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E-man Part II: Application of Neural Networks for Classification of Bauxite

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Dedicated to Dr V Anantha Ramam, Professor of Chemistry, Andhra University, Visakhapatnam, India

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ABSTRACT

E-man (Evolution of Mimics of Algorithms of Nature) comprises of mapping of processes in nature (animate/inanimate) onto mathematical algorithmic domain. The software implementation of mimicking nature in functioning of brain, foraging, social interaction, hereditary, evolution and mating brought renaissance in parametric/nonparametric data processing into information in all science/ engineering/ technological research. The classification of bauxite based on ICP-MS chemical elemental quantification in different locations is modeled using single layer perceptron (SLP-) neural network (NN) procedure with Trajan software. The processing of data set (NP=30) using five rock types in central and northern blocks with IPS, a fast solution choice of Trajan, resulted in SLP with eight hidden neurons. The classification results endorse the superiority of data driven NN over soft PC analysis. A progressive classification data analysis of high quality instrumental data is performed from hard linear correlation, soft dimension-reduction of correlated variables (PCA) and model free data driven supervised NN, a subset of natural intelligent computational paradigm. The two classes are unequivocally detected employing training, verification and test protocols.

Keywords: Geochemistry, transition metal/lanthanides, ICP_MS, Neural network, PCA, bauxite, classification, E-man, ore-benefaction

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INTRODUCTION

Geochemistry of mineral/ore processes is complex and difficult to model from first principles. Instrumental analysis, however, increased the accuracy of detection and quantification of chemical elements or even speciation. Classification, a sub-goal of pattern recognition of minerals from different geographic location is critical in ore benefaction. Ore grade estimation is an interdisciplinary complex task and it is time consuming phase in mining projects. The difficulty arises as a result of structural complexities in mineral/ore deposits and hybrid artificial intelligence-2 (AI2) methods have become an integral path of this challenge for geologists/mining engineers/geochemical experts. The complex tasks are better solved by multiple paradigms viz. NNs statistical/mathematical methods, which is beneficial and apt in routine geochemical exploration. Tahmasebi and Hezarkhani [1] reported that co-active-neuro-genetic-fuzzy inference system (CA-NN-GA-FIS) is faster and accurate compared to the individual component methods in modeling of Sungun Copper deposit (Iran). In this study, a co-active neuro-FIS NN along with GA is employed to optimize NN weights, learning rate, momentum and number of membership functions for each input. The prediction of grade of offshore placer gold deposit with Co-evolutionary-RBF-NNs is better than FFNN and ordinary kriging methods [2]. GA is used to partition the input matrix into training, calibration and validation datasets and the center/width are refined by EA using the concept of cooperative-coevolution.

Ziaii [3] reported GA – NN-FIS to identify geochemical anomalies to separate zone dispersed from that of blind mineralization and found Takagi, Sugeno and Kang (TSK) type FIS with five layered FFNN is superior to other classification methods like metallometry zonality and BPNN. Ruilin [4] and Lowndes used NN and fault tree analysis to predict the risk in underground mining in deep Chinese coal seams considering geological conditions. The prediction of reservoir parameters in petroleum industry excelled [5] simple GA and NNs. The result is smallest error and highest CC when ensemble or committees of NNs and GA with a new selection of female chromosomes (Jafari) are the modules of the hybrid model.

In continuation of our studies in computational chemical sciences, we pursue the application of E-man [6], a comprehensive set of nature mimicking algorithms reported over the last half a century in geochemical research. Earlier kineto-metrics [7,8], pisci-metrics [9], dieteto-metrics, medicino-metrics and nano-metrics, enviro-metrics [10,11] and applications of chemometrics were reported from this laboratory [12-14]. In this communication, we report the results of classification of Bauxite from different locations using principal component analysis (PCA) and neural networks (NNs).

MATERIALS AND METHODS

Hardware and software: An Inspiron 1525-laptop with dual core processer is used and MATLAB (version 4.2c.l for windows environment) from Math Works Inc [15] is employed to develop programs and generate graphic outputs. SEDA (statistical exploratory data analysis) and PCA are performed with in-house software. Software package Trajan 4.0 [16] is used for developing data driven SLP-NN models. This package has an additional advantage of providing intelligent problem solver (IPS) to generate a large set of NN-models automatically.

*Dataset***:** The samples of bauxite and other associated minerals are collected from two different locations viz. central block and northern block near Damanjodi, Orissa state. The data set consists of concentrations of 30 chemical elements. The samples from different

environments of bauxite mine viz. Khondolite (Khond), partially altered , Khondlites (Pak) , Lithomarge (Litho), lower bauxite (Bxt.II) , upper bauxite (Bxt.I) and Laterite cap (Lat) are collected. ICP-MS is employed to analyze different rare earth elements (REE) and trace elements. Table 1 describes primary instrumental data along with Latitude of location and name of the chemical element.

