Formulating a Mathematical Model for the E-Nose Application through Genetic Algorithm (GA)

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ABSTRACT
From a technical and commercial point of view it is found that electronic sensing technologies have emerged significant progresses over the last few decades. The potentiality of reproducing human senses by sensor arrays and pattern recognition systems is termed as electronic sensing. E-Nose provides an industry-specific management resolution for the perpetual and real-time monitoring of environmental odor and air quality resulting in higher profit and improved community relations. The device constitutes arrays of effective and rapid acting chemical sensors, supplemented by patented electronics and software. Chemicals in the air are identified by the sensor arrays, registering complex odor images in real time. By means of wireless connection or lines a permanent record is sent to the computer, where it is detected, computed and alarms for inconsistent events were sent or else it can be indicated by some displacement. Electronic nose instruments are exploited by research and development laboratories, quality control laboratories, process & production department's of environmental protection, all these are done for the detection of volatile organic compounds in air, water and soil samples, and the measurement and comparison of the effects of manufacturing process on products are also determined. In this paper, An E-Nose is proposed to identify the gas component. For this process, the soft computing technique called Genetic algorithm is used. This provides an optimized weight to identify the gas component by means of the input concentration range and SMAC/hr (units in ppm). The intended Technique is evaluated with different training samples and results are produced.

Keywords
Electronic nose, odor, electronic sensing, concentration range and SMAC, volatile organic compounds, Genetic algorithm (GA).

1. INTRODUCTION
Nowadays, sensor for gaseous molecules plays a significant role in monitoring the environment, controlling chemical processes, and in medical applications. Electronic Nose (E-nose) is a device used to detect and identify the odors/vapors. Although it has been in the market for several years, its size is large and also it is high-priced [3]. In an ever-growing world, the electronic devices are duplicating every other sense of perception; the sense of smell is lagging behind. But still, there has been a significant increase in the need for detecting odors, to replace the human job of sensing and quantification. Several important applications fall in the category where humans cannot meet the risk in smelling the substance.

In many fields, the detection of volatile organic compounds (VOCs) has become a serious task as the fast evaporation rate and toxic nature of VOCs and working close to human life could be dangerous at high concentration levels in air for the health of human beings. In fact, the VOCs are also considered as the main reason for allergic pathologies, skin, and lung diseases [7]. Some necessary applications such as continuous monitoring, medical applications, etc., allow humans to perform tasks that were once considered as unfeasible. The fast paced technology has helped to develop sophisticated devices that have brought the electronic nose to small sizes with superior capabilities. The trend is such that there will be precise, qualitative, and quantitative measurements of odor in the near future. The growth of gas sensors is a field of great activity. Especially, the electronic noses are used for process control, quality control in the food and beverage industry, pollution monitoring, and airport security. [1]

Unpleasant odor or malodor has been regarded as an indicator of potential risks to human health but not necessarily the direct trigger of health effects. Thus, development of E-nose for medical diagnostics has become one of the important issues in the biomedical engineering research now days [2]. Electrical properties will be changed when the sensors react with odorant [3]. A chief concern of scientists is global warming, largely due to huge emissions of carbon dioxide (CO2) which is considered as one of the main greenhouse gases inducing a warming climate, CO2 concentration in the atmosphere is under special analysis of many weather services in the world. Suburban areas continue to grow rapidly and are potentially an important land-use category for anthropogenic carbon-dioxide emissions [4].

The core component of an E-Nose is an array of non-specific chemical sensors. An odor examines and stimulates many of the sensors in the array and extracts characteristic response pattern. The sensors inside e-Nose can be made up of various technologies, but in all cases certain physical property are to be measured and a set of signals is generated [6]. It consists of a set of different gas sensors which can detect different toxic gasses. Output of sensor array is connected with encoder circuit and gas sensors often respond to an open range of gas species and are therefore only partially selective [5]. Generally, source localization is done by the support of electronic nose and mobile vehicles since robotic techniques are getting mature. However, certain problems could occur during specific situations, such as instantaneous emission and complex landscape environment [8]. If gas sensor array discovers any toxic gasses of dangerous level of lethal concentration, then processor will switch on the exhaust fan in the laboratory [5]. The toxin gasses in the room are to be collected in a proper manner and should be removed by means of appropriate techniques.

