# Gas Discrimination for Mobile Robots

*To my parents, my grandmother*
*and all the rest of my family*

*Örebro Studies in Technology 41*

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*Title:* Gas Discrimination for Mobile Robots.

*Publisher*: Örebro University 2010
www.publications.oru.se
trycksaker@oru.se

*Printer:* Intellecta Infolog, Kållered 11/2010

ISSN 1650-8580
ISBN 978-91-7668-762-8

# Abstract

The problem addressed in this thesis is discrimination of gases with an array of partially selective gas sensors. Metal oxide gas sensors are the most common gas sensing technology since they have, compared to other gas sensing technologies, a high sensitivity to the target compounds, a fast response time, they show a good stability of the response over time and they are commercially available. One of the most severe limitation of metal oxide gas sensors is the scarce selectivity, that means that they do not respond only to the compound for which they are optimized but also to other compounds. One way to enhance the selectivity of metal oxide gas sensors is to build an array of sensors with different, and partially overlapping, selectivities and then analyze the response of the array with a pattern recognition algorithm. The concept of an array of partially selective gas sensors used together with a pattern recognition algorithm is known as an electronic nose (e-nose).

In this thesis the attention is focused on e-nose applications related mobile robotics. A mobile robot equipped with an e-nose can address tasks like environmental monitoring, search and rescue operations or exploration of hazardous areas. In e-noses mounted on mobile robots the sensing array is most often directly exposed to the environment without the use of a sensing chamber. This choice is often made because of constraints in weight, costs and because the dynamic response obtained by the direct interaction of the sensors with the gas plume contains valuable information. However, this setup introduces additional challenges due to the gas dispersion that characterize natural environments. Turbulent and chaotic gas dispersal causes the array of sensors to be exposed to rapid changes in concentration that cause the sensor response to be highly dynamic and to seldom reach a steady state. Therefore the discrimination of gases has to be performed on features extracted from the dynamics of the signal. The problem is further complicated by variations in temperature and humidity, physical variables to which metal oxide gas sensors are crossensitive. For these reasons the problem of discrimination of gases when an array of sensors is directly exposed to the environment is different from when the array of sensors is in a controlled chamber.

This thesis is a compilation of papers whose contributions are two folded. On one side new algorithms for discrimination of gases with an array of sensors directly exposed to the environment are presented. On the other side, innovative experimental setups are proposed. These experimental setups enable the collection of high quality data that allow a better insight in the problem of discrimination of gases with mobile robots equipped with an e-nose. The algorithmic contributions start with the design and validation of a gas discrimination algorithm for gas sensors array directly exposed to the environment. The algorithm is then further developed in order to be able to run online on a robot, thereby enabling the possibility of creating an olfactory driven path-planning strategy. Additional contributions aim at maximizing the generalization capabilities of the gas discrimination algorithm with respect to variations in the environmental conditions. First an approach in which the odor discrimination is performed by an ensemble of linear classifiers is considered. Then a feature selection method that aims at finding a feature set that is insensitive to variations in environmental conditions is designed. Finally, a further contribution in this thesis is the design of a pattern recognition algorithm for identification of bacteria from blood vials. In this case the array of gas sensors was deployed in a controlled sensing chamber.

# Acknowledgements

First, I would like to express my gratitude to my supervisors Amy Loutfi and Silvia Coradeschi for giving me the opportunity to join the Mobile Robotics Lab at the Applied Autonomous Sensors Systems (AASS) at Örebro University. I would like to thank especially Amy for the guidance in writing scientific articles and this thesis. I am also grateful to my opponent and committee members for having accepted to review this thesis. A big thanks goes to Achim Lilienthal that, despite not being officially my supervisor, invested a lot of time for helping me with suggestions, fruitful discussions and revision of my publications.

During autumn 2009 I visited the lab of Hiroshi Ishida at the Tokyo University of Agriculture and Technology. I would like to thank Prof. Ishida for inviting me to his lab and for sharing with me his expertise. I also thank Yuichiro Fukazawa, Yuta Wada and the other members of the lab for being not only colleagues but also good friends.

I have to thank a lot Kicki Ekberg and Barbro Alvin for helping me in the organization of my numerous trips. Many thanks also for the help in avoiding many of the bureaucratical pitfalls I found on my way.

I would like to thank (in alphabetical order) Krzysztof Charusta, Marcello Cirillo, Robert Krug, Kevin LeBlanc, Karol Niechwiadowicz, Federico Pecora, Matteo Reggente, Todor Stoyanov and all the PhD students at AASS for being very good friends. Most of the highlights of this last three years would not have happened without them.

My gratitude goes also to the senior researchers at AASS, in particular to Henrik Andreasson and Dimitar Dimitrov, for the very interesting scientific discussions. A big thanks goes to Per Sporrong and Bo Lennart Silfverdal for the great effort in setting up the robot and the electronic noses used in the experiments. Special thanks to Bo Lennart for supervising me in designing circuit boards. I would like to thank Bo Söderquist and Lena Barkman for providing the material for the bacteria identification experiments.

I want to acknowledge also the windsurfers in Örebro, especially Tadas Mikalauskas and Richard Ström, for the fantastic afternoons in which Hjälmaren has been our playground.

Finally, big gratitude goes to my family and my friends back home because they always make me feel their presence, especially when I need it.

# List Of Publications

This thesis is a compilation of publications. The publications are referenced in the text using the labels indicated in the following list:


PAPER I *Marco Trincavelli, Matteo Reggente, Silvia Coradeschi, Hiroshi Ishida, Amy Loutfi and Achim J. Lilienthal*, **Towards environmental monitoring with mobile robots**, in: Intelligent Robots and Systems, 2008. IROS 2008. IEEE/RSJ International Conference on, pages 2210 - 2215, 2008

PAPER II *Marco Trincavelli, Silvia Coradeschi and Amy Loutfi*, **Classification of odours with mobile robots based on transient response**, in: Intelligent Robots and Systems, 2008. IROS 2008. IEEE/RSJ International Conference on, pages 4110 - 4115, 2008

PAPER III *Marco Trincavelli, Silvia Coradeschi and Amy Loutfi*, **Online Classification of Gases for Environmental Exploration**, in: Intelligent Robots and Systems, 2009. IROS 2009. IEEE/RSJ International Conference on, pages 3311 - 3316, 2009

PAPER IV *Marco Trincavelli, Silvia Coradeschi and Amy Loutfi*, **Classification of Odours for Mobile Robots Using an Ensemble of Linear Classifiers**, in: OLFACTION AND ELECTRONIC NOSE: Proceedings of the 13th International Symposium on Olfaction and Electronic Nose, Brescia, pages 475 - 478, 2009

PAPER V *Marco Trincavelli, Silvia Coradeschi and Amy Loutfi*, **Odour classification system for continuous monitoring applications.** (2009), in: Sensors and Actuators B: Chemical, 139:2(265 - 273)

PAPER VI *Achim J. Lilienthal, Matteo Reggente, Marco Trincavelli, Jose Luis Blanco Claraco and Javier Gonzalez Jimenez*, **A Statistical Approach to Gas Distribution Modelling with Mobile Robots – The Kernel DM+V Algorithm**, in: Intelligent Robots and Systems, 2009. IROS 2009. IEEE/RSJ International Conference on, pages 570 - 576, 2009

Paper VII *Marco Trincavelli and Amy Loutfi*, **Feature Selection for Gas Identification with a Mobile Robot**, in: Robotics and Automation, 2010. ICRA'10. IEEE International Conference on, pages 2852 - 2857, 2010

Paper VIII *Marco Trincavelli and Amy Loutfi*, **An inspection of signal dynamics using an open sampling system for gas identification**, in: Robotics and Automation, 2010. ICRA'10. IEEE International Conference on, Workshop in Networked and Mobile Robot Olfaction in Natural, Dynamic Environments, 2010

Paper IX *Marco Trincavelli, Silvia Coradeschi, Amy Loutfi, Bo Söderquist and Per Thunberg*, **Direct Identification of Bacteria in Blood Culture Samples using an Electronic Nose** (2010), in: Biomedical Engineering, IEEE Transactions on(to appear)

Paper X *Yuta Wada, Marco Trincavelli, Yuichiro Fukazawa and Hiroshi Ishida*, **Collecting a Database for Studying Gas Distribution Mapping and Gas Source Localization with Mobile Robots** (2010), in: International Conference on Advanced Mechatronics 2010(to appear)

All the publications have been reprinted with permission.

# Contents

# Chapter 1
# Introduction

The ability to monitor and identify gases is required in a variety of applications ranging from air pollution monitoring, food and beverage quality assessment, medical diagnosis, exploration of hazardous areas and search and rescue operations. Various technologies for gas sensing are available and the gas sensors can be deployed in many different setups in order to fulfill the application dependent requirements. For applications like food quality assessment and medical diagnosis, where the accurate analysis of a small amount of gas is the main challenge, gas sensors are often placed in a sensing chamber isolated from the outside environment in order to try to minimize interfering factors and enhance the robustness and accuracy of the measurement process. Instead, for applications like air pollution monitoring or inspection of hazardous areas where the main challenges are the localization of a source of pollution or the creation of a map of the gas distribution, gas sensors are deployed either in a sensor network that covers the area of interest or on a mobile platform that can transport them. In this scenario gas sensors are most often directly exposed to the environment they are analyzing and perform continuous measurements. This is mainly due to the fact that sampling systems are bulky and many platforms would not be able to transport them. Also, it is possible that the dynamic response of the sensor when directly exposed to the environment contains information about the nature of the plume. This information can be extracted in order to perform parallel tasks such as gas source localization, but is otherwise unavailable if the sensor is enclosed in a chamber. Moreover a setup with sensors that continuously sample the environment is more suited to meet time constraints that arise in certain applications, for example when a robot continuously moves and cannot stop for collecting gas samples. We refer at the setup where sensors are placed in a measurement chamber isolated from the environment as closed sampling system and at the setup where sensors are directly exposed to the environment in order to continuously sample it as open sampling system.

Signals collected when an array of sensors is used in a closed sampling system have different characteristics with respect to signals collected with an array in an open sampling system. Variables like the exposure of the sensors to the analyte, temperature and humidity are controllable in the closed sampling system setup while they can only be observed in the open sampling system. In a closed sampling system the sensors are often exposed to a step in the concentration of the analyte, in order to be able to observe the dynamic behaviour of the sensors to a fixed stimulus. Moreover variables like temperature and humidity, to which many sensors are cross-sensitive, are stabilized in order to enhance the repeatability of the measurement process. In an open sampling system the sensors are instead exposed to fast changes in concentration due to the turbulent nature of gas plumes in natural environment. Moreover temperature and humidity changes might influence the sensors response. Given these differences in the signal, the problems of gas identification and quantification look completely different in these two setups.

The problem addressed in this Ph.D. thesis is the discrimination of gases with an array of low cost compact gas sensors with particular attention to applications that require an open sampling system. Most of the original contributions presented in this thesis use metal oxide (MOX) gas sensors. MOX gas sensors have a relatively large response time, and in most of applications they are modelled as first order sensors. Normally 3-5 seconds are needed for the sensor to stabilize on a value when exposed to a compound and few minutes are needed in order to recover to the original value after the exposure. Therefore the sensor response does not correspond to instantaneous gas concentration due to the dynamics introduced by the sensor itself. As a consequence, in a highly dynamic and turbulent environment where a stable steady state is normally not reached, the analysis of the transient phase is necessary. It often happens that multiple sensor responses are collected in a sequence without the sensor recovering to the baseline state. Moreover changes in environmental variables like temperature and humidity, to which most of the gas sensors are cross-sensitive, introduce an additional degree of complexity in the problem.

Gas discrimination with an open sampling system has not been thoroughly addressed in literature. Though this is a relevant problem since much of the work done for other gas sensing applications would get benefit. For example most of the works in gas sensing networks and mobile robotics olfaction have been developed under the assumption of a single predefined analyte (most often ethanol). This limits the applicability of these results in real scenarios where this assumption is unrealistic. Mobile robotics olfaction is the sub-field of robotics that deals with robots equipped with gas sensors and other sensing modalities (often an anemometer) that make them able to monitor the presence and dispersion of volatile chemicals. Typical tasks addressed by gas sensing robots are gas source localization, gas plume tracking and source declaration and gas distribution mapping. The capability of discriminating gases would enable to extend these tasks to the presence of multiple, heterogeneous gas sources. With gas discrimination capabilities a gas sensing robot would be able to perform gas distribution mapping in presence of multiple different gas sources, to localize a specific gas source in presence of interfering gas sources and to track the gas plume of a specific compound.

While achieving the aforementioned tasks is a long term objective of this work, the specific objective in this thesis has been to make a first step towards gas discrimination with a mobile robot by analyzing the problem of identification using an open sampling system. These investigations have been done primarily on the robotic platform and secondarily in controlled conditions. The specific contributions of this thesis are:

- Design and implementation of a gas discrimination algorithm with an open sampling system. Analysis of the performance of the algorithm with respect to variables like e.g. distance of the sensor array from the gas source (Paper II, Paper V).
- Implementation of a discrimination algorithm that runs online on the robot and provides inputs to a path planner that can therefore optimize the movement of the robot with respect to gas discrimination (Paper III).
- Demonstration of the influence of the movement of the robot and experimental setup on the collected signal. Formulation of a classification and a feature selection strategy that enhances the performance of the gas discrimination algorithm (Paper IV, Paper VII).
- Collection of large dataset in various conditions for studying of the problem of classification of odors with an open sampling system. The collected data can be used also to study other problems like gas source localization or gas distribution mapping (Paper I, Paper VI, Paper VIII, Paper X).
- Design of an algorithm for rapid identification of bacteria from blood vials through an electronic nose (Paper IX).

## 1.1 The Structure of this Thesis

The structure of the thesis is as follows:

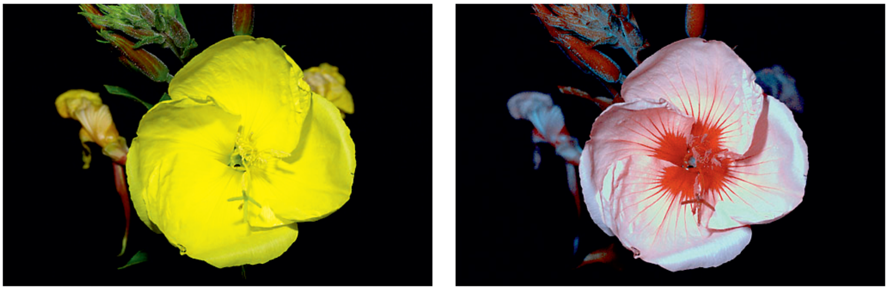
**Chapter 2** Gives a general introduction on the field of machine olfaction. The first part of the chapter describes the functional parts of an electronic nose, while the second part presents some of the most relevant applications of the electronic nose. This chapter is purely based on bibliography.

**Chapter 3** Presents the problem of gas discrimination with particular focus on the analysis of the dynamic response of an array of gas sensors. The first part of the chapter presents different techniques for extracting features that capture the dynamics of a signal collected with a gas sensor. Then, a case study in which the electronic nose is used for identifying bacteria in blood vials is presented. The last part of the chapter shifts the attention on the analysis of a signal collected with a gas sensor array directly exposed to the environment.

**Chapter 4** Introduces the topic of gas discrimination in the context of mobile robotics olfaction. The contributions related to mobile robotics olfaction are presented in detail in this chapter. The chapter concludes with an overview of related topics in mobile robotics olfaction.

# Chapter 2
# Machine Olfaction and Electronic Nose

The concept of electronic nose (e-nose) has been introduced in the early 1980's [1]. In the beginning the ambition of the e-nose research community has been to mimic human olfaction and while this ambition remains, 30 years later we find that the applications whereby artificial olfaction has mostly contributed are those where the e-nose technology acts as a complementary sense to the human nose. For example e-noses can detect explosives [2] or air contaminants like CO [3] that are undetectable by human nose. Röck et al. in [4] use a metaphor in order to compare an electronic nose and a human nose. They say that the comparison of an electronic nose with a human nose is in the best case like the comparison of an eye of a bee with a human eye. Both the eye of a bee and the eye of a human are sensors for electromagnetic waves. What makes them different is the spectrum of frequencies that they can detect. Indeed the eye of a bee is blind for a part of the visible spectrum (wavelengths close to red) but it is sensitive for ultraviolet wavelengths. This can cause a completely different perception of the same entity. Figure 2.1 gives an example of how a flower is perceived when ultraviolet light is added to the image through the use of a UV filter compared to when only visible wavelengths are considered. The "bulls-eye" with stripes is visible only in the ultraviolet spectrum, while it is completely transparent in the visible spectrum. The correlation between human odour impressions and electronic nose measurements is hard to achieve and it makes sense only in limited and well defined scenarios. Therefore the term electronic nose might be misleading and it is important to always keep in mind the differences between the electronic and the biologic aspects of olfaction. In this thesis the term electronic nose is used not because of the relation to



(a) Visible Light (b) UV Light

**Figure 2.1:** Picture of an Oenothera biennis L. with a normal camera 2.1(a) and with a camera with a UV filter 2.1(b). Notice that UV light does not have a color and therefore the attention should be focused rather on the difference in the patterns than in the colors.

biological olfaction but rather because the signal to be analyzed is a fingerprint of a volatile chemical compound[1].