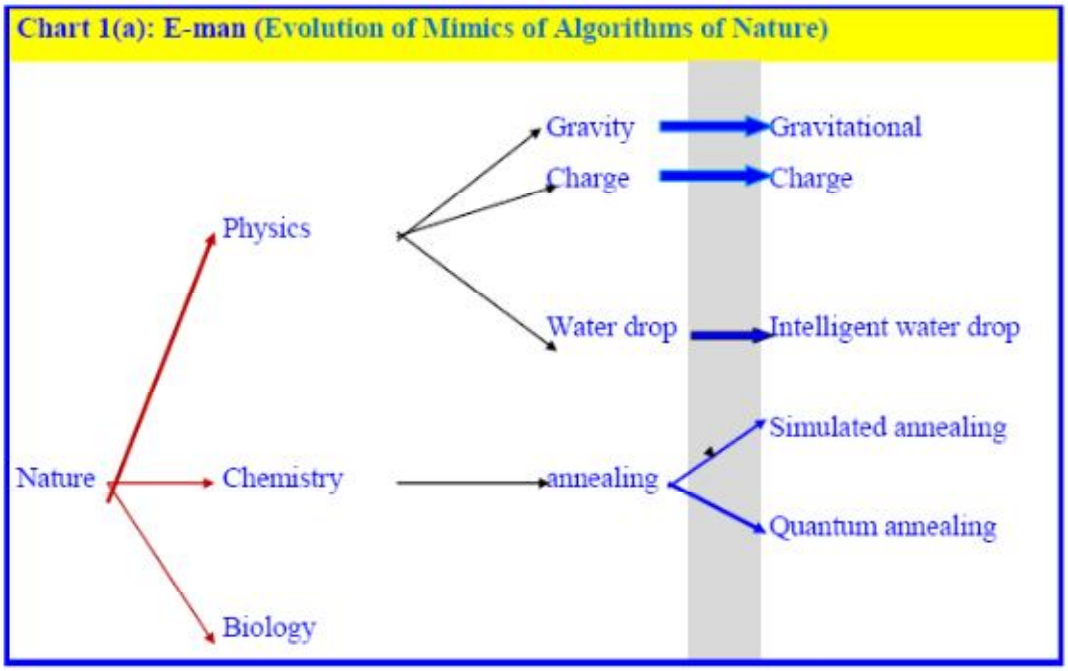
Table 1: Quantities of chemical elements by ICP_MS in two blocks of bauxite

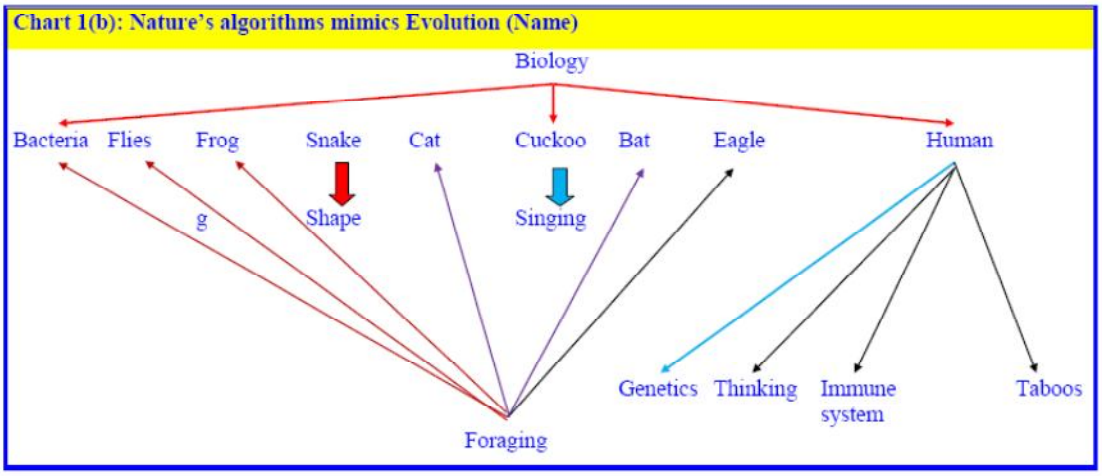
		Central Block						Northern Block					
	trace/ REE	**Lat**	**Bxt.1**	**Bxt.11**	**Litho**	**PAK**	**Khon**	**Lat**	**Bxt.1**	**Bxt.11**	**Litho**	**PAK**	**Khond**
1	Sc	27.53	30.25	15.8	32.22	35.79	76.94	19.73	18.7	17.04	26.37	33.19	35.2
2	Co	19.45	13.38	10.14	10.01	12.23	13.55	18.67	10.2	10.82	10.22	13.64	13.9
3	Ni	26.71	23.56	12.92	29.25	36.66	68.73	25.48	15.9	14.77	31	50.24	65.0
4	Cu	40.16	48.46	24.75	49.47	48.3	116.8	28.23	37.1	30.66	28.39	41.46	187
5	Zn	63.69	90.46	43.78	47.54	41.9	100.8	58.00	58.9	56.79	55.74	51.1	79.0
6	Ga	59.21	57.65	56.67	53.44	55.29	64.4	65.46	65.7	59.81	55.58	68.81	79.0
7	Rb	4.72	3.48	1.4	0.26	0.45	2.63	3.15	0.24	0.5	0.69	1.25	3.79
8	Sr	11.7	9.84	7.16	9.4	6.67	12.48	20.96	6.35	4.36	10.1	9.11	20.43
9	Y	5.1	5.34	3.42	4.8	4.21	14.29	9.43	4.46	2.36	6.1	6.16	35.22
10	Zr	166.5	435.38	112.99	81.78	72.94	61.01	171.44	100.	139.88	121	93.76	66.94
11	Cs	0.1	0.14	0.05	0.06	0.09	0.07	0.1	0.01	0.02	0.05	0.09	0.08
12	Hf	8.53	12.69	6.75	3.59	3.08	2.54	8.68	5.35	8.26	3.81	3.32	2.34
13	Ta	2.95	3.68	2.4	1.67	1.72	2.48	3.51	3.03	2.83	1.37	1.61	2.21
14	Pb	38.8	21.53	13.53	33.14	32.36	40.69	79.73	30.9	10.68	22.76	22.52	26.14
15	Th	88.96	74.94	86.88	55.27	51.66	41.89	91.47	96.3	87.41	42.54	52.54	34.84
16	U	2.64	2.27	1.87	1.02	0.99	2.8	2.27	1.14	1.5	1.01	1.05	1.48
17	La	33.59	37.41	28.4	49.61	55.6	73.71	30.01	33.5	22.87	24.86	36.35	77.81
18	Ce	58.99	87.1	53.21	80.91	99.61	176.5	60.66	73.8	42.2	31.4	48.46	171.46
19	Pr	6.41	7.36	6	9.12	9.86	18.76	6.43	6.56	4.86	5.2	7.99	18.13
20	Nd	23.02	25.14	21.72	26.71	29.68	62.17	24.08	27.7	16.28	17.25	23.85	64.17
21	Sm	3.57	4.2	3.92	4.48	4.48	11.92	4.73	4.78	3.05	3.87	3.37	13.03
22	Eu	0.42	0.32	0.37	0.61	0.44	1.26	1.53	1.19	0.75	2.4	1.37	2.87
23	Gd	3.65	3.14	2.39	3.75	3	8.45	3.41	3.26	1.69	3.91	2.85	8.23
24	Tb	0.34	0.23	0.21	0.32	0.23	0.75	0.39	0.33	0.16	0.53	0.37	0.96
25	Dy	1.51	1.39	0.95	1.5	1.13	3.78	1.43	1.51	1.11	2.72	2.19	5.84
26	Ho	0.2	0.22	0.14	0.014	0.12	0.4	0.23	0.23	0.14	0.22	0.24	0.91
27	Er	0.76	0.67	0.45	0.39	0.38	0.87	0.77	0.51	0.26	0.4	0.59	1.36
28	Tm	0.1	0.1	0.08	0.07	0.07	0.22	0.11	0.11	0.05	0.08	0.09	0.35
29	Yb	0.98	0.9	0.54	0.78	0.8	1.79	1	0.55	0.46	0.57	0.7	2.84
30	Lu	0.15	0.14	0.08	0.09	0.07	0.21	0.14	0.08	0.07	0.1	0.08	0.39

