

Research Article

Prediction of Microwave-Assisted Extraction to Determine Zinc in Fish Muscles Using Support Vector Machine and Artificial Neural Network

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Abstract: In this study, the support vector machine and the artificial neural network are adopted in the microwave-assisted extraction method to determine the amount of zinc in fish muscle samples. In the experiment, the irradiation power, irradiation time, nitric acid concentration and temperature are set as independent variables while the amount of zinc was considered as a function of the four factors. By comparing the RMS error and the training time of the support vector machine and the artificial neural network, the most suitable predicting model can be determined. The results show that the MLFN model with 7 nodes performed the best with the lowest RMS error of 1.21 and 100% prediction accuracy.

Keywords: Artificial neural networks, microwave-assisted extraction, predicting accuracy, support vector machine

INTRODUCTION

Nowadays, the Microwave-Assisted Extraction (MAE) technology is mainly used as an extraction method for its advantages of shorter time, higher extracting rate, less solvent and higher production efficiency (Hao *et al.*, 2000; Mansour and Mostafa, 2011). Also, it is a combination of advanced microwave and traditional solvent extraction (Montgomery, 2004).

Artificial Neural Networks (ANNs) are a highly simplified complex of neurons used in the modeling of different kinds of biological networks (Sharma *et al.*, 2008). It works on the principle that data is received by the input layers, processed in a non-linear way and is given out by the output layers (Bas and Boyaci, 2007). With the capacity of recognizing and reproducing the cause-effect relationships in the input-output system, ANNs are capable of modeling the most complicated systems (Montgomery, 2004; Manohar and Divakar, 2005).

Support Vector Machines (SVMs) are machine learning models that are able to analyze data and form non-linear classification. Given a set of training examples, a SVM training algorithm establishes a model that can assign different examples to one or more categories.

Currently, there have already been studies using ANN models in the experimental design (Yang *et al.*, 2014; Desai *et al.*, 2008; Basri *et al.*, 2007; Lou and Nakai, 2001; Bourquin *et al.*, 1998). Basri *et al.* (2007) applied ANN models in the lipase-catalyzed synthesis of palm-based wax ester and suggested ANN models as

an superior techniques than the Response Surface Methodology (RSM), which is another modeling and analyzing method using mathematical and statistical techniques. Also, ANN models are found to have better predictive and analytical abilities in the comparison with the RSM (Pareek *et al.*, 2002). In 2011, Mansour GhaffariMoghaddam also compared the performance of the RSM and the ANN in predicting the microwave-assisted extraction process of determining zinc in fish muscles (Montgomery, 2004).

In order to have a better understanding of amount of zinc in fish muscles, we choose the SVM and the ANN to predict the zinc amount by Flame Atomic Absorption Spectrometry (FAAS) in fish samples based on the study of Mansour.

MATERIALS AND METHODS

Experimental: According to Mansour's research, a 3-level four factor Box-Behnken experimental design was employed to establish the model. Also, the artificial network used the same experimental data used for RSM design.

In the experiment, the nitric acid concentration (1-3 mol/L), irradiation power (500-700 W), irradiation time (20-40 min) and temperature (80-120°C) were input variables. The statistical result is shown as follows in Table 1.

ANN models: Artificial Neural Networks (ANN) (Hopfield, 1998; Yegnanarayana, 2009; Dayhoff and

Table 1: Descriptive statistic of the variables for 29 samples of microwave-assisted extraction procedure to determine zinc in fish muscles

Item	Irradiation power (W)	Temperature (°C)	Time (min)	HNO ₃ concentration (mol/L)	Amount of zinc (µg/g)
Maximum	700	120	40.0	3.00	24.9
Minimum	500	80	20.0	1.00	19.3
Range	200	40	20.0	2.00	5.6
Average	600	100	30.0	2.00	22.2
Standard deviation	65.5	13.1	6.55	0.65	1.39

