

# Calibration transfer and drift counteraction in chemical sensor arrays using Direct Standardization

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## Abstract

Inherent variability of chemical sensors makes it necessary to calibrate chemical detection systems individually. This shortcoming has traditionally limited usability of systems based on Metal Oxide gas sensor arrays and prevented mass-production for some applications. Here, aiming at exploring calibration transfer between chemical sensor arrays, we exposed five twin 8-sensor detection units to different concentration levels of Ethanol, Ethylene, CO, or Methane. First, we built calibration models using data acquired with a master unit. Second, to explore the transferability of the calibration models, we used Direct Standardization to map the signals of a slave unit to the space of the master unit in calibration. In particular, we evaluated the transferability of the calibration models to other detection units, and within the same unit measuring days apart. Our results show that signals acquired with one unit can be successfully mapped to the space of a reference unit. Hence, calibration models trained with a master unit can be extended to slave units using a reduced number of transfer samples, diminishing thereby calibration costs. Similarly, signals of a sensing unit can be transformed to match sensor behavior in the past to mitigate drift effects. Therefore, the proposed methodology can reduce calibration costs in mass-production and delay recalibrations due to sensor aging. Acquired dataset is made publicly available.

*Keywords:* Chemical sensors, Calibration transfer, MOX sensors, electronic nose, Direct Standardization, Public Dataset

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## 1. Introduction

Devices composed of an array of unspecific chemical gas sensors coupled with machine learning algorithms have been proposed to solve large diversity of tasks, although such devices found limited use beyond laboratory settings and they are still far from fulfilling industry requirements [1, 2]. Inherent variability of chemical gas sensors degrades the performance of calibration models when transferred to other sensing systems [3]. Hence, calibration needs to be performed for each system individually, even if the chemical detection platform includes the same number and type of sensors. As a result, mass-production is unfeasible and calibration transfer between systems has been identified as one of the main obstacles towards wide-spread deployment [4].

Unlike sensor drift and robustness, which were studied thoroughly during the last decade [5, 6, 7, 8, 9, 10], calibration transfer between chemical gas sensor arrays received much less attention from the research community, even though calibration is an expensive and time-consuming process. An efficient calibration transfer methodology would map the spaces of two sensing systems by means of a small set of transfer samples. Such transformation would enable the use of a calibration model built for one instrument (master) to build another calibration model for the slave instrument. As the number of transfer samples would be smaller than the number of calibration samples, such methodology would reduce the cost of calibrating new systems, thereby alleviating the road to industrial applications for systems based on chemical sensor arrays.

Calibration transfer techniques have been explored in spectroscopic instruments to preserve models in time or update the models after hardware replacement. The different strategies that are found in the literature can be divided in two groups [11]. First, standardization methods attempt at mapping system space at measurement time back to system space during calibration. Direct Standardization (DS) and Piecewise Direct Standardization (PDS) are two prominent examples of methodologies of this group [12, 13]. Second, other methodologies aim at removing variation in the responses of different instruments (or the same instrument at different measurement times) to cancel out dissimilarity, such as Orthogonal Signal Correction (OSC) and Generalized Least Squares Weighting (GLSW) [14, 15, 16, 17]. The success of calibration transfer techniques made them suitable for being extended to other sensory

31 systems.

32 Pioneering studies on calibration transfer between chemical detection systems were fo-  
33 cused on classification problems. In early 2000s, Balaban et al. used two commercially  
34 available systems based on polymeric sensors to measure milk samples [18]. They explored  
35 three methodologies to transform data acquired with one sensing unit to the space of another  
36 unit: Simple coefficient, coefficient with intercept, and a matrix transformation (which ac-  
37 tually is equivalent to DS). They found that the latter was the most satisfactory approach.  
38 Tomic et al. used five units of a quartz micro balance sensor array [19]. They tested an  
39 approach that includes a linear regression to compensate each sensor individually, and a mul-  
40 tivariate approach based on partial least squares regression that compensates the whole set  
41 of sensors. Both methodologies could successfully remove signal shift, showing slightly better  
42 performance the univariate method. In another study, again Tomic et al. attempted calibra-  
43 tion transfer for milk sample classification [20]. They used a hybrid device that combined  
44 two sensing principles: field-effect transistors and Metal Oxide (MOX) gas sensors. They  
45 explored how to compensate the entire replacement of the sensor array that took place be-  
46 tween two series of measurements. Multiplicative drift correction and component correction  
47 showed similar performance to transfer the signals from the slave unit to the space of the  
48 master unit. More recently, Shaham et al. showed the feasibility of mapping responses from  
49 sensor arrays composed of different technologies: quartz microbalance and conducting poly-  
50 meric sensors [21]. They evaluated principal components regression, partial least squares,  
51 neural networks and tessellation-based linear interpolation. The best results were obtained  
52 with neural networks, although the quality of the result was dependent on the direction of  
53 the mapping.

54 Only recently calibration transfer techniques have been used in regression tasks. In con-  
55 trast to classification tasks, regression is a more challenging problem, but also offers a more  
56 sensitive measure of the quality of the calibration transfer. Lei Zhang et al. presented a  
57 methodology for on-line calibration transfer [22]. They built six twin units: a master unit  
58 and five slave units. Each unit was composed of four MOX gas sensors along with tempera-  
59 ture and humidity sensors. They fit univariate linear regression curves between each of the  
60 slave units and the master unit to transform the signals acquired with slave units to the space  
61 of the master unit. Although the units were exposed to formaldehyde, benzene and toluene,

62 only the former was used as reference for calibration transfer. Their results show that a sim-  
63 ple homogeneous linear transformation provides good signal mapping between sensing units.  
64 In another study by Deshmukh et al., the authors proposed calibration transfer between two  
65 chemical sensor arrays by means of box-behnken design and robust regression [23]. Two  
66 twin systems with six MOX gas sensors each were built and tested simultaneously. Artificial  
67 neural network models were built with the master unit to predict the concentration of four  
68 compounds relevant for the paper industry: hydrogen sulfide, methyl mercaptan, dimethyl  
69 disulphide, and dimethyl sulphide. The authors showed that the calibration model developed  
70 for the master system, built upon 100 calibration samples, can be transferred to the slave unit  
71 using a smaller set of 27 transfer samples, resulting in a faster calibration of the slave system.  
72 Finally, in a very recent work, Yan and Zhang developed three twin devices that included  
73 eight MOX sensors each [24]. They employed windowed piecewise direct standardization to  
74 transform the variables from the slave device to match the master unit. They tested their  
75 approach on six regression tasks: acetone, hydrogen or ammonia mixed with synthetic air or  
76 exhaled air. Although the complexity of the generated dataset, the authors did not merge  
77 different compounds and backgrounds in the tasks, building regression models for one single  
78 compound.

