CHAPTER 6

Artificial Intelligence (AI) Based Tools for Predicting the Removal Efficiency of Heavy Metals by Adsorption

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Abstract

The two most popular artificial intelligence (AI) techniques namely, artificial neural networks (ANN) and support vector machines (SVM) have been applied for predicting the removal efficiency of heavy metals like Copper (II), Arsenic (III), Lead (II), etc. in an adsorption process using low cost biosorbents. A comparison has been made between ANN, SVM and multiple linear regression (MLR) models based on the statistical parameters such as: correlation coefficient (R), average absolute relative error (AARE) etc. SVM is found to be the better predictive model than the commonly used MLR model and ANN model. Hence, its results are more accurate and generalized.

Keywords

Artificial Intelligence (AI), Artificial Neural Networks (ANN), Support Vector Machines (SVM), Adsorption, Biosorption.

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1. Introduction

Pollution due to heavy metals has become a major issue in many countries and this problem is becoming more serious every as the concentration of heavy metals is found to continually exceed the permissible standards. This is caused by heavy metals which are not biodegradable and toxic and thus are a great threat to the environment and human life. The major cause of increased heavy metals concentration in the environment is the effluents from many industries. Some of the prominent industries are: fuels related, fertilizer, iron and steel, leather, mining, petroleum refining etc. [1]. Most commonly found heavy metals in the effluents are: toxic metals (such as Hg, Cr, Pb, Zn, Cu, Ni, Cd, As, Co, Sn, etc.), precious metals (such as Pd, Pt, Ag, Au, Ru etc.) and radio nuclides such as U, Th, Ra, Am, etc. [2, 3]. These heavy metals are responsible for various serious health problems like brain damage, liver and kidney damage, break down of nervous system, lung cancer, bronchitis etc. Due to the severe impact of these metals on both environment and human health, removal and recovery of heavy metals from effluent streams is essential.

Several methods are being employed for the removal of these heavy metals coming from industrial effluents such as chemical precipitation, membrane filtration, ion exchange, activated carbon adsorption, evaporation etc. Recently, the biosorption process which is adsorption on a biosorbent has been found to offer an attractive substitute to these existing methods [4, 5]. Besides being economical it has several advantages as compared to other conventional techniques such as high metal removal efficiency, minimization of chemical and toxic sludge or biological sludge which can be easily disposed of, minimum requirement of additional nutrients, easy regeneration of biosorbent and metal recovery [6, 7, 3].

Biosorption of heavy metal removal is greatly affected by various parameters such as nature of biomass and its concentration, contact time between solution containing metal and the biomass, temperature, surface area to volume ratio, initial metal ion concentration, metal affinity to biosorbent and pH of the solution [8]. Heavy metal removal efficiency predictions are made by using several techniques like MLR, ANN, genetic algorithm (GA) etc. [9, 10, 11]. Recently, support vector machines (SVM) have been developed that are being applied for classification and regression termed as a support vector classification (SVC) and support vector regression (SVR). SVM possesses

many advantages over traditional ANN. While ANN suffers from multiple local solution, SVM gives unique, optimal and global solution for quadratic problems. Only two parameters need to be selected, upper bound and kernel parameter. The use of a structural risk minimization (SRM) principle in SVM provides a good generalization performance. There are many past studies which show the superiority of SVM over ANN [12, 13, 14, 15].

SVR now finds many applications for the prediction of many real world problems like time series prediction, predicting thermal–hydraulic performances in compact heat exchangers, predicting the auto-ignition temperatures of the organic compounds, atmospheric temperature prediction, predicting heat transfer coefficient and circulation rate in a thermosiphon reboiler etc. [16, 17, 18, 19, 20, 21].

This chapter mainly focuses on the application of artificial intelligence tools, primarily SVR, to predict the removal efficiency of heavy metals during the adsorption process using low cost biosorbents. The first section of this chapter introduces the adsorption process as used for heavy metal removal from waste water. The second section discusses the basic principle and theory of the two most popular artificial intelligence techniques i.e. ANN and SVM. This is followed by a third section which presents three different case studies for the prediction of the removal efficiency of heavy metals: Cu (II), As (III) and Pb (II) using SVR for all the three cases and ANN for predicting the removal efficiency of Pb (II) only. Comparison of the results is made with the conventional MLR method. Further, for the case of Pb (II), the prediction performance of these three models is assessed in the light of existing theory and the experimental findings. The same along with the conclusions are presented in the last section.

1.1 Adsorption

Adsorption is essentially a surface phenomenon, the substance which gets adsorbed on to the surface is called adsorbate which may either be a liquid or gas on the other hand the surface usually a solid on to which this adsorbate gets adsorbed is referred as adsorbent. As adsorption being the surface phenomenon entirely different from absorption which is a bulk phenomenon, adsorbate permeates deeply into the adsorbent i.e. the whole volume of the material is involved in the absorption process. The term sorption includes both the process namely absorption and adsorption. The adsorption process is basically used to remove individual component from liquid or gas mixture. The component to be removed is physically or chemically bonded to a surface. Thus, adsorption may be categories into physical adsorption and chemical adsorption.

Physical Adsorption or Physisorption

When the force of attraction between adsorbate and adsorbent is of the order of weak Vanderwaal force, the process is called physical adsorption or physisorption. In physisorption the enthalpy change is very low, typically 20-40 KJ/mol. It takes place at low temperature and as the temperature increases, the physisorption process decreases.

Chemical Adsorption or Chemisorption

When the force of attraction between adsorbate and adsorbent is similar to those present in chemical bonding, the process is called chemical adsorption or chemisorptions. As compared to physisorption, the enthalpy change associated with chemisorptions is very high i.e. around 200-400 KJ/mol. Chemisorption first increases with temperature and then decreases.