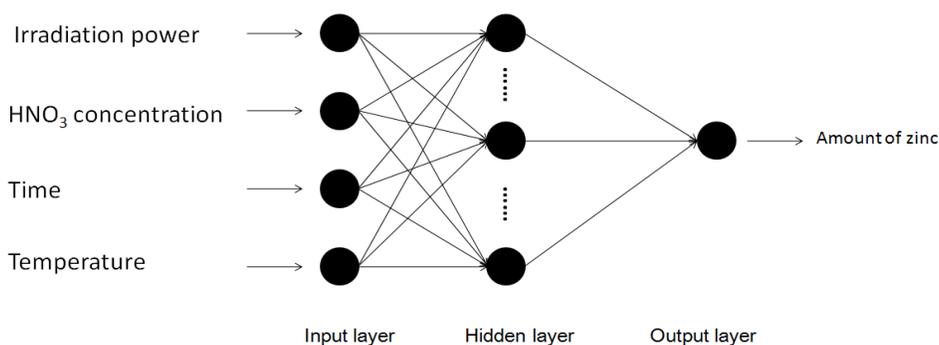


Fig. 1: Schematic structure of an MLFN in our research

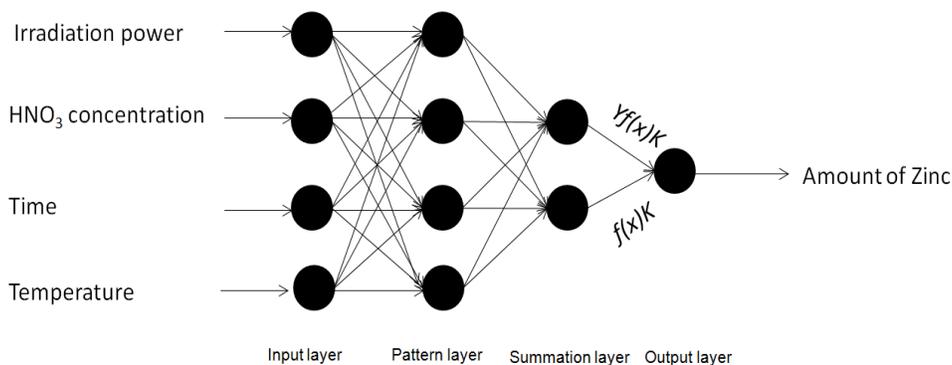


Fig. 2: Schematic structure of a GRNN in our research

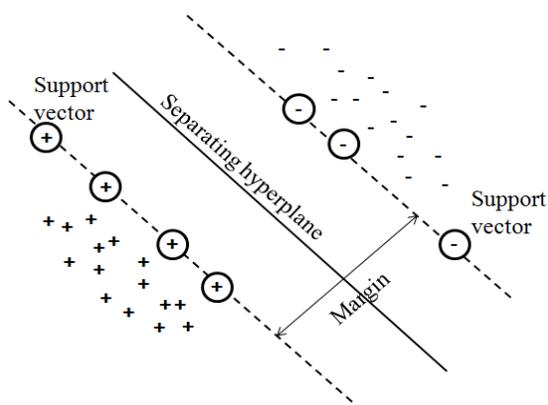


Fig. 3: The support vectors determine the position of the optimal hyperplan

DeLeo, 2001) are a series of statistical learning algorithms that can be capable of estimating and approximating once given a large amount of inputs. Inspired by the way biological nervous systems process

information, ANNs can learn by examples, improving their performance and achieving a certain responses in a parallel processing style. Though, there is a discrepancy between biological neural networks and the ANNs, for the ANNs may have multiple layers of direction logic, using algorithms in control determining and function organizing. Usually comprised of neurons which can compute values under different circumstances, ANNs have the ability of machine learning and pattern recognizing. In modeling, when the data is too complex or too much to be process by mankind, the ANNs are a perfect alternative in inferring a function from observation.

