

**Abstract:** This study aims to develop an intelligent modeling approach for accurately predicting compaction characteristics of cohesive soils across compaction energy (CE) levels. A comprehensive database of 1001 observations falling within the theoretical bounds was created through experimental investigation encompassing sieve analysis, hydrometer analysis, liquid limit ( $w_L$ ), plastic limit ( $w_P$ ), specific gravity ( $G_s$ ), and compaction tests on natural soil samples and literature review, encompassing diverse cohesive soils, CE levels, and compaction characteristics. Multiple machine learning techniques, including Extreme Gradient Boosting (XGBoost), Random Forest (RF), Gene Expression Programming (GEP), Multi Expression Programming (MEP), Artificial Neural Networks (ANN), and Multiple Linear Regression (MLR), were applied to develop predictive models. XGBoost demonstrated superior performance in predicting maximum dry density ( $\gamma_{dmax}$ ) and optimum moisture content ( $w_{opt}$ ) as evaluated by statistical indicators and external validation and compared with existing models in the literature. The models effectively captured the influence of key parameters, highlighting the primary role of CE and  $w_L$ , the secondary role of plastic limit ( $w_P$ ), the tertiary role of plasticity index ( $I_P$ ) and fines activity ( $A_F$ ), and the quaternary role of soil gradation in predicting and influencing the compaction characteristics of cohesive soils. This approach enables accurate global modeling of cohesive soil compaction across varying CE levels, providing a valuable tool for geotechnical engineers and researchers to determine compaction characteristics for a known CE level using basic soil properties used for soil classification.

**Keywords:** Machine learning; XGBoost; Compaction; Cohesive soils; Big geotechnical data

## 1. Introduction

Compaction control is a crucial factor that governs the engineering properties of fine-grained soils also referred to as cohesive soils, across various earthwork projects, including the construction of foundation structures, roads, compacted clay liners, earthen dams, nuclear repositories, and embankments, among others (Wang and Yin, 2020; Zhu et al., 2024). To attain desired engineering characteristics through optimal densification in a project, the soil density and moisture content are benchmarked against the maximum dry density ( $\gamma_{dmax}$ ) and optimum water content ( $w_{opt}$ ) obtained through a compaction test (Horpibulsuk et al., 2009). The field compaction parameters are benchmarked against the parameters obtained at specified CE levels linked with the standard and modified proctor tests to obtain the degree of compaction ( $D_c$ ) (Ran et al., 2024). Thus, compaction parameters are crucial in designing and commencing the compaction process in earthwork, while simultaneously establishing a standard for quality control and assurance (QA/QC) during field operations (J. Li et al., 2024; Ma et al., 2024; Tarantino and De Col, 2008). However, the testing methodologies required to obtain these parameters are characterized by labor-intensive and tedious procedures, necessitating a substantial quantity of representative material for the examination, factors linked to escalating project time and cost (Teramoto et al., 2024; Wang et al., 2020). Furthermore, this challenge is exacerbated by the adoption of test protocols standardized across various conceptual compaction energy (CE) levels, i.e., standard or modified, which may or may not align with actual field conditions (Alzubaidi et al., 2024; Jia et al., 2024). In practical applications, compaction energy (CE) levels can vary significantly, either adhering to established conceptual levels or being set at project-specific levels. This variability underscores the need for efficient methods to determine compaction characteristics across a range of CE levels. Recent research by Miller and Vahedifard (2024) and Spagnoli and Shimobe (2020) has highlighted this necessity, emphasizing the importance of adaptable compaction assessment

techniques. Furthermore, there is a growing demand for methods to accurately determine the compaction state at arbitrary CE levels in the field. This is crucial for assessing the  $D_c$  achieved under various field conditions, which often differ from laboratory settings. In large-scale projects, to mitigate errors, field values of compaction characteristics are also increasingly being evaluated using samples retrieved from different field locations at arbitrary CE levels during the compaction process (Blanco, 2015). This underscores a need for an expedited method for the prediction of compaction parameters at arbitrary CE levels to reduce the testing requirements for QA/QC (Deng et al., 2024; Miller and Vahedifard, 2024).

For quick estimation of compaction characteristics, several researchers have established methods to determine  $\gamma_{dmax}$  and  $w_{opt}$  of cohesive soils using Atterberg's limits, i.e., liquid limit ( $w_L$ ), plastic limit ( $w_P$ ), and plasticity index ( $I_P$ ) (Al-Khafaji, 1993; Farooq et al., 2016; Ito and Komine, 2008; Khalid and Rehman, 2018; Sridharan and Nagaraj, 2005; Tilahun et al., 2024; Wang and Yin, 2020). Most of the past correlations were established for a singular conceptual CE designated by the ASTM, i.e., standard (592.3 kN-m/m<sup>3</sup>) or modified (2693.3 kN-m/m<sup>3</sup>) or either unspecified CE; thereby, their application for an arbitrary CE or even to the conceptual CE designated by other standards, e.g., BS which involve a slight variation in CE than ASTM, is restricted (Blotz et al., 1998; Gurtug and Sridharan, 2004; Prakash et al., 2024). Attempts have been made to incorporate CE alongside other input parameters to predict the compaction characteristics of cohesive soils. Nevertheless, some models, e.g., Farooq et al. (2016) have treated CE as a constant rather than an independent input parameter, thereby compromising their predictive capability across various CE levels. Meanwhile, certain models developed for multiple CE levels not only highlight limitations in the range of CE levels in their dataset but also yield a dataset featuring CE application across inconsistent soil samples, thereby undermining the actual sensitivity of CE as a parameter within the models (Gurtug and Sridharan, 2004; Wang and Yin, 2020). Addressing this issue necessitates a dataset

characterized by not only a broad spectrum of CE levels but also the systematic application of multiple CE levels to various homogeneous soil samples to broaden the compaction modeling horizon vis-a-vis CE (Najdi, 2023). Additionally, previous models have often utilized a limited set of input parameters such as  $w_L$  and  $w_P$  for predicting compaction parameters, potentially neglecting output variability imparted by other influencing factors (Ali et al., 2024; Spagnoli and Shimobe, 2020). Moreover, in different models, disparities arise in the assigned relative sensitivity of the input parameters, highlighting the necessity for more expansive incorporation of diverse parameters within the modeling framework to enhance generalizability. Nonetheless, for the sake of convenience in prediction, these input parameters should ideally be derived from simplified procedures. Furthermore, different existing models are typically applicable only within a limited range of cohesive soil plasticity, owing to their development based on a restricted dataset (Associates et al., 2016; Wang et al., 2023). Consequently, they lack the requisite generality to encompass the full spectrum of cohesive soil plasticity from low to high ranges (Agus et al., 2010; Ito and Komine, 2008). Therefore, it is imperative to devise global models that are founded upon expansive datasets incorporating a comprehensive array of plasticity indices, CE levels, grain size distribution parameters, and pertinent compaction attributes. By explicitly accounting for CE, models can bridge the gap between controlled laboratory conditions and variable field applications, improving their practical utility and adaptability to different geotechnical scenarios (Dialmy et al., 2024). This approach enables more precise predictions of  $\gamma_{dmax}$  and  $w_{opt}$  across a spectrum of energy levels, contributing to more efficient compaction processes and enhanced quality control in field applications (Miller and Vahedifard, 2024). Meanwhile, conventional regression-based modeling strategies used in existing models often yield diminished predictive efficacy, especially on a large dataset owing to their incapacity to effectively account for the antagonistic interactions or complex interplay among multiple parameters, underscoring the need for a more robust modeling framework.

Machine learning (ML) has emerged as a potent tool for predictive modeling, particularly in handling large datasets and input parameters (Rehman et al., 2024; Zhang et al., 2021). Various approaches have been devised, including black box, grey box, and white box techniques, which have evolved alongside advancements in neural networks, evolutionary, and decision tree-based ML algorithms (Khatti and Grover, 2023; ur Rehman et al., 2022). These ML-based methodologies have found extensive application in the modeling of geotechnical or geological databases. However, the inherent high variability within these datasets owing to antagonist response and complex interplay between different geological properties to define the response of geomaterials often leads to disparate predictive performances when employing specific ML techniques (Shi and Wang, 2021). To establish dependable models for geotechnical or geological databases, it is imperative to employ multiple techniques and robust modeling procedures to identify the most effective predictive models (Karpatne et al., 2019). Furthermore, when utilizing ML algorithms, careful consideration must be given to ensuring that the models adhere to the defined theoretical geotechnical framework. This is particularly crucial when modeling compaction characteristics, as not only high predictive accuracy is indispensable as these parameters serve as guidelines for QA/QC, but it also demands accurate prediction of parameter combinations, such as  $\gamma_{dmax}$  and  $w_{opt}$ , within the theoretical boundary of 100% degree of saturation ( $S_{\gamma dmax}$ ), aspects often neglected in past models (Spagnoli and Shimobe, 2020; Tarantino and De Col, 2008; Tatsuoka and Gomes Correia, 2018). These aspects demand a systematic and extensive database, a robust modeling framework, and critical evaluation of developed models not only based on conventional key performance indicators (KPIs) but also against typical and customized external validation indices (EVIs).

Considering the preceding discourse, the current study establishes an extensive database for modeling the compaction characteristics of soils through a customized testing regimen and comprehensive literature review. The compilation of this database involves subjecting identical

soil samples to multiple CEs, ensuring adherence to specified geotechnical theoretical bases to facilitate effective modeling frameworks. Further, by employing a suite of modeling techniques, including two variants of decision tree-based ML technique (i.e., Extreme Gradient Boosting (XGBoost) and Random Forest (RF)) encompassing enhanced black box technique, two variants of evolutionary ML technique (i.e., Genetic Expression Programming (GEP) and Multi Expression Programming (MEP)) encompassing gray box technique, along with two conventional methods such as Artificial Neural Networks (ANN) featuring standard black box ML technique and Multi-Linear Regression (MLR) featuring white box technique, a series of models were developed. These models underwent rigorous statistical assessment utilizing established KPIs to identify the most robust ones, subsequently validated against independent datasets using both typical and customized EVIs, and benchmarked against the existing models. Subsequently, the most optimal model was proposed and scrutinized for its internal modeling mechanisms, offering insights of interest to researchers and practitioners in the field. By providing a modeling strategy applicable to any CE level, including specified levels like standard and modified proctor, the current study presents a more versatile and potentially global solution for predicting compaction characteristics in place of doing laborious testing, ultimately benefiting the engineering community in optimizing soil compaction practices (Najdi, 2023). The predicted  $\gamma_{dmax}$  at standard or modified Proctor effort can serve as the reference for calculating the  $D_c$  for typical earthworks while the estimated  $w_{opt}$  for the anticipated field compaction effort can guide moisture conditioning of fill materials (Miller and Vahedifard, 2024). By predicting local  $\gamma_{dmax}$  values across a site, spatial variations in achievable density can be assessed, allowing for more targeted compaction efforts. Furthermore, estimated compaction parameters can inform initial earthwork planning and specifications potentially streamlining the project timeline and reducing preliminary costs.

## 2. Database Descriptions and Analysis

The establishment of the database was based on a comprehensive testing regimen and a systematic review of pertinent literature. The criteria delineating the inclusion of observations are derived from the specific objectives delineated within the ambit of this study. Each observation admitted into the modeling database necessitates the application of at least two distinct CE levels to homogenous soil specimens. Furthermore, to ensure the theoretical integrity of the modeling data, a criterion is enforced whereby the combination of the  $\gamma_{dmax}$  and  $w_{opt}$  is selected such that the  $S_{\gamma_{dmax}}$  does not surpass the theoretical threshold of 100%. Moreover, to maintain technical coherence within the modeling dataset, cohesive soils are operationally defined in accordance with ASTM D2487 specifications, which mandate the fines content ( $F_{200}$ ) equal to or exceeding 50%. The calculation of CE levels adheres to prescribed standards, with a concerted effort expended towards encompassing a broad spectrum of such levels through an exhaustive data search. Additionally, the database is constructed primarily utilizing natural soil samples, the majority of which exhibit  $w_L$  and  $I_P$  below 100%, although a subset exceeding this threshold is also incorporated to enrich the modeling horizon. It is imperative to underscore that, for the validation dataset sourced from literature, a judicious selection process was employed, wherein datasets adhering to both the aforementioned limits and those deviating from them were considered, thereby facilitating an assessment of the models' applicability across a wider array of soil compositions and characteristics.

### 2.1. Test results data

To construct the database, a comprehensive testing program was developed, involving the collection of 156 soil samples from diverse locations within the Indus Plain, obtained from depths ranging between 1-2 meters. This selection aimed to encompass a broad spectrum of fine-grained soils for analysis. The characterization of these soil samples involved grain size

distribution analysis conducted through both sieve analysis (ASTM D422) and hydrometer analysis (ASTM D7928), alongside Atterberg's limit tests adhering to ASTM D4318-95A. The outcomes of the grain-size distribution analysis revealed that all examined soil samples were classified as cohesive soils having fines ( $F_{200}$ ) in a range of 50-100%, with grains such as gravel, sand, silt, and clay distributed within defined ranges: 0% to 10%, 0% to 50%, 42% to 90%, and 10% to 58%, respectively. Atterberg's limit testing illustrated  $w_L$  and  $w_P$  spanning from 15% to 78% and 9% to 26.6%, respectively, and  $I_P$  ranging from 1.63% to 60% (Fig. 1). These parameters collectively facilitated the categorization of soils into distinct subcategories, delineated as ML, CL-ML, CL, and CH according to ASTM D2487 (Fig. 1). Notably, the ML subset exhibited  $w_L$  values ranging from 15% to 29% and  $I_P$  values from 0% to 5%, whereas the CL-ML subset demonstrated  $w_L$  values between 19% and 28%, with  $I_P$  values ranging from 4% to 7%. The CL subset presented  $w_L$  and  $I_P$  ranges of 30% to 48% and 7.7% to 26.5%, respectively, while the CH subset displayed ranges of 52% to 78% for  $w_L$  and 27.5% to 60% for  $I_P$ . Furthermore, the clay activity ( $A_c$ ), defined as the ratio of  $I_P$  to clay fraction, exhibited a range of 0.16 to 1.3 across all samples. This parameter has been utilized in previous models as an input; however, its determination necessitates the hydrometer test, a labor-intensive and time-consuming procedure coupled with Atterberg's limit test. Consequently, in the interest of modeling simplicity and circumventing reliance on the hydrometer test, the current study introduces an alternative parameter, namely fines activity ( $A_F$ ), defined as the ratio of  $I_P$  to the fraction passing through the  $F_{200}$ . This parameter can be swiftly determined via sieve analysis and Atterberg's limit test and was observed to range from 0.017 to 0.625 for the tested samples. Thus, the testing dataset illustrates the collection of a diverse array of cohesive soil samples for this investigation.

Subsequently, these soil samples underwent soil compaction tests using standard CE of 593 kN-m/m<sup>3</sup> as per ASTM D-698 and modified CE of 2700 kN-m/m<sup>3</sup> as per ASTM D-1557. The

relationship between the  $\gamma_d$  and  $w$  was plotted as a compaction curve, from which the  $\gamma_{dmax}$  and  $w_{opt}$  were determined as shown in Figure 2. Standard compaction tests, yielded  $\gamma_{dmax}$  and  $w_{opt}$  within a range of 13.5 kN/m<sup>3</sup> to 19.5 kN/m<sup>3</sup> and 10% to 25%, respectively. For CL, ML, CL-ML, and CH soils,  $\gamma_{dmax}$  values ranged from 14.3 kN/m<sup>3</sup> to 18.8 kN/m<sup>3</sup>, 15.9 kN/m<sup>3</sup> to 19.3 kN/m<sup>3</sup>, 16.3 kN/m<sup>3</sup> to 19.5 kN/m<sup>3</sup>, and 13.5 kN/m<sup>3</sup> to 16.7 kN/m<sup>3</sup>, respectively. Correspondingly,  $w_{opt}$  values for CL soils ranged from 11% to 21.8%, while for ML, CL-ML, and CH soils,  $w_{opt}$  ranged from 10.5% to 19.9%, 10% to 18.9%, and 14.5% to 25%, respectively (Fig. 2(a)). Furthermore, modified compaction tests, as illustrated in Figure 2b, yielded compaction parameters, including  $\gamma_{dmax}$  and  $w_{opt}$ , which fell within the ranges of 16 kN/m<sup>3</sup> to 20.4 kN/m<sup>3</sup> and 8.4% to 16.6%, respectively. These parameters were further delineated for each soil subgroup, with  $\gamma_{dmax}$  values ranging from 16.6 kN/m<sup>3</sup> to 20.4 kN/m<sup>3</sup> for CL, 17.8 kN/m<sup>3</sup> to 20 kN/m<sup>3</sup> for ML, 18 kN/m<sup>3</sup> to 20.4 kN/m<sup>3</sup> for CL-ML, and 13.5 kN/m<sup>3</sup> to 16.7 kN/m<sup>3</sup> for CH. Corresponding  $w_{opt}$  values ranged from 9% to 16.6% for CL, 8.4% to 13.5% for ML, 8.4% to 13% for CL-ML, and 12.8% to 16% for CH. Thus, a total of 312 sets of observations were yielded for the database based on this experimental program. Additionally, specific gravity ( $G_s$ ) tests were conducted following ASTM D-854, revealing values ranging from 2.7 to 2.83. The  $G_s$  values were subsequently utilized to ascertain the zero air void line and  $S_{\gamma_{dmax}}$  as follows:

$$S_{\gamma_{dmax}} = \frac{\gamma_{dmax}}{G_s \cdot \gamma_w - \gamma_{dmax}} \times (w_{opt} \cdot G_s) \quad (1)$$

where  $\gamma_w$  is the unit weight of water. The results indicated that all combinations of  $\gamma_{dmax}$  and  $w_{opt}$  exhibited  $S_{\gamma_{dmax}}$  lesser than the theoretical range of 100% saturation and nearly over 80%. It is important to note that compaction tests, such as the standard and modified Proctor tests, generally target an optimal saturation range of close to 80%–90% for cohesive soils, with around 80% often being the minimum for desirable engineering properties (e.g., low

permeability) (Miller and Vahedifard, 2024; USDA, 2000). However, the actual saturation range mainly depends on the soil type and CE level.

