

Inductive Classifying Artificial Network for Fly Ash Type Categorization

M.C.Nataraja , M.A.Jayaram, C.N.Raikumar

Abstract- Nowadays, fly ash is a common ingredient of concrete and may constitute up to 50% by weight of the total binder material. Incorporation of fly ash in Portland-cement concrete is highly desirable due to technological, economic, and environmental benefits. This article demonstrates the use of artificial intelligence neural networks for the classification of data. ICAN stands for Inductive Classifying Artificial Network and is used to conveniently describe Kohonen's Self-organizing feature map (SOFM) for fly ash type categorization using chemical attributes as inputs. Eight chemical attributes have been considered in classification as these play their role in performance of concrete. The application of ICAN permitted to differentiate three main groups of fly ashes. This is in contrast to ASTM classification of fly ashes into F and C classes based on percentage of Calcium Oxide (CaO) alone. Three one-dimensional ICANs of 16 neurons, 24 neurons and 32 neurons were explored. The overall classification results of all the three simple models were significant and encouraging.. The data pertaining to fly ash were collected from standard published works. The categories formed by ICAN were then correlated with their performance in High Volume Fly Ash Concrete System [HVFAC].

Index Terms- Fly Ash, High Volume Fly Ash Concrete System, ICAN, Self-organizing feature map.

I. INTRODUCTION

Fly ash is a common ingredient of concrete and may constitute up to 50% by weight of the total binder material. Incorporation of fly ash in Portland-cement concrete is highly desirable due to technological, economic, and environmental benefits. Published literature contains a large amount of data on properties of structural concrete containing 10 to 30 percent fly ash by weight of the total cementitious material (i.e. cement + fly ash) .For most structural applications except mass concrete, the fly ash content is often limited to 20-30%.

Manuscript received January 10,2006. This work is part of the ongoing research work on applications of soft computing techniques in concrete technology.

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The quality of fly ash is often specified by standards in terms of fineness, loss on ignition and limitation of its chemical constituents. However, to the concrete technologist and the design engineer, the more important factors are the influences of fly ash on properties such as workability, heat of hydration, strength or durability. Besides the effects of fly ash on the properties of concrete, fly ash also affects the cost of the concrete product. The cost of fly ash is generally one-third [1]. High volume fly ash concrete [HVFAC] is ideally suited for rigid pavement construction to meet the projected needs of interstate highway & major constructions in India [2,3]. This paper reports an attempt made to classify the fly ashes into groups using the available copious data. Such grouping of data is useful for a concrete technologist for expeditious use of certain kinds of fly ashes in HVFAC system.

This paper reports an attempt made to classify the fly ashes into groups using the available copious data. Such grouping of data is useful for a concrete technologist for expeditious use of certain kinds of fly ashes in HVFAC system. However, chemical composition of fly ashes is considered in this work as they play a significant role in fly ash concrete and also there is variability in their proportions.

II. BACKGROUND

There exists a considerable variability in concrete related characteristics of fly ashes between typical low-calcium and typical high-calcium fly ashes. At present ASTM specifications call low calcium "class F" fly ashes and high-calcium "class-C" fly ashes. Low calcium fly ashes have their origin in bituminous coal while high calcium fly ashes are due to burning of coals with high limestone. However, this classification emphasizes percentage of calcium oxide only and discounts other chemical constituents. The differences in chemical composition of these two kinds of fly ashes are palpable. The silica contents of high-calcium fly ashes are somewhat variable [3]. Alumina contents may not be as variable. Iron oxide contents of low calcium are usually higher than that of high calcium fly ashes. The major distinction between the two groups is CaO content. A CaO content upto 29% is reported in the literature. Fly ashes with intermediate CaO contents have their origin in sub-bituminous coals. The remaining chemical contents like MgO, SO₃,K₂O, Na₂O₃ and TiO₂ are often considered to be of less importance, but this is not necessarily so[4]. The MgO contents of high calcium fly ashes are usually quite high. Higher SO₃ contents in high calcium fly ashes may reflect either readily soluble alkali sulphates or calcium sulphates or both. Many low calcium fly ashes have

