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Utilizing an Innovative Deep Learning Technique for Predictive Modeling and Response Analysis in the Context of Spent Catalyst Bioleaching

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Abstract

Utilizing microorganisms, spent catalyst bioleaching is a technique for extracting precious metals or other materials from used catalysts. Chemical processes can be accelerated by catalysts without consuming any of the materials involved. Reaching a high level of selectivity for the desired metals might be problematic. Using a leaching solution to dissolve or remove the molybdenum (Mo) from the catalyst material is the first step in the leaching process. Mo is extracted at a lesser rate than other metals by the use of acidophiles in the bioleaching of used catalysts. Mo-leaching with alkaline chemicals or other microbes has been investigated as a potential solution to this issue. This research optimization using Stochastic Gradient Descent (SGD) and Dynamic Deep Neural Network (DDNN) method was trained to predict the data on using Escherichia coli, Mo bioleaching from the wasted catalyst. Response modeling was used to investigate how metal extraction varied with changes in temperature, residence time, pulp density and particle size. The DDNN method is used to prevent over fitting on the training set throughout the training process. Using the coefficient of determination R^2 score, the optimal network architecture was determined and tested on a test dataset. The most successful network was determined to have a two-layer hidden layer architecture with a logistic activation function (R^2 = 0.978).

Keywords: Spent Catalyst, Bioleaching, Chemical, Stochastic Gradient Descent Dynamic, DDNN, Mo-leaching

Full length article **Corresponding Author*, e-mail: jaspreet.sidhu.orp@chitkara.edu.in

1. Introduction

The massive amount of high-metal industrial waste created has forced the industry to search for recycling solutions in situations when basic mineral supplies are depleted or restricted. Modern research on metal extraction is focused on secondary metal resources while emerging technologies are supporting main metal resources in response to the increasing need for metals globally. For any recycling technique to be expanded for a full-scale operation for recovering metal values, it must be economical and environmentally beneficial [1]. A biotechnological answer to this problem is presented by the idea of wasted catalyst bioleaching. The use of microorganisms in biological leaching, a method for removing precious metals from ores, is expanded to include wasted catalysts. This procedure is in line with the ideas of the circular economy and green chemistry yet it differs from conventional disposal methods [2]. Solid catalysts are utilized for processing crude oil in an oil refinery to produce higher-quality petroleum products. These solid catalysts are composed of metals in the form of oxides of metals, metal sulfides, nickel, aluminum, molybdenum, zinc and cobalt, among others. When solid catalysts are used in the refining of crude oil, they lose their

ability to be used again and these results in a waste product known as a waste catalyst [3]. Specialized microorganisms, bacteria, are used in spent catalyst bioleaching to target and remove valuable elements from the wasted catalyst matrix in a targeted manner. Through their interactions with the catalyst's material, these microbes can change or break down the substance's architecture in a manner that makes it easier to extract rich results in reduced environmental toxicity, using wasted secondary sources such as catalysts of the aforementioned metals is metals or other resources [4]. This strategy helps to create a more sustainable and profitable industrial landscape by providing a way to recover resources while simultaneously reducing the negative environmental impact of conventional disposal techniques [5]. The use of biotechnological methods for the handling of wasted catalysts highlights the increasing significance of environmentally and financially sustainable solutions in industrial processes. In addition to reducing waste, spent catalyst bioleaching has the potential to unlock the latent value of wasted catalysts, supporting more ethical and sustainable industrial procedures [6]. The incorporation of spent catalyst bioleaching into industrial processes might become a crucial tactic for making the most use of available resources and reducing the environmental effect of the chemicals and metallurgy sectors as this field's development and research continue [7]. Significant amounts of coke and metals can be found in the spent catalysts generated from both procedures. In the wasted hydro-processing catalyst, the concentrations of depositing elements are greater. After fulfilling their catalytic role in industrial processes, spent catalysts often include priceless metals like molybdenum. Utilizing microorganisms, such as fungus or bacteria that are acidophilic, bioleaching is an eco-friendly substitute for traditional chemical leaching techniques in which metals are extracted selectively [8]. Moreover, the rates of metal recycling are poor even in affluent nations necessitating the development of systems that enable high recycling rates. Because it lowers the need for fundamental mineral resources, lowers the cost of purchasing a new catalyst and very advantageous [9]. Regeneration is feasible when the catalyst's activity falls below the permissible threshold. However, it is not always achievable. The catalyst activity falls to values below what is considered acceptable after a few rounds of reuse coupled with regeneration and further regeneration cannot be economically viable known as "spent catalysts," these catalysts are disposed of as solid trash. Globally, an estimated 4 x 108 kg of wasted catalysts is produced each year [10]. The study [11] offered using machine learning (ML) techniques might eliminate the need for expensive and time-consuming trials to determine the ideal circumstances for the bioleaching procedures, which are complicated and time-consuming. ML is a branch of artificial intelligence that has been shown to be accurate, dependable and economical in a range of settings. Random forest regression yielded the best results out of 40 regression-based machine-learning algorithms and it was used to create an effective bioleaching process model. The research [12] presented work showcases the capability of cyanogenic bacteria to extract platinum group metals (PGM) from spent automotive catalysts (SAC) by bioleaching. Bacillus megaterium and Pseudomonas fluorescence were the two mesophiles used in the bioleaching of PGM from SAC. Studies on leaching under various circumstances were conducted to look into the production of cyanide and its function in PGM solubilization. The research [13] looked at how ultrasonic assistance with nitric acid pre-treatment affected the amount of PGMs that cyanogenic bacteria were able to leach. Using ultra sonication and acid pre-treatment, SAC specimens were first made free of competitive elements that can interfere with the PGM-cyanidation process following bioleaching. It was determined that an ultrasound power of 80%, a nitric acid concentration of 6M, an ultrasound duration of 50 minutes and an ultrasound wavelength of 37 kHz were the ideal pre-treatment settings.

