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Relating Sensor Responses of Odorants to Their Organoleptic Properties by Means of a Biologically-Inspired Model of Receptor Neuron Convergence onto Olfactory Bulb

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Abstract. We present a neuromorphic approach to study the relationship between the response of a sensor/instrument to odorant molecules and the perceptual characteristics of the odors. Clearly, such correlations are only possible if the sensing instrument captures information about molecular properties (e.g., functional group, carbon chain-length) to which biological receptors have affinity. Given that information about some of these molecular features can be extracted from their infrared absorption spectra, an attractive candidate for this study is infrared (IR) spectroscopy. In our proposed model, high-dimensional IR absorption spectra of analytes are converted into compact, spatial odor maps using a feature clustering scheme that mimics the chemotopic convergence of receptor neurons onto the olfactory bulb. Cluster analysis of the generated IR odor maps reveals chemical groups with members that have similar perceptual characteristics e.g. fruits, nuts, etc. Further, the generated clusters match those obtained from a similar analysis of olfactory bulb odor maps obtained in rats for the same set of chemicals. Our results suggest that convergence mapping combined with IR absorption spectra may be an appropriate method to capture perceptual characteristics of certain classes of odorants.

6.1 Introduction

Smell is the most primitive of the known senses. In humans, smell is often viewed as an aesthetic sense, as a sense capable of eliciting enduring thoughts and memories. For many animal species however, olfaction is the primary sense. Olfactory cues are extensively used for food foraging, trail following, mating, bonding, navigation, and detection of threats (Axel 1995). Irrespective of its purpose i.e., as a primary sense or as an aesthetic sense, there exists an astonishing similarity in the organization of the peripheral olfactory system across phyla (Hildebrand and Shepherd 1997). This suggests that the biological olfactory system may have been optimized over evolutionary time to perform the essential but complex task of recognizing odorants from their molecular features, and generating the perception of smells.

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Inspired by biology, artificial systems for chemical sensing and odor measurement, popularly referred to as the 'electronic nose technology' or 'e-noses' for short, have emerged in the past two decades. A number of parallels between biological and artificial olfaction are well known to the e-nose community. Two of these parallels are at the core of sensor-based machine olfaction (SBMO), as stated in the seminal work of Persaud and Dodd (1982). First, biology relies on a population of olfactory receptor neurons (ORNs) that are broadly tuned to odorants. In turn, SBMO employs chemical sensor arrays with highly overlapping selectivities. Second, neural circuitry downstream from the olfactory epithelium improves the signal-to-noise ratio and the specificity of the initial receptor code, enabling wider odor detection ranges than those of individual receptors. Pattern recognition of chemical sensor signals performs similar functions through preprocessing, dimensionality reduction, and classification/regression algorithms.

Most of the current approaches for processing multivariate data from e-noses are direct applications of statistical pattern recognition and chemometrics techniques (Gutierrez-Osuna 2002). In this book chapter, we focus on an alternative approach: a computational model inspired by information processing in the biological olfactory system. This neuromorphic approach to signal processing represents a unique departure from current practices, one that could move us a small step beyond multivariate chemical sensing and in the direction of true machine olfaction: relating sensor/instrumental signals to the perceptual characteristics of the odorant being sensed.

6.2 Odor Representation in the Early Stages of the Olfactory Pathway

The first stage of processing in the olfactory pathway consists of a large array (~10-100 million) of olfactory receptor neurons (ORNs), each of which selectively expresses one or a few genes from a large (100-1,000) family of receptor proteins (Buck and Axel, 1991; Firestein, 2001). Each receptor is capable of detecting multiple odorants, and each odorant can be detected by multiple receptors, leading to a massively combinatorial olfactory code at the receptor level. It has been shown (Alkasab et al. 2002; Zhang and Sejnowski 1999) that this broad tuning of receptors may be an advantageous strategy for sensory systems dealing with a very large detection space. This is certainly the case for the human olfactory system, which has been estimated to discriminate up to 10,000 different odorants (Schiffman and Pearce, 2003). Further, the massively redundant representation improves signal-to-noise ratio, providing increased sensitivity in the subsequent processing layers (Pearce et al. 2002).

Receptor neurons relay their responses downstream to the olfactory bulb (OB) for further processing. Receptor neurons expressing the same receptor gene converge onto one or a few glomeruli (GL) (Mori et al. 1999; Laurent 1999), which are spherical structures of neuropil at the input of the OB. This form of convergence serves two computational functions. First, massive summation of multiple ORN inputs averages out uncorrelated noise, allowing the system to detect odorants below the detection threshold of individual ORNs (Pearce et al., 2002). Second, chemotopic organization leads to a more compact odorant representation, an odor map that encodes odor identity/ quality (Friedrich and Korsching 1997). The generated odor maps have also been shown to correlate with the overall odor percept (Leon and Johnson 2003; Uchida et al., 2000). Hence we will focus on these convergence circuits in this study.