RESULTS AND DISCUSSION

E-man (Evolution of Mimics of Algorithms of Nature) translates a part of natures' processing ability into computational algorithmic format. These computational intelligent modules excelled in performance in solving classification, functional approximation, multi-object optimization compared to many advanced mathematical and statistical methods. The new era started with neural networks in 1940; now expanded into a cover imbibing or leaving all

earlier paradigms much below the base and setting a new era (numerical as well literal) data processing technology. The inspiration of E-man is form multiple matured paradigms viz. biology, physics, chemistry etc, (Chart 1).



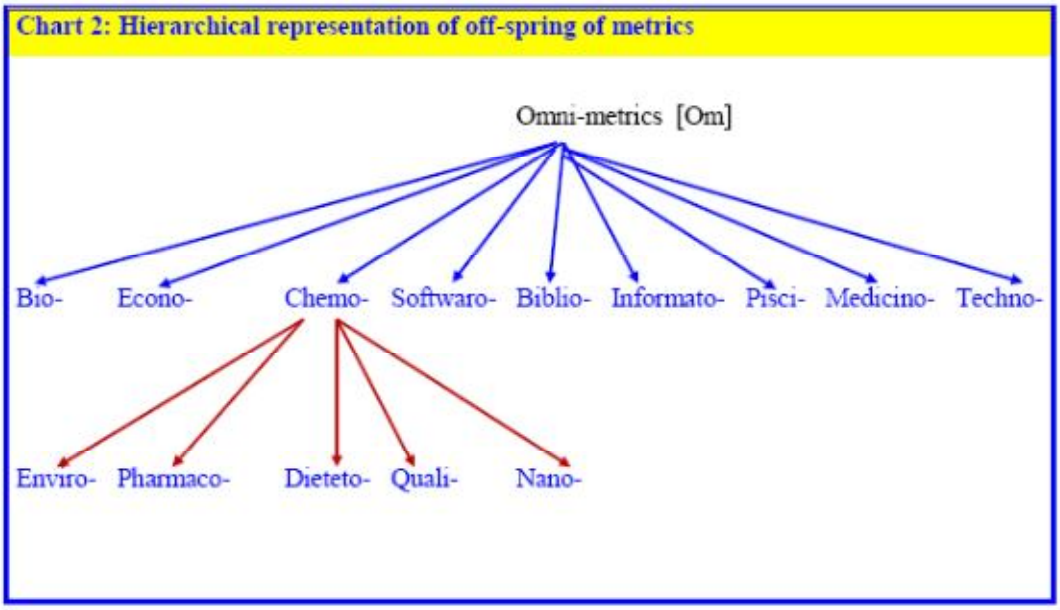


Confining the activity of nature from a bird's eye point of view to a human being lifecycle, GA and GP are well practiced tools in solving instrumental data analysis even in chemistry. NNs and fuzzy logic are unavoidable mathematical paradigms started with an

