

# A novel artificial intelligence approach for regolith geochemical grade prediction using multivariate adaptive regression splines

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## ARTICLE INFO

### Article history:

Received 28 December 2021

Revised 31 January 2022

Accepted 9 February 2022

### Keywords:

Multivariate adaptive regression spline  
Artificial intelligence techniques  
Kriging geostatistical technique  
Ashanti belt  
Geochemical grade prediction

## ABSTRACT

The necessity for applying a potent analytical regolith geochemical grade estimator is driven by the reality of mineral exploration. This is because many exploration geologists rely upon the classical geostatistical method of Kriging which oftentimes do not produce accurate predictions due to the complexity of interactions between geological features and spatial variables. In this study, a novel non-linear data-driven approach known as Multivariate Adaptive Regression Spline (MARS) is proposed as an effective predictive tool to unravel regolith geochemical complexities. The proposed MARS approach was used to predict regolith geochemical grade from a thick regolith cover in the Tarkwaian paleo-placer of the South-Western Ashanti belt in Ghana. Out of the 891 samples, the data was partitioned into 70% training (model development) and 30% testing (model validation). The proposed MARS result was compared with three other artificial intelligence techniques (i.e., radial basis function neural network, backpropagation neural network and generalised regression neural network) and kriging geostatistical technique. Based on the test results, MARS had the highest correlation coefficient ( $R = 0.9675$ ) and the least statistical error metrics ( $RMSE = 0.7791$ ,  $MAE = 0.6014$ , and  $\rho = 0.0472$ ). The implementation of the MARS approach in regolith geochemical grade estimation domain has yielded outstanding and promising results. The MARS superiority was evident in its calibration strength, prediction accuracy, robust interaction of variables and overcoming the black box system of ANN. Thus, the proposed MARS approach could be an excellent tool in regolith geochemical grade estimation workflow when fully integrated with exploration tasks.

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## 1 Introduction

The future of mining and mining-related industries looks bleak as governments and investors struggle to add an ounce to existing production mines. Over the past decade, there has been a tremendous decline in exploration activities and collapse or near-collapse of existing mines. This worrying trend has not escaped the attention of the geoscience industry. Indeed, the discovery of economic mineral deposits has dwindled significantly (Barnett and Williams, 2012) hence the need to salvage the situation.

Generally, exploration is preoccupied with integrating relevant datasets and utilising various techniques to discover subtle surface

indications of mineralisation. The most pertinent decision, according to Barnett and Williams (2012), is deciding where to focus attention on the ocean of barren and prospecting areas. Accordingly, one of the most fundamental and crucial tasks in regional-scale geochemical exploration involves the delineation of exploration targets using soil, stream sediment and lithochemical geochemical data (Carranza and Hale, 1997; Cheng, 2007; Carranza, 2011; Afzal et al., 2013; Parsa et al., 2016; Ghezelbash and Maghsoudi, 2018; Ghezelbash et al., 2018; Liu et al., 2018). This will usually lead to regolith geochemical models and possibly mineral deposit discovery. Ghana located in tropical zones is endowed with thick regolith, i.e., a layer of weathered residual soil mass that covers most of the South Ashanti lode auriferous belt (Griffis et al., 2002), has proven to be a source of favourable ore enrichment (Griffis et al., 2002; Carranza et al., 2009). However, geoscientists usually are challenged with the ability to model

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and predict favourable targets for final follow-up. To circumvent the situation, the use of data mining, Geographic Information System (GIS) and geostatistical techniques have aided in geochemical data processing, grade estimation and anomaly detection (Moyeed and Papritz, 2002; Misra et al., 2007; Rossi and Deutsch, 2014; Ghandhi and Sarkar, 2016). The fundamental design and interpretation of lithochemical target generation mineral prospectivity mapping and grade predictions and estimation have been discussed in detail by various authors (Marjoribanks, 2010; Carranza and Sadeghi, 2010; Porwal et al., 2010; Chilès and Delfiner, 2011; Rossi and Deutsch, 2014; Keyan et al., 2015; Ghandhi and Sarkar, 2016).

In the last two decades, geostatistical modelling with GIS has been used to establish measures of spatial continuity or variability for ore grade estimation. This hybrid modelling has become the standard and most widely used technique for regional geochemical target generation and mineral resource estimation (Hale and Plant, 1994; Goovaerts, 1997; Isaaks and Srivastava, 1988; Isaaks and Srivastava, 1989; Hale, 2000; Chilès and Delfiner, 2011; Rossi and Deutsch, 2014; Ghandhi and Sarkar, 2016). It is a well-known fact that geostatistical modelling is known for its kriging techniques and has led to growing complexities in the handling of relationships between geological attributes (Hastie et al., 2009; Rossi and Deutsch, 2014). Despite its fame and versatility, geostatistical techniques have been plagued with certain setbacks such as its inability to model universally complex non-linear spatial relationships (Breiman, 2001; Moyeed and Papritz, 2002; Strebelle, 2002; Tahmasebi and Hezarkhani, 2012; Misra et al., 2007; Rossi and Deutsch, 2014). Besides, geostatistical techniques usually require the satisfaction of certain modelling assumptions such as stationarity, linearity and normality of dataset. Also, geostatistical modelling can be time-consuming and computationally expensive due to the complexity of cumbersome data processing (Strebelle, 2002; Leathwick et al., 2006; Misra et al., 2007; Samanta and Bandopadhyay, 2009). Moreover, in highly heterogeneous and sparse data situations, geostatistical models find it challenging to produce good results and as a result perform poorly in that regard (Samanta et al., 2004; Dutta et al., 2010).

To overcome these setbacks, there is, therefore, the need to apply an alternative method for geochemical ore grade predictions. The literature is replete with the use of several machine learning methods such as Artificial Neural Network (ANN) aimed at geochemical grade estimation and target generation (Harris et al., 2001; Brown et al., 2000; Harris et al., 2003; Porwal et al., 2003; Nykänen, 2008; Carranza and Sadeghi, 2010; Oh and Lee, 2010; Ibrahim et al., 2021) and ore grade estimation (Skabar, 2005; Samanta and Bandopadhyay, 2009; Tahmasebi and Hezarkhani, 2010). The suitability of the ANN has increased its application to geochemical data processing, analysis, interpretation and detection of geochemical anomalies due to its strength in processing non-linear variable relationships. While ANN requires extensive datasets, its training and design are computationally expensive and sometimes the results get stuck in local optima due to the gradient descent training algorithms used. In addition to that, ANN black box system has made it mathematically "unattractive" because the functional relationship between input and target variables cannot be established between the modeller and the user (Breiman, 2001; Leathwick et al., 2006). In view of these mathematical inconveniences in ANN, several researchers have adopted other machine learning techniques such as Support Vector Machine (SVM) (Zuo and Carranza, 2011; Abedi et al., 2012), Random Forest (RF) (Rodriguez et al., 2015; Carranza and Laborte, 2016), Extreme gradient boosting (Ibrahim et al., 2021), Decision tree (Reddy and Bonham-Carter, 1991; Chen et al., 2014) and hybrid ANN techniques (Adaptive Neuro Fuzzy Inference System (ANFIS), genetic algorithm-ANN (GA-ANN). These methods have been pro-

posed by various researchers and have proven their strength over the ANN methods in ore grade estimation (Samanta et al., 2004; Porwal et al., 2004; Mahmoudabadi et al., 2009; Tahmasebi and Hezarkhani, 2009; Yu et al., 2012; Chatterjee et al., 2010).

Zuo (2017) stated that machine learning has been applied in geosciences but in a limited scope and thus more applications to demonstrate its advantages and uniqueness in solving complex integrated geological datasets should be explored. This study proposes the Multivariate Adaptive Regression Splines (MARS) developed by Friedman (1991) as a novel alternative predictive tool for regolith geochemical grade estimation. The proposed MARS approach (Smith, 1982; Friedman, 1991) is a specialised form of multivariate regression algorithms that builds hierarchical models using stepwise selection and a set of basis functions. MARS can produce data-driven, localised multiple non-linear regression models wherein each region, a simple hyperplane is built and linked to each other. In addition, the MARS does not impose any underlying modelling assumptions on the dependant and predictor variables, hence, does not require class relationships on the predictor-dependant variables of interest (Quirós et al., 2009; Hastie et al., 2009).

The MARS has demonstrated its robustness against many ANN methods due to its exceptional analytical speed and intuitive capabilities that avoid fine-tuning of several parameters and slow convergence, which has been the case of ANN (Abraham et al., 2000; Moisen and Frescino, 2002; Yang et al., 2003; Yang et al., 2004; Leathwick et al., 2005). In addition to that, the MARS approach overcomes the black box system of ANN by providing a functional relationship between response and explanatory variables. Despite the widespread use of MARS and other machine learning techniques in geosciences, the situation is even alarming with respect to the six principal auriferous gold Belts in Ghana (Griffis et al., 2002), where the strength of MARS and other machine learning techniques, in general, are yet to be explored in the potentials of Ghana's rich greenstone/volcanic gold deposits. Therefore, the proposed MARS technique in this study is targeted at providing a fast, timely, and reliable regolith geochemical grade estimation, with minimum prerequisite for modelling skills and assumptions.

The simplified computational and functional capabilities of MARS (Hastie et al., 2009) as a proposed technique was tested against the benchmark machine learning methods of Radial Basis Function Neural Network (RBFNN), Backpropagation Neural Network (BPNN) and Generalised Regression Neural Network (GRNN) to demonstrate its robustness and easy interpretability of predicted results. Furthermore, this study compares the predictive capabilities of machine learning algorithms (i.e., MARS, RBFNN, BPNN and GRNN) to the classical geostatistical modelling technique of ordinary kriging.