6.3 Infrared Absoption Spectroscopy

Though very little is known about the molecular determinants of an odorant, it is widely believed that each glomerulus (to which similar ORNs converge) acts as a "molecular feature detector" that identifies a particular molecular property, such as type and position of a functional group (Mori et al. 1999) or carbon chain-length (Sachse et al., 1999). Information about these molecular features can be extracted from their IR absorption spectra, making IR absorption spectroscopy an attractive candidate for this study.

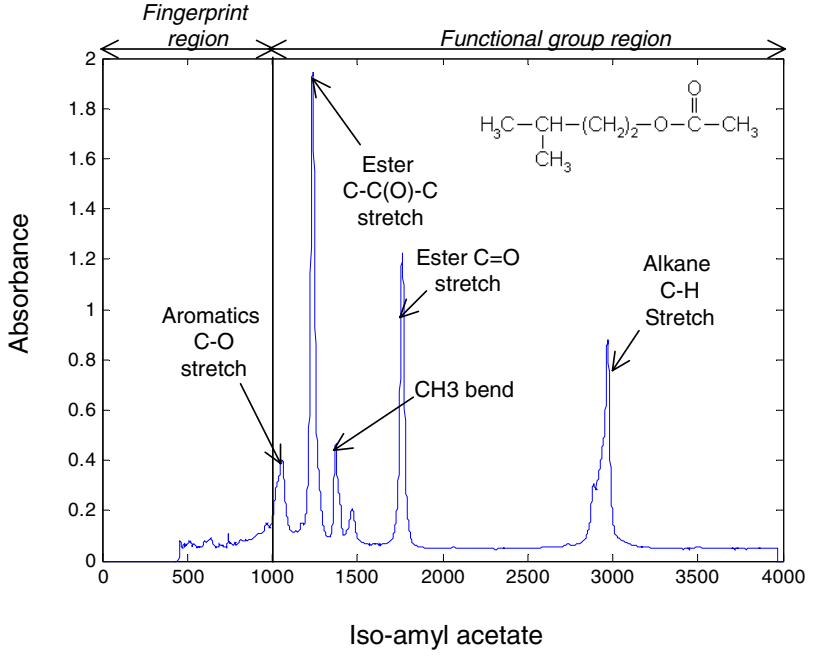

Fig. 6.1. IR absorption spectrum of iso-amyl acetate (an ester with a fruity smell). Each peak is labeled by the functional group responsible for the absorption.

Infrared radiations are electromagnetic waves whose wavelength lies in the region between the visible light and microwaves. When exposed to IR rays, molecules tend to absorb these radiations at wavelengths where the radiant energy matches the energy of their intra-molecular vibrations. In IR spectroscopy, differences in molecular structure and inter-atomic bonds between chemicals are exploited to generate unique IR absorption spectra that are rich in analytical information (Nogueira et al. in press). The entire IR spectrum comprises of three non-overlapping regions, each with a distinct purpose: (1) the far-IR region (400-10 cm^{-1}), used for rotational spectroscopy, (2) the mid-IR region (4000-400 cm^{-1}), which provides information about molecular rotations-vibrations, and (3) the near-IR region (12800-4000 cm^{-1}), used for studying molecular overtones and certain combination vibrations. Of particular interest is the

mid-IR region, which is further subdivided into the so-called "functional-group" (4000-1500 cm^{-1}) and "fingerprint" (<1500 cm^{-1}) regions. The former contains information about the functional groups that are present in the molecule (e.g., alcohols, aldehydes, ketones, esters etc.,), whereas the latter contains a global absorption pattern that is unique to each organic compound. A sample IR spectrum (iso-amyl acetate; an ester with a fruity smell) obtained from the National Institute of Standards and Technology (NIST) Chemistry Web Book database (Linstrom and Mallard 2003) is shown in Figure 6.1. Different peaks in the absorption spectrum correspond to the various molecular features present in iso-amyl acetate.

We use a database comprising of IR absorption spectra (wave number range 0 – 4000 cm^{-1}) of ninety-three chemicals obtained from NIST (Linstrom and Mallard 2003). Each feature in the absorption spectrum indicates the intensity of light absorbed by a molecule at a particular wavenumber, thus defining a high dimensional odor signal of 4,000 features.

6.4 Modeling Receptor Neuron Convergence

To process high-dimensional experimental data from infrared spectroscopy we adapt the ORN convergence model presented by us earlier (Gutierrez-Osuna 2002; Raman et al., 2006). Briefly, this model is based on three principles: (i) ORNs with similar affinities project onto neighboring GL, (ii) GLs in OB are spatially arranged as a two-dimensional surface, and (iii) neighboring GL tend to respond to similar odors (Meister and Bonhoeffer 2001; Johnson and Leon 2000). Therefore, a natural choice to model the ORN-GL convergence is the self-organizing map (SOM) of Kohonen (1982).

To form a chemotopic mapping, we must first define a selectivity measure upon which IR absorption features can be clustered together. In this work, this is accomplished by treating the IR absorption at a particular wavelength across a set of odorants as an affinity vector:

$$IR_i = \left[IR_i^{O_1}, IR_i^{O_2}, ..., IR_i^{O_C} \right] \tag{6.1}$$

where IR_i^O is the IR absorption at wavenumber *i* for odor O, and C is the number of odorants (C = 93 in this study).

