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Increasing the separability of chemosensor array patterns with Hebbian/anti-Hebbian learning

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Abstract

The olfactory bulb is able to enhance the contrast between odor representations through a combination of excitatory and inhibitory circuits. Inspired by this mechanism, we propose a new Hebbian/anti-Hebbian learning rule to increase the separability of sensor-array patterns in a neurodynamics model of the olfactory system: the KIII. In the proposed learning rule, a Hebbian term is used to build associations within odors and an anti-Hebbian term is used to reduce correlated activity across odors. The KIII model with the new learning rule is characterized on synthetic data and validated on experimental data from an array of temperature-modulated metal-oxide sensors. Our results show that the performance of the model is comparable to that obtained with Linear Discriminant Analysis (LDA). Furthermore, the model is able to increase pattern separability for different concentrations of three odorants: allyl-alcohol, *tert*-butanol, and benzene, even though it is only trained with the gas sensor response to the highest concentration.

Keywords: Contrast enhancement; Hebbian; Anti-Hebbian; KIII model; Gas sensor-array

1. Introduction

The olfactory system has been optimized over evolutionary time to allow animals detect and interpret the information from volatile molecules in the environment. The striking similarity between the olfactory system across phyla seem to imply that its architecture has been shaped to reflect basic properties of olfactory stimuli [1]. This suggests that the underlying mechanisms of the olfactory system could be of practical use to process signals from gas sensor arrays.

Motivated by this idea, our long-term research objective is to develop biologically inspired computational models for chemical sensor arrays. In this paper, we focus on the ability of the olfactory bulb to improve the separability of odor representations. The olfactory bulb receives direct inputs from olfactory receptor neurons in the epithelium, and reshapes this information through excitatory–inhibitory circuits, increasing the contrast across odor representations [2]. This article presents a learning rule to apply this computational function to gas sensor-array patterns. The proposed learning rule is validated on the KIII model of Freeman et al. [3,4]. The KIII is a neurodynamics model of the olfactory system that encodes odor information through dynamic attractors. In recent years, computational models using this coding strategy have been shown to have resistance to noise and higher storage capacity [5,6,7]. However, with a few exceptions [8–10], the KIII model has gone largely unnoticed in the machine olfaction literature.

2. Contrast enhancement through Hebbian/anti-Hebbian learning

Contrast enhancement in the olfactory bulb is performed through the inhibition of mitral cells by nearby granule interneurons [11]. This inhibition has the effect of reducing the molecular tuning range (i.e., the number volatile molecules detected) of a mitral cell relative to that of olfactory receptor neurons, effectively orthogonalizing patterns across odors. It is well known that this computational function can be achieved by means of anti-Hebbian learning [12]. The anti-Hebbian learning rule is the opposite of the Hebbian rule [13], and states that the strength of the connection between two neurons should decrease when both

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activate simultaneously:

$$\Delta w_{kl} = -x_k x_l \tag{1}$$

where x_k and x_l are the kth and lth inputs to the system. The application of this rule to a laterally connected network leads to a decorrelation of the input channels in the system.

We propose a learning rule that combines Hebbian and anti-Hebbian terms to achieve both robustness to sensor failures and enhanced pattern separability, respectively. Assuming a pattern recognition problem with N odor patterns $p^i = [x_1^i x_2^i, ..., x_M^i]^T; 1 \leq i \leq N$, and a recurrent network with M fully laterally connected neurons, the strengths of the lateral connections are computed with the following off-line expression:

$$w = \overbrace{\sum_{i=1}^{N} p^i (p^i)^T}^{\text{Hebbian}} - \overbrace{\sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq i}}^{N} p^i (p^j)^T}^{\text{anti-Hebbian}} \tag{2}$$

The first term in Eq. (2) is the Hebbian rule, which strengthens the connection between neurons that are active *within* a pattern. The second term is the anti-Hebbian component, which reduces the connection weights between neurons that are active for multiple patterns, on the average reducing the overlap *across* patterns. Negative mitral-to-mitral connections are avoided by forcing to zero all elements in Eq. (2) that become negative.

