

## Prediction of Zeta Potential of Decomposed Peat via Machine Learning: Comparative Study of Support Vector Machine and Artificial Neural Networks

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Zeta potential is crucial for practical applications in electrochemistry. However, the precise determination of zeta potential of decomposed peat is complex and has high requirements to related instruments. Previous study shows that zeta potential of decomposed peat can be predicted by back-propagation (BP) neural network. However, it lacks available comparisons and neglects the importance of the decomposed stages of peat and the required training times. Here, to extend this research, we propose a series of novel machine learning techniques including support vector machine (SVM) and artificial neural networks (ANNs) to predict the zeta potential of decomposed peat. Four indicators including hydrated radius (nm), cation valence, concentration (mol/L) and pH are set as independent variables while zeta potential (mV) is set as the dependent variable. The SVM, general regression neural network (GRNN) and multilayer feed-forward neural networks (MLFNs) are developed in different decomposed stages, including the slightly decomposed peat, the highly decomposed peat and all decomposed peat. Results show that separating the models based on the decomposed stages have better prediction results than taking all decomposed peat in one model. During our studies, the SVM is the best model for the prediction to the slightly decomposed peat (RMS error: 2.37, training time: 1s), while the GRNN is the best model for the prediction to the highly decomposed peat (RMS error: 2.20, training time: 1s).

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**Keywords:** Zeta potential; decomposed peat; support vector machine; artificial neural networks.

## 1. INTRODUCTION

In the field of electrochemistry, zeta potential, the electric potential in the interfacial double layer at the location of the slipping plane, is the potential difference between the stationary layer of fluid attached to the dispersed particle and the dispersion medium [1-3]. Studies show that zeta potential is mainly caused by the net electrical charge contained in the region bounded by the slipping plane and influenced by the location of it [4-8]. With the development of electrochemical technology, there are currently several determination methods for zeta potentials, including electro-osmosis, electrophoresis, streaming potentiometry and ultrasonic method [1].

Zeta potential is a crucial indicator of the stability of colloidal dispersions [9-14]. For the decomposed peat, zeta potential also plays a crucial role in related studies. However, in practical applications, the exact determination of zeta potential of decomposed peat is complex and requires a series of operations and necessary electrochemical instruments, which wastes too much time and manpower. To reduce experimental works, previous studies used back-propagation (BP) neural network to predict the zeta potential of decomposed peat in the presence of different cations [15]. However, this study only discussed one possible model for the prediction, which neglected necessary comparisons with different artificial neural networks (ANNs) and other powerful machine learning techniques. Also, the decomposed stages and the effects of number of neurons to the required training time were also neglected. Therefore, to improve the prediction technique, it is necessary for us to find out a better model that takes all these neglected items into consideration, including i) prediction effects of different models; ii) errors of testing and required training times of the models and iii) numbers of neurons (numbers of nodes) in the hidden layers of ANNs. Here, to find out a better model for the prediction of zeta potential of decomposed peat, we use novel machine learning techniques including novel ANNs and support vector machine (SVM) to develop a series of prediction models for decomposed peat in the presence of different cations. Two stages of decomposed peats defined by the classification method [15] including the slightly and the highly decomposed peats are taken into different considerations. Selections of results are based on the comprehensive performances of different models, including the change regulation of results of ANNs with different nodes. Comparisons are made among different models according to the testing results, which contain the root mean square error (RMS error), training time and prediction accuracy.

## 2. MATERIALS AND METHODS

### 2.1 Introduction to Experiments

According to previous research [15], the determination of zeta potential of decomposed peat is highly related to four indicators that can be obtained by easy measuring process, including hydrated radius (nm), cation valence, concentration (mol/L) and pH. To develop a series of machine learning models, in our study, these four indicators are set as independent variables, while zeta potential (mV) is set as the dependent variable. Experimental data is provided by Asadi's research, including 65 data groups of the slightly decomposed peat and 66 data groups of the highly decomposed peat [15].

