

Detection of characteristic clusters in IMS-Spectrograms of exhaled air polluted with environmental contaminants

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Abstract Detection of special disease markers in exhaled breath is a method becoming more and more relevant in medical diagnostic. The test environment plays a big role in the analysis of exhaled air when using ion mobility spectrometry (IMS). Environmental contaminants appear also in exhaled air of test persons, potentially even in other forms than in the ambient air. Different ways to deal with these environmental factors will be discussed and our method of choice will be presented. It was possible to identify specific fingerprints for dedicated features of probands as well as for specific environmental pollution. By using statistical evaluation it was also possible to identify characteristic features of probands notwithstanding the environmental burden for correct assignment into specific groups, reaching correct classification rates above 0.85.

Keywords Exhaled breath · Disease marker · Cross validation · Support vector machine · Environment

Introduction

A study searching for markers of a specific group (or disease, for example: lung cancer), collecting the exhaled air of

test and control group in two different environments, will surely find significant differences between these two groups. The problem is then to clarify the source of the differences. The question whether they are environment- or group-specific markers, can often not be answered.

To measure the ambient air and subtract it from exhaled air measurements does not solve the problem because it is not clear how specific substances act in the human body and therefore significant differences caused by the environment can still be found [1]. Furthermore it is possible that environmental pollutants are originally from the exhaled air and therefore a subtraction will distort the original results.

In addition to the easy to understand problem of place there is also a problem of time, when the two groups were measured in the same environment but on different days (or on different times of day) the same problem occurs [2], because the environmental parameters of the best laboratory cannot maintain constant.

Excluding environmental-related markers from exhaled air by cleaning processes, for example breathing through a filter, is difficult and time-consuming [3]. In case of certain disturbances of the ventilatory system it takes between 10 to 15 min to remove all environmental markers from the exhaled air. This is well known from pulmonary function test like nitrogen wash-out or oxygen-wash-in [4]. Therefore a software-based evaluation of exhaled markers would be more practicable.

The basic idea for such an evaluation is to mix the measurement environments (or times) for both groups. Environmental conditions should be mixed due to daytime, location and eating-habits as a minimum.

Surely, a correlation between environmental parameters and the study groups can still occur, especially for small group sizes, but this is random and will likely be identified by cross validation.

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