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Investigation of Electronic Nose Sensor Drift Correction Methods and Their Application to Environmental Samples

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Sensor drift is one of the main problems connected to gas sensors, and is one of the main responsible of their limited diffusion and adoption for different real-life applications. For this reason, different algorithms have been proposed in literature for drift mitigation. This paper has the main objective of giving an overview of the methods that can be applied in order to correct sensor responses relevant to real environmental odours and investigating some of those methods that were identified as most suitable for the desired application. The two methods that were considered for the experimental work are the PCA component correction and the Orthogonal signal correction methods. For the application of the first method, different calibrants were investigated, finally selecting acetone and ammonia as the most suitable compounds for the electronic nose calibration. The preliminary results obtained prove both methods to be robust towards small calibration set sizes and show a good performance in improving improve data clusterization and discrimination.

1. Introduction

The electronic nose is an instrument capable of simulating human olfaction in odour detection and classification. Its detection system simulates olfactory receptors through an array of gas chemical sensors with partial specificity, which respond to volatile compounds with perturbations of their physical properties (Di Carlo & Falasconi, 2012); while systems for data elaboration reproduce olfactory bulbs activity for signal compression and brain functions for odour classification.
The electronic nose does not perform a chemical analysis of the odorous samples, but it provides a global characterization through a specific olfactory pattern. This feature allows the analysis of complex mixtures, such as environmental samples from landfills, refineries or other industrial activities (Capelli et al., 2014).
One of the main criticalities aspect that has limited the electronic noses diffusion in everyday applications up to now is gas sensor drift, i.e. a gradual change of sensor response over time (Holmberg & Artursson, 2002), which causes a decrease of instrument sensitivity and selectivity over time. This problem becomes particularly critical in the case of electronic noses used for environmental odour monitoring in the field, where the variability of the atmospheric conditions makes sensor responses even more unstable, and thus drift extremely undesired and hardly identifiable.
Different drift correction methods have been presented in literature. All of them involve the estimation of drift trends, involving or not the use of specific calibrants, and propose different techniques for drift compensation, such as suppression of drift direction from the measurement set or definition of correction factors to be applied to signal responses.
This paper investigates the possibility to apply literary methods for the correction of sensor responses relevant to real environmental odours and presents preliminary results of their application.

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2. Drift correction methods

2.1 General overview

The sensor drift is defined as “a small temporal variation of the sensor response exposed to the same analyte under identical conditions” (Di Carlo and Falasconi, 2012). Drift causes a decrease in sensor sensitivity and selectivity over time and affects measurement reproducibility.
The main factors responsible for sensor drift are sensors aging due to thermochemical fatigue after successive gas expositions, thermo-mechanical degradation, environmental factors (temperature, humidity and ambient pressure variations) and sensor surface poisoning.
In literature, several methods for drift correction have been proposed. Those methods, which differ in complexity and field of applications, can be roughly classified into the following three different groups:

- Sensor signal pre-processing methods are used for a first correction of the raw sensor response and they are always the initial step of more complex techniques. Those include for instance Baseline manipulation (Gardner and Bartlett, 1999) and Frequency domain filtering (Feng et al., 2011);
- Periodic calibration methods base drift estimation on sensors response to reference standards (i.e. calibrants), which are periodically analysed to evaluate changes in sensor response. Examples are PCA/PLS Component Correction (Artursson et al., 2000) and Multivariate Component Deflation (Gutierrez-Osuna, 2000);
- Attuning methods deduce drift components directly from training data and remove those directions from the dataset. Those include Independent Component Correction (Di Natale et al., 2002), Orthogonal Signal Correction (Wold et al., 1998) and Adaptive methods, i.e. Neural Networks (Zuppa et al., 2004).

Based on a literature study, Principal Component Analysis (PCA) component correction and Orthogonal signal correction (OSC) have been evaluated as the most suitable methods to be further investigated for drift correction in the analysis of environmental odour samples. Those methods are therefore described more in detail in the following sections.

2.2 PCA component correction

Since aging effects cause most of the drift, PCA component correction assumes that drift has a preferred direction in the measurement space. This drift direction is estimated referring to sensor responses to a calibrant, and then removed from the measurement space to mitigate drift effects on sensor responses.
PCA is a linear supervised learning pattern-recognition technique, usually employed in conjunction with cluster analysis. In other words, PCA rotates the original coordinate system along the direction of maximum variance (Misra et al., 2002).
The PCA component correction estimates a loading vector p from reference measurements by PCA analysis, which uses the correlation among sensors to transform the multivariate space into a subspace that preserves the maximum variance of the original space in the minimum number of dimensions. Then, the score matrix T for samples is determined by projecting responses relevant to sample analyses on p (Artursson et al., 2000). The drift correction is operated by subtracting the bilinear expression tpT from the original data.

