A SUPER-LEARNER MACHINE LEARNING MODEL FOR A GLOBAL 1 2 PREDICTION OF COMPRESSION INDEX IN CLAYS 3 Esteban Díaz^{1*}, Giovanni Spagnoli² 4 ¹ Departamento de Ingeniería Civil, Escuela Politécnica Superior, Universidad de Alicante, P.O. 5 Box 99, E-03080 Alicante, Spain, esteban.diaz@ua.es 6 ² DMT GmbH & Co. KG, Am TÜV 1, 45307 Essen, Germany, spagnoli giovanni@yahoo.de, 7 giovanni.spagnoli@dmt-group.com; ORCID: 0000-0002-1866-4345 8 * Corresponding author. 9

10 Abstract

Settlement of structures is determined by the stiffness of the soil where they are built. 11 12 Compression index (c_c) quantifies the compressibility of the soil and is a key parameter in the 13 design of geotechnical structures. To predict the value of c_c in clay soils, a global database of 14 more than 1000 data points was collected and analysed. Liquid limit, plasticity index, natural 15 water content, and initial void ratio were considered as predictor variables. A super-learner 16 machine learning model was developed to predict c_c from these variables. The model 17 demonstrated a reasonable predictive performance and was subsequently integrated into an online tool. Additionally, four symbolic regression expressions were obtained to relate c_c with some of 18 19 the input variables when not all data are available, providing simple and practical alternatives for c_c , estimation. This study provided two major contributions: (1) the non-local nature of the data 20 21 expands the scope and generalizability of the findings, and (2) the availability of the proposed 22 algorithm through an online application ensures its accessibility for geotechnical engineers, 23 enhancing the work's practical applicability and intrinsic value.

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Keywords: machine learning; compression index; liquid limit; plasticity index; natural water
content; initial void ratio; clay.

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29 1. Introduction

Compression index (c_c), which is the slope of the linear section of the $e - \log \sigma'$ plot (and is 30 31 dimensionless), and the coefficient of consolidation (c_v) , primarily define the compressibility 32 properties of fine-grained soils (Craig 2004). c_c is a crucial parameter for characterizing soil 33 compressibility and deformation behaviour under load. It is commonly used in geotechnical 34 engineering to estimate the settlement and deformation of soil structures, such as foundations and 35 embankments (Das 2021). Soils with a higher c_c tend to be more compressible and deformable under load, whereas soils with a lower c_c are less compressible and have a greater capacity to 36 37 withstand deformation when they are loaded. The c_c value in soils is obtained through the 38 oedometer test, which is relatively time-consuming and results in higher costs when compared to 39 standard index tests. Since Atterberg limits initially characterize soils, these state parameters have been used to establish correlations with various other engineering properties of soils. Furthermore, 40 41 plasticity is influenced by the electrochemical behaviour of clay minerals (Carter and Bentley 42 1991) in the same way as c_c (Onyejekwe et al. 2015). For this reason, several attempts were made 43 in the past to correlate basic geotechnical properties with c_c . Numerous authors provided linear 44 equations relating c_c to the liquid limit (LL) of soils (e.g. Azzouz et al. 1976; Bowles 1979; Park 45 and Lee 2011; Sridharan and Nagaraj 2000; Terzaghi et al. 1967; Tsuchida 1991). On the other 46 hand, plasticity index (PI), was also correlated with c_c (Sridharan and Nagaraj 2000; Wroth and 47 Wood 1978). Additionally, many correlations based on a linear relationship with natural water content (w) were proposed (e.g. Azzouz et al. 1976; Koppula 1981; Rendon-Herrero 1980). The 48 49 relationship with initial void ratio (e_0) was examined by Nishida (1956), Hough (1957) and 50 (Bowles 1979), among others. Other studies included more than one index property in the 51 estimation of c_c , such as w and LL (Koppula 1981) or e_0 and LL (Al-Khafaji and Andersland 1992). However, when these correlations were tested with new data, they exhibited significant 52 scatter, with deviations reaching up to 30% (Spagnoli and Shimobe 2020), suggesting a lack of 53 54 universally applicable validity. They are applicable within specific limits and should be restricted 55 to the soil type or location where they were validated (Verbrugge and Schroeder 2018). Using 56 these correlations in different conditions may lead to unsatisfactory outcomes (Onyejekwe et al. 57 2016). To address the limits of classic regression approaches in geotechnical engineering, the 58 application of machine learning (ML) algorithms have been extensively developed, 59 demonstrating improved performance for predicting several soil engineering properties compared to traditional statistical methods (e.g. Bardhan et al. 2023; Bardhan et al. 2021; Dam Nguyen et 60 al. 2022; Díaz and Tomás 2021; Salvatore et al. 2022; Singh et al. 2023; Trong et al. 2021). 61 62 However, it is important to be aware of the limitations and uncertainties associated with ML 63 approaches before applying them to real-world geotechnical engineering projects. Numerous studies (Baghbani et al. 2022; Zhang et al. 2023; Zhang et al. 2022) have exposed these 64 65 limitations, which are primarily: a) the scarcity of high-quality data, b) the difficulty in interpreting the models, and c) the lack of generalization. Regarding data availability, 66 67 geotechnical data can be costly and often incomplete or uncertain. This can lead to ML models that are not as accurate or reliable as desired. Another limitation of ML is the interpretability of 68 69 the models (i.e., black box). ML models are often complex and nonlinear, making it challenging 70 to understand the relationship between input data and output predictions. Finally, due to the 71 inherent heterogeneity and spatial variability of soil deposits, it is difficult for empirical models 72 trained on limited datasets to reliably extrapolate beyond the geographic scope represented by 73 those data. Therefore, while ML shows great potential to complement traditional approaches in 74 geotechnical engineering, it is crucial to address these limitations before the implementation of 75 any ML model.

