Sensor Evaluation in a Breath Analysis System

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***Abstract*—Breath analysis systems contain arrays of correlated chemical sensors. For such systems, sensor selection is needed. From the process of sensor selection, some insight behind the performance of different sensor arrays can be gotten. Thus, we can know more about the sensors, which could help us with the selection work in turn. In this paper, a breath analysis system for diabetes diagnosis with 16 sensors is described. Based on this system, several methods are proposed to evaluate the importance, unique discriminant information and redundancy of each sensor. They are based on the results of exhaustive sensor selection. These methods are made convenient to observe and draw intuitive conclusions. They are applied to the breath analysis system and some useful discoveries about the sensors in the system are made accordingly.**

Keywords—chemical sensor; sensor evaluation; breath analysis; diabetes diagnosis; e-nose

I. INTRODUCTION

An electronic nose (e-nose) is an instrument that combines gas sensor arrays and pattern analysis techniques for the detection, identification, or quantification of volatile compounds [1]. Generally, e-noses contain a set of chemical sensors responding to various gases with different sensitivity. There could be large correlationship among the responses of the sensors, thus some sensors are redundant. Removing the useless sensors can not only improve the performance of the classifier, but also reduce the cost of the device [2].

Researchers have developed many techniques to select useful sensors from the original sensor array. Yin et al. [3] used Wilks lambda-statistic coupled with elimination transform to pick sensors with high discriminant ability. Bag et al. [4] applied a rough set-based approach which could simultaneously classify the data as well as optimize the array. In [5], the authors tried to utilize neural network sensitivity analysis for this task. Linear discriminant analysis (LDA) based sensor selection technique had also been proposed to estimate the contribution weight of each sensor, followed by subset selection [6]. Traditional method such as genetic algorithm (GA) was also a good choice [2].

All of these methods have succeeded in providing optimized sensor arrays with higher accuracy and smaller size. Many of them could also estimate the importance of each sensor by either weights or an order of sensors [3-6]. However, these importance indices do not have clear meanings. Sometimes questions such as "how much the accuracy will improve by adding this sensor" may be raised. Besides, we may also be interested in the inter-relationships between sensors, e.g. "given the presence of sensor S2, how much will the accuracy change by adding sensor S1?" "Does sensor S1 have very similar performance to S2?" From the answers to these questions, useful messages can be inferred about the importance, unique discriminant information and redundancy of the sensors in our prediction task. These messages help us to select better array in turn.

To answer these questions, a direct and reliable way is to analysis the results of an exhaustive search among all possible sensor combinations. For an e-nose with N sensors, the number of experiments to carry out during searching is 2^N-1. For example, if N = 13, the experiment number is 8191. In fact, this number is affordable for modern computers if the time cost for each experiment is not too much. This exhaustive searching method is suitable for the cases in [4-6], since the e-noses have no more than 13 sensors. This method can also ensure to select the optimal array.

In this paper, we propose several techniques based on exhaustive searching to evaluate the sensors so as to infer their importance, unique discriminant information and redundancy. The experiments are carried out with a breath analysis system. It has 16 sensors to measure the volatile organic compounds (VOCs) in breath. 167 breath samples from healthy subjects and 151 from diabetics have been collected. This dataset is used to test the sensor evaluation methods. Several useful conclusions will be drawn after the evaluation.

The remainder of this paper is organized as follows: Section II describes the breath analysis system in detail; Section III introduces the idea of our sensor evaluation methods. The analysis results and a few discussions will be provided in Section IV. Section V concludes the paper.

II. SYSTEM DESCRIPTION

The proposed breath analysis system includes a device to measure breath and a set of data analysis algorithms. In this section, we will first introduce the framework of the breath analysis device. The key part of the device, the sensor array, will be described next. After that the process of breath collection and measurement will be shown. Finally, a brief introduction will be given about the data analysis algorithms.