The article [14] proposed method for recovering precious metals, such as rare earth elements (REE), from commercial or consumer trash, which is bioleaching using organic acids. When agricultural or food scraps are utilized as the bioleaching agents' carbon substrates synthesis, bio hydrometallurgy can be a profitable and ecologically responsible method of recycling rare earth elements. An obstacle to REE bioleaching using organic acid is the partial transformation of a carbon base into an ideal combination of organic acids that has a high capacity to extract REEs. Native acidophilic bacteria from hot, acidic springs and mine drainage were gathered for this study's bioleaching tests [15]. On a variety of minerals, the native acidophilic bacteria were cultivated. To investigate bioleaching over time, uninoculated controls were used to assess variations in the amounts of heavy metals, pH and Eh. Therefore, depending on the kind of minerals, temperature and other factors, as well as the microorganisms' origin, the characteristics of bioleaching differed substantially. To represent and forecast these intricate bioleaching tendencies, we used an artificial neural network (ANN) model. Study [16] offered the ecologically sound preparation of the possibility of enabling the extraction of metals linked to platinum from spent three-way catalysts (TWC) *Acidithiobacillusthiooxidans* has been investigated for its ability to bioleach aluminum by acid. When contrasted with elemental sulfur that is sold for business, the synthesis of acid by A. thiooxidans was enhanced by the use of biogenic sulfur derived from desulfurization bioreactors. In comparison to a control batch made using commercial H_2SO_4, the lixiviation capacities of biogenic acid-containing bacteria and biogenic acid-containing bacteria in an exponential or stationary state were examined. Recycling old batteries is feasible both environmentally and economically, as the study [17] provide at their essential metal composition found. Conventional hydrometallurgical and pyro metallurgical extraction techniques need dangerous chemicals or require a lot of energy. It has been proposed that bioleaching manganese from discarded batteries as a secondary resource can accomplish two goals: lessen environmental impact and create income from waste. Along with being a straightforward process that generates less dangerous by-products, a bioleaching process can function with lower operational expenses, energy and water use. An effective acidithiobacillus caldus UVS10 bioleaching strain was produced in this investigation. The metallic biological leaching performance of “A. caldus UVS10 to spent FCC catalyst (SFCCC)” was assessed using batch and bioreactor testing. Batch outcomes of the experiment indicated that the SFCCC. Elevated SFCCC pulp density impeded metal leaching. A. caldus UVS10 generated an acidic environment

where Sb leaching was suppressed. The extracellular polymeric substances (EPS) have much larger La, V, Ni and Ce contents than the intracellular counterparts [18]. Utilizing three strains of Aspergillus, the bioleaching of aluminum (Al) metallic material from the used the initiator was studied in the study. Various spending catalyst loading densities were used for bioleaching in batch culture mode. By utilizing A. foetidus with 0.8% (w/v) catalysts loading, the maximum Al bioleaching efficiency of 88.43% was achieved and the rise in catalyst loading further reduced the efficiency. Furthermore, to facilitate the bioleaching of the catalyst utilized, molasses was employed as a low-priced carbon source at different attentions [19]. The article [20] proposed a unique adaption process was used to explore the *Acidithiobacillus ferrooxidans* and *Acidithiobacillus thiooxidans* bioleaching two precious metals, nickel (Ni) and cobalt (Co), lithium-ion batteries (LIBs) from abandoned laptops. Various biological leaching techniques were used, such as bioleaching of A. ferrooxidans and A. thiooxidans in one step and two steps in the wasted medium. It was assessed how the silver ion affected the Co and Ni bioleaching using these techniques. Additionally, a unique strain adaptation strategy was developed in response to the hazardous solid portion of the powdered battery, which led to bioleaching and a very quick adaption period. In this study, we utilize predictive modeling and reaction analysis in the context of bioleaching from wasted catalysts

2. Materials and Methods

In this section, we detail the use in the context of spent catalyst bioleaching for response analysis and predictive modeling. Fig.1 depicts the flow of the proposed method.

