SIZE PREDICTION OF SILVER NANOPARTICLES USING ARTIFICIAL NEURAL NETWORK

A DISSERTATION
SUBMITTED IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE AWARD OF THE DEGREE
OF

MASTER OF TECHNOLOGY
IN
NANOSCIENCE AND TECHNOLOGY

Submitted by:
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MAY, 2022

CANDIDATE'S DECLARATION

I, Anubhab Biswas, 2K20/NST/01 of M. Tech Nanoscience and Technology, hereby declare that the project Dissertation titled "***Size Prediction of Silver Nanoparticles using Artificial Neural Network***" which is submitted to the Department of Applied Physics, Delhi Technological University, Delhi in partial fulfillment of the requirement for the award of the degree of Master of Technology, is a review of literature and not copied from any source without proper citation. This work has not previously formed the basis for the award of any Degree, Diploma Associateship, Fellowship or other similar title or recognition.

Place: Delhi **ANUBHAB BISWAS**

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CERTIFICATE

I hereby certify the Project Dissertation titled "***Size Prediction of Silver Nanoparticles using Artificial Neural Network***" submitted by Anubhab Biswas, 2K20/NST/01, Department of Applied Physics, Delhi Technological University, Delhi in partial fulfillment of the requirement for the award of the degree of Master of Technology, is a record of the project work (a review only) carried out by the student under my supervision. To the best of my knowledge, this work has not been submitted in part or full for any degree or Diploma to this University or elsewhere.

Place: Delhi

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ACKNOWLEDGEMENT

I would like to express my profound gratitude to the Dept. of Applied Physics, Delhi Technological University and especially to my supervisor Dr. M.S. Mehata for all the support and guidance he provided throughout the course of my work.

ABSTRACT

The study emphasized the estimation and prediction of the size of silver nanoparticles, which are prepared via green synthesis, using the concept of an artificial neural network. A certain number of recordings of a suitable, thoroughly conducted experiment was taken into account, in which parameters like concentration of plant extract, reaction temperature, the concentration of silver nitrate and stirring duration were taken as input, whereas the size of silver nanoparticles was taken as the undisputed output. After taking all the possible parameters into account, we have been able to design an artificial neural network controller using the MATLAB platform, based completely on back propagation algorithm. After rigorous training of the ANN controller and adjusting the relevant network-based controller parameters, it is found to be performing close enough to expect. And as a result, we have also been able to determine the contribution of each factor involved in tuning the size of silver nanoparticles formed or prepared. We believe this proposed model can contribute to a greater extent when it comes to exploration of a wide range of applications and to exploration of possibilities of reduction of requirement of materials to a huge extent to produce silver nanoparticles with desirable sizes under optimised condition.

Keywords: Artificial neural networks (ANN); MATLAB; back propagation algorithm (BPA)

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LIST OF ABBREVIATIONS

ANN	: Artificial Neural Network
MSE	: Mean Squared Error

1. INTRODUCTION

1.1 Introduction to silver nanoparticles

Silver nanoparticles have been genuinely one of the interesting subjects of research for the researchers in modern times because of their multiple unique properties, e.g., optical, electrical and microbial. The production of nano-particles via modern tools has genuinely emerged as one of the most significant applications in the healthcare field, catering especially to multiple diversified demands of bio and pharma sectors [7].

The modern concept of nanotechnology, though, has a history that dates way back to the ninth century, when gold and silver nanoparticles were indeed used to get utilized by the craftspeople from Mesopotamia, in order to produce a scintillating effect over the surface of pots. Still, the first ever science-based illustration of nano-particle properties was given by none other than Michael Faraday. In contrast, the term 'nanotechnology' was put on the table for the first time by Richard Feynman in 1959, which marked the beginning of a modern era of nanotechnology [7, 9].