79 The above mentioned approaches confirm the feasibility to map, by means of a set of  
80 transfer samples, the signal spaces of different sensing units. This transformation enables  
81 the model built with calibration samples acquired with the master unit to be used with  
82 the slave device, thereby reducing calibration costs. Nevertheless, previous methodologies  
83 that considered regression tasks, to the best of the authors' knowledge, did not explore  
84 cross-sensitivity to other volatiles. Basically, although the sensing units were exposed to  
85 different volatiles, for each compound, a regressor was trained separately using the samples  
86 of the selected compound to quantify its concentration, and the resulting models were not  
87 tested with the other volatiles. This can yield to overoptimistic results as the models may  
88 predict high concentration levels of the calibrating gas when samples composed of other  
89 compounds are presented. Moreover, previous contributions did not consider repetitions  
90 of the same sensing unit in time. Hence, whether transferred models degrade in time or  
91 whether calibration transfer techniques can be applied to the same device periodically to  
92 alleviate drift effects remain open questions. Finally, some of the previous datasets do not

93 exactly replicate the scenario of building calibration models for standalone sensing units.  
94 Datasets were generated by placing the different units together on the experimental setup,  
95 acquiring the data for all the devices (master and slave units) simultaneously. This is not  
96 realistic since, in industrial production, one may need to calibrate slave devices while the  
97 master unit is not available. As a result, changes in uncontrolled environmental conditions  
98 (temperature and relative humidity) may increase sensor response variability between units.  
99 In other experimental setups, twin units shared sensor conditioning electronics, and therefore,  
100 sensing units cannot be considered completely independent devices.

101 The goal of the present work is to study calibration transfer between MOX sensor arrays  
102 on a realistic scenario that also includes sensor drift. In contrast to previous approaches, our  
103 methodology relies on a multiclass regression model that is trained and tested using samples  
104 of different compounds, and therefore, incorporates prediction errors due to miss-classification  
105 and cross-sensitivity. To target this goal, we generated a complete dataset that was acquired  
106 by exposing five stand-alone sensing units to 4 gases at 10 different concentration levels in  
107 a period of 22 days. A total of 640 measurements was performed to obtain, to the best of  
108 our knowledge, the largest dataset designed for calibration transfer purposes. Furthermore,  
109 the acquired dataset is made available to the research community for further study and  
110 benchmark of methodologies <sup>1</sup>. The remainder of the paper is organized as follows. We  
111 present the experimental setup (Section 2) and the methodology to generate the dataset  
112 (Section 3), followed by the results (Section 4) and the conclusions of this work (Section 5).

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<sup>1</sup>The dataset will be made publicly available upon acceptance of the manuscript

## 113 2. Experimental setup

### 114 2.1. Detection units

115 Conductometric gas sensors, and in particular MOX sensors, are a popular choice due to  
116 their cost-efficient design, easy operation, sensitivity, fast response, and number of volatiles  
117 that can be detected [25]. Moreover, several options can be found in the market, facilitating  
118 sensor integration in arrays. The sensing principle of MOX sensors relies on the absorption or  
119 desorption of a gas on the sensitive layer, which induces a change in the sensor conductivity.  
120 The composition of the sensing layer and the operating temperature of the sensor, which is  
121 usually controlled with a built-in heater, determine its sensitivity to the different volatiles. A  
122 MOX sensor operating at a different temperature behaves differently and can be, effectively,  
123 considered as a new virtual sensor. Hence, in order to increase the receptive range of detection  
124 systems, usually, different types of sensors (and/or sensors working at different temperatures)  
125 are included in the arrays. Although different types of sensors are designed to detect different  
126 target volatiles, the non-specificity of the sensors makes them sensitive to wide spectrum of  
127 analytes.

128 In order to obtain different sensing units with similar specifications, we implemented five  
129 independent, stand-alone chemical detection platforms following the same design. Each plat-  
130 form can hold 8 MOX sensors and integrates custom-designed electronics for sensor control  
131 and signal conditioning. In particular, each sensing unit included 4 different types of commer-  
132 cially available sensors (Figaro USA Inc., Glenview, USA) to generate multivariate responses  
133 to the different presented stimuli. The control electronics allowed setting the operating tem-  
134 perature of each sensor individually by means of a pulse width modulated signal applied to  
135 the heater of each sensor. Table 1 shows the sensor types included in each sensing unit along  
136 with the corresponding mean voltage induced in the heater. Note that the repetitions of the  
137 same sensor type are operating at different temperatures. As a result, each channel ( $CH$ ) of  
138 the sensing units holds a sensor with unique configuration (sensor type and voltage in the  
139 heater). To minimize the variability within the different units, the configuration was repeated  
140 in all the units: the sensors of the same type and operating temperature were always placed  
141 on the same channel of the respective boards.

142 In summary, following the same system design and implementation, we designed and built

143 5 detection units composed of 8 MOX sensors each.

Table 1: Types of MOX sensors (provided by Figaro Inc.) and corresponding voltage induced in the heater.

Channel	Sensor type	Voltage in sensor heater
0	TGS2611	5.65 V
1	TGS2612	5.65 V
2	TGS2610	5.65 V
3	TGS2602	5.65 V
4	TGS2611	5.00 V
5	TGS2612	5.00 V
6	TGS2610	5.00 V
7	TGS2602	5.00 V

144 *2.2. Gas mixing station and data acquisition*

145 Variations in the composition of gas mixtures induce changes in the MOX sensor’s con-  
146 ductivity. We developed an experimental setup to acquire continuously the conductivities of  
147 a 8-sensor array while the gas conditions are controlled. The complete setup consists of a  
148 data acquisition platform, a power control module, and a chemical delivery system. For an  
149 accurate and reproducible data generation, the system was fully operated by a computerized  
150 environment.

151 The gas delivery system was based on three independent fluidic branches, each of them  
152 controlled by a Mass Flow Controller (MFC) system. The first fluidic branch was used to  
153 control the flow of dry air, whereas the other two branches were free to be connected to any  
154 pressurized gas cylinder. The gases were supplied by Airgas Inc. in calibrated pressurized gas  
155 cylinders. The three branches met together to obtain the desired gas mixtures. MFC were  
156 set to induce the desired concentration levels while keeping the total flow at 400 *ml/min*.  
157 The sensor array was placed in a 60 – *ml* sealed chamber with 8 openings in its bottom that  
158 fit with the standard TO-5 package. Finally, the resulting mixture passed through the mea-  
159 surement chamber continuously before being collected by the exhaust system. The sensors’  
160 conductivities were acquired continuously at 100 *Hz* throughout the complete experiment.