2.1. Microorganisms

The bioleaching process used E. coli DH5α. Maximum cell density was reached by growing the culture before the catalyzed waste was added in a two-step bioleaching procedure. A 2% v/v inoculation of an actively developed E. coli culture was added to 100 mL of 250 mL conical flasks with LB miller broth, which, using an incubation shaker running at 150 rpm, were incubated at 25, 30, or 37 °C. LB medium was used to generate plates with nutrients on them for counting colony-forming units (CFUs) of Escherichia coli. The flasks were refilled with a catalyst after a 24-hour growth of the culture period.

2.2. Spent catalyst

Catalyst with a size range of less than 75, 75–100 and more than 100μm was powdered and dry-screened via sieves.

2.3. The bioleaching technique

Over the course of 30 days, various pulp densities, particle sizes and temperatures were used for bioleaching. To assess how these characteristics affected bioleaching, a mathematical model was used for the collected data. Samples of 2 milliliters were taken out of the culture flasks for analysis of metals at pre-arranged intervals. Duplicates of every experiment were performed. Employing optical emission spectroscopy with inductively coupled plasma, the concentrations of heavy metals were determined.

2.4. Activations

This research assessed three distinct activation functions: rectified linear unit (ReLU), tanh and logistic. Non-linear functions like logistic and tanh restrict the output inside the intervals of 0 to 1 and −1 to 1, accordingly. Contrarily, ReLU is a linear activation function that gets rid of values that are negative.

$$ReLU(w) = \max(0, w) \quad (1)$$

$$logistic(x) = 1/(1 + f^{-w}) \quad (2)$$

$$\tanh(w) = \frac{(f^{w} - f^{-w})}{(f^{w} + f^{-w})} \quad (3)$$

The training set and test set were randomly selected from the dataset that was made available for mathematical modeling. After modeling, the system was assessed using a set of tests, which included the data points of 10%. As the name implies, the training set was utilized to train the DDNN and included 90% of the available data points.

2.5. Data range and interface modeling

Four input variables were utilized to assess the impact on Mo-bioleaching: temperature (T) (25, 30 and 37 °C), pulp density (PD) (0.5, 0.75 and 1%) and particle size (PS) (< 75, 75–100 and > 100 μm) and duration of bioleaching (t). The collection of data gathered in this way was utilized to train the DDNN. These are the crucial bioleaching prospective factors, which is why they were assessed for modeling. The research's coding and all of its data will be available to the public.

2.6. Stochastic Gradient Descent and Dynamic Deep Neural Network (SGD-DDNN)

SGD-DDNN may propose to train a dynamic neural network with the ability to dynamically modify its design by utilizing SGD as the optimization technique. Combining these two may result in effective training and enhanced performance in situations where the ideal network topology is unknown or subject to change over time.

2.6.1. Dynamic Deep neural network (DDNN)

The interpretation of an idea by a DDNN is the main topic of this section. Neurons in a DDNN are arranged in a series of layers, with each layer's neuron activations serving as an input. The neurons then carry out a basic calculation, such as adding up the weighted total of the input and activating a nonlinear function. From the input to the output, the network's neurons carry out a sophisticated nonlinear mapping. Using a method known as error back propagation, each neuron's weight is modified to determine this mapping based on the data. Fig.2 displays a neural network's architectural layout.

2.6.2. Network optimization using stochastic gradient descent (SGD)

In a linear model, the stochastic gradient descent approach was utilized for network optimization. More sophisticated DDNN networks were trained using this algorithm. A significant simplification is provided by the SGD method. Rather than calculating the gradient of $F_m(e_x)$,using one randomly selected sample as the basis for each iteration, this gradient is estimated.

$$x_{k+1} = x_s - \gamma_s \nabla_x R(y_s, x_s) \quad (4)$$

Every iteration's random selection of instances determines the stochastic process $\{x_s, s = 1, \ldots\}$.It is anticipated that even the noise created by this streamlined process acts as expected by the literature on stochastic approximations, which has explored the convergent process of SGD. Generally, diminishing gains that meet the requirements are needed for convergence outcomes.

$$\Sigma_s \gamma_s^2 < \infty and \Sigma_s \gamma_s = \infty \quad (5)$$

Under moderate circumstances, the Robbins-Siegmund theorem offers a way to achieve virtually certain convergence, even in situations where the function of losses is not differentiated. The SGDs speed of convergence is constrained by the noisy estimation of the genuine gradient. The parameter estimate's variance occurs when the gains drop off too slowly and $x_s$declines uniformly slowly. When the profits decrease too soon, the parameter estimate's expectation $x_s$approaches the ideal state relatively slowly. The best convergence speed is attained utilizing gains under adequate regularity conditions$\gamma_s{}^{\sim s-1}$. Subsequently, the residual error expectation falls at a comparable rate, that is, $E_{\rho\sim s-1}$. The gradients are multiplied by a positive definite matrix $\Gamma_s$in the second-order stochastic gradient descent (2SGD), This gets close to the Hessian's inverse

$$x_{s+1} = x_s - \gamma_s \Gamma_s \nabla_x R(y_s, x_s) \quad (6)$$

Regretfully, this alteration does not lessen the random noise, which enhances the variation of wt. Even with better variables, the residual error expectation declines as s^{-1}that is$E_{\rho\sim s-1}$.