Multiple efforts are reportedly being made across the globe to innovate and develop eco-friendly technologies to further produce less harmful and non-toxic products with the help of green nano-technology and bio-technology. Mentioning about biotechnological tools, nanobiotechnology is achieving enormous recognition in the modern era, owing to its capability to attune metals at the nanoscale, which effectively modifies their various properties. Nanoparticles produced via biological methodologies or green technology are expected to possess assorted natures with comparatively higher permanence and congruous proportions since they are manufactured mainly via single-step procedures [7].

Researchers are also found to have been reportedly emphasizing vapor phase synthesis of nanoparticles, which is found to have provided immense control in attaining desirable morphology and non-agglomerated nanoparticles that too with the narrow-size distribution. Since not enough inquisitions on the aspects influencing the synthesis of nanoparticle and their characterization have been carried out, this review has emphasized this very aspect [9].

1.2 Neural networks

As far as this study is concerned, the development of a mathematical model to carry out the estimation of the size of the silver nanoparticles and the establishment of the correlation of the factors influencing the morphology of synthesized nanoparticles becomes vital. Artificial neural networks (ANNs) are computerised programs designed to carry out simulation of neurons in the human brain and how it processes and handles data [5, 13].

ANNs are generally used or deployed to unravel the non-linear relationship between inputs and outputs. One of the main merits of ANNs is its immense capability to deliver efficient and optimized performance when it comes to estimation of the size of silver nanoparticles as well as determination of the contribution of each parameter to the size of silver nanoparticles.

The aim of the study was to carry out a sensitivity based analysis in order to evaluate the impact of input variables in the form of amount of plant extract, reaction temperature, stirring duration and molar concentration of silver nitrate in the considered green synthesis over the morphology and size of silver nanoparticles produced [1,5].

2. DATA COLLECTION AND METHODOLOGY

2.1 Data set and selection

Recognizing the relevant parameters of green synthesis, which influence the size or morphology of silver nanoparticles is an important step of mathematical modeling and optimization, if not the most important. Shabanzadeh investigated the green synthesis of silver nanoparticles using *Vitax negundo L* extract [4, 13] They actually ended up stating that the size of silver nanoparticles was found to be influenced mainly by four input parameters named plant extract, reaction temperature, stirring duration and molar concentration of silver nitrate.

Table 3.1 summarizes the details of 30 odd practical observations made based on operational conditions of literature. Given data has been evenly divided into multiple testing and training sets to achieve the optimized performance of the ANN controller and achieve stable results, eventually indicating a contribution of each factor to the size of silver nanoparticles [3, 4].

2.2 Analysis based on ANN modelling

The ANN-based analysis has been undertaken using MATLAB software to model complex non-linear relationships between given multiple inputs and single output parameters. 30 odd experiments were considered for training ANN, in which parameters like plant extract, reaction temperature, stirring duration and molar concentration of silver nitrate were taken as input variables into account. In contrast, the size of silver nanoparticles was taken as an output variable into account. Training of neural network was eventually carried out using feed-forward back propagation algorithm with hyperbolic tangent sigmoid function as the transfer function for hidden as well as for output layers [3,21].

In order to introduce a learning function for the prepared networks, the Levenberg-Marquardt learning methodology was eventually adopted. Also, in order to unravel the network architecture as well as to make sure overfitting does not occur, we began from the minimum number of neural units up to the smallest possible number of neurons, generating a network controller with the highest possible predictability, with no overfitting phenomena taking place [4, 13].

Therefore, the concepts of correlation coefficient and mean square error were eventually utilized to make sure the quality of training procedure and the predictability of the designed model were not compromised. From the network selected out of the multiple networks prepared (based on predictability and performance), the relative contribution of each input variable to the output variable was eventually determined [3, 4, 13].

