ML model indicates that longitudinal reinforcement (ρ_l), shear span–effective depth ratio (a/d), and compressive concrete strength (f_{ck}) have a relatively lower impact on shear resistance. Therefore, altering these features may not have a significant impact on the predicted shear resistance of the beam.

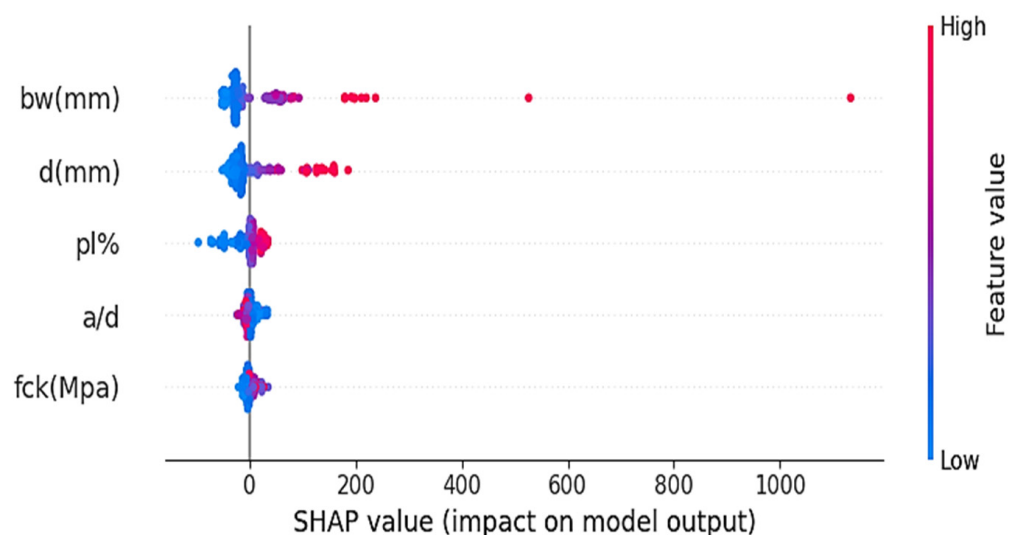


Figure 7. SHAP summary plot for XGB model.

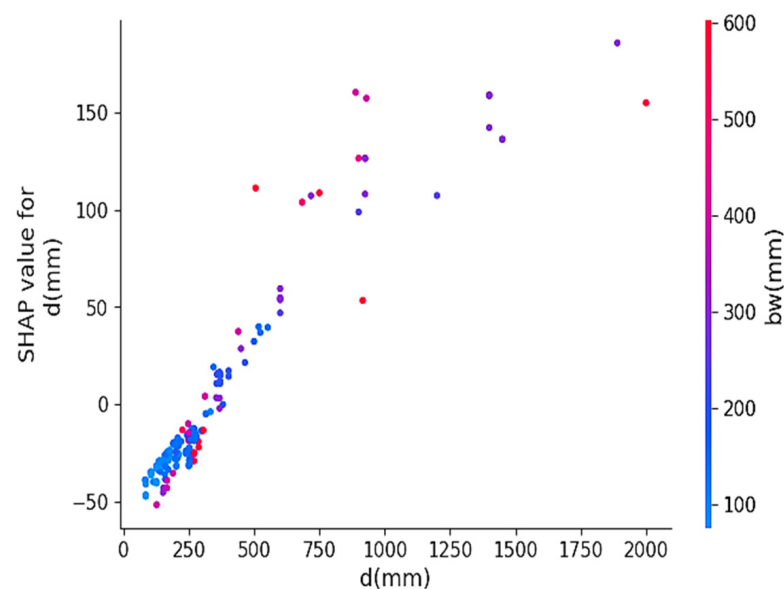
Figure 8a illustrates a positive linear correlation between the SHAP (Shapley additive explanation) value and lower values of effective depth (d) for beams of small widths (represented by blue points). However, as the effective depth increases from 500 mm to 2000 mm, this relationship becomes nonlinear, particularly for beams of medium and large widths (represented by purple and red points). For slender beams without shear reinforcement, the shear resistance generally increases with increasing compressive strength, especially for beams with small depths (as denoted by the blue points in Figure 8b). Nevertheless, a discernible scatter in the effect of f_{ck} on the shear resistance is noticeable when the concrete strength exceeds 60 MPa.