substantially more K_2O than Na_2O . On the other hand, many high calcium fly ashes have more Na_2O than K_2O . The other attribute is percentage loss- on- ignition [Loi]. The value of this is a reflection of the efficiency of combustion process. However, the values of Loi for high calcium fly ashes are usually very low. Fineness measured in terms of percentage passing 45 μ m sieve is another property. It has been reported that the contents of the coarse particles is often substantially lower in high calcium than in low calcium fly ashes. The pozzolonic activity index, as measured with cement after 28 days of curing at slightly elevated temperature is almost always substantially higher for high-calcium than low-calcium fly ashes [1,4]. It is concluded that except for the calcium content, variations in the other chemical constituents of fly ash appeared to have no effect on its reactivity [5]. The particle size distribution is important parameter governing the reactivity of fly ash. For low calcium fly ashes the reactivity was found to be directly proportional to the amount of particles <10 μ m, and inversely proportional to particles >45 μ m. High calcium fly ashes seem to be relatively less sensitive to particle size distribution [5]. Though quoted in the list of attributes, the pozzolanic activity index does not provide a useful yardstick for grading the relative reactivity of fly ashes [4,5].

III. SIGNIFICANCE OF THE WORK

There have been many reported applications of neural networks in civil engineering [6]. In particular, an attempt to classify soils by using feed forward neural network with back propagation learning algorithm is also reported [7]. The primary objective of this work is to categorize fly ashes from different sources into distinct groups mostly based on its chemical constituents. The so formed groups were then correlated with their performance in High Volume Fly Ash Concrete System [HVFA] from the available literature. The scope of the research work is limited to about 80 sets of data garnered through literature. Some reasons for using ICAN- a self-organizing neural network in this research include:

- Ability to detect irregularities in input and adapt responses accordingly.
- Use of competition to naturally cluster data without supervision.
- Similarity to the well-understood k-means statistical algorithm, which seeks to maximize inter-cluster distances.

IV. KOHONEN MAPS

The self-organizing map (SOFM) network performs unsupervised learning [8]. It is a neural network that forms clusters of neurons that reflect similarities in the input vector. It is a mapping that is defined implicitly and not explicitly. This is desirable because this investigation is not restricted to any particular application or predefined categories. Input vectors are presented sequentially in time

without specifying the output. Because of this fact, there is no way of predicting which neuron will be associated with a given class of input vectors. This mapping is accomplished after training the network. The SOFM has a sequential structure starting with the d input vectors (input neurons) \mathbf{x} , which are received by the n neurons in parallel and are scaled by the weight vector \mathbf{w} . Thus the weight matrix is the size of n neurons by d inputs. The n neurons are then entered into competition where only one neuron wins. The architecture of the SOFM is illustrated in figure 1. SOFM employs the concept of topological neighborhoods, which are equidistant neuron neighborhoods centered around a particular neuron. The neighborhood distance matrix for a one-dimensional case using four neurons is:

0	1	2	3
1	0	1	2
2	1	0	1
3	2	1	0

It can be seen that the distance of a neuron from itself is 0, the distance of a neuron from its immediate neighbor is 1, and so on. Unlike simple competitive learning, the weights of the neighborhood neurons are updated in addition to the weights of the winning neuron. The steps in training the SOFM can be outlined as follows:

- Step 1. Initialize weights randomly.
- Step 2. Present new input.
- Step 3. Compute distances between input and neuron weights.
- Step 4. Competitive selection of the neuron with the minimum distance.
- Step 5. Update neuron weights to winning neuron and neighborhood neurons.
- Step 6. Continue iterating by going through steps 2-5.

In describing the training algorithm, it is useful to understand the weight structure of the network. Each neuron has the same number of weights \mathbf{w} as the dimension of the input vector \mathbf{x} . The weight structure for each neuron can then be viewed as a matched filter competing against other neurons. A matched filter has the impulse response tuned to input so that it produces the maximal signal [9]. The overall weight structure can be viewed as an array of matched filters with each neuron's weights being adjusted on the basis of current weights and the goodness- of- match of the input.