Recently, numerous studies have employed ML algorithms to predict c_c from some parameters 76 77 related to this property showing promising results (e.g. Desai et al. 2009; Kalantary and Kordnaeij 78 2012; Kumar and Rani 2011; Nesamatha and Arumairaj 2015; Samui et al. 2012). Alam et al. (2014) compiled a database of 125 clay samples, which included w, LL, e_0 , and PI as input 79 80 variables and created an Artificial Neural Network (ANN) model to predict c_c . Kumar and Rani (2011) also used an ANN to predict c_c , considering 41 samples with the following input variables: 81 82 fine contents, LL, PI, maximum dry density, and optimal moisture content. Park and Lee (2011) 83 developed an artificial neural network (ANN) model by utilizing 947 consolidation tests

84 performed on soil samples gathered from 67 construction sites in the Republic of Korea. They 85 considered as input variables, w, LL, PI, e_0 , specific gravity of soil particles (G_s), and weight 86 percentage of sand, silt and clay. Benbouras et al. (2019) developed an ANN model with 373 oedometer test samples to correlate c_c with wet density, w, e_0 , fine content, LL, PI, and soil type. 87 88 The dataset utilized in this research comprised samples gathered from various projects executed 89 in the city of Algiers (Algeria). Zhang et al. (2021) used a Random Forest algorithm that utilized 90 a database with 311 samples, encompassing three input variables (LL, PI, e_0). Asteris et al. (2022) 91 introduced extreme learning machine models that applied Manta ray foraging optimization to 92 predict c_c from void ratio at liquid limit, LL and PI. It should be noted that the void ratio at LL is 93 a parameter that is not usually available in the design phases of geotechnical projects, whereas 94 e_0 , is more frequently encountered. Long et al. (2023) established a relationship between c_c and 95 w, LL, PI, e_0 , and G_s using Tree-Based Techniques from 391 samples from Northern Iran. 96 However, all these approaches have, to a greater or lesser extent, a local character, or a relatively 97 small number of samples. All the studies presented either rely on a limited dataset, or the collected 98 samples have a local nature (i.e., they come from the same area or country), or they do not have 99 a direct application because they are based on ML algorithms. Many engineers lack knowledge 100 of the programming language or specific software required to utilize the proposed algorithms. 101 Therefore, the main objective of this work is threefold: 1) to create an algorithm based on a dataset 102 with a large number of samples, 2) to ensure these samples are collected worldwide to eliminate 103 any local bias, and 3) to design the proposed algorithm in a way that any geotechnical engineer 104 can easily use it. The present paper took advantage of ensemble learners, to develop and validate 105 an accurate prediction model for forecasting the compression index of clay soils for a large 106 number of data (1008) collected worldwide. Subsequently, this model was deployed to a user-107 friendly web application. This paper is structured as follows. A brief summary of the experimental 108 database is given in Section 2. The machine learning process performed is presented in Section 109 3. Later, in Section 4, the main results obtained are studied and interpreted by evaluating the 110 super-learner machine learning model. Section 5 describes the online tool deployed. An analysis

of the dataset using Symbolic Regression is included in Section 6. The final section (Section 7)ends the paper and presents the main conclusions obtained.

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114 2. Database description and analysis.