In addition, the shear resistance increases with beam width, especially within the range of 60 to 500 mm (as depicted in Figure 8c). On the other hand, Figure 8d indicates that the shear resistance increase is not observed when ρ_l falls within the range of 0–1%, particularly for beams with large effective depths. Conversely, a slight increase in shear strength is observed for beams with small effective depths and longitudinal reinforcement ranging from 0 to 3%. However, as the longitudinal reinforcement exceeds 3%, the effect

on shear strength becomes indistinct. In general, an increase in the ratio of shear span to effective depth results in a reduction in SHAP value. Nevertheless, this trend becomes less discernible as a/d increases beyond 4 (as shown in Figure 8e).

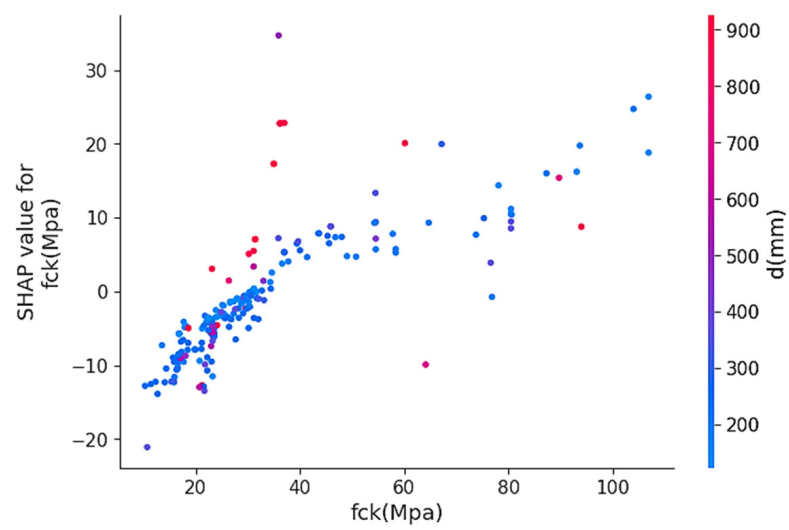
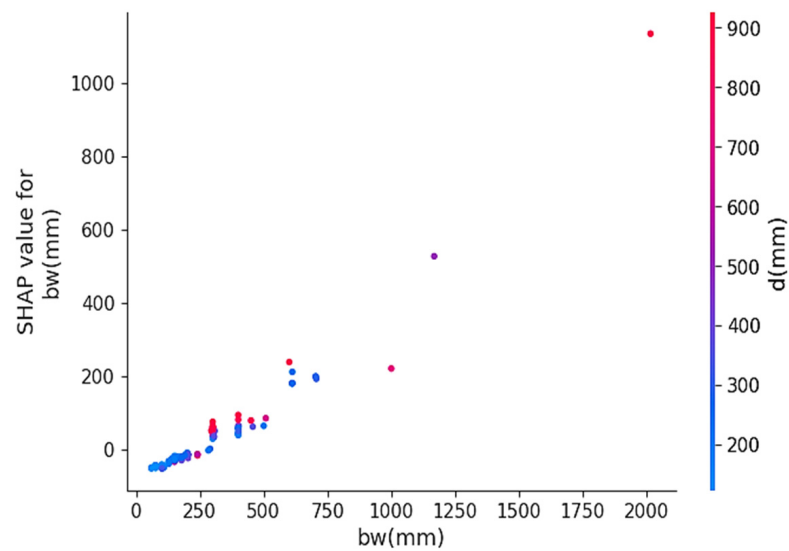
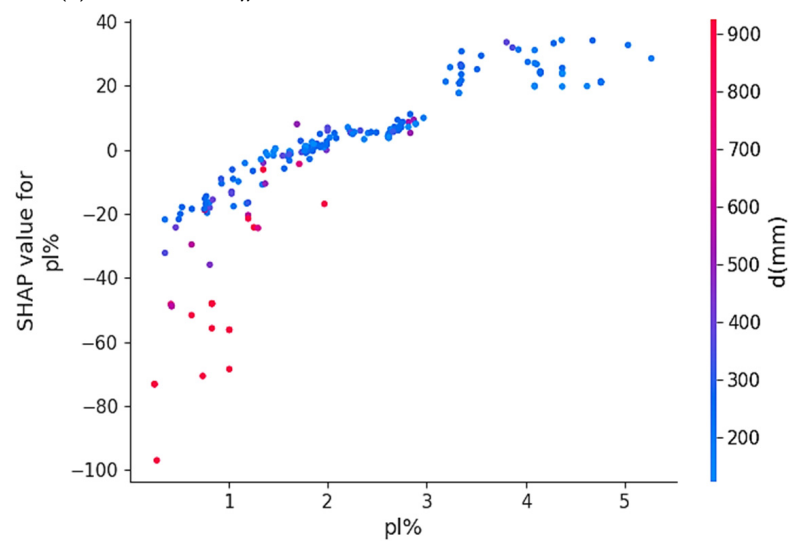
To summarize, the findings presented in Figure 8 suggest that the shear resistance of reinforced concrete beams is influenced by various factors, such as effective depth, compressive strength, beam width, longitudinal reinforcement, and the ratio of shear span to effective depth but the performance of these factors largely depends on the effective depth and beam width only.