Given that the feature map is initialized with random weights \mathbf{w} for all the neurons, a distance measure, $d(\mathbf{x}, \mathbf{w}_i)$ can be used to define the goodness-of-match between a particular weight vector \mathbf{w}_i and the input vector \mathbf{x} . The distance measure used can be correlation, Euclidian, city-block, or other statistical measures. If the Euclidian distance is used, then the winning neuron from the competition is found at each iteration k by using the following equation:

$$\| \mathbf{x}(k) - \mathbf{w}_c(k) \| < \| \mathbf{x}(k) - \mathbf{w}_i(k) \| . \forall i \quad (1)$$

Where neuron c is the winning neuron. The network weights are then updated as follows:

$$w_i(k+1) = \begin{cases} w_i(k) + \alpha(k)[x(k) - w_i(k)], i \in N_c(k) \\ w_i(k), i \notin N_c(k) \end{cases} \quad (2)$$

Where N_c defines the neuron neighborhood and $\alpha(k)$ is the learning rate at each iteration. The weight updating equation shows that $d(\mathbf{x}, \mathbf{w}_i)$ is decreased for N_c while those outside N_c are left unchanged. The neighborhood size and the learning rate both decrease with increase in the number of training iterations. Typically, $\alpha(k)$ start near 1 and go down to 0.1. The size N_c can start out as large as the greatest distance between weight vectors, and decrease until the neighborhood defines only one neuron.

An interesting feature of SOFM is that the distances between neurons can be interpreted as statistical frequency distributions. In a fully trained network, if input vectors occur with varying frequencies, the feature map will also allocate neurons to an area in proportion to the frequency of input vectors [10]. Another interesting feature of SOFM is that the weights become topologically similar to the input vectors. In a sense, the final weights are analogous to class templates and can be plotted for visual interpretation. Because of this feature, the SOFM is less like a black box and more like an automated k-means statistical clustering algorithm.

The choice of the particular SOFM configuration is not a precise science and involves engineering judgment. The two major design parameters are dimension of the network and the number of neurons. As cited in [11], powerful results have been obtained by just using one- and two-dimensional topologies. The training parameters are the learning rate and the number of training iterations. The initial learning rate may be between 0 and 1, and the value of 0.2 was chosen based on experience. Kohonen [8] cites the use of 10,000 –1,00,000 training iterations as typical, and recommends that the number of training cycles should be at least 500 times the number of output neurons. In this study, for all the topologies considered (8-16, 8-24 and 8-32), the training was stopped at 10,000 iterations as the winning neurons were found to be stable.

V. APPLICATION

The chemical composition of fly ashes plays a significant role in HVFAC. But, the important factor that has hindered the widespread use of ashes is their variability. No two ashes are completely alike. The need to characterize them in terms of their chemical, mineralogical composition and host of other parameters relevant to engineering use is urgent and real [11]. However, in this study, only eight chemical attributes of the fly ashes were considered.

Data for this classification work was availed from the listed references [13-30]. In all, about 80 sets of data were

gathered. The eight chemical attributes of fly ash considered for classification are listed in the table 1. Among these attributes, the sulphur dioxide is predominant in high calcium fly ashes and was found to be not appreciable in low calcium fly ashes. The reverse was the trend in the case of Titanium oxide i.e, appreciable percentage of titanium oxide was reported in low calcium fly ashes. Therefore, they are together taken as one attribute. Among these 80 data sets, eight records were rejected due to non-availability

of data concerned to some chemical compositions. Some references even contained the information about the source of the fly ash also. The remaining 72 data sets were normalized and shuffled for their random arrangement. The program coded in C++ was executed in Turbo C++ IDE.