It is widely known that regolith mapping logging codes contain numerous categorical variables, which are mostly subjective. Some of these geological features are alteration, weathering, lithological codes and oxidation. To overcome the issue of subjectivity, this study focuses on a data-driven approach, using the spatial dataset of Easting (E), Northing (N) and Elevation (Z) that define the positions of the various sample points as the input variables and gold (Au) value as the output. This study uses MARS as a novel technique to improve the prediction accuracy of interaction between Au and spatial features (E, N, Z) within the placer environments. This will be achieved by: (a) inspiring confidence and reliability of MARS as a useful universal data-driven model for regolith geochemical grade estimation; (b) accurately predicting Au values within regolith geochemical features critical for the Tarkwaian paleo-placer exploration of the South-Western Ashanti belt; and (c) demonstrate the robustness of MARS models against other benchmark methods (BPNN, RBFNN and GRNN) investigated.

## 2. Geological setting

Ghana is predominantly underlain and hosted by metamorphosed greenschist rock of the paleoproterozoic (ca. 2300–1900 Ma) age (Boher et al., 1992; Taylor et al., 1992; Davis et al., 1994; Oberthür et al., 1998; Allibone et al., 2002) and related to Eburnean orogenic cycle (Griffis et al., 2002). Much of the historical and detailed description of the geological and structural setting of Ghana is provided in these studies (Junner, 1940; Kesse, 1985; Hirdes et al., 1993; Loh and Hirdes, 1996; Griffis, 1998). The study area falls within the Tarkwaian paleoplacer within the prolific South-Western Ashanti orogenic lode gold belt system.

### 2.1. Geology and mineralisation style of the Tarkwaian

The study area is located within the Tarkwaian group, which forms part of the West African Craton. It is covered largely by the Birimian volcanic and metasediments. The Birimian Supergroup underlining the Tarkwaian Group consists of metamorphosed lava and pyroclastic rocks, which contains abundant grey wacke (meta siltstone and sandstone), phyllites and intrusive rocks. The Tarkwaian group consists of a thick sequence of clastic metasedimentary rocks that have suffered low grade regional metamorphism, shearing and altering by hydrothermal solution (Kesse, 1985). The higher grades are uncommon and are often associated with intrusive rocks. Locally, the mine is situated along the southern end of the Tarkwa syncline (basin) of the Tarkwaian Group. Gold mineralisation occurs in a sedimentary sequence known as the Banket Formation.

The Banket Reef zone comprises a sequence of individual beds of quartz conglomerates (Banket beds), breccia conglomerates, meta-sandstones (quartzite) and grits. All the known gold mineralisation is associated with the conglomerates and is found within the matrix that binds the pebbles together (Griffis et al., 2002). The Tarkwaian group consists of a thick sequence of clastic meta-sedimentary rocks that have suffered low-grade regional metamorphism, shearing and altering by hydrothermal solution (Kesse, 1985). The higher grades are uncommon and are often associated with intrusive rocks. The Tarkwaian group is subdivided into four main groups: Kawere Formation, Banket Formation, Tarkwa Phyllite Formation and Huni Formation (Fig. 1). The Basal Kawere Group is predominantly polymictic, poorly sorted sandstone and conglomerates and varies in thickness between 250 m and 700 m, which contain low economic gold mineralisation (Ewusi et al., 2017).

The overlying Banket Formation comprises conglomerates, made up of volcanic clasts and Birimian quartz pebbles, with intercalated cross-bedded sandstones. The Banket Formation hosts the Tarkwa Placer gold deposit (<100 m thick gold zone), attains an estimated maximum thickness of 600 m and grades upwards into the Tarkwa Phyllite Formation, which is about 400 m thick. The Phyllites grades conformably into the uppermost Huni Formation, which consists of approximately 1400 m thick sequence of sandstones with interbedded phyllites and quartzites, intruded by minor dolerite sills (Kesse, 1985; Strogen, 1991; Griffis et al., 2002; Pigois et al., 2003; Perrouty et al., 2012).

## 3. Overview of methods

In this section, the theoretical concept of the proposed MARS technique is briefly presented. Also presented are the Kriging technique and the various benchmark machine learning techniques (BPNN, RBFNN, and GRNN), which have been successfully applied to grade estimation.

### 3.1. Multivariate adaptive regression splines

MARS is a form of regression analysis introduced by Jerome Friedman for solving classification and regression problems (Friedman, 1991). The method can select and transform variables automatically and can easily recognise and identify their potential interactions. The MARS approach fits the stepwise linear basis function of the form  $(x-a)_+$  and  $(a-x)_+$  as shown in Eq. (1).

$$Y = (x - a)_+ = \begin{cases} x - a, & \text{if } x > a \\ 0, & \text{otherwise} \end{cases}; \quad Y = (a - x)_+ = \begin{cases} a - x, & \text{if } a > x \\ 0, & \text{otherwise} \end{cases} \quad (1)$$

where “+” means positive part and  $a$  is an arbitrary threshold value. Here, the MARS breaks the data into step-functions having a knot at the value  $a$ , that imposes a locally non-linear relationship. These two functions are direct mirror pairs such that a collection of basis functions,  $C$ , of non-linear pattern for every input  $x_j$  with an observable knot of  $x_{ij}$  of that input (Eq. (2)) is formed in a continuous chain of functions (Hastie et al., 2009).

$$C = \{(x_j - a)_+, (a - x_j)_+\}, \quad a \in \{x_{1j}, x_{2j}, \dots, x_{Nj}\}; \quad j = 1, 2, \dots, p \quad (2)$$

The MARS model building involves the forward and backward selection stages. In the forward stage, MARS builds a flexible piecewise model by dividing the solution space into various intervals of predictor parameters which are hierarchical (Hastie et al., 2009). This is accomplished by building knots with an analytical construct known as the basis function. The knot building stops after a specified upper limit is attained. Usually, the initial MARS model typically overfits the data (with so many knots) so a later backward pruning is followed to delete the redundant knots. The MARS final predictive model thereby has the general form as expressed in Eq. (3).

$$f(x) = \beta_0 + \sum_{m=1}^M \beta_m h_m(x) \quad (3)$$

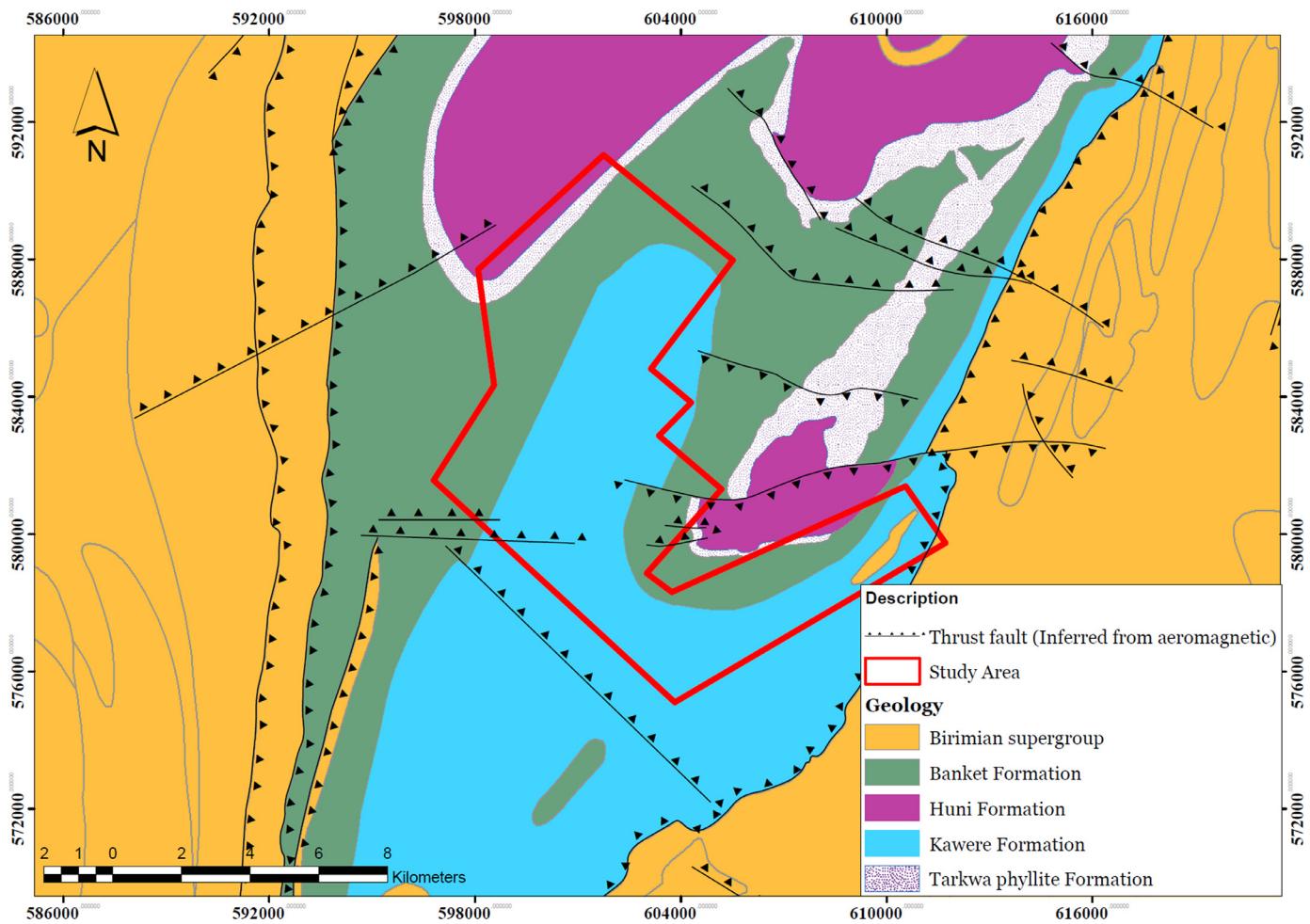
where  $h_m(x)$  is the  $m^{th}$  basis function,  $\beta_0$  is the constant term,  $M$  is the number of basis functions,  $\beta_m$  is the coefficient corresponding  $h_m(x)$ . The final stage involves determining the optimal model of which MARS typically uses the Generalised cross-validation (GCV) criterion (Friedman, 1991; Hastie et al., 2009; Kuhn and Johnson, 2013) on the data, defined in Eq. (4).

