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Covariance Matrix Adaptation Evolutionary Strategy for Drift Correction of Electronic Nose Data

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Abstract. Electronic Noses (ENs) might represent a simple, fast, high sample throughput and economic alternative to conventional analytical instruments [1]. However, gas sensors drift still limits the EN adoption in real industrial setups due to high recalibration effort and cost [2]. In fact, pattern recognition (PaRC) models built in the training phase become useless after a period of time, in some cases a few weeks. Although algorithms to mitigate the drift date back to the early 90 this is still a challenging issue for the chemical sensor community [3]. Among other approaches, adaptive drift correction methods adjust the PaRC model in parallel with data acquisition without need of periodic calibration. Self-Organizing Maps (SOMs) [4] and Adaptive Resonance Theory (ART) networks [5] have been already tested in the past with fair success. This paper presents and discusses an original methodology based on a Covariance Matrix Adaptation Evolution Strategy (CMA-ES) [6], suited for stochastic optimization of complex problems.

METHODS AND RESULTS

The proposed drift correction algorithm is summarized in Figure 1. The fundamental idea is to adaptively correct the drift within a given time frame (window) for prorogating the validity of the classification model built in the calibration phase. Windows (W_n) are small such that the drift can be assumed to be linear. The linear transformation represented by a Correction Matrix (CM) is continuously and slowly evolved to follow the drift variations over time. The adaptation is obtained using the CMA-ES, applied to minimize the sum of the distances of each classified sample from the centroid of the related training class. This objective function measures how much the drift-corrected samples deviate from the class distributions learnt during the calibration phase. Different distance functions were tested.

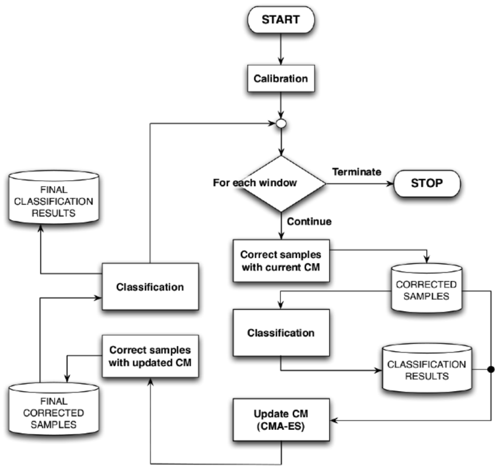

FIGURE 1. Conceptual flow chart of the drift correction algorithm.

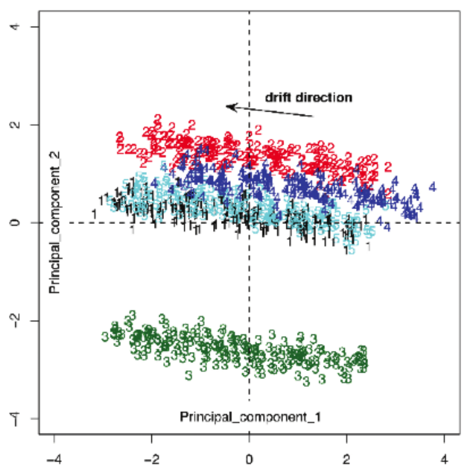

FIGURE 2. PCA of simulated electronic nose data affected by uniform drift. 1000 samples were generated (100 training, 900 test); 18 time windows were used, each including 50 test samples.

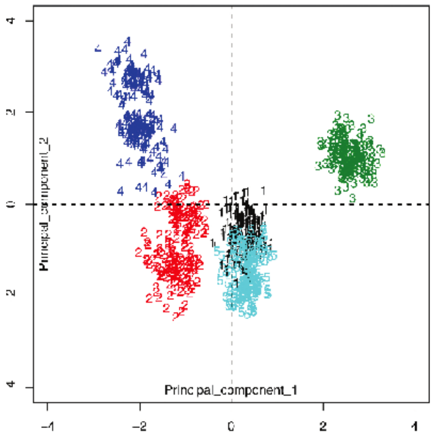

FIGURE 3. PCA of corrected data by using the adaptive drift correction CMA-ES algorithm. Mahalanobis distance was used in the definition of the CMA-ES objective function.

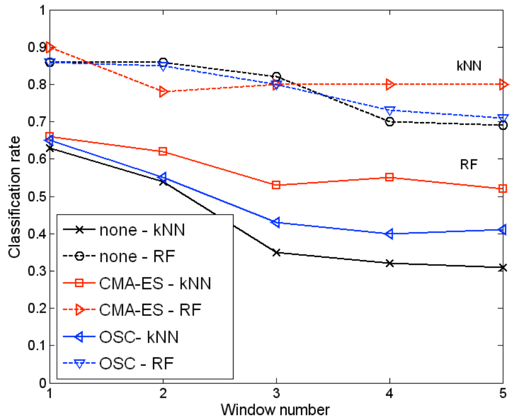

FIGURE 4. Classification results on experimental data at different time frames for: (i) original data (no drift correction), (ii) CMA-ES based drift correction method (Mahalanobis distance), and (iii) OSC drift correction method. Two different classifiers are compared, i.e. kNN and Random Forests (RF).

The proposed methodology was validated on two datasets: (a) simulated data affected by uniform drift (see Figure 2); (b) experimental data obtained at the SENSOR lab with the EOS835 EN (545 samples of 5 organic vapors measured by static headspace sampling). Four cross-validated classifiers were tested together with the drift correction method: kNN, PLS, ANN and Random Forest (RF). Orthogonal Signal Correction (OSC) based drift correction [3] was used as state of the art comparison technique.

For simulated data, we observed that, due to drift, the classification performance degrades from 100% (W1) down to 20% (W18), while by applying the proposed drift correction the classification rate remains above 95% up to W11 and then decays, being still to 80% at W18. The PCA plot of corrected samples (Figure 3) shows how strongly the drift effect can be mitigated by the implemented approach.

Experimental data were also affected by strong drift. Figure 4 shows that CMA-ES approach allows to achieve superior classification rates w.r.t. uncorrected data. The new method performs better than OSC correction, especially in the long term. Gathered results also corroborate the hypothesis that the proposed methodology can systematically adapt to drift even when the amount of data is relatively small and CMA-ES can flexibly work well with different types of classifiers (e.g. kNN or RF).

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