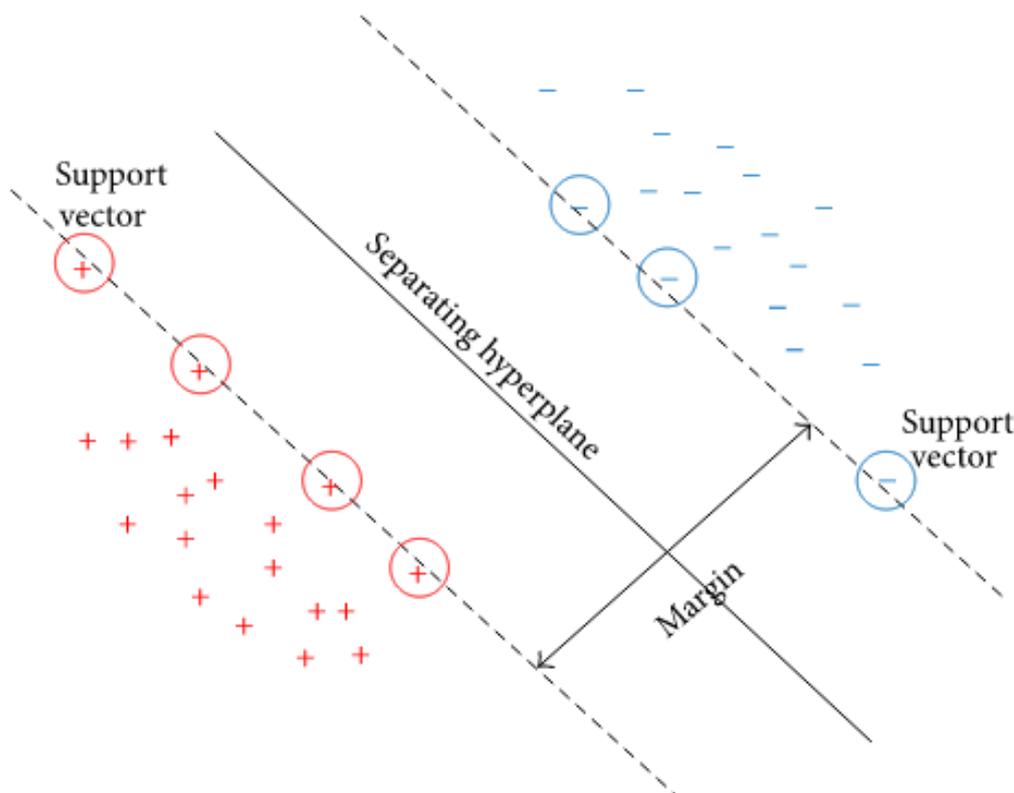
Statistical experimental results of the determination of zeta potential of decomposed peat are shown in Table 1.

**Table 1.** Statistical experimental results of the determination of zeta potential of decomposed peat (data extracted from Asadi's research [15]).

Statistical item	Hydrated radius (nm)	Cation valence	Concentration (mol/L)	pH	Zeta potential (mV)
Minimum	0.33	1	0.0001	2.790	-32.37
Maximum	0.48	3	0.0010	11.77	-1.500
Average	0.39	N/A	0.0034	7.260	-15.69

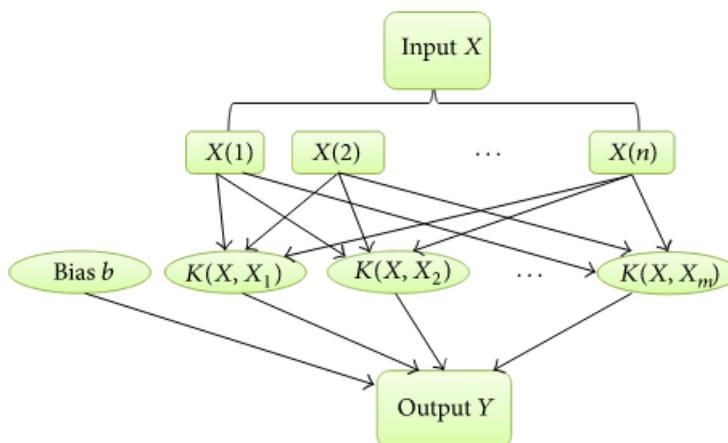
### 2.2 Support Vector Machine (SVM)

SVM is a powerful machine learning technique mainly on the basis of statistical learning theory [16]. Based on the limited information of samples between the complexity and learning ability of models, this theory has an outstanding ability of global optimization for improving generalization. In terms of linear separable binary classification, finding the optimal hyperplane, a plane that separates all samples with the maximum margin, is the main principle of SVM [17, 18]. The plane not only helps improve the predictive ability of the model, but also helps reduce the error which occurs occasionally when classifying. Figure 1 [19] shows the optimal hyperplane, with “+” representing the samples of type 1 and “-” representing the samples of type -1.