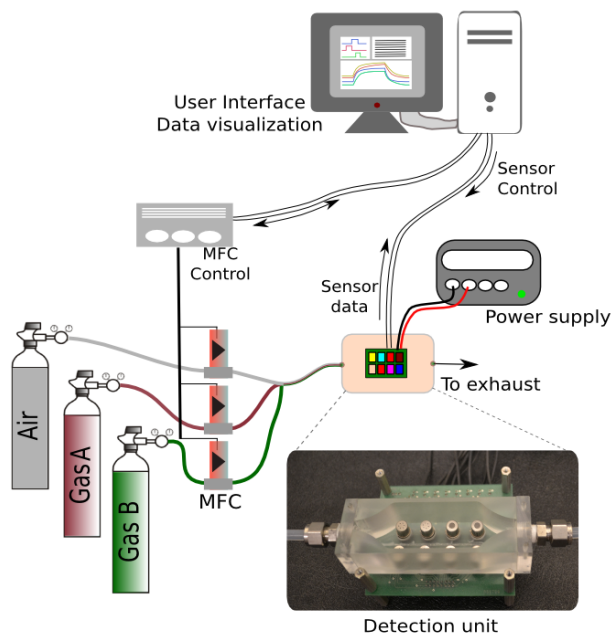


Figure 1: Experimental setup with one of the detection units. By means of a set of three MFC the total flow was kept constant at  $400 \text{ ml/min}$  in the measurement chamber, while different concentration levels of Ethanol, Methane, Ethylene, and Carbon Monoxide were presented to the sensor unit. We built 5 stand-alone sensor units following the same design. Each unit is composed of eight MOX sensors and was tested individually.

161 Figure 1 shows a diagram of the experimental setup along with one of the implemented  
 162 detection units.

163 Hence, by means of a set of three MFCs and the acquisition system, the sensor array was  
 164 exposed to controlled gas conditions, while the sensors' conductivities were recorded. At the  
 165 end of the measurement, we acquired 8 time-series that were indicative of the presented gas  
 166 conditions.

### 167 2.3. Experimental protocol

168 The same experimental protocol was followed to measure the response of the 5 chemical  
 169 detection platforms. Each day, a different unit was tested, which included the presentation  
 170 of 40 different gas conditions, presented in random order. In particular, the board under test  
 171 was exposed to 10 concentration levels of Ethanol, Methane, Ethylene, and Carbon Monoxide.  
 172 The gas mixtures were generated with calibrated gas cylinders at different concentrations:  
 173  $1000 \text{ ppm}$  for Carbon Monoxide and Methane, and  $500 \text{ ppm}$  for Ethylene and Ethanol. Table  
 174 2 shows the tested concentration levels for each volatile. Moreover, the sensory units were



175 tested several times over a period of 22 days (see Table 3).

Table 2: Tested analytes and corresponding concentration setpoints. Each volatile was presented at 10 concentration levels.

Analyte	Concentration levels (ppm)
Ethylene	12.5, 25.0, 37.5, 50.0, 62.5, 75.0, 87.5, 100.0 , 112.5, 125.0
Ethanol	12.5, 25.0, 37.5, 50.0, 62.5, 75.0, 87.5, 100.0 , 112.5, 125.0
Carbon Monoxide	25.0, 50.0, 75.0, 100.0 , 125.0 ,150.0, 175.0, 200.0, 225.0 , 250.0
Methane	25.0, 50.0, 75.0, 100.0 , 125.0 ,150.0, 175.0, 200.0, 225.0 , 250.0

Table 3: Days in which each detection platform was tested.

	Days tested
Unit 1	4,10,15,21
Unit 2	1,7,11,16
Unit 3	2,8,14,17
Unit 4	3,9
Unit 5	18,22

176 The design of the experiment was the same for the four tested volatiles: First, a constant  
177 flow of air (carrier gas) circulated through the sensing chamber for 50 s. This step constitutes  
178 a preliminary stabilization phase, which served to measure the baseline of the sensor response.  
179 Second, the carrier gas was mixed with the selected volatile at the desired concentration level.  
180 The resulting gas mixture circulated during 100 s. Finally, the vapor was purged out from  
181 the test chamber by re-circulating only clean air during the subsequent 450 s. Therefore, the  
182 total duration of each experiment was 600 s. Once the recovery phase was complete, a new  
183 measurement could restart. The order of the concentration levels and the order of the tested  
184 volatiles were selected randomly for each experiment and day.

185 In summary, the acquired dataset, which was generated over the course of 22 days, includes  
186 640 different measurements, distributed in five sensing units exposed to four volatiles at ten  
187 different concentration levels each volatile.

### 188 3. Methodology

#### 189 3.1. Calibration models

190 We evaluated the ability of calibration models built with one chemical detection unit  
191 (master) to predict the concentration level of samples presented to other (slave) sensing  
192 units. In order to build the calibration models, we concatenated the response of the 8  
193 sensors contained in the same unit. The acquired signals were downsampled to 300 samples  
194 per measurement to alleviate computational costs. This would be equivalent to acquire the  
195 sensors' responses at a sampling frequency of 0.5  $Hz$ . Hence, for each measurement, we  
196 concatenated 2400 features in a vector.

197 The calibration models were trained to identify the presented compound and its con-  
198 centration level. Using functions in scikit-learn library [26], we built two-layer calibration  
199 models: First, a Support Vector Machine (SVM) classifier was trained to predict the gas  
200 type presented to the sensor array. The models were trained to classify the four different  
201 classes (gas types) using one-versus-all approach. We opted for SVM-based classifiers due  
202 to their proven success in gas classification problems [27]. Moreover, in a previous study  
203 that we carried out using the same design for the detection unit, we explored the ability of  
204 different classifiers to predict the presence-absence of ethylene in different backgrounds [28].  
205 LDA, k-NN, Perceptron, and SVM did show similar classification accuracy when trained and  
206 tested under the same conditions. However, SVM classifiers seemed to show higher flexibil-  
207 ity to correctly classify samples at lower concentration levels than the calibration samples.  
208 Other works that explored several models to classify data from MOX sensor arrays also re-  
209 sult in similar performances for different models. For example, detection of potato soft rot  
210 was explored using a set of 12 MOX gas sensors. Predictive models based on LDA, MARS,  
211 RBF SVM, Random forests and C5.0 were built. With similar performance, RBF SVM and  
212 LDA appeared to be the best suited models for early discrimination of healthy controls from  
213 infected samples [29].

214 Second, we trained four Support Vector Regression (SVR) to estimate the concentration  
215 of each compound. The output of the classifier determined which regression model was  
216 employed to estimate the concentration of an unknown sample. Therefore, the predicted  
217 output, as well as the presented sample, can be represented in a 4-component vector, which

218 is a convenient representation to compute prediction error. In fact, the error of the predicted  
219 sample was computed by means of the Euclidean distance from the presented sample:

$$Error = dist\left(\vec{x}_{presented}, \vec{x}_{predicted}\right) \quad (1)$$

220 We selected one sensing unit as master device and we utilized the measurements performed  
221 in one day to build a calibration model. From the 40 available measurements, we selected 20  
222 measurements as calibration samples. In particular, the concentration levels 2,4,6,8, and 10  
223 for each of the compounds were used to build the calibration model. Therefore, the classifier  
224 was trained with 20 calibration samples, and 5 samples were utilized to train each regression  
225 model. The models were trained such that a 5-fold cross-validation error was minimized.  
226 The rest of the concentration levels (1,3,5,7, and 9) were set aside to test the performance  
227 of the model within the same board and repetition (test samples). In order to perform the  
228 calibration transfer between sensing units (transfer samples), we only considered a subset of  
229 the calibration samples: concentration levels 4 and 8. Therefore, in contrast to the master  
230 unit which is calibrated using 20 calibration samples, a slave unit would be calibrated using  
231 only 8 transfer samples (2 from each compound). This represents a 60 % reduction of the  
232 required number of samples to calibrate a new unit.

