Describing Non-selective Gas Sensors Behaviour via Logical Rules

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Abstract - **This work presents an ongoing research aimed at interpreting the responses of non-selective gas sensors (such as metal oxide resistive ones) in terms of simple IF THEN rules. In particular, it is shown how a logical combination of the output of three extremely low-cost sensors, namely MQ131, MQ136 and TGS2602, can be arranged to produce IF THEN inferences able to discriminate among CO, SO_2 and NH_3 emissions. The outcome is quantitatively similar to that obtained with high-selective and costly chemical sensors. The experimental results, albeit grounding on an empirical base, seem to support the idea that smart compositions of low-cost sensors are able to manifest surprising discrimination abilities.**

Keywords - gas discrimination, low-cost sensors, IF THEN rules.

I. INTRODUCTION

Electronic noses are progressively disseminating throughout both the business-to-business and business-to-consumer market for the number of application domains they spawn. Alcohol testers, air quality monitoring stations [1] food ripeness detectors [2] and even lung cancer sniffers [3] are all examples of this progression. The total cost of such devices is made of two chief components: signal acquisition, processing and transmission unit on the one hand and sensing unit on the other. The latter may significantly affect the final price when high-selective responses, precise and accurate performances are required. Of course, choosing cheaper solutions entails a conundrum.

Low-cost oxide-based resistive sensors are well known to be sensitive to a wide spectrum of gases and air contaminants (this, in principle, is not a drawback); however, their selectivity is generally low [4] thus providing an ambiguous response in terms of individual components of the gas mixtures. Consequently, if high selectivity is needed by the application, the only commercially available option is to buy extremely expensive sensors.

This work presents some empirical results aimed at validating the following hypothesis: it is possible to discriminate among different gas emissions by logically combining the output of low-cost sensors appropriately. The outcome should be as much close as possible to that obtained by employing high-selective and costly chemical sensors.

Therefore, wide-spectrum sensitivity is turned into an advantage because it allows one to provide a multi-detection device at extremely low-cost. Commercial prototyping of this kind of device is currently involving the set of three sensors MQ131, MQ136 and TGS2602 to discriminate among CO, SO_2 and NH_3 emissions.

Paper layout is organized as it follows. Section II overviews the principal approaches published in the literature to tackle with gas discrimination problems. Section III presents two different approaches to gas discrimination, i.e., classification and disambiguation; the latter is used in this paper and analyzed from the perspective of logics. Then, the experimental setting and the proposed approach are described in Section IV; finally, conclusions are drawn in Section V.

II. RELATED WORK

Several techniques have been proposed in the literature to address the problem of low selectivity in low-cost sensors. With reference to tin oxide chemical sensors, two typical measurement strategies are employed [5]: multi-sensor arrays or dynamic measurements based on a single sensor. The latter mainly includes modulation in operating temperature by pulsed or oscillated heating.

A lot of works can be found on temperature modulation in semiconductor gas sensing [6-8]. The modulation is well known to provide more information than static measurement with a mode of a constant operating temperature. Sears et al. [9] suggest several advantages that can arise from the application of a heating voltage pattern. Among all, due to the different reaction rates of various analyte gases at different temperatures, a cyclic temperature variation can be used to characterize unique signatures for each gas.

Unfortunately, temperature modulation requires an intense (hence expensive) pre-calibration phase because of different kinds and patterns of temperature modulation that have to be tried in order to minimize cross-sensitivity effects. For this reason, some sort of signal post-processing is generally applied.

Signal processing attempts to extract information hidden in raw data attenuating the effect of the different sources of noise that can occur during measurements such as cluttered or dynamic background [10]. In [11], a systematic approach for automatic signal processing, evaluation and optimization of gas sensors with temperature cycles is proposed.

In very recent times, signal processing has been coupled with multi-array sensor setups. Initial promising results for example have been obtained in real-time breath monitoring applications with micro-sensor arrays [12]. In that case, the

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signal processing technique is based on standard statistical dimensionality reduction and classification algorithms.