3. Contrast enhancement in the KIII

The proposed learning mechanism is implemented on the KIII, a neurodynamics model of the olfactory system developed by Freeman and colleagues over the last 30 years [3,4]. The KIII reproduces electroencephalographic (EEG) recordings in the olfactory system by modeling the oscillatory behavior of neuron populations [4]. The topology of the model, shown in Fig. 1, is based on the physiology of the mammalian olfactory system [3,14]. Each node in the KIII represents a population of neurons, modeled by a second order differential equation, and each edge models the interaction between two populations. The

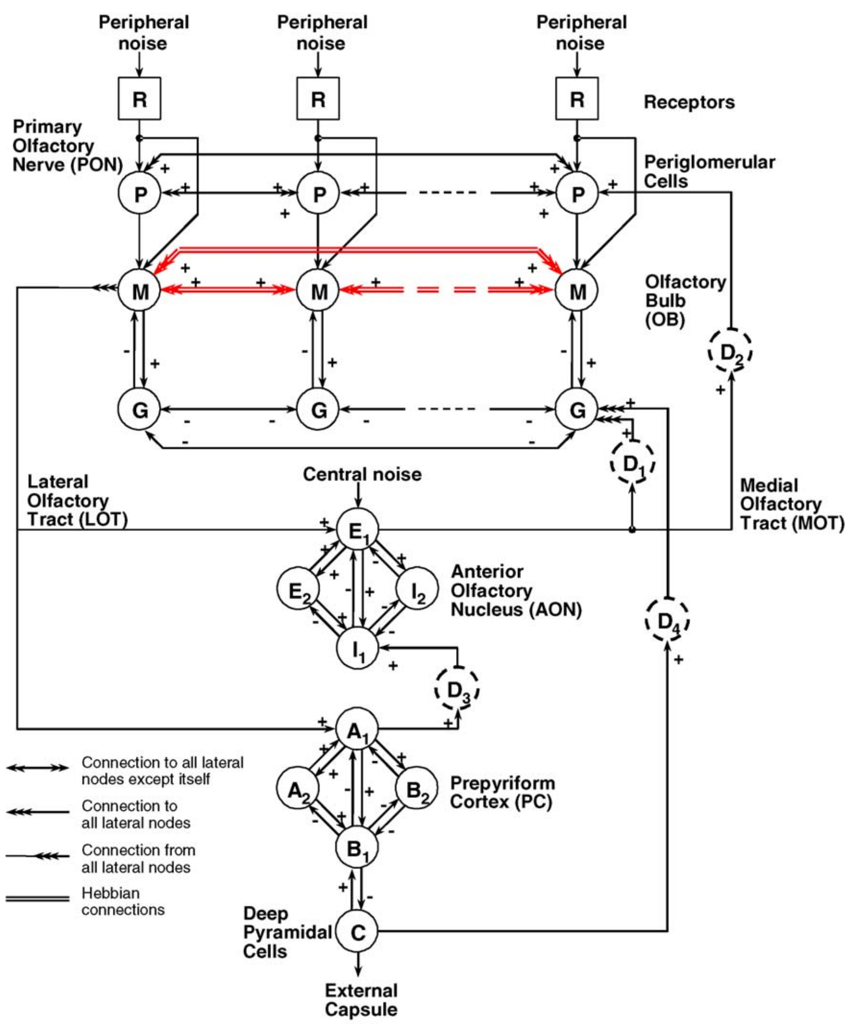

Fig. 1. The KIII model architecture. The KIII model is built after the basic architecture and building blocks of the olfactory system: R olfactory receptor neurons; P periglomerular cells; M mitral cells; G granule cells; E and I cells from the anterior olfactory nucleus; A and B are cells from piriform cortex; C deep pyramidal cells. M-to-M connections are learnable and are trained with the proposed Hebbian/anti-Hebbian rule (Eq. (2)).

strength of this interaction is controlled by a weight, which is positive when the connection is excitatory and negative if the connection is inhibitory.

Odor stimuli are presented to the system as a pattern through an input layer of receptors. Each receptor defines an input channel, and is connected to an oscillator (also known as a reduced-KII set) consisting of one mitral and one glomerular ensemble. Patterns are stored by means of a layer of Hebbian lateral connections between mitral ensembles [15]. Thus, the model can be used as an associative memory to recover incomplete or corrupted stimuli.

In the absence of an external stimulus, the KIII channels follow an aperiodic oscillatory behavior known as a basal state [16]. When an input is presented, the system moves into a global attractor in state space, which can also be observed as pseudo-periodic oscillations in the output channels. The amplitude of the oscillations at each channel depends on the activation level of its receptor input, but is also influenced by other receptors as a result of the lateral connections. The output pattern of the KIII is commonly taken to be the amplitude or RMS of the oscillations of each channel [3].