ambitious prototype product namely 'artificial brain'. The realization of this goal even after fifty years of concerted efforts is tiny. But, its impact in modeling F16 airplane and rat brain [18] is astounding. Much more real sparkles are in solving multi-conflicting-objective optimization of non-convex, non-differentiable, multivariate-multi-response functions with a large number of equality and inequality constraints. Artificial immune system and taboo search are other powerful procedures adapted from natural disease immune system and social interaction. Jafari [5] proposed a new procedure to select chromosomes in artificial genetic algorithm. The label of selected male chromosome and population diversity (of the previous generation) are the input to a FIS aimed at selection of female chromosome for recombination. This approach of looking for a female chromosome in sexual selection avoids premature convergence in GA.

The word metrics refers to measurement and the amalgamation of mathematical sciences with other fields resulted in the hybrid disciplines with the suffix metrics which can be brought under an umbrella of omni-metrics (om) [19] described in a hierarchical tree structure (Chart 2).

Chart 2: Hierarchical representation of off-spring of metrics



The correlation coefficients calculated with corr.m are shown in Table 2. In the central block, CCs are high among Laterite, Bauxite1 (lower) and bauxite2 (upper). The correlations are decreased with lithomarge and partially altered Khondalites. But, with Khondalites the correlations are poor. This indicates that except in khondalites, in other rocks the chemistry showing good correlations. Khondalite being the host rock it is expected that the chemistry might be different than the ore. The very high to high correlations among bauxites at two different levels, Laterite cap, lithomarge and PAK suggests that all these rocks the mineral content may be present. In the northern block also the correlation coefficients are very high to high different litho units except for khondalite as in the case of central block.

The linear correlation coefficient between explanatory variable space is crucial to prune X variables and indicated the need for orthogonalisation to alleviate the problems of multi collinearity. The correlation between response and explanatory variable space, ANOVA and MANOVA reflect explainability of the variable of response with the model.

The validity of regression coefficients endorses the acceptability of the models for generalization with a possibility to interpret the regression parameters on a physico chemical basis. The residual analysis rules out the outliers, trend (an artifact of model error) and the dependability of the model within the measurement precision. The cross validation (LOO, L-kO) and influential statistics estimates the efficacy of data points on the model. The gross limitation of these hard parametric models are that no real data set adheres to the necessary conditions of distributions of regression parameters and the presence of normal noise only in the response.

Table 2 : Linear correlation matrix of ICP_MS data in central and northern blocks

(a) Central block

	Lat	Bxt.1	Bxt.11	Litho	Pak	Khond
Lat	1					
Bxt.1	0.92	1				
Bxt.11	0.97	0.85	1			
Litho	0.88	0.71	0.89	1		
Pak	0.81	0.63	0.83	0.99	1	
Khond	0.58	0.4	0.59	0.87	0.91	1
	Lat	Bxt.1	Bxt.11	Litho	Pak	Khond

(a) North block

	Lat	Bxt.1	Bxt.11	Litho	Pak	Khond
Lat	1					
Bxt.1	0.91	1				
Bxt.11	0.94	0.94	1			
Litho	0.94	0.88	0.95	1		
Pak	0.88	0.92	0.90	0.95	1	
Khond	0.47	0.64	0.49	0.53	0.69	1

Singular value decomposition (SVD): SVD transforms matrix or second order tensor of real numbers (X) into three matrices, U, S and V. U is called row designee and V corresponds to column designee and the diagonal elements of S are singular values reflecting the influence of rows and columns and their product $U*S*V^T$ reproduces X [20]. The linear dependency of rows and/or columns is reflected in very small values of S. The process of pruning the number of S is affected by deleting all zero and insignificant singular values as well their corresponding vectors in U and V. This procedure, called truncated SVD, retains all the information in the linearly independent variables. The matrices U and V are orthogonal. The object modules (om_firex.m) to calculate the number of significant (linearly) independent singular values/Eigen values exemplified with simulated data sets is given in Chart 3. SVD is the best choice to invert a matrix compared to determinant based methods.

