

Dynamic neural network architectures for on field stochastic calibration of indicative low cost air quality sensing systems

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ABSTRACT

In the last few years, the interest in the development of new pervasive or mobile implementations of air quality multisensor devices has significantly grown. New application opportunities appeared together with new challenges due to limitations in dealing with rapid pollutants concentrations transients both for static and mobile deployments. In this work, we propose a **Dynamic Neural Network (DNN) approach to the stochastic prediction of air pollutants concentrations by means of chemical multisensor devices.** DNN architectures have been devised and tested in order to tackle the cross sensitivities issues and sensors inherent dynamic limitations. Testing have been performed using an on-field recorded dataset from a pervasive deployment in Cambridge (UK), encompassing several weeks. The results obtained with the dynamic model are compared with the response of the static neural network and the performance analysis indicates the capability of the on-field dynamic multivariate calibration to ameliorate the static calibration approach performance in this real world air quality monitoring scenario. Interestingly, results analysis also suggests that the improvements are more significant when pollutants concentration changes more rapidly.

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1. Introduction

Recently, new sensing technologies and systems for achieving a truly pervasive air quality (AQ) monitoring capability in cities are being developed [1]. The primary driver is actually the current coarse grained and sparse AQ measuring mesh that is based on costly and cumbersome conventional analyzers. These are challenged by the need for obtaining a detailed and representative map of the true concentrations of pollutants in the city. **As a matter of fact, the current approach is clearly unable to cope with the local complex chemical and fluid dynamic effects occurring in the urban landscape.** Emission of air pollutants is caused by different anthropogenic processes which can be categorized into source groups like car traffic, industry, power plants, and domestic fuel. Emitted air pollutants are dispersed and diluted in the atmosphere [2]. Chemical reactions producing, for example, photochemical ozone, occur frequently [3,4]. Dispersion and dilution of air pollutants are strongly influenced by meteorological conditions, especially by wind direction, wind speed, turbulence, and atmospheric stability. Topographical characteristics and urban structures like street

canyons, for example, have a significant influence on these meteorological parameters. Eventually, along with chemical reactions, dispersion and dilution processes result in an ambient air pollution distribution which shows concentrations of different substances significantly varying with regard to time and space.

Low cost chemical multisensory devices seem a promising answer to the needs; however their performances are hindered by several issues including specificity and stability of transducers. Actually, chemical microsensors devices are, in general, subjected to interferent gases that either boost, or depress, their response, to the target gas [5]. For this reason, any attempt to rely on a monovariate calibration procedure neglecting interferents influence is prone to failure [6]. Information on interferent gases should be exploited by calibration procedure in order to solve this issue. Chemical microsensors response generally changes in time due to several effects including poisoning and environmental variables sensitivity [7]. As a consequence, long term stability is a significant concern given the need to reduce maintenance burden on a pervasive network of AQ analyzers.

Although the lab based calibration approach, pioneered in [38], allows for fully controlling the range and the ratios of pollutant concentrations to which the sensor array is subject, the exact reproduction of field atmosphere is actually precluded by its inherently complex nature. The number of different pollutants and interfer-

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ents concentrations to consider, in order to cover the experimental space and fully characterize sensors response, may easily explode. For example, in Ref. [39], Zhang et al., tried to adequately cover possible RH and T variation ranges using twelve different value combinations at different pollutant concentrations. Eventually, they generated more than 100 samples while in lab calibrating their multisensor device for single pollutant concentration estimation (formaldehyde) in indoor air quality applications. The straightforward use of on-field recorded data may allow solving this issue. On the other hand the concentrations ranges, in this case, are out of the researcher's control. Moreover it could, in principle, reflects a local situation limiting the use of the data for the deployment in different locations. Nonetheless, **multivariate calibration with on-field data is being currently reported as an efficient tool** [6,8].

Actually, **machine learning (ML) is a promising approach to obtain a multivariate calibration** [8]. Flexibility of ML tools can be a decisive asset compared with parametric techniques that require the assumption of a specific hard model form.

Non-linearity in a data set can be detected with graphical methods but identification of its source is more challenging and sometimes impossible. Thanks to their ability to learn and derive input-output relationships from the presentation of a set of training samples, ML tools avoid the time-consuming and possibly expensive task of hard model identification. Generalization property of ML tools, that is, the capability of a model to produce a valid estimate of the correct output when a totally new input is presented, is a further driver advocating its use with on field recorded data [37]. However, a major drawback is the possibility to overfit calibration data negatively affecting generalization capabilities. Most machine learning can perform at least as well as any other technique in terms of prediction, but a major criticism remains their black-box nature. Model interpretation for a Neural Network, for example, is still considered much more complex than for PLS or PCR models. This is due to the operations (summation and projection on transfer function) performed subsequently in the hidden and output layer, that prevent one from deriving simple analytical expressions between input and output variables.

The usually proposed methodologies, however, are trained to produce instantaneous calibration that do not consider the typically slow and sometimes non-linear (in time) dynamic behavior of chemical sensors [6,9]. In our specific scenario this means that significant but relatively short pollution bursts, due for example to moving car or trucks emissions, traffic light related stops, passage of plumes occurring in static deployments or plume crossing by a mobile sensors, could be filtered out, masking the real magnitude of the phenomena. This may, in turn, affects time average indicators used for pollution evaluation. Of course these limitations become extremely significant for mobile applications like personal pollution exposition evaluation. In fact, mobile platforms, as they navigate relatively to the source, may cross pollutants plume several times, experiencing sudden and rapid gas concentration transitions [10]. A rapid detection of the concentration changes is hence paramount for personal exposure quantification.

In this view, rapid transient response analysis is extremely relevant. In order to capture the information contained in the dynamics of the gas sensors, artificial olfaction practitioners relies on a fixed, predefined and controlled experimental protocol. Typically, before and after sample presentation, the sensor array is exposed to a gas reference (clean air) to capture the rising and decaying signal transients [5,11]. Then, the complete set of acquired time series, or a set of features extracted from the time series [7,12–15,31] itself, is used to train a calibration model [16,17]. In both case, such a calibration methodology requires to capture the sensors signals over a measurement time defined beforehand during a controlled variation of the pollutants concentrations and environmental variables. As a result, the model prediction for a new sample can only be provided

after such a measurement is complete. This process, however, is extremely difficult to reproduce when operating in the field requiring complex delivery systems. It is necessary to alternate the gas sample with the reference baseline and the composition of the gas samples has to remain constant, during the whole sample presentation. In open sampling systems the sensor array is exposed directly to the environment with no measurement test chamber, making the system sensitive to flow turbulence [18]. A method that is able to provide continuous and accurate prediction according to the present and past states of the sensor array would be better suited for such applications [34–36]. Only a few works have explored quantitative prediction algorithms for continuous gas concentration estimation with fast varying concentration inputs. Usually, they were based on a regressor with tapped-delayed input to provide a finite and fixed memory to the system.

In particular, tapped-delay predictors have been explored with linear (finite impulse response filters) and polynomial regressors (Wiener regressors) (Refs. [19,33]), neural networks [20–22], or support vector regressors (Refs. [21,32]).

In Ref. [19], Pardo et al., among the firsts, proposed and compared different nonlinear inverse dynamic models of gas sensing systems for quantitative measurements. With respect to our scenario, a measurement chamber is used to obtain the gas sensor readings, which implicitly modifies the dynamic properties of the measured signals, and the acquisition frequency is too low (one sample per minute) to reflect the fast and highly dynamic changes of the gas concentration in open sampling systems. Anyway, we couldn't find any work based on the use of faster on field analyzer.