115 The collection of the dataset is the first step in the building of a machine learning model. In the present work, the experimental database of c_c (1008 samples) comprised 913 samples from 116 117 research papers (Alhaji et al. 2017; Benbouras et al. 2019; Kalantary and Kordnaeij 2012; LCPC 118 1977; McCabe et al. 2014; Mitachi and Ono 1985; Widodo and Ibrahim 2012), and 95 samples 119 from authors' own data. This database has samples of different countries as Nigeria, Ireland, 120 Spain, Iran, Indonesia, France, Algeria, Bangladesh, among others. In the same way, the database has soils with low plasticity to very high plasticity. In fact, LL ranges from 17.1% to 199.0% and 121 122 PI from 2.0% to 82.0%. On the other hand, the database included soils with very high 123 compressibility and soils with low compressibility according to e_0 values (ranging from 0.279 to 7.114). This fact is also corroborated, by examining the values of c_c varying these between 0.013 124 125 and 2.2. Finally, the w values, also varies widely ranging from 8% to 244.1%. Based on all the above, the database includes a significant amount of data and a wide range of them, making it 126 127 suitable for a reliable study. The final dataset can be found in Table S1 (accessible online), which 128 includes details such as references, soil type, mineralogy, and origin when available. Furthermore, 129 the dataset includes both the actual c_c values and those obtained by the super-learner ML model. 130 The main statistics of the compiled database are shown in Table 1.

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	LL (%)	PI (%)	e	w (%)	c _c
Samples	1008	947	1008	1008	1008
Mean	46.49	21.78	0.817	29.73	0.236
Standard deviation	15.90	9.83	0.467	17.06	0.210
Minimum	17.10	2.00	0.279	8.00	0.013
25 th percentile	36.00	15.07	0.598	21.00	0.143
Median	44.85	22.03	0.712	25.40	0.180
75 th percentile	54.14	28.05	0.852	31.20	0.246
Maximum	199.00	82.00	7.114	244.10	2.200



Table 1. Descriptive statistics of the data analysed.

134 Figure 1 shows box plots for LL, PI, e_0 , w and c_c of the database. Box plots are used to visualize 135 data dispersion, which was split into quartiles. The method is used to detect outliers (if any), data symmetry, dispersion, and skewness (Reagan and Kiemele 2008). The box in a box plot shows 136 the interquartile range (IQR), with the bottom and top of the box representing the 25th and 75th 137 percentiles, respectively. The whiskers extend to the final data value inside the inner fence, which 138 139 is 1.5 times the IQR from the box's edge. The height of the box represents the interquartile range. 140 Outliers are defined as data points extending to 3×IQR (Reagan and Kiemele 2008). Some points 141 in Figure 1 are identified as outliers, mainly corresponding to high values of the variables. The 142 analysis of these box plots reveals the wide range of variation and high dispersion of the variables 143 studied clearly related to the worldwide character of the compiled database. For a better 144 interpretation of Figure 1, the data included in Table 1 can be consulted.

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Figure 1. Box plots of the variables considered.

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149 The scatter plots of the considered parameters are depicted in Figure 2, to show a descriptive 150 overview of the data distribution. These plots indicate a positive relationship between c_c and the 151 rest of the variables. This fact implies, to a greater or lesser extent, that an increase in the 152 considered input variables tends to proportionally increase c_c . This relationship is clearer in 153 variables as e_0 and w and more diffuse in LL and PI. Finally, a strong relationship between e_0 154 and w must also be noted.

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Figure 2. Scatter plots and distribution histograms of the variables.

159 These linear trends can be quantified numerically using the Pearson correlation coefficient (r) and 160 a correlation matrix. A correlation matrix is a table showing the correlation values, which measure 161 the degree of linear relationship between each pair of variables. Correlation values can be between 162 -1 and +1. If the two variables tend to increase or decrease at the same time, the correlation value

is positive. In Table 2 is shown the correlation matrix providing an overview of the Pearson correlation coefficient. From the analysis of the table, it can be verified that the same relationships established previously in a visual manner are the ones that obtain the highest correlation values. Indeed, a strong and positive correlation is shown between c_c and e_0 (r=0.87) and w (r=0.89), and a somewhat less strong and also positive correlation between c_c and LL (r=0.66). Between c_c and PI, the correlation is low and positive (r=0.34). On the other hand, there is a strong and positive correlation between e_0 and w (r=0.92).

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	LL	PI	e ₀	W	C _c
LL	1.00				
PI	0.92	1.00			
e_0	0.61	0.23	1.00		
w	0.64	0.28	0.92	1.00	
c _c	0.66	0.34	0.87	0.89	1.00

171Table 2. Correlation matrix of the variables considered. Note that the values indicated

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correspond to the Pearson correlation coefficient (r).

