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Machine learning brings new insights for reducing salinization disaster

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This study constructs a machine learning system to examine the predictors of soil salinity in deserts. We conclude that soil humidity and subterranean CO_2 concentration are two leading controls of soil salinity—respectively explain 71.33%, 13.83% in the data. The (R^2 , root-mean-square error, RPD) values at the training stage, validation stage and testing stage are (0.9924, 0.0123, and 8.282), (0.9931, 0.0872, and 7.0918), (0.9826, 0.1079, and 6.0418), respectively. Based on the underlining mechanisms, we conjecture that subterranean CO_2 sequestration could reduce salinization disaster in deserts.

KEYWORDS

salinization disaster, principal components analysis (PCA), artificial neural network (ANN), long short-term memory (LSTM), subterranean CO_2 sequestration

1 Introduction

Soil salinization is one major type of land desertification and degradation in the world, which is a disaster to global resources and ecology (Dehaan and Taylor, 2002; Metternicht and Zinck, 2008; Li et al., 2014; Singh, 2015; Savich et al., 2021). Such disaster not only brought great impact and serious losses to food production, but also hindered the sustainable development of agriculture (Kotb et al., 2000; Amezketa, 2006; Rengasamy, 2016; Okur and Örçen, 2020; Hassani et al., 2021). The influences of soil salinization disaster to other aspects of society and economy are also inevitable (Schofield et al., 2001; Ghollarata and Raiesi, 2007; Ding et al., 2011; Wang and Li, 2013; Nachshon, 2018; Yang et al., 2020). The disaster leads to a low rate of soil utilization and a sharp decline of forests (De Pascale et al., 2005; Li-Xian et al., 2007; Xiaohou et al., 2008; Bouksila et al., 2013; Wu et al., 2014; Teh and Koh, 2016; Zhou et al., 2017; Li et al., 2018; Zhuang et al., 2022). Ecologists have made great efforts to develop theory and methodology for reducing soil salinization disaster (Lavado and Taboada, 1987; El Harti et al., 2016; Wang et al., 2019). But until now, the degree of global soil salinization is still increasing (Tian and Zhou, 2000; Aragüés et al., 2015; Jesus et al., 2015).

Considering its threats to the earth environments, any theory and methodology for reducing soil salinization disaster is worthy to be discussed (Welle and Mauter, 2017). In the era of artificial intelligence, machine learning has been introduced in the frontier of earth science (Jiang et al., 2018; Huang et al., 2020a; Huang et al., 2020b; Chang et al., 2020; Huang et al., 2020c). The machine learning system is mainly composed of input layer, output layer and hidden layers (Chahal and Gulia, 2019). After obtaining a training set, the learning system can extract effective features (LeCun et al., 2015). These features are connected by artificial neurons (Hao et al., 2016). The neurons receive data from the input layer, make computation with



assigned weights—passed through the activation function in the hidden layers, and finally work out the results in the output layer (Coşkun et al., 2017). By testing the trained network, we can assess the errors between the outputs and correct results (Kato et al., 2016). Some latest researches constructed 3-stages learning systems (the training stage, validation stage and testing stage) to improve the generalization capability (Gatos et al., 2019; Skrede et al., 2020; Zhuang et al., 2021).

Our objectives of this study are 1) to construct a machine learning system and examine the predictors of soil salinity in a desert by this learning system, 2) to evaluate the most interpretable proportion of the leading predictors, which will highlight the unneglectable contribution of the subterranean CO₂ concentration to soil salinity, and 3) to analyze the underlining mechanisms for such contribution and according to these mechanisms, to present new insights for reducing salinization disaster in deserts. The organization of the whole paper is as follows. In Section 2, we will construct the machine learning system for examining the predictors, along with some preliminaries and the driven data. Principal components analysis (PCA) is integrated with the artificial neural network (ANN) and long-short term memory (LSTM). Performance of PCA-ANN-LSTM will be presented and the leading predictors will be determined in Section 3. We will also assess the largest proportion of two leading predictors in explaining soil salinity and further clarify their leading roles. Based on the results from PCA-ANN-LSTM calibrations, in Section 4, some new insights will be expanded for reducing soil salinization disaster and the underlining mechanisms will be theoretically analyzed. The conclusions and next research priorities are presented in Section 5.

