

1 **A new CPT virtual calibration chamber in sand based** 2 **on Machine learning algorithms**

3 Mingpeng Liu^a, Enci Sun^b, Ningning Zhang^a, Fengwen Lai^{c,*}, Raul Fuentes^a

4 ^a Institute of Geomechanics and Underground Technology, RWTH Aachen University,
5 Germany.

6 ^b School of Qilu Transportation, Shandong University, Jinan 250061, China.

7 ^c Faculty of Civil Engineering and Geosciences, Delft University of Technology, Delft,
8 2628 CN Delft, The Netherlands.

9 * Corresponding author. Email address: F.Lai-1@tudelft.nl (Fengwen Lai)

10 **Abstract**

11 Interpretation of Cone Penetration Tests (CPTs) still relies greatly on empirical
12 correlations that are mostly developed in resource-demanding and time-consuming
13 calibration chambers. This paper presents a CPT virtual calibration chamber using
14 machine learning approaches. For such purpose, the multilayer perceptron (MLP) and
15 long short-term memory (LSTM) neural networks are implemented to predict the cone
16 resistance (q_c) profiles under various soil states and testing conditions. The Bayesian
17 optimization (BO) is first adopted to find the optimal neural network hyperparameters
18 of MLP and LSTM. Thereafter, the BO-MLP and BO-LSTM networks are trained with
19 the available data from published datasets. Further comparison and validation of the
20 prediction results are carried out against numerical results obtained from a Coupled
21 Eulerian-Lagrangian (CEL) model. The results show that BO reduces the prediction
22 error of the neural networks by 73.1% (MLP) and 59.5% (LSTM) in the training set as
23 well as 44.4% (MLP) and 40% (LSTM) in the testing set compared to that without BO.
24 The established machine learning models are proven competent to reproduce the q_c
25 profiles with the coefficient of determination (R^2) of 98.65% (MLP) and 98.51%
26 (LSTM) in the training set as well as 95.13% (MLP) and 94.65% (LSTM) in the testing

27 set. Apart from matching the numerical model results in terms of accuracy, the proposed
28 methods show a much greater computational efficiency. Eventually, to showcase the
29 use of this new virtual calibration chamber, the predicted q_c are used to obtain a new
30 relationship to predict the relative density, D_r , of the sand. The improved correlation
31 has an R^2 of 92.7% compared to all data, including those generated by the machine
32 learning method and experiments, and 88.3% compared to the pure experimental data.
33 This is a better generalization than other previously suggested relationships.

34

35 **Keywords:** cone penetration test, virtual calibration chamber, Bayesian optimization,
36 multilayer perceptron neural network, long short-term memory network

37 **1. Introduction**

38 The cone penetration test (CPT) is one of the most common and popular in-situ test
39 tools for site characterization [1]. One notable advantage of CPT is to quickly obtain
40 continuous and reproducible soil testing records (cone resistance q_c and sleeve friction
41 f_s) with minimal disturbance compared to laboratory element testing [2]. The cone
42 resistance profile from the CPT is widely used to interpret soil properties. However,
43 many CPT-based interpretations of soil parameters still greatly rely on empirical
44 correlations [3]. The majority of these correlations are presented from the results of
45 calibration chamber tests where the soil state and properties can be well-controlled [4].
46 However, calibration chamber testing is resource-demanding and time-consuming. As
47 a consequence, available CPT data from calibration chamber tests is still scarce, which
48 leads to some of the presented empirical correlations being only valid for specific soil
49 types or specific conditions (e.g., over-consolidation ratio) [5].

50

51 To remediate the above shortage of CPT data in calibration chambers, analytical
52 modeling (e.g., cavity expansion theory [6, 7]) and numerical simulations (e.g.,
53 Coupled Eulerian-Lagrangian (CEL) method [8, 9] and discrete-element method (DEM)

54 [10]) have been proposed to estimate q_c profiles for various types of soils. However,
55 the complicated formulations contribute to a gap between analytical solutions and
56 practical use. The numerical solutions are also notoriously difficult due to expensive
57 computational costs and non-trivial calibration for constitutive models [11, 12],
58 although the DEM has been previously presented as a solution for virtual calibration
59 chambers [10].

60

61 With the advances made in hardware and software over the past decades, machine
62 learning (ML) approaches may be an attractive alternative possessing a strong ability
63 to utilize the raw (existing) data for prediction without any prior assumptions [13].
64 Multiple attempts have been made towards the application of ML-based models in
65 geotechnical practice relevant to the CPT, e.g., prediction of bearing capacity of piles
66 [14], soil type classification [15-17], soil parameter identification [18], and evaluation
67 of soil liquefaction potential [19, 20]. However, for CPT profile prediction that depends
68 largely on the depth (overburden stress) and soil type, a non-linear mapping capable of
69 catering to sequence loading situations may be more suitable. In this regard, two
70 possible ML options are multilayer perceptron (MLP) and long short-term memory
71 (LSTM) neural networks [21]. Zhang et al. [22] and Guan and Yang [23] successfully
72 applied the LSTM model to reproduce the constitutive responses of sands under both
73 monotonic and cyclic loading. Wang and Sun [24] combined LSTM with a multiscale
74 framework to capture the hydro-mechanical coupling effects of porous media.
75 Habibagahi and Bamdad [25] and Kohestani and Hassanlourad [26] employed MLP to
76 describe the mechanical properties of carbonate sand and unsaturated soil. Their results
77 demonstrated that MLP and LSTM both have great potential in predicting nonlinear-
78 mapping datasets. Hence, we hypothesize that MLP and LSTM neural networks are
79 capable of reproducing and predicting CPT resistance profiles in calibration chamber
80 tests.

81

82 The selection of hyperparameters is a critical task for the construction of ML-based
83 models (particularly for neural networks). There are currently no well-established
84 methods to tune the optimal hyperparameters, which means that typically these are
85 obtained by a trial-and-error [23]. To address this drawback, some researchers [27, 28]
86 have used Bayesian optimization (BO) that has been applied to geotechnical problems
87 to give optimal hyperparameters for various networks. For example, Tao et al. [28]
88 integrated Bidirection LSTM neural networks with BO to predict excavation-induced
89 responses. Zhang et al. [29] used the BO-optimized neural network to present a
90 modeling strategy for developing prediction models of soil properties. Hence, this paper
91 combines the MLP and LSTM neural networks with Bayesian optimization (i.e., BO-
92 MLP and BO-LSTM) to quickly reproduce and predict the CPT profile in calibration
93 chamber tests, and to discuss their applications in soil interpretation based on the
94 predicted CPT data.

95

96 The paper aims at developing accurate, and computationally efficient, virtual
97 calibration chambers to generate q_c profiles of the CPT in sand. First, we briefly
98 introduce MLP, LSTM, and BO algorithms to illustrate the fundamentals of Bayesian-
99 optimized neural networks. Subsequently, the BO-MLP and BO-LSTM models are
100 developed and trained by feeding observed data, and their performance is then
101 evaluated by the testing dataset. The developed models are further compared with the
102 validated solutions from the Coupled Eulerian Lagrangian (CEL) method. Eventually,
103 an example is given to show how the developed models are used to correlate cone
104 resistance with soil properties and to enhance the empirical equations.

105 **2. Fundamentals of machine learning approaches**

106 **2.1 Multilayer perceptron (MLP)**

107 The multilayer perceptron is one of the most popular artificial neural networks for

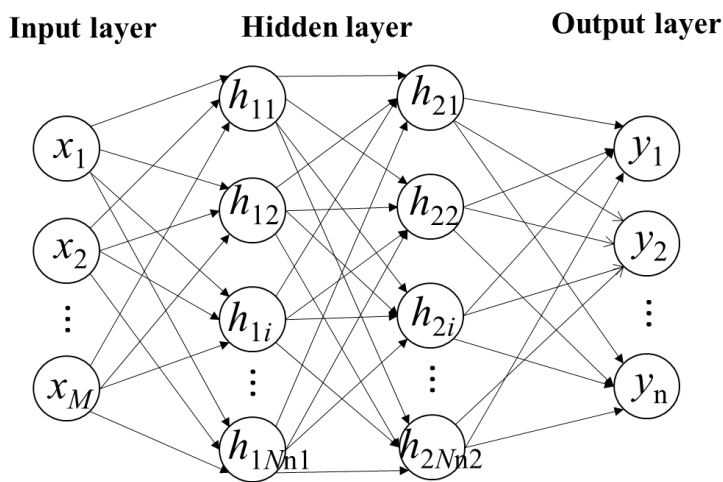
108 modelling and predicting complex non-linear responses and processes [26]. Fig. 1
 109 shows a typical MLP structure consisting of one input layer, one or more hidden layers,
 110 and one output layer. A set of neurons are arranged in each layer and connected through
 111 weights and bias. The numbers of hidden layers and neurons in each layer are not
 112 constant and need to be optimized. The input data are firstly presented through the input
 113 layer and then pass through the hidden layer(s) being processed by the neural network
 114 to eventually predict values for the output layer. This process can be expressed
 115 mathematically by considering a feedforward propagation process that uses input \mathbf{x} to
 116 estimate the output \mathbf{y} :

$$117 \quad \mathbf{h}_1 = f(\mathbf{W}_1 \mathbf{x} + \mathbf{b}_1) \quad (1-1)$$

$$118 \quad \mathbf{h}_2 = f(\mathbf{W}_2 \mathbf{h}_1 + \mathbf{b}_2) \quad (1-2)$$

$$119 \quad \mathbf{y} = \mathbf{W}_3 \mathbf{h}_2 + \mathbf{b}_3 \quad (1-3)$$

120 The formulas (1-1) and (1-2) represent two hidden layers, where \mathbf{h}_1 and \mathbf{h}_2 are the results
 121 of the first and second hidden layer, respectively; \mathbf{W}_1 , \mathbf{W}_2 , \mathbf{W}_3 represent the weight
 122 matrices, and \mathbf{b}_1 , \mathbf{b}_2 , \mathbf{b}_3 are the bias vectors; f represents the activation function. The \mathbf{h}_1
 123 and \mathbf{h}_2 include the result of each neuron and $\mathbf{h}_1 = [h_{11}, h_{12}, \dots, h_{1i}, \dots, h_{1N_{n1}}]$ and $\mathbf{h}_2 =$
 124 $[h_{21}, h_{22}, \dots, h_{2i}, \dots, h_{2N_{n2}}]$, where N_{n1} and N_{n2} are the number of neurons of the first and
 125 second hidden layer.



126

127 Fig. 1. Structure of a general MLP. x_1, x_2, \dots, x_M represent the elements in input vector \mathbf{x} ; $y_1,$

128 y_2, \dots, y_n represent the elements in output vector \mathbf{y} .