**Figure 1.** Support vectors determine the position of the optimal hyperplane [19].

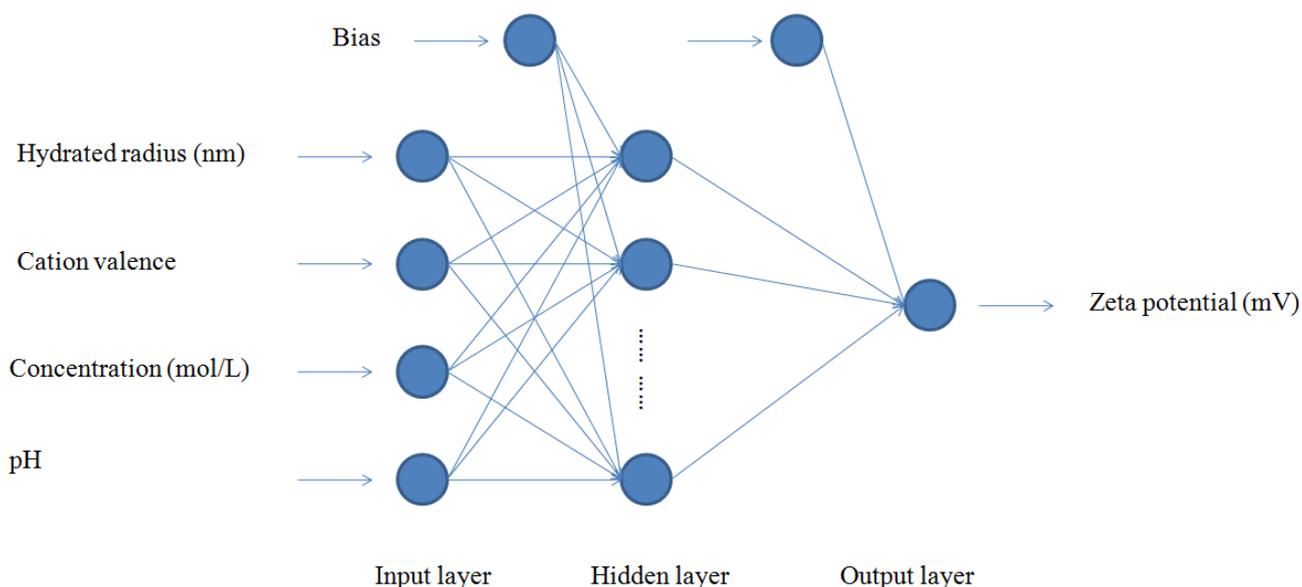
Figure 2 illustrates the main structure of a typical SVM [19]. The letter “ $K$ ” represents kernels [20]. As it can be seen from Figure 2, it is a small subset extracted from the training data by relevant algorithm that consists of the SVM. For applications, choosing suitable kernels and appropriate parameters is of great importance to get a good prediction accuracy. Nevertheless, there is still no existing international standard for users to choose these parameters. Under most circumstances, the comparison of experimental results, the experiences from copious calculating, and the use of cross validation that is available in software package are able to help us solve this problem in a relatively reliable way [19,21,22].



**Figure 2.** Main structure of a support vector machine [19].

### 2.3 Artificial Neural Networks (ANNs)

ANNs [23-25] are statistical learning algorithms with the functions of estimation and approximation based on a large number of inputs. ANNs are inspired from the biological neural networks especially the brain. They are different from networks with only one or two layers of single direction logic, using algorithms in control determining and function organizing. Interconnected artificial neural networks usually consist of neurons that can calculate values from inputs and adapt to different situations. Therefore, ANNs are capable of machine learning and pattern recognition. Due to the characters mentioned above, ANNs have gained wide popularity in inferring a function from observation especially when the data or the task is too complicated to be dealt with human brains. Figure 3 presents a schematic structure of a typical ANN for the prediction of zeta potential, which contains the input layer, hidden layer and output layer. The four independent variables are considered as neurons in the input layer in this study, including hydrated radius (nm), cation valence, concentration (mol/L) and pH, while the dependent variable, the zeta potential is considered as the only output neuron in the output layer.



**Figure 3.** Schematic structure of an ANN for the prediction of zeta potential.

### 3. RESULTS AND DISCUSSION

#### 3.1 Model Development

Here, we use novel machine learning techniques to analyze the experimental results provided by previous research [15]. 80% data group was set as the training set, while 20% data group was set as the testing set. The SVM was developed by the Matlab software. The ANNs were constructed by the NeuralTools<sup>®</sup> software (trial version, Palisade Corporation, NY, USA). General regression neural network (GRNN) [26-28] and multilayer feed-forward neural network (MLFN) [29-31] were chosen as the algorithms of ANNs.

The RMS error, required training time and prediction accuracy (under the tolerance of 30%) were used as indicators to measure the performances of the SVM and ANNs. The number of nodes of MLFNs were set from 2 to 25, from which we could find out the change regulation of the MLFNs when dealing with the development processes. Three groups of models were developed respectively, including the slightly decomposed peat (Table 2), the highly decomposed peat (Table 3) and all decomposed peat (which contains both slightly and highly decomposed peats, Table 4).