3. Results and discussion

To investigate the effects of temperature, pulp density, residence duration and particle size, bioleaching data was gathered at many data points. The training approach for DDNN modelling of the bioleaching data was carried out in accordance with the described methodology. Preprocessing experimental biological leaching data, optimizing the network as well as choosing the right network and parameters are all part of the training procedure. The parts that follow go into further depth about these stages. A DDNN was used for modeling that is non-linear after a direct framework was used to describe the bioleaching information. To investigate how standardization affects the influence of the input variables in bioleaching, a linear model was developed. It's crucial to remember that the linear model in this case is a very simple DDNN with no hidden layers.

3.1. Standardization of data for bioleaching modeling of wasted catalysts

Data from a linear model was fitted to catalyst bioleaching and random values produced by the system were used to initialize weights (θ1, θ2, etc.). The fitted model was contrasted to the collection of data to calculate the error and use the gradient descent technique, an optimization method utilized to reduce a function of cost, which was utilized to reduce the sum of square errors for the fit of the model. In this instance, the cost function was the sum of the squares of the mistakes, which was reduced by an iterative process. Mo extraction is said to grow in tandem with increases in the values of temperature (T) and duration of residence (t), according to positive coefficient calculations. More influence on metal extraction is indicated by a greater coefficient value calculated for t. A decline in bioleaching is predicted by negative coefficients of PD and PS for the reasons listed below. Above a certain threshold, the quantity of metal that can be extracted from the same source quantity of metabolites or leachate rises when the amount of catalyst (measured in grams) in the leachate (100 ml) is increased. This poses a threat to microorganisms. Reduced metabolite concentration and a decreased percentage of bioleaching (Y) are the outcomes of the ensuing decrease in the number of microbes. Lower PD results in greater metabolite concentrations due to microbial proliferation. Table 1 displays the CFU count that was used to track how PD affected microbial growth.

3.2. Non-linear models in DDNN

The bioleaching data's linear modeling produced an R^2 value of 0.88, indicating that there was no linear distribution. As it was previously mentioned, DDNN can be used for Bioleaching and other non-linear biological process models. However, DDNN is more appropriate for data modeling sets in which the data spreading is uncertain. A DDNN network can be trained to predict the output given a history dataset. In this study, data from Bioleaching using wasted catalyst was installed to non-linear models using DDNN. To produce the output (or response), weights and inputs are combined to create the activating or transmission functions. Mathematical functions called activation functions (logistic, tanh, ReLU, etc.) introduce non-linearity into the system and use thresholds to regulate the output value. The ultimate output of the neuron is the value that the activation function provides. Using DDNN makes modelling non-linear relations simpler than with existing techniques. Since all DDNNs have neurons, connections amongst neurons and functions for activation, we all share a common property. Nonetheless, variances occur due to changes in the amount of hidden layers and neurons. Using modelling of the current data set based on trial and error, the ideal quantity of neurons and layers is identified. A neural network's parallel architecture, improved ability to describe systems that are not linear and capacity for learning to produce generalized models makes it a potent computing