129

130 Typically used activation functions are sigmoid, hyperbolic tangent (tanh), rectified
131 linear unit (Relu), and leaky Relu activation functions [30]. The weight matrices W as
132 well as the bias vectors b are randomly initialized first and then updated through a
133 training process. The training implementation of MLP can be considered into two
134 phases: forward calculation and backward propagations using the Back-propagation
135 algorithm. During the forward process, the value of each hidden neuron is calculated
136 by summing up the values of input neurons multiplied by corresponding connection
137 weights. The error between the output and the real values can be calculated and then
138 minimized by the backward algorithm that updates the connection weights. A full
139 explanation of MLP neural networks can be found in the literature [31].

140 **2.2 Long short-term memory neural network (LSTM)**

141 LSTM is a typical class of recurrent neural networks (RNNs), which have been widely
142 used to model time-dependent phenomena. The outputs of RNN depend on inputs of
143 the network from not only the current time step but also previous time steps, thereby
144 presenting the ability to predict future information related to previous inputs and
145 enabling its application in modeling sequential problems. By introducing a memory cell
146 in place of the neurons, LSTM can overcome the shortcoming of gradient vanishing or
147 exploding in the back-propagation algorithm in traditional RNNs.

148

149 The typical structure of an LSTM memory cell is displayed in Fig. 2. The memory cell
150 has three gates (forget gate f^t , input gate i^t , and output o^t) which are employed to control
151 the information flow. First, the output at the previous time step h^{t-1} in a memory cell
152 and the input at current time step x^t are used to calculate the forget gate f^t , input gate i^t ,
153 output o^t , and the storage cell \tilde{c}^t , as shown in Eqs. (2-1) to (2-4). Then, the forget gate
154 f^t acts on the memory cell state at the previous time step c^{t-1} , while the input gate i^t acts
155 on the storage cell at the current time step \tilde{c}^t , as shown in Eq. (2-5). The f^t and i^t

156 together determine whether the information should be discarded or stored and update
 157 the current memory cell state \mathbf{c}^t . Eventually, the output \mathbf{o}^t decides the final output values
 158 \mathbf{h}^t , as shown in Eq. (2-6). The specific formulas are shown as follows:

159
$$\mathbf{i}^t = \sigma(\mathbf{W}_i \mathbf{x}^t + \mathbf{U}_i \mathbf{h}^{t-1} + \mathbf{b}_i) \quad (2-1)$$

160
$$\mathbf{f}^t = \sigma(\mathbf{W}_f \mathbf{x}^t + \mathbf{U}_f \mathbf{h}^{t-1} + \mathbf{b}_f) \quad (2-2)$$

161
$$\mathbf{o}^t = \sigma(\mathbf{W}_o \mathbf{x}^t + \mathbf{U}_o \mathbf{h}^{t-1} + \mathbf{b}_o) \quad (2-3)$$

162
$$\tilde{\mathbf{c}}^t = \tanh(\mathbf{W}_c \mathbf{x}^t + \mathbf{U}_c \mathbf{h}^{t-1} + \mathbf{b}_c) \quad (2-4)$$

163
$$\mathbf{c}^t = \mathbf{f}^t \otimes \mathbf{c}^{t-1} + \mathbf{i}^t \otimes \tilde{\mathbf{c}}^t \quad (2-5)$$

164
$$\mathbf{h}^t = \mathbf{o}^t \otimes \tanh(\mathbf{c}^t) \quad (2-6)$$

165 where \mathbf{W}_i , \mathbf{W}_f , \mathbf{W}_o , and \mathbf{W}_c represent the weight matrices corresponding to the inputs
 166 within different gates; \mathbf{U}_i , \mathbf{U}_f , \mathbf{U}_o , and \mathbf{U}_c represent the weight matrices corresponding
 167 to the output at the previous time step with different gates; \mathbf{b}_i , \mathbf{b}_f , \mathbf{b}_o , and \mathbf{b}_c denote bias
 168 matrices of each gate, σ is the sigmoid activation function, and \otimes signifies the element-
 169 wise product of vectors.

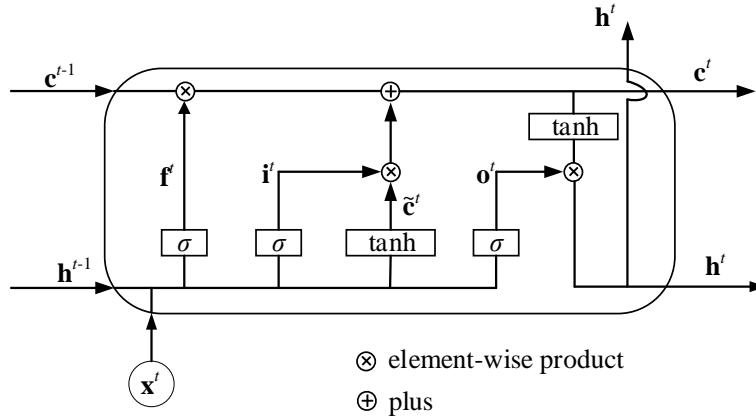


Fig. 2. Structural diagram of a LSTM memory cell

172 2.3 Bayesian Optimization

173 Although applying LSTM or MLP to predict CPT cone resistance profiles is promising,
 174 the selection of hyperparameters for a neural network often needs to be optimized by
 175 hand. To solve this problem, this paper adopts a global optimization algorithm,
 176 Bayesian optimization (BO), to select a superior combination of model

177 hyperparameters locating the minima of the model error. BO adopts the probabilistic
 178 surrogate model to fit real objective functions, where the next most likely point is
 179 selected for evaluation according to fitting results. The historical information is used to
 180 reasonably reduce the evaluation time and to improve search efficiency. The framework
 181 mainly includes two core parts: the probabilistic surrogate model and the acquisition
 182 function, which will be introduced in more detail in the following.

183 **2.3.1 Probabilistic surrogate model**

184 The surrogate model is developed using a widely-used Gaussian process [28] with the
 185 assumption that the responses obey a multidimensional normal distribution.
 186 Correspondingly, a prior distribution with the mean value being equal to 0 can be
 187 constructed by a Gaussian regression:

$$188 \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \sim N \left(0, \begin{bmatrix} k(x_1, x_1) & \dots & k(x_1, x_n) \\ \vdots & \ddots & \vdots \\ k(x_n, x_1) & \dots & k(x_n, x_n) \end{bmatrix} \right) \quad (3)$$

189 where k denotes the covariance function; x_1, \dots, x_n represents input values (i.e.,
 190 hyperparameters in MLP and LSTM); and y_1, \dots, y_n are the response output values.
 191 Through the training set, the updated value y_* can be obtained through a posterior
 192 formula:

$$193 P(y_* | y) \sim N(K_* K^{-1} y, K_{**} - K^{-1} K_*^T) \quad (4)$$

194 where K is the covariance matrix of the assumed prior distribution; K_* is the
 195 covariance matrix of the observed set and K_{**} is the covariance matrix of new-added
 196 samples. The Gaussian regression model can be continually updated through y_* :

$$197 \begin{bmatrix} y \\ y_* \end{bmatrix} \sim N \left(0, \begin{bmatrix} K & K_*^T \\ K_* & K_{**} \end{bmatrix} \right) \quad (5)$$

198 This process considers the relationship of y_N and y_{N+1} and builds the input-output
 199 function, providing the basics of parameter searching.

200 **2.3.2 Acquisition function**

201 Acquisition functions are employed to select the next probable point that enables the
202 model's best performance. The acquisition function can obtain the posterior distribution
203 through the observed dataset $D_{1:n}$, thereby guiding the next evaluation point x_{n+1} .
204 Expected Improvement (EI), which is the most widely-used acquisition function, is
205 employed in this study:

$$206 \quad \alpha_n(x, D_{1:n}) = (v^* - \mu(x))\phi\left(\frac{v^* - \mu(x)}{\sigma_n(x)}\right) + \sigma_n(x)\phi\left(\frac{v^* - \mu(x)}{\sigma_n(x)}\right) \quad (6)$$

207 where α_n is the expectation; v^* is the current optimum function value; ϕ is the
208 standard normal distribution probability density function; σ and μ are variance and
209 mean values, respectively.

210 **2.4 Bayesian Optimized MLP/LSTM**

211 Using BO to the selection of the hyperparameters of MLP and LSTM can be considered
212 into the following formula:

$$213 \quad x^* = \arg \min f(x), x \in X \quad (7)$$

214 where $f(x)$ is the objective function; x represents a group of hyperparameters; X denotes
215 the space of hyperparameters combination; and x^* signifies the x that makes $f(x)$ obtain
216 an optimized solution. We use the mean squared error (MSE) of the response from a
217 neural network as the objective function $f(x)$:

$$218 \quad \text{MSE} = \frac{1}{n} \sum_{i=1}^n (\tilde{y}_i - y_i)^2 \quad (8)$$

219 where n represents the number of output elements, and \tilde{y}_i and y_i denotes the predicted
220 and true values of a neural network, respectively.

221

222 In summary, the paper uses this Gaussian process to proxy the hyperparameter
223 combination x to neural networks. The posterior distribution is obtained according to
224 the observed dataset. Furthermore, the next evaluation point is selected by the EI
225 acquisition function, then iteratively modifying the prior information. Thereby the

226 surrogate model can be improved step by step and eventually attains the optimal
227 hyperparameter combination.

228 **3. Implementation of BO-MLP and BO-LSTM**

229 **3.1 Data source and processing**

230 The selected cone resistance profiles from previously reported calibration chamber tests
231 are summarized in Table 1, in which cases 1-45 are experimental results and cases 46-
232 64 are derived from numerical simulations. It is known that the CPT results are
233 influenced by various factors. In this paper, five well-recognized important factors
234 greatly affecting q_c profiles are considered: the relative density D_r , effective vertical
235 stress σ_v , lateral earth pressure coefficient K_0 , saturation condition (dry or saturated),
236 and boundary condition (BC) [32, 33]. The five commonly used boundary conditions
237 (BC1 - BC5) were further summarized in Table 2. Of note, these boundary conditions
238 are represented with numbers 1 – 5 in the dataset, respectively. It is assumed that the
239 above five influencing factors of CPT in calibration chambers are considered constant
240 throughout the penetration process [33].

241

242 One essential requirement for applying neural networks is the one-to-one mapping
243 relationship between input data and output data. For the two neural networks MLP and
244 LSTM, the input data consisted of the above variables, as well as the depth z^t at the
245 current step t , while the output was the current-step cone resistance q_c^t . In this way, the
246 $q_c - z$ profiles were processed into the corresponding relationship. For each q_c curve, the
247 initial whole profile was processed into 100 points using interpolation. As can be seen
248 in Table 1, a total of 64 groups of data were used for training and testing the network.
249 52 groups (5200 points) were employed to train the machine learning network, while
250 the rest 12 groups (1200 points) with the “*” symbol in Table 1 were selected as the
251 testing dataset to evaluate whether the model overfits or underfits. Note that the testing

252 set has considered different relative densities, vertical stresses, and K_0 conditions, as
 253 well as saturation and boundary conditions.