Here, Multilayer feed-Forward Neural networks (MLFN) (Svozil *et al.*, 1997; Li *et al.*, 2014a) (Fig. 1) and General Regression Neural Networks (GRNN) (Specht, 1991; Goulermas *et al.*, 2007; Khan *et al.*, 2007; Baxt 1991; Hoskins and Himmelblau, 1998; Li *et al.*, 2014b; Kandirmaz *et al.*, 2014) (Fig. 2) were used for developing alternative models for seeking the

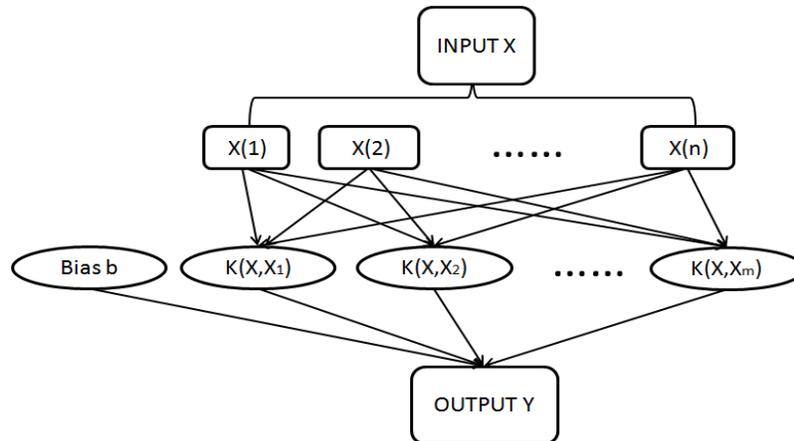


Fig. 4: The main structure of support vector machine

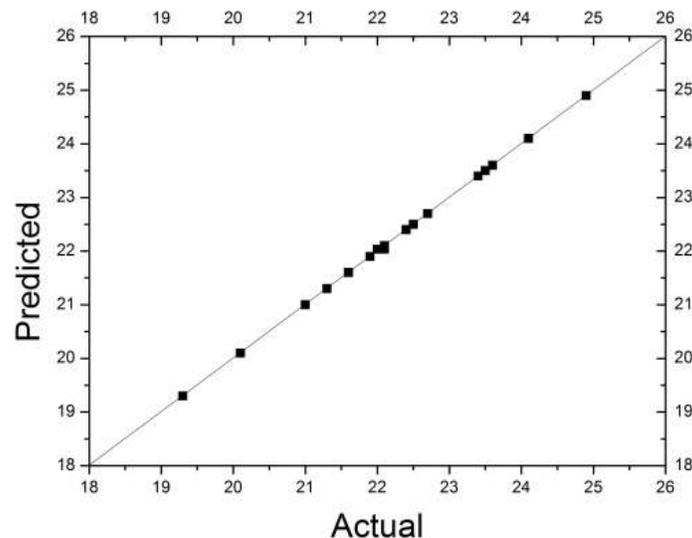


Fig. 5: Predicted values versus actual values about the raining results of the MLFN-2

optimal conditions for lipase production and bacterial growth.

SVM model: Support Vector Machine (SVM) is a learning algorithm on the principle of statistical learning theory (Deng *et al.*, 2012). Based on the limited information from samples between the complexity and learning ability of models, this theory is highly capable of global optimization in generalization improving. In regard to linear separable binary classification, the essential principle of SVM is to find the optimal hyperplane, a plane that separates all samples with the maximum margin (Zhong *et al.*, 2013; Shen *et al.*, 2012). The plane can improve the predictive ability of modeling and simultaneously reduce the errors in classifying. Figure 3 illustrates the optimal hyperplane, with “+” indicating the samples of type 1 and “-” representing the samples of type -1.

The main structure of SVM is shown in Fig. 4. The letter “K” stands for kernels (Kim *et al.*, 2005). As can

be seen from the figure, it is a small subset extracted from the training data by relevant algorithm that is composed of the support vector machine. In order to improve the predictive accuracy in classification, it is important to choose suitable kernels and appropriate parameters. However, there currently exists no mature international standard for us to choose these parameters. In most circumstances, we can overcome that problem by comparing the experiment results, judging from the copious calculating experiences and using available cross validation in software package (Fan *et al.*, 2008; Guo and Liu, 2010).