**Table 2.** Machine learning models for the prediction of zeta potential of the slightly decomposed peat.

Model	RMS Error	Training Time	Prediction Accuracy
SVM	2.37	0:00:01	100%
GRNN	3.23	0:00:01	84.6%
MLFN: 2 Nodes	2.64	0:00:39	92.3%
MLFN: 3 Nodes	2.40	0:00:44	100%
MLFN: 4 Nodes	3.14	0:00:46	84.6%
MLFN: 5 Nodes	2.43	0:00:56	92.3%

MLFN: 6 Nodes	3.09	0:01:04	84.6%
MLFN: 7 Nodes	2.83	0:01:09	92.3%
MLFN: 8 Nodes	3.43	0:01:22	84.6%
MLFN: 9 Nodes	5.16	0:01:39	69.2%
MLFN: 10 Nodes	4.61	0:01:55	76.9%
MLFN: 11 Nodes	6.29	0:01:51	69.2%
MLFN: 12 Nodes	5.96	0:02:04	69.2%
MLFN: 13 Nodes	5.81	0:02:27	69.2%
MLFN: 14 Nodes	2.93	0:02:40	84.6%
MLFN: 15 Nodes	3.45	0:03:03	84.6%
MLFN: 16 Nodes	8.72	0:03:26	61.5%
MLFN: 17 Nodes	5.03	0:03:35	76.9%
MLFN: 18 Nodes	4.33	0:03:34	76.9%
MLFN: 19 Nodes	3.15	0:03:56	84.6%
MLFN: 20 Nodes	6.33	0:04:09	69.2%
MLFN: 21 Nodes	4.21	0:04:54	76.9%
MLFN: 22 Nodes	3.54	0:05:19	84.6%
MLFN: 23 Nodes	4.43	0:05:34	76.9%
MLFN: 24 Nodes	3.95	0:06:10	76.9%
MLFN: 25 Nodes	3.25	0:06:30	84.6%

Table 2 shows that the SVM and MLFN with 3 nodes have the lowest RMS errors (2.37 and 2.40 respectively) and the highest prediction accuracies (both 100%). The SVM and GRNN have the shortest training times (both 1s). In sum, the SVM is the most suitable model for the prediction of zeta potential of the slightly decomposed peat because of its low RMS error, high prediction accuracy and short required training time.

**Table 3.** Machine learning models for the prediction of zeta potential of the highly decomposed peat.

Model	RMS Error	Training Time	Prediction Accuracy
SVM	2.71	0:00:01	92.3%
GRNN	2.20	0:00:01	100%
MLFN: 2 Nodes	3.16	0:00:40	84.6%
MLFN: 3 Nodes	2.91	0:00:42	92.3%
MLFN: 4 Nodes	2.85	0:00:52	92.3%
MLFN: 5 Nodes	4.77	0:00:58	76.9%
MLFN: 6 Nodes	2.57	0:01:06	92.3%
MLFN: 7 Nodes	3.48	0:01:08	84.6%
MLFN: 8 Nodes	2.22	0:01:29	100%
MLFN: 9 Nodes	3.29	0:01:42	84.6%
MLFN: 10 Nodes	4.24	0:01:50	76.9%
MLFN: 11 Nodes	6.38	0:01:59	69.2%
MLFN: 12 Nodes	3.08	0:02:27	84.6%
MLFN: 13 Nodes	4.83	0:02:38	76.9%

MLFN: 14 Nodes	4.65	0:02:47	76.9%
MLFN: 15 Nodes	3.92	0:03:01	84.6%
MLFN: 16 Nodes	4.90	0:03:13	76.9%
MLFN: 17 Nodes	4.75	0:03:54	76.9%
MLFN: 18 Nodes	5.53	0:04:10	69.2%
MLFN: 19 Nodes	6.25	0:05:08	69.2%
MLFN: 20 Nodes	4.71	0:05:42	76.9%
MLFN: 21 Nodes	3.77	0:05:23	84.6%
MLFN: 22 Nodes	3.39	0:06:38	84.6%
MLFN: 23 Nodes	3.73	0:06:33	84.6%
MLFN: 24 Nodes	5.23	0:07:26	69.2%
MLFN: 25 Nodes	10.19	0:09:24	0.00%