254 Table 1. Summary of used cases of calibration chamber test

Case No.	D_r	σ_v (MPa)	K_0	Saturation condition	Boundary condition (BC)	Reference
1	0.878	0.100	0.450	Dry	5	Kluger et al. [34]
2	0.748	0.200	0.450	Dry	5	
3	0.838	0.100	0.450	Saturated	5	
4*	0.78	0.200	0.450	Saturated	5	
5	0.952	0.100	0.450	Dry	5	
6	0.97	0.100	0.450	Saturated	5	
7	0.668	0.200	0.450	Saturated	5	
8*	0.606	0.200	0.450	Dry	5	
9	0.918	0.200	0.450	Saturated	5	
10	0.918	0.200	0.450	Dry	5	
11	0.650	0.056	0.393	Dry	5	Huang and Hsu. [33]
12	0.840	0.056	0.393	Dry	5	
13	0.250	0.160	0.463	Dry	5	
14	0.500	0.160	0.463	Dry	5	
15*	0.650	0.160	0.463	Dry	5	
16	0.840	0.160	0.463	Dry	5	
17	0.500	0.056	0.786	Dry	1	
18	0.500	0.056	0.786	Dry	5	
19*	0.650	0.056	0.786	Dry	1	
20	0.650	0.056	0.786	Dry	5	
21	0.840	0.056	0.786	Dry	1	
22	0.840	0.056	0.786	Dry	5	
23	0.500	0.070	0.400	Dry	1	Lech Bałachowski [35]
24*	0.500	0.100	0.400	Dry	1	
25	0.500	0.150	0.400	Dry	1	
26	0.500	0.200	0.400	Dry	1	
27	0.500	0.350	0.400	Dry	1	
28	0.500	0.400	0.400	Dry	1	
29	0.800	0.050	0.400	Dry	1	
30	0.800	0.070	0.400	Dry	1	
31	0.800	0.100	0.400	Dry	1	
32	0.800	0.150	0.400	Dry	1	
33	0.800	0.250	0.400	Dry	1	
34*	0.800	0.300	0.400	Dry	1	
35	0.800	0.400	0.400	Dry	1	

36	0.800	0.050	0.400	Dry	3	
37	0.800	0.070	0.400	Dry	3	
38*	0.800	0.150	0.400	Dry	3	
39	0.800	0.200	0.400	Dry	3	
40*	0.800	0.250	0.400	Dry	3	
41	0.330	0.025	1.000	Saturated	1	
42	0.330	0.050	1.000	Saturated	1	
43*	0.330	0.100	1.000	Saturated	1	Pournaghiazar et al. [5]
44	0.610	0.030	1.000	Saturated	1	
45	0.610	0.050	1.000	Saturated	1	
46	0.718	0.150	0.500	Dry	3	
47*	0.615	0.150	0.500	Dry	3	Chen et al. [4]
48	0.395	0.150	0.500	Dry	3	
49	0.231	0.150	0.500	Dry	3	
50	0.23	0.100	1.000	Dry	3	
51*	0.63	0.100	1.000	Dry	3	
52	0.86	0.100	1.000	Dry	3	Schnaid. [36]
53	0.65	0.075	0.500	Dry	3	
54	0.65	0.150	0.500	Dry	3	
55	0.65	0.300	0.500	Dry	3	
56	0.752	0.060	1.000	Dry	1	
57	0.752	0.100	1.000	Dry	1	
58	0.768	0.200	1.000	Dry	1	
59*	0.776	0.300	1.000	Dry	1	Arroyo et al. [37]
60	0.784	0.400	1.000	Dry	1	
61	0.907	0.100	1.000	Dry	1	
62	0.914	0.140	1.000	Dry	1	
63	0.922	0.200	1.000	Dry	1	
64	0.929	0.300	1.000	Dry	1	

255 Note: ‘*’ represents the testing dataset.

256

Table 2. Five boundary conditions in the calibration chamber

Boundary conditions	Top and bottom boundary		Lateral boundary	
	Stress	Strain	Stress	Strain
BC1	Constant	-	Constant	-
BC2	-	0	-	0
BC3	Constant	-	-	0
BC4	-	0	Constant	-
BC5	Constant	-	Servo-controlled	

257

258 It is known that the quality of input data could significantly affect the predictive
 259 performance of machine learning models. Normalization is preferably adopted to
 260 rescale variables with different scales to lower their influence on the model performance
 261 and also reduce computational costs. The following equation was used to normalize the
 262 input data to the common range of 0 ~ 1:

$$263 \quad x_{\text{norm}} = \frac{x - x_{\text{min}}}{x_{\text{max}} - x_{\text{min}}} \quad (9)$$

264 where x is the raw input variables before normalization, x_{norm} is the input variables after
 265 normalization, x_{min} and x_{max} are the minimum and maximum values of the input
 266 variables, respectively. Besides, in many cases, especially DEM simulations [37], the
 267 q_c profile usually exhibited large oscillations, which can decrease the quality of training
 268 data. Therefore, a sliding window approach was used to smooth data before input into
 269 neural networks and therefore reduce the fluctuation in q_c curves to all groups [38]. The
 270 value of smoothed x_s can be calculated by:

$$271 \quad x_s = \frac{1}{t} \sum_{i=n-t+1}^n x_i \quad (10)$$

272 where t = window size. The average value of datasets within a window is assigned as
 273 the new value of the studied parameter. The datasets within a window consist of current
 274 and former $(t-1)$ values. It should be noted that the first $(t-1)$ and the last $(t-1)$ points
 275 cannot form a complete window, thereby values of such points maintain constant.
 276 Larger window size can generate a smoother sequential curve, but it is much more likely
 277 to deviate from the original curve. The window size is thus set as four in this study for
 278 maintaining the reliability and smoothness of the datasets.

279 **3.2 Neural network structures**

280 **3.2.1 MLP**

281 The MLP structure in this paper contains 4 layers: one input layer, two hidden layer
 282 layers, and one output layer, as shown in Fig. 1. The main hyperparameters of the MLP
 283 are listed in Table 3. For training the MLP, three important hyperparameters are to be

284 optimized using BO: the number of nodes in the first and second hidden layer (N_{n1} and
 285 N_{n2}) as well as the initial learning rate (η_{MLP}). Furthermore, we set the range of N_{n1} and
 286 N_{n2} as 1-20 to decrease the complexity of the network structure, thereby preventing
 287 overfitting in the training set. The Levenberg-Marquardt algorithm is employed to
 288 optimize the weight and bias matrices [39], and the Tanh activation function is also
 289 adopted for hidden layers. The maximum number of training epochs was chosen as 200,
 290 but we also used the early-stop method to prevent overfitting, by which the training
 291 process will stop if the normalized MSE (MSE after data normalization) reaches the
 292 target precision of 5E-4. The two neural networks are implemented in Matlab R2022b
 293 toolboxes.

294 Table 3. Main hyperparameters of MLP network.

Hyperparameter	Description	Value
N_h	Number of hidden layers	2
N_{n1}	Number of nodes in the first hidden layer	[1, 20] [#]
N_{n2}	Number of nodes in the second hidden layer	[1, 20] [#]
Optimizer	Algorithm for optimizing weights and biases	Levenberg–Marquardt
MaxEpochs	Maximum number of rounds used for training	200
η_{MLP}	Initial learning rate	[1E-5, 1E-2] [#]

295 Note: “#” represents the hyperparameters to be optimized by Bayesian Optimization.

296
 297 The discrepancy between prediction values and target values was measured by using
 298 the mean squared error (MSE, see Eq. 8) as the loss function. Besides, the fitting effect
 299 is also quantified by the coefficient of determination:

$$R^2 = 1 - \frac{\sum_{i=1}^n (y_i - \tilde{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2} \quad (11)$$

301 where \bar{y} is the mean true value and other parameters are the same as in Eq. (8).

302 3.2.2 LSTM

303 The LSTM structure contains four layers: a sequence input layer, one LSTM layer,
 304 followed by a fully connected layer, and eventually the regression layer. The main
 305 hyperparameters of the LSTM are listed in Table 4. Herein, three hyperparameters: the

306 number of nodes in the hidden layer, the initial learning rate, and the L2 regularization
307 parameter are determined with the aid of BO. The optimization ranges are also given in
308 Table 4. During the optimization process, Relu was chosen as the activation function
309 for the LSTM layer, and the adaptive moment estimation (Adam) optimizer is utilized
310 due to its superiority [40]. The batch size used for each training iteration is set to 100
311 because every q_c profile has 100 points [38]. The number of epochs needs to be
312 sufficiently large to ensure the loss value that can converge at a constant value. However,
313 due to the use of BO in this paper, the epoch should not be too large to prevent
314 overfitting and therefore was set to 300 [22, 23, 38].

315 Table 4. Main hyperparameters of LSTM model.

Hyperparameter	Description	Value
N_h	Number of hidden layers	1
N_n	Number of nodes in the hidden layer	[1, 20] [#]
Optimizer	Algorithm for optimizing weights and biases	Adam
η_{LSTM}	Initial learning rate	[1E-4, 1E-2] [#]
L2	L2 regularization parameter	[1E-5, 1E-2] [#]
MaxEpochs	Maximum number of rounds used for training	300
N_b	The batch size used for each training iteration	100

316 Note: “#” represents the hyperparameters to be optimized by Bayesian optimization.

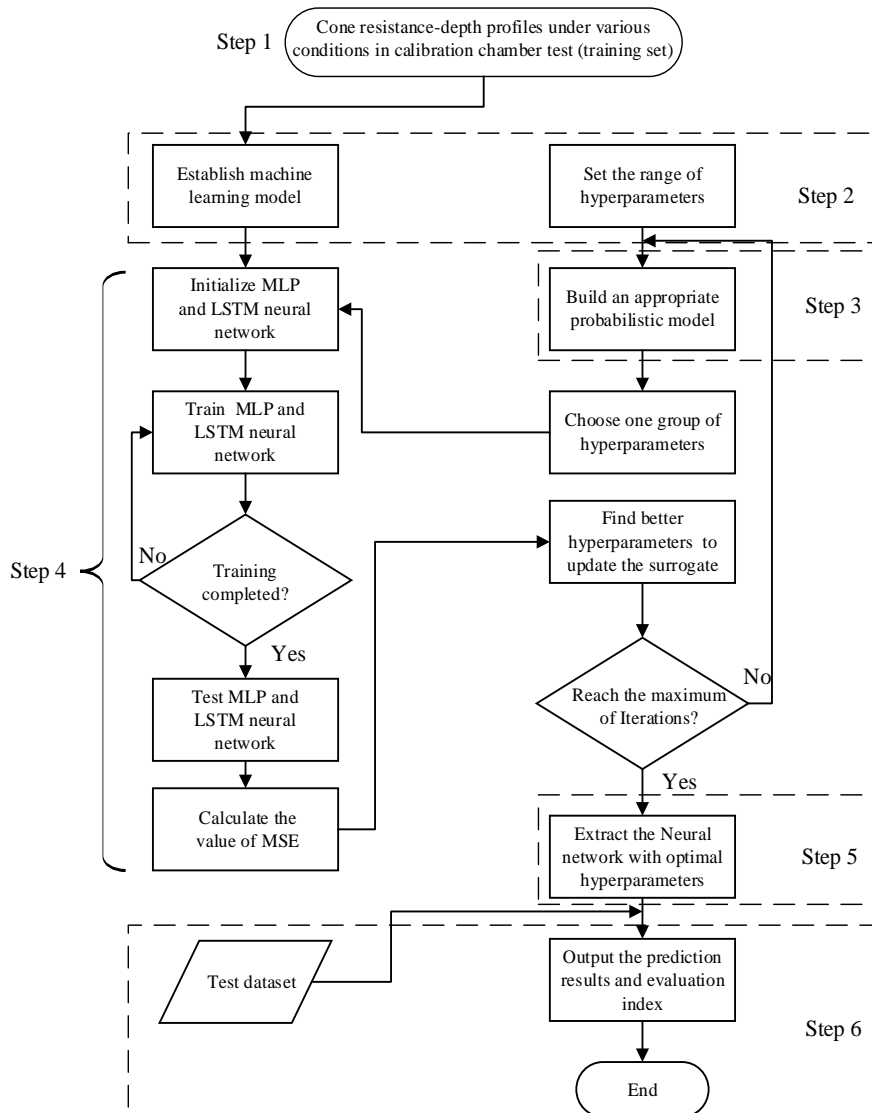
317 3.3 BO-MLP/BO-LSTM modelling

318 Fig. 3 presents a flowchart showing the BO-MLP and BO-LSTM modelling process. It
319 can be described by six main steps:

- 320 • Step 1: Obtain the raw datasets under different soil and penetration conditions, as
321 presented in Section 3.1. Then, normalize the dataset, and separate it between
322 training and testing datasets.
- 323 • Step 2: Establish the MLP and LSTM neural networks. Then determine the
324 hyperparameters of network models and set the range of hyperparameters to be
325 optimized. The details for this step can be found in Section 3.2.
- 326 • Step 3: Build the Bayesian optimization model. Neural network models are
327 regarded as the objective function in optimization, while the MSE given in Eq. (8)

328 is determined as the evaluation function.

- 329 • Step 4: Training the neural network under the current combination of
- 330 hyperparameters with the training set. The value of the evaluation function under
- 331 the current combination of hyperparameters is calculated and then returned to BO.
- 332 According to the probabilistic surrogate model and acquisition function, the next
- 333 group of hyperparameters is selected for a new round of training until reaching the
- 334 maximum number of iterations.
- 335 • Step 5: Output the combination of hyperparameters with the best model
- 336 performance after BO. Then use these hyperparameters to train the neural network.
- 337 • Step 6: Input the testing dataset into the trained network to evaluate the working
- 338 performance of the established neural network.

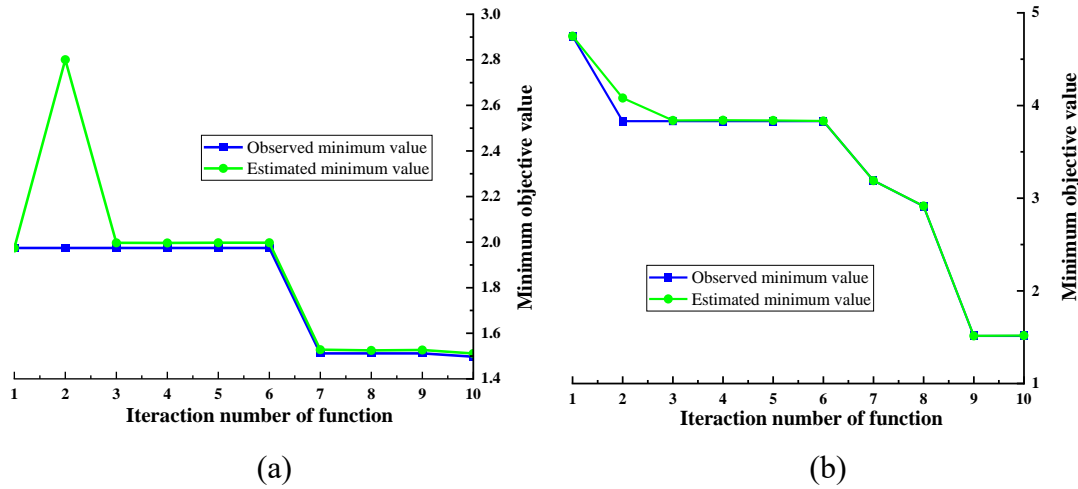


339

341 4. Performance of the machine learning models

342 4.1 Effectiveness of Bayesian optimization

343 When using BO to optimize the neural networks, the iteration number of the objective
 344 function is set to 10 for preventing overfitting [41]. The process is displayed in Fig. 4.
 345 With the process of Bayesian optimization, the minimum objective value (i.e., the MSE
 346 of the neural network) decreases to a small value, signifying a good performance
 347 achieved by using BO. The combination of hyperparameters, after optimization, for the
 348 MLP neural network was determined to be $N_{n1}=8$, $N_{n2}=4$, $\eta_{MLP}=1.31E-3$, while for
 349 the LSTM neural network they are $N_n=16$, $\eta_{LSTM}=5.2E-3$, $L2=1.2E-3$. These
 350 hyperparameters were then used to train the neural networks.

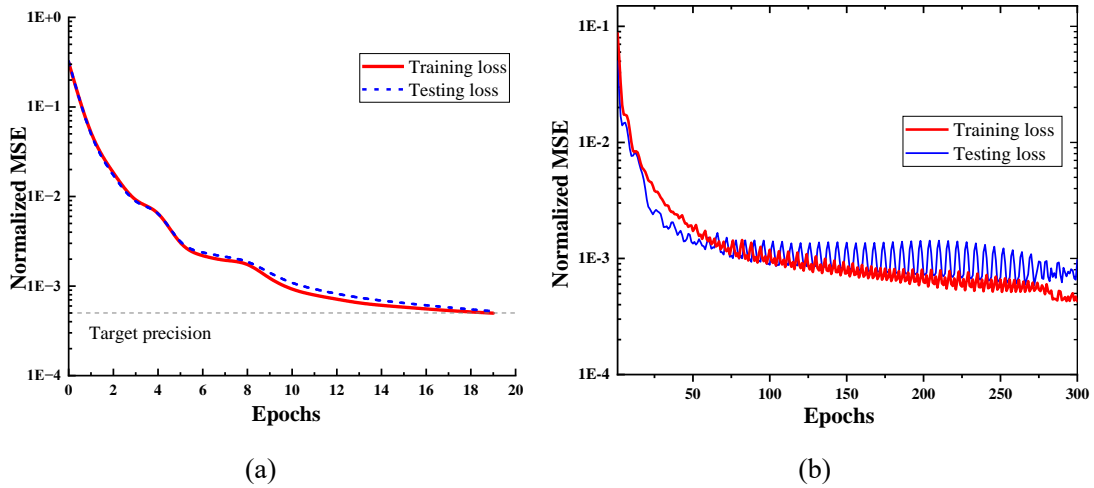


351 Fig. 4. Process of Bayesian optimization for (a) MLP model and (b) LSTM model

352

353 The normalized loss function MSE of the two models with the optimized
 354 hyperparameters are shown in Figs. 5(a) and 5(b), respectively. For both models, the
 355 normalized MSE rapidly reduces to a relatively small value. For MLP, the normalized
 356 MSE reaches the target precision at epoch 19, which mainly benefits from the adopted
 357 Levenberg-Marquardt algorithm that can rapidly converge to optimal solutions [39];
 358 the normalized MSE of the LSTM reaches a relatively constant value at the end of

359 training. The evaluation indexes of BO-MLP and BO-LSTM are listed in Table 5.
 360 Besides, the MSE and R^2 of MLP and LSTM without optimization are also shown in
 361 Table 5, in which the errors of neural networks achieve an obvious reduction while the
 362 fitting degree R^2 has an increase after the Bayesian optimization. The MSE reduces by
 363 73.1% (MLP) and 59.5% (LSTM) in the training set as well as 44.4% (MLP) and 40%
 364 (LSTM) in the testing set; the R^2 increases by 0.83% (MLP) and 0.88% (LSTM) in the
 365 training set, and 1.05% (MLP) and 0.76% (LSTM) in the testing set. The loss functions
 366 and evaluation indexes show that the Bayesian optimization performs well in selecting
 367 hyperparameters for the neural networks.



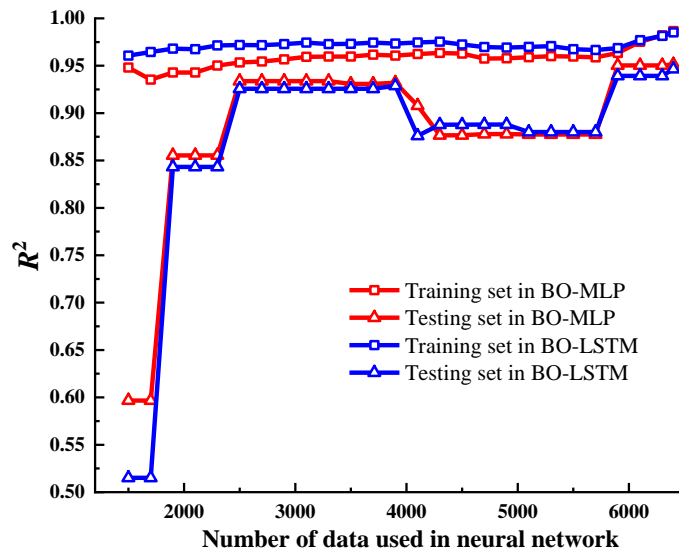
368 Fig. 5. Evolution of normalized MSE against epochs during model training for (a) MLP model and
 369 (b) LSTM model.

370 Table 5. Evaluation index for different models

Model	MSE (MPa)		R^2	
	Training	Testing	Training	Testing
BO-MLP	2.0006	4.8272	0.9865	0.9513
BO-LSTM	2.2200	5.0109	0.9851	0.9465
MLP	3.4720	6.9720	0.9782	0.9408
LSTM	3.5412	7.0001	0.9763	0.9389

371
 372 To further evaluate whether the optimized hyperparameters in neural networks are
 373 suitable to the used cases, Fig. 6 shows the variation of R^2 with the number of data used
 374 in neural networks. It can be observed that R^2 in the training set is maintained at a high

375 level exceeding 95% for two neural networks. However, the R^2 of the testing set
 376 increases with the number of used data from a low level (59.6% and 51.5%) to a
 377 relatively high level of more than 90%. But the used cases 41 to 55 (corresponding to
 378 4100-5500 on x-axis in Fig. 6) decrease the R^2 of the training set, which may attribute
 379 to that the results of cases 41 to 55 are not so identical to other research, thereby
 380 reducing the overall quality of the dataset. For the eventually used 64 cases, the R^2 of
 381 both training and testing sets reach the highest level, indicating that the adopted cases
 382 in this study are adaptive to the constructed neural networks.