3.1. Hebbian/anti-Hebbian learning in the KIII model

Whereas the use of Hebbian learning in the KIII model is well established [15], application of anti-Hebbian learning is non-trivial because of the oscillatory nature of the KII sets: the interaction between laterally connected oscillators is a vector operation. Therefore, depending on the relative phase of the two oscillators, it is possible for an inhibitory connection to have an excitatory effect. This problem has also been reported in other oscillatory neural systems [17]. To address this problem, the proposed learning rule (Eq. (2)) combines an anti-Hebbian term with a Hebbian term. The role of the Hebbian term is two-fold. First, it provides positive mitral-to-mitral connections, which are subsequently reduced by an anti-Hebbian term. Second, it preserves the associative-memory function of the KIII, allowing the model to learn odor-specific attractors.

4. Comparison with other methods

To evaluate the new Hebbian/anti-Hebbian rule, the performance of the KIII model is compared to that of three additional procedures: a Hopfield network [18], a KIII with only Hebbian learning, and Linear Discriminant Analysis (LDA) [19]. The first two procedures are associative memories, and were chosen to determine the extent to which the proposed learning rule can improve the performance of a model trained with Hebbian learning. LDA was used to provide a reference on the pattern separability that can be obtained with linear models; LDA is known to find the optimum projection for Gaussian likelihoods with equal covariances [19] by maximizing the Fisher Discriminant Function introduced below. In turn, the pattern separability of the raw inputs was used as a lower bound of performance for the models (Fig. 2).

Pattern separability was measured with the Fisher Discriminant Ratio [19]. Assuming a c-class problem with same number of elements per class, the Fisher Discriminant Function was computed following the expression [20]:

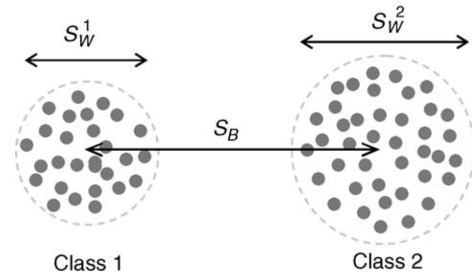

Fig. 2. Illustration of the between class-scatter S_B, and within class-scatter S_W^1, S_W^2 for a two-class problem.

$$J = \frac{\mathrm{tr}(S_B)}{\mathrm{tr}(S_W)} \tag{3}$$

where S_B is the between-class scatter, and S_W is the within-class scatter:

$$S_B = \sum_{i=1}^{c} (\mu_i - \mu)(\mu_i - \mu)^t \tag{4}$$

$$S_W = \sum_{i=1}^{c} \overbrace{\sum_{y \in C_i} (y - \mu_i)(y - \mu_i)^t}^{S_W^i} \tag{5}$$

μ_i is the mean of class i, μ the pooled mean, and C_i is the set of samples from class i. The between-class scatter is a measure of the distance between the mean of each one of the classes, and the within-class scatter is a measure of the spread of each class. Thus, class separability is directly proportional to S_B and inversely proportional to S_W, as captured by the objective function in Eq. (3).

4.1. Synthetic binary problem

The KIII with Hebbian/anti-Hebbian learning and the other 3 procedures were presented with a 3-class problem with 16-dimensional binary inputs. Fig. 3 shows the three overlapping binary patterns (A, B, C) used as training patterns. Test patterns were generated by randomly mutating bits of the 16-dimensional patterns. Six levels of noise were considered by mutating 1–6 bits of the input pattern, which corresponds to a 6–37% change of the original pattern. One thousand examples were generated for each noise level.

Fig. 4 shows the pattern-separability obtained by the four procedures and that available at the input. The separability J is plotted as a function of the amount of noise that was introduced to the input patterns. The KIII-Hebbian/anti-Hebbian

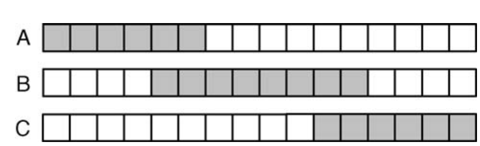

Fig. 3. Overlapping binary patterns used to test the pattern separability of the model.