$$GCV(\lambda) = \frac{\sum_{i=1}^n (y_i - \hat{h}_\lambda(x_i))^2}{\left(1 - \frac{P(\lambda)}{n}\right)^2} \quad (4)$$

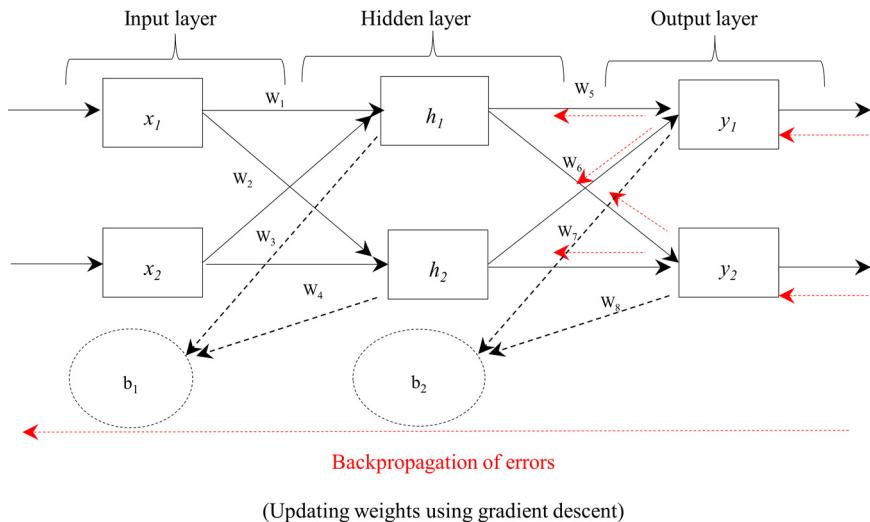
where  $\lambda$  is the number of terms,  $y_i$  is the  $i^{th}$  response variable,  $\hat{h}_\lambda(x_i)$  is the fitting response,  $P(\lambda)$  is the effective number of parameters in the model and  $n$  is the number of observations. It must be noted that  $P(\lambda)$  is generally related to the number of basis functions,  $d$  is the penalty term of the model, and  $k$  represents the flexibility or complexity of the model. It follows that  $P(\lambda) = r + kd$ . According to Hastie et al. (2009),  $k$  is defined between  $2 < k < 3$ .

### 3.2. Backpropagation neural network

The BPNN architecture consists of input, hidden and output arranged in a feed-forward manner (Fig. 2). The technique can also be described as a universal nonlinear multilayered feed-forward function approximator (Ahmadian, 2016) that adapt weights of layer connections continuously after each training process. The weight adjustment is based on the error difference between the predicted and expected results. Each layer initialises with a weight



**Fig. 1.** Simplified stratigraphic sequence map and geological map of south-western Ghana.

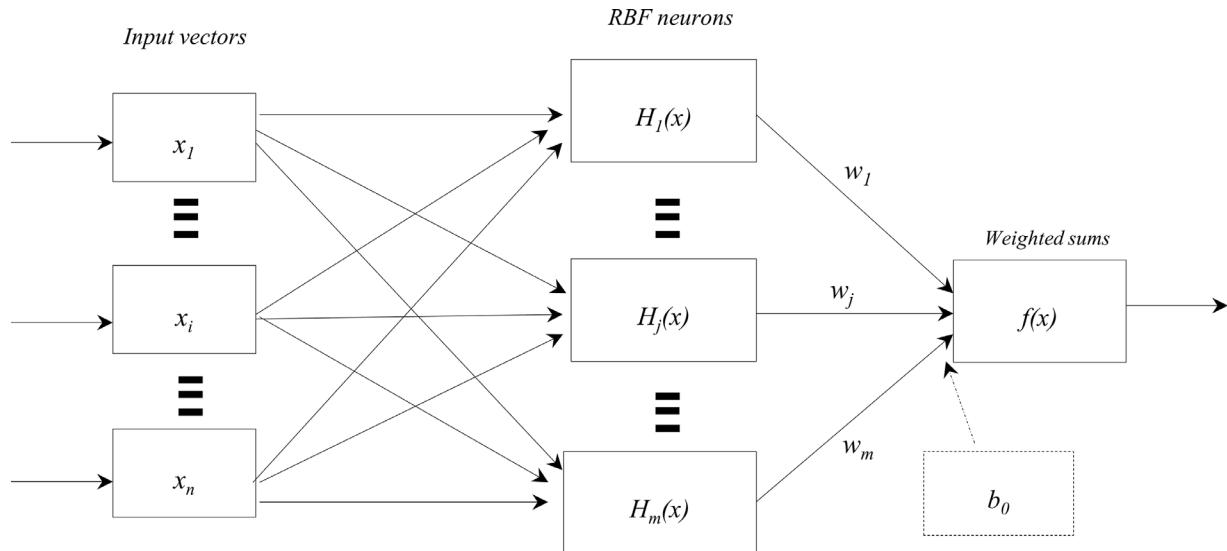


**Fig. 2.** Backpropagation neural network architecture.

matrix ( $w_{ij}$ ), a bias ( $b_i$ ) and an output, ( $y_i$ ) vector. Typically, the computational process of the BPNN involves two stages (i.e., the forward and backward phase).

The forward phase involves computing the signal of the output neurons. This is achieved through a systematic sequence of inputs, applying weights and “squashing” with activation function and given predicted signal. Here, each neuron receives a set of

inputs ( $x_i$ ) to the input layer, performs a dot product with the weights matrix, bias vector ( $b_i$ ) and transfer it into the hidden layer. In the hidden layer, an activation function is applied to the outputs from the input layer. In this study, the hyperbolic tangent transfer function which gives values within the range of -1 to 1 (Karlik and Olgac, 2010; Mueller and Massaron, 2016) was used in the hidden layer. The results from the hidden layer are then sent



**Fig. 3.** Radial basis function neural network architecture.

to the output layer for further processing. The same computation process in the hidden layer is repeated for the output layer neurons to produce the predicted outputs.

The backward phase involves computing error (difference between predicted and desired outputs) and backpropagating (reversing) to modify the connected weights, starting from output layers with the objective of minimising the error function (Fig. 2). The backpropagating process iterates until the error margin reached an acceptable limit.

### 3.3. Radial basis function neural network

RBFFNN is a form of multilayered feed-forward network. It was originated from Powell (1977), introduced and formulated by Broomhead and Lowe (1988), and Moody and Darkin (1989). Its versatility and uniqueness in solving function estimation, pattern recognition and classification problems have been demonstrated by several authors (Poggio and Girosi, 1990; Chen et al., 1991; Bishop, 1991; Musavi et al., 1992; Chang and Lippmann, 1993; Haykin, 1994; Roy and Miranda, 1995; Bishop, 1995; Behnia, 2007; Quirós et al., 2009; Patra et al., 2015). Specifically, the RBFFNN has also been applied to ore grade estimation (Kapageridis and Derby, 1998) and prospectivity mapping (Nykänen, 2008). The RBFFNN architecture consists of an input layer, a non-linear hidden layer activation function called radial basis function (RBF) and a linear activation function for the output layer (Fig. 3). The RBF consists of only one hidden layer that contains the transfer function, unlike the BPNN where several hidden layers can be used.

The input variables correspond to the number of neurons in the input layer. First, the input neurons, \$x\_n\$, feed the values to the hidden layer in a vector space. Now the input vector is connected to the computational neurons in the hidden layer with Gaussian radial basis activation function (Eq. (5)), which is inversely related to the distance from the centers of neurons (Hagan et al., 1996; Haykin, 1999).

$$\varphi(x) = \exp\left(-\frac{\|x_i - c_m\|^2}{2\sigma_m^2}\right), \quad m = 1, 2, \dots, q \quad (5)$$

where \$\varphi\$ is the Gaussian RBF, \$\sigma\$ is the spread (variance) responsible for the smoothness of the activation function, \$x\_i\$ is the input vector, \$c\_m\$ is the centre vector of the \$m^{th}\$ activation centre and \$\|x\_i - c\_m\|\$ is the distance between the input and the centre of the function. The \$\sigma\$ and \$c\_m\$ in each RBF dimension, network

weight parameters of the output layer and the optimal number of hidden layer neurons are determined during the network training Haykin, 1999). Here, the centers of the RBFs of the network are specified through either gradient descent learning, random selection (Broomhead and Lowe, 1988; Poggio and Girosi, 1990), or self-organising methods such as the k-means clustering technique (Moody and Darkin, 1989). The Euclidean norm \$\|\cdot\|\$ is used to express the distance of data points to the centre of each neuron (this is within the same dimensional space as the inputs). The respective weights, centers and the spread are trained using the following learning rules as given in Eqs. (6)-(8).

$$w_{mn}(k+1) = w_{mn}(k) + \eta e(k) h_m(k) \quad (6)$$

$$c_{mi}(k+1) = c_{mi}(k) + \eta e(k) w_{mn} h_m \frac{\|x_i(k) - c_{mi}(k)\|}{\sigma_m^2(k)} \quad (7)$$

$$b_m(k+1) = b_m(k) + \eta e(k) w_{mn} h_m \frac{\|x(k) - c_m(k)\|^2}{\sigma_m^3(k)} \quad (8)$$

where \$\eta\$ is the learning rate, \$e(k)\$ is the error in \$k^{th}\$ sampling, \$w\_{mn}\$ is the connect weight between \$n^{th}\$ output node, \$m^{th}\$ is the basis function and \$b\_m\$ is the width vector. The network's weight parameter is computed and updated for each neuron from the calculated distance using the recursive least squares parameter identification technique (Nekoukar and Beheshti, 2010; Senapati and Dash, 2013). Finally, predictions are made by the weighted sum of the RBFs' outputs and weights of each neuron and optimal spread. Hence, the outputs of the hidden layer are weighted \$w\_m\$ and output function \$f(x)\$ (Haykin, 1999) is computed as given in Eq. (9).

$$f(x) = \sum_{m=1}^q w_m \varphi(\|x_i - c_m\|) + b \quad (9)$$

where \$b\$ is bias vector with weight nodes, \$w\_1, w\_2, \dots, w\_q\$.