In Ref. [16], Muezzinoglu et al. proposed an approach to accelerate the odor processing using transient features. Recording the response of metal-oxide sensors array, subjected to a specific analyte in a constant flow, they computed the correlation among a transient features and the steady-state resistance. This correlation was used to accelerate standard quantification and classification of analytes.

Again, in Ref. [23], the group of D'Amico and Marco proposed a so-called ARMA (Auto Regressive Moving Average) system and multi-exponential models, for reducing the time necessary to calibrate a sensor array, taking into account the behavior of a metal oxide (MOX) semiconductor gas sensor. A dynamic model based on multi-exponential decays allowing a net reduction of the calibration time is introduced and discussed. Nevertheless, since the focus is on the calibration of MOX sensors, the dynamic models are only applied to the rise transient signals recorded in Closed Sampling Systems over long time periods (over 800 s). Moving average and Linear system model identification approaches are compared by Vembu et al. with Support Vector Machines using specific devised time series kernels [42]. Tests have been executed by recording temperature optimized MOX responses in a simulated wind tunnel facility. Results highlighted the performance advantage of the proposed approach.

De Vito et al. in Ref. [21], proposed a dynamic calibration based on a tapped delay NN architecture operating on instantaneous and past sensor response samples. In their experimental settings, training samples were obtained by rapidly changing concentrations of multiple gases and environmental conditions. Tests were conducted in the same lab settings confirming the capability of such architectures in improving quantification performance in presence of a slow sensors dynamics. However, in such an architectures the memory is fixed by the length of the TD line (or duration of the delay) and has to be optimized in calibration phase. The effectiveness of this methodology in real world setting where duration and dynamic characteristics of transients are unpredictable is at least controversial and has never been proved.

In Refs. [24,25], the authors proposed the use of reservoir computing (RC) algorithms to overcome the slow temporal dynamics of

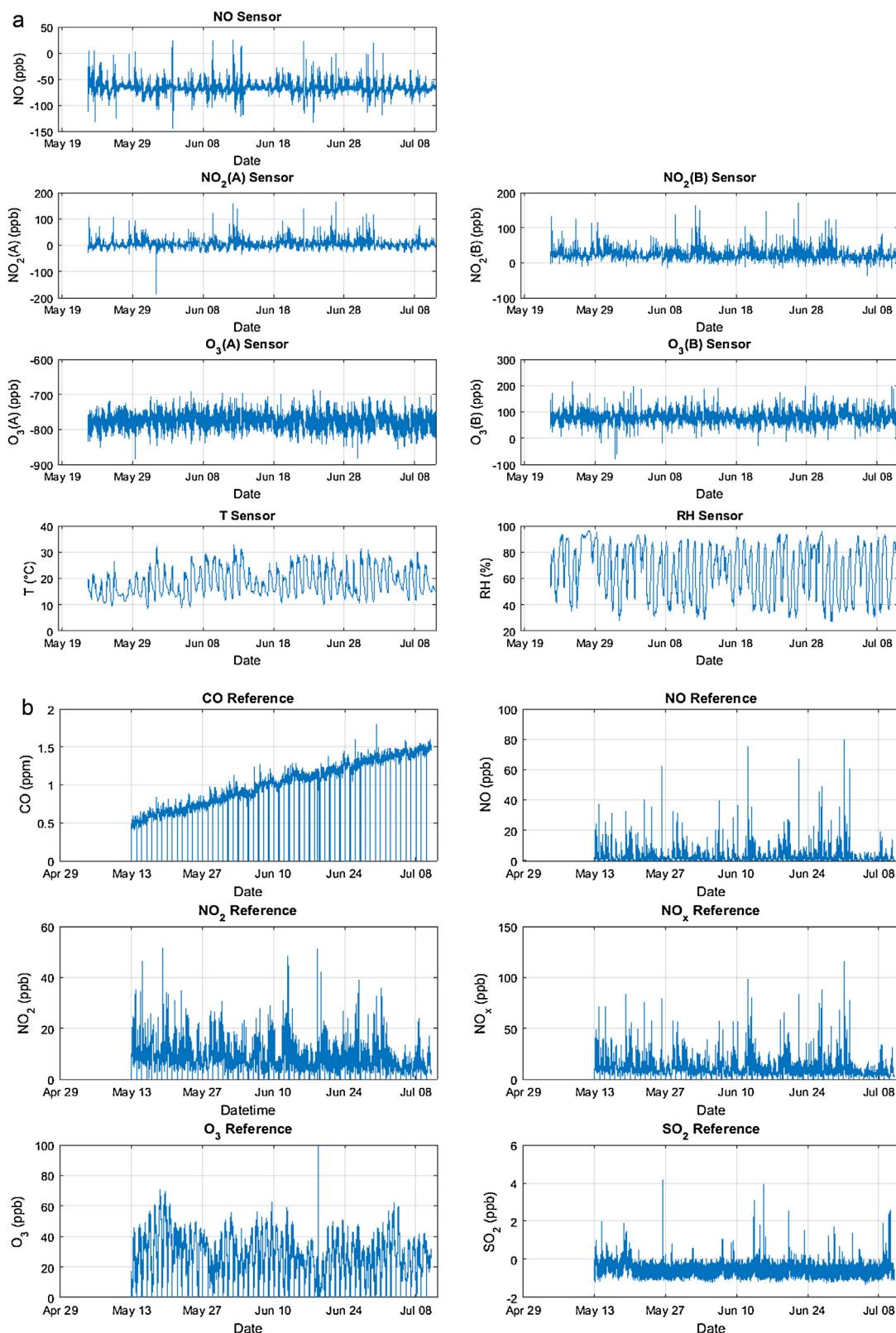


Fig. 1. (a) Plot of uncalibrated SnaQ EC Sensors Data (Temperature Correction apply) versus time (seconds), plus Temperature (T) and Humidity (RH) sensors. The daily oscillation pattern is evident. (b) Plot of reference concentration data (Roof Dataset). The CO concentration data present a linear drift (with) time and it is not used in this work.

chemical sensor arrays, allowing identification and quantification of chemicals of interest continuously and reducing measurement delays. Moreover, the proposed architecture allows to automati-

cally “learn” the time delay line length and density reducing the needed optimization efforts. The provided results were based on two datasets: one generated with synthetic data and the other