2 The machine learning system

2.1 The learning mechanisms

The learning mechanisms depend on not only the problem itself but also the components of the data. As stated in Section 1, the considered problem is to construct a machine learning system for examining the potential predictors of soil salinity in a desert by this learning system. That is, the input data of the system is environmental variables (meteorological, soil, and subterranean factors), while the output data is soil salinity. These data were collected from the Manas River Basin of Xinjiang Uygur autonomous region, which is located at the southern periphery of the Gubantonggut Desert, China, as shown in Figure 1. We established five stations by integrating 13 sensors to collect the meteorological, soil and subterranean data, including the CO₂ concentration 3 m beneath the soil (Cs) and 10 cm above the soil (Ca), the soil temperature (Ts), humidity (Hs), alkalinity (pH) and salinity (Y) at 10 cm depth, the atmospheric temperature (Ta), humidity (Ha), air pressure (AP), wind speed (WS), wind direction (WD), rainfall (R), and groundwater level (WL). In order to develop a novel deep neural network to detect the potential environmental controls of soil salinity, Y is employed as the dependent variable of the network and the other 12 environmental factors are naturally employed as independent variables. The basic learning mechanisms of a neural network can be described as follows. The neuron input x was calculated from the model established in (Zhuang et al., 2021).

Alternatively, we integrated the principal component analysis (PCA) and the artificial neural network (ANN) to examine the potential control of Cs, where PCA was improved by the singular value decomposition (SVD) (Van Loan, 1976; Klema and Laub, 1980; Paige and Saunders, 1981; Mandel, 1982; Stewart, 1993). Suppose Θ^i is the weight matrix and g(x) is the activation function. Let $z^{(j)}$ be the pulses to the *jth* layer, which results in $a^{(j)}$. Let $h_{\theta}(x)$ be the result in the output layer.

That is,

$$z^{(j)} = \Theta^{(j)} a^{(j-1)}, a^{(j)} = g(z^{(j)})$$
(1)

Hence the learning mechanisms can be formulated as

$$\begin{bmatrix} x_0\\ x_1\\ x_2\\ \dots \end{bmatrix} \rightarrow \begin{bmatrix} a_0^{(1)}\\ a_1^{(1)}\\ a_2^{(1)}\\ \dots \end{bmatrix} \rightarrow \begin{bmatrix} a_0^{(2)}\\ a_1^{(2)}\\ a_2^{(2)}\\ \dots \end{bmatrix} \rightarrow \begin{bmatrix} a_0^{(3)}\\ a_1^{(3)}\\ a_2^{(3)}\\ \dots \end{bmatrix} \rightarrow \dots \rightarrow \begin{bmatrix} a_0^{(j)}\\ a_1^{(j)}\\ a_2^{(j)}\\ \dots \end{bmatrix} \rightarrow \begin{bmatrix} h_\theta(x)_1\\ h_\theta(x)_2\\ h_\theta(x)_3\\ \dots \end{bmatrix}$$
(2)

and

$$h_{\theta}(x) = \begin{bmatrix} h_{\theta}(x)_{1} \\ h_{\theta}(x)_{2} \\ h_{\theta}(x)_{3} \\ \cdots \end{bmatrix} = a^{(j)}$$
(3)

where the backpropagation process is monitored by the loss function

$$J(\Theta) = -\frac{1}{m} \sum \left(Y^T . *log \left(h_\theta(x) \right) . * \left(1 - Y^T \right) \right)$$
(4)

2.2 The learning processes

Differing from (Zhuang et al., 2021), we further introduce a braininspired mechanism in the learning processes. That is, we further improve SVD-PCA-ANN by long-short-memory neural network (LSTM) (Salman et al., 2018; Ali et al., 2020; Ahmad and Zhang, 2022; Gao, 2022; Rusnac and Grigore, 2022) and proposed a novel deep neural network PCA-ANN-LSTM to detect the potential environmental controls of soil salinity in the desert. The output of the SVD-PCA-ANN will not be directly input into LSTM. Instead, we utilize the errors data of the SVD-PCA-ANN model as the input data of LSTM. That is, we employ LSTM for learning and reducing the errors to improve the robustness when detecting the potential environmental controls of soil salinity and analyzing the contributions of the subterranean CO_2 concentration to the soil salinity.