### 3.4. Generalised regression neural network

GRNN was first introduced by Specht (1991) and related to the probabilistic neural classifier. A GRNN is similar to RBFFNN with slight variation in its architecture and computational procedures (Ahmadian, 2016; Hannan et al., 2010). For example, within the training dataset, the GRNN set one neuron to each sample with a very fast learning rate because it does not require an iterative

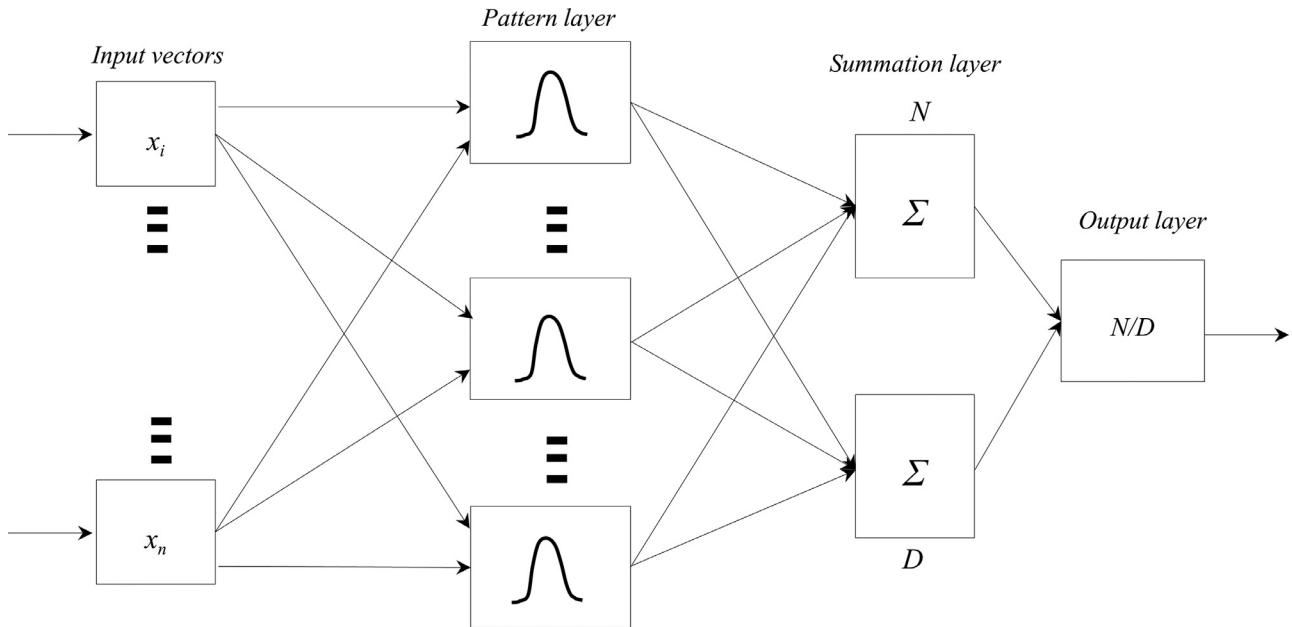


Fig. 4. Generalised regression neural network architecture.

procedure to produce results as has been observed in the Probabilistic Neural Network (PNN), RBFNN and BPNN (Hannan, 2010). This enables the GRNN to be less sensitive to the training dataset (Subramanian and Saraswathi, 2012). A GRNN network architecture consists of four basic layers: input layer, pattern layer, summation layer and output layer, as shown in Fig. 4.

The first layer, which is only a distribution unit, is fully connected to the pattern layer with one more node than the output layer. Each sample within the training data will influence every point that is being predicted by GRNN. The pattern layer, which is the first hidden layer, takes on the scaled measurement variables  $x$  from the input layer. The pattern layer consists of an  $N$  number of training samples where each node is represented by a  $x_i$  input vector. The input vector is associated with the assigned vector with the  $j^{th}$  training sample data point. Within each node, the input vector is subtracted from the assigned vector to the node,  $x_i$ , that is squared by the node. The result is then fed into a non-linear radial basis kernel function (Hannan et al., 2010). The outputs from the pattern hidden layer are passed onto the summation layer (second hidden unit).

The summation layer has two parts, the Numerator ( $N$ ) and Denominator ( $D$ ) Eq. (11)). The  $N$  part contains the summation of the multiplication of the first hidden layer outputs and the observed training output,  $y_i$  corresponding to  $x_i$ . The input of the second node ( $D$ ) is the summation of the first hidden layer activation function. Finally, the fourth layer is the output layer which receives the two outputs from the summation layer and merely divides ( $N/D$ ) to yield an estimate or prediction result of  $f(x)$  (Jang et al., 1997). The GRNN can generalise for new inputs after adequately learning from the training datasets. The GRNN output is computed using Eqs. (10) and (11).

$$d_i^2 = (x - x_i)^T (x - x_i) \quad (10)$$

$$f(x) = \frac{\sum_{i=1}^n y_i \exp\left(-\frac{d_i^2}{2\sigma^2}\right)}{\sum_{i=1}^n \exp\left(-\frac{d_i^2}{2\sigma^2}\right)} = \frac{N}{D} \quad (11)$$

where  $e^{-d_i^2/2\sigma^2}$  is the Gaussian activation function,  $d_i^2$  is the Euclidean distance between the training vector,  $x_i$ , and the input sample  $x$ , and  $\sigma$  is the spread (variance) responsible for the smoothness of the GRNN.  $f(x)$  is the predicted outputs of the network.

### 3.5. Kriging interpolation

Kriging resembles a non-parametric local fitting model that restricts the mapping of the model through variogram structure to a neighbourhood of datasets (Misra et al., 2007; Rossi and Deutsch, 2014). In kriging, the prediction of an unknown value at a location is obtained by linearly weighting the data points near to that particular location using the variogram structure of the spatial attribute (Moyeed and Papritz, 2002; Misra et al., 2007; Rossi and Deutsch, 2014; Ghandhi and Sarkar, 2016). amongst the numerous kriging estimators, the most versatile and common estimation technique is ordinary kriging (Rossi and Deutsch, 2014), although different kriging methods are becoming popular in recent years. By construction, kriging and its variants is a minimum error estimator (Rossi and Deutsch, 2014), and according to Srivastava (1987), no other set of weights can estimate lower variance than kriging. While least-squares optimisation is the valuable property of kriging, there are cases where minimum variance may be the wrong optimisation criteria to use (Srivastava, 1987). In this study, the most widely used ordinary kriging estimation method was used. Eq. (12) expresses the generalised form of the kriging interpolation technique.

$$\hat{z}(x_0) = \sum_{i=0}^n (\lambda_i z(x_i)) \quad (12)$$

where  $\lambda_i$  is an unknown weight for the measured value at the  $i^{th}$  location,  $x_0$  is the prediction location,  $n$ , denotes the number of measured values,  $\hat{z}(x_0)$  is the estimate at an un-sampled location,  $x_i$  is the measured value at the  $i^{th}$  location.

In ordinary kriging, the  $\lambda_i$  does not depend only on the difference in distance between predicted and measured locations, but on the total spatial arrangements of the measured locations. Typically, kriging interpolation is achieved through (i) estimating statis-

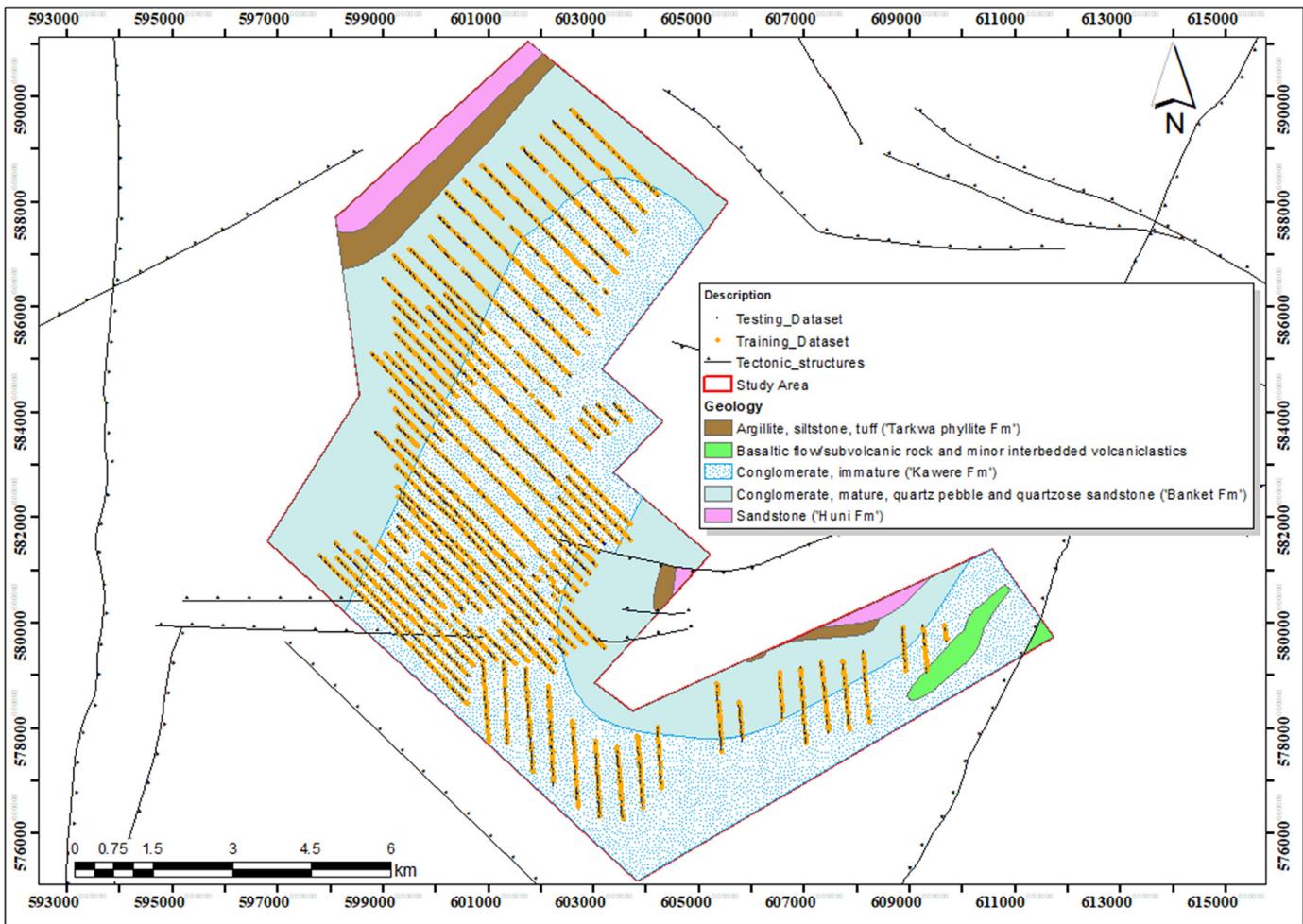


Fig. 5. Sampling points of the study area showing training and testing datasets.