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The equations obtained by linear regression for the cases with the highest value of Pearsoncorrelation coefficient are (Equations 1 to 3):

177	$c_c = 0.393e_0 - 0.0842$	(1)
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- 178 $c_c = 0.011w(\%) 0.0905$ (2)
- 179 $e_0 = 0.0252w(\%) + 0.0687$ (3)
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- 181 The coefficient of determination (\mathbb{R}^2) of each of the three equations above presented is 0.76, 0.80, 182 0.85, respectively. Equation 3 is very interesting, as the e_0 value can be estimated by w, 183 considering that e_0 relates the soil structure with its geologic history (Onyejekwe et al. 2015).
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185 **3. Machine learning procedure.**

186 **3.1. Model selection process.**

187 According to the analysis of the dataset carried out in the previous section, PI has 61 data less 188 than the rest of the variables. To match the number with the rest of the variables, a data imputation 189 technique was used. This is a technique widely used in ML algorithms for dealing with missing 190 values and it has been used in geotechnical issues satisfactorily (e.g. Aydın et al. 2023; Díaz et al. 191 2023). For the imputation of values, a multivariate feature imputation algorithm has been chosen 192 (Little and Rubin 2019; Van Buuren and Oudshoorn 2000). This technique uses the information 193 of all of the available features in order to estimate the missing value of one variable by considering 194 samples which have a similar situation in terms of all of the features in the dataset. After imputing 195 the missing data, an outlier detection analysis was conducted using the one-class SVM algorithm 196 developed by Schölkopf et al. (1999) and successfully employed in similar works (e.g. Díaz et al. 197 2023). This algorithm is a method designed to identify outliers and anomalies within a dataset, 198 utilizing the principles of traditional Support Vector Machines (SVM). The core idea behind SVM 199 is to identify a hyperplane that maximizes the separation between different classes within the 200 dataset. Once this hyperplane is established, new data points can be classified based on their 201 position relative to the hyperplane. In the case of the one-class SVM, there is only one class, and 202 it defines the hyperplane for normal data points while classifying data points located outside the 203 hyperplane as outliers. Upon applying this algorithm, 9 outliers were identified. These 9 data 204 points were thoroughly examined, but no anomalous values in their properties were observed. 205 Therefore, due to their limited number, it was decided not to remove them from the dataset. With 206 the final dataset including 1008 records of each variable, a machine learning algorithm selection 207 process was carried out using the k-fold cross-validation technique (with k=10). The results of 208 this selection process are shown in Table 3, ordering the selected algorithms, from best to worst

performance considering four statistical indicators, mean absolute percentage error (MAPE),
coefficient of determination (R²), root mean squared error (RMSE), and mean absolute error
(MAE). Three algorithms, all of them based on decision trees, outperform over the rest: Extra
Trees Regressor (Geurts et al. 2006), Random Forest Regressor (Ho 1995), and Gradient Boosting
Regressor (Friedman 2001).

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Model	RMSE	MAPE	MAE	R ²
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Extra Trees Regressor	0.0767	0.2521	0.0466	0.87
Random Forest Regressor	0.0776	0.2534	0.0473	0.86
Gradient Boosting Regressor	0.0781	0.2529	0.0478	0.86
Huber Regressor	0.1050	0.2766	0.0559	0.75
Light Gradient Boosting Machine	0.1059	0.2831	0.0576	0.74
K Neighbors Regressor	0.1000	0.2919	0.0578	0.75
AdaBoost Regressor	0.0876	0.3427	0.0581	0.81
Ridge Regression	0.1084	0.3106	0.0610	0.74
Linear Regression	0.1117	0.3106	0.0613	0.72
Least Angle Regression	0.1117	0.3106	0.0613	0.72
Bayesian Ridge	0.1113	0.3124	0.0616	0.72
Decision Tree Regressor	0.0966	0.3296	0.0622	0.79
Elastic Net	0.1040	0.3307	0.0625	0.74
Orthogonal Matching Pursuit	0.1034	0.3471	0.0654	0.74
Lasso Regression	0.1170	0.3479	0.0668	0.68
Lasso Least Angle Regression	0.1170	0.3479	0.0668	0.68
Passive Aggressive Regressor	0.1232	0.3562	0.0728	0.63

²¹⁵ *Table 3. Performance of base machine learning models obtained by k-fold cross validation.*

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This process was carried out with the variables without normalization. But it should be noted that the same algorithm selection process was also performed normalizing the variables using the minmax method, which scales each variable individually between zero and one. The results of this process normalizing the variables, were exactly the same in the three models with the best performance.

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223 **3.2. Model development.**

To ensure a proper generalization of the algorithms, it is good practice to assess their performance on unknown data. For this purpose, the dataset was divided into two groups (training and test) with an 80/20 partition. Subsequently, the three algorithms with the best performance were subjected to a tuning process of their hyperparameters to maximize their performance. For this
purpose, the particle swarm optimisation (Kennedy and Eberhart 1995) was used. This is a
computational technique which optimises problems by iteratively improving candidate solutions
(aka particles). The results of this optimization are shown in Table 4, in terms of R², RMSE, and
MAE and with the result in both in the training and in the test set.

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Model	Set	R ²	MAE	RMSE
Extra Trees	Training	0.92	0.034	0.059
Regressor	Test	0.92	0.040	0.055
Random Forest	Training	0.92	0.039	0.061
Regressor	Test	0.92	0.041	0.055
Gradient Boosting	Training	0.93	0.038	0.056
Regressor	Test	0.91	0.042	0.058

Table 4. Summary of performance metrics of the trained machine learning algorithms.