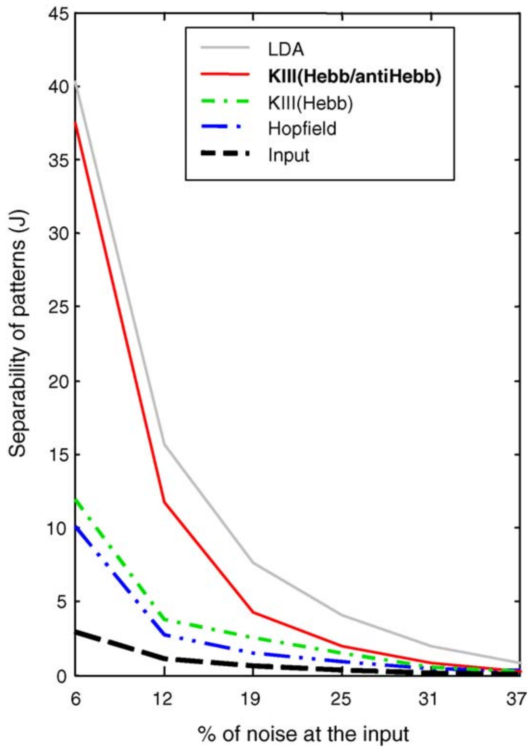

Fig. 4. Separability of the output patterns against the level of noise introduced in the input patterns. Separability of the output patterns of LDA, KIII-Hebbian/anti-Hebbian, KIII-Hebbian, Hopfield output, along with the separability of the raw input.

clearly outperforms the KIII-Hebbian and the Hopfield network, approaching the performance of LDA. It is important to note that the KIII model and the Hopfield model deal exclusively with positive-defined patterns. LDA is not subject to this constraint: LDA output patterns can (and do) have positive and negative values, affording a larger between-class scatter than that obtained with the KIII model. Despite the constraints, the proposed KIII Hebbian/anti-Hebbian model is still able to perform close to LDA.

Several mechanisms are responsible for the increase of separability obtained by the KIII models and the Hopfield network. The Hopfield network and the KIII-Hebbian model are able to increase the separability of the input patterns through pattern completion. This mechanism is able to partially restore the stored patterns from the noisy version presented at the input, reducing the within-class scatter, S_W. The KIII-Hebbian/anti-Hebbian takes advantage not only of the pattern completion mechanism, but also of the overlap and crosstalk reduction mechanisms. Crosstalk is the interference of other stored patterns in the retrieval of any stored pattern. Both mechanisms allow the system to increase the between class-scatter S_B of the input patterns, consequently increasing its separability.

5. Sensor array-pattern validation

The KIII-Hebbian/anti-Hebbian was finally validated on experimental data from a gas sensor array with four MOS sensors (TGS2600, TGS2610, TGS2611, and TGS2620) [21]. A delivery system was used to expose the sensors to the dynamic headspace of three analytes: allyl-alcohol (A), *tert*-butanol (B), and benzene (C) at five different concentrations. To increase the information content of the sensor response, the MOS sensors were modulated in temperature [22] with a ramp profile on the heater voltage from 2 to 4.5 V over a period of 200 s. Fig. 5 shows the response of the TGS2610 sensor to the five different concentrations of each analyte. Using this excitation profile, we collected a database of sensor response patterns for the three analytes (A, B, C), five concentrations per analyte, and five repetitions each; each repetition was collected on a different day to determine whether or not the sensors patterns were repeatable.

The temperature-modulated response of the four MOS sensors at the highest concentration was concatenated to form a single pattern, and used to train the KIII. Each pattern was previously normalized individually to have a maximum value of one and decimated to obtain 64 samples per sensor response. This preprocessing is necessary to balance the inputs to the KIII, and ensures that the model operates in a well-behaved dynamic region. Fig. 6(a)–(c) shows the concatenated response from two (TGS2610, TGS2611) of the four sensors; only two sensors were used here in order to facilitate visualization. Even though the sensors provide a unique response pattern to each analyte, there is also a significant degree of overlap that shadows the most relevant discriminatory information. Fig. 6 (right column) shows the output of the KIII to the three analytes; the KIII is able to noticeably reduce the overlap across patterns and enhance the channels (i.e., operating temperatures) with highest selectivity. The response pattern for analyte A is highly reduced