The necessity to further integrate with LSTM in the learning processes can be explained as follows. In ANN, it is assumed that the output only depends on the current input, which is not true in the real world (Gu et al., 2019). LSTM allows us to infer the potential relationships among the content of the context, because it is a recurrent neural network (RNN)—the output depends on the current input and memory (Klimov et al., 2020; Huang et al., 2021; Li et al., 2022; Gorgij et al., 2023). The basic idea of RNN is to build a hidden state for acquiring the information at the previous time point

and the global parameters are calculated from the current time and all previous memories. Each cell in RNN shares these parameters to reduce the amount of calculation. For LSTM, the current input is linked with the state of the hidden layers in the previous time through three gates—the input gate (information adding), forgetting gate (information discarding) and output gate (Robinson and Zaffaroni, 1997).

A sketch of the learning processes is shown in Figure 2, which construct cells in the machine brain (O'Doherty et al., 2011; Wang et al., 2020; Wang et al., 2021; Wang et al., 2022). We can understand the LSTM learning process with the cells' states. For a cell state C_{t-1} with the input x_t and hidden state h_{t-1} , let σ be the sigmoid function. The retaining or discarding ratio is

$$f_t = \sigma \Big(W_f [h_{t-1}, x_t] + b_f \Big) \tag{5}$$

where b_f is the bias at the current cell state.

Define the trained cell i_t and the corresponding cell state \tilde{C}_t as

$$i_{t} = \sigma(W_{i}[h_{t-1}, x_{t}] + b_{i}), \tilde{C}_{t} = \tanh(W_{C}[h_{t-1}, x_{t}] + b_{C}).$$
(6)

Then updates of the cell state can be formulated as

$$C_{t} = f_{t} * C_{t-1} + i_{t} * \tilde{C}_{t}$$
(7)

and the calculation formula for the next hidden state is

$$h_{t} = \sigma(W_{o}[h_{t-1}, x_{t}] + b_{o}) * \tanh(C_{t}).$$
(8)

The pseudocode of the whole learning processes based on the PCA-ANN-LSTM algorithm is shown in Figure 3, where the detailed steps to detect environmental controls of soil salinity in the desert are carried out through the machine learning framework characterized in Figure 2. In order to exclude the interactions among the 12 factors, we employ partial least squares regression (PLSR) and will compare the performance of PLSR-ANN and PCA-ANN with the proposed method.

The following three indices are calculated to quantify the robustness of PCA-ANN-LSTM in previewing the possible environmental controls of soil salinity, which are also utilized in the comparison with PCA-ANN and PLSR-ANN. For a reliable comparison, the input data was uniformly divided into three subsets for all the learning processes—one for the training stage (half of the data), one for the validation stage (one-quarter of the data).

(1) The coefficient of determination:

$$RMSE = \sqrt{\frac{\sum_{i} (y_{i} - y_{i}')^{2}}{N}}$$
(9)

(2) The root-mean-square error:

$$R^{2} = 1 - \frac{\sum_{i} (y_{i} - y'_{i})^{2}}{\sum_{i} (y_{i} - \bar{y})^{2}}$$
(10)

(3) The ratio of prediction to deviation:

$$RPD = \frac{\left(\sum y_i^{\prime 2} - \left[\sum \frac{y_i^{\prime 2}}{n}\right] / (N-1)\right)^{1/2}}{\left(\sum_i (y_i - y_i^{\prime})^2 - \left\{\left[\sum (y_i - y_i^{\prime})\right]^2 / N\right\} / N-1\right)^{1/2}}$$
(11)

where y_i is the true value, y'_i is the predicted value, \bar{y} is the average of the true value, and N is the number of environmental variables.



3 Performance of the system

3.1 Efficiency of the learning processes

The contributions of twelve potential predictors to soil salinity in linear (PCA) and non-linear (ANN) relationships were determined together within a minute, implying a high efficiency of the main learning processes (LSTM only learned the errors from PCA-ANN). The learning results indicate that all the considered factors (i.e., environmental variables) can potentially influence the variation in the data of soil salinity in deserts, as shown in Figure 4. The first leading contributor is Hs and the contribution of Hs to soil salinity is 71.33%. The underlining mechanisms are easy to be understood. The status of soil salinization in deserts is restricted by the law of soil water and salt movements. Salt in soil moves with soil water-salt is transported to the surface with water in the evaporation process, and after evaporation, salt accumulates in the surface soil. The water infiltrated by rainfall in deserts can also bring salt to the deep soil layers. For a long time, there is no rainfall in the desert, the salt brought to the surface by evaporation is much more than the salt brought to the deep soils by infiltration leaching, the soil is in a salt accumulation state and salinization is aggravated.