Three topologies 8-16, 8-24 and 8-32 were considered to pick out the best possible one. The number of output neurons was set as multiples of input neurons. It is recommended that [31] before learning process starts, SOM coefficients should be sized and ascertained. These parameters govern the network-learning rate, learning iteration, process and weight updating, etc. The following are the parameters that must be ascertained before training the network:

- Kohonen output neurons. This is the estimation of number of kohonen cells. The output neurons were considered as multiples of input neurons. Three combinations 8-16, 8-24 and 8-32 were explored.
- Learning coefficient. The learning coefficient must be estimated before the network actually undergoes learning. After sufficient learning cycles, it was estimated that the learning rate would start from 0.2 for the best training of the network to achieve good results.
- Number of SOM steps. This is the number of learning iterations. Typically, this should be around 30 times the number of training vectors. However, after observing the performance of the network after sufficient training and comparison of results, it was assumed to be 10,000.
- Neighborhood size. The neighborhood size is used in the self-organizing phase of the learning when the winning PE and all its neighbors move toward the input PE. Neighborhood sizes of 5, 4 and 3 were used in all the topologies mentioned.
- Epoch size. Epoch size is the number of training vector counts after which the network weights and parameters are updated. It is recommended that the epoch should be less than or equal to the number of vectors in currently specified training file. However, the epoch size chosen was 100. The parameters are summarized in table 2.

VI. RESULTS

All feature maps tested had the following general characteristics. First, the input vector was composed of 8 components corresponding to the chemical compositions. Second, the number of training iterations was the same for

all feature maps. The feature maps considered are of the topology 8-16, 8-24 and 8-32. Even though some trials involving as little as 3000 iterations were performed, the resulting feature maps did not exhibit convergent characteristics.

Table 1: Chemical Attributes considered

Sl No	Attribute [%]	Sl No.	Attribute [%]
1	Silicon dioxide (SiO ₂)	5	Magnesium Oxide (MgO)
2	Aluminum Oxide (Al ₂ O ₃)	6	Sodium oxide (Na ₂ O ₃)
3	Ferric Oxide (Fe ₂ O ₃)	7	Potassium Oxide (K ₂ O)
4	Calcium Oxide (CaO)	8*	Sulphur oxide or Titanium Oxide.

*-Any one that has higher % is selected

Table 2: SOFM coefficients

Coefficients	Values
Learning coefficient	0.2
Neighborhood Sizes	5,4 and 3
Epoch size	100
Learning iterations	10000

Therefore, based on the recommendations of other researchers and on experience, the number of training iterations was chosen to be 10,000. A 2.4GHz personnel computer was used for implementing ICAN, and the training took only a few minutes for each feature map configuration. In all the three cases, three distinct clusters resulted from the training; the representative classes as guided by winning neurons. The training set composed of 72 records. A segment of data and the classification are listed in table 3. The overall classification rate is defined as the percentage of fly ashes that was classified correctly. The result was significant and encouraging in small sized SOFM (8-16) when compared with other two SOFMs. The average percentage classification was found to be as high as 95% in case of 8-16 topology, 80% in case of 8-24 and 77% in case of 8-32 topology. Figure 2 shows a schematic view of three-group classification in terms of winning neurons found in feature map of topology 8-16. The details of overall classification result are appended in Table 4. In all the three topologies, the fly ash group with very low calcium content was classified with relatively high percentage classification. The performance evaluation of these groups and range of values in some chemical

attributes that proved to be sensitive during classification is presented in Table 5. The other attributes and their values seem to be overlapping over different groups.

A. Sensitivity of important attributes

Four chemical attributes, i.e., SiO₂, Al₂O₃, CaO and SO₃/TiO₂ were found to be sensitive during the classification process. To convalidate this observation, three different SOFMs of topologies 4-8, 4-12 and 4-16 were tested with randomly arranged data sets. All the topologies conclusively proved that these attributes are in fact more crucial in the classification. A sample segment of data consisting of these four attributes and the winning neurons are presented in table 6. The published research work on high volume fly ash concrete [13-30] emphasizes the quantum of calcium oxide in fly ash as the decisive parameter in long-term performance of high volume fly ash concrete. Therefore, the sensitivity of classification lies in the correlation of other attributes with that of calcium oxide. In order to get a visual clue of correlation among group sensitive attributes, two-dimensional combinations of calcium oxide – silicon oxide, calcium oxide – ferric oxide and calcium –sulphur oxide (or Titanium oxide) were considered. Figure 3 shows correlation between calcium oxide and silicon oxide. In this plot, higher percentage of calcium oxide corresponds to lower amount of silicon dioxide and vice versa with moderate percentage ranges of both in the midst. In fig 4, the correlation between calcium oxide and ferric oxide is not that marked. There is a fair correlation between calcium oxide and sulphur oxide/titanium oxide as portrayed in fig 5.