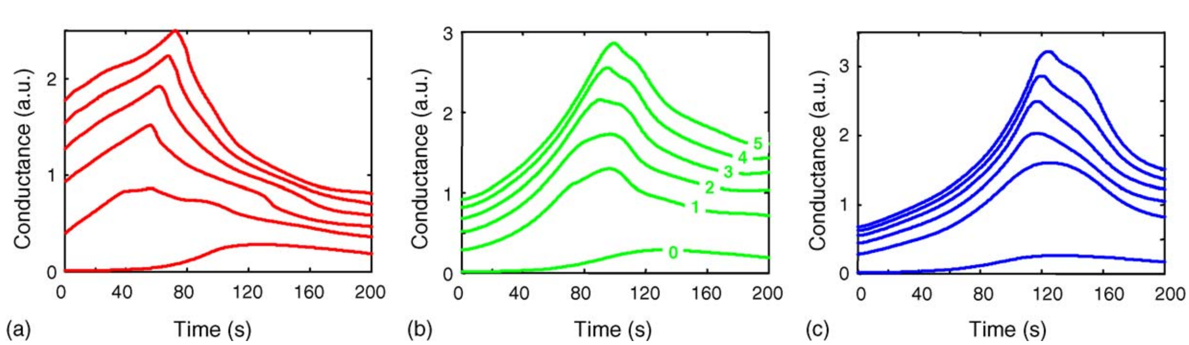

Fig. 5. Response of a TGS2610 sensor to five different concentrations of allyl-alcohol (a), *tert*-butanol (b), and benzene (c). The bottom curve in each plot is the sensor response to air. The heather voltage was modulated using a ramp profile (2 to 4.5 V; 200 s).

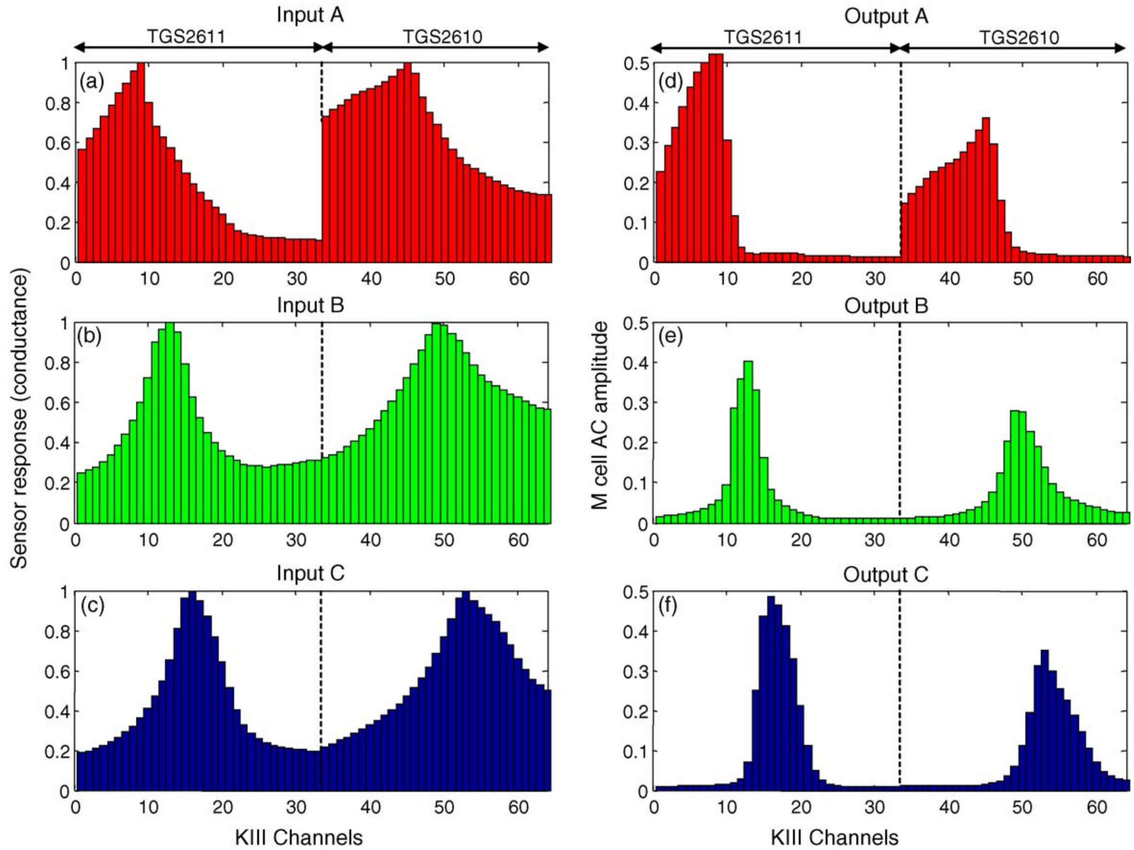

Fig. 6. Contrast enhancement in the KIII with experimental data from gas sensors. The left column shows the original sensor response to the three analytes, which serves as the input to the KIII. The right column shows the corresponding output of the KIII (i.e. ac amplitude in mitral cells).