The major difference between physisorption and chemisorption include [22]:

- Physisorption is basically a reversible process and does not require any activation energy while chemisorption is an irreversible process and requires high activation energy.
- Chemisorption is highly selective and occurs only between certain active surface and adsorbent where as physisorption occurs on all surfaces if the conditions are favorable.
- Physisorption results in forming multimolecular layer while chemisorptions process proceeds in a monomolecular layer.
- Heat of adsorption for physisorption process is low on the other hand for chemisorption heat of adsorption is high.

The most commonly used industrial adsorbents are activated carbon, silica gel, molecular sieves, alumina, clay mineral and synthetic polymers etc. as they provide large surface areas per unit weight. A good adsorbent should have the following properties [23]:

- High porosity, high selectivity and large surface area per unit weight.
- Thermal, mechanical and chemical stability.
- Low pressure drop over the adsorber bed.
- Low fouling, no side reaction and easy regeneration.
- Low cost.

Applications of adsorption

Some of the important applications of adsorption are listed below [24, 25]:

- Separation of gaseous mixture, chemicals and air.
- Purification of liquids and water, softening of hard water, removal of impurities from liquid and gas etc.
- Removal of coloring matter from solution.
- Volatile organic compound (VOCs) removal from the polluted air.
- Production of high vacuum.
- Using activated charcoal for the preparation of gas masks to avoid poisonous gases like CO, CH₄ etc.
- It plays a vital role in controlling the environmental pollution especially the control of 'greenhouse gases' like CH₄, CO₂, N₂O etc., thus, helps in reducing global warming.

Factors affecting the adsorption process

There are various factors which affect the adsorption process [26]:

- Nature of the adsorbent: The type of adsorbent used in the adsorption process plays an important role in the adsorption rate such as the chemical nature of adsorbent surface, its specific area and the extent of porosity. Since, adsorption is a surface phenomenon, the larger the surface area of the adsorbent, the larger is its capacity for adsorption.
- Temperature and Pressure: Adsorption is an exothermic process, therefore with the decrease in temperature, the rate of adsorption increases. Further adsorption of a gas is accompanied by decrease in pressure, the rate of adsorption increases as the pressure increases. Whereas decrease in pressure leads to desorption. Thus, the decrease in temperature and increase of pressure both leads to an increased rate of adsorption.
- Nature of the gas: The type of gases used also affects the adsorption process such as chlorine, sulphur dioxide and ammonia are more easily adsorbed because of weak Vander wall forces compared to oxygen, hydrogen and nitrogen. The rate of adsorption is in direct proportion to the critical temperature of gases and these gases have high critical temperature.

The amount of heavy metal removed during adsorption process is evaluated either in terms of adsorption capacity/metal uptake or heavy metal removal efficiency. In order to obtain the adsorption capacity, the amount of metal ions adsorbed per unit mass of adsorbent is determined using the following equation [27, 28]:

$$q_e = \frac{V(C_o - C_f)}{m}$$

Where, q_e , V , m , C_o and C_f represent the metal ions adsorbed per adsorbent at equilibrium (mg/g), volume of solution (L), mass of adsorbent (g), the initial metal ions concentration in the solution (mg/L), final metal ions concentration in the solution (mg/L) respectively.

Heavy metal ion removal efficiency can be calculated with the amount of metal ions which gets adsorbed on the adsorbent and the available amount of metal ions in the solution as given by the equation below:

$$\text{Heavy metal removal efficiency (\%)} = \frac{\text{Heavy metal ions removed}}{\text{Heavy metal ions remaining}} * 100$$

2. An Overview of Artificial Intelligence (AI) Techniques

Artificial intelligence is the simulation of human intelligence processes by machines i.e. making the computer behave like humans. These processes include learning, reasoning, problem solving, perception, planning etc. Particular applications of AI include expert systems, speech recognition, and machine vision.

This section describes two very popular computational intelligence techniques namely, artificial neural networks (ANN) and support vector machines (SVMs).

2.1 Artificial Neural Networks (ANN)

Artificial neural networks are parallel processing computer algorithms inspired by the working of the human brain. The basic components of neural networks is composed of neurons and weights (bias). The neural networks architecture is made up of an input layer, one or more hidden layers and the output layer. The input layer receives the information and conveys this information/data to the hidden layer and does not carry any activation or transfer function. Hidden layers are sometimes called as “black boxes” as they are within the networks and no direct connection exists to the external environment [29]. The output layer processes the outcome of the hidden layer using some activation function [30] and then finally it sends the calculated output to the user. The most widely used activation functions are: linear function, piecewise linear function, tangent hyperbolic function, threshold function and sigmoidal (S shaped) function. The neural networks structure can be of three types [31, 32, 33, 34, 35]: if the input layer is directly connected to the output then it is often called a single-layer network, and if some hidden layer exists between the input and the output layer then it is called a multi-layer network as shown in Figs. 1 and 2. A feed forward network with one or more hidden layers as well as with feedback loop is termed as a recurrent network i.e. output of the network is fed back to its input layer as shown in Fig 3. The number of neurons at the input and

output layers is decided by the nature of the problem and the no. of neurons as the hidden layer is generally decided by the trial and error method. Too few neurons lead to an inadequately fit-to the data and problem of under fitting arises while too many neurons lead to an over fit-to the data and have poor generalizability [36].

Figure 1. Single layer feed-forward NN (FFNN)

Figure 2. Multi layer feed-forward NN (FFNN)

Figure 3. A recurrent network

Neural learning

Learning in neural networks basically refers to the method of modifying the weight of the connections between the nodes. Learning may be classified as supervised learning, unsupervised learning and reinforced learning. In supervised learning, the desired set of output (target) is available for each set of input. The weights of the connection are modified till the output of the response and target matches, otherwise the network produces an error. Whereas in unsupervised learning, no desired output (target) is available and the network adjusts its weight according to the input, and reinforced learning is in between the supervised and unsupervised learning. The desired output of the response is not compared with the target and it provides the information of the computed result, whether it is correct or not. Network weights are adjusted to have a good performance (based on certain criteria) and are rewarded while the other parts of ANN are penalized [37, 38].