2. GENETIC ALGORITHM
In 1970, John Holland proposed the Genetic Algorithm (GA). GA modeled on the process of natural selection for stressing

biological evolution is a stochastic search algorithm [17]. GAs has become substantial as they are formulated by promising search and optimization methods for complex engineering optimization problems. GA is used to grasp the intention of availability, allowing for installation and upholding expenses [19]. GAs are used for simulating the natural genetic operators in parallel with global search techniques [20].

Crossover and mutation are two frequently used genetic operators. Crossover is a mixing operator that combines genetic material from chosen parents. Mutation behaves as a background operator and is applied to find the unexplored search space by arbitrarily altering the values at one or more locations of the chosen chromosome [21]. Selection is a technique for choosing individuals (strings) for reproduction consisting with their fitness [22]. Genetic algorithm automatically obtains and stores the required knowledge related to the search space during its search process as Compared to that of the conventional search algorithms which requires certain external forces. Moreover, GE self-adaptively handles the whole search process by means of random optimization technique [23]. GA requires more memory but it works faster than the Simulated Annealing Algorithm [18].

Spacecraft Maximum Allowable Concentrations

SMACs provide guidance on chemical exposures during both normal as well as emergency operations in aboard spacecraft. Generally SMAC comprise of short term and long term, in short term SMACs the concentrations of airborne substances such as a gas and vapor does not comprises the concert of precise errands by astronauts during emergency conditions or cause severe toxic effects in long term SMACs are intended to avoid adverse health effects and to prevent any noticeable changes in the crews' concert under continuous exposure to chemicals for as long as 180 days

Data needed for developing the SMACs in Astronautically hygiene comprised of

- Chemical-physical characterization of the toxic chemical
- Animal toxicity studies
- Human clinical studies
- Accidental human exposures
- Epidemiological studies
- In-vitro toxicity studies
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3. RELATED RECENT RESEARCHES: A REVIEW

David C. Wedge *et al*. [9] have discussed that Electronic noses (e-noses) are increasingly being used as vapour sensors in a wide range of application areas. E-noses made up of arrays of organic field-effect transistors (OFETs) are particularly valuable due to the range and diversity of the information which they provide concerning analyst binding. Their study has demonstrated that arrays of OFETs, when combined with a data analysis technique using Genetic Programming (GP), can selectively detect airborne analysts in real time. The use of multiple parameters – on resistance, off current and mobility – collected from multiple transistors coated with different semiconducting polymers has given dramatic improvements in the sensitivity (true positive rate), specificity (true negative rate), and speed of sensing. Computer-controlled data collection allows the identification of analytes in real-time, with a time-lag between exposure and detection of the order of 4s.

Chatchawal Wongchoosuk *et al*. [10] have described a portable electronic nose (E-nose) which is based on hybrid carbon nanotube-SnO_2 gas sensors. The hybrid gas sensors have been fabricated using electron beam (E-beam) evaporation by means of powder mixing. The instrument has used feature extraction techniques including integral and primary derivative, which lead to higher classification performance as compared to the classical features (ΔR and $\Delta R/R0$). It was shown that the doping of carbon nano tube (CNT) has improved the sensitivity of hybrid gas sensors, while the quantity of CNT has a direct effect on the selectivity to volatile organic compounds, i.e., methanol (MeOH) and ethanol (EtOH). The real-world applications of this E-nose have also been demonstrated. Based on the proposed methods, this instrument can monitor and classify 1vol % of MeOH contamination in whiskeys.

Muhammad Rivai *et al*. [11] have presented a type of odor identification system, which combines gas chromatography (GC) and electronic nose techniques. The system comprises a GC column and a 10-MHz quartz crystal microbalance sensor producing a unique pattern for an odor in time domain. The proposed method has offered the advantages of substantially reduced size, interferences, and power consumption in comparison to existing odor identification system. Several odors of organic compounds have been introduced to judge the selectivity of the system. Principle component analysis method has been used to visualize the classification of each odor in two-dimensional space. The proposed system could resolve common organic solvents, including molecules of different classes (aromatic from alcohols) as well as those within a particular class (methanol from ethanol) and also fuels (premium from pertamax). The neural network can be taught to recognize the odors tested in the experiment with identification rate of 85%. Therefore, the system has taken the place of human nose, especially for poisonous odor evaluations.