A. Framework of the Device

Fig. 1 shows the main framework of the breath analysis device. The gas sensors in our sensor array include an electrochemical ammonia (NH3) sensor, a photo ionization

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detector (PID) sensor and 12 metal oxide semiconductor (MOS) sensors. The MOS sensors work in a relatively high temperature which is not suitable for the NH3 and PID sensors, so separate small gas rooms were made for the NH3 and PID sensors. Breath or fresh air is drawn from outside and pumped into the gas rooms by a micro vacuum pump. According to our experiments, the contamination and carryover in the pump is negligible.

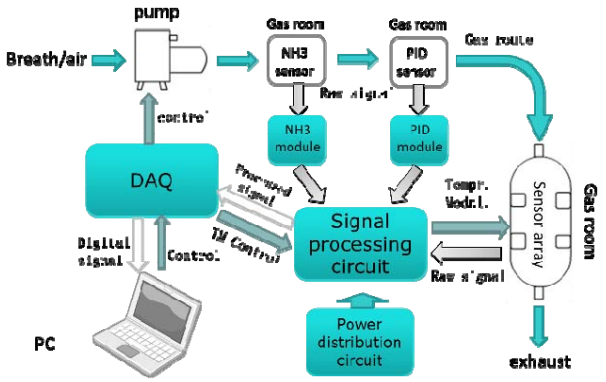

Fig. 1. Main framework of the proposed device.

The gas passes the gas room for the NH3 sensor, the PID sensor and the MOS sensors successively. It is worth noting that instead of the common box-shaped gas chamber, we designed a column-shaped gas chamber for the 12 MOS sensors, see Fig. 2. The internal shape of the chamber is cylindrical so as to allow gases to flow smoothly. The external shape is hexagon, which is convenient for the fastening of the sensor modules. The sensors are embedded on the six facets of the chamber. In this design, the gas concentration on the head space of each sensor is similar, and the size of the chamber is miniature.

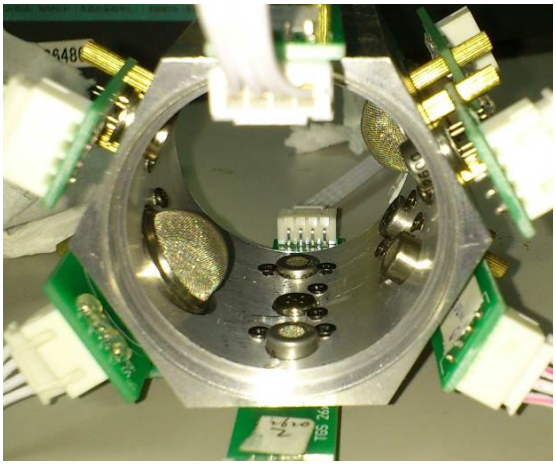

Fig. 2. A snapshot of the column-shaped gas chamber.

The signal of the NH3 and PID sensors are transmitted to the signal processing circuit through transmitting modules. The signal processing circuit magnifies and filters the responses of all the sensors. Finally, a data acquisition card digitizes the processed signals and transmits them to a computer using a USB cable. On the other way round, the computer sends control signals to the data acquisition card to control the on/off of the pump and the modulation voltage of the temperature modulated sensors. The whole device is powered by a 12V power adapter. The power is sent to each unit by a power distribution circuit.

B. Sensor Array

There are 16 sensors in our device. Besides the NH3 sensor, the PID sensor and the 12 MOS sensors, a humidity sensor and a MEMS mass flow sensor are also utilized. Table I is a list of these sensors. When choosing these candidate sensors, we focused on commercially available sensors because they are easier to acquire, more robust and have a good variety. The diversity of the candidates were augment by choosing sensors from different companies and of different types, sensitive spectrums and measurement ranges. We also paid attention to choose some sensors that have higher sensitivity to our target compounds such as acetone. Our references included sensor datasheets and previous studies [6, 7].