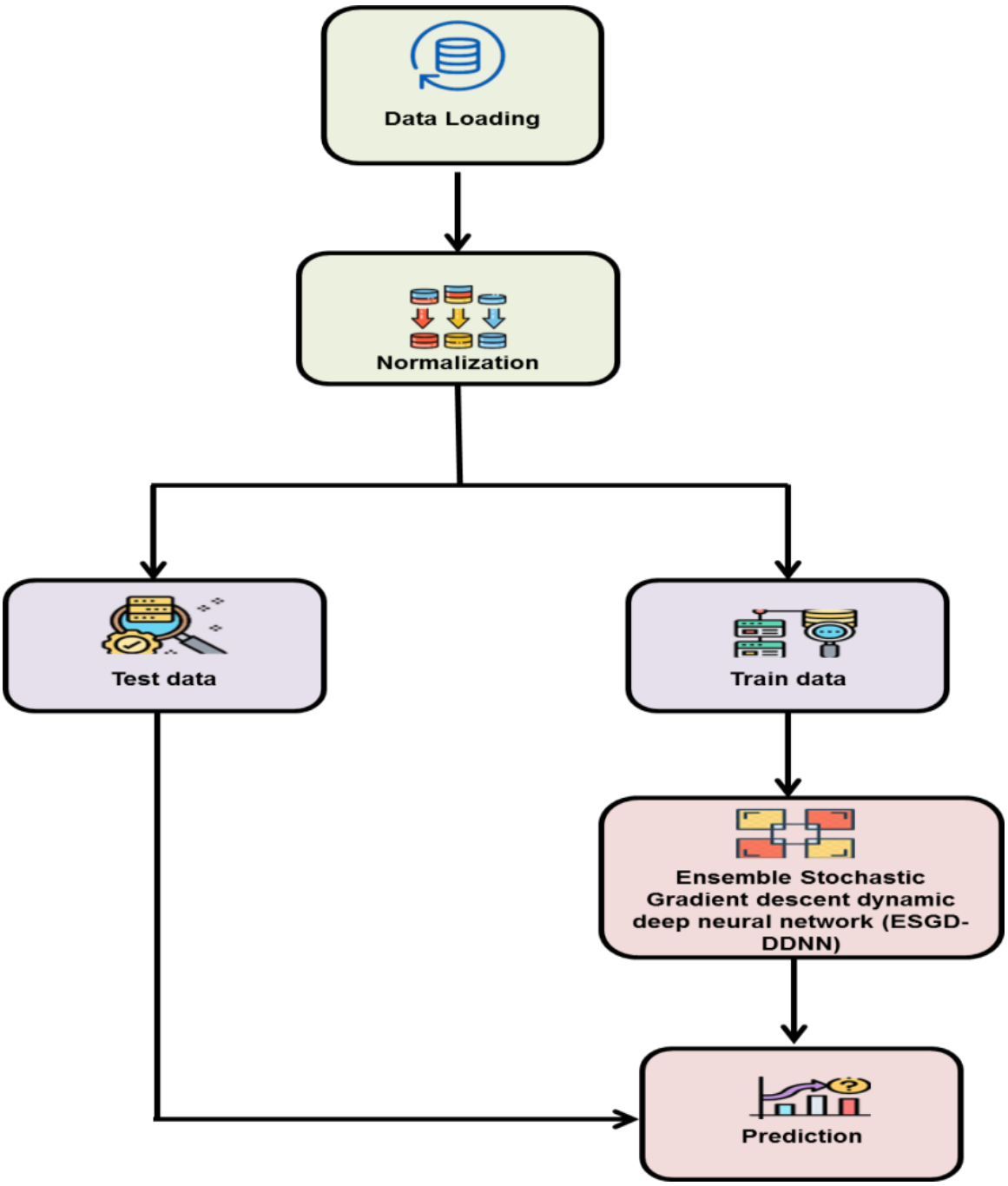

Figure 1. Procedure flow for the proposed method

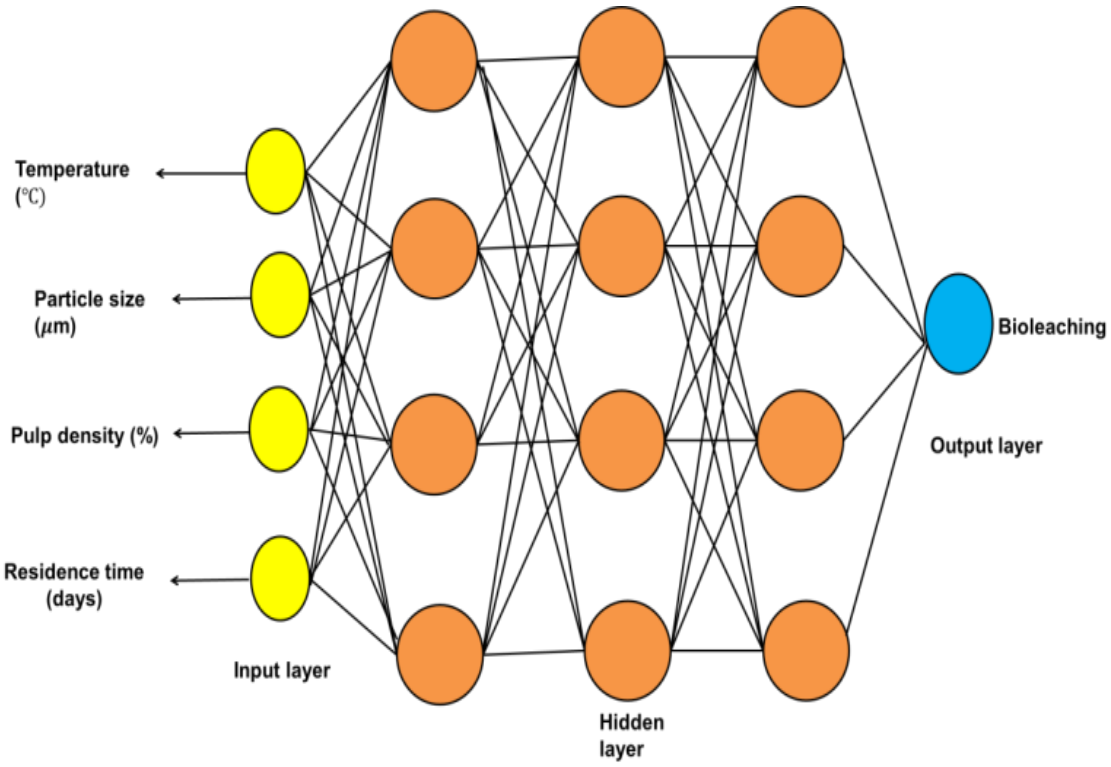

Figure 2. Architecture of DDNN

Table 1. Plate count with different pulp densities

Pulp density (PD)	Plate count days (t) after the insertion of the wasted catalyst					
	0	**1**	**4**	**10**	**15**	**20**
25%	4200	5000	700	100	80	50
	3800	4000	300	80	50	48
50%	4000	1000	-	10	2	*
	3800	1600	-	30	4	*
100%	4000	1400	200	-	*	-
	3900	1200	100	-	*	-

Table 2. Forecast by a trained network with a range of activation function

T (days)	PS (μm)	T (℃)	PD (%)	Bioleaching (%)	Bioleaching prediction (%)		
					ReLU	tanh	Logistic
6	>80	35.00	1.00	22.10	20.87	21.55	21.91
10	77	35.00	0.75	40.80	41.56	41.70	39.33