VII CONCLUDING REMARKS

Self-organized maps are proved to be an effective technique to group fly ashes from various sources around the world. Grouping is according to similarity. This work has shown that there can be three broad groups of fly ashes named as *low calcium*, moderate calcium and *high calcium* fly ashes. The grouping achieved demonstrates several advantages for incorporating self-organizing maps into the development of indexing equations with reduced parsimony [32]. The established data groups demonstrate following benefits:

- The data can be correlated and grouped easily.
- The data groups evolved using ICAN can be refined using supervised learning techniques like Radial Basis Function (RBF) networks [32].
- The groups evolved can be evaluated for their performance in high volume fly ash concrete system.

Table 3: Sample data and its classification as guided by winning neurons in different ICANs

Sample No.	SiO ₂	Al ₂ O ₃	Fe ₂ O ₃	CaO	MgO	Na ₂ O	K ₂ O	SO ₃ /TiO ₂	Winning Neurons in ICANs		
									8-16	8-24	8-32
1	60.4	29.4	4.35	0.80	0.41	0.26	0.93	1.92	6	8	12
2	62.7	28.5	3.97	0.78	0.40	0.23	0.89	1.90	6	8	12
3	59.9	30.9	3.40	0.87	0.44	0.24	1.01	1.92	6	1	12
4	61.6	27.0	4.38	1.02	0.61	0.24	1.13	1.64	6	8	12
5	42.0	22.0	28.0	3.00	1.0	0.30	1.30	1.00	7	1	17
6	34.0	19.0	6.00	29.0	5.0	0.10	0.30	3.00	0	20	0
7	49.4	19.8	3.67	11.5	2.4	1.30	0.53	0.74	12	13	6
8	47.1	23.0	20.4	1.2	1.17	0.54	3.16	0.67	7	8	12
9	55.7	20.4	4.61	10.7	1.53	4.65	1.00	0.38	13	14	17
10	48.4	27.0	6.6	8.5	2.0	0.5	1.0	1.3	12	14	18
11	44.9	36.6	5.7	9.8	2.1	0.65	0.0	0.64	12	13	18
12	56.8	28.2	5.3	3.0	5.2	0.14	0.0	0.70	7	13	12
13	40.7	17.9	29.9	2.8	1.1	0.7	1.60	1.30	6	13	12
14	53.4	22.0	6.3	6.8	2.0	2.9	0.67	0.50	12	14	6
15	57.6	29.0	5.2	0.3	1.1	0.2	2.90	0.20	6	8	12
16	52.2	27.4	9.2	4.4	1.0	0.5	0.68	0.45	7	1	6
17	50.9	28.9	5.4	2.4	0.9	0.4	2.54	0.40	6	8	12
18	46.2	31.3	8.5	1.8	0.70	0.50	1.9	0.50	7	8	12
19	38.4	13.0	20.6	14.6	1.40	3.30	2.04	3.30	13	14	17
20	39.5	19.5	5.7	24.7	3.4	1.80	0.21	1.80	0	20	0
21	36.0	19.8	5.0	27.2	4.9	3.15	1.72	3.15	0	20	0
22	50.5	17.2	5.9	15.8	3.1	1.0	0.82	1.00	13	14	7
23	45.1	22.2	15.7	3.77	0.9	0.58	1.52	1.40	6	1	12
24	53.6	27.4	7.74	2.88	0.99	0.38	2.42	0.37	6	8	12
25	52.4	23.4	4.70	13.4	1.33	3.60	0.60	0.80	13	14	17

Table 4. ICAN overall classification results

	Low calcium Fly ash Group 1	Medium Calcium Fly ash Group 2	High Calcium Fly ash Group 3
SOFM-1, 8-16	99%	92%	94%
SOFM-2, 8-24	94%	64%	85%
SOFM-3, 8-32	81%	63%	78%

Table 5: Ranges of Sensitive Chemical Attributes of the Groups and Performance Evaluation