## **2.2. Literature-based data**

The research methodology encompassed a meticulous review of existing literature encompassing over 500 publications to select the most suitable one for data extraction. This process commenced by pinpointing relevant scholarly works using tailored keywords corresponding to the study's aims, such as maximum dry density, optimum moisture content, compaction energy, standard and modified tests as well as variations like reduced modified/standard, plasticity, and grain size distribution, etc. Databases like Web of Science, Scopus, and Google Scholar were extensively searched to locate pertinent published literature. Initially, abstracts of the selected studies were screened to determine their relevance, followed by a comprehensive evaluation vis-a-vis the current study's objectives through in-depth reading. Additionally, references cited within the searched studies were scrutinized to ensure any overlooked but relevant literature was included. Finally, as mentioned earlier, the extracted data underwent thorough scrutiny to identify and remove any outliers that exceeded the theoretical conditions and other predefined thresholds established for the current study. As a result, 681 data observations were finalized to be included in the modeling dataset mainly from a diverse range of literature from 1959-2020 (i.e., (Agus et al., 2010; Aldaood et al., 2015; Associates et al., 2016; Bello, 2013; Benson and Trast, 1995; Blotz et al., 1998; Daniel and Trautwein, 1994; Farooq et al., 2023, 2016; Gurtug and Sridharan, 2004; Horpibulsuk et al., 2009, 2008; Hussain, 2017; Ito and Komine, 2008; McRae, 1959; Mehmood et al., 2011; Miller et al., 2002; Osinubi and Nwaiwu, 2005; Osinubi et al., 2006; Osinubi and Bello, 2011; Perez N et al., 2013; Prasanna et al., 2020; Sabat, 2015; SAPEI et al., 1996; Sengupta et al., 2017; Sridharan and Gurtug, 2004; Taha and Kabir, 2005; Tinjum et al., 1997; Tripathy et al., 2005; Woon-Hyung Kim and Daniel, 1992; Yilmaz et al., 2016; Yogeshraj Urs and Prasanna, 2023;

Yusoff et al., 2017) ). Atterberg's limit testing illustrated  $w_L$  and  $w_P$  ranging from 15.3% to 608% and 6% to 48.3%, and  $I_P$  spanning from 1.6% to 570.1% (Fig. 1). The soil classification was ranged in CL, ML, CH, MH and CL-ML in these samples as per ASTM D2487. Meanwhile, Sand and  $F_{200}$  were observed to be in the range of 0% to 50% and 50% to 100%, respectively, with  $A_F$  spanned from 0.001 to 11.4. Meanwhile, vast CE levels were procured in the dataset from literature ranging from 202 kN-m/m<sup>3</sup> to 10832.1 kN-m/m<sup>3</sup>. Meanwhile, the  $\gamma_{dmax}$  and  $w_{opt}$  were in the range of 10.9 % to 22.5 % and 5.2% to 45%, respectively, with no datapoint exceeding theoretical  $S_{\gamma dmax}$  over 100%. The description of the modeling dataset by amalgamating the testing dataset and the aforementioned literature dataset is presented in Table 1 and Figure 3. Moreover, within the context of literature, 139 datasets were obtained that met all the specified selection criteria for this study, with the exception of having undergone at least two distinct CE levels on identical samples and some observations having  $F_{200}$  less than 50%. These data points were excluded from the modeling database used for both the model training and testing processes. However, they were reserved for the external validation of the models due to their ability to provide a diverse validation horizon. The compilation of this dataset primarily originated from studies spanning the years 1993 to 2022 (e.g., (Akcanca and Aytekin, 2012; Al-Hussaini, 2017; Al-Khafaji, 1993; Burton et al., 2015; Clariá and Rinaldi, 2007; Daniel and Wu, 1993; Delage et al., 2011; Duong et al., 2014; Fox et al., 2014; Günaydın, 2009; Inci et al., 2003; Khalid et al., 2019; Kiliç et al., 2016; Lim and Miller, 2004; Othman and Benson, 2011; Rehman et al., 2017; Sawangsuriya et al., 2009; Shafiee, 2008; Shelley and Daniel, 1993; Taïbi et al., 2008; Vassallo et al., 2007; Vega and McCartney, 2015; Wang et al., 2017; Yang et al., 2022; Zhang et al., 2015). A detailed statistical description of the validation database sourced from the literature is presented in Table 1.

### 2.3. Data and input analyses

The database comprising 1001 observations was established through the amalgamation of testing data and literature-based data for model testing and training, encompassing a wide range of soil classification and compaction-related parameters (Fig. 3). The selection of input parameters was conducted based on theoretical relevance, ease of testing and statistical significance. Initially, four sets of input parameters were identified in the database for the input analysis based on theoretical relevance including Atterberg's limits ( $w_L$ ,  $w_P$ , and  $I_P$ ), grain size (Sand fraction (Sand),  $F_{200}$ ,  $A_c$ , Silt, Clay, and  $A_F$ ), physical property ( $G_s$ ) and compaction (CE). The  $w_L$  can be obtained through standard tests outlined in ASTM D4318-95A, specifically through Method A, i.e., Casagrande apparatus or Method B, i.e., fall cone apparatus. Similarly, the  $w_P$  can be determined through plastic limit test following the ASTM D4318-95A, also allowing for the calculation of the  $I_P$  as the difference between  $w_L$  and  $w_P$ . The Sand and  $F_{200}$  can be assessed through sieve analysis testing in accordance with ASTM D6913. Additionally, the  $A_F$  is calculated by dividing the  $I_P$  by  $F_{200}$ . For CE, the standard laboratory formula is given by  $CE = \frac{\text{Number of blows} \times \text{Number of layers} \times \text{Weight of hammer} \times \text{Height of drop}}{\text{Volume of mold}}$ , as specified in ASTM D697 and ASTM D1557 and for field a different formula can be employed  $CE = \frac{\text{Drawbar pull} \times \text{Number of passes} \times \text{Number of lifts for 0.31 m depth}}{\text{Drawbar width}}$  as per Johnson and Sallberg (1960). Thus, the selection of these parameters limits the testing requirements for obtaining input parameters to only sieve analysis and Atterberg limit tests, since CE does not require additional testing and can be calculated using formulas based on the specific compaction task. Further, these parameters, being essential to soil classification, offer engineers an initial, interpretable insight into soil properties, which is critical for envisaging the engineering behavior of soils. Parameters such as Silt, Clay, and  $A_c$  which require hydrometer analysis and  $G_s$ , were not further considered, as their incorporation would necessitate testing in excess of the basic requirements of USCS and AASHTO soil classification systems for model input despite their potential relevance to compaction characteristics. However, considering the theoretical

relevance of  $G_s$  for soil compaction, it was indirectly used to determine  $S_{\gamma_{dmax}}$ , which is included to evaluate the theoretical validity of the compaction parameters and various EVIs.

The statistical examination of the dataset utilized for model training and testing has revealed considerable variability across all pertinent input parameters, namely  $w_L$ ,  $w_P$ ,  $I_P$ , Sand,  $F_{200}$ ,  $A_F$ , and CE, as delineated in Table 1 and Figure 4. Kernel Density Estimation (KDE) plots illustrate the probability density ( $P_d$ ) distribution, portraying a consistent trend of  $P_d$  elevation from low to high plasticity ranges, which are representative of prevalent natural cohesive soils worldwide. Furthermore, a congruent trend in  $P_d$  is observed across parameters  $w_L$ ,  $A_F$ , and  $I_P$ . Sand and  $F_{200}$  parameters also demonstrate notable variability, with heightened  $P_d$  evident at both lower and higher value ranges for sand, and predominantly at higher values for  $F_{200}$ . CE exhibits considerable variance, characterized by two instances of elevated  $P_d$  levels. Conversely, output parameters,  $\gamma_{dmax}$  and  $w_{opt}$ , demonstrate extensive variance within defined theoretical bounds, with heightened  $P_d$  occurring at central values for both. Subsequent analysis employing excess kurtosis indicates that all input and output parameters exhibit Leptokurtic distributions, except for sand and  $F_{200}$ , which manifest slightly Platykurtic distributions (Table 1). Moreover, skewness analysis reveals right-skewed distributions for all parameters, except for  $F_{200}$  and  $\gamma_{dmax}$ , which exhibit slight left-skewedness. This analysis underscores a high degree of symmetry in the distribution patterns of input and output parameters, albeit with minor exceptions.

Furthermore, a meticulous correlation analysis was conducted, involving the generation of both correlational and Pearson correlation coefficient (PC) matrices to scrutinize the interrelationships among the input and output variables, as illustrated in Figure 5. This comprehensive examination unveiled that no individual input parameter exhibits a significantly elevated or negligible correlation i.e.,  $PC < 0.1$ , as quantified by the PC, with the output parameter. This observation suggests that no single parameter singularly possesses the capacity

to yield a substantial correlation with the output parameter, indicating the presence of a multifaceted relationship. Moreover, the assessment of correlations among the input variables revealed moderate to low PC values, indicative of a diminished likelihood of multicollinearity among the input parameters. Notably,  $\gamma_{dmax}$  and  $w_{opt}$  demonstrated a significantly high PC and a linear relationship, underscoring a discernible synchronization between these parameters, thereby reflecting the coherence and reliance of the dataset. Based on these insights, it was ascertained that all input parameters designated for inclusion exhibited reasonable statistical robustness. Additionally, in the context of ML-based modeling, the analysis of input parameters necessitates consideration vis-a-vis the number of data points, as a larger dataset provides a broader modeling horizon, while a greater number of statistically suitable input parameters contributes to enhanced predictive accuracy. However, a balanced ratio of at least 5 data points per input parameter is deemed desirable (ur Rehman et al., 2022); for the present dataset, this ratio stands at 143, exceeding the prescribed threshold value.

### 3. Modeling and Evaluation Methods

Figure 6 presents the overall methodology of the current study. Drawing upon input analysis that accounts for both physical and statistical significance, the input parameters employed comprise sieve analysis, Atterberg's limits, and compaction-based parameters. The output parameters can be expounded with input parameters as follows.

$$\gamma_{dmax} = f(w_L, w_P, I_P, \text{Sand}, F_{200}, A_F, CE) \quad (2)$$

$$w_{opt} = f(w_L, w_P, I_P, \text{Sand}, F_{200}, A_F, CE) \quad (3)$$

Furthermore, in order to construct machine learning (ML) based models, the database underwent partitioning into training and testing sets at a ratio of 70% to 30%. Additionally, an independent dataset constituting approximately 14% of the total data was reserved for external validation, distinct from the modeling process. A comprehensive array of ML methodologies was employed, encompassing three variants of black-box techniques, including the enhanced

decision tree-based modeling approaches including Boosting Programming (i.e., XGBoost) and RF, alongside a conventional feed-forward ANN. Grey-box techniques were represented by two variants: Genetic Programming (i.e., GEP) and Evolutionary Programming (i.e., MEP). In addition, multiple linear regression (MLR) which is a white-box technique, was included as a baseline for comparison with other techniques.

Figures 7-10 present the algorithm architecture of different ML algorithms designed for this study. Extreme Gradient Boosting (XGBoost) is an advanced decision tree-based machine learning algorithm known for its efficiency and effectiveness in solving supervised learning problems to develop predictive models (Fig. 7). By utilizing a gradient-boosting framework, XGBoost sequentially combines weak learners, typically decision trees, to form a strong ensemble model, making it a superior variant compared to other decision tree-based techniques (Chen and Seo, 2023). It incorporates regularization methods like Lasso (L1) and Ridge (L2), which help prevent overfitting and enhance generalization by applying penalties to the coefficients' magnitudes. Additionally, XGBoost is optimized for high performance, offering parallel and distributed computing capabilities that enable fast training on large datasets and help capture complex data patterns. It also provides customizable parameters and feature importance scores, making it a flexible and interpretable choice for various domains, especially geotechnical databases. The XGboost algorithm developed for the current study can be mathematically expounded as follows.

$$O_i = \sum_{i=1}^n L(y_i, \hat{y}_i) + \sum_{k=1}^K \Omega(f_k) \quad (4)$$

$$\Omega(f_k) = \gamma T + L_1 + L_2 \quad (5)$$

where  $O_i$  is the objective,  $\Omega(f_k)$  is the regularization function,  $L(y_i, \hat{y}_i)$  is the loss function, with  $n$  representing the number of training samples,  $K$  is the number of trees and  $\gamma T$  defines the thickness of the decision tree. Random Forest (RF) is another powerful ensemble learning

algorithm that constructs multiple decision trees during training, each trained on a random subset of the data and features using a bagging technique (Fig. 8). Similar to XGBoost, RF offers insights into feature importance and robustness against overfitting through the aggregation of predictions. However, unlike XGBoost, which uses gradient boosting and regularization, RF relies on the diversity of decision trees and bagging to achieve predictive power. Gene Expression Programming (GEP) is a gray-box machine learning method inspired by genetic evolution, utilizing regression and neural techniques to solve complex problems. It iteratively adjusts parameters to optimize performance and employs expression trees to represent nonlinear entities (Fig. 9). GEP has shown promising results in handling complex geotechnical data, making it a suitable choice for the current modeling study. Multi-Expression Programming (MEP), another evolutionary modeling approach, uses fixed-length binary strings to encode multiple computer programs within a single chromosome. MEP applies a fitness evaluation process to generate the most optimal solution through recombination and mutation of chromosomes (Fig. 10). Artificial Neural Networks (ANN) are black-box models where data flows through interconnected nodes across layers, learning complex patterns from input data via activation functions applied to the weighted sum of inputs. A feed-forward ANN model is utilized in this study to test various black-box methods on the geotechnical dataset. Meanwhile, Multiple Linear Regression (MLR) is a widely used statistical method that models the relationship between a dependent variable and multiple independent variables; it estimates the coefficients that best fit the data.

This selection facilitated a comprehensive exploration of ML modeling paradigms on the established geotechnical database for compaction modeling. Multiple models were iteratively developed through algorithmic refinement and parameter optimization across the spectrum of employed techniques. The models exhibiting superior statistical performance were identified through a meticulous evaluation process. The most refined models derived from each ML

technique further underwent meticulous examination and comparison, predicated upon a variety of absolute and relative statistical KPIs. The ML-based model's performance underwent evaluation through distinct categories of key performance indices (KPIs). This includes error indices such as root mean squared error (RMSE), relative root mean square error value (RRMSE), mean absolute error (MAE), and mean absolute percentage error (MAPE). Additionally, correlation and efficiency indices, comprising Nash-Sutcliffe efficiency coefficient (NSE), Kling-Gupta efficiency coefficient (KGE), correlation coefficient ( $R^2$ ), residual sum of square (RSS), norm of residual (NR) and adjusted correlation coefficient (adj  $R^2$ ), and PC were analyzed as per Rehman et al., (2022). These indices have been chosen to encompass relative and absolute statistical perspectives, facilitating a comprehensive model performance analysis. Additionally, variance analysis (ANOVA) was performed on the developed models to assess their statistical integrity including F-value and  $\text{prob} > F$ .