Other approaches employ gray-box models for predicting metal oxide sensor response as in [13]; in this case selectivity enhancement is reached thanks to parametric models. This, however, requires a specific knowledge of the underlying electrochemical and thermodynamic aspects.

III. DIFFERENT APPROACHES TO GAS DISCRIMINATION

The problem of correctly attributing low-cost sensor response to one gas from the list of the putative ones can be handled from multiple perspectives. Two of these are considered in the following: classification and signal disambiguation.

A. Classification-based approaches

In principle, the task of assigning a class label to a pattern can be viewed as a classification problem [14], hence the expected output is a classifier that minimizes inter-class and intra-class distance. However, several riddles hinder the correct classification of gases when low-cost sensors are employed. For example: provided timesheets often show an underestimation of the number and the range of sensed gases; furthermore, sensor drift determines non-steady behavior even when similar emission stimuli are supplied thus invalidating the calibration phase.

A high desirable condition is that function boundaries allow for proper discrimination among output classes. In other words, linear separability should be always pursued to avoid misclassification.

Starting from the work of Rumelhart and McClelland [15] it is well-known that 3-layer feed-forward networks are capable of forming any possible complex decision boundary (the so-called property of 'Universal Approximation'). For this valuable property, a number of reference works in the literature applying neural networks as a computational tool for gas discrimination [16][17][18][19][20][21].

Notwithstanding, linear separation of data in case of gas mixtures can be hardly obtained. In fact, to achieve perfect classification, all the possible concentration combinations should be exploited, which is impractical and in contrast with the objective of an affordable sensor price, at least from the manufacturer's point of view. For this reason, metal oxide sensors seem unable to produce a true quantitative information of gaseous concentrations, especially in normal operating conditions.

B. Disambiguation-based approaches

In a recent paper [22], the problem of cross-sensitivity has been accounted from a different viewpoint. It has been considered as a disambiguation process driven by algorithmic rules that come from the observation of the sensor datasheets and simple hypotheses on sensor behavior. The basic idea grounds on the hypothesis that, if the same gas is actually measured by two or more sensors, then their estimated concentrations will be similar, with an accuracy related to the number of concordant sensors. The same consideration can be drawn for every possible gas detected by the sensors so that a simple ranking strategy is applied. If the level of agreement among sensors about a supposed measured gas is above a certain confidence threshold, then the gas is considered to be a good candidate for the disambiguation process.

C. Blending classification and disambiguation approaches

The current paper tries to take benefit from the two above-mentioned approaches of gas discrimination as either a classification or disambiguation problem. The proposed one deals in fact with both separability (hence classification) and semantics (hence disambiguation). To achieve this goal, logical combinations of the output of three extremely low-cost sensors are employed. They represent a simple means to characterize sensor behaviors in intuitive linguistic terms, as it happens with fuzzy logic [23] descriptions. In the following, the proposed approach is presented in more detail.

IV. PROPOSED LOGIC-BASED APPROACH

It is fair to assume that any empirically-driven scientific methodology is based on the following steps:

1. observations and pre-processing (i.e., of measurable signals);
2. theoretical hypothesis formulation from observations;
3. consequent hypothesis validation;
4. theory formulation (hypotheses become verified rules);

If applied with care (possibly after several iterations) the steps above should lead to some verifiable (inductive) inference (i.e., a theory) about the phenomenon under scope. Hence, the result is a *description* of the analyzed phenomenon after some kind of classification and validation phase. It is noteworthy that none of the traditional Computational Intelligence [24] techniques such as neural networks or fuzzy logic seem to provide a complete coverage of all the previous points at the same time.

In [25], a heuristic for extracting IF THEN rules form signal measurements has been presented with reference to temperature time-series analysis. In this paper, the same heuristic is used for gas discrimination.

IF THEN rules are widely used in expert systems [26] for representing knowledge in a structured and logical way; their application to the field of sensor measurements is indeed quite a novel engagement in the literature.