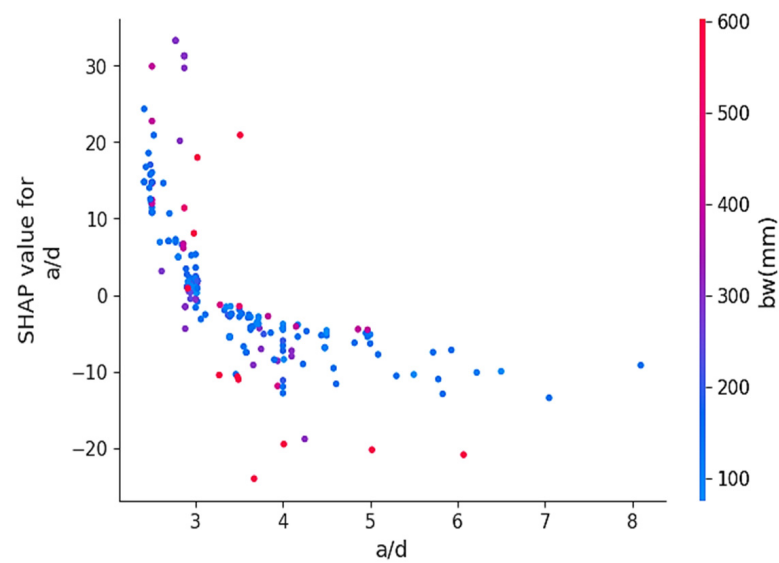
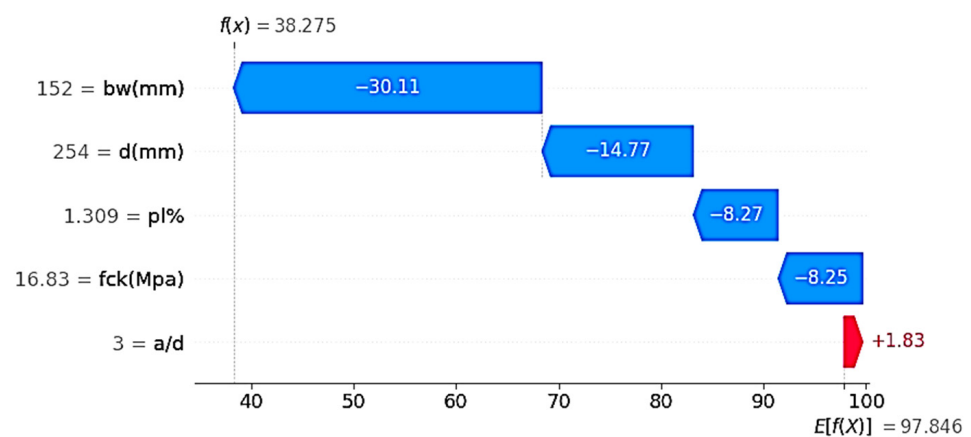
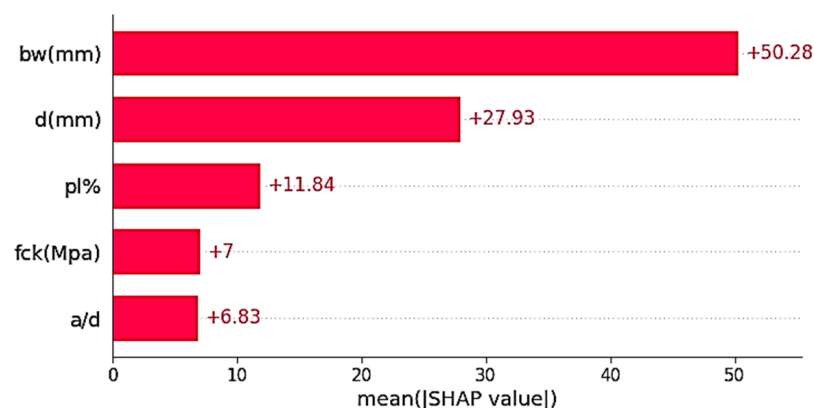
In Figure 9, the SHAP waterfall plot is presented as a sequence of horizontal bars, where each bar represents the contribution of a particular feature to the overall prediction. These bars are arranged in descending order based on their magnitude of impact. Figure 9 illustrates the contribution of each feature to the model's output for a specific instance of the beam data displayed as a horizontal bar, with the length of the bar indicating its impact on the prediction. According to Figure 9, the beam width and effective depth are the most significant factors in determining shear strength, as they have long blue bars. In contrast, the shear span to effective depth feature has a negative impact on the shear strength prediction, as indicated by its shorter red bar. Figure 10 displays the SHAP bar plot, which is an effective tool for understanding the importance of different features in predicting the outcome of a machine learning model. The plot is created using the mean SHAP values of each feature across all iterations (196 test sets). Each feature is represented by a horizontal bar, with the length of the bar corresponding to the feature mean SHAP value. The bars in the SHAP bar plot are arranged in descending order based on their size, with the feature that has the greatest mean SHAP value appearing at the top of the graph. Conversely, the feature with the smallest mean SHAP value appears at the bottom of the graph. Figure 10 highlights the beam geometrical features as the most significant features in predicting shear strength. This suggests that factors such as the beam width and effective depth have the greatest impact on the outcome of the ML model.