Subsequently, the performance of these optimized models, as determined by the designated criteria, was compared with that of existing models in the literature, utilizing the modeling dataset. Additionally, both the optimized and the literature-based models underwent further validation procedures utilizing an independent validation dataset, and their performance was assessed using standard and customized EVIs. To further validate the credibility of the proposed model, an additional dataset comprising 139 observations sourced from existing literature was utilized. This dataset served to assess the predictive efficacy of the proposed model, comparing its performance with that of established models documented in prior literature some of which even used this validation dataset in their modeling process. Various standard EVIs, including the coefficient of determination ( $R$ ), the correlation coefficient ( $R_m$ ), and the slopes of regression lines ( $k$  and  $k'$ ), along with their corresponding indices ( $R_0$  and  $R_0'$ ), were methodically assessed in this comparative analysis as per Rehman et al., (2024). Additionally, customized EVIs were developed to assess the compaction characteristics,

including Normalized Absolute Percentage Error (NAPE) and Outlier  $S_{\gamma_{dmax}}$  ( $S_{\gamma_{dmax}(ol)}$ ). NAPE is defined mathematically as follows:

$$NAPE = \left| \frac{E_i - M_i}{((E_i + M_i)/2)} \right| \times 100 \quad (6)$$

NAPE was further customized for the  $w_{opt}$  and  $\gamma_{dmax}$  in accordance with AS 1289.5.1.1 and AS 1289.5.2.1 standards, which stipulate that NAPE should not exceed 20% and 4% for the former and latter, respectively, for more than 5% of prediction samples in a validation dataset, with certain exceptions in high plastic clays (Spagnoli and Shimobe, 2020). Furthermore,  $S_{\gamma_{dmax}(ol)}$  is defined when Eq. 1 for any model prediction for the combination of  $w_{opt}$  and  $\gamma_{dmax}$  yields a value exceeding 100% or less than 0 (Tarantino and De Col, 2008). This ensures the theoretical validity of the developed model by verifying its adherence to the theoretical bounds of the soil saturation state.  $S_{\gamma_{dmax}(ol)}$  and the outlier NAPE ( $NAPE_{ol}$ ) for  $w_{opt}$  and  $\gamma_{dmax}$  can be defined as follows:

$$NAPE_{ol} = \frac{k_{NAPE(ol)}}{n} \times 100 \quad (7)$$

$$S_{\gamma_{dmax}(ol)} = \frac{k_{S\gamma_{dmax}(ol)}}{n} \times 100 \quad (8)$$

where  $k_{(ol)}$  denotes the count of outliers for each index, taking into account the pertinent theoretical bounds.

Finally, the most sophisticated model was proposed, marking the culmination of a rigorous process in selecting the optimal ML-based models for this study. Furthermore, the modeling mechanism of the proposed model was subjected to thorough analysis through Shapley additive explanations (SHAP) analysis on the modeling dataset and parametric and sensitivity evaluations on the assumed ranged dataset.

## 4. Results and Discussion

### 4.1. Model Development

#### 4.1.1. XGBoost model

An extensive XGBoost modeling approach was utilized to construct a robust predictive model for predicting  $\gamma_{dmax}$  and  $w_{opt}$  parameters. Model training procedures were conducted to attain optimal settings that yield high predictive accuracy while mitigating model complexity. By meticulously fine-tuning the model parameters and iteratively refining the algorithmic settings, a level of predictive accuracy was achieved that closely mirrors experimental values. This optimization process was achieved by establishing specific thresholds for model complexity parameters and varying algorithmic parameters within these bounds. Optimal settings were determined wherein the number of trees was limited to 100, each with a depth of 6, and a learning rate of 0.30 was employed. Additionally, the fraction of features and regularization constant were constrained to 1.00. Through iterative refinement, the best-performing model was identified based on these algorithmic constraints. The optimal model for  $\gamma_{dmax}$  showed a high level of accuracy in the prediction aligning with experimental observations (Fig. 11a). Both training and testing data points and trend lines exhibited minimal deviation from the ideal 45-degree line remaining within the  $\pm 5\%$  reference error band with  $R^2$  of 0.99 and 0.99, respectively (Table 2), indicative of strong model performance. Similarly, the predictive accuracy of  $w_{opt}$  was demonstrated through XGBoost modeling, with the predicted values closely matching experimental observations mainly remaining within the  $\pm 5\%$  reference error band of the 45-degree line with  $R^2$  of 0.98 and 0.98 for testing and training databases, respectively (Fig. 12a). Notably, trend lines for both predicted and experimental data points remained consistent with the 45-degree line, further affirming the model's reliability. The close alignment between the trend lines of testing and training datasets for both models and the 45-degree line suggests that the model generalizes well to unseen data and model is interpretable

and aligns well with domain knowledge. This also indicates that the model has learned the underlying patterns in the data without overfitting the training set. These findings and statistical KPIs as manifested in Table 2 underscore the high predictive accuracy and interpretability afforded by the developed XGBoost models in predicting  $\gamma_{dmax}$  and  $w_{opt}$  parameters. XGBoost model is highly applicable when prediction accuracy of compaction characteristics is critical, and the data shows complex, non-linear relationships.

#### 4.1.2. RF model

An RF modeling approach was undertaken to develop models for  $\gamma_{dmax}$  and  $w_{opt}$ , involving meticulous fine-tuning of model parameters and iterative refinement of algorithmic settings. Through this process, optimal models were obtained based on their predictive performance and complexity considerations. Notably, the optimal model for  $\gamma_{dmax}$  exhibits minimal deviations between predicted and experimental values, as evidenced by their proximity to the 45-degree line within  $\pm 5\%$  reference error band across both testing and training datasets with  $R^2$  of 0.93 and 0.83, respectively. Additionally, while slight deviations are observed at extreme values, the trend lines for both datasets largely align with the 45-degree line (Fig. 11b). Similarly, the optimal RF model for  $w_{opt}$  demonstrates a comparable performance, with minimal deviation between predicted and experimental values across testing and training datasets yielding  $R^2$  of 0.95 and 0.92, respectively, and trend lines consistent with the 45-degree line (Fig. 12b). These analyses and statistical KPIs of the developed models in Table 2 highlight a good performance of the optimal RF models for  $\gamma_{dmax}$  and  $w_{opt}$ . The RF model's performance also suggests a good balance between accuracy and generalizability for the prediction of  $\gamma_{dmax}$  and  $w_{opt}$ . Its ensemble nature allows it to capture non-linear relationships while maintaining robustness against overfitting. This makes the RF model particularly suitable for scenarios where both predictive power and model generalizability are desired.

#### 4.1.3. GEP model

A wide-ranging GEP modeling methodology was employed to optimize genetic operators, constants, and general parameters. This optimization procedure was facilitated through a stepwise GEP modeling strategy, iteratively transitioning from simpler to more complex algorithmic parameters to enhance predictive performance. The attainment of the optimal model configuration necessitated meticulous adjustment of mutation, inversion, genetic recombination, uniform recombination, and constant fine-tuning rates, resulting in respective values of 0.00138, 0.00546, 0.000277, 0.00755, and 0.00206. Upon thorough evaluation, the optimal GEP model for predicting  $\gamma_{dmax}$  exhibited a moderate degree of dispersion between predicted and experimental values across both testing and training datasets centered around the 45-degree line with  $R^2$  of 0.77 and 0.71, respectively. It is noteworthy that the trend lines for both datasets displayed deviations, characterized by underestimation at higher values and overestimation at lower values (Fig. 11c). A similar trend was observed in the estimation of  $w_{opt}$  with  $R^2$  of 0.78 and 0.71 for training and testing datasets, respectively (Fig. 12c). These observations and statistical KPIs (Table 2) suggest that the GEP models predict  $\gamma_{dmax}$  and  $w_{opt}$ , reasonably aligning with experimental observations while manifesting a moderate degree of discrepancies. The performance of the GEP model indicates its potential for capturing the underlying patterns in the data. However, the observed deviations in  $\gamma_{dmax}$  and  $w_{opt}$  predictions suggest that the model may be struggling to fully represent the complexity of the relationships between variables in the current dataset. This model could be particularly useful in situations where a balance between interpretability and predictive power is required, and insights into the data structure are needed, especially when a more flexible model is desired, albeit with some limitations in accuracy.

#### 4.1.4. MEP model

MEP modeling was employed to achieve optimal models for  $\gamma_{dmax}$  and  $w_{opt}$  by varying the algorithmic parameters and applying multiple evolutionary iterations. The configuration of the MEP algorithm involved the establishment of two subpopulations, each composed of 1000 iterations. It implemented a crossover probability of 0.9 and incorporated a tournament size of 2. Based on the statistical KPIs, the best-performing MEP models for  $\gamma_{dmax}$  and  $w_{opt}$  were finalized. The optimal MEP model predictions for  $\gamma_{dmax}$  showed a considerable level of scatteredness in comparison to experimental values for both testing and training datasets around the 45-degree line, with  $R^2$  values of 0.65 and 0.61, respectively (Fig. 11d). The trend lines of both testing and training datasets underscore considerable underestimation at higher values and overestimation at lower values. A similar trend was observed for the  $w_{opt}$  prediction by the optimal MEP model, with slightly improved  $R^2$  values of 0.71 and 0.66, respectively, for the training and testing datasets (Fig. 12d). These analyses and statistical KPIs of both optimal MEP models for  $\gamma_{dmax}$  and  $w_{opt}$  (Table 2) demonstrate considerably low prediction accuracy, generalizability, and interpretability. However, this model offers simplicity, ease of interpretation, and an evolutionary prediction stream, its applicability may be limited to scenarios where slightly less accurate estimates of  $\gamma_{dmax}$  and  $w_{opt}$  are sufficient.

#### 4.1.5. ANN model

The feedforward ANN model was constructed with a variable number of neurons ranging from 10 to 100 per hidden layer. The selection of this range aimed to strike a balance between model complexity and efficacy, as excessively high neuron counts tend to yield intricate and burdensome models. Optimal performance was attained when employing 100 neurons, coupled with an  $\alpha$ -value of  $10^{-4}$ . The ANN model developed for predicting  $\gamma_{dmax}$  exhibited a discernible discrepancy between predicted and experimental values, as evidenced by respective  $R^2$  values of 0.70 for both the training and testing datasets (Fig. 11e). Notably, trend line analysis revealed

a tendency towards overestimation at lower values and underestimation at higher values. A similar pattern was observed in the prediction of  $w_{opt}$  by the optimal ANN model, yielding  $R^2$  values of 0.71 and 0.66 for the training and testing datasets, respectively (Fig. 12e). These analyses, along with statistical KPIs presented in Table 2, collectively suggest that the feedforward ANN models exhibit relatively low accuracy, generalizability, and interpretability, particularly concerning predictions of  $\gamma_{dmax}$  and  $w_{opt}$ . The model's performance and its tendency to overestimate at lower values and underestimate at higher values suggest that it may be particularly useful in mid-range predictions of  $\gamma_{dmax}$  and  $w_{opt}$ . In practical applications, this ANN model could be employed in preliminary soil compaction assessments or as part of a larger ensemble of models to provide a comprehensive view of soil behavior.

#### 4.1.6. MLR model

MLR was also utilized in this study, as it stands as the most prevalent technique in the existing literature for developing predictive models concerning  $\gamma_{dmax}$  and  $w_{opt}$ . However, the MLR approach yielded models displaying substantial deviations in the prediction of  $\gamma_{dmax}$ , as indicated by relatively low  $R^2$  values of 0.55 and 0.54 for the training and testing datasets, respectively (Fig. 11f). Notably, both the training and testing dataset trend lines exhibited significant overestimation and underestimation in comparison to the 45-degree line at low and high values. A parallel pattern emerged in the prediction of  $w_{opt}$  using MLR, albeit with marginally enhanced  $R^2$  values of 0.63 and 0.71 for the training and testing datasets, respectively (Fig. 12f). These analyses, in conjunction with statistical KPIs (Table 2), collectively underscore the limited accuracy and generalizability exhibited by MLR models in predicting  $\gamma_{dmax}$  and  $w_{opt}$ . This suggests that while MLR is simple and interpretable, its applicability in the current context is limited. The model's performance could potentially be improved through feature engineering but more complex ML models are better suited for this particular problem.

## 4.2. Performance analysis

### 4.2.1. Performance analysis of developed models

The performance of the best models from all the applied ML techniques was evaluated to identify the most suitable models for further analysis, based on the statistical KPIs presented in Figure 13 and Table 2. Regarding correlation and efficiency indices (i.e.,  $R^2$ , PC, adj  $R^2$ , KGE, and NSE), the model performance showed a significant improvement in the order of MLR, MEP, ANN, GEP, RF, and XGBoost for both  $\gamma_{dmax}$  and  $w_{opt}$ . All models exhibited better performance on the training dataset compared to the testing dataset for both categories of models. XGBoost demonstrated the smallest reduction in performance from the training to the testing dataset for both  $\gamma_{dmax}$  and  $w_{opt}$ , followed by ANN, MLR, RF, GEP, and MEP for  $\gamma_{dmax}$  (Fig. 13a), and RF, GEP, MEP, and ANN for  $w_{opt}$  (Fig. 13b). These correlation and efficiency indices clearly indicate that the XGBoost model outperforms other models (Table 2), as all these indices are close to unity, demonstrating high prediction accuracy (Figure 13). The RF model also performed excellently in terms of correlation and efficiency indices. However, all other models showed values below 0.9 for these indices. These results highlight that black-box decision-tree-based ML techniques effectively approximate predicted values to experimental values in the current geotechnical database (Shi and Wang, 2021).

The performance analysis was further conducted using multiple error indices (i.e., MAE, MAPE, MSE, RMSE, and NRMSE), covering both absolute and relative statistical perspectives. The models' performance was consistent with the results from correlation and efficiency indices for both testing and training datasets for  $\gamma_{dmax}$  and  $w_{opt}$  (Table 2 and Fig. 13). The models' performance improved in terms of error indices in the order of MLR, MEP, ANN, GEP, RF, and XGBoost for both  $\gamma_{dmax}$  and  $w_{opt}$ . The XGBoost model outperformed all the models, yielding error indices close to zero (Table 2 and Figure 13). The RF model also showed relatively low error indices compared to other models except XGBoost. Higher error indices

were observed for GEP, MEP, ANN, and MLR. Furthermore, XGBoost exhibited exceptionally low NR and RSS, with RF showing the second-best performance, while other models showed high values indicating larger residuals in predictions. These analyses emphasize the extremely low prediction error by XGBoost and the reasonable performance of RF on the current database. Nevertheless, all models demonstrated satisfactory performance, as evidenced by high F-values and low Prob>F in the ANOVA, with XGBoost showing the highest F-value followed by RF. Based on the comprehensive performance across all statistical KPIs, XGBoost exhibited exceptionally high prediction accuracy outperforming all the models. At the same time, the RF model also showed reasonable performance compared to other models except XGBoost for both  $\gamma_{dmax}$  and  $w_{opt}$ . Thus, XGBoost and RF models are shortlisted for further evaluation.

#### *4.2.2. Performance analysis of shortlisted and existing models*

The performance of existing models in the extant literature (e.g., (Al-Khafaji, 1993; Blotz et al., 1998; Farooq et al., 2016; Günaydın, 2009; Gurtug and Sridharan, 2004; Ito and Komine, 2008; Sridharan and Nagaraj, 2005; Wang and Yin, 2020)) for predicting  $\gamma_{dmax}$  and  $w_{opt}$ , either with CE as an input parameter or without specifying bounds for any particular CE level, was evaluated using the current training and testing datasets used for the model development to compare with the proposed ML models, i.e., XGBoost and RF, developed in this study. All existing models exhibited substantial deviations between predicted and experimental  $\gamma_{dmax}$  and  $w_{opt}$  values from the 45-degree line, with these deviations significantly exceeding the reference  $\pm 5\%$  error band, indicating inferior performance compared to XGBoost and RF (Figs. 12a, b; 13 a, b; 14a; 15a). This finding suggests that the applicability of existing models is limited to certain thresholds but to a larger spectrum of cohesive soils and CE levels. Furthermore, performance comparisons based on correlation indices ( $R^2$  and PC) and error indices (MAE, RMSE) revealed suboptimal performance of all the existing models and excellent performance

of the proposed models for predicting  $\gamma_{dmax}$  and  $w_{opt}$ , when combining the training and testing datasets used previously (Figs. 14b, c; 15b, c). XGBoost outperformed all other models based on this big data showing a wider application range. The Taylor diagram analysis further confirms that XGBoost predicts  $\gamma_{dmax}$  and  $w_{opt}$  with the least deviation and the highest correlation strength, followed by RF (Fig. 16). In contrast, all existing models demonstrated a larger deviation from experimental values in their predictions, with a standard deviation exceeding 2 (Fig. 16). This indicates a low fidelity of these models in predicting accurate results. The superior performance of XGBoost and RF in comparison to existing models underscores their robustness and reliability in capturing the underlying patterns in this big dataset, as evidenced by their proximity to the experimental values on the Taylor diagram. It is noteworthy that while all MLR-based models demonstrated a high degree of deviation, the MEP-based model by Wang and Yin (2020) outperformed the other existing models but still exhibited inferior performance to the MEP model developed in the current study demonstrating the effectiveness of training the model on a big database (Figs. 14 and 15 and Table 2). The superior performance of XGBoost and RF compared to existing models can be attributed to their training on a larger dataset encompassing a broad spectrum of soil plasticity, classification, and CE levels (Chen and Seo, 2023). It is also important to note that the part of the database used in this performance analysis also serves as a parent database, necessitating further verification of these models as presented in the following section.