Most of the research in the electronic nose field has focused on discrimination and quantification of gases. With respect to classical analytic techniques that aim at identifying and quantifying every compound of a given sample, the electronic nose extracts instead a signature of the sample that can be used to identify it but provides little or no information about the components of the gas mixture that composes the sample. Despite this lack of power with respect to traditional techniques the electronic nose technology, due to its ease of use and low cost, has obtained interest in areas ranging from medical diagnosis to food and beverage quality assurance, detection of explosives, environmental monitoring and industrial process monitoring [4]. It is expected that such a wide range of applications results in the development of a multitude of different solutions for all the functional parts of an electronic nose, namely the sensor array, the sampling system and the pattern recognition algorithm. Sections 2.1, 2.2 and 2.3 will give a brief overview of the most common solutions adopted for these functional parts, paying particular attention to the ones relevant for robotics applications. A summary of the applications where the electronic nose has been most successful is given in Section 2.4.

## 2.1 The Sensor Array

Chemical sensing is a process that aims at getting an insight about the chemical composition of a system. In this process an electrical signal results from the interaction of the chemical species in the system and the sensor. There are various

[1]In this thesis the term *gas discrimination* is used instead of the term *odour discrimination* in order to stress the fact that we are detecting volatile chemical substances. These substances might be odourless, i.e. not perceivable by human olfaction.

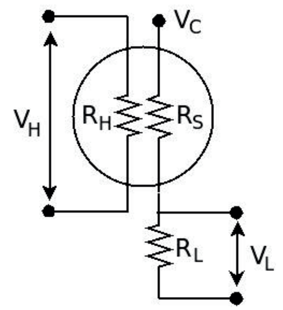



**Figure 2.2:** Electrical schema of a MOX gas sensor.

families of sensors based on different transduction principles. The most common are thermal sensors, mass sensors, electrochemical sensors, potentiometric sensors, amperometric sensors, conductometric sensors and optical sensors [5]. An exhaustive review of the different sensors technology is out of the scope of this thesis and therefore only the two technologies that are used in the original works presented in this thesis will be introduced: the metal oxide gas sensors (conductometric family) and the MOSFET gas sensors (potentiometric family).

### 2.1.1 The Metal Oxide Gas Sensor

The metal oxide (MOX) gas sensors are by far the most widely used in electronic nose applications as well as in mobile robotics olfaction. The most prominent reasons for this are that they are commercially available, they show good stability over time, they have a relatively fast response and they have a higher sensitivity than most other sensing technologies. MOX gas sensors are conductometric sensors, that means that a change in the conductance of the oxide is measured when a gas interacts with the sensing surface. The change in conductance is usually linearly proportional to the logarithm of the concentration of the gas [6]. There are two types of MOX sensors: $n$-type ($SnO_2$,$ZnO$) which respond to reducing gases like $H_2$, $CH_4$, $CO$, $C_2H_5$, $C_2H_5OH$, $(CH_3)_2CHOH$ or $H_2S$ and p-type ($NiO$,$CoO$) which respond to oxidizing gases like $O_2$, $NO_2$, and $Cl_2$ [5]. The action of a MOX sensor results from chemosorption and redox reactions at the surface. Since the rate of such reactions is dependent on the temperature, it is clear that the temperature of the sensing surface considerably affects the sensor characteristics [6]. Typical temperatures for the sensing surface of MOX sensors lie between 300°C and 500°C. Selectivity is obtained either by doping the sensing surface with different additives or by setting different operating temperature. It has also been demonstrated that introducing a dynamic operating temperature further enhances the selectivity of the sensor [6].

Figure 2.2 shows a schematic of a MOX sensor. $R_H$ and $R_S$ are respectively the heater and the sensor resistances, while $R_L$ is the load resistance that is applied in series to $R_S$ in order to be able to read it. $V_H$ is the voltage applied to the heating resistance and it is proportional to the operating temperature, $V_C$ is the reference voltage for the measurement, while $V_L$ is the voltage drop on $R_L$. In order to calculate the value of the sensor resistance (inverse of the sensor conductance - the quantity that changes when the sensor responds) the following formula is applied:

$$R_S = \frac{V_C - V_L}{V_L} \times R_L \tag{2.1}$$

### 2.1.2 The MOSFET Gas Sensor

The MOSFET sensor is a metal-insulator-semiconductor device introduced by Lundström et al. in 1975 [7]. Its structure is shown in Figure 2.3. When certain molecules in the gas phase reacts at the catalytic surface (indicated as *selective layer* in Figure 2.3), certain products of the reactions may polarize and adsorb at the metal surface. Some products like $H_2$ might diffuse through the catalytic metal and form dipoles at the metal-insulator interface. The polarized species at the insulator surface and polarized hydrogen atoms at the metal-insulator interface form a dipole layer, which adds to the electric field between the metal and the semiconductor. This change in the electric field causes a change in the work functions of the metal and oxide layers and this translates in a change of the threshold voltage of the MOSFET. In practice, the sensor response is measured as the change in the voltage applied to the gate of the MOSFET required in order to keep a constant current through the transistor.

Figure 2.4 displays the response of 3 MOX gas sensors and 3 MOSFET gas sensors contained in the sensor array of the NST 3220 Emission Analyzer,

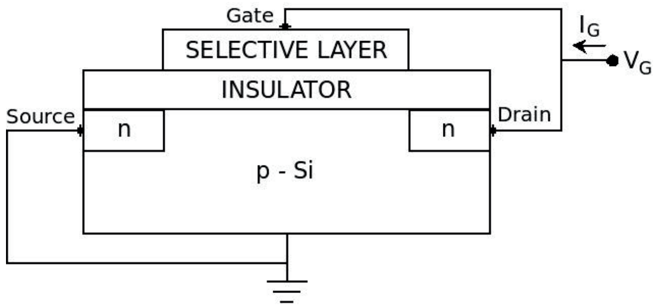



**Figure 2.3:** Electrical schema of a MOSFET gas sensor.

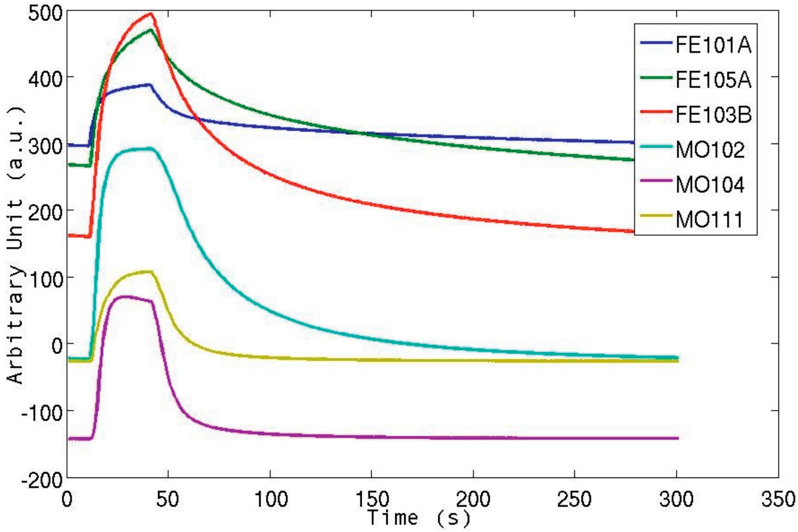



**Figure 2.4:** Sensor response collected with 6 of the sensors of the array present in the NST emission analyzer when exposed to the volatile products of the metabolism of *Pasteurella multocida*. The sensors starting with the prefix FE are MOSFET sensors, while the ones starting with the MO prefix are metal-oxide sensors. The sample has been collected using a three-phase sampling technique where the baseline has been collected for 10 seconds, then the headspace of the vial containing the infected blood has been sampled for 30 seconds and finally the array has been exposed for 260 seconds to dry air in order to recover the initial state.

Applied Sensors, Linköping. The NST 3220 Emission Analyzer has a closed sampling system.

The main advantages of MOX sensors are the fast response and recovery times and the limited price, while the disadvantages are the limited number of detectable substances, the scarce selectivity and the high operating temperature that results in large power consumption. MOSFET sensors are small, cheap, CMOS integrable but they suffer from large baseline drift due to the large dependency of the response on humidity and especially temperature. For this reason MOSFET sensors are mainly suitable for use in controlled environments [8].

## 2.2 The Sampling System

The handling and delivery system determines the modality in which the array of sensor is exposed to the gas to be analyzed. The choice of an appropriate sampling system can significantly enhance the capability and reliability of an electronic nose. Various techniques like sample flow system, preconcentrator systems, GC column, static system and open sampling system have been proposed in literature. In a sample flow system the sensors are placed in the gas flow and normally the three phase sampling strategy is adopted. This strategy, which consists in exposing the sensors array to a step in concentration of the analyte after being exposed to a reference gas, is very popular since it allows to collect a dynamic response of the sensor in addition to the steady state [9]. It has been demonstrated that the dynamics of the sensor response contains useful information for gas discrimination and quantification purposes [10]. A preconcentrator tube is often used when the sensitivity of the sensor is too low to meet the requirements of the application considered. In a preconcentrator, first the tube accumulates the vapor and then a heat pulse is applied to the tube to desorb the concentrated vapor, and therefore a higher concentration is obtained [11]. In other applications the most problematic aspect might be that the required selectivity is difficult to reach only with an array of gas sensors. In this case Zampolli et al. [12] proposed a hybrid system in which the array of sensors is located at the end of a micromachined GC column. The separation obtained by the GC column significantly enhances the selectivity of the sensor array. In a static system the steady state response of a sensor exposed to a gas at constant concentration is measured.

The systems mentioned above are considered closed systems, since the sensors are in a chamber and therefore the exposure of the sensors to the samples can be accurately controlled. In some applications where a rapid concentration change should be captured or where a complete sampling system is too bulky, expensive or energy consuming the sensors are directly exposed to the gas in a so called open sampling system. In mobile robotic olfaction literature most of the mobile robots have been equipped with gas sensors with an open sampling system [13]. In the mobile robotics related work presented in this thesis the array of sensors has been used with an open sampling system.

## 2.3 The Pattern Recognition Algorithm

Gas sensors suffer from a number of shortcomings like lack of selectivity, long and short term drift, nonlinearities in the response, and slow response and recovery time. These limitations, together with the variability associated with the sampling system and the small amount of data that is often available due to economical reasons, contribute to make the problem of classifying and then further quantifying chemical substances with an electronic nose a difficult one. Therefore, much work has been done in order to design appropriate pattern recognition algorithms for gas discrimination and quantification with electronic noses [10, 14].

The pattern recognition algorithm for electronic noses can be subdivided in two distinct families: the biologically inspired algorithms and the statistically based pattern recognition algorithms. Biologically inspired algorithms try to formulate mathematical models of the olfactory pathways that process the signals coming from the olfactory receptors. Given the impressive olfactory ability of many animals, it can be speculated that understanding the biological olfactory system could be beneficial for the development of electronic noses. Therefore, when biologists understand new computational principles underlying olfaction, different processing stages in the olfactory pathway are mathematically modelled and applied to gas sensors data [14]. Since the works presented in this thesis will be based on statistically based pattern recognition algorithm, the description of biologically inspired algorithms is out of the scope of this thesis, but a good review of the biologically inspired olfactory models can be found at [15], while a more recent model of the olfactory system of insects can be found at [16].

Statistically based pattern recognition algorithms are related to classic multivariate analysis and they often consists of four phases namely signal conditioning, feature extraction, dimensionality reduction and classification or regression.

**Signal Conditioning** Signal conditioning is a broad term that defines a series of operations performed on the raw sensor data in order to increase the signal-to-noise ratio of the signal before extracting features and design a pattern recognition model.

One of the most serious limitations of gas sensors is the drift problem, that can be observed as variation in the sensor response when exposed to identical vapors under identical conditions. A very common preprocessing technique to cope with this problem is baseline manipulation. This means that before exposing the array of sensors to the target gas, the array is exposed to a reference gas and the response of the array is recorded (baseline value). Once the baseline value is available one of three baseline correction methods is normally applied: differential (baseline value subtracted from sensor response), relative (ratio between the sensor response and the baseline value) and fractional (subtract the baseline value from the sensor response and then divide by the baseline value) [17]. The choice of the baseline correction technique depends mostly on the transduction principle used by the sensors in the array. Scaling or normalization techniques can be used in order to ensure that sensor response amplitudes are comparable (no sensor overwhelms the others because the amplitude of its response is much larger) and to limit the effect of concentration changes in case of a gas discrimination problem.

**Feature Extraction** Feature extraction is the procedure of extracting parameters that are descriptive of the sensor array response. This can be seen as a first step of reducing the dimensionality of the learning problem. Feature extraction techniques for arrays of gas sensors can be subdivided in two families: steady state features, that use only the steady state phase of the sensor response, and transient features, that use the whole dynamics of the sensor response. Various works in literature advocate the superiority of transient based features on static features [18, 19]. Given the central importance of features that capture the dynamics of the sensor response, especially for electronic noses with an open sampling system we defer the detail description of this topic to Chapter 3.

**Dimensionality Reduction** The small amount of data that is often available together with the fact that the responses of the gas sensors in an array are highly correlated can create problems related with high dimensionality and redundancy. If redundant or noisy information is not removed before trying to learn a model, the problem of the *Curse of Dimensionality* [20] may arise. This refers to the fact that for high-dimensional spaces it is difficult to collect enough samples to attain a high enough density in order to obtain a valid estimate for a function or a discriminant. The most common way of dealing with this problem is to reduce the dimensionality of the feature space by either projecting the original $N$ dimensional space into a $M$ dimensional one where $M < N$ (feature projection), or selecting $M$ out of the $N$ original features (feature selection).

The most commonly used techniques for feature projection are Principal Component Analysis (PCA) and Linear Discriminant Analysis (LDA). PCA is an unsupervised technique that finds the directions that capture most of the variance contained in the original data, while LDA is a supervised technique that finds the directions that minimize the average distance among points belonging to the same class while maximizing the average distance among the centroids of different classes [17]. PCA is often used as a visualization tool for representing high dimensional spaces in 2-3 dimension that capture the most of the variance in the data. Given the high correlation in the responses of different gas sensors, usually the first 2-3 principal components can capture more than 90% of the variance in the data, and therefore PCA is a valuable tool for exploratory analysis of data collected with gas sensors. An interesting approach for exploiting the directions found by PCA for reducing the dimensionality of an array of gas sensors is presented in [21].

Feature selection methods proposed in literature fall into two main categories, the *filter* approaches and the *wrapper* approaches [22]. The filter based methods produce a ranking of the features based on an optimality criterion and then select the first $M$ features in the ranking, where $M$ can be arbitrarily chosen. Wrapper methods instead use the prediction performance of a given classifier to assess the relative usefulness of subsets of variables. Since the number of possible feature subsets of $N$ features is $2^N$, an exhaustive search is unfeasible even for small $N$. Therefore wrapper algorithms use a search heuristic to perform a partial exploration of the feature subsets space. An example of feature selection applied to an electronic nose is presented in [23].

**Classification/Regression** The last step of the pattern recognition algorithm is building a model that will be able to efficiently solve the problem of gas discrimination or quantification. Usually the gas discrimination problem is formalized as a classification problem, where the objective is to create a decision rule which optimally partitions the data space into regions that will be assigned to the different classes. In cases where it is needed to have a confidence measure on the decision, models that can provide an estimation of the posterior probability are preferred. An extensive review of statistically based classifiers used in electronic noses can be found at [14]. Probably the most commonly used classifier for electronic nose applications is the multi layer perceptron (MLP), an artificial neural network [24]. Another widely used classifier is the K Nearest Neighbor (KNN). The KNN is a nonparametric density estimation model that can be used both for classification and for regression problems [25]. Recently, the attention has been moved to kernel methods and in particular to the Support Vector Machine (SVM) [26]. The SVM has many appealing characteristics with respect to other classification methods, of which probably the most relevant is that the SVM is formulated as a convex optimization problem. This implies the fact that the error function that is minimized during training has only one minimum (global) and moreover the training algorithm can be executed much faster than for example the backpropagation algorithm that is often used to train MLPs. For what concerns gas quantification, the problem can be formalized either as a regression problem or a classification problem. In the first case the concentration will be treated as a real valued variable while in the second case the concentration is discretized into intervals and each interval is considered as a separate class. The most widely used regression methods for gas quantification are multiple linear regression (MLR) and partial least squares (PLS) [27].

## 2.4 Applications of the Electronic Nose

In this section a brief description of the most important applications of the electronic nose in the areas of medical diagnosis, food and beverage, and environmental monitoring will be given. Concerning robotic applications the discussion is deferred to Chapter 4. The purpose of this section is not to give a complete review of applications of electronic noses but to mention the works that are either relevant for this thesis or they try to connect the field of electronic nose with other, more established, fields like analytical chemistry. For an exhaustive review please refer to [4, 28, 29, 30].

### 2.4.1 Medical Diagnosis

In ancient times smell was an important sense for diagnosing diseases. According to the Greek physician Hippocrates (ca. 460 BC – ca. 370 BC) "You can learn a lot just by smelling your patients with the unaided nose". However, modern diagnostics techniques do not rely any more on the olfactory perception of the physician but they are based on physical, chemical and biological analysis. Human olfactory perception is indeed highly subjective and therefore not suitable as a diagnosis method according to modern criteria. However, a non-intrusive device that could perform a fast analysis of volatile compounds generated by infections or metabolic diseases would be valuable. An electronic nose could be for example used as a complement for laboratory analysis, that are often very time consuming and expensive. Probably the most successful medical application of the e-nose is presented by Persaud et. al. in [31], where an array of conducting polymer gas sensors is used to monitor urinary tract infections (UTI) and bacterial vaginosis (BV). In this study HS-GC-MS is used to identify acetic acid as a marker for both UTI and BV, then an array of conducting polymer sensors calibrated on the detection of acetic acid is developed. Finally a pattern recognition algorithm is developed in order to interpret the response of the array. This study is particularly interesting since it links classic analytical chemistry techniques with electronic noses. The validity of this study is confirmed by the FDA approval for the use of the devices developed in this study as aids to clinical diagnosis in the USA.