383

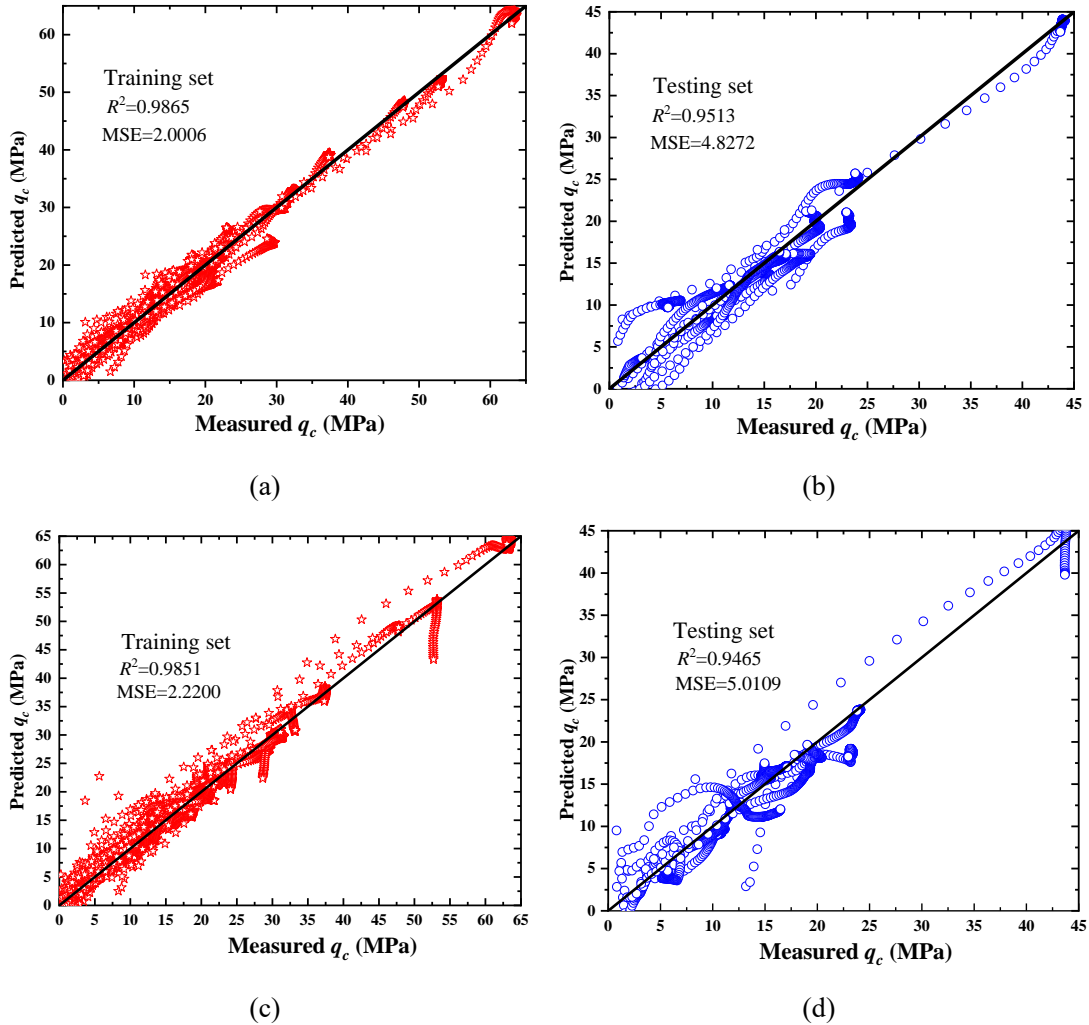
384

Fig. 6. R^2 of training and testing sets with the number of data used in neural networks

385 4.2 Evaluation of the developed models

386 To evaluate the performance of the established machine learning models, the predicted
 387 q_c values obtained from the two neural networks versus the measured data of all the 64
 388 groups are presented in Fig. 7 for the BO-MLP and BO-LSTM models. As expected in
 389 the training set, the predicted q_c values from the neural networks are close to the
 390 measured values. The R^2 of the training set is 98.65% and 98.51%, respectively for
 391 MLP and LSTM models. Besides, the regression errors MSE in the training set are
 392 2.0006 and 2.2200 for the two networks, respectively. The R^2 values for the evaluation
 393 against the unseen testing set are 95.13% and 94.65%, respectively for MLP and LSTM,
 394 while the MSE values are 4.8272 and 5.0109, respectively. In summary, the regression

395 plots in Fig. 7 show that the MLP and LSTM neural networks both perform well in
 396 predicting cone resistances among the selected raw datasets. But in some cases, the
 397 predictions still have some discrepancies with the measured values. A reasonable
 398 explanation might be that the fitting degree of neural networks cannot reach 100% and
 399 thereby hard for the ML model to fit all discrepancies [38]. This means there are some
 400 prediction points deviated from the original results.



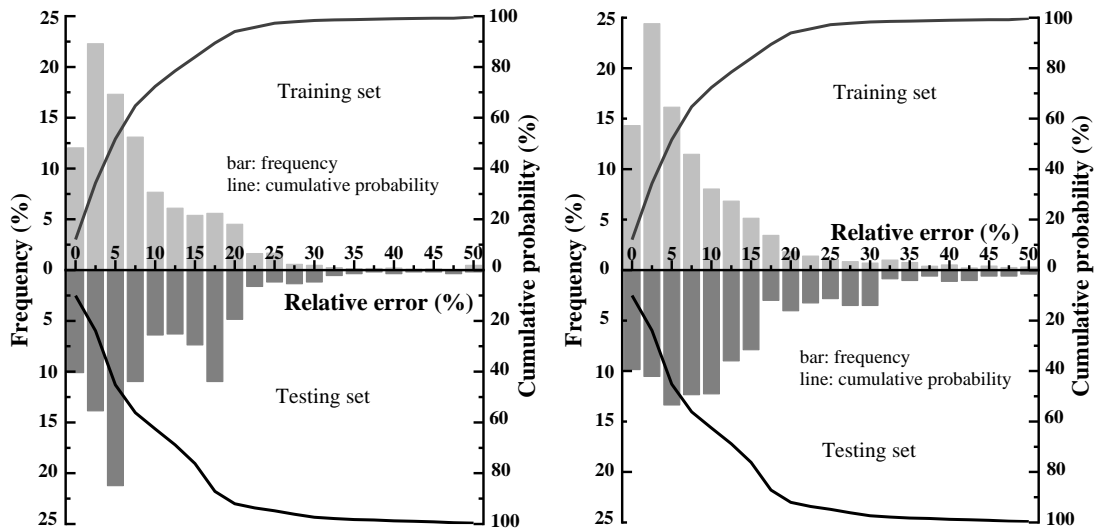
401 Fig. 7. Measured cone resistances against predicted values from the two neural networks in (a)
 402 training set in BO-MLP network, (b) testing set in BO-MLP network, (c) training set in BO-LSTM
 403 network, and (d) testing set in BO-LSTM network

404
 405 To evaluate the performance of developed models more comprehensively, the relative
 406 error (RE) is employed to reflect the deviation percentage between measured values

407 and predictions:

$$408 \quad \text{RE} = \left| \frac{\hat{y}_i - y_i}{y_i} \right| \quad (12)$$

409 where the parameters are the same as in Eq. (8). Fig. 8 depicts the frequency and
 410 cumulative probability of relative error distribution for all data in BO-MLP and BO-
 411 LSTM models. In the training set of two neural networks, about 13.5% of total points
 412 show a high convergence around the standard line of 0% error. This value is about 10%
 413 for the testing set. The relative errors under 7.5% account for the majority of datasets
 414 with a cumulative probability larger than 60% for both training and testing sets. Besides,
 415 most (about 95%) of the total points show a relative error lower than 20%, proving that
 416 the prediction by the ML-based models can be highly accepted for calibration chamber
 417 tests. However, there are still a small number of points with errors greater than 30%.
 418 These are believed to be within the discrepancies between different scholars even under
 419 similar experimental situations. For example, cases 38 and 46 in Table 1 have similar
 420 experimental conditions, but the stable q_c of case 38 is 11.4 MPa while in case 46 the
 421 value is 21.5 MPa. This discrepancy would decrease the precision of machine learning
 422 to the overall dataset, thereby causing a large error. Only if other variables that
 423 explained this discrepancy were included (i.e., instrument accuracy in the
 424 measurements) the machine learning algorithm could be improved. This is however
 425 impractical within the scope of this paper.



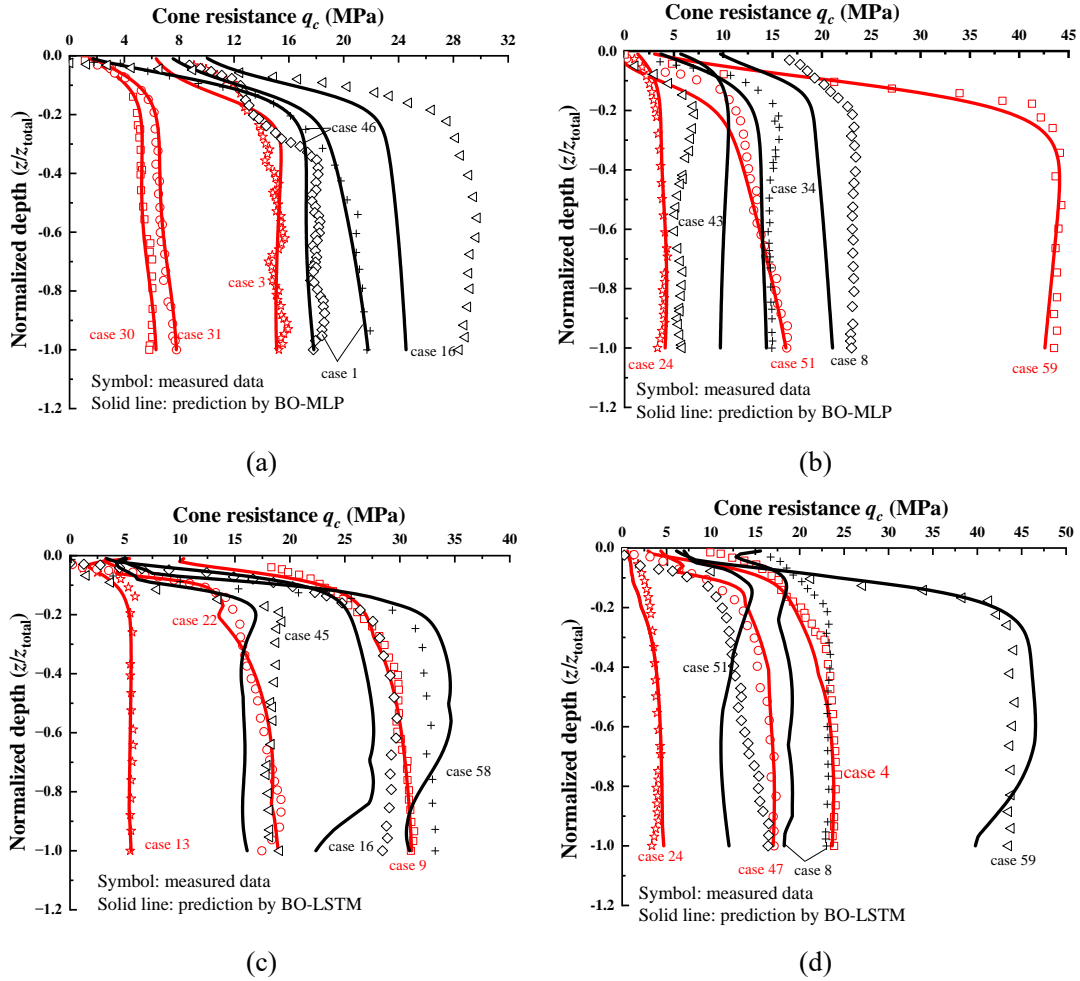
(a)