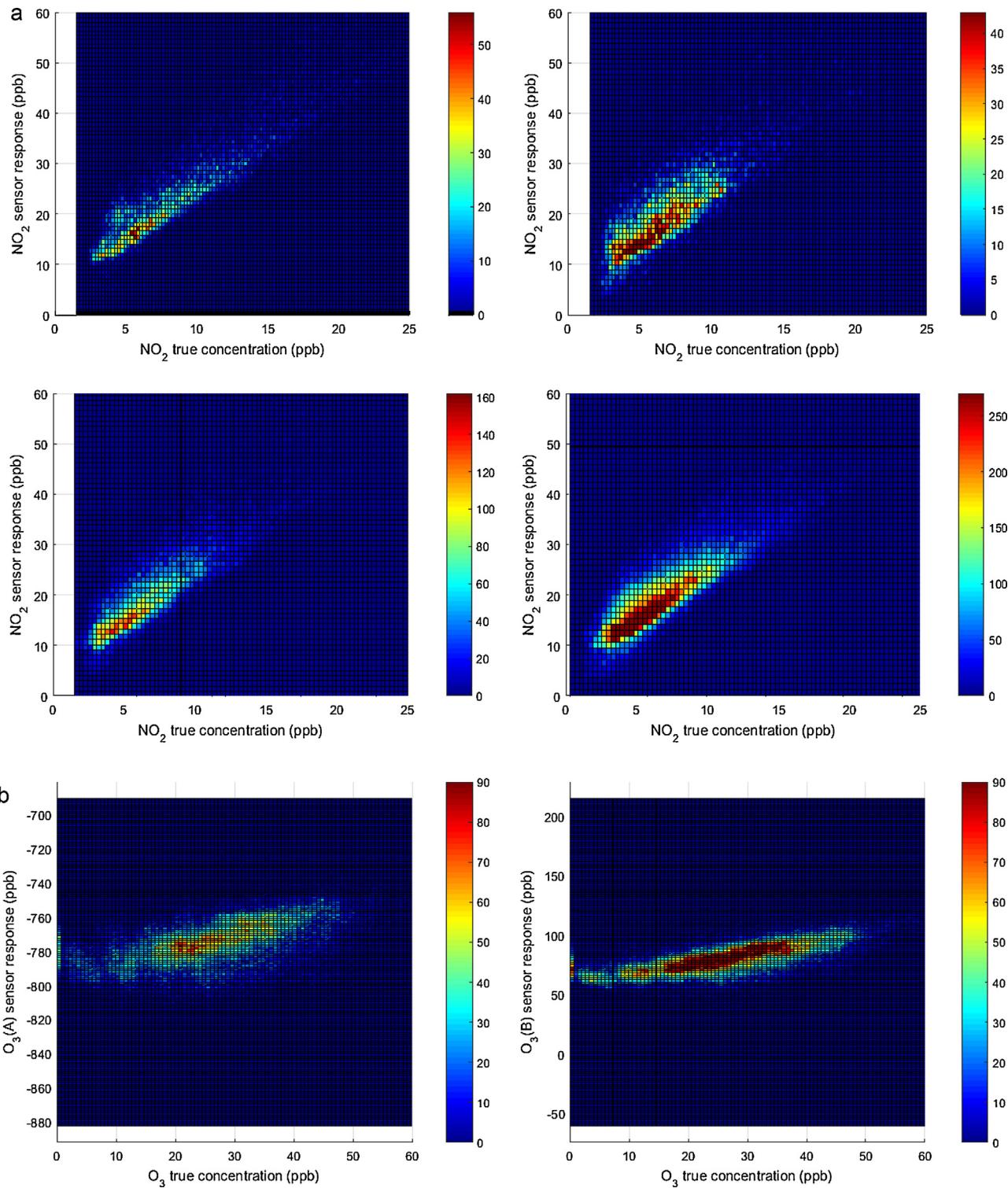


Fig. 2. (a): Data distribution shows significant correlation among target gas concentration and sensor raw values, for NO₂ gas concentration (color code is the histogram of the readings). The first figure shows a scatter plot in the first week ($R=0.88$), the second, provides the relationship as computed during the fourth week ($R=0.81$). The third picture relates with third and fourth week, below used as test set ($R=0.82$). Finally, the fourth picture shows correlation plot over the entire dataset ($R=0.85$). (b): Data distribution shows inferior correlation among target gas concentration and sensor raw values for O₃ gas concentration (color code reflects histogram of the readings). The first figure shows the correlation among target gas and O₃ (A) sensor response ($R=0.51$), the second, considers O₃(B) sensor response ($R=0.67$).

acquired from actual gas sensors. They recorded time series of MOX sensors while exposed to binary gas mixtures where concentration levels changed randomly over time.

In the robotics framework, several efforts have been produced for gas mapping and quantitative calibration using partially

controlled environments. Recently, Monroy et al. described an interesting multicentre effort to provide a probabilistic quantification approach based on Gaussian process [41]. They validate the approach within a simulated field environment, in which ethanol is emitted and transported by an air flow towards MOX sensors

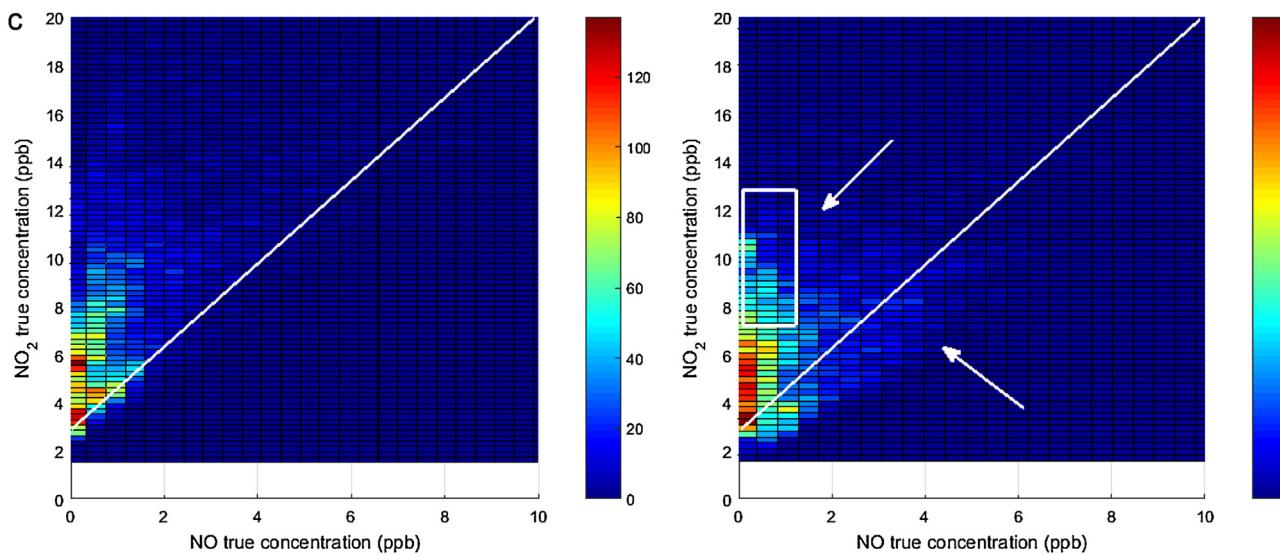


Fig. 2. (c): Mutual distribution of reference data for NO and NO₂. Evidence of complex relationship among the two gases is observed in different weeks with low correlation data ($R=0.55$ in the first and $R=0.52$ in the fourth week). During the fourth week, in particular, the picture shows significant differences with the appearance of a number of occurrences in the two highlighted areas (area inside the white rectangle and below the white line) that were barely populated in the first week.

located in a room. A Photo-Ionization Device (PID) VOC sensor is used as a reference.

Summarizing, to the best of our knowledge, dynamic calibration approaches, known for lab based measurements, has never been validated for on-the-field deployed chemical multisensor devices where they have to deal with the uncontrollable exposure to multiple analyte concentrations over several weeks.

In our opinion, the lack of high speed validated reference measurements is one of the primary factor limiting this development. As a matter of fact, most of the reference stations provide validated readings of hourly concentrations averages limiting validation of high sampling frequency devices. Furthermore, in order to reduce issues and errors related with turbulent flow exposure of both indicative and reference measurement systems, both systems has to analyze the same air almost simultaneously.

In this contribution, we can analyze the results of a calibrated multisensing device that was co-located with a 1 min sampling frequency conventional analyzer deployed on the field in the city of Cambridge (UK) for several weeks. We propose and test a Dynamic Neural Network approach as a dynamic multivariate calibration tool in a real world deployment, thus extending the results available for static multivariate on-field approaches. Section 2 describes the experimental settings and the results of a preliminary data analysis. Section 3 describes the proposed calibration methodology, whose results are presented in Section 4. Finally, in Section 5, conclusions are drawn.