Another quite developed medical application of the electronic nose is the identification of bacteria from bacteria cultures. Bacteria cultures are an in-vitro isolated system whose analysis is easier and much more repeatable than other setups that have to be in contact with the patient like breath analysis for example. The most relevant works dealing with bacteria identification in blood cultures with an e-nose are [32, 33, 34]. More recently the project Mednose, a collaboration between Örebro University and Örebro University Hospital in the Novamedtech framework, aims at the development of a fully fledged instrument for rapid bacteria identification that complements traditional bacteria identification techniques based on bacteria cultures (Paper IX). One relevant specification of this project is that the developed prototype has to fulfill the tests for obtaining the CE Mark approval for In Vitro Diagnostics (IVD) devices and can therefore be used in a hospital as a tool for diagnosis support. Details about the algorithm developed in this project are given in Section 3.1.4.

## 2.4.2 Food Quality Monitoring

Electronic noses have been proposed in the food and beverage industry for addressing applications like inspection of the nature and quality of ingredients, supervision of the manufacturing process and spoilage detection of foodstuff. Probably the most studied deterioration process with an electronic nose is fish spoilage. The biochemical processes that take place after the death of the fish and specific volatiles that are produced by these processes are well known. The main responsible for the spoilage of fish is the growth of microorganisms [35], which is dependent on extrinsic and intrinsic factors. The most relevant extrinsic factors are temperature and composition of the atmosphere, while the fish species is what determines the most relevant intrinsic factors (poikilotherm nature, aquatic environment, post mortem pH of the flesh, concentration of non-protein nitrogen and trimethylamine oxide). Therefore, the spoilage of different fish species in different storage conditions is dominated by different microorganisms, primarily Vibrionaceae, *Shewanella putefaciens*, *Pseudomonas* spp., *Photobacterium phosphoreum*, *Lactobacillus* spp. and *Carnobacterium* spp [35]. As already pointed out in the previous section, the different microorganisms produce different metabolites. The difference in the metabolites is reflected in changes in the sensor response of an appropriate array of sensors [28].

### 2.4.3 Environmental Monitoring

In the last decades, given the increase in awareness of the negative effects of pollution on human health and quality of the environment, environmental monitoring has become more and more important. The electronic nose has often been proposed as a cheap alternative to analytical chemistry techniques to detect pollutants in the ambient atmosphere or in the headspace of water [4]. Other projects, more closely related to the content of this thesis, aim at collecting gas measurements to create a gas distribution map or find the source of a gas plume [30].

For what concerns air pollution monitoring, the substances that are commonly measured by air pollution stations in town are $NO_2$, suspended particulate matter (SPM), $O_x$, $SO_2$ and CO. Currently, pollution monitoring stations installed in towns are mounting very expensive gas analyzers and therefore their number is limited. This implies that the resolution of the measurement is sparse, hindering the accuracy of the mapping/source localization process. This limitation can be overcome by a network of cheap and reliable sensors. Maruo et. al. presented a work where the $NO_2$ distribution in Sapporo is monitored with an optical sensor [36]. A network of 10 sensor nodes has been placed around the intersection of two main roads, and the variations in the temporal and spatial variations in the $NO_2$ concentration are analyzed on a hourly basis. In [37] the concentration of $NO_2$ in the area of the Tokyo Institute of Technology has been monitored with semiconductor gas sensors. The sensor nodes were equipped also with a temperature and humidity sensor in order to measure these variables and to compensate for their effect on the sensor response.

Mobile robots equipped with gas sensors can provide an enhancement in the performance of sensor networks for environmental monitoring. Indeed, two of the main limitations of sensor networks are the coarse spatial resolution and the non-adaptive sensors placement. These limitations can be overcome if the sensors are mounted on a mobile robot (Paper VI). Moreover mobile robots with gas sensing capabilities could also be able to track a gas plume to its source and then perform an appropriate action for repairing the damage. The discussion about mobile robots with olfactory capabilities is deferred to Chapter 4.

## 2.5 Discussion

This chapter is by no means a comprehensive review of the field of machine olfaction. The first part of this chapter gives an introduction of the functional parts of an electronic nose. The aim of this part is introducing the aspects that constitute the basis of the original contributions presented in the next chapters.

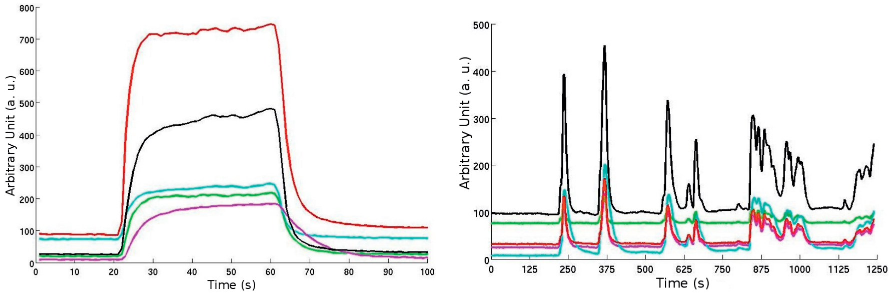
The second part of the chapter presents the applications of artificial olfaction that, in the opinion of the author, can have the highest impact. The works presented in this section have been selected because they try to connect the research in electronic nose with other, more established fields, like analytical chemistry. This, in the opinion of the author constitutes a step forward with respect to works in which a dataset of electronic nose responses are collected and then a machine learning algorithm is applied in order to discover some pattern or correlation in the dataset, without understanding the mechanisms underlying the process under examination. Indeed only by understanding the physical and chemical processes underlying a certain phenomenon or at least by having a clear idea of the chemical compounds relevant for the specific application one can be sure that the solution proposed is really capturing the essence of the problem. Otherwise there is always the risk that the results observed are due to contingent factors that are not taken into account. In the opinion of the author purely machine learning based approaches are a good proof of concept that the electronic nose is a suitable instrument for addressing a certain application. Then, once the proof of concept has been successfully obtained, the attention should be moved towards explaining the phenomena that caused the correlations that have been observed.

# Chapter 3
# Towards Open Sampling Systems

This chapter addresses the problem of discrimination of gases through the analysis of the dynamics of the response of an array of gas sensors. At first a brief summary of the methods for extracting features that can capture the dynamics of a signal collected with a closed sampling system is presented. At the end of the summary, the only contribution of this thesis that deals with a closed sampling system, the identification of bacteria in blood vials using an electronic nose, is presented as a case study. Then, an investigation of the properties of the signal collected with an open sampling system in controlled conditions is presented. The chapter is concluded with a discussion on the results obtained in the investigation.

Recall, the main goal of this thesis is to develop gas discrimination algorithms for e-noses that have an open sampling system, with particular interest to mobile robotics olfaction applications. Before starting the technical discussion of the problem it is beneficial to make some qualitative considerations about the differences between a signal collected with a closed sampling system (three-phase sampling strategy) and a signal collected with an open sampling system. A signal collected with an e-nose mounted on a mobile robot and a signal collected with the same e-nose in a small chamber using the three-phase strategy are displayed in Figure 3.1. The e-nose is an array of 5 MOX gas sensors. The robot on which the e-nose is mounted performed a sweeping trajectory in a large room where a cup filled with ethanol was placed. More details about this experimental setup are given in Section 4.1.

The first difference between the two signals is that, given the open sampling system, the signal collected with the robot does not have the three phases typical of a signal collected by an e-nose with a closed sampling system. This is because there is no step in the concentration of the analyte induced by a sampling mechanism but the changes in concentration are due to the turbulence




(a) Closed sampling system (b) Open sampling system

**Figure 3.1:** Response of a sensor array composed by 5 metal oxide gas sensors. In subfigure (a) the sensors are in a small chamber and the three phase sampling strategy is used. In subfigure (b) the sensors are mounted on a mobile robot and are placed in an actively ventilated tube. Adapted from Paper V.

and advection of the airflow that transports the gas in environments characterized by a high Reynolds number. These changes in concentration have a much faster dynamics than the metal oxide gas sensors themselves and therefore the gas sensor response never reaches a steady state. For this reason, an algorithm for performing gas discrimination or quantification in such a setup has to be able to extract information from the dynamics of the sensor response since a steady state in the response is never observed. The lack of a controlled exposure of the sensor array to the target gases, that in closed sampling systems allows segmenting the signal into three phases, introduces the additional complication of not having any trivial segmentation of the signal into different phases. In most of the articles on which this thesis is based, this problem is addressed by a segmentation policy that is based on the assumption that every patch of gas that hits the sensor array causes a peak in the response. The segmentation algorithm, together with the other parts of the gas discrimination algorithms are described in Chapter 4. Algorithms that can perform gas discrimination on the early phase of the transient are beneficial also for electronic noses with closed sampling systems [38], especially if quick gas discrimination is desirable. Indeed, if the initial transient phase contains enough discriminatory information, the lengthy acquisition time needed for the sensor to reach the steady state can be avoided. Indeed, even for metal oxide gas sensors that have a relatively quick response, a measurement cycle (response + recovery of the sensors to initial state) takes at least five minutes to be completed. If a gas can be identified in the early phase of a response then the sample can be removed before the steady state is reached, causing a speedup also in the recovery phase.

This chapter begins with a brief review of the general problem of analysis of the dynamic response of an array of gas sensors in a closed sampling system (Section 3.1). Section 3.1.4 presents the results of a study where an electronic nose with a closed sampling system uses static as well as dynamic information to improve the identification of bacteria in blood samples. Section 3.2 moves the discussion to the investigation of the properties of a signal collected with an open sampling system under controlled conditions. Section 3.3 concludes the chapter with a discussion on the results concerning gas discrimination with an open sampling system.

## 3.1 Dynamic Feature Extraction in the Presence of Steady State

A sensor response can be seen as time series of length N. The problem of gas discrimination/quantification can therefore be seen as a classification/regression problem in an N dimensional space, where every sensor response is represented by a point. In most of the cases, the number of sensor responses M available for analyzing the problem of interest is much smaller than N. From a geometrical point of view we have M points in an N dimensional space and, given that $M << N$, the density of points is very low. It is well known that the estimation of a function (discriminant or regression) in a high dimensional space (or in a space with a very low density of points) is a difficult problem and therefore the dimensionality of the space have to be reduced before applying any machine learning algorithm. The most common methodology to cope with this problem is to extract features from the signal that can capture the information that is relevant for successfully performing the function estimation task. Only few features are extracted from a sensor response and therefore the dimensionality of the space where the estimation is performed is drastically reduced.

There are in general three approaches for compressing the information contained in a sensor response in order to capture the dynamic of the signal: subsampling procedures, extraction of ad-hoc transient parameters and extraction of model based parameters. In the literature there are various works that compare these different feature extraction methods and, in the opinion of the author, the most significative are [39, 19, 25]. It is important to notice that a further step of dimensionality reduction might be needed. Indeed not all the features extracted from all sensors might carry useful information or many of the feature might be highly correlated. This additional dimensionality reduction step is normally carried out either by projecting the samples on a lower dimensional space (feature extraction) or by selecting a subset of the available feature (feature selection). A feature selection technique for gas discrimination in mobile robotics application has been developed in Paper VII. Details about the contribution and feature selection techniques in general are presented in Chapter 4, which is dedicated to the mobile robotics related contribution.

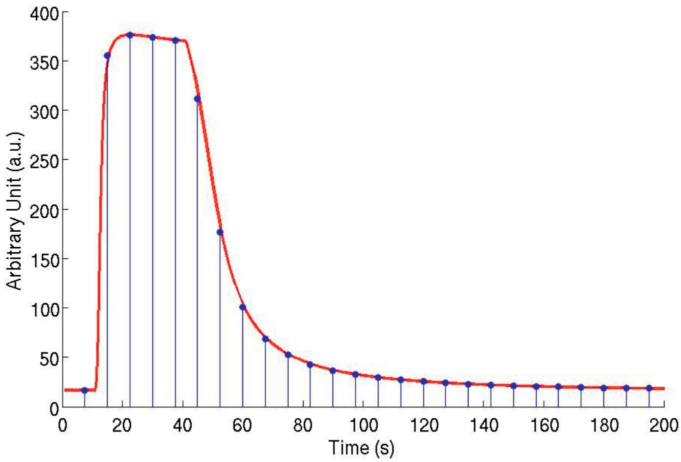



**Figure 3.2:** Response of the sensor MO110 of the NST 3220 Emission Analyzer (Applied Sensors) when exposed to the volatile metabolite of *Escherichia Coli*. The original response has been sampled at the frequency of 2 Hz. The stem plot shows a subsampling where every fifteenth has been kept. Notice that for graphical reasons only the first 200 s of the total response (260 s) have been plotted.

### 3.1.1 Subsampling Procedures

Probably the most straightforward way to capture the dynamics of a sensor response is to sub-sample the sensor response. In this case the dynamic information is represented implicitly in the correlation of the sensor values at different times. This technique can be seen as an extension of the static feature extraction techniques that just consider the sample (or an average of some samples) at the end of the gas exposure phase. Figure 3.2 gives a graphical interpretation of this technique. It should be noted that in certain sensor technologies like metal-oxide gas sensors, the transient in the gas exposure phase is much faster than the one in the recovery phase. Therefore the subsampling should be more fine-grained in the gas exposure phase than in the recovery phase. Indeed, observing Figure 3.2 where a uniform subsampling strategy has been used, it is quite straightforward to notice how only one sample in the steep part of the transient in the gas exposure phase has been kept, compared to at least six samples in the steep part of the transient in the recovery phase.

### 3.1.2 Ad-hoc Transient Parameters

A wide range of heuristic parameters might be extracted from the response of a gas sensor. Figure 3.3 depicts three of the most common: the maximum value of the sensor response, the maximum value of the derivative of the sensor

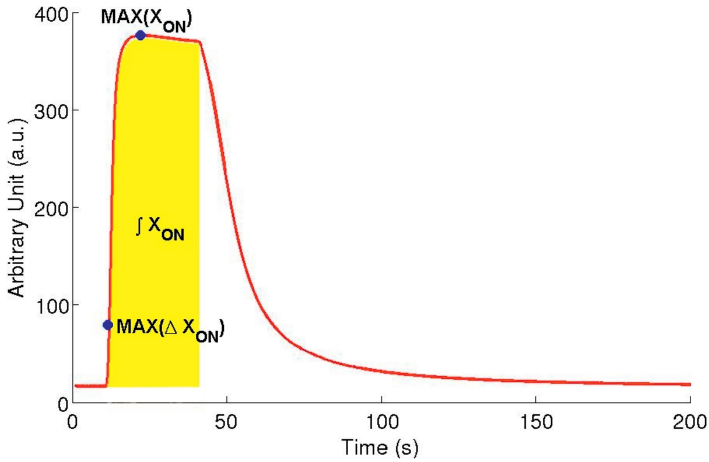



**Figure 3.3:** Response of the sensor MO110 of the NST 3220 Emission Analyzer (Applied Sensors) when exposed to the volatile metabolite of *Escherichia Coli*. The original response has been sampled at the frequency of 2 Hz. Three ad-hoc features are depicted: the maximum value of the response, the maximum value of the derivative and the integral of the response phase. Notice that for graphical reasons only the first 200 s of the total response (260 s) have been plotted.

response and the integral of the sensor response in the gas exposition phase. Other feature can be rise or decay time and derivatives or integrals of the signal taken at different times. A list of the most common ad-hoc feature can be found in [39].

More recently Martinelli et al. [40] proposed to extract features from the phase plot of the sensor response. The phase plot they consider has the sensor response and its derivative as state variables. A number of features like area and higher-order moments are extracted from the phase plot.

It is particularly interesting the work presented by Muezzinoglu et al. in [38] where they present a dynamic feature based on an exponential moving average technique. This feature is particularly interesting since it is possible to modulate the time at which the feature will be available through a parameter. The choice of this value is a tradeoff between the speed in the availability of the feature and the information content. Another interesting aspect is that this feature shows a good correlation with the steady state response of the sensor, and therefore it can be argued it has similar information content.

