

# Cancellation of chemical backgrounds with generalized Fisher's linear discriminants

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## Abstract

This article presents a signal-processing technique capable of canceling the effect of background chemicals from the multivariate response of a sensor array. We propose a generalization of the Fisher's eigenvalue solution that minimizes the discrimination between undesirable chemicals and a neutral reference. The proposed technique is a generalization of an earlier model that was limited to the removal of single volatiles. A reformulation of class memberships allows the new model to cancel the effect of both single and mixture backgrounds. The model is validated on experimental data from an array of temperature-modulated metal-oxide sensors exposed to binary and ternary mixtures.

## INTRODUCTION

Sensory adaptation is a mechanism by which an organism reduces its sensitivity to constant or strong stimuli, thus preventing sensory overflow and improving the ability to detect new inputs [1]. Two forms of adaptation can be recalled from everyday life. Upon exiting a building on a sunny day one is initially blinded by the intensity of the light, but the retina rapidly adapts to the new lighting conditions. Similarly, a person entering a coffee shop is immediately greeted by the smell of fresh ground coffee, but that sensation vanishes after a few minutes.

The objective of our work is to develop a computational model for chemical sensor arrays capable of mimicking the effects of olfactory adaptation to specific stimuli. Such capability would have a broad impact in sensor arrays as a mechanism to remove background odors (e.g., matrix

effects) and enhance the selectivity of the system towards the interesting components in a given chemical detection problem. To this end, in [2] we have presented a statistical pattern recognition model that was able to cancel the effect of single volatiles. The present work is a generalization of the earlier model that is capable of removing the effect of both single and mixture backgrounds.

## SENSORY ADAPTATION AS A SUBSPACE PROJECTION

Our approach to sensory adaptation is illustrated in Fig. 1(a). The multivariate response of a sensor array, denoted by feature vector  $x$ , is projected onto a low dimensional subspace  $y$  by means of a linear transformation  $W(\omega)$  that minimizes contributions from the adapting stimulus  $\omega$ . The computational function that this transformation performs is best described with an example. Consider a sensory system designed to detect the presence of three analytes (A, B, C), which may appear in mixtures, and a neutral (N). Assume that the system has been exposed to analyte A for a long period of time. As illustrated in Fig. 1 (b), the system should then display decreased sensitivity to the adapting stimulus: the response to analyte A becomes close to the neutral, and the response to mixtures containing analyte A approaches that to the novel components in the mixture (e.g., the mixture A+B becomes similar to analyte B alone). This computational function is consistent with results from olfactory psychophysics showing that, under adaptation to one of the mixture components, the sensory system shifts the perceived quality towards the remaining component(s) in the mixture [3, 4].

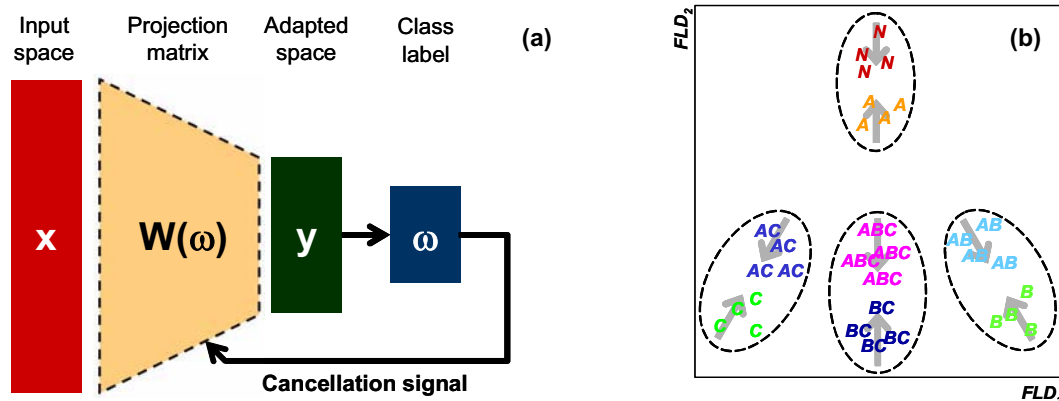


Fig. 1. (a) Sensory adaptation as a subspace projection: the sensor-array response  $x$  is projected onto subspace  $y$  that minimizes the discrimination of previous stimulus  $\omega$  from a neutral. (b) Removal of background chemical A in a ternary mixture problem. The projection is formed by grouping class labels so as to reduce the contribution of the adapting stimulus.