Model development: The ANN prediction models were constructed by the NeuralTools[®] software (trial version, Palisade Corporation, NY, USA) (Pollar *et al.*, 2007; Friesen *et al.*, 2011; Vouk *et al.*, 2011). The GRNN and MLFN module are adopted as the training modules.

The RMS error and training time are chosen as the indicators to measure the performances of ANN models

(Table 2). The nodes of MLFN models were set from 2 to 50. The change regulation of the MLFN models can be seen from the different nodes of models when dealing with the development process.

Table 2 indicates that the SVM, GRNN and MLFN with 7 nodes have comparatively low mean RMS errors (1.23, 1.55 and 1.21, respectively). Here, we discuss the availability of the GRNN and MLFN respectively.

RESULTS AND DISCUSSION

Comparison between the GRNN and MLFN: As can be seen from the Table 2, with the increase of nodes, the RMS errors and training time of MLFN models changed a lot, which is due to the fluctuating character of typical MLFN models. What should be mentioned is

that (Table 2) the results of different MLFN models are not fixed because the computer chooses different original values at random. However, it is undeniable that the MLFN model may have a comparatively better result (relatively lower RMS error and shorter training time) with a relatively low number of nodes than most of the MLFN models. Researchers need to use related software to select the best model among all the low number of nodes in practical application. Furthermore, among all the MLFN models, the MLFN model with 7 nodes is with the lowest RMS error and relatively shorter training time. Therefore, we consider the MLFN model with 7 nodes is the most suitable artificial neural network for the prediction of the micro-assisted extraction procedure to determine the zinc in fish muscles.

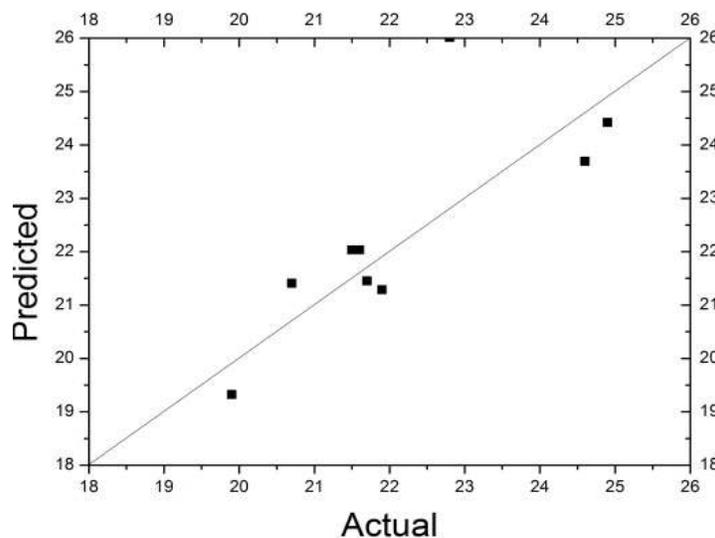


Fig. 6: Predicted values versus actual values about the testing results of the MLFN-7