The various steps involved for the development of ANN model are listed below [39, 40, 41, 42]:

1. Collection of data as input and output variables for a specified problem.
2. Data preprocessing i.e. scaling or normalization of data.
3. Dividing the whole data set into training, testing and validation sets.

4. Selecting ANN architecture i.e. the type of ANN, no. of hidden layers, no. of neurons at the input layer, hidden layer and the output layer, type of activation function at the hidden layer and the output layer.
5. Neural networks training:
 - (a) A training set is used to adjust the weight and bias.
 - (b) A Validation set is used to check the generalization performance and when to stop the training process.
 - (c) A test set is used to check the performance of the developed ANN model based on some statistical parameters.

2.2 Support Vector Machines (SVMs)

Support vector machines (SVMs) are a set of related supervised learning methods [43, 44] originally developed for classification purposes i.e. support vector classification (SVC). However, it's application has now been extended to regression problems [45, 46, 47]. SVM is based on machine learning theory and enhances the accuracy of prediction while avoiding an over-fit to the data. Basically, SVM is superior than the conventional techniques like ANN on the following counts [48, 49, 12]: (a) only two parameters need to be selected i.e. upper bound and the kernel parameter, (b) unique, optimal and global solution for quadratic programming problem, and (c) implementation of structural risk minimization (SRM) principle provides good generalization performance [50]. Thus, SVM overcomes the problem of over fitting explicitly. Robustness of SVM is achieved by considering absolute, instead of quadratic values of the errors. As a consequence, the influence of outliers is less pronounced [51]. Because of these advantages, SVM has found many applications [52, 53].

Theory and Basic Principles

Fitting a regression function, $y = f(x)$ in a ϵ -SVR model is the basic goal so as to accurately predicts the targets $\{y_i\}$ corresponding to a set of input samples, $\{x_i\}$, With the given training data set as $D = \{(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)\}$, where $x_i \in R^N$ is a vector of input variables and $y_i \in R^N$ is the corresponding scalar output (target) value.

For the case of a linear function, SVR approximates the relationship between the output and input parameters given by:

$$f(\mathbf{x}, \mathbf{w}) = (\mathbf{w} \cdot \mathbf{x} + b) \quad (1)$$

Where, $\mathbf{w}$ expresses the weight vector and $\mathbf{b}$ refers to a constant called bias.

However, for non-linear problems of the real world where the input data cannot be correlated to the required output linearly, the following linear model can be constructed for high-dimensional feature space using a nonlinear mapping function $\phi(\mathbf{x})$ [54]:

$$f(\mathbf{x}, \mathbf{w}) = (\mathbf{w} \bullet \phi(\mathbf{x}) + b) \quad (2)$$

Where, $\phi(\mathbf{x})$ is the function termed feature and $(\mathbf{w} \bullet \phi(\mathbf{x}))$ the dot product in the feature space F.

The regression problem is equivalent to minimizing the following regularized function:

$$\text{Minimize: } R(f) = C \frac{1}{N} \sum_{i=1}^N L_{\epsilon} (y, f(x, w)) + \frac{1}{2} \|\mathbf{w}^2\| \quad (3)$$

$$L_{\epsilon}(y, f(\mathbf{x}, \mathbf{w})) = \begin{cases} 0 & \text{if } |y - f(\mathbf{x}, \mathbf{w})| \leq \epsilon \\ |y - f(\mathbf{x}, \mathbf{w})| - \epsilon & \text{otherwise} \end{cases} \quad (4)$$

In Eq. (3), the first term represents the empirical error and the term C gives a measure of the trade-off between the training or empirical error and the model flatness given by the second term of the said equation. Eq. (4) defines the ϵ -insensitive loss function proposed by Vapnik [56, 57]. The loss function assumes a zero value in the ϵ -insensitive zone and as a result it does not penalize the prediction errors with magnitudes smaller than ϵ . However, practically it is not possible to establish a function, $f(\mathbf{x}, \mathbf{w})$ with errors less than ϵ . In that case, some allowance for errors has to be considered, which can be represented in terms of slack variables ξ and ξ^* . These slack variables have non-zero values outside the ϵ -insensitive zone and measure the deviation from the boundaries of the ϵ -insensitive zone (penalty).

Thus after introducing the slack variables ξ and ξ^* , SVR is formulated as minimization of the following convex optimization problem:

$$\text{Minimize} \quad \frac{1}{2} \|\mathbf{w}^2\| + C \sum_{i=1}^N \xi_i + \xi_i^{(*)} \quad (5)$$

Subject to

$$(y_i - \mathbf{w} \bullet \phi(\mathbf{x}) - b) \leq \epsilon + \xi_i, \quad (6)$$

$$(\mathbf{w} \bullet \phi(\mathbf{x}) + b - y_i) \leq \epsilon + \xi_i^{(*)}, \quad \xi_i, \xi_i^{(*)} \geq 0 \quad (7)$$

The above optimization problem can be transformed into a dual problem by incorporating Lagrangian multipliers α and α^* as follows:

Maximize

$$L_d(\alpha_{i,j}^{(*)}) = -\frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N (\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) \times (\phi(\mathbf{x}_i) \bullet \phi(\mathbf{x}_j)) - \varepsilon \sum_{i=1}^N (\alpha_i - \alpha_i^*) - \sum_{i=1}^N (\alpha_i + \alpha_i^*) y_i \quad (8)$$

Subject to constraints

$$C \geq \alpha_i, \alpha_i^* \geq 0 \text{ and } \sum_{i=1}^N y_i (\alpha_i - \alpha_i^*) = 0 \quad (9)$$

By solving this convex quadratic programming problem (QP), the coefficients α and α^* in Eq. (8) are obtained. Only the non-zero coefficients, and the corresponding input vectors, $\mathbf{x}_i$, are called support vectors (SVs). These SVs are the most informative data points that compress the information content of the training set, thereby representing the entire SVR function.