2.3 Orthogonal signal correction

OSC is an attuning method, which was first proposed by Wold et al. (1998) for NIR spectra correction, and then several algorithms were developed to improve its performance. This method does not involve the use of a calibrant but operates the drift correction dividing data relevant to real samples into a calibration set and a prediction set.
For data processing, first two matrixes X and Y are defined, whereby X is the matrix for the independent and Y the matrix for the independent variables, respectively. After that, this technique focuses on removing by suppression the non-relevant information of the response in matrix X (i.e. the variance of X that is not correlated to the variation of the dependent variable Y), thus reducing the influence of long-term drift on sensor responses.
Since only information orthogonal to Y is removed, signal correction removes as little information as possible, preserving relevant information for odour detection and classification (Laref et al., 2017).
This paper refers to the OSC algorithm proposed by the Wise implementation. This algorithm first searches by PCA for the direction of maximum variance of the data X, then orthogonalizes the PCA score vector t with respect to matrix Y. The vector resulting from orthogonalization captures the highest possible amount of variance of X (Padilla et al., 2010).
Subsequently, the partial least square (PLS) method is applied to calculate the weights w as to minimize the covariance between X and Y, so to get as close to orthogonality between t and Y (Wold et al., 1998). This allows to estimate scores T and loadings P vectors, containing information not related to Y.
Finally, the correction (TP’) is subtracted from matrix X to remove drift.

3. Material and methods

3.1 The electronic nose used for the study

The electronic nose involved in this research is a commercial model produced by SACMI, i.e. the EOS507c (Dentoni et al., 2012).
The instrument is equipped with six MOS sensors (n-type doped semiconductors), which differ in terms of morphology and operating temperature. The sensor array works at the temperature of 450°C to reduce the semiconductors resistance and maximize the sensor response.
The instrument is also equipped with an automatic calibration system, which operates a daily check of sensor performance. More precisely, the device checks the sensor response to a fixed concentration of a reference odorant ("standard"), i.e. n-butanol, and performs a signal correction with respect to this standard.
The EOS507c instrument also includes a reference air generation system that operates a filtration of the ambient air on activated carbon, periodically regenerated and substituted, to restore the signal after samples analysis.
During operation, a vacuum pump continuously pulls the reference air into the sensor chamber to create a baseline for the sensor response. During analysis, the sample-handling unit exposes the sensors to the odorant, producing a transient response as the VOCs interact with the sensors active material. A steady state condition is usually reached in a few minutes. During this interval (i.e. the response time of the sensor array), the sensors response is recorded and delivered to the signal-processing unit. Then, the reference air is again fluxed to the sensor array to restore the reference line and prepare sensors for a new measurement cycle.

3.2 Samples

Real environmental samples used for testing literary methods selected are representative of two target olfactory classes (i.e. A and B) relevant to an industrial activity.
Since periodic calibration methods involve the use of calibrants for the estimation of drift components, compounds representative of common environmental odours were considered as possible reference compounds.
In particular, this paper presents test carried out with acetone, ammonia and n-butanol. Acetone and ammonia were selected because they are very common constituents of real environmental samples (Eusebio et al., 2016). N-butanol is not so common in environmental emissions, but it is the referent odorant for dynamic olfactometry, and this is the historical reason why it is currently used as reference substance for the electronic nose used in this research.
Hydrogen sulphide was also considered as a possible calibrant, since it is one of the main constituents of environmental emissions responsible for odour nuisance. However, it was decided to exclude it from further investigations, because of its toxicity, and also because it has a very low odour threshold, which makes it scarcely detectable by common gas sensor (Eusebio et al., 2016).
Table 1 reports the calibrant samples preparation methods and the concentrations tested.