To our surprise, Cs is the second leading contributor and its contributions to soil salinity is 13.83%. The possible mechanisms could be linked with the soil CO_2 absorption processes. Such absorption was frequently observed in deserts ecosystems and has been attributed to abiotic processes. One conjecture of these abiotic

processes is that CO₂ reacts with moisture in the soil to form carbonic acid and dissolve calcium carbonate. But such reaction is not enough to explain the absorption intensity. Another conjecture is that the absorbed CO₂ has gone into deep cycles. If these conjectures were true, then soil salinity and subterranean CO2 concentration will be linked in the reaction and deep cycles. The learning results indicated that the contribution of Cs to soil salinity is approximated to a sum of the contributions the other ten potential predictors (the sum value is 14.84%). It is also worthy to note that Ca (with a contribution=3.56%) and WS (contribution=3.77%) are also leading factors. Their contributions are almost equal and the total contribution of them two (7.33%) is approximated to the total contribution of the rest eight factors (7.51%). But some of the rest eight factors (e.g., pH) have been thought to be closely related to soil salinity. Hence, it is quite necessary to prove the robustness of the learning system, which will be done in Section 3.2.

3.2 Robustness of the learning system

The coefficient of determination (R^2), the root-mean-square error (RMSE) and the ratio of prediction to deviation (RPD) of the learning system at the training, validation, and testing stages with 200 epochs are respectively shown in Figures 5–7, and the optimized values are shown in Table 1.

The lower R^2 values of PCA-ANN at the training stage ($R^2 = 0.9891$), the validation stage ($R^2 = 0.9844$) and the testing stage ($R^2 = 0.9844$)

Input: the datasets $X = \{x_1, x_2, x_3, ..., x_m\}, Y$. Output: PCA-ANN-LSTM with a robust prediction. Processes: For all $x_m \in X$ do 1. $x_{\nu} - \overline{x_{\nu}}$ end 2. Compute the matrix covMat = np.cov(meanRemoved, rowvar=0) 3. Calculate the eigenvalues and eigenvectors of the covariance matrix by SVD 4. Sort the eigenvalues from largest to smallest, select the largest k of them and respectively use the corresponding k eigenvectors as column vectors for PCA. 5. Transform the data into a new space constructed by k feature vectors. 6. Obtain the dataset $\mathbf{D} = \{(X_k, Y_k)\}$ and set the learning rate $\boldsymbol{\eta}$ for ANN 7. Random initializes all connection weights and thresholds within (0,1) 8. Repeat for all $(X_k, Y_k) \in D$ do Calculates the output of the current sample $\widehat{y_k}$ based on the current parameters and $f(x) = \frac{1}{1+e^{-x}}$; Calculate the gradient parameter $oldsymbol{g}_I$ of the output layer neurons ; Calculate the gradient parameter e_h of the hidden layer neurons; Update the weights w_{hJ} , v_{ih} and thresholds θ_J , γ_h of the hidden layer to the output layer; end until the SVD-PCA-ANN model converges. 9. Obtain the basic results of Ypredict for a further correction 9. Calculate Y_{loss} = Y_{predict} - Y_{true} 10. Construct the forgetting, input, and output gates of LSTM, respectively, which is sumarrized as $g(x) = \sigma(\omega x + b)$, σ =sigmoid, ω =weighting matrix, b=bias 11. Update the weights ω , **b** and thresholds θ_I , γ_h of the hidden layer to the output layer of PCA-ANN-LSTM. 12. Correct \overline{Y}_{loss} and obtain the final predicted result $\overline{Y}_{predict} = Y_{predict} + \overline{Y}_{loss}$ FIGURE 3 Pseudocode of the learning processes based on PCA-ANN-LSTM.