tical dependence using variography and covariance functions and (ii) predicting unknown locations. Variography, however, is used to fit a model for use in kriging interpolation. The semi-variogram can be written in the form (Eq. (13)):

$$\gamma(x_0) = \frac{1}{2N(x_0)} \sum_{i=0}^n [z(x_i) - z(x_i + x_0)]^2 \quad (13)$$

where  $N(x)$  is the number of pairs for lag separation,  $x$ . Fitting empirical semi-variogram models involves function approximators such as Gaussian, spherical, linear, exponential and circular models. The spherical model is the most commonly used variogram model (Rossi and Deutsch, 2014; Haldar, 2013) due to its positive definite functions. In this study, we used the spherical semi-variogram model (Eq. (14))

$$\gamma(x_0) = \begin{cases} 0, & x_0 = 0 \\ k_0 + k, & x_0 > \alpha \\ k_0 + k \left( \frac{3x_0}{2\alpha} - \frac{1}{2} \left( \frac{3x_0}{2\alpha} \right)^3 \right), & 0 < x_0 \leq \alpha \end{cases} \quad (14)$$

where  $k_0$  is the nugget effect/constant (natural or analytical error),  $k_0 + k$  is the sill (total variance where the empirical variogram appears to level off),  $k$  is the structure variance and  $\alpha$  is the range (distance where maximum variability between samples is reached).

#### 4. Statistical evaluation of model performance

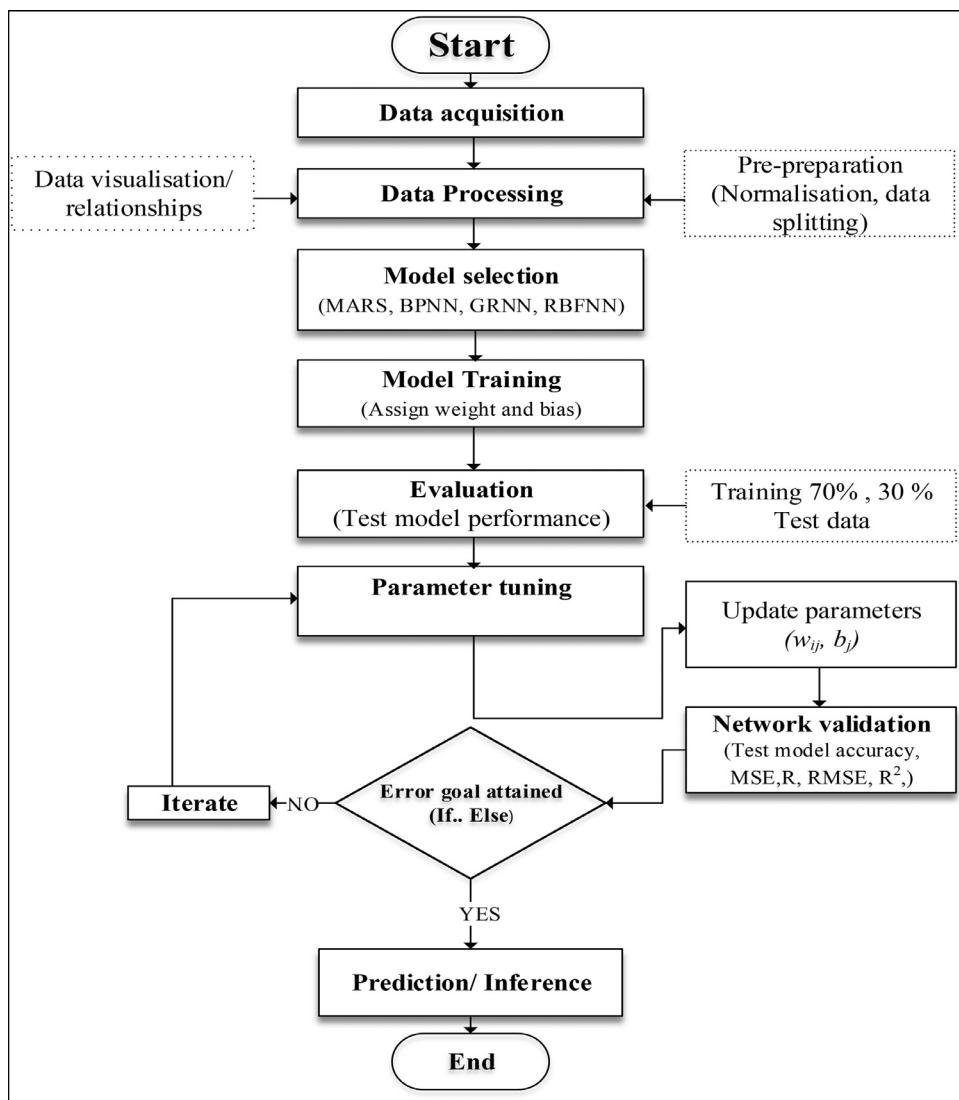
In this study, various performance measures were used as a criterion for ranking and evaluating the viability of the developed models. Four statistical evaluating parameters namely: Correlation Coefficient ( $R$ ), Root Mean Squared Error (RMSE), Mean Absolute Error (MAE), and Correlation Index ( $\rho$ ) were considered (Smith, 1982; Friedman, 1991; Hastie et al., 2009). These statistical performance metrics are expressed mathematically (Asuero et al., 2006; Milani and Benasciutti, 2010; Gandomi et al., 2011; Savaux and Bader, 2015; Chai and Draxler, 2014; Gandomi et al., 2015; Hasanipanah et al., 2016) in Eqs. (15)-(18).

$$MAE = \frac{1}{N} \sum_{i=1}^N |A_i - E_i| \quad (15)$$

$$RMSE = \left( \frac{1}{N} \sum_{i=1}^N (A_i - E_i)^2 \right)^{1/2} = \sqrt{MSE} \quad (16)$$

$$R = \frac{\sum_{i=1}^N (A_i - \bar{A})(E_i - \bar{E})}{\left( \sum_{i=1}^N (A_i - \bar{A})^2 \right)^{1/2} \left( \sum_{i=1}^N (E_i - \bar{E})^2 \right)^{1/2}} \quad (17)$$

$$\rho = \frac{RRME}{R + 1} \quad (18)$$



**Fig. 6.** Model-building flowchart.

where  $\bar{A}$  is the mean of the measured values  $A_i$ ,  $\bar{E}$  is the mean of the predicted  $E_i$ ,  $N$  is the total number of samples and RRME is the Relative Root Mean Square.

## 5. Results and discussion

### 5.1. Data acquisition and pre-processing

Litho-geochemical surveys are usually undertaken to target areas for the advanced stage. The surveys typically involve the collection of soil, rock and/or stream sediment samples. A total of 891 soil sediment samples were taken from the study area of about 54 sq. km on 20 m spacing sampling points at an average depth of 0.8 m (Fig. 5). This district-scale soil geochemical project was undertaken to delineate high prospectivity zones. The grid line spacing was generally 200 m. The traverse lines were orientated on NW-SE bearing across the regional lineation trends (Fig. 5). The samples were analysed for gold using aqua-regia digestion low level ( $2 \leq \text{limit} \leq 1000 \text{ ppb}$ ) technique. Aqua regia is commonly used because it dissolves elemental gold as well as breakdown iron and manganese oxides, oxy-hydroxides, carbonates, sulphates, sulphides and many types of clay. It will not release elements or minerals included within quartz (including silcrete) or other in-

soluble silicates or dissolve resistant minerals such as chromites, rutile, cassiterite, ilmenite and zircon (Fletcher, 1981; Potts, 1987; Thompson and Walsh, 1989).

A rigorous quality control/analysis procedure was followed by inserting a field duplicate at baren quartz (blank). About 97% of the blank samples fell below the detection limit suggesting barely no contamination. Analysis of pair of samples using simple regression and half absolute relative deviation plots showed a coefficient of correlation of 15% indicating a very low precision. This may be due to the high heterogeneity and nugget effect of the paleo-placers. In this study, a total of 891 data points consisting of gold (Au) and positional coordinates (Easting, Northing, Elevation) in the Universal Transverse Mercator (UTM30N) projection system was obtained through field measurements and used. Table 1 presents the statistical description of the dataset.