Table 1: Calibrant samples preparation methods and concentrations

Compound	Preparation method	Concentration tested
N-butanol	Sampling from bottle at 60ppm	60 ppm
Acetone	Dilution from headspace: 30mL liquid in 7L air, stored at 25°C and 60% RH for 1h	39 ppm
Ammonia	Sampling from bottle at 19ppm	19 ppm

4. Results

4.1 Data processing

PCA component correction and OSC were adopted for drift correction of real environmental samples representative of two different olfactory classes, i.e. A and B.
Sensor signals recorded during the analyses of real samples and calibrants were elaborated in terms of resistance ratio R_0/R, where R_0 is the resistance value at time zero and R is the resistance value recorded at the end of the measure, when the sensor signal reaches a plateau.

4.2 PCA component correction

As already mentioned, the PCA component correction method involves the use of a calibrant for drift estimation. As a first strep, this technique was adopted to identify which one, among the tested reference compounds, was the most representative of the real samples to be corrected. Indeed, as a general rule, an effective calibrant should be as similar as possible to real samples in order to optimize drift estimation and correction. For this purpose, responses relevant to the analyses of environmental samples and reference compounds carried out in different days were processed by PCA to estimate drift directions (Figure 1). This allowed to visualize and compare the drift trends relevant to the different classes considered.

As shown in Figure 1, drift trends estimated for samples A and B are very similar to those obtained for ammonia and acetone, respectively.

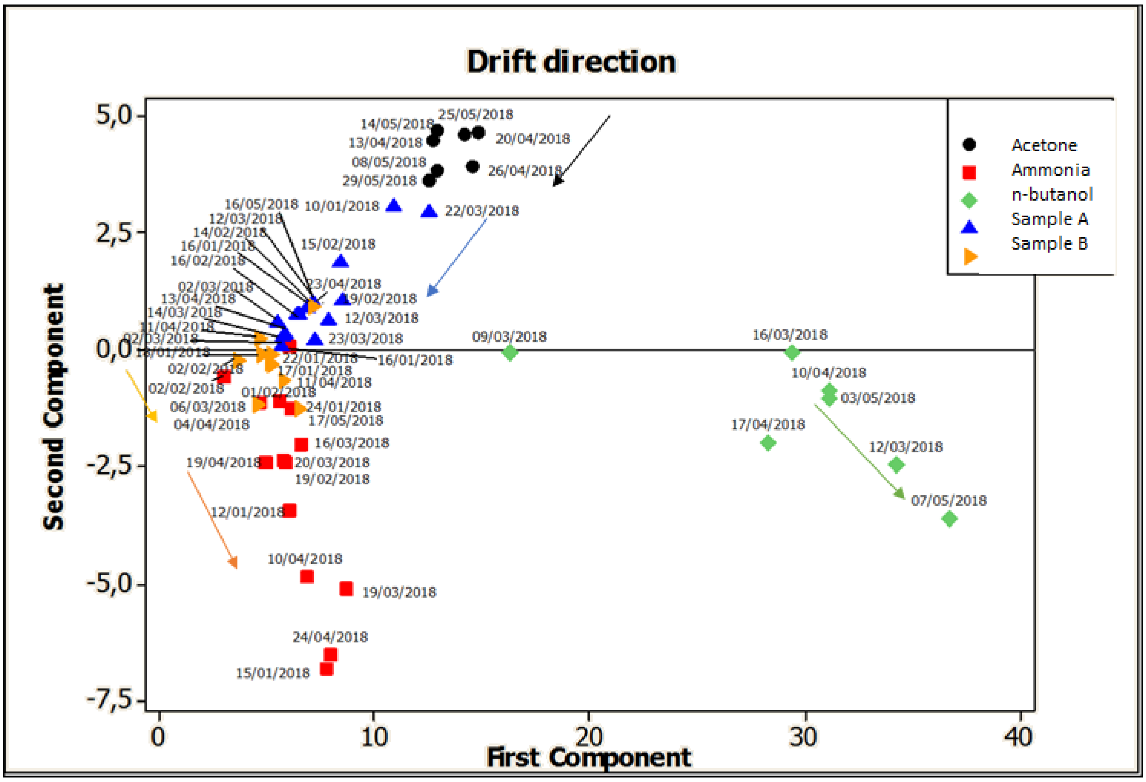

Figure 1. Drift directions of real samples and calibrant analyses

Therefore, these two compounds were chosen as calibrants and the drift correction was operated by subtracting both drift directions estimated from the dataset. Figure 2 reports graphical representations of discrimination between olfactory classes A and B before and after drift correction.

It can be observed that after drift correction by application of this method, clusterization of samples belonging to the same class is improved.

