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Towards Drift Correction in Chemical Sensors Using an Evolutionary Strategy

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ABSTRACT
Gas chemical sensors are strongly affected by the so-called *drift*, i.e., changes in sensors' response caused by poisoning and aging that may significantly spoil the measures gathered. The paper presents a mechanism able to correct drift, that is: delivering a correct unbiased fingerprint to the end user. The proposed system exploits a state-of-the-art evolutionary strategy to iteratively tweak the coefficients of a linear transformation. The system operates continuously. The optimal correction strategy is learnt without a-priori models or other hypothesis on the behavior of physical-chemical sensors. Experimental results demonstrate the efficacy of the approach on a real problem [1].

Categories and Subject Descriptors
I.2 [**Computing Methodologies**]: Artificial Intelligence; I.5.4 [**Computing Methodologies**]: Pattern Recognition-Applications

General Terms
Algorithms

Keywords
Drift correction, Artificial olfaction, Evolutionary Strategies

1. INTRODUCTION
Gas detection instruments are increasingly needed for industrial health and safety, environmental monitoring, and process control. During the operating life sensing materials undergo irreversible modifications due to poisoning and aging, causing sensors' selectivity decreases. This phenomena is usually referred to as *sensor drift* and it afflicts almost all kinds of sensors, including pressure sensors, pH sensors, conductivity sensors. Drift correction algorithms are not new in the field but currently the only effective counteraction to prevent negative effects of drift is in fact frequent sensor calibration. However, while this approach is rather simple to implement for physical sensors where the quantity to be measured is exactly known, chemical sensors pose a series of challenging problems. Indeed, in chemical sensing, the choice of the calibrant strongly depends on the specific application and, when the sensing device is composed of a number of cross-correlated sensors, a univariate signal correction is not feasible. This paper proposes a methodology for an evolutionary adaptive drift-correction module. The work stems from a previous, and successful, attempt to create a drift-resistant classifier [1]. The proposed approach seems to be effective towards drift correction.

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2. BACKGROUND
2.1 Pattern Classification
In supervised classification a set of previously classified items, usually referred to as *training set*, is used to build (train) a prediction model able to classify a set of unknown samples denoted as *test set*. Dimensionality reduction techniques are also employed for data visualization in order to have a preliminary insight of the multidimensional pattern distribution, where the most used technique is principal component analysis (PCA) [2].

2.2 Drift correction in chemical sensing
Current solutions for drift correction [4] fall into three main categories: use of calibrants to return the classifier to its original state, attune the classifier with proper feature selection/extraction to reduce drift effects, and use of adaptive models to real-time update the classifier. Adaptive models try to on-line adjust the classifier by taking into account pattern changes due to drift effects [3]. All the proposed solution are limited by the loss of generalization and are not able to correct time evolving drift effects. More recently, we presented an adaptive methodology based on CMA-ES [1]. Under such schemes, newly recognized data can be used to retrain the classifier or fed the CMA-ES.

3. PROPOSED METHODOLOGY
Figure 1 sketches the architecture of the proposed drift correction framework. It is composed of a set of different conceptually separated blocks collaborating in the correction process. The first block implements a *linear transformation*