2. Experimental settings

The Dataset here used has been extracted from a specific deployment of multisensory devices (SnaQ systems, see Ref. [26] for detailed description of the deployment) developed by a partnership led by the Center for Atmospheric Sciences (CAAS) of University of Cambridge (UK). The multisensory device is equipped with the following sensors units:

- two different NO₂ EC sensor units (Alphasense NO₂-B4 termed in the following as NO₂(A) and NO₂(B));
- one NO Alphasense EC sensor unit (Alphasense NO-B4);
- two different O₃ Alphasense EC sensor units (Alphasense O₃-B4 termed in the following as O₃(A) and O₃(B));

- T, RH sensor units;
- wind speed and direction unit.

One of the devices, deployed in the city Centre of Cambridge, was located on the roof of the Chemical Dept. together with a conventional reference station operated by CAAS. This station relies on chemiluminescence and spectrometer based analyzers. While the sampling period of the SnaQ system was set at 20 s, the reference station provides ground truth readings of target gases at 60 s intervals. The conventional station target gases were CO, NO, NO₂, NO_x, O₃, SO₂ and Total Oxidants gases. It is worth to note that electrochemical sensors, when operating at low ppb levels, are also prone to interference issues. Specifically for the SnaQ sensors, a known cross sensitivity is reported for, respectively, O₃ and NO₂ [27,28].

Two different experimental methodologies concerning time-frame harmonization procedures have been considered. A preliminary work has been carried out by averaging three instances of raw sensor readings belonging to the 60 s interval before each conventional analyzer sample. In this work, instead we considered all raw instantaneous sensors readings for calibration purposes, comparing the estimations results with the conventional analyzer samples when available (one out of three sensor readings).

Baseline and temperature correction by datasheet procedure have been implemented. Furthermore, a preprocessing step has been conducted to delete reference station calibration periods during the night.

In order to build a suitable dataset, five weeks of continuous measurements have been extracted by the available recordings. The first week of measurements (10 ksamples) have been set apart as a training set for statistical machine learning tools, while the remaining four weeks of data have been used for validation (10 ksamples) and testing purposes (30 ksamples). This partition allows for evaluating the performance of the trained model including possible medium term sensors drift effects.

2.1. Preliminary data analysis

Early data analysis revealed that the monitored zone has significant daily variations of RH and T. In particular, it was frequent to observe daily variation of RH from 20% to 80% and temperatures varying from 10 °C to 25 °C (see Fig. 1a). Of course this

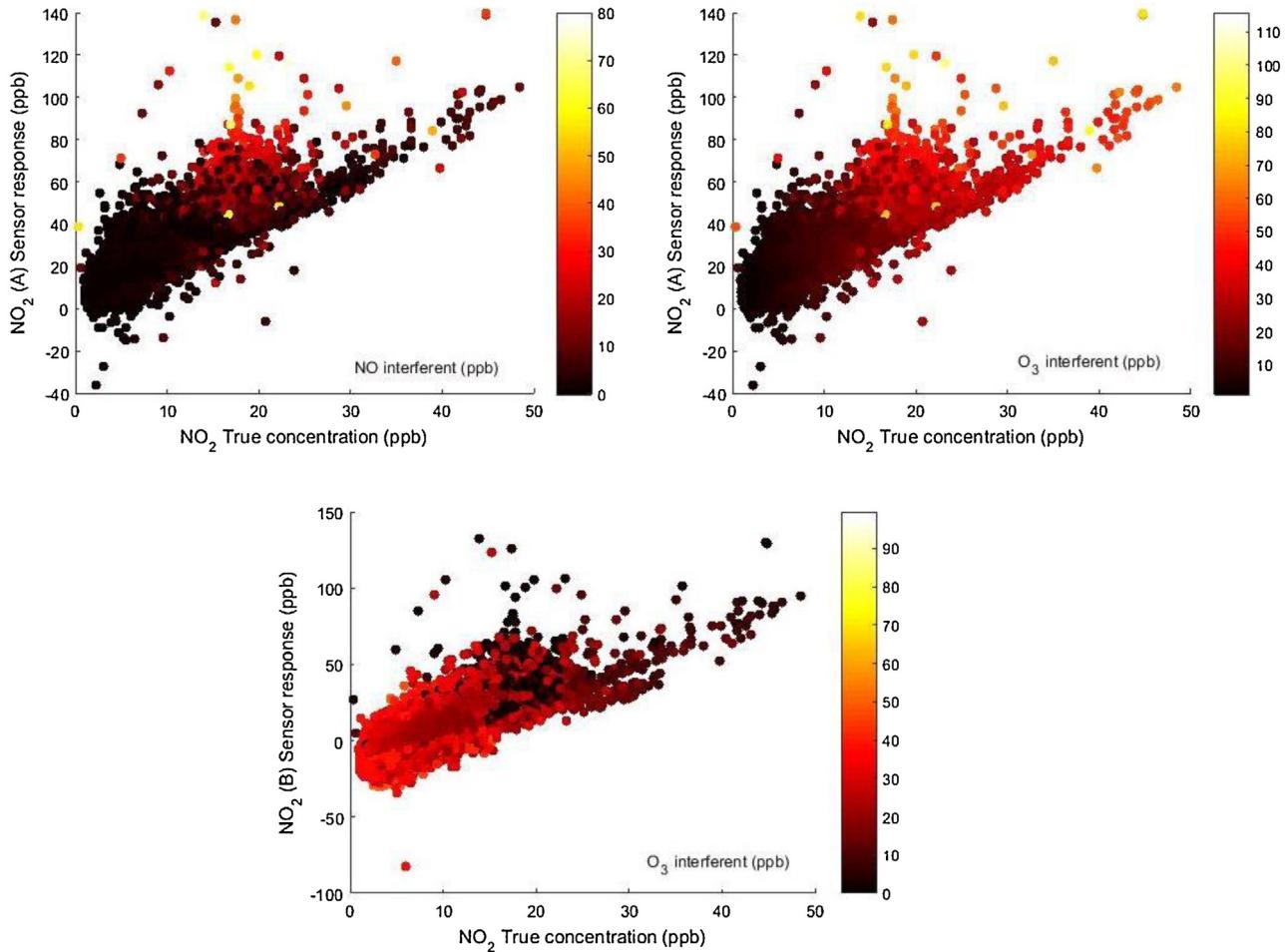


Fig. 3. Scatterplot of NO₂ concentration, considering: (a) NO as interferent (NO₂ (A) sensor reading); (b) O₃ as interferent (O₃ (A) sensor reading); (c) O₃ as interferent (NO₂ (B) and O₃ (B) sensors readings). Dot color encodes the concentration of the interferent gas (ppb).

prove challenging for the microsensors array subjected to varying environmental conditions. In the same period, the minimum temperature recorded was less than 8 °C, with the maximum being about 30 °C.

The Roof conventional analyzer dataset (Fig. 1b), generally depicts a high sensitivity of the SnaQ sensors and significant correlation among sensors raw values and target gases, except for O₃ sensors (Fig. 2a and b). However, evidence of concept drifts is present (Fig. 2c). Furthermore the relationship among some of the sensors and their target gas seems to show clues of the above mentioned cross sensitivities. Actually in Fig. 3a it is possible to observe a positive shift in the response of NO₂(A) sensor, in presence of relatively high NO concentrations. In presence of different concentrations of O₃, NO₂(A) and NO₂(B) seems to modify their response very differently.

3. Dynamic multivariate calibration

The considered multivariate calibration technique includes the use of dynamic and nonlinear supervised machine learning tools. We focused our attention on DNNs in order to exploit their capability to build a dynamic multivariate model of the sensor response. Actually, our aim is to use them to overcome static network limitations in high speed transients evaluation simultaneously tackling sensors cross-specificities. Since, DNNs can be designed to operate as a multivariate regression so to provide pollutant concentration estimations on the basis of raw sensor readings.