### 3.1.3 Model Based Parameters

A third way to capture the dynamic information contained in the response of a gas sensor is to fit an analytical model to it and then use the parameters of the model as features. Many types of models have been proposed, ranging from autoregressive models, to polynomial, multi-exponential, sinusoidal (Fourier expansion) and wavelets. Given the exponential nature of the transient response of a gas sensor, the multi exponential models are the most often used. Indeed the sum of exponential functions represents the different reactions that take place when the gas is sampled and absorbed by the sensing surface. In the multi exponential model, the response is modeled by a sum of K exponential functions that can be expressed by the following formula:

$$f(t) = \sum_{i=1}^{K} A_i e^{-t/\tau_i} \tag{3.1}$$

The task of modelling a time series with the sum of exponential functions is an ill-conditioned problem. Indeed, unlike the sinusoidal functions used in Fourier analysis or most of the families of functions used in wavelet analysis, exponential functions do not provide an orthogonal expansion. This implies that the problem of the determination of the coefficients $\{A_i, \tau_i, i = 1 \ldots K\}$ of

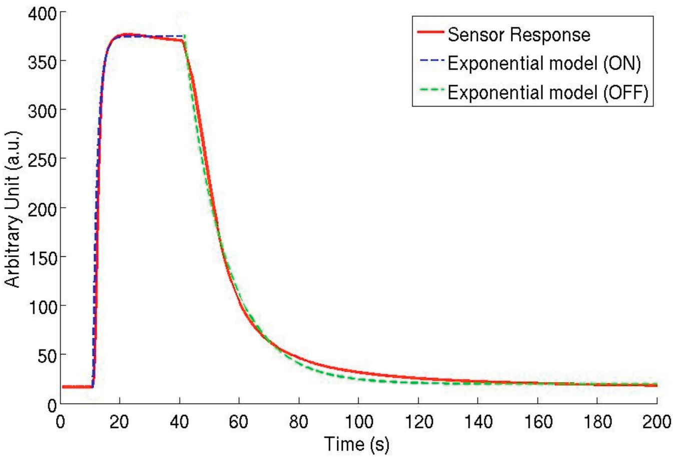



**Figure 3.4:** Response of the sensor MO110 of the NST 3220 Emission Analyzer (Applied Sensors) when exposed to the volatile metabolite of *Escherichia Coli*. The original response has been sampled at the frequency of 2 Hz. The dashed lines show two exponential models fitted respectively to the sampling and to the recovery phase of the signal. Notice that for graphical reasons only the first 200 s of the total response (260 s) have been plotted.

the model from a finite time and finite precision time series does not have a unique solution. Moreover, an additional problem is the determination of the number of exponential models K to be used in the fit. An extensive analysis of the problem of fitting a multi exponential model to the response of a gas sensor can be found at [18]. Figure 3.4 displays the fit of an exponential model to the response of a metal oxide gas sensor. It can be noticed how the fit of a single exponential ($K = 1$ - both for the response and for the decay phase) is not perfect and therefore, for obtaining better feature extraction the number of exponential used in the fit should be increased.

### 3.1.4 Case Study: Bacteria Identification with an Electronic Nose

Sepsis, also known as blood poisoning or septicemia, is caused by the presence of micro-organisms in the blood such as bacteria. With the current techniques used in hospitals, based on bacteria culturing, the identification of the bacterium causing the infection is a lengthy procedure that takes up to 4-5 days. An early diagnosis would allow the usage of antibiotics tailored on the identified bacteria from the first stages of the treatment instead of wide spectrum antibiotics that weakens the immunitary system of the patient. This would translate in a better treatment in terms of shortened hospitalization time and, in the most severe cases of sepsis, in saving human lives.

The project Mednose (Novamedtech framework), is a collaboration between Örebro University and Örebro University Hospital and aims at developing an electronic nose for the fast identification of the bacterium causing sepsis. The work presented in Paper IX describes the details about the pattern recognition algorithm developed for discriminating 10 different bacteria (selected by microbiologists at Örebro University Hospital as main responsible for Sepsis) using a general purpose electronic nose (NST Emission Analyzer, Applied Sensors, Linköping). A prototype of an electronic nose tailored on the bacteria identification problem is currently under development. The proposed algorithm can be summarized in five steps:

**Feature Extraction** The feature extracted are the static response of the sensor and the average derivative of the first 3 seconds of the response. These two features capture both the static and the dynamic information of the signal.

**Dimensionality reduction** In order to reduce the dimensionality of the feature space the linear discriminant analysis (LDA) is used.

**Classification** The classification algorithm that has been considered in this work is the Support Vector Machine (SVM) [41]. The SVM is a popular kernel based algorithm that projects the data into a high dimensional space in which the problem is solved using a maximum margin linear classifier.

The linear decision boundaries in the high dimensional feature space are in general non linear decision boundaries in the original feature space. One of the most important properties of support vector machines is that the estimation of the model parameters is a convex optimization problem and therefore any local solution is also a global optimum. Many variations of the original model of SVM have been proposed, both for classification and regression problems. The model used in this work is the soft margin SVM with Gaussian kernel. The SVM is by definition a binary classifier, though it is possible to extend it to the multiclass case using different approaches. In this work the *one-versus-one* approach is used.

**Posterior Probability Estimation** An estimation of the posterior probability for a sample belonging to each of the classes considered is obtained by fitting a sigmoid to every pairwise decision hyperplane found by the SVM classifier. These pairwise coupled posterior probabilities are then ensembled using the second method proposed in [42] in order to get a multiclass posterior probability.

**Ensembling Decisions** The estimation of the posterior probability from ten consecutive measurements of the same sample are treated as a random sample. A decision is taken only if there is a class whose average of the posterior probability across the ten samples is significantly superior than all the other ten.

The sampling cycle used in this work, as in most e-nose based systems, is composed by three phases: baseline acquisition, odour sampling and recovery to initial state. In the baseline acquisition phase the sensor array is exposed to a reference gas (air in this case) for 10 seconds and the value of the sensors is recorded. During the odour sampling phases the headspace in the analysis bottle is injected into the sensor chamber for 30 seconds. After this, the sensors are exposed again to the reference gas for 260 seconds in order for the sensors to recover the value they had during the baseline acquisition phase. The total length of the sampling cycle is five minutes. The sampling cycle is repeated ten times in a row and we refer to a series of ten consecutive sampling cycles as a measurement. A measurement sequence is composed by one measurement for every type of bacteria. The whole data set is composed by 12 measurement sequences, 6 done with a first batch of bacteria cultures and six done with a second batch one week later. Blood samples within a batch came from the same source and different sources were used between batches.

The proposed algorithm has been validated with a 12-fold cross validation on the collected data set. In every fold, one sequence of measurements have been left out and used for testing the algorithm trained with the remaining eleven sequences. Table 3.1 shows the performances obtained in the twelve measurement sessions. It is evident how measurement sessions 1 and 7 obtain

| # Session | Response Features | Response and Derivative Features |
|---|---|---|
| 1 | 73% | 69% |
| 2 | 91% | 99% |
| 3 | 93% | 98% |
| 4 | 100% | 100% |
| 5 | 100% | 100% |
| 6 | 100% | 100% |
| 7 | 65% | 64% |
| 8 | 88% | 97% |
| 9 | 97% | 100% |
| 10 | 100% | 100% |
| 11 | 98% | 99% |
| 12 | 97% | 96% |

**Table 3.1:** Classification accuracy for the twelve measurement sessions. Taken from Paper IX.

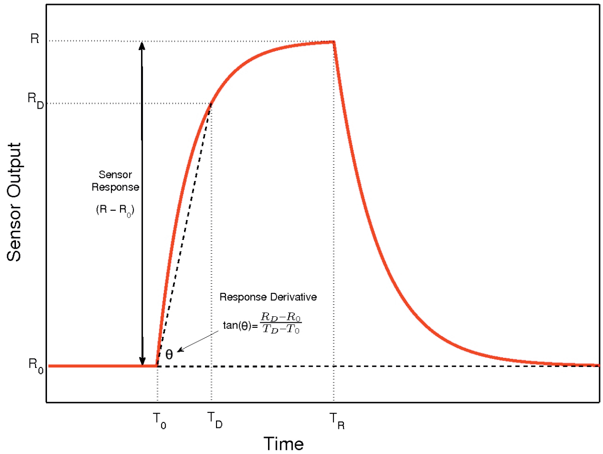



**Figure 3.5:** Graphical interpretation of the two feature extraction methods used in this work. Taken from Paper IX.

a performance much worse than the other sessions. This can be explained by the fact that these two sessions are the ones recorded in the beginning of the two experiment batches. Therefore, we can suppose that this degradation of performance can be due to interference in the measuring system, like humidity deposited on the sensors surface, the sensors were not fully warmed or stagnant air was present in the sampling system. For this reason session 1 and 7 are removed from the subsequent analysis.

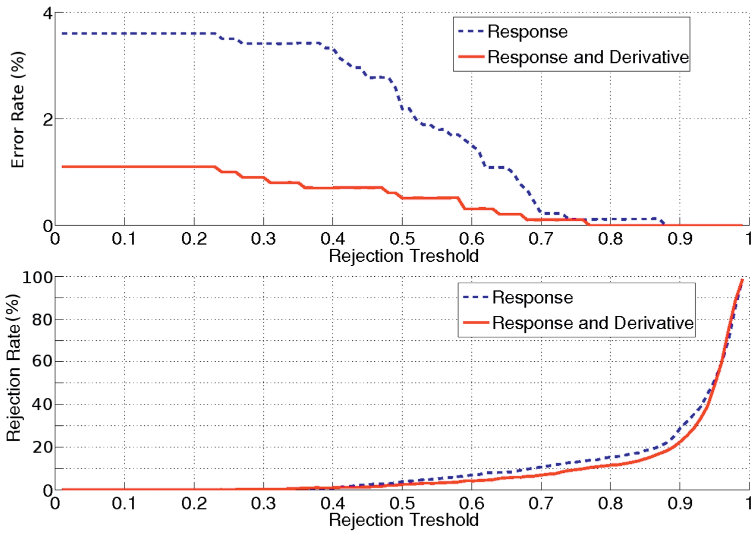



**Figure 3.6:** Performance of the classification algorithm with a varying rejection threshold. The upper figure shows the error rate and the lower figure the rejection rate. The dashed lines represent the performance obtained by the algorithm that uses only the response based features, while the solid lines represent the performance obtained by the algorithm that uses both the response and derivative based features. These results have been obtained using a leave one out cross validation. Taken from Paper IX.

As already mentioned, two features are extracted, from the dynamic response of every sensor: the static response of the sensor and the average derivative of the first 3 seconds of the response. Figure 3.5 displays a graphical interpretation of the two features. Given that the time interval on which the derivative is averaged is fixed (3 s), this feature is directly proportional to the value of the sensor after 3 seconds. Therefore the use of these two features is equivalent to perform a subsampling strategy sampling the sensor response after 3 and 30 seconds of exposure to the sample. Figure 3.6 displays the results obtained by the classification algorithm in case only the steady state value is used and in case both the features are considered. It can be observed how the addition of the derivative based features diminishes the error to roughly its third part over the entire rejection threshold spectrum without increasing the rejection rate. This is yet another confirmation that the dynamic characteristics of the signal contain useful information for the discrimination of gases.

Figure 3.7 shows how the errors are spread across measurement cycles. It can be observed how the number of errors made during the first measuring cycle is larger than the errors in the other cycles. This can be due to the fact that the purging procedure of the nose at the end of a measuring cycle is not perfect

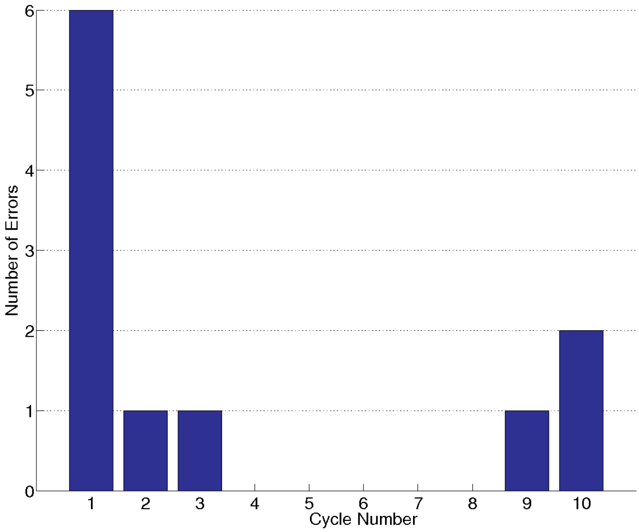



**Figure 3.7:** Number of errors committed by the classification algorithm in the different measuring cycles for the data set where sequences 1 and 7 have been removed. It is evident how the first measurement cycle is more subject to erroneous decisions. Taken from Paper IX.

and therefore some leftover from the previous sampling cycle is still there. This effect is particularly evident in the first measuring cycle since the bacteria that was smelled in the cycle before was different.

Results from ensembling the decisions for the data set without sequence 1 and 7 are shown in Figure 3.8. It is important to notice how neglecting the first cycle improves the performance of the ensemble. This confirms that the first cycle contains additional noise with respect to the subsequent cycles. Figure 3.8 displays only the rejection rate since the error is constantly zero. After only 4 sampling cycles perfect discrimination is obtained as both the error and rejection rate are zero. More details and results can be found in Paper IX.

## 3.2 Investigation of the Signal Dynamics for E-Noses with an Open Sampling System

To the knowledge of the author, the first paper addressing gas discrimination with an open sampling system is [43]. In this work an array of 4 metal oxide gas sensors is mounted on a mobile robot whose task is to navigate to a specific gas source. The feature extraction technique proposed in this work is the Discrete Wavelet Transform (DWT). The authors claim that only 4 seconds of exposure of the array to the target analyte are sufficient in order to perform reliable

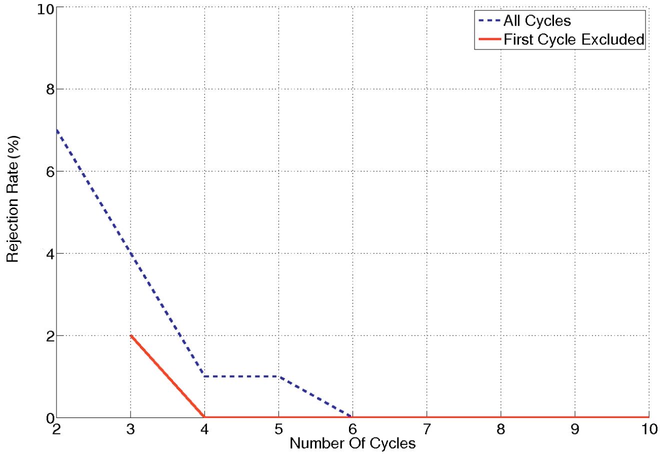



**Figure 3.8:** Performance of the ensembled classification algorithm with a varying number of measuring cycles for the data set where sequences 1 and 7 have been removed. Only the rejection rate is shown since the error is constantly zero. The dashed lines represent the performance obtained by the algorithm that uses all the measuring cycles, while the solid lines represent the performance obtained by the algorithm that neglects the first measurement cycle. Notice that the dashed line starts from cycle two and the solid line from cycle three. This is because at least two samples are needed to calculate an uncertainty. Taken from Paper IX.

identification. Though, the work presented in that paper is not very detailed and contains some clear mistakes. For example the resistance of a n-type metal oxide gas sensor decreases when exposed to some reducible gas, while from one of the figures displayed it seems the opposite. Moreover, the experimental setup and the data processing algorithm are not described in detail. Therefore the validity of the results presented is not clear.

Martinez et. al. in 2006 [44] propose a biomimetic robot for tracking a specific gas plume. This paper addresses both the problem of navigation towards a gas source and gas discrimination in order to be able to navigate towards a specific source. The navigation system is based on the comparison of the signals collected by two spatially separated e-noses places at either side of the robot. The odor discrimination algorithm is based on a spiking neural network using a synchronization coding scheme. The spiking neural network is a biologically inspired computational model that falls out of the scope of this thesis, for more details refer for example to [45]. The methods presented in this paper for gas discrimination and plume tracking are interesting but the experimental setup seems inadequate to demonstrate the claims. Indeed the arena is small compared to the dimension of the robot (the width of the arena is only 4 times

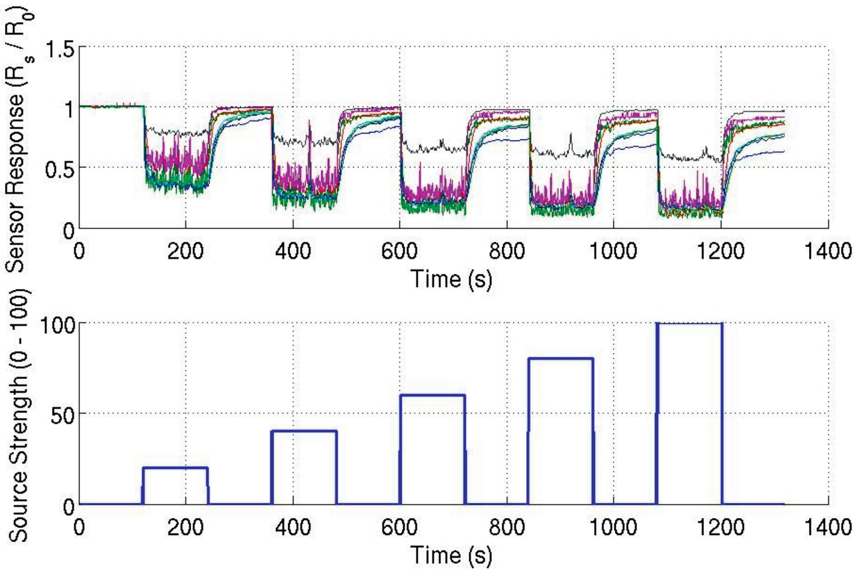



**Figure 3.9:** Sensor response obtained for the experiment in which the gas source emits steps of increasing intensity of ethanol. The sensor response is defined as the instantaneous sensor resistance divided by the value of the resistance measured during the baseline acquisition. Taken from Paper VIII.

the width of the robot) and the two tasks of gas discrimination and gas plume tracking are examined in two different experiments. Therefore it is never really demonstrated that the robot can track a specific gas plume until its source.

In [46] the rapid fluctuations in the concentration of the analyte due to turbulence were reproduced using the gas generator described in [47]. An array of 4 QCM sensors is used to discriminate muscat and apple flavors. The signal processing is carried out using standard techniques like short time Fourier transform (feature extraction), and learning vector quantization (classification).