### 233 3.2. Direct Standardization

234 Direct Standardization is a multivariate transfer technique by which one sample in the new  
235 space (sample measured with the uncalibrated system) is mapped to the reference space (same  
236 sample measured with the reference instrument). The relationship of the transformation is  
237 given by:

$$S_{master} = S_{slave}F \quad (2)$$

238 where  $S_{master}$  and  $S_{slave}$  are the response matrices of the transfer samples (also called  
239 standardization samples) acquired with the master and the slave devices. Both response  
240 matrices have as many rows as transfer samples used to perform the transformation, and as  
241 many columns as the number of features of each sample. Then, the transformation matrix  
242  $F$  can be estimated from the pseudo-inverse matrix of the transfer samples. Finally, new  
243 samples can be transformed to the reference space by means of the transformation matrix.

244 DS assumes that all the variations in the signals are caused by the variability of the  
245 sensing devices. However, since the experiment setups to deliver chemical samples also suffer  
246 from some uncertainty, any variation in the sample concentration will be incorporated in  
247 the transformation matrix as well. Moreover, DS also assumes a linear relationship between  
248 the signals from both instruments. Despite such limitations, DS is a transfer technique that  
249 has been successfully applied to near-infrared spectroscopy. The reader is referred to the  
250 literature for more details [30, 31].

## 251 4. Results

### 252 4.1. Sensor variability

253 For each measurement, we acquired 8 signals that embody the response of the sensor  
254 array to the presented gas conditions. Figure 2 shows that the acquired signals indeed follow  
255 the changes in the composition of the gas sample. Moreover, different stimuli induce different  
256 sensors' responses.

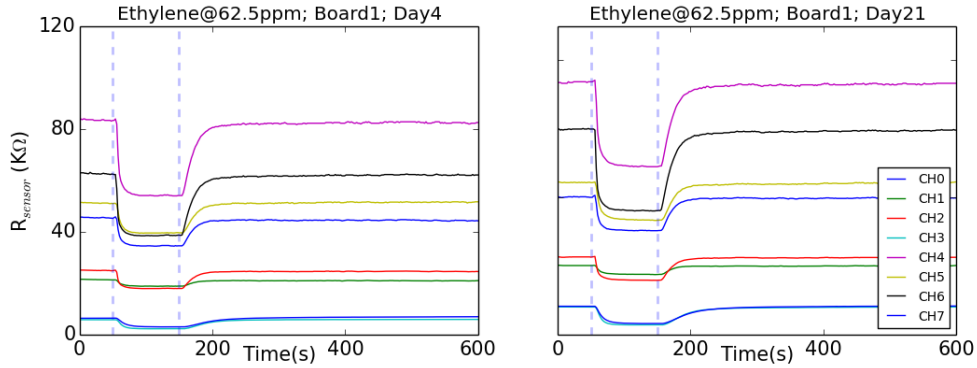
257 Although the design of the detection platforms is the same for all the boards, the variabil-  
258 ity of sensors disperses the responses of the sensing units. Note, for example, that baseline  
259 shifts are more prominent between different boards (see Fig. 2b) than the baseline shifts  
260 within the same board (see Fig. 2a), even if the experiments were more distant in time (17  
261 days compared to two consecutive days). Also, the sensitivity of the sensors of the same type  
262 varies from one unit to another (see channels 4,5,6 in Fig. 2b). Therefore, from a simple  
263 visual inspection of the acquired signals, one can confirm the variability of the sensors, both  
264 across units of the same type and across time.

265 We utilized the model of Clifford-Tuma [32, 33] to quantify the sensor variability. Based  
266 on experimental observations, the model describes the sensor resistance ( $R_S$ ) as a function  
267 of the gas concentration ( $c$ ) and the sensor resistance in air ( $R_0$ ). At operating temperature,  
268 the model can be simplified to [34, 35]:

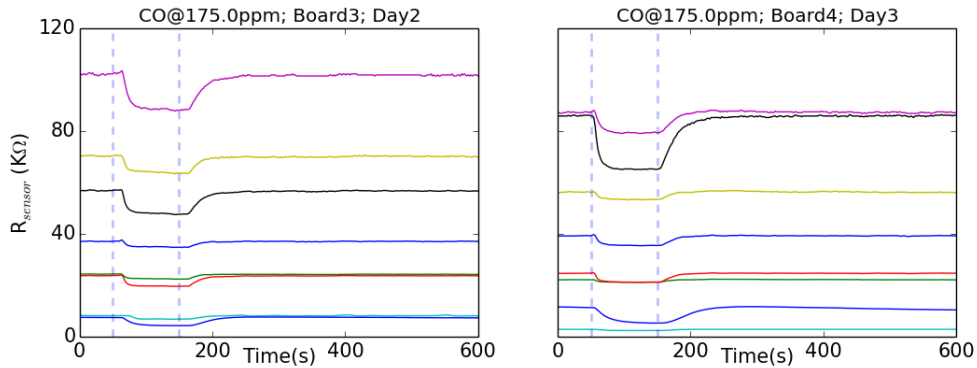
$$\log\left(\frac{R_0 - R_S}{R_S}\right) = \log(s) + \beta \log(c) \quad (3)$$

269 where both,  $s$  and  $\beta$  are parameters that depend on the analyte under test and the sensor's  
270 operating temperature.

271 Using the ten concentration levels of each compound that we acquired each day for each  
272 sensor, we fitted the sensors' responses according to Eq. 3. Therefore, for each sensor, we  
273 obtained 64 pairs of values that are indicative of the variation on the sensor's behavior across  
274 units and across time. Figure 3 shows the estimated value for  $\beta$  for the five sensors placed  
275 in the channel 3 of the sensing boards. The fitted functions for the five sensors are also  
276 presented for CO and Ethylene. The sensitivity to the different volatiles can be considered  
277 as the chemical signature of the sensor. However, from Fig. 3 one can conclude that the



(a) Reproducibility within the same unit



(b) Reproducibility within different units

Figure 2: Acquired time series for different detection units under different gas conditions. The sensors are able to follow the changing gas conditions (dashed vertical lines indicate start/stop of selected gas release). Each volatile induces a different response to the sensor array. Although the design of each sensing unit is the same, the acquired signals differ significantly from one board to another (note prominent baseline shifts and different sensor sensitivities to the same stimuli in the bottom panel).