**Table 1. Indicator variables prior to and following adaptation**

Class	(a) Prior to adaptation				(b) Adaptation to $\vec{\eta} = (\eta_A \ \eta_B \ \eta_C)$			
	$\gamma_A^N$	$\gamma_B^N$	$\gamma_C^N$	$\gamma_N^N$	$\gamma_A^{\vec{\eta}}$	$\gamma_B^{\vec{\eta}}$	$\gamma_C^{\vec{\eta}}$	$\gamma_N^{\vec{\eta}}$
A	1	0	0	0	$1-\eta_A$	0	0	$\eta_A$
B	0	1	0	0	0	$1-\eta_B$	0	$\eta_B$
C	0	0	1	0	0	0	$1-\eta_C$	$\eta_C$
AB	1	1	0	0	$1-\eta_A$	$1-\eta_B$	0	$\min(\eta_A, \eta_B)$
AC	1	0	1	0	$1-\eta_A$	0	$1-\eta_C$	$\min(\eta_A, \eta_C)$
BC	0	1	1	0	0	$1-\eta_B$	$1-\eta_C$	$\min(\eta_B, \eta_C)$
ABC	1	1	1	0	$1-\eta_A$	$1-\eta_B$	$1-\eta_C$	$\min(\eta_A, \eta_B, \eta_C)$
N	0	0	0	1	0	0	0	1

The adapting projection  $W(\omega)$  proposed in this work is based on a reformulation of Fisher’s linear discriminant analysis (LDA). LDA is a supervised dimensionality-reduction technique that finds a linear projection  $y=Wx$  such that the discrimination of classes in the projection space  $y$  is maximized. It can be shown [5] that the rows of  $W$  are the eigenvectors corresponding to the largest eigenvalues of the matrix  $S_W^{-1}S_B$ , where  $S_W$  and  $S_B$  are the within-class and between-class scatter matrices, respectively, defined by:

$$\mu_q = \frac{1}{n_q} \sum_{x \in \omega_q} x \quad \text{and} \quad \mu = \frac{1}{n} \sum_{\forall x} x \quad (1)$$

$$S_W = \sum_{q=1}^Q \sum_{x \in \omega_q} (x - \mu_q)(x - \mu_q)^T \quad (2)$$

$$S_B = \sum_{q=1}^Q (\mu_q - \mu)(\mu_q - \mu)^T \quad (3)$$

where  $Q$  is the number of classes,  $n$  is the total number of examples in the dataset,  $\mu_q$  and  $n_q$  are the mean vector and number of examples of class  $\omega_q$ , respectively, and  $\mu$  is the mean vector of the entire distribution.

To mimic olfactory adaptation to A, we modify the definition of classes in equations (1-3) such that discrimination is directed towards the grouping of odors in Fig. 1 (b). Similarly, adaptation to mixture AB (see Fig. 4(d)) can be achieved by maximizing the separability between groups  $\{A,B,AB,N\}$  and  $\{C,AC,BC,ABC\}$ .

For simplicity, we derive an analytical solution for a chemical space with three components and a neutral. Formally, we define a vector of indicator variables  $\vec{\gamma}^N(x) = (\gamma_A^N \ \gamma_B^N \ \gamma_C^N \ \gamma_N^N)$ , where  $\gamma_\omega^N = 1$  if sample  $x$  contains chemical(s)  $\omega$ , and zero otherwise (see Table 1(a)). The superscript  $N$  (for NNeutral) denotes that the LDA projection has not undergone adaptation. For a given adaptation scenario, we also define an adaptation vector  $\vec{\eta} = (\eta_A \ \eta_B \ \eta_C)$ , where  $0 \leq \eta_\omega \leq 1$  denotes the degree of adaptation of the system to analyte  $\omega$ . Adaptation is then