The work presented in [46] is of particular interest for this thesis since it inspired the experimental setup described in Paper VIII. This setup enables a ground truth on the compound (and its concentration) that is interacting with the sensors in a specific moment. In this way it would be possible to get a deeper insight in the behaviour of the sensors when exposed to abrupt changes of compound/concentration. In this setup the experiments are carried out in a $5 \text{ m} \times 5 \text{ m} \times 2 \text{ m}$ room where an artificial airflow of approximately $0.1 \text{ m/s}$ is induced. The airflow is created using two arrays of four fans (standard microprocessor cooling fans), one placed on the floor and one on the wall. The gas source is an odour blender, a device described in [48] that can mix up to 13 odour components from arbitrary recipes using PWM modulated solenoid valves. This odour blender enables abrupt switches of compound and concentration allowing the generation of rapidly changing controlled signals. The outlet of the olfactory blender is placed on the floor 0.5 m upwind with respect to an array of 11 metal oxide gas sensors and a photo ionization detector (ppbRAE2000, RAESystems). The purpose of the photo ionization detector is to obtain calibrated measurements in the proximity of the metal oxide gas sensor array. These calibrated measurements serve as ground truth for concentration estimation algorithms. Moreover the controlled airflow and the fixed distance of the sensor array from the gas source enable an exact estimation on which substance is hitting the sensor array at every instant. These two facts provide a ground truth on the compound (and its concentration) that is causing the sensor response. The two compounds selected for these experiments are ethanol and 2-propanol. These two substances have been chosen since they are both heavier than air (they form a plume at ground level) and they have a saturated vapor pressure in the same order of magnitude. Having a similar saturated vapor pressure is relevant because the odour blender samples the vials containing the compounds directly from the headspace and this implies that a similar saturated vapor pressure would translate in similar concentration emitted by the odour blender for the two substances. This strengthens the fact that a successful gas discrimination is possible due to the real selectivity of our sensor array and not to differences in the concentration of the two compounds. In order to create a database that allows to study the dynamic behaviour of the sensors when consecutively exposed to different analytes, two different gas emitting strategies have been used. In the first strategy only one analyte is used at the time. The gas source emits clean air for two minutes and the signal of sensors during this period is assumed as baseline. Then for two additional minutes the compound (ethanol or 2-propanol) is emitted at 20% of gas source strength. After which the gas source will emit clean air for 2 minutes. This schema is repeated with source strength 40%, 60%, 80% and 100%. In the second strategy the gas source emits clean air for the first 2 minutes as in the previous strategy. However, rather than continuing to switch between air and a target analyte, the source switches between the two target analytes, namely ethanol and 2-propanol, every 2 minutes. A total of 10 switches between the two analytes is performed. The intensity of the source is chosen randomly in among 20%, 40%, 60%, 80%, 100%. At the end of the experiment the source emits clean air for 2 minutes. A graphical representation of the gas source intensity together with the response of the sensors array for the two emitting strategies is displayed in Figure 3.9 and 3.10.

Analyzing Figures 3.9 and 3.10 it is possible to observe how the sensors, due to the rapid changes in concentration generated by turbulence, never reach a steady state in the same way they do in controlled sampling systems (chamber or flow system). Though, we can observe that after an initial transient phase that takes place when the gas source changes either the analyte or the intensity of emission, the response of the sensor fluctuates around a value. Therefore

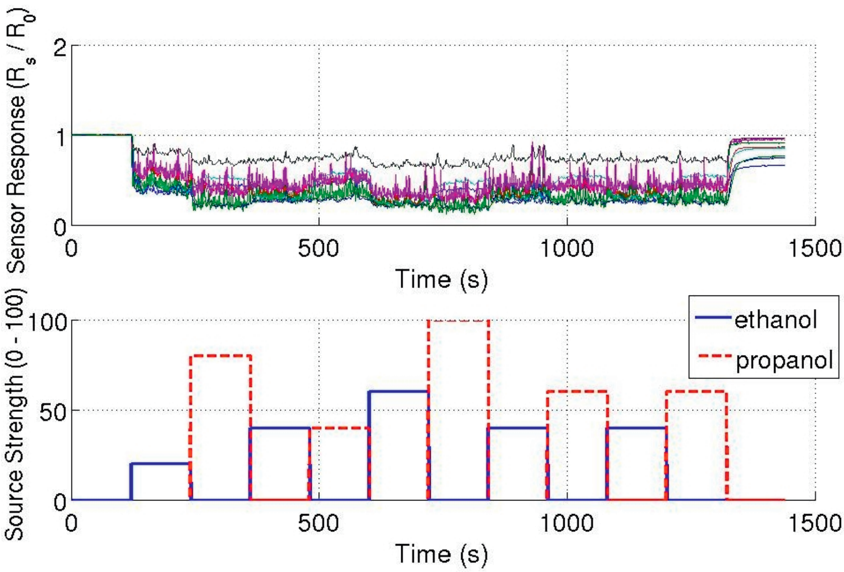



**Figure 3.10:** Sensor response obtained for the experiment in which the gas source emits ethanol and 2-propanol in alternation with random intensity. The sensor response is defined as the instantaneous sensor resistance divided by the value of the resistance measured during the baseline acquisition. Taken from PAPER VIII.

it is interesting to compare the discrimination ability of these two "states" in the signal: signals which are in transient due to switching between analyte, and signals which have fluctuations around a base value after the transient due to switching has occurred. In order to analyze this aspect we calculate how long the sensors take to stabilize around a new value after an intensity/analyte change. An exponential function is fitted to every segment of signal in which the gas source emits an analyte with constant intensity (two minutes) and a time constant $\tau$ is estimated. The transient in between two substances or intensities is considered concluded after a time constant $\tau$ of the slowest sensor has passed (after the switch).

Figure 3.11 shows a PCA plot of all the samples that have been collected after the response of the sensor array has stabilized around a new value. It is possible to notice that the responses collected when the array is exposed to the 3 compounds considered are still well clustered, despite that the turbulence introduces oscillations in the response. This is an indication that, once the sensor has passed the transient phase due to a substance or source intensity change, the fluctuations in the signal due to turbulence do not necessarily prevent the analyte from being identified. In this condition a static system, i.e. a system whose decision at time t depends only on the sensor response at time t, would pro-

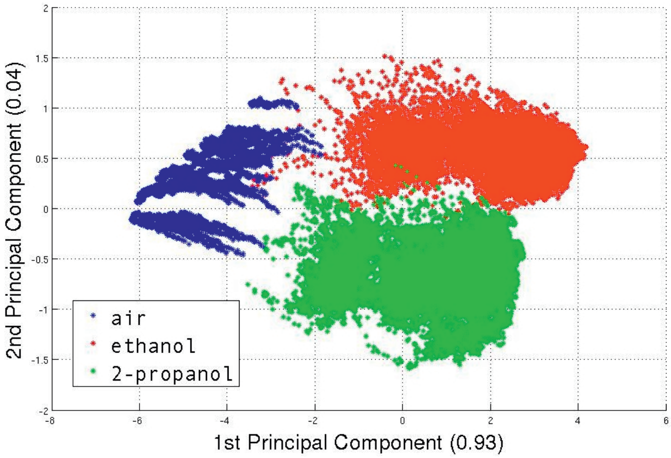



**Figure 3.11:** Samples collected when the transient due to a substance switch is over. Taken from Paper VIII.

vide satisfactory identification performances. For what concerns the transient phase (the time elapsed from the substance switch is less than $\tau$) the situation looks different, as can been seen in Figure 3.12. In this case the clusters overlap significantly, indicating that identification with a static system would be problematic. However, dividing the samples according to the substance from which

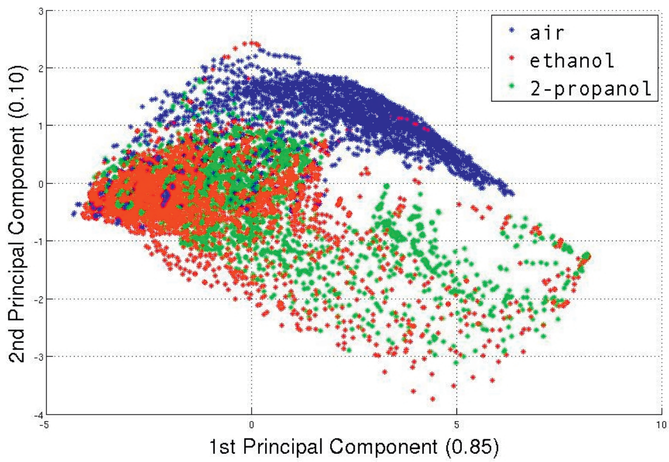
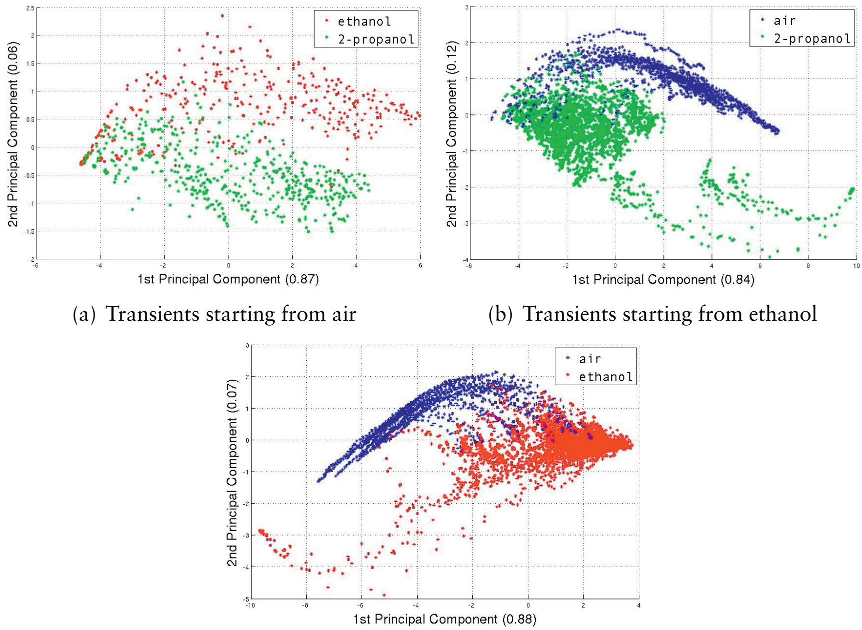



**Figure 3.12:** Samples collected during the transient due to a substance switch. Taken from Paper VIII.




(a) Transients starting from air

(b) Transients starting from ethanol

(c) Transients starting from propanol

**Figure 3.13:** PCA plot of the transients divided according to the substance they start from. Taken from PAPER VIII.

the transient starts changing the situation as shown in Figure 3.13, and a PCA analysis with the first two components suggest good discrimination ability.

In order to verify the applicability of the results to an array of sensors mounted on a mobile robot a series of experiments has been carried out in the same room. The mobile robot experiments are described in PAPER X.

## 3.3 Discussion

Probably one of the most crucial aspects of research in electronic noses with an open sampling system is the design of the experiments. Technical difficulties in designing experiments that enable to study and develop systems for airborne chemical monitoring are due to various reasons.

One reason is that the dispersion of chemicals in natural environment is difficult to observe since most chemicals produce an invisible plume. Plus, given the chaotic dispersal of a gas in natural environment, the plume is also difficult to predict in a generic setting. Moreover, environmental conditions are often very variable and therefore experiments are hard to repeat. Thus it is difficult to obtain a ground truth that can be used to validate experimental results. In order to overcome this limitation, often experiments are carried out under controlled conditions that enable to obtain a ground truth that simplifies the analysis of the experimental data. Another advantage of controlling experimental conditions is that the repeatability of the experiments is increased. On the other hand, it is hard to predict how the results obtained in experiments carried out under controlled conditions extend to uncontrolled environments. Experiments performed with uncontrolled environmental conditions are interesting because they for sure constitute a good benchmark for the system to be developed. Indeed the ultimate goal of research in electronic noses with an open sampling system is to produce systems that can be deployed in a multitude of settings where environmental conditions are not controllable (e.g. environmental monitoring in towns). The experimental setup in often a result of a tradeoff between controlled experimental conditions, that enable deep insight in the data and ease of analysis, and uncontrolled experimental conditions, that enable the collection of data that are more similar to the one that the final system would have to cope with.

This tradeoff has been central in the design of the experiments presented in this thesis. From a chronological perspective, first a series of experiments with a gas sensing robot has been carried out (described in detail in Section 4.1). These experiments have been conducted in different environments under uncontrolled conditions. After developing the algorithms presented in Chapter 4, the experiments under controlled environmental conditions have been performed. Those experiments enabled the observation of the sensor response when the sensors array is exposed to abrupt changes in analyte and/or concentration. Abrupt changes of analyte interacting with the sensors surface might occur in case the sensors are deployed in a location where more than one gas source is present. Therefore the ability of coping with this situation is useful for addressing tasks like multiple gas source localization or gas distribution mapping in presence of multiple heterogeneous gas sources. Another important observation enabled by the controlled experimental setup is that the discrimination problem becomes much simpler when the sensors have been exposed for long enough time to an analyte, despite turbulence does not allow the sensor response to stabilize on one level. In the experiments under controlled conditions this long exposure could be achieved by introducing a stable unidirectional airflow, but in environments where the airflow is uncontrolled this long exposure time cannot be guaranteed. Therefore, it may be important to perform the identification when the sensor is in the transient phase that occurs just after the exposure of the sensor to a substance, even if the sensor have been previously exposed to a different compound without possibility of recovery between the two exposures.

# Chapter 4
# Mobile Robotics Olfaction

This chapter presents the contributions of this thesis related to mobile robotics olfaction. The attention is therefore moved from the analysis of the problem of discrimination of gases with an open sampling system per se, to the implications of having the e-nose mounted on a mobile robot. At first the experimental setup that has been used to collect data is presented, then the algorithmic contributions are analyzed in detail. At last a brief panoramic of related research topics in mobile robotics olfaction is given, with particular attention to the problem of gas distribution mapping since one of the contributions of this thesis is in that field.

Gas sensing with mobile robots is a relatively recent research area that started in the beginning of the 1990s. Chemical sensing capabilities would allow mobile robots to acquire functionalities that cannot be obtained with other sensing modalities. Robots with olfactory capabilities can for example monitor polluted areas (Paper I), detect gas leaks or find explosives [49].

The tasks that have been addressed by research in mobile robotics olfaction are mainly three: gas source localization, gas distribution mapping and trail guidance. The works that address gas source localization can be further categorized with respect to the approach, either gas plume tracing and gas source declaration or gas distribution model based source localization or the sensing modalities available, either with or without using local wind airflow information. To the knowledge of the author the latest review of the field is [13]. In 2008, Kowadlo and Russell presented another review [50], but in this case the scope is limited gas source localization methods.

One of the key challenges for chemical sensing robots is to determine the way in which the gas is dispersed. The Reynolds number is a dimensionless number that can be used to characterize different flow regimes. It gives a measure of the ratio of inertial forces to viscous forces and consequently quantifies the relative importance of these two types of forces for given flow conditions. At low Reynolds numbers, where viscous forces are dominant, the flow regime will be laminar and it will be characterized by a smooth fluid motion, while at high Reynolds number, where inertial forces dominate, turbulent flow occurs which tends to produce random eddies, vortices and other flow instabilities. Gas dispersal in turbulent airflow occurs mainly through advection caused by the fluid flow itself. That is the reason why many gas sensing robots have been equipped with an anemometer that can provide local information on the airflow. Given these considerations, it is understandable how a robot that has to be able to successfully localize a gas source or produce a gas distribution map has to be designed taking in consideration the environment in which it will be deployed.

Together with the difficulties introduced by chaotic gas dispersal, additional challenges are introduced by the sensing device. MOX gas sensors are the most common sensor technology in mobile robotics olfaction because they have a relatively fast response and recovery time, a high sensitivity, a good stability over time and they are commercially available. It is important to notice that, despite MOX based sensor have faster dynamics than other gas sensing devices, the dynamics of MOX sensors is still too slow to be able to capture fluctuations in concentration due to turbulent airflow. This fact, together with cross-sensitivity to temperature and humidity, prevents from interpreting the sensor readings as true gas concentration readings. Another significant drawback of MOX sensors is the lack of selectivity. This makes the gas discrimination problem non-trivial.

Gas discrimination with mobile robots is still a relatively unexplored field. Indeed only a handful of works address it [43, 44, 51]. As already mentioned in Chapter 3, when the array of sensors is deployed in an open sampling system, as is the case with most of olfactive mobile robots, the dynamics induced by the turbulent airflow is too fast for allowing the sensor to reach a steady state. In this chapter, we will move our attention from the analysis of the discrimination of gases with an open sampling system per se, to the contribution related to the fact that the array of sensors is installed on a mobile robot. Section 4.1 describes the experimental setup that has been designed to study the problem of gas discrimination with mobile robots. Following Sections focus the attention on algorithmic contributions. In particular Section 4.2 presents the gas discrimination algorithm, Section 4.3 describes how the gas discrimination algorithm can provide input to the robot's path planner in order to optimize the gas discrimination performance. Section 4.4 presents a feature selection algorithm for optimizing the generalization performance of the gas discrimination algorithm with respect to varying environmental conditions. The chapter is concluded by Section 4.5 that provides a quick overview of other research topics in mobile robotics olfaction.