15	>80	28.00	1.00	36.21	34.48	34.35	33.18
20	>80	35.00	0.50	58.35	61.02	60.40	58.16
25	78	35.00	0.50	67.06	63.85	64.87	64.83
30	75	35.00	0.75	72.89	71.09	71.12	70.36

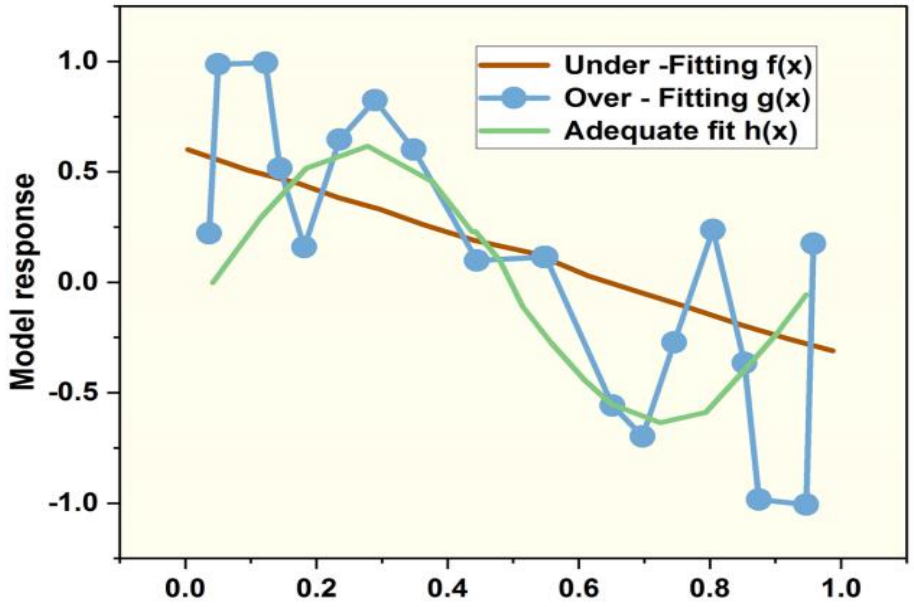

Figure 3. Underfitting, Overfitting, adequate fit

Table 3. Three activation functions' average R^2score values

No. of hidden layers	*tanh*			ReLU			Logistic		
1	.923 (.033)	.972 (.017)	.970 (.011)	.8578 (.043)	.933 (0.055)	.931 (0.057)	.948 (.028)	.965 (.024)	.978 (.018)
2	0.886 (.052)	0.976 (0.008)	0.984 (0.008)	.867 (.039)	.980 (0.012)	.983 (0.012)	0.789 (.083)	0.891 (.093)	.905 (.069)
3	0.812 (.142)	.945 (.051)	.951 (.049)	.907 (.043)	0.970 (0.027)	.975 (0.024)	0.829 (.089)	0.796 (.120)	.892 (.067)