### 4.3. External validation

The shortlisted models, namely XGBoost and RF, along with existing models from the current literature, were validated using an independent dataset of 139 observations obtained from previous studies. This dataset, which spans a wide range of statistical input and output parameters (Table 1), was not used in the model testing and training phases, thus termed as an independent dataset. It was observed that XGBoost predicted the  $\gamma_{dmax}$  and  $w_{opt}$  values within a

673  $\pm 5\%$  reference error band, whereas all other models exhibited greater deviations (Fig. 17).  
 674 Taylor diagram analysis further confirmed these findings, indicating that XGBoost predicted  
 675  $\gamma_{dmax}$  and  $w_{opt}$  values closest to the experimental results, followed by the RF and the MEP model  
 676 by Wang and Yin (2020) (Fig. 18). Most existing models showed significant deviations in  $\gamma_{dmax}$   
 677 and  $w_{opt}$ , highlighting their lower fidelity in prediction accuracy. The external validation was  
 678 extended to assess the models' ability to yield a combination of  $\gamma_{dmax}$  and  $w_{opt}$  that breaches the  
 679 threshold  $S_{\gamma dmax}$  value, i.e., higher than 100% or equal to or lower than 0%. It was observed that  
 680 all models tended to produce some  $S_{\gamma dmax}$  values outside theoretical bounds at certain instances,  
 681 except for XGBoost, which consistently predicted  $\gamma_{dmax}$  and  $w_{opt}$  values close to the  
 682 experimental data without breaching theoretical limits (Fig. 19). This indicates that other  
 683 models are prone to unacceptable results, while XGBoost effectively captures minimal  
 684 prediction error and remains within the desired bounds of  $70\% < S_{\gamma dmax} < 100\%$  as of  
 685 experimental values (Fig. 19). This performance is mainly attributed to the screened database  
 686 used for model development, which excluded observations yielding unacceptable  $S_{\gamma dmax}$   
 687 combined with the sophisticated training ability of XGBoost demonstrated on the current  
 688 database to maintain minimal error indices and close proximity with experimental values.  
 689 Further external validation was conducted by assessing the performance of the models on the  
 690 independent dataset using standard Evaluation Indices (EVIs) (i.e., R,  $R_m$ , k, k',  $R_0$ , and  $R_0'$ )  
 691 and customized EVIs ( $NAPE_{ol}$  and  $S_{\gamma dmax(ol)}$ ) for  $\gamma_{dmax}$  and  $w_{opt}$ , as presented in Tables 3 and 4,  
 692 respectively. The results indicate that XGBoost maintains all the EVIs within desirable ranges  
 693 set to demonstrate high prediction accuracies, whereas the other models struggle to do so,  
 694 failing in some or all EVIs. This demonstrates the superior prediction accuracy of XGBoost  
 695 and its robust capability to perform global predictions of cohesive soil compaction within  
 696 acceptable limits. In contrast, the other models exhibit certain limitations, failing to  
 697 consistently achieve desirable EVI metrics. These findings highlight the efficacy of XGBoost

in modeling complex soil compaction parameters, reinforcing its potential for broader applications in geotechnical engineering. The comprehensive evaluation underscores the model's ability to generalize well across diverse datasets, thus providing reliable predictions. This superior performance can be attributed to the advanced algorithmic structure of XGBoost, which effectively captures nonlinear relationships and interactions within the data coupled with training on a big and systematic dataset, resulting in higher fidelity and precision (Chen and Seo, 2023; Shi and Wang, 2021). Consequently, XGBoost stands out as a reliable tool for predicting  $\gamma_{dmax}$  and  $w_{opt}$ , offering significant improvements over traditional and other ML models in this domain.

#### **4.4. Model explanation and modeling mechanism analysis**

##### *4.4.1. Proposed model explanation*

The XGBoost model is a black box, making it difficult to interpret it in terms of mathematical formulations for predictions. To improve interpretability, SHAP analysis was used, based on modeling data used in this study. SHAP assigns rank values to input features for individual predictions, offering insight into how input features, i.e., Atterberg's limit, gradation parameters and compaction effort affect predictions of  $\gamma_{dmax}$  and  $w_{opt}$ . (X. Li et al., 2024). The SHAP summary plots for the prediction of the XGBoost model proposed for  $\gamma_{dmax}$  and  $w_{opt}$  in this study are presented in Figures 20 (a) and (b), respectively. In SHAP summary plots, the horizontal axis represents SHAP values, which indicate the extent to which each input feature pushes the prediction higher (positive SHAP values) or lower (negative SHAP values). Each row corresponds to an input feature, and each dot represents a SHAP value for a particular observation. The color gradient from blue (low feature values) to red (high feature values) shows how the magnitude of each input feature's value affects the model's output.

721 The CE feature has a particularly strong impact on  $\gamma_{dmax}$  and  $w_{opt}$ . Low values significantly  
 722 reduce the prediction of  $\gamma_{dmax}$  and increase the prediction of  $w_{opt}$ , as indicated by a cluster of  
 723 blue dots with negative and positive SHAP values, respectively. Conversely, high values of CE  
 724 push the prediction upward and downward for  $\gamma_{dmax}$  and  $w_{opt}$ , respectively, indicating that this  
 725 feature is a key driver for increasing  $\gamma_{dmax}$  and decreasing  $w_{opt}$ .  $w_L$  also shows a substantial  
 726 influence on both  $\gamma_{dmax}$  and  $w_{opt}$ . High values of  $w_L$  increase the prediction of  $\gamma_{dmax}$  and low  
 727 values decrease it; meanwhile, a reverse response was observed for  $w_{opt}$ . This feature has a  
 728 relatively wide distribution for both  $\gamma_{dmax}$  and  $w_{opt}$ , indicating interactions with other features  
 729 or nonlinear effects.  $w_P$  displays a balanced spread around zero for both  $\gamma_{dmax}$  and  $w_{opt}$ , with  
 730 high values associated with a slight increase in  $\gamma_{dmax}$  and low values linked to a decrease in  
 731 the prediction of  $\gamma_{dmax}$ ; meanwhile, a reverse trend was observed for  $w_{opt}$ . This distribution  
 732 pattern suggests that  $w_P$  has a moderate but consistent effect on both  $\gamma_{dmax}$  and  $w_{opt}$  since  
 733 clustering is closer to zero SHAP value as compared CE and  $w_L$ . Moreover, CE has a consistent  
 734 impact on both  $\gamma_{dmax}$  and  $w_{opt}$ . In contrast,  $w_L$  and  $w_P$  have slightly varying degrees of impact  
 735 on  $\gamma_{dmax}$  and  $w_{opt}$ , with a stronger influence on  $w_{opt}$  than on  $\gamma_{dmax}$ .  $I_P$  has a also mixed influence  
 736 on compaction characteristics, with high values leaning toward increasing  $\gamma_{dmax}$ , while low  
 737 values slightly decrease; a reverse trend was observed for  $w_{opt}$ . However, the distribution  
 738 pattern of  $I_P$  shows an interaction with other features and more clustering close to zero showing  
 739 less impact than CE,  $w_L$  and  $w_P$ .  $A_F$ , on the other hand, shows a less pronounced impact for  
 740 both  $\gamma_{dmax}$  and  $w_{opt}$ ; the values cluster around zero, meaning it slightly affects the predictions.  
 741 The Sand and  $F_{200}$  features also show a los impact on  $\gamma_{dmax}$  and  $w_{opt}$ , as most SHAP values are  
 742 concentrated near zero, indicating these features have little effect on the models' output in  
 743 comparison to CE,  $w_L$ ,  $w_P$ , and  $I_P$ . Moreover, the occasional and frequent occurrence of red and  
 744 blue dots across negative and positive SHAP values for input features suggests that the impact  
 745 of each feature is influenced by its interactions with other features for different instances in

predicting  $\gamma_{dmax}$  and  $w_{opt}$ , thereby helping to bridge gaps in prediction and enhance prediction accuracy.

Overall,  $w_L$  and CE stand out as the most influential features playing a primary role in predicting  $\gamma_{dmax}$  and  $w_{opt}$ .  $w_P$  has a secondary role, with moderate effects that mirror  $w_L$ 's trend in predicting compaction parameters.  $I_P$  and  $A_F$ , have a tertiary and  $F_{200}$ , and Sand exhibits a quaternary role. This shows that the proposed XGBoost aligns with geotechnical principles, as increased CE allows particles to rearrange efficiently at lower moisture levels and decrease the void spaces significantly resulting in high  $\gamma_{dmax}$ .  $w_L$  shows a strong positive correlation with  $\gamma_{dmax}$  and  $w_{opt}$ , reflecting that soils with higher  $w_L$  require more water for optimal compaction due to their greater water-holding capacity and undergo less densification while  $w_P$  and  $I_P$  also mirror this impact in a comparatively less pronounced manner. The small impact of  $F_{200}$  and Sand suggests that grain size distribution shows low influence over compaction characteristics compared to Atterberg's limit and CE for cohesive soils but their impact somewhat influences the impact of other peoperties.

#### 4.4.2. Parametric analysis

A parametric analysis was conducted by maintaining all parameters at their minimum values and varying individual input parameters to observe the impact on the model's performance, as illustrated in Figure 21. This analysis revealed that in the XGBoost model, the  $w_{opt}$  increases while the  $\gamma_{dmax}$  decreases with increases in  $w_L$ ,  $w_P$ , and  $I_P$ , with  $w_L$  exerting the most significant influence among them. Specifically, the impact of  $w_L$  is pronounced at approximately 100%, after which its influence becomes negligible. The variables Sand and  $F_{200}$  demonstrated inverse effects relative to each other and slightly impacted compaction parameters. This effect was significant only when Sand was below 50% and  $F_{200}$  exceeded 50%, highlighting that the model accounts for the impact within the fine-grained soil boundary defined by ASTM D2487,

given the data limitations for cohesive soils. Furthermore, the CE increased  $\gamma_{dmax}$  and decreased  $w_{opt}$ , consistent with basic soil mechanics principles. However, this impact was significant only for CE values below 5000 kN-m/m<sup>3</sup>, after which it became less significant. The variable  $A_F$  exhibited a slight impact on  $\gamma_{dmax}$  and  $w_{opt}$ , primarily at lower values. The XGBoost model consistently performed without anomalies, whereas the RF model exhibited some irregularities. For instance, with CE values, the RF model showed a decrease in  $w_{opt}$  up to 2500 kN-m/m<sup>3</sup>, followed by an increase up to 5000 kN-m/m<sup>3</sup>. Similar irregularities were observed for  $F_{200}$  and Sand in the RF model. These irregularities can be regarded as the reason for the inferior performance of RF than XGBoost.

Additionally, the model's efficacy was evaluated by examining the combination of predicted  $\gamma_{dmax}$  and  $w_{opt}$  to assess its impact on  $S_{\gamma dmax}$ , by varying  $G_s$  within the theoretical bounds of 2.65 and 2.9 for cohesive soils (Fig. 22). The XGBoost model consistently yielded theoretically valid results, did not produce a combination that resulted in  $S_{\gamma dmax}$  exceeding 100% for any instance. In contrast, the RF model frequently produced  $S_{\gamma dmax}$  values surpassing 100%. This demonstrates the robust underlying modeling mechanism of the XGBoost model, enabling it to accurately predict  $\gamma_{dmax}$  and  $w_{opt}$  while adhering to theoretical constraints.

#### 4.4.3. Sensitivity analysis

The sensitivity analysis using the assumed database used in parametric analysis revealed that in the XGBoost model, all input parameters possess a certain  $S_i$ , validating the input analysis conducted for this study (Figure 23). Notably,  $w_L$  and CE emerged as the most sensitive parameters for  $\gamma_{dmax}$  and  $w_{opt}$ , similar to the SHAP analysis. Consequently, the XGBoost model is suitable for application across a range of cohesive soil classifications and varying CE levels, accommodating a wide range of variations in these two most significant input features. The  $S_i$  for the XGBoost model varied in the order of  $w_L$ , CE,  $w_P$ ,  $I_P$ ,  $A_F$ , Sand and  $F_{200}$  for  $\gamma_{dmax}$ , and CE,  $w_L$ ,  $w_P$ ,  $I_P$ ,  $A_F$ ,  $F_{200}$ , and Sand for  $w_{opt}$  (Fig. 22). This indicates a robust modeling process

employed by the XGBoost algorithm, which mathematically bounds different parameters with distinct schemes for  $\gamma_{dmax}$  and  $w_{opt}$ , thereby accurately predicting these values.

## 5. Practical Application

The proposed method in this study for predicting  $\gamma_{dmax}$  and  $w_{opt}$  at arbitrary CE levels has significant implications for field applications in geotechnical engineering and construction projects. In large-scale earthwork operations, where soil properties can vary considerably across the site, this method offers a more efficient alternative to traditional laboratory and field testing for each location. By utilizing readily available soil parameters such as  $w_L$  and  $w_P$ , field engineers can quickly estimate location-specific compaction characteristics, potentially reducing the time and cost associated with extensive laboratory testing. This approach is particularly valuable in projects where discrepancies between laboratory-derived and field-observed compaction parameters are common. Furthermore, the method allows for a more nuanced approach to compaction control by enabling the redefinition of the compaction degree based on site-specific predicted  $\gamma_{dmax}$  values that account for variable field CE levels. This redefinition could lead to a more accurate assessment of compaction adequacy across heterogeneous sites, potentially optimizing compaction efforts and improving quality control processes. Moreover, the ability to estimate compaction parameters at arbitrary CE levels also opens up possibilities for adaptive compaction strategies, where equipment settings and pass numbers can be adjusted in real time based on local soil conditions and predicted optimal compaction parameters (Miller and Vahedifard, 2024). A particularly significant application of this method is in achieving efficient compaction by adjusting the water content of fill material to match the  $w_{opt}$  at the field CE level. The proposed method allows for the prediction of  $w_{opt}$  corresponding to the estimated field CE, enabling more precise moisture content adjustments. This capability can lead to optimized compaction efforts and improved soil performance. However, it's important to note that to fully leverage this advantage, it is

necessary to develop reliable means of evaluating the field CE level, albeit different methods are available in literature as proposed by Johnson and Sallberg, (1960). Additionally, this method could facilitate the development of more sophisticated specifications for earthwork projects, allowing for variable compaction requirements that are tailored to specific areas within a site based on their unique soil properties and the estimated field CE level. Such an approach could result in more efficient use of resources, improved overall compaction quality, and potentially reduced construction time and costs. However, implementation of this method in field practice would require careful calibration and validation against traditional methods which can be done in future research. Also, the proposed XGBoost model exposes the complex feedback loops that govern soil compaction. For instance, the model shows that increasing CE boosts  $\gamma_{dmax}$  by facilitating particle rearrangement and reducing void spaces at lower moisture levels. Meanwhile, the parametric study also uncovers a threshold effect, where CE becomes less effective beyond a certain point. Similarly, while soils with higher  $w_L$  require more moisture to achieve optimal compaction, their increased water-holding capacity paradoxically limits their ability to densify effectively. The model trained on a global dataset also provides insights into the categorization of soil properties to influence the compaction characteristics of the cohesive soil useful for controlling compaction in fields based on soil properties.

## 6. Conclusions,

The current study provides a comprehensive approach for the global modeling of compaction parameters at arbitrary CE levels using an extensive database established through testing and literature surveys. The following are the main findings of this study.

- Different ML techniques showed inconsistent performance with the current database. The optimal XGBoost model had the lowest prediction deviation for  $\gamma_{dmax}$  and  $w_{opt}$ , followed by the RF model. In contrast, GEP, MEP, ANN, and MLR models had higher deviations. Statistical KPIs confirmed these results, reflecting the complexity of the

geotechnical data and the varying effectiveness of different modeling techniques. This suggests that no single ML method universally performs best for geotechnical databases, and tailored performance analysis may be needed for different datasets.