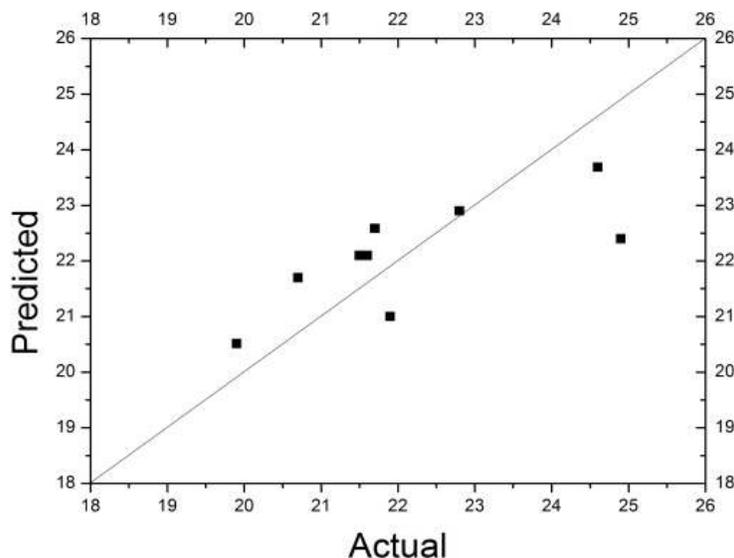


Fig. 7: Predicted values versus actual values about the testing results of the SVM model

Table 2: Best net search in different ANN models

Model type	Mean RMS error	Training time	Prediction accuracy (%)
SVM	1.23	0:00:00	100
GRNN	1.55	0:00:00	100
MLFN 2 Nodes	1.91	0:00:26	100
MLFN 3 Nodes	2.57	0:00:27	100
MLFN 4 Nodes	1.59	0:00:35	100
MLFN 5 Nodes	2.31	0:00:40	100
MLFN 6 Nodes	2.46	0:00:53	100
MLFN 7 Nodes	1.21	0:01:07	100
MLFN 8 Nodes	3.27	0:01:31	88.89
MLFN 9 Nodes	3.46	0:01:56	88.89
MLFN 10 Nodes	4.43	0:02:34	77.78
MLFN 11 Nodes	1.75	0:03:12	100
MLFN 12 Nodes	1.34	0:04:04	100
MLFN 13 Nodes	6.09	0:05:30	88.89
MLFN 14 Nodes	2.82	0:06:54	100
MLFN 15 Nodes	2.38	0:10:31	100
MLFN 16 Nodes	2.31	0:51:30	100
MLFN 17 Nodes	4.54	0:55:33	77.78
MLFN 18 Nodes	2.42	0:58:31	100
MLFN 19 Nodes	2.41	1:03:00	100
MLFN 20 Nodes	4.50	0:01:36	77.78
MLFN 21 Nodes	7.32	0:01:41	33.33
MLFN 22 Nodes	4.57	0:01:46	77.78
MLFN 23 Nodes	6.16	0:01:53	88.89
MLFN 24 Nodes	6.43	0:01:56	77.78
MLFN 25 Nodes	7.19	0:02:01	44.44
MLFN 26 Nodes	13.57	0:02:09	44.44
MLFN 27 Nodes	9.24	0:02:10	55.56
MLFN 28 Nodes	8.30	0:02:13	77.78
MLFN 29 Nodes	9.51	0:02:21	44.44
MLFN 30 Nodes	9.98	0:02:28	55.56
MLFN 31 Nodes	7.25	0:02:30	77.78
MLFN 32 Nodes	3.61	0:02:33	88.89
MLFN 33 Nodes	11.42	0:02:38	44.44
MLFN 34 Nodes	10.26	0:02:45	66.67
MLFN 35 Nodes	11.60	0:02:48	33.33
MLFN 36 Nodes	7.61	0:03:00	55.56
MLFN 37 Nodes	12.07	0:03:01	44.44
MLFN 38 Nodes	11.32	0:03:07	44.44
MLFN 39 Nodes	16.16	0:03:09	55.56
MLFN 40 Nodes	11.75	0:03:15	66.67
MLFN 41 Nodes	15.22	0:03:17	33.33
MLFN 42 Nodes	10.02	0:03:24	44.44
MLFN 43 Nodes	8.59	0:03:26	44.44
MLFN 44 Nodes	8.51	0:03:35	44.44
MLFN 45 Nodes	10.48	0:03:37	44.44
MLFN 46 Nodes	10.27	0:03:46	44.44
MLFN 47 Nodes	9.21	0:03:54	44.44
MLFN 48 Nodes	12.34	0:03:51	55.56
MLFN 49 Nodes	9.45	0:04:00	66.67
MLFN 50 Nodes	23.62	0:04:02	33.33