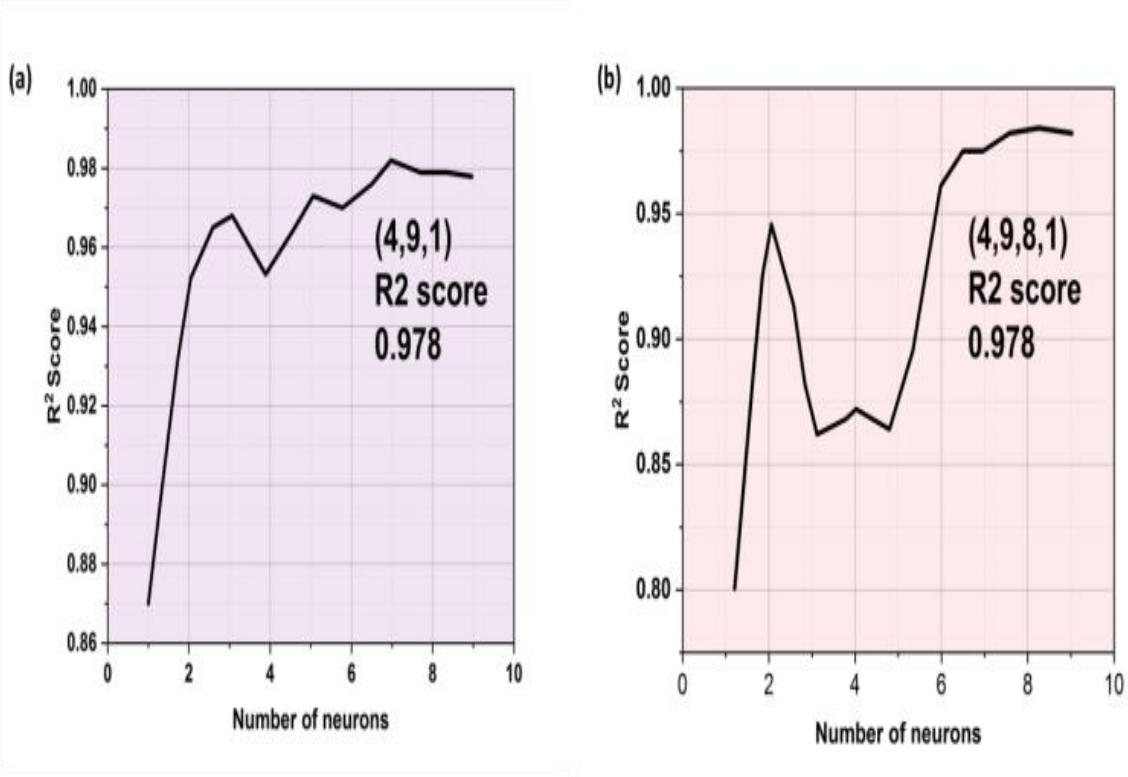

Figure 4. R^2 score versus neuron count, using activation function of logistics (a) 1 hidden layer (b) 2 hidden layer