(b)

426 Fig. 8. Frequency and cumulative probability of relative error in (a) BO-MLP network and (b)
427 BO-LSTM network.

428

429 Fig. 9 shows the comparison between the predicted q_c profiles by MLP and LSTM
430 neural networks with the experimental data. Every subplot in Fig. 9 shows three good
431 predictions (red lines) and three worst cases (black lines). It can be seen from Fig. 9
432 that both in the training and testing set, the variation tendency of cone resistance with
433 the normalized depth z/z_{total} (ratio of the current penetration depth over the total
434 penetration depth) can be successfully reproduced by two neural networks during
435 penetration processes. Given that coefficient of determination R^2 has reached relatively
436 large values for training and testing datasets, many cases can be well predicted by neural
437 networks. But some cases still display obvious errors between measured values and
438 predictions, especially for these worst cases, as displayed in the black lines in Fig. 9.
439 Such as the example of case 43 in Fig. 9(b), the true stable q_c is about 5 MPa while the
440 prediction reaches 10 MPa, resulting in the relative error of 50%. These worst cases
441 lead to the RE in Fig. 8 larger than 30%. Besides, the cone resistance at the bottom of
442 penetration, in some cases, presents the tendency of reduction, as displayed in cases 16
443 and 58 in Fig. 9(c). The main reason behind this phenomenon might be that some
444 calibration chamber tests with flexible bottom boundaries cause a decrease in cone
445 resistance around the bottom of the chamber [34]. The established neural networks
446 learned this feature, thereby causing the resistance reduction at the bottom of
447 penetration in some cases. In addition, some experimental results like case 8 show large
448 errors and singular points where the q_c curve did not start from the original point, which
449 may explain the points outside the 30% error in Fig. 8. In summary, the established
450 machine learning models are proven capable of predicting the cone resistance profiles
451 in calibration chamber test with an acceptable fitting degree.



452 Fig. 9. Comparison of measured data with prediction profiles from ML model in (a) training set of
 453 BO-MLP; (b) testing set of BO-MLP; (c) training set of BO-LSTM; (d) testing set of BO-LSTM.
 454 Red lines represent better predictions by neural networks while black lines represent the worst
 455 cases.

456 5. Further validation and application of the trained models

457 5.1 Validation with numerical solutions

458 This section aims to further compare the neural networks with numerical solutions for
 459 new (not given in Table 1) cases. These new cases are designed to consider the variation
 460 of relative density, vertical effective stress, and saturation conditions of sand, as listed
 461 in Table 6. Numerical simulations to install the CPT in the calibration chamber for these
 462 cases are then performed to provide cone resistance profiles. Details on the CEL model

463 setup and soil constitutive relationships are shown in Appendix A and B, respectively.

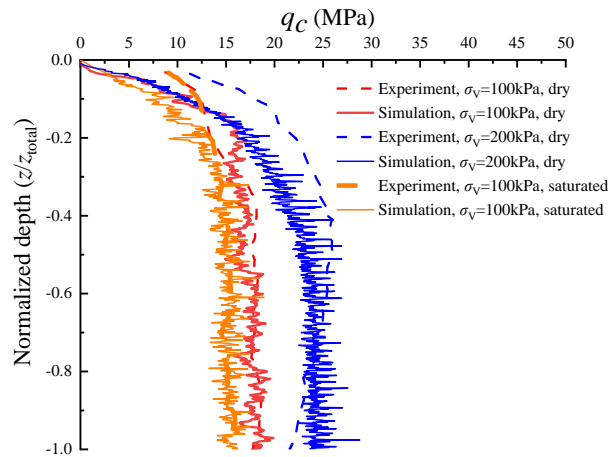
464

Table 6. New cases to be validated by numerical modelling.

No.	D_r	σ_v (MPa)	K_0	Saturation condition
1	0.563	0.13	0.42	Dry
2	0.82	0.15	0.45	Saturated
3	0.734	0.09	0.5	Dry
4	0.8	0.16	0.38	Dry

465

466 The CEL model is first compared and validated against calibration chamber tests
 467 conducted by Kluger et al. [34] in Ticino sand. Their testing results under two vertical
 468 effective stresses σ_v of 100 kPa and 200 kPa are shown in Fig. 10. It can be seen from
 469 Fig. 10 that the numerical solutions are in good agreement with testing results, giving
 470 confidence that the CEL modelling can provide the reliable q_c profiles in calibration
 471 chamber tests.



472

473 Fig. 10. Comparison of the simulated cone resistance with the experimental results of Kluger et al.

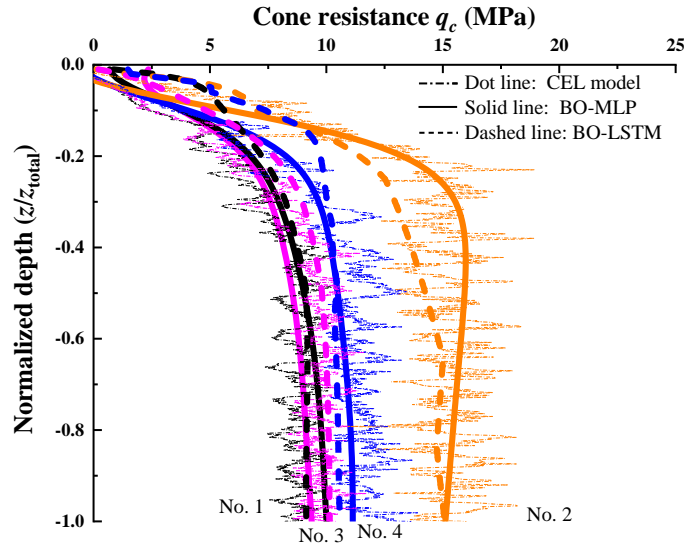
474

[34].

475

476 Fig. 11 shows the comparisons of cone resistance profiles obtained from the two neural
 477 networks and the numerical simulation for the artificial cases in Table 6. The q_c profiles
 478 obtained from the machine learning models are fair close to the numerical simulations,
 479 although some cases like No. 2 in Table 6 still show discrepancies between the two
 480 methods. However, the stable values of cone resistance achieve a better agreement

481 between the numerical simulation and the neural networks. One has to be aware that
 482 the application of the validated models still requires complex model set-up and time-
 483 consuming running. In contrast, a well-trained neural network can quickly (typically a
 484 few seconds) create reliable q_c curves under certain soil conditions.



485

486

Fig. 11. Comparison of neural networks with CEL model in predicting unseen cases.

487 5.2 Application: relating q_c with soil properties

488 As mentioned before, most of the existing correlations between q_c and soil properties
 489 (e.g., relative density D_r) were presented through a limited number of datasets for
 490 specific soil types. The trained neural networks have been proven as a reliable approach
 491 to quickly extend the database of CPT in calibration chambers, therefore the corrections
 492 of these correlations can be made based on the extended database based on the machine
 493 learning models. This section shows an example to potentially improve the $D_r - q_c$
 494 correlation using the neural networks developed in this study.

495

496 Table 7 summarizes four reported correlations of $D_r - q_c$. Here, the normalized cone
 497 resistance of $Q = (q_c - \sigma_v) / \sigma_v$ was introduced to consider the influence of vertical stress
 498 whenever available. Fig. 11 presents the deduced correlations of $D_r - Q$ from Eqs. (13)
 499 to (16). The 864 groups of $D_r - Q$ generated from the developed neural networks are
 500 also shown in Fig. 12. Note that only the constant q_c values from cone resistance profiles

501 are used to relate soil properties, and the ML results are the average values of BO-MLP
502 and BO-LSTM. The previous experimental results of Bolton and Gui [42] and
503 Jamiolkowski et al. [43] are also presented in Fig. 12. The existing empirical formulas
504 often only match with the corresponding experimental data used for fitting but deviate
505 from others. Conversely, the predictive database from neural networks has considered
506 different soil types and test conditions (see Table 1).

507

Table 7. Summary of representative correlations of D_r - q_c - σ_v

Empirical formula	Empirical coefficient	Reference
$D_r = \frac{1}{c_2} \ln \left[\frac{q_c}{c_0(\sigma_v)^{c_1}} \right]$ (13)	$C_0 = 60, C_1 = 0.7, C_2 = 2.91$	Lunne and Christoffersen (1983) [44]
$D_r = C_2 \log_{10} \left[\frac{\frac{q_c}{p_a}}{\left(\frac{\sigma_v}{p_a}\right)^{c_1}} - 1 \right]$ (14)	$C_1 = 0.5, C_2 = 68, p_a$ is the atmospheric pressure	Kulhawy and Mayne (1990) [45]
$D_r = AQ + B$ and $Q = \frac{q_c - \sigma_v}{\sigma_v}$ (15)	$A = 0.2831, B = 32.964$	Bolton and Gui (1993) [42]
$D_r = A_0 + B_0 \ln \left[\frac{q_c}{(\sigma_v)^{0.5}} \right]$ (16)	$A_0 = -1.292, B_0 = 0.268$	Jamiolkowski et al. (2003) [3]

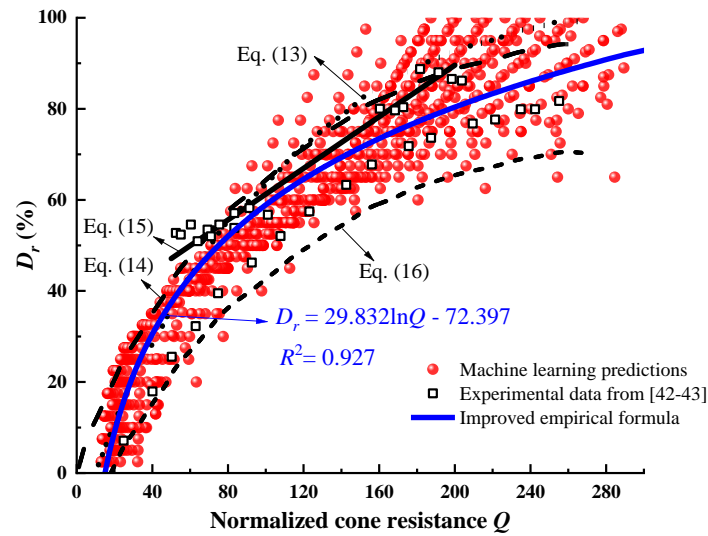
508

509 Comparison with the dataset from the developed neural networks finds that the linear
510 regression of Eq. (15) works not so well in fitting all these data, especially for D_r lower
511 than 50%. Eq. (16) underestimates the relative density from normalized cone resistance
512 and is close to the lower bound of the dataset. The logarithmic form of Eqs. (13) and
513 (14) conform better to the D_r - Q relationship. Nevertheless, Eq. (14) overestimates
514 slightly the dataset for values of D_r lower than 50% while Eq. (15) overestimates
515 slightly the dataset for values larger than 50%. For pure experimental data in Fig. 12,
516 the R^2 of Eqs. (13) to (16) are 68.7%, 71.3%, 75.6%, and 65.2%, respectively. This
517 conclusion illustrates that traditional empirical equation regarding a specific soil type
518 has some limitations when expanded to other soil states. However, with the help of the
519 ML model, we can generate hundreds of D_r - Q points for practical application.
520 Consequently, a new correlation of D_r - Q by curve fitting to all the data in Fig. 12 is
521 given below:

522

$$D_r = 29.832 \ln Q - 72.397 \quad (17)$$

523 Eq. (17) has a high fitting degree of 92.7% to all D_r - Q points. For the pure experimental
 524 data in Fig. 12, Eq. (17) still has a relatively high R^2 value of 88.3%. It is believed that
 525 the improved Eq. (17) is more reliable since the database used for the fitting included
 526 not only the published experimental data but also a large amount of data from the
 527 developed ML models. In the future, if more datasets of calibration chamber tests can
 528 be provided to further train the ML models, more convincing ML models can be trained
 529 for enhancing practical application.