Group	SiO ₂	CaO	SO ₃	TiO ₂	Performance/ utility in concrete [As found in references]
	[%]	[%]	[%]	[%]	
1	53-63	0.6-3.00	..NA..	0.8-2.3	Mostly as a micro-aggregate, very low strength development at early ages. No significant pozzolonic activity. For normal strength concrete, the replacement could be up to 60%, for high strength concrete it could be only up to 20%. Reduction in workability and demand for large quantities of super plasticiser.
2	39-52	3.0-18.0	0.8- 2.5	..NA..	Replacement could be up to 50%. Significant improvement in strength after 90 to 365 days. Decrease in average pore diameter in concrete. Excellent durability against freezing and thawing. Strength of concrete is sensitive to particle size distribution in fly ash, low elastic modulus value, and demands high dosages of super plasticiser for good workability. Reactivity is governed by fineness.
3	30-40	16-29	2.5-3.0	..NA..	Excellent mechanical properties of concrete. However, high expansion with high SO ₃ , severe volume instability, appearance of ettringite in some cases, excellent compressive and flexural strength. The reactivity is not governed by the fineness of the particles. Most of the fly ashes of this category can be used for structural grade concrete in quantities up to 40% replacement of cement.

Table 6: Sensitive attributes and their grouping as guided by winning neurons.

Sample No.	SiO ₂	Fe ₂ O ₃	CaO	SO ₃ /TiO ₂	Winning neurons in different ICANs		
					4-8	4-12	4-16
1	60.4	4.35	0.80	1.92	0	1	7
2	62.7	3.97	0.78	1.90	0	1	7
3	59.9	3.40	0.87	1.92	0	1	7
4	61.6	4.38	1.02	1.64	0	1	7
5	42.0	28.0	3.00	1.00	7	2	6
6	34.0	6.00	29.0	3.00	1	8	13
7	49.4	3.67	11.5	0.74	7	8	6
8	47.1	20.4	1.2	0.67	0	2	6
9	55.7	4.61	10.7	0.38	7	2	6
10	48.4	6.6	8.5	1.3	7	2	6
11	44.9	5.7	9.8	0.64	7	2	6
12	56.8	5.3	3.0	0.70	0	1	7
13	40.7	29.9	2.8	1.30	0	2	7
14	53.4	6.3	6.8	0.50	7	2	6
15	57.6	5.2	0.3	0.20	0	1	7
16	52.2	9.2	4.4	0.45	7	2	7
17	50.9	5.4	2.4	0.40	0	1	7
18	46.2	8.5	1.8	0.50	7	1	7
19	38.4	20.6	14.6	3.30	7	8	13
20	39.5	5.7	24.7	1.80	1	8	13
21	36.0	5.0	27.2	3.15	1	8	13
22	50.5	5.9	15.8	1.00	7	8	13
23	45.1	15.7	3.77	1.40	7	1	6
24	53.6	7.74	2.88	0.37	0	1	7
25	52.4	4.70	13.4	0.80	7	2	7