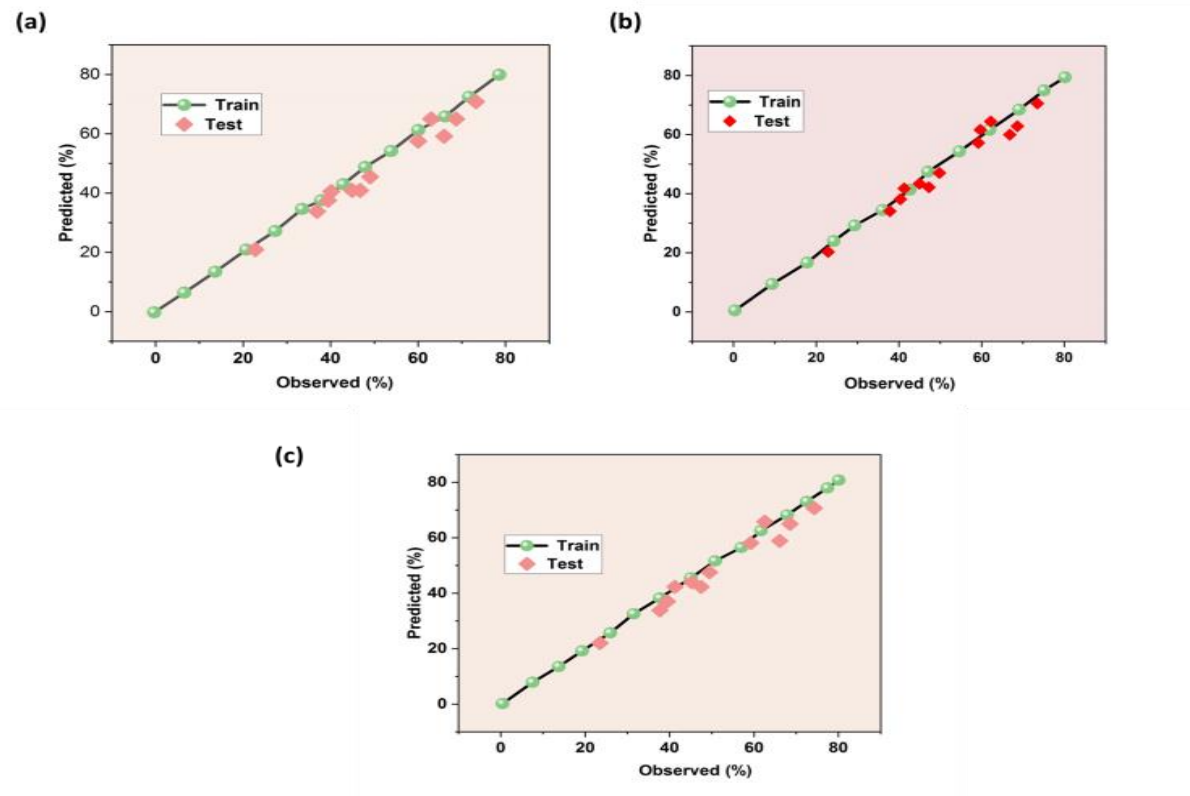

Figure 5 (a) Logistic predictions value, (b) ReLU predictions value and (c) tanh predictions value

tool. The predicted values and the test dataset derived from the three purposes of activation are shown in Table 2.

3.3. Bioleaching using wasted catalyst modelling

As seen in Fig. 2, a DDNN design for wasted catalyst bioleaching comprises four input variables in the input layer, a few hidden layers and an output layer. ReLU has been employed in the area of deep learning and has been shown to be effective in modelling. The utilized tanh and sigmoid functions, it has produced superior model fitting for biological systems. The issue of the model that is either over fitted or under fitted occurs while modelling a dataset. A simpler model is more likely to create underfitting, while a more complex model produces overfitting. Instances of over fitting, under fitting and a good fit for randomly chosen data points are shown in Fig.3. Various network designs using the three activation mechanisms yielded the highest R^2 score. The optimal model had two secret layer configurations (4, 9, 8 and 1); use the first concealed layer has nine neurons, whereas the second layer contains eight and it was generated by the network using the function of logistic activation. The optimal model with a tanh activation function has an arrangement of three hidden layers (4, 9, 7, 1, 1) and a comparable R^2 score of 0.978. With an R^2 value of 0.979 and a three layer of hidden design (4, 8, 4, 7, 1), using a ReLU function in the network offered the greatest match. For the provided training data set, the algorithm identified the ideal model as ReLU. Then, utilizing the test dataset that was chosen at random, the R^2scores of those models were assessed. For the test dataset that has not yet viewed, logistic, tanh and ReLU models yielded R^2 values of 0.970, 0.960 and 0.963 each. The training model's capacity to generalize to new data is shown by higher R^2 scores. E.Coli bioleaching modeling has not been the subject of any investigations. Nevertheless, these outcomes are similar to the R^2 values that have been reported in other bioleaching methods, which vary from 0.83 to 0.99. Based on its greatest R^2 score, even with unseen data, the model of logistics was determined to be the most suitable model for the given objective. The variance in R^2 of three predefined activation processes is used to score and three rates for neurons 2, 5 and 8 are shown in Table 3. It was noted that the network with the highest R^2 score is not the one with the most complexity. Fig. 4 displays the difference of the R^2 score based on the number of neurons in the hidden layer. One hidden layer, the fluctuation of the R^2 value with the quantity of neurons is seen in Fig. 4 a. Nine neurons were chosen for the first hidden layer and based on the fluctuation of R^2 value with neurons, the first layer of nine neurons has a high 0.978 R^2 value. Figure 4 b illustrates how the number of neurons affects the R^2 score in the case of two hidden layers. Nine neurons were chosen for the first hidden layer, while the image illustrates the fluctuation of R^2 score with neurons in the second layer. When the system configuration is (4, 9, 8, 1) the R^2 score rises to 0.978, even more with two hidden layers. Fig. 5 shows the observed and projected values for the top three models, which were chosen according to the training R^2 value. The training and test samples exhibit a strong connection with the anticipated and

actual values. The R^2 scores for all three functions were quite high. Nonetheless, the logistic model outperformed the others and it is considered the test set as the most effective model with training for bioleaching using a catalyst.

4. Conclusion

In summary, recovered precious metals from abandoned catalysts can be recovered by a sustainable and promising method called wasted catalyst bioleaching. The research looked at how experimental bioleaching data was simulated and explored the effect of significant variables, including pulp densities, particle sizes, residence times and temperatures. With the use of the SDG algorithm and several activations, such as logistic, ReLU and tanh, the network's number of neurons and layers that are hidden was optimized. The experimental and anticipated values showed a strong connection. An R^2 score of 0.978 was obtained by the optimal design with logistic activation. The genetic diversity of the microbial communities engaged in Mo bioleaching can be better understood in the future via metagenomic research.

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