Chart 3(a): Matlab object modules (om) for SVD and eigen analysis

```
function [u,s,v,singularValues] = om_svd(x)
    [u,s,v] = svd(x);
    singularValues = diag(s);
```

```
function [er,lr,ec,lc,facr,facc] = om_evf(x)
% Eigen values
    [er,lr] = eig(x*x');
    [ec,lc] = eig(x'*x);
% Factor analysis
    facr = er * lr.^0.5;
    facc = ec * lc.^0.5;
```

```
function expl2(x)
[u,s,v,singularValues]  = om_svd(x)
[p_expl,fi,re,ie,xe,rms]= om_firex(s);
```

```
function om_xcal_svd(x)
    [u,s,v] = svd(x);  [nsv,c]= size(s);
    for i = 1:min(size(s))
      xcal = u(:,1:i)*s(1:i,1:i)*v(:,1:i)';
```

```
                                    res = x-xcal;
                                    i,[res]     %pause
                                  end
```

```
% dem_svd
  diary off
 !del dem_svd.out
 diary dem_svd.out
   x = eye(2);  expl2([x]);
   x1 = [1:2]';x= [x1 , x1]; expl2([x]);
   x = [1 2 3 4;3 4 9 13; 5 7 10 15];expl2([x]);
   x = eye(2);  expl2([x;x]);
   x = eye(2);  expl2([x x]);
  diary off
```

```
function [p_expl,find,re,ie,xe,rms] =
om_firex(sMatrix)
        s = diag(sMatrix);
        sum_s  = sum(s);
        p_expl = s./sum_s *100.;
        [ns,cs] = size(s);no = [1:ns]';

% Number of significant hidden roots i.e.
%         Singular or eigen values or
%         factors

  for ii = 1: ns-1
     npe = ii;
     sum1 = sum(s(npe+1:ns));
     n = ns;
%
     re(ii,1) = sqrt(sum1/ns/(ns-npe));
     ie(ii,1) = re(ii,1) * sqrt(npe/ns);
     xe(ii,1) = re(ii,1) * sqrt((ns-npe)/ns);
     find(ii,1) = re(ii,1)/(ns-npe)^2;
     rms(ii,1)  = sum1/ns/ns;
  end
```

Chart 3(b): Correlation (linear) matrix and singular values, their explainability

X	Correlation matrix	No	Singular Values	%_explain ability	Cum_%_explain ability
1 0 0 1	x1 1.00 x2 -1.00 1.00 ---------- x1 x2	1 2	1.00 1.00	50.00 50.00	50.00 100.00
1 1 2 2	x1 1.00 x2 1.00 1.00	1 2	3.16 0.00	100.00 0.00	100.00 100.00
1 2 3 4 3 4 9 13 5 7 10 15	x1 x2 x3 x4 ---------- x1 1.00	1 2 3	26.47 1.7 0.43	92.26 6.25 1.50	92.26 98.50 100.00

	x2 0.99 1.00 x3 0.92 0.87 1.00 x4 0.94 0.89 1.00 1.00 --- x1 x2 x3 x4				

Chart 3(c) : U, S and V matrices

X	U	S	V
1 1 2 2	-0.44 -0.89 -0.89 0.44	3.16 0 0 1.5e-016	-0.707 -0.707 -0.707 0.707
1 0 0 1	1 0 0 1	1 0 0 1	1 0 0 1
1 2 3 4 3 4 9 13 5 7 10 15	-0.20 0.08 -0.97 -0.62 -0.77 0.07 -0.75 0.62 0.21	26.4 0 0 0 0 1.7 0 0 0 0 0.43 0	-0.22 0.48 0.65 -0.54 -0.31 0.79 -0.48 0.24 -0.52 -0.29 -0.48 -0.64 -0.76 -0.25 0.33 0.49

Chart 3(d): Calculated X matrix (Xcal) with 1 to N singular values

X	Xcal(1:3)		
	Number of singular values		
	1	2	3
1 1 2 2	4.4e-016 4.4e-016 6.6e-016 6.6e-016	3.3e-016 5.51e-016 6.6e-016 6.6e-016	---
1 0 0 1	0 0 0 1	0 0 0 0	---
1 2 3 4 3 4 9 13 5 7 10 15	-0.20 0.31 0.15 -0.17 -0.64 -1.10 0.40 0.36 0.59 0.83 -0.37 -0.25	-0.27 0.19 0.20 -0.13 0.02 -0.02 -0.02 0.01 0.06 -0.04 -0.04 0.03	1.1e-16 -8.8e-16 -8.8e-16 -1.7e-15 1.7e-15 -1.7e-15 -1.7e-15 -3.5e-15 2.6e-15 -1.7e-15 0 -1.7e-15

Singular values of data matrices with individual/cumulative percent explainability are incorporated in Table 3.

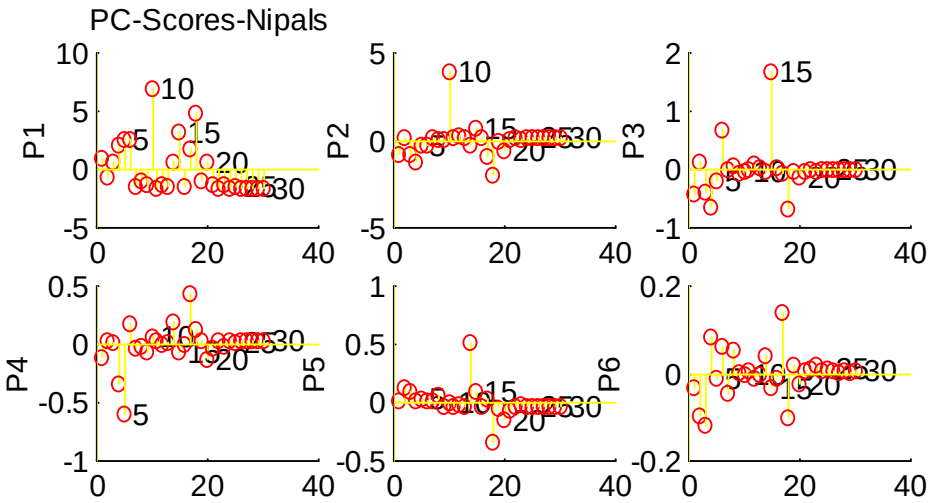
Table 3: Singular values (s), % Explainability (PE) of ICP_MS data