The convergence model operates as follows. The SOM is presented with a population of IR absorption features (corresponding to each wavenumber), each represented by a vector in C-dimensional affinity space, and trained to model this distribution. Once the SOM is trained, each IR absorption feature is then assigned to the closest SOM node in affinity space, thereby forming a convergence map from which the response of each SOM node is computed as:

$$SOM_j^O = \sum_{i=1}^{N} W_{ij} IR_i^O \tag{6.2}$$

where N is the number of IR features (N = 4,000 in this study), and W_{ij}=1 if IR_i converges to SOM_j and zero otherwise.

To help visualize this model, Fig. 6.2. illustrates a problem with absorption spectra of three odors (labeled as A, B and C). The affinities at different wavenumbers are shown

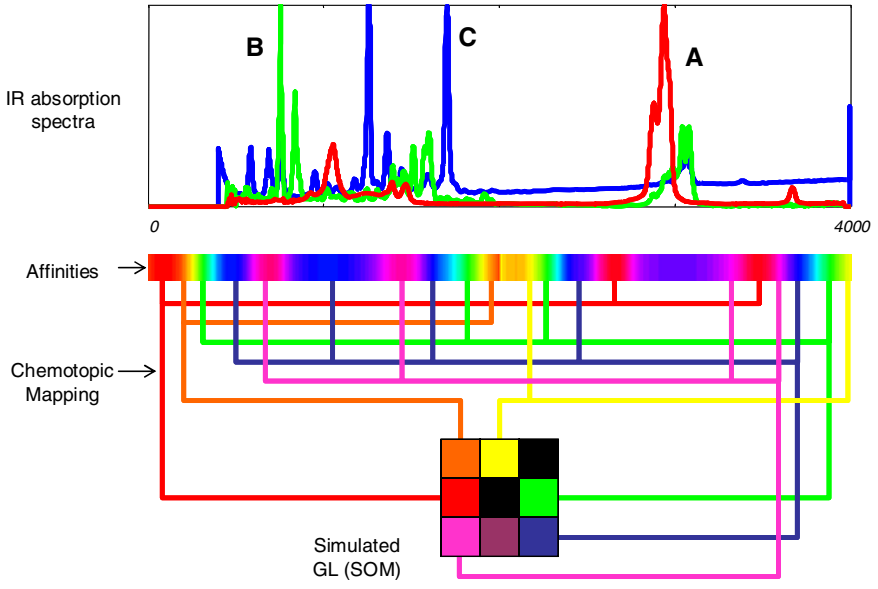

Fig. 6.2. Illustration of chemotopic convergence: the relative response to three analytes (labeled A, B and C) is used to define the wavenumbers' affinities (shown as a colorbar). IR wavenumbers with similar affinities project to the same SOM node as a result of chemotopic convergence. Activity across the SOM lattice can be considered as an artificial odor map.

as a colorbar below the IR spectra[1]. The chemotopic mapping is achieved by assigning features (i.e., IR wavenumbers) with similar affinities to the same SOM node. The activity of the entire SOM lattice is then considered as an artificial odor map.

This convergence model works well when the different sensors are reasonably uncorrelated, since the projection of sensor features across the SOM lattice approximates a uniform distribution, i.e., maximum entropy (Lancet et al. 1993; Laaksonen et al. 2003). Unfortunately, the population of sensors created through IR absorption spectra tends to be over-sampled. As a result, a few SOM nodes tend to receive the majority of input, which capture the "common-mode" response of the sensor, overshadowing the most discriminatory information. To avoid this issue, the activity of each SOM node is normalized by the number of sensor features that converge onto it:

$$SOM_j = \frac{\sum_{i=1}^{N} W_{ij} IR_i}{\sum_{i=1}^{N} W_{ij}} \tag{6.3}$$

Note that this solution is not driven by biological plausibility but largely by the limitations of the sensors.

[1] This is a simplification to illustrate the concept, as the actual affinity space in this case is three dimensional.

6.5 Results

To generate artificial odor maps, a population of 4,000 pseudo-sensors generated from the IR spectrum is projected chemotopically onto a 10x10 SOM lattice (100 nodes). The odor images are then low-pass filtered using a 5x5 Gaussian kernel.