Nowadays, electronic noses (E-nose) become popular in industry. There are a few types of E-noses which are used to detect odorant and gases such as surface acoustic wave (SAW) device, optical sensor, metal oxide semiconductors (MeOX), and carbon black polymer composite. Electronic nose is a device that can be mimicking biological human nose, which can detect and differentiate types of odorant. Fauzan Khairi Che Harun *et al.* [12] have focused on how to fabricate carbon black polymer composite gas sensor. In addition, constant current source circuit has been designed to act as interface circuitry so that the change of resistance when exposed to the gas can be observed via Lab VIEW. Besides that, the characteristics of each sensor have been observed and studied. This is to ensure the fabricated sensor gives the same responds with actual sensor. The result from the experiments has shown that the fabricated carbon black polymer composite gas has the potential to detect and respond just like the actual gas sensor.

Huichun Yu *et al*. [13] have proposed the potential of the electronic nose to monitor Longjing tea different grade based on dry tea leaf, tea beverages and tea remains volatiles was studied. The original feature vector was obtained from the response signals of the E-nose, and was analyzed by principal component analysis (PCA). To decrease the data dimension and optimize the feature vector, the front five principal component values of the PCA were extracted as the final feature vectors by PCA. The linear discrimination analysis (LDA) and the back propagation neural network (BPNN) were proposed to identify Long jing tea grade. The results showed that the discrimination results and testing results for the tea grade were better based on the tea beverages than those based on the tea leaf and the tea remains based on the new five feature vectors; both of the LDA and BPNN methods attain better discrimination for the tea grades based on the tea beverages and the analysis results of the two methods were accordance.

The e-nose technology has enormous potentialities for in site monitoring of off-odors. However a number of limitations are associated with the properties of chemical sensors, the signal processing performances and the real operating conditions of the environmental field. In order to appraise the time evolution of the sensors and the effect on the results of an electronic nose, experimentation has been performed during more than 3 years on two identical sensor arrays. The two arrays contain the same six Figaro sensors and are in the same sensor chamber of the e-nose system. Both arrays have worked continuously, without break. A.C. Romain *et al*. [14] have proposed technique which describes the drift of some TGS sensors for 7 years as well as the difference in the temporal behavior of identical sensors and the consequence on the e-nose results after the sensor replacement in the sensors array. A correction of the drift and of the replacement effect is applied and the classification results are exposed, with and without correction.

M. Castro et al. [15] have reported that the original design of a proposed type of electronic nose (e-nose) consisting of only five sensors made of hierarchically structured conductive polymer nanocomposites (CPC). Each sensor benefits from both the exceptional electrical properties of carbon nanotubes (CNT) used to build the conductive architecture and the spray layer by layer (sLbL) assembly technique, which provides the transducers with a highly specific 3D surface structure. Excellent sensitivity and selectivity were obtained by optimizing the amount of CNT with five different polymer matrices: poly (caprolactone) (PCL), poly (lactic acid) (PLA), poly (carbonate) (PC), poly (methyl methacrylate) (PMMA) and biobased polyester (BPR). The ability of the resulting e-nose to detect nine organic solvent vapours (isopropanol, tetrahydrofuran, dichloromethane, n-heptane, cyclohexane, methanol, ethanol, water and toluene), as well as biomarkers for lung cancer detection in breath analysis, has been demonstrated. Principal component analysis (PCA) proved to be an excellent pattern recognition tool to separate vapour clusters

Z. Haddi *et al*. [16] have proposed the potential of an electronic nose to differentiate the geographical origin of the Moroccan virgin olive oils based on their volatile profile was investigated. An electronic gas sensor array system composed of 6 metal oxide semiconductor sensors was used to generate a chemical fingerprint (pattern) of the volatile compounds present in olive oils. Multivariate statistical approach showed good discrimination between the classes of the 27-sample of the dataset population. The results of this study provide promising perspectives for the use of a low-cost and rapid system for the verification of geographical origin of the olive oils based on their volatile profile.