TABLE I. DETAILED SENSOR INFORMATION

No	Model	Function	Range	Company
1	D6F-P0001A1	Gas mass flow rate	0-100 (mL/min)	Omron Inc. Japan
2	NH3 3E 100 SE	NH3	0-100 (ppm)	City Inc. UK
3	piD-TECH 200	VOCs	1-200	Baseline-Mocon Inc. USA
4	TGS826	NH3, VOCs	30-300	Figaro Inc. Japan
5	TGS2610D	VOCs, H2	500-10000	
6	TGS2602	VOCs, NH3, H2S	1-30	
7	TGS2600-TM	H2, VOCs, CO	1-100	
8	GSBT11	VOCs	1-1000	Ogam Inc. Korea
9	TGS2602-TM	VOCs, NH3, H2S	1-30	Figaro Inc. Japan
10	WSP2111-TM	VOCs, H2	5-40	Winsen, China
11	WSP2111	VOCs, H2	5-40	
12	HTG3515CH	Humidity	10~95 (RH%)	Humirel Inc. France
13	TGS2610C	VOCs, H2	500-10000	Figaro Inc. Japan
14	TGS822	VOCs, H2, CO	50-5000	
15	TGS2600	H2, VOCs, CO	1-100	
16	SP3S-AQ2	VOCs, H2, CO	1-1000	FIS Inc. Japan

Temperature modulation (TM) is a way of using the MOS sensors. Instead of giving the sensors a constant heating voltage as usual, this method periodically modulates the heating voltage. It has been proved that this method can increase the discriminability and selectivity of MOS sensors [9]. Although it has been used a lot to classify different chemicals, TM has never been applied in breath analysis systems. So three MOS sensors in our array (TGS2600, TGS2602 and WSP2111) were copied, with one copy of each

sensor operated under TM. We wish to explore if they would outperform the original ones. In Table I, the suffix "-TM" indicates that the sensor is a temperature modulated sensor.

Sampling Procedure

When collecting the breath sample from either a healthy or a diabetes subject, he/she is asked to exhale into a 600 mL Tedlar® gas bag through a disposable mouthpiece. After that, the gas bag is plugged onto the connector of the device to let the software control the device to finish the measurement of the breath. The measurement consists of 4 stages, including:

1) *Baseline stage (1 s):* The baseline values of the sensors are recorded for future data preprocessing.
2) *Injection stage (7 s):* The pump opens, breath is drawn from the gas bag to the gas room at a constant speed.
3) *Reaction stage (56 s):* The pump is off, the sensors continue reacting with the gas particles.
4) *Purge stage (80 s):* The pump opens again, fresh air is drawn into the gas room to push the breath gas out.

Data Analysis

In this paper, sensors are evaluated based on their performance on the task of classification between healthy and diabetes samples. Before classification, the samples need to be preprocessed first. The preprocessing is made up of 3 steps: baseline removing, gas amount compensation and humidity compensation. For each of the chemical sensors, the baseline value is estimated by its average response in the baseline stage. Then it is subtracted from the response of the corresponding sensor. Gas amount and humidity compensation is used to compensate the fluctuation of gas amount and humidity among samples. First, several acetone samples were collected with different gas amount and humidity. Then two linear models were built to describe each sensor's dependency on gas amount and humidity, respectively. Finally the breath samples were compensated using these models and the responses of mass flow sensor and humidity sensor in the samples. The details of the compensation algorithm can be found in [10].

Next, principle component analysis (PCA) is used to extract a smaller set of features from the preprocessed responses of 14 chemical sensors (except the mass flow sensor and the humidity sensor). A critical coefficient of PCA is the ratio of variance that can be explained by the extracted features. In this paper, the ratio is set to be 99.99%. Finally, support vector machine (SVM) with a Gaussian kernel is adopted to do the final classification. Details of these algorithms can be found in many related papers or textbooks.