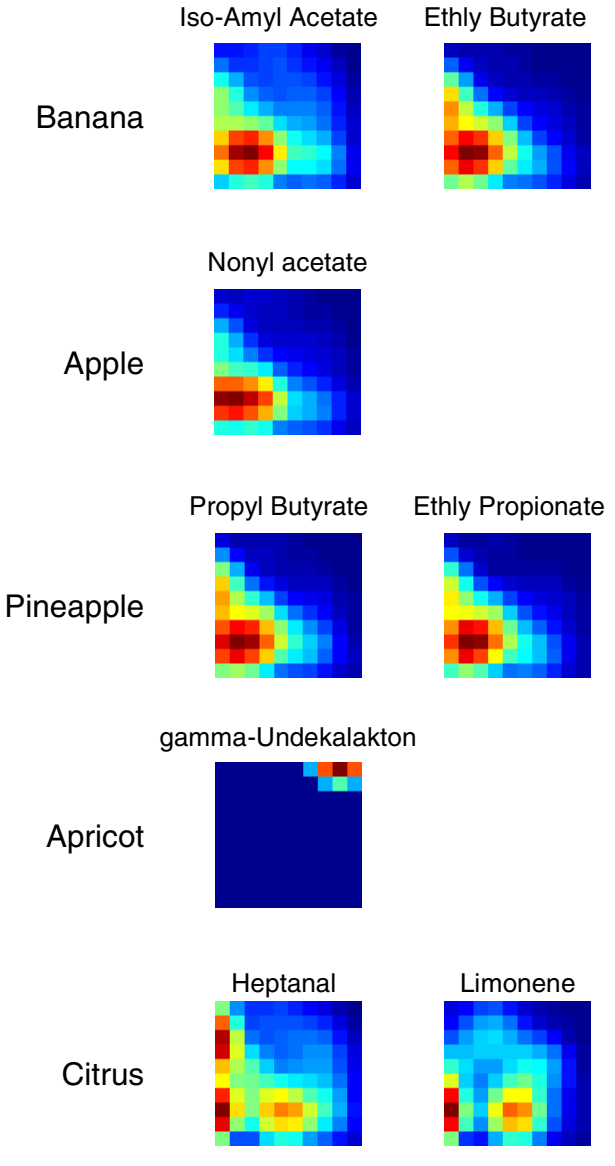

Fig. 6.3. Odor maps generated from the IR spectrum using the chemotopic convergence model for ten different smell percepts: i) banana, ii) pineapple, iii) apple, iv) apricot, v) citrus, vi) nuts, vii) cheese, viii) sweat, ix) minty and x) fat.

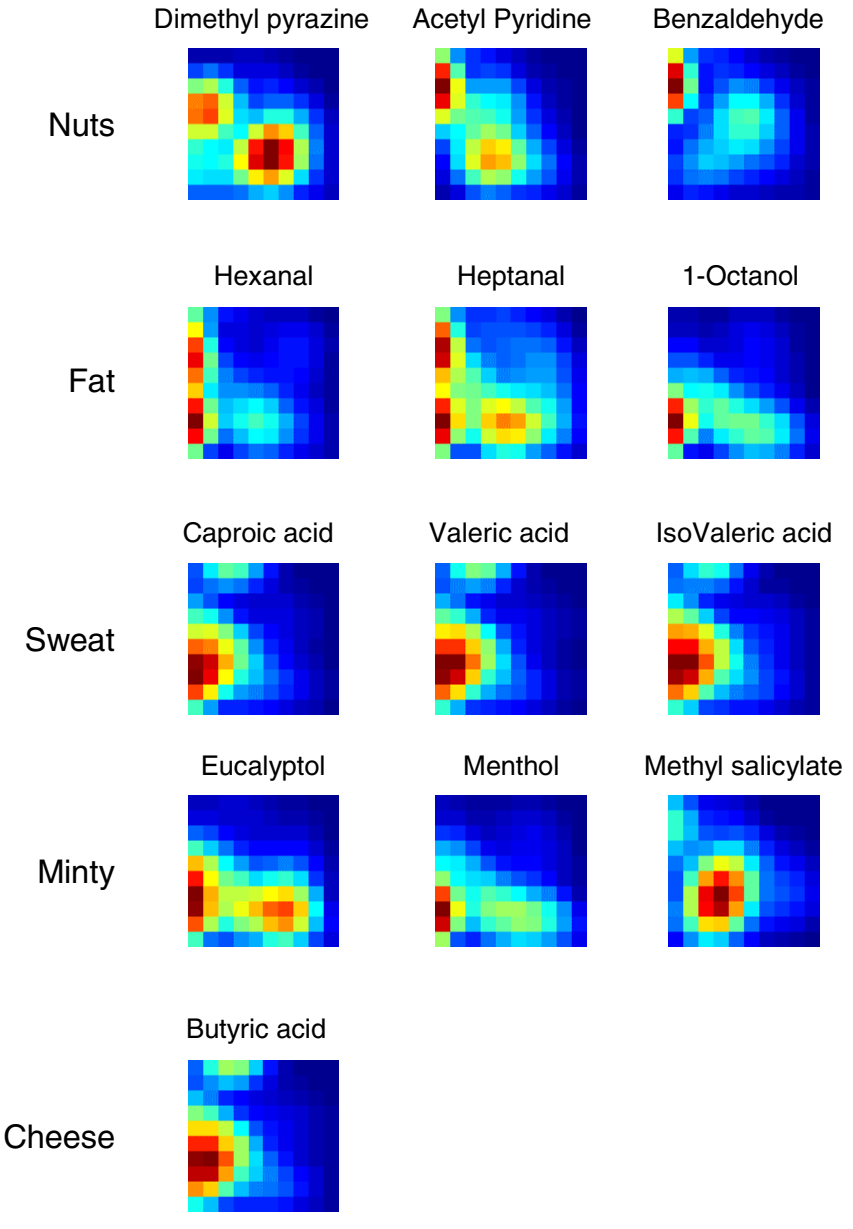

Fig. 6.3. (*continued*)

Fig. 6.3. shows the odor maps for ten different smell percepts[2] from the IR database. The following observations can be made based on the odor images obtained from their IR absorption spectrum:

[2] The organoleptic descriptors were obtained from Flavornet.