The expanded form of the SVR is thus given as:

$$f(\mathbf{x}, \alpha_i, \alpha_i^*) = \sum_{i=1}^{N_{sv}} (\alpha_i - \alpha_i^*) (\phi(\mathbf{x}_i) \bullet \phi(\mathbf{x}_j)) + b \quad (10)$$

However, for the above-mentioned problem [Eq. (10)], the inner product in the feature space needs to be calculated. But with the increase in the input dimensions, the computation in the high-dimensional feature space becomes a computationally complicated problem (curse of dimensionality). Such a problem of contradiction between high dimensions and computational complexity can be overcome by using the kernel trick or defining appropriate kernel functions in place of the dot product of the input vectors in high-dimensional feature space. The kernel function is used to compute directly the inner product from the input space, rather than in the high dimensional feature space. Kernel functions provide a way to avoid the curse of dimensionality.

The most commonly used kernel functions include linear function, polynomial function, Gaussian function, and sigmoid function, spline, etc. [58]. The Gaussian function is a widely used kernel function as it can map the input space sample set into a high dimensional feature space effectively and is good for representing the complex nonlinear relationship between the input and output samples. Furthermore, only one variable (the width parameter) is there to be defined [21, 19]. Considering the above advantages, the Gaussian radial basis function (RBF) is chosen as the kernel function in this work and the expression is given as:

$$K(x, x_i) = \exp\left(-\frac{\|x - x_i\|^2}{\sigma^2}\right) \quad (11)$$

Where, σ denotes the width of the RBF and $\gamma = \frac{1}{2\sigma^2}$

Thus by applying the kernel function, the basic SVR function modeling the data obtained by using the above-mentioned maximization function is then given by:

$$f(\mathbf{x}, \alpha_i, \alpha_i^*) = \sum_{i=1}^{N_{sv}} (\alpha_i - \alpha_i^*) K(\mathbf{x}, \mathbf{x}_i) + b \quad (12)$$

The bias parameter, b , can be obtained by applying Karush–Kuhn–Tucker (KKT) conditions.

SVR modeling procedure

The computational procedure for SVR modeling can be broadly divided into five stages [59, 60, 61]:

1. The first step is to collect the data set as independent input variables and the target output variable.
2. Thereafter, the data set is normalized and then divided into a training data set and test data set in the ratio of 8:2.
3. Once the training data set is selected and normalized, the next step is to optimize the model and kernel parameters using grid search methodology with K-fold cross validation.
4. Establishment of final SVR model is carried out using the obtained optimal parameters.
5. The performance of the obtained SVR model is evaluated and validated in terms of the statistical evaluation parameters such as average absolute relative error (AARE), root mean square error (RMSE), coefficient of determination (R^2) etc., comparing the prediction performance with models existing in literature and in the light of existing theory.

3. Application of AI Techniques

The following sections discuss three case studies for the prediction of the removal efficiency for Cu (II), As (III) and lead (II) by applying AI techniques like ANN and SVM and the comparison of the results with MLR.

CASE STUDY – I

PREDICTION OF Cu (II) BIOSORPTION EFFICIENCY

In this study, an effort has been made to assess the performance of a developed SVR-based model for predicting the biosorption efficiency of Cu(II) ions on the litter of a

natural trembling poplar (*Populus tremula*) forest (LNTPF) as a low-cost and abundant biosorbent vis-à-vis an MLR model using the same data set extracted from published literature [62].

Analysis of the MLR model

As per the existing theory, it has been found that the Cu(II) biosorption efficiency (%) depends on pH (a_1), temperature (a_2), particle size (a_3), agitating speed (a_4), initial Cu(II) concentration (a_5), adsorbent concentration (a_6), and the contact time (a_7). The following MLR model equation has been obtained:

$$y = -8.3357 + 11.0513 (a_1) + 0.3574 (a_2) - 30.3253 (a_3) + 0.0608 (a_4) - 0.2541 (a_5) + 5.9614 (a_6) + 0.06619 (a_7)$$

The independent variables are found to be significant into the regression.

Figure 4. Performance of MLR model using training data and test data for prediction of Cu(II) biosorption efficiency (%).

Performance assessment of the MLR model has been carried out based on statistical parameters namely, AARE, R², RMSE, SD and MRE. A comparison between the predicted values of Cu(II) biosorption efficiency (%) by the MLR model and those calculated from the experimental data using the training dataset and the test dataset is shown in the Fig. 4. An AARE of 5.514 %, R² of 0.8708, RMSE of 0.0733, SD of 14.0785 and MRE of 0.0527 on the training data are obtained while the corresponding

values for the test data are: 5.327 % AARE, 0.8965 R², 0.0665 RMSE, 12.94 SD and 0.0525 MRE. It can be seen that the MLR model has consistent prediction ability. In fact, the model gives an improved generalized performance on the test data set.

Analysis of the SVR-based model

The entire dataset of 197 samples is divided into two non-repetitive groups as the training dataset and the testing dataset using the simple random sampling (SRS) technique, in the ratio of 8 (158 data points): 2 (39 data points), respectively. Thereafter, using the same training data set, a SVR-implementation known as “ ϵ -SVR” in the open software LIBSVM library [63] on MATLAB platform has been used to develop the SVR-based model. The generalization ability of the SVR model has been assessed using the virgin test data set.

RBF kernel has been used in this study because of its good general performance and the requirement of few parameters to be adjusted [58]. For achieving the optimal values of the SVR model hyper-parameters (C and ϵ) and the kernel parameter (γ), grid search methodology with 10-fold cross validation has been carried out on the training data set by considering a wide range of these parameters: C [2^5 , 2^{15}], γ [2^{-15} , 2^2] and ϵ [2^{-15} , 2^4]. The optimal values of the model parameters for the SVR model are given in Table 1.

Table 1. Optimal parameters for SVR-based model for Cu (II) biosorption efficiency in a biosorption Process.