The obtained rules are considered as "self-descriptors" of the observed signals since they manifest knowledge in the form of logical implications built upon numerical hypotheses on the input data without any external knowledge source available. Although quite at an early stage, this simple methodology has a relevant aspect: the output (i.e., rules) is built over the same alphabet of the input space (signals) by means of numerical hypotheses. Alternatively speaking, input-output mapping is performed through measurable hypotheses. At the end of the validation process, verified hypotheses become IF THEN rules, hence they provide a (logical) description of the observed input.

Since such methodology is general, it can be employed for gas discrimination, which is the aim of this paper. Consequently, numerical hypotheses applied over low-cost

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gas sensor output signals can be used to infer on the kind of gas actually being sensed. In other words, given *N* sensors as input, the expected output should be a set of IF THEN rules of the type:

IF $hyp(sensor_1)$ **AND** $hyp(sensor_2)$ … **AND** $hyp(sensor_N)$

THEN gas_x **OR** gas_y … **OR** gas_z *are being measured*

where hyp() is a predicative function defined as follows:

$$hyp(sensor_x) = \begin{cases} 1 & \text{if hyp is verified for sensor } x \\ 0 & \text{otherwise} \end{cases}$$

A pictorial representation of the proposed approach is drafted in Figure 1.

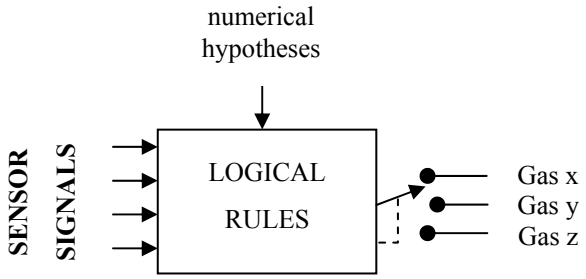

Figure 1. Conceptual schema of the proposed approach.

A. Experimental setting

The experimental setting has been built around three extremely low-cost sensors (see Figure 2 for more details), namely: Hanwei MQ131 and MQ136, Figaro TGS2602.

In all these sensors, the sensing material is a metal oxide semiconductor (generally tin oxide). When the sensing layer is heated at a certain temperature in the air, oxygen is adsorbed on the crystal surface with a negative charge. As quoted in [6] by withdrawing electron density from the semiconductor surface, adsorbed oxygen gives rise to Schottky potential barriers at grain boundaries, and thus increases the resistance of the sensor surface. Reducing gases decrease the surface oxygen concentration and thus decrease the sensor resistance. The overall process causes a decrease in the resistance R_s of the sensing layer that can be measured against a standard value R_0 gathered at optimal test condition. Sensor datasheets are given as R_s/R_0 values against part-per-million (ppm) concentrations.

Experiments have been carried by directly exposing the device acquisition unit to small quantities of different gaseous contaminants. Emissions have been produced in sequence to stimulate subgroups of the chosen sensor triplet. Emissions have been the following: first, carbon monoxide (CO); second, sulfure dioxide (SO_2); third, a mix of the first two ($CO+SO_2$); fourth, ammonia (NH_3).

Actually, we purposely did not use any test chamber for the experiment since our objective was mainly to discriminate among classes of emissive phenomena rather than exactly computing the ppm values of the induced gases. All emission events have been tagged with a timestamp. This assured a correct synchronization between the emitted gases and the observed sensor responses.

B. Pre-processing

A brief sequence of pre-processing steps has been applied over raw data, namely: 1) normalization; 2)extraction of the first derivative; 3) extraction of the absolute value.

In the normalization step, the dataset is transformed so that each signal is brought at mean zero with unary standard deviation. This allows for comparing the dynamics of the signals on the same scale. The consequence is the loss of absolute values, which is however outside the scope of the paper and is left to a future work on the subject.

In the second processing step, sensor dynamics is emphasized by considering the first derivatives as relevant features in the signal characterization process.

In the last processing step, absolute values obtained from the previous step are taken, so that oscillatory behaviors of the first derivatives are eliminated.

The effect of the three processing steps on input data is displayed in Figure 3.