(i) Esters that smell like tropical fruits (banana and pineapple) produce similar odor maps, which are different from the maps of chemicals with apricots or citrus fruits descriptors,
(ii) *Citrus* odor maps are similar to those that smell *Fatty*,
(iii) *Sweat* and *Cheese* also produce similar odor maps, and,
(iv) Methyl salicylate and Menthol, which are both minty, produce distinct odor maps.

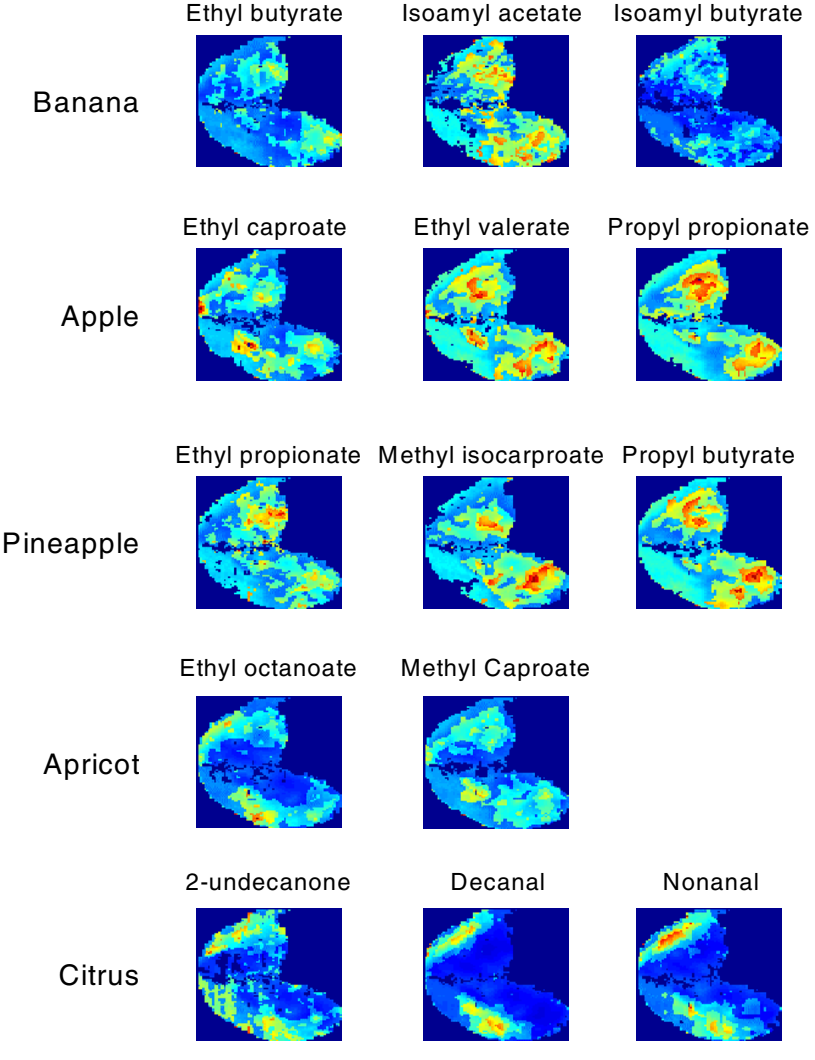

Fig. 6.4. Odor maps obtained in the rat olfactory bulb[3] for the same ten smell percepts

[3] A database of odor maps from the rat olfactory bulb is available at http://leonlab.bio.uci.edu/