on the right hand side of the two peaks (located in channels 9 and 44) since that region is highly overlapping with the response to analytes B and C. On the other hand, the same sensor response maintains activity on the left hand side of the peaks because this area contains discriminatory information of analyte A on the original sensor response. Since the response pattern for analyte B has large overlap with the other two response patterns on both sides of the peaks (channels 13 and 49), the KIII narrowly sharpens the activity of this pattern around its peaks (Fig. 6). Finally, the sensor response pattern for analyte C is sharpened also around the two peaks (channels 16 and 53), which is where discriminatory information for this analyte is highest.

We performed a more systematic study of the pattern separability achieved with the KIII model using the entire database. As in the previous section, model performance was measured using the Fisher discriminant ratio (J). The KIII model was trained with the sensor–array response at the highest concentration of each analyte, and subsequently tested with the entire database. Fig. 7 shows the pattern separability at the input and output of the KIII as a function of analyte concentration. Pattern separability increases with concentrations. This is due to two reasons. First, the analytes become more separable at increasing concentrations. This is clearly shown by the lower curve in Fig. 5. Second, the KIII is likely to display better performance at concentrations close to the one it was trained on (the highest one in our case). However, the model is able to increase pattern separability at all the lower concentrations as well, as can be observed in Fig. 7.

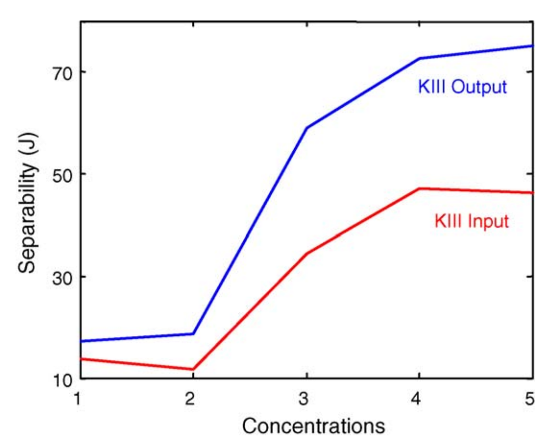

Fig. 7. Pattern separability at the input and output of the KIII on a database of analytes at different concentrations. The model was trained using only the sensor patterns at high concentration.

6. Discussion

This paper has presented a Hebbian/anti-Hebbian learning rule to increase the separability of gas sensor-array patterns. The proposed rule is implemented in Freeman's KIII model.

The model with the new learning rule has been characterized with a synthetic binary problem comparing it with three other procedures. The model is validated with gas sensor response of four MOS sensors to three analytes: allyl-alcohol, *tert*-butanol, and benzene, at different concentrations.

The model has been characterized with a synthetic problem with binary patterns. The proposed learning rule has been shown to increase the separability (Fisher discriminant ratio) of the output patterns with respect to that available at the input. This is achieved by both a decrease of the within-class scatter and the increase of the between-class scatter of the output distribution. It is worth to notice that the simulated dataset in Section 4.1 consisted of isotropic likelihoods and, therefore, all discriminatory information was contained in the mean of the distribution. This type of distribution was used to ensure a fair comparison between the two KIII models and the Hopfield model, which are limited to first-order statistics, and LDA, which can also consider second-order statistics.

The model has also been validated on the response of four MOS sensors to three analytes: allyl alcohol, *tert*-butanol, and benzene, at different concentrations. Our results have shown that the model is able to increase the separability of gas-sensor-array patterns, and also generalizes well across concentration levels.

The main objective of this work is to model signal-processing strategies in the olfactory pathway, and apply them to the processing of chemosensor arrays. As with other biologically inspired approaches, the question often arises as to whether or not these methods can (or should) outperform statistical approaches. If the probability density function for each class is available, the optimum performance is given by the Maximum A Posteriori (MAP) classifier: assign examples to the class with highest posterior probability [19]. To the extent that these probabilities are available, no other form of classification (biologically inspired or otherwise) can outperform a MAP classifier. Thus, given that the classes in Fig. 3 are unimodal and have similar noise properties, the LDA performance shown in Fig. 4 should be taken as a good *approximation* of the upper bound on performance for any classification approach. Improved performance should be expected for biologically inspired models in problems where the input dimensionality matches that available in the olfactory system [23]; it is in these high-dimensional spaces where statistical approaches do not scale well.

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Biographies

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