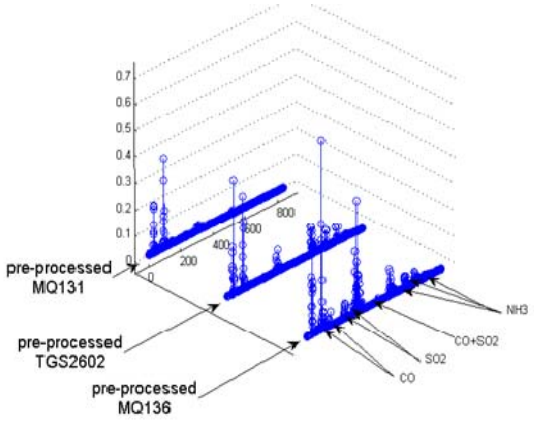

Figure 3. Synopsis of the three signals after all the pre-processing steps.

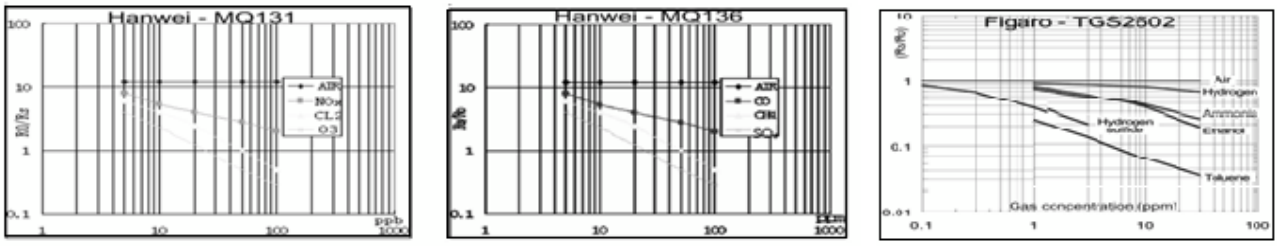

Figure 2. Datasheet of the employed sensors.

C. Defining numerical hypotheses over the dataset

After the pre-processing step, data are given in input to the logical block for gas selection.

Logical rules are defined by means of numerical hypotheses on data, as discussed above. The chosen hypothesis is a very simple one: it is defined by the following function:

$$hyp\big(datum(k)\big)=\begin{cases}1 & \text{if datum}(k)\geq\vartheta\\ 0 & \text{otherwise}\end{cases}$$

where datum(k) is an input sample at time k and θ is a parametric threshold.

It is interesting to note that, depending on the value of θ, hypotheses can be true or false, i.e., below or above certain levels the hypothesis function may switch from one logical state to another. This means that an IF THEN rule of the type defined above can be verified only in certain subsets of the dataset.

Furthermore, it is important to stress that the logical state (true or false) is obtained only by means of *measures*, without explicitly knowing the analytical form of the underlying datum function. This allows for analyzing, in principle, any given measurable signal.

Parameter θ provides one degree of freedom to the definition of the logical block. Of course, more than one parameter can be considered; however, for the sake of simplicity, only one parameter is taken in this paper.

D. Finding the best parametric configuration

The choice for optimal θ has been led by the estimation of another parameter, referred to as the *coverage index* (CI).

The coverage index of an IF THEN rule is simply defined as the number of samples where the rule is verified divided by the dataset cardinality. In formulae:

$$\mathrm{CI}(Rule_i)=\frac{\#\text{samples where } Rule_i \text{ is verified}}{|\,\text{Dataset}\,|}$$

Similarly, the *total coverage index* (TCI) represents the fraction of samples in the dataset covered by at least one of the IF THEN rules representing the knowledge base.

TCI varies from 0 (no rule) to 1 (when rules completely partition the dataset). TCI can be reckoned by means of the following formula:

$$\mathrm{TCI}(KB)=\sum_{i=1}^{|KB|}\bigcup_{\text{Dataset}}\mathrm{CI}(Rule_i)$$

There can be samples in the dataset firing more than one rule; this means that there can be rule activation patterns that partially or totally overlap over the dataset.