530

531

Fig. 12. Correlation between relative density and normalized cone resistance.

532 6. Conclusion

533 This study introduces a Bayesian-optimized machine learning approach using neural
 534 networks for predicting cone resistance profiles in calibration chamber tests performed
 535 on sand. We began by training the neural networks using 52 groups (5200 points) taken
 536 from the results in the literature, followed by validation of the results using a testing
 537 data set consisting of 12 groups (1200 points). Bayesian optimization was used to obtain
 538 the hyperparameters of both the MLP and the LSTM networks, and in particular the
 539 number of neurons per layer and the initial learning rate.

540

541 The prediction of the cone resistance q_c , had a coefficient of determination (R^2) for the

542 training set of 98.65% (MLP) and 98.51% (LSTM), and an MSE of 2.0006 (MLP) and
543 2.2200 (LSTM). In the training dataset, the R^2 and MSE values were 95.13% (MLP)
544 and 94.65% (LSTM), and 4.8272 (MLP) and 5.0109 (LSTM) respectively. Further
545 comparisons were carried out using the results of a Coupled Eulerian-Lagrangian model
546 for other soils not covered in the experimental results, which also gave good results.

547

548 Finally, the validated machine learning model was deployed to generate unseen
549 scenarios, correlating cone resistance (q_c) with the relative density of sand to prove the
550 validity of the derived results. The model is derived from 864 groups (cases) generated
551 using the ML model and is tested against literature models. The obtained R^2 value
552 versus experiments mentioned in the literature is 88.3%, which indicates its ability to
553 generalization.

554

555 In conclusion, we have demonstrated that neural networks can be applied to provide
556 general models that could serve the purpose of virtual calibration chambers. This
557 approach outperforms other previously published calibration chambers based on
558 numerical models as they provide pseudo-real-time models, and therefore, it is orders
559 of magnitude more computationally efficient. Besides, this work can be extended to
560 more CPT-based material parameter interpretations such as soil strength and stiffness
561 parameters using other machine learning-based approaches.

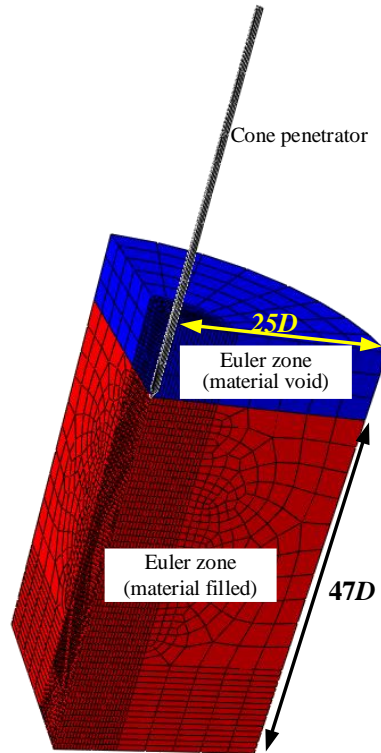
562 **Appendix A. CEL model set-up**

563 The CEL model for a calibration chamber test is shown in Fig. A1. The CPT probe has
564 a standard diameter of $D = 36$ mm and an apex angle of 60° [4]. The cone penetrometer
565 was modeled by a Lagrangian body and discretized using C3D8R elements with a total
566 number of 202. Eulerian material was employed to model the soil with large
567 deformation. As the symmetry of the model test, only a 1/4 size model was established.
568 A soil domain of $25D$ in radial direction and $47D$ in depth direction was sufficient to

569 avoid boundary effects [4]. The central rectangular area of approximately $5.5D$ was
570 densified to ensure the calculation accuracy. The mesh size in the dense field was set as
571 $0.125D \times 0.27D$ in radial and vertical directions, respectively. The upper part of
572 model represents the initially void region but could be filled by the movement of
573 materials into elements during penetration, while the lower part is filled fully with
574 materials. The soil domain was discretized by the EC3D8R elements with a total
575 number of 12968 with reduced integration and hourglass control.

576

577 The bottom boundary of the soil domain was restrained in the vertical direction, and
578 the lateral boundary was constrained in both horizontal directions (BC3). Two dynamic-
579 explicit steps were employed to simulate the penetration process in sand, in which the
580 first geostatic step is used to establish the initial stress field and balance the geostatic
581 stress for sand. According to Table 6, the corresponding σ_v and K_0 were applied to
582 generate the soil stress field. In the validation with an experiment in Fig. 10, the lateral
583 earth pressure coefficient K_0 was set to be 0.45, which was consistent with the selected
584 calibration chamber tests. The relative density was calculated by the initial void ratio
585 [4]. In the second step, the modelling of CPT penetration under a constant vertical
586 velocity of 0.2 m/s was performed. The contact between the cone/shaft and soil was
587 modelled using a surface-to-surface discretization with a frictional coefficient of $\mu =$
588 0.22.



589

590

Fig. A1. CEL model for calibration chamber

591 **Appendix B. Soil constitutive relationship**

592 The hypoplastic (HP) constitutive model for sand proposed by Gudehus [46] and
 593 Wolffersdorff [47] was employed to model soil constitutive behavior. An extension of
 594 the concept of intergranular strain proposed by Niemunis and Herle [48] was
 595 established to account for the accumulation effects and hysteretic behavior in small
 596 strain stiffness cases. The Ticino sand was chosen to fill the chambers. The
 597 experimental drained triaxial shear data on Ticino sand conducted by Rorato et al. [49]
 598 is shown in Fig. B1 for dense sand with a constant initial void ratio $e_0=0.612$ under
 599 different confining pressure σ_c . A set of HP model parameters of the Ticino sand are
 600 summarized in Table B1. For calibration, Fig. B1 also gives the predicted constitutive
 601 relationships of Ticino sand modelled by HP model parameters in Table B1. From Fig.
 602 B1, although some small differences between the experimental and the numerical data
 603 are found, the HP model parameters listed in Table B1 are considered to be enough

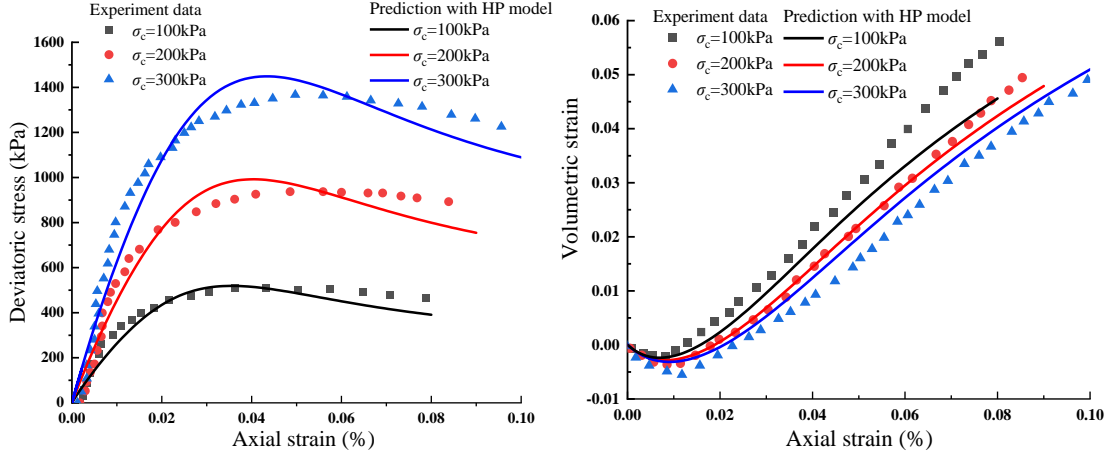
604 reasonable, and hence can be used to run the following models.

605

606 To incorporate the effect of pore water pressure generated in the saturated sand, this
 607 paper employed the method by Qiu and Grabe [50]. The changes in pore water pressure
 608 p_w are determined by the state equation of pore pressures and the balance of mass:

$$609 \quad \dot{p}_w = \frac{K_w}{n} \dot{\varepsilon}_v \quad (B1)$$

610 where K_w is the bulk modulus of water is derived 2.1 GPa; n is the porosity; ε_v is the
 611 volumetric strain. $K_w=0$ means dry sand while $K_w>0$ signifies saturated condition. The
 612 HP model and Eq. (B1) are employed to describe the constitutive relationship of sand
 613 and are incorporated using a VUMAT subroutine.



614

615 (a) Stress-strain relationship

615 (b) Volumetric response

616 Fig. B1. Comparison between the experiment data and simulation with hypoplastic model

617

Table B1. Hypoplastic material parameters for Ticino sand

Parameter	Value
Critical state friction angle, φ_c	31°
Granular hardness, h_s (MPa)	2000
Material constant, n	0.29
Minimum void ratio at zero pressure, e_{d0}	0.57
Critical void ratio at zero pressure, e_{c0}	0.94
Maximum void ratio at zero pressure, e_{i0}	1.1
Material constant, α	0.16
Material constant, β	1.65
Maximum value of intergranular strain, R	0.00033
Material constant, m_R	5

Material constant, m_T	2
Evolution of intergranular strain, β_r	0.5
Parameter controlling stiffness degradation during monotonic deformation, χ	6

618 Acknowledgments

619 The authors would like to acknowledge the funding support by the China Scholarship
620 Council (CSC).

621 Data availability

622 Data will be made available on request. The datasets and machine learning models are
623 available in <https://github.com/MingpengLiu/BO-MLP-and-BO-LSTM>.