III. Sensor Evaluation Methods

Cumulative Sensor Importance

Many sensor selection algorithms are capable of giving each sensor an estimation of importance/weight/contribution. For example, the estimation may come from some intermediate values of the classifier [5, 6]. However, if the prediction accuracy of every possible sensor array is available, we can get a more reliable importance evaluation. The question is, how to evaluate the sensor importance from these accuracy values?

When we have the prediction accuracy of every possible sensor array, it is easy to sort the arrays according to the descending order of the accuracy values. The first few items of this sorted list may be like Table II. A reasonable intuition is that the sensor in the rank 1 array must be important. But because the prediction algorithm may not be perfect, and that large correlation exists among chemical sensors, some important sensor may not be present in the rank 1 array. Besides, what is the importance order of the sensors in the rank 1 array?

Following the evaluation criterion known as "cumulative match score" [11], we propose a criterion named "cumulative sensor importance" (CSI). For each sensor, its occurrence in the top K ranked arrays is counted and denoted as CSI(K). A sensor with high importance should occur more in the top ranked arrays than those with low importance. So CSI can be used to indicate the importance of the sensors. Curves of CSI(K) with K as the x-axis can be plotted. Thus, by observing these curves' height, we can get the importance order of all the sensors.

TABLE II. An Example of ohe Array Rank List

Rank	Sensors	Accuracy
1	s7,s8,s9,s10,s11,s16	0.923
2	s7,s8,s9,s10,s11	0.922
3	s3,s4,s7,s8,s9,s10,s11	0.919
…	…	…

Average Accuracy Improvement

The average accuracy improvement (AAI) intends to answer such a question: "how much will the accuracy improve by adding a certain sensor?" For instance, we already have an array A which doesn't contain the sensor S. The prediction accuracy for A is acc(A). So the accuracy improvement after adding sensor S is acc(A ∪ S)-acc(A). Since A1 could be any array without S, it is better to average this improvement for all possible A's. So AAI(S) is defined by this average accuracy improvement of sensor S.

If we can use the prediction accuracy to estimate the discriminating information of an array, AAI(S) somehow reflects the average of unique discriminating information in S, subtracting the noise or redundancy in S. This is because the accuracy is likely to increase only if S contains some unique discriminating information that the original array doesn't have. Or, in other words, S should contain some complementary information. If compared to the discriminative information it can bring, S introduces more noise or redundancy to the prediction algorithm, AAI(S) could even be negative.

As a result, we could also draw a scatter plot for all the sensors, with the accuracy of each single sensor as the x-axis, and the AAI of each sensor as the y-axis. Suppose the accuracy of each single sensor reflects the total discriminating information of the sensor, then the sensors in the right part of

this plot are those with high discriminating information by themselves, while those in the upper part are those with more unique discriminating information. When selecting sensors, it is reasonable that we first select those in the upper right corner of the scatter plot, followed by the ones in the upper part. When discarding sensors, those in the lower left corner should be the first choices.

Sensor Inter-relationship

The AAI reflects the average of the unique discriminating information of a sensor. Sometimes we are interested in relationships between sensors pairs, e.g. "compared to sensor S2, does S1 contain any unique discriminating information?" This could be estimated by sensor accuracy improvement (SAI). We define SAI(S1, S2) = acc(S1 ∪ S2)-acc(S2). The reason is that only if S1 has some unique discriminating information that the S2 does not have, acc(S1 ∪ S2) is likely to be larger than acc(S2). If compared to the discriminative information it can bring, S1 introduces more noise or redundancy to the prediction algorithm, SAI(S1, S2) could even be negative.

In an opposite aspect, we may wonder if sensor S1 is very similar to S2. If so, one of them is likely to be redundant and can be discarded. The similarity could be estimated by algorithms such as correlation or mutual information between the features of two sensors, but the result is not task-specific. Our real goal is to evaluate if the two sensors contribute analogously to our prediction task. Therefore, it is better to use the prediction accuracy to judge the similarity. Suppose there is an array A which contains neither S1 nor S2. If acc(A ∪ S1) is close to acc(A ∪ S2) for every possible A, then S1 has similar performance to S2 for this prediction task. Thus, the sensor accuracy similarity (SAS) can be defined as SAS(S1,S2) = 1-mean(abs(acc(A ∪ S1) - acc(A ∪ S2))), where the operation "abs" means the absolute value and "mean" means averaging over all possible A's.

