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"Chemical gamut" and implications for describing the analytical capability of sensor arrays

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Abstract:

There is a general lack of systematic, generally applicable metrics for expressing the capability of arrays of partially selective sensors for chemical analysis. Such metrics would allow for objective comparison of widely different array technologies and efficient optimization of such arrays for uncertain, complex sensing tasks. This work explores the use of concepts and formalisms from the field of color theory for use in describing analytical capability of chemical sensor arrays.

Key words: Sensor Arrays, Quality Metrics, Selectivity, Optimization, Color Theory

Introduction

A central perceived benefit of arrays of partially selective sensors (i.e. machine olfaction) is the idea that such devices will provide greater selectivity against complex, unknown chemical backgrounds. In essence, the idea is that adding more and more sensors with complementary response to an array will enable progressively greater analytical capability, at some point potentially even rivaling the analytical power of laboratory instruments. However, the extent to which this is possible is not well understood, nor is the specific mechanisms by which analytical capabilities emerge from such systems. While it is straightforward to empirically evaluate sensor (and sensor array) capabilities for well-defined, simple sensing tasks, theoretical methods to quantitatively express the overall analytical power of sensor arrays against a wide range of potential tasks remain an open question.

One novel way to address this problem is to examine the literature for analogous systems in other fields of study. For instance, color theory and the mathematics of color vision has been an area of active research for more than one hundred years and has been extensively reported in the scientific literature.[1] Color perception in humans is generated from the responses of an array of the three distinct photoreceptor neurons, each of which exhibits a different spectral response function. Thus, the essentially infinite range of possible spectral stimuli leads to a finite range of perceivable colors known as a "gamut" and described by a chromaticity diagram. Differentiating between stimuli on the basis of perceived color is limited by both uncertainty in neural response (measurement noise) and by the unavoidable ambiguity introduced by mapping a high-dimensional space of possible stimuli to a measurement space of reduced dimension. Spectral stimuli that produce indiscernible color perceptions are known as "metamers." Fonseca and Samengo have described theoretically how uncertainty in color perception arises from specific neural array characteristics and subsequently, how a color gamut can be transformed into a space with a uniform error metric. [2,3] Pike described how color gamuts can be extended to systems with an arbitrary number of unique photoreceptors. [4]

Analogy to Chemical Sensor Arrays

The analogy to arrays of partially-selective chemical sensors is clear. In this case, a high-dimensional space of possible *chemical* stimuli is mapped by a given sensor array to a *chemical* gamut describing the span of stimuli rendered discernible by the array. As with color perception, these systems exhibit metamerism as chemical stimuli that are indiscernible by the sensor array. These metamers can be understood as potential sources of false positives in chemical detection tasks, and perceptual error metrics within a sensor array's gamut as fundamental limitations to its capability as a general-purpose analytical device for chemical measurement.

Here, surface acoustic wave sensors are used as an example system to illustrate this concept. The compound-specific sensitivity of individual SAW sensors is driven by a linear solvation energy relationship that is, in turn, driven by five molecular parameters. [5] In this work, molecular structures for more than 200,000 compounds were extracted from the NIST11 mass spectral library and LSER coefficients were estimated for each compound using Absolv from ACD/Labs. Partition coefficients for each compound were estimated for 21 different polymer sensor coatings as described in [6]. Note that partition coefficient is used here as a proxy for relative compound-specific sensitivity, and that the absolute sensitivity of a SAW sensor will also depend on additional physical properties of the sensor.

Visualization of Sensor Array Capability

Figure 1 depicts how the library compounds are distributed in three-dimensional normalized response spaces corresponding to four separate configurations of three-sensor SAW arrays. These distributions varied widely among the 1,330 possible three sensor configurations, leading to significantly different capabilities. A given level of sensor measurement error implies a resolution metric in the space. Additionally, it can be seen that sensor array configuration imposes varying mappings of adjacency between individual compounds from the library, and thus varying instances of metamerism that depend on sensor configuration. Careful examination of this can uncover the fundamental limitations imposed by sensor array design in a quantitative fashion.

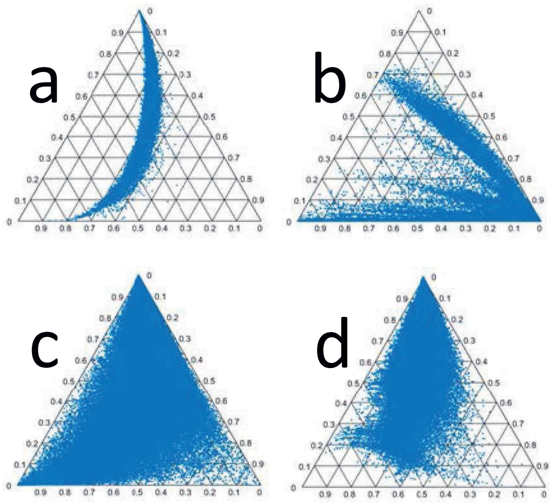

Fig. 1. Chemical gamut diagrams for four different three-sensor SAW array configurations.

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