Our attempt was to empirically find the minimum number of rules (depending on parameter θ) with the total coverage index closest to 1. For this to be achieved, an iterative procedure has been run varying the value of θ. Good results have been found for θ = 0.3 with TCI=1 obtained by means of the four rules expressed in Table 1, while an image showing all four rules activation patterns is framed in Figure 4.

TABLE I. LOGICAL RELATIONSHIPS FOUND AMONG SENSORS WITH THRESHOLD PARAMETER = 0.3. N.A. STAYS FOR NOT AVAILABLE. A MINUS SIGN IN APEX INDICATES LOW CREDIBILITY

Rule ID	KNOWLEDGE BASE (for θ=0.3)							
	IF STATEMENT			THEN STATEMENT				CI %
	MQ 131	TGS 2602	MQ 136	SO_2	NH_3	CO	other	
1	F	F	T	T	T^-	T^-	N.A.	4.9
2	F	T	F	N.A.	T	N.A.	N.A.	1.4
3	T	T	T	N.A.	N.A.	T	N.A.	2.7
4	F	F	N.A.	T	N.A.	N.A.	T	93.7

Each row from Table I represents a true IF THEN rule. Antecedents (i.e., arguments of the IF statement) are hypotheses on samples coming from sensors; consequents (i.e., arguments of the THEN statement) are True/False values over the hypothesis that a certain gas is actually being sensed. These last hypotheses have been verified in a supervised manner by windowing the emission events around the tagged timestamp of the experiment phase. For any given rule, if the number of firing events in the window of a gas emission was too low (less than 5% of the window length) then the predicate variable was considered insensitive to that gas. If the number of firing event was comprised between 5% and 50% of the window length, then the predicate value was assigned a low credibility.

To be more clear, the first row of Table I represents the following statement:

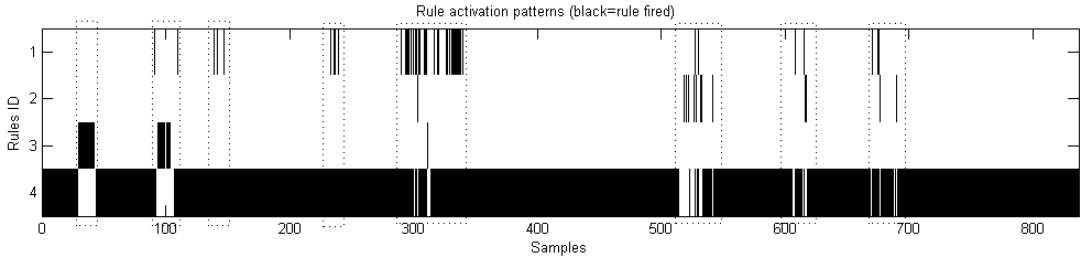

Figure 4. Rule activation patterns (rules correspond to logical relationship reported in Table I).

Rule 1:

IF MQ131< 0.3 **AND** TGS2602< 0.3 **AND** MQ136 >= 0.3

THEN SO_2 **OR** NH_3 **OR** (with low credibility) CO (with low credibility)

This means that every time the (preprocessed) values of MQ131 and TGS2602 are below 0.3 and those of MQ136 are above or equal to 0.3 then all the three gases are possibly being sensed: SO_2, NH_3 or CO, having the latter two cases a low credibility.

Rules may also provide very poor pieces of information like in **Rule 4:**

IF MQ131< 0.3 **AND** TGS2602< 0.3

THEN SO_2 **OR** something unknown

where the interpretation is that if both MQ131 and TGS2602 values are below 0.3 then *either* we are in presence of SO_2, *or* we are not capable of ascribing sensor behavior to one of the considered gases.

Of course, having multiple gases in output is not a desirable condition since it represents an ambiguous response. Notwithstanding, disambiguation can be partially dealt with by means of simple considerations.

E. Disambiguating sensor response

Rule 2 and 3 account respectively for NH_3 and CO. This means that they do not need further disambiguation. If we want our system to be able to detect also SO_2 emissions, some kind of rule post-processing has to be carried out. In particular, Rule 1 can be simplified assuming to disregard NH_3 and CO response due to their low credibility.