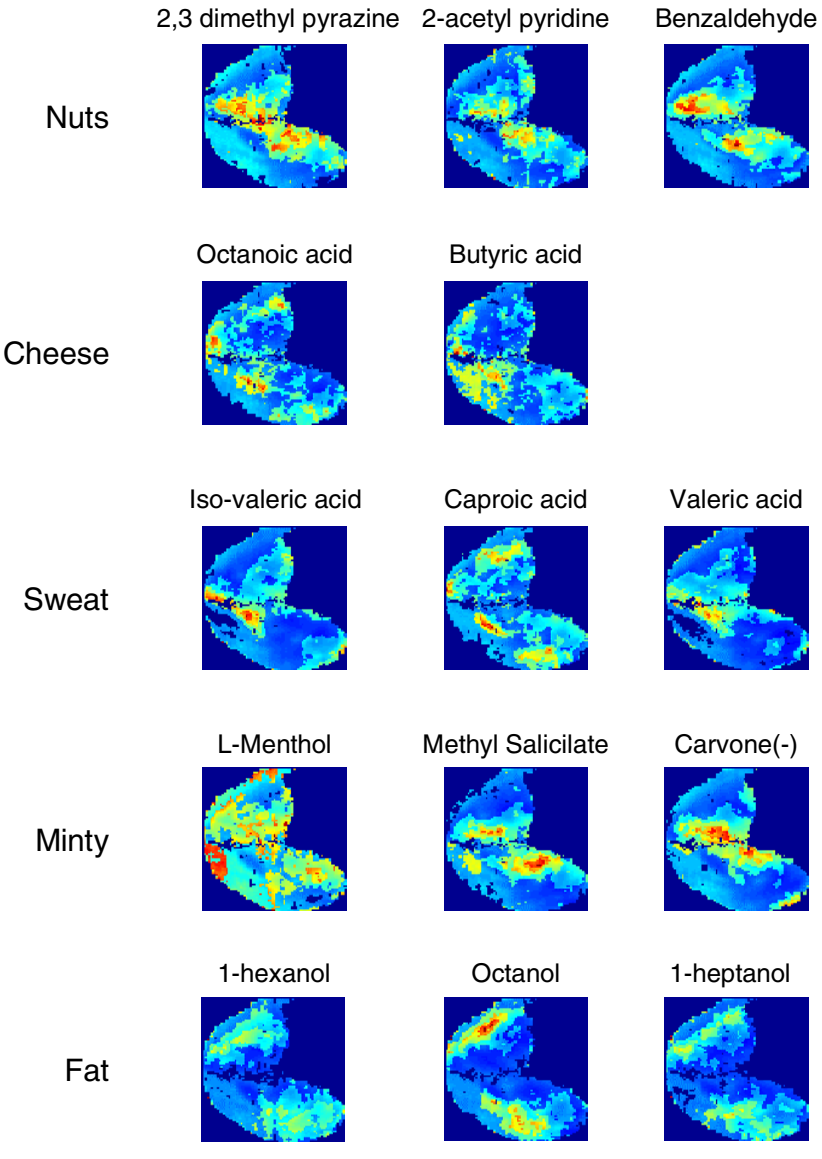

Fig. 6.4. (*continued*)

Spatial odor images for these compounds in the dorsal part of rat OB are shown in Figure 6.4. These odor maps were obtained using optical imaging techniques involving 2-deoxyglucose uptakes in the dorsal part of the rat olfactory bulb (Johnson and Leon 2000). Similar to the images obtained from the IR spectra, esters with tropical fruit smells produce similar activation patterns across the OB, which is different from chemicals with apricot and citrus descriptors. Odor maps for Citrus and Fat descriptors,

Table 6.1. List of odorants and their perceptual properties

Odorant number	Odorant name	Perceptual characteristics
1	Acetyl Pyridine	Nuts
2	Iso-amyl acetate	Fruits
3	Benzaldehyde	Nuts
4	Butanoic acid or Butyric acid	Cheese
5	2,3 Dimethyl pyrazine	Nuts
6	Ethyl Butyrate	Fruits
7	Ethyl Propionate	Fruits
8	Heptanal	Citrus, Fatty
9	Heptanol	Fatty
10	Hexenal	Fatty
11	Hexanoic acid or Caproic acid	Sweat
12	Hexanol	Fatty
13	Methyl Salicylate	Minty
14	Octanol	Fatty
15	Pentanoic acid or Valeric acid	Sweat
16	Propyl Butyrate	Fruits
17	Iso-Valeric acid	Sweat

Sweat and Cheese descriptors overlap similar to the IR-generated odor maps. Minty smelling Methyl salicylate and Menthol produced distinct odor maps.
Hierarchical cluster analysis of the seventeen chemicals, shown in Table 1, present in both the *NIST-IR* dataset and the rat OB image dataset reveal similar groupings, as shown in Figures 6.5a and 6.5b. In both cases, four distinct clusters can be identified that correspond to the following four smell descriptors: *Fruits*, *Cheese* or *Sweat*, *Fat* or *Citrus* and *Nuts*. Interestingly, methyl salicylate, which smells *Minty*, is grouped with the nuts category in both cases. Hexanoic acid, which is a fatty acid that smells like *Sweat*, is grouped under *Fat* or *Citrus* smell descriptor using the rat OB images and in the *Sweat* cluster using IR odor maps.

These results suggest that convergence mapping, combined with IR absorption spectra, may be an appropriate method to capture perceptual characteristics of certain classes of odorants.

6.6 Discussion

What molecular features contribute to the overall percept of smell still remains an open question in olfaction. Three theories have been proposed in an attempt to relate molecular properties of an odorant with its overall quality: vibrational, steric, and odotope theories (Dyson 1938; Moncrieff 1949; Shepherd 1987). The vibrational theory first proposed by Dyson (1938), revisited first by Beck and Miles (1947) and

later by Wright (1982) and Turin (1996) (Lefingwell 2002), suggests that vibrations due to stretching and bending of odor molecules are the determinants of odor identity and quality[4]. On the other hand, the steric theory initially put forth by Moncrieff (1949) and later extended by Amoore (1970) (Lefingwell 2002) proposes that odor quality is determined by the shape and size of the odorant molecules. More recently, the odotope or weak shape theory was proposed by Shepherd (1987). According to this theory, odor quality is determined by various molecular features of an odorant (commonly referred to as odotopes), such as carbon chain length or different functional groups.