Comparison between the GRNN and MLFN: The ANN models are firstly compared to each other because they share the same mechanism. Firstly, we take into consideration the results of GRNN. From Table 2, we can see that the GRNN model has a short training time, compared to most of the MLFN models. One the one hand (Table 2) the RMS error of the GRNN is 100% which indicates an utmost accuracy. On the other hand, according to the principles of the GRNN, it also has a high reproducibility. Also, the robustness of the GRNN models can be seen by repeating the experiments for the GRNN models.

The mean RMS error and training time should be taken into consideration when comparing the MLFN

models with different numbers of nodes. In this study, we define that among all the MLFN models, the one with a lower RMS error or with a shorter training time at the same time can be considered as the better one. Thus, from Table 2, although with a comparatively longer training time, the MLFN with 7 nodes has the lower RMS error than the GRNN model. And in a computer with higher performance, the differences of the training times can be overlooked in a certain range of nodes of MLFN. Therefore, here we still consider the MLFN model with 7 nodes to be the better one than the GRNN model (with the RMS error of 1.21).

Comparison between the MLFN-7 and SVM: Here, availability of the MLFN-7 is presented by the typical examples of the training and testing results and the testing results of the SVM are also illustrated. Figure 5 and 6 are used for the illustration of the training and testing results of the MLFN-7, while Fig. 7 is used for the illustration of the testing results of the SVM. The MLFN-7 and SVM share the same training and testing sets.

In order to show the capacity for recall of the MLFN-7 model for microwave-assisted extraction procedure to determine zinc, Fig. 5 is used for illustrating the training results of the MLFN-7.

Figure 5 shows that the MLFN-7 is strongly capable of recalling the non-linear fitting process. The predicted values can accurately fit the actual values (Fig. 5a), which indicates a high decency in the non-linear fitting effects of the model.

We use the data set which has not been used for the training process to validate the MLFN-7. Results are shown in Fig. 6. Figure 6 shows the predicted results during the testing process. Predicted values are close to the actual values (Fig. 6a). Results present the robustness and availability of the MLFN-7 during the testing process.

In terms of the testing results of the SVM, the precision and robustness of the SVM in the prediction section can be shown in Fig. 7. From Fig. 7 we can see that the testing result of SVM is more analogical and precise, compared to the testing results of the MLFN-7. Also, we can see that the testing results of the SVM are quite similar to those of the MLFN-7.

To compare the MLFN-7 with the SVM, we should firstly pay attention to the fact that the MLFN-7 chooses its original values randomly during the training process, which will result in different results in repeated experiments. Compared with the MLFN-7 model, the repeatable results of the SVM models are better because of its principle and algorithm. However, irrespective of the fluctuations of the RMS errors, results of repeated experiments show that still the MLFN-7 has a high robustness because the MLFN fluctuations are in a controllable range. When comparing the training time of the three models, both the GRNN model and the

SVM model have a shorter training time than those of the MLFN models in the experiment process. However, since nowadays the required time for machine learning process can be dramatically reduced by a faster calculation machine, the training time of the MLFNs with low nodes can also be ignored on a high-performance computer. Therefore, after considering the RMS error and the prediction accuracy, the MLFN-7 should be taken as the most suitable machine learning model in the prediction of the microwave-assisted extraction procedure to determine zinc in fish muscles.

CONCLUSION

We successfully find that machine learning techniques including SVM and ANNs are useful for the prediction of the microwave-assisted extraction to determine zinc in fish muscles. Results show that the SVM and MLFN with 7 nodes have relatively low RMS errors while the GRNN and SVM have the shortest required training times. The best prediction accuracy (30% tolerance) presented in the MLFN-2 model (100%). Our research successfully shows that machine learning techniques like the SVM and ANNs can be precisely applied for the prediction of the microwave-assisted extraction to determine zinc in fish muscles.

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