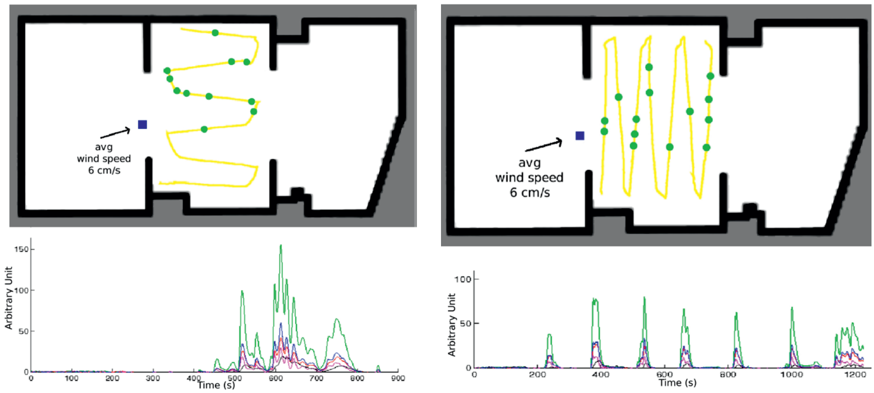
## 4.1 The Experimental Setup

In the papers (Paper I, Paper II, Paper III, Paper IV, Paper V, Paper VI, Paper VII) the experimental setup using a mobile olfactory robot is the same. The robot used is an ATRV-JR all terrain robot equipped with the Player Robot

| Model | Gases Detected | Quantity |
|---|---|---|
| Figaro TGS 2600 | Hydrogen, Carbon Monoxide | 2 |
| Figaro TGS 2602 | Ammonia, Hydrogen Sulfide, VOC (volatile organic compound) | 1 |
| Figaro TGS 2611 | Methane | 1 |
| Figaro TGS 2620 | Organic Solvents | 1 |

**Table 4.1:** Gas sensors used in the electronic nose.

Device Interface [52]. Player provides both the interface to the sensors and the actuators, and high level algorithms to address robotic tasks such as localization (amcl driver) and navigation (vfh and wavefront drivers). Apart from a laser range scanner (SICK LMS 200) used for localization and navigation, the robot is equipped with an electronic nose and an anemometer. The electronic nose is an actively ventilated aluminum tube containing an array of five metal oxide gas sensors, mounted in front of the robot at a height of 0.1 m on the ground. Table 4.1 lists the sensors included in the array and their target compounds.

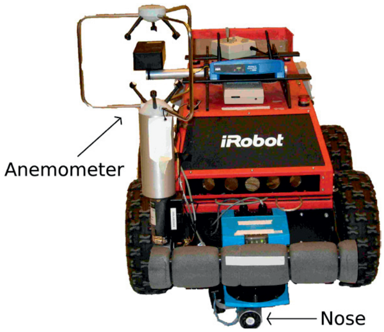



(a) E-W sweeping (b) N-S sweeping

**Figure 4.1:** Upper: Example run where the analyte was respectively ethanol (a) or isopropyl (b). When the robot sweeps N-S it continuously enters and exits the plume, while when it sweeps E-W it stays in the plume for longer time. The arrow shows the average direction and magnitude of the wind flow. The square indicates the position of the source. The solid line is the trajectory of the robot. The circles are locations in which a sensor response was obtained. Lower: sensor readings collected during the run. Adapted from Paper II.

In Paper I the e-nose was mounted at 0.34 m above the ground and the sensor TGS 4161 (electrochemical sensor for $CO_2$ detection) was included in the array. In the experiments on which all the rest of the publications are based, the TGS4161 sensor has been removed since it did not show any sensitivity to the analytes considered in the experiments. Moreover, the position of the nose has been lowered because the three compounds of interest, namely ethanol, acetone and isopropyl are heavier than air and therefore form a plume close to the ground. By positioning the nose 0.1 m above the ground the number of "gas hits" was increased.

Experiments have been performed in three different locations using four moving strategies which attempt to vary the interaction of the robot with a possible plume. In all experiments the robot was moving with a speed of 0.05 m/s. The gas source was a cup full of the analyte placed on the ground. The first location that has been considered is a large closed room in which the robot followed a sweeping trajectory with two orthogonal orientations that are named N-S and




(a) The robot with the electronic nose and the anemometer

(b) The robot in the large room

(c) The robot in the courtyard

**Figure 4.2:** The robot and snapshots from two experimental runs in different locations. Adapted from Paper VII.

E-W. Figure 4.1 provides a graphical representation of the two paths followed by the robot together with the signal collected during two experimental runs.

The second set of experiments has been carried out in a small classroom whose door has been left open. In this environment the robot performed two different types of spiral path: a spiral without any stops from the beginning to the end of the experiment and a spiral with stops when a gas is detected, at which point the robot stands static until enough information is obtained to perform a classification (more details about these moving strategies are provided in Section 4.3). The rooms were ventilated after each experimental run in order to avoid gas accumulation. The last experimental location was a courtyard with an uneven grass surface. In this case the robot performed a spiral movement stopping when a gas is detected similar to the one performed in the classroom.

Figure 4.2 shows a picture of the robot and two snapshots of the robot in action, once in the large room and once in the courtyard. Table 4.2 summarizes the five different experimental configurations. The experiments have been repeated multiple times (more than 100) with three different target substances. It is important to notice that during one experimental run multiple responses were collected. When the signals are segmented with the algorithm illustrated in Figure 4.3, we obtain a total of 592 responses evenly distributed among the three classes.

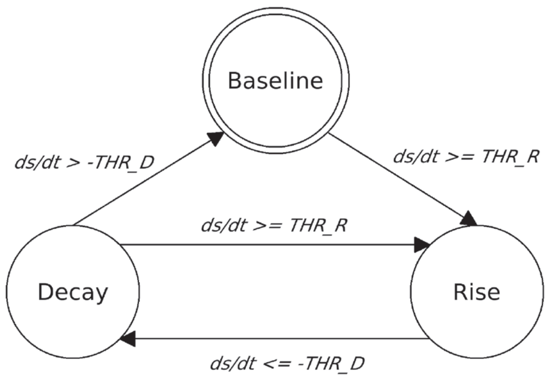



**Figure 4.3:** Finite State Machine that illustrates the segmentation algorithm. The first derivative is denoted as ds/dt and the threshold for the rise and decay are THR_R and THR_D respectively. Two different thresholds are needed since the rise and decay phase have a different time constant. Taken from PAPER III.

## 4.2 Algorithms for Transient Based Gas Discrimination

As already mentioned in Section 3.2, a gas discrimination algorithm for an e-nose with an open sampling system has to be able to perform the identification on the transient phase of the signal. Indeed without a closed sampling system the exposure of the sensor array to the analyte cannot be controlled. Therefore instead of being exposed to a step in concentration under controlled temperature and humidity (three-phase sampling strategy), as most commonly happens for e-noses with a closed sampling system, the sensor array would be exposed to continuous changes in concentration due to the turbulent nature of airflow carrying the analyte to the sensors. In this setup it becomes relevant to identify the parts of the signal that contain the information for performing the identification. The approach that has been used in the works presented in this thesis is to segment the responses due to patches of gas that hit the sensors. The basic observation is that when a patch of gas hits the sensors it causes a response, and a simple approach based on the first derivative of the signal can isolate the responses due to the gas patches. The segmentation algorithm can be efficiently explained with the finite state machine in Figure 4.3. A complete response to a patch is considered to be the ensemble of a consecutive rise and decay phase.

Once the segmentation is performed, different feature extraction methods (FFT, DWT, and polynomial curve fitting), baseline manipulation techniques (differential, fractional, relative) and normalization techniques (vector normalization, vector autoscaling, dimension autoscaling) are used. In Paper V a factor analysis using multiway ANOVA is performed in order to evaluate which of these techniques (or combination of techniques) performs best on the data collected with the mobile robot.

An additional comment is needed on the segmentation policy. The proposed approach is based on the observation that when a patch of gas hits the sensors it causes a response, and a simple approach based on the first derivative of the signal can isolate the responses due to the gas patches. However, this policy of isolating gas patches is not optimal since it is not guaranteed that all the gas patches contain enough information to be correctly identified. Therefore the gas discrimination algorithm presented in Paper II and Paper III provides not only a decision but also an estimation of the posterior probability of each sample belonging to the classes of interest. This posterior probability can be used as a confidence measure on the classification outcome. For example it is possible to introduce a threshold that, if not met by the maximum of the posterior probabilities, the sample is rejected and not classified. The model used for estimating the posterior probabilities is the Relevance Vector Machine (RVM). For what concerns the intermediate parts of the algorithm, namely baseline preprocessing, feature extraction and data normalization, standard techniques were used and therefore their discussion is deferred to the papers in attachment.

More interesting at this point is an analysis of the implications of introducing a posterior probability estimation together with a rejection threshold, and furthermore a closer look on which responses are more difficult to be classified.

As a first analysis of the classification performance (Paper II), a leave-one-out cross validation is performed. The results are shown in Figure 4.4. This graph displays the classification error rate and the rejection rate for different values of the rejection threshold. We can observe how the error rate decreases for increasing rejection thresholds. This means that the calculation of the posterior probabilities is meaningful since raising the rejection threshold we discard more erroneously classified samples than correct ones. Another observation is that the DWT based features outperform the FFT based ones. Indeed, a lower classification error is obtained for every rejection threshold maintaining approximately the same rejection rate. This means that the DWT provides a description of the signal that contains more discriminatory information than the FFT. A more interesting aspect is to analyze how the classification performance varies with the distance between where the sensors response is collected and the gas source. Figure 4.5 shows a scatter plot of the correctly classified responses for varying rejection threshold for the RVM classifier. The scatter plots give a spatial representation of the classification performance where the location of the gas source is marked by the square. Correctly classified responses are

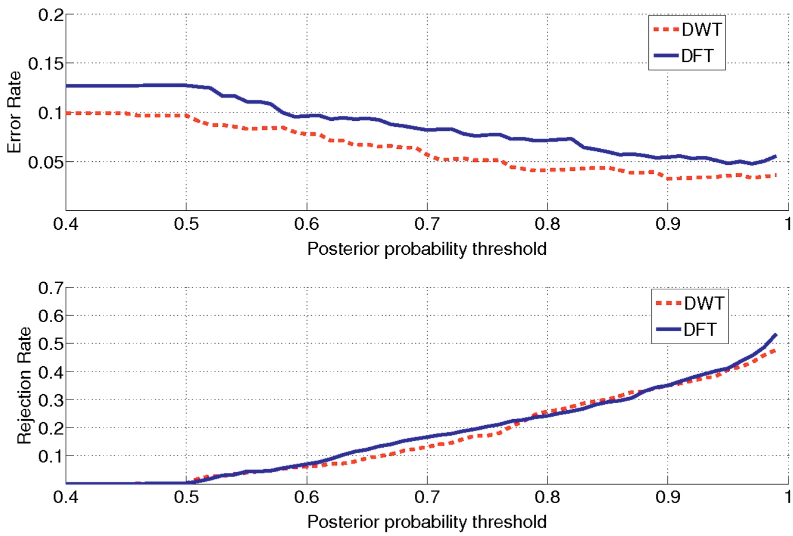



**Figure 4.4:** Classification and rejection rate of the classifier with a varying rejection threshold. The dashed line represents a classifier trained with DWT based features, while the solid line represents a classifier trained with FFT based features. Taken from Paper II.

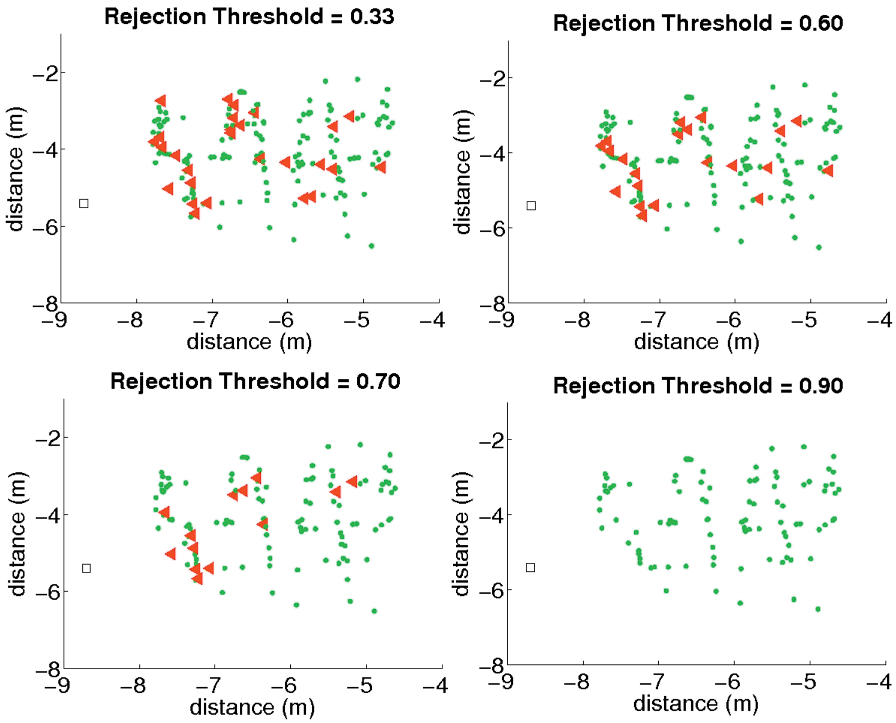



**Figure 4.5:** Scatter plot of the sensor responses classified with the RVM. The circles represent correctly classified responses, while the triangles are the errors. The distances on the axes are expressed in meters. The data depicted in this figure have been collected in the large room environment using two different sweeping strategies (Experimental setup 1 and 2 according to Table 4.2). Taken from PAPER V.

indicated by the smaller circles whereas incorrectly classified responses are indicated by red triangles. Note that successful classification is not only obtained in close proximity to the source but also at distances of approximately 4 meters from the source. Another interesting feature to note is that the misclassified responses are not necessarily concentrated far from the location of the gas source. This suggests that it is not only possible to use an open sampling system but also to use this method in an open environment where the position of the gas source is not known in advance.

In order to gain insight into how the characteristics of the transient affect classification performance, two measures $\gamma$ and $\eta$ are extracted. These measures are defined as:

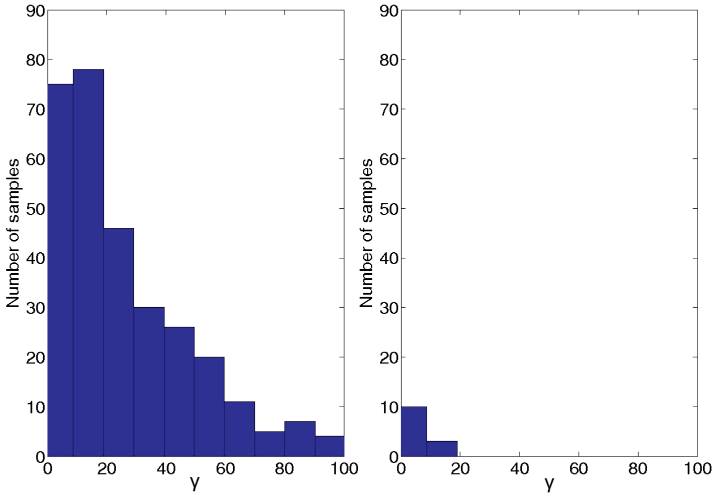



**Figure 4.6:** Left: The histogram of the correctly classified samples with respect to $\gamma$. Right: The histogram of the incorrectly classified samples with respect to $\gamma$. Taken from Paper II.

$$\gamma = \frac{\sum_{t=1}^{N} \mu_n}{N} \tag{4.1}$$

$$\eta = \max \mu_n - \min \mu_n \qquad \textit{where} \tag{4.2}$$

$$\mu_n = \frac{\sum_{s=1}^{S} X_{n,s}}{S} \tag{4.3}$$

The first measure $\gamma$ captures the distance of the transient from the baseline response. Here, $\mu_t$ represents the mean of all the values of all sensors at reading $n$ for a particular transient. $N$ is the total number of readings in a transient and $S$ is the total number of sensors. The second measure $\eta$ is based on the amplitude of the transients calculated by the difference of the minimum and the maximum value of $\mu_n$. Therefore in Figure 4.6 the histogram can be used to depict the correct classifications (seen on the left-hand figure) and incorrect classification (right), with the value of $\gamma$ on the x-axis. Here, incorrect classifications primarily occur on transients close to the baseline (i.e. lower mean values).

In Figure 4.7 a histogram is used to depict the correct classifications and incorrect classifications with value $\eta$ shown on the x-axis. Transients which have higher amplitudes, where the sensors have had longer exposure to a gas, are classified correctly.

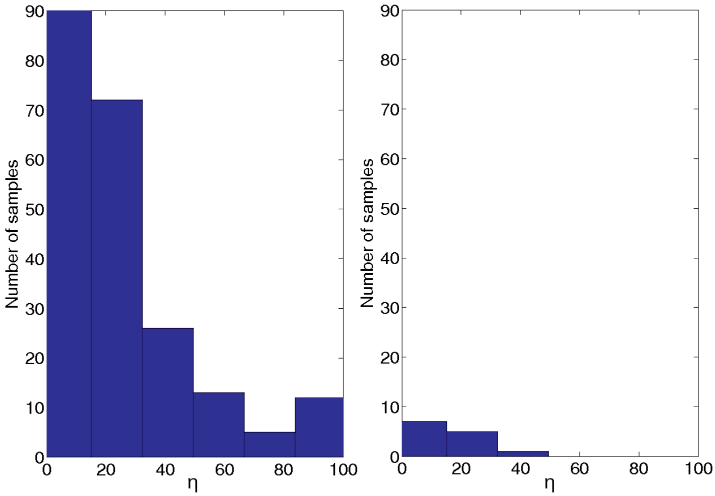



**Figure 4.7:** Left: The histogram of the correctly classified samples with respect to η. Right: The histogram of the incorrectly classified samples with respect to η. Taken from Paper II.

Combining these two results we can see that errors are concentrated in transients which have a small amplitude and are close to the baseline. To achieve good classification, we prefer either a transient with high amplitude or smaller transients that occur in sequence after one another without a complete recovery. It is important to note that these results are validated with the assumption that only one gas is present, but they can be related to the ones presented in Paper VIII. The scenario presented in Paper VIII is more general since the sensors are exposed to different analytes without the possibility to recover in between the two exposures. However, despite this different assumption, both results confirm the fact that samples collected when the sensors have been exposed to a compound for long enough time are easier to classify. Though, achieving a long exposition time of the sensors to the analyte is not a trivial problem. Therefore, the interest in being able to discriminate gases in the first phase of the transient due to the sudden exposure to an analyte or to a compound switch is still intact.