achieved by subtracting  $\vec{\eta}$  from  $\vec{\gamma}^N(x)$ , as described in Table 1(b), to form adapted indicator variables  $\vec{\gamma}^{\vec{\eta}}(x)$ . From here, adapted mean, within-group and between-group covariance matrices can be defined as:

$$\mu_p^{\vec{\eta}} = \frac{\sum_{\forall x} x \gamma_p^{\vec{\eta}}(x)}{\sum_{\forall x} \gamma_p^{\vec{\eta}}(x)}; \quad \mu^{\vec{\eta}} = \frac{1}{P} \sum_{p=1}^P \mu_p^{\vec{\eta}} \quad (4)$$

$$S_W^{\vec{\eta}} = \sum_{\forall x} \left( x - \frac{\sum_{p=1}^P \mu_p^{\vec{\eta}} \gamma_p^{\vec{\eta}}(x)}{\sum_{p=1}^P \gamma_p^{\vec{\eta}}(x)} \right)^2 \quad (5)$$

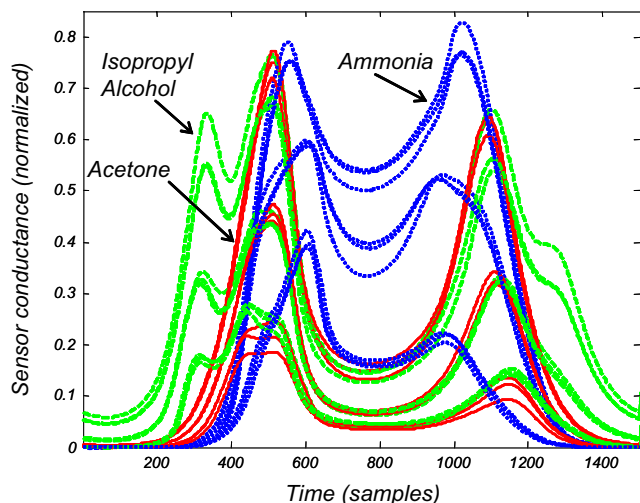
$$S_B^{\vec{\eta}} = \sum_{p=1}^P (\mu_p^{\vec{\eta}} - \mu^{\vec{\eta}})^2 \quad (6)$$

where  $p = [1..P]$  is the set of primary analytes, including the neutral (e.g.,  $P=4$  for the example in Table 1). Note that equations (4-6) are equivalent to (1-3), except for examples are now weighted by their adapted indicator variables  $\vec{\gamma}^{\vec{\eta}}(x)$ . As a result, each adaptation vector  $\vec{\eta}$  leads to a different set of eigenvalues of  $(S_W^{\vec{\eta}})^{-1}S_B^{\vec{\eta}}$ . For the particular case  $\vec{\eta} = (0 \ 0 \ 0)$ , the eigen-solution is a projection where the mixtures have patterns that are the average of their constituent analytes (i.e., mixture AB projects halfway between analytes A and B), as illustrated later in Fig. 3. In all other cases, the eigen-solution is a projection that reduces the contribution of the adapting analyte(s), as illustrated earlier in Fig. 1(b).

### EXPERIMENTAL SETUP

The proposed algorithm was validated on a sensor array with four Figaro metal-oxide chemoresistors (2602, 2610, 2611 and 2620) [6]. To improve the information content of the array, the sensors were temperature modulated using a sinusoidal heater voltage (0-7 V; 2.5min period) [7]. The sensor response was sampled with a frequency of 10Hz.