(a) Effect of d

Figure 8. Cont.

(b) Effect of f_{ck} (c) Effect of b_w (d) Effect of pl **Figure 8.** Cont.

(e) Effect of a/d **Figure 8.** SHAP dependence plots for XGB shear model.**Figure 9.** SHAP waterfall plot for XGB shear model.**Figure 10.** SHAP bar plot for XGB shear model.

7.7. Partial Dependence Plot

The partial dependence plot showing the relative importance of input features in predicting the shear strength is presented in Figure 11. The insights gleaned from Figure 11 evidently corroborate the findings following the SHAP analysis discussed previously in Section 7.6. From these plots, it can be observed that an increase in the geometrical

properties (b_w and d) of the beam lead to a corresponding increase in the prediction of the shear capacity. While the increase in ρ_l and f_{ck} shows a marginal increase in shear prediction, the latter tends to slightly decrease with an increase in a/d . As noted earlier, the input features selected for this analysis are the major factors influencing the shear capacity of beams without stirrups.

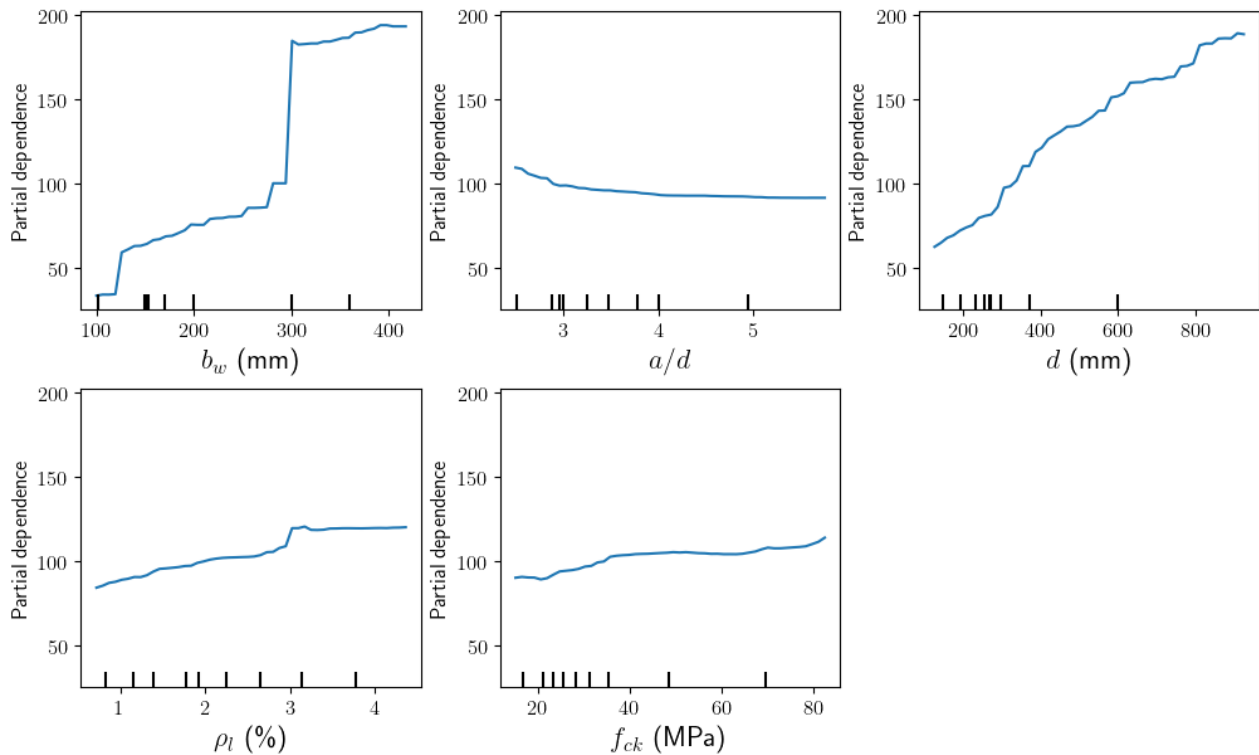


Figure 11. Partial dependence plot of input features used in XGB shear model.

8. Mechanical Model Shear Result Discussion