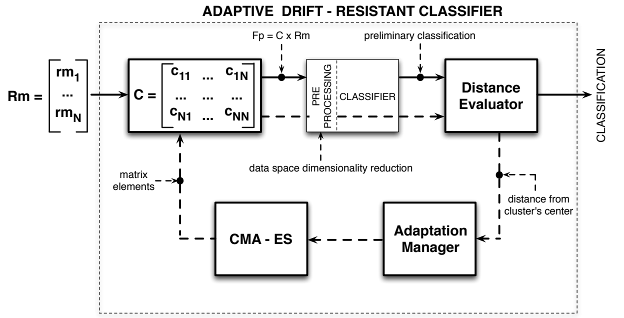

Figure 1: Conceptual architecture of the drift corrector

C transforming a raw drifted measure Rm into a drift-free fingerprint $Fp = C \times Rm$. Initially C is set to the identity matrix so that no modification is applied to Rm. We therefore assume a negligible drift during the training phase and in the very beginning of the experiment. The second block is a *standard classifier* that receives the drift-free fingerprint and provides as output its classification. In order to cope with complex datasets this block usually performs dimensionality reduction to decrease the number of considered variables. The prediction provided by the classifier is used by the *distance evaluator* module to compute the distance between the fingerprint and the centroid of the related class. Whenever the computed distance D is contained between a lower threshold T_l and an upper threshold T_u, the *adaptation manager* activates a CMA-ES for slightly tweaking the elements of the correction matrix C in order to further reduce the distance of the fingerprint from the selected centroid. The rationale is that drift effects change gradually over few measures. If a fingerprint has a distance from its related centroid lower than T_l, no modification of the current correction matrix is required. On the other hand, if the distance is higher than T_u the fingerprint is unreliable and it is not worth using it for modeling the drift. The use of the history mechanism is more efficient than the *inertia* coefficient exploited in [1] since it is less influenced by the timings of the measures. In order to avoid oscillation in the drift correction, the distance between the fingerprint F_p calculated with the actual linear transformation C, and the fingerprint $\bar{F}_p$ calculated with the new linear transformation $\bar{C}$ is required to be smaller than the distance between F_p and the centroid of its cluster. Solutions not complying with this requirements are discarded in the CMA-ES.

3.1 Evaluation function

The proposed evolutionary strategy exploits the euclidean distance in the N-dimensional feature space between the current fingerprint F_p and the centroid C_m of the related class to build a specific evaluation function, as follows:

$$D = Fp - Cm = \sqrt{(Fp_1 - Cm_1)^2 + \cdots + (Fp_N - Cm_N)^2}$$

4. EXPERIMENTAL RESULTS

The proposed approach has been experimentally validated on a real data set collected using the EOS835 electronic nose composed of 6 chemical MOX sensors. The main goal of the performed experiments is to determine the capability of the electronic nose to identify five pure organic vapors, namely: ethanol (1), water (2), acetaldehyde (3), acetone (4), ethyl acetate (5). The measuring campaign is developed in five different sessions carried out in a period of time of about one month, while the whole data set is composed of 100 samples as the training set and 445 samples as the test set. PCA analysis clearly shows the presence of sensor drift in the considered data set, i.e. shift of samples in a direction over the time. Measures of the test set tend to drift toward a direction that is perfectly visible on the first two principal components. This phenomenon leads to an overlapping of the different classes and, consequently, to a loss of classification performance as time goes on. The classifier used in the experience is a linear discriminant analysis (LDA) classification algorithm implemented using the R scripting language, while the adaptation block is implemented in C and PERL. A preliminary classification of the test set has been performed with the LDA classifier without drift compensation. It has classified about 90% of the test set correctly. The proposed approach, called *drift_reduction* has been also compared with the results obtained with the adoption of the robust classifier presented in [1]. Clearly, this is an effect of the drift. As visible from the data, the drift reduction system has the ability of reducing the effect of the drift that affects the test set allowing a good level of classification. In general the system has the tendency to leave less errors in the test set with respect to the robust classifier. From this point of view, the previous approach may not only leave wrong fingerprints in the test set but in some cases it may introduce new errors.

5. CONCLUSIONS

This paper presented a drift corrector based on an evolutionary strategy. The work enhances a drift-resistant classifier presented in [1] and completes its main deficiency. Namely, that it enhanced the power of the classification without an internal representation of the drift. As a result, fingerprints were pushed toward unrealistic directions achieving better separation. But nothing sensible could be derived as a conclusion whether the classifier was not applicable. The proposed approach, on the contrary, is able to deliver a consistent flow of corrected measures where the effect of the drift has been removed. Such measures may be later exploited to perform feature extraction, characterization or further classification.

6. ACKNOWLEDGMENTS

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