The sensor array was exposed to the static headspace of mixtures from three analytes: acetone (*A*), isopropyl alcohol (*B*) and ammonia (*C*), at three dilution levels in distilled water (the neutral). The lowest dilution of the analytes was 0.3 v/v% for acetone, 1.0 v/v% for isopropyl alcohol and 33 v/v% for ammonia. These baseline dilutions were chosen so that the average isothermal response (i.e., a constant heater voltage of 5V) across the four sensors was similar for the three analytes, thus ensuring that they could not be trivially discriminated. Two serial dilutions with a dilution factor of 1/3 were also acquired, resulting in 24 samples per day (7 mixtures × 3 concentrations, plus 3 neutral samples). The process was repeated on three separate days, for a total of 72 samples. The temperature modulated response of one of the sensors to the three concentrations of the single analytes is shown in Fig. 2. The sinusoidal heater voltage starts at 0V at  $t=0$  samples, reaches a maximum of 7V at  $t=750$  sa., and returns to 0V at  $t=1500$  sa. Each analyte leads to a unique pattern, defined by the amplitude and location of a maximum in conductance. Two maxima are easily resolved in the case of isopropyl alcohol.

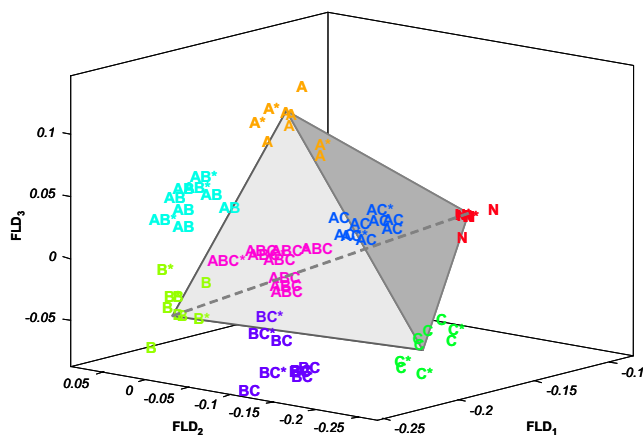


**Fig. 2. Temperature modulated response of a MOS sensor to the three analytes at three concentrations. Three replicates per analyte and concentration are shown to illustrate the repeatability of the patterns. Mixtures are not shown to avoid clutter.**

## RESULTS

In order to form a feature vector for each example, the temperature-modulated response of each sensor was decimated down to 5 samples by taking the sensor conductance at intervals of 37.5 seconds during the 2.5 minute temperature cycle in Fig. 2. As a result, a 20-dimensional feature vector was obtained for each example (5 samples × 4 sensors). The dataset was split into a training set containing two-thirds of the data (48 examples) and a test set with one-third (24 examples). In all adaptation results that follow, eigenvalues for the projections were computed using only training data.

Fig. 3 shows the projection of training and test data onto the three largest eigenvalues of  $(S_w^{\bar{\eta}})^{-1} S_B^{\bar{\eta}}$  in the absence of adaptation (i.e.,  $\bar{\eta} = (0 \ 0 \ 0)$ ). As a result of the grouping imposed by the indicator variables, the examples arrange as a tetrahedron whose vertices are defined by the single analytes (A,B,C,N). It is interesting to note how mixture samples project at or near the mean of the constituent analytes, a symmetry imposed by the grouping of analytes in equations (4-6).



**Fig. 3. Three-dimensional projection that results from the non-adapted indicator variables in Table 1(a). Analytes organize in a topographic fashion along the vertices and edges of a tetrahedron.**

Fig. 4(a) illustrates partial removal of volatile A with adaptation vector  $\bar{\eta} = (0.5 \ 0 \ 0)$ . As a result, samples from odor A approach those of the neutral, whereas mixtures AB, AC and ABC become closer to B, C, and BC, respectively. Fig. 4(b) illustrates full removal of volatile B with adaptation vector  $\bar{\eta} = (0 \ 1 \ 0)$ . As a result, samples of B, BC, AB and ABC overlap entirely with the neutral, C, A, and AC, respectively. Fig. 4(c) shows partial removal of mixture AC with adaptation vector  $\bar{\eta} = (0.30 \ 0 \ 0.60)$ . As a result, samples of A, C and AC project closer to the neutral, their distance being inversely proportional to the adaptation parameter. Note how mixture AC is both approaching the neutral and becoming closer to A. Finally, Fig. 4(d) shows full removal of mixture AB  $\bar{\eta} = (1.00 \ 1.00 \ 0)$ . As a result, samples of A, B and AB are confounded with the neutral, and the remaining samples map close together. In the latter case, only the first discriminant projection (FLD<sub>1</sub>) is meaningful since the grouping leads to a binary discrimination problem and, as a result, the between-group scatter matrix becomes of rank one (i.e., the second eigenvalue is zero.)