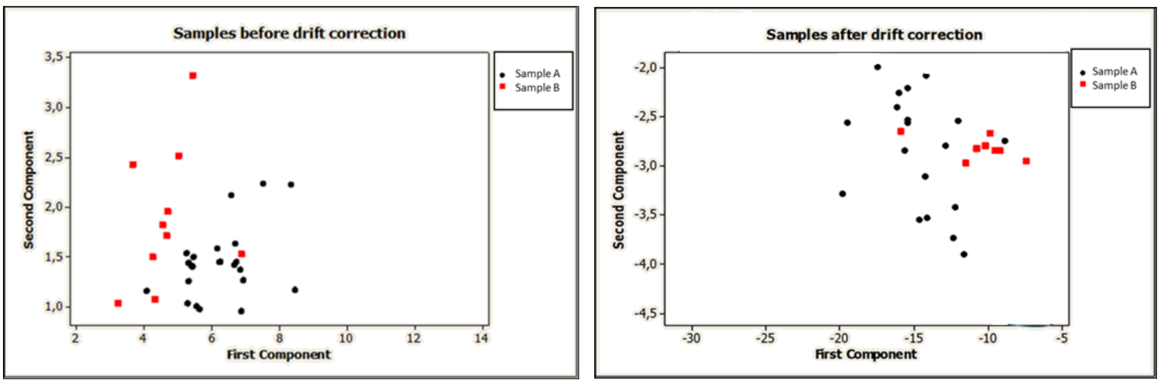

Figure 2. Sample discrimination before (left) and after (right) PCA component correction

4.3 Orthogonal signal correction

For the application of this method, the dataset relevant to the analyses of real environmental samples was divided into a calibration set and a prediction set. Samples of the calibration set were used to preditct drift trends to be subtracted from the prediction set. Figure 3 shows the discrimination between classes A and B before and after drift correction, which proves the capability of this method of improving sample clusterization.

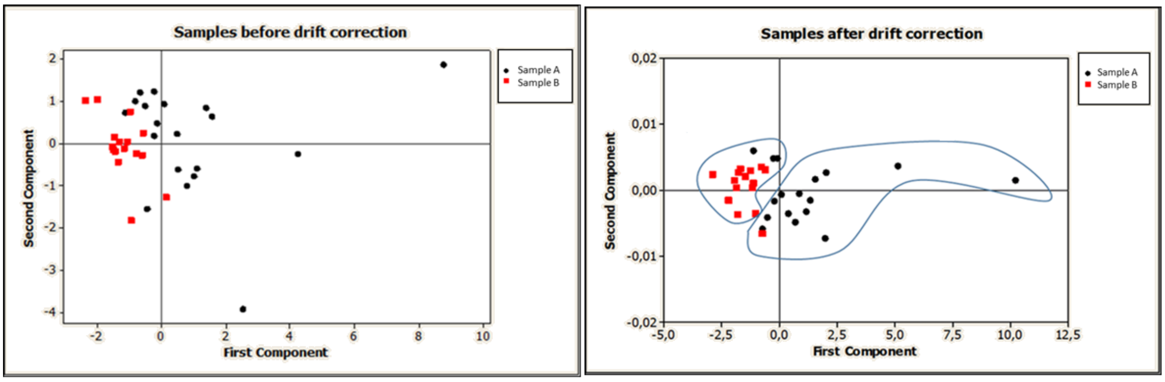

Figure 3: Sample discrimination before (left) and after (right) orthogonal signal correction

5. Conclusions

Among the different drift correction methods proposed in the scientific literature, this paper investigated the capability of PCA component correction and Orthogonal signal correction methods to mitigate drift effects in environmental samples. Both pre-processing methods are robust regarding small calibration set sizes and show a good performance in improving improve data clusterization and discrimination.
PCA component correction is also a suitable technique for the selection of specific calibrants to be used for drift correction. The choice of a suitable calibrant is a crucial aspect for the effective application of periodic calibration methods, because it directly affects the method performance. As a consequence, calibrants should be as similar as possible to the real samples to be analysed, in order ensure that drift trends of calibrant and real samples are highly correlated.
The sensor response processing (i.e. the feature extraction) also has an important influences on the method performance. Therefore, sensor signal pre-processing techniques may be combined with PCA and OSC to optimize sample clusterization.
Future works should further study the possible software improvements to be applied in order to make the drift correction methods more effective. One possibility would also be to use combinations of the tested compounds as calibrants to correct drift in variable blends.

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