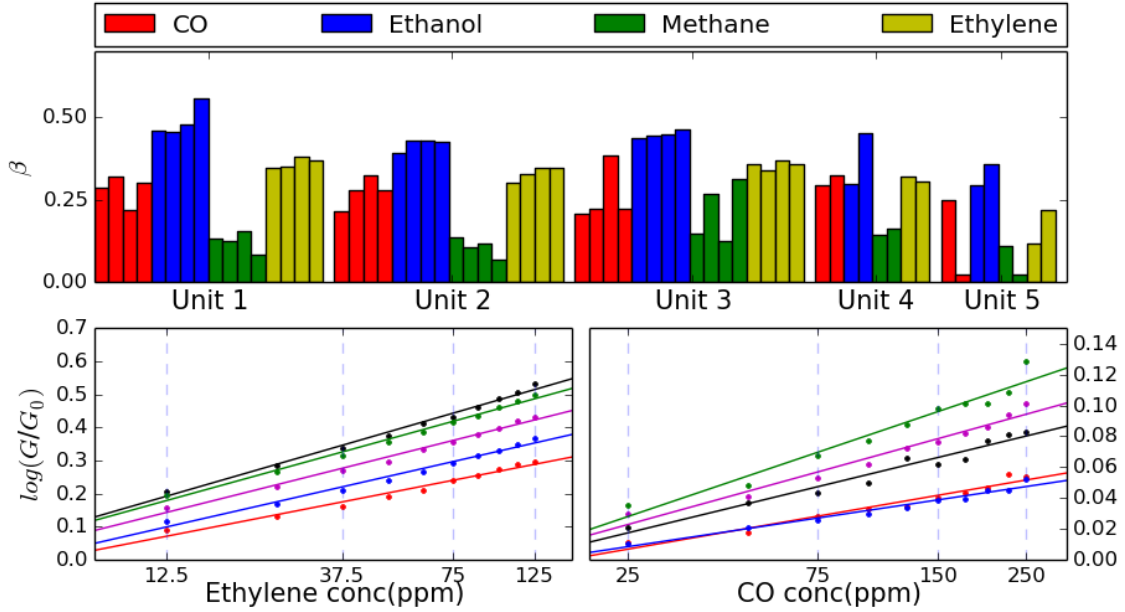


Figure 3: Clifford-Tuma model was used to fit acquired data and estimate  $s$  and  $\beta$  for each sensor and volatile. Top panel shows  $\beta$  for the five sensors of the same type placed in the channel CH3 of the five units. Each sensor is identified by the unit it belongs to (see label *Unit* 1 – 5). Parameter  $\beta$  is presented for the four gases (grouped in colors) and for the number of repetitions of each condition. Bottom panels show fitted models along with acquired data, confirming the quality of the fit. Each color represents a different sensor of the same type. The slope of each linear fit corresponds to a  $\beta$  value presented in the top panel.

278 behavior of the sensors changes across boards and also within the same sensor, since each  
 279 repetition was measured days apart.

#### 280 4.2. Signal mapping

281 We collected data with a master unit and compared the acquired data with the signals  
 282 from a slave unit exposed to the same conditions. Figure 4 shows the captured signals with  
 283 the master unit and the slave unit when Ethylene at 10 concentration levels was presented.  
 284 From a visual inspection, one can confirm the variability between captured signals for sensors  
 285 of the same type: For example, the steady state corresponding to the highest concentration  
 286 level (125 ppm) for the master unit would correspond to a much lower concentration level  
 287 (50 ppm) for the slave unit. This mismatch between sensors' sensitivities would limit the  
 288 prediction ability of the calibration models. However, after applying DS, with only two  
 289 transfer samples, the responses captured with the slave unit are successfully mapped to the  
 290 space of the master unit.

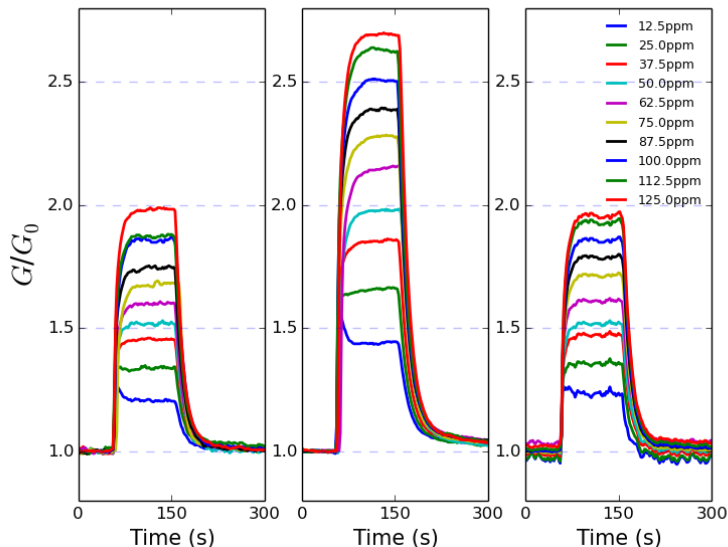


Figure 4: Signals captured for a sensor of the same type (CH7) using a master unit (left) and a slave unit (middle) exposed to Ethylene at different concentration levels. The sensitivity of the sensors differs significantly from unit to unit. The signals captured with the slave unit after DS transformation (right) are mapped to the signals captured with the master.

291 To visualize the captured signals before and after DS transformation, and compare the  
 292 signal spaces of slave and master unit, we projected captured signals using Principal Com-  
 293 ponent Analysis (PCA) for data visualization at a lower dimension space. We applied PCA  
 294 on the data captured with a master unit (see Fig. 5). The first two Principal Components  
 295 for the master unit were plotted. Then, using the same data projection, data acquired with  
 296 a slave unit was added to the plot. One can conclude that the data is grouped in clusters  
 297 for each compound. Every cluster spreads out from a region that represents *clean air* to  
 298 higher concentration levels. Moreover, data acquired with the slave unit results in clusters  
 299 with different sizes and angles from the origin. However, after DS transformation, the data  
 300 from slave unit is better aligned with respect to the master datapoints. This confirms the  
 301 ability of DS to map slave data to the space of a master unit using only two transfer samples  
 302 per volatile.

### 303 4.3. Calibration transfer

#### 304 *Transfer between devices*

305 We built a calibration model selecting a sensing unit as master device and using only cal-



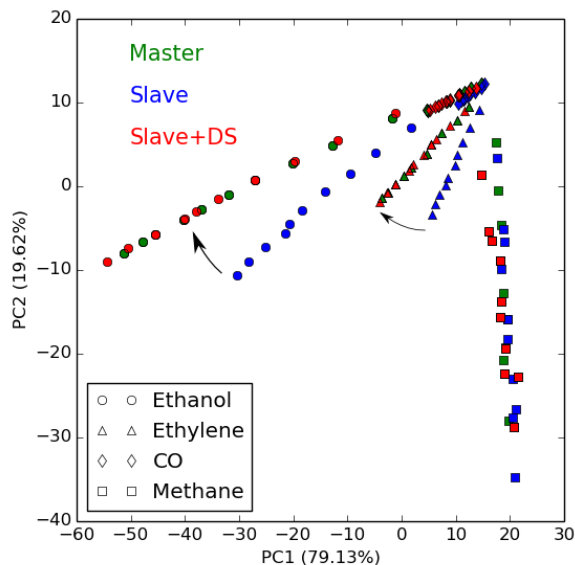


Figure 5: PCA transformation of the signals captured with the master unit (green). Signals from the slave unit (blue) are represented using the same projection. After DS, data captured with the slave unit (red) is successfully transformed to the space of the master unit.