## DISCUSSION

Fig. 3 provides an intuitive explanation of the subspace projection mechanism to sensory adaptation. By rotating the tetrahedron in Fig. 3, one can find a two-dimensional view where the contributions of a given analyte are reduced. The method proposed in this article operates in a

similar fashion by projecting from original feature space, which affords as many degrees of freedom for the rotation as dimensions (20 in the case of our database).

The method is able to simulate different degrees of adaptation to both single analytes and mixtures. In the absence of adaptation, the method seeks a projection where pattern additivity is preserved (e.g.,  $x_{AB}=x_A+x_B$ ). It is also important to note the stability of the method, demonstrated by the ability to produce projections that generalize well to unseen test data.

The method has been validated on an experimental dataset containing binary and ternary mixtures. The next stage of this work is to evaluate the ability of the method to remove background odors and matrix effects in complex application scenarios.

### ACKNOWLEDGMENTS

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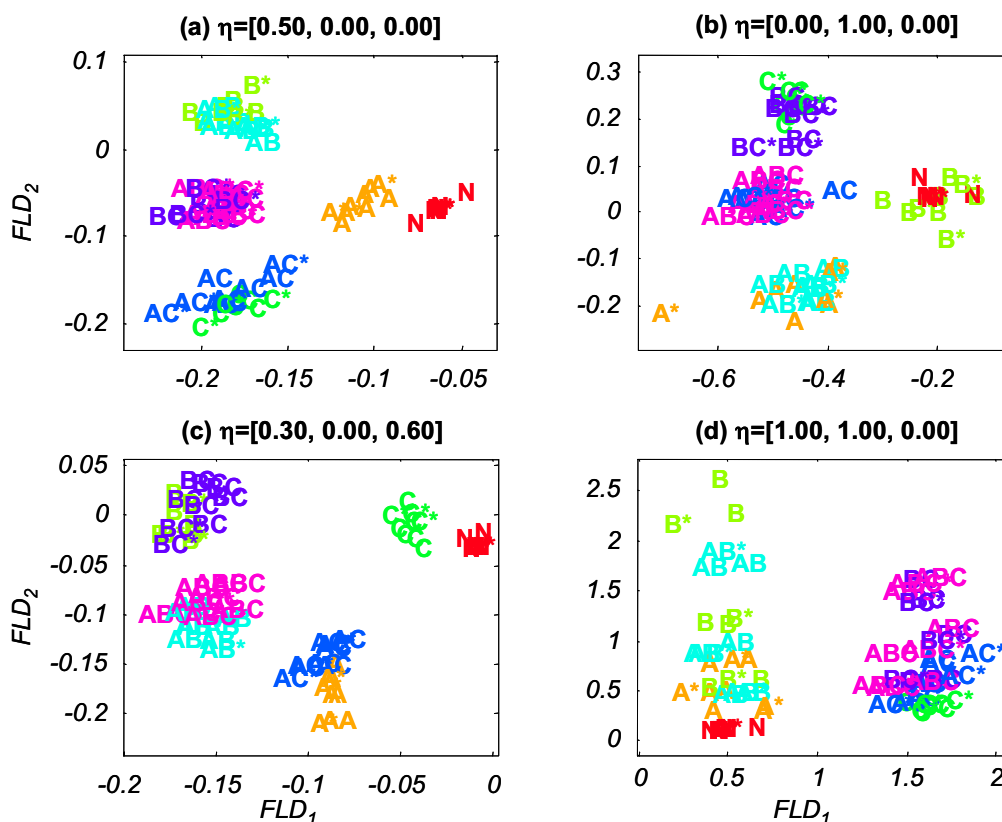


Fig. 4. Examples of background cancellation: (a) partial removal of volatile A (b) full removal of volatile B, (c) partial removal of mixture AC, and (d) full removal of mixture AB. Both training examples and test examples (denoted by an asterisk \*) are shown to illustrate the generalization properties of the projection.