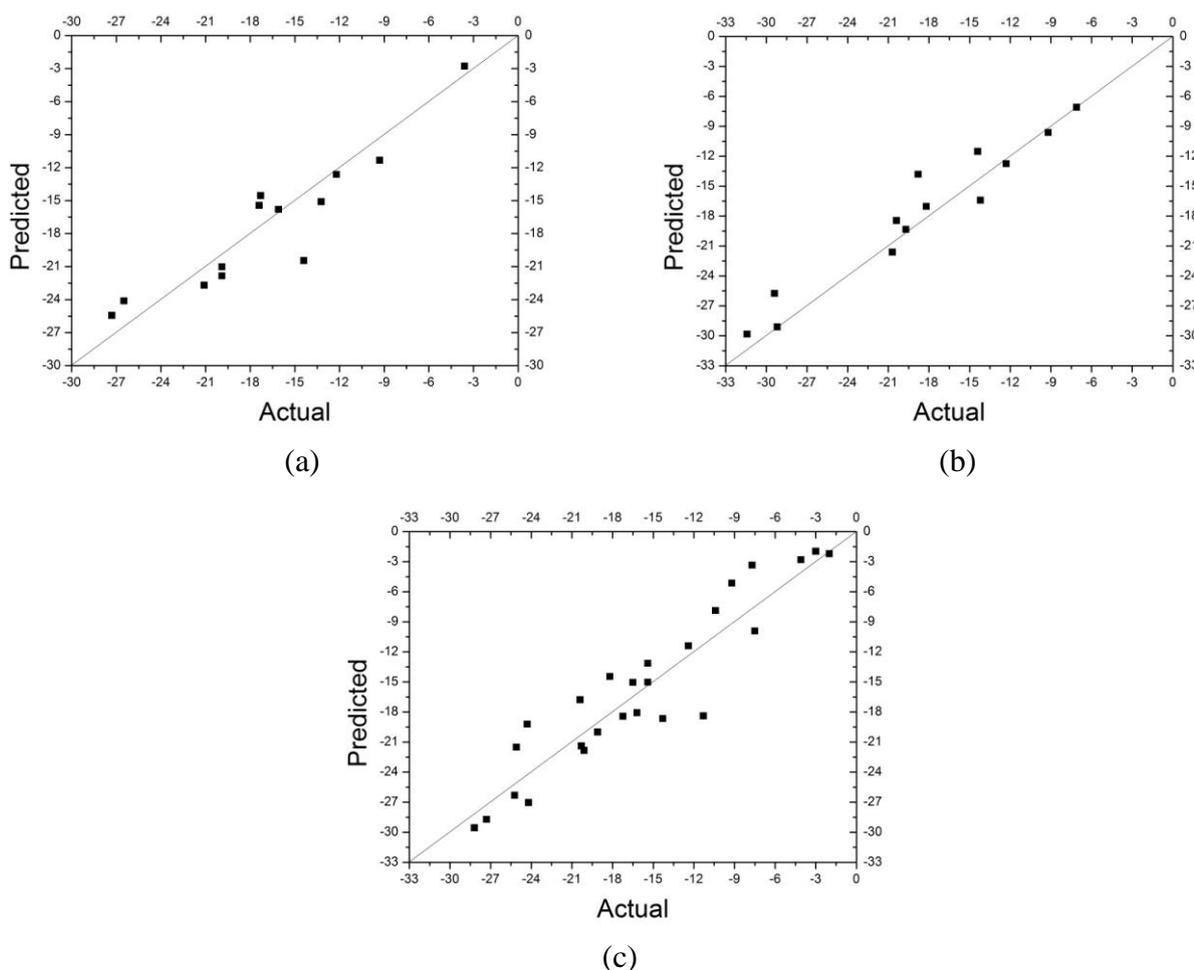
Table 3 shows that the GRNN and MLFN with 8 nodes have the lowest RMS errors (2.20 and 2.22 respectively) and the highest prediction accuracies (both 100%). However, the MLFN with 8 nodes required a much longer training time than that of the GRNN. Therefore, the GRNN is considered as the most suitable model for the prediction of zeta potential of the highly decomposed peat.

**Table 4.** Machine learning models for the prediction of zeta potential of all (both slightly and highly) decomposed peats.