Table 5 indicates that the statistical moment of Tran’s fracture mechanics-based model performs better in predicting shear strength, based on its low bias (1.02) and low variability (16%). In contrast, the models from Cladera et al. [6,62] are also mechanical-based models that consider shear mechanisms, but differ from fracture mechanics-based models in that they do not rely on crack propagation analysis or incorporate concepts such as crack opening, crack slip, aggregate size, and fracture energy. However, the structural mechanics model relies solely on the beam geometry and material properties, as well as loading and boundary conditions, to predict the behaviour of the structure.

Table 5. Statistical parameters of model factors for mechanical shear models across the entire dataset.

	Counts	Mean	Std	CoV (%)	Min	Max	Q1	Q2	Q3
MF_{CCC}	784	1.14	0.28	25	0.28	2.23	1.02	1.16	1.28
MF_{MASM}	784	1.11	0.28	25	0.31	2.28	0.98	1.13	1.25
MF_{NLT}	784	1.02	0.16	16	0.57	1.98	0.94	1.06	1.17

Table 6 measures the strength and direction of the linear relationship between the mechanical model’s model factor realizations and the shear parameters. MF_{NLT} appears to not correlate with any shear parameter, while MF_{MASM} only shows weak negative correlation with the concrete strength, and MF_{CCC} appears to be weakly negatively correlated with the ratio of shear span to effective depth and the longitudinal reinforcement ratio.