- The XGBoost model outperformed existing models and RF in predicting  $\gamma_{dmax}$  and  $w_{opt}$ , both using the established database and an independent dataset, meeting all evaluation criteria. Its superior performance highlights the effectiveness of training on a comprehensive database and XGBoost's robust framework, resulting in minimal prediction error within theoretical bounds. Predicted  $\gamma_{dmax}$  and  $w_{opt}$  values for  $S_{\gamma_{dmax}}$  remained consistently within 100% across different CE levels, while other models exceeded this threshold, indicating the need for careful consideration when using them.
- By combining SHAP analysis with real modeling data, the XGBoost model reveals how CE, soil plasticity and gradation influence  $\gamma_{dmax}$  and  $w_{opt}$ . The analysis emphasizes the primary roles of CE and  $w_L$ , with CE increasing  $\gamma_{dmax}$  and decreasing  $w_{opt}$ , and  $w_L$  having the opposite effect.  $w_P$  play a secondary role in prediction, with moderate impacts that align with the trends of  $w_L$ .  $I_P$  and  $A_F$  play a tertiary role, and  $F_{200}$  and Sand show a small impact, confirming their quaternary role in prediction. Meanwhile, all these parameters combined result in high prediction accuracy, helping to fill the gaps in the predictions. The model shows insignificant irregularities from these trends during parametric analysis across a wide range of input feature values. Sensitivity analysis further confirms the model's adaptability across various soil plasticity ranges and CE levels. The current modeling approach allows engineers to focus on the most influential factors and thresholds, effectively optimizing compaction for cohesive soils.

The proposed method for predicting  $\gamma_{dmax}$  and  $w_{opt}$  at varying CE levels offers a promising solution to enhance field compaction practices, especially in large-scale projects, by providing a more efficient alternative to traditional, labor-intensive measurement techniques. Predicting

compaction parameters at arbitrary CE levels is particularly useful in the field, as it allows for more flexible and accurate adjustments to compaction efforts based on site-specific conditions. This approach, based on readily available soil properties, could improve compaction quality, optimize resource usage, and offer a more accurate assessment of compaction in heterogeneous field conditions. Meanwhile, future work should focus on developing reliable methods for estimating field CE, validating this modeling approach in the field, and expanding it to different soil types, i.e., granular soils.

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### **Competing interests**

The authors declare that they have no competing interests

### **Availability of code**

The codes of the proposed models are available at <https://github.com/ZiaurRehman16/Soil-Compaction-Model.git>.

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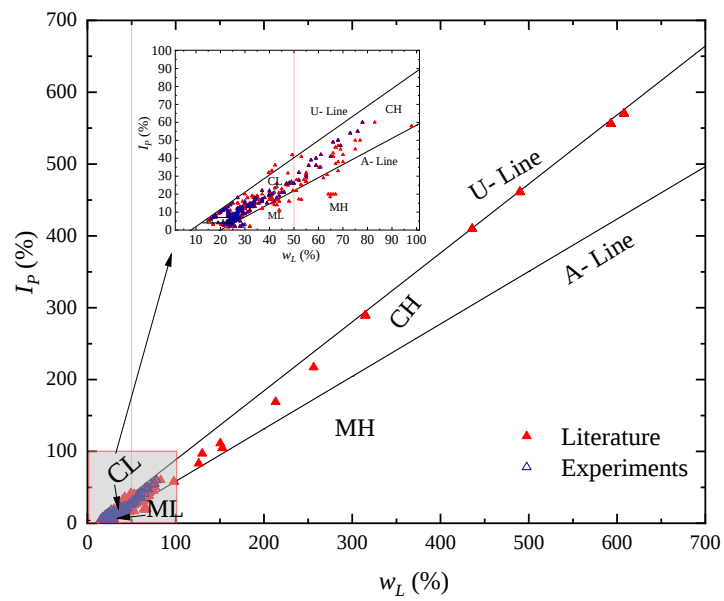
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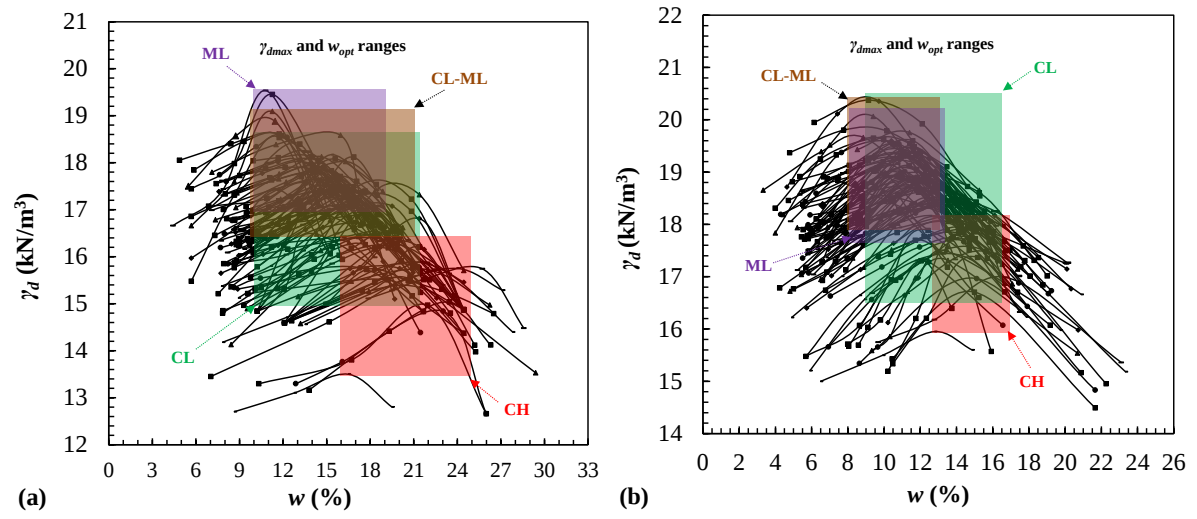
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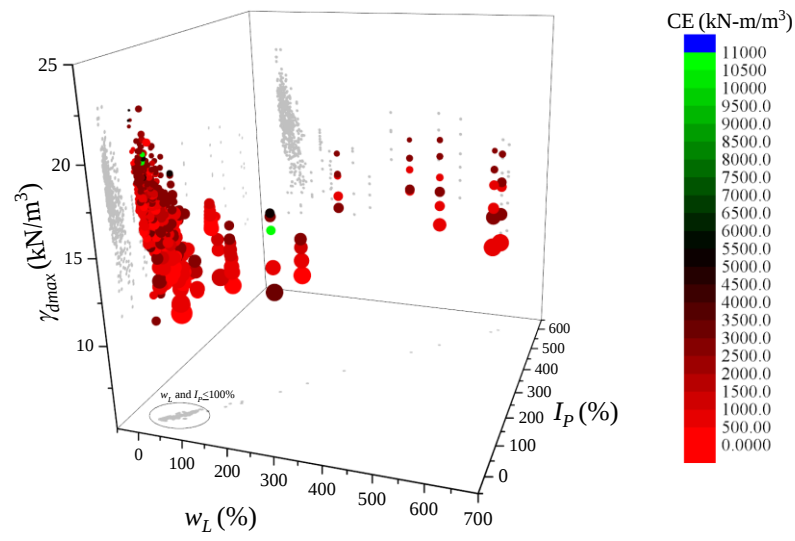
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**Fig. 1:** Soil classification data orientation on A-line plasticity chart

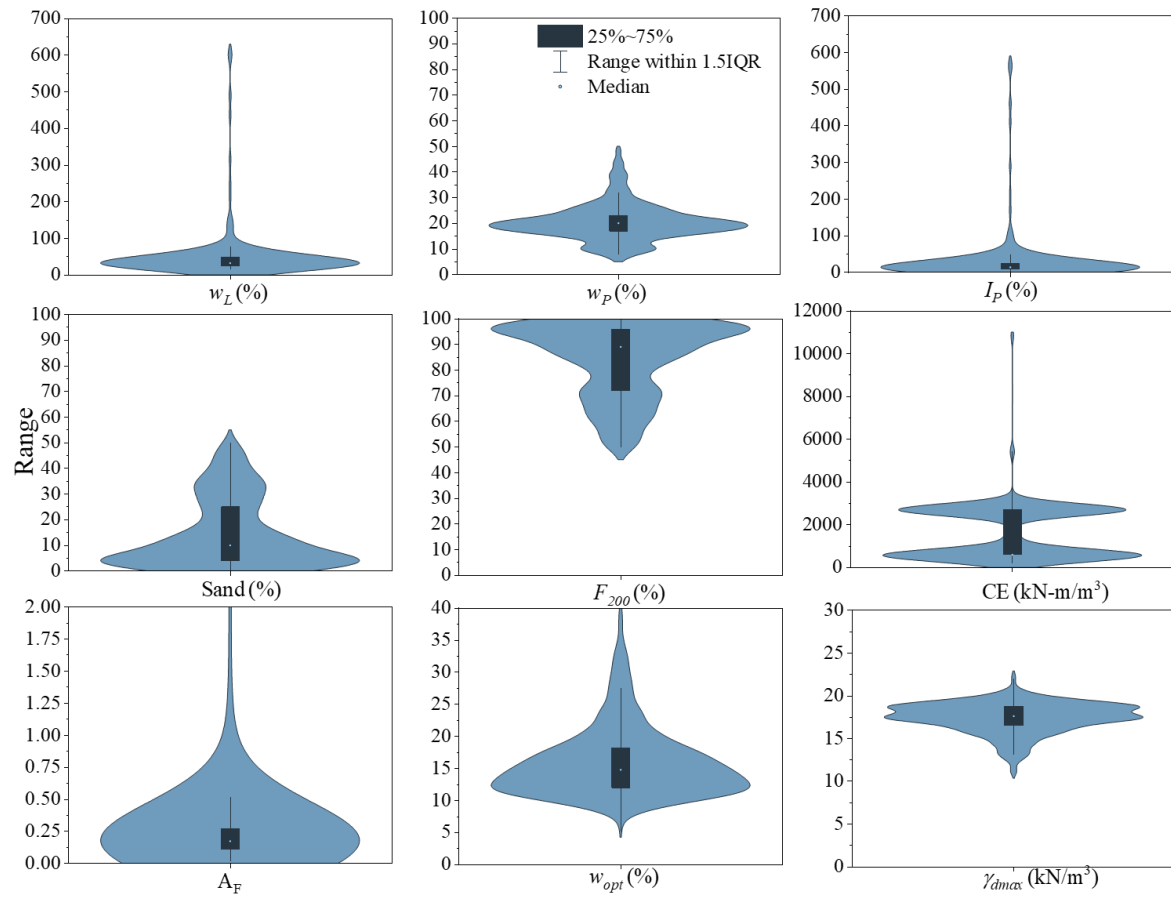


**Fig. 2:** Relationship between  $\gamma_d$  and  $w$  of tested samples (a) standard compaction tests; (b) modified compaction tests

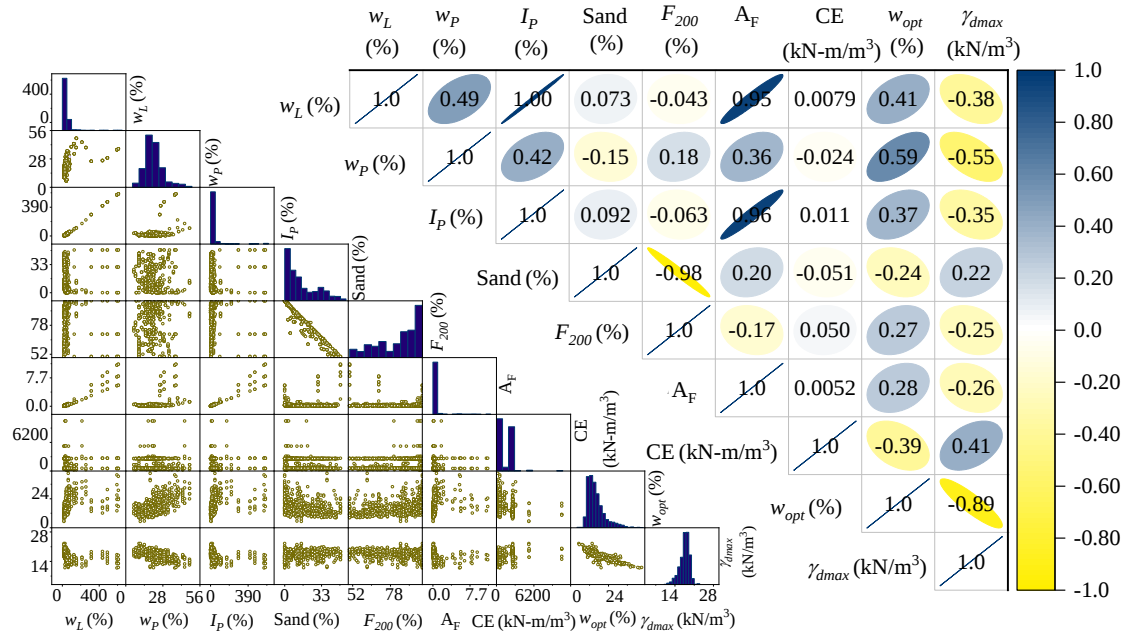


Symbol size proportional to  $w_{opt}$  (%): scaling factor 0.5

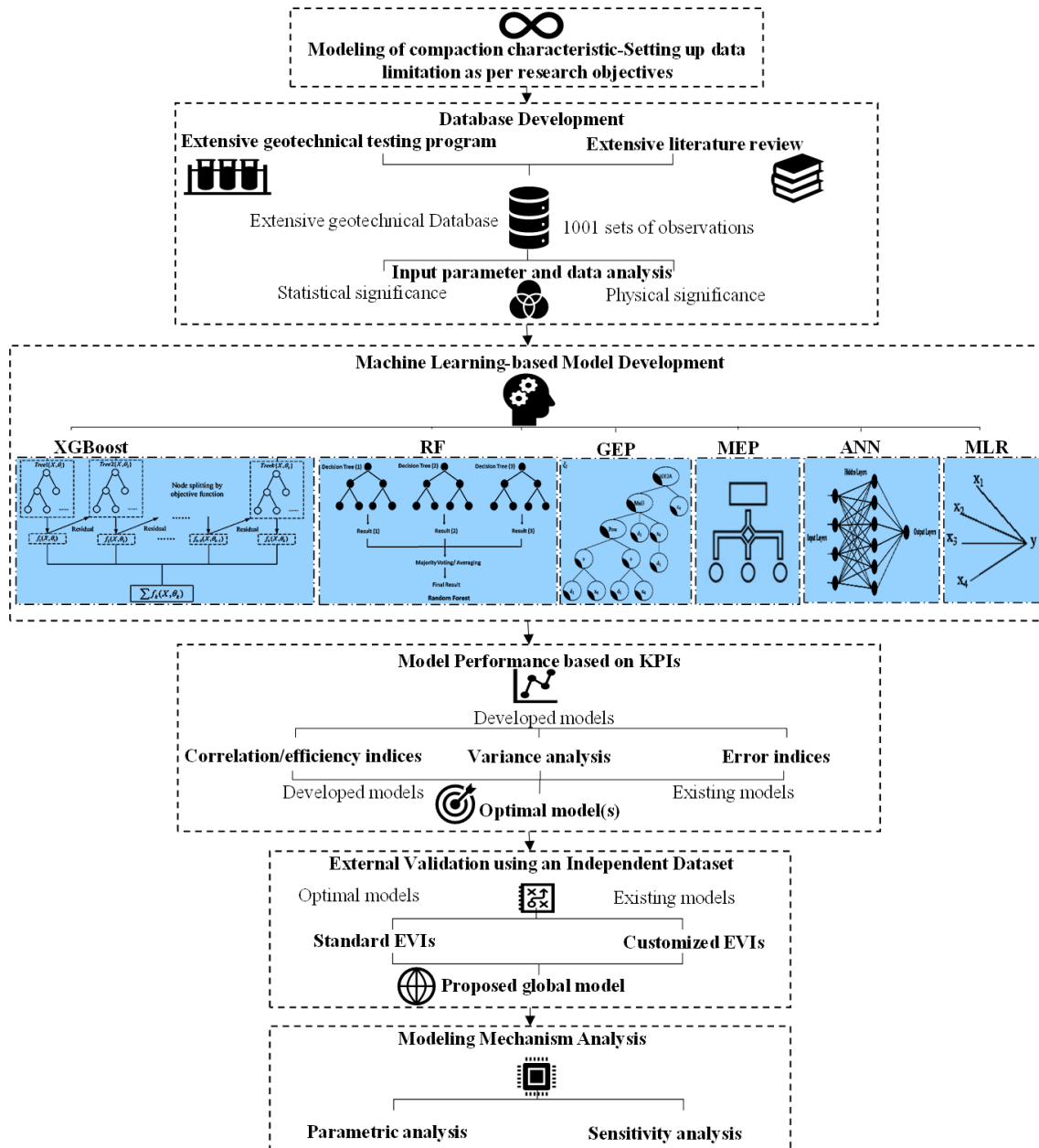
**Fig. 3:** Modeling data orientation



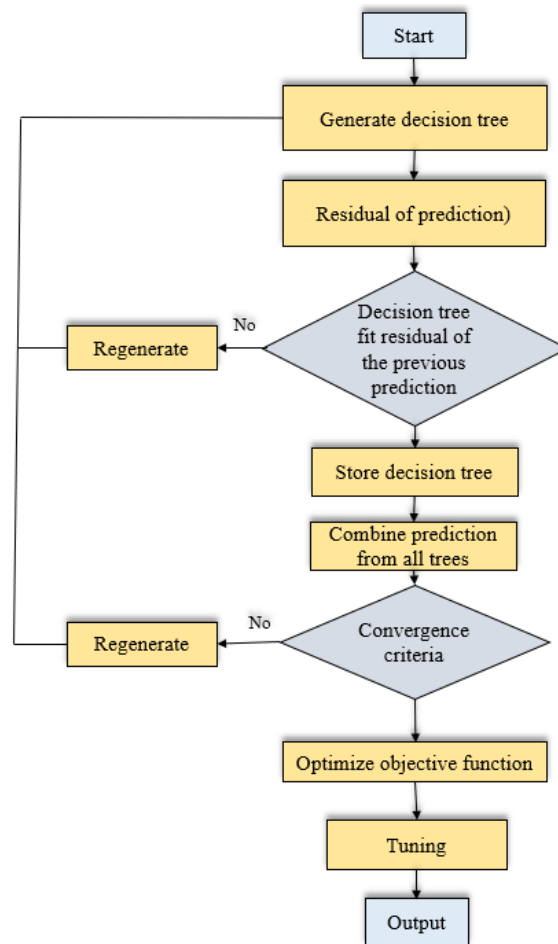
**Fig. 4:** Violin plots of the established database for modeling