0.9764) means accurate predictions. Epochs in Figure 5 has displayed the learning processes. The learning system not only indicates a high prediction accuracy, but also indicates small errors. The RMSE values of the learning system at the training, validation, and testing stages are 0.0849, 0.1086, 0.1198, respectively. This is a degree of dispersion (not an absolute error), which further demonstrated the effectiveness of the learning system. Epochs in Figure 6 also reflect the stability of the learning system, RPD is introduced to build a new emergency response process in decision-making and make up for the disadvantages of R^2 and RMSE. The RPD values of the learning system at the training, validation, and testing stages are 1.4568, 1.1042, 0.9703, respectively. This finally demonstrated the robustness of the learning system.

As a cross validation, the R^2 , RMSE, RPD values were also calculated when PCA is replaced by PLSR. PLSR is also based on a linear relationship and differing from PCA, PLSR excludes the interactions among the twelve environmental factors. Performance of PLSR-ANN at the training stage ($R^2 = 0.9952$, RMSE = 0.0522, RPD = 2.3451), the validation stage ($R^2 = 0.9922$, RMSE = 0.0787, RPD = 1.4763) and the testing stage ($R^2 = 0.9868$, RMSE = 0.0688,

RPD = 1.7906) indicate more accurate predictions. These results are a little better than the performance of PCA-ANN. The final performance of the whole system PCA-ANN-LSTM is better than both PCA-ANN and PLSR-ANN. The R^2 values of PCA-ANN-LSTM at the training, validation, and testing stages are 0.9924, 0.9931, 0.9826, respectively. The RMSE values of PCA-ANN-LSTM at the training, validation, and testing stages are 0.0123, 0.0872, 0.1079, respectively. The RPD values of PCA-ANN-LSTM at the training, validation, and testing stages are 8.282, 7.918, 6.0418, respectively. Therefore, the learning system PCA-ANN-LSTM is recommended for subsequent studies when examining potential predictors of soil salinity in deserts.

4 Discussions

Soil salinity has been widely used to describe the degree of soil salination, but in the previous studies, the dynamics of soil salinity are few linked with the CO_2 concentration above or under the ground (Singh, 2016). A series of latest studies have demonstrated abiotic soil CO_2 absorption in the alkaline land, which is closely related with salts in the soil (Chen et al., 2013). Until now, the mechanisms of such CO_2 absorption have not been fully understood. Results from the present





study indicate that subterranean CO_2 concentration and the atmospheric CO_2 concentration around the soil can both influence soil salinity in deserts. These results also present further evidences for the conjecture that the abiotic CO_2 absorption by saline-alkali soils were resulted from subterranean CO_2 sequestration in reaction of soil salts, CO_2 , and moisture.

We hence further hypothesize that the soil salination processes in deserts could be affected by such a subterranean CO_2 sequestration, since based on this new hypothesis, the underlining reaction of salts, CO_2 , and moisture in the soil would further link the dynamics of subterranean CO_2 concentration with soil salinity. Alternatively, we

further hypothesize that the abiotic soil CO_2 absorption in deserts could influence the subterranean CO_2 concentration. If this hypothesis were true, the results from the learning system would be wellexplained. During the reaction of salts, CO_2 , and moisture in different soil layers, soil salinity is changing (Wang et al., 2016a), where both subterranean CO_2 concentration and the atmospheric CO_2 sequestration can play significant roles. This brings new insights for reducing salination disaster. Hypothesizing that we can reduce salinization disaster through the new insights, we can mediate the subterranean CO_2 concentration through the CO_2 storage and sequestration technologies. In response to the global climate





Accuracy evaluation index		R^2	RMSE	RPD
Training	PLSR-ANN	0.9952	0.0522	2.3451
-	PCA-ANN	0.9891	0.0849	1.4568
-	PCA-ANN-LSTM	0.9924	0.0123	8.282
Validation	PLSR-ANN	0.9922	0.0787	1.4763
	PCA-ANN	0.9844	0.1086	1.1042
	PCA-ANN-LSTM	0.9931	0.0872	7.0918
Testing	PLSR-ANN	0.9868	0.0688	1.7906
	PCA-ANN	0.9764	0.1198	0.9703
	PCA-ANN-LSTM	0.9826	0.1079	6.0418

change, the world has made commitments on the peak of CO_2 emissions and the targets to achieve carbon neutrality (Chapin et al., 2006; Wang et al., 2015a). Under this goal, as an important technological approach to achieve large-scale low-carbon utilization of fossil energy, CO_2 capture, utilization and storage technology has become a hot research topic (Tapia et al., 2018). It was recognized that the geological storage potential of CO_2 is great, and the deep soil layers present the main space for CO_2 storage (Orr, 2018). Collaborating this technology with the above hypothesis, subterranean CO_2 capture, utilization and storage not only can help us to achieve carbon neutrality, but also can help us to influence the soil salinization processes.