Both SAI and SAS can be described with a matrix, where each row and each column correspond to a sensor. SAI(i, j) is an estimation of the unique discriminating information of sensor i that the sensor j does not have. SAS(i, j) is an estimation of the similarity between sensor i and j. The larger SAS(i, j), the more similar. It is easy to know that SAI(i, i) = 0, SAS(i, i) = 1. SAI(i, j) ≠ SAI(j, i), but SAS(i, j) = SAS(j, i).

In this chapter, we introduced our methods to compute the cumulative sensor importance and average accuracy improvement for each sensor, as well as sensor accuracy improvement and sensor accuracy similarity between each pair of sensors. Each measurement can be plotted to a figure, which is convenient for us to observe and draw intuitive conclusions. While traditional sensor selection methods only tell us which sensors are important, these methods give us more insight and tell us why certain sensors are important and some should be discarded. These conclusions come from analyzing the exhaustive searching results of a certain task, followed by cumulating or averaging, so they are more reliable and more specific for the task. In the next chapter, these methods will be used to analyze the data collected by our breath analysis system, followed by a detailed discussion.

IV. Experiments and Discussion

Experiment Configuration

167 breath samples from healthy subjects and 151 from diabetics is collected. To classify between healthy and diabetes samples, half of samples are randomly picked from both class to form the training set. The rest of the samples formed the test set. We ran the classification 50 times and calculate the average accuracy for sensor performance evaluation.

There are 14 chemical sensors in our breath analysis system. The NH3 sensor is ignored since it is irrelevant to our task and generates little response for all the samples. Thus, there are 13 sensors to evaluate altogether. 8191 arrays need to be tested. The program was ran on the Matlab v8.0 software on a computer with 2.4GHz, 8 core CPU and 16GB RAM. The parallel function of Matlab was used to accelerate the program. It took 8.8h to test the 8191 arrays. This time cost is acceptable for our task. If the sensor number becomes larger, it will be impractical to test all the arrays. However, some filter algorithms can be used to exclude some sensors before testing.

Sensor Evaluation Results

Fig. 3 shows the cumulative sensor importance of the evaluated 13 sensors. For clarity, the sensors' names have been replaced by their number. One can check Table I for correspondence. From Fig. 3, it is clear that sensor 9,10,7,8,11 and 4 are the most important ones, since for the same K, their CSI(K) is higher, indicating that they appear more in the top K arrays.

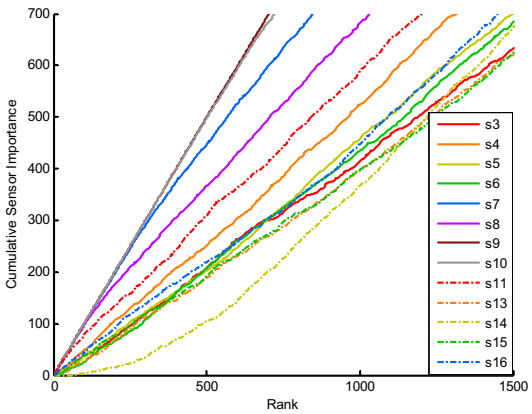

Fig. 3. Cumulative sensor importance (CSI) for all sensors.

From Fig. 4 we can get similar conclusions. The average accuracy improvement (AAI) of sensor 9,7,10,8 and 4 are the highest ones. Sensor 9 can improve the accuracy by 4% on average. This AAI list is not identical to CSI, since AAI averaged over the accuracy of all the arrays, while in the CSI figure only the top 1500 arrays are shown. The sensor 3,13,15

and 16 have negative AAI values, indicating that on average they introduce more noise and redundancy than discriminating information. The AAI is basically proportional to the accuracy of each single sensor. But for sensor 14 and 15, although they have higher single accuracy than sensor 8 and 4, their AAI is lower than sensor 8 and 4. This is probably because sensor 14 and 15 have some discriminating information, but much of it is overlapped with other sensors, the unique discriminating information left is less than sensor 4 and 8.