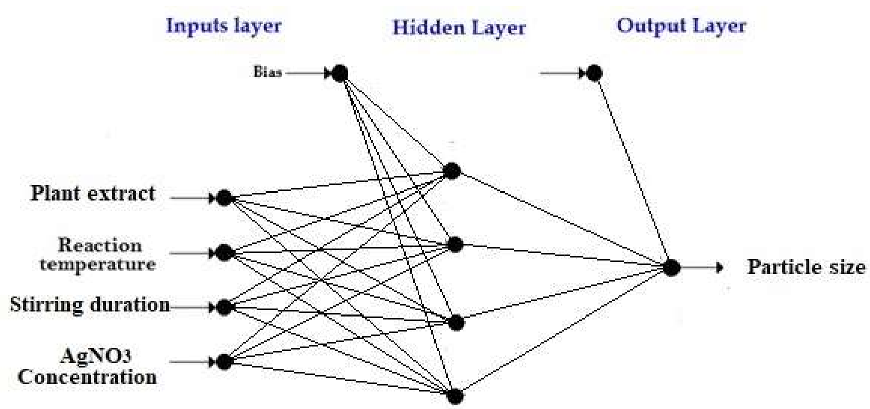

Figure 2.1: Architecture of ANN utilized to estimate the particle size of silver nanoparticles.

3. RESULTS AND DISCUSSION

3.1 Data analysis using ANN

A neural network consisting of four neurons representing plant extract, reaction temperature, stirring duration, and molar concentration of silver nitrate as input variables. One neuron representing the size of silver nanoparticles formed as an output variable and four more neurons present in the hidden layer has been successfully designed and modeled. The weight and bias values were successfully determined while considering sigmoid transfer function, especially for the hidden layer [2,3].

And ultimately, we decided to undertake the connection-weight approach, as it is found to be offering the best possible methodology for carrying out precise quantification of variable importance. The mentioned technique successfully identified the relevance of each input variable participating in the neural network, which showcases any correlation at every possible level with the outcome [3,19].

Table 3.1 represents experimental data for the preparation of silver nanoparticles carried out via green synthesis, where plant extract, reaction temperature, stirring duration and molar concentration were taken as input variables [4].

Table 3.1: Experimental data for the synthesis of silver nanoparticles.

No.	Plant extract (g in 100ml water)	Reaction temperature (°C)	Stirring duration (hr)	Molar concentration of silver nitrate (in 100ml water)	Size of nanoparticles (nm)
1	0.1	25	48	0.1	27
2	0.1	30	48	0.2	28
3	0.1	40	48	0.5	29
4	0.1	50	48	1	29
5	0.1	60	48	1.5	31
6	0.1	70	24	2	32
7	0.25	25	24	0.1	25
8	0.25	30	24	0.2	26
9	0.25	40	24	0.5	26
10	0.25	50	24	1	27
11	0.25	60	12	1.5	27
12	0.25	70	12	2	29
13	0.25	25	12	0.1	18
14	0.5	30	12	0.2	19
15	0.5	40	12	0.5	21
16	0.5	50	6	1	21
17	0.5	60	6	1.5	24
18	0.5	70	6	2	24
19	0.75	25	6	0.1	15
20	0.75	30	6	0.2	16
21	0.75	40	3	0.5	18
22	0.75	50	3	1	19
23	0.75	60	3	1.5	20
24	0.75	70	3	2	21
25	1	25	3	0.1	16
26	1	30	1	0.2	16
27	1	40	1	0.5	17
28	1	50	1	1	18
29	1	60	1	1.5	18
30	1	70	1	2	19

Fig. 3.1 represents the graphical representation of the designed ANN model based on the comparison between predicted and practical values, showing the proposed model fits perfectly well with data extracted from the conducted experiment.