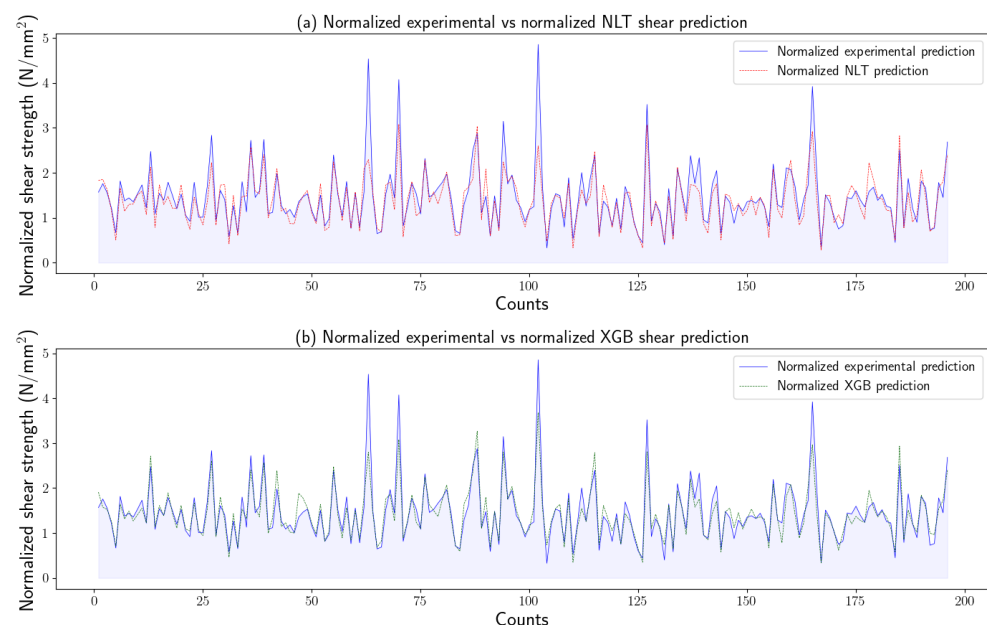
Table 6. Pearson correlation matrix of mechanical shear model factors with shear parameters.

	Pearson Correlation Coefficient (r)				
	b_w (mm)	a/d	d (mm)	ρ_l (%)	f_{ck} (MPa)
MF _{CCC}	0.039	−0.24	0.14	−0.22	−0.13
MF _{MASM}	−0.032	−0.17	0.033	−0.061	−0.21
MF _{NLT}	0.086	0.083	0.12	−0.18	−0.0038

9. Juxtaposition of the Statistical Results of the Mechanical Shear Model and ML-Based Shear Model

To ascertain the degree of similarity between the predictions provided by the ML algorithm and the mechanics-based shear models, a comparative analysis was conducted using the test dataset. Specifically, the analysis focused on identifying the optimal predictor of shear strength in both scenarios. The result of this investigation revealed that the predictions obtained through the fracture mechanics-based model developed by Tran [61] were comparable to those generated through the XGB ML shear model, as evidenced by the statistical moment analysis presented in Table 7. While it was noted that the ML-based model produced more accurate shear estimates with less variability than its mechanical counterpart, the latter was found to be 7% more conservative than the former and exhibited a marginal increase in shear estimate variation (17%). Additionally, an examination of the percentiles of the model factor realizations suggested that the respective prediction distributions were highly similar.

Figure 12 illustrates that at higher values of shear, both ML-based models and mechanical models behave similarly through underpredicting the shear strength. Generally, it can be deduced from Figure 12 that the XGB model provides estimates that are less conservative compared to the mechanical shear model (NLT), but they both follow the same predictive pattern.

**Figure 12.** Line chart overlaying the experimental shear prediction with the (a) Tran [61] model and (b) XGB prediction.

The reliability of the shear strength prediction generated by the XGB model was confirmed by assessing the probability distribution and probability plots, as presented in Figure 13. Specifically, the distribution of the XGB model follows a normal distribution, indicating a high degree of accuracy and consistency in its predictions. While the model

factor realization of the 196 test data points following Tran’s shear model may appear to fit a lognormal distribution, a closer examination revealed that the deviation from a normal distribution was minimal and of no implication in its reliability prediction.

Table 7. Juxtaposition of statistical parameters of model factors between XGB and Tran [61] shear models.