The sensor accuracy improvement (SAI) matrix is drawn in Fig. 5. For easy reading, pseudo-color is used to represent values. Red indicates large positive SAI values, while blue indicates large negative values. The i'th row and j'th column of this matrix is SAI(i,j), which means that adding sensor i to sensor j, the prediction accuracy will increase SAI(i,j). We can see that sensor 9,7,10 (the s9, s7, s10 row) and so on have relatively large SAI values along all the columns. This is a hint that they has some unique discriminating information that every other sensors do not have. This is consistent to our observation from CSI and AAI. Another finding is that SAI(s7,s15)>0 but SAI(s15,s7)<0. This is a hint that the discriminating information in s15 is a subset of that in s7.

To estimate the redundancy between sensors, we plot the sensor accuracy similarity (SAS) matrix in Fig. 6. A red-color grid (i, j) in this figure means that sensor i and j have very similar performance, thus one of them may be redundant and can be discarded. For clarity reason, the order of row and column has been rearranged to cluster sensors with close SAS values. As we can see, sensor 13,5,3,15 and 16 have large SAS values between one another. This possibly means that they have highly correlated responses. An interesting fact is that from Fig. 4 we know none of them has much unique discriminating information and from Fig. 3 we know none of them is very important. Keeping one of them in the array is enough. Sensor 11, 14, 6, 4 and 8 also have some correlationship between each other, but not as much as sensor 13 and so on. Sensor 10,7 and 9 are really different from other sensors. They contain much unique discriminating information and adding them to the array will make big differences to the accuracy of this task.

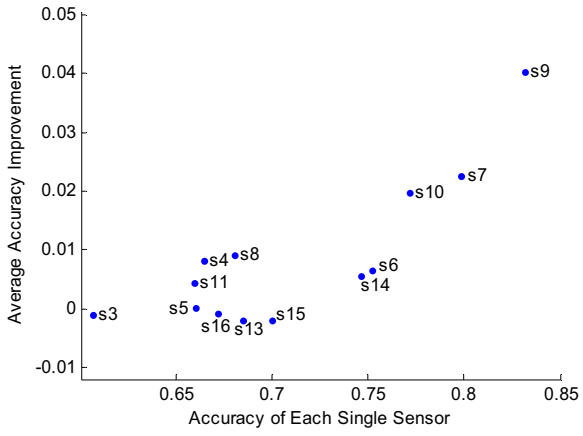

Fig. 4. Accuracy of each single sensor vs. average accuracy improvement (AAI).

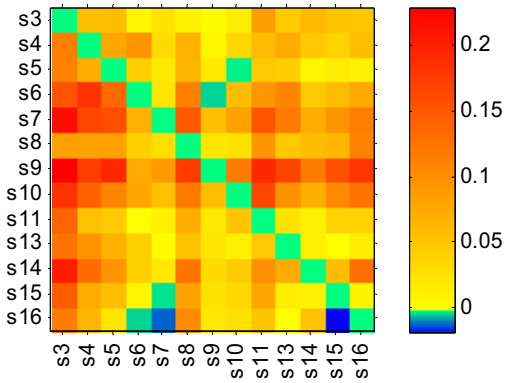

Fig. 5. Sensor accuracy improvement (SAI) matrix.