Model	RMS Error	Training Time	Prediction Accuracy
SVM	3.02	0:00:01	92.3%
GRNN	3.38	0:00:01	92.3%
MLFN: 2 Nodes	3.15	0:01:12	92.3%
MLFN: 3 Nodes	3.45	0:01:16	92.3%
MLFN: 4 Nodes	3.54	0:01:17	92.3%
MLFN: 5 Nodes	4.43	0:01:30	84.6%
MLFN: 6 Nodes	3.31	0:01:53	92.3%
MLFN: 7 Nodes	4.97	0:02:02	84.6%
MLFN: 8 Nodes	5.63	0:02:19	76.9%
MLFN: 9 Nodes	4.14	0:02:26	84.6%
MLFN: 10 Nodes	5.69	0:02:39	76.9%
MLFN: 11 Nodes	4.14	0:02:45	84.6%
MLFN: 12 Nodes	5.69	0:02:57	76.9%
MLFN: 13 Nodes	4.68	0:03:10	84.6%
MLFN: 14 Nodes	4.65	0:03:28	84.6%
MLFN: 15 Nodes	5.78	0:03:40	76.9%
MLFN: 16 Nodes	6.03	0:03:54	69.2%
MLFN: 17 Nodes	7.88	0:04:11	30.1%
MLFN: 18 Nodes	9.30	0:04:42	30.1%
MLFN: 19 Nodes	8.02	0:04:38	30.1%
MLFN: 20 Nodes	7.17	0:04:42	30.1%
MLFN: 21 Nodes	14.05	0:04:56	0.00%

MLFN: 22 Nodes	14.54	0:06:12	0.00%
MLFN: 23 Nodes	10.94	0:06:23	0.00%
MLFN: 24 Nodes	15.70	0:06:03	0.00%
MLFN: 25 Nodes	20.99	0:05:41	0.00%

Table 4 shows that the SVM has the lowest RMS error (3.02) and the shortest required training time (1s). However, it can be apparently seen that results presented in Tables 2 and 3 are generally better than those in Table 4, with generally lower RMS errors and higher prediction accuracies. This phenomenon indicates that the best prediction results may appear when prediction models for the slightly and the highly decomposed peats are developed respectively. If the two stages of decomposed peats are used for making a united model (like the models presented in Table 4), the learning process may be confused because the zeta potentials of the two stages of decomposed peats may have different relationships with the independent variables we chose.



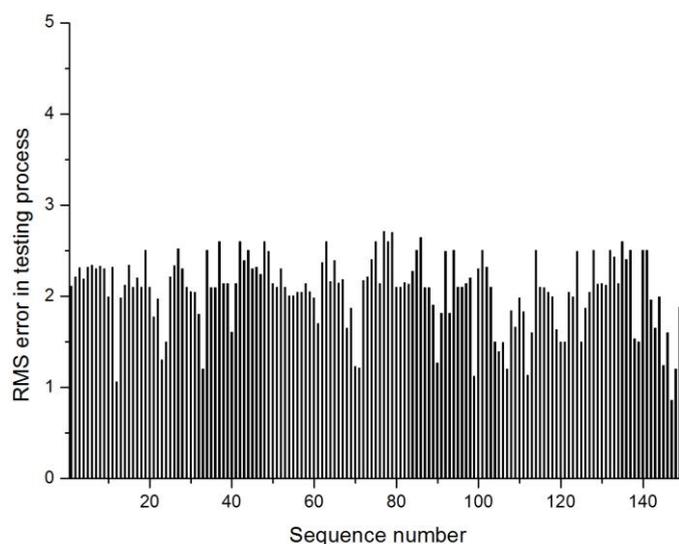
**Figure 4.** Testing results of three zeta potential prediction models. a) SVM for the slightly decomposed peat; b) GRNN for the highly decomposed peat; c) SVM for all decomposed peat.

To make the discussion more intuitionistic, Figure 4 is illustrated to show the testing results of the best models in Tables 2, 3 and 4, respectively. It shows that the predicted values of the SVM for the slightly decomposed peat [Figure 4 (a)] and the GRNN for the highly decomposed peat [Figure 4

(b)] are relatively closer to their actual values than those of the SVM for all decomposed peat [Figure 4 (c)]. Therefore, the SVM is shown as the best model for the prediction of zeta potential for the slightly decomposed peat, while the GRNN is shown as the best model for that of the highly decomposed peat.