## 4.3 Olactory driven Path Planning

Mobile robots can be valuable instruments for environmental monitoring or inspection of dangerous areas. Particularly in cases where hazardous contaminants are involved, mobile robots can play an important role in assessing the presence of dangerous substances, identifying their character, quantifying their concentration and localizing the source of the substance. Chemical and air-

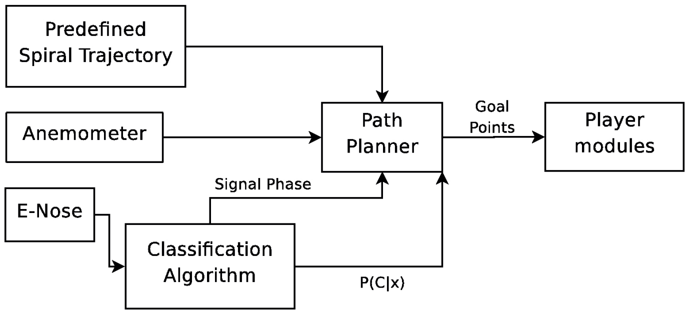
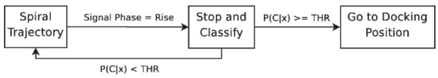


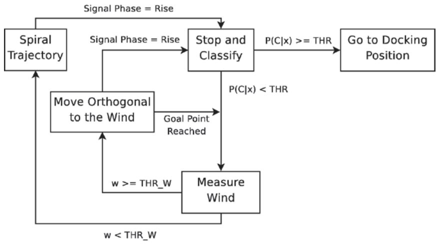

**Figure 4.8:** Software architecture of the exploration system. Taken from PAPER III.

flow sensors, the sensing modalities that have been mostly used for addressing exploration tasks, take point measurements. This means that, unlike range sensors, the variable of interest can be measured only at the location of the sensor. Therefore the mobile robot serves an important role to bring the sensor system to an area where good measurements can be obtained. From now on the attention will be focused on the task of gas discrimination, i.e. determining which compound, among a pool of known compounds, is polluting the area of interest. We assume that only one compound is present at the time. PAPER III presents a set of works that aims at exploiting the capability of the robot of performing gas discrimination online in order to provide to the path planner information that can optimize the exploration and translate into a quicker and more robust identification of the polluting substance. Figure 4.8 displays a block diagram of the software structure designed for this purpose. This structure has been inspired by the results described in PAPER II. There it was noted that, with respect to classification performance, it is beneficial that the robot stays in the gas plume as long as possible (at least until enough confidence on the gas discrimination is obtained). Therefore the classification algorithm has been implemented in order to run online while the exploration is being performed and provide information to the path planning algorithm. In particular the robot starts performing a spiral trajectory that covers the area of inspection until the segmentation module of the classification algorithm detects a response from the gas sensor. At this point the robot stops and collects a whole response being inside the plume. Then a classification is performed and in case high confidence is obtained (posterior probability of one of the classes greater than 0.95) then the exploration is declared finished and the robot goes back to the docking position. Otherwise the exploration is continued until the next response is collected.

Two algorithms for continuing the exploration have been proposed: in the first case the robot continues to follow the predefined spiral trajectory (Fig-




(a) Path planning strategy that makes use only of the electronic nose




(b) Path planning strategy that makes use both of the electronic nose and the anemometer

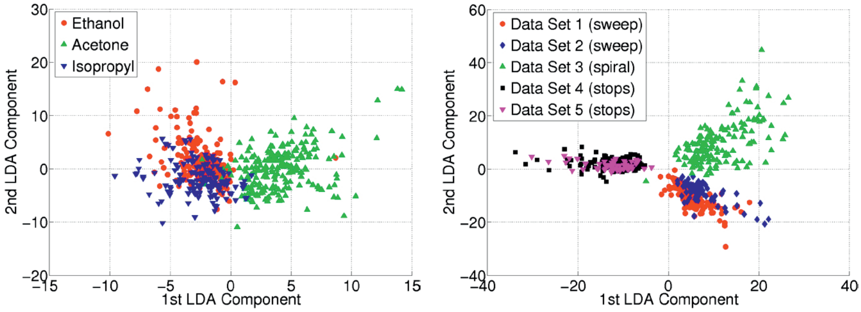
**Figure 4.9:** Olfaction driven path planning strategies. Taken from Paper III.

ure 4.9(a)), while in the second case the robot navigates perpendicular to the wind in order to try to reacquire the gas plume (Figure 4.9(b)). For details about these two algorithms refer to Paper III. Both these strategies have demonstrated to be beneficial with respect to both the exploration time (by allowing an incomplete exploration is quite obvious that the exploration time is reduced) and the classification performance. Though, the efficiency of the strategy in which the robot travels perpendicular to the wind is still to be proven. Indeed, since in a indoor environment the local wind information is chaotic there can be large differences in the direction and intensity of the wind in neighbouring points. Therefore the trajectory followed by the robot when traveling perpendicular to the wind is characterized by some randomness. Consequently, before ascertaining the efficacy of the algorithm, a deeper study and analysis of a navigation strategy given the wind information is needed in future study. Nevertheless, the basic ingredients for achieving gas discrimination in an online context whilst actively exploring the environment have been developed in this work.

## 4.4 Feature Selection for Gas Discrimination with Mobile Robots

At this point, we have collected a dataset of gas sensor responses generated by three different compounds, in five different experimental conditions. Experimental conditions differ for either the robot moving strategy or the experimental location. Table 4.2 summarized the performed experimental runs.

In Paper IV it was observed that the experimental conditions heavily influence the signal collected by the mobile robot. In that work, after the segmentation algorithm presented in Section 4.2, a second order polynomial was fitted to the each sensor response. The coefficients of the fitted polynomial were considered as features to be fed to the subsequent parts of the algorithm. Figure 4.10 shows the LDA projection of the responses collected in the experiment listed in Table 4.2. LDA is a supervised dimensionality reduction method that




(a) LDA with respect to the compound

(b) LDA with respect to the experimental condition

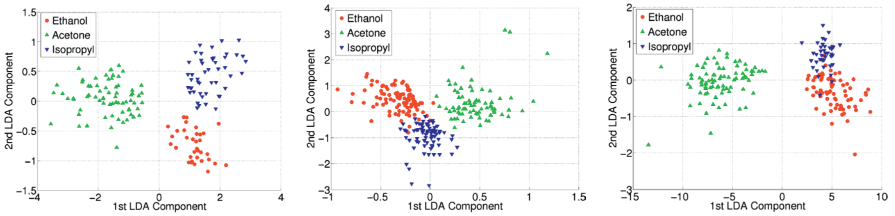
**Figure 4.10:** LDA projections of the collected data set. Taken from Paper IV.

minimizes the average distance among points belonging to the same class while maximizing the distance among the centers of different classes. In particular Figure 4.10(a) displays the LDA considering the compound as a target label while Figure 4.10(b) displays the LDA considering the experimental condition as a target label.

It is noticeable how the clusters formed for the robot movement label are more separated and compact than those formed by the compound label. This suggests a classification algorithm that, implicitly, first recognizes the robot movement and then the compound. Once the robot movement has been recognized the classification becomes much easier, as we can see from Figure 4.11 that displays the LDA with respect to the compounds when the responses collected with the three different movements are considered separately. This algorithm was implemented as an ensemble of linear classifiers that obtained a 89%

| Experimental Setup | Location | Moving Strategy | Number of Runs |
|---|---|---|---|
| 1 | Large Room | Sweep N-S | 15 |
| 2 | Large Room | Sweep E-W | 15 |
| 3 | Classroom | Spiral | 18 |
| 4 | Classroom | Spiral with Stops | 72 |
| 5 | Courtyard | Spiral with Stops | 16 |

**Table 4.2:** Summary of the experimental conditions in which the data have been collected.




(a) Spiral movement (b) Spiral with stops movement (c) Sweep movement

**Figure 4.11:** LDA projections for the dataset partitioned into the different robot movements. Taken from PAPER IV.

of correct classifications. As a term of comparison we used a SVM with RBF kernel working on the whole dataset that obtained 75% correct classification.

These results form the basis of the work presented in PAPER VII. Indeed the solution of first recognizing the exploration condition and then the compound is suboptimal. For discrimination on a mobile robot to be generic, it is necessary to find a set of features which are independent of the experimental setup. In this way, we can enable the possibility to train a mobile robot on a specific gas in one environment and deploy the robot in another environment having different properties and/or having different interaction with the plume. These features acquire particular importance when the robot has to be deployed for a search and rescue operation or for exploration in an unknown environment. The general approach we consider in this paper for dealing with the above problem is to extract features from the sensor signals and select features that show regularity across the experimental setups while providing enough discrimination between different analytes. The measure chosen to formulate this concept is the mutual information. Mutual information has its origin in information theory and provides a measure of mutual dependence of two random variables. The mutual information, $I(X, Y)$, in between two random variables $X$ and $Y$ can be calculated according to the following formula:

$$I(X, Y) = \int_Y \int_X P(X, Y) \log \frac{P(X, Y)}{P(X)P(Y)} dXdY \tag{4.4}$$

Mutual information is lower bounded by the value zero, obtained in case the two variables are independent and upper bounded by the entropy of one of the two random variables in case they are coincident. In PAPER VII mutual information is used as an index to measure the dependency between a feature and either the compound label or the experimental setup label. The dependency between a feature and the compound label can be considered a measure of its discriminative power and therefore it is a positive feature, while the dependency between a feature and the experimental setup label can be considered a measure of the variability of a feature across different experimental condition, which is something we want to penalize. Two feature selection approaches, one filter and one wrapper have been proposed.

In the filter approach each feature f is ranked according to the following score:

$$\gamma(f) = \frac{I(f,S)^{\alpha}}{I(f,C)} \tag{4.5}$$

where S is the experimental setups vector, C is the analyte labels vector, I is the mutual information between two random variables and $\alpha$ is a parameter that modulates the relative importance of the two factors. The best features in the set have the smallest values for $\gamma$. It is important to notice that for $\alpha = 0$, the expression degenerates to $\gamma(f) = I(f;C)^{-1}$ and therefore we would select the features with the highest mutual information with respect to the class vector, that is equivalent to the traditional information theoretic ranking criterion. For increasing values of $\alpha$ we tend to prefer features that do not carry any information about the experimental setup and therefore are more robust to changes in the environment or in the moving strategy of the robot. The joint and marginal distributions ($P(f;C)$,$P(f;S)$,$P(f)$,$P(C)$ and $P(S)$) used in the calculation of the mutual information are estimated using histogram techniques.

In the wrapper approach we propose a modification to the Backward Elimination algorithm. Indeed one of the weak points of the Backward Elimination algorithm is that many features would be good candidates for elimination since the performance of the subsets of the remaining features does not drastically change. Rather than perform an uninformed choice on which feature to eliminate (since they are equivalent with respect to our criterion), we isolate the features which obtain a comparable classification accuracy. These features are then ranked according to the mutual information with respect to the experimental setup and the highest ranked feature is permanently eliminated. Technical details of the algorithm can be found in PAPER VII.

The algorithms proposed have been evaluated performing a 5-fold cross validation where every fold has been formed by taking all the samples collected in a specific experimental setup. This evaluation scheme has been chosen in order to analyze the ability of the system to generalize and perform well in an unknown experimental setup. Figure 4.12 gives the classification performance obtained selecting features with the proposed filter approach with $\alpha = 10$ and with $\alpha = 0$ (based only on the mutual information between the features and the labels). The optimal value of $\alpha$ has been iteratively evaluated. The error bars display the average performance across the 5 folds together with the standard deviation. We can notice that the proposed filter clearly outperforms the filter based solely on the mutual information with the classes. Moreover the proposed approach obtains in average a smaller standard deviation for the performance across the fold. This is important because it shows how the feature subsets obtained with the proposed filter are more robust with respect to variations in the data. Figure 4.13 shows the classification performance obtained by

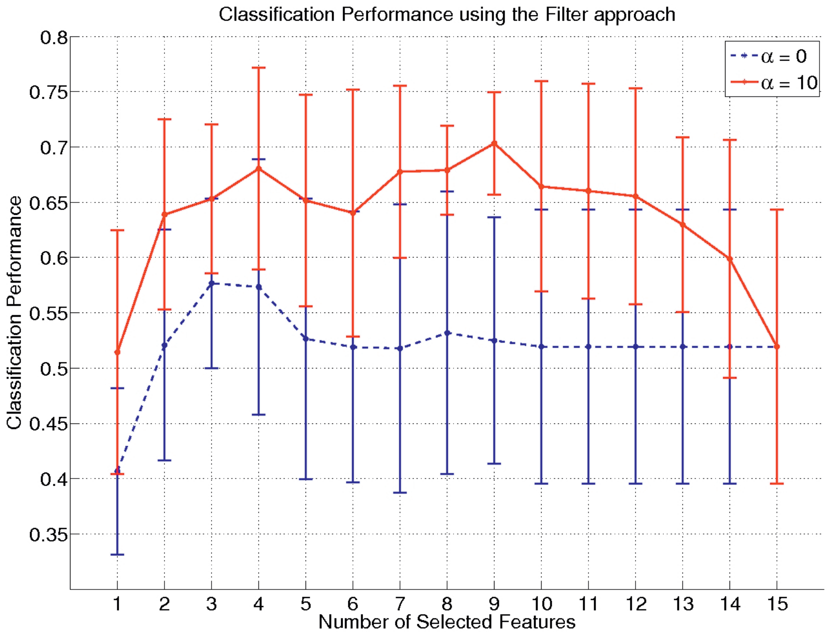



**Figure 4.12:** Error bars displaying average and standard deviation of the performance of the classifier obtained selecting the features using the filter approach. The lines represent the performance of the proposed approach with $\alpha = 10$ and $\alpha = 0$. Notice that $\alpha = 0$ is a filter based only on the mutual information between each feature and the labels vector. Taken from Paper VII.

the proposed wrapper approach compared with a wrapper that in case of ties selects to eliminate the first feature in the list. In the proposed approach features are considered equally ranked if the classification performance differs by less than $\epsilon = 0,2\%$ (given that we have 592 samples, each sample contributes for $0,16\%$). Also in this case we can see how the proposed approach outperforms the traditional one both with a higher average performance and with a lower standard deviation for the performance across the folds.

Comparing the performances of the two proposed approaches we can notice that the number of features yielding the best classification performance is 9-10. Also, the wrapper outperforms the filter both for average classification performance and small variance in between the folds. This has to be expected since the wrapper approach scores the features according to the performance of the target classifier (in contrast with the filter approach that uses a score that is independent from the classifier). The main drawback of the wrapper approach is that it is computationally more expensive since it requires a training of the classifier for every feature subset to be evaluated.

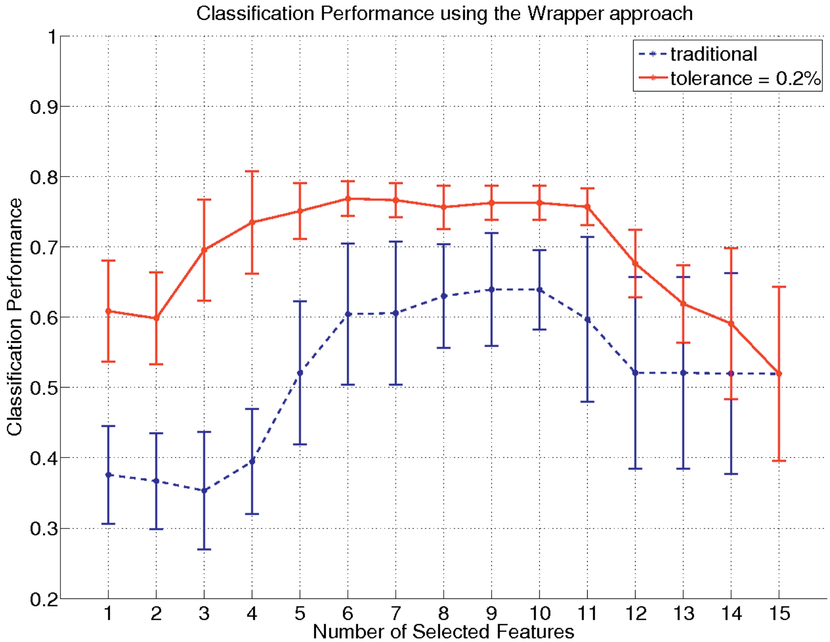



**Figure 4.13:** Error bars displaying average and standard deviation of the performance of the classifier obtained selecting the features using the wrapper approach. The solid line represents the performance of the proposed approach while the dashed line represents the performance of a wrapper that eliminates the feature that when removed obtains the highest classification performance. In case of a tie the wrapper eliminates the first feature of the list. Taken from Paper VII.

To further analyze the results it is also possible to examine the regularity between the ranking of the features across the different sensors and the coefficients of the model (a second order polynomial in this case) that we fit to the sensor response. By analyzing the rankings obtained by the groups as random variables it is possible to get some insight on how a specific sensor/coefficient contributes to the classification task. Paper VII contains the details of this analysis.