In this work, we tested the performance of two particular architectures, comparing the obtained results with the commonly used static Feed Forward Neural Network (FFNN). The first selected dynamic architecture has been a **Time Delay Neural Network** (TDNN); a **Nonlinear Autoregressive with exogenous inputs network** (NARX) was the second [30]. DNNs architectures include a tapped delay line that allows using as inputs both past sensor readings and past output values. In this way they can exploit the informative contents of both sensors and process dynamics.

3.1. Feed forward neural network

FFNN is the most popular and most widely used neural model in many practical applications. It consists of a (possibly large) number of simple neuron-like processing *units*, organized in *layers*. Every unit in a layer is connected with all the units in the previous layer. These connections are not all equal: each connection may have a different strength or *weight*. The weights on these connections encode the knowledge of a network. Often the units in a neural network are also called *nodes*. The structure of a feedforward neural network is represented in Fig. 4a.

In this work, we considered a FFNN model, with a sigmoid activation function for the neurons in the hidden layer. The network core was based on a Matlab® *tansig* neurons hidden layer with a single output layer designed to provide estimation of a single pollutant every 1 min [29]. Model complexity is basically controlled

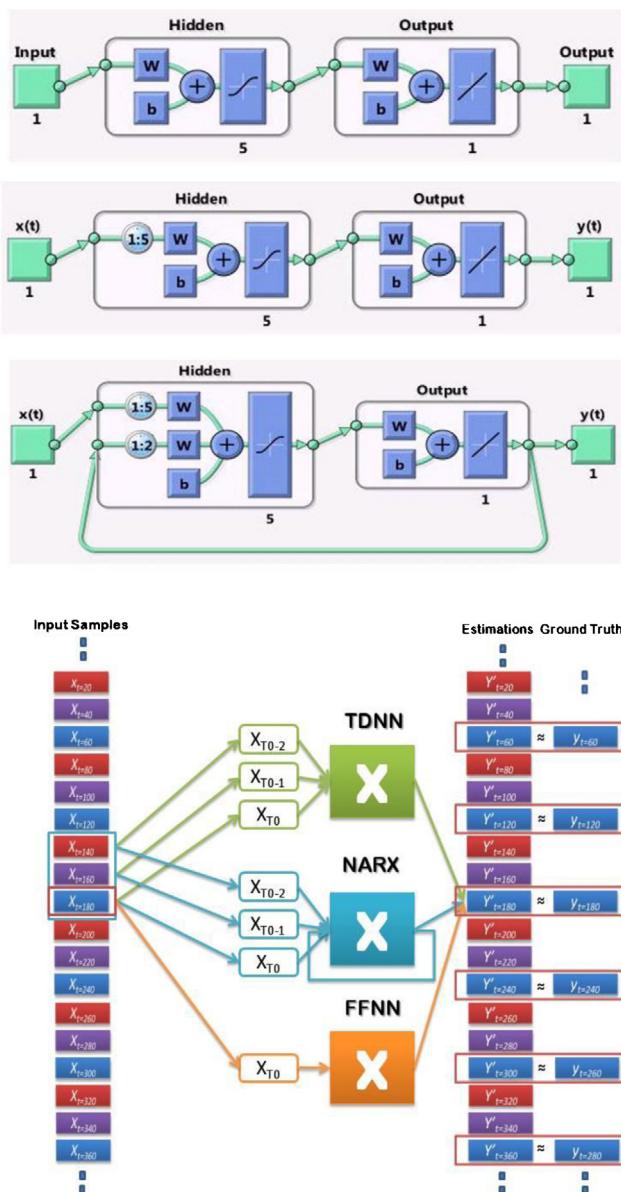


Fig. 4. Relevant examples of FFNN (a), TDNN with $TDL = 5$ (b), NARX with $TDL = 5$, $FDL = 2$ (c) networks architecture. (d) Depicts the *modus operandi* of the three architectures while estimating y_t with y_t' by using the input samples x_t with unfolded timeline. In particular, the depicted TDNN and NARX networks have $TDL = 3$ and $FDL = 1$. Note that ground truth comparison, and hence performance estimation, is only possible at reference station sample rate (1 min) while in principle, the networks could estimate pollutant concentration every time a new input sample become available (20 s).

by the number of hidden layer neurons. In our experiments, We have let it vary in the $HN = [3,5,10]$ set.

3.2. Tapped delay neural network

TDNN consists of a feedforward network with a tapped delay line at the input [30]. This allows the network to have a finite dynamic response to time series sensors data. In our framework, it can be used to analyze and exploit sensor dynamics. A TDNN is typically described as a layered network in which the input of a layer is buffered for several time steps and then fed to the input layer (see Fig. 4b). By the introduction of T time delays, each neuron has access to n input values, corresponding to different sensors array instantaneous response $x(t-nT), \dots, x(t)$.

Summarizing the model complexity is controlled by both TD line length (TDL) and the number of hidden layer. In this paper we have let them vary in the $TDL = [3,6,9]$ and $HN = [3,5,10]$ sets, respectively.

3.3. Nonlinear autoregressive with exogenous inputs network

The NARX net is a nonlinear autoregressive neural model which has exogenous inputs. These systems model the dynamic of a variable (time series) as depending on its past values and on the current and past values of external driving input (exogenous inputs).

Practically, the NARX network is a recurrent dynamic network, with feedback connections affecting several layers of the network. The model is based on the linear Autoregressive with Exogenous input (ARX) model, and it is well suited to model nonlinear dynamic systems. It is commonly used in time-series modelling. As for the training of the NARX network, it is noteworthy to highlight that the true output is available during the training of the network. Therefore, this value can be used instead of the estimated output during the training phase. This architecture is illustrated in Fig. 4c. Summarizing the model complexity of our NARX networks is controlled by input delay (TDL) and feedback lines lengths (FDL) and by the number of hidden layer. In this paper we have let them vary in the $TDL = [3,6,9]$, $FDL = [2,5]$ and $HN = [3,5,10]$ sets, respectively.

3.4. Performance estimation procedure

The three above mentioned architecture have been tested for their capability to model and generalize sensors response to target gas concentration relationships. Dataset have been partitioned in training (1 week), validation (1 week) and test set (3 weeks), as described in Section 2. The network training procedure was based on backpropagation with Levenberg-Marquardt algorithm [40]. The validation set have been used for model complexity optimization e.g. selecting the best performing number of hidden layer neurons, tapped delay length and feedback delay line length. Optimization has been conducted by brute force exploration of model complexity spaces, described by model complexity hyperparameters sets, for the three architectures. For this reason, a total number of 30 different NNs architectures (3FFNN + 9TDNN + 18NARX) have been generated, trained and tested. Mean relative error (MRE) defined as the sample mean of the ratio between absolute prediction error and true concentration value, mean absolute error (MAE) defined as the sample mean of absolute prediction error, Standard Deviation (STD) of the absolute prediction error and correlation coefficient (CC) have been used as performance indicators. Tests set have been used to extract generalization performance indicators. Each training and procedure has been repeated 30 times so to reduce the uncertainty in performance indicators computation induced by the random choice of networks initial weights, by averaging. Best performing networks architectures for FFNN, TDNN and NARX networks, defined by their hyperparameters t-uple, have been selected to be compared.

Obtained differences among indicators have been tested for statistical significance at 0.05 confidence level. Specifically, Two-Sample t -test with Unequal Variance for computed MAEs has been used assuming a normal distribution for computed MAEs populations. This t -test returns a test decision for the null hypothesis that indicators comes from independent random samples from normal distributions with equal means and unknown and unequal variances. The needed normality assumption have been positively validated using Kolmogorov-Smirnov normality test at 0.01 confidence level for all the obtained MAE estimations (FFNN, TDNN and NARX) over the performed 30 repetitions.