624 References

- 625 [1] Liyanapathirana, D.S. Arbitrary Lagrangian Eulerian based finite element analysis
626 of cone penetration in soft clay. *Computers and Geotechnics*, 2009, 36(5): 851-860.
- 627 [2] Hamann, T., G. Qiu and J. Grabe. Application of a Coupled Eulerian–Lagrangian
628 approach on pile installation problems under partially drained conditions. *Computers*
629 *and Geotechnics*, 2015, 63: 279-290.
- 630 [3] Jamiolkowski, M., D. Lo Presti and M. Manassero. Evaluation of relative density
631 and shear strength of sands from CPT and DMT, in *Soil behavior and soft ground*
632 *construction*. 2003. 201-238.
- 633 [4] Chen, Z., M. Huang and Z. Shi. Application of a state-dependent sand model in
634 simulating the cone penetration tests. *Computers and Geotechnics*, 2020, 127: 103780.
- 635 [5] POURNAGHIAZAR, M., A.R. RUSSELL and N. KHALILI. The cone penetration
636 test in unsaturated sands. *Géotechnique*, 2013, 63(14): 1209-1220.
- 637 [6] Mo, P.-Q., A.M. Marshall and H.-S. Yu. Interpretation of cone penetration test data
638 in layered soils using cavity expansion analysis. *Journal of Geotechnical and*
639 *Geoenvironmental Engineering*, 2017, 143(1): 04016084.

- 640 [7] Cudmani, R. and V. Osinov. The cavity expansion problem for the interpretation of
641 cone penetration and pressuremeter tests. *Canadian Geotechnical Journal*, 2001, 38(3):
642 622-638.
- 643 [8] Susila, E. and R.D. Hryciw. Large displacement FEM modelling of the cone
644 penetration test (CPT) in normally consolidated sand. *International Journal for*
645 *Numerical and Analytical methods in geomechanics*, 2003, 27(7): 585-602.
- 646 [9] Wang, D., B. Bienen, M. Nazem, et al. Large deformation finite element analyses
647 in geotechnical engineering. *Computers and Geotechnics*, 2015, 65: 104-114.
- 648 [10] Zhang, N., M. Arroyo, M.O. Ciantia, et al. Standard penetration testing in a virtual
649 calibration chamber. *Computers and Geotechnics*, 2019, 111: 277-289.
- 650 [11] Fan, S., B. Bienen and M. Randolph. Stability and efficiency studies in the
651 numerical simulation of cone penetration in sand. *Géotechnique Letters*, 2018, 8(1): 13-
652 18.
- 653 [12] Yu, H., H. Zhou, B. Sheil, et al. Finite element modelling of helical pile installation
654 and its influence on uplift capacity in strain softening clay. *Canadian Geotechnical*
655 *Journal*, 2022, 0(0): null.
- 656 [13] Zhang, P. A novel feature selection method based on global sensitivity analysis
657 with application in machine learning-based prediction model. *Applied Soft Computing*,
658 2019, 85: 105859.
- 659 [14] Alkroosh, I.S., M. Bahadori, H. Nikraz, et al. Regressive approach for predicting
660 bearing capacity of bored piles from cone penetration test data. *Journal of Rock*
661 *Mechanics and Geotechnical Engineering*, 2015, 7(5): 584-592.
- 662 [15] Wang, H., X. Wang, J.F. Wellmann, et al. A Bayesian unsupervised learning
663 approach for identifying soil stratification using cone penetration data. *Canadian*
664 *Geotechnical Journal*, 2018, 56(8): 1184-1205.
- 665 [16] Erharter, G.H., S. Oberhollenzer, A. Fankhauser, et al. Learning decision
666 boundaries for cone penetration test classification. *Computer-Aided Civil and*
667 *Infrastructure Engineering*, 2021, 36(4): 489-503.

- 668 [17] Rauter, S. and F. Tschuchnigg. Identification of soil strata from in-situ test data
669 using machine learning. in International Conference of the International Association for
670 Computer Methods and Advances in Geomechanics. 2022: Springer.
- 671 [18] Pham, B.T., T.-A. Hoang, D.-M. Nguyen, et al. Prediction of shear strength of soft
672 soil using machine learning methods. *Catena*, 2018, 166: 181-191.
- 673 [19] Ahmad, M., X.-W. Tang, J.-N. Qiu, et al. Application of machine learning
674 algorithms for the evaluation of seismic soil liquefaction potential. *Frontiers of*
675 *Structural and Civil Engineering*, 2021, 15: 490-505.
- 676 [20] Samui, P. Liquefaction prediction using support vector machine model based on
677 cone penetration data. *Frontiers of Structural and Civil Engineering*, 2013, 7: 72-82.
- 678 [21] Guan, Q.Z., Z.X. Yang, N. Guo, et al. Finite element geotechnical analysis
679 incorporating deep learning-based soil model. *Computers and Geotechnics*, 2023, 154:
680 105120.
- 681 [22] Zhang, P., Z.Y. Yin, Y.F. Jin, et al. An AI-based model for describing cyclic
682 characteristics of granular materials. *International Journal for Numerical and Analytical*
683 *Methods in Geomechanics*, 2020, 44(9): 1315-1335.
- 684 [23] Guan, Q.Z. and Z.X. Yang. Hybrid deep learning model for prediction of
685 monotonic and cyclic responses of sand. *Acta Geotechnica*, 2022.
- 686 [24] Wang, K. and W. Sun. A multiscale multi-permeability poroplasticity model linked
687 by recursive homogenizations and deep learning. *Computer Methods in Applied*
688 *Mechanics and Engineering*, 2018, 334: 337-380.
- 689 [25] Habibagahi, G. and A. Bamdad. A neural network framework for mechanical
690 behavior of unsaturated soils. *Canadian Geotechnical Journal*, 2003, 40(3): 684-693.
- 691 [26] Kohestani, V.R. and M. Hassanlourad. Modeling the Mechanical Behavior of
692 Carbonate Sands Using Artificial Neural Networks and Support Vector Machines.
693 *International Journal of Geomechanics*, 2016, 16(1): 04015038.
- 694 [27] Alizadeh, B., A.G. Bafti, H. Kamangir, et al. A novel attention-based LSTM cell
695 post-processor coupled with bayesian optimization for streamflow prediction. *Journal*

696 of Hydrology, 2021, 601: 126526.

697 [28] Tao, Y., H. Sun and Y. Cai. Predictions of deep excavation responses considering
698 model uncertainty: integrating BiLSTM neural networks with Bayesian updating.
699 International Journal of Geomechanics, 2022, 22(1): 04021250.

700 [29] Zhang, P., Z.-Y. Yin and Y.-F. Jin. Bayesian neural network-based uncertainty
701 modelling: application to soil compressibility and undrained shear strength prediction.
702 Canadian Geotechnical Journal, 2021, 59(4): 546-557.

703 [30] Zhang, P., Z.-Y. Yin and Y.-F. Jin. State-of-the-Art Review of Machine Learning
704 Applications in Constitutive Modeling of Soils. Archives of Computational Methods in
705 Engineering, 2021, 28(5): 3661-3686.

706 [31] Dai, H. and C. MacBeth. Effects of Learning Parameters on Learning Procedure
707 and Performance of a BPNN. Neural Networks, 1997, 10(8): 1505-1521.

708 [32] Yang, Z., R. Jardine, B. Zhu, et al. Sand grain crushing and interface shearing
709 during displacement pile installation in sand. Géotechnique, 2010, 60(6): 469-482.

710 [33] Huang, A.-B. and H.-H. Hsu. Cone penetration tests under simulated field
711 conditions. Geotechnique, 2005, 55(5): 345-354.

712 [34] Kluger, M.O., S. Kreiter, F.T. Stähler, et al. Cone penetration tests in dry and
713 saturated Ticino sand. Bulletin of Engineering Geology and the Environment, 2021,
714 80(5): 4079-4088.

715 [35] Bałachowski, L. Penetration resistance of Lubiatowo sand in calibration chamber
716 tests. Archives of Hydro-Engineering and Environmental Mechanics, 2006, 53(4): 311-
717 329.

718 [36] Schnaid, F. A study of the cone-pressuremeter test in sand. 1990, University of
719 Oxford.

720 [37] ARROYO, M., J. BUTLANSKA, A. GENS, et al. Cone penetration tests in a
721 virtual calibration chamber. Géotechnique, 2011, 61(6): 525-531.

722 [38] Zhang, P., Z.-Y. Yin, Y. Zheng, et al. A LSTM surrogate modelling approach for
723 caisson foundations. Ocean Engineering, 2020, 204: 107263.

- 724 [39] He, S. and J. Li. Modeling nonlinear elastic behavior of reinforced soil using
725 artificial neural networks. *Applied Soft Computing*, 2009, 9(3): 954-961.
- 726 [40] Ruder, S. An overview of gradient descent optimization algorithms. arXiv preprint
727 arXiv:1609.04747, 2016.
- 728 [41] Huang, Y., Y. Wang, Z. Xu, et al. Prediction and variable importance analysis for
729 small-strain stiffness of soil based on ensemble learning with Bayesian optimization.
730 *Computers and Geotechnics*, 2023, 162: 105688.
- 731 [42] Bolton, M. and M. Gui. The study of relative density and boundary effects for cone
732 penetration tests in centrifuge. 1993: University of Cambridge, Department of
733 Engineering.
- 734 [43] Jamiolkowski, M. New developments in field and laboratory testing of soils. in
735 Proc. 11th. Int. Conf. on SMFE., San Francisco, CA, 1985. 1985.
- 736 [44] Lunne, T. and H.P. Christoffersen. Interpretation of cone penetrometer data for
737 offshore sands. in *Offshore Technology Conference*. 1983: OTC.
- 738 [45] Kulhawy, F.H. and P.W. Mayne. Manual on estimating soil properties for
739 foundation design. 1990, Electric Power Research Inst., Palo Alto, CA (USA); Cornell
740 Univ., Ithaca
- 741 [46] Gudehus, G. A comprehensive constitutive equation for granular materials. *Soils
742 and foundations*, 1996, 36(1): 1-12.
- 743 [47] Von Wolffersdorff, P.A. A hypoplastic relation for granular materials with a
744 predefined limit state surface. *Mechanics of Cohesive-frictional Materials: An
745 International Journal on Experiments, Modelling and Computation of Materials and
746 Structures*, 1996, 1(3): 251-271.
- 747 [48] Niemunis, A. and I. Herle. Hypoplastic model for cohesionless soils with elastic
748 strain range. *Mechanics of Cohesive-frictional Materials: An International Journal on
749 Experiments, Modelling and Computation of Materials and Structures*, 1997, 2(4): 279-
750 299.
- 751 [49] Rorato, R., M. Arroyo, A. Gens, et al. Image-based calibration of rolling resistance

752 in discrete element models of sand. *Computers and Geotechnics*, 2021, 131: 103929.
753 [50] Qiu, G. and J. Grabe. Explicit modeling of cone and strip footing penetration under
754 drained and undrained conditions using a visco-hypoplastic model. *geotechnik*, 2011,
755 34(3): 205-217.

756