It is important to note that IR absorption spectroscopy is in fact the basis of the vibrational theory of olfactory reception. This theory has been found to be limited in terms of explaining structure-odor relationships (Rossiter 1996). First, enantiomers, molecules that form non-superimposable mirror images of each other, have identical IR absorption spectrum, yet they can smell differently. e.g., the S- and R- enantiomers

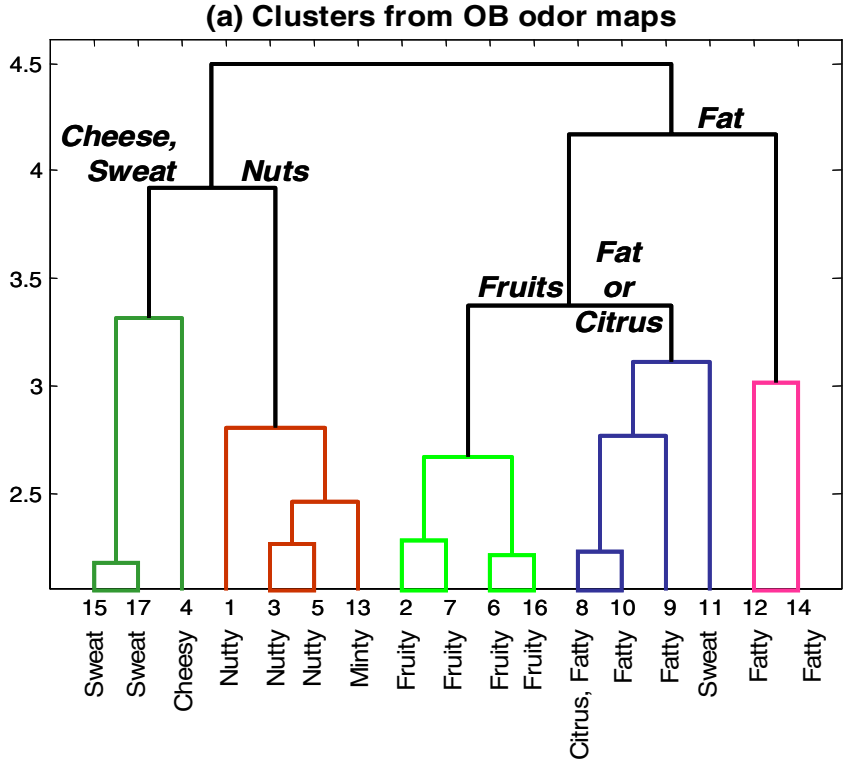

Fig. 6.5. Dendrograms (complete-linkage) revealing similar clusters a) from OB odor maps b) from artificial odor maps formed from their IR absorption spectra. The seventeen common chemicals found in both databases used in this study are listed in Table 6.1.

[4] Readers are referred to (Keller and Vosshall 2004) where using psychophysical tests the authors have found that vibrational theory alone cannot explain the overall smell of an odorants.

