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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.

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 impredictable 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