Typically, as with all machine learning techniques, a very large dataset for computations is required in order to generalise globally and make very good predictions. This involves a method of fine-tuning at the training and testing phases. In this study, a structured procedure used in the final tuning of the model is to divide the dataset for training and testing purposes (Lantz, 2015; Kuhn and Johnson, 2013). Therefore, the entire 891 data points used in this study were partitioned into training (70%) and testing (30%) sets,

**Table 1**  
Summary statistics of the data.

Parameter	Sample point	Min.	Max.	Mean	Std. Dev.	Skewness	Kurtosis
Au (ppb)	891	4.00	23.00	7.71	2.87	1.86	4.79
Easting (m)	891	597,962.94	609,705.51	601,344.45	2200.90	1.53	2.48
Northing (m)	891	576,487.24	589,666.81	582,751.53	3206.33	0.13	-0.96
Elevation (m)	891	24.50	176.01	59.73	21.40	2.35	8.46

**Table 2**  
Test results of the various MARS models developed based on different orders of interactions.

Model Number	FBF	Order of Interaction	Training		Testing	
			MSE	R	MSE	R
1	30	0	1.6868	0.8827	1.8495	0.8973
2	30	1	0.7252	0.9513	0.9342	0.9495
3	30	2	0.6271	0.9581	0.7507	0.9596
4	30	3	0.6271	0.9581	0.7507	0.9596
5	50	0	1.5037	0.8962	1.8102	0.9000
6	50	1	0.5569	0.9629	0.7842	0.9578
7	50	2	0.5034	0.8725	0.6367	0.8704
8	50	3	0.5034	0.9664	0.6367	0.9659
9	60	0	1.4608	0.8992	1.7076	0.9056
10	60	1	0.5245	0.9650	0.7345	0.9605
11	60	2	<b>0.4785</b>	<b>0.9682</b>	<b>0.6070</b>	<b>0.9675</b>
12	60	3	0.4785	0.9682	0.6070	0.9675

representing 624 and 267 sets. The training set was used for the model building, while the testing set was applied to test or validate the performance of the trained model. It is important to note that there are no universally accepted criteria for splitting the dataset. Fig. 6 provides information on the model development phases.

To avoid the likelihood of potential overfitting or underfitting, the training data was carefully selected to give a representation of the study area. Hence, the training-testing data selection was made through the stratified hold-out random sampling procedure, which has been widely adopted in machine learning predictions (Saltelli et al., 2008; Hastie et al., 2009; Koyuncu and Kadilar, 2009; Koyuncu, 2013; Singh et al., 2015). During the preprocessing phase, the datasets were normalised to ensure constant variability and prevent being skewed by certain attributes with large values. This is valid due to differences in the range of physical quantities and units of the data set used. In this study, the dataset was normalised in the range of [0–1] using Eq. (19) (Mueller and Hemond, 2013):

$$N_i = a + \frac{[(x_i - A)(b - a)]}{B - A} \quad (19)$$

where  $N_i$  is the normalised data,  $a$  and  $b$  are minimum and maximum scales respectively, that are set at 0 and 1.  $x_i$  is the measured normalising data,  $A$  and  $B$  are the minimum and maximum data values of the entire dataset.

## 5.2. Proposed MARS model development

In this study, the input parameters were Easting (E), Northing (N) and Elevation (Z) and Au grade value was used as the output parameter in the MARS model development. In all, twelve different MARS models with varying basis functions were developed based on different piecewise order of interactions. In this study, the 0, 1st and 2nd order piecewise interactions were carried out. In the 0 order there is no interaction between predictor variables while for the 1st and 2nd orders, there are possible interactions between predictor variables up to two or more linear members. The essence of testing different orders of interactions is to determine the op-

timal MARS model whose prediction performance is greatly influenced by the order of interactions used. Table 2 presents the training and testing results of the various MARS models developed based on the different order of interactions and the total number of basis functions used at the forward stage designated as FBF. All the MARS models were trained with zero penalty and 3rd degree of freedom for knot optimisation.

Finally, the optimal MARS model was determined based on the premise that the model should attain the least RMSE, MARE and highest R values (Table 2). From Table 2, it can be observed that the R varied within 0.9500 and 0.9600 for the various MARS models. Slight overfitting was observed at zero interaction, predicting R values between 0.8827 and 0.9065. The MSE values were in the range 0.400 and 0.900 for the interactive models, and from 1.400 to 1.700 for zero-order interactions. Because all the interactive models gave an R value very close to 1 and an MSE value close to 0, suggest MARS capability to overcome complex geospatial relationships and accurately predict geochemical grades of placer deposits. The presence of interactions is so significant in building an accurate model for Au predictions and not simply additive. Again, it indicates that MARS has the capability to capture complex and nonlinear relationships of datasets without prior assumptions about the underlying functional relationship between the predictor variables and output response (Zhang, 2019).

The final optimal MARS model (Eq. (20)) at the forward phase had 60 basis functions (see Table 2), but after backward pruning (deleting redundant knots in a step-wise regression manner), an optimum 35 basis functions was achieved. The same results were produced by both the 2nd and 3rd orders interactions as shown in Table 2. Due to model performance and simplicity, the 2nd order was selected as the optimal MARS model with its respective equations shown in Table 3. Therefore, the piecewise 2nd order interaction which comprises of product between the predictor variables (E, N, Z) and basis functions, can be observed in Table 3. According to the training and testing results presented in Table 2, the MARS model has demonstrated its capability in accurately predicting regolith geochemical grade values in a paleo-placer environment. Furthermore, it is obvious that the MARS model has been able to

**Table 3**  
Details of the selected optimal MARS model.

$\beta_m$	Model Equation	Coefficients ( $h_m$ )	$\beta_m$	Model equation	Coefficients ( $h_m$ )
BF2	max(0, 0.733 - N)	44.71	BF31	max(0, E - 0.274) * BF18	352.04
BF4	max(0, 0.283 - Z)	-44.41	BF32	max(0, 0.274 - E) * BF18	-106.58
BF5	max(0, E - 0.868) * BF4	-181.96	BF33	max(0, Z - 0.336) * BF8	-1616.76
BF6	max(0, 0.868 - E) * BF4	90.98	BF35	max(0, N - 0.329) * BF28	-577.65
BF7	max(0, E - 0.278) * BF1	449.27	BF37	max(0, N - 0.537) * BF28	-1420.61
BF9	max(0, N - 0.303) * BF6	-196.41	BF40	max(0, 0.242 - N) * BF27	302.72
BF11	max(0, N - 0.304) * BF4	92.24	BF41	max(0, Z - 0.321)	26.93
BF13	max(0, E - 0.156) * BF2	-334.04	BF43	max(0, E - 0.182) * BF17	-346.01
BF14	max(0, 0.156 - E) * BF2	212.02	BF45	max(0, E - 0.362) * BF3	152.30
BF15	max(0, Z - 0.207) * BF1	73.14	BF46	max(0, 0.3620 - E) * BF3	33.39
BF17	max(0, N - 0.603)	37.23	BF47	max(0, Z - 0.164) * BF31	-288.12
BF19	max(0, E - 0.272)	38.15	BF48	max(0, 0.164 - Z) * BF31	657.35
BF20	max(0, 0.272 - E)	-38.52	BF51	max(0, N - 0.171) * BF49	191.74
BF21	max(0, Z - 0.611)	-35.06	BF52	max(0, 0.171 - N) * BF49	-268.67
BF23	max(0, E - 0.375) * BF15	-1681.24	BF54	max(0, 0.409 - E) * BF12	-607.00
BF29	max(0, N - 0.510) * BF28	2410.75	BF55	max(0, E - 0.544)	7.18
BF30	max(0, 0.510 - N) * BF28	-760.57	BF57	max(0, Z - 0.472) * BF56	-51.37
			BF60	max(0, 0.283 - N) * BF42	-75.54

**Table 4**  
Comparison of MARS model and other machine learning methods testing results.

Method	Performance criteria			
	R	RMSE	MAE	$\rho$
MARS	0.9675	0.7791	0.6481	0.0497
BPNN	0.9665	0.7920	0.6585	0.0506
RBFNN	0.9616	0.8766	0.7683	0.0561
GRNN	0.9435	1.0236	0.8106	0.0661

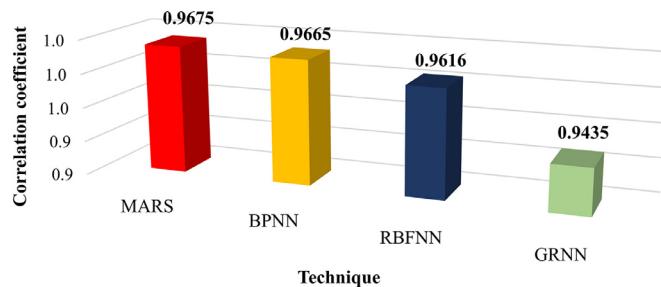
learn the complex relationship existing between the regolith geochemical characteristics with gold (Au) values. Hence Eq. (20) can intuitively generalise correctly for un-sampled prospective areas with high accuracy.

$$Au = 4.12429 + \sum_{m=1}^{35} \beta_m h_m(x) \quad (20)$$

### 5.3. Comparison of MARS model and other investigated techniques

The applied BPNN, RBFNN and GRNN methods have over the years been extensively studied and applied in literature as benchmark techniques for comparison with other machine learning methods in geosciences and other related disciplines (Ziggah et al., 2016; Arthur et al., 2020; Poulton, 2002; Van der Baan and Jutten, 2000). Hence, the present authors saw it as an opportunity to apply and compare them to the proposed MARS technique. To test the strength of MARS with these benchmark machine learning methods, we selected the same datasets for training and testing. Table 4 presents a summary statistical performance comparison based on the testing data for the MARS, BPNN, RBFNN and GRNN.