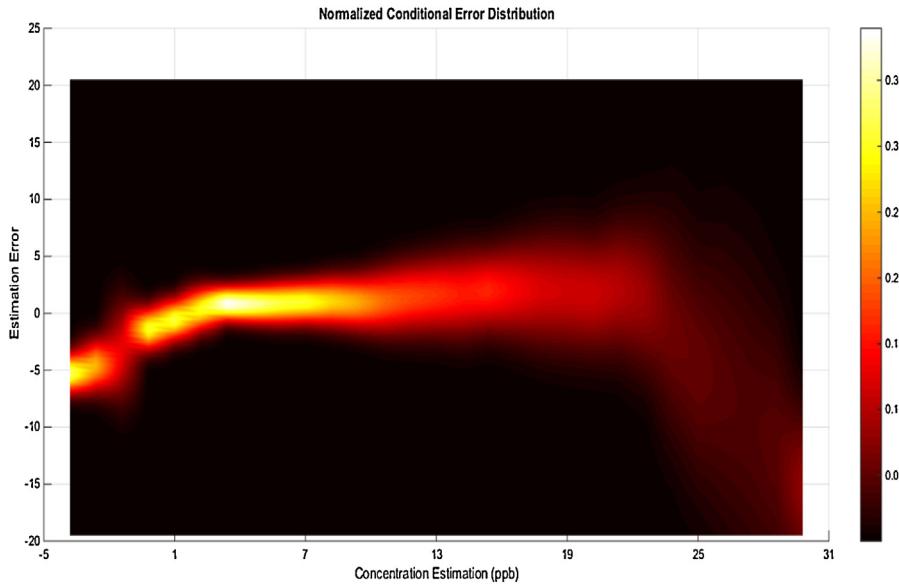


Fig. 5. Example of the normalized empirical conditional error distribution for the TDNN. Probability distribution of error $e = (y - y')$ given concentration estimation y' have been fitted with Gaussian distribution profiles for every interval a_i . Prediction error bias is non-zero at both the extremes of estimated concentration distribution while standard deviation become visibly wider at high estimated concentration values. Normality assumption have been positively tested with Kolmogorov Smirnov test.

Validation Set Performance (MAE) – NARX FDL = 2				Validation Set Performance (MAE) – NARX FDL = 5			
HN	MAE (ppb)			HN	MAE (ppb)		
10	1.36	1.28	1.30	10	1.32	1.22	1.19
5	1.24	1.26	1.23	5	1.30	1.18	1.27
3	1.31	1.32	1.22	3	1.26	1.33	1.25
TDL				TDL	3	6	9

Fig. 6. Validation set MAE averaged on the 30 repetitions as computed for NARX architecture with Feedback delay line length equal to 2 (left) and 5 (right). Bold values indicate the best performing hyperparameters combination.

3.5. Uncertainty analysis

Our aim is to provide the sensor node with a methodology to extract locally or remotely precise and accurate target gas concentration estimation, however, the availability of uncertainty estimations will provide definitely more complete information to the user.

Actually, neural networks does not provide a direct methodology for estimation of uncertainty, yet it could be estimated empirically by means of an error distribution estimation procedure, executed using the validation set. To this purpose, by partitioning the relevant values range for target gas in equal intervals a_i , for each execution of training-validation-test procedure, we have computed the empirical predictive error (err) distribution, given target concentration estimation y' :

$$p(err|y' \in a_i) \quad , (1)$$

over the validation samples. In this work, we chose the number of intervals to be 30.

For each relevant value of a_i , such empirical distribution has been fitted with a Gaussian model (see Fig. 5). Then, mean $\mu_{a_i}^{err}$ and standard deviation $\sigma_{a_i}^{err}$ of the fitted distribution have been used to obtain biased uncertainty bars for estimation performed at time t , using a coverage factor of 1σ :

$$\mu_{a_i,t}^{err} - c(\sigma_{a_i}^{err}) \leq (y'(\bar{x}, t) - y(t)) \leq \mu_{a_i,t}^{err} + c(\sigma_{a_i}^{err}) \quad , (2)$$

where $y'(\bar{x}, t)$ is the network output, $y(t)$ is the target gas real concentration and \bar{x} is the sensor array instantaneous response.

In this way, the user can be provided by both concentration estimation and prediction uncertainty. To this purpose, in the following, estimation charts have been superimposed with the obtained biased uncertainty bars.

Finally, the Negative Log Predictive Density (NLPD) measure (see Ref. [43]) have been used for testing the performance of obtained confidence intervals estimations. The NLPD, is a regression performance index designed for evaluating uncertainty estimations for generative models or, in general, of every machine learning approaches providing a posteriori conditional distributions. The action of the index is dual inasmuch it both penalize over and under-confident estimations, i.e. estimation with over narrow and over wide a posteriori distributions and their relative confidence intervals spread with respect to actual estimation error magnitudes. Under gaussian assumptions, it can be computed as

$$NLPD = \frac{1}{2N} \left\{ \sum_{t=1}^N \left[\log(var_t) + \frac{(y(t) - \mu_t)^2}{var_t} \right] \right\} + c \quad (3)$$

where var_t is the predictive a posteriori variance, μ_t is the predictive mean i.e. the expected value of the a posteriori distribution. Constant c is independent of μ_t and var_t and here is set to $\log(2\pi)/2$.

Table 1

Results obtained upon averaging 30 different executions of the proposed architectures by the use of different subsets of the complete chemical sensor array (+environmental variables) at respective best hyperparameter combination. HN = Hidden Number, TDL = Tapped Delay Length and FDL = Feedback Delay Length. Bold values indicates best performance.

Neural Net	Input (Sensors)	Hyper Parameters	NO ₂ concentration estimation MAE (ppb)	MRE	NLPD
FFNN	NO, NO ₂ , O ₃ , Rh, T	HN = 5	1.50(std = 0.06)	0.25	2.15(std = 0.03)
	NO, NO ₂ , O ₃	HN = 5	1.58(std = 0.04)	0.28	1.98(std = 0.01)
TDNN	NO, NO ₂ , O ₃ , Rh, T	HN = 5, TDL = 0:6	1.27 (std = 0.10)	0.22	1.78 (std = 0.05)
	NO, NO ₂ , O ₃	HN = 5, TDL = 0:6	1.33(std = 0.05)	0.24	1.78(std = 0.02)
NARXNN	NO, NO ₂ , O ₃ , Rh, T	HN = 5, TDL = 0:6, FDL = 1:5	1.30(std = 0.15)	0.21	1.82(std = 0.10)
	NO, NO ₂ , O ₃	HN = 5, TDL = 0:6, FDL = 1:5	1.40(std = 0.10)	0.24	1.87(std = 0.21)