Property to be predicted	C	$\gamma = 1/2\sigma^2$	ϵ	Kernel type	Type of Loss function	Number of support vectors	Number of training points
Biosorption efficiency	32768	0.01195	0.0625	RBF	ϵ - insensitive	104	158

After optimization of the SVR parameters, the model output for the training and test data has been plotted in Fig. 5. It is evident that both the predicted values for the training data as well as the test data lie close to the ideal fit line. Table 2 exhibits the model evaluation parameters of the SVR-based model for both the training data as well as the test data. The close proximity to each other of the model evaluation parameters for the training data and test data testify to the excellent prediction performance and also to the high generalization ability of the SVR-based model.

Figure 5. SVR simulation of Cu(II) biosorption efficiency(%) in a biosorption process with optimal parameters using training data and test data.

Table 2. Model evaluation parameters for SVR-based model using the training data and the test data.

SVR Model evaluation parameter	Train data	Test data
AARE (%)	2.07	1.97
R	0.9881	0.9879
RMSE	0.0011	0.0007
SD	14.837	13.2689
MRE	0.0206	0.0199
Q^2_{LOO} (Train data), Q^2_{ext} (Test data)	0.9763	0.9759

Comparison of SVR-based model with the MLR model.

A comparison was made of the prediction performances of the developed MLR model with the SVR-based model. Fig. 6 clearly illustrates the superior prediction performance of the SVR-based model. Table 3 exhibits the relevant model evaluation parameters for the two modeling methods on the test data set. It can be easily surmised that the SVR-based model is a vastly improved model than the MLR model. Further, in terms of

absolute deviation (AD) values, the SVR-based model again scores over the MLR model as shown in Table 4 and 5.

Figure 6. Comparison of SVR model with MLR model for prediction of Cu(II) biosorption efficiency (%) in a biosorption process using test data.

Table 3. Model evaluation parameters for SVR-based model and MLR model using the test data.

SVR Model evaluation parameter	SVR-based model	MLR model
AARE (%)	1.97	5.33
R^2	0.9760	0.8965
RMSE	0.0007	0.0665
SD	13.2689	12.9434
MRE	0.01994	0.0525

Table 4 illustrates the distribution of predicted data points of Cu (II) biosorption efficiency by the SVR-based model in terms of absolute deviation (AD) for the training data. The SVR-based model was found to predict nearly 92.4 % data points within an absolute deviation of less than 5 % and a total of 97.5 % data points within an absolute deviation of less than 10%. Only 2.5 % data points have an AD of more than 10%. Whereas, the MLR-based model was observed to predict only 65.1% data points within

an absolute deviation of less than 5 % and a total of 86.2% data points within an absolute deviation of less than 10%. Only 13.8% data points have an AD of more than 10%.

Table 5 depicts the distribution of predicted data points of Cu (II) biosorption efficiency by MLR and SVR-based model in terms of absolute deviation for the test data set. It is observed that the SVR based model predicts nearly 92.3% data points within an absolute deviation of less than 5% and all the data points fall within an absolute deviation of no more than 10%. While, the MLR-based model predicts nearly 56.4 % data points within an absolute deviation of less than 5 % and a total of 84.6 % data points within an absolute deviation of less than 10%. Only 15.4 % data points have an AD of more than 10%. This shows that the SVR-based model is highly accurate and has good generalization ability.

Table 4. Percentage distribution of predicted data points of Cu (II) biosorption efficiency by MLR model and SVR- based model in terms of absolute deviation (AD) for training data.

Absolute deviation (AD) (%)	% of SVR model predicted values	Cumulative score	% of MLR model predicted values	Cumulative score
AD< 2	76.6	76.6	27.2	27.2
2<AD< 5	15.8	92.4	37.9	65.1
5<AD< 10	5.1	97.5	21.1	86.2
AD>10	2.5	100	13.8	100
Total	100		100	

Table 5. Percentage distribution of predicted data points of Cu (II) biosorption efficiency by MLR model and SVR- based model in terms of absolute deviation (AD) for test data.

Absolute deviation (AD) (%)	% of SVR model predicted values	Cumulative score	% of MLR model predicted values	Cumulative score
AD< 2	61.5	61.5	23.1	23.1
2<AD< 5	30.8	92.3	33.3	56.4
5<AD< 10	7.7	100	28.2	84.6
AD>10	00.00		15.4	100
Total	100		100	

CASE STUDY II

PREDICTION OF ARSENIC (III) BIOSORPTION EFFICIENCY

In this study biosorption efficiency of As (III) ions has been predicted with the developed SVR-based model and the MLR model. Biosorption data for the present work have been taken from available published literature [64] where the input parameters are taken as: initial As (III) concentration, biosorbent dosage, contact time and temperature. The whole dataset of 81 samples are divided into a training dataset and a testing dataset using the simple random sampling (SRS) technique, in the size ratio of 80% (65 data points) and 20% (16 data points) respectively.

Analysis of the MLR model

From the literature [64] we found that biosorption of As (III) (y) depends on initial As (III) concentration (m_1), biosorbent dosage (m_2), contact time (m_3) and temperature (m_4) and the following MLR model equation has been obtained:

$$y = 54.5550 - 0.3314 (m_1) + 1.3083 (m_2) + 0.2120 (m_3) + 0.2442 (m_4)$$

These independent variables are found to play a significant role into the regression.

Figure 7: Performance of MLR model using a training data and a test data for predicting the biosorption efficiency of As(III).

Performance assessment of the MLR model for the prediction of biosorption efficiency As (III) based on statistical parameters like AARE, R, RMSE, SD and MRE. A comparison between the predicted values of As(II) biosorption efficiency by the MLR model and those calculated from the experimental data using the training dataset and the test dataset is shown in the Fig. 7 and Table 6.