306 ibration samples. The prediction ability of the model was evaluated using the test samples  
 307 that were acquired the same day with the master. We also evaluated the calibration models  
 308 with the test samples but acquired with the rest of the devices (slave). We repeated the  
 309 process until all the units and repetitions were selected to build a calibration model (master)  
 310 and tested with the rest of the devices and repetitions. For each configuration, we computed  
 311 the cross validation error (internal error in training), the error with the test samples of the  
 312 same unit and day, and the error with the samples acquired with other units. To evaluate the  
 313 error with other units, we input the raw signals as they were acquired and the signals after  
 314 DS transformation. Figure 6 shows the distributions of obtained prediction errors after 200  
 315 repetitions (samples acquired with unit 5 when exposed to methane were discarded as acqui-  
 316 sition issues resulted in corrupted signals). Since the ranges of presented concentrations were  
 317 not the same for each volatile, errors in the volatiles that were presented at higher concen-  
 318 trations bias the total prediction error. In order to balance the contribution of each volatile  
 319 to the prediction error, the prediction errors were normalized to the maximum concentration  
 320 level presented for each gas. Therefore, in Fig. 6, prediction errors are presented as a relative  
 321 error with respect to the maximum concentration for each volatile. Table 4 details the first

322 and third quartiles of the distribution of errors in *ppm* for each volatile.

323 Several conclusions can be drawn from Fig. 6 and Table 4. First, the trained models show  
324 good generalization since the differences between the error in internal validation and the  
325 error with test samples are not significant. Second, the ability of the calibration models to  
326 predict the concentration of new samples decays when the measurements are performed with  
327 other sensing units. Although for some repetitions one still obtains errors in the predictions  
328 of the same order than when using the master unit, there are noticeable occasions in which  
329 the errors increase dramatically. These high concentration errors result in uncertainty on  
330 the quality of the prediction in test. However, after a DS transformation, using only two  
331 transfer samples, the prediction ability is improved. Actually, prediction errors after DS  
332 transformation are comparable to the errors obtained with test samples (with the master  
333 unit). The median of the error decreases from 17% to 4.7% when DS is applied. The latter is  
334 only slightly higher than the error obtained measuring the same day with the master: 3.9%,  
335 which provides a performance limit for the prediction accuracy of the models.

336 In order to confirm the flexibility of our approach, we evaluated the same methodology  
337 using a different calibration model and several calibration transfer techniques. First, we used  
338 Principal Least Squares (PLS) instead of SVR models. Obtained classification accuracies  
339 showed that SVR outperforms PLS when testing the models with the same unit (12% for  
340 PLS versus 3.9% for SVR). However, the accuracy of the predictions when the models are  
341 transferred to another unit becomes similar for both classifiers (19.2% for PLS, and 17.0%  
342 for SVR). This result indicates that the variability between boards is prominent with respect  
343 to the choice of the regression model. Finally, when DS was introduced to perform data  
344 transfer, accuracies similar to same-unit same-day predictions were recovered: 12.6% for  
345 PLS and 4.7% for SVR. This confirms the ability of DS to recover the prediction accuracy  
346 of different classifiers when extended to other boards.

347 Second, we explored the ability of other calibration transfer techniques. In particular,  
348 we evaluated PDS, OSC, and GLSW that are already implemented in the *PLS\_Toolbox*  
349 [36]. Following the same methodology, and using SVR regression, we compared the obtained  
350 accuracy to DS. Table 5 shows first/third quartiles of the distribution of errors in *ppm* for  
351 each volatile. Prediction errors for the tested calibration transfer strategies show that the  
352 selection of the strategy does not change dramatically prediction accuracies. Best accuracy

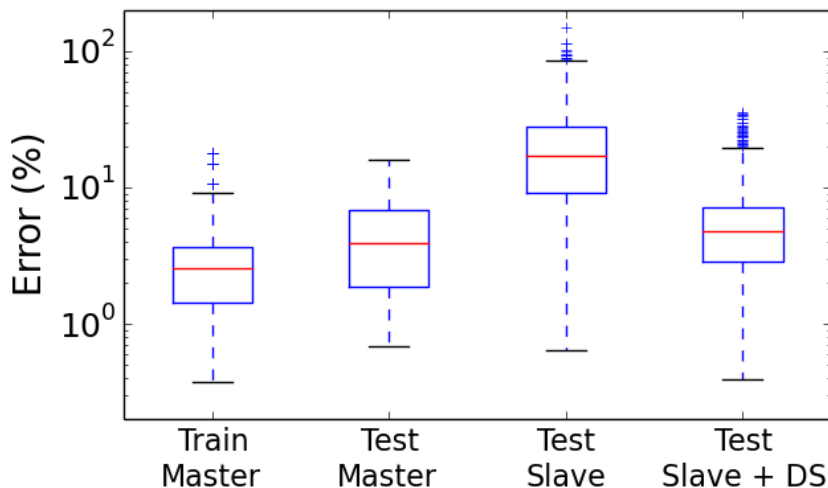


Figure 6: Prediction error distribution of the calibration models when evaluated with data from master/slave units. Error in training (internal validation using samples from the master unit). Prediction error using unseen test samples acquired with the master unit. Prediction error testing samples acquired with slave units, before and after DS transformation. Errors were normalized to the highest concentration level presented for each volatile. Whiskers represent the limit for samples that are further than 3 times the interquartile range from the lower/upper quartiles.

353 predictions were obtained with DS and PDS. Although the simplicity of DS transformation  
 354 and its rapid execution in a microprocessor, results confirm the ability of DS to map two  
 355 sensor spaces.

356 *Transfer within the same device*

357 We tested whether DS can be used to alleviate sensor drift. Similarly to results presented  
 358 in Fig. 6, we applied the signal transformation to measurements acquired with the same unit  
 359 but measured days apart. In particular, we built the calibration models with the calibration

Table 4: Prediction errors for each volatile in training, testing on the same unit, testing on slave units, and testing on slave units after DS. [First Quartile, Third Quartile]

(ppm)	CO	Ethanol	Ethylene	Methane
Train	[7.8,19]	[2.6,4.3]	[1.6,3.4]	[2.9,5.8]
Same unit	[11,21]	[2.3,9.3]	[2.2,3.4]	[3.2,8.1]
Other unit	[36,97]	[16,40]	[12.5,32]	[9.9,29]
Other unit + DS	[13,27]	[4.7,9.4]	[2.7,5.5]	[5.2,14]

Table 5: Prediction errors for each volatile, testing on slave unit after different transfer strategies. [First Quartile, Third Quartile]

(ppm)	CO	Ethanol	Ethylene	Methane
DS	[13,27]	[4.7,9.4]	[2.7,5.5]	[5.2,14]
PDS	[12,29]	[4.6,11]	[2.7,5.3]	[5.2,13]
OSC	[14,40]	[6.5,15]	[4.2,12]	[6,14]
GLSW	[15,36]	[3.5,11]	[3.4,7.4]	[9,16]

360 samples acquired one day (one unit). To quantify the accuracy of the prediction models, we  
 361 tested the models with test samples acquired the same day than the calibration samples, and  
 362 also with samples acquired other days. Figure 7 shows prediction errors in training and using  
 363 samples acquired other days. One can conclude that DS transformation results in prediction  
 364 error drop.