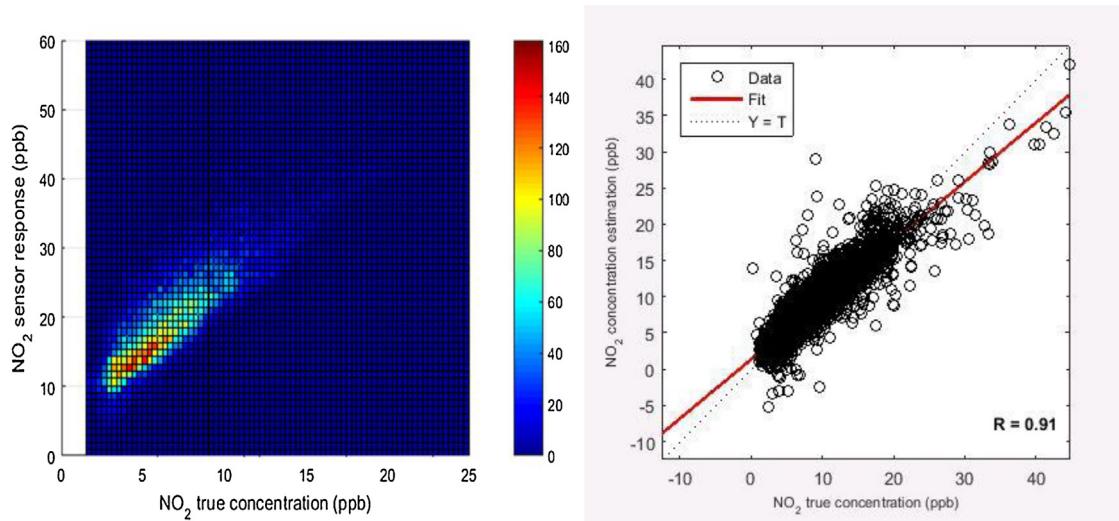


Fig. 7. NO₂ concentration estimation versus ground truth correlation plot (TDNN). The picture shows the compact distribution of estimations around true concentrations (left) and the high correlation rate ($R = 0.91$) among them (right). Comparing these results with Fig. 2a, the improvement wrt the uncalibrated sensor reading is evident. On the left, color indicates number of occurrences of the (y,y') couple.

4. Results

In this work, we specifically report the results of testing the DNN (TDNN and NARX) architectures with a focus on targeting NO₂ concentration estimation comparing them to the results obtained by a static FFNN operating on the same problem with same inputs. We use NO, NO₂, O₃, RH and T high speed sensor response measurements as input variables for filling the delay lines of the tested dynamic architectures ($T_s = 20$ s) while the FFNN have been fed with response samples obtained with $T_s = 1$ min. Error performance for all the architectures have been computed on instantaneous ground truth readings at $T_s = 1$ min for which the reference values have been obtained by conventional analyzers station (see Fig. 4d).

Results of model optimization have allowed the selection of the best performing hyperparameters t-uple for each network class. Surprisingly the best number of hidden layer neurons have been found to be 5 for all the three network classes. For the TDNN networks, the best performing TD length was found to be 6, so the best TDNN was the HN = 5, TDL = 6 network. Finally, for the NARX class, the best input delay line length was also found at 6 while the feedback delay line for the NARX network was best performing at length 5, so the best NARX network was the HN = 5, TDL = 6, FDL = 5 (see Fig. 6).

The resulting best network architectures performances have been selected and compared using results obtained over the test set with the described 30x averaging procedure. In Table 1, we report the results of the comparison tests of the selected models. Results show a significant advantage of the dynamic approach with respect to the static FFNN, with the TDNN emerging as the best performing

approach. The results of significance test of the observed differences at 0.05 level confirm this finding. In particular, the obtained p value ($<10^{-5}$) allowed sufficient evidence to reject the null hypothesis (equal averaged MAE) for FFNN and NARX computed MAEs comparison. The same, *a fortiori*, applied for the FFNN and TDNN comparison ($p < 10^{-10}$). The test results does not allow for deeming the observed difference between TDNN and NARX, in the average, as significant at 0.05 level.

The TDNN advantage is best summarized with a percentage gain of $16 \pm 4\%$ on mean absolute error value over the three weeks test period obtained by FFNN. The NARX advantage is more limited, having been found setting at $13 \pm 5\%$ over FFNN computed MAE. Furthermore, for TDNN and NARX net, we have obtained a correlation coefficient r equal to 0.91 and 0.88, respectively, while FFNN reported a r equal to 0.84. Furthermore, it is worth to note that dynamic networks are also capable to express better confidence interval as witnessed by a lower value of the NLPD loss function.

All this finding collectively support a numerically and statistically significant advantage of the dynamic architectures over static FFNN for the calibration of chemical multisensory nodes in this setting.

In Table 1 we also show results obtained by neglecting information coming from environmental sensors (RH and T sensors). Surprisingly, they show that, notwithstanding the performed datasheet temperature correction procedure, environmental conditions readings still conveyed significant information for reducing estimation error. In fact, multivariate calibration including RH and T readings always perform better than the corresponding, same architecture, environmentally unaware system.

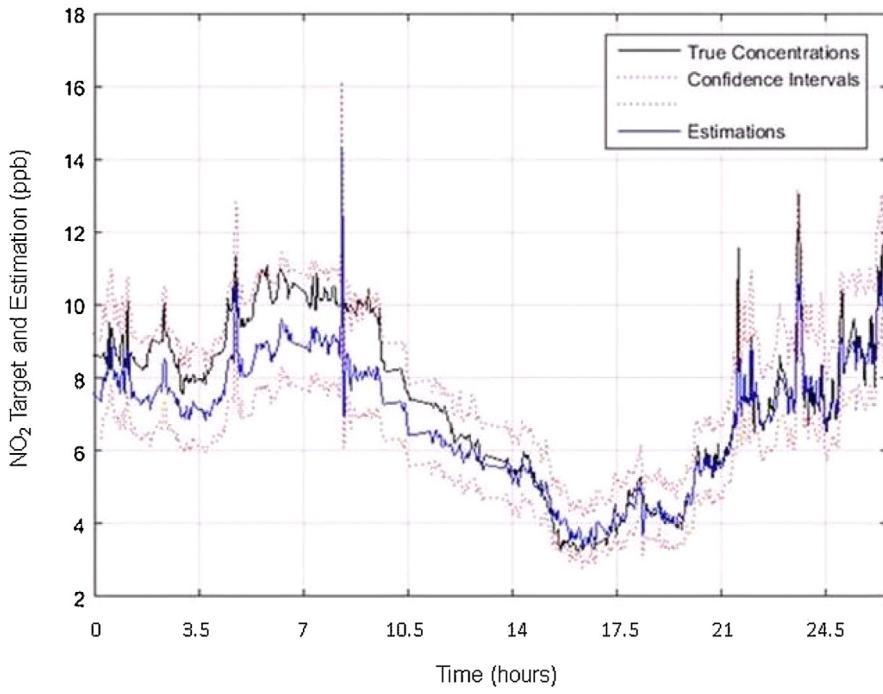


Fig. 8. NO₂ concentration estimation performed by TDNN over a temporal subset of test set data (26 h) with confidence intervals.

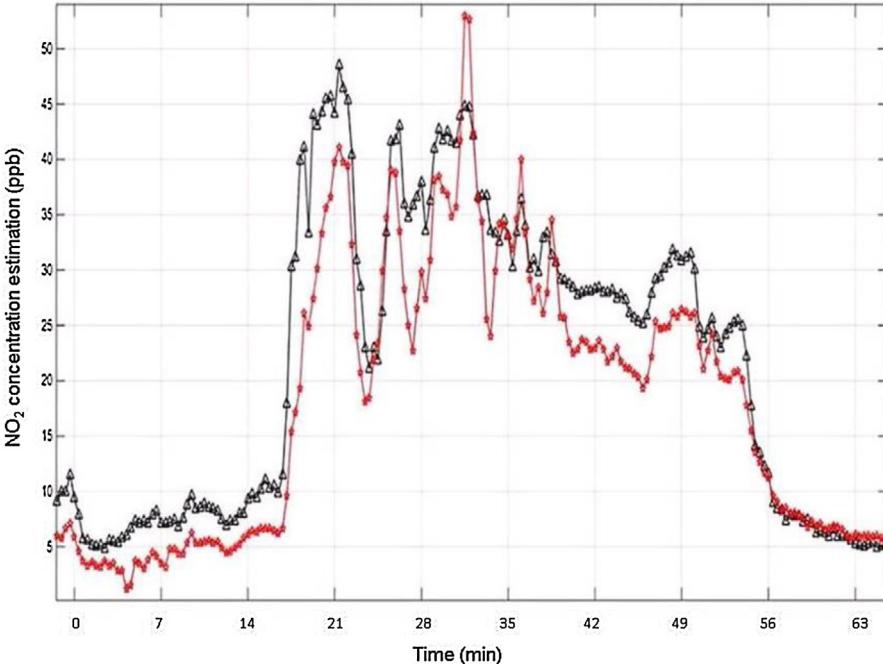


Fig. 9. The network exhibits a very quick response to very rapid transient that challenges the sensors dynamic characteristics.(For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article). (Black = true concentration, red = TDNN estimation).