Table 6: Model evaluation parameters for MLR model using the training data and the test data

MLR Model evaluation parameter	Train data	Test data
AARE (%)	2.3206	1.74
R	0.9066	0.8775
RMSE	0.0275	0.0233
SD	4.7056	4.1988
MRE	0.0231	0.0177
Q^2_{LOO} (Train data), Q^2_{ext} (Test data)	0.8217	0.7533

Analysis of the SVR-based model

Similar procedure as discussed in “Case Study I” were used to develop the SVR model by grid search methodology with a 10-fold cross validation. The obtained optimal values of the model parameters are given in Table 7.

Table 7. Optimal parameters for SVR-based model for biosorption efficiency of As (III).

Property to be predicted	C	$\gamma = 1/2\sigma^2$	ε	Kernel type	Type of loss function	Number of support vectors	Number of training points
Biosorption efficiency(%)	32768	0.055	0.0848	RBF	ε - insensitive	46	65

The training and test course has been constructed using the training data set and test data set as shown in the Fig. 8 and Fig. 9 respectively. One can observe that the predicted data points for the training as well as for testing set lies very close to the experimental data. Further, it can be clearly seen that the SVR prediction results are much improved over the test data set.

Figure 8. Training course curve for the Prediction of As(III) biosorption efficiency(%)

Figure 9. Test course curve for the Prediction of As(III) biosorption efficiency(%)

Comparison of SVR-based model with the MLR model

A comparison of the prediction performances of the developed MLR model with the SVR-based model is shown in Table 8 and Fig. 10.

Table 8. Model evaluation parameters for SVR-based model and MLR model using the test data.

SVR Model evaluation parameter	SVR-based model	MLR model
AARE (%)	0.5591	1.74
R	0.9905	0.8775
RMSE	5.6418E-05	0.0233
SD	3.6245	4.1988
MRE	0.00562	0.0177

Figure 10. Comparison of SVR model with the MLR model using the test data set.

Table 9 illustrates the distribution of predicted data points of As (III) biosorption efficiency by the SVR-based model in terms of absolute deviation for the training data set. It has been found that the SVR-based model predicts nearly 90.7 % data points within an absolute deviation of less than 1 %. Only 9.23 % data points within an absolute deviation of less than 5% and no deviation have been found above an AD of more than 5%. Whereas, it is observed that the MLR-based model predicts nearly 95.38% data

points within an absolute deviation of less than 5 % and a total of 4.6% data points have an AD of more than 5%.

Table 10 depicts the distribution of predicted data points of As (III) biosorption efficiency by MLR and SVR-based model in terms of absolute deviation for the test data set. It is observed that the SVR based model predicts nearly 56.25% data points within an absolute deviation of less than 1% and all the data points fall within an absolute deviation of no more than 5%. While, the MLR-based model predicts nearly 25 % data points within an absolute deviation of less than 1 % and a total of 93.75 % data points within an absolute deviation of less than 5%. Only 6.25 % data points have an AD of more than 5%.

Table 9. Percentage distribution of predicted data points of the sorption efficiency of As (III) by MLR model and SVR- based model in terms of absolute deviation (AD) for the training data set.

Absolute deviation (AD) (%)	% of MLR model predicted values	Cumulative score	% of SVR model predicted values	Cumulative score
AD< 1	20	20	90.7692	90.7692
1<AD< 5	75.3846	95.3846	9.2308	100
AD>5	4.6154	100	0.00	
Total	100		100	

Table 10. Percentage distribution of predicted data points of the sorption efficiency of As (III) by MLR model and SVR- based model in terms of absolute deviation (AD) for test data.

Absolute deviation (AD) (%)	% of MLR model predicted values	Cumulative score	% of SVR model predicted values	Cumulative score
AD< 1	25	25	56.25	56.25
1<AD< 5	68.75	93.75	43.75	100
AD>5	6.25	100	0.00	
Total	100		100	

CASE STUDY - III

PREDICTION OF THE SORPTION CAPACITY OF LEAD (II)

To predict the sorption capacity of Lead (II) using an agricultural by-product ‘tree fern’, as a low cost biosorbent, similar procedure has been adopted as discussed in earlier case studies. Biosorption data for SVR, MLR and ANN model have been taken from the available published literature [65, 66]. The entire dataset consisting of 145 samples are divided into training dataset and testing dataset using the simple random sampling (SRS) technique, in the size ratio of 80% (116 data points) and 20% (29 data points) respectively. Finally developed SVR model has been evaluated and validated on the basis of statistical parameters as well as by comparing it with the commonly used multiple linear regression (MLR) model and ANN model.

Analysis of the MLR model

The MLR model was developed for predicting the sorption capacity of lead (II) ions (y) with the independent input parameters being: initial lead ion concentration (x_1), temperature (x_2), pH (x_3) and contact time (x_4).

The following MLR model equation has been obtained through MS-Excel (2007):

$$y = -141.8444 + 0.0398 (x_1) + 0.4826 (x_2) + 2.8756 (x_3) + 0.1336 (x_4)$$

The independent variables are found to be significant into the regression.

In this study, performance of the developed MLR model for the training and test data set is shown in the Fig. 11 as well as also, given in the Table 11. It can be seen from Table 11 that the performance of the MLR model for test data set (unseen data) is poor as compared to the training data set.

Table 11. Model evaluation parameters for MLR model using the training data and the test data.

MLR Model evaluation parameter	Train data	Test data
AARE (%)	21.1178	25.0056
R	0.78661	0.7613
RMSE	0.0469	0.1188
SD	8.3075	8.3246
MRE	0.1745	0.1799
Q^2_{LOO} (Train data), Q^2_{ext} (Test data)	0.6153	0.5764

Figure 11. Performance of MLR model using training data and test data for predicting the sorption capacity of lead(II).