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235 With the tuned algorithms, they were ensembled to improve their predictive capacity. Among the existing approaches, the super-learner algorithm (Laan et al. 2007) was chosen. The super-learner 236 237 algorithm is a type of ensemble method that applies stacked generalization to k-fold cross-238 validation. It combines multiple prediction models (base learners) by assigning different weights 239 to these models to find their optimal combination and produce a single best prediction function. 240 Thus, the predictions of the base learners are used to train a regression model (meta learner) that 241 assigns relative weights to the predictions of each base-model. In this case, and after a process of 242 trial and error, the best results were obtained using the tuned Extra Trees Regressor and Gradient Boosting Regressor algorithms as base learners, and the tuned Random Forest Regressor 243 244 algorithm as meta learner. It must be indicated that the meta learner was trained on the base 245 models' predictions as well as the original training data. The performance metrics resulting in the 246 super-learner machine learning model, are shown in Table 5.

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Model	Set	\mathbb{R}^2	MAE	RMSE
Super-Learner	Training	0.93	0.034	0.057
	Test	0.93	0.039	0.053

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 Table 5. Summary of performance metrics of the super-learner machine learning model.

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As can be seen the super-learner machine learning model improved slightly the predictions of thebest of the three selected algorithms (Table 4).

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252 **4. Results.**

4.1. Analysis of the super-learner ML model for predicting c_c .

254 The prediction accuracy of the super-learner machine learning model is evaluated using training 255 and test datasets. Figure 3 shows the scatter plots for the actual values of c_c (x-axis) versus the predicted values of c_c (y-axis). This figure shows that the vast majority of data are located close 256 257 to the no error line, indicating a good agreement between the predicted and measured values. Additionally, in Figure 3 are included the values of R^2 on both the training and test datasets. These 258 259 values (0.93 in both sets) are indicative of a high predictive capacity, and since they are the same, 260 it is assured a correct behaviour of the model in unseen data, discarding overfitting issues. The 261 predictive performance of the selected model was also evaluated based on the anteriorly defined performance metrics (MAE and RMSE). In the training dataset, MAE and RMSE values of 0.034 262 263 and 0.057 were obtained, respectively. In the test set, these values were similar (MAE of 0.039 264 and RMSE of 0.053). These metrics are summarized in Table 5 (previous section) for both the 265 train and test datasets. Additionally, the a20-index (Apostolopoulou et al. 2020; Asteris et al. 266 2021a; Asteris et al. 2021b) was calculated. The a20-index offers the advantage of having a clear 267 engineering interpretation, indicating the percentage of samples that meet the predicted values 268 within a $\pm 20\%$ deviation from the experimental ones. The values obtained in the training and test 269 sets were 73.45% and 71.27%, respectively, showing a similar and reasonable performance for 270 the prediction of c_c .



Figure 3. Scatter plot showing graphical performance of the super-learner machine learning
model in (a) training set, and (b) test set. The identity line (i.e., no error line) and the best fit
line were included in both figures.

In order to evaluate the results of the adopted model, a residuals study was performed. The 277 278 residuals were defined as the difference between the predicted and actual value obtained by the 279 super-learner model. In Figure 4 are shown the residuals for both the training and test datasets 280 with two different visualizations, a scatter plot, and a histogram distribution. An inspection of this 281 figure shows that for the two datasets considered, the residuals are concentrated around zero and 282 have Gaussian distributions (i.e., residuals are normally distributed) and, thus, there are not many 283 outliers. These facts are indicative of a robust algorithm with a great generalization ability and do 284 not reveal significant issues in the predictions.



287 Figure 4. Residuals scatter plot and histogram distribution in (a) training set and (b) test set of

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the super-learner machine learning model.

Figure 5 compares the experimental and predicted c_c values on the test set (unseen data). The prediction performance of the testing set, according to what was previously discussed, was very good. Figure 5 shows that the super-learner machine learning model, can accurately capture the

- evolution of the actual values, the prediction results are consistent, and the difference between the
 minimum and maximum predicted values is relatively small. No large deviations are observed in
 a general manner, affecting only isolated samples.
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301 4.2. Sensitivity analysis.