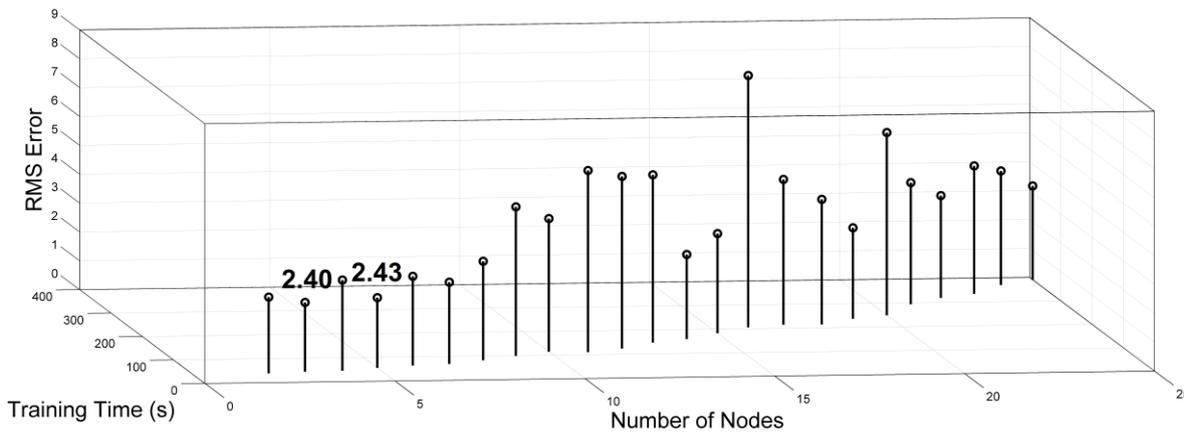
### 3.2 Robustness Analysis for ANNs

According to the principles of the SVM, it has an excellent robustness, which means that it has a good reproducibility. However, the randomness in the initial process is one of the characteristics of ANNs, which leads to different results in repeated experiments. Now that the results presented in this article has shown that the GRNN is the best for the highly decomposed peat, the reproducibility of the GRNN still cannot be neglected. To test the robustness of the GRNN in predicting the zeta potential of the highly decomposed peat, 150 repeated experiments were done (Figure 5). They show that although there exists fluctuations, the changes of RMS errors are stable, indicating that the GRNN is robust in predicting the zeta potential of the highly decomposed peat using the provided data. Therefore, the GRNN is proved to be available in practical applications.

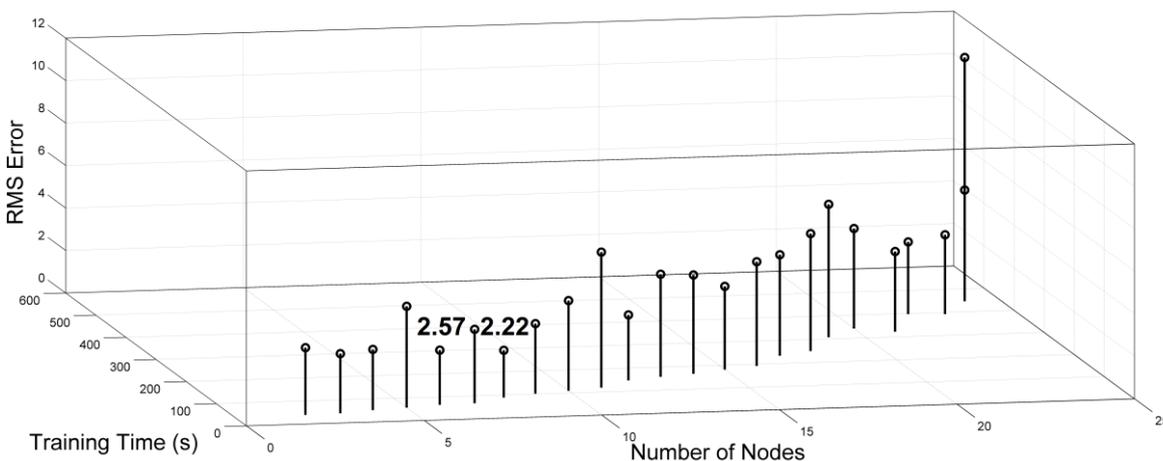


**Figure 5.** Repeated experimental results of the GRNN in predicting the zeta potential of the highly decomposed peat.

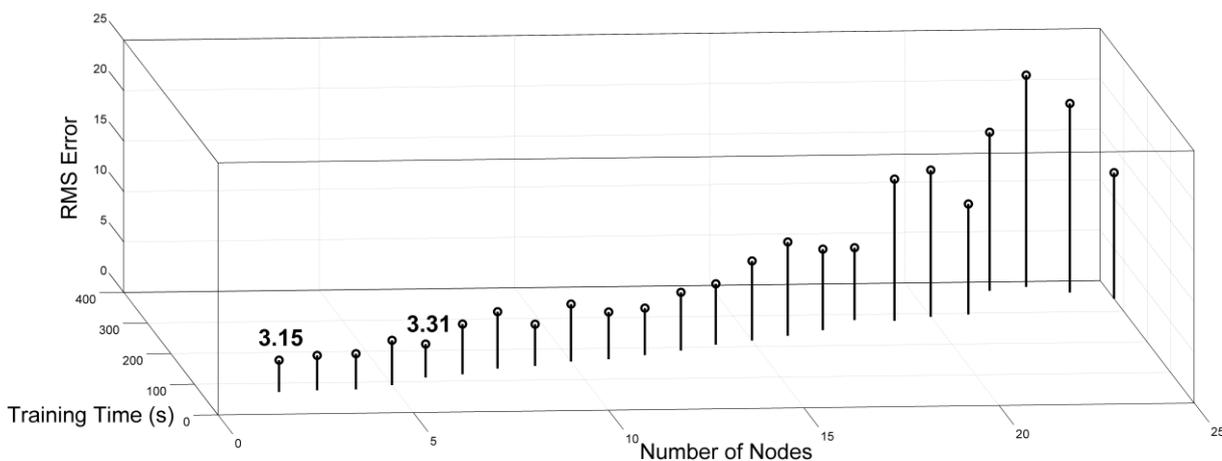
In our study, the SVM and ANNs are constructed by different softwares. Although the MLFNs are generally not as precise than the SVM and GRNN in this research, it is also clear that it can be a suitable alternative model for the prediction without a Matlab software. However, RMS errors and required training times of MLFNs are significantly different with different nodes. To show the change regulation of the MLFNs, here, we present the results of MLFNs of Tables 2, 3 and 4 in a three-dimensional way (Figure 6).