In Table 2, we additionally report similar conditions occurring for estimations of other target gases including O₃ and NO_x. For all target gases, dynamic multivariate calibration with TDNN always obtain best scores with respect to static multivariate approach (FFNN) and static nonlinear univariate approach obtained feeding a FFNN only with target gas related sensor response.

From a visualization point of view, Fig. 7 shows the improved correlation among NO₂ true values and multivariate estimations with respect to raw NO₂ sensor data correlation plot (see Fig. 2).

Moreover, in Fig. 8, we show an example of stochastic estimation of NO₂ concentration performed by the TDNN architecture. It shows the precise estimations outputted by the network as well as the confidence intervals as computed with the approach depicted in the previous sections. With the proposed architecture each estimation is completed by the confidence interval that is associated with the estimated value.

Finally, in Figs. 9 and 10, we address the capability of DNN to follow significantly fast transient with limited precision losses. In

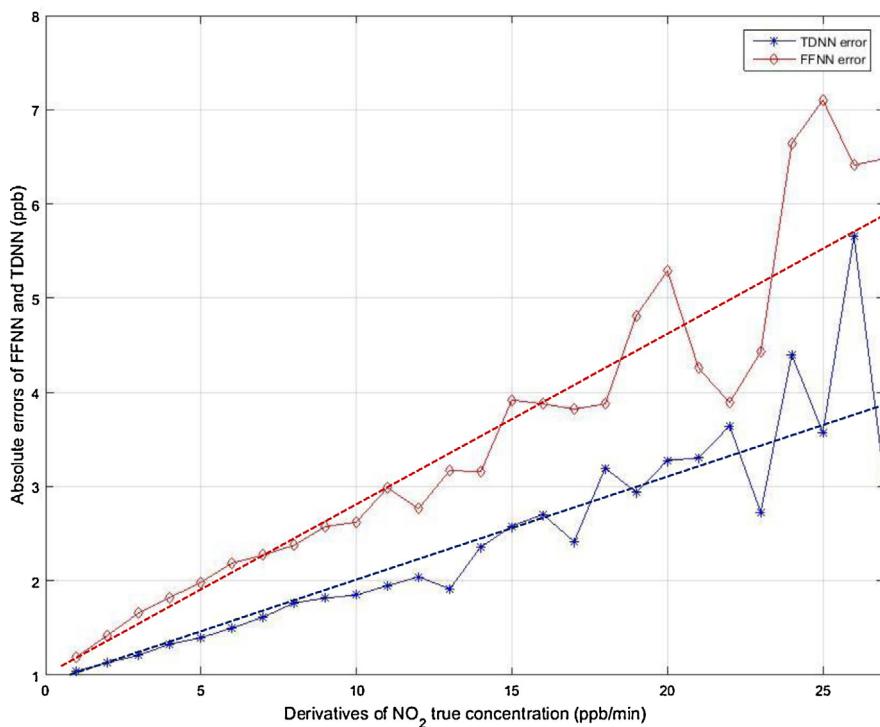


Fig. 10. Comparison of average absolute error distribution trends given the absolute derivative of the NO₂ target gas concentration (ppb/min) for dynamic (below) and static network. The TDNN network is capable of achieving a significant reduction of the estimation error wrt the static FFNN network. This behavior is enhanced when the target gas concentration changes quickly and high values of absolute derivative can be measured.

Table 2

Comparison of the results obtained, respectively, with Univariate, Multivariate and Dynamic Multivariate Calibration (TDNN) while estimating different pollutants. Bold values indicates best performance.

Target	Calibration Methodology	MAE (ppb)	STDERR (ppb)	CC (ppb)	MRE (perc)
NO ₂	Static Univariate	1.68	1.75	0.80	31%
NO ₂	Static Multivariate (FFNN)	1.50	1.69	0.84	25%
NO ₂	Dynamic Multivariate (TDNN)	1.27	1.32	0.91	22%
O ₃	Static Univariate	8.30	6.87	0.50	90%
O ₃	Static Multivariate (FFNN)	7.90	5.21	0.82	70%
O ₃	Dynamic Multivariate (TDNN)	7.45	5.10	0.83	42%
NO _x	Static Univariate	2.14	2.65	0.82	31%
NO _x	Static Multivariate (FFNN)	1.95	2.39	0.85	29%
NO _x	Dynamic Multivariate (TDNN)	1.37	1.61	0.94	20%

particular, in Fig. 10, we depict the values of the mean absolute errors (*y* axis) obtained partitioning the test set with respect to the target gas absolute first derivative value approximation (*x* axis):

$$\frac{|\Delta y(t)|}{\Delta t} = \frac{|y(t + \Delta t) - y(t)|}{\Delta t} = \frac{|y(t_{i+1}) - y(t_i)|}{\Delta t} \quad (4)$$

with $t_i \in [t_0, T]$, $i = 1, \dots, n$, n = number of samples in the test set, $y(t)$ = target gas concentration (NO₂, in our case).

We compare the static FFNN and the TDNN dynamic network response to rapid transients occurring at different absolute first derivative values. It can be observed that the TDNN is significantly more accurate than the FFNN in following the high speed variation of the target phenomena (NO₂ concentration). In particular, the faster is the variation of the target variable, the more significant is the enhancement in concentration estimation accuracy that can be achieved by this dynamic architecture.

To this regard, it can be observed that, TDNN absolute error is always smaller than FFNN error, but the differences increase with the absolute derivative values. This confirms that the dynamic

model is able to improve the dynamic response to rapid transient with respect to the static model.

5. Conclusions

In this work, we proposed a dynamic neural networks approach to improve the stochastic estimation of pollutant concentrations by chemical multisensory network devices in real world deployment scenario. Two different dynamic architectures have been trained and tested by relying on a multi-weeks deployment data and compared with state of the art static FFNN approach. A procedure for empirically estimating concentration prediction uncertainty have also been described and used for enhancing prediction semantic value. This procedure is not dependent on the particular computational intelligence approach and could be applied to different calibration approaches. Results, confirming lab based evidences (see [21,24]), show that dynamic neural networks, by capturing the dynamic behavior of the sensors array, improve the results obtainable by static neural networks over on the field recorded data. This improvement affect both accuracy and uncertainty estimations. This improvement may prove decisive in meeting the Data Quality Objective for indicative measurements as expressed by EC 2008 Air Quality directive (see Table 2 for NO₂ and NO_x). This on field validation is shown, to the best of our knowledge, for the first time in literature. Moreover, Dynamic on field calibration show up as a possible approach to novel issues emerging in mobile and pervasive air quality monitoring deployments with regards to rapid transients. In these cases, our results show that the performance advantage is particularly evident and actually increase when the target gas concentration is rapidly changing. As a secondary result, our data suggests that sensor readings environmental correction procedures for electrochemical sensors should be further improved in order to completely remove the residual environmental effects on sensor responses that we indirectly measured. It is worth to note that this has been achieved with a relatively simple architecture that has

an interestingly efficient knowledge representation allowing for on board implementations. Performance analysis on long term deployments are now under evaluation and future works will focus on the effects of sensor dynamic analysis in drift counteraction capabilities of nonlinear on field calibration approaches.

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