302 Subsequently, a sensitivity analysis of the parameters involved in the super-learner ML model 303 was conducted. This analysis employed Sobol's method (Sobol 1990), a technique for assessing 304 the significance of input parameters in computational models. Sobol's method evaluates their 305 impact on the output by quantifying their contribution to output variance. Within this method, the 306 First-order sensitivity indices (S1) measure the influence of each variable in isolation while 307 holding all other variables constant. Total-order sensitivity indices (ST) encompass not only the 308 individual effects of each variable but also their interactions with other variables on the output. 309 The results of this analysis are collected in Table 6, showing that e_0 was the most influential 310 variable, with a ST of 0.839, implying that it had the greatest effect on the variability of the 311 model's output. Following e_0 , w emerged as the second most important factor in this analysis (ST = 0.122). Next, LL possessed a moderate ST, with a value of 0.066. Finally, PI exhibited the 312

lowest ST, with a value of 0.018. The values of ST and S1 for each variable were similar,
suggesting that the majority of the influence of the variables on the model's output was attributed
to their individual effects rather than complex interactions among them.

Variable	ST	S1
LL	0.066	0.064
PI	0.018	0.016
e_0	0.839	0.802
W	0.122	0.080

³¹⁷ Table 6. Sensitivity analysis of variables using Sobol's method comparing the Total (ST) and

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First-Order (S1) Sensitivity Indices for input variables.

320 After establishing the significance of the variables, an analysis was conducted to understand the 321 impact of variations in these inputs on the overall results. Initially, partial dependence plots for single input features were analysed to visualize the relationship between individual input variables 322 323 and the output variable in a regression model. These plots are instrumental in understanding how 324 a single input variable influences the output while holding other variables constant. The results of 325 this analysis are displayed in Figure 6 in terms of partial dependence (average predicted effect). 326 For the variables LL and PI, an increasing trend was observed, with some fluctuations, indicating 327 a positive and near linear relationship with c_c . In the case of variable e_0 , a very strong growth 328 trend was noted until $e_0=2.5$, after which the impact stabilizes. This suggests that within this range 329 of values (up to $e_0=2.5$), small variations in e_0 will cause a significant impact on the value of c_c , 330 clearly indicating that the relationship is not linear. As for w, a similar pattern to e_0 was observed, 331 but with a lesser impact on the value of c_c , with the effect becoming stable around values of 110%. 332



Figure 6. Partial dependence plots for single input features in terms of the average predicted
effect. Note that the figure has a dual x-axis, with the upper one for e₀ and the lower one for the
variables LL, PI and w.

338 Finally, partial dependence plots for pairs of input features were computed. These plots are 339 designed to illustrate the joint influence of input feature pairs on the model's predictions, offering 340 insights into their collective impact on the output variable. They assist in elucidating complex 341 interactions between input features and the model's response. These graphs depicting the pairs of 342 variables LL and PI, as well as w and e_0 , are presented in Figure 7. The graphs showing the 343 remaining variable pairs are included in Figure S1. From this analysis, it was established that most 344 of the impact on the model's output can be attributed to the individual effects of the variables, 345 rather than complex interactions among them. In the LL and PI pair (Figure 7a), as well as in the w and e_0 pair (Figure 7b), some interaction was observed, although not excessively significant. 346 347 These conclusions were consistent with the Sobol analysis.



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Figure 7. Partial dependence plots for pairs of input features. a) LL - PI and b) $w - e_0$.

In conclusion, the analyses conducted highlighted that the most significant variable in the model was e_0 , which also caused the most substantial changes in the predicted value of c_c , both individually and in terms of interactions between pairs of variables.

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355 **4.3. Overfitting analysis**

356 One of the common challenges encountered in ML models is overfitting. This occurs when a 357 model performs exceptionally well in replicating the data used for its development and training. 358 However, when applied to input parameter values outside those used during development and 359 training, the model may generate highly unusual predictions. To analyse the overfitting of a ML 360 model, there are several techniques, highlighting the works of Asteris et al. (2019) or Armaghani 361 and Asteris (2021), where the final model is checked with datasets in which the inputs gradually 362 increase in value as they are tests made for a subsequent analysis. In this study, it is not like this 363 since the inputs do not increase gradually as they were tests conducted on soils where the values 364 of the input variables do not follow a gradual pattern. Thus, alternative techniques were chosen 365 to enable the identification of overfitting in a model. To this end, the difference in model 366 performance between the training set and the test set was initially assessed. In this case, a very 367 small difference was observed between the training and test errors (Table 5), indicating that there 368 was no evidence of overfitting. Alternatively, analysing the residuals can provide insights into potential overfitting in the model. Specifically, the residuals of the train and test sets were 369

370 analysed based on the following criteria: a) size: if the test residuals are significantly larger than 371 the train residuals, it is a sign of overfitting; b) variance: if similar variances exist in train and test, 372 it is indicative that the model generalizes well, not evidencing overfitting; and c) correlation: if 373 the residuals are correlated, it is a sign that the model is learning patterns that are not relevant for 374 predicting the dependent variable, which is a sign of overfitting. In this case, the size of the 375 residuals and their variance were given by the mean and standard deviation, respectively. The 376 correlation of the residuals was carried out through the Durbin-Watson test, which is a method to 377 detect the presence of autocorrelation among the residuals in regression analysis. The value of the 378 Durbin-Watson statistic varies between 0 and 4. A value close to 2 suggests that there is no 379 autocorrelation; values less than 2 indicate positive autocorrelation; and values greater than 2 380 indicate negative autocorrelation. The summary of this analysis is shown in Table 7.