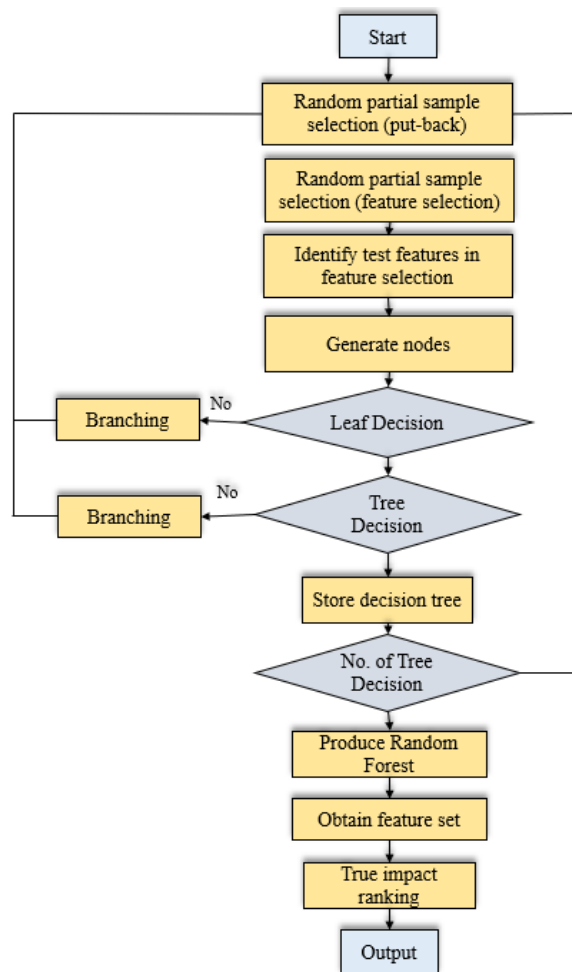
**Fig. 5:** Correlational and Pearsons correlation coefficient matrices of input and output parameters



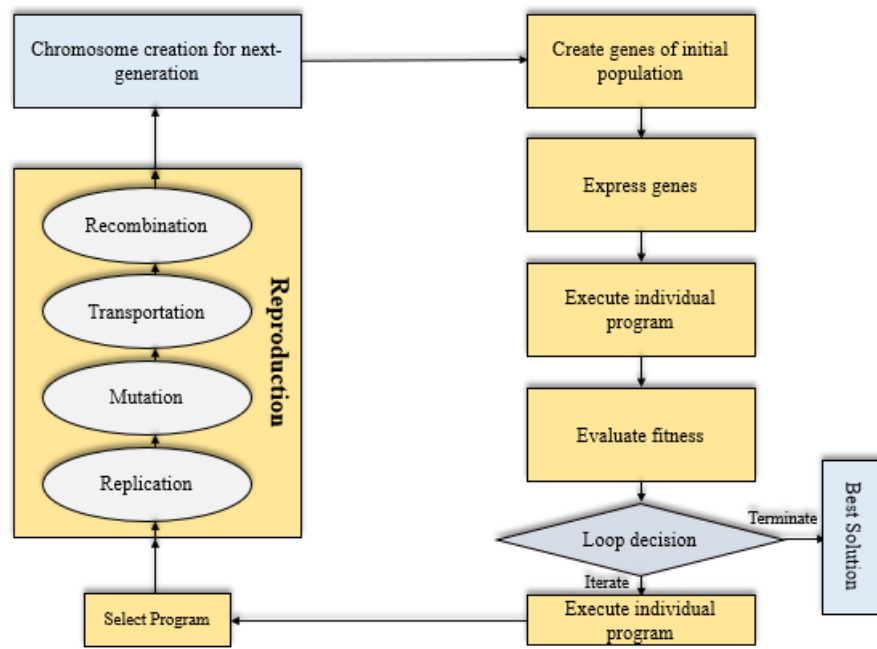
**Fig. 6:** Methodology of the current study



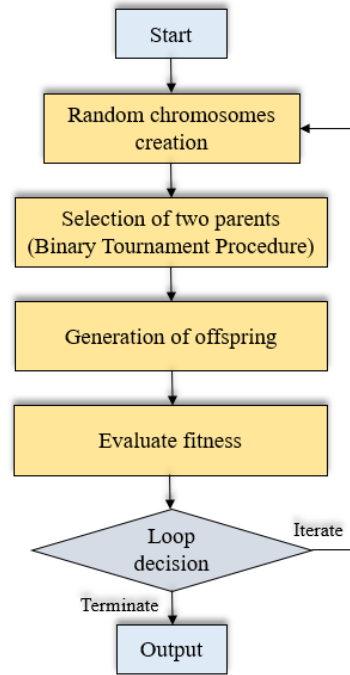
**Fig. 7:** XGBoost algorithm architecture