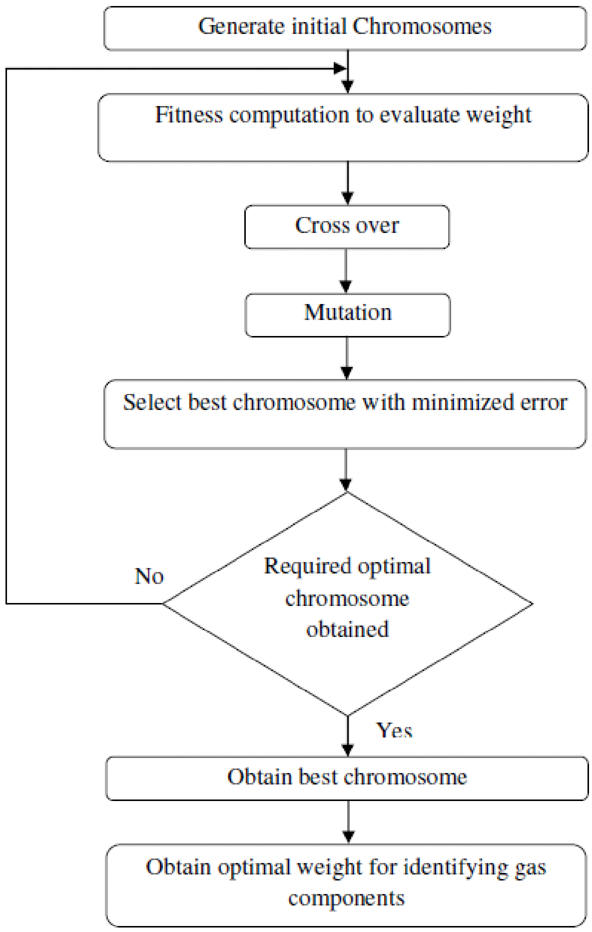
4. PROPOSED METHOD

In recent decades, electronic sensing techniques have significant progress in both the commercial and technical aspects. The term electronic sensing means the ability of reproducing human senses by sensor arrays and pattern recognition systems. E-Nose provides an industry-specific management solution for the continuous and real-time monitoring of environmental odor and air quality resulting in higher profit and improved community relations. In this paper we utilize genetic algorithm to compute the optimized weight. The upcoming sessions of this section clearly explain the progression in detail.

$$F(x_j) = c + \lambda_j \left(\frac{1}{1+\exp\left(1-\sum_{i=0}^{N-1} x_i \psi_{ik}\right)} \right) \qquad (1)$$

Where $F(x_j)$ = Fitness value; c = 0.5; λ_j and ψ_{ik} = Weights: x_i = i^{th} elements of fitness value.

4.1 Genetic Algorithm based Optimized Weight for Identifying Gas Components



4.1.1 Generation of Chromosomes

Initially, generate N_p number of random chromosomes each having N_s number of genes. The randomly generated chromosomes can be determined as shown in eqn (2)

$$W_s^{(k)} = \left\{\omega_0^{(k)}, \omega_1^{(k)}, \omega_2^{(k)}, \Lambda, \omega_{N_s-1}^{(k)}\right\} 0 \le k \le N_p - 1, \quad 0 \le s \le N_s - 1 \qquad (2)$$

Here, N_p - No of Chromosome, N_s - No of genes in Chromosome and $\omega_s^{(k)}$ represents the s^{th} gene of the k^{th} chromosome with generated values of in the range of $(0-1)$.

Fitness Computation

To compute the fitness, apply all the obtained weights from the eqn (2) and the obtained inputs (concentration value and SMAC) in to eqn (1). Here error minimization is the fitness function which is shown below

$$Err_e = (Ep - Md)$$
$$s = \sum_{m=1}^{N_m} Err_e^m$$
$$\mu = \frac{s}{N_m}$$

If min (μ)
Select the chromosome
End

Where, Ep – Experimental value; Md – model value ; Err_e - Error Element ; s- sum of error Elements ; N_e - No of Elements; μ - Mean of error elements which is also said to be Fitness.

From the above pseudo code, select N_x no of chromosomes to be applied with the genetic operation crossover, mutation.

4.1.2 Crossover and Mutation

Crossover and mutation are significant genetic operators of the genetic algorithm. Amid dissimilar types of crossover, the two-point crossover is engaged here at a cross over rate Cr_t. In the two-point crossover, two points are selected on the parent chromosomes by means of the equations (3) and (4). The genes in between the two points Cr_1 and Cr_2 are then interchanged between the parent chromosomes to obtain $N_p / 2$ children chromosomes. The crossover points Cr_1 and Cr_2 are determined as follows

$$Cr_1 = \frac{|W_s^{(k)}|}{N_s} \tag{3}$$

$$Cr_2 = Cr_1 + \frac{|W_s^{(k)}|}{N_s} \tag{4}$$

The child chromosomes are obtained and the mutation process is to be held on these chromosomes. This process is repeated until the minimized error is to be obtained regarding to threshold value, which is said to be the best chromosome and sort those sets in ascending order then evaluates them by means of its error value.