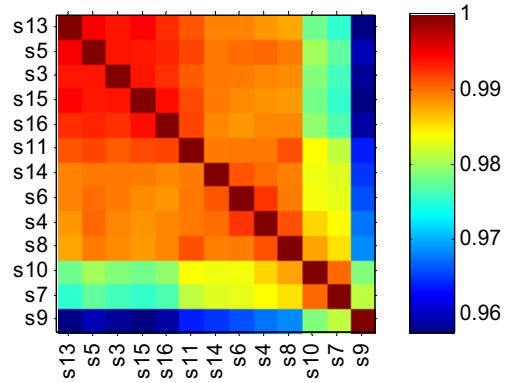

Fig. 6. Sensor accuracy similarity (SAS) matrix.

Discussion

In this section, the evaluation results will be related with some prior knowledge about the sensors to see if it will bring more discoveries on the sensors.

- From the 4 evaluation techniques it is found that sensor 9,7 and 10 (particularly sensor 9) are the most important sensors, contains the most unique discriminant information than other sensors and are not redundant at all. They are all temperature modulated sensors. Their performance is much better than their counterpart without TM, i.e. sensor 6,15 and 11. SAI(15,7) and SAS(6,9) are even negative (see Fig. 5), which is to say that compared to the TM version, the non-TM version of the 2 sensors contains only noise and redundancy. In conclusion, temperature modulation can be applied to breath analysis systems and it can greatly improve the performance of MOS sensors.

- Sensor 8,4,6 have medium importance, unique discriminant information and moderate redundancy. Actually, in our pilot experiments, these 3 sensors have high sensitivity to acetone, which is the main biomarker of diabetes. This fact can explain their importance.
- Sensor 13,5,3,15,16 and 11 contain high redundancy and low unique discriminant information. This is consistent to the fact that the sensitivity features in their datasheets are very similar. Sensor 5 and 13 have very similar performance according to Fig. 6, which is possibly because that they both belong to the TGS2610 series.
- The 4 figures above show that the PID sensor (sensor 3) is not a good choice for our task. It is because that a PID sensor is sensitive to a wide range of analytes [8], thus have poor selectivity.
- From the discussions above, we have more knowledge on the sensor selection results now. Although the best sensor array is sensor 7, 8, 9, 10, 11, 16 according to exhaustive searching, it is not the only choice. It can be inferred that sensor 7,9,10 are essential; sensor 16 could be replaced by another one in sensor 5, 13, 15; sensor 8, 4, 6 are better kept; sensor 11 and 14 are optional; sensor 3 should be discarded.
- In its datasheet, sensor 14 has high sensitivity to acetone. The datasheet of sensor 8,4 and 6 do not include any content about acetone. But in our experiments, sensor 14's sensitivity of acetone is not comparable to the latter 3 sensors. This is maybe because that the latter 3 sensors are not designed to sense acetone, so it is not written in their datasheet. This finding shows that when selecting sensors for e-noses, the datasheets are not completely reliable, since they do not show the sensors' sensitivity to every analyte.

V. Conclusion

In this paper, a breath analysis system for diabetes diagnosis is introduced. Four techniques are developed to evaluate the sensors' performance. The cumulative sensor importance shows the importance order of the sensors. The average accuracy improvement displays the accuracy improvement brought by a sensor. The sensor accuracy improvement tells us the accuracy gain by combining one sensor with another. The sensor accuracy similarity shows the likeness of performance between two sensors. Different from traditional sensor selection methods which focus on selecting the best array, the proposed statistics aim at judging the importance, unique discriminating information and redundancy of each sensor based on the exhaustive search results of all the possible sensor arrays.

The key step of using these techniques lies in comparing the results to prior knowledge about the sensors. It can bring us more insight and tell us why certain sensors are important and some should be discarded, thus provide new aspects for selecting sensors. We have tested these techniques on our data and draw some useful conclusions. The conclusions themselves may not be very helpful for other researches since they are specific for our task. But the analysis methods are suitable to analyze all systems with an array of sensors, especially when different sensors have correlation. The heavy computation cost needed to do the exhaustive search is an obstacle. A possible solution is to filter out some irrelative sensors in advance. Future works may include applying some other methods to replace exhaustive searching, such as genetic algorithms.

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