	Central Block			North Block			Total		
No	s	%E	CPE	s	%E	CPE	s	%E	CPE
1	144.1	82.84	82.84	147.3	84.63	84.63	284. 4	80.33	80.33
2	24.7	14.2	97.04	19.68	11.31	95.95	43.17	12.2	92.53
3	3.88	2.23	99.27	3.617	2.07	98.02	18.5	5.22	97.75
4	0.78	0.448	99.72	2.033	1.16	99.19	4.43	1.25	99.01
5	0.43	0.24	99.96	1.254	0.72	99.91	2.555	0.72	99.73
6	0.068	0.039	100	0.1506	0.086	100	0.963	0.27	100

Eigen Vector Analysis (EVA): The data matrix in chemical analysis is in general rectangular, for example, the concentrations of chemical elements at different geological locations. In multivariate calibration with a spectrophotometer the absorbances of calibration samples at different wavelengths form a matrix of observations $A_{Sample,\ wavelengths}$. EVA and FA are used to find the number of the responsible factors contributing to the response data matrix. They are related to SVD.

Principle Component Analysis (PCA): It is a variant of looking at data matrix in a transformed space to arrive at minimum number of linear combination of data vectors either in column or row space. It is applicable to unsupervised data like that of ICP for chemical elements of geological sample. The algorithm of PCA proceeds in searching for the maximization of variance direction [$\max(X^T*X)$] in the column space. The distance along the best fit straight line (X= T*P+ error) is the first Principle Component (PC). It is obtained by computing largest Eigen vectors of X^T*X, a square symmetric matrix. The scores of PC(1) are the coordinates of the point along PC1 axis. The contribution of first PC is substracted from the data and a new PC is calculated as before. This results in the second PC uncorrelated with the first. NIPALS algorithm for PCA [21] is used and Fig 1 shows the PC-scores for the dataset. The distribution of metal ions in North and central zones are given in PC#1 vs PC#2 plots (Fig.2). Some of elements are overlapping in the PC space. The results of PC model will be improved by applying nonlinear PC analysis. However, SLP-NNs imbibe linear and nonlinear PC as well discriminate analysis.