365 We also evaluated the feasibility of a transferred calibration model to be transferred again.  
 366 In other words, we explored whether calibration models can be concatenated in a sequential  
 367 chain of calibration transfers. To test multiple transfer of calibrations, we selected a master  
 368 unit (Unit #3) and a slave unit (Unit #1). First, the calibration model built with the master  
 369 was transferred to the slave unit. Second, the calibration model was transferred again to  
 370 compensate drift within the same slave unit. Figure 8 shows the prediction error of the slave  
 371 unit when the master calibration model is used to predict new samples, with and without  
 372 DS transformation. The prediction error is significantly increased when the model is directly  
 373 used to evaluate samples from another board, and it remains at approximately 30 % for all  
 374 the tested time period. However, if the signals are mapped by means of DS transformation,  
 375 the prediction errors remain of the same order than in the master unit. Therefore, master  
 376 calibration models can be transferred to slave units, which in turn can be transferred at  
 377 desired time intervals to counterattack sensor drift.

### 378 *Continuous monitoring applications*

379 In the previously explored scenarios, either when calibration transfer was evaluated be-  
 380 tween different sensing units or within the same unit, we considered that the complete signals  
 381 were available. However, such assumption is not realistic for continuous monitoring applica-  
 382 tions, in which the sensing unit is measuring continuously the environment and a reference

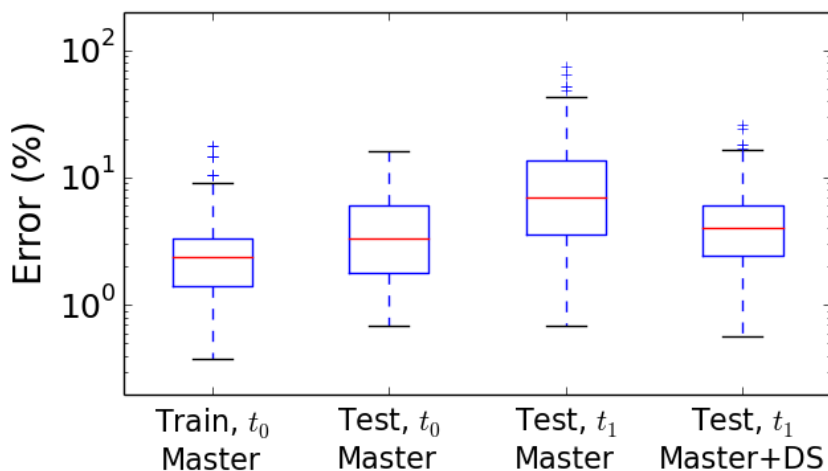


Figure 7: Prediction error distribution of the calibration models when evaluated with samples from the same unit acquired at different times. The sensor array, after some time, can be considered as another virtual device with deviated specifications with respect to the original system. Error in training (internal validation using training samples). Prediction error using unseen test samples acquired the same day than the training samples. Prediction error testing samples acquired days apart (before and after DS transformation). Errors were normalized to the highest concentration level presented for each volatile. Whiskers represent the limit for samples that are further than 3 times the interquartile range from the lower/upper quartiles.

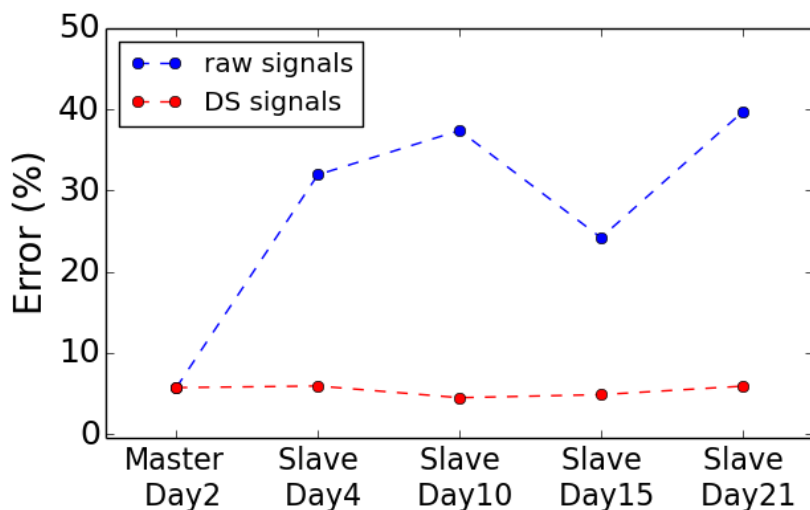


Figure 8: Prediction error when the master calibration model is transferred several times. The master model is transferred to a slave unit, and the resulting model is transferred again to mitigate drift effects. When the signals are mapped with a DS transformation, the prediction errors retain the error of the master unit.

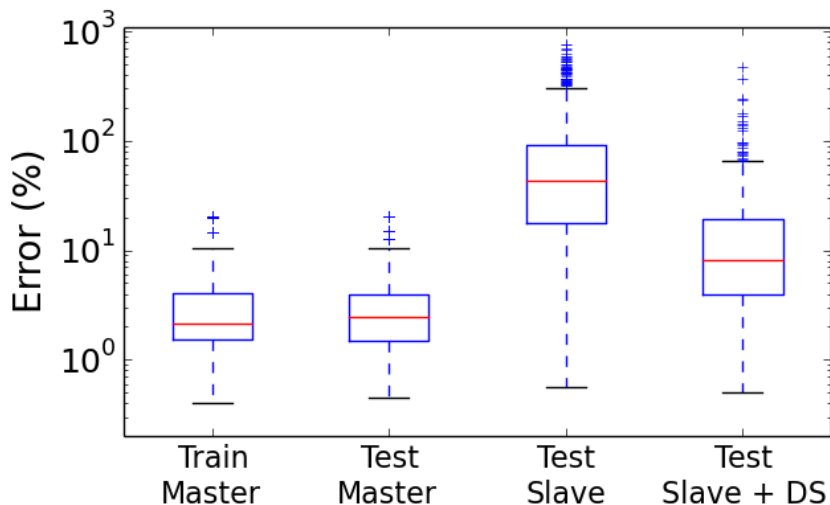


Figure 9: Prediction error distribution of the calibration models for continuous monitoring scenarios. Baseline and transient parts of the signal are not considered. Error in training (internal validation using samples from the master unit). Prediction error using unseen test samples acquired with the master unit. Prediction error testing samples acquired with slave units, before and after DS transformation. Errors were normalized to the highest concentration level presented for each volatile. Whiskers represent the limit for samples that are further than 3 times the interquartile range from the lower/upper quartiles.

383 is not presented before measuring a new sample. Therefore, baseline and transient portions  
 384 of the signal are not acquired systematically at the beginning of each new measurement. To  
 385 simulate monitoring tasks, we only considered the steady state portion of the signal and we  
 386 repeated the same methodology to evaluate the calibration transfer between units. Figure 9  
 387 shows prediction errors when baseline and transient portions of the signal are omitted. It can  
 388 be seen that the prediction errors increase up to 8 times the highest concentration level. Al-  
 389 though DS transformation reduces prediction error, the calibration models do not guarantee  
 390 an accuracy within the same order of magnitude of the presented concentrations.