	Counts	Mean	Std	CoV (%)	Min	Max	Q1	Q2	Q3
MF_{XGB}	196	1.00	0.14	14	0.38	1.72	0.91	1.00	1.06
MF_{NLT}	196	1.07	0.18	17	0.68	1.97	0.95	1.03	1.16

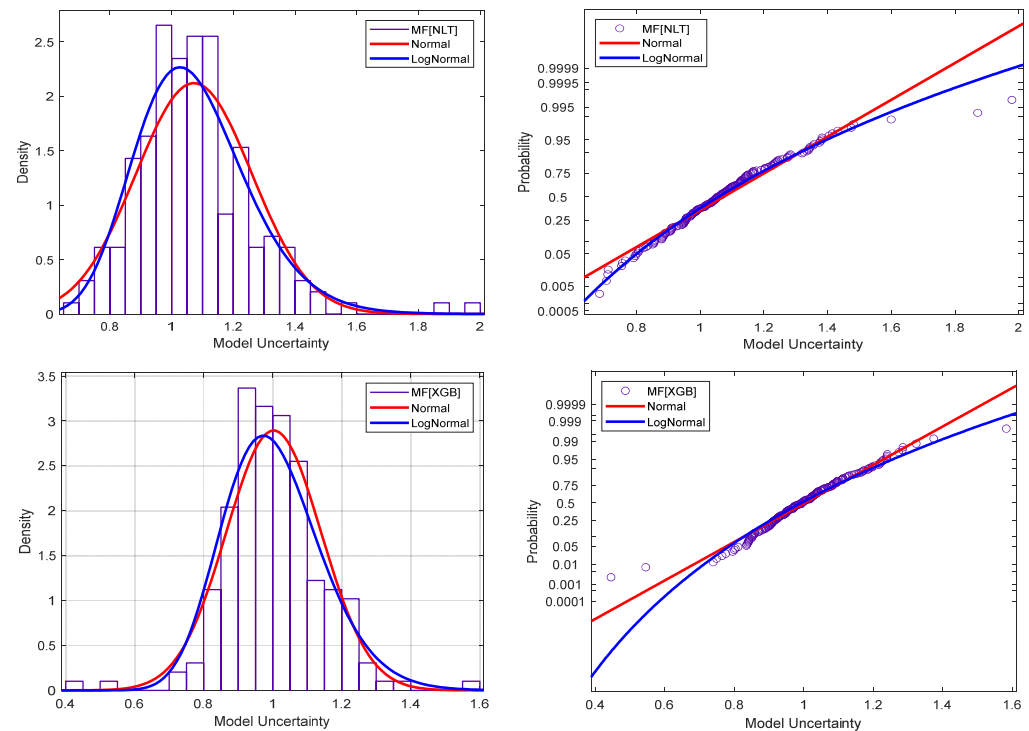


Figure 13. Probability distribution function and probability plot.

From the probability plot presented in Figure 13, it can be observed that there are some points that do not align with the lower tail of either of the distribution curves for the model uncertainty of the XGB shear model. These points may be called the cut-off points or boundary conditions in the use of the XGB shear model in this study. This may be due to various reasons. Firstly, the algorithm may have been poorly trained in regions representing the lower tail of the distribution (corresponding to high shear values) of the model error due to the paucity of data in this range. Additionally, the XGB model tends to overly estimate the shear capacity in these regions, leading to unconservative shear predictions. The use of a more robust and diverse dataset that better represents the extreme tails of the distribution may potentially mitigate this limitation by improving the model’s generalization and accuracy across all ranges of shear values.