(a)



(b)



(c)

**Figure 6.** Change regulation of MLFNs in different number of nodes. Prediction of zeta potentials for (a) the slightly decomposed peat, (b) the highly decomposed peat and (c) all decomposed peat.

Figure 6 shows that in all the three prediction duties, RMS errors of the MLFNs are comparatively stable in low nodes and the required training times generally increase with the increase of the number of nodes. Meanwhile, the RMS errors in high number of nodes are not stable enough. Therefore, if we have to use an MLFN as an alternative, the MLFNs with low number of nodes can be considered.

### 3.3 Comparisons with Previous Studies

To make comprehensive comparisons between our models and previous approaches, the discussion should be divided into two parts. The first part is the comparisons between machine learning techniques and the conventional measurements for zeta potentials. The second part is the comparisons among different machine learning techniques for zeta potentials.

So far, there are various conventional approaches for measuring zeta potentials. In many different cases, some of these approaches have been widely-used in relevant fields, including the use of Smoluchowski equation [32], the use of the relationship between measured electrical signals and zeta potentials [33,34], the use of effects of ions to the zeta potentials [35] and electrophoresis technique [36]. However, all these approaches require a large number of experimental and calculation works, which have high requirements to experimental instruments and meanwhile, waste too much time and manpower. In contrast, based on the "learned" experimental data, machine learning techniques have comparatively better performances to predict the zeta potential in our cases due to its powerful capacity of finding out the relationship between independent and dependent variables. When the training process of a model is completed, users can only input the values of independent variables obtained by simple determination processes, and then the precise predicted results can be outputted automatically and quickly. Here, we use the decomposed peat as a typical example, showing that machine learning techniques have strong potentials for practical applications to measure zeta potentials. Also, with the development of computer science, machine learning models now can be developed using user-friendly softwares or packages [19,21,22,37,38]. Based on the reasons above, machine learning, our novel techniques for measuring zeta potentials, have significant advantages when being compared with other conventional popular approaches.

In terms of machine learning techniques, according to previous studies [15], the BP neural network with 19 nodes in its hidden layer was also useful for the prediction of zeta potential for decomposed peat, with an RMS error 2.50. However, on the one hand, their study didn't notice that the slightly and the highly decomposed peats can be separated and be predicted in different models respectively, which may obtain better prediction results. In fact, we can note that in the non-linear fitting process, the fitting results can be easily disturbed because the experimental conditions and the independent variables for the slightly and the highly decomposed peats are the same, which is also a reason why results presented in Table 4 are not as good as those presented in Tables 2 and 3. On the other hand, the BP neural network with 19 nodes in its hidden layer requires a comparatively high required training time due to the principles of an ANN, which is difficult for users to develop the model. Our study successfully shows that separating the peats into two decomposed stages and taking

the required training times into consideration can help us obtain better machine learning models for the prediction of the zeta potential. In addition, the use of the SVM also shows that as a novel and strong machine learning tool, SVM has great potential applications in electrochemical field. Further related studies should not only discuss the availability of ANNs, but also introduce the results of SVM when predicting. Only by making comparisons among ANNs, SVM and other prediction models, can we define the most suitable models in related prediction studies.

#### 4. CONCLUSION

Here, we successfully show that better machine learning prediction models of zeta potential of decomposed peat can be obtained by separating the decomposed peat into two stages, the slightly and the highly decomposed peats. Models are proposed respectively to find out the best prediction results for zeta potentials of the two stages. Results show that the SVM is the most suitable model for the prediction of zeta potential of the slightly decomposed peat while the GRNN is the most suitable model for the prediction of zeta potential of the highly decomposed peat due to their low RMS errors, high prediction accuracies and short training times.

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