Analysis of ANN model

The schematic representation of neural networks architecture shown in Fig. 12. comprises of: (1) input layer (independent variables), (2) hidden layers, (3) and the output layer (dependent variables). Three layered multiple feed forward neural networks (4:12:1) have been used for modeling of the sorption capacity of lead (II) with 4 – neuron for initial lead ion concentration (mg/L), temperature ($^{\circ}\text{C}$), pH of the solution and contact time (min) at the input layer, 12 – neuron at hidden layer and 1- neuron for the sorption capacity at the output layer. The entire data set of 145 samples is partitioned into three subsets consisting training dataset, 65% (data), validation dataset, 15% (data) and test dataset, 20% (data). The numbers of input and output neurons are set according to the nature of the problem whereas an appropriate number of neuron in the hidden layer has been chosen by trial and error method as insufficient neurons may cause under fitting while too many neurons might lead to over fitting [67, 68, 69]. The training of the ANN model is carried out with the complete input data set to the network till the MSE is minimized [70, 71, 72, 73]. A model should be trained properly in order to have its high correlation coefficient (R) close to 1 and low MSE. The ANN toolbox present in MATLAB has been used in this study to develop the model.

Figure 12. Schematic representation of ANN architecture.

Fig. 13 demonstrates that both the predicted values for the training data as well as the test data lie close to the ideal fit line. Table 12 exhibits the model evaluation parameters of the ANN model for both the training data as well as the test data.

Figure 13. Performance of ANN model using training data and test data for predicting the sorption capacity of lead(II).

Table 12. Model evaluation parameters for ANN model using training and the test data.

Model evaluation parameter	Train data	Test data
AARE (%)	4.4545	4.941
R	0.9889	0.9845
RMSE	0.0048	0.0587
SD	8.2293	7.9204
MRE	0.0444	0.0912
$Q^2_{\text{LOO}}(\text{Train data}), Q^2_{\text{ext}}(\text{Test data})$	0.9826	0.9779

Analysis of the SVR-based model

An SVR model with the same data set of 145 samples is developed using the procedure described in the previous case studies, the obtained optimal values of the SVR model parameter is given below in Table 13.

Table 13. Optimal parameters for SVR-based model for sorption capacity of Lead (II).

Property to be predicted	C	$\gamma = 1/2\sigma^2$	ε	Kernel type	Type of loss function	Number of support vectors	Number of training points
Sorption capacity [mg/g]	32768	0.058	0.09	RBF	ε -insensitive	70	116

After optimizing the SVR parameters, training course curve and test course has been constructed as shown in Fig. 14 and Fig. 15 respectively.

Figure 14. Training course curve for predicting the sorption capacity of lead (II) using SVR.

Figure 15. Test course curve for predicting the sorption capacity of lead (II) using SVR.

A comparison between the predicted values of the sorption capacity of lead (II) by the SVR-based model and those calculated from the experimental data using the training

dataset and the test dataset has been shown in the Fig. 16 and the model evaluation parameters are given in the Table 14.

Figure 16. SVR simulation of sorption capacity (mg/g) of lead (II) ions with optimal parameters using training data and test data set.

Table 14. Model evaluation parameters for SVR-based model using training and the test data.

SVR Model evaluation parameter	Train data	Test data
AARE (%)	3.9874	3.3816
R	0.9901	0.9914
RMSE	0.0041	0.0025
SD	8.2529	7.8962
MRE	0.0399	0.0338
$Q^2_{\text{LOO}}(\text{Train data}), Q^2_{\text{ext}}(\text{Test data})$	0.9800	0.9845

Comparison of SVR-based model with ANN and MLR model

Prediction performance of the developed SVR-based model has been compared with the ANN and the MLR model as shown in Fig. 17. Table 15 clearly depicts the superior prediction performance of the SVR-based model.

Figure 17. Comparison of SVR model with MLR and ANN model for predicting the sorption capacity (mg/g) of lead (II) ions using the test data set.

Table 15. Model evaluation parameters for SVR-based model, ANN and MLR model using test data set.

Model evaluation parameter	SVR-based model	ANN model	MLR model
AARE (%)	3.38	4.941	25.01
R	0.9915	0.9845	0.7613
RMSE	0.0025	0.0587	0.1188
SD	7.8962	7.9204	8.3246
MRE	0.0338	0.0912	0.1799

Table 16 illustrates the distribution of predicted data points of lead (II) sorption capacity by SVR-based model in terms of absolute deviation for the training data set. It has been found that the SVR-based model predicts nearly 77.58 % data points within an absolute deviation of less than 5 % and a total of 91.37 % data points within an absolute deviation of less than 10%. Only 0.86 % data points have an AD of more than 20%. Whereas, it is observed that the ANN model have 69.83 percent data points within an absolute deviation of less than 5 % and a total of 86.21 per cent data points within an absolute deviation of less than 10%. Only 96.55% data points have an AD of more than 20%.

MLR-based model predicts nearly 14.65% data points within an absolute deviation of less than 5 % and a total of 36.2% data points within an absolute deviation of less than 10%. Only 31.03% data points have an AD of more than 20%.

Table 17 depicts the distribution of predicted data points of lead (II) sorption capacity by MLR and SVR-based model in terms of absolute deviation for the test data set. It is observed that the SVR based model predicts nearly 86.2% data points within an absolute deviation of less than 5% and a total of 93.10 % data points within an absolute deviation of less than 10% and all the data points fall within an absolute deviation of not more than 20%. While, it is found that ANN model have 79.31 percent data points within an absolute deviation of less than 5 % and a total of 96.55 % data points within an absolute deviation of less than 10%. Only 3.44% data points have an AD of more than 20%.

MLR-based model predicts nearly 20.68 % data points within an absolute deviation of less than 5 % and a total of 37.93 % data points within an absolute deviation of less than 10%. Only 31.03 % data points have an AD of more than 20%. This shows that the SVR-based model is highly accurate and has good generalization ability for the unseen test data set.

Table 16 Percentage distribution of predicted data points of the sorption capacity of lead (II) by MLR model and SVR- based model in terms of absolute deviation (AD) for training data.