10. Conclusions and Recommendations

This study investigated the suitability of mechanics-based and optimized ML-based models in the shear strength prediction of slender beams without stirrups. The following conclusions were drawn from this study:

- i. In exploring the efficiency of fracture mechanics-based shear models compared to the empirical models and traditional structural mechanics, this study shows that the fracture mechanics-based models achieved a more accurate and reliable shear

- strength prediction. The models are focused on crack development and propagation; as such, they exhibit greater transparency, resulting in a perfect understanding of the interactions between various shear transfer mechanisms and the shear failure process. As a result, the models have better precision in shear strength characterization, making them very suitable for design.
- ii. While the ML models highlighted the robustness of fracture mechanics in predicting shear strength, this study also emphasizes the importance of paying attention to beam geometry, especially that of effective depth and beam width, because, through explainable AI methods, these factors significantly impact shear strength. With the results obtained, it can be recommended that fracture mechanics-based models should be adopted in design codes due to their accurate prediction of shear strength compared to other models, such as empirical, strength-based, and semi-empirical models.
 - iii. The crack width and depth largely affect the overall shear strength, as shown by the mechanisms. However, further research on the shear model is recommended to explore the effect of residual tensile strength and aggregate interlock on slender beams without stirrups. Moreover, future studies can investigate the relationship between shear transfer mechanisms and beam width, especially for beams without stirrups. Such a study can help to enhance the precision of fracture mechanics-based models.

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Conflicts of Interest: The authors declare no conflicts of interest.

Appendix A

Table A1. Optimal hyperparameters of models.

Model	Hyperparameter Grid	Optimal Hyperparameters
SVM	C: 0.001, 0.01, 0.1, 0.5, 1, 2	2
	Kernel: Linear, Rbf, Poly, Sigmoid	Linear
	Scale: Auto, Gamma	Gamma
	Degree: 2, 3	2
	Epsilon: 0, 0.01, 0.1, 0.5, 1, 2	0.5
RF	N estimators: 64, 80	64
	Criterion: squared error, absolute error, Poisson	squared error
	Max depth: 40, 50, 37, 35	37
	Min samples split: 3, 5, 2	2
	Min impurity decrease: 0.00001, 0.005, 0.000008	0.000008
	Min samples leaf: 1, 2	1
	Max features: auto, sqrt, log2	Auto
	Max leaf nodes: 30, 40, 45, 50	45
	Bootstrap: True, False	True
	Random state: 101, 73, 80	73

Table A1. Cont.

Model	Hyperparameter Grid	Optimal Hyperparameters
Model	Hyperparameter grid	Optimal hyperparameters
DT	Criterion: squared error, absolute error, Poisson, Friedman MSE Splitter: Best, Random Max depth: [40, 50, 60, 70, 80, 90, 100] Min samples split: 3, 5, 10, 20, 25 Min impurity decrease: [0.00001, 0.005, 0.000008] Min samples leaf: [1, 2, 3, 4, 5] Max features: auto, sqrt, log2 Max leaf nodes: [3,5,10,15,30,40]	Squared error Random 40 3 0.000008 1 Auto 40
AB	n_estimators: [50, 100, 200, 500] learning_rate: [0.01, 0.005, 0.5, 0.1, 1] loss: ['linear', 'square', 'exponential'] max_depth: [3, 5, 7] random_state: [25, 45, 73, 101]	50 0.5 exponential 5 random_state = 101
GB	n_estimators: [50, 100, 150] max_depth: [2, 3, 4, 5] learning_rate: [0.1, 0.05, 0.01] loss: ['squared_error', 'absolute_error', 'Huber', 'quantile'] criterion: ['friedman_mse', 'squared_error'] min_samples_split: [2, 3, 4] max_features: ['auto', 'sqrt', 'log2']	n_estimators: 150 max_depth: 3 learning_rate: 0.1 loss: 'Huber' criterion: 'squared_error' min_samples_split: 2 max_features: log2
XGB	n_estimators: [50, 100, 120, 150] max_depth: [2, 5, 7, 10] learning_rate: [0.1, 0.05, 0.01] reg_lambda: [1, 0.1, 0.01] reg_alpha: [0, 1, 0.1, 0.01] min_child_weight: [1, 0.5, 2, 3] gamma: [0, 0.01, 0.1, 0.5] subsample: [0.5, 0.7, 1]	n_estimators: 100 max_depth: 7 learning_rate: 0.1 reg_lambda: 1 reg_alpha: 0 min_child_weight: 1 gamma: 0.1 subsample: 1
ANN	Numberof hidden layers Learning rate The activation function in both layers Optimizer Loss function Mini-batch size Epochs	2 0.01 ReLU Adam Optimizer MSE 16 500

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