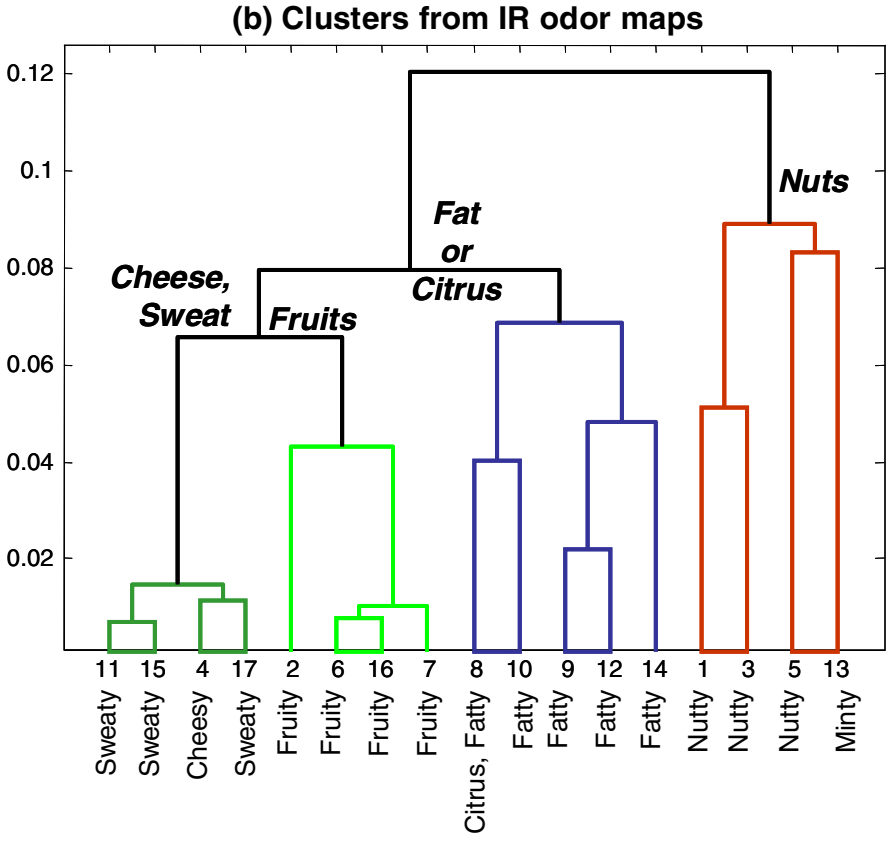

Fig. 6.5. (*continued*)

of carvone have smells of caraway and spearmint, respectively. Second, isotopic substitution affects the IR spectrum but does not change the perceived smell. Hence it is important to realize that, in the general case, it will not be possible to predict the organoleptic properties of chemicals from their IR absorption spectrum alone. Nevertheless, IR spectroscopy has been successfully employed in the food and beverage industry for determining their chemical composition (fat, fiber, moisture, carbohydrates etc.,), demonstrating that this method might be well suited for process monitoring and control in these applications (Li-Chen et al. 2002; Anderson et al. 2002; Osborne and Fearn 1988).

The neuromorphic scheme employed an affinity space to cluster sensor features with similar selectivity. Conventional statistical pattern recognition approaches for clustering operate in the feature space, where each input dimension corresponds to a particular feature (or sensor). Figure 6.6a shows a hypothetical example where multiple samples from two odorants (A, B) have been sampled with a two-sensor array (S1, S2). Samples that belong to the same (odor) class cluster together in feature space, as shown in Fig. 6.6. a. In contrast to feature space, each dimension in affinity space corresponds

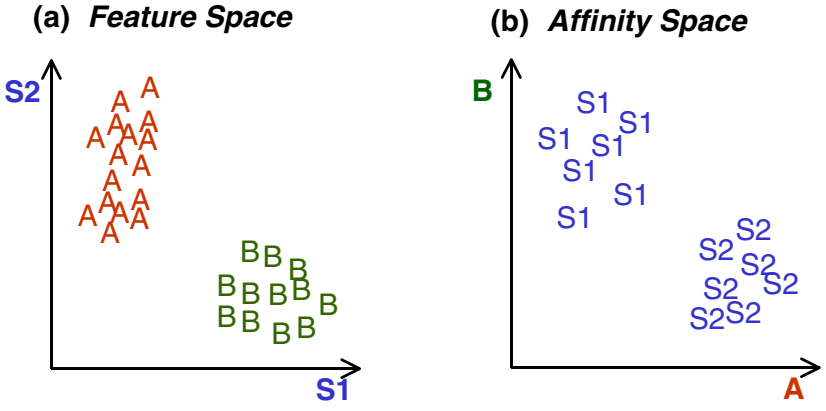

Fig. 6.6. Clustering in feature space and in affinity space. (a) Samples of the same class produce similar response across sensor array, and therefore cluster together in feature space. (b) Features that produce similar response to different odors (classes) cluster together in the affinity (class) space.

to a particular (odor) class. Features that provide similar information regarding the different classes cluster together in the affinity space. As an example, in Fig. 6.6. b all features of type S_1 provide high response to class B and low response to class A; as a result they can be clustered together. In contrast, all features of type S_2 provide high response to class A and low response to class B, therefore form a separate cluster. This basic principle underlies the proposed chemotopic convergence model. A more detailed treatment on the novelty of this approach and its formulation as a dimensionality reduction technique can be obtained from Perera et al. (2006)[5].

6.7 Summary

We have presented a neuromorphic approach for correlating instrumental/sensor data of odorants with their organoleptic properties. This approach comprised of two complementing components: (1) a model of early olfactory processing, which provides odor images that are qualitatively similar to those observed in the OB of animals, and (2) an instrument (IR spectroscopy) that provides high-dimensional data and captures some information consistent with the odotope theory. Our results show that artificial odor maps of chemicals generated from their IR absorption spectra form clusters that match those obtained by clustering the rat OB images of the same set of chemicals. More interestingly, each of these clusters uniquely identified a specific smell descriptor: *Fruits*, *Cheese* or *Sweat*, *Fat* or *Citrus* and *Nuts*. Though encouraging, our results are preliminary at best, as our analysis is limited to those odorants that are common among the NIST and Leon Lab's databases. Further investigations are required to study the relationships among the three representations of an odorant:

[5] A related approach to evaluate contribution of a single element in a sensor array has been independently proposed by Niebling and Muller (1995).

stereo-chemical molecular features (Pelosi and Persaud 2000), olfactory bulb images (Johnson and Leon 2000), and organoleptic descriptors (Dravnieks 1985). However, as rightly pointed out by Sell (2006), the complexity of the problem might make such relationships hard to uncover.

Acknowledgments

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