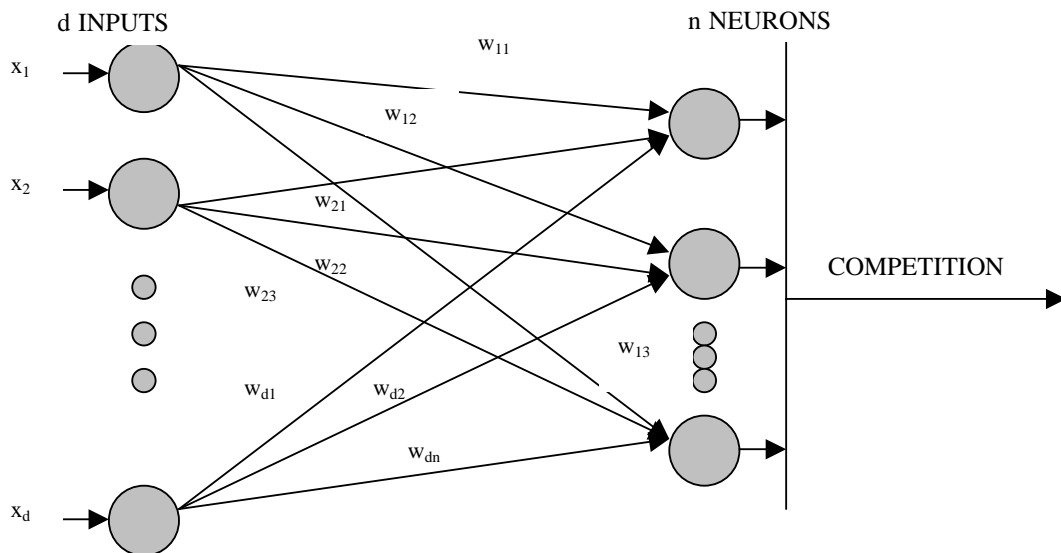


Fig.1. One-dimension Self-organizing feature map architecture

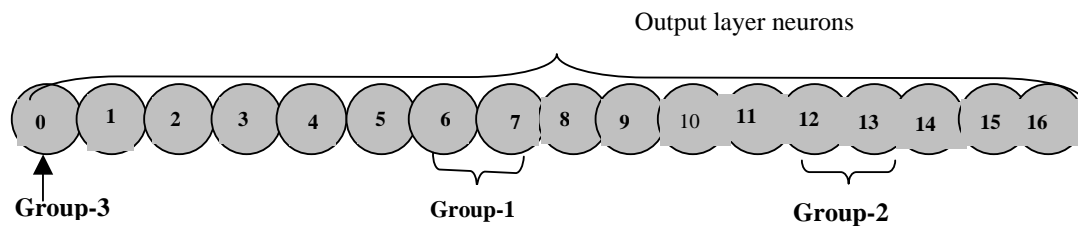


Fig.2. Winning neurons guiding the grouping (feature map topology: 8-16)