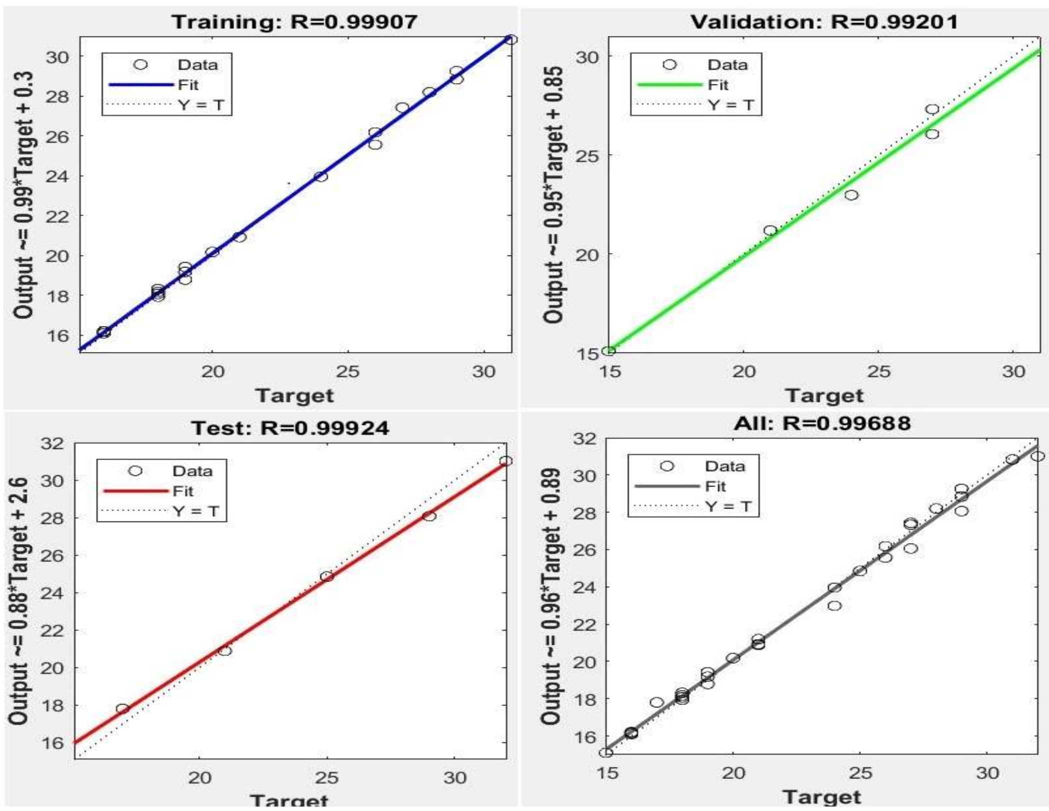

Figure 3.1: Observed versus predicted values for training, validation, testing and all data sets.

Fig. 3.2 represents the Mean Squared Error (MSE) of data sets of training, validation and testing taking place, and eventually, the best validation performance is found to be 0.41448 at epoch 6 or 6th iteration.

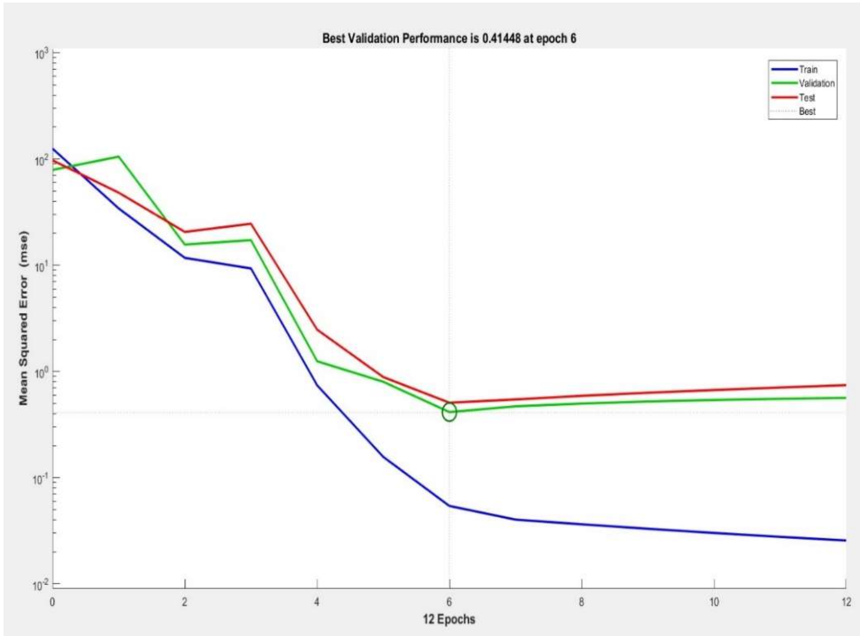

Figure 3.2: Mean squared error of data sets of training, validation and testing.