Fig 1: PC scores of ICP-MS data



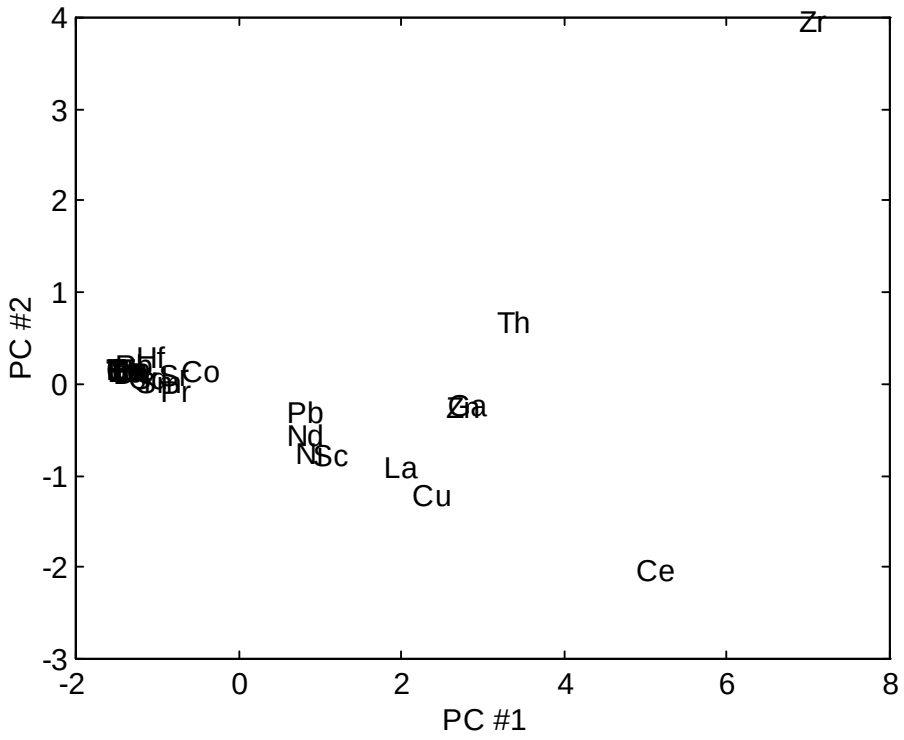


Fig 2a: PC#1 vs. PC#2 North block

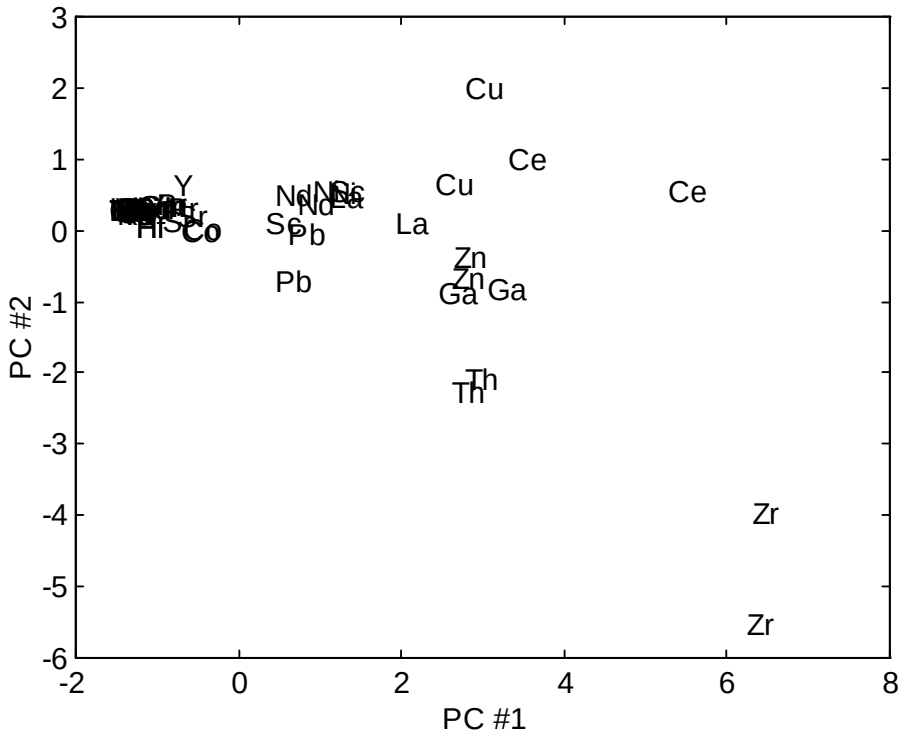


Fig 2: PC#1 vs. PC#2 for Central Blocks

Neural networks (NNs): Neural networks are data driven models accepting attribute-, binary- and floating point- (real and complex) input. This approach does not require a priori or posterior statistical distribution/ density function of data or noise and even a model to start with. A set of transfer (mathematical/statistical/fuzzy) functions operating on multivariate user input data maps into output. It is not only an imbibing methodology in the sense that it mimics many of earlier model driven models, but gracefully performs I(nput)→O(utput) mapping in multi-dimensional non-linear hyper space with discontinuities, knots etc. Fig. 3 incorporates a few neural network architectures popular over the last half a century. The process never fails, in other words the model never collapses even with high noise of any statistical distribution, but performance of the system diminishes.

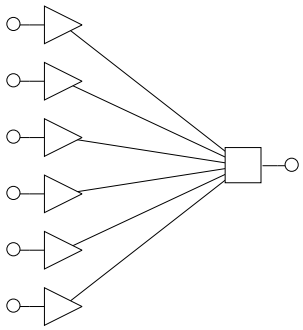
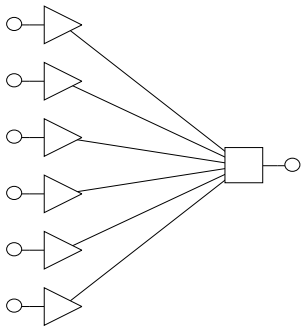
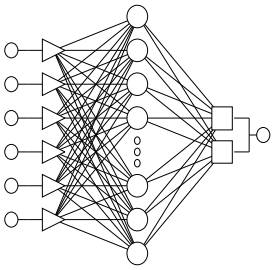
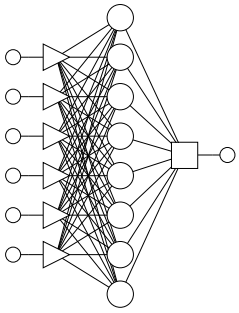
Linear-NN	**Non-Linear (SLP)-NN**
	
Probabistic-NN	**Radial_Basis_Function-NN**
	

Fig : 3 Typical neural network architectures used in geochemistry

A single layer perceptron NN is used to train the classification patterns.

Intelligent Problem Solver (IPS) of Trajan: IPS is an automated procedure in arriving at optimum set of architectures for a data set. It is a fast solution finder even for a novice. The option, 'advanced' is for experts, wherein the types of NNs, number of layers, CPU time limit, performance, and training/testing of data sets can be opted based on the need. The results can be exported to Excel, Word or Statistica package for further analysis. The inferences are only a guideline and further runs are to be carried out varying the type of training algorithms, epochs and parameters specific to the network chosen. The results of classification for typical NN run are in Table 4.

The classification statistics for the training set in central block correctly classified 15 elements out of 16 and 13 out of 14. The wrong (mis-) classification in each class is only one. A detailed inspection of dataset split into training, verification and testing shows (Table 4b), the number of misclassified elements is totally four. The classification result can be refined by increasing data set size, number of samples of each class and by resorting to hybrid NNs.

Table 4(a): Classification statistics (a) central block (NN-41 : MLP, 6-8-1)

	Tr	
	C1	**C2**
Total	**16**	**14**
Correct	**15**	**13**
Wrong	**1**	**1**
Unknown	**0**	**0**
C1	**15**	**1**
C2	**1**	**13**

Although hybridization of even 4 to 6 methods [3] are in vogue, fusion technologies and research/expert/SAP/sure-but examine mode hardware hungry software is the need of the hour. This approach enables application intensive disciplines to obtain results from the state of the art data driven processing. Ensemble or committee of NNs output different results for the same task. The generalization of performance increases through simple averaging, gating network, stacking, SVM and GA. Saridakis [22] reviewed the fusion of FIS, GA and NN and their success to address hard-to-solve tasks and the benefits hitherto not realized.