Absolute Deviation AD (%)	% of MLR model predicted values	Cumulative score	% of ANN model predicted values	Cumulative score	% of SVR model predicted values	Cumulative score
AD< 5	14.6552	14.6552	69.8276	69.8276	77.5862	77.5862
5<AD< 10	21.5517	36.2069	16.3793	86.2069	13.7931	91.3793
10<AD< 20	32.7586	68.9655	10.3448	96.5517	7.7586	99.1379
AD>20	31.0345	100	3.4483	100	0.8621	100
Total	100		100		100	

Table 17 Percentage distribution of predicted data points of the sorption capacity of lead(II) by MLR model, ANN and SVR- based model in terms of absolute deviation (AD) for test data set.

Absolute Deviation AD (%)	% of MLR model predicted values	Cumulative score	% of ANN model predicted values	Cumulative score	% of SVR model predicted values	Cumulative score
AD< 5	20.6897	20.6897	79.3103	79.3103	86.2069	86.2069
5<AD< 10	17.2414	37.9310	17.2414	96.5517	6.8965	93.1035
10<AD< 20	31.0345	68.9655	0.00	96.5517	6.8965	100
AD>20	31.0345	100	3.4483	100	0.00	
Total	100		100		100	

Performance Assessment of the Commonly Used MLR Model, ANN And SVR-Based Model in the Light of Existing Theory and Experimental Findings

A. Effect of initial conc. of lead (II)

Experiments were performed at constant condition (pH 4.9, temperature = 20° C, agitating speed = 300 rpm) to show the effect of various initial concentration of lead (II) on the sorption capacity of lead (II). It was observed that the sorption capacity of lead (II) initially increases due to ion exchange with the surface of cations on the tree fern and afterwards, it slows down representing a gradual uptake of cation exchange at the inner surface. The equilibrium sorption capacity increases from 18.2 to 41.5 mg/g, as initial lead (II) concentration vary from 74.1 to 350 mg/l.

Prediction of sorption capacity of lead (II) by SVR-based model, ANN and MLR model is shown in the Fig. 18 and it is found that the SVR-based model shows fair agreement with the experimental results and thus, it can be said that SVR-based has the best prediction ability and generalizability than ANN and MLR model.

Figure 18 (a)-(e). Effect of initial lead (II) ion concentrations on the sorption capacity (mg/g) of lead against contact time (pH 4.9, temperature = 20° C, agitating speed = 300 rpm).

B. Effect of temperature on sorption capacity of lead (II)

The effect of various temperatures on sorption capacity of lead (II) shown in Fig. 19 has been obtained by experiments performed with a constant condition (pH 4.9 initial lead concentration 200 mg/L, agitating speed = 300 rpm). Sorption capacity increases with an increase in solution temperature from 278 K to 318 K. However, the equilibrium sorption capacity was hardly affected by increased temperature. The values of rate constant were found to increase from 9.18×10^{-4} to 0.103 g/mg.min with an increase in the solution temperature from 278 K to 318 K.

The variation in temperature influenced the time required to reach saturation with excellent agreement between the experimental and the predicted curves. It is observed that the SVR-based follows the same trends of the experimental results and is the better predictive model than the other two.

Figure 19 (a)-(e). Effect temperatures on the sorption capacity (mg/g) of lead against contact time (pH 4.9 initial lead concentration 200 mg/L, agitating speed = 300 rpm).

C. Effect of pH on sorption capacity of lead (II)

Ho [66] had performed the experiments at constant condition (initial lead concentration 200 mg/L, temperature = 20° C, agitating speed = 300 rpm) to show the effect of pH on sorption capacity of lead (II). The obtained results shown in Fig. 20 demonstrate that the sorption was initially fast and then slowed until equilibrium was reached, it is believed that ion exchange may have occurred in the beginning state of sorption. It was also found that at low pH, surface of the tree fern becomes positively charged and as pH increased more ligands (neutral molecule) of tree fern gets attracted to the positively charged lead ion.

Predicting the effect of pH on sorption capacity of lead (II) by the SVR-based model, ANN and MLR and the data showed good compliance with the SVR model.

Figure 20 (a)-(e). Effect pH on the sorption capacity (mg/g) of lead against contact time (initial lead concentration 200 mg/L, temperature = 20° C, agitating speed = 300 rpm).

4. Conclusions

Artificial intelligence techniques such as ANN and SVM have been applied to predict the heavy metals removal efficiency in adsorption process and the results thus obtained have been compared with those obtained by MLR. Three case studies have been studied for the removal of heavy metals like Cu (II), As (III) and lead (II). It has been observed that the prediction performance of SVR is the best as compared followed by ANN and MLR, in that order. It is also found that the SVR model most effectively predicts the behavior of the complex interaction process of lead (II) removal from waste water under various experimental conditions, followed by the ANN model. Good prediction results from these AI techniques can be helpful in a more efficient design and fabrication of an efficient waste water treatment plant for treating heavy metal rich effluent.

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Nomenclature

b	Bias term
C	Cost function
C_0	Initial Cu(II) concentration, mgL^{-1}
F	High-dimensional feature space
$f(\mathbf{x})$	Regression function
$K(\mathbf{x}_i, \mathbf{x}_j)$	Kernel function
L	Lagrangian function (dual form)
Q^2_{ext}	Leave-one-out cross validation on the test set
Q^2_{LOO}	Leave-one-out cross validation on the training set
W	Weight vector
x_i	Input vector
y_i	Output vector

Greek symbols

σ	Width parameter of RBF kernel
ε	Loss function
γ	Regularization parameter
α and α^*	Lagrange multipliers
$\phi(\mathbf{x}_i)$	Mapping function to high dimensional feature space for input vector $\mathbf{x}$

Abbreviations

AARE	Average absolute relative error
AD	Absolute deviation

ANN	Artificial neural networks
MSE	Mean square error
RMSE	Root mean square error
SD	Standard deviation
MRE	Mean relative error
MLR	Multiple linear regression
SVM	Support vector machine
SVR	Support vector regression

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