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Set	Mean	Standard deviation	Durbin–Watson statistic
Training	0.0003	0.05730	1.95
Test	-0.0038	0.05301	1.87

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Table 7. Summary of residual metrics in the training and test sets.

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From the analysis of the results, it was evident that the mean of the residuals is very close to zero for both sets, which is good as it suggested that there is no systematic bias in the predictions. The standard deviations were also comparable, indicating that the dispersion of errors was similar in both sets. The Durbin-Watson values were close to 2, implying that the residuals exhibited independence. According to the results obtained in the residual analysis, there is no evidence of overfitting from this perspective.

Although none of the conducted analyses indicated signs of overfitting in the model, an additional analysis was undertaken by perturbing the input values of the test set. In this analysis, a random perturbation of $\pm 1\%$ was applied to the test set data (including all input variables) to simulate natural variability and assess the robustness of the model and its propensity for overfitting. Subsequently, the super-learner ML model was tasked with making predictions on both the original test set and the perturbed test set to evaluate how the model reacted to disturbances in the 396 input data. A model that is excessively sensitive to small perturbations in the data might be 397 overfitting, meaning it has learned to adjust to the particularities and noise of the training set, 398 rather than capturing general trends. The results of this analysis are presented in Figure 8, where 399 the scatter plot revealed an almost perfect correlation (R^2 of 0.999) between the original and 400 perturbed predictions. The histogram showed that the average changes in predictions due to 401 perturbations were minimal, with a mean of 0.0036, suggesting significant stability of the model 402 against minor variations in the data. As a conclusion of this analysis, the model was highly robust 403 and showed low sensitivity to disturbances in the input data. Therefore, the three conducted 404 analyses concluded that the super-learner ML model exhibited strong generalization abilities, 405 capturing underlying trends rather than fitting to specific noises or peculiarities of the training 406 data.

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413 **4.4.** Comparison of the super-learner ML model with geotechnical correlations.

In order to assess the performance of the proposed model, a comparative analysis was conductedusing the database compiled for this study. This analysis involved nine empirical correlations for

estimating c_c with a global scope. The results are depicted in Figure S2 as a scatter plot, 416 417 showcasing the comparison between each correlation's predictions and the actual values from the 418 comprehensive dataset. Additionally, in this figure, the formulas of the tested correlations are 419 included. The super-learner ML model proposed in this work clearly achieved the best performance overall, with the highest R² score, lowest RMSE, and lowest MAE (Figure S2a). In 420 contrast, the Sridharan and Nagaraj (2000) correlation (Figure S2b) performed very poorly, with 421 a negative R² score (-0.79), high RMSE (0.281), and high MAE (0.257), clearly showing it did 422 423 not work well for this dataset. Other correlations such as Azzouz et al. (1976) (Figure S2e), Rendon Rendon-Herrero (1980) (Figure S2g), and Koppula (1981) (Figure S2f) achieved 424 moderate results, with R² scores around 0.7, RMSE values around 0.10, and MAE values around 425 426 0.06. The Wroth and Wood (1978) (Figure S2c), Bowles (1979) (Figure S2h), and Al-Khafaji and 427 Andersland (1992) (Figure S2i) correlations demonstrated low performance, characterized by low 428 R^2 scores around 0.20, RMSE values around 0.19, and high MAE values. Additionally, the Koppula (1981) (Figure S2j) correlation also had poor outcomes, with negative R² scores, high 429 430 RMSE, and high MAE. It is noteworthy that some correlations, such as Sridharan and Nagaraj 431 (2000) (Figure S2b and d), Koppula (1981) (Figure S2f and j), and in less extent, Wroth and Wood 432 (1978) (Figure S2c), consistently predicted values significantly above the actual ones. 433 Conversely, correlations like Al-Khafaji and Andersland (1992) (Figure S2i) and Bowles (1979) 434 (Figure S2h) tended to predict consistently below the actual values. Furthermore, the four 435 expressions obtained through Symbolic Regression in this study (Equations 4 to 7) also exhibited 436 superior performance metrics compared to the analysed correlations. In summary, the model 437 proposed in this paper was unequivocally the most accurate and effective for this dataset.