From Table 4, the predicted R for the MARS model perfectly match the observed Au values within the study area (paleo-placer deposit) by 96.82%. This was closely followed by the BPNN, RBFNN and GRNN. In comparison to other artificial intelligence models, MARS has demonstrated its superiority against the other methods by its highest R value (Fig. 7). The RMSE and MAE have widely used performance measures in statistics to evaluate the closeness of a model prediction to the observed data (Willmott and Matsuura, 2005). Again, MARS demonstrated its predictive accuracy over the BPNN, RBFNN and GRNN methods with producing the



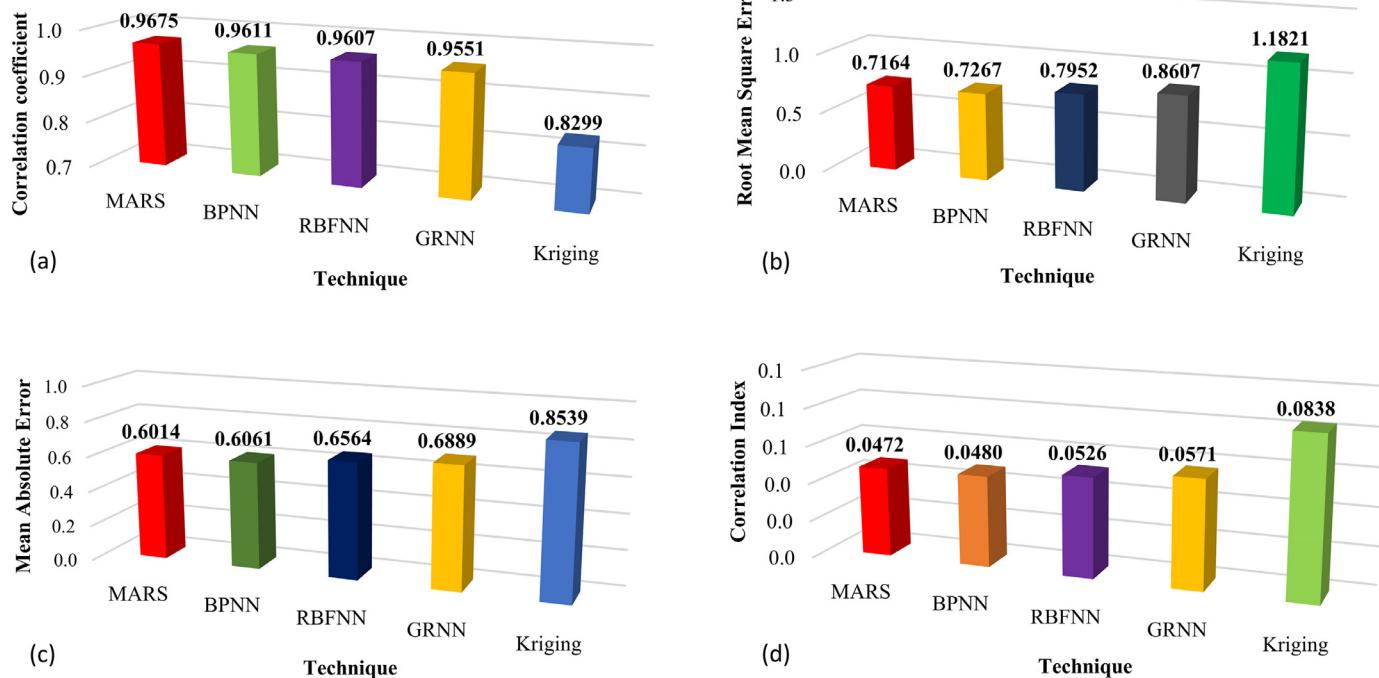
**Fig. 7.** Performance comparison of MARS and other machine learning techniques based on R.

least RMSE and MAE values (Table 4). A lower correlation index,  $\rho$  also indicates a more precise model. As observed from Table 4, the  $\rho$  value for the proposed MARS model produced 0.0497 while BPNN, RBFNN and GRNN predicted 0.0506, 0.0561 and 0.0661, respectively.

Based on the overall analyses, the proposed MARS model comparatively has the strongest calibration abilities. That is, given the testing dataset, the MARS exhibited an excellent prediction tendency than the other machine learning techniques investigated in this study. This can be attributed to the capability of the MARS to capture inherent complex high pattern relationships within predictor parameters amongst the training and the testing datasets (Zang and Goh, 2016).

Further, the optimum models of the MARS, BPNN, RBFNN and GRNN were compared with the classical kriging method. In order to create uniformity and consistency in comparison, the 891 datasets were used as testing datasets in the optimum trained MARS, BPNN, RBFNN and GRNN models. The kriging estimation was done through experimental variography modelling. The variography utilised a spherical model, twelve lags, and assumed anisotropy. Table 5 summarises the results based on MARS, BPNN, RBFNN, GRNN and the Kriging method. Interestingly, the proposed MARS approach achieved the best in all aspects of the performance indicators values indicated by a maximum R value and a minimum error (i.e., RMSE, MAE and  $\rho$ ). Graphical presentation of the predictive strength of the MARS technique against other techniques is shown in Fig. 8(a-d).

Fig. 9(a-e) compares the measured Au with the predicted models for all the methods investigated in this study. The plot shows an excellent correlation of the measured and the predicted Au



**Fig. 8.** Performance of the various techniques based on: (a)  $R$ ; (b) RMSE; (c) MAE; and (d) correlation index ( $\rho$ ).

**Table 5**  
Comparison of all developed models and performance indicators.

Method	Performance criteria (Accuracy for Testing sets)			
	RMSE	$R$	MAE	$P$
MARS	0.7164	0.9675	0.6014	0.0472
BPNN	0.7267	0.9611	0.6061	0.0480
RBFNN	0.7952	0.9607	0.6564	0.0526
GRNN	0.8607	0.9551	0.6889	0.0571
Kriging	1.1821	0.8299	0.8539	0.0838

for the MARS model, demonstrating its efficiency over the models. From Fig. 9(a), almost 96.7% of the variation of the measured Au (ppb) data is explained by the MARS model. This was closely followed by BPNN (96.5%), RBFNN (95.9%) and GRNN (94.6%) as shown in Fig. 9(b-d), respectively. However, OK achieved the least performance by only explaining 89.4% of the variation in the measured Au data as shown in Fig. 9(e). The MARS model produced similar estimates of the  $R$  value with the rest of the neural network models, and even generalised very well for extreme Au values.

Fig. 10 shows a combined line plot of the measured and predicted Au for all the models. It is worth noting that all the models show an excellent prediction at various ranges of sample index. This plot also reveals very interesting subtle information with respect to the performance of the machine learning models against the classical ordinary kriging methods. In comparison with the results obtained for the other methods, the MARS model gave an excellent prediction where the predicted Au values were more consistent with the observed values. This generalisation can be attributed to the better and more versatile learning capabilities of MARS models against the other models. In terms of regolith geochemical gold prediction, the authors with no doubt demonstrated MARS' remarkable performance against other machine learning models (GRNN, BPNN and RBFNN) and kriging geostatistical ap-

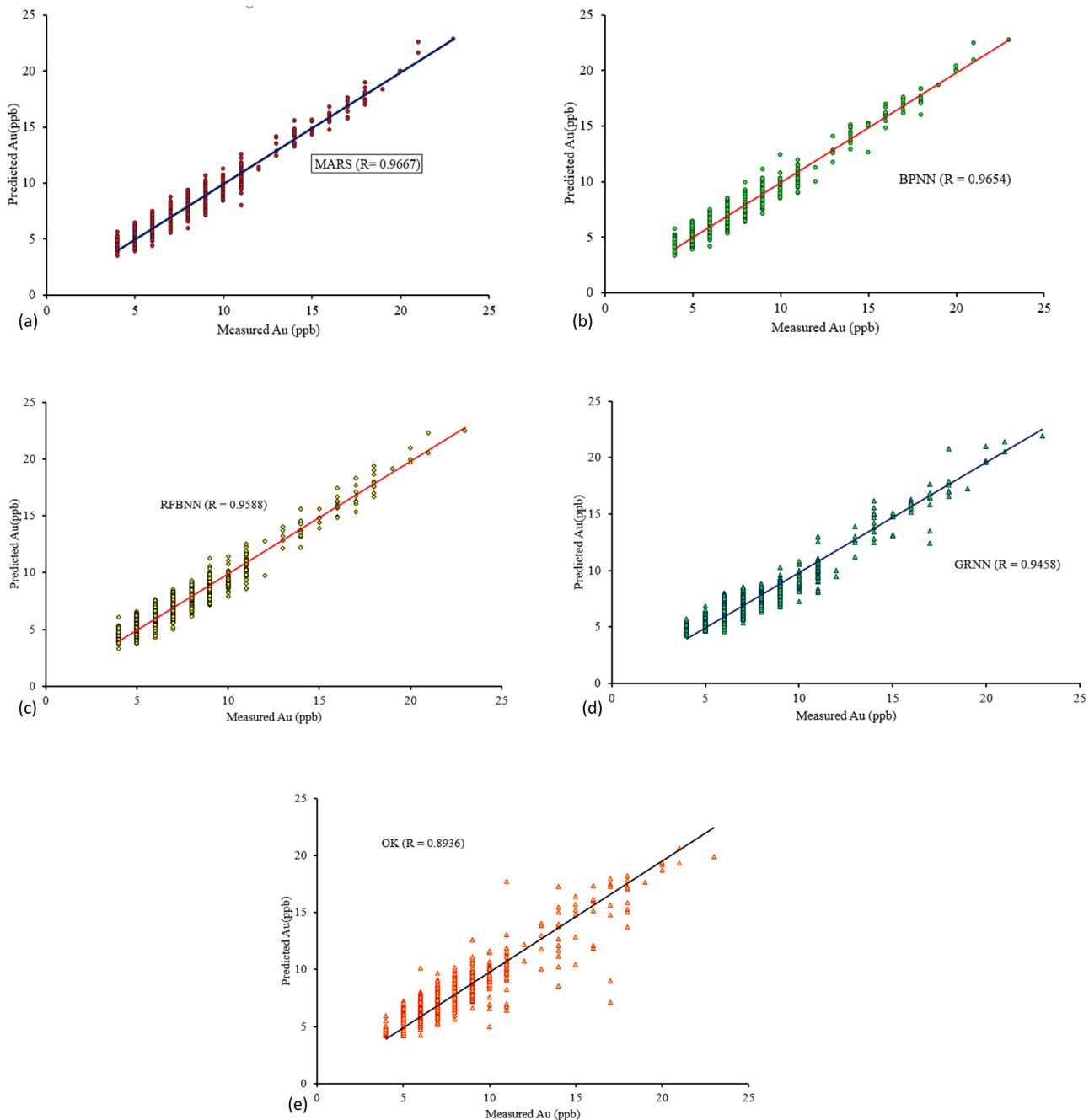
proaches. Indeed, these results indicated that the MARS model is better suited for Au prediction in the study area.