Soil salinization and desertification are both disasters resulted from surface environmental changes, which not only depend on climate conditions, but also closely related to the role of groundwater (Amezketa, 2006). This study further links soil salinization in deserts with subterranean CO₂ concentration and advances a new hypothesis (Sunda and Cai, 2012). Since subterranean CO2 sequestration and soil salinization process can both be influenced by the reaction of salts, CO2, and moisture in the soil (Schlesinger, 2001), our hypothesis sounds reasonable. Nevertheless, we still need some direct evidences from isotopic analysis to further demonstrate that the soil salination processes in deserts could be affected by such a subterranean CO₂ sequestration (Inglima et al., 2009). Deserts are extremely arid areas and occupy more than 20% of the earth's land area (Chen et al., 2014). Due to high temperature, drying and strong evaporation, upwelling is the dominant process of soil water in the deserts, while the leaching and desalination processes are weak (Kowalski et al., 2008; Serrano-Ortiz et al., 2010; Sanchez-Cañete et al., 2011). These processes formed a large area of saline-alkali land in deserts and in deep soil layers around the groundwater, there are good conditions for reaction of salts, CO2, and moisture (Stone, 2008). But there are still some outstanding questions for subsequent studies. How to assess the intensity of such reaction? How to quantify the contribution of changing processes in subterranean CO₂ concentration to the reaction? How much these processes can affect the soil salinization processes? Are these coupled processes enough to explain the apparent CO_2 absorption? If not, where has the missing CO_2 gone? Can it be attributed to some capnophiles in the deep soil layers? If these questions were appropriately addressed, then our hypothesis would be verified and make a real contribution to reduce salinization disaster in deserts.

Benefitting from the rapid development of various kinds of sensors, the subterranean processes can be further explored by different kinds of signals or images (Wang et al., 2016b). These sensors present a good base to obtain enough data for machine learning. But the mechanisms of the abiotic CO_2 absorption are still poorly understood and the soil salinity might be influenced by many other factors (Wang et al., 2015b). It is still quite necessary to integrate a series of sensors for acquiring other meteorological, soil and subterranean data. The additional data not only can present a better understanding of the whole story about soil salinization, but also can motivate researches on the effects of various environmental factors on the subterranean CO_2 concentration in other arid ecosystems and researches on the mechanisms for the abiotic soil CO_2 absorption (Rey et al., 2012; Rey, 2014; Wang et al., 2016c). Physically-based modelling (Guo et al., 2020; Medina et al., 2021) is also a next research priority.

5 Conclusion

Subterranean CO_2 concentration and the atmospheric CO_2 concentration around the soil surface can both influence soil salinity in deserts, which presents further evidence for a conjecture in the previous studies—the abiotic CO_2 absorption by saline-alkali soils in deserts were resulted from subterranean CO_2 sequestration in reaction of soil salts, CO_2 , and moisture. Based on this conjecture, we

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advance a new hypothesis—the soil salination processes in deserts could be affected by such a subterranean CO_2 sequestration. Since the underlining reaction of salts, CO_2 , and moisture in the soil would further link the dynamics of subterranean CO_2 concentration with soil salinity. Due to strong water-salt processes in deserts, the water in the deep soil layers move upward [resp. downward] in the dry season [resp. the rainy season], and then react with salts and CO_2 in the capillary. The story sounds well. But we need further evidences. A better understanding of the whole story is still quite necessary.

Data availability statement

The raw data supporting the conclusion of this article will be made available by the authors, without undue reservation.

Author contributions

PA and WW were mainly responsible for data collection, code convenience and paper writing as the core contributor of this paper. ZZ and LC assisted in the completion of experiments and data table compilation. WW led the project and conceive the main idea of this research. CX was responsible for the guidance of the experimental code and the language polishing of the paper.

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Conflict of interest

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