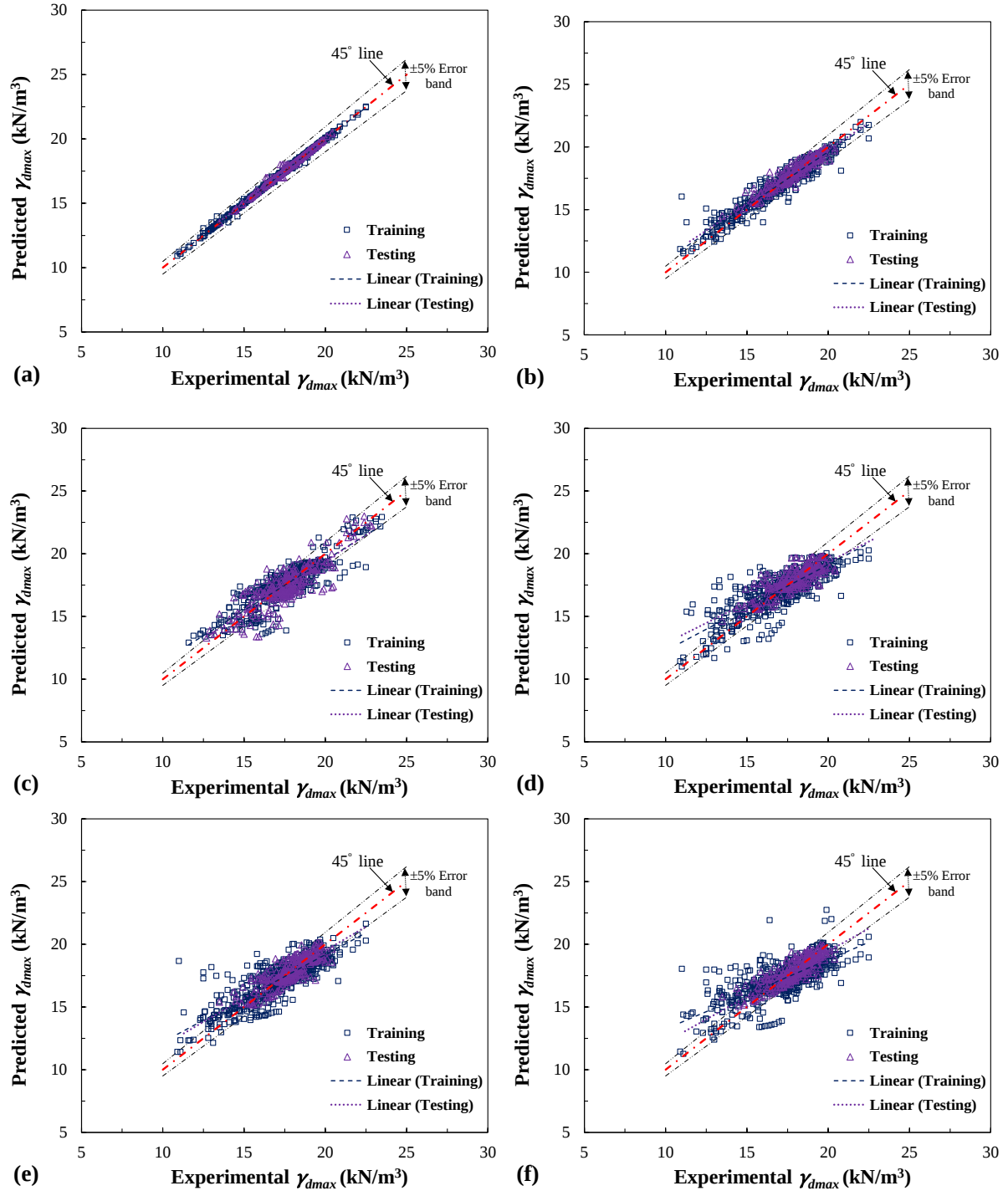
**Fig. 8:** RF algorithm architecture



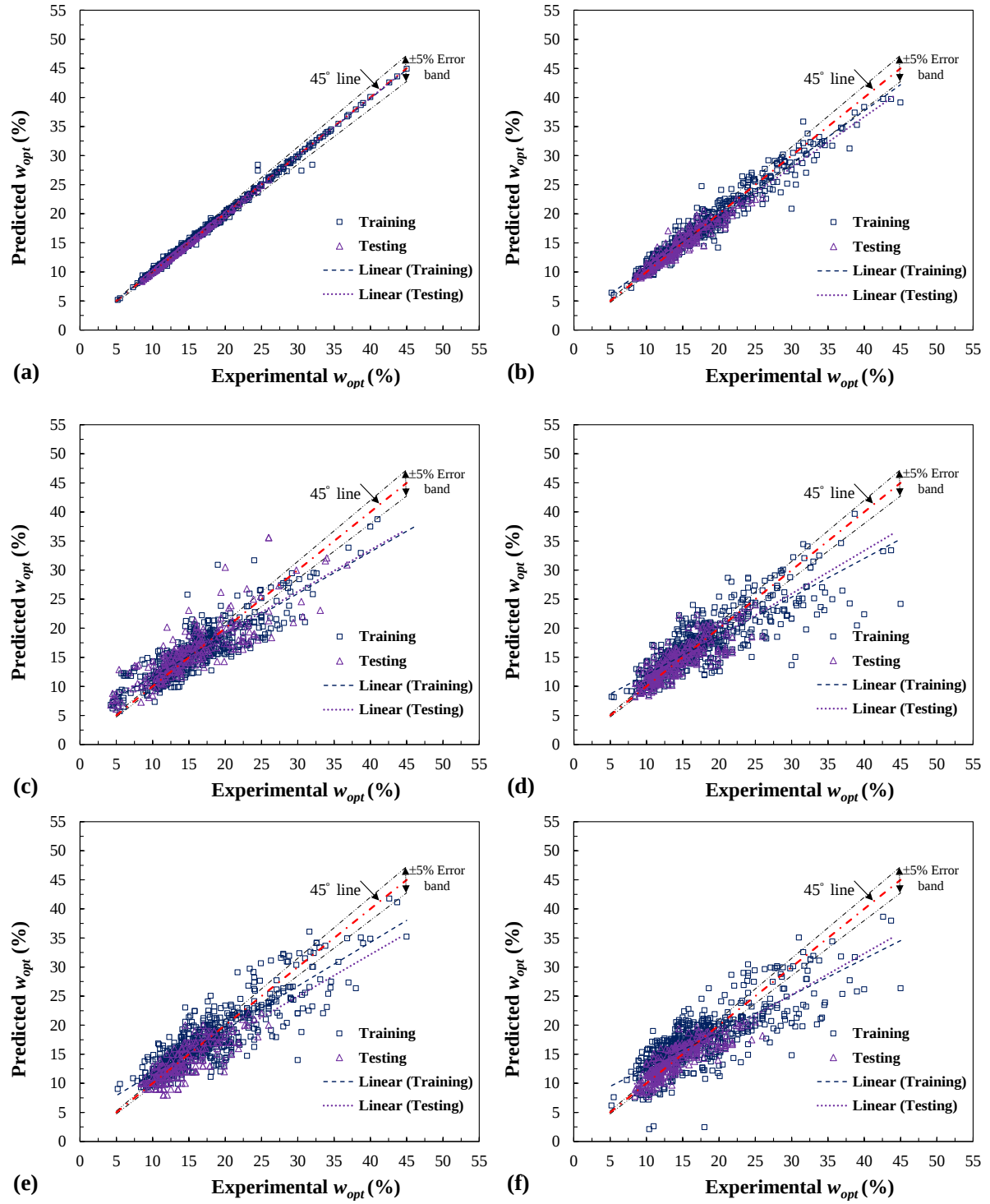
**Fig. 9:** GEP algorithm architecture



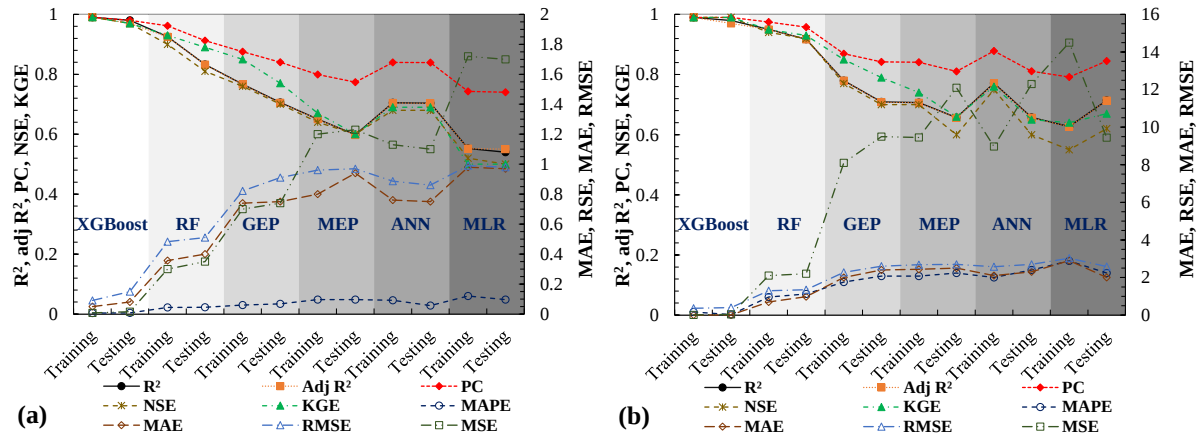
**Fig. 10:** MEP algorithm architecture



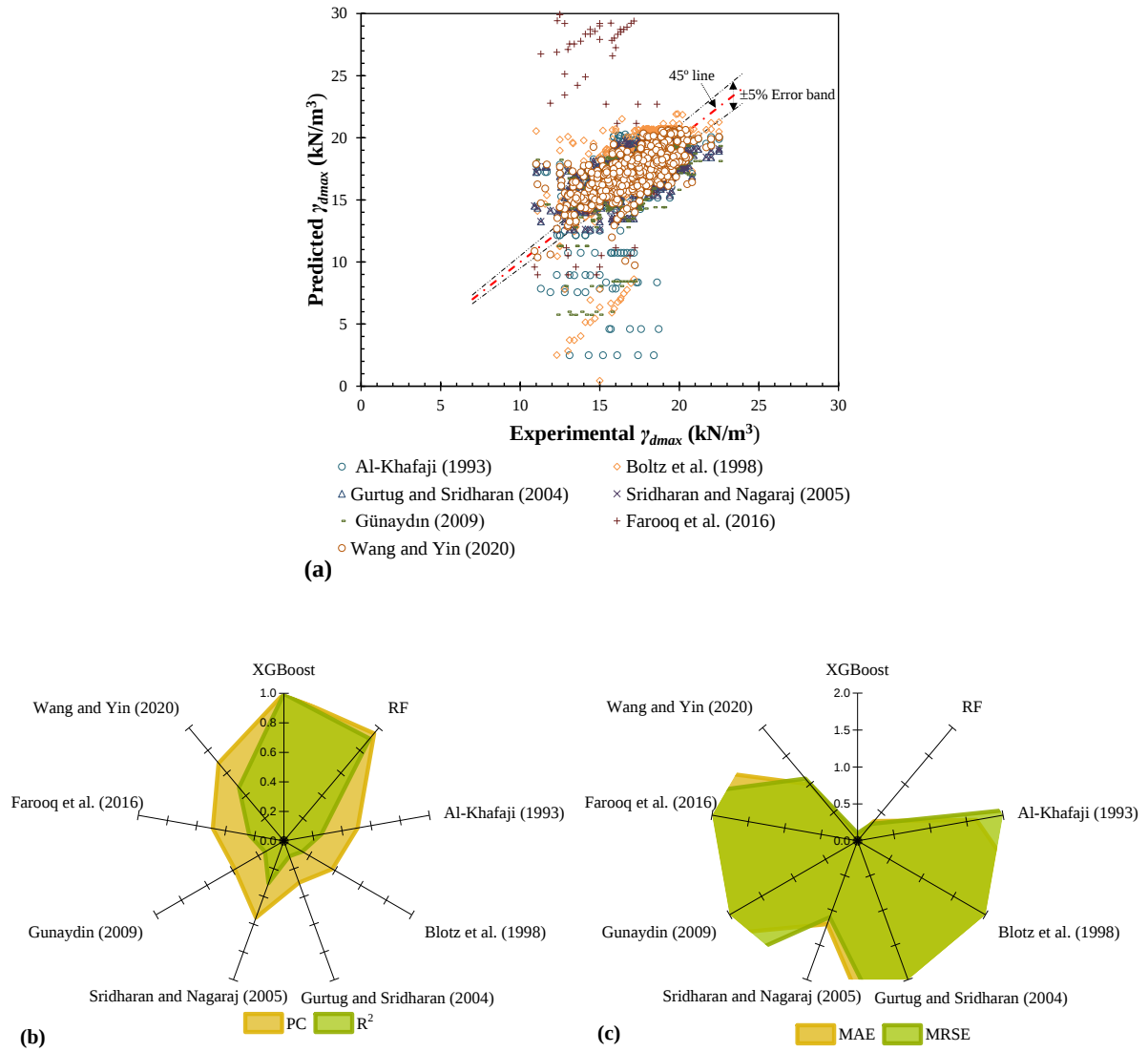
**Fig. 11:**  $\gamma_{dmax}$  model training and testing (a) XGBoost; (b) RF; (c) GEP; (d) MEP; (e) ANN; (f) MLR



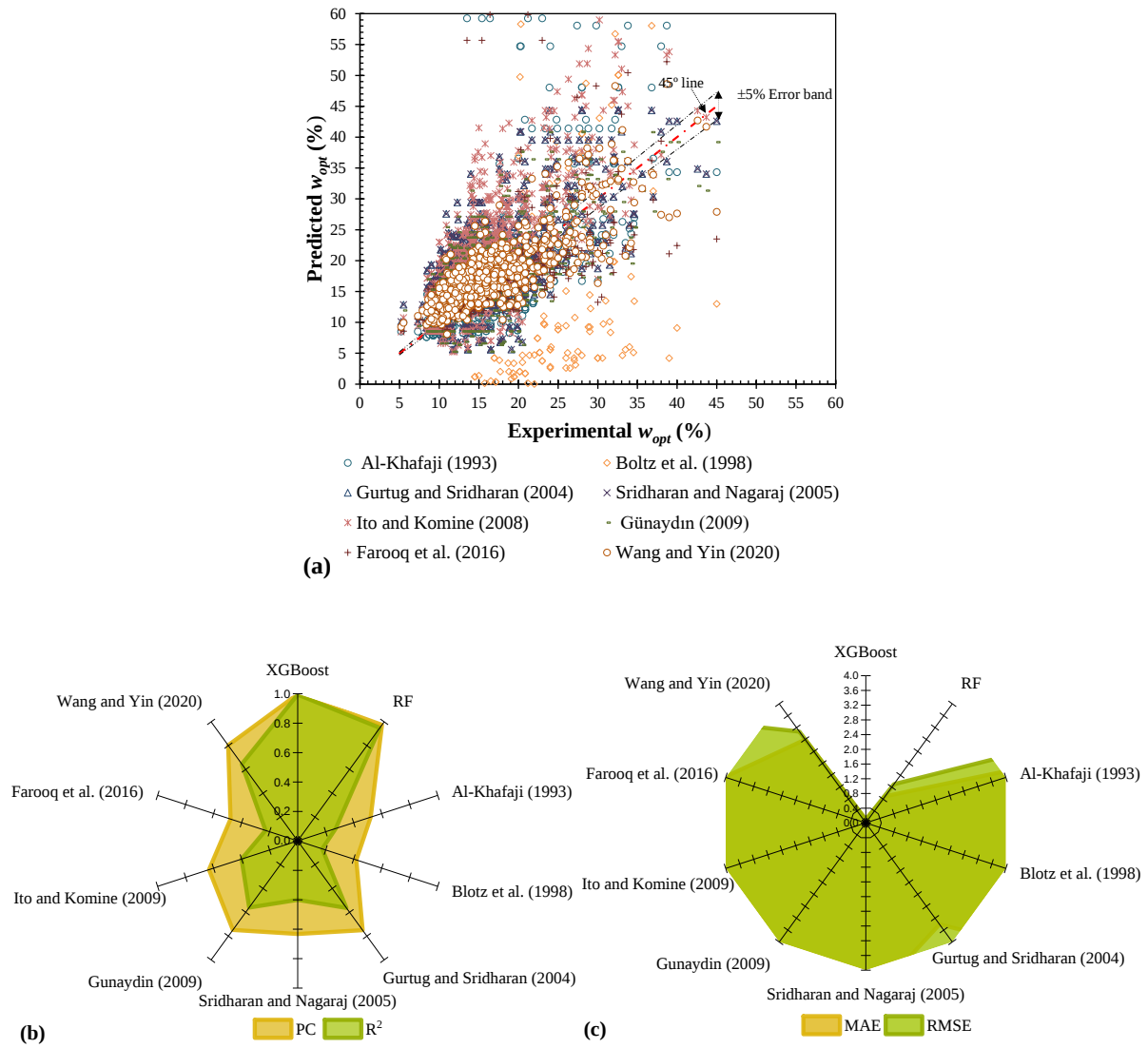
**Fig. 12:**  $w_{opt}$  model training and testing (a) XGBoost; (b) RF; (c) GEP; (d) MEP; (e) ANN; (f) MLR



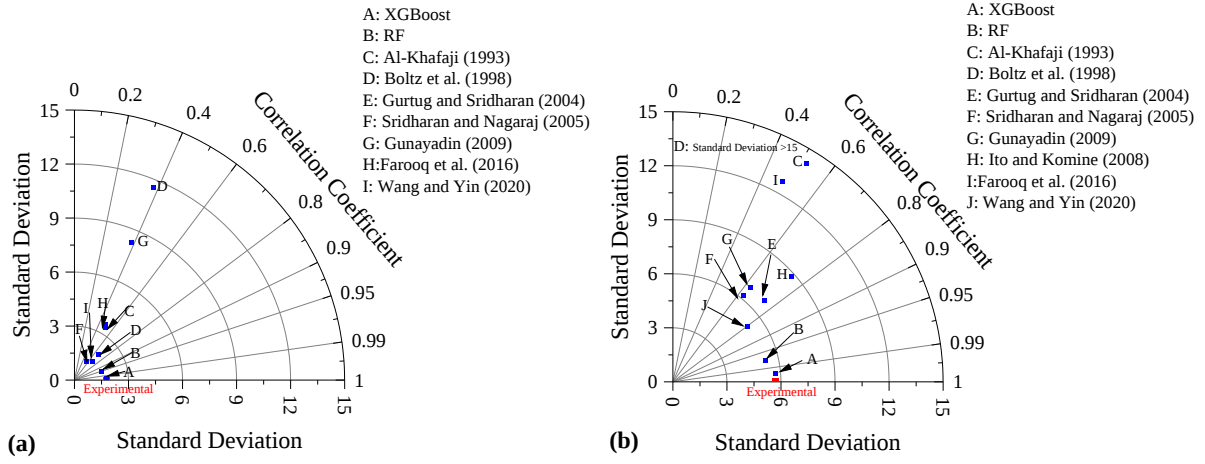
**Fig. 13:** Performance comparison of developed models (a) for  $\gamma_{dmax}$ ; (b) for  $w_{opt}$



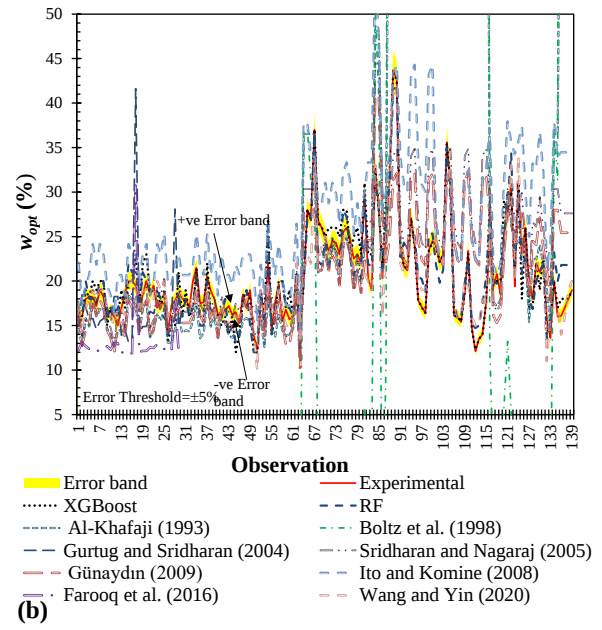
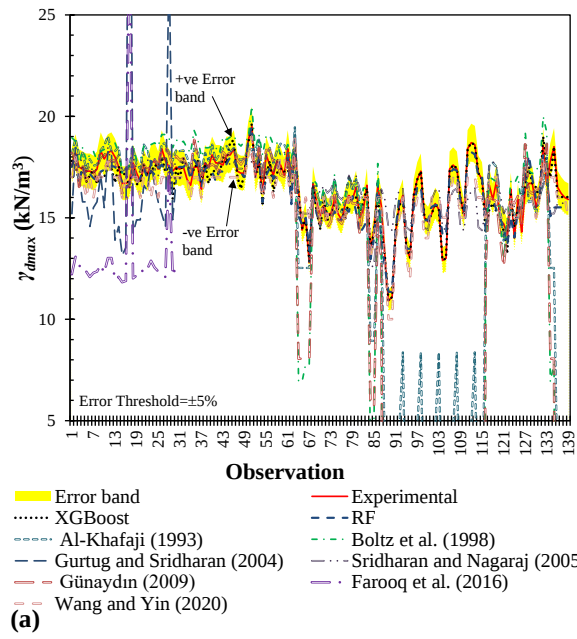
**Fig. 14:** Performance comparison of shortlisted models with existing models for  $\gamma_{dmax}$  (a) scatter plot; (b) correlation indices; (c) error indices



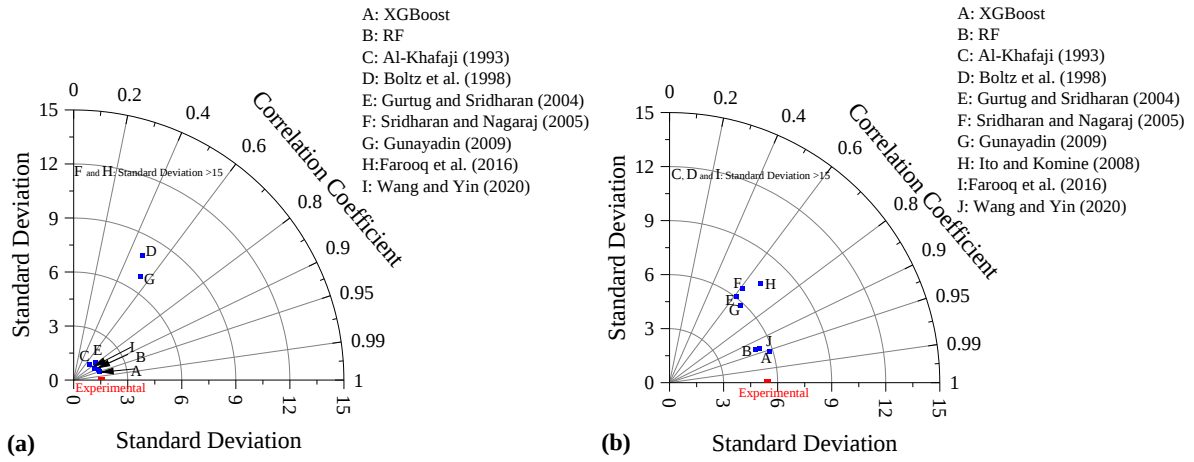
**Fig. 15:** Performance comparison of shortlisted models with existing models for  $w_{opt}$  (a) scatter plot; (b) correlation indices; (c) error indices



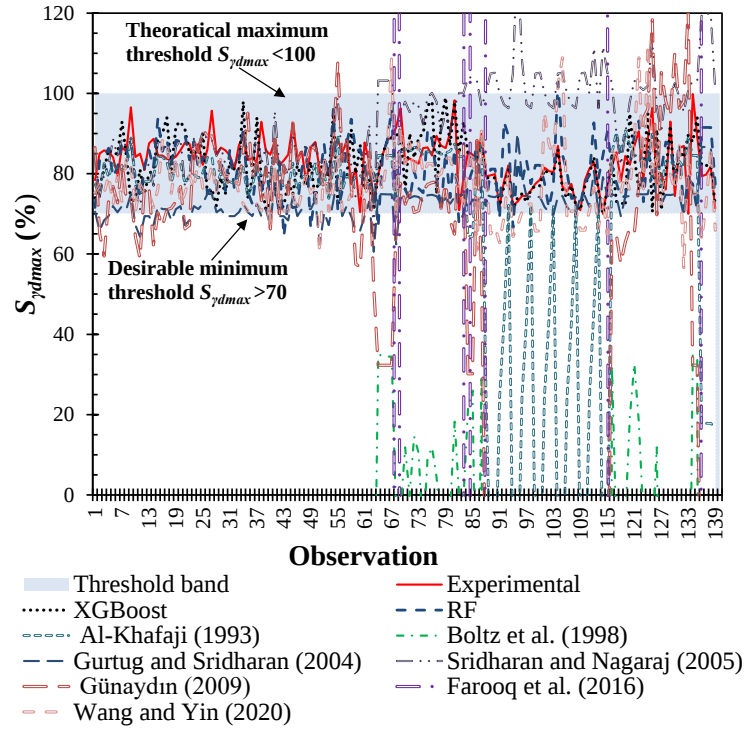
**Fig. 16:** Performance comparison of shortlisted models with the existing models through the Taylor diagram a) for  $\gamma_{dmax}$ ; (b) for  $w_{opt}$