4.1.3 Selection of best Chromosomes

After the progression is completed $iter_{\max}$ number of times, the best chromosome is chosen from the obtained chromosomes. Here the best chromosome is the one that has the minimum error value. Then, the best chromosome's genes are sorted in the mounting order and the chromosome that has the minimum errors is selected as the best gene. Thus, by means of genetic algorithm the optimized weight for identifying gas components are adjusted

$$F(x_j) = 0.5 + \lambda_{j(best)} \left(\frac{1}{1 + \exp\left(1 - \sum_{i=0}^{N-1} x_i \psi_{ik(best)}\right)} \right) \tag{5}$$

From the process, we have obtained the optimal weights (eqn (5)) for the concern concentration range and the SMAC value inputs hence we identify the particular element through our work with the aid of the resultant value. By obtaining the proper weights that aid to obtain the mathematical model for the further process.

5. RESULT AND DISCUSSION

The proposed technique is used to formulate a mathematical model is genetic algorithm and was implemented in the working platform MATLAB. Initially blind mathematical model is generated by utilizing the experimental result and with the aid of genetic algorithm technique optimized weight is obtained which is used to compute the mathematical model and is said to be optimized mathematical model to identify the reference number to the corresponding components.

Table 1. Reference Table

Concentration range tested (ppm)	SMAC (ppm)	Reference number	Targeted compound
10 – 50	30	1	Benzene
10 – 130	2000	2	Ethanol
50 – 525	50	3	Freon
0.006 – 0.06	1	4	Indole
3000 – 7000	5300	5	Methane
10 – 300	30	6	Methanol
75 – 180	400	7	Propanol
30 – 60	16	8	Toluene
10 – 50	30	9	Ammonia
50 – 510	0.4	10	Formaldhyde

The obtained Experimental values are tabulated in the above tabular column with the aid of this tabular column only the whole mathematical model is generated

Table 2. Optimized Weight for Different Elements

Element	Concentration range Tested in (ppm)	1 hr SMAC (ppm)	Optimized weight		Fitness	Reference Number
			$\lambda_{j(best)}$	$\psi_{ik(best)}$		
Benzene	11 25 48	30	0.99688	0.294773	0.503121	1
Ethanol	15 89 111	2000	0.993428	0.142282	1.506572	2
Freon	55 222 500	50	0.99461	0.996881	2.50539	3
Indole	0.006 0.01 0.05	1	0.998595	0.92621	4.011204	4
Methane	3500 5000 6500	5300	0.998143	0.633544	4.501857	5
Methanol	18 150 298	30	0.999669	0.10604	5.501906	6
Propanol	80 155 175	400	0.996463	0.279633	6.503537	7
Toluene	35 50 55	16	0.993736	0.63315	7.506264	8
Ammonia	15 35 55	30	0.994016	0.391825	8.505984	9
Formaldhyde	55 350 500	0.4	0.998937	0.432619	9.501063	10

In the table 2 various range of compound values are utilized to test the generated mathematical model from this we obtained optimized weights $\lambda_{j(best)}$ and $\psi_{ik(best)}$, fitness value and their correspondent reference value for the components which are all clearly tabulated in the above table 2

True positive: An element 'A' is identified as A.

False positive: Another element 'B' is identified as element A.

True negative: Element 'B' is identified as element B.

False negative: Element 'A' is identified as some other element B.

Where

A- Target Element.

B- Other Element.

$$Sensitivity = \frac{Number\ \text{of True Positives}}{\text{Number of True Positives} + \text{Number of False Negatives}} \quad (6)$$

$$Specificity = \frac{Number\ \text{of True Negatives}}{\text{Number of True Negatives} + \text{Number of False Positives}} \quad (7)$$

$$Accuracy = \frac{(\mathrm{TP}+\mathrm{TN})}{\mathrm{TP}+\mathrm{TN}+\mathrm{FP}+\mathrm{FN}} * 100 \quad (8)$$

$$False\ Positive\ Rate\ (FPR) = \frac{\mathrm{FP}}{\mathrm{N}} = \frac{FP}{(FP+TN)} \quad (9)$$

$$Positive\ \text{Predictive Value}\,(PPV) = \frac{TP}{(TP+FP)} \quad (10)$$

$$Negative\ \text{Predictive Value}\,(NPV) = \frac{TN}{(TN+FN)} \quad (11)$$

$$False\ \text{Discovery}\ Rate\ (FDR) = \frac{FP}{(FP+TP)} \quad (12)$$

$$Mathews\,\text{CorrelationCoefficient}(\mathrm{MCC}) = \frac{(\mathrm{TPTN} - \mathrm{FPFN})}{\sqrt{\mathrm{PNP'N'}}} \quad (13)$$