#### 5.4. Sensitivity and multicollinearity analysis

Sensitivity analysis was carried out to identify predictive variables that have a significant impact on the observed variable (Sorentino and Barnett, 1994). This further serves as quality assurance and contributes to the defensibility of model-based analysis (Saltelli et al., 2000; Saltelli et al., 2004; Saltelli et al., 2008). Statistical techniques used to test the significance of predictor variables are not well developed for artificial neural networks. One of the advantages of the MARS approach is its ability to make feature selections on the predictor variables. Hence, the sensitivity analysis was carried out using the MARS technique. To identify input predictor variables that participate in interactions with each other, MARS uses the ANOVA decomposition method. Fig. 11 shows the relative importance of the input parameters (Easting, Northing and Elevation) on the output (Au) in the model development process. According to Fig. 11, the UTM(N) parameter was selected as the dominant input parameter, which contributes to 100% of the predicted model. This was closely followed by Easting (88.14%) and Elevation (82.44%) respectively. By virtue of the sensitivity analysis results, it can also be deduced that all the input parameters contributed significantly to the model building.

Multicollinearity analysis was performed to determine how the input and output variables are correlated to each other. In diagnosing multicollinearity, the study used the Variance Inflation Factor (VIF) index (Stine, 1995; Akinwande et al., 2015) to measure how much the variance of an estimated regression coefficient has increased due to collinearity (Stine, 1995; Akinwande et al., 2015). The VIF (Eq. (21)) is mathematically expressed as:

$$VIF_m = \frac{1}{1 - R_m^2} \quad (21)$$



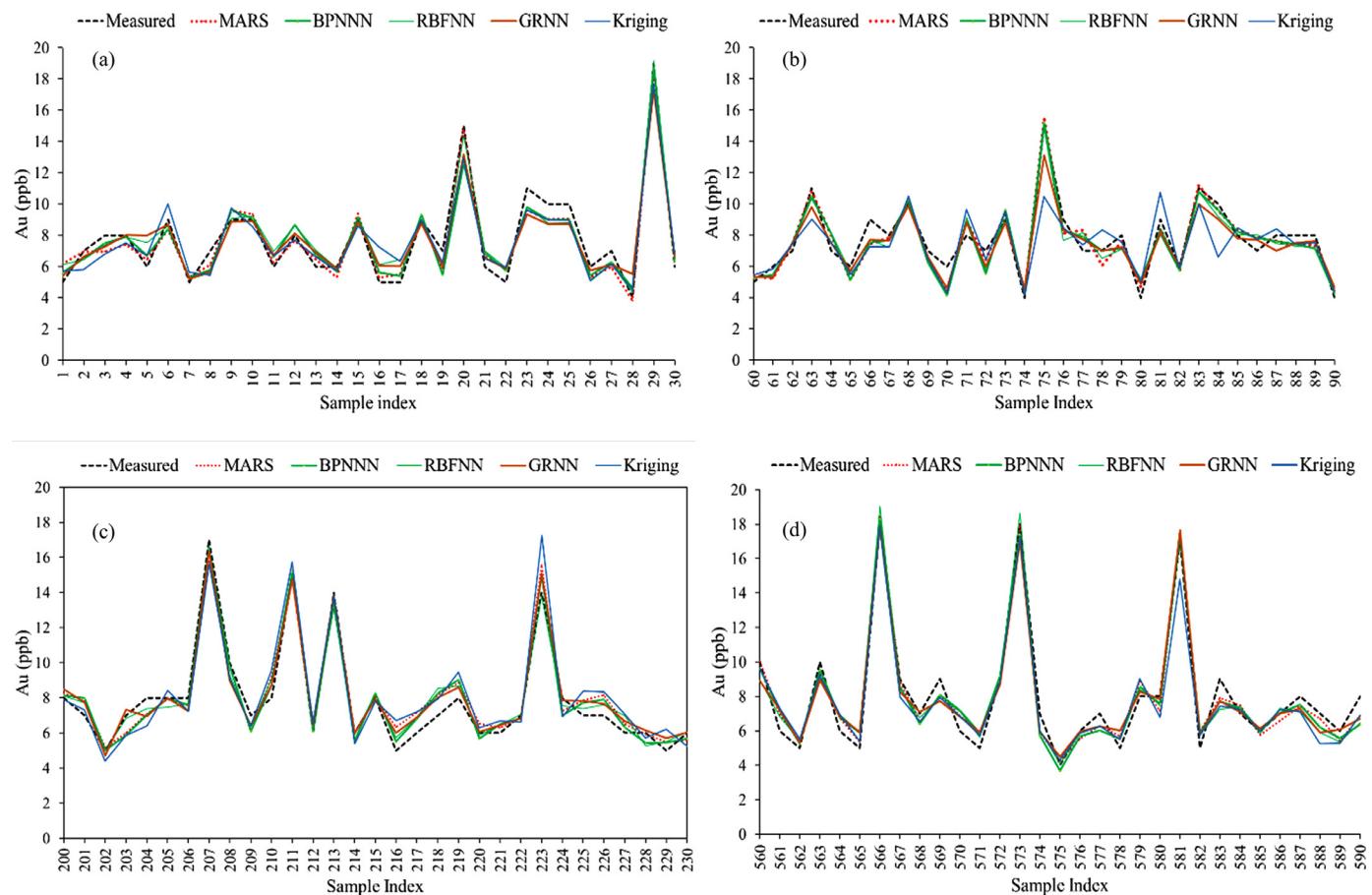
**Fig. 9.** Measured versus predicted Au (ppb) values using different models: (a) MARS; (b) BPNN; (c) RBFNN; (d) GRNN; and (e) OK.

**Table 6**  
Multicollinearity indexes for predictor variable.

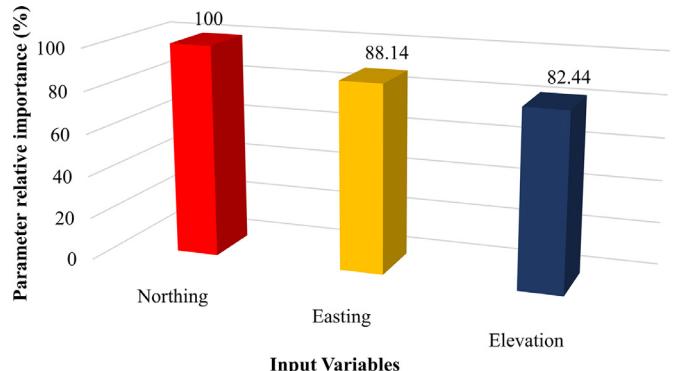
Analysis	Easting coordinate	Northing coordinate	Elevation
Variance Inflation Factor	1.0031	1.0103	1.0201

where  $R^2$  of the  $m^{th}$  variable is the coefficient of determination obtained through regressing the input variables. Table 6 summarises the result of the VIF. VIF of 1 shows that none of the factors is correlated meaning there is no multicollinearity existing amongst the predictors. For moderately correlated factors, VIF should lie between 1 and 5. Moreover, if VIF is greater than 10, then the assumption is that the model coefficient is poorly estimated due

to strong multicollinearity. It can be observed from Table 6, that the Easting, Northing and Elevation coordinates (input parameters) produced a VIF of approximately 1. The interpretation is that these input parameters do not exhibit any multicollinearity amongst them but rather correlate well with the output parameter (Au). To this end, it can be stated that all three input parameters were suitable for use in the formulation of the various Au predictive models.



**Fig. 10.** Comparison of measured and predictive models of Au values by subsampling of (a) 1 up to 30; (b) 60–90; (c) 200–230; and (d) 560–590 samples.



**Fig. 11.** Relative importance of the input variables.

## 6. Conclusions

Over the years, the empirical method of Kriging has been widely used for regolith geochemical grade estimation. A review of previous studies indicates that the Kriging approach oftentimes does not produce satisfactory results. Therefore, this study applied the MARS as a novel approach to regolith geochemical grade estimation within the Tarkwaian district. The proposed MARS approach was compared with three standard ANN methods (BPNN, RBFNN and GRNN) and empirical method (Kriging). These modelling techniques were applied to the regolith geochemical dataset to aid in accurate estimation and prediction of Au value within

the Tarkwaian paleoplacer deposit. The performance of the methods was evaluated using statistical indicators such as  $R$ , RMSE, MAE and  $\rho$ . The major findings are:

The statistical results revealed that the MARS technique gave superior results as compared to the BPNN, RBFNN, GRNN and Kriging. This was evident from the results where MARS had the lowest values of RMSE (0.7164), MAE (0.6014),  $\rho$  (0.0472) as well as highest  $R$  (0.9675) value.

It can be inferred from the reported results that the MARS approach can learn the intricacies and complex relationships existing between the regolith geospatial parameters ( $E$ ,  $N$  and  $Z$ ) with gold (Au) values. These results have shown that the proposed MARS approach is useful for predicting Au with some degree of certainty.

Furthermore, the sensitivity and multicollinearity test revealed that the geospatial input parameters were equally qualified to be used in the development of the predictive models.

Overall, the present study has provided clear insight into the strength and robustness of MARS in predicting Au anomalies in a highly complex regolith geochemical environment. The authors are intrigued by the performance of the MARS model and therefore has the exciting fervour to propose the MARS modelling technique. This outcome may prove quite useful for the mining and exploration industry when MARS could be an effective computational tool to unravel regolith geochemical complexities. This is because MARS has shown all the favourable characteristics to be adopted as a tool for the analysis of regolith geochemical datasets due to (a) its self-adaptive strength, (b) robust interactive variables, (c) computational efficiency and (d) accuracy and reliable predictions.

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Acknowledgements

The authors would like to thank Anglogold Ashanti Iduapriem, Tarkwa for providing the data and other logistics for the success of this research.

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