Of course, this is only an empirical approach aimed at showing the problem of disambiguation at a coarse scale. More formal approaches go beyond the scope of the paper; for example, the reader may refer to a previous work [22].

F. Testing results with high-cost chemical sensors

For testing purposes, the discrimination abilities of the logic block has been compared with the output of high-cost chemical sensors. In particular, two SensoriC sensors for CO and SO_2 detection respectively have been used for this aim. These two sensors are approximately between one and two orders of magnitude more costly than the low-cost ones. Their response to the events of CO and SO_2 is depicted in Figure 5.

G. Dataset heteroschedasticity

In order to have a further estimate of the inner correlation among sensors, dataset heteroschedasticity (i.e., the property of measured samples to represent a population with equal variance) has been assessed through the Barlett's test [27]. The test, computed on raw data coming from the triplet, has shown that (with reference to the proposed experiment) the number of dimensions necessary to explain the non-random variations in data is 3. The same result has been obtained by means of the principal component analysis [28].

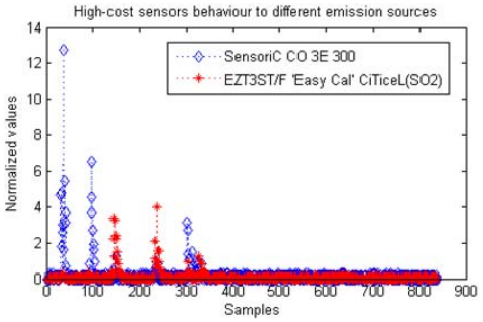

Figure 5. Rule activation patterns
(rules correspond to the logical relationships reported in Table I).

This assessment defines the putative minimum number of IF THEN rules needed to best explain our data. As shown before, four IF THEN rules were empirically found.

H. Theoretical aspects and future developments

Since IF THEN rules are logical statements, they guarantee logical coherence in their respective domain of validity. For example, assuming that "IF A AND B THEN C" is true in a certain interval, this implies that, in the same interval, "IF A AND B THEN NOT C" cannot be verified. In other words, the proposed logical approach to signal interpretation, provides a coherent framework for gas discrimination.

Another key point, is the type of numerical hypothesis to apply over incoming data. For the sake of simplicity, only one parameter has been used for tuning purposes. However, it is fair to assume that, the more parameters used, the more discriminatory the type of rules found.

Starting from these observations, it is interesting to note that the proposed approach stays amid a wide number of fields, such as measurements, computational intelligence, logics. Measurements become valuators of hypotheses over data, thus allowing for a jump from the numerical world to the logic-symbolic one.

V. CONCLUSION

In this work, the novel hypothesis of logically combining low-cost metal oxide sensor responses by means of IF THEN inference rules has been presented for gas discrimination purposes. Observational experiments have been made to support this claim. In particular, it has been shown how a triplet of low-cost sensors (namely, MQ131, MQ136 and TGS2602) is sufficient for discriminating three different classes of emissions (CO, SO_2 and NH_3).

This paper is built upon the theoretical and practical expertise gained from previous works in the mixed fields of measurement and computational intelligence. As far as the electrochemical and thermodynamic aspects are concerned, a temperature-humidity calibration phase was performed digitally on raw data basing on the available MQ131, MQ136 and TGS2602 datasheet information and using high-sensitivity temperature and humidity sensor output as ground-truth reference. As for the information processing aspects, the computationally-lightweight rule extraction

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mechanism presented in [25] allowed for producing a coherent knowledge base with a very small number of valid rules (four in our case). Since the obtained rules are *logical*, when they account for conflicting behaviors, this means that they certainly do not occur in the same sampling time.

To cap it all, the noteworthy principle behind our proposal is that gas discrimination abilities gained with low-cost sensors can be surprisingly similar to that obtained with high-cost counterparts. This idea, although grounding by now only on an empirical base, seems to open a promising perspective in the research field of both measurements and intelligent information systems.

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