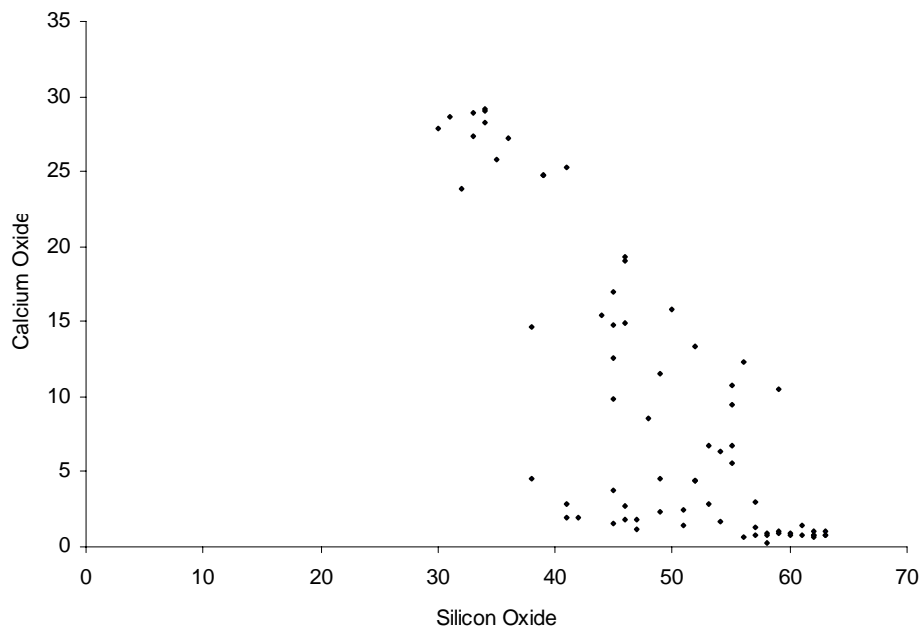


Fig 3. Correlation between Calcium -oxide and Silicon Oxide

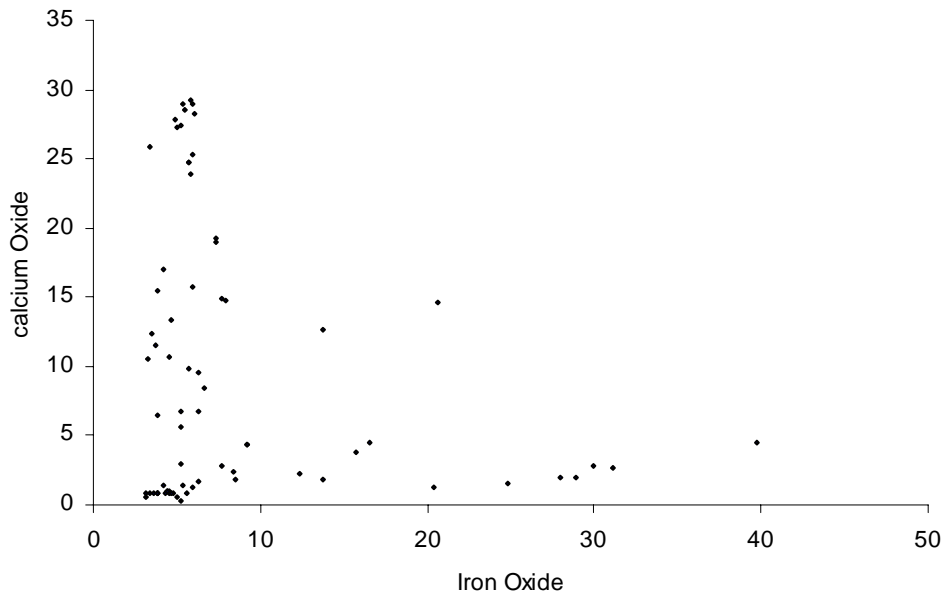


Fig 4. Correlation between Calcium oxide and ferric oxide

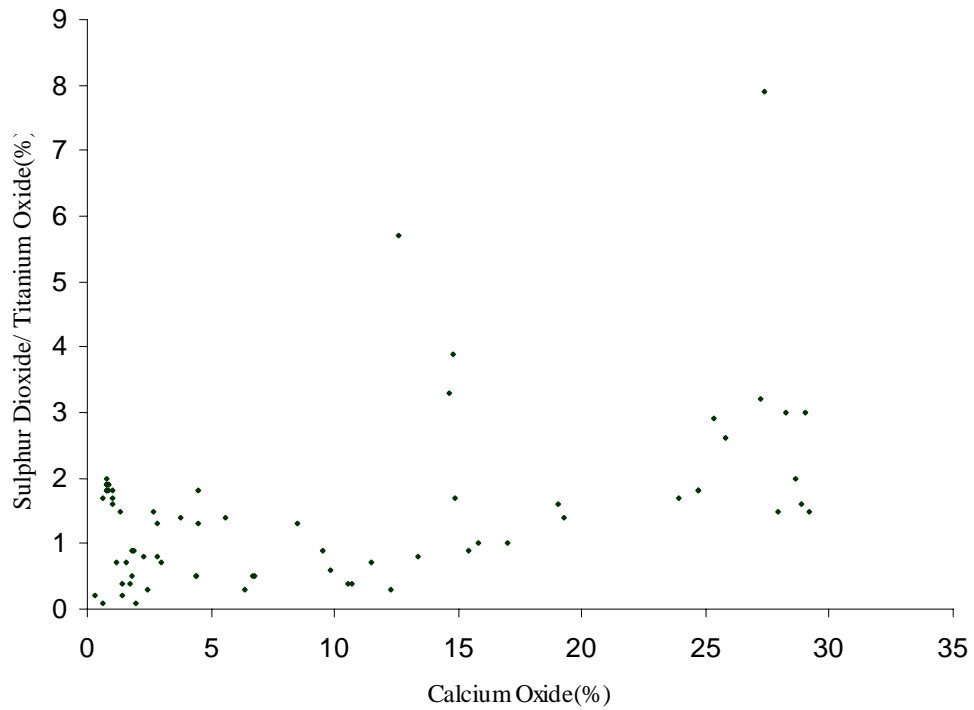


Fig.5. Correlation between calcium oxide and Sulphur Dioxide /titanium oxide

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