438

439 **5. Online tool developed**

440 Machine learning models have seen their use increase exponentially in recent years due to their 441 high performance on the predictions and for their ability of discovering robust patterns in complex 442 datasets. However, their application is usually difficult because it is necessary to know the trained 443 algorithm fully, with all its hyperparameters and to know the tools with which it has been 444 developed (e.g., programming language or specific software). This means that currently, many 445 machine learning researches do not have a great practical application. In this study, an online 446 application has been developed to facilitate the non-expert user, the usage of the machine learning 447 model presented here, becoming one of the few studies that offers a practical implementation of 448 the trained machine learning algorithm. Figure 9 shows the graphical user interface of the 449 developed prediction tool, which is located at https://huggingface.co/spaces/EstebanDC/Compression_Index. In this tool, the value of c_c of a 450 451 clay soil can be easily obtained by the user, defining the input values (i.e., LL(%), (PI %), w(%)452 and e_0). Once these values are introduced, the compression index is calculated using the optimized 453 super-learner ML model. This online tool can be used on any device with an internet connection 454 (computers, tablets, or smartphones).

455



456



Figure 9. Application developed with the trained super-learner machine learning model.

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459

461 6. Symbolic regression

In addition to the analysis carried out using the machine learning models presented previously, the dataset was analysed using Symbolic Regression. The aim of this analysis is to propose mathematical expressions, which relate c_c with some of the input variables. These expressions can be applied alternatively to the super-learner machine learning model when data for all the input variables are not available. Symbolic Regression-based approaches provide alternative machine learning methods that are recently gaining popularity. These approaches, as other ML algorithms, learn patterns from observed data and they have a great advantage over other ML algorithms due to their interpretability and explanation capabilities. Symbolic Regression attempts to explain a target variable by multiple input variables using a mathematical expression involving of a predefined set of basic computation functions. In this study, a symbolic regressor based on Feynman's path integral formulation from quantum field theory (Broløs et al. 2021) was applied. With this approach, four expressions (Equations 4 to 7) were obtained, and their performance metrics are presented in Table 8.

476
$$c_c = 1.95 - 2.04 \tanh(1.82(0.204e_0 - 1)^2)$$
 (4)

 $c_c = 1.72e^{-4.02(1-0.209e_0)^4 - 0.599(0.00363LL - 1)^2} + 0.0513$ (5)

 $c_c = 3.32e^{-3.82(1-0.219e_0)^2 - 2.0e^{-9.78(1-0.244e_0)^2 - 0.237(-0.0135PI-1)^2}} - 0.0409$ (6)

482
$$c_c = 2.67e^{-1.99(1-0.209e_0)^2 - 0.406(0.00286w-1)^2} - 0.26$$
 (7)

- 484 With *w*, LL, and PI expressed in %.

Equation	Set	R ²	MAE	RMSE
4	Training	0.85	0.049	0.083
4	Test	0.87	0.042	0.065
5	Training	0.86	0.047	0.072
	Test	0.86	0.049	0.088
6	Training	0.86	0.047	0.078
	Test	0.91	0.043	0.063
7	Training	0.85	0.048	0.082
	Test	0.92	0.047	0.068

489

490 Symbolic Regression approach gets good prediction performance, albeit being less accurate than 491 the trained super-learner machine learning model, although presenting moderately long training 492 times. Alternatively to the Equations 4 to 7, those obtained by linear regression and included in 493 section 2 (Equations 1 to 3) can be used, although they offer worse metrics than those obtained 494 by Symbolic Regression. These expressions must be fed with values of the input variables within 495 the ranges with which the algorithm has been trained, since the behaviour outside these ranges is 496 unknown.

497

498 **7.** Conclusions.

499 This study proposes a novel super-learner ML algorithm that provides a reliable and accurate 500 model for predicting c_c , a key parameter in engineering applications. This algorithm is reasonably 501 capable of predicting the value of c_c based on variables previously related to this parameter (i.e., 502 LL, PI, e₀ and w). To this aim, a database was built including more than 1000 samples collected 503 worldwide, in order to reduce the local character of the proposals presented. The high and 504 satisfactory error metrics, including R², MAE, RMSE, and a20-index, demonstrate the model's 505 robust performance, particularly considering the global nature of the dataset and the dispersion in 506 the input variables. To facilitate the use of the model, a user-friendly prediction tool has been 507 deployed online (https://huggingface.co/spaces/EstebanDC/Compression_Index). Additionally, 508 four symbolic regression expressions have been proposed for cases where all input parameters 509 are not available. A comparative analysis was carried out using the compiled database against 510 global empirical correlations, demonstrating that super-learner ML model was the most accurate and effective for this dataset. The global scope of this study and the development of an online tool 511 512 enhance the proposed algorithm's applicability and value beyond other methods in the field, 513 thereby making it more useful for geotechnical engineers. Future work will focus on expanding 514 the dataset and updating the model to increase its generalization ability and application range. 515 Finally, it is important to exercise caution when applying the model or expressions beyond the 516 specified input variable ranges, as this can lead to predictions of questionable reliability, a 517 common issue with predictive algorithms.

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- 520 Availability statement
- 521 The data that support the findings are available from the corresponding author upon reasonable
- 522 request.

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