Table 3.2 shows the values of input-hidden connection weights as well as hidden-output connection weights respectively of the proposed and designed Artificial Neural Network.

Table 3.2: Values of input-hidden and hidden-output connection weights.

w1 — 4x4 double

	1	2	3	4
1	-2.4569	0.0490	3.4222	2.0448
2	-2.5953	0.3536	-0.3190	-2.4195
3	0.3728	0.3299	-1.1966	-0.4554
4	-1.2099	2.3459	-0.4574	0.2262

w2 — 1x4 double

	1	2	3	4
1	-0.1626	-0.2465	-1.0657	0.2548
2				

Table 3.3 shows the values of input-hidden connection biases as well as hidden-output connection biases respectively of the proposed and designed Artificial Neural Network.

Table 3.3: Values of input-hidden and hidden-output connection biases.

b1 (4x1 double)

	1	2
1	6.8427	
2	-1.2170	
3	-0.7429	
4	2.0905	

b2 (1x1 double)

	1	2	3
1	-0.2484		

3.2 Statistical analysis

In this study, statistical analysis preferably refers to exploring variable importance or contribution of each input parameter involved in the considered green synthesis of silver nanoparticles, to the output using ANN. Table 3.4 represents the determination of variable importance of input, involved in the preparation of nanoparticles, corresponding to output, based on the connection-weight approach [5, 25].

Table 3.4: Determination of contribution of each input parameter to output.

X \ Y	Hidden A	Hidden B	Hidden C	Hidden D
Input 1	-2.4569	0.0490	3.4222	2.0448
Input 2	-2.5953	0.3536	-0.3190	-2.4195
Input 3	0.3728	0.3299	-1.1966	-0.4554
Input 4	-1.2099	2.3459	-0.4574	0.2262

X

	Hidden A	Hidden B	Hidden C	Hidden D
Output	-0.1626	-0.2465	-1.0657	0.2548

X \ Y	Hidden A	Hidden B	Hidden C	Hidden D
Input 1	0.3994	-0.0120	-3.6470	0.5210
Input 2	0.4219	-0.0871	0.3399	-0.6164
Input 3	-0.0606	-0.0813	1.2752	-0.1160
Input 4	0.1967	-0.5782	0.4874	0.0576

$$Input_X = \sum_{Y=A}^{E} Hidden_{XY}$$

	Importance	Rank
Input 1	-2.7386	4
Input 2	0.0583	3
Input 3	1.0173	1
Input 4	0.1635	2

CONCLUSION

We managed to innovatively design an artificial neural network with success, which was meant to explore the contribution, or variable importance of each input parameter corresponding to the size of silver nanoparticles in the form of an output prepared via green synthesis based on *Vitax negundo L* extract [4, 5]. The ANN design was also found to be inherently capable of estimating the size of synthesized silver nanoparticles, with emphasis on the determination of variable prominence of each input parameter corresponding to the output. The determination of the variable importance of input parameters was mainly carried out using the connection-weight approach, with stirring duration found to be contributing the most, followed by molar concentration, reaction temperature, and plant extract [5].

We decided to undertake this approach over other similar quantifying approaches like Garson's algorithm, Partial derivatives, Input perturbation, Sensitivity Analysis, etc. It has been found that the Connection weight approach possesses the ability to offer the comparatively best possible methodology to carry out quantification of variable importance with a lot of accuracy and precision [3, 25].

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