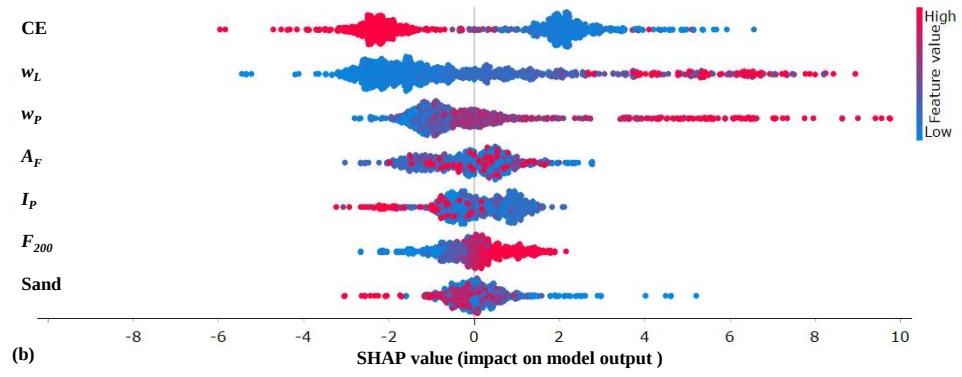
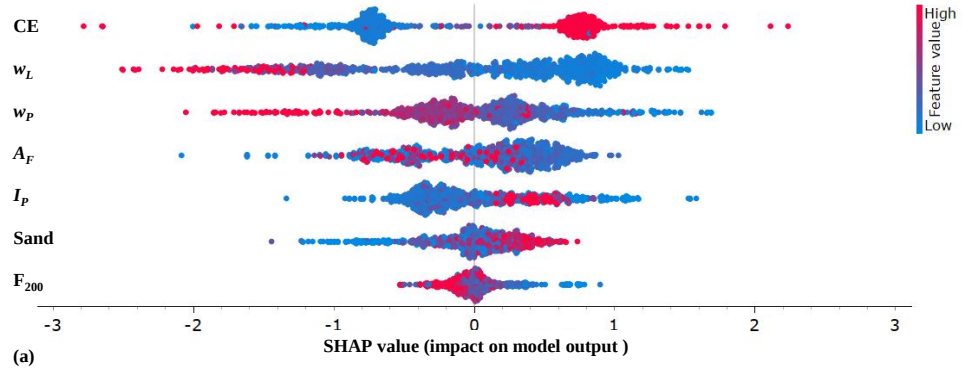
**Fig. 17:** External validation of shortlisted models and comparison with existing models (a) for  $\gamma_{dmax}$ ; (b) for  $w_{opt}$



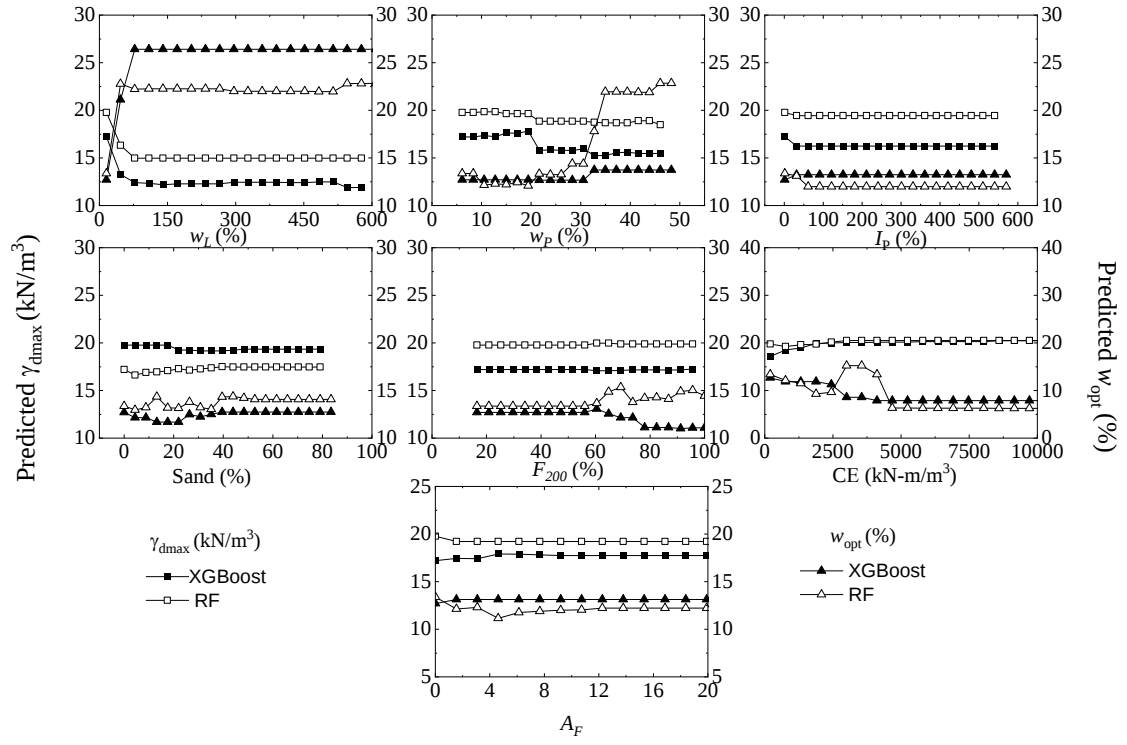
**Fig. 18:** External validation of shortlisted models and comparison with existing models through the Taylor diagram (a) for  $\gamma_{dmax}$ ; (b) for  $w_{opt}$



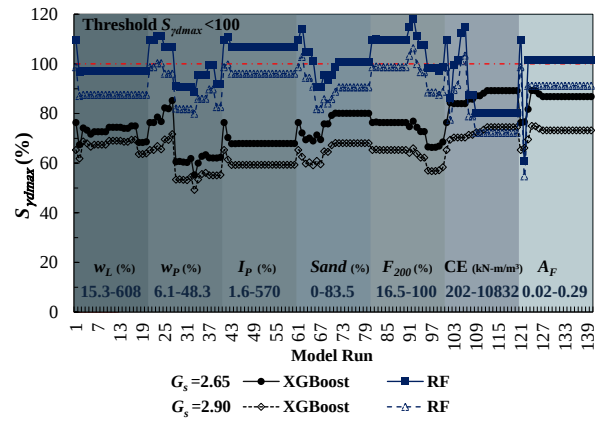
**Fig. 19:** External theoretical validation of shortlisted models and comparison with existing models through  $S_{\gamma dmax}$  analysis



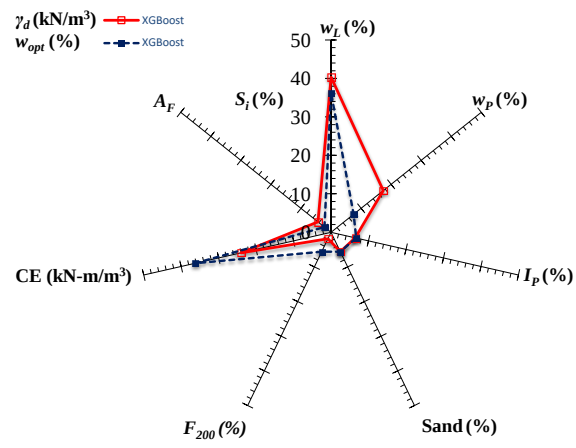
**Fig. 20:** XGBoost model explanation with SHAP analysis (a) for  $\gamma_{dmax}$ ; (b) for  $w_{opt}$



**Fig. 21:** Parametric analysis of XGBoost model and comparison with RF



**Fig. 22:** Parametric analysis of XGBoost model and comparison with RF to analyze theoretical validation using  $S_{y\text{dmax}}$



**Fig. 23:** Sensitivity analysis of input parameters for proposed models

Table 1: Overview of the dataset used for modeling and validation

|                                                             |                    | $w_L$   | $w_P$ | $I_P$   | Sand  | $F_{200}$ | CE                  | $A_F$ | $w_{opt}$ | $\gamma_d$        | $S_{ydlmax}$ |
|-------------------------------------------------------------|--------------------|---------|-------|---------|-------|-----------|---------------------|-------|-----------|-------------------|--------------|
|                                                             |                    | %       | %     | %       | %     | %         | kN-m/m <sup>3</sup> | -     | %         | kN/m <sup>3</sup> | %            |
| Model Training and Testing Data<br>(Testing and literature) | Maximum            | 608.0   | 48.3  | 570.1   | 50.0  | 100.0     | 10832.1             | 11.4  | 45.0      | 22.5              | 97.1         |
|                                                             | Minimum            | 15.0    | 6.1   | 1.6     | 0.0   | 50.0      | 202.0               | 0.001 | 5.2       | 10.9              | 50.2         |
|                                                             | Count              | 1001    | 1001  | 1001    | 1001  | 1001      | 1001                | 1001  | 1001      | 1001              | 1001         |
|                                                             | Mean               | 53.5    | 20.5  | 32.9    | 14.8  | 83.9      | 1614.5              | 0.4   | 16.1      | 17.5              | 76.1         |
|                                                             | Median             | 32.0    | 20.0  | 14.0    | 10.0  | 89.0      | 594.0               | 0.2   | 14.8      | 17.6              | 75.0         |
|                                                             | Standard Deviation | 82.2    | 7.2   | 78.9    | 13.6  | 14.4      | 1280.6              | 1.2   | 5.7       | 1.8               | 8.5          |
|                                                             | Variance           | 6758.1  | 52.2  | 6227.8  | 184.9 | 206.4     | 1639813.7           | 1.5   | 32.4      | 3.2               | 72.0         |
|                                                             | Range              | 592.7   | 42.2  | 568.5   | 50.0  | 50.0      | 10630.1             | 11.4  | 39.8      | 11.6              | 49.5         |
|                                                             | Excess kurtosis    | 28.6    | 2.0   | 30.2    | -0.4  | -0.6      | 11.6                | 43.4  | 3.2       | 0.9               | 0.0          |
|                                                             | Skewness           | 5.2     | 1.0   | 5.4     | 0.9   | -0.8      | 2.0                 | 6.3   | 1.6       | -0.8              | 0.1          |
| External Validation Data (Literature)                       | Maximum            | 550     | 48.3  | 480     | 83.5  | 100.0     | 2693.0              | 29.1  | 43.7      | 37                | 98.9         |
|                                                             | Minimum            | 23.0    | 12.0  | 3.4     | 0.0   | 16.5      | 551.0               | 0.03  | 12.1      | 12.3              | 70.0         |
|                                                             | Count              | 139     | 139   | 139     | 139   | 139       | 139                 | 139   | 139       | 139               | 139          |
|                                                             | Mean               | 153.1   | 24.6  | 128.5   | 19.7  | 80.0      | 882.2               | 2.2   | 20.3      | 16.4              | 83.2         |
|                                                             | Median             | 49.4    | 23.0  | 26.0    | 13.0  | 87.0      | 593.0               | 0.3   | 18.6      | 16.8              | 83.9         |
|                                                             | Standard Deviation | 196.8   | 7.2   | 192.2   | 19.7  | 20.0      | 726.4               | 4.2   | 5.4       | 2.0               | 6.0          |
|                                                             | Variance           | 38733.3 | 51.4  | 36945.8 | 388.6 | 399.3     | 527597.7            | 17.7  | 28.9      | 4.0               | 35.7         |
|                                                             | Range              | 527.0   | 36.3  | 476.7   | 83.5  | 83.5      | 2100                | 29.0  | 31.6      | 24.7              | 29.9         |
|                                                             | Excess kurtosis    | 0.3     | 0.3   | 0.3     | 0.8   | 0.6       | 2.9                 | 13.4  | 4.3       | 21.1              | 0.3          |
|                                                             | Skewness           | 1.4     | 0.8   | 1.4     | 1.2   | -1.2      | 2.2                 | 3.1   | 1.8       | -3.4              | 0.0          |

Table 2: Evaluation of developed models based on KPIs

[illegible]

Table 3: External validation analysis of proposed and existing models for  $\gamma_{dmax}$  (kN/m<sup>3</sup>)

| Dataset         | Statistical Parameters |                |                             |                               |           |           |       |                    |                                             |
|-----------------|------------------------|----------------|-----------------------------|-------------------------------|-----------|-----------|-------|--------------------|---------------------------------------------|
|                 | R <sup>2</sup>         | R <sub>m</sub> | R <sub>0</sub> <sup>2</sup> | R <sub>0</sub> ' <sup>2</sup> | k         | k'        | MAE   | NAPE <sub>ol</sub> | S <sub><math>\gamma_{dmax(ol)}</math></sub> |
| Desirable range | >0.9                   | >0.5           | around 1                    | around 1                      | 0.85-1.15 | 0.85-1.15 | <3    | ≤5                 | 0                                           |
| A               | 0.91                   | 0.65           | 0.99                        | 0.99                          | 0.99      | 0.84      | 0.30  | 4.3                | 0.0                                         |
| B               | 0.84                   | 0.51           | 0.99                        | 0.99                          | 0.98      | 0.80      | 0.40  | 10.1               | 0.7                                         |
| C               | 0.29                   | 0.06           | 0.90                        | 0.90                          | 0.82      | 0.10      | 3.86  | 37.4               | 8.6                                         |
| D               | 0.21                   | 0.04           | 0.90                        | 0.90                          | 0.20      | 2.32      | 15.54 | 56.7               | 84.9                                        |
| E               | 0.59                   | 0.26           | 0.94                        | 0.94                          | 0.94      | 0.85      | 1.23  | 51.1               | 0.0                                         |
| F               | 0.51                   | 0.19           | 0.93                        | 0.93                          | 1.00      | 0.69      | 0.81  | 28.1               | 30.2                                        |
| G               | 0.21                   | 0.04           | 0.90                        | 0.90                          | 0.39      | 1.53      | 11.11 | 35.6               | 25.8                                        |
| H               | 0.23                   | 0.04           | 0.90                        | 0.90                          | 1.71      | 1.17      | 12.57 | 94.9               | 100                                         |
| I               | 0.77                   | 0.42           | 0.98                        | 0.98                          | 0.98      | 0.93      | 0.70  | 25.9               | 3.6                                         |

A=XGBoost; B= RF; C= Al-Khafaji (1993); D= Boltz et al. (1998); E=Gurtug and Sridharan (2004); F= Sridharan and Nagaraj (2005); G= Günaydin (2009); H: Farooq et al. (2016); I: Wang and Yin (2020)

Table 4: External validation analysis of proposed and existing models for  $w_{opt}$  (%)

| Dataset         | Statistical Parameters |       |          |          |           |           |      |             |                |
|-----------------|------------------------|-------|----------|----------|-----------|-----------|------|-------------|----------------|
|                 | $R^2$                  | $R_m$ | $R_0^2$  | $R_0'^2$ | k         | k'        | MAE  | $NAPE_{ol}$ | $S_{ydmx(ol)}$ |
| Desirable range | >0.9                   | >0.5  | around 1 | around 1 | 0.85-1.15 | 0.85-1.15 | <3   | $\leq 5$    | 0              |
| A               | 0.92                   | 0.70  | 0.99     | 0.99     | 1.00      | 0.85      | 1.2  | 3.1         | 0.0            |
| B               | 0.88                   | 0.60  | 0.99     | 0.99     | 1.00      | 0.87      | 1.5  | 5.0         | 0.7            |
| C               | 0.11                   | 0.01  | 0.9      | 0.9      | 1.75      | 8.88      | 18.0 | 44.0        | 8.6            |
| D               | 0.08                   | 0.01  | 0.8      | 0.8      | 3.03      | 117.72    | 71.4 | 97.3        | 84.9           |
| E               | 0.45                   | 0.15  | 0.9      | 0.9      | 1.01      | 1.81      | 3.4  | 31.6        | 0.0            |
| F               | 0.37                   | 0.10  | 0.9      | 0.9      | 1.09      | 1.95      | 4.0  | 30.9        | 30.2           |
| G               | 0.37                   | 0.10  | 0.9      | 0.9      | 1.00      | 2.51      | 3.9  | 35.9        | 25.8           |
| H               | 0.45                   | 0.15  | 0.9      | 0.9      | 1.30      | 0.33      | 6.8  | 58.7        | NA             |
| I               | 0.08                   | 0.01  | 0.9      | 0.9      | 1.68      | 5.56      | 16.5 | 30.9        | 100            |
| J               | 0.86                   | 0.50  | 0.98     | 0.98     | 0.97      | 0.69      | 1.6  | 6.0         | 3.6            |

A=XGBoost; B= RF; C= Al-Khafaji (1993); D= Boltz et al. (1998); E=Gurtug and Sridharan (2004); F= Sridharan and Nagaraj (2005); G= Günaydin (2009); H: Ito and Komine (2020); I: Farooq et al. (2016); J: Wang and Yin (2020)