## 391 5. Discussion and conclusions

392 We built five twin sensing units that included eight MOX gas sensors each. We exposed the  
393 units to the same chemical conditions such that each day the device under test was exposed  
394 to 40 mixtures of air with Ethylene, CO, Ethanol, or Methane at 10 concentration levels  
395 each. The result is a dataset that is unique since it was generated with 5 standalone sensing  
396 units that were exposed to the gas conditions separately, with several repetitions across time.  
397 Therefore, the generated dataset is suitable to study sensor diversity, calibration transfer  
398 techniques between units and time drift effects. Moreover, the dataset is made publicly  
399 available.

400 We explored sensor tolerance by fitting sensor responses to the Clifford-Tuma model and  
401 comparing the obtained sensitivities. Our results show a mismatch between the responses  
402 of sensors of the same type. In particular, sensor mismatch becomes prominent in baseline  
403 shifts. Actually, such sensor variability is confirmed by the sensor manufacturer. MOX gas  
404 sensors provided by Figaro [37] exhibit significant tolerance on sensor resistance measured  
405 in air (baseline) and sensitivity: According to the *TGS2602* data sheet, for example, sensor  
406 baseline ranges between  $10K\Omega$ – $100K\Omega$  and the relative change in sensor resistance at 10 *ppm*  
407 of Ethanol ranges between  $0.15 - 0.5\Omega/\Omega$ .

408 Our results showed that the mismatch between sensors limits calibration models trans-  
409 ferability from a master unit to a slave unit. We built hierarchical calibration models that  
410 included a classifier to determine the gas type and regressors to estimate the concentration  
411 level of the presented chemical compounds. Such calibration models allowed us to quantify  
412 the quality of calibration transfer considering the combined task of compound identification  
413 and concentration quantification. We found that calibration models become inefficient when  
414 are used to evaluate samples acquired with other units. However, DS transformation success-  
415 fully maps slave signals to the space of the master unit, thereby enabling calibration transfer  
416 between units.

417 We showed that DS successfully applies a signal transformation across twin units and  
418 within the same unit measuring days apart. This result confirms that calibration transfer  
419 techniques can be also applied to compensate drift. Actually, a device after some time can be  
420 considered as another virtual device with deviated specifications with respect to the original

421 system. Hence, one can easily adopt calibration transfer strategies to counteract drift. We  
422 also showed that calibration transfers can be concatenated and that slave units preserve, with  
423 no significant increase, prediction errors of the master. This scenario of multiple calibration  
424 transfers would be very desirable for mass production of units: One could train calibration  
425 models, which could be transferred between units or within the same unit at different times.  
426 As a result, a network of standards keeping track of the distance in terms of the number of  
427 calibration transfers performed from the original master would be available.

428 Although DS applies linear transformation to map signals between units, non-linear be-  
429 havior captured by the calibration model trained with the master unit is still being transferred  
430 to the calibration model for the slave unit. We remark, that in fact, calibration models that  
431 we trained are non-linear (SVM with RBF kernels, for example). We explored the accuracy  
432 of the transferred models with two transfer samples per compound. Although the number  
433 of transfer samples could be increased, the cost of the calibration for the slave unit would  
434 be higher and the expected improvement in the performance is marginal. Actually, in our  
435 dataset, as shown in the PCA decomposition, the samples corresponding to each gas appear  
436 aligned. Therefore, two points from the master and the slave spaces will suffice to map the  
437 signals to the new space. Hence, although the simplicity of DS, we showed that it can be  
438 used to transfer calibrations between devices and it can help to mitigate drift effects, thereby  
439 delaying recalibration of the devices as well. However, sensor systems with higher non-linear  
440 behavior or larger variability between units may need larger number of transfer samples to  
441 map sensor spaces using a more dense grid of transfer samples.

442 We also explored continuous monitoring scenario by considering only steady state portion  
443 of the signal. The results showed that one needs to include a reference measurement (clean  
444 air, for example) before sample presentation to successfully map the signals from the slave  
445 unit to the master space. To deal with continuous inputs, regressors with tapped-delayed  
446 or non-linear transformation of temporally varying input signals to a higher dimension have  
447 been proposed [38, 39, 40, 41, 42]. A route to apply calibration transfer in devices that  
448 sample continuously would be the combination of such approaches with DS transformation.

449 Finally, we tested the performance of different popular methods for calibration transfer,  
450 namely DS, PDS, OSC, and GLSW. Our results indicate that, although the selection of  
451 the methodology does not change classification accuracy dramatically, DS and PDS are the



452 methods that provide best calibration transfer among units. This result is in agreement  
453 with recent studies on calibration transfer based on MOX sensor arrays [43] and NIR spec-  
454 troscopy database [11]. In the mentioned works, DS or PDS also outperform other explored  
455 calibration transfer methodologies. This may yield to think that DS, or PDS, are the best  
456 calibration transfer techniques. However, other calibration transfer techniques may provide  
457 better results when examined on sensing systems with different cross-sensitivity among their  
458 sensing elements, in calibrations performed with higher number of training samples or train-  
459 ing conditions, or when the number of transfer samples becomes larger. The best choice for  
460 calibration transfer is probably database sensitive and providing guidelines for its selection  
461 requires further study on databases, acquired with sensory systems of different technologies  
462 and for different classification or regression tasks.

463 All in all, for a successful calibration transfer, one needs to acquire transfer samples with  
464 the slave unit. Provided that the calibration model for the master unit is already available,  
465 slave units trained with smaller set of transfer samples coupled with DS provide similar  
466 prediction error than when they are trained with all the set of calibration samples. The lower  
467 number of samples needed to build a calibration model will reduce the cost of calibration  
468 of new units, alleviating thereby industrial costs. Moreover, calibration transfer techniques  
469 could be coupled with other calibration methodologies that aim at reducing calibration costs  
470 by selecting the best training examples, or with active sampling strategies to adapt operating  
471 sensor temperature to mirror sensor behaviors [44, 45, 46].

## 472 **Acknowledgments**

473 This work was partially funded by the Spanish MINECO program, under grants TEC2014-  
474 59229-R (SIGVOL) and PCIN-2013-195 (SENSIBLE), and from the European Community's  
475 ENIAC Joint Undertaking program, under Grant agreement no. 621272 (SAFESENS). JF,  
476 LF, AGG, and SM are part of a consolidated research group recognized by the Generalitat  
477 de Catalunya (2014-SGR-1445). JF acknowledges grant 2013 Beatriu de Pinós-B 00190. We  
478 thank Dr. Emre Neftci for his helpful comments and reviewing the manuscript.

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619 the brain, and chemical sensing and machine olfaction applications based on bio-inspired  
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627 using microsystem technologies. Dr. Marco research has produced over 100 articles in peer-  
628 reviewed archival journals.