## 4.5 Related Topics in Mobile Robotics Olfaction

Most of the works in mobile robotics olfaction have been developed under the assumption of a single predefined analyte. The capability of discriminating gases would enable to extend those results to scenarios in which more than one compound is present. For example a gas sensing robot would be able to perform gas distribution mapping in presence of multiple different gas sources, to localize a specific gas source in presence of interfering gas sources or to follow a specific chemical trail. This section gives a brief overview of the works that would benefit from the introduction of gas discrimination capabilities.

Some early works start appearing in the beginning of the 1990s. These works focus on gradient following strategies for gas plume tracing. The applicability and reproducibility of the results obtained is unclear since no explicit description of the environmental condition is given. Indeed these works start from the assumption that gas disperses due to diffusion leading to a stable and smooth chemical concentration. For ground robots this assumption is unrealistic since natural environment is dominated by turbulent flow and therefore no smooth concentration gradient to follow is available. Therefore in the next sections we will focus our attention on later works that paid more attention to the description of the environmental conditions and therefore to the actual complexity of gas dispersal. Section 4.5.1 presents works related to gas distribution mapping, Section 4.5.2 deals with gas source localization and Section 4.5.3 gives an overview on works dealing with chemical trail tracing.

### 4.5.1 Gas Distribution Mapping

Gas distribution mapping is the task of deriving a truthful representation of the observed gas distribution from a set of spatially and temporally distributed measurements of relevant variables, foremost gas concentration, but also wind and temperature, for example. Building gas distribution models is a very challenging task since many realistic scenarios are characterized by a high Reynolds number and therefore gas disperses by turbulent advection. This results in a concentration field that consists of fluctuating, intermittent patches of high concentration. Given this consideration, an exact description of the gas distribution is an intractable problem, though it is possible to describe turbulent gas distribution *on average* under certain assumptions [53]. It is important to notice that the maps obtained in most of the works that can be found in literature that use metal oxide gas sensors, are obtained from the raw sensor response and thus cannot be directly interpreted as concentration maps. Indeed metal oxide gas sensors are cross sensitive to temperature and humidity and have a slow response time (much slower than what would be needed to be able to follow the fluctuations in concentration due to turbulence). For these reasons their readings cannot be directly interpreted as concentration measurements. Thus, the preferred solution in most of the works in literature is to calculate a *gas distribution map* instead of a true *gas concentration map*.

Probably the most straightforward method to create a time-averaged gas distribution model is to perform measurements for a prolonged time with a grid of gas sensors deployed on the area to inspect [54]. The main advantage of performing simultaneous measurements with a grid of stationary sensors is the reduced time needed to obtain measurements over the area of inspection, while the main drawbacks are the need for calibration to match the sensitivity of the different sensors, the lack of flexibility in the sensor positioning and the increasing cost with the size of the area to cover.

Instead of using a grid of sensors, gas measurements can also be performed in succession by placing a sensor on a mobile platform. This approach is particularly appealing in case of a gas source with constant delivery and stable environmental conditions. Mounting a sensor on a mobile platform has several advantages, of which the most relevant are the flexibility and adaptiveness of the sensor position, the possibility of tracing a gas plume, the possibility to adapt to changes in the environment and the possibility of exploring an unknown area (installing a sensor network in advance in disaster area is unfeasible). The main drawback is the impossibility to get simultaneous measurement at different places. This limitation implies to assume stable environmental conditions for being able to perform gas distribution mapping or at least the need of a mechanism to discover any change to the environment in order to understand that part of the measurement are out of date and therefore need to be discarded.

After having examined the main modalities for data acquisition, the attention is focused on the algorithmic aspect of gas distribution mapping focusing mainly on the algorithms developed for small scale gas distribution mapping with mobile robots. Two approaches are predominant: the model based and the statistical based. Model based algorithms infer the parameters of an analytical model from the measurements. The application of truthful fluid dynamics model is often unfeasible in practical situations (lack of boundary conditions and computationally too expensive). Therefore rather unrealistic simplifications have to be applied to the models in order to remove part of the complexity. For example, the gas distribution model used in [54] makes the assumption of an unidirectional wind field where the time-averaged wind speed is constant and the wind turbulence is isotropic and homogeneous.

Statistical based algorithms try instead to learn a predictive model of a measurement $z$ at the query location $x$

$$p(z \mid x, x_{1:n}, z_{1:n}) \tag{4.6}$$

given a set of measurements $z_{1:n}$ taken at locations $x_{1:n}$. Probably the simplest method for small scale statistical based gas distribution map is presented in [55]. In this work the gas distribution map was obtained applying bi-cubic and triangle-based cubic interpolation. The main problem with these interpolation methods is that there is no means of "averaging out" instantaneous response fluctuations since every measurement appear independently in the gas distribution map and thus the representation tends to get more and more jagged while new measurements are added. Another approach proposed by Hayes et al. [56] is to calculate a 2D gas histogram where "gas hits", that is sensor readings above a threshold, are accumulated. The main weak points of this algorithm are that the information gathered from the sensor is reduced to binary "hits" and all the information contained in the average sensor readings is discarded. Moreover this method requires perfectly even coverage of the area of interest. Lilienthal and Duckett presented a kernel extrapolation distribution mapping ("Kernel DM") that can be seen as an extension of the histogram method. The concentration field is represented in the form of a grid map. Spatial integration is carried out by convolving sensor readings and modelling the information content of the point measurements with a Gaussian kernel [57]. The kernel can be seen as a model of the information content of a measurement about the average concentration with respect to the point of measurement. Intuitively, the information content decreases with increasing distance from the point of measurement. This algorithm does not require perfectly even coverage of the area of inspection but, due to the slow sensor dynamic of MOX sensors, either one has to consider only measurements when the robot stands still or the robot path has to average out the distortion component due to the direction of the movement (in this case the distribution will be more stretched and blurred but not deformed).

An interesting extension (PAPER VI) of the "Kernel DM" algorithm is the "Kernel DM+V" that, together with the mean of the distribution, it estimates also the variance. Two main points make the estimation of the variance particularly interesting. First, studies in literature propose that the maximum of the variance map is a more accurate predictor of the location of the gas source than the maximum in the distribution mean map. Second, and probably more interesting, the estimated variance provides a tool for evaluating the obtained model by measuring how well unseen measurements are predicted. The score calculated for this purpose is the negative log predictive density (NLPD) that is the average negative log likelihood assuming a Gaussian posterior. Evaluating a distribution model has always been problematic in the field of gas distribution mapping. Indeed, considering the fact that is very difficult to obtain ground truth measurement, gas distribution models have often been evaluated with their capability to infer hidden parameters like the gas source location or independently measured mean concentrations. However, an estimator of the prediction capability of the model is a more principled tool for evaluating and comparing different models. Moreover such a measure, not only allows a better ground truth evaluation, but enables as well the learning of the parameter model (kernel size) from the data. The details on the estimation of the model and the NLPD are in PAPER VI.

Recent developments of the "Kernel DM+V" algorithm from Reggente and Lilienthal extend the algorithm to estimate a 3D map [58] and to include in the mapping process information coming from an anemometer placed in proximity of the gas sensors [59]. The wind information is integrated by giving the kernel an elliptical shape and modifying the orientation of the ellipse according to the wind direction.

### 4.5.2 Gas Source Localization

Gas source localization is by far the most studied problem in mobile robotics olfaction. Many taxonomies of the gas source localization methods are possible depending on:

- Environmental conditions: laminar airflow, turbulence dominated environment with strong unidirectional airflow, turbulence dominated environment with weak chaotic airflow, diffusion dominated environment (e.g. underground [60]).
- Sensor modalities: the robot is equipped only with gas sensors or with other sensor modalities that can provide useful information for localizing the gas source. The most commonly used sensor modalities are an airflow sensor (anemometer) or cameras that can help the robot in recognizing the gas source in case some prior information on shape/colour of the gas source is available.
- Biologically inspired or statistical based search strategies.
- Plume model based strategies or model free strategies.
- Single robot or multiple robot strategies.

To make a complete review of the research area of gas source localization is out of the scope of this thesis. For this reason the attention will be focused on works that were published after the two comprehensive studies published in 2006 and 2008 [13, 50]. Before starting the discussion it is important to notice that localizing a gas source does not necessarily imply moving towards it. Indeed the robot might, instead of moving towards the gas source, travel towards locations where a measurement could provide valuable information for reducing the uncertainty on the source position (and this does not always coincide with traveling towards the gas source).

Probably, the most influential and revolutionary article in the field of gas source localization is [61]. This paper introduces *Infotaxis* as a search strategy for a chemical source in a chaotic environment. In contraposition with *Chemotaxis* and *Anemotaxis* two of the most common strategies for searching a chemical source, *Infotaxis* does not use any local concentration gradient or local airflow information. This is a big theoretical advantage above the aforementioned methods, since in turbulent environments the signal-to-noise ratio for these two variables is very low. The concept at the basis of *Infotaxis* is entropy, the central concept of information theory. *Infotaxis* interprets a sequence of gas “hits” separated by voids where the concentration gas is below the limit of detection, as a message transmitted by the source to the searcher with strong noise due to the chaotic nature of turbulent environment. The decoding of the message can be interpreted as calculating the posterior probability distribution of the unknown location of the source. Entropy is a quantity that measures how spread out a probability distribution is, and goes to zero when the probability distribution takes only one value. In case this probability distribution models the unknown location of a gas source and its entropy is zero, it means that the location of the gas source is known exactly. Since the searcher estimates the probability distribution of the location of the gas source from the data he has available (the history of the gas encounters), the goal is to try to collect information that provide the largest decrease of entropy, i.e. the biggest amount of information on the location of the gas source. In [61] it is also observed how infotactic trajectories feature "zigzagging" and "casting" movements similar to those observed in the flight of moths, that has being the source of inspiration for many other algorithms developed for gas plume tracking. In [61] only simulated experiments are presented, but Moraud and Martinez in [62] provide an experimental validation of infotaxis with real robots that successfully localize, a heat source (the transport mechanism of heat is very similar to the one of chemicals in environments where advection clearly dominates over diffusion, but temperature sensors have a faster dynamics than chemical sensors).

Lochmatter et al. presented systematic evaluation and comparison of three bioinspired algorithms for plume tracking described in the literature, namely the *casting*, *surge-spiral* and *surge-cast* algorithms. The comparison is carried out both in simulation [63], with experiments carried out in a wind tunnel with real robots [64] and even theoretically under simplifying assumptions [65]. The algorithms are compared in terms of success rate and distance overhead when tracking the plume up to the source. Overall, the algorithms based on upwind surge yield significantly better performance than pure casting. Interesting extensions of these evaluations are presented in [66], where the algorithms are evaluated in presence of obstacles and in [67], where the performance of the same three algorithms is evaluated in the context of a non-cooperating multi-robot system.

### 4.5.3 Chemical Trail Following

Stigmergy is a mechanism that allows the coordination of actions within the same agent or across different agents by means of traces left in the environment. A well known example is given by ants that mark the path to a source of food with a chemical trail [68]. Chemical markings are particularly suited to store temporal information due to their naturally fading intensity. For example chemical marking could be used as a barrier for signaling areas that have already been wiped to an autonomous cleaning robot.

In contrast to the task of following a gas plume, the effect of turbulence and airflow advection is considerably reduced in the case of trail following because the distance between the sensor and the source is small. In the experimental work published in this area the height of the gas sensors on the ground was in the order of 10 $mm$ [13]. According to [70], chemical trails placed on the floor are covered by a layer of laminar airflow. Though, this layer is so thin that state of the art robots cannot perform gas measurements in this region. However the proximity of the sensors to the gas source (the trail) causes a pretty large concentration difference between the situation where the sensors are on the trail and when the sensors are outside. This is normally not the case in experiments where a gas plume has to be traced and a distant gas source has to be localized. In [69] it has been proposed a device, depicted in Figure 4.14, to further enhance the concentration gradient encountered between the trail and non-trail region. This device draws air from the floor to the sensor inlet and blows air in the opposite direction around the sensor inlet in order to create an "air curtain". However, the efficacy of this device has been questioned by Larionova et al. in [71], and it is currently unclear whether the different results have been obtained because of small differences in the implementation of the air curtain or to differences in the tasks considered (detecting a narrow trail in [69] versus a comparatively wide area in [71]).

All other works in the area focus mainly on designing an algorithm that implements a trail following strategy. Particular attention is devoted to enhance the robustness against gaps or imperfection in the trail or faulty sensor readings. Most of the works assume the presence of two gas sensors which sample the analyte in the proximity of the ground [70, 72, 73]. In [71] a strategy based on

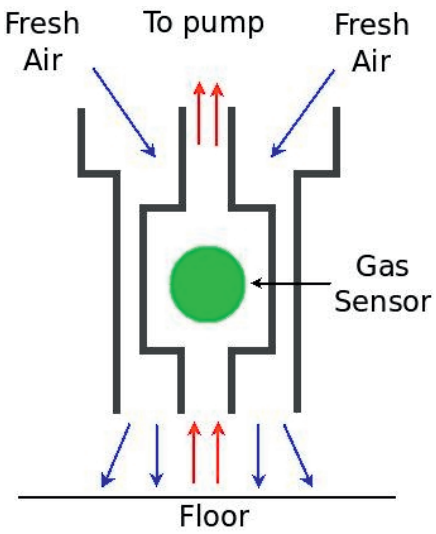



**Figure 4.14:** Device for creating an air curtain. The flux of fresh air is represented by blue lines, while the flux of air to be analyzed by the gas sensor is represented by red lines. The curtain of fresh air is blown towards the floor around the air that is drawn to the sensor. Adapted from [69].

a single gas sensor is presented. An in-depth description of these algorithms is out of the scope of this work and therefore the interested reader is can find a good comparative description in [13].

# Chapter 5
# Conclusions

In this thesis we analyzed the problem of gas discrimination with an array of partially selective gas sensors, paying particular attention to applications where the sensors are mounted on a mobile robot. In robotics applications the gas sensors are usually installed in an open sampling system because an open sampling system is cheap, light and easy to carry, and mostly because the sensors needs to be directly exposed to the environment since the dynamics of the interaction between the sensors and the gas plume, that cannot be captured with a closed sampling system, contains valuable information for example like the distance of the gas source.

In mobile robotics olfaction research, the experimental process is crucial. Indeed only a careful design and an accurate description of the experimental setup can give a good applicability to the result of this kind of research. Indeed, depending on the considered environment the olfactory device can have completely different requirements. Design of experiments to study mobile robotics olfaction is one of the contributions of this thesis. Experiments for mobile robotics olfaction are technically challenging to design because phenomena related to gas dispersion are difficult to observe and control. Therefore mobile robotics olfaction experiments are often the result of a tradeoff between two different requisites: having an experimental setup that is as close to the deployment environment of the system as possible and having a setup where many of the variables are controlled and therefore it enables a deeper understanding of the experimental data. In the work described in this thesis, experiments have been at first carried out in various environments, both indoor and outdoor, without introducing any modification aimed at controlling the airflow or other environmental variables. These experiments provide a good test bed for algorithms that are supposed to work in a general setting and not only in simplified environments. On the other hand these experiments, due to the complexity of the phenomena that govern gas distribution, provide only a limited insight on the collected data. For this reason it is particularly hard to get a ground truth on what is happening at the sensor level since the airflow that carries the gas is chaotic and is hard to predict where the gas patches would "hit" the sensors. In order to obtain data that enables a better ground truth, a series of experiments where the airflow and the gas source emissions are controlled have been designed. Probably a combined observation of the data collected according to the two different philosophies would enable a step forward in the design of an olfactory mobile robot.

Focusing the attention on the algorithmic contributions of this thesis, the main point of interest have been the problems related to the discrimination of gases when the e-nose is deployed on a mobile platform. Discrimination of gases with an e-nose having an open sampling system is a relatively unexplored field and it presents different challenges with respect to discrimination of gases when the sensor array is contained in a closed sampling system. When an array of sensors is deployed in an open sampling system it is exposed to a turbulent airflow that carries the gases to be analyzed. Therefore the sensor response is influenced both by the environment where the robot is deployed and by the movement of the robot. Indeed these two factors determine the way an odor plume is formed and the way the robot interacts with the plume. In this thesis, first it is proposed a gas discrimination algorithm for e-noses with an open sampling system. The classification results are then analyzed in order to try to understand how to improve the quality of the collected data by optimizing the movement of the robot. For the sake of correct gas discrimination, it was observed that being in the proximity of a gas source would not help. Instead, a moving strategy that can keep the robot inside the gas plume for enough time to get sufficient exposure of the array of sensors to the gas would help in collecting sensor responses that are easier to classify. This has been accomplished by running the gas classification algorithm online and designing two olfactory driven path planning strategies.

After having performed more than hundred experimental runs in different locations and with the robot moving according to different trajectories, a large database of sensor responses was available. Analyzing the database, it became clear that experimental location and the movement strategy of the robot influence the characteristics of the collected signal. The first approach proposed to cope with this is to build an ensemble of classifiers in which first, the experimental setup is identified and the compound is identified only in a second moment. This solution is suboptimal in the sense that it supposes that the robot will be deployed in an already known environment. Therefore this result has been improved by proposing a feature selection algorithm that selects a feature set that not only has discrimination capability but is also regular across different experimental setups.

An additional contribution presented in this thesis is related to the use of the electronic nose for medical diagnosis. The electronic nose is proven as an appropriate instrument for identify ten different kinds of bacteria from blood samples. Robustness and accuracy in the identification is achieved by extracting features that can capture the dynamics of the signal and by ensembling the classification of multiple consecutive sampling cycles.

Future research will center around the integration of the gas discrimination algorithms presented in this thesis with algorithms for gas source localization, gas distribution mapping or gas plume tracking. This will enable the robot to address tasks like localization of a specific gas source, create a distribution map of multiple gases and track a specific gas plume in presence of interfering gas plumes.

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