APPLICATION

Data from more sampling locations and larger datasets and analysis with self organizing map (SOM), learning vector quantization (LVQ), neural gas (NG), and unsupervised/supervised auto-resonance theory (ART) will probe deep into geochemical prospects.

CONCLUSION

The bauxite ore grade and quality is studied with ICP-MS in central and north blocks of deposit. The elemental concentration data matrix is analyzed with (linear) exploratory data analysis. The data are highly correlated in the vertical space from Khondolite to the laterite cap. In each block trace and REE are separated through PCA. The partial success is due to nonlinear interactions. NN, a data driven non-linear model developer (without any a prior

Table 4b: Classification statistics for training (Tr), verification (Ve) and test (Te) set

C1: Trace elements C2 : Lanthanides

	Tr		Ve		Te	
	C1	C2	C1	C2	C1	C2
Total	9	6	3	4	4	4
Correct	8	6	3	3	3	3
Wrong	1	0	0	1	1	1
Unknown	0	0	0	0	0	0
C1	8	0	3	1	3	1
C2	1	6	0	3	1	3

model-driven-model to start with), distinguishes central and north blocks. Even, SLP-NN is superior to PCA for linearly inseparable classification of clusters. The preliminary results with advanced supervising (LVQ, X-ARTMAP) and non-supervisory (X-SOM, ART) and

hybrid approaches involving GA, EA and honey bee mating algorithm are promising to pursue with additional data and a priori knowledge.

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REFERENCES

[1] P. Tahmasebi, A. Hezarkhani, Computers & Geosciences, **2012**, 42, 18-27.
[2] B. Samanta, S. Bandopadhyay, Computers & Geosciences, **2009**, 35, 1592-1602.
[3] M. Ziaii, F. Doulati Ardejani, M. Ziaei, Ali A. Soleymani, Applied Geochemistry, **2012**, 27, 663-676.
[4] Z. Ruilin, Ian S. Lowndes, International Journal of Coal Geology, **2010**, 84, 141-152.
[5] S.A. Jafari, S. Mashohor, M. Jalali Varnamkhasti, J. Petroleum Science and Engineering, **2011**, 76, 217-223.
[6] R. Sambasiva Rao and V. Anantha Ramam, Ch. V. Kameswara Rao and K. Rama Krishna, in P. Sasi Bhushana Rao, Climate change impact on environmental and human health, 11-12 February, 2011, Visakhapatnam (India), Gayatri vidya parishad, Visakhapatnam, **2011**, 27-43.
[7] G. Nageswara Rao, V. Ananta Ramam, S. Satyanarayana Rao and R. Sambasiva Rao, J. Ind. Chem. Soc., **1998**, 75, 236-47.
[8] V. Anantha Ramam, G. Nageswara Rao, S. V. Rama Sastri, R. Sambasiva Rao, Ind J Chem. **1997**, 36A, 964-969.
[9] I. Suryanarayana, A. Braibanti, R. Sambasiva Rao, V. Ananta Ramam, D. Sudarsan and G. Nageswara Rao, Fisheries Research, **2008**, 92, 115-139.
[10] A. Braibanti, R. Sambasiva Rao, A. Ravindra Babu, and G. Nageswara Rao, Ann. Chim. Rome, **1995**, 85, 17-29.
[11] A. Braibanti , G. Nageswara Rao , S. B. Jonnalagadda , D. Sudarsan , R.Sambasiva Rao, Ann. Chim. (Rome) **2001**, 91, 29-39.
[12] K. Sambasiva Rao and R. Sambasiva Rao, J Korean Phys. Soc., **1998**, 32, S1850-S1851.
[13] A Braibanti, R.Sambasiva Rao, V. Ananta Ramam, G. Nageswara Rao, V. Panakala Rao Ann. Chim, **2005**, 95, 291-301.
[14] M. Venkata Subba Rao, V. Ananta Ramam, V. Muralidhara Rao, R. Sambasiva Rao, Asian J Chem., **2010**, 22, 5937-5950.
[15] *MATLAB 4.2C*, (*The Maths Works Inc.*) 24, Boston, USA.
[16] TRAJAN software Ltd., Trajan house, 68 lesbury close, Chester-le street, co. Durham, DH2.3SR England.
[17] R. Sambasiva Rao, K. Rama Krishna and V. Ananta Ramam, Volume I: State-of-art of Layered Neural networks, Volume 2: Applications of Neural networks in Pharmaceutical and Environmental Chemistry, Himalaya Publishing House, Bombay (Under publication).
[18] R. H. Markram, Nature Reviews-Neuroscience, **2006**, 7, 153-160.
[19] R. Sambasiva Rao, Unpublished.

[20] E. Fisicaro, A. Braibanti, R. Sambasiva Rao, C Compari, A Ghiozzi, G. Nageswara Rao, Talanta **1998**, 45, 1267-79.
[21] Laila H. Abdel Rehman, K. Sambasiva Rao, G. Nageswara Rao, R. Sambasiva Rao, J. Ind. Council. Chemists, **2001**, 17, 33-50.
[22] K. M. Saridakis, A. J. Dentsoras, Advanced Engineering Informatics, **2008**, 22, 202-221.