Table 3. Performance Analysis for the Proposed System with Different Elements

Component	TP	TN	FP	FN	sensitivity	FPR	accuracy	Specificity	PPV	NPV	FDR	MCC
Benzene	5	1	0	4	56	0	60	100	100	20	0	30.4
Ethanol	8	1	0	0	100	0	100	100	100	100	0	94.3
Freon	4	2	1	3	57	33.33333	60	67	80	40	20	19.9
Indole	7	1	0	0	100	0	100	100	100	100	0	93.5
Methane	8	1	0	1	89	0	90	100	100	50	0	62.9
Methanol	10	1	0	1	91	0	92	100	100	50	0	64.3
Propanol	11	1	1	1	92	50	86	50	92	50	8	41.7
Toluene	12	1	0	0	100	0	100	100	100	100	0	96.1
Ammonia	7	2	1	0	100	33.33333	90	67	88	100	13	72.0
Formaldhyde	8	1	0	0	100	0	100	100	100	100	0	94.3

Receiver Operating Characteristic

ROC (Receiver operating characteristic) is the graphical representation drawn between True Positive and False Positive, False Positive rate is plotted in the X axis and True Positive rate is plotted in the Y axis which is showed in the below graphical format. The graph which laid out of the Y axis (i.e.) True Positive rate represent that the Specificity values does not meet the targeted output.

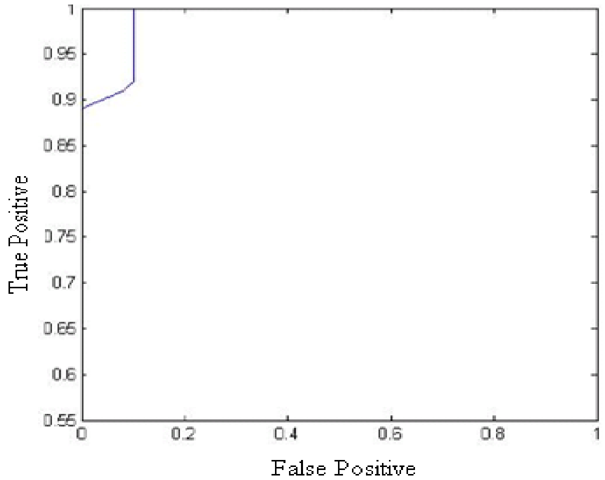


Fig.1 (Performance analysis of true positive and false negative)

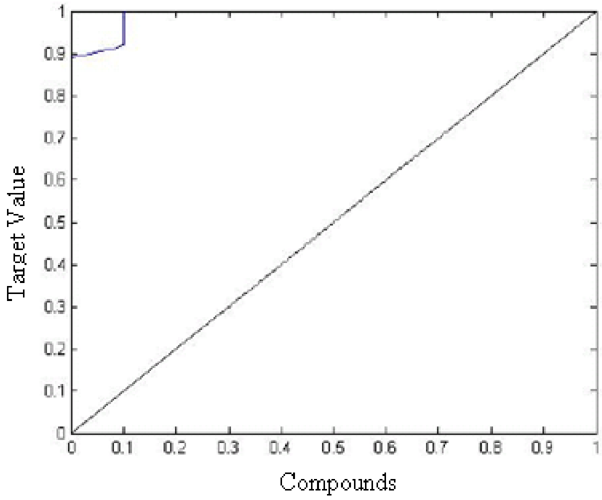


Fig. 2 (Performance analysis of true positive false negative with respect to targeted value)

In the above graph the targeted values and the compounds in the x-axis and y- axis were plotted respectively, from that we obtained graph as linear. The aforementioned graph clearly explained the difference in targeted value and the experimented result

6. CONCLUSION

An effective system has been proposed to identify an element with the aid of a mathematical model For generating a mathematical model a blind eqn (1) is utilized and with the aid of the experimental value an optimized weight is generated using genetic algorithm once the optimized weight is identified then that optimized weight is applied in the generated mathematical model. In the evaluation process different concentration range and the SMAC values are inputted to identify the element. Hence with the aid of the concentration range and the SMAC value the reference values is obtained with this reference value correspondent compound are identified